Supporting Information

Catalytic Arene *meta*-C–H Functionalization Exploiting a Quinoline Based Template

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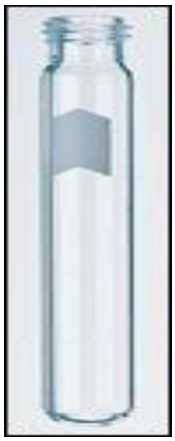
1. General Consideration

1.a.Reagent Information: Unless otherwise stated, all the reactions were carried out under aerobic condition in screw cap reaction tubes. All the solvents were bought from Aldrich/Alfa Aesar (India)/TCI (India)/Merck in a sure-seal bottle and were used as received. Palladium acetate was purchased from Alfa Aesar. Silver acetate was bought from Loba Chemicals and *N*-Ac-gly-OH is obtained from Alfa aesar (India). HFIP was received from TCI (India). All the benzyl chlorides and bromides were bought from Aldrich/Alfa Aesar (India)/TCI (India)/Spectrochem. For column chromatography, silica gel (100–200 mesh) from SRL Co. was used. A gradient elution using pet ether and ethyl acetate was performed based on Merck aluminium TLC sheets (silica gel $60F_{254}$).

1.b. Analytical Information: All isolated compounds are characterized by ^{1}H NMR, ^{13}C NMR spectroscopy. Copies of the ^{1}H NMR, ^{13}C NMR can be found in the supporting information. Nuclear magnetic resonance spectra were recorded either on a Bruker 500 or 400 MHz instrument. All ^{1}H NMR experiments are reported in units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) in the deuterated solvent, unless otherwise stated. All ^{13}C NMR spectra were reported in ppm relative to $CDCl_3$ (77.23 ppm), unless otherwise stated, and all were obtained with ^{1}H decoupling. High-resolution mass spectra (HRMS) were recorded on a micro-mass ESI TOF (time of flight) mass spectrometer.

1.c. Description of Reaction Tube:



Pictorial description of reaction tube for *meta*-olefination and acetoxylation reaction: Fisherbrand Disposable Borosilicate Glass Tubes (16*125mm) with Threaded End (Fisher Scientific Order No. 1495935A) [left]; Kimble Black Phenolic Screw Thread Closures with Open Tops (Fisher Scientific Order No. 033407E) [right]; Thermo Scientific National PTFE/Silicone Septa for Sample Screw Thread Caps (Fisher Scientific Order No. 03394A) [right].

2. Experimental Section

2.a. General Procedure

General Procedure A: *meta*-mono-Olefination of sulphonic esters

An oven-dried screw cap reaction tube was charged with a magnetic stir-bar, substrate (0.2 mmol, 1.0 equiv), olefin (0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (10 mol%, 0.02 mmol, 4.4 mg), *N*-Ac-Gly-OH (20 mol%, 0.04 mmol, 4.7 mg), and AgOAc (2.0 equiv, 0.4 mmol, 66.7 mg) were taken. Subsequently, HFIP:DCE (1:1, 2 mL) was added and the reaction mixture was stirred vigorously for 24-48 h at rt-80 °C. The reaction mixture was then diluted with EtOAc and filtered through celite pad. After evaporation of the solvent, the crude mixture was purified by column chromatography using silica gel (100-200 mesh size) and petroleum ether/ethyl acetate as the eluent. (Olefination reactions with 3-substituted arene compounds have been carried out in only HFIP solvent for improved yield)

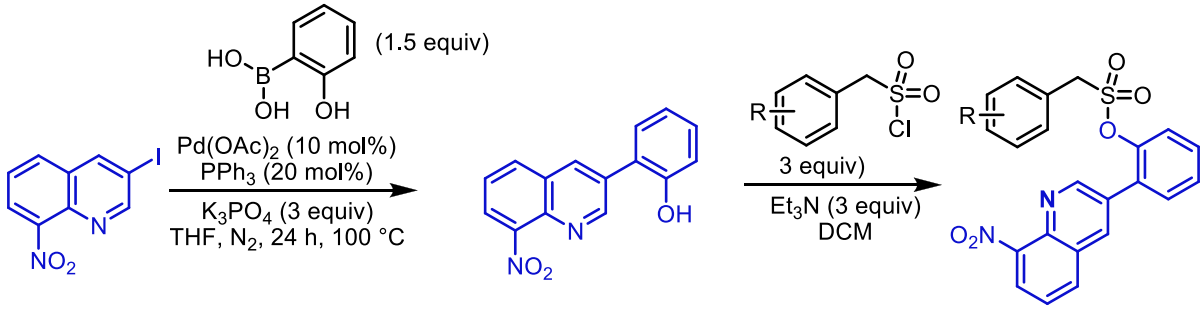
General Procedure B: *meta*-di-olefination of sulphonic esters

The *mono*-olefinated product has been utilized as the substrate for the hetero-di-olefination. An oven-dried screw cap reaction tube was charged with a magnetic stir-bar, mono-olefianted product as substrate (0.1 mmol, 1.0 equiv), olefin (0.3 mmol, 3.0 equiv), $Pd(OAc)_2$ (10 mol%, 2.2 mg), *N*-Ac-Gly-OH (20 mol%, 2.3 mg), and AgOAc (0.2mmol, 2.0 equiv, 33 mg) were taken. Subsequently, HFIP (1 mL) was added and the reaction mixture was stirred vigorously for 24 h at a preheated oil bath of 80 °C. The reaction mixture was then diluted with EtOAc and filtered through celite pad. After evaporation of the solvent, the crude mixture was purified by column chromatography using silica gel (100-200 mesh size) and petroleum ether/ethyl acetate as the eluent.

General Procedure C: *meta*-Acetoxylation of sulphonic esters

An oven-dried screw cap reaction tube was charged with a magnetic stir-bar, substrate (0.2 mmol, 1.0 equiv), $Pd(OAc)_2$ (10 mol%, 0.02 mmol, 4.4 mg), *N*-Ac-Gly-OH (20 mol%, 0.04 mmol, 4.7 mg) and $PhI(OAc)_2$(0.8 mmol, 4.0 equiv, 257.6 mg) were taken. Subsequently, HFIP (2 mL) and 100 μL Ac_2O were added. The reaction mixture was placed on a preheated oil bath of 80 °C and stirred vigorously for 24-36 h. The reaction mixture was then diluted with EtOAc and filtered through celite pad. After evaporation of the solvent, the crude mixture was purified by column chromatography using silica gel (100-200 mesh size) and petroleum ether/ethyl acetate as the eluent.

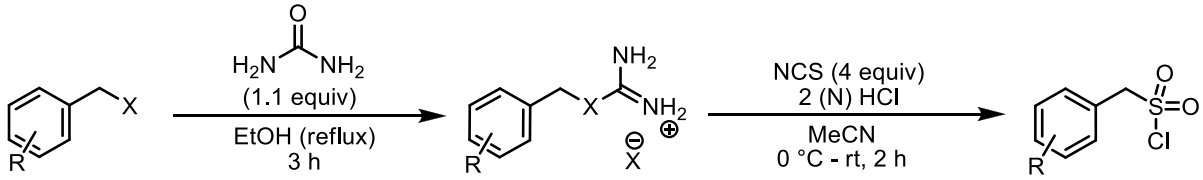
Procedure D: Synthesis of directing group and substrates



Step 1: In an oven-dried screw cap reaction tube, charged with a magnetic stir-bar,3-iodo-8-nitroquinoline (1.0 equiv), 2-hydroxyphenylboronic acid (1.5 equiv), $Pd(OAc)_2$ (10 mol%), PPh_3 (20 mol%) and K_3PO_4 (3.0 equiv) were added. Then the closed reaction tube was evacuated and backfilled with N_2 for three times and THF (3 mL per 1 mmol) as solvent was added using syringe. The reaction mixture was submerged in a preheated 100 °C oil bath and allowed for vigorous stirring for 24 hours. After 24 hour, reaction mixture was allowed to cool and diluted with EtOAc and extracted with brine solution. The organic layer was dried over Na_2SO_4 and concentrated by evaporation. Concentrated organic part was purified by column chromatography. Yellow crystalline compound was isolated in 75% yields using 15% ethyl acetate and pet ether mixture as an eluent.

Step 2: In an oven dried 100 mL round bottom flask, phenol (1 equiv) was dissolved in DCM (5 mL DCM permmol phenol) and Et_3N (3.0 equiv) was added drop wise and allowed to stir for 15 min at room temperature. Followed by, sulphonyl chloride (3.0 equiv) was added portion wise very slowly at 0 °C. The reaction mixture was then stirred at room temperature for overnight and upon complete consumption of phenol DCM was dried under vacuum. The residue was diluted with EtOAc and was with brine solution. The organic part was dried over Na_2SO_4, and purified by column chromatography.

Procedure E: Synthesis of sulfonyl chloride from benzyl chloride/bromide[1]



Step 1: In an oven dried 250 mL round bottomed flask charged with magnetic stir-bar, thiourea (11 mmol , 1.1 equiv, 836 mg) was taken in absolute ethanol (30 mL) followed by the corresponding benzyl chloride/bromide (10 mmol , 1.0 equiv) was added. The reaction mixture was refluxed for 3 h. After cooling the reaction mixture, the solvent was dried under reduced pressure which result a white solid. The solid was directly used for the next step directly.

Step 2: In a clean round bottomed flask charged with stirbar, *N*-chlorosuccinimide (40 mmol, 4.0 equiv, 5.34 g) was added to MeCN (20 mL). 2(N) HCl(2.8 mL) was then added to the solution. The reaction mixture was stirred on an ice cooled water bath for 15 min. The solid salt obtained from the first step was added slowly to this reaction mixture and stirred vigorously. The addition led to an exothermic reaction. However the temperature was maintained below 25 °C. Upon forming a clear solution the mixture was warmed to the room temperature and stirred for 2 h. The reaction was evaporated under reduced pressure to remove the acetonitrile. The remaining solution was diluted with water and extracted with ethyl acetate. The organic portion was dried over anhydrous Na_2SO_4. The solution was concentrated under reduced pressure and purified through column chromatography.

2.b.Optimization

2.b.I. Optimization for*meta*-olefination reaction:

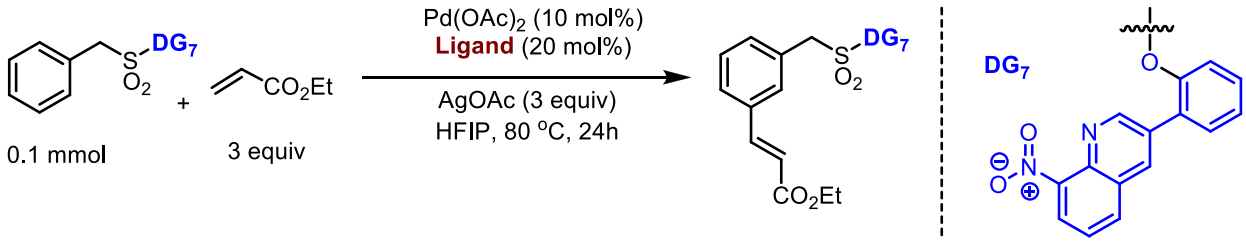


Table S1: Optimization by varying ligands:

Entry	Ligands	% Yield (NMR)	Ratio (mono:di)
1	***N*-Ac-Gly-OH**	**86**	**1.5:1**
2	*N*-Ac-Phe-OH	37	11:1
3	*N*-Ac-Val-OH	18	8:1
4	*N*-Ac-Leu-OH	38	15:1
5	*N*-Boc-Leu-OH	32	15:1
6	*N*-Boc-Phe-OH	28	>20:1
7	*N*-Ac-Ala-OH	<10	-
8	Boc-Gly-OH	15	>20:1
9	Boc-isoleucine	<5	-
10	For-Gly-OH	<5	-
11	Boc-Val-OH	<10	-
12	Boc-Ala-OH	<10	-
13	*N*-acetyl methionine	<10	-
14	Ac-Gly-ethylester	-	-
15	Glycine	<5	-
16	*Z*-Phe-OH	<5	-

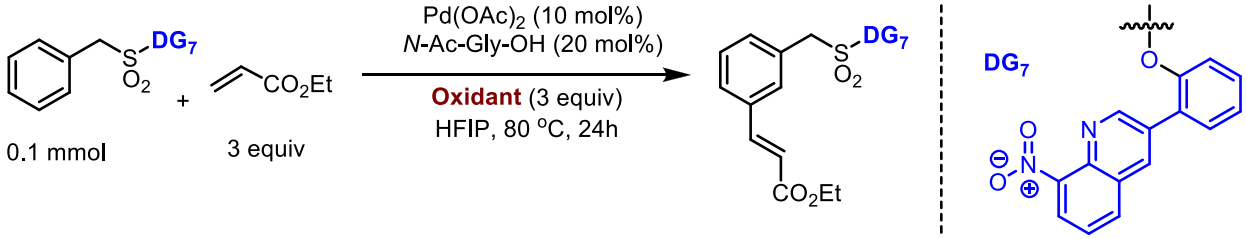


Table S2: Oxidant optimization:

Entry	Oxidant	% Yield(NMR)	Ratio (*mono:di*)
1	**AgOAc**	**86**	**1.5:1**
2	Ag_2CO_3	70	2:1
3	$AgSO_4$	45	5:1
4	AgO	<20	-
5	$K_2S_2O_8$	-	-
6	*p*-Benzoquinone	-	-
7	$Cu(OAc)_2$	-	-
8	$CuCl_2$	-	-

9	MnO_2	-	-

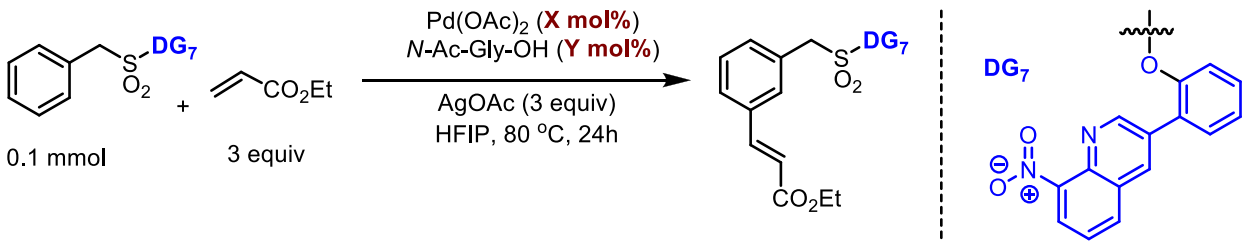


Table S3: Optimization by varying catalyst loading (palladium and ligand amount):

Entry	Pd- Loading (mol%)	Ligand Amount (mol%)	% Yield (NMR)	Ratio (*mono:di*)
1	2	4	50	7:1
2	4	8	70	2:1
3	6	12	74	2:1
4	8	16	79	2:1
5	**10**	**20**	**86**	**1.5:1**
6	15	30	87	1:1
7	20	40	87	1:1

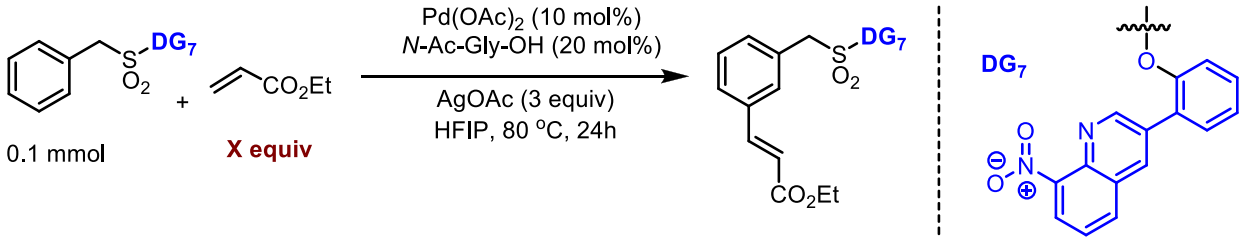


Table S4: Olefin amount variation:

Entry	Olefin Amount (equiv)	% Yield (NMR)	Ratio (*mono:di*)
1	1	57	7:1
2	1.2	65	3:1
3	1.4	76	3:1
4	1.6	80	2.5:1
5	1.8	85	2:1
6	**2.0**	**86**	**2:1**
7	2.5	87	1.5:1
8	3.0	86	1.5:1

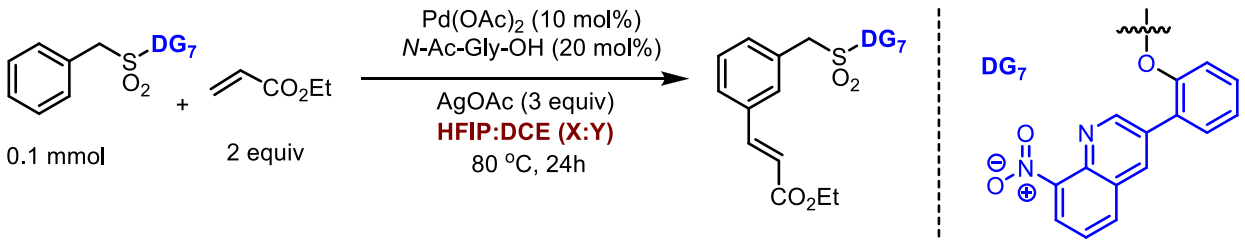


Table S5: Solvent combination screening:

Entry	HFIP/DCE (µl)	% Yield (NMR)	Ratio (*mono:di*)
1	500:0	86	2:1
2	400:100	85	3:1
3	300:200	81	3:1
4	**250:250**	**80**	**3:1**
5	200:300	78	3:1
6	100:400	72	3.5:1
7	50:450	64	5:1
8	0:500	0	-

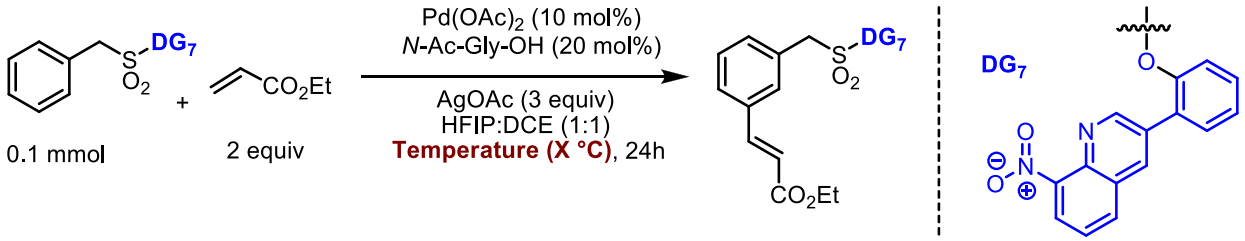


Table S6: Temperature optimization:

Entry	Temperature (°C)	% Yield (NMR)	Ratio (*mono:di*)
1	**RT**	**55**	**>10:1**
2	35	68	2:1
3	40	70	2:1
4	45	75	2:1
5	50	78	2:1
6	80	80	3:1
7	100	87	1:1
8	130	61	1:1

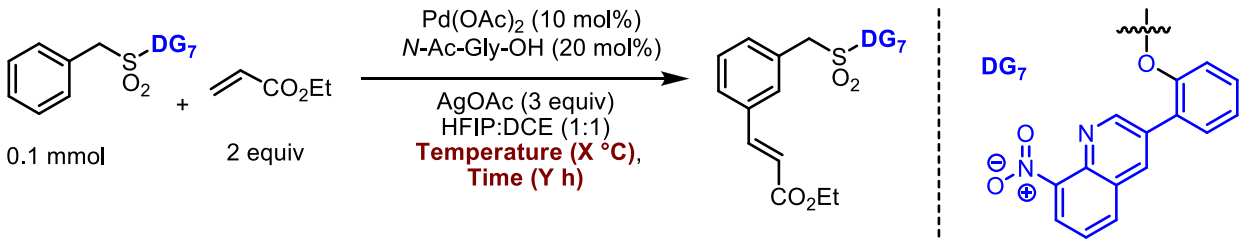


Table S7: Temperature and time optimization:

Entry	Temperature (°C)	Time (h)	% Yield (NMR)	Ratio (*mono:di*)
1	RT	12	34	>20:1
2	RT	24	55	>10:1
3	RT	30	63	>10:1
4	RT	36	70	10:1
5	**RT**	**48**	**75**	**7:1**
6	50	48	87	1:1
7	80	48	90	1:1
8	100	48	89	1:1

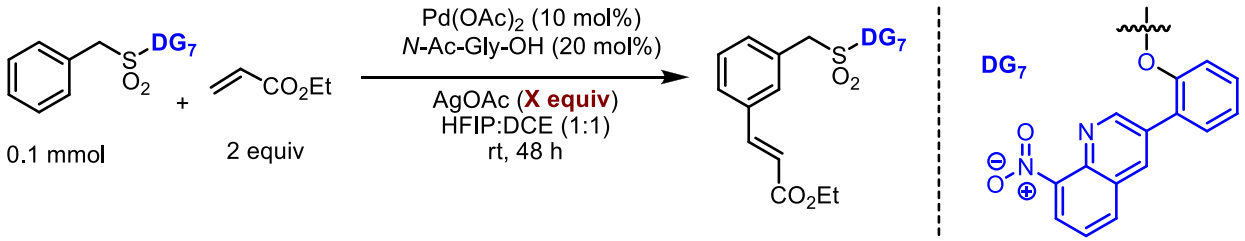


Table S8: Oxidant amount optimization:

Entry	Oxidant Amount (equiv)	% Yield (NMR)	Ratio (*mono:di*)
1	0.5	35	10:1
2	1.0	70	7:1
3	1.5	70	7:1
4	**2.0**	**75**	**7:1**
5	2.5	75	7:1
6	3.0	75	7:1

2.b.II. Optimization for*meta*-acetoxylation reaction:

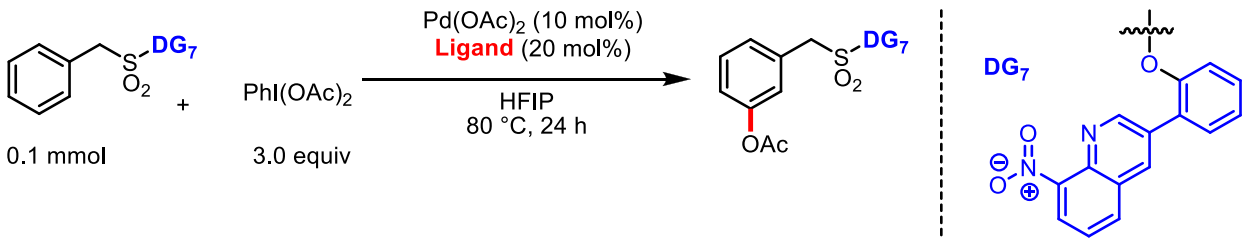


Table S9: Oxidant optimization:

Entry	Ligands	% Yield (NMR)	Ratio (mono:di)
1	***N*-Ac-Gly-OH**	**60**	**>20:1**
2	*N*-For-Gly-OH	36	>20:1
3	*N*-Ac-Val-OH	18	>20:1
4	*N*-Ac-Phe-OH	44	>20:1
5	*N*-Ac-Ala-OH	20	>20:1
6	*N*-Boc-Phe-OH	<10	-
7	*N*-Boc-Val-OH	<5	-
8	*N*-Boc-Gly-OH	<5	-
9	*N*-Boc-isoleucine	<5	-
10	Ac-Gly-ethylester	<10	-
11	Glycine	<10	-
12	N-Ac-Leu-OH	54	>20:1

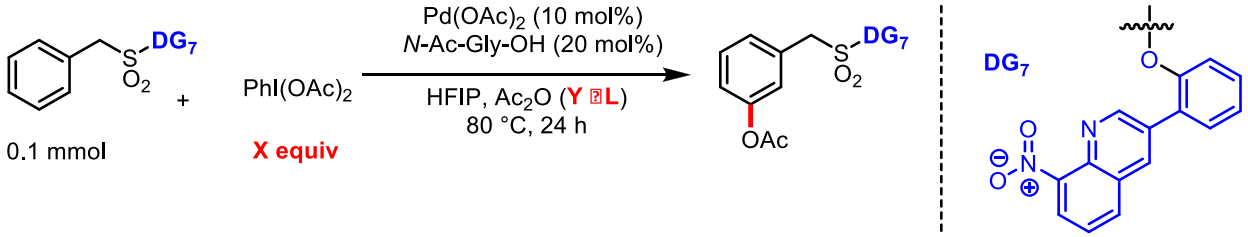


Table S10: $PhI(OAc)_2$ and Ac_2O amount variation:

Entry	$PhI(OAc)_2$(equiv)	Ac_2O (µL)	% Yield (NMR)	Ratio (mono:di)
1	1.0	-	25	>20:1
2	2.0	-	32	>20:1
3	2.5	-	50	>20:1
4	3.0	-	60	>20:1
5	3.5	-	65	>20:1
6	4.0	-	69	>20:1
7	5.0	-	65	>20:1
9	4.0	50	70	>20:1
10	4.0	75	71	>20:1
11	**4.0**	**100**	**75**	**>20:1**
12	4.0	120	76	<20:1

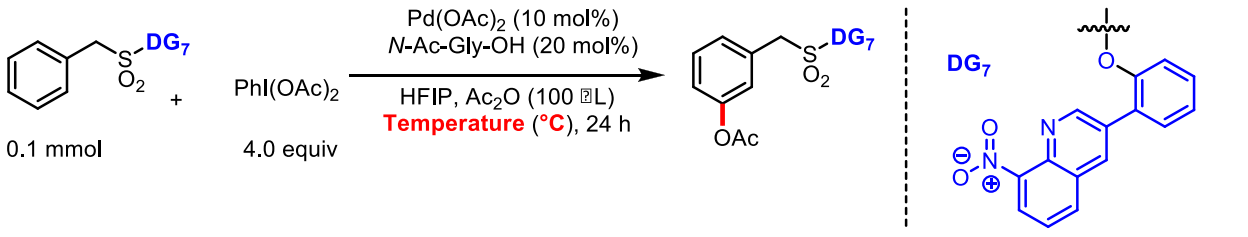


Table S11: Temperature optimization:

Entry	Temperature (°C)	% Yield (NMR)	Ratio (mono:di)
1	RT	<10%	-
2	50	30	>20:1
3	60	52	>20:1

4	70	68	>20:1
5	**80**	**75**	**>20:1**
6	90	76	>20:1
7	100	80	<20:1

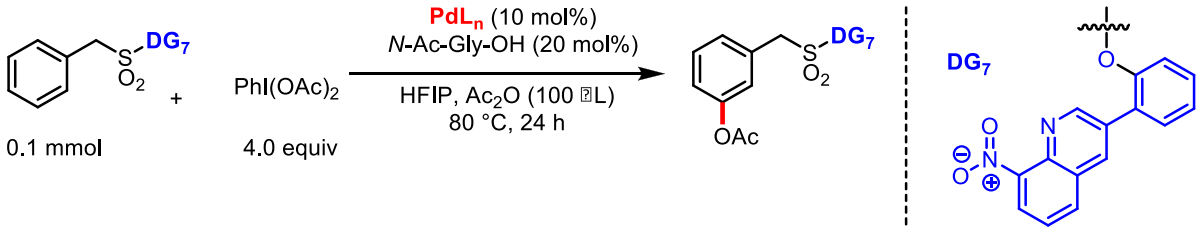


Table S12: Pd-salt variation:

Entry	Pd-Salt	% Yield (NMR)	Ratio (mono:di)
1	**$Pd(OAc)_2$**	**75**	**>20:1**
2	$PdSO_4$	-	>20:1
3	$Pd(PPh_3)_4$	40	>20:1
4	$Pd(CH_3CN)_2Cl_2$	20	>20:1
5	$Pd_2(dba)_3$	35	>20:1
6	$PdCl_2$	-	>20:1

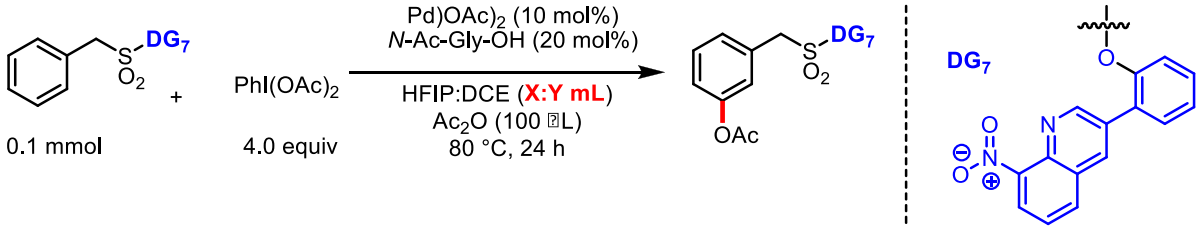


Table S13: Oxidant optimization:

Entry	HFIP:DCE (mL)	% Yield (NMR)	Ratio (mono:di)
1	**1.0:0**	**75**	**>20:1**
2	0.8:0.2	70	>20:1
3	0.6:0.4	61	>20:1
4	0.5:0.5	56	>20:1
5	0.4:0.6	40	>20:1
6	0.2:0.8	20	>20:1
7	0:1.0	-	-

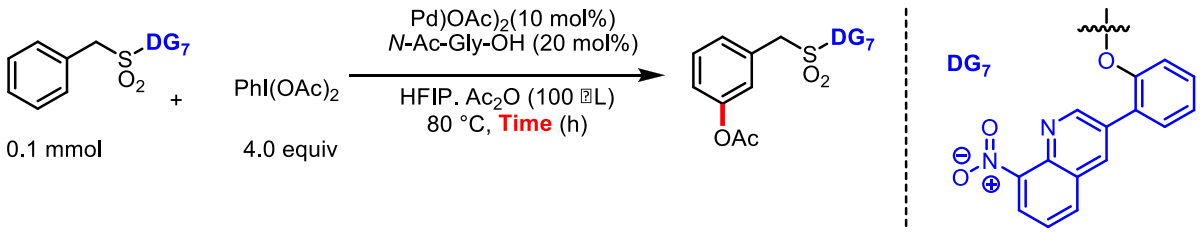
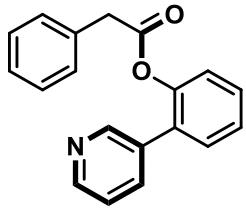


Table S14: Time optimization:

Entry	Time (h)	% Yield (NMR)	Ratio (mono:di)
1	12	40	>20:1
2	16	53	>20:1
3	**24**	**75**	>20:1
4	30	76	>20:1
5	**36**	**78**	**<20:1**
6	48	80	<20:1

2.c. Characterization:

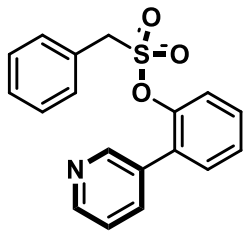


2-(pyridin-3-yl)phenyl 2-phenylacetate :

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (dd, *J* = 2.2, 0.7 Hz, 1H), 8.52 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.65 (d, *J* = 7.3 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.43 (q, *J* = 7.3 Hz, 3H), 7.36 (dd, *J* = 5.0, 1.7 Hz, 3H), 7.23 (dd, *J* = 6.9, 3.3 Hz, 3H), 3.76 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.78, 148.12, 136.91, 132.97, 130.94, 129.74, 129.57, 129.41, 128.87, 128.68, 127.50, 127.06, 126.85, 123.14, 41.44.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{19}H_{16}NO_2$: 290.1175, found 290.1170.

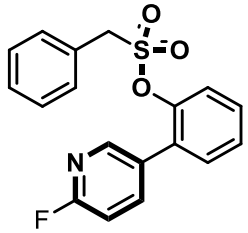


2-(pyridin-3-yl)phenylphenylmethanesulfonate (DG_1):

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 – 8.73 (m, 1H), 8.63 (dd, *J* = 4.7, 1.6 Hz, 1H), 7.84 – 7.77 (m, 1H), 7.46 – 7.30 (m, 9H), 7.28 (s, 1H), 4.17 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.97, 149.01, 146.33, 136.94, 132.93, 131.95, 131.43, 130.84, 129.87, 129.36, 129.04, 127.66, 126.81, 123.36, 123.29, 57.55.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{18}H_{16}NO_3S$: 326.0845, found 326.0841.

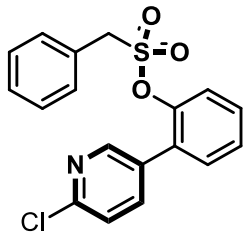


2-(6-fluoropyridin-3-yl)phenylphenylmethanesulfonate (DG_2):

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 2.3 Hz, 1H), 7.83 (td, *J* = 8.1, 2.5 Hz, 1H), 7.44 – 7.36 (m, 6H), 7.35 – 7.31 (m, 3H), 7.27 (dd, *J* = 6.1, 4.6 Hz, 2H), 6.89 (dd, *J* = 8.5, 2.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.77, 146.21, 142.21, 142.13, 131.51, 131.13, 130.91, 130.08, 129.53, 129.17, 127.75, 126.89, 123.36, 109.49, 109.12, 57.70.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{18}H_{15}FNO_3S$: 344.0751, found 344.0755.

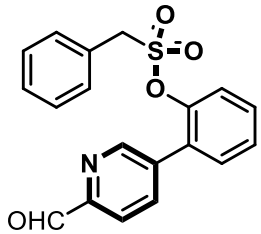


2-(6-chloropyridin-3-yl)phenylphenylmethanesulfonate(DG_3):

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 2.1 Hz, 1H), 7.68 (dd, *J* = 8.2, 2.4 Hz, 1H), 7.43 – 7.33 (m, 7H), 7.30 – 7.26 (m, 3H), 4.31 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.97, 150.01, 149.75, 146.05, 139.62, 131.85, 131.45, 130.91, 130.28, 129.57, 129.20, 127.81, 126.83, 124.06, 123.44, 57.70.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{18}H_{14}ClNNaO_3S$: 382.0275, found 382.0278.

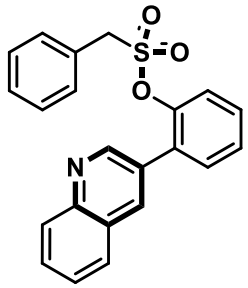


2-(6-formylpyridin-3-yl)phenylphenylmethanesulfonate (DG_4):

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.12 (s, 1H), 8.88 – 8.71 (m, 1H), 7.96 – 7.79 (m, 2H), 7.53 – 7.13 (m, 9H), 4.30 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.19, 151.69, 150.46, 145.98, 137.81, 137.19, 131.44, 131.32, 130.89, 130.69, 129.55, 129.17, 127.91, 126.79, 123.58, 121.39, 57.66.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{19}H_{16}NO_4S$: 354.0800, found 354.0790.

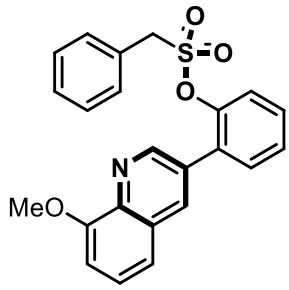


2-(quinolin-3-yl)phenylphenylmethanesulfonate(DG_5):

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (d, *J* = 2.2 Hz, 1H), 8.25 (d, *J* = 1.9 Hz, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.78 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.61 (ddd, *J* = 14.1, 7.6, 4.1 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.46 – 7.36 (m, 3H), 7.24 – 7.13 (m, 5H), 4.15 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 151.12, 147.51, 146.59, 136.30, 132.13, 131.91, 130.78, 130.22, 130.14, 129.97, 129.53, 129.33, 128.98, 128.37, 127.81, 127.75, 127.33, 126.79, 123.37, 57.72.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{22}H_{18}NO_3S$: 376.1007, found: 376.1005.

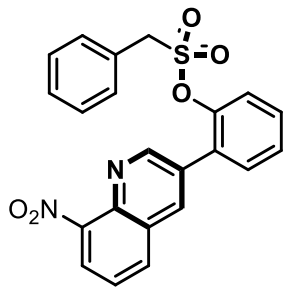


2-(8-methoxyquinolin-3-yl)phenylphenylmethanesulfonate(DG_6):

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.06 (s, 1H), 8.24 (s, 1H), 7.52 (dd, *J* = 17.1, 8.9 Hz, 2H), 7.44 (d, *J* = 6.4 Hz, 4H), 7.20 (dt, *J* = 16.7, 6.7 Hz, 5H), 7.12 (d, *J* = 7.6 Hz, 1H), 4.14 (s, 3H), 4.11 (s, 2H).

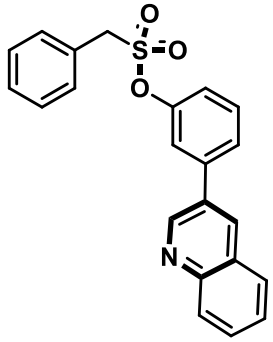
^{13}C NMR (126 MHz, $CDCl_3$) δ 149.88, 146.59, 136.21, 132.00, 131.91, 130.87, 130.84, 130.01, 129.30, 128.98, 128.96, 127.76, 127.61, 126.76, 123.49, 120.08, 108.25, 77.48, 77.23, 76.98, 57.70, 56.29.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{23}H_{20}NO_4S$: 406.1113, found: 406.1112.

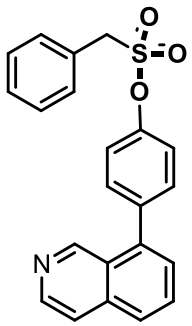


2-(8-nitroquinolin-3-yl)phenylphenylmethanesulfonate(DG_7):

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.08 (d, *J* = 2.1 Hz, 1H), 8.28 (d, *J* = 2.1 Hz, 1H), 8.07 (d, *J* = 7.5 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.9 Hz, 1H), 7.49 – 7.40 (m, 3H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.22 – 7.15 (m, 5H), 4.30 (s, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 153.26, 148.28, 146.21, 138.57, 136.15, 132.61, 131.97, 131.75, 131.24, 130.66, 130.49, 129.28, 128.93, 128.55, 127.87, 126.67, 125.88, 124.19, 123.40, 57.63.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{22}H_{17}N_2O_5S$: 421.0858, found: 421.0853.

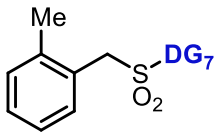


3-(quinolin-3-yl)phenylphenylmethanesulfonate (DG_8):
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (d, *J* = 2.2 Hz, 1H), 8.24 (d, *J* = 1.9 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.80 – 7.71 (m, 1H), 7.61 (t, *J* = 7.8 Hz, 2H), 7.54 – 7.46 (m, 3H), 7.46 – 7.40 (m, 3H), 7.35 – 7.28 (m, 1H), 7.18 (dd, *J* = 8.1, 1.6 Hz, 1H), 4.60 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.98, 149.49, 147.67, 140.07, 133.94, 132.40, 131.17, 130.78, 130.12, 129.81, 129.65, 129.28, 128.27, 128.02, 127.53, 127.39, 126.21, 121.78, 121.15, 115.72, 57.36.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{22}H_{18}NO_3S$: 376.1001, found: 376.1006.



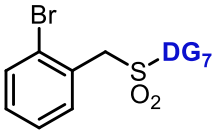
4-(isoquinolin-8-yl)phenylphenylmethanesulfonate(DG_9):

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 (s, 1H), 8.59 – 8.54 (m, 1H), 7.88 – 7.81 (m, 1H), 7.76 – 7.68 (m, 2H), 7.55 – 7.40 (m, 8H), 7.26 (s, 2H), 4.61 (s, 2H).
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{22}H_{18}NO_3S$: 376.1001, found: 376.1004.

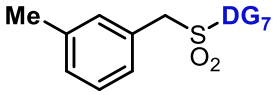


2-(8-nitroquinolin-3-yl)phenyl o-tolylmethanesulfonate (3a)

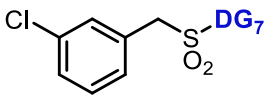
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (d, *J* = 2.2 Hz, 1H), 8.31 (t, *J* = 5.8 Hz, 1H), 8.07 (t, *J* = 6.9 Hz, 1H), 8.02 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.49 – 7.42 (m, 3H), 7.36 – 7.32 (m, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.09 (tt, *J* = 6.8, 3.4 Hz, 1H), 7.05 – 6.98 (m, 2H), 4.36 (s, 2H), 2.20 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 153.31, 146.17, 138.69, 138.27, 136.20, 132.61, 132.11, 131.85, 131.74, 131.52, 131.05, 130.58, 129.60, 128.57, 127.94, 126.51, 125.91, 125.12, 124.23, 123.64, 55.18, 19.56.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{23}H_{19}N_2O_5S$: 435.1015, found: 435.1010.



2-(8-nitroquinolin-3-yl)phenyl (2-bromophenyl)methanesulfonate (3b):
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.2 Hz, 1H), 8.30 (d, *J* = 2.2 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.03 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.50 – 7.42 (m, 4H), 7.38 (dt, *J* = 6.8, 3.4 Hz, 1H), 7.30 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.09 (td, *J* = 7.5, 1.3 Hz, 1H), 7.02 (td, *J* = 7.7, 1.7 Hz, 1H), 4.57 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.28, 148.43, 145.92, 138.68, 136.19, 133.46, 132.62, 132.50, 132.02, 131.84, 131.58, 130.88, 130.59, 128.53, 128.05, 127.91, 126.91, 125.86, 125.63, 124.14, 123.69, 56.91.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{22}H_{15}BrN_2NaO_5S$: 520.9777, found: 520.9771.

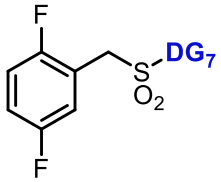


2-(8-nitroquinolin-3-yl)phenyl m-tolylmethanesulfonate (3c):
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (d, *J* = 2.2 Hz, 1H), 8.31 (d, *J* = 2.2 Hz, 1H), 8.09 (d, *J* = 7.5 Hz, 1H), 8.02 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.66 (t, *J* = 7.9 Hz, 1H), 7.49 – 7.43 (m, 3H), 7.40 (dd, *J* = 7.0, 5.7 Hz, 1H), 7.09 – 6.97 (m, 4H), 4.25 (s, 2H), 2.22 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 153.34, 146.28, 138.87, 138.68, 136.18, 132.67, 132.01, 131.79, 131.41, 131.32, 130.56, 130.18, 128.87, 128.59, 127.93, 127.77, 126.48, 125.88, 124.74, 124.27, 123.54, 57.68, 21.35.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{23}H_{19}N_2O_5S$: 435.1015, found: 435.1008.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{22}H_{14}F_2N_2NaO_5S$: 479.0483, found: 479.0485.



2-(8-nitroquinolin-3-yl)phenyl (3-chlorophenyl)methanesulfonate (3g):
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.30 (d, *J* = 1.4 Hz, 1H), 8.13 (d, *J* = 7.5 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.55 – 7.46 (m, 4H), 7.23 (d, *J* = 4.1 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 4.28 (s, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 153.25, 146.01, 138.72, 136.13, 134.84, 132.62, 131.95, 131.37, 130.68, 130.65, 130.26, 129.64, 128.86, 128.58, 128.11, 126.11, 126.04, 124.32, 123.51, 56.98.

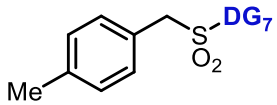
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{22}H_{15}ClN_2NaO_5S$: 477.0282, found: 477.0285.



2-(8-nitroquinolin-3-yl)phenyl (2,5-difluorophenyl)methanesulfonate (3l):

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.05 (d, *J* = 2.2 Hz, 1H), 8.31 (d, *J* = 2.2 Hz, 1H), 8.09 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.09 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.05 (dd, *J* = 8.3, 1.2 Hz, 1H), 8.05 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.66 (d, *J* = 7.7 Hz, 1H), 7.51 – 7.48 (m, 2H), 7.48 – 7.44 (m, 1H), 6.98 (ddd, *J* = 8.2, 5.4, 2.8 Hz, 1H), 6.87 (tdt, *J* = 9.3, 8.0, 4.7 Hz, 1H), 4.35 (s, 2H

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.15, 145.91, 138.69, 136.14, 132.80, 132.57, 132.25, 132.17, 131.96, 131.90, 131.45, 130.64, 128.99, 128.89, 128.51, 128.18, 126.00, 124.27, 123.45, 118.63, 117.18, 50.31.

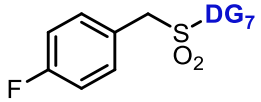


2-(8-nitroquinolin-3-yl)phenyl p-tolylmethanesulfonate (3n):

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.13 (s, 1H), 8.32 (s, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 1H), 7.50 – 7.36 (m, 4H), 7.09 (d, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 4.26 (s, 2H), 2.25 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.39, 148.32, 146.36, 139.46, 138.65, 136.20, 132.63, 132.02, 131.77, 131.15, 130.62, 130.53, 129.74, 128.62, 127.88, 125.89, 124.27, 123.57, 123.45, 57.47, 21.34.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{22}H_{15}FN_2NaO_5S$: 461.0577, found: 461.0570.

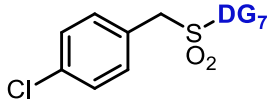


2-(8-nitroquinolin-3-yl)phenyl (4-fluorophenyl)methanesulfonate (3o):

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (d, *J* = 2.2 Hz, 1H), 8.28 (d, *J* = 2.2 Hz, 1H), 8.11 (dt, *J* = 4.6, 2.3 Hz, 1H), 8.02 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.67 (dd, *J* = 8.2, 7.6 Hz, 1H), 7.52 – 7.40 (m, 4H), 7.21 – 7.16 (m, 2H), 6.91 – 6.85 (m, 2H), 4.26 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.32, 148.31, 146.09, 138.66, 136.13, 132.62, 132.55, 131.99, 131.85, 131.26, 130.62, 128.55, 128.04, 126.06, 124.43, 123.49, 122.61, 116.25, 116.07, 56.83.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{23}H_{19}N_2O_5S$: 435.1015, found: 435.1008.

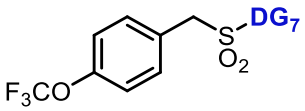


2-(8-nitroquinolin-3-yl)phenyl (4-chlorophenyl)methanesulfonate (3p):

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (t, *J* = 3.7 Hz, 1H), 8.28 (d, *J* = 2.1 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.00 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.66 (t, *J* = 7.9 Hz, 1H), 7.49 – 7.39 (m, 4H), 7.17 – 7.11 (m, 4H), 4.26 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.25, 148.21, 146.08, 138.58, 136.08, 135.59, 132.53, 131.99, 131.88, 131.84, 131.13, 130.57, 129.23, 128.50, 128.04, 126.07, 125.25, 124.45, 123.39, 56.84.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{22}H_{15}ClN_2NaO_5S$: 477.0282, found: 477.0288.

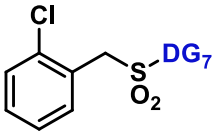


2-(8-nitroquinolin-3-yl)phenyl (4-(trifluoromethoxy)phenyl)methanesulfonate (3q):

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 2.2 Hz, 1H), 8.32 (d, *J* = 2.2 Hz, 1H), 8.04 (ddd, *J* = 12.7, 7.9, 1.2 Hz, 2H), 7.67 – 7.60 (m, 1H), 7.50 – 7.42 (m, 3H), 7.36 – 7.32 (m, 1H), 7.26 (s, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 4.29 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.24, 149.87, 148.18, 146.19, 138.53, 136.10, 132.49, 132.37, 131.92, 131.81, 131.08, 130.54, 128.52, 128.04, 126.06, 125.45, 124.32, 123.23, 121.25, 56.70.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{23}H_{15}F_3N_2NaO_6S$: 527.0495, found: 527.0492.

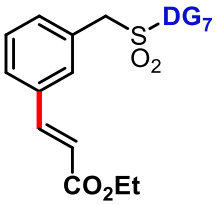


2-(8-nitroquinolin-3-yl)phenyl (2-chlorophenyl)methanesulfonate (8b):

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 – 9.03 (m, 1H), 8.29 (d, *J* = 2.1 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.05 – 7.98 (m, 1H), 7.67 – 7.61 (m, 1H), 7.50 – 7.42 (m, 4H), 7.30 – 7.27 (m, 1H), 7.20 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.10 (td, *J* = 7.7, 1.7 Hz, 1H), 7.04 (td, *J* = 7.5, 1.3 Hz, 1H), 4.54 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.24, 148.40, 145.95, 138.65, 136.17, 135.17, 132.59, 132.52, 132.01, 131.83, 131.53, 130.74, 130.56, 130.08, 128.52, 128.00, 127.27, 125.86, 125.11, 124.13, 123.58, 54.40.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{22}H_{15}ClN_2NaO_5S$: 477.0282, found: 477.0280.



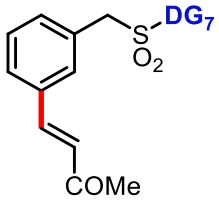
(E)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (2a):

The compound was synthesized following the general procedure A in 0.2 mmol scale at room temperature for 48 hour. The pure compound was purified through silica column using ethyl acetate: petroleum ether (20:80) mixture as the eluent. Whitesolid. Yield 75%; (mono:di 7:1) 68 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (d, *J* = 2.0 Hz, 1H), 8.26 (d, *J* = 2.0 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.99 (d, *J* = 8.3 Hz, 1H), 7.64 (t, *J* = 7.9 Hz, 1H), 7.48 (m, 5H), 7.34 (d, *J* = 4.5 Hz, 2H), 7.24 – 7.16 (m, 2H), 6.29 (d, *J* = 16.0 Hz, 1H), 4.30 (s, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.70, 153.17, 148.34, 146.03, 143.23, 138.58, 136.02, 135.22, 132.54, 132.18, 131.90, 131.87, 131.33, 130.56, 130.08, 129.57, 128.76, 128.49, 128.02, 127.60, 125.91, 124.19, 123.46, 119.55, 60.78, 57.21, 14.46.

HRMS (*m*/*z*): $[M + H]^+$calcd for $C_{27}H_{23}N_2O_7S$: 519.1226, found: 519.1224



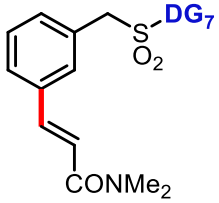
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-(3-oxobut-1-enyl)phenyl)methanesulfonate(2b):

The compound was synthesized following the general procedure A in 0.2 mmol scale at room temperature for 48 hour. The pure compound was purified through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Whitesolid. Yield 65%; (mono:di 13:1) 59 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.01 (d, *J* = 1.8 Hz, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 8.05 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.98 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.62 (t, *J* = 7.9 Hz, 1H), 7.52 – 7.39 (m, 4H), 7.37 – 7.33 (m, 2H), 7.29 (d, *J* = 16.3 Hz, 1H), 7.20 (dd, *J* = 7.8, 5.5 Hz, 2H), 6.55 (d, *J* = 16.3 Hz, 1H), 4.31 (s, 2H), 2.33 (d, *J* = 11.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 198.37, 153.15, 148.29, 145.91, 142.05, 138.51, 136.00, 135.23, 132.56, 132.40, 131.89, 131.29, 130.58, 130.26, 129.62, 128.99, 128.49, 128.07, 128.04, 127.66, 125.92, 124.16, 123.47, 57.14, 27.75.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{26}H_{20}N_2NaO_6S$: 511.0934, found: 511.0937.



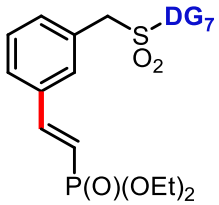
(E)-2-(8-nitroquinolin-3-yl)phenyl(3-(3-(dimethylamino)-3-oxoprop-1-enyl)phenyl)-methanesulfonate(2c):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as brown viscous liquid through silica column using ethyl acetate: pet ether (50:50) mixture as the eluent. Yield 74%, 77 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 8.05 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.97 (d, *J* = 4.8 Hz, 1H), 7.62 (t, *J* = 7.9 Hz, 1H), 7.48 – 7.38 (m, 5H), 7.37 – 7.30 (m, 2H), 7.15 (dd, *J* = 6.5, 2.2 Hz, 2H), 6.81 (d, *J* = 15.5 Hz, 1H), 4.29 (s, 2H), 3.15 (s, 3H), 3.04 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.43, 153.14, 148.20, 145.99, 141.03, 138.50, 136.12, 136.05, 132.63, 131.87, 131.81, 131.46, 131.27, 130.53, 129.75, 129.38, 128.69, 128.48, 128.00, 127.39, 125.94, 124.21, 123.43, 118.69, 57.24, 37.60, 36.09.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{23}N_3NaO_6S$: 540.1200, found: 540.1191.



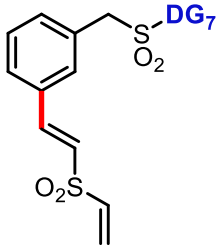
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-(diethoxyphosphoryl)vinyl)phenyl)methane-sulfonate(2d):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (60:40) mixture as the eluent. Yield 72%, 84 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.0 Hz, 1H), 8.28 (d, *J* = 2.1 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.01 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.68 – 7.63 (m, 1H), 7.48 – 7.42 (m, 4H), 7.38 – 7.31 (m, 3H), 7.19 (dd, *J* = 4.8, 1.7 Hz, 2H), 6.24 – 6.15 (m, 1H), 4.28 (s, 2H), 4.17 – 4.07 (m, 4H), 1.34 (t, *J* = 7.1 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.20, 148.37, 147.40, 147.34, 146.09, 138.61, 136.09, 135.83, 135.60, 132.56, 132.21, 131.95, 131.86, 131.36, 130.61, 129.86, 129.57, 128.52, 128.50, 128.08, 127.56, 126.05, 124.24, 123.51, 116.65, 114.75, 62.20, 62.14, 57.26, 16.61, 16.55.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{28}H_{27}N_2NaO_8PS$: 605.1118: 372.1795, found: 605.1111.



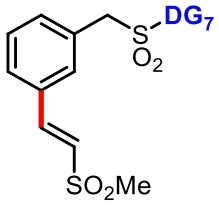
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-(vinylsulfonyl)vinyl)phenyl)methanesulfonate (2e):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (35:65) mixture as the eluent. Yield 40%, 43 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (d, *J* = 2.1 Hz, 1H), 8.26 (d, *J* = 2.1 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.01 (dt, *J* = 7.0, 3.5 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.51 – 7.47 (m, 2H), 7.46 – 7.42 (m, 2H), 7.42 – 7.36 (m, 1H), 7.34 (s, 1H), 7.31 (dt, *J* = 6.9, 1.7 Hz, 1H), 7.26 – 7.18 (m, 2H), 6.76 – 6.61 (m, 2H), 6.51 – 6.40 (m, 1H), 6.15 – 6.08 (m, 1H), 4.30 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.14, 148.35, 145.85, 143.06, 138.55, 137.62, 136.03, 133.28, 133.14, 132.58, 131.95, 131.39, 130.67, 130.54, 129.89, 129.38, 128.50, 128.18, 127.99, 126.88, 126.17, 124.30, 123.54, 57.03.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{26}H_{20}N_2NaO_7S_2$: 559.0604, found: 559.0598.



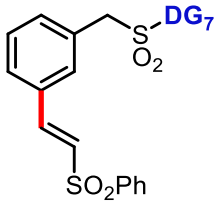
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-(methylsulfonyl)vinyl)phenyl)methanesulfonate (2f):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (40:60) mixture as the eluent. Yield 62%, 65 mg mono olefinatedsolid product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.99 (d, *J* = 2.1 Hz, 1H), 8.26 (d, *J* = 2.1 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.1 Hz, 1H), 8.03 – 8.00 (m, 1H), 7.66 (t, *J* = 7.9 Hz, 1H), 7.49 (q, *J* = 3.7 Hz, 2H), 7.47 – 7.42 (m, 2H), 7.40 (t, *J* = 11.1 Hz, 1H), 7.36 (s, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 7.25 (s, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 15.5 Hz, 1H), 4.30 (s, 2H), 3.04 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.14, 148.28, 145.79, 142.53, 138.49, 136.03, 133.19, 132.95, 132.62, 131.93, 131.36, 130.66, 130.53, 129.82, 129.36, 128.48, 128.17, 127.99, 127.64, 126.13, 124.28, 123.53, 57.02, 43.32.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{25}H_{20}N_2NaO_7S_2$: 547.0604, found: 547.0611.



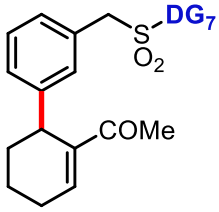
(E)-8-nitro-3-(2-((3-(2-(phenylsulfonyl)vinyl)benzylsulfonyl)methyl)phenyl)quinoline (2g):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (50:50) mixture as the eluent. Yield 71%, 83 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, *J* = 2.1 Hz, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 8.05 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.99 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.95 – 7.90 (m, 2H), 7.66 – 7.59 (m, 2H), 7.55 (t, *J* = 7.5 Hz, 2H), 7.46 (ddd, *J* = 12.2, 5.9, 3.9 Hz, 5H), 7.32 – 7.27 (m, 2H), 7.20 (dd, *J* = 6.3, 4.2 Hz, 2H), 6.81 – 6.76 (m, 1H), 4.28 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.14, 148.35, 145.85, 143.06, 138.55, 137.62, 136.03, 133.28, 133.14, 132.58, 131.95, 131.39, 130.67, 130.54, 129.89, 129.38, 128.50, 128.18, 127.99, 126.88, 126.17, 124.30, 123.54, 57.03.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{30}H_{23}N_2O_7S_2$: 587.0947, found: 587.0947.



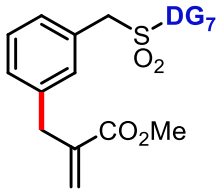
(S)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-acetylcyclohex-2-enyl)phenyl)methanesulfonate (2h):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as viscous compound through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 70%, 76 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 2.1 Hz, 1H), 8.35 (d, *J* = 2.1 Hz, 1H), 8.11 – 8.04 (m, 2H), 7.68 – 7.63 (m, 1H), 7.44 (tdt, *J* = 11.2, 7.5, 3.9 Hz, 3H), 7.18 – 7.06 (m, 4H), 7.01 (d, *J* = 8.7 Hz, 2H), 4.26 (d, *J* = 2.4 Hz, 2H), 3.95 (s, 1H), 2.37 (dd, *J* = 16.9, 5.1 Hz, 1H), 2.18 (s, 3H), 1.80 (tdd, *J* = 12.9, 5.6, 3.2 Hz, 2H), 1.67 – 1.59 (m, 1H), 1.40 (dddd, *J* = 23.4, 13.1, 10.4, 7.1 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 198.63, 153.43, 148.41, 146.54, 146.29, 142.98, 140.75, 138.70, 136.21, 132.70, 132.09, 131.66, 131.23, 130.56, 130.14, 129.12, 128.98, 128.71, 128.41, 127.85, 126.51, 125.92, 124.21, 123.50, 57.93, 38.35, 31.18, 26.26, 25.89, 16.87.

HRMS (*m*/*z*): $[M + Na]^+$ calculated. for $C_{30}H_{26}N_2NaO_6S$: 565.1404, found: 565.1399.



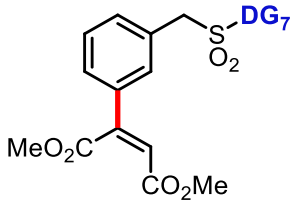
Methyl 2-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)benzyl)acrylate (2i):

The compound was synthesized following the general procedure A in 0.2 mmol scale at room temperature for 48 hour. The pure compound was purified as viscous compound through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 65%, 67 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (d, *J* = 2.1 Hz, 1H), 8.32 (d, *J* = 2.1 Hz, 1H), 8.08 (ddd, *J* = 7.0, 3.9, 1.0 Hz, 1H), 8.03 (t, *J* = 6.2 Hz, 1H), 7.66 (dd, *J* = 10.2, 5.5 Hz, 1H), 7.45 (qd, *J* = 9.0, 4.4 Hz, 3H), 7.33 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.14 – 7.04 (m, 4H), 6.19 (s, 1H), 5.43 (d, *J* = 0.9 Hz, 1H), 4.26 (s, 2H), 3.67 (s, 3H), 3.51 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.28, 153.33, 148.35, 146.30, 139.80, 139.59, 138.66, 136.17, 132.65, 132.02, 131.77, 131.46, 131.29, 130.55, 130.11, 129.12, 128.81, 128.60, 127.95, 126.90, 126.77, 125.94, 124.27, 123.52, 57.64, 52.11, 37.95.

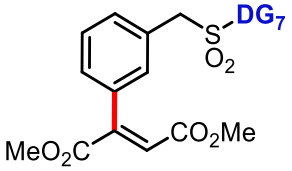
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{22}N_2NaO_7S$: 541.1040, found: 541.1041.



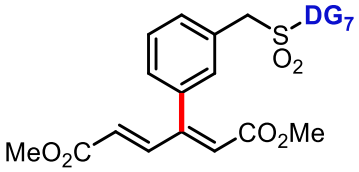
Dimethyl 2-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)maleate (2j):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 120 °C for 36 hour. The pure compound was purified as pale white solid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 55%, 62 mg mono olefinated product was isolated.

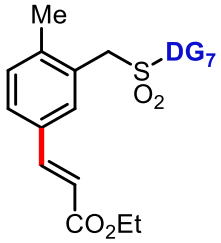
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.16 (d, *J* = 2.2 Hz, 1H), 8.38 (d, *J* = 2.2 Hz, 1H), 8.09 – 8.05 (m, 2H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.50 – 7.41 (m, 4H), 7.25 – 7.23 (m, 2H), 7.22 – 7.18 (m, 2H), 7.02 (s, 1H), 4.28 (d, *J* = 6.5 Hz, 2H), 3.76 (s, 3H), 3.55 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.38, 165.43, 153.43, 148.33, 146.45, 143.13, 138.69, 136.24, 134.76, 132.69, 132.05, 131.67, 131.44, 131.25, 130.98, 130.61, 130.08, 129.66, 128.67, 128.60, 127.96, 126.48, 125.98, 124.31, 123.64, 57.60, 53.19, 52.16.



Dimethyl 2-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)maleate (2k):
The compound was synthesized following the general procedure A in 0.2 mmol scale at 120 °C for 36 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 82% (mon:di – 7:1), 80 mg mono olefinated product was isolated.
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.0 Hz, 1H), 8.27 (d, *J* = 2.0 Hz, 1H), 8.09 – 8.06 (m, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.9 Hz, 1H), 7.48 – 7.40 (m, 4H), 7.35 (s, 1H), 7.31 (d, *J* = 7.3 Hz, 1H), 7.25 – 7.17 (m, 2H), 6.21 (s, 1H), 4.29 (s, 2H), 3.89 (s, 3H), 3.78 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.03, 165.35, 153.25, 148.38, 147.76, 146.03, 138.66, 136.09, 134.09, 132.63, 131.94, 131.92, 131.39, 130.64, 129.78, 128.99, 128.56, 128.14, 127.92, 127.73, 126.02, 124.29, 123.57, 118.51, 57.20, 53.04, 52.38.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{28}H_{22}N_2NaO_9S$: 585.0938, found: 585.0933.



(2Z,4Z)-dimethyl3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)hexa-2,4-dienedio-ate (2l):
The compound was synthesized following the general procedure A in 0.2 mmol scale at 120 °C for 36 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (28:72) mixture as the eluent. Yield 35%, 41 mg mono olefinated product was isolated.
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 – 9.05 (m, 1H), 8.65 (dd, *J* = 16.1, 0.8 Hz, 1H), 8.32 (d, *J* = 2.1 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.04 (dt, *J* = 12.2, 3.9 Hz, 1H), 7.68 – 7.60 (m, 1H), 7.52 – 7.43 (m, 4H), 7.41 – 7.37 (m, 1H), 7.21 – 7.12 (m, 3H), 5.94 – 5.87 (m, 1H), 5.74 (d, *J* = 16.1 Hz, 1H), 4.30 (s, 2H), 3.79 (s, 3H), 3.74 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.78, 165.71, 153.27, 151.36, 148.33, 146.12, 140.06, 139.19, 138.63, 136.09, 132.56, 132.07, 131.89, 131.36, 131.31, 131.01, 130.63, 129.82, 129.41, 128.61, 128.11, 128.04, 127.31, 126.05, 124.34, 123.72, 123.50, 57.35, 52.16, 52.03.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{30}H_{24}N_2NaO_9S$: 611.1095, found: 611.1097.



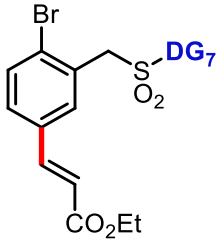
(*E*)-ethyl 3-(4-methyl-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4a):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as pale whitesolid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 90%, 96 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.04 (d, *J* = 1.9 Hz, 1H), 8.26 (d, *J* = 1.8 Hz, 1H), 8.07 (d, *J* = 7.5 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.62 (t, *J* = 7.9 Hz, 1H), 7.49 (ddd, *J* = 10.8, 6.5, 3.4 Hz, 1H), 7.43 (dd, *J* = 18.0, 10.2 Hz, 4H), 7.28 (s, 1H), 7.20 (t, *J* = 10.9 Hz, 1H), 7.06 (d, *J* = 7.9 Hz, 1H), 6.23 (d, *J* = 16.0 Hz, 1H), 4.35 (s, 2H), 4.25 (dd, *J* = 14.0, 6.8 Hz, 2H), 2.21 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.92, 153.14, 148.40, 145.93, 143.26, 140.55, 138.64, 136.07, 132.86, 132.54, 132.02, 131.88, 131.70, 131.62, 131.44, 130.64, 128.80, 128.49, 128.08, 125.95, 125.91, 124.20, 123.67, 118.54, 60.72, 54.74, 19.58,14.51.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{28}H_{24}N_2NaO_7S$: 555.1196, found: 555.1198.



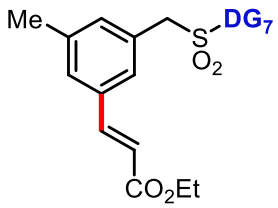
(*E*)-ethyl 3-(4-bromo-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4b):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 82%, 74 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.97 (d, *J* = 2.1 Hz, 1H), 8.23 (d, *J* = 2.1 Hz, 1H), 8.03 (d, *J* = 7.4 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.49 (ddd, *J* = 12.8, 7.9, 6.6 Hz, 2H), 7.45 – 7.36 (m, 4H), 7.29 (t, *J* = 10.7 Hz, 1H), 7.12 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.21 (d, *J* = 16.0 Hz, 1H), 4.53 (s, 2H), 4.22 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.52, 153.11, 145.69, 141.95, 138.58, 136.07, 134.29, 134.09, 132.57, 131.97, 131.93, 131.64, 131.58, 130.66, 129.74, 128.44, 128.19, 127.67, 127.15, 125.87, 124.16, 123.70, 120.16, 60.95, 56.40, 14.50.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{27}H_{22}BrN_2O_7S$: 597.0326, found: 597.0324.



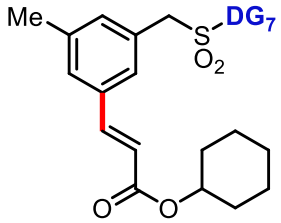
(*E*)-ethyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4c):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour in HFIP. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 94%, 100 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.04 (d, *J* = 2.1 Hz, 1H), 8.27 (d, *J* = 2.1 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.45 (tt, *J* = 18.7, 10.5 Hz, 5H), 7.14 (s, 2H), 7.02 (s, 1H), 6.28 (d, *J* = 16.0 Hz, 1H), 4.28 – 4.21 (m, 4H), 2.22 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.83, 153.19, 148.29, 146.03, 143.48, 139.62, 138.56, 136.05, 135.11, 133.08, 132.65, 131.89, 131.35, 130.59, 129.64, 128.48, 128.06, 127.34, 125.90, 124.31, 123.55, 119.24, 60.77, 57.18, 21.20, 14.49.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{28}H_{24}N_2NaO_7S$: 555.1196, found: 555.1199.



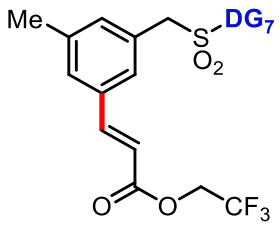
(*E*)-cyclohexyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)-acrylate (4d):

The compound was synthesized following the general procedure A in 0.1 mmol scale at 80 °C for 24 hour in HFIP solvent. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 92%, 54 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (d, *J* = 2.2 Hz, 1H), 8.27 (d, *J* = 2.2 Hz, 1H), 8.06 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.98 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.60 (dt, *J* = 12.2, 6.1 Hz, 1H), 7.48 – 7.42 (m, 4H), 7.42 – 7.36 (m, 1H), 7.14 (s, 2H), 7.01 (s, 1H), 6.28 (d, *J* = 16.0 Hz, 1H), 4.91 – 4.82 (m, 1H), 4.26 (s, 2H), 2.22 (s, 3H), 1.90 (dd, *J* = 9.1, 4.0 Hz, 2H), 1.76 (dd, *J* = 8.8, 3.6 Hz, 2H), 1.60 – 1.52 (m, 1H), 1.50 – 1.42 (m, 2H), 1.42 – 1.32 (m, 2H), 1.32 – 1.24 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.22, 153.13, 148.21, 146.01, 143.12, 139.55, 138.51, 136.02, 135.14, 132.98, 132.63, 131.86, 131.83, 131.31, 130.55, 129.59, 128.44, 128.03, 127.27, 125.88, 124.27, 123.51, 119.79, 73.00, 57.13, 31.86, 25.54, 23.94, 21.16.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{32}H_{30}N_2NaO_7S$: 609.1666, found: 609.1666.



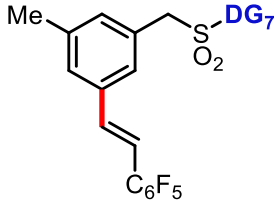
(*E*)-2,2,-difluoroethyl3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4e):

The compound was synthesized following the general procedure A in 0.1 mmol scale at 80 °C for 24 hour in HFIP solvent. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 89%, 52 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (d, *J* = 2.1 Hz, 1H), 8.27 (d, *J* = 2.2 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.98 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.64 – 7.59 (m, 1H), 7.53 – 7.47 (m, 3H), 7.47 – 7.44 (m, 2H), 7.18 (s, 1H), 7.16 (s, 1H), 7.07 (s, 1H), 6.32 (d, *J* = 16.0 Hz, 1H), 4.72 (t, *J* = 13.7 Hz, 2H), 4.27 (s, 2H), 2.26 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 164.99, 153.17, 148.34, 146.00, 145.96, 139.85, 138.56, 136.01, 134.48, 133.74, 132.59, 131.95, 131.92, 131.37, 130.63, 129.93, 128.50, 128.11, 127.56, 127.53, 125.90, 124.27, 123.57, 116.85, 60.57 (q, *J* = 365 Hz), 57.10, 21.20.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{32}H_{30}N_2NaO_7S$: 609.1666, found: 609.1664.



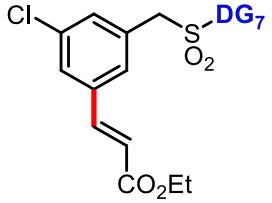
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-methyl-5-(perfluorostyryl)phenyl)methanesulfonate (4f):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour in HFIP solvent. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (15:85) mixture as the eluent. Yield 77%, 96 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (d, *J* = 1.9 Hz, 1H), 8.30 (d, *J* = 1.9 Hz, 1H), 8.05 (d, *J* = 6.9 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.52 – 7.42 (m, 4H), 7.22 – 7.12 (m, 3H), 6.98 (s, 1H), 6.82 (d, *J* = 16.8 Hz, 1H), 4.29 (s, 2H), 2.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.20, 148.26, 146.10, 139.50, 138.57, 137.13, 136.25, 136.17, 136.07, 132.64, 131.88, 131.31, 130.59, 128.52, 128.45, 128.05, 127.25, 126.41, 125.79, 124.23, 123.55, 113.61, 57.31, 21.25.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{31}H_{20}F_5N_2O_5S$: 627.1008, found: 627.0999.



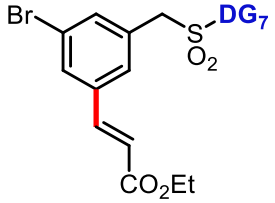
(*E*)-ethyl 3-(3-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)-acrylate (4g)

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour in HFIP solvent. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 90%, 99 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, *J* = 1.9 Hz, 1H), 8.30 (dd, *J* = 12.7, 2.1 Hz, 1H), 8.09 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.01 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.65 (dd, *J* = 8.1, 7.6 Hz, 1H), 7.52 – 7.48 (m, 2H), 7.47 (dt, *J* = 4.0, 2.2 Hz, 2H), 7.41 – 7.35 (m, 1H), 7.32 (t, *J* = 1.6 Hz, 1H), 7.20 (dd, *J* = 3.2, 1.6 Hz, 2H), 6.32 – 6.27 (m, 1H), 4.30 – 4.22 (m, 4H), 1.34 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.32, 153.13, 148.28, 145.87, 141.64, 138.63, 136.90, 136.03, 135.49, 132.63, 132.00, 131.80, 131.32, 130.67, 129.24, 128.67, 128.47, 128.33, 128.25, 126.04, 124.46, 123.51, 121.03, 61.01, 56.56, 14.45.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{21}ClN_2NaO_7S$: 575.0650, found: 575.0654.



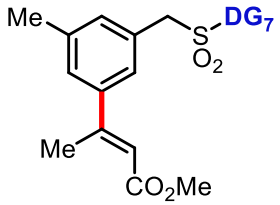
(*E*)-ethyl 3-(3-bromo-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4h):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour in HFIP solvent. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 92%, 110 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.06 (s, 1H), 8.28 (s, 1H), 8.08 (d, *J* = 7.4 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.52 – 7.42 (m, 5H), 7.36 (d, *J* = 18.5 Hz, 2H), 7.25 (s, 1H), 6.29 (d, *J* = 16.0 Hz, 1H), 4.28 – 4.20 (m, 4H), 1.33 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.28, 153.12, 148.26, 145.88, 141.53, 138.62, 137.10, 136.03, 134.65, 132.65, 131.99, 131.77, 131.60, 131.30, 130.66, 129.45, 128.76, 128.47, 128.24, 126.04, 124.46, 123.49, 123.40, 121.04, 60.99, 56.48, 14.44.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{27}H_{22}BrN_2O_7S$: 597.0326, found: 597.0368.



(*E*)-methyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)but-2-enoate (4i):

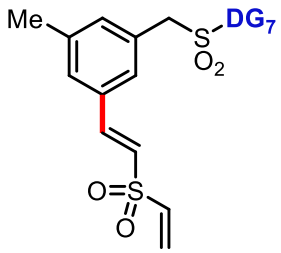
The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour in HFIP solvent. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 73%, 74 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (t, *J* = 4.2 Hz, 1H), 8.32 (d, *J* = 2.2 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.01 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.51 – 7.42 (m, 4H),

7.15 (s, 1H), 7.12 (s, 1H), 7.02 (s, 1H), 5.97 (d, J = 1.2 Hz, 1H), 4.25 (s, 2H), 3.74 (s, 3H), 2.44 (d, J = 1.2 Hz, 3H), 2.25 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.17, 154.81, 153.25, 148.27, 146.18, 142.84, 139.26, 138.59, 136.08, 132.62, 132.01, 131.96, 131.88, 131.29, 130.61, 128.54, 128.22, 128.08, 126.86, 125.95, 125.87, 124.34, 123.55, 117.37, 57.42, 51.38, 21.36, 18.02.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{28}H_{24}N_2NaO_7S$: 555.1196, found: 555.1199.



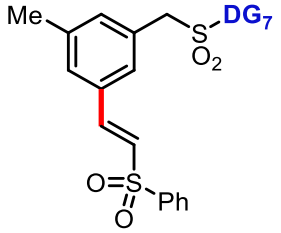
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-methyl-5-(2-(vinylsulfonyl)vinyl)phenyl)methanesulfonate (4j):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour in HFIP. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (40:60) mixture as the eluent. Yield 58%, 64 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (d, J = 1.4 Hz, 1H), 8.27 (d, J = 2.1 Hz, 1H), 8.11 – 8.05 (m, 1H), 8.01 (d, J = 8.3 Hz, 1H), 7.66 (td, J = 8.2, 1.9 Hz, 1H), 7.53 – 7.43 (m, 4H), 7.34 (d, J = 15.4 Hz, 1H), 7.13 (s, 1H), 7.11 (s, 1H), 7.07 (s, 1H), 6.74 – 6.59 (m, 2H), 6.43 (dd, J = 16.6, 2.0 Hz, 1H), 6.10 (dd, J = 9.8, 1.3 Hz, 1H), 4.26 (s, 2H), 2.22 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.08, 148.26, 145.88, 143.27, 140.01, 138.48, 137.69, 136.02, 134.14, 133.01, 132.61, 131.93, 131.89, 131.38, 130.63, 130.13, 129.16, 128.45, 128.14, 127.80, 127.75, 126.51, 126.14, 124.33, 123.54, 56.98, 21.16.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{22}N_2NaO_7S_2$: 573.0761, found: 573.0766.

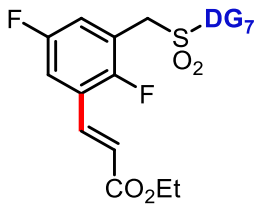


(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-methyl-5-(2-(phenylsulfonyl)vinyl)phenyl)methanesulfonate (4k):

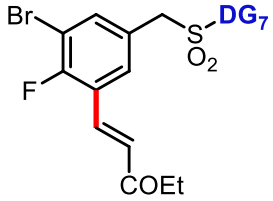
The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate:pet ether (50:50) mixture as the eluent. Yield 86%, 103 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, J = 1.5 Hz, 1H), 8.27 (d, J = 2.0 Hz, 1H), 8.05 (dd, J = 7.5, 1.1 Hz, 1H), 7.99 (d, J = 8.2 Hz, 1H), 7.94 – 7.88 (m, 2H), 7.64 – 7.59 (m, 2H), 7.57 – 7.51 (m, 2H), 7.51 – 7.46 (m, 2H), 7.46 – 7.38 (m, 3H), 7.10 (s, 2H), 7.04 (s, 1H), 6.77 (d, J = 15.4 Hz, 1H), 4.24 (s, 2H), 2.21 (s, 3H).

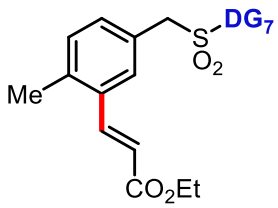
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.04, 148.20, 145.90, 141.36, 140.59, 139.94, 138.45, 136.04, 134.00, 133.67, 132.97, 132.61, 131.91, 131.83, 131.34, 130.60, 130.02, 129.54, 128.41, 128.23, 128.12, 127.84, 127.62, 126.14, 124.34, 123.51, 56.92, 21.12.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{31}H_{24}N_2NaO_7S_2$: 623.0917, found: 623.0915.



(*E*)-ethyl 3-(2,5-difluoro-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)-acrylate (4l):
The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour in HFIP solvent. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 85%, 94 mg mono olefinated product was isolated.
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.05 (s, 1H), 8.31 (s, 1H), 8.09 (d, *J* = 7.3 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.65 (t, *J* = 7.7 Hz, 1H), 7.56 (d, *J* = 16.2 Hz, 1H), 7.51 (s, 2H), 7.48 (d, *J* = 11.2 Hz, 2H), 7.11 (s, 1H), 7.01 (s, 1H), 6.40 (d, *J* = 16.2 Hz, 1H), 4.37 (s, 2H), 4.28 (q, *J* = 7.0 Hz, 2H), 1.35 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.19, 153.10, 148.34, 145.83, 138.66, 136.10, 134.84, 132.55, 132.05, 131.88, 131.47, 130.69, 128.49, 128.30, 126.07, 124.40, 123.49, 123.18, 123.14, 120.23, 120.03, 116.33, 116.13, 61.15, 50.27, 14.46.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{20}F_2N_2NaO_7S$: 577.0857, found: 577.0852.



(*E*)-ethyl 3-(3-bromo-2-fluoro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-phenyl)acrylate (4m):
The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (32:68) mixture as the eluent. Yield 72%, 86 mg mono olefinated product was isolated.
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.08 (d, *J* = 2.0 Hz, 1H), 8.29 (dd, *J* = 17.3, 2.2 Hz, 1H), 8.10 (d, *J* = 7.5 Hz, 1H), 7.99 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.67 (t, *J* = 7.9 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.48 (dt, *J* = 5.8, 2.3 Hz, 2H), 7.43 (dd, *J* = 9.1, 7.0 Hz, 2H), 7.36 – 7.32 (m, 1H), 6.66 (d, *J* = 16.4 Hz, 1H), 4.22 (s, 2H), 2.70 (q, *J* = 7.2 Hz, 2H), 1.16 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 200.45, 153.17, 148.30, 145.83, 138.66, 136.52, 136.02, 132.53, 132.37, 132.36, 132.02, 131.81, 131.32, 130.75, 130.22, 130.17, 130.07, 128.47, 128.36, 126.20, 124.94, 124.55, 123.60, 110.95, 56.05, 34.65, 8.14.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{20}BrFN_2NaO_6S$: 621.0102, found: 621.0109.



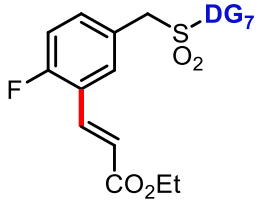
(*E*)-ethyl 3-(2-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4n):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 43%, 46 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (d, *J* = 2.1 Hz, 1H), 8.32 (d, *J* = 2.1 Hz, 1H), 8.09 (d, *J* = 7.5 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.78 (d, *J* = 15.9 Hz, 1H), 7.65 (td, *J* = 7.8, 3.8 Hz, 1H), 7.50 – 7.43 (m, 4H), 7.39 (d, *J* = 1.1 Hz, 1H), 7.09 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.23 (d, *J* = 15.9 Hz, 1H), 4.30 – 4.21 (m, 4H), 2.32 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.90, 153.33, 148.30, 146.26, 141.26, 139.00, 138.63, 136.22, 134.31, 132.65, 131.98, 131.87, 131.56, 131.20, 130.65, 128.66, 128.61, 128.07, 125.97, 124.83, 124.41, 124.39, 123.54, 120.62, 60.87, 57.18, 19.75, 14.51.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{28}H_{24}N_2NaO_7S$: 555.1196, found: 555.1197.



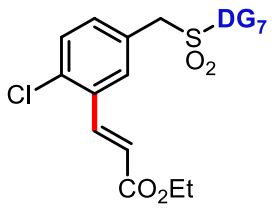
(*E*)-ethyl 3-(2-fluoro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4o):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (28:72) mixture as the eluent. Yield 75% (mono:di – 10:1), 73 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.09 (d, *J* = 2.0 Hz, 1H), 8.26 (d, *J* = 2.1 Hz, 1H), 8.09 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.98 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.57 (d, *J* = 16.2 Hz, 1H), 7.52 – 7.44 (m, 4H), 7.39 (dd, *J* = 6.7, 2.1 Hz, 1H), 7.21 – 7.15 (m, 1H), 6.92 (dd, *J* = 9.9, 8.7 Hz, 1H), 6.40 (d, *J* = 16.2 Hz, 1H), 4.30 – 4.22 (m, 4H), 1.33 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.57, 162.57, 160.53, 153.22, 148.21, 145.94, 138.57, 136.08, 135.98, 133.74, 133.66, 132.53, 131.91, 131.39, 131.37, 131.28, 130.66, 128.49, 128.16, 126.09, 124.51, 123.54, 123.33, 123.24, 122.18, 122.12, 117.15, 116.97, 60.98, 56.52, 14.46.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{21}FN_2NaO_7S$: 559.0946, found: 559.0949.



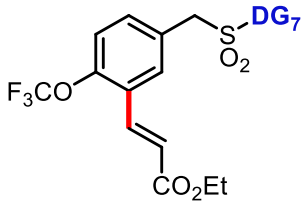
(*E*)-ethyl 3-(2-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4p):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 50%, 55 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 2.1 Hz, 1H), 8.27 (d, *J* = 2.1 Hz, 1H), 8.10 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.98 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.87 (d, *J* = 16.0 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.53 – 7.43 (m, 5H), 7.24 (d, *J* = 4.2 Hz, 1H), 7.15 – 7.11 (m, 1H), 6.30 (d, *J* = 16.0 Hz, 1H), 4.30 – 4.22 (m, 4H), 1.34 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.29, 153.25, 146.01, 139.27, 138.65, 136.06, 133.58, 132.78, 132.53, 131.93, 131.84, 131.22, 130.86, 130.68, 129.78, 128.49, 128.22, 126.15, 126.07, 124.58, 123.54, 122.19, 61.04, 56.68, 14.46.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{27}H_{21}ClN_2NaO_7S$: 575.0650, found: 575.0651.



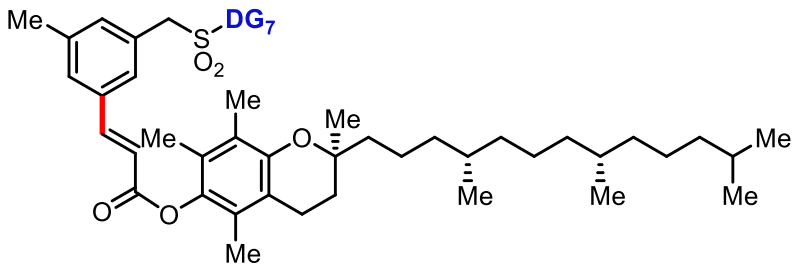
(*E*)-ethyl 3-(5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-2-(trifluoromethoxy)-phenyl)acrylate (4q):

The compound was synthesized following the general procedure A in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 65%, 78 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.14 (d, *J* = 1.8 Hz, 1H), 8.30 (t, *J* = 13.4 Hz, 1H), 8.12 – 7.98 (m, 2H), 7.79 – 7.69 (m, 1H), 7.69 – 7.62 (m, 1H), 7.57 – 7.38 (m, 5H), 7.28 (dd, *J* = 9.7, 7.6 Hz, 1H), 7.16 (dd, *J* = 8.5, 1.4 Hz, 1H), 6.38 (d, *J* = 16.1 Hz, 1H), 4.35 – 4.20 (m, 4H), 1.35 – 1.31 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.24, 153.31, 148.38, 148.05, 146.17, 136.18, 136.09, 133.30, 132.48, 131.96, 131.93, 131.24, 130.72, 130.47, 128.62, 128.26, 126.19, 126.02, 124.49, 123.46, 122.66, 121.74, 61.07, 56.66, 14.44.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{28}H_{21}F_3N_2NaO_8S$: 625.0863, found: 625.0868.



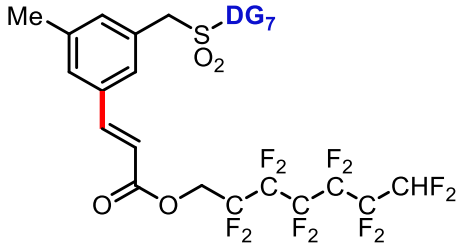
(*E*)-((S)-2,5,7,8-tetramethyl-2-((4S,8S)-4,8,12-trimethyltridecyl)chroman-6-yl) 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (5a):

The compound was synthesized following the general procedure A in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 87%, 76 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.09 (d, *J* = 2.2 Hz, 1H), 8.32 (d, *J* = 2.2 Hz, 1H), 8.09 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.02 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.66 (dd, *J* = 15.9, 8.2 Hz, 2H), 7.51 (ddd, *J* = 5.9, 3.9, 1.4 Hz, 2H), 7.49 – 7.45 (m, 2H), 7.26 – 7.25 (m, 1H), 7.23 (s, 1H), 7.07 (s, 1H), 6.58 (d, *J* = 16.0 Hz, 1H), 4.28 (s, 2H), 2.61 (t, *J* = 6.7 Hz, 2H), 2.27 (s, 3H), 2.11 (s, 3H), 2.05 (s, 3H), 2.01 (s, 3H), 1.86 – 1.74 (m, 3H), 1.63 (d, *J* = 17.5 Hz, 3H), 1.59 – 1.47 (m, 4H), 1.47 – 1.32 (m, 6H), 1.18 – 1.02 (m, 8H), 0.86 (dd, *J* = 8.7, 6.8 Hz, 14H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.49, 153.25, 149.68, 148.39, 146.11, 145.16, 140.62, 139.81, 138.63, 136.11, 135.06, 133.44, 132.62, 131.98, 131.91, 131.41, 130.66, 129.89, 128.55, 128.13, 127.61, 127.44, 126.97, 126.02, 125.23, 124.34, 123.63, 123.28, 118.39, 117.63, 75.29, 57.26, 39.57, 37.60, 37.49, 32.98, 28.19, 25.02, 24.66, 22.93, 22.84, 21.27, 20.83, 19.96, 19.90, 13.26, 12.41, 12.07.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{55}H_{68}N_2NaO_8S$: 939.4594, found 939.4511.



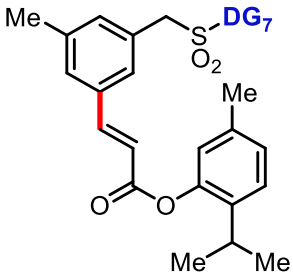
(*E*)-2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)-phenoxysulfonyl)methyl)phenyl)acrylate (5b):

The compound was synthesized following the general procedure A in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 74%, 65 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (d, *J* = 2.1 Hz, 1H), 8.27 (d, *J* = 2.2 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.98 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.64 – 7.59 (m, 1H), 7.53 – 7.42 (m, 5H), 7.18 (s, 1H), 7.16 (s, 1H), 7.07 (s, 1H), 6.32 (d, *J* = 16.0 Hz, 1H), 6.07 (tt, *J* = 51.9, 5.1 Hz, 1H), 4.72 (t, *J* = 13.7 Hz, 2H), 4.27 (s, 2H), 2.26 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.05, 153.20, 148.37, 146.13, 145.97, 139.88, 138.59, 136.03, 134.49, 133.79, 132.60, 131.96, 131.39, 130.65, 129.98, 128.52, 128.14, 127.61, 127.53, 125.91, 124.29, 123.61, 116.80, 57.11, 21.21.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{33}H_{23}F_{12}N_2O_7S$: 819.1029, found: 819.1007.



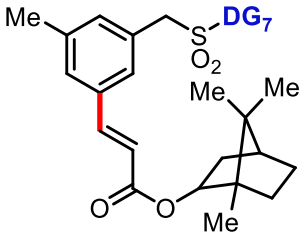
(*E*)-2-isopropyl-5-methylphenyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (5c):

The compound was synthesized following the general procedure A in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (27:73) mixture as the eluent. Yield 89%, 57 mg mono olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.09 (d, *J* = 2.1 Hz, 1H), 8.32 (d, *J* = 2.1 Hz, 1H), 8.09 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.54 – 7.45 (m, 4H), 7.26 (d, *J* = 1.0 Hz, 1H), 7.23 (dt, *J* = 11.5, 5.8 Hz, 2H), 7.10 – 7.03 (m, 2H), 6.89 (s, 1H), 6.55 (dd, *J* = 16.0, 2.7 Hz, 1H), 4.28 (s, 2H), 3.03 (dt, *J* = 13.7, 6.8 Hz, 1H), 2.34 (s, 3H), 2.27 (s, 3H), 1.22 (dd, *J* = 6.9, 2.4 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.57, 153.21, 148.34, 148.05, 146.06, 145.37, 139.79, 138.59, 137.31, 136.78, 136.08, 134.90, 133.52, 132.61, 131.94, 131.91, 131.37, 130.64, 129.91, 128.52, 128.12, 127.61, 127.46, 127.38, 126.66, 125.97, 124.31, 123.58, 122.91, 118.32, 57.19, 29.88, 27.31, 23.28, 21.24, 21.05.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{36}H_{32}N_2NaO_7S$: 659.1822, found: 659.1823.



(*E*)-2-isopropyl-5-methylphenyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (5d):

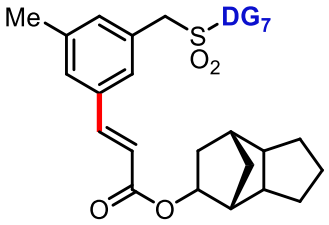
The compound was synthesized following the general procedure A in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 80%, 51 mg mono olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.2 Hz, 1H), 8.29 (d, *J* = 2.2 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.99 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.50 – 7.45 (m, 4H), 7.38 (d, *J* = 16.0 Hz, 1H), 7.15 (s, 2H), 7.01 (s, 1H), 6.27 (d, *J* = 16.0 Hz, 1H), 4.79 (dd, *J* = 7.5, 4.0 Hz, 1H), 4.26 (s, 2H), 2.24 (s, 3H), 1.93 – 1.80 (m, 2H), 1.78 (t, *J* = 4.0 Hz, 1H), 1.62

– 1.54 (m, 1H), 1.25 (d, *J* = 5.0 Hz, 1H), 1.23 – 1.16 (m, 1H), 1.15 – 1.08 (m, 1H), 1.06 (s, 3H), 0.90 (s, 3H), 0.87 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.43, 153.21, 146.07, 143.20, 139.65, 138.60, 136.09, 135.22, 133.06, 132.66, 131.91, 131.38, 130.63, 129.74, 128.51, 128.10, 127.33, 127.28, 125.94, 124.34, 123.60, 119.85, 81.47, 57.22, 49.10, 47.20, 45.26, 39.06, 33.95, 27.26, 21.23, 20.34, 20.27, 11.74.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{37}H_{40}N_2NaO_6S$: 663.2499, found: 663.2499.



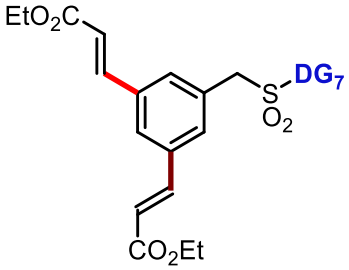
(*E*)-dicyclopentanyl-3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-phenyl)acryl-ate (5e):

The compound was synthesized following the general procedure A in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 95%, 61 mg mono olefinatedproduct was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.05 (d, *J* = 2.0 Hz, 1H), 8.28 (d, *J* = 2.1 Hz, 1H), 8.11 – 8.06 (m, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.63 (td, *J* = 7.9, 2.0 Hz, 1H), 7.50 – 7.44 (m, 4H), 7.38 (d, *J* = 16.0 Hz, 1H), 7.14 (s, 2H), 7.01 (s, 1H), 6.27 (d, *J* = 16.0 Hz, 1H), 4.67 (t, *J* = 10.9 Hz, 1H), 4.25 (s, 2H), 2.23 (s, 3H), 2.22 – 2.12 (m, 2H), 2.10 – 2.03 (m, 1H), 1.89 – 1.71 (m, 5H), 1.52 – 1.46 (m, 1H), 1.37 (q, *J* = 11.0 Hz, 2H), 1.23 (dt, *J* = 12.3, 5.9 Hz, 1H), 1.04 – 0.91 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.67, 153.21, 148.32, 146.05, 143.12, 139.63, 138.60, 136.07, 135.21, 133.02, 132.66, 131.91, 131.38, 130.62, 129.68, 128.50, 128.08, 127.29, 125.93, 124.33, 123.59, 119.80, 57.22, 47.48, 46.41, 43.20, 39.80, 39.33, 32.22, 31.88, 29.66, 27.93, 21.23.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{36}H_{34}N_2NaO_7S$: 661.1979, found: 661.1955.



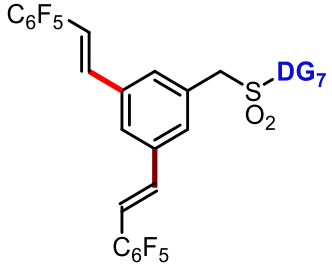
(2*E*,2'*E*)-diethyl 3,3'-(5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-1,3-phenylene)diacrylate (7a):

The compound was synthesized following the general procedure B in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (25:75) mixture as the eluent. Yield 68%, 42 mg homo-di-olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (d, *J* = 2.0 Hz, 1H), 8.26 (d, *J* = 2.0 Hz, 1H), 8.09 – 8.06 (m, 1H), 8.00 – 7.96 (m, 1H), 7.62 (t, *J* = 7.9 Hz, 1H), 7.50 (dd, *J* = 7.3, 4.5 Hz, 4H), 7.46 (t, *J* = 3.6 Hz, 3H), 7.34 (s, 2H), 6.35 (d, *J* = 16.1 Hz, 2H), 4.31 (s, 2H), 4.27 (q, *J* = 7.1 Hz, 4H), 1.35 (t, *J* = 7.1 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.51, 153.12, 148.32, 145.88, 142.39, 138.59, 136.05, 136.00, 132.58, 132.00, 131.85, 131.38, 131.15, 130.68, 128.47, 128.44, 128.28, 128.24, 125.99, 124.40, 123.59, 120.57, 60.97, 56.89, 14.49.

HRMS (*m*/*z*): $[M + H]^+$calcd for $C_{32}H_{29}N_2O_9S$: 617.1594, found: 617.1587



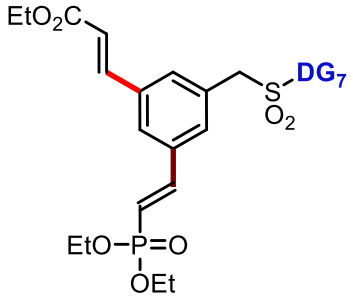
2-(8-nitroquinolin-3-yl)phenyl (3,5-bis(perfluorostyryl)phenyl)methanesulfonate (7b):

The compound was synthesized in 0.1 mmol scale at 80 °C for 24 hour. The di-olefnated product was obtained while the model substrate, phenylmethanesulfonate (**1**),was treated with the standard condition of procedure B. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (18:82) mixture as the eluent. Yield 73%, 59 mg homo-di-olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (d, *J* = 2.2 Hz, 1H), 8.29 (d, *J* = 2.2 Hz, 1H), 8.03 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.95 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.61 – 7.50 (m, 3H), 7.50 – 7.44 (m, 2H), 7.42 (s, 1H), 7.32 (s, 2H), 7.28 (s, 1H), 7.24 (s, 1H), 6.90 (d, *J* = 16.8 Hz, 2H), 4.36 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.15, 148.35, 145.98, 138.62, 137.98, 136.02, 135.52, 135.47, 135.39, 132.60, 132.01, 131.87, 131.38, 130.69, 129.06, 128.53, 128.22, 126.40, 125.78, 124.21, 123.64, 114.75, 112.01, 57.16.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{38}H_{18}F_{10}N_2NaO_5S$: 827.0669, found: 827.0647.



(*E*)-ethyl 3-(3-((E)-2-(diethoxyphosphoryl)vinyl)-5-((2-(8-nitroquinolin-3-yl)phenoxy-sulfonyl)meth-yl)phenyl)acrylate (7c):

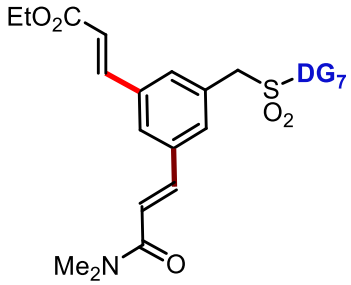
The compound was synthesized following the general procedure B in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (55:45) mixture as the eluent. Yield 65%, 44 mg hetero-di-olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.02 (d, *J* = 2.0 Hz, 1H), 8.29 (d, *J* = 2.0 Hz, 1H), 8.07 (d, *J* = 7.4 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.50 – 7.45 (m, 5H), 7.43 –

7.29 (m, 4H), 6.35 – 6.22 (m, 2H), 4.29 – 4.23 (m, 4H), 4.17 – 4.10 (m, 4H), 1.35 (dt, *J* = 10.6, 7.1 Hz, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.46, 153.08, 148.30, 146.52, 146.46, 145.90, 142.34, 138.55, 136.03, 135.99, 132.56, 131.96, 131.85, 131.38, 131.13, 131.06, 130.68, 128.46, 128.37, 128.26, 127.89, 126.09, 124.37, 123.60, 120.51, 62.29, 62.25, 60.94, 56.87, 16.63, 16.58, 14.47.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{33}H_{34}N_2O_{10}PS$: 681.1666, found: 681.1666



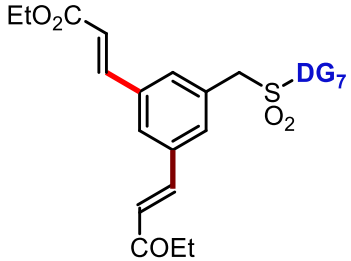
(*E*)-ethyl 3-(3-((E)-3-(dimethylamino)-3-oxoprop-1-enyl)-5-((2-(8-nitroquinolin-3-yl)-phenoxysulfonyl)meth-yl)phenyl)acrylate (7d):

The compound was synthesized following the general procedure B in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (50:50) mixture as the eluent. Yield 88%, 54 mg hetero-di-olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.96 (d, *J* = 2.1 Hz, 1H), 8.24 (d, *J* = 2.0 Hz, 1H), 8.04 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.97 (d, *J* = 8.3 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.50 – 7.47 (m, 3H), 7.46 – 7.38 (m, 4H), 7.33 (s, 1H), 7.28 (s, 1H), 6.89 (d, *J* = 15.4 Hz, 1H), 6.30 (d, *J* = 16.0 Hz, 1H), 4.31 (s, 2H), 4.25 (q, *J* = 7.1 Hz, 2H), 3.20 (s, 3H), 3.06 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.52, 166.29, 153.03, 148.21, 145.80, 142.54, 140.31, 138.46, 136.96, 135.97, 135.73, 132.60, 131.95, 131.82, 131.34, 131.31, 130.63, 130.36, 128.43, 128.25, 128.17, 127.88, 125.96, 124.32, 123.52, 120.14, 119.73, 60.88, 56.82, 37.71, 36.20, 14.47.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{32}H_{30}N_3O_8S$: 616.1748, found: 616.1742.



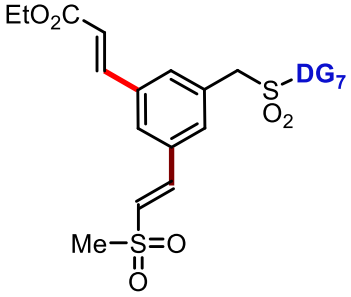
(*E*)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-5-((E)-3-oxopent-1-enyl)phenyl)acrylate (7e):

The compound was synthesized following the general procedure B in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 68%, 41 mg hetero-di-olefinated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.98 (d, *J* = 2.1 Hz, 1H), 8.25 (d, *J* = 2.0 Hz, 1H), 8.06 (d, *J* = 7.5 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.51 – 7.43 (m, 6H), 7.35 (t, *J* = 7.6 Hz, 3H), 6.66 (d, *J* = 16.2 Hz, 1H), 6.34 (d, *J* = 16.0 Hz, 1H), 4.32 (s, 2H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.70 (q, *J* = 7.3 Hz, 2H), 1.34 (dd, *J* = 9.4, 4.8 Hz, 3H), 1.16 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 200.68, 166.50, 153.08, 148.28, 145.77, 142.39, 139.90, 138.51, 136.27, 135.96, 132.59, 132.00, 131.87, 131.32, 131.17, 130.68, 128.46, 128.24, 127.75, 125.97, 124.31, 123.58, 120.49, 60.96, 56.84, 34.53, 14.48, 8.23.

HRMS (*m*/*z*): $[M+Na]^+$ calculated for $C_{32}H_{28}N_2NaO_8S$: 623.1464, found: 623.1468.



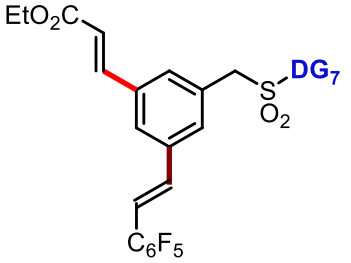
(*E*)-ethyl 3-(3-((E)-2-(methylsulfonyl)vinyl)-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-phenyl)acrylate (7f):

The compound was synthesized following the general procedure B in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (40:60) mixture as the eluent. Yield 71%, 44 mg hetero-di-olefinated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, *J* = 2.1 Hz, 1H), 8.24 (d, *J* = 2.1 Hz, 1H), 8.08 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.00 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.55 (ddd, *J* = 8.8, 7.6, 1.7 Hz, 2H), 7.48 – 7.41 (m, 5H), 7.37 (d, *J* = 4.2 Hz, 2H), 7.01 – 6.97 (m, 1H), 6.34 – 6.29 (m, 1H), 4.32 (s, 2H), 4.27 (q, *J* = 7.1 Hz, 2H), 3.10 (s, 3H), 1.35 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.36, 153.03, 145.56, 141.93, 141.70, 136.24, 135.94, 133.89, 132.62, 132.06, 131.98, 131.93, 131.72, 131.43, 130.77, 128.85, 128.75, 128.57, 128.47, 128.34, 126.16, 124.41, 123.66, 120.89, 77.55, 77.23, 76.91, 61.04, 56.71, 43.32, 14.50.

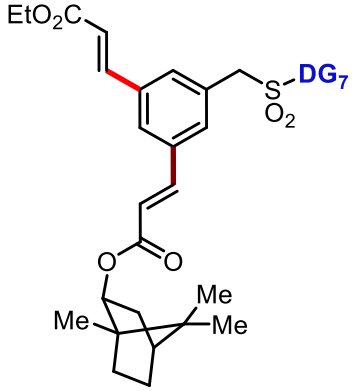
HRMS (*m*/*z*): $[M+H]^+$calcd for $C_{30}H_{27}N_2O_9S_2$: 623.1152, found: 623.1153



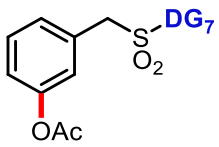
(*E*)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-5-(perfluorostyryl)-phenyl)acrylate (7g):

The compound was synthesized following the general procedure B in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 85%, 60 mg hetero-di-olefinatedproduct was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.02 (d, *J* = 2.2 Hz, 1H), 8.27 (d, *J* = 2.1 Hz, 1H), 8.04 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.96 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.62 – 7.56 (m, 1H), 7.54 – 7.48 (m, 3H), 7.48 – 7.43 (m, 3H), 7.34 (s, 1H), 7.30 (s, 1H), 7.23 (t, *J* = 11.1 Hz, 1H), 6.89 (d, *J* = 16.8 Hz, 1H), 6.36 (d, *J* = 16.0 Hz, 1H), 4.34 (s, 2H), 4.27 (q, *J* = 7.1 Hz, 2H), 1.35 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.57, 153.11, 148.28, 145.90, 142.68, 138.56, 138.04, 135.99, 135.90, 135.13, 132.60, 131.99, 131.83, 131.35, 130.66, 130.33, 130.01, 128.48, 128.34, 128.20, 127.17, 125.87, 124.29, 123.58, 120.27, 114.94, 60.94, 56.97, 14.48.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for$C_{35}H_{23}F_5N_2NaO_7S$: 733.1038, found: 733.1035.

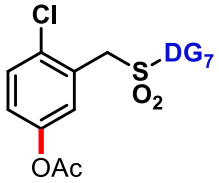


(*E*)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-5-((E)-3-oxo-3-((2R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yloxy)prop-1-enyl)phenyl)acrylate (7h):
The compound was synthesized following the general procedure B in 0.1 mmol scale at 80 °C for 24 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (30:70) mixture as the eluent. Yield 86%, 62 mg hetero-di-olefinated product was isolated.
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (d, *J* = 2.2 Hz, 1H), 8.28 (d, *J* = 2.2 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.99 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.52 – 7.39 (m, 7H), 7.35 (s, 1H), 7.33 (s, 1H), 6.37 (d, *J* = 7.8 Hz, 1H), 6.33 (d, *J* = 7.8 Hz, 1H), 4.80 (dd, *J* = 7.3, 4.2 Hz, 1H), 4.33 – 4.22 (m, 4H), 1.86 (dd, *J* = 6.9, 3.8 Hz, 1H), 1.80 – 1.69 (m, 4H), 1.63 – 1.55 (m, 1H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.18 – 1.11 (m, 1H), 1.07 (s, 3H), 0.90 (s, 3H), 0.87 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.50, 166.08, 153.12, 145.95, 142.41, 142.12, 136.16, 136.07, 136.01, 132.55, 131.99, 131.87, 131.40, 131.17, 130.68, 128.49, 128.41, 128.27, 128.24, 126.02, 124.37, 123.60, 121.15, 120.58, 81.69, 60.96, 49.13, 47.22, 45.29, 39.05, 33.97, 27.26, 20.33, 14.49, 11.73.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{40}H_{41}N_2O_9S$: 725.2527, found: 725.2521.

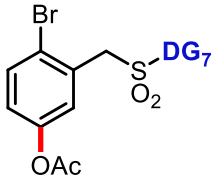


3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9a):
The compound was synthesized following the general procedure C in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as white solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 75%: 72 mg *meta*-acetoxylated product was isolated.

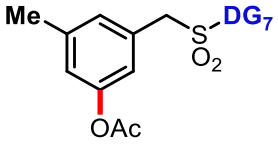
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (dd, *J* = 7.2, 2.2 Hz, 1H), 8.29 (dd, *J* = 6.7, 2.2 Hz, 1H), 8.07 (dt, *J* = 7.5, 1.9 Hz, 1H), 8.03 – 7.99 (m, 1H), 7.66 – 7.59 (m, 1H), 7.49 – 7.40 (m, 3H), 7.37 (ddd, *J* = 8.2, 4.8, 2.6 Hz, 1H), 7.19 (dd, *J* = 13.3, 5.4 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 7.02 (t, *J* = 1.9 Hz, 1H), 6.98 – 6.92 (m, 1H), 4.28 (s, 2H), 2.26 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.31, 153.27, 150.88, 148.31, 146.12, 138.63, 136.09, 132.66, 131.91, 131.80, 131.30, 130.56, 129.95, 128.55, 128.18, 128.08, 128.00, 125.88, 124.22, 123.95, 123.51, 122.73, 57.11, 21.20.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{24}H_{19}N_2O_7S$: 479.0913, found: 479.0910.



4-chloro-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9b):
The compound was synthesized following the general procedure C in 0.2 mmol scale at 100 °C for 24 hour. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 60%: 62 mg *meta*-acetoxylated product was isolated.
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 – 9.03 (m, 1H), 8.35 – 8.27 (m, 1H), 8.12 – 8.06 (m, 1H), 8.03 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.69 – 7.61 (m, 1H), 7.51 – 7.43 (m, 4H), 7.21 (dd, *J* = 9.7, 6.5 Hz, 1H), 7.12 (d, *J* = 2.7 Hz, 1H), 6.88 (td, *J* = 8.5, 2.5 Hz, 1H), 4.50 (d, *J* = 8.4 Hz, 2H), 2.25 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.09, 153.27, 149.26, 148.41, 145.89, 138.70, 136.14, 132.68, 132.02, 131.96, 131.90, 131.54, 130.84, 130.65, 128.55, 128.14, 126.23, 125.87, 125.57, 124.24, 123.68, 54.16, 21.19.
HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{24}H_{17}ClKN_2O_7S$: 551.0082, found: 551.0084.



4-bromo-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9c):
The compound was synthesized following the general procedure C in 0.2 mmol scale at 80 °C for 24 hour. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 64%: 71 mg *meta*-acetoxylated product was isolated.
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.0 Hz, 1H), 8.31 (dd, *J* = 9.1, 2.0 Hz, 1H), 8.12 – 8.05 (m, 1H), 8.05 – 8.01 (m, 1H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.51 – 7.42 (m, 4H), 7.38 (d, *J* = 8.7 Hz, 1H), 7.13 (d, *J* = 2.7 Hz, 1H), 6.81 (dt, *J* = 8.2, 4.1 Hz, 1H), 4.54 (s, 2H), 2.25 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.00, 153.27, 149.90, 145.85, 138.68, 136.16, 134.15, 132.69, 131.95, 131.89, 131.54, 130.65, 128.53, 128.15, 128.09, 125.86, 125.59, 124.42, 124.23, 123.72, 121.96, 56.64, 21.19.
HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{24}H_{17}BrKN_2O_7S$: 594.9571, found: 594.9593.



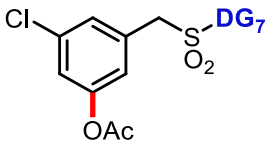
3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9d):

The compound was synthesized following the general procedure C in 0.2 mmol scale at 80 °C for 36 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 78%: 77 mg *meta*-acetoxylated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (dd, *J* = 8.3, 2.2 Hz, 1H), 8.32 (dd, *J* = 6.2, 2.3 Hz, 1H), 8.11 – 8.07 (m, 1H), 8.05 – 8.00 (m, 1H), 7.68 – 7.60 (m, 1H), 7.52 – 7.39 (m, 4H), 6.88 (t, *J* = 3.4 Hz, 1H), 6.82 (s, 1H), 6.77 (s, 1H), 4.24 (s, 2H), 2.25 (s, 3H), 2.20 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.47, 152.34, 149.86, 147.38, 145.21, 139.51, 137.69, 135.11, 131.69, 130.96, 130.82, 130.37, 129.60, 127.96, 127.59, 127.03, 126.82, 124.87, 123.27, 122.62, 122.48, 120.04, 56.22, 28.89, 20.25.

HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{25}H_{20}KN_2O_7S$: 531.0623, found: 531.0628.



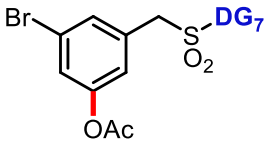
3-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9e):

The compound was synthesized following the general procedure C in 0.2 mmol scale at 80 °C for 36 hour. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 68%: 70 mg *meta*-acetoxylated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.08 (d, *J* = 2.2 Hz, 1H), 8.28 (dd, *J* = 7.9, 2.2 Hz, 1H), 8.11 (dt, *J* = 8.5, 4.3 Hz, 1H), 8.03 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.48 (ddd, *J* = 11.6, 3.9, 2.9 Hz, 4H), 7.07 (t, *J* = 1.6 Hz, 1H), 6.95 (t, *J* = 1.9 Hz, 1H), 6.91 (t, *J* = 1.7 Hz, 1H), 4.24 (s, 2H), 2.27 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 168.96, 153.25, 151.25, 145.89, 138.70, 136.08, 135.23, 132.74, 131.95, 131.82, 131.37, 130.68, 129.37, 128.53, 128.22, 128.08, 126.02, 124.49, 123.58, 123.38, 122.46, 56.55, 21.18.

HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{24}H_{17}ClKN_2O_7S$: 551.0082, found: 551.0079.



3-bromo-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9f):

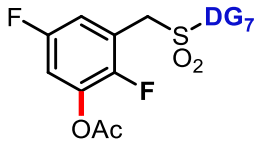
The compound was synthesized following the general procedure C in 0.2 mmol scale at 90 °C for 36 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 74%: 82 mg *meta*-acetoxylated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.05 (t, *J* = 14.9 Hz, 1H), 8.27 (d, *J* = 10.9 Hz, 1H), 8.15 – 8.07 (m, 1H), 8.02 (t, *J* = 9.6 Hz, 1H), 7.66 (dt, *J* = 11.6, 7.9 Hz, 1H), 7.56 – 7.40 (m, 4H),

7.20 (s, 1H), 7.09 (d, J = 11.1 Hz, 1H), 6.95 (d, J = 10.8 Hz, 1H), 4.25 – 4.19 (m, 2H), 2.24 (dd, J = 20.7, 17.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 168.95, 153.26, 151.26, 148.34, 145.92, 138.73, 136.08, 132.76, 131.97, 131.83, 131.41, 130.94, 130.69, 129.65, 128.55, 128.23, 126.23, 126.04, 124.50, 123.59, 122.95, 122.82, 56.48, 21.17.

HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{24}H_{17}BrKN_2O_7S$: 594.9571, found: 594.9591.



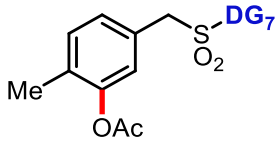
2,5-difluoro-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9g):

The compound was synthesized following the general procedure C in 0.2 mmol scale at 80 °C for 36 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 50%: 51 mg *meta*-acetoxylated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.07 (d, J = 2.2 Hz, 1H), 8.32 (d, J = 2.2 Hz, 1H), 8.12 – 8.09 (m, 1H), 8.05 (dd, J = 8.3, 1.2 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.51 – 7.45 (m, 4H), 6.89 (ddd, J = 8.0, 4.9, 3.1 Hz, 1H), 6.80 (ddd, J = 8.7, 8.0, 5.0 Hz, 1H), 4.37 (s, 2H), 2.32 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.83, 153.20, 148.55, 148.36, 145.86, 138.73, 136.12, 132.66, 131.99, 131.89, 131.55, 131.33, 130.69, 128.54, 128.29, 128.22, 125.99, 124.43, 123.56, 115.59, 115.78, 113.31, 113.11, 96.33, 50.19, 20.60.

HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{24}H_{16}F_2KN_2O_7S$: 553.0278, found: 553.0279.



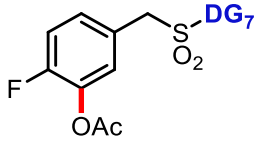
2-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9h):

The compound was synthesized following the general procedure C in 0.2 mmol scale at 80 °C for 36 hour. The pure compound was purified as solid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 43%: 43 mg *meta*-acetoxylated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (d, J = 2.0 Hz, 1H), 8.32 (d, J = 1.8 Hz, 1H), 8.09 (d, J = 6.8 Hz, 1H), 8.02 (d, J = 7.9 Hz, 1H), 7.65 (t, J = 7.8 Hz, 1H), 7.50 – 7.42 (m, 3H), 7.42 – 7.37 (m, 1H), 7.06 (d, J = 7.8 Hz, 1H), 6.98 (d, J = 7.9 Hz, 1H), 6.95 (s, 1H), 4.25 (s, 2H), 2.29 (s, 3H), 2.08 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.20, 153.39, 149.54, 146.24, 138.66, 136.18, 132.70, 131.95, 131.89, 131.79, 131.73, 131.20, 130.59, 129.78, 128.62, 128.31, 128.00, 125.87, 125.50, 124.29, 123.58, 56.99, 20.92, 16.17.

HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{25}H_{20}KN_2O_7S$: 531.0623, found: 531.0625.



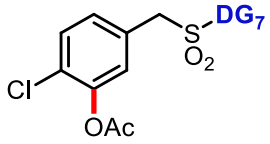
2-fluoro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9i):

The compound was synthesized following the general procedure C in 0.1mmol scale at 80 °C for 36 hour. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 52%: 26 mg *meta*-acetoxylated product was isolated.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.28 (s, 1H), 8.10 (d, *J* = 7.3 Hz, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.66 (t, *J* = 7.8 Hz, 1H), 7.47 (dd, *J* = 13.7, 7.6 Hz, 3H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.12 – 7.01 (m, 2H), 6.96 (t, *J* = 9.0 Hz, 1H), 4.34 – 4.18 (m, 2H), 2.31 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 168.24, 153.37, 136.11, 132.61, 131.95, 131.89, 131.30, 130.67, 129.56, 129.50, 128.59, 128.12, 127.33, 126.34, 126.04, 124.90, 124.42, 123.56, 117.42, 117.31, 56.61, 20.62.

HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{24}H_{17}FKN_2O_7S$: 535.0372, found: 535.0377.



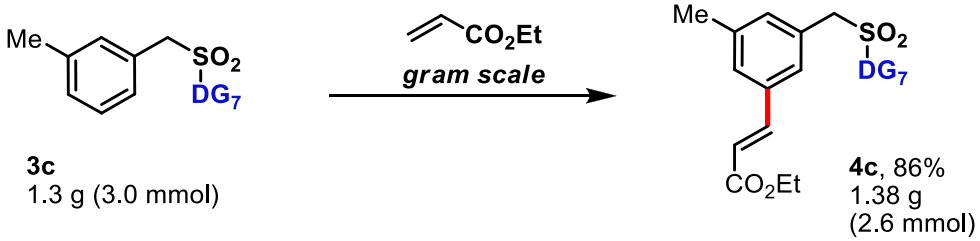
2-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9j):

The compound was synthesized following the general procedure C in 0.2 mmol scale at 80 °C for 24hour. The pure compound was purified as viscous liquid through silica column using ethyl acetate: pet ether (20:80) mixture as the eluent. Yield 39%: 40 mg *meta*-acetoxylated product was isolated.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (d, *J* = 2.2 Hz, 1H), 8.28 (d, *J* = 2.1 Hz, 1H), 8.12 – 8.09 (m, 1H), 8.01 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.51 – 7.45 (m, 3H), 7.42 (t, *J* = 5.6 Hz, 1H), 7.15 (tdd, *J* = 6.5, 4.2, 2.2 Hz, 1H), 7.08 (d, *J* = 2.0 Hz, 1H), 7.03 (dd, *J* = 8.3, 2.1 Hz, 1H), 4.25 (s, 2H), 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.45, 153.35, 148.30, 147.35, 146.05, 138.69, 136.11, 132.64, 132.02, 131.88, 131.23, 130.87, 130.67, 129.35, 129.19, 128.58, 128.16, 126.85, 126.08, 126.06, 124.50, 123.57, 56.63, 20.74.

HRMS (*m*/*z*): $[M + K]^+$ calculated for $C_{24}H_{17}ClKN_2O_7S$: 551.0082, found: 551.0086.

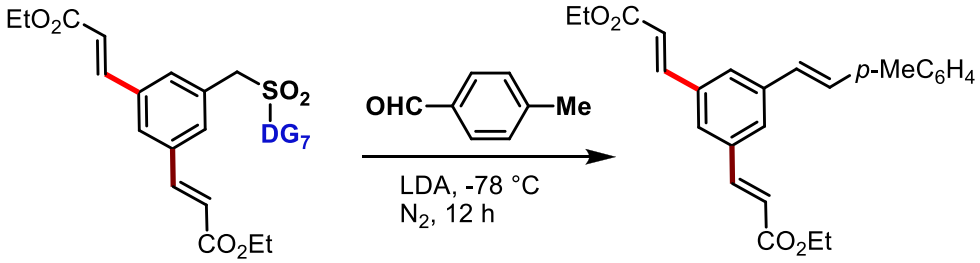


3c
1.3 g (3.0 mmol)

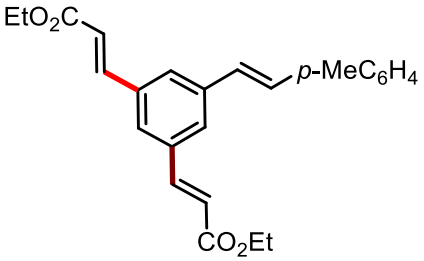
4c, 86%
1.38 g
(2.6 mmol)

Procedure for gram scale reaction: In an oven dry round bottomed flask all the solid reagents were added sequentially; $Pd(OAc)_2$ (10 mol%, 67 mg), *N*-Ac-Gly-OH (20 mol%, 70 mg), and AgOAc (2.0 equiv, 6.0 mmol, 1.0 g) was taken and followed by 3.0 mmol (1.3 g) of *m*-tolylmethanesulfonate ester (**3c**) was added. To the mixture 6 mL of HFIP and ethyl acrylate (3.0 equiv, 9.0 mmol, 0.95 mL) were added. The reaction mixture was then placed on a preheated 80 °C oil bath and stirred for 24 hour. The reaction mixture was then diluted with EtOAc and filtered through celite pad. After evaporation of the solvent, the crude mixture was purified by column chromatography using silica gel (100-200 mesh size) and pure compound was isolated as white solid by petroleum ether/ethyl acetate (75:25) as the eluent. Yield: 86% (1.38 g).

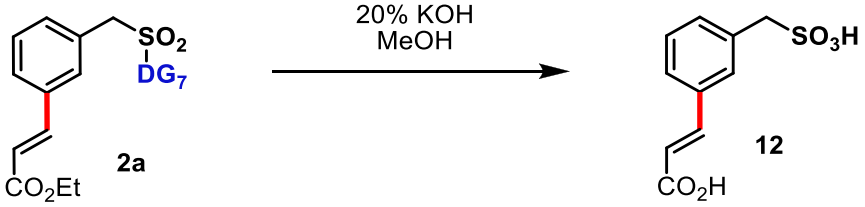
2.d. Application



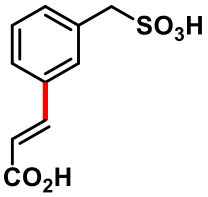
Procedure:[2] 0.25 mL freshly prepared LDA solution (2M in THF) was diluted with THF (5 mL) in a flame dry round bottomed flask, charged with a magnetic stir bar. The solution was then cooled to -78 °C. In an another round bottomed flask a solution of 4-methylbenzaldehyde (0.3 mmol) and homo-di-olefinated product (**7a**, 0.2 mmol) was made in 20 mL dry THF. The solution was added slowly to the LDA/THF solution at -78 °C. Then the reaction mixture was allowed to attain room temperature and stirred overnight. The reaction mixture was quenched with saturated NH_4Cl solution and extracted with EtOAc. The combined organic layer was dried over Na_2SO_4. The desired compound was purified by column chromatography using silica gel (100-200 mesh size) and petroleum ether/ethyl acetate as the eluent.



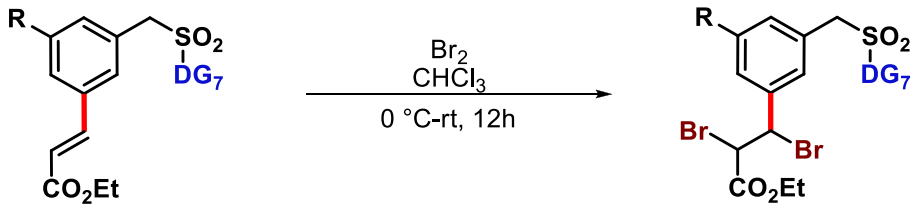
(2*E*,2'*E*)-diethyl 3,3'-(5-(4-methylstyryl)-1,3-phenylene)diacrylate (10):
Pure compuoud was isolated as white solid in 70% yield, 82 mg by column chromatography using ethylacetate:petroleum ether (1:99) as eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 16.0 Hz, 2H), 7.62 (d, *J* = 1.2 Hz, 2H), 7.51 (s, 1H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 7.9 Hz, 2H), 7.16 – 7.00 (m, 2H), 6.50 (d, *J* = 16.0 Hz, 2H), 4.28 (q, *J* = 7.1 Hz, 4H), 2.37 (s, 3H), 1.36 (t, *J* = 7.1 Hz, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.88, 143.81, 139.02, 138.38, 135.64, 134.04, 130.63, 129.70, 127.43, 126.81, 126.36, 126.15, 119.61, 60.84, 21.48, 14.50.
HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{25}H_{26}NaO_4$: 413.1723, found: 413.1728.



Procedure:[1c] Olefinated compound **2a** (0.2 mmol, 103 mg) was dissolved in 5 mL of 20% KOH in MeOH solution and the reaction mixture was stirred for overnight at room temperature. After completion of the reaction (checked by TLC), methanol was removed in vacuo and a white solid appeared. Then the crude solid was washed with ethyl acetate for three times. After washing, solid di-acid **12** was obtained quantitatively.



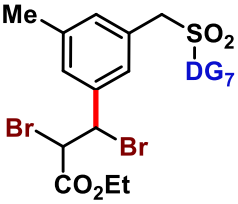
(*E*)-3-(3-(sulfomethyl)phenyl)acrylic acid (12):
Yield 83% (40 mg)
^{1}H NMR (400 MHz, D_2O) δ 7.41 (d, *J* = 11.0 Hz, 2H), 7.34 – 7.16 (m, 3H), 6.38 (d, *J* = 16.0 Hz, 1H), 4.03 (s, 2H).
^{13}C NMR (101 MHz, D_2O) δ 175.27, 160.62, 140.02, 135.52, 132.69, 131.26, 129.45, 127.12, 125.05, 56.65.



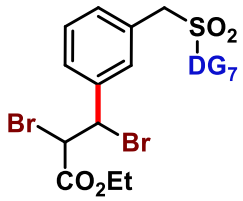
11

R = Me; **13**, 92%
R = H; **14**, 94%

Procedure:[3] Bromine (2.0 equiv, 0.2 mmol) was added dropwise to a solution of olefinated product **11** (0.1 mmol) in chloroform (2 mL) at 0 °C. The reaction mixture was allowed to warm to room temperature and was stirred until complete consumption of starting material. The mixture was quenched with saturated sodium thiosulfate solution, and then the layers were separated. The aqueous layer was extracted with chloroform. Then the combined organic extract was dried ($MgSO_4$) and purified by column using EtOAc/petroleum ether (15:85). And white solid was obtained in quantitative yield.



Ethyl 2,3-dibromo-3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenylsulfonyl)methyl)phenyl)propane-ate (13):
Yield: 92%, **(**63.5 mg)
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (t, *J* = 3.1 Hz, 1H), 8.26 (d, *J* = 2.2 Hz, 1H), 7.96 (ddd, *J* = 5.0, 3.3, 1.3 Hz, 2H), 7.57 – 7.51 (m, 1H), 7.41 – 7.38 (m, 1H), 7.36 – 7.32 (m, 2H), 7.23 – 7.19 (m, 1H), 7.10 – 7.07 (m, 1H), 7.05 (s, 1H), 6.97 (s, 1H), 5.15 (d, *J* = 11.7 Hz, 1H), 4.67 (d, *J* = 11.7 Hz, 1H), 4.27 – 4.21 (m, 2H), 4.16 (s, 2H), 2.18 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 167.75, 153.36, 148.35, 146.33, 139.87, 138.67, 138.61, 136.13, 132.58, 132.48, 131.99, 131.74, 131.24, 130.56, 129.98, 128.63, 128.03, 127.66, 127.49, 126.02, 124.29, 123.57, 62.84, 57.35, 50.01, 46.90, 21.31, 14.03.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{28}H_{25}Br_2N_2O_7S$: 690.9749 found: 690.9743.



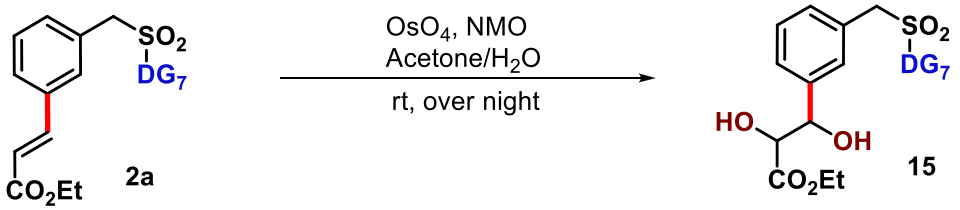
Ethyl2,3-dibromo-3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)propanoate (14):

Yield: 94% (63.5 mg)

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (d, *J* = 2.1 Hz, 1H), 8.34 (d, *J* = 2.1 Hz, 1H), 8.11 – 8.05 (m, 2H), 7.71 – 7.65 (m, 1H), 7.51 – 7.43 (m, 3H), 7.37 – 7.32 (m, 2H), 7.31 – 7.26 (m, 2H), 7.24 (t, *J* = 5.7 Hz, 1H), 5.25 (d, *J* = 11.7 Hz, 1H), 4.74 (d, *J* = 11.7 Hz, 1H), 4.38 – 4.28 (m, 4H), 1.38 – 1.34 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.76, 153.43, 148.46, 146.31, 138.85, 138.76, 136.18, 132.64, 132.05, 131.80, 131.66, 131.30, 130.64, 130.57, 129.77, 129.27, 128.70, 128.08, 127.73, 126.08, 124.34, 123.58, 62.95, 57.43, 49.82, 46.96, 14.10.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{27}H_{23}Br_2N_2O_7S$: 676.9593, found: 676.9587.



Ethyl 2,3-dihydroxy-3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)propaneate (15):[4]

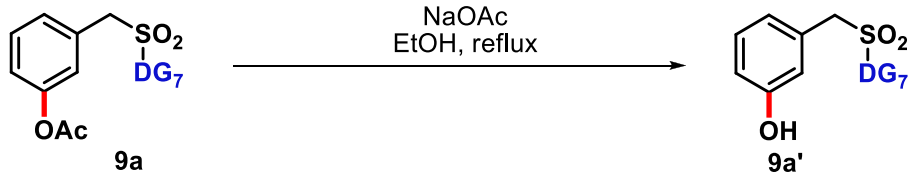
Yield: 78% (43 mg)

Procedure: To a solution of cinnamate (**2a**) (0.1 mmol, 52 mg) in a mixture of acetone (1 mL), and H_2O (1 mL) were added NMO (0.2 mmol, 2.0 equiv, 23.4 mg) and OsO_4 (2% by *wt*in H_2O, 0.01 mmol, 125 mg) and the mixture was stirred at room temperature for overnight. After completion of the reaction EtOAc and saturated solution of $Na_2S_2O_3$ were added to the reaction mixture. The aqueous layer was extracted with EtOAc, and the combined organic layer was washed with brine solutioin, and dried over Na_2SO_4. The solvent was removed under reduced pressure and the pure compound was obtained by column chromatography on silica gel eluted with petroleum ether/EtOAc (30:70) to afford the 1,2-dihydroxy compound **15**as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (d, *J* = 2.2 Hz, 1H), 8.24 (d, *J* = 2.2 Hz, 1H), 8.10 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.03 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.53 – 7.47 (m, 3H), 7.47 – 7.40 (m, 2H), 7.26 (s, 1H), 7.04 (dt, *J* = 7.5, 2.9 Hz, 2H), 5.09 – 5.04 (m, 1H), 4.43 – 4.35 (m, 3H), 4.34 – 4.28 (m, 2H), 3.82 (d, *J* = 6.4 Hz, 1H), 3.62 (t, *J* = 6.3 Hz, 1H), 1.33 (t, *J* = 7.1 Hz, 3H).

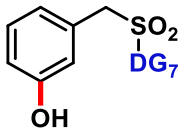
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.61, 153.35, 147.79, 145.33, 141.84, 138.00, 136.21, 132.98, 132.28, 131.89, 131.47, 130.68, 130.15, 129.06, 128.80, 128.79, 128.19, 127.70, 126.97, 125.93, 124.76, 124.24, 74.71, 74.18, 62.33, 57.57, 14.37.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{27}H_{25}N_2O_9S$: 553.1281, found: 553.1281.



9a 9a'

Procedure:[5] To the stirred solution of acetoxylated compound (**9a,** 1.0 equiv) in EtOH (5 mL/mmol), NaOAc (10 equiv) in H_2O (2.5 mL/mmol) was added and the reaction mixture was refluxed for overnight. After completion of reaction, The mixture was diluted with H_2O and extracted with ethyl acetate. The organic layer was dried over Na_2SO_4 and the pure product was isolated as white solid by column chromatography using petroleum:ethyl acetate (75:25) as eluent.

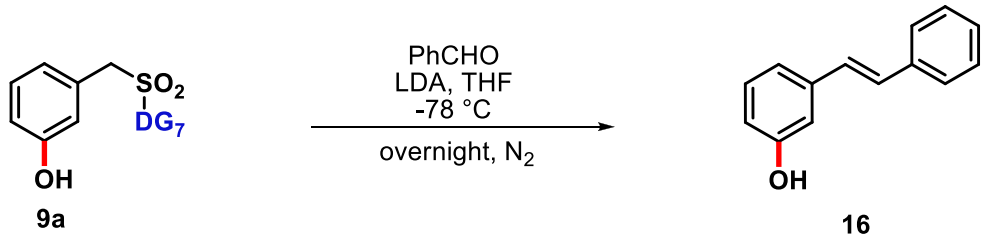


2-(8-nitroquinolin-3-yl)phenyl (3-hydroxyphenyl)methanesulfonate (9a'):

^{1}H NMR (400 MHz, MeOD) δ 8.98 (d, *J* = 2.1 Hz, 1H), 8.42 (d, *J* = 2.0 Hz, 1H), 8.13 (t, *J* = 7.8 Hz, 2H), 7.70 (t, *J* = 7.9 Hz, 1H), 7.56 (dd, *J* = 6.7, 2.5 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.36 (dd, *J* = 7.6, 1.7 Hz, 1H), 6.93 (t, *J* = 7.9 Hz, 1H), 6.69 (s, 1H), 6.63 (d, *J* = 7.6 Hz, 1H), 6.58 (dd, *J* = 8.2, 1.8 Hz, 1H), 4.44 (s, 2H).

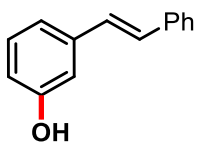
^{13}C NMR (101 MHz, CD_3CN): δ 158.32, 154.41, 149.66, 147.86, 139.33, 137.63, 133.68, 133.31, 133.25, 132.80, 131.80, 131.17, 130.04, 129.80, 129.23, 127.56, 124.90, 124.36, 123.54, 118.83, 117.36, 58.00.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{22}H_{17}N_2O_6S$: 437.0807, found: 437.0803.



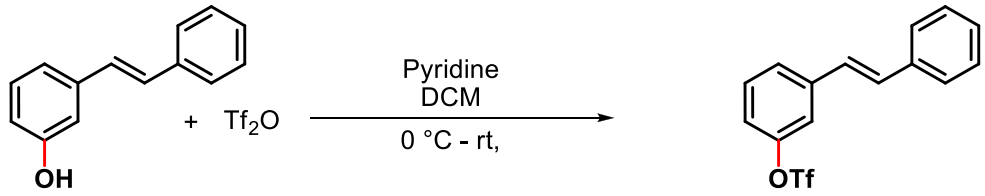
9a 16

Procedure:[2] Freshly prepared LDA solution (0.15 mL/mmol; 2M in THF) was taken in a flame dry round bottomed flask, charged with a magnetic stir bar. The solution was then cooled to -78 °C. In an another round bottomed flask a solution of benzaldehyde (2.0 equiv) and phenol (**9a'**, 1.0 equiv) was made in dry THF (10 mL/mmol). The solution was added slowly to the LDA/THF solution at -78 °C. Then the reaction mixture was allowed to attain room temperature and stirred overnight. The reaction mixture was quenched with saturated NH_4Cl solution and extracted with EtOAc. The combined organic layer was dried over Na_2SO_4. The desired compound was purified by column chromatography using silica gel (100-200 mesh size) and petroleum ether/ethyl acetate(98:2) as the eluent.



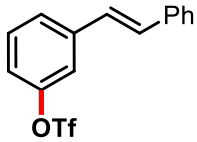
(*E*)-3-styrylphenol (16):

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.47 (m, 2H), 7.39 – 7.32 (m, 2H), 7.26 (s, 2H), 7.13 – 7.04 (m, 3H), 7.01 – 6.97 (m, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 4.83 (s, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.00, 139.33, 137.36, 130.09, 129.43, 128.91, 128.45, 127.96, 126.78, 119.69, 114.88, 113.17.
HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{14}H_{13}O$: 197.0966, found:197.9627.

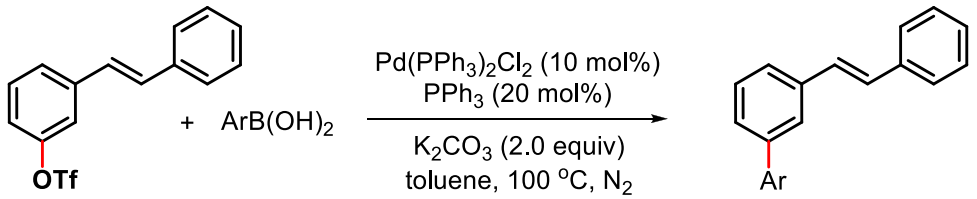


16 **17**

Procedure:[6] To a solution of (*E*)-3-styrylphenol **16** (1 equiv) in dry dichloromethane anhydrous pyridine (1.5 equiv) was added at 0 °C and stirred for 15 min, followed by triflic anhydride (2.0 equiv) was added. After allowing the reaction mixture to attain room temperature, the reaction mixture was stirred for overnight. The reaction was quenched with saturated aqueous bicarbonate solution and extracted with DCM. The organic layer was dried over sodium sulfate, concentrated to dryness under reduced pressure, and purified by column chromatography using petroleum ether as eluent. Pure compound was isolated as colourlessliquid in 92% yield.



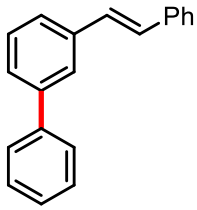
(E)-3-styrylphenyl trifluoromethanesulfonate (17):
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.49 (m, 3H), 7.47 – 7.35 (m, 4H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.19 – 7.03 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.27, 140.44, 136.63, 131.50, 130.60, 129.03, 128.60, 127.00, 126.70, 126.55, 120.10, 119.12.
GC-MS (*m/z*): 328.1 $[M]^+$.



17 **18**

Procedure: In an oven dried reaction tube charged with magnetic stir bar, triflate (**17**, 0.1 mmol, 1.0 equiv), $Pd(PPh_3)_2Cl_2$ (10 mol%, 0.01 mmol, 7.0 mg), PPh_3 (20 mol%, 0.02 mmol, 5.2 mg), K_2CO_3 (0.2 mmol, 2.0 equiv, 27.6 mg) and aryl boronic acid (0.15 mmol, 1.5 equiv) have been taken. The reaction tube was closed by a screw capfor evacuation and back filled with N_2 for three times. Then 2 mL of dry toluene was added to the reaction mixture and placed in a preheated oil bath at 100 °C. The reaction mixture was stirred vigorously for 24 h. The reaction mixture was allowed to cool to room temperature and filtered through the celite

pad. The filtrate was concentrated under reduced pressure and pure product was isolated by column chromatography using petroleum ether as the eluent.



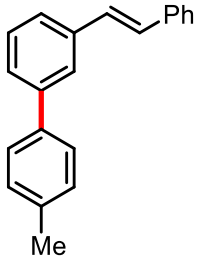
(*E*)-3-styrylbiphenyl (18a):

Yield: 76%, (19.5 mg)

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.68 – 7.62 (m, 2H), 7.60 – 7.42 (m, 7H), 7.39 (t, *J* = 7.6 Hz, 3H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.20 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.93, 141.32, 138.00, 137.47, 129.31, 129.26, 128.99, 128.92, 128.79, 127.92, 127.62, 127.42, 126.77, 126.74, 125.64, 125.59.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{20}H_{16}Na$: 279.1150, found: 279.1153.



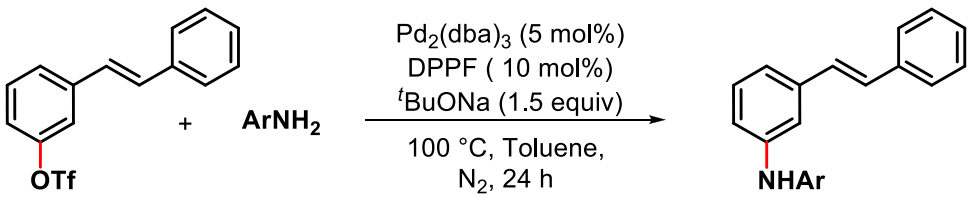
(*E*)-4'-methyl-3-styrylbiphenyl (18b):

Yield: 70% (19 mg)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (t, *J* = 1.6 Hz, 1H), 7.57 – 7.51 (m, 4H), 7.48 (ddt, *J* = 7.3, 5.5, 1.5 Hz, 2H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.41 – 7.34 (m, 2H), 7.28 (ddd, *J* = 5.6, 3.1, 1.2 Hz, 3H), 7.17 (s, 2H), 2.41 (s, 3H).

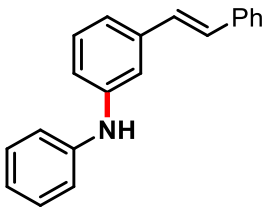
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.86, 138.44, 137.97, 137.53, 137.42, 129.72, 129.27, 129.19, 128.92, 128.90, 127.89, 127.25, 126.77, 126.58, 125.48, 125.32, 21.34.

HRMS (*m*/*z*): $[M + Na]^+$ calculated for $C_{21}H_{18}Na$: 293.1306, found: 293.1301.



Procedure:[7] In an oven dried reaction tube charged with magnetic stir bar, aryl amine (0.2 mmol, 2.0 equiv), $Pd_2(dba)_3$ (5mol%, 0.005 mmol, 4.5 mg), DPPF (10 mol%, 0.01 mmol, 5.5 mg), ^{t}BuONa (0.15 mmol, 1.5equiv, 14.4 mg) have been taken. The reaction tube was closed by a screw cap for evacuation and back filled with N_2 for three times. Then 2 mL of dry toluene was added to the reaction mixture was stirred vigorously at 85 °C. In another reaction tube a solution of triflate (0.1 mmol, 1.0 equiv) was made in degassed toluene and added drop wise to the previous mixture.The reaction mixture was stirred vigorously for 24 h. The

reaction mixture was allowed to cool to room temperature and filtered through the celite pad. The filtrate was concentrated under reduced pressure and pure product was isolated by column chromatography using petroleum ether as the eluent.



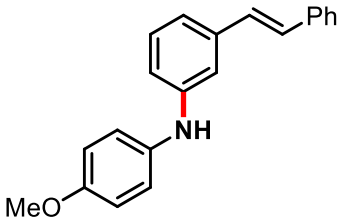
(*E*)-N-phenyl-3-styrylaniline (19a):

Yield: 71% (19.5 mg)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.4 Hz, 3H), 7.37 (t, *J* = 7.6 Hz, 3H), 7.31 – 7.26 (m, 1H), 7.24 – 7.21 (m, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.08 (dd, *J* = 10.9, 5.8 Hz, 4H), 6.99 (s, 1H), 6.77 – 6.71 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.06, 139.27, 137.35, 130.07, 129.55, 129.35, 128.90, 128.46, 127.94, 126.76, 119.60, 119.28, 115.71, 114.91, 113.17.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{20}H_{17}NNa$: 294.1256, found: 294.1259.



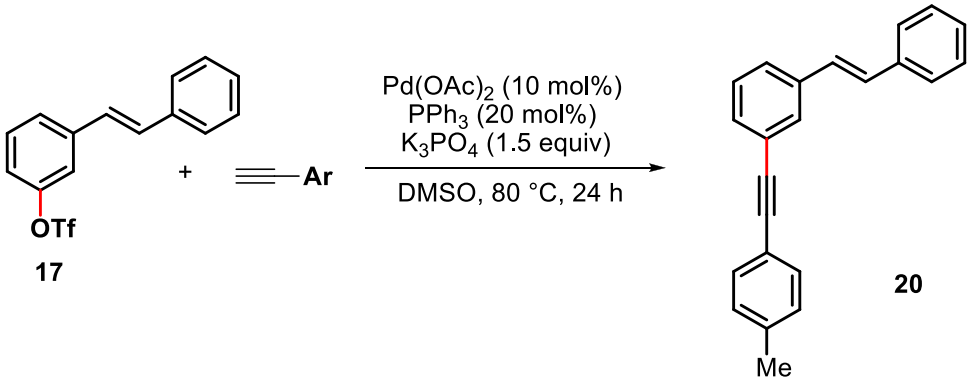
(*E*)-N-(4-methoxyphenyl)-3-styrylaniline (19b):

Yield: 66% (20 mg)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 16.0 Hz, 1H), 7.51 – 7.48 (m, 2H), 7.42 (dd, *J* = 5.0, 1.8 Hz, 2H), 7.35 (dd, *J* = 10.3, 4.7 Hz, 2H), 7.20 (t, *J* = 7.9 Hz, 1H), 7.11 (dd, *J* = 6.9, 1.9 Hz, 2H), 7.06 (d, *J* = 8.6 Hz, 1H), 7.04 (s, 1H), 7.01 (d, *J* = 7.3 Hz, 1H), 6.90 – 6.87 (m, 2H), 5.53 (s, 1H), 3.82 (s, 3H).

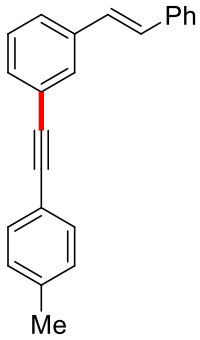
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.56, 137.57, 135.04, 130.73, 129.20, 129.08, 128.87, 128.62, 127.78, 126.72, 125.65, 122.68, 118.24, 115.38, 114.95, 113.75, 55.81.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{21}H_{20}NO$: 302.1545, found: 302.1530.



Procedure:[8] Aryl triflate (**17**, 0.1 mmol, 1.0 equiv), 4-ethynyltoluene (0.15 mmol, 1.5 equiv), $Pd(OAc)_2$ (10 mol%, 0.01 mmol, 2.2 mg), PPh_3 (20 mol%, 0.02 mmol, 5.2 mg) and K_3PO_4,

(0.15 mmol, 1.5 equiv, 31.8 mg) was taken in a reaction tube and 2 mL of DMSO was added under N_2 atmosphere. The reaction mixture was stirred for 24 h at 80 °C. After completion of the reaction the reaction mixture was diluted with water and extracted with diethyl ethr. The organic layer was washed with brine and dried over Na_2SO_4. Evaoration of the solvent followed by purification have been done by column chromatography and the pure compound (**20**) was isolated as solid using petroleum ether as the eluent.



(*E*)-1-styryl-3-(p-tolylethynyl)benzene (20):

Yield: 81% (24 mg)

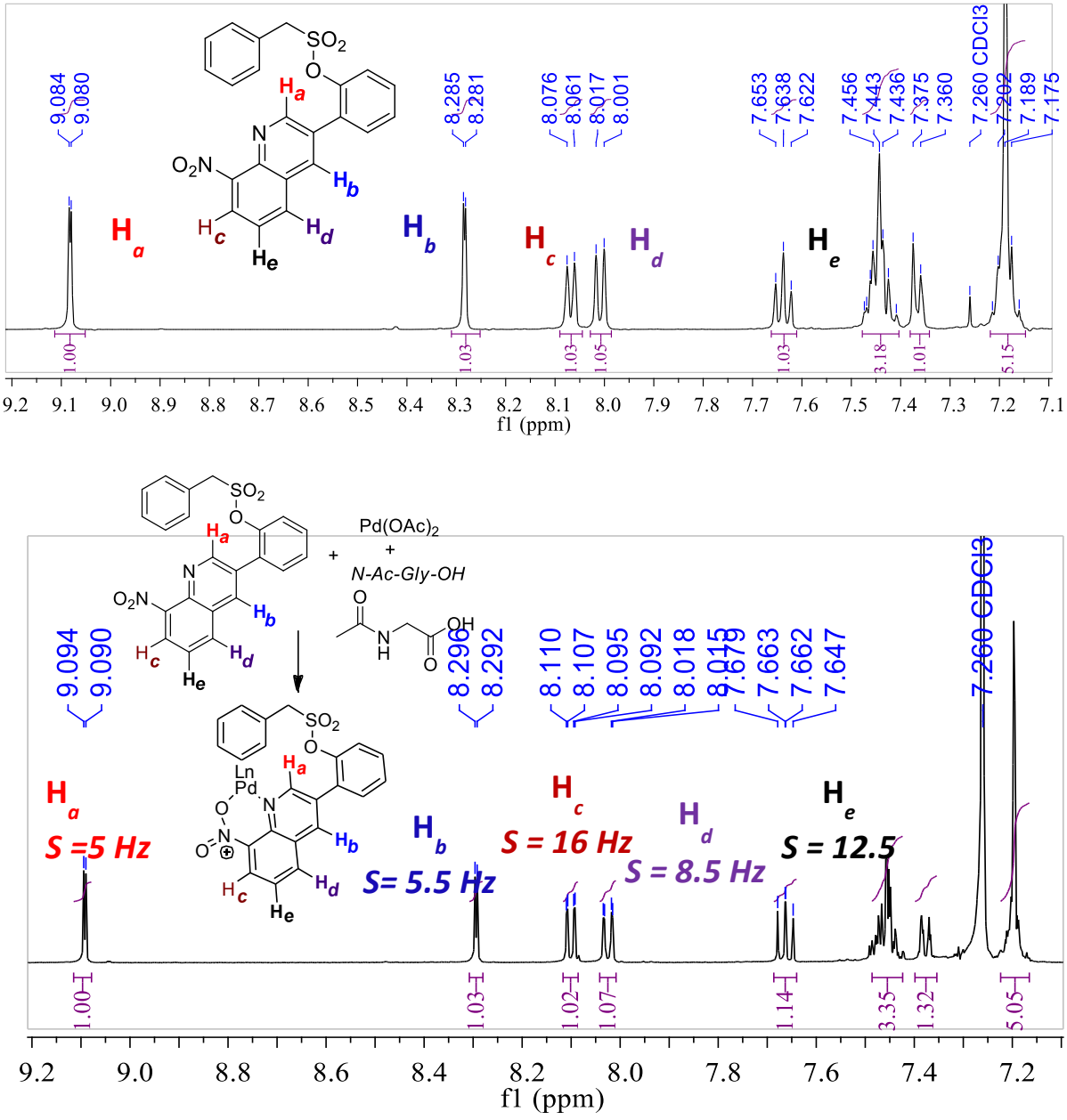
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.56 – 7.51 (m, 2H), 7.48 (t, *J* = 8.4 Hz, 3H), 7.45 – 7.41 (m, 1H), 7.41 – 7.32 (m, 3H), 7.31 – 7.27 (m, 1H), 7.19 (t, *J* = 8.8 Hz, 2H), 7.16 – 7.06 (m, 2H), 2.39 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.71, 137.73, 137.32, 131.77, 130.82, 129.70, 129.69, 129.38, 128.96, 128.91, 128.06, 126.83, 126.57, 124.09, 120.34, 89.91, 88.85, 21.76.

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{23}H_{18}Na$: 317.1306, found: 317.1305.

2.e. NMR study:

In an oven dry reaction tube charged with clean magnetic stir bar equimolar amount of substrate (0.05mmol, 21 mg, 1.0 equiv), *N*-Ac-Gly-OH (0.1 mmol, 11 mg, 2.0 equiv) and $Pd(OAc)_2$ (0.05 mmol, 11 mg, 1.0 equiv) was taken and to that 0.5 mL HFIP was added. The reaction mixture was then stirred vigorously for 3 h at 80 °C. Then the reaction mixture was taken out and NMR of the mixture was analyzed immediately. Comparing the proton shift of the reaction mixture and substrate, we concluded that the reasonable ^{1}H shift of directing groups (specifically the ^{1}H shift of 8-nitroquinoline moiety) indicating a weak coordiantion may be operative during the course of the reaction. In other word, quinoline group could be involved in coordinating to the palladium centre during the reaction which resulted a down field shift in proton NMR.



**(S stands for the shift in Hz)*

Figure S1: NMR study to interfere metal-directing group interaction

2.f. ESI-MS study:

$Pd(OAc)_2$ was dissolved in CH_3CN and HFIP mixture (1:1, 1 mL) in a oven dried reaction tube then substrate (**1a**, 0.05 mmol, 21 mg), *N*-Ac-Gly-OH (0.1 mmol, 11 mg), was added to the solution of $Pd(OAc)_2$. The mixture was stirred for 3 h at 80 °C. After that ESI-MS spectrum was recorded. In mass spectrum, a CH_3CN-Pd-substrate adduct such as [**CH_3CN-Pd-1a**] was appeared as a possible intermediate species with desired isotopic pattern.

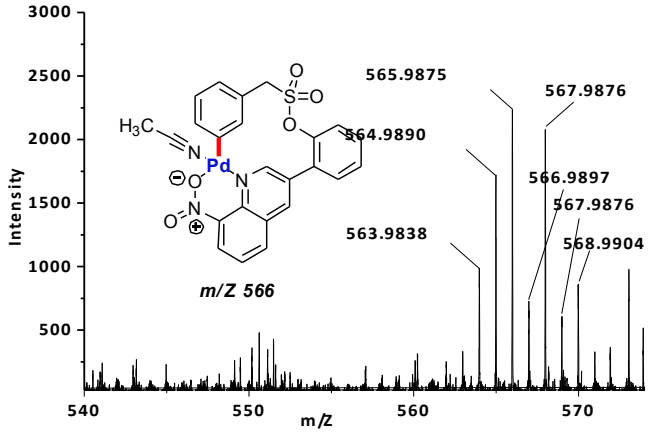


Figure S2: Palladium-Substrate (**1a**) adduct in ESI-MS study [**CH_3CN-Pd-1a**] m/Z = 566.

To verify further the observed intermediate of the reaction, **1a** was replaced with a methyl substituted substrate (**3c**). Similar adduct has been detected. The observation found to be consistent while solvent, CH_3CN has been replaced by CD_3CN.

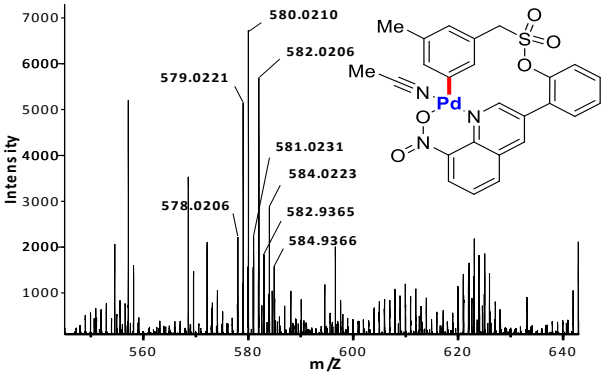


Figure S3: Palladium-Substrate (**3c**) adduct in ESI-MS study [**CH_3CN-Pd-3c**] m/Z = 580.

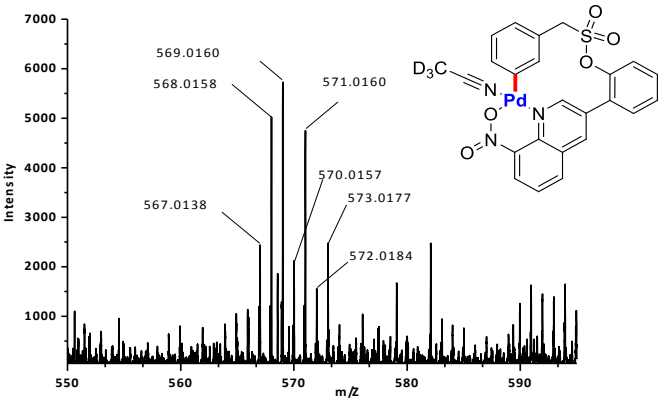


Figure S3: Palladium-Substrate (**1**) adduct in CD_3CN in ESI-MS study **[CD_3CN-Pd-1a**]: m/Z = 569

2.g. Kinetic Experiment:

Table S15: Kinetic experiment

	Substrate	Olefin	$Pd(OAc)_2$	*N*-Ac-Gly-OH	AgOAc	HFIP:DCE

Run 1	**0.1mmol**	0.1 mmol	10 mol%	20 mol%	0.1 mmol	1 mL
Run 2	**0.05mmol**	**0.1 mmol (2 equiv)**	10 mol%	20 mol%	0.1 mmol	1 mL
Run 3	0.05 mmol	**0.2 mmol (4 equiv)**	10 mol%	20 mol%	0.1 mmol	1 mL
Run 4 (**D-1**)	**0.05 mmol (Deuterated substrate D-1)**	0.1 mmol (2 equiv)	10 mol%	20 mol%	0.1 mmol	1 mL

*Reaction carried out at room temperature to avoid the formation of *di*-product.

Determination of order with respect to substrate: Comparing Run 1 and Run 2

Run 1: 0.1 mmol

x_1- 0.1559, y_1- 0.0979

x_2- 1.2714, y_2- 0.0924

$dx = x_2-x_1 = (1.2714 - 0.1559) = 1.1155$

$dy = y_2-y_1 = (0.0924 - 0.0979) = -0.0055$

$R_1 = dy/dx = -0.0055/1.1155 = -0.0049$

Run 2: 0.05 mmol

X_1- 0.3284, Y_1- 0.0494

X_2- 2.2892, Y_2- 0.0452

$DX = X_2-X_1 = (2.2892 - 0.3284) = 1.9608$

$DY = Y_2-Y_1 = (0.0452 - 0.0494) = -0.0042$

$R_2 = DY/DX = -0.0042/1.9608 = -0.0021$

We know

Rate = $dy/dx = k[substrate]^a[olefin]^b$

Now, $R_1/R_2 = \{dy/dx\}_{run1}/\{DY/DX\}_{run2} =$

$\{k[substrate]^a_{Run1}[olefin]^b_{run1}\}/\{k[substrate]^a_{run2}[olefin]^b_{run2}\}$

At t=0; $[olefin]_{run1} = [olefin]_{run2}$

- $R_1/R_2 = [substrate]^a_{run1}/[substrate]^a_{run2}$
- $-0.0049/-0.0021 = [substrate]^a_{run1}/[substrate]^a_{run2}$

⇨ $2.33 = [\text{substrate}]^{a}_{run1}/[\text{substrate}]^{a}_{run2}$

At t=0; $[\text{substrate}]^{a}_{run1}/[\text{substrate}]^{a}_{run2} = [0.1/0.05]^{a} = 2^{a}$

So, $2.33 = 2^{a}$

log(2.33) = alog(2)

0.3673 = a*0.3010

So, a = 1.22

Which indicates that the reaction rate with respect to substrate is **one**.

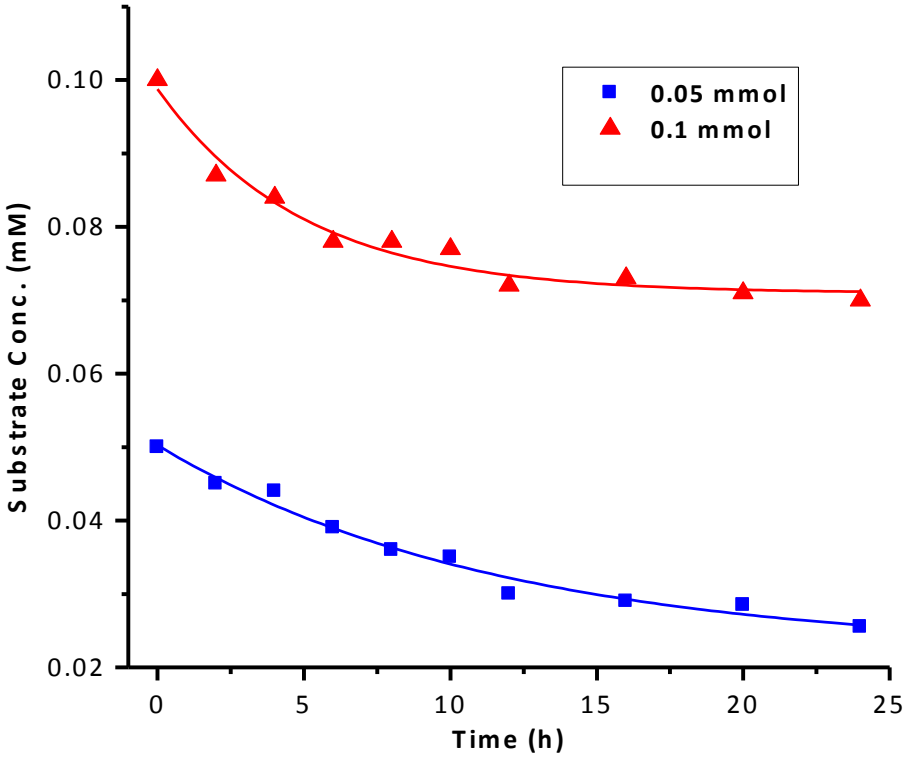


Figure S4: Determination of order with respect to substrate

Determination of order with respect to olefin: Comparing Run 2 and Run 3

From Run 2 we have seen that

$R_2 = DY/DX = -0.0042/1.9608 = -0.0021$

From Run 3:

$X_1' = 0.2022$, $Y_1' = 0.0497$

$X_2' = 1.7091$, $Y_2' = 0.0465$

$DX' = X_2' - X_1' = (1.7091 - 0.2022) = 1.5069$

$DY' = Y_2' - Y_1' = (0.0465 - 0.0497) = -0.0032$

Hence, $R_3 = DY'/DX' = (-0.0032/1.5069) = -0.002123$

So slope of Run 2 and Run 3 is same following the same route to calculate the order with respect to olefin;

Rate = dx/dy= $k[substrate]^a[olefin]^b$

Now, $R_2/R_3=\{dy/dx\}_{run2}/\{DY/DX\}_{run3} = \{k[substrate]^a{}_{Run1}\ [olefin]^b{}_{run1}\}/\{k[substrate]^a{}_{run2}\ [olefin]^b{}_{run2}\}$

At t=0; $[Substrate]_{run1}= [Substarate]_{run2}$

- ⇨ $R_2/R_3 = [olefin]^b{}_{run2}[olefin]^b{}_{run3}$
- ⇨ $-0.0021/-0.0021 = [olefin]^b{}_{run2}/[olefin]^b{}_{run3}$
- ⇨ $1 = [olefin]^b{}_{run2}/[olefin]^b{}_{run3}$

At t=0; $[olefin]^b{}_{run2}/[olefin]^b{}_{run3}= 2$

So, $1 = 2^b$

log(1) = blog(2)

0 = b*0.3010

So, b = 0

Which implies that the reaction order with respect to olefin is **zero**, i.e.the rate is independent on the amount of olefin.

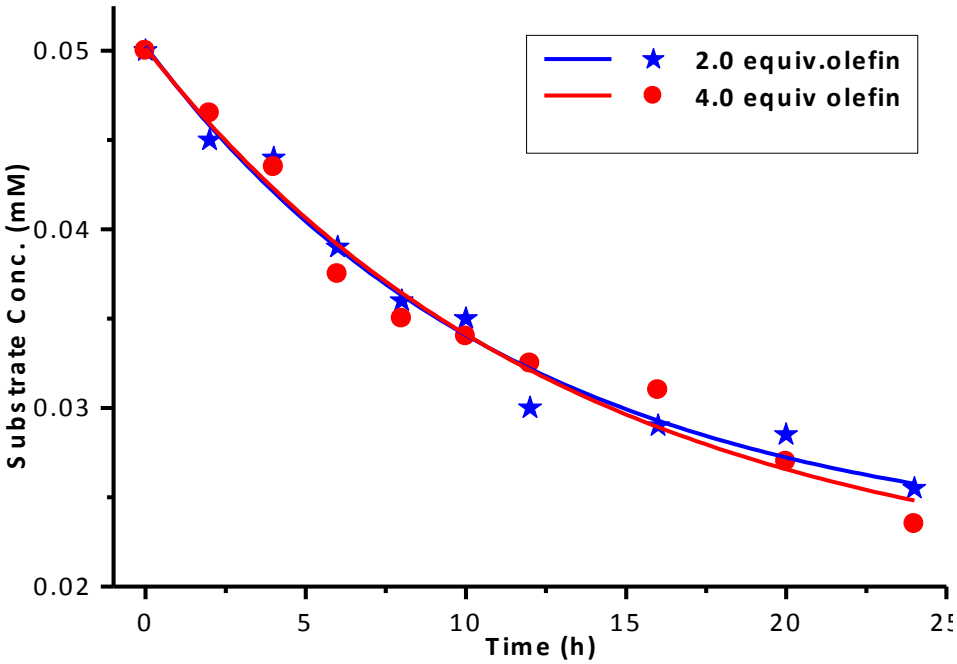
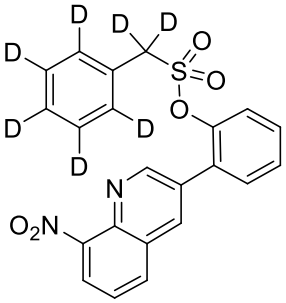


Figure S5: Determination of order with respect to olefin

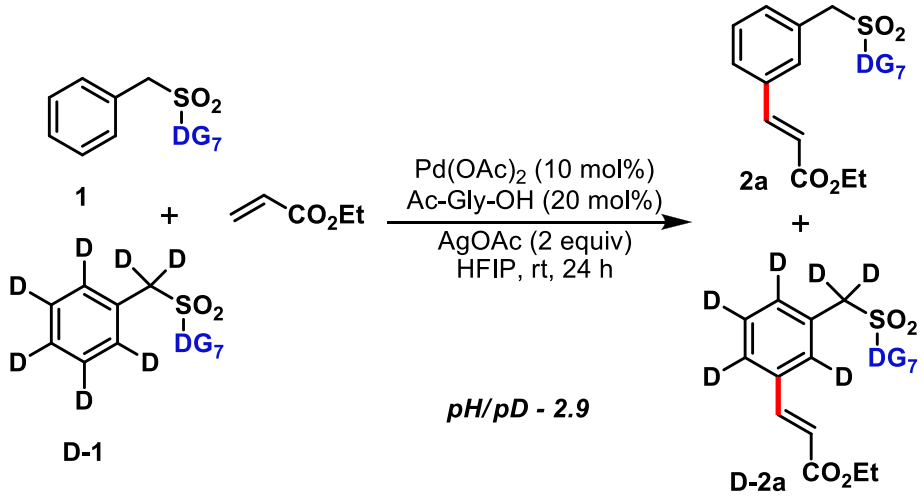
2.h. Intermolecular KIE experiment:



^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (d, *J* = 2.0 Hz, 1H), 8.29 (d, *J* = 2.1 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 8.02 (d, *J* = 8.3 Hz, 1H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.49 – 7.41 (m, 3H), 7.39 – 7.34 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.31, 147.40, 145.24, 137.68, 135.14, 131.61, 131.01, 130.79, 130.30, 129.53, 129.13 (d), 127.77 (d), 127.58, 127.35 (d), 126.91, 125.43 (d), 124.90, 123.20, 122.46, 56.33 (t).

HRMS (*m*/*z*): $[M + H]^+$ calculated for $C_{22}H_{10}D_7N_2O_5S$: 428.1298, found: 428.1295.



An oven-dried screw cap reaction tube was charged with a magnetic stir-bar, phenylmethanesulfonate ester **1**,(0.1 mmol, 42 mg), deuterated-phenylmethanesulfonate ester**D-1** (0.1 mmol, 43 mg), olefin (0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (10 mol%, 4.4 mg), *N*-Ac-Gly-OH (20 mol%, 4.7 mg), and AgOAc (2.0 equiv, 66 mg) were taken. Subsequently, HFIP:DCE (1:1, 2 mL) was added and the reaction mixture was stirred vigorously for 48 h at room temperature. The reaction mixture was then diluted with EtOAc and filtered through celite pad. After evaporation of the solvent, the crude mixture was purified by column chromatography using silica gel (100-200 mesh size) and 20:80 petroleum ether:ethyl acetate was used as the eluent. P_H/P_D was calculated from 1H NMR spectrum of the isolated product. From NMR spectrum product distribution *pH/pD*was found 2.9.

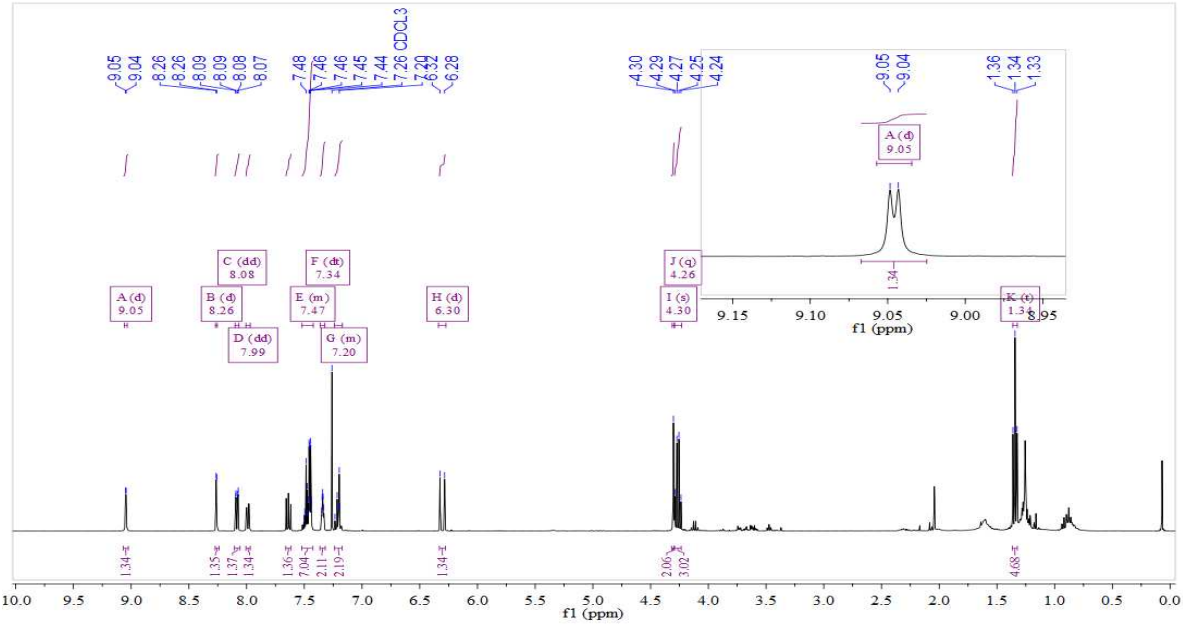


Figure S6: Determination of P_H/P_D

In this spectrum peak at 9.05 ppm is corresponds to the nitroquinoline group and total integration is 1.34 which is also true for the doublet (at 6.30 ppm) coming from the styrenyl proton. Among this 1.34 proton, one proton is coming from compound **2a** is rest 0.34 is the contribution of deutarated substrate **D-2a**. And hence [$_PH/_PD$] = 1/0.0.34 = 2.9

Determination of K_H/K_D: Comparing Run 2 and Run 4

Run 2: 0.05 mmol

X_1- 0.3284, Y_1- 0.0494

X_2- 2.2892, Y_2- 0.0452

DX = X_2-X_1 = (2.2892 - 0.3284) = 1.9608

DY = Y_2-Y_1 = (0.0452 - 0.0494) = -0.0042

R_2 = DY/DX = -0.0042/1.9608 = -0.0021

Run 4: 0.05 mmoldeuterated substrate (D-1)

x_1= 1.5050, y_1 = 0.0482
x_2= 2.9088, y_2 = 0.0466
dx = x2 – x1 = 2.9088 - 1.5050 = 1.4038
dy= y2 – y1 = 0.0490 – 0.0479 = -0.0016
R_4 = dy/dx = -0.0016/1.4038 = -0.0011
We know
Rate = dy/dx= k[substrate]^a[olefin]^b
Now, R_2/R_4 ={ DY/DX }$_{run2}$/{dy/dx }$_{run4}$ = {K_H[substrate] ^{a} $_{Run2}$ [olefin] ^{b} $_{run2}$}/{K_D[substrate] ^{a} $_{run4}$ [olefin] ^{b} $_{run4}$}
At t=0; [olefin] $_{run2}$= [olefin] $_{run4}$ and [substrate] $_{run2}$ = [substrate] $_{run4}$

⇨ $R_2/R_4 = K_H/K_D = -0.0021/-0.0011 = 1.9$

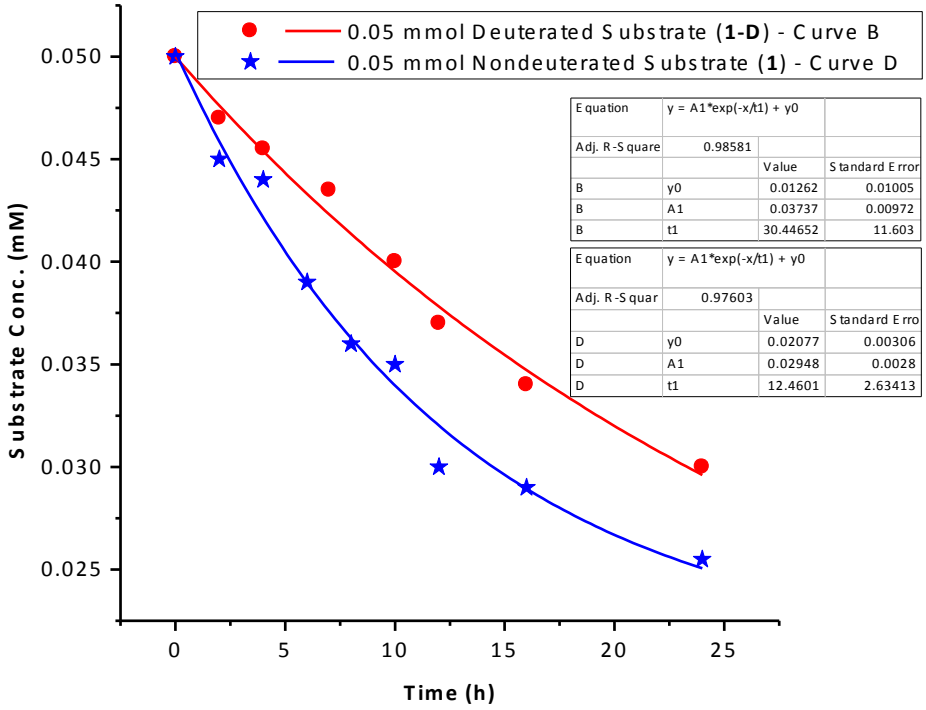
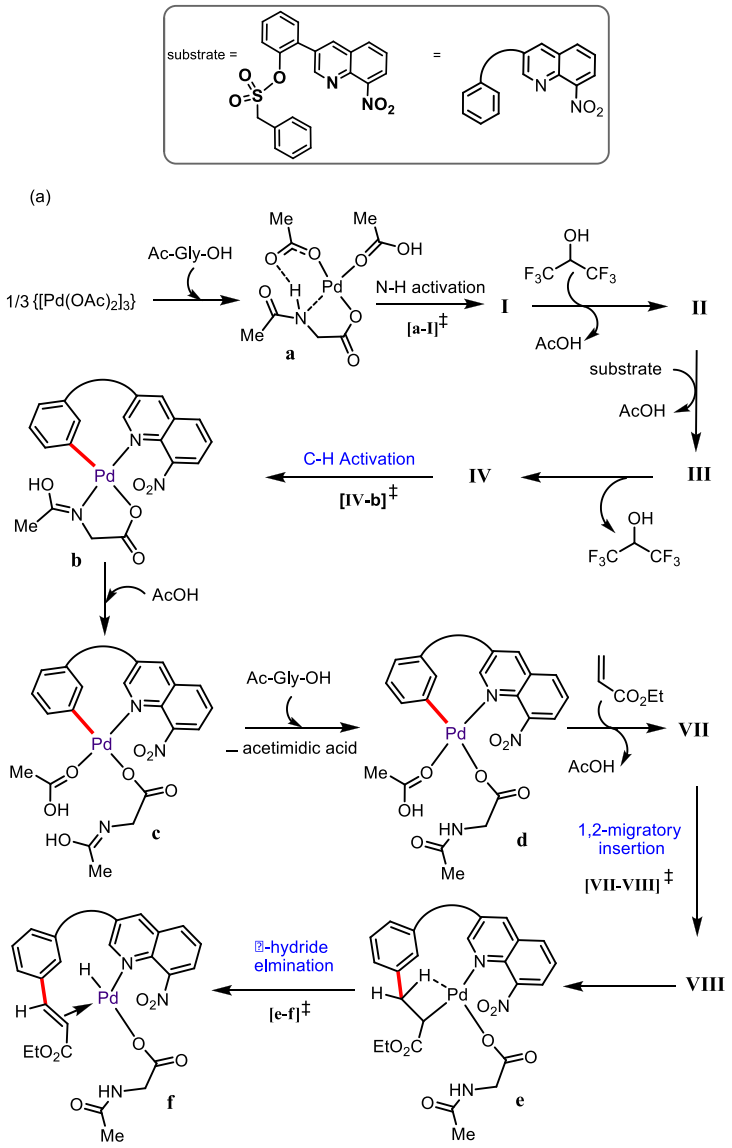


Figure S7: Determination of K_H/K_D

3. Computational Methods

Computations were performed using Gaussian09 (Revision D.01) suite of quantum chemical program.[9]The transition states were verified by examining whether it has a unique imaginary frequency representing the desired reaction coordinate. Intrinsic reaction coordinate (IRC) calculations were additionally carried out to further characterize the true nature of the important transition states.[10]Graphical representation of the optimized geometries are created by using CYLView.[11] All the relative energies (kcal/mol) were calculated with respect to the separated reactants.

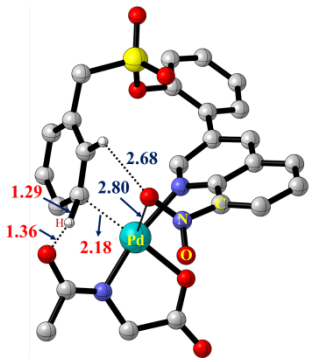
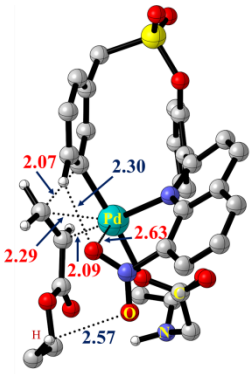
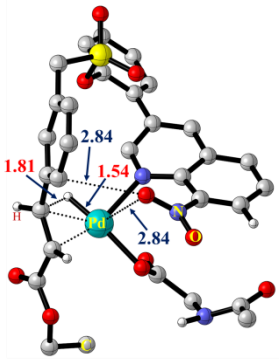
3.a. Detailed mechanistic steps involved in olefination reaction



Scheme S1: Detailed intermediate steps

3.b. Optimized geometries of the important transition states

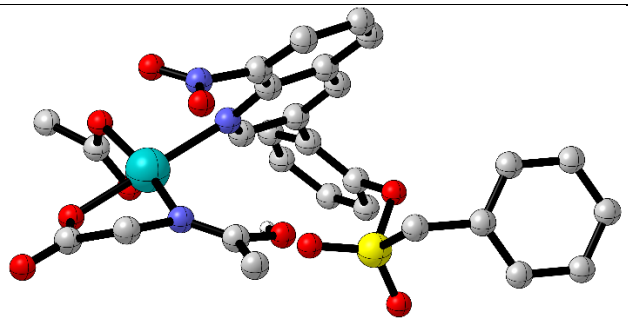
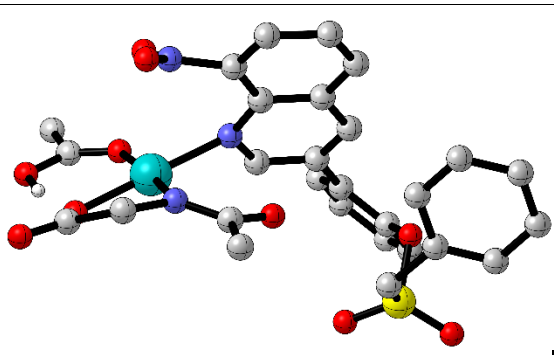
Table S16: Optimized geometries

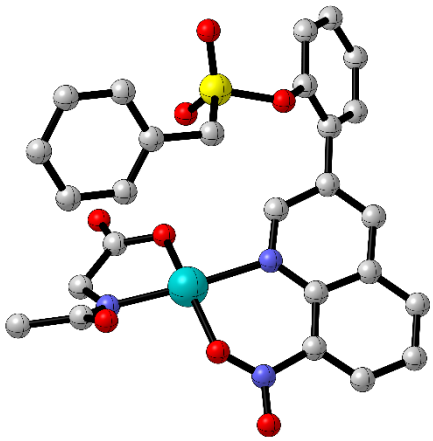
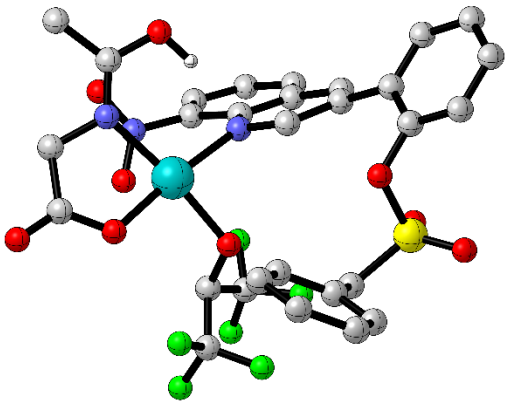
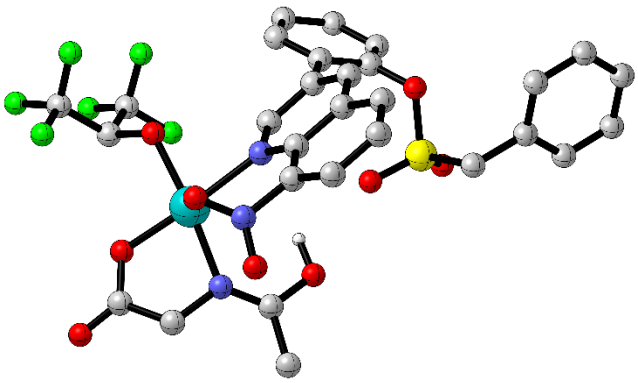
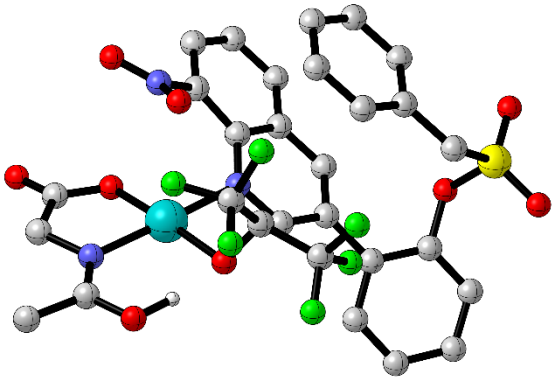
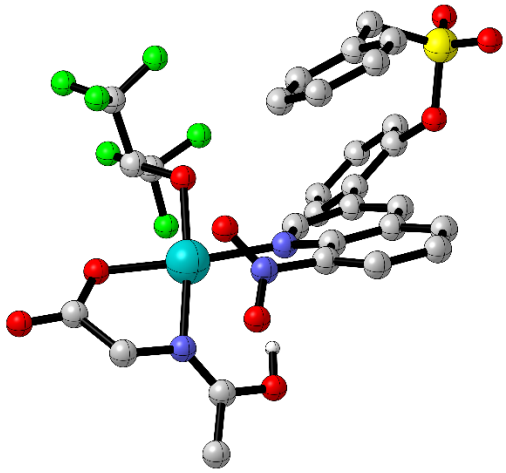
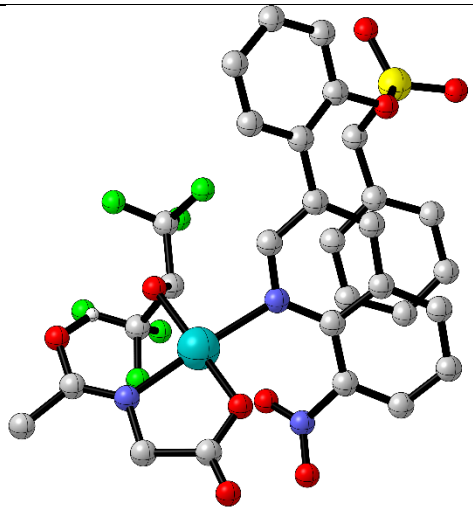
 C–H activation [**IV-b**]‡	 Olefin insertion [**VII-VIII**]‡	 *β*-hydride elimination [**e-f**]‡

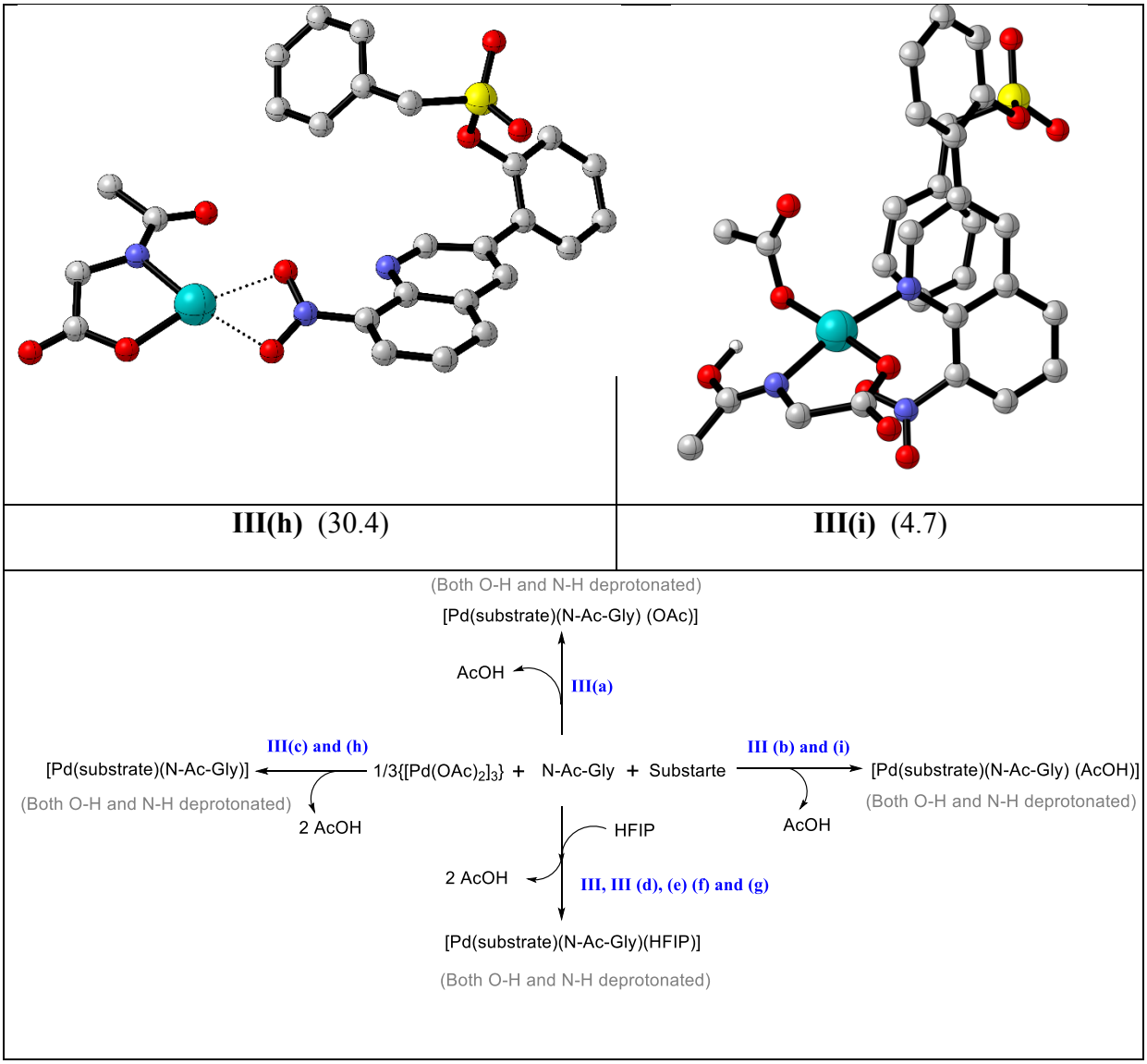
***Transiton state geometries obtained at the M06/6-31G**, SDD(Pd) level of theory**

3.c.Different binding modes between palladium acetate, *N*-acetylglycine ligand and substrate

Table S17: Optimized geometries of different binding modes between palladium acetate, N-acetyl glycine ligand and the substrate obtained at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G**//M06/6-31G** level of theory and the corresponding Gibbs free energies (in kcal/mol).

	
III(a) (9.6)	**III(b)** (8.5)

	
III(c) (14.0)	**III(d)** (10.3)
	
III(e) (10.4)	**III** (2.6)
	
III(f) (11.6)	**III(g)** (3.0)



Scheme S2: Illustration of how the relative Gibbs free energies of different binding modes (as shown in Table S17) of catalyst, ligand and substrates are computed

3.d. C–H Activation Models

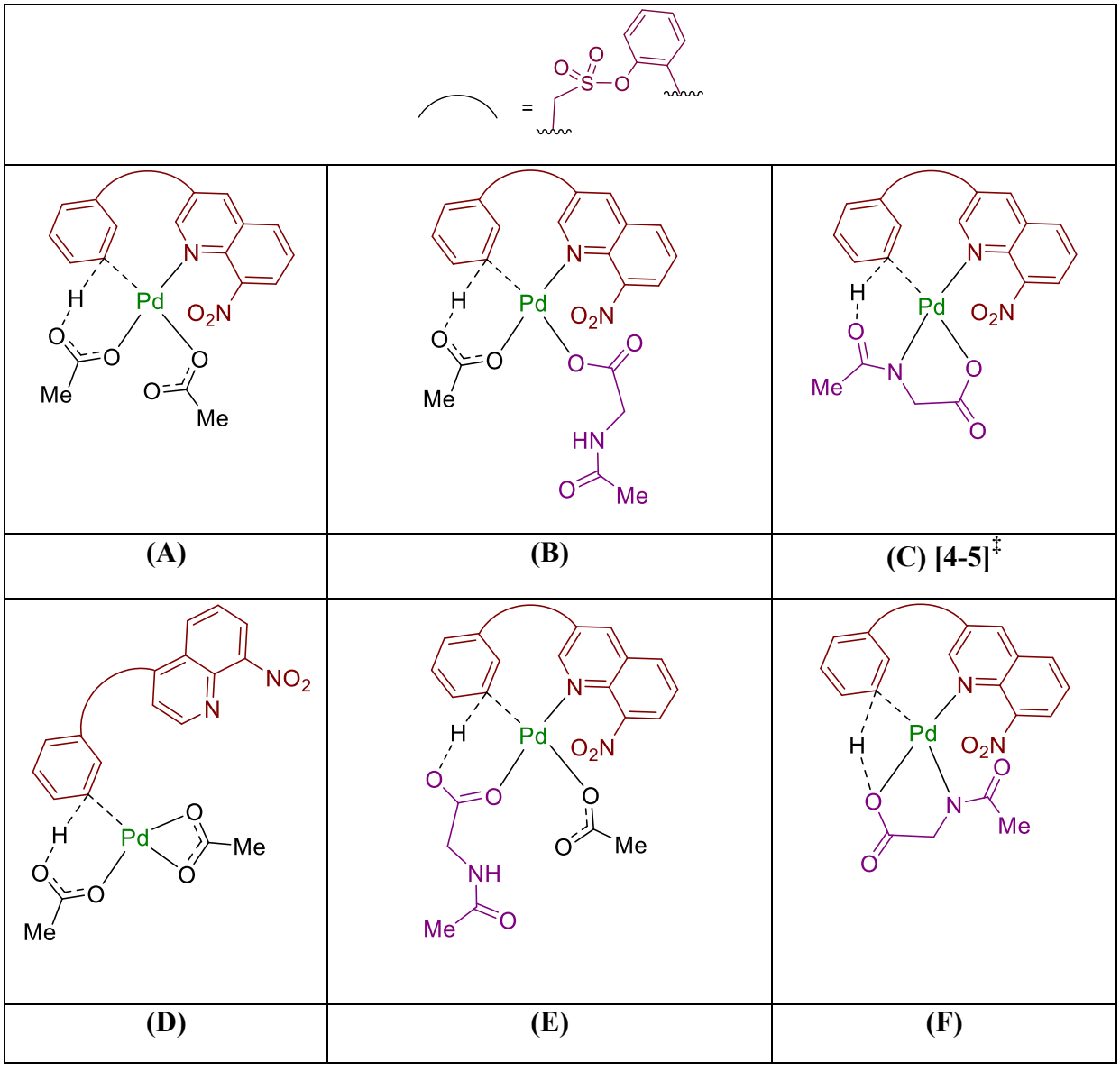
Table S18: Relative Gibbs Free Energies (in kcal/mol) of the C–H Activation Transition States at the *meta-, ortho*-and *para-* Positions Obtained at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G**//M06/6-31G** Level of Theory

Mode of C–H activation[a]	*meta-*	*ortho-*	*para-*
A	25.6	33.2	22.6
B	25.0	36.5	22.2
C	**21.8**	32.8	22.9
D	37.0	33.5	36.7
E	26.1	36.6	27.4

F	56.1	62.6	57.5
G	26.3	36.1	27.8

[a]SeeTable S19for details of these binding modes. The lowest energy possibility (**C**) is shown in bold font type.

Table S19: *meta* C-H bond activation transition states obtained at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G**//M06/6-31G** level of theory. (Similar possibilities for the *ortho*- and *para*-C–H bond activation were also examined and the computed data is provided in Table S17).



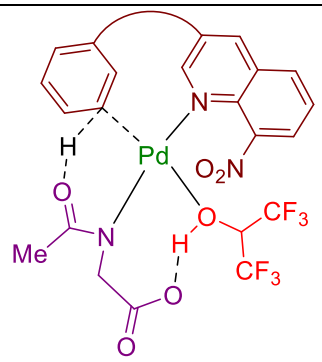
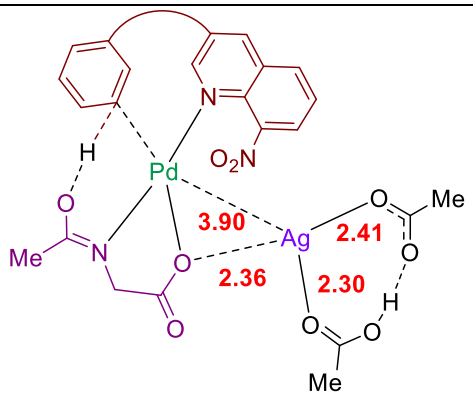
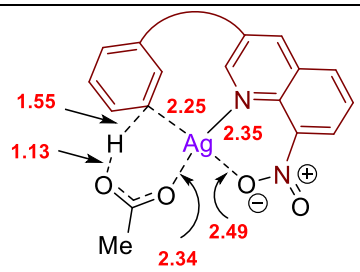
		
(G)	**(H)** 23.1 kcal/mol	**(I)** 28.8 kcal/mol[12]

Table S20: Energetics of Various Species Involved in the Catalytic Cycle Computed at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G**,SDD(Pd)//M06/6-31G**,SDD(Pd) Level of Theory

Stationary Points	Total Energy	Stationary Points	Total Energy
$[Pd(OAc)_2]_3$	-1754.125986	**II**	-1582.142215
Substrate-**1**	-1730.762457	**III**	-3083.949447
Ligand	-436.8757687	**IV**	-2294.368782
HFIP	-789.5300087	**[IV-b]**‡	-2294.35374
AcOH	-228.9731031	**b**	-2294.379387
Substrate-**2** (olefin)	-345.5744617	**c**	-2523.354903
$[AgOAc]_2$	-750.8489252	**d**	-2523.374801
AgOAc	-375.3915089	**VII**	-2639.977314
$[AgOAc.HFIP]_2$	-2329.958543	**[VII-VIII]**‡	-2639.969199
		VIII	-2640.009943
a	-1021.576704	**e**	-2639.996198
[a-I]‡	-1021.564145	**[e-f]**‡	-2639.981611
I	-1021.577629	**f**	-2639.984206

Table S21: Energetics of Various Species of Stationary Point **(III)** Computed at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G**,SDD(Pd)//M06/6-31G**,SDD(Pd) Level of Theory

Stationary Point **(III)**	Total Energy	Stationary Point **(III)**	Total Energy

III(a)	-2523.370273	**III**	-3083.949697
III(b)	-2523.372453	**III(f)**	-3083.935267
III(c)	-2294.368028	**III(g)**	-3083.949447
III(d)	-3083.932562	**III(h)**	-2294.339047
III(e)	-3083.929150	**III(i)**	-2523.382959

Table S22: Energetics of Various Mode of C–H activation are Computed at the $SMD_{(\varepsilon=16.7)}$/M06/6-31G**,SDD(Pd)//M06/6-31G**,SDD(Pd) Level of Theory

Mode of C-H activation	*meta*	*ortho*	*para*
	Total Energy		
A	-2315.43694	-2315.425049	-2315.438938
B	-2523.345309	-2523.328582	-2523.350687
C	-2294.35374	-2294.336536	-2294.353957
D	-2315.410802	-2315.419308	-2315.416384
E	-2523.338294	-2523.322493	-2523.341104
F	-2294.299699	-2294.288701	-2294.297372
G	-3083.905376	-3083.888413	-3083.902035
H	-2898.784668		
I	-2106.14555		

3.e. *meta*-C–H activation transition state plot for showing non-covalent interactions

The transition state geometries, as given in 3.b, convey an important interaction between the quinoline nitro group and the palladium center. The contact distances between the $–NO_2$ group and Pd are found to be in the range from 2.6 to 2.8 Å. Another interaction is between the $–NO_2$ oxygen and the $C_{sp2/sp3}$–H of the aryl ring of the substrates. A graphical illustration of these weak interactions, generated using the non-covalent interaction plot, is shown below.[13] It is interesting to note that the substituents such as $–NO_2$ and –OMe at the C-8 position of the quinoline ring offers improved yields of *meta*olefinated products as compared to unsubstitutedquinolines.

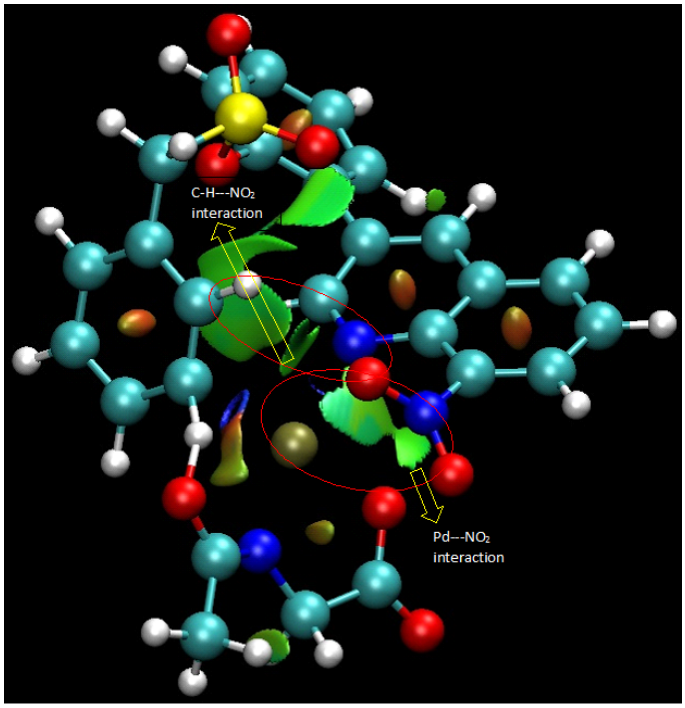
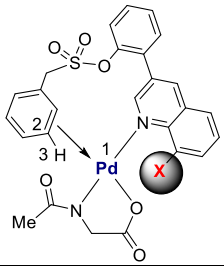


Figure S8:*meta*-C–H activation transition state plot

3.f. Calculation of natural charges

We have computed the natural charges on the carbon and hydrogen atoms of the pre-reacting complexes of the C–H activation transition states, shown as C-2 and H-3 in Table S23, by using natural population analysis (NPA).[14] The relative nucleophilicities and electrophilicities of the C-2 and H-3 atoms of the aryl ring can be approximately compared using the computed NPA changes. It appears that the C-8 substituent on the quinoline ring is able to influence the charge on palladium, which in turn, results in a minor change in C-2 and H-3 atoms that are involved in the C–H activation (Table S23). In both –NO_2 and –OMe substituted quinolines, H-3 becomes more protic while C-2 becomes relatively more nucleophilic as compared to the theunsubstituted case. These trends suggest that the substituted quinolines are likely to be better directing groups for improving efficiency of *meta*-C–H activation of arenes.

Table S23: Natural charges on important atoms in the respective pre-reacting complexes of the *meta*-C–H activation transition states

	X=	Pd(1)	C(2)	H (3)
	-NO2	0.513	-0.282	0.328
	-OMe	0.530	-0.257	0.310
	-H	0.522	-0.243	0.304

4. Reference

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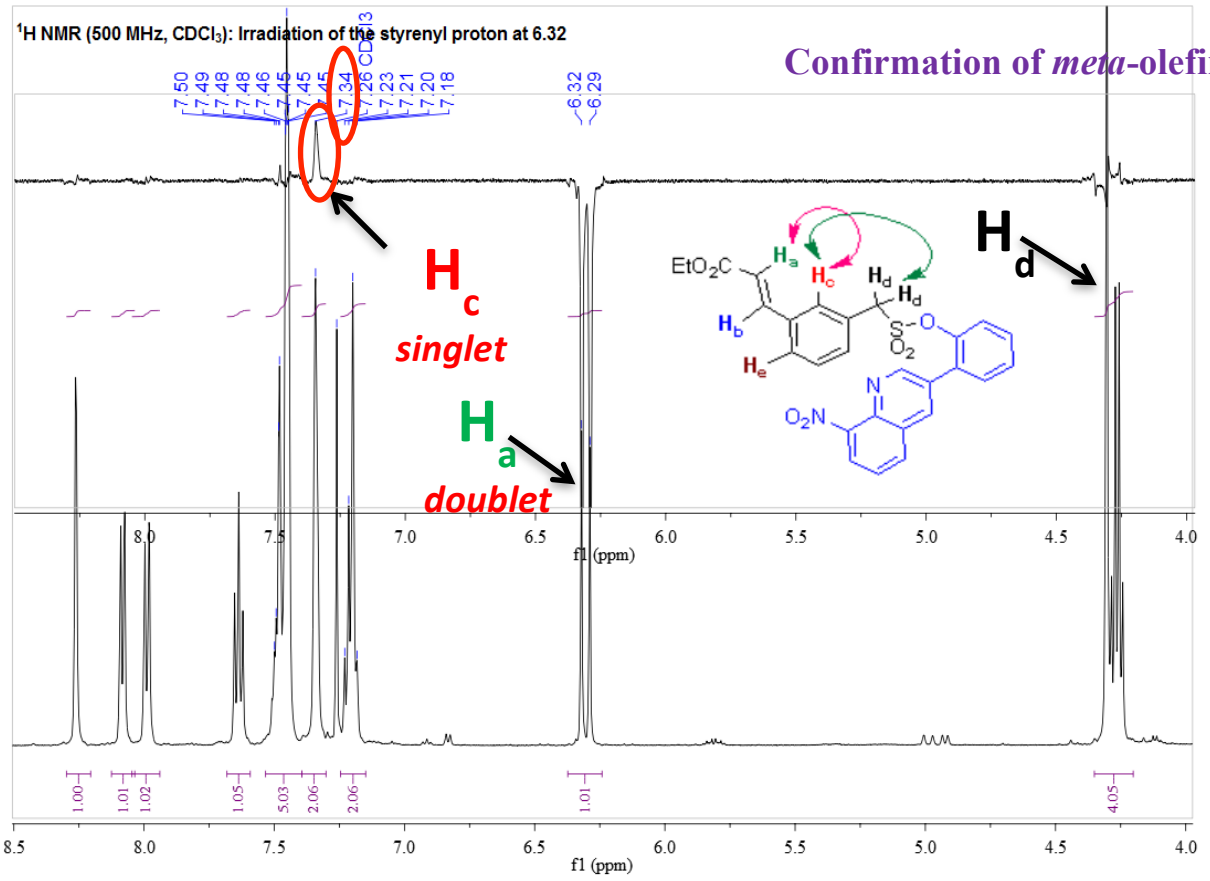
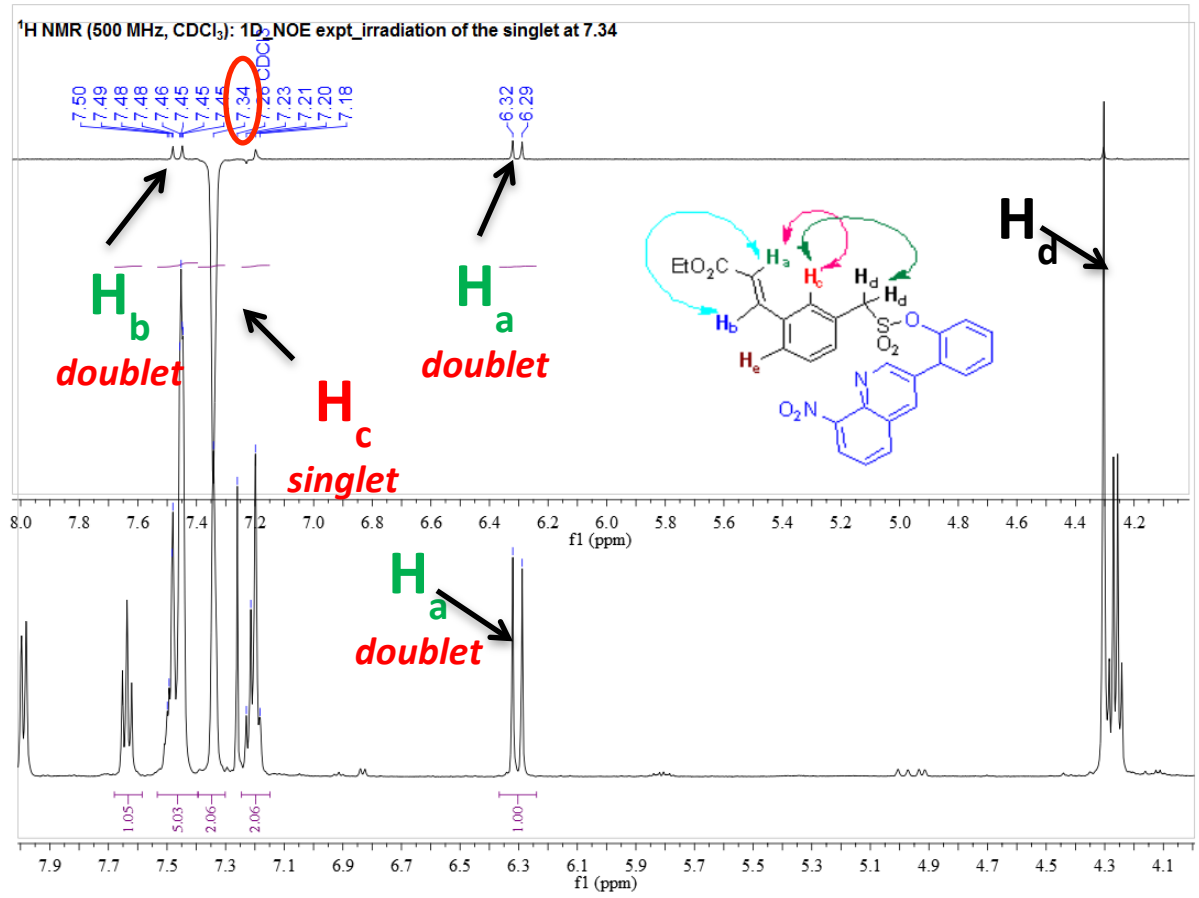
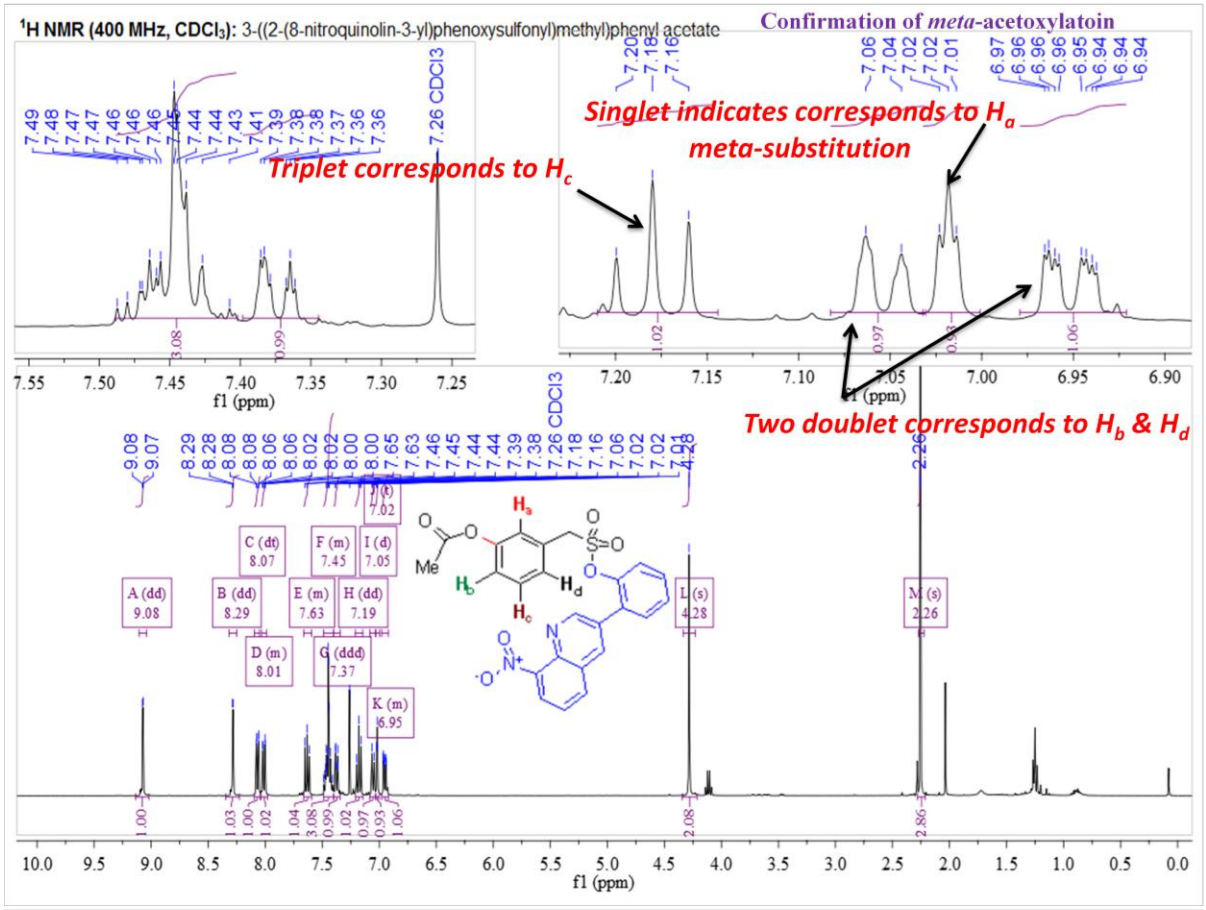
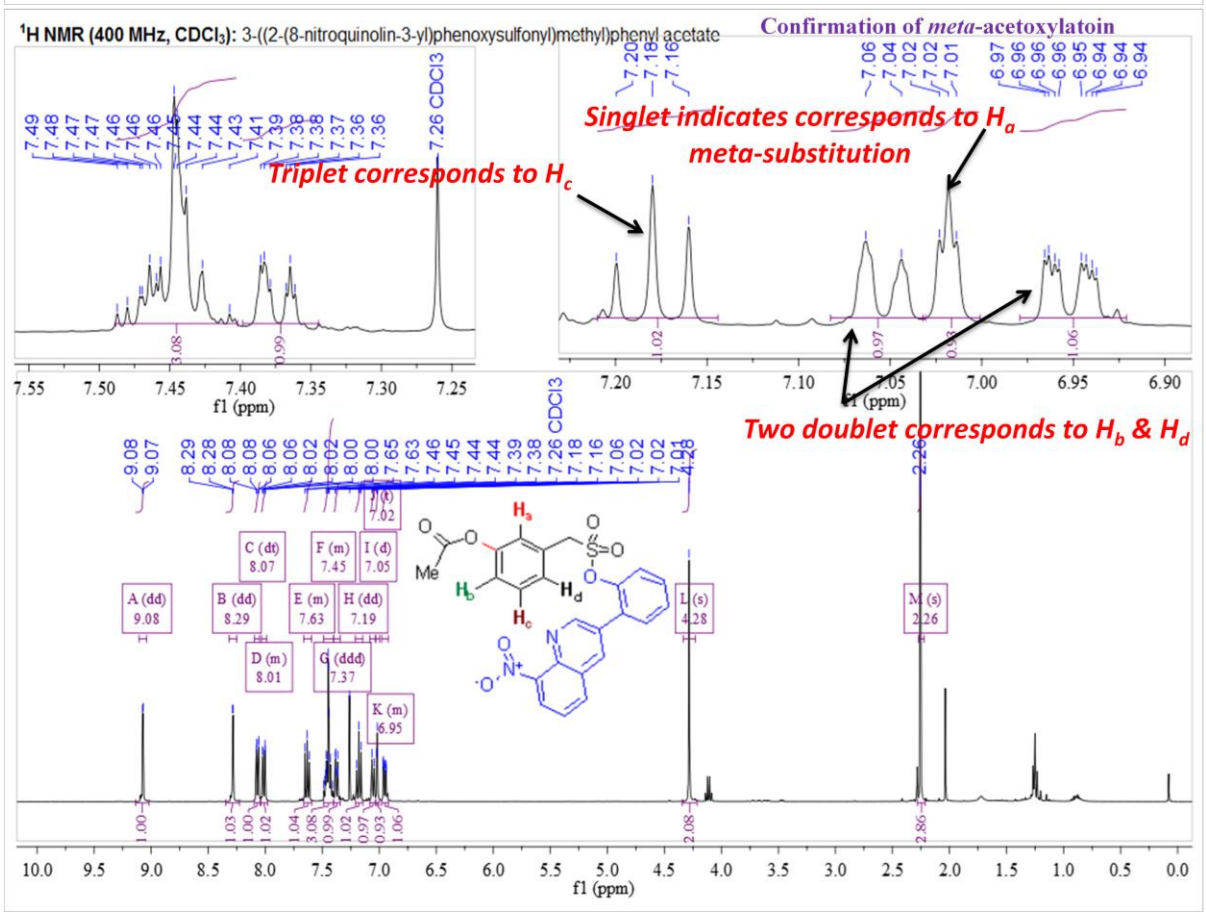
5. NMR Spectra

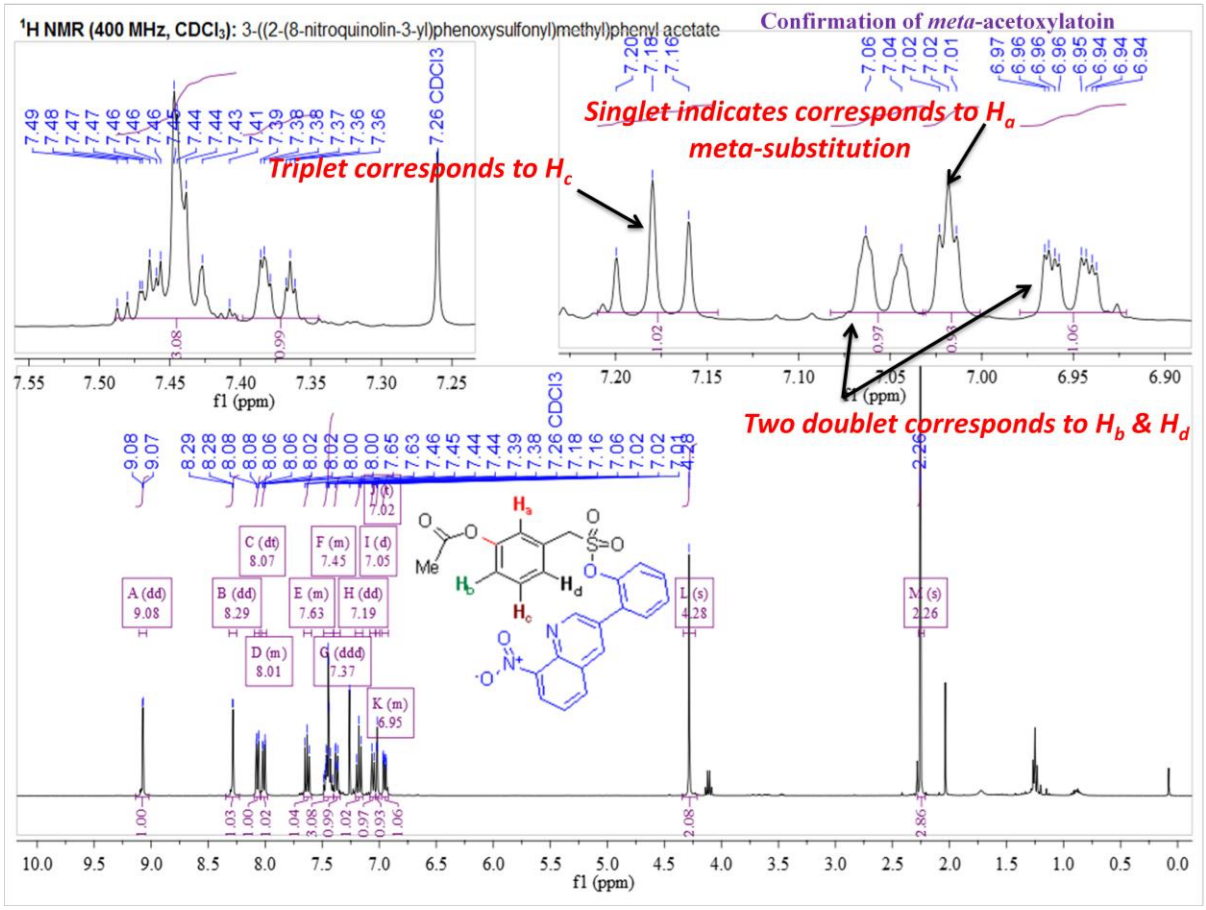
Confirmation of *meta*-olefination

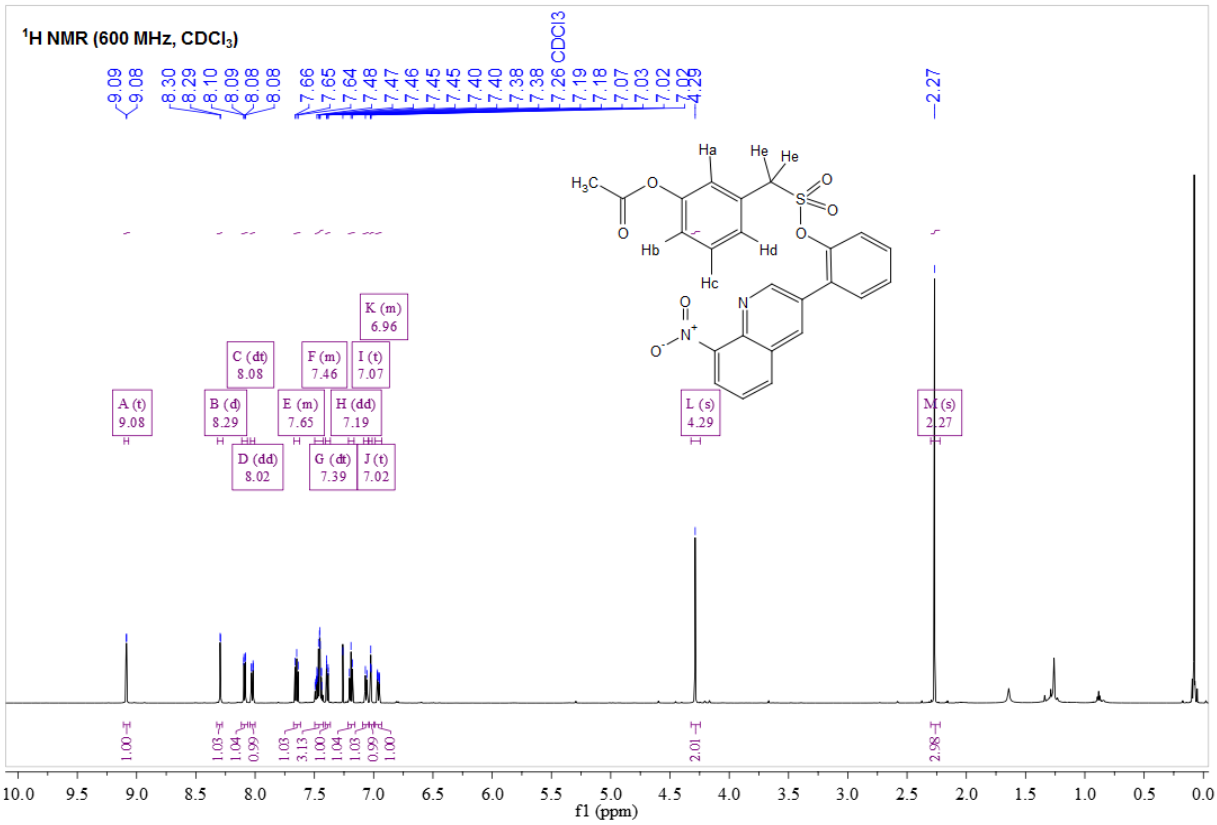




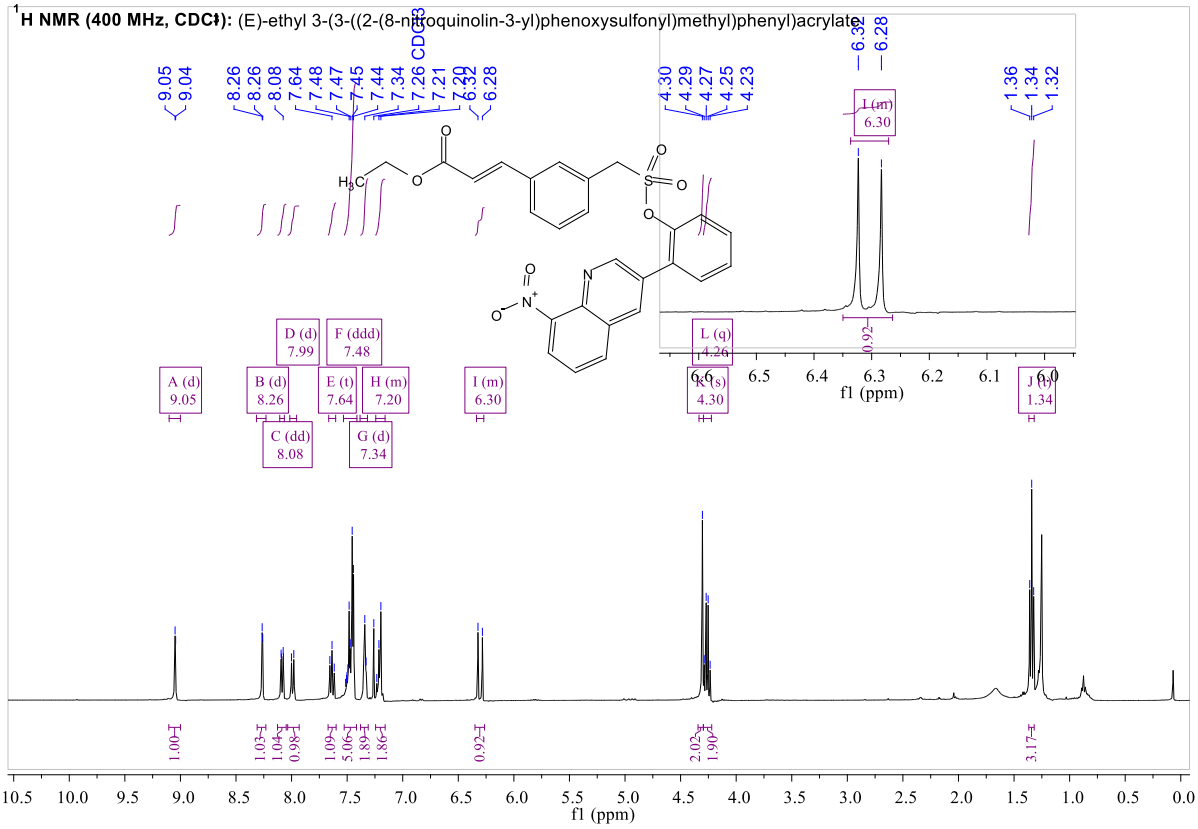

¹H NMR (400 MHz, CDCl₃): 3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate
Confirmation of meta-acetoxylatoin
Singlet indicates corresponds to Ha
meta-substitution
Triplet corresponds to Hc
Two doublet corresponds to Hb & Hd
f1 (ppm)

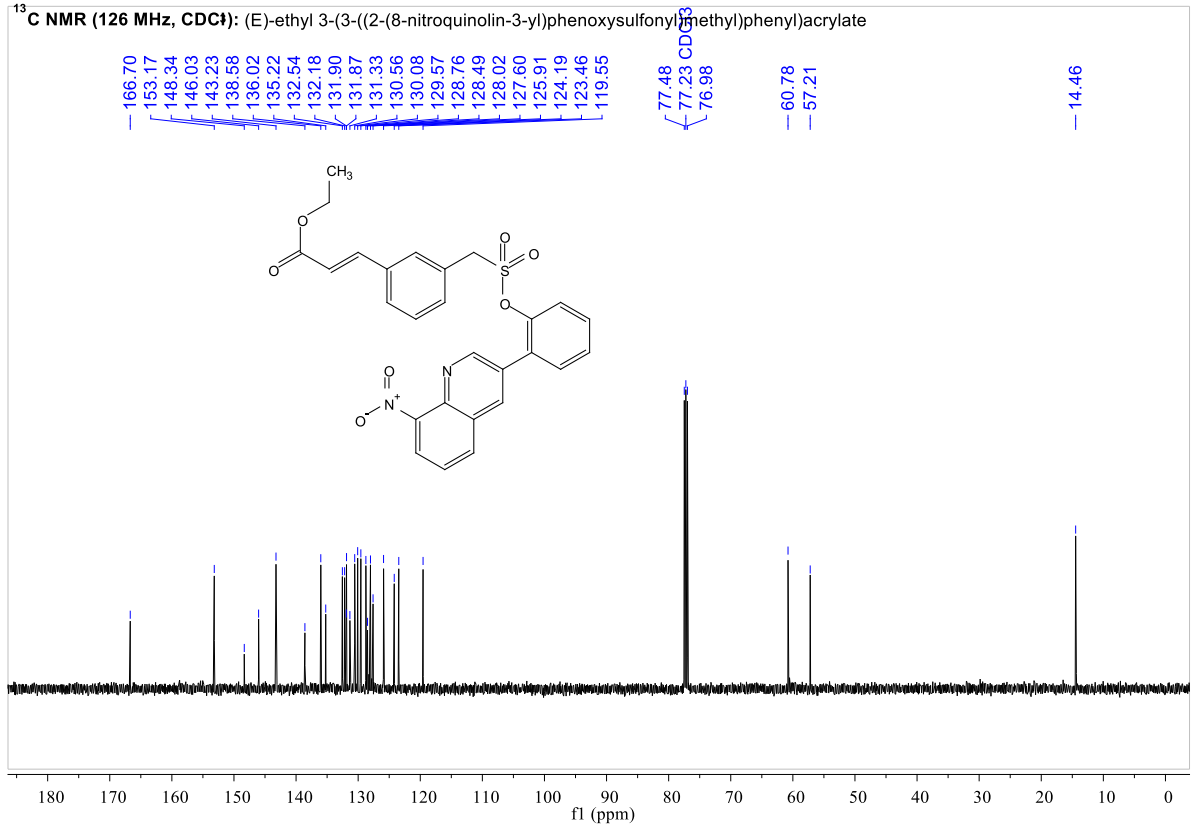

¹H NMR (400 MHz, CDCl₃): 3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate
Confirmation of meta-acetoxylatoin
Singlet indicates corresponds to Ha
meta-substitution
Triplet corresponds to Hc
Two doublet corresponds to Hb & Hd
f1 (ppm)


¹H NMR (400 MHz, CDCl₃): 3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate
Confirmation of meta-acetoxylatoin
Singlet indicates corresponds to Ha meta-substitution
Triplet corresponds to Hc
Two doublet corresponds to Hb & Hd
f1 (ppm)

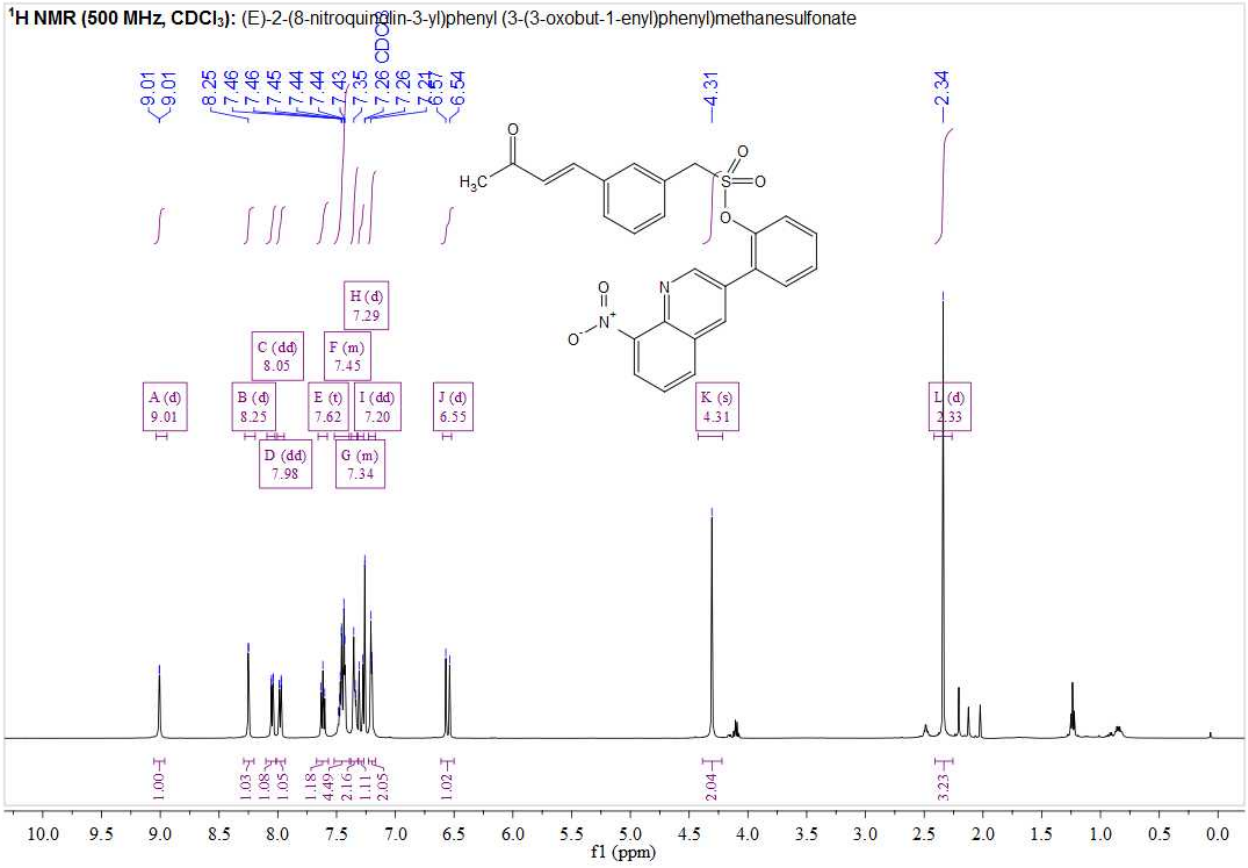

¹H NMR (600 MHz, CDCl₃)
f1 (ppm)

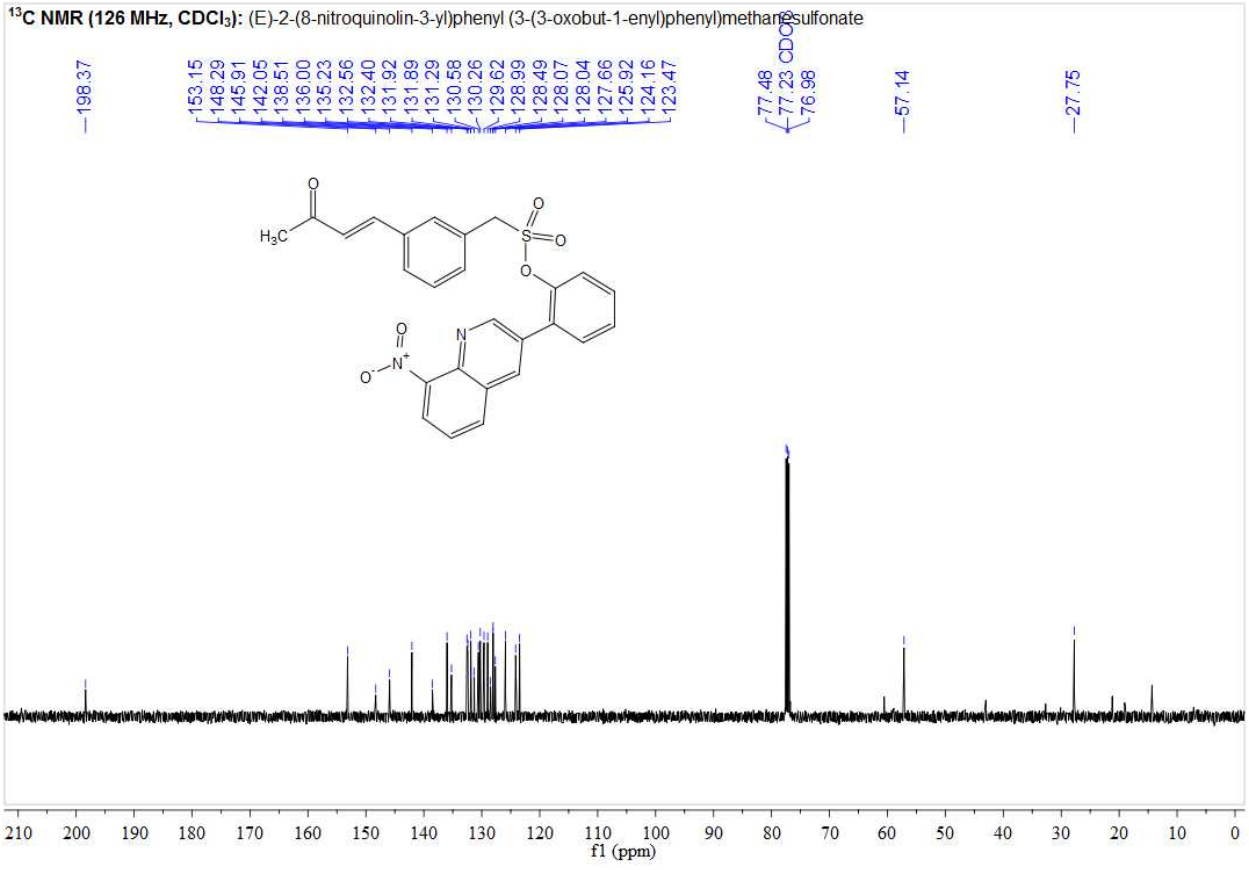
(*E*)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (2a).



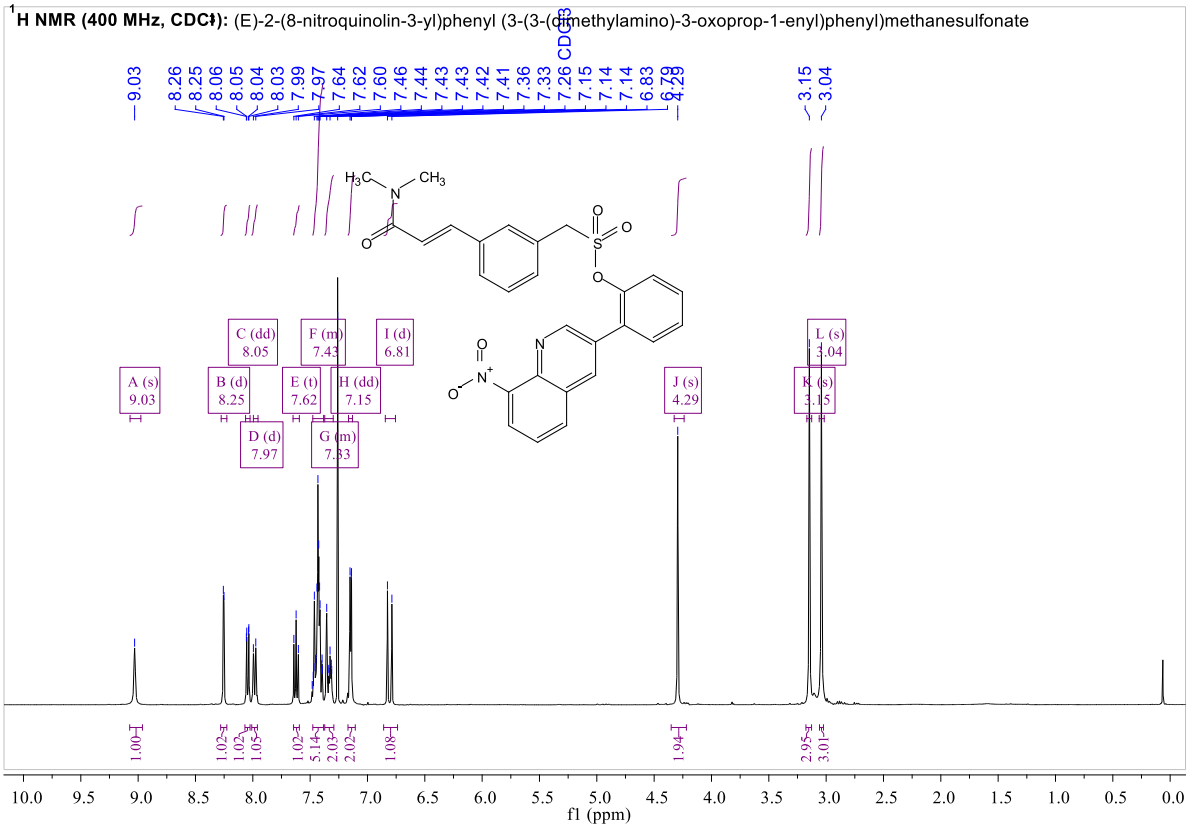


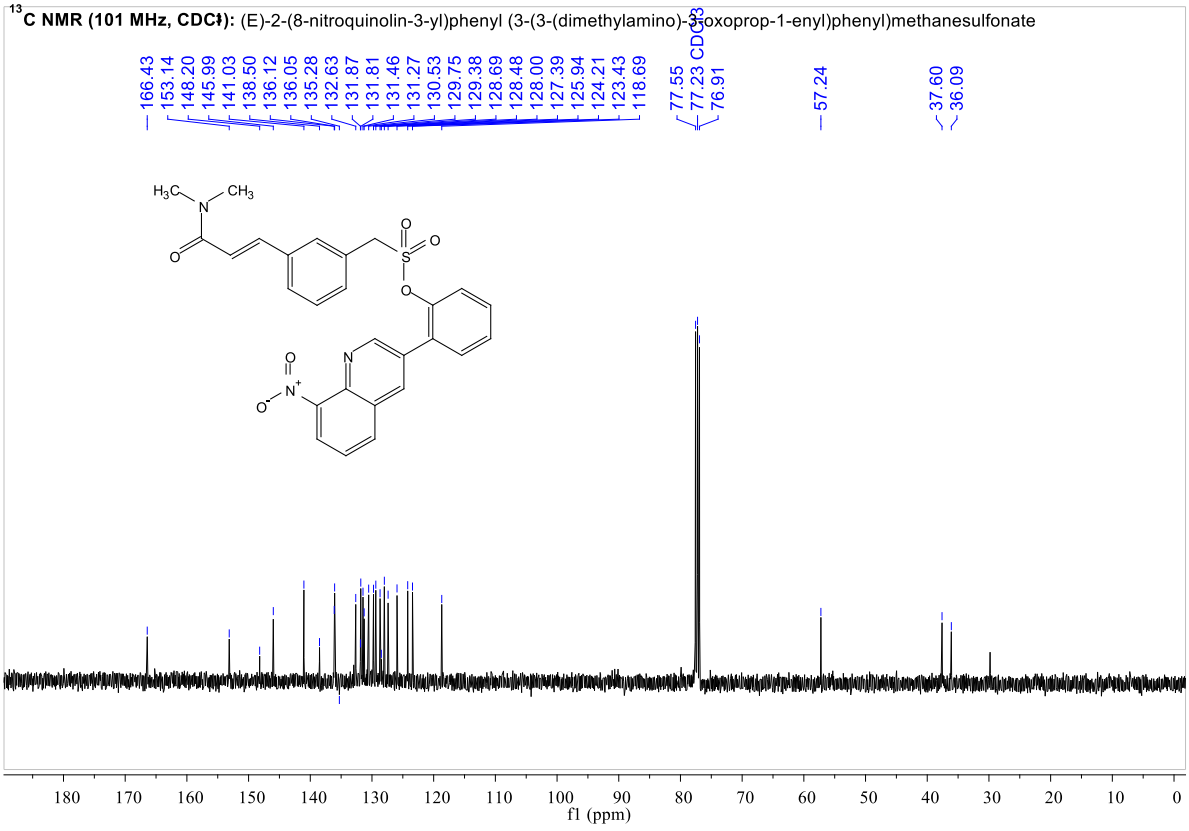
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-(3-oxobut-1-enyl)phenyl)methanesulfonate (2b):



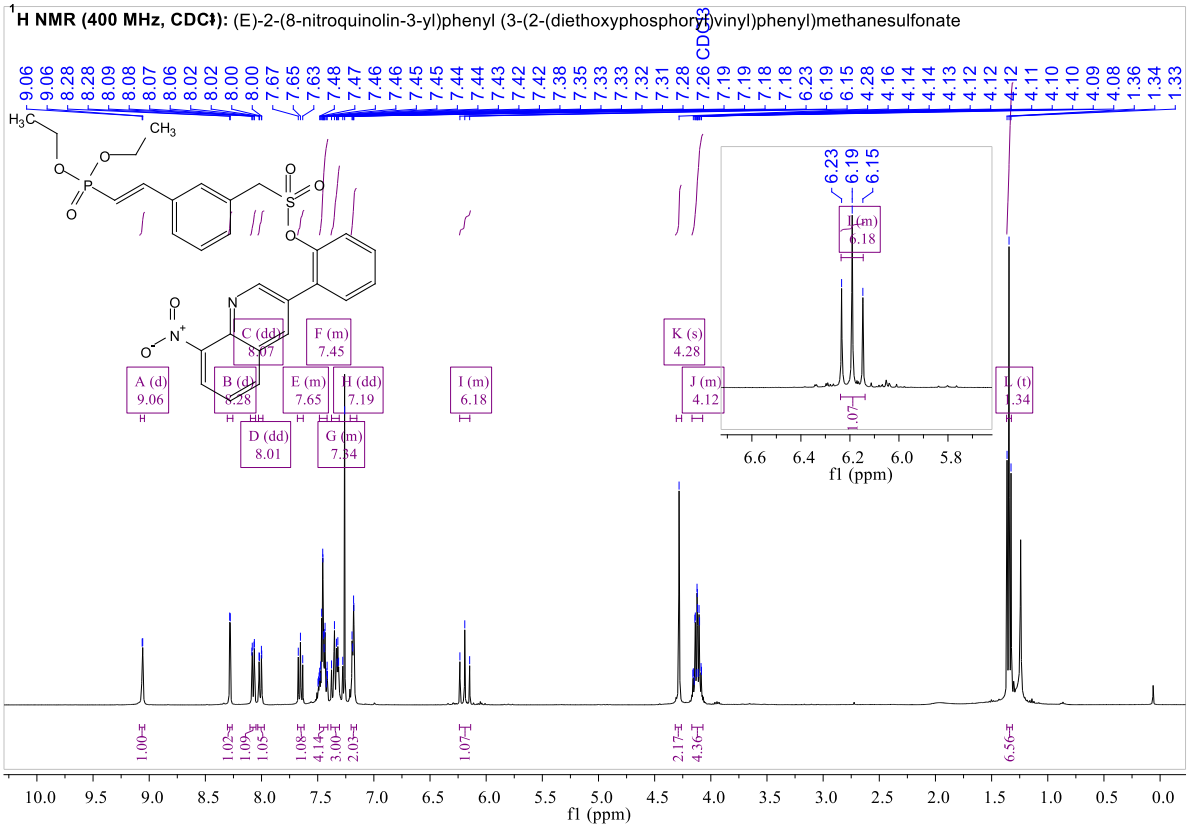


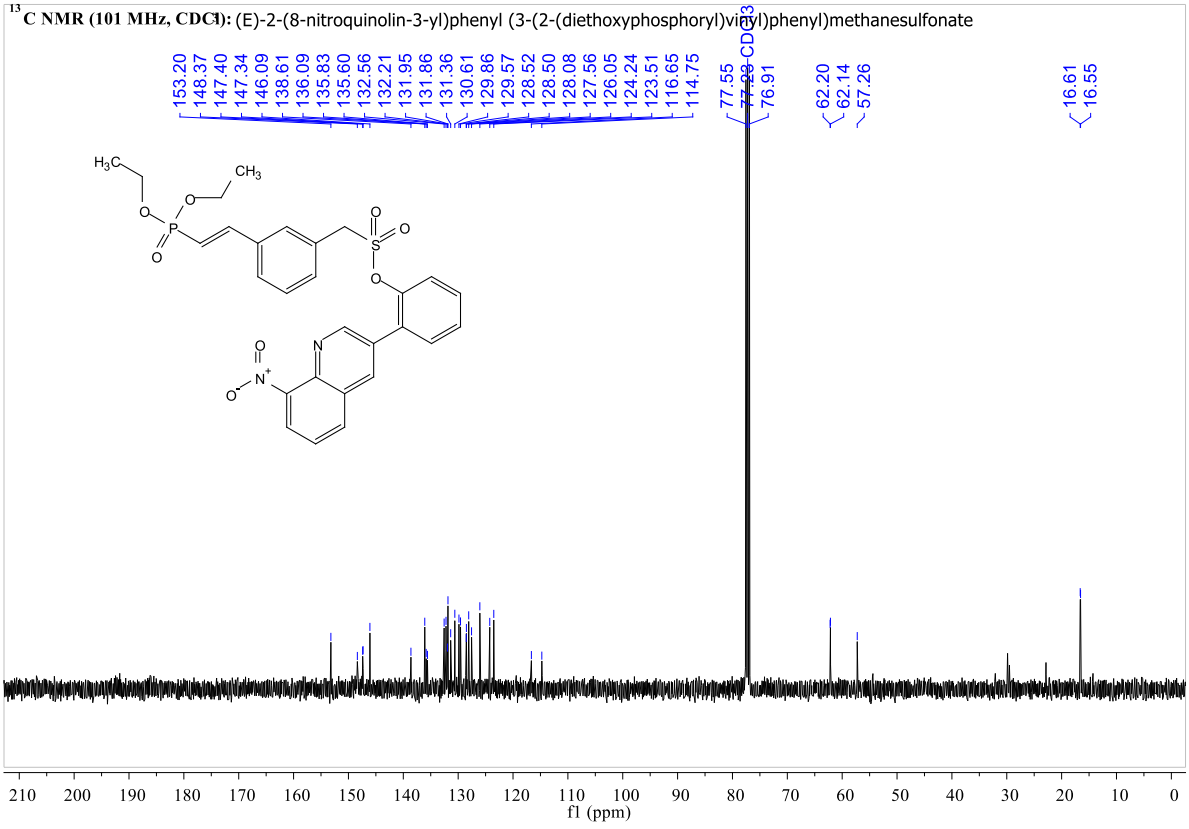
(E)-2-(8-nitroquinolin-3-yl)phenyl(3-(3-(dimethylamino)-3-oxoprop-1-enyl)phenyl)-methanesulfonate (2c):



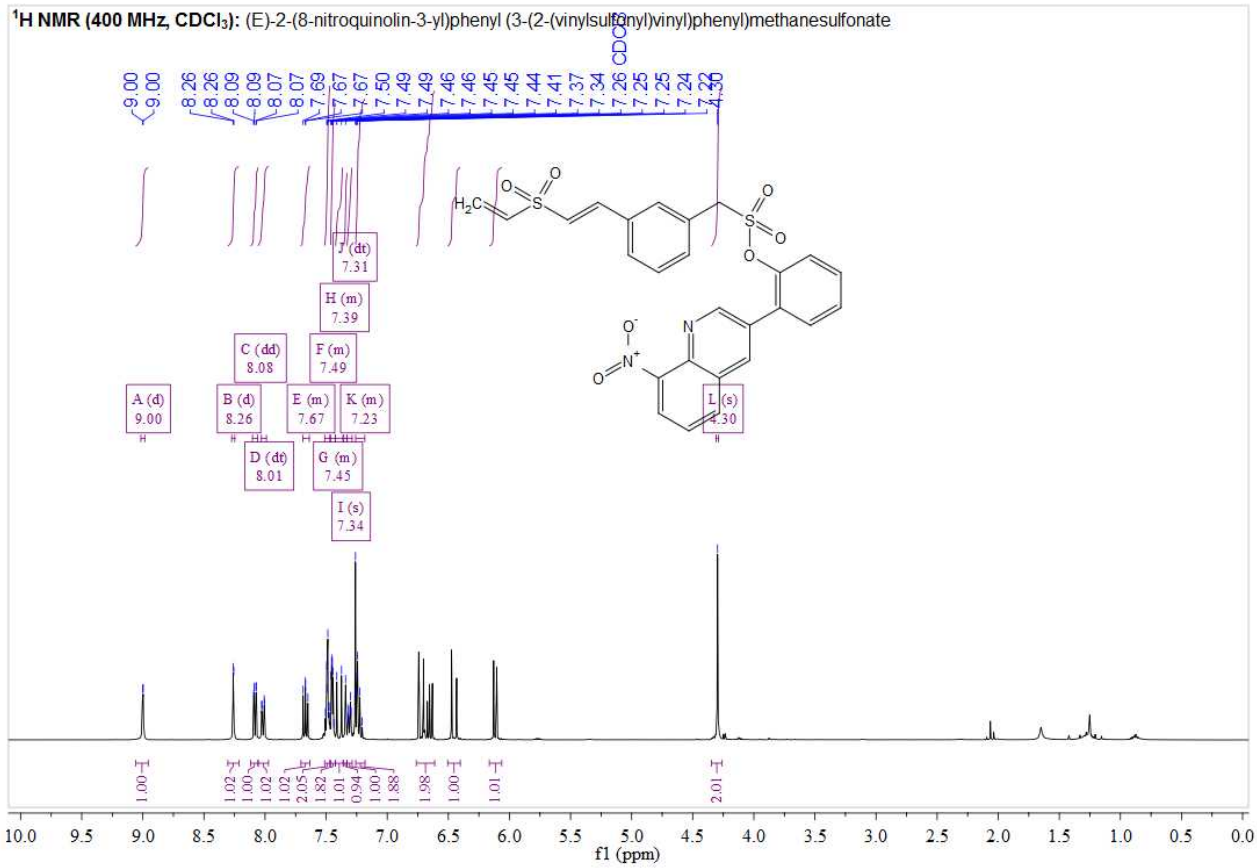


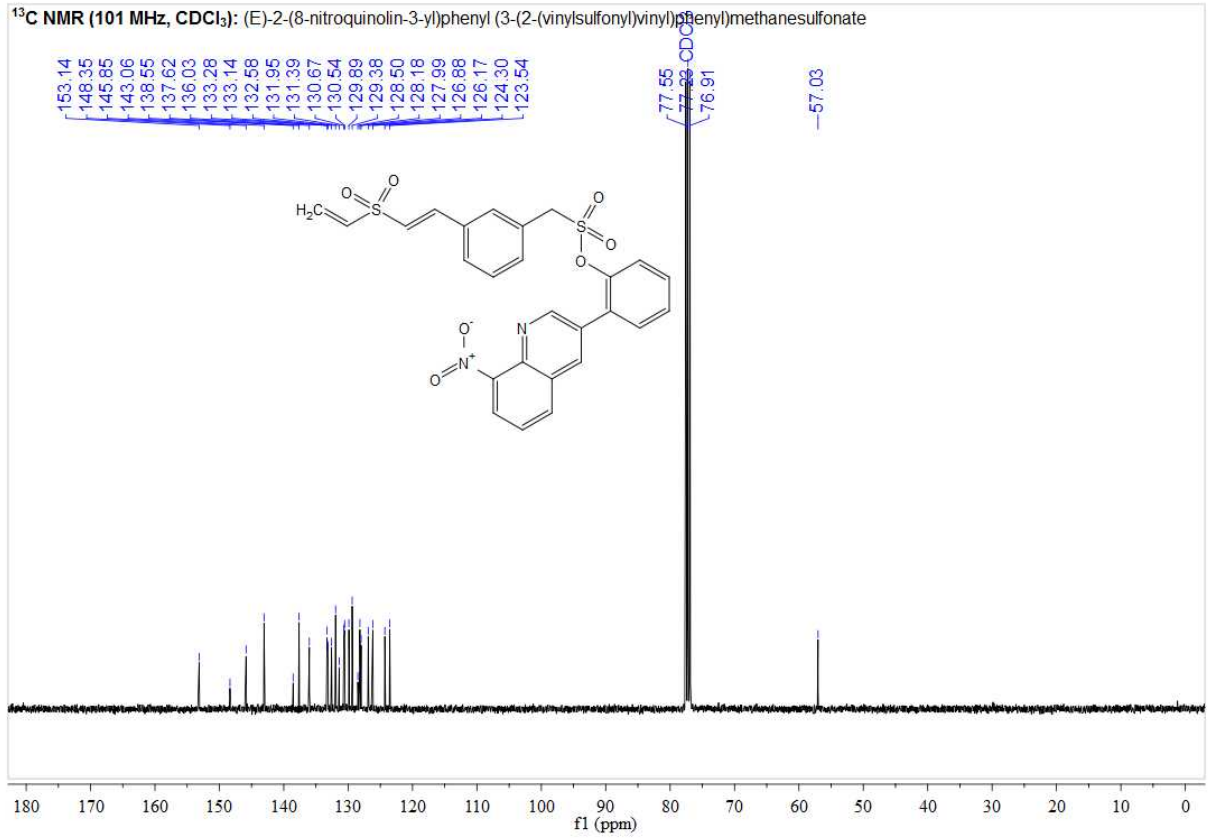
(E)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-(diethoxyphosphoryl)vinyl)phenyl)methane-sulfonate (2d):



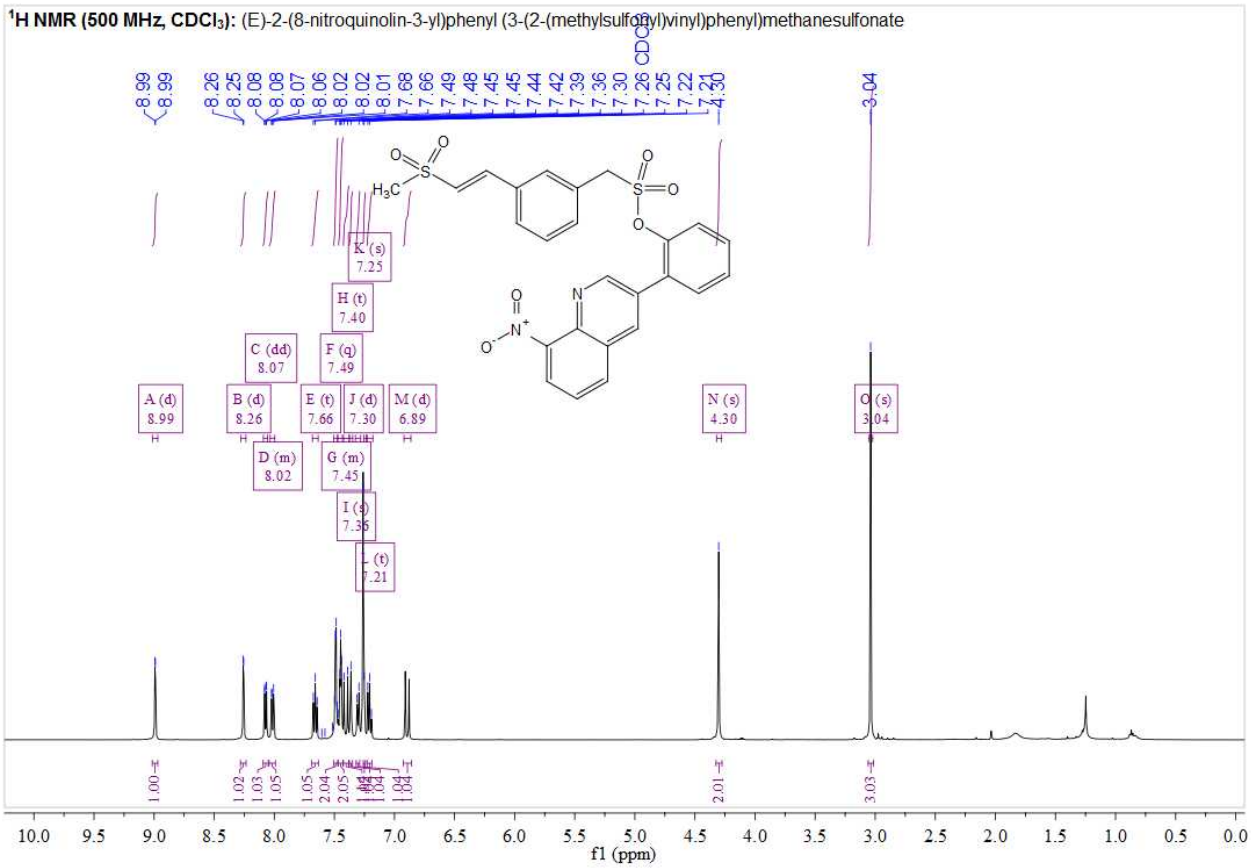


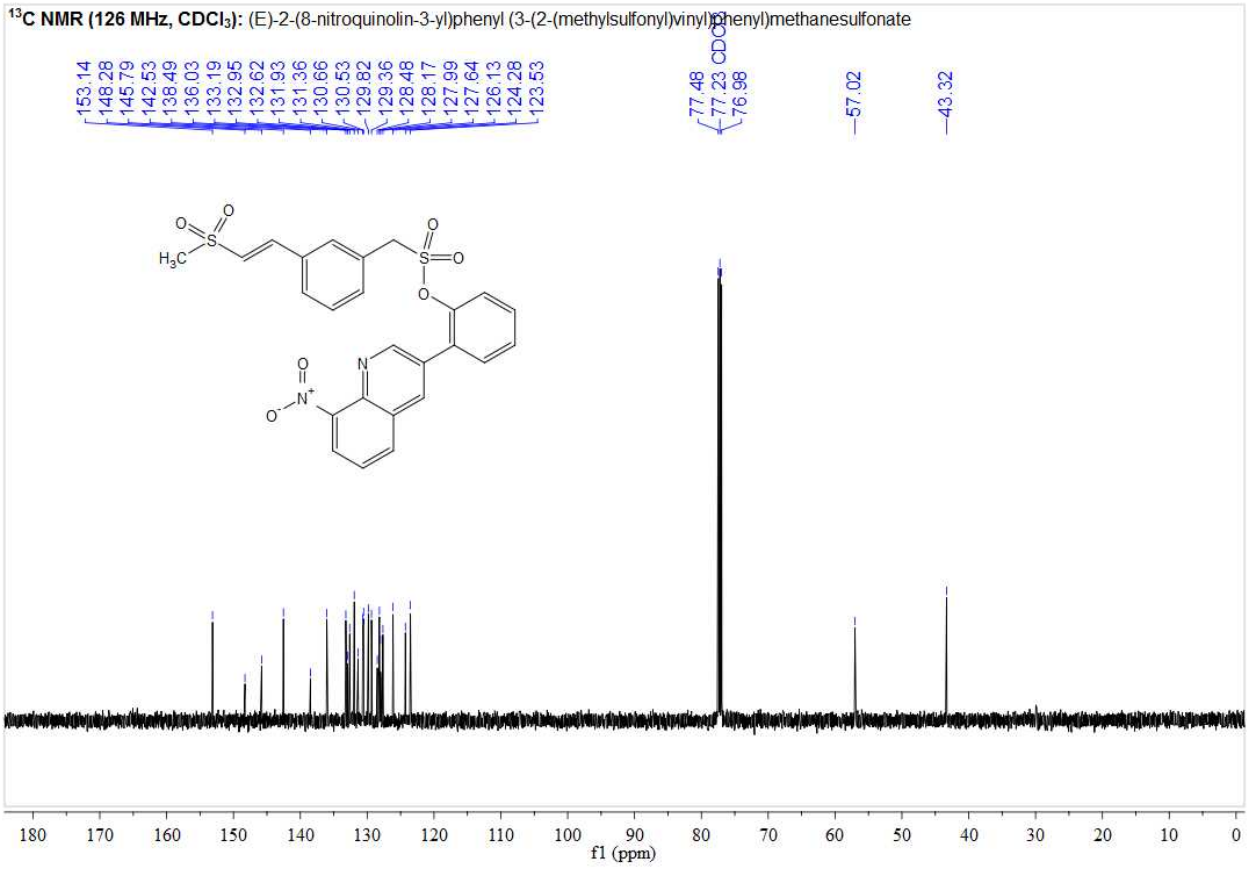
(E)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-(vinylsulfonyl)vinyl)phenyl)methanesulfonate (2e):



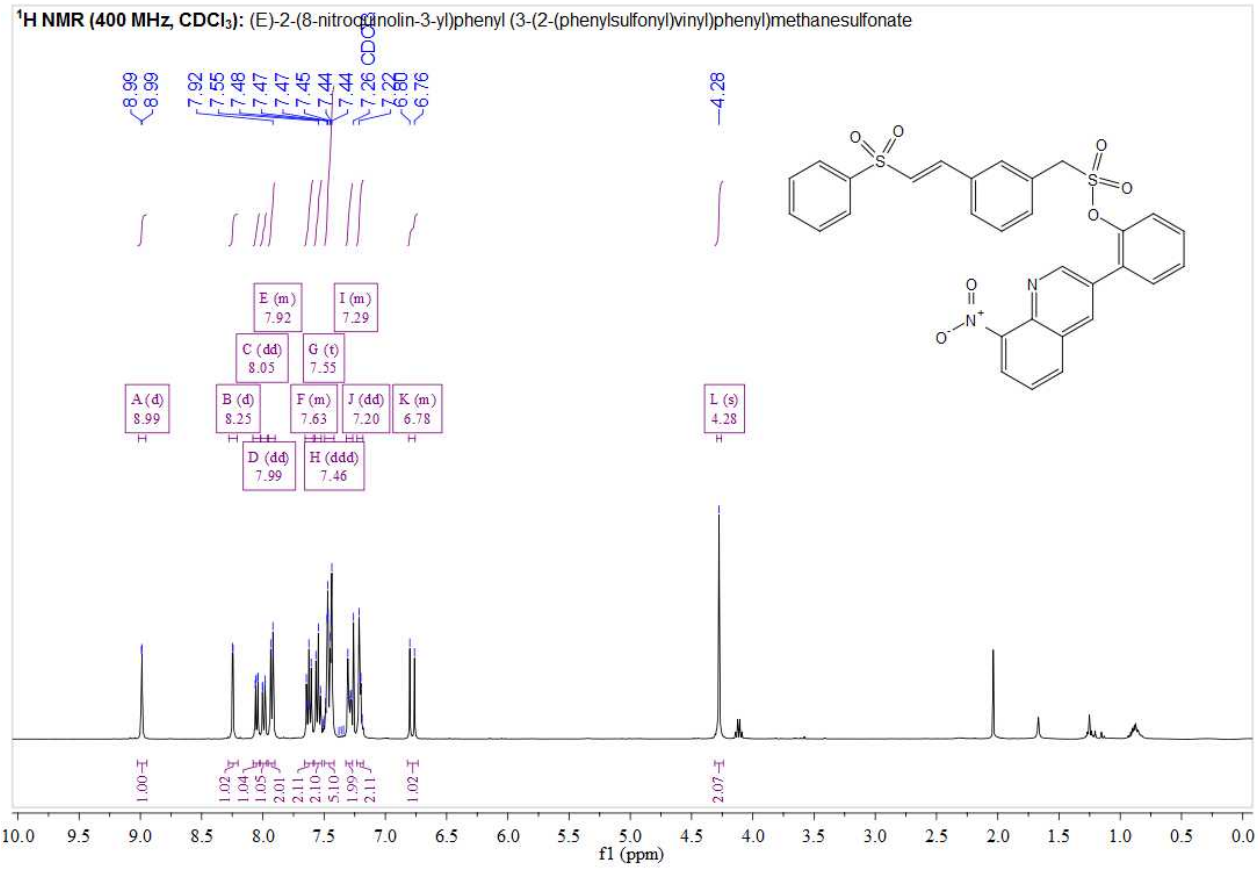


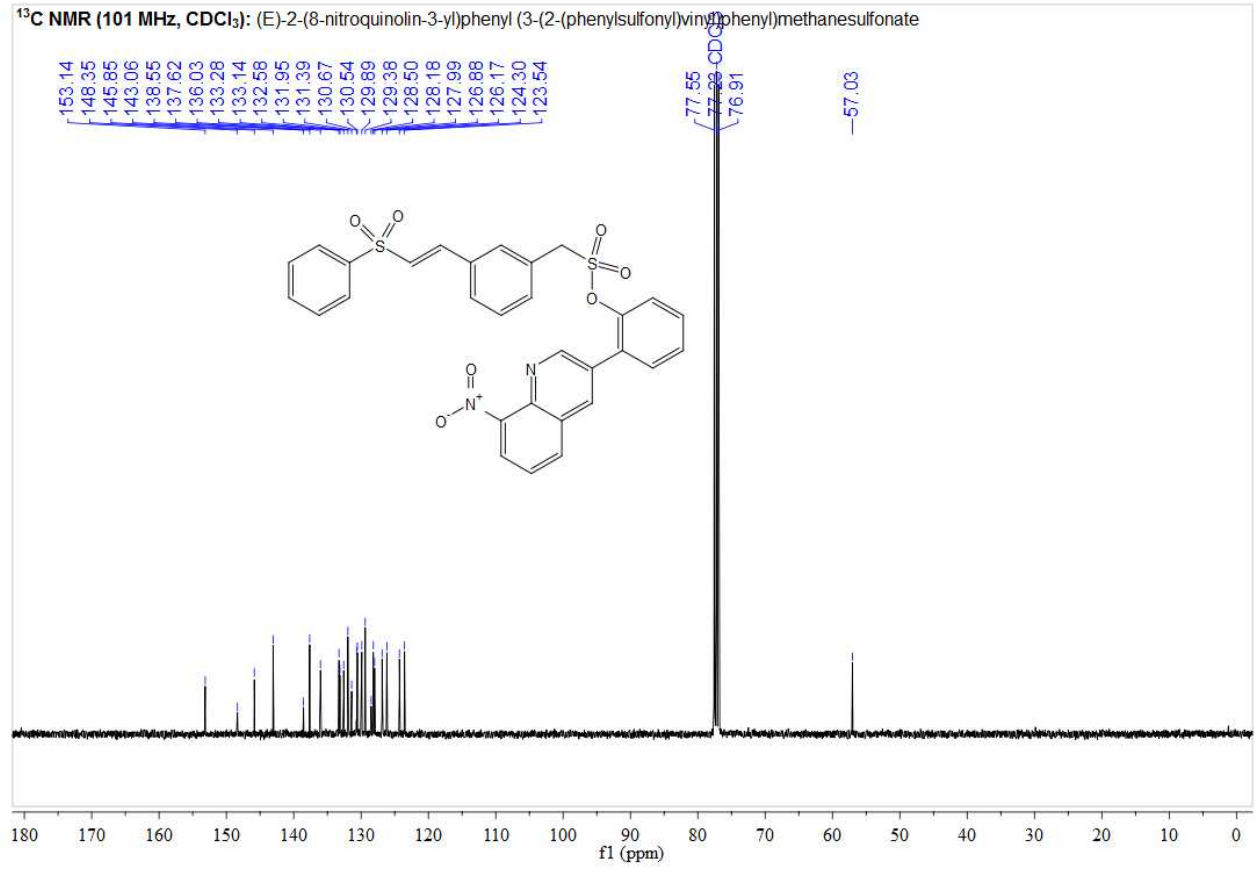
(E)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-(methylsulfonyl)vinyl)phenyl)methanesulfonate (2f):



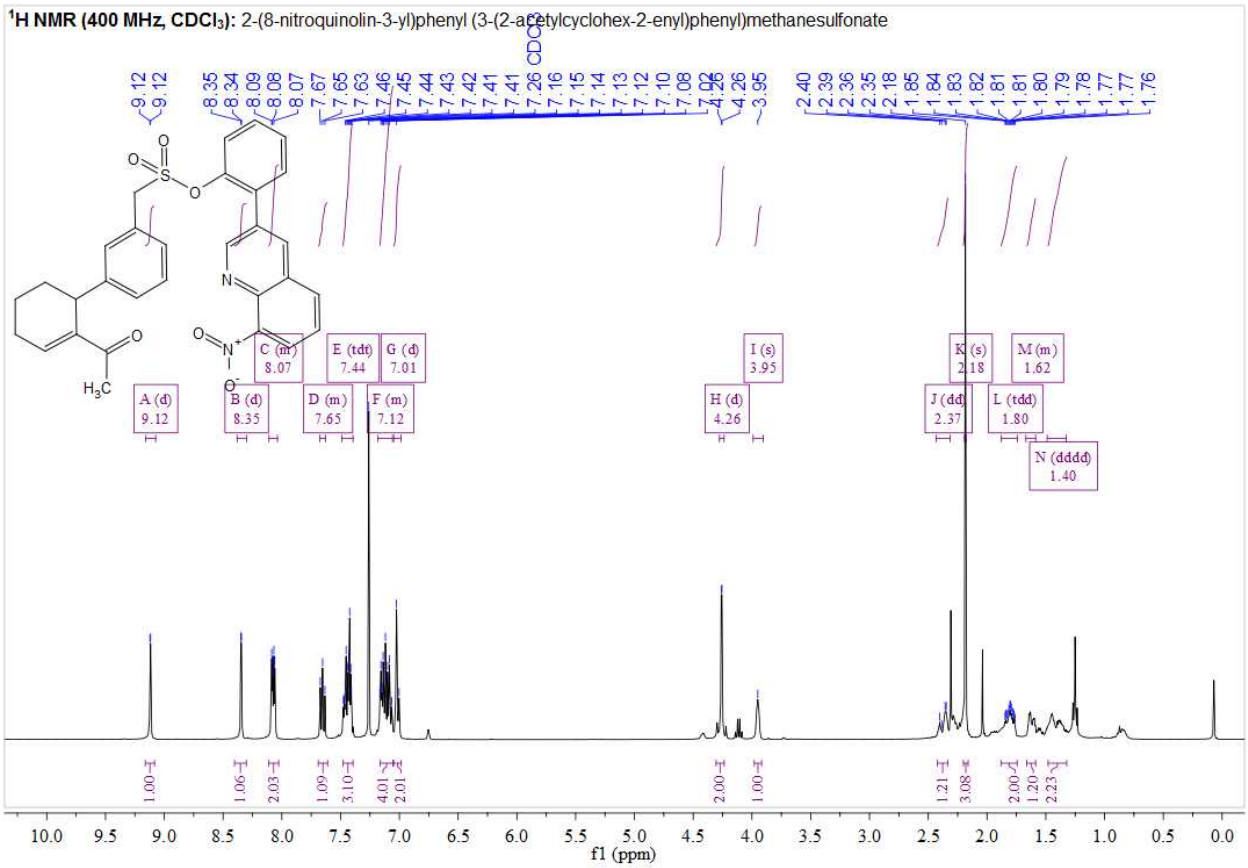


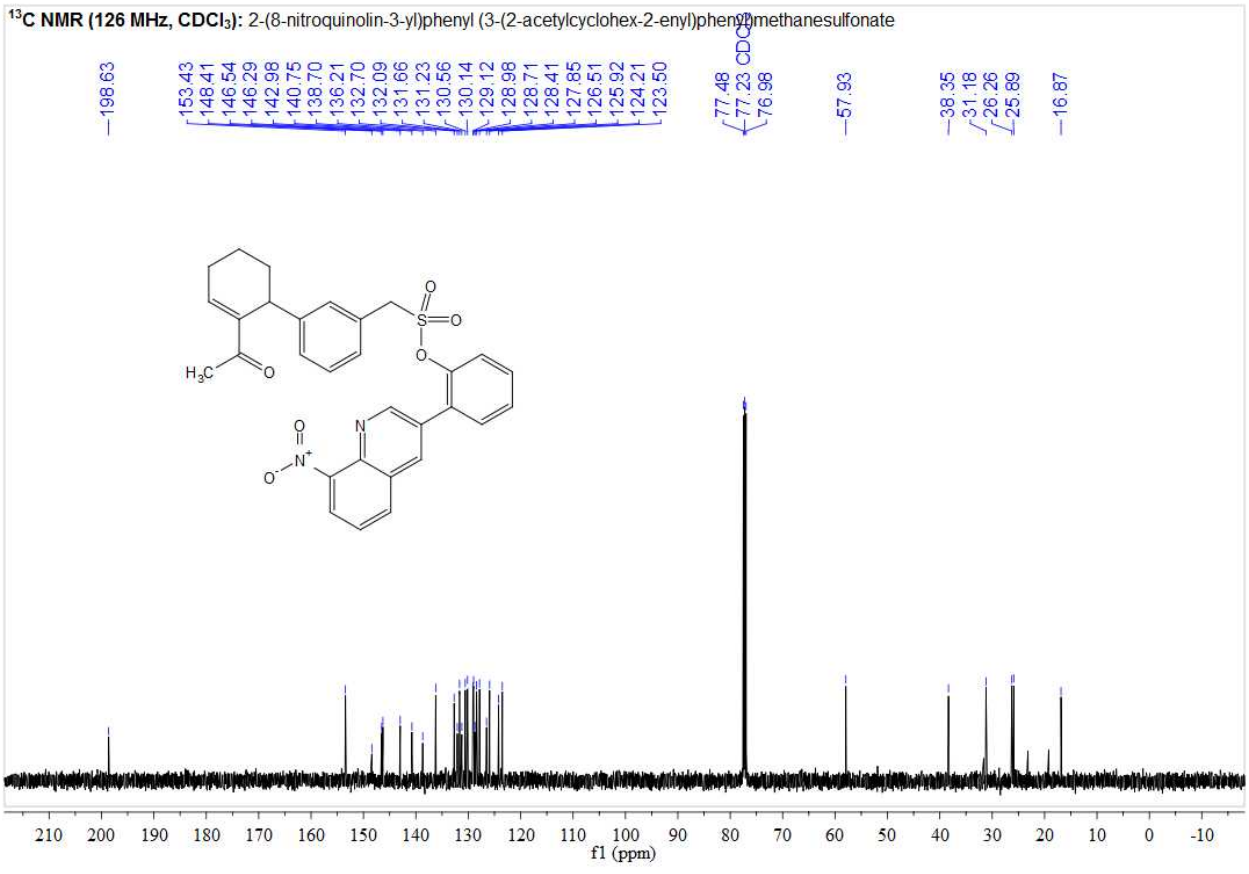
(E)-8-nitro-3-(2-((3-(2-(phenylsulfonyl)vinyl)benzylsulfonyl)methyl)phenyl)quinoline (2g):



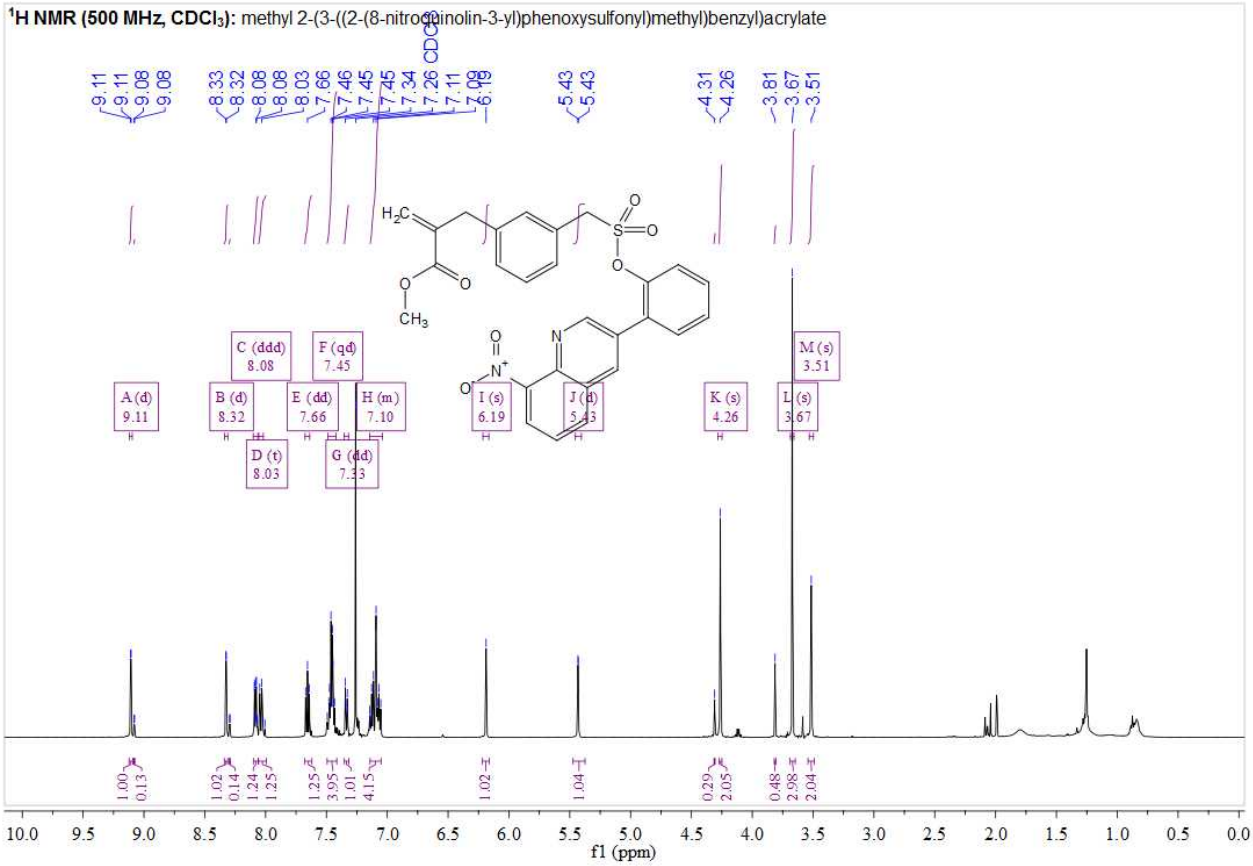


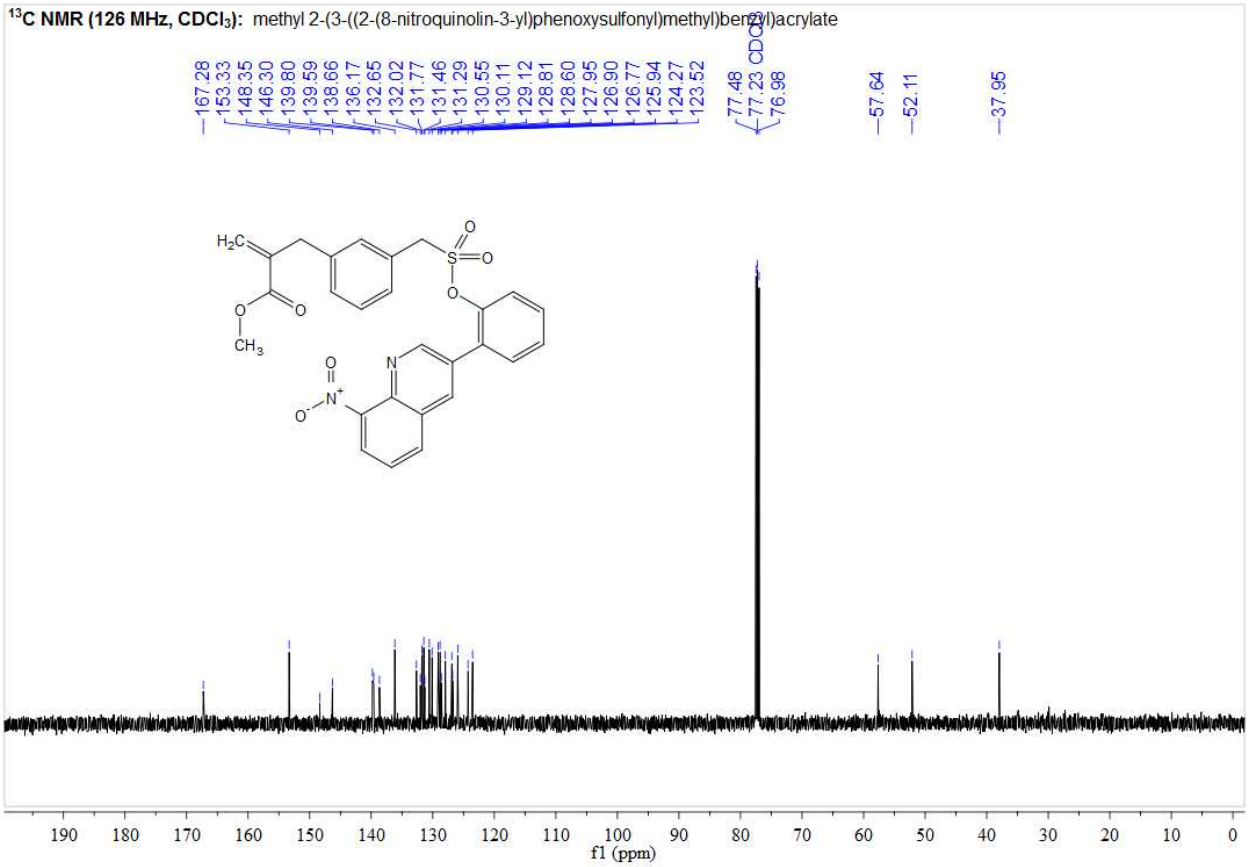
(*S*)-2-(8-nitroquinolin-3-yl)phenyl (3-(2-acetylcyclohex-2-enyl)phenyl)methanesulfonate (2h):



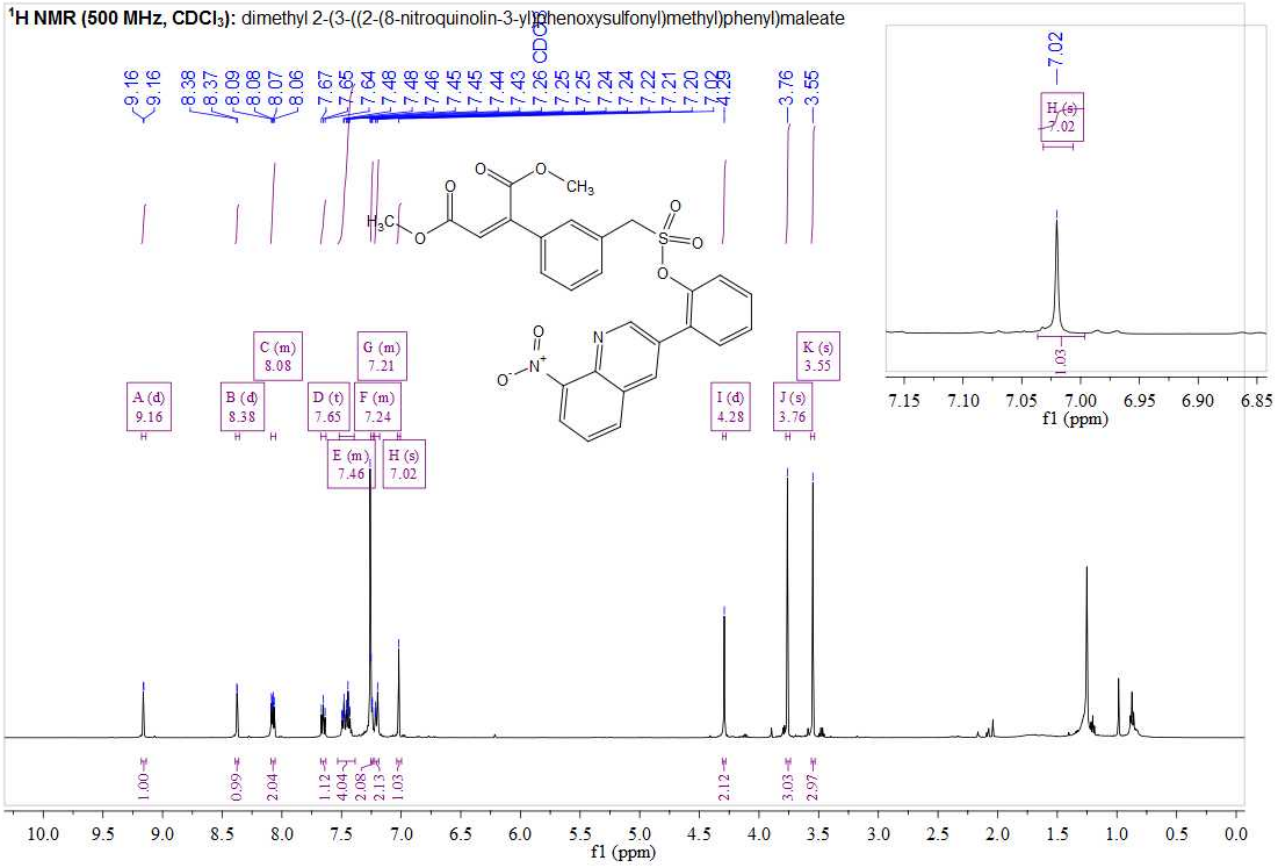


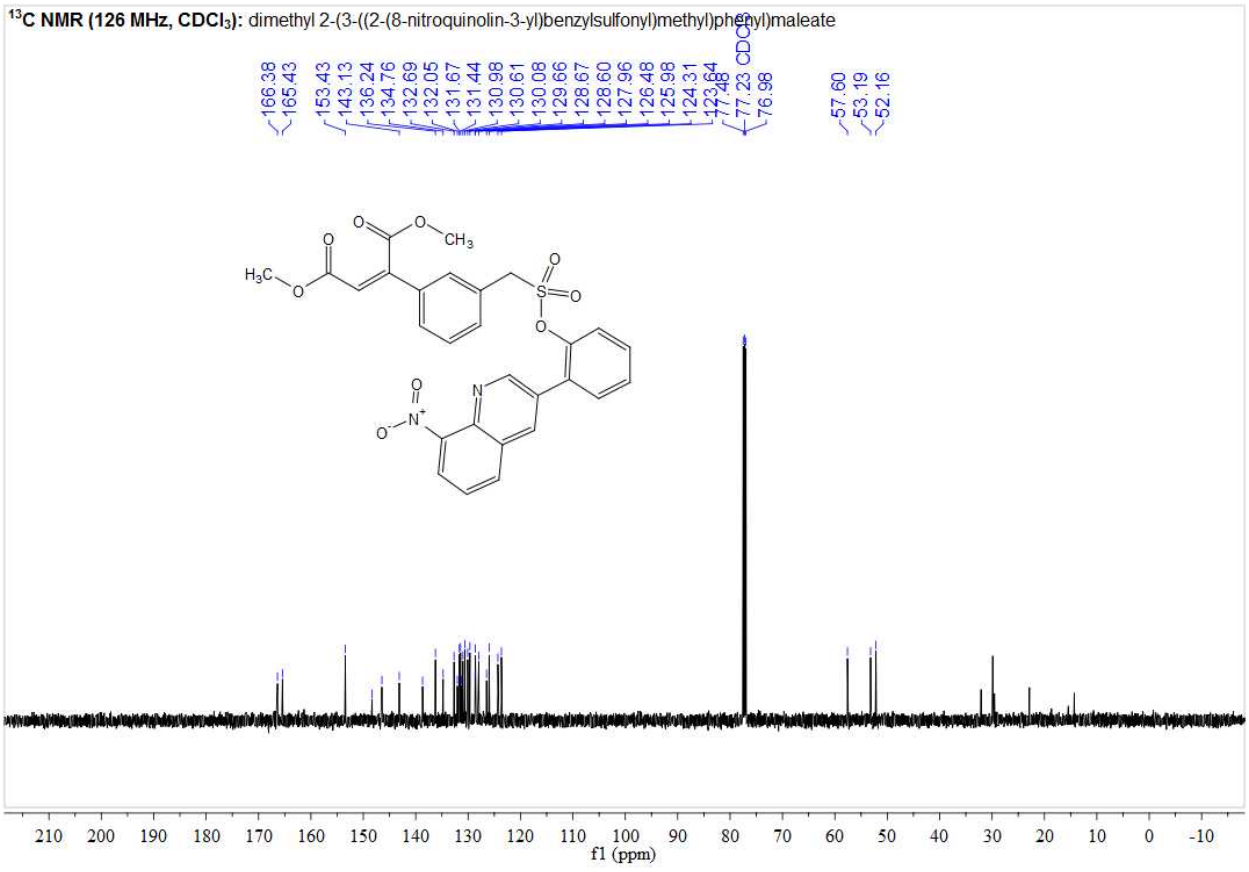
Methyl 2-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)benzyl)acrylate (2i):



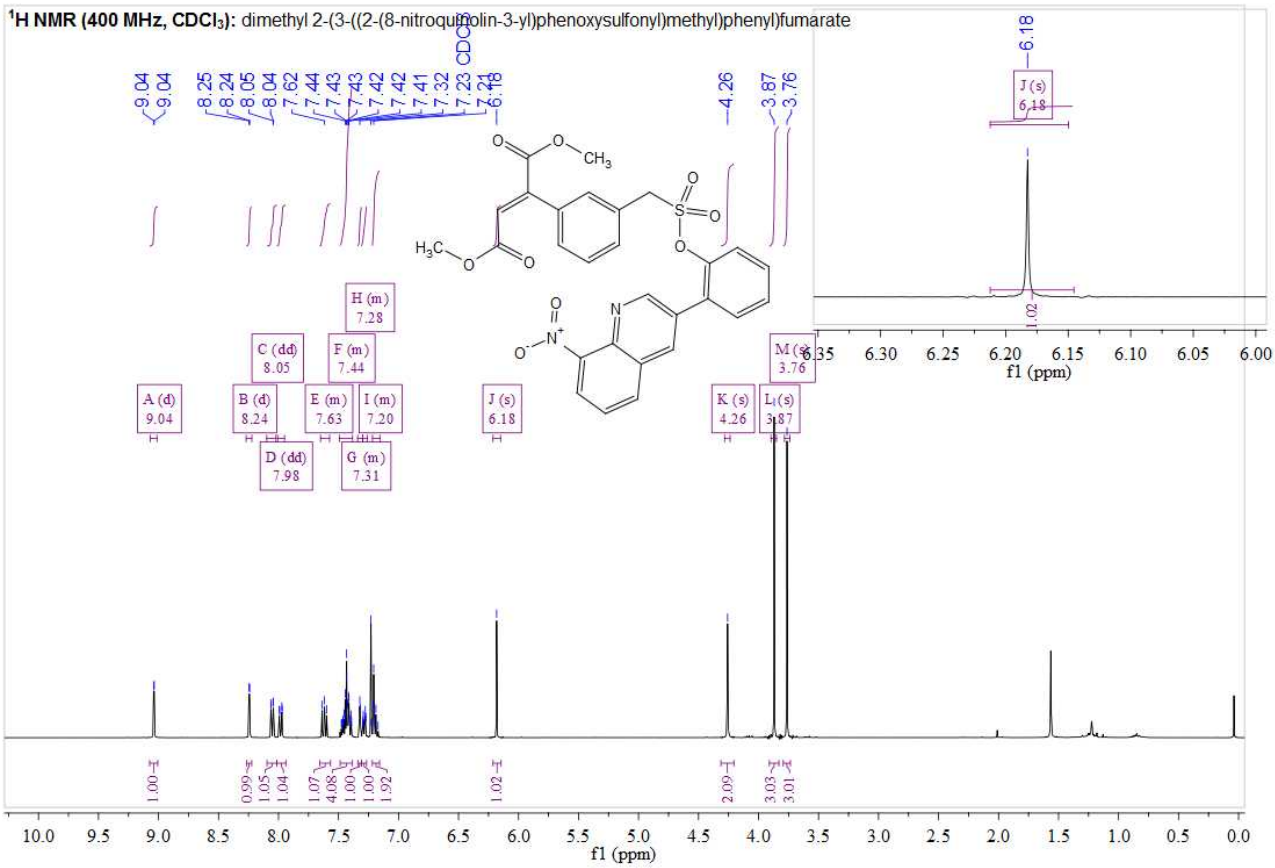


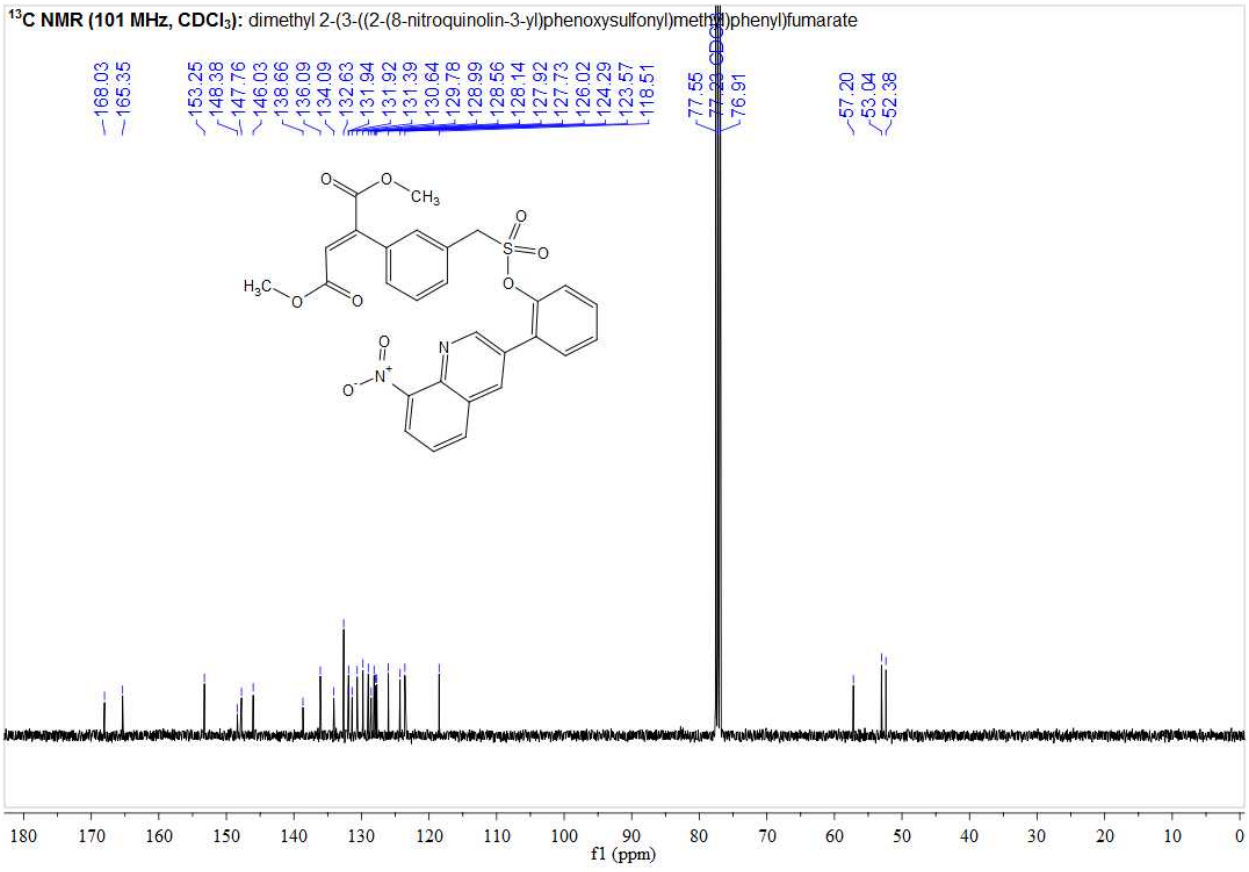
Dimethyl 2-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)maleate (2j):



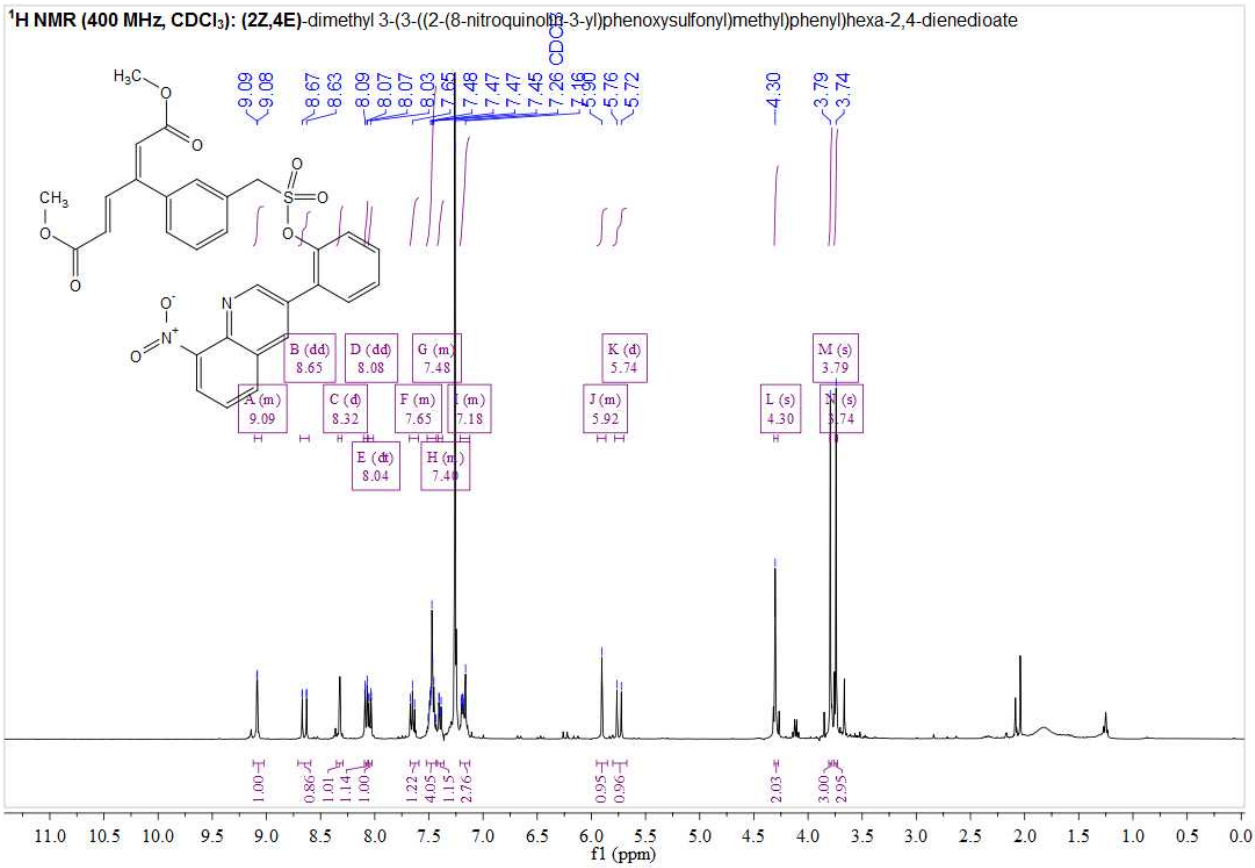


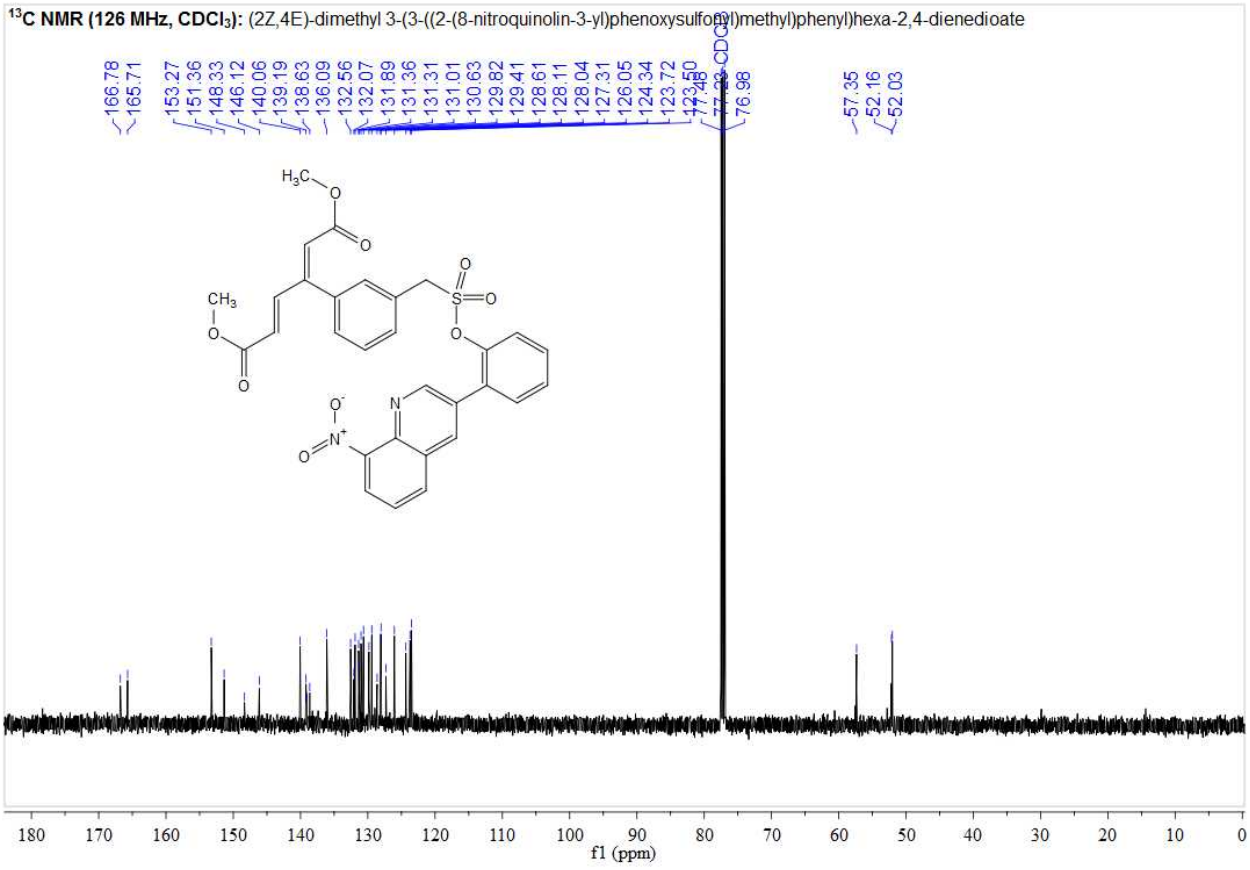
Dimethyl 2-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)maleate (2k):



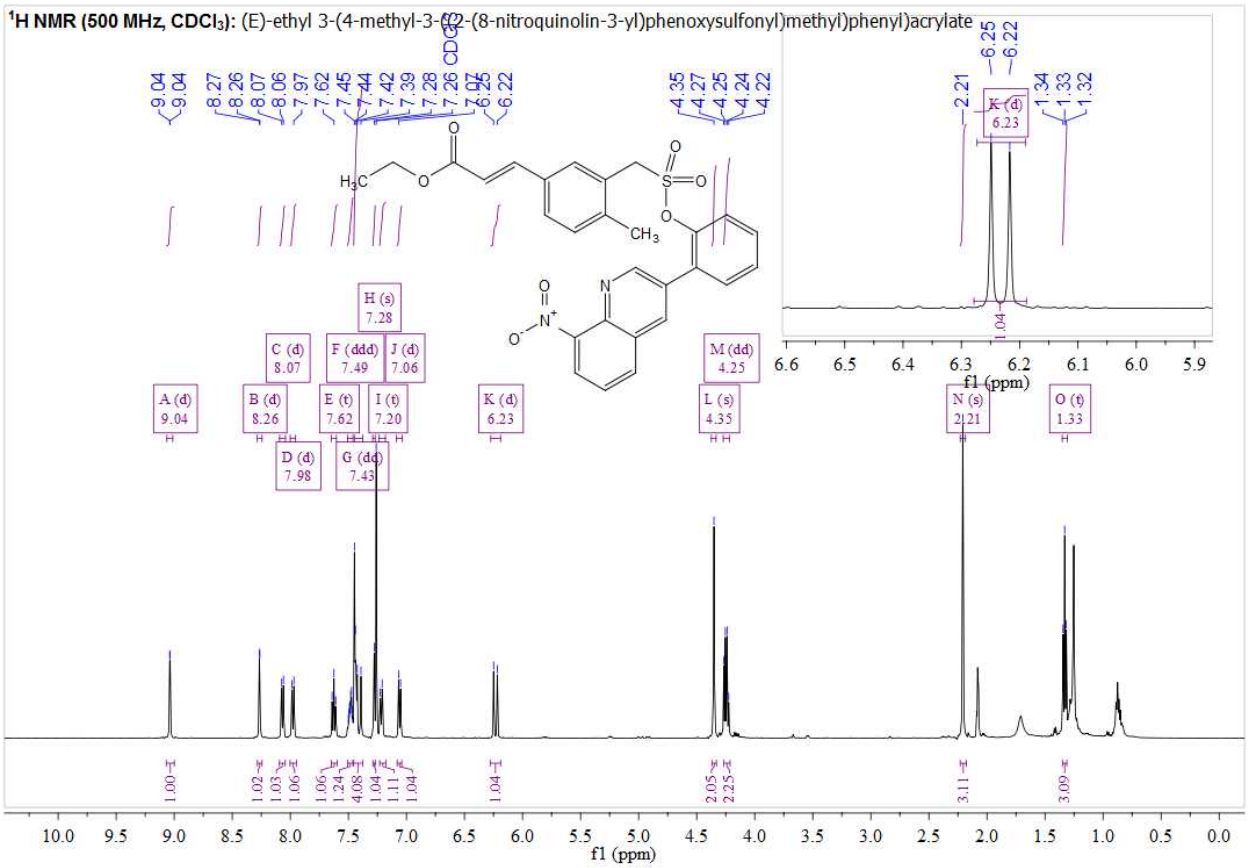


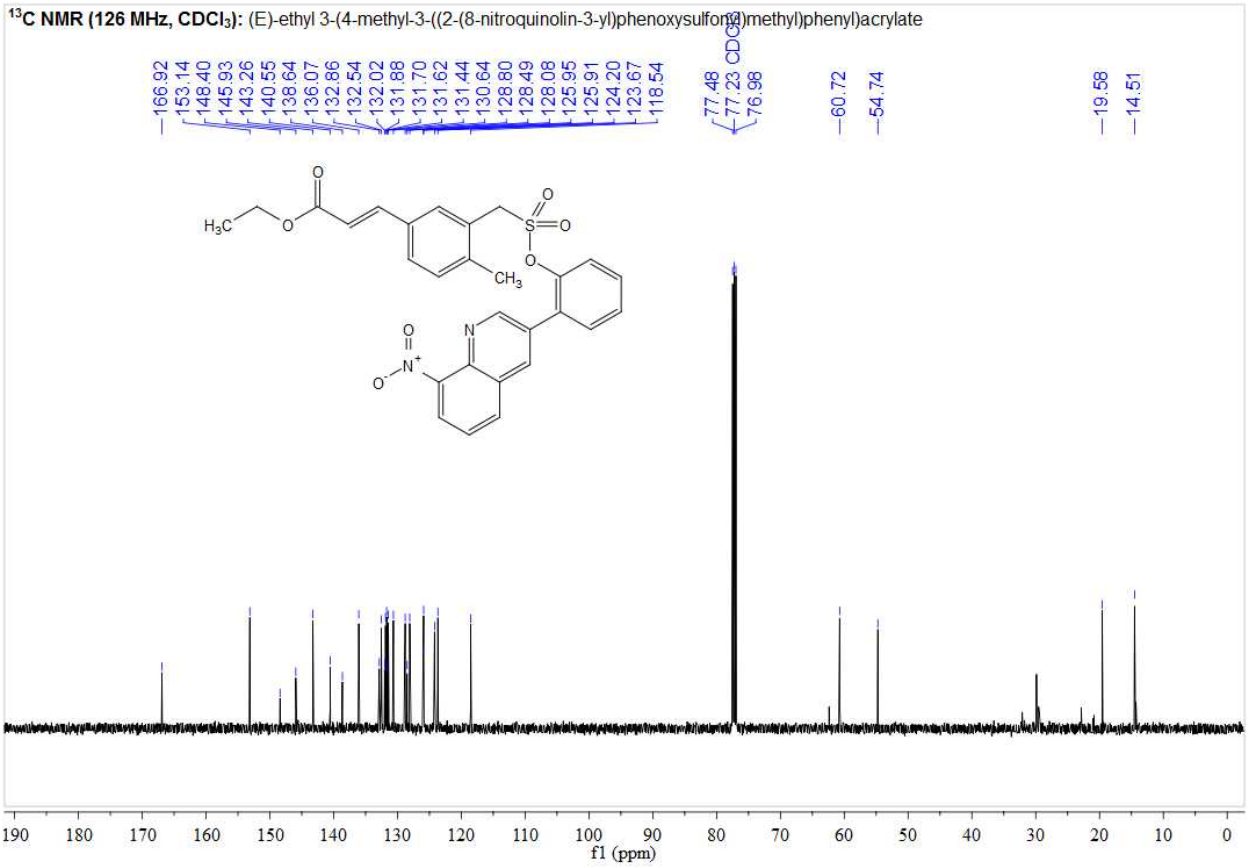
(2Z,4Z)-dimethyl3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)hexa-2,4-dienedio-ate (2l):



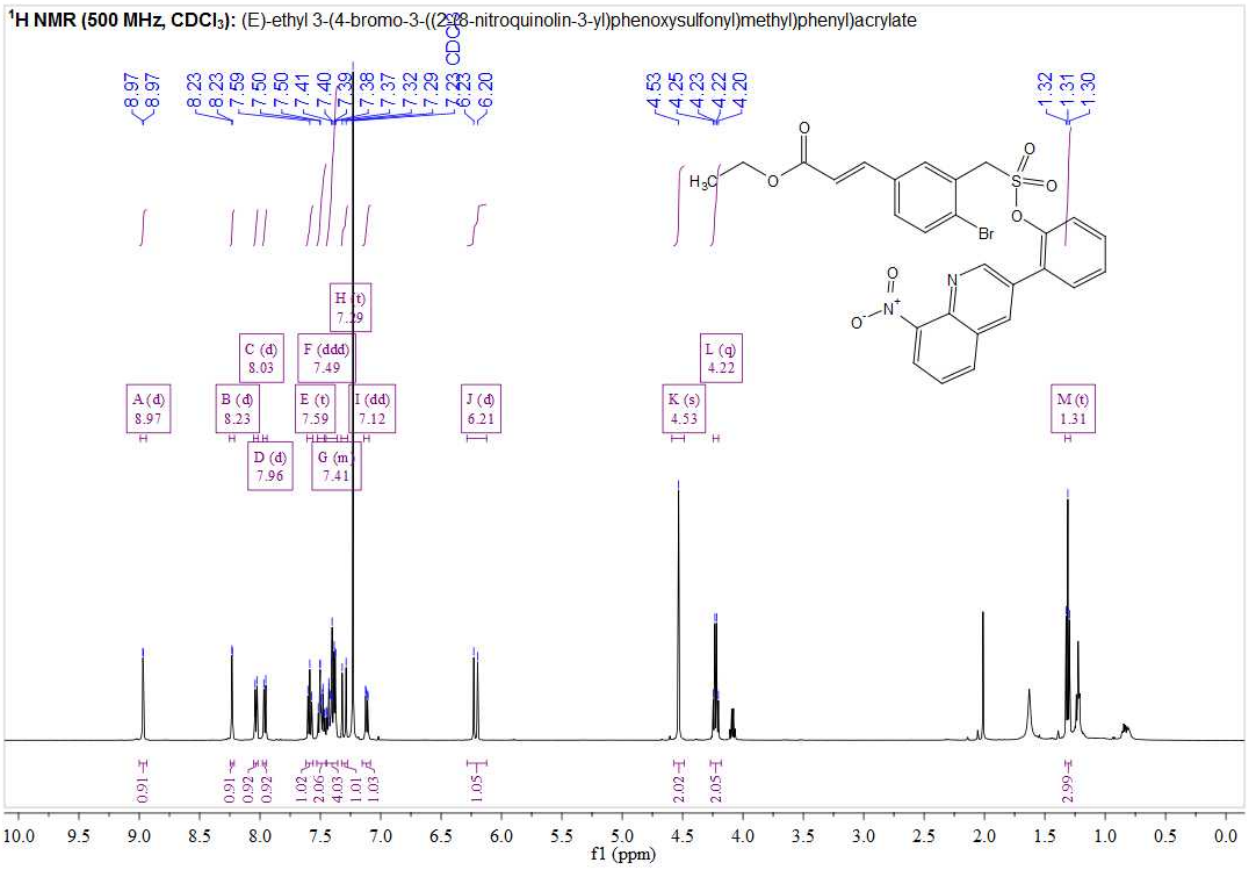


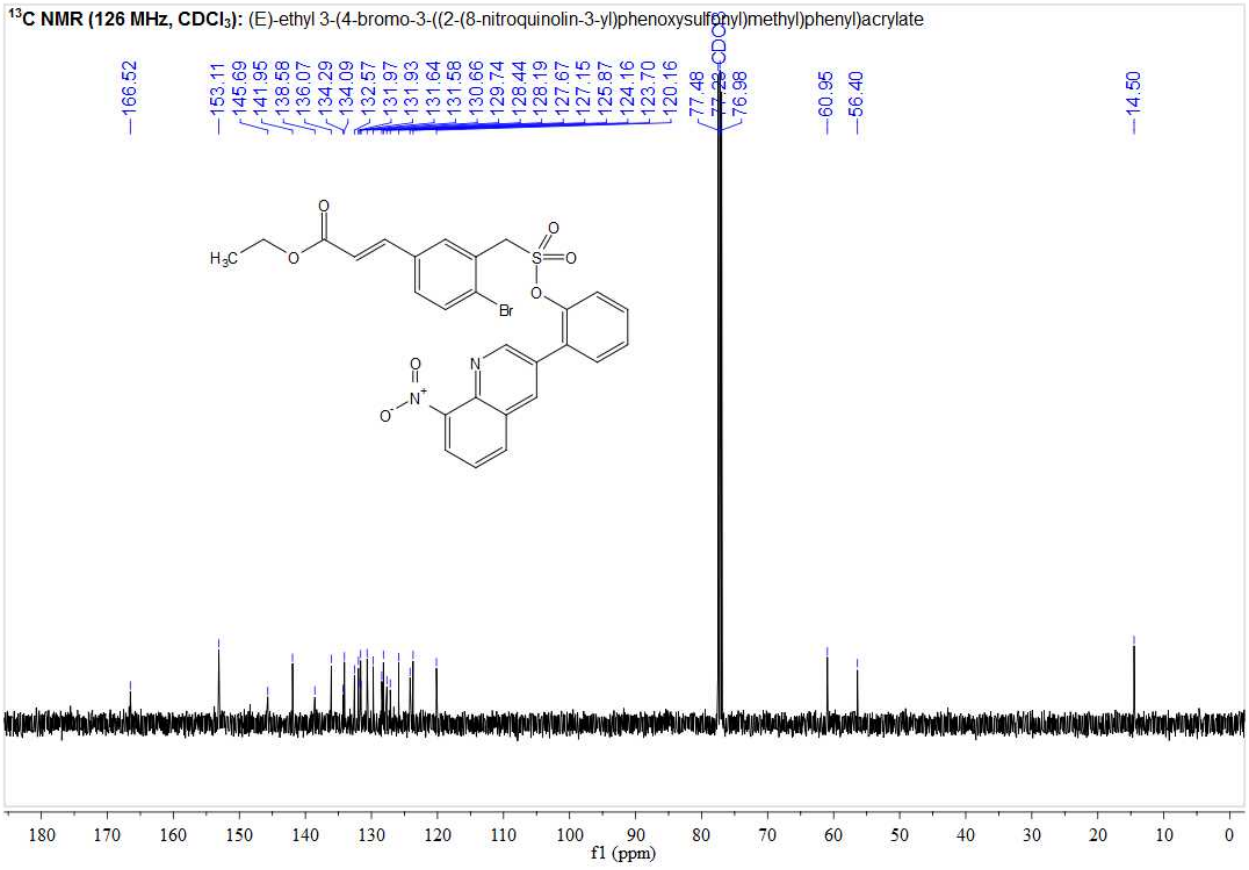
(*E*)-ethyl 3-(4-methyl-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4a):



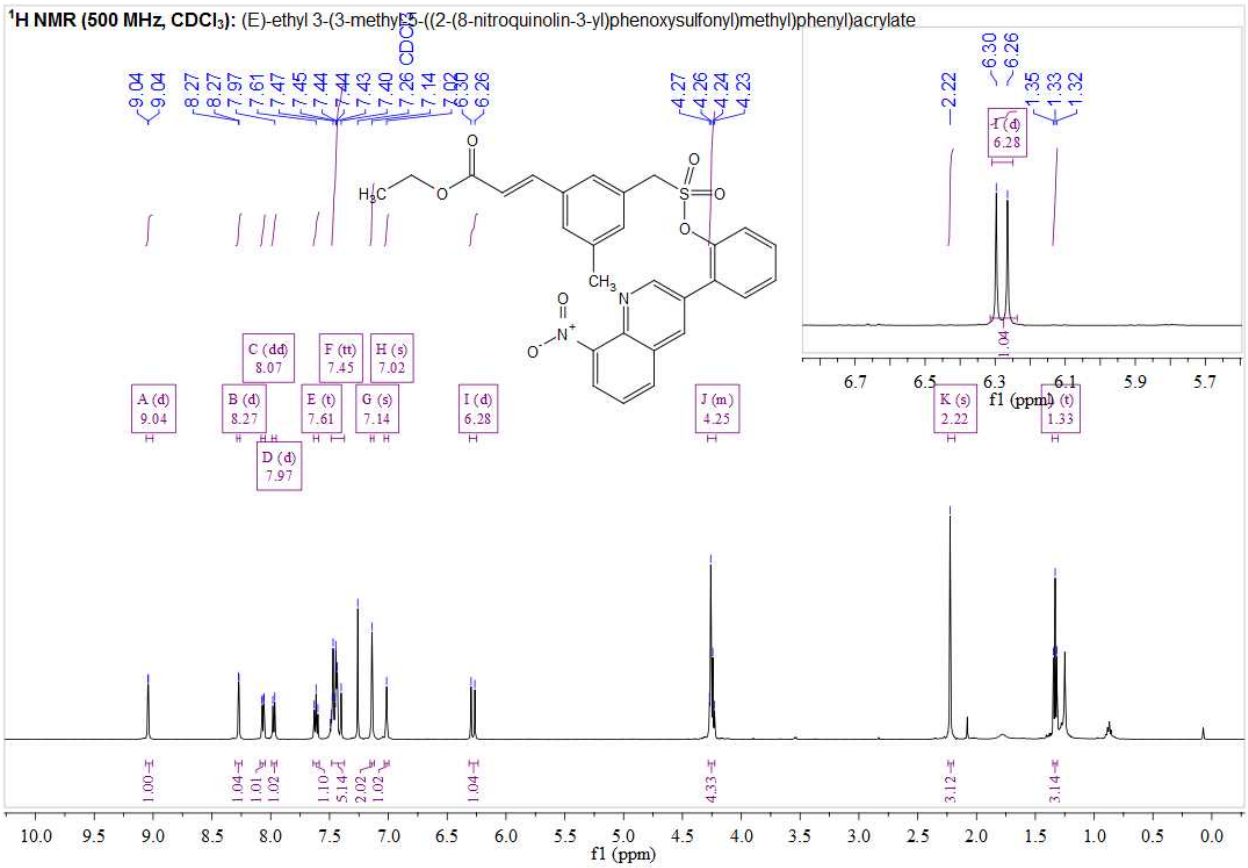


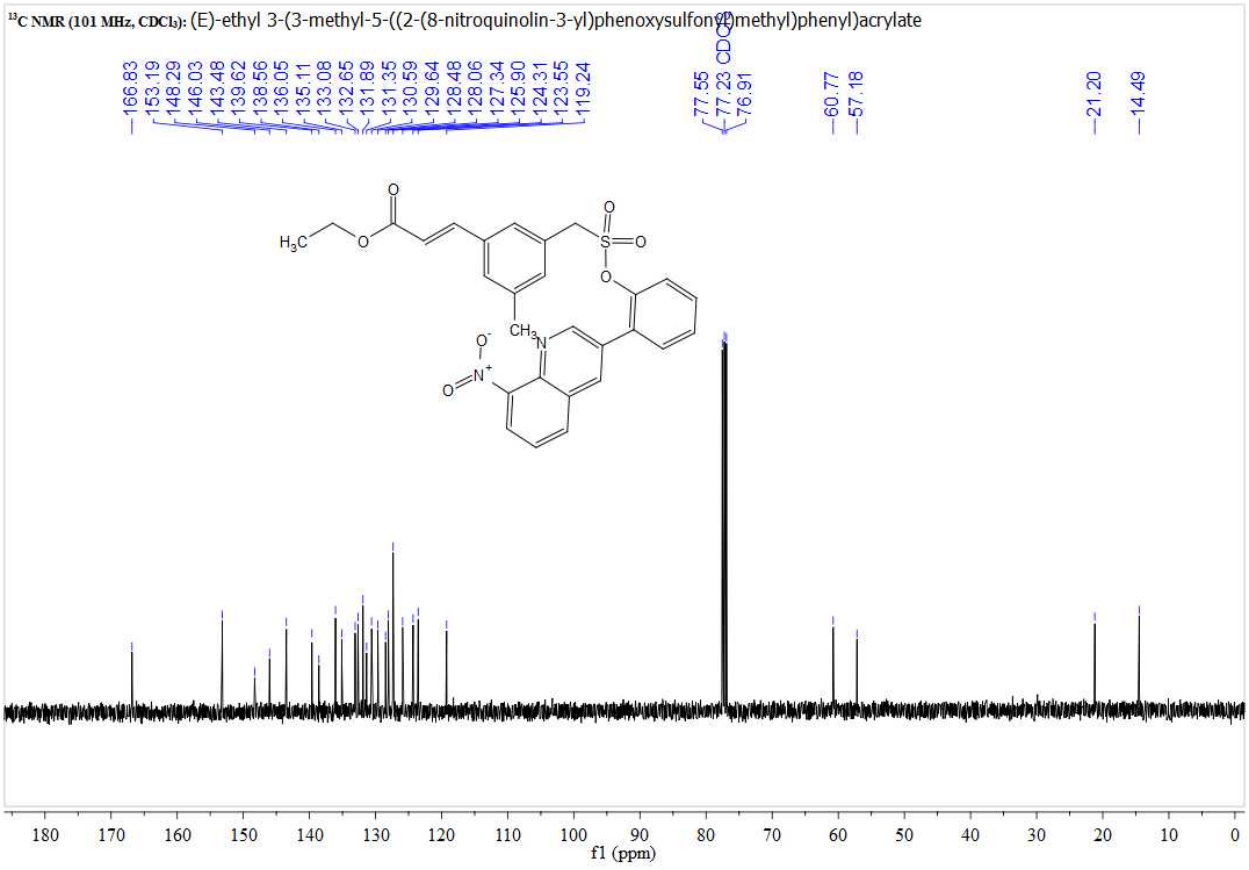
(*E*)-ethyl 3-(4-bromo-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4b):



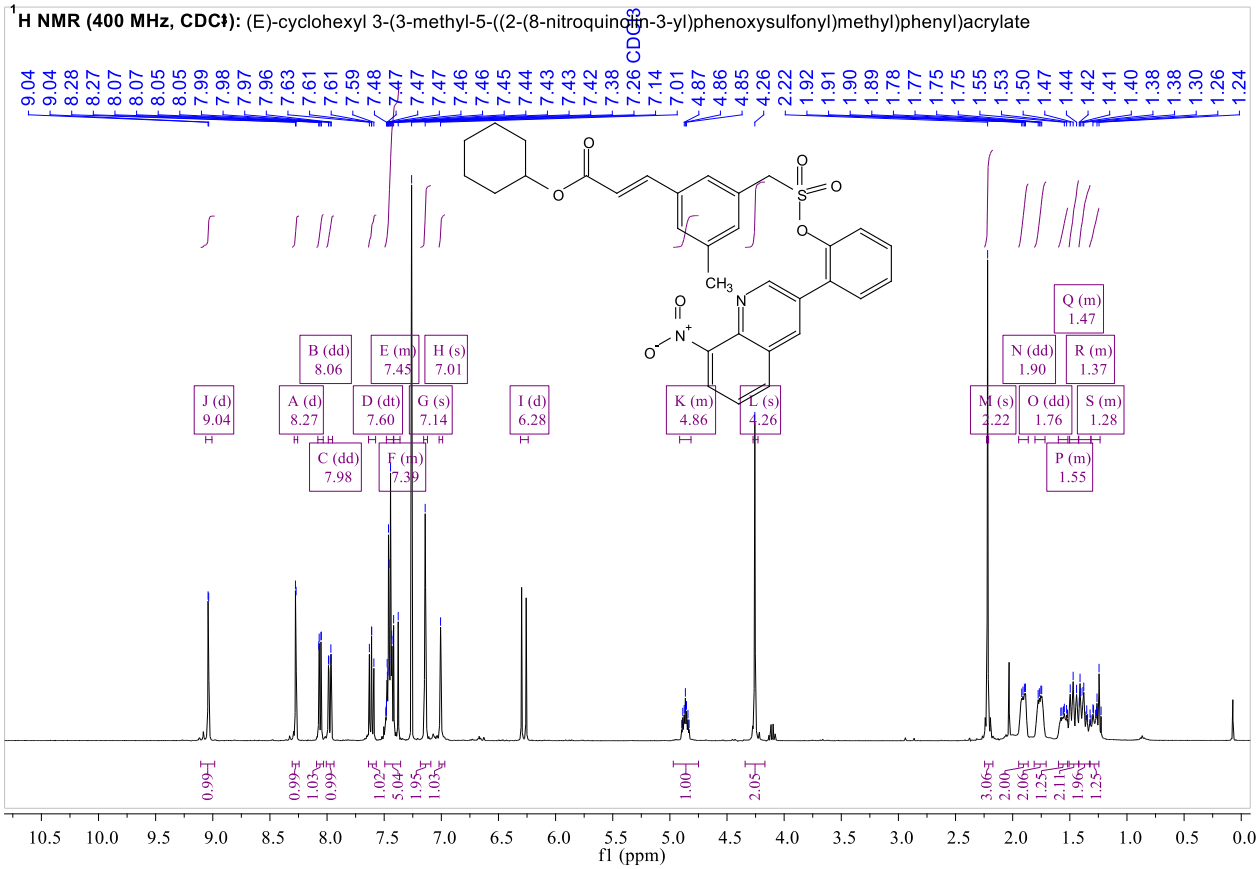


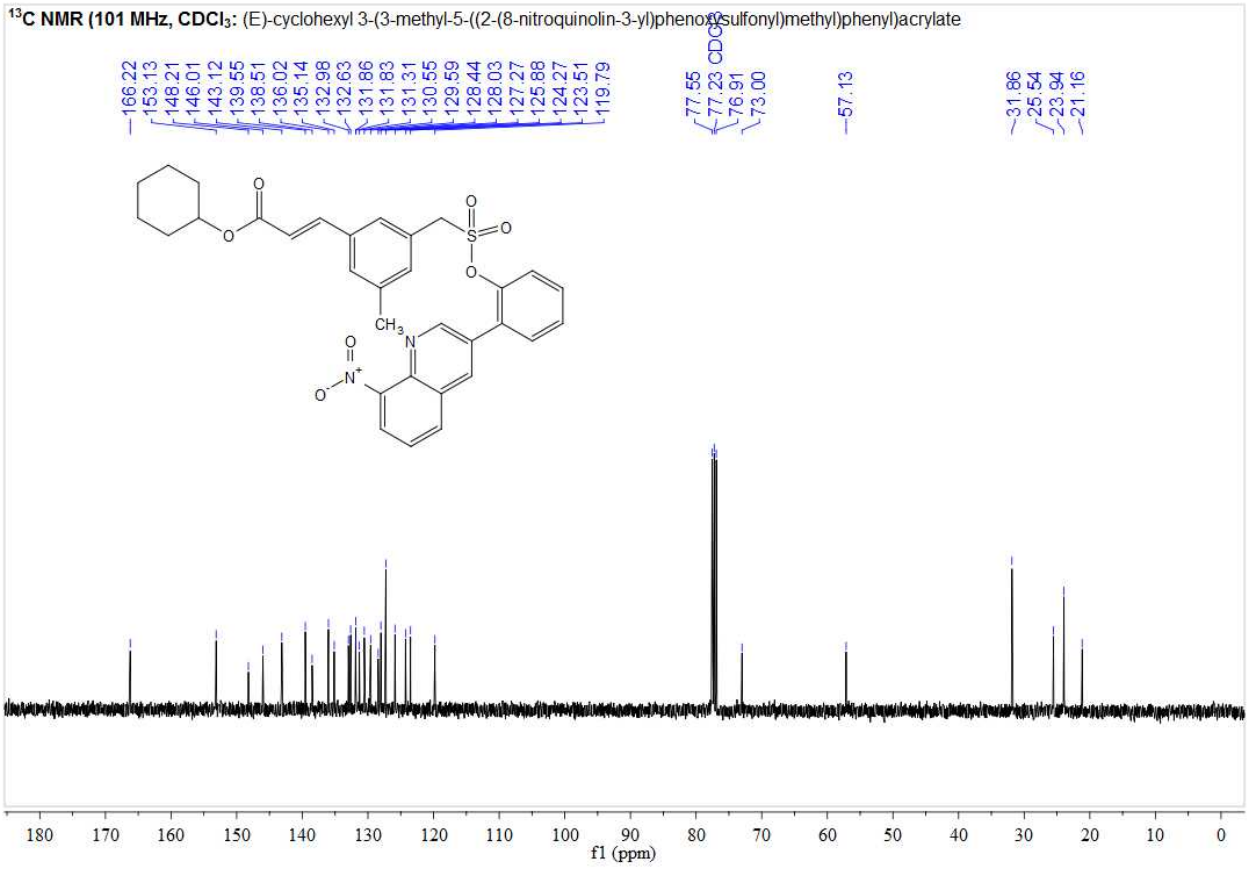
(*E*)-ethyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4c):



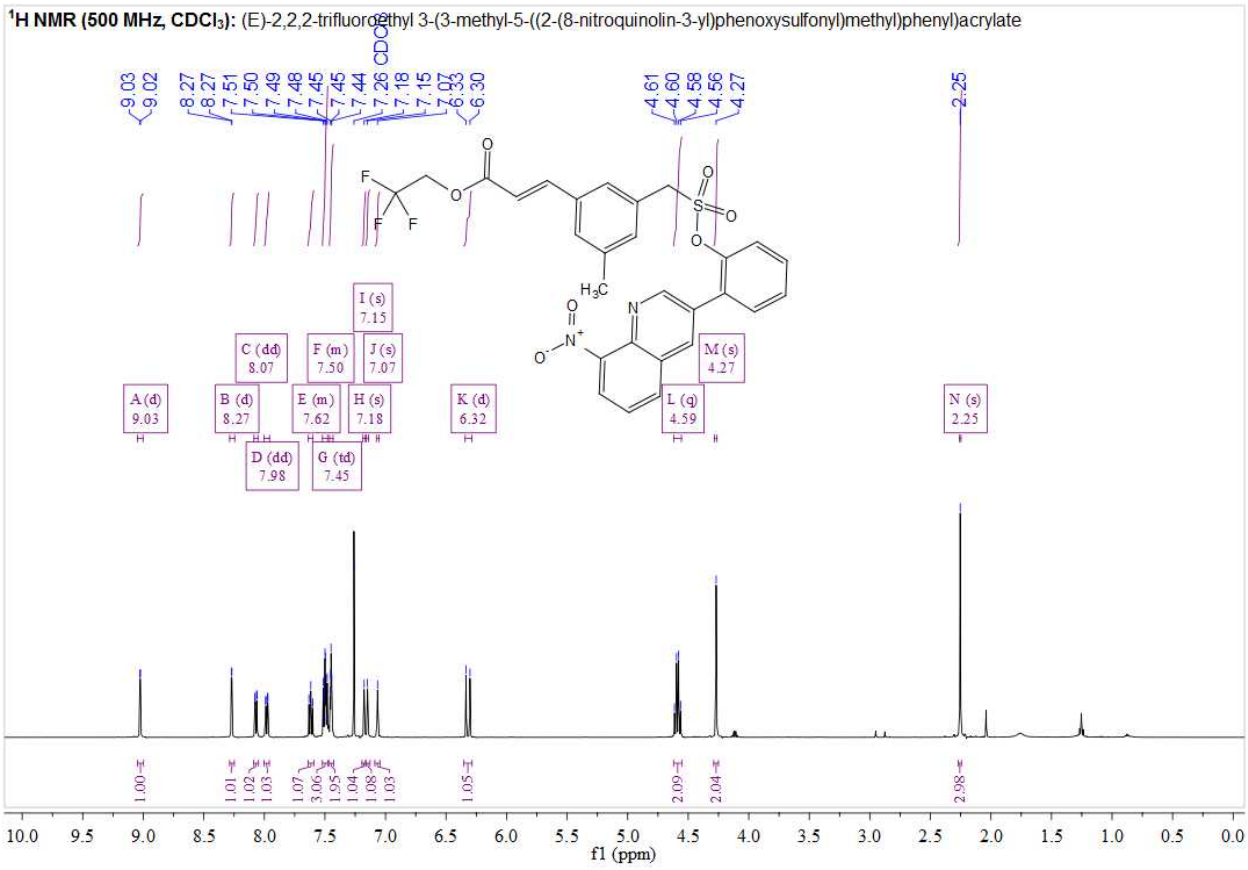


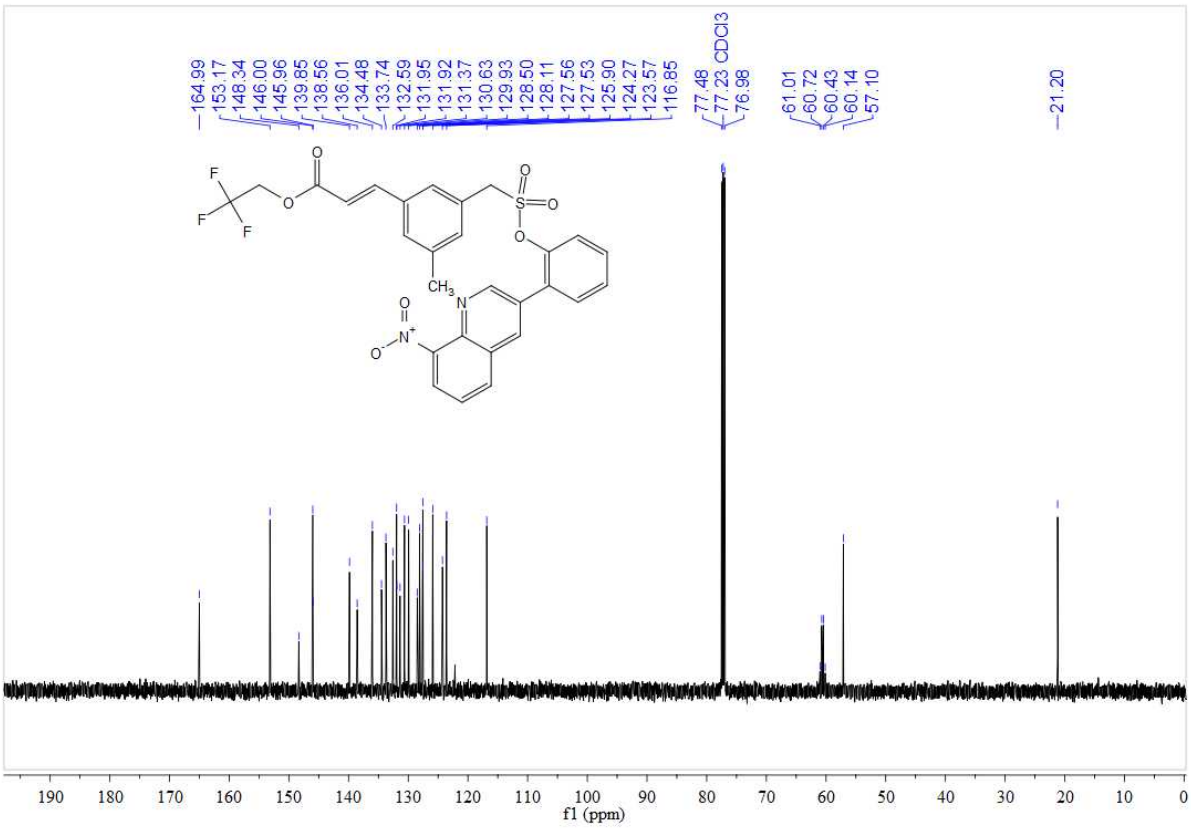
(*E*)-cyclohexyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)-acrylate (4d):



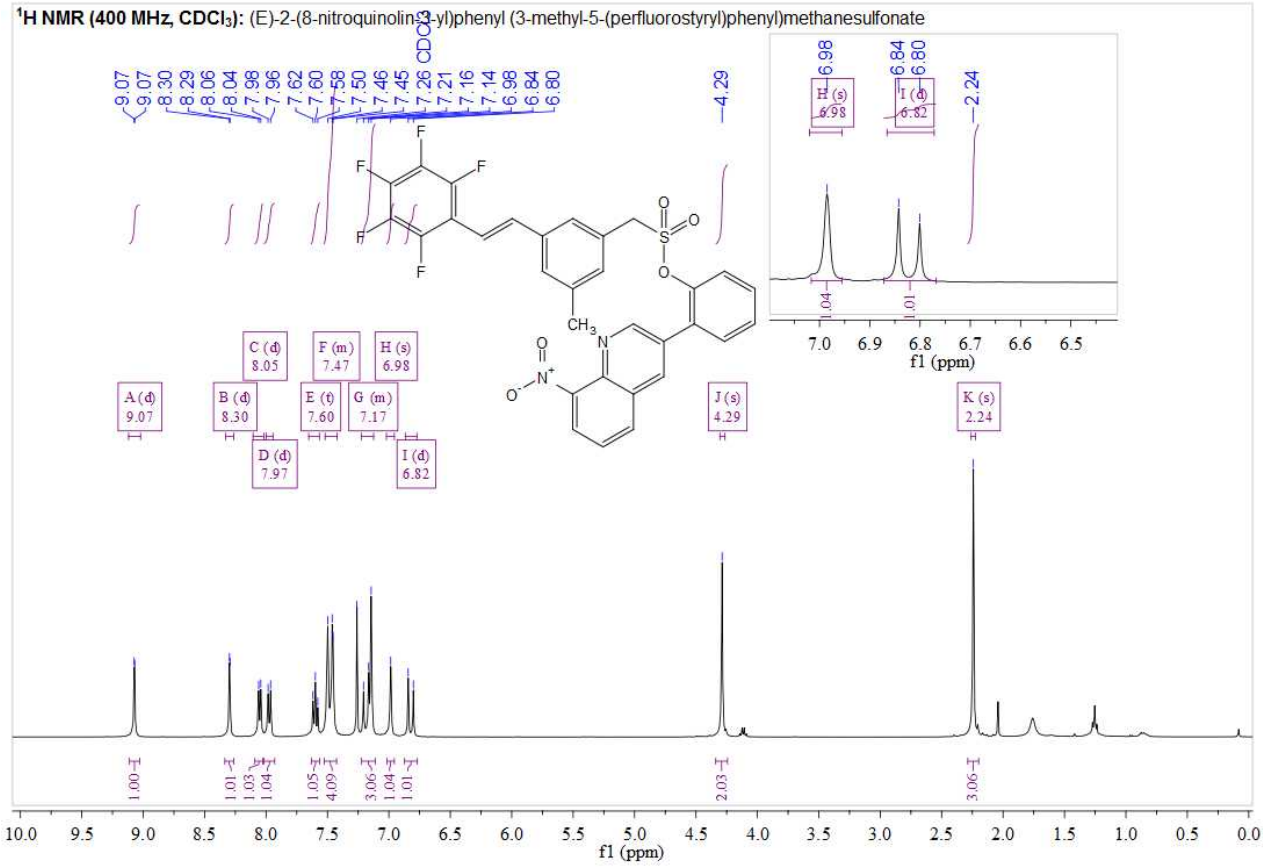


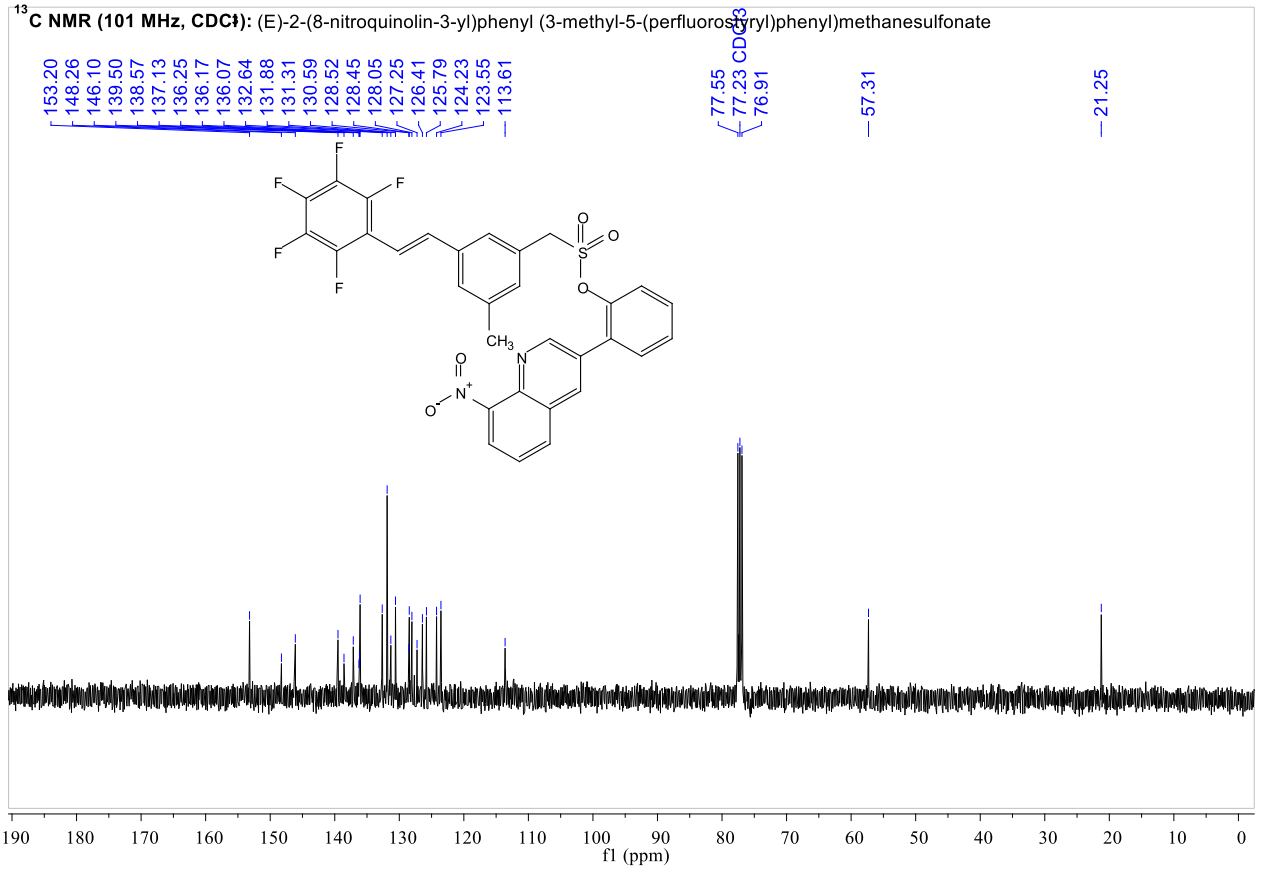
(*E*)-2,2,-difluoroethyl3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4e):



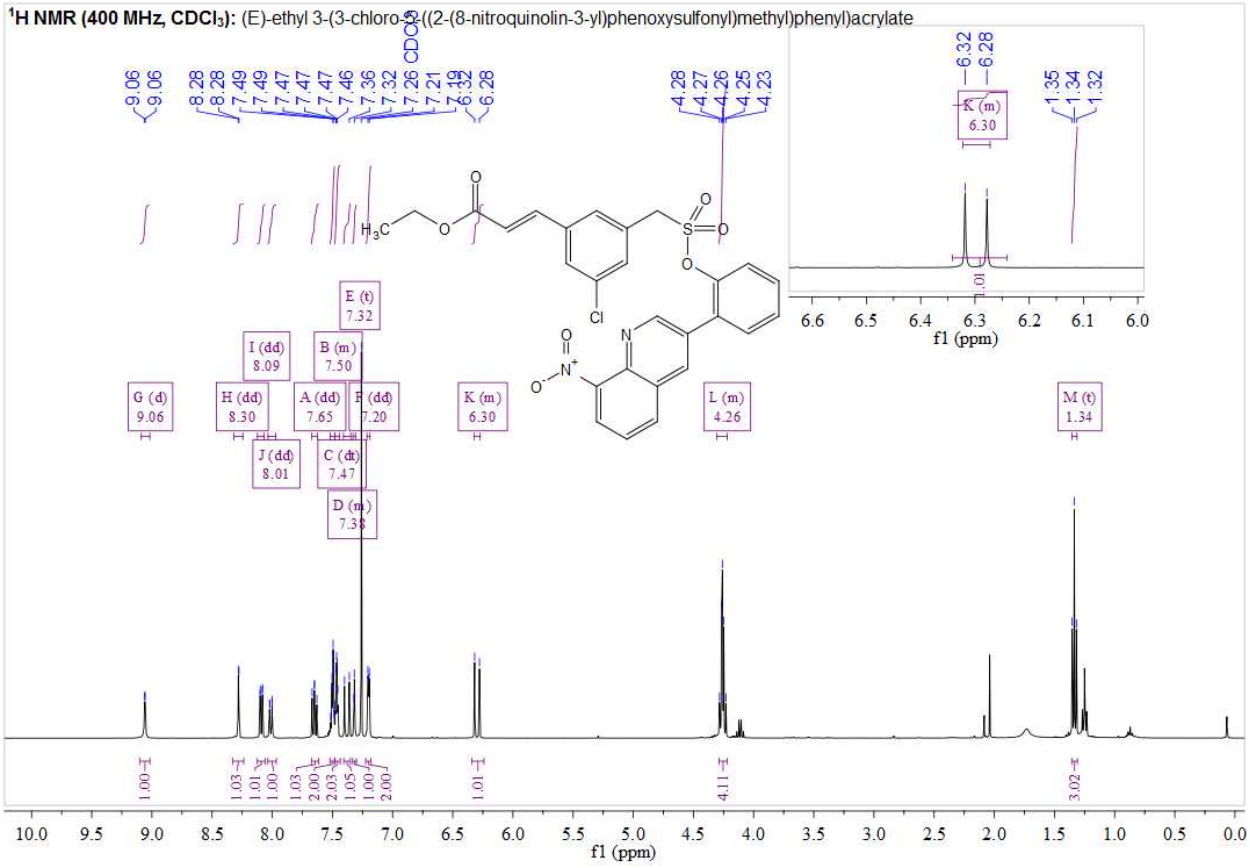


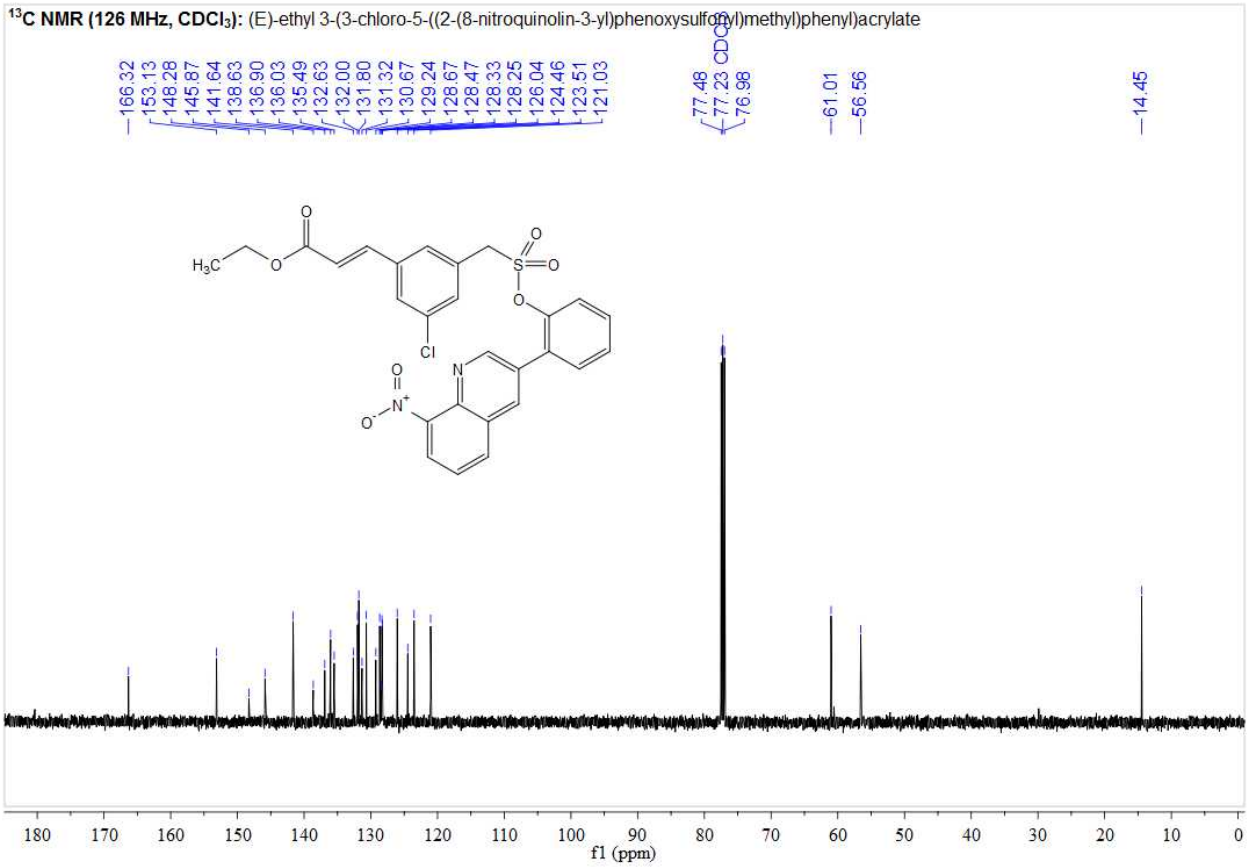
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-methyl-5-(perfluorostyryl)phenyl)methanesulfona-te(4f):



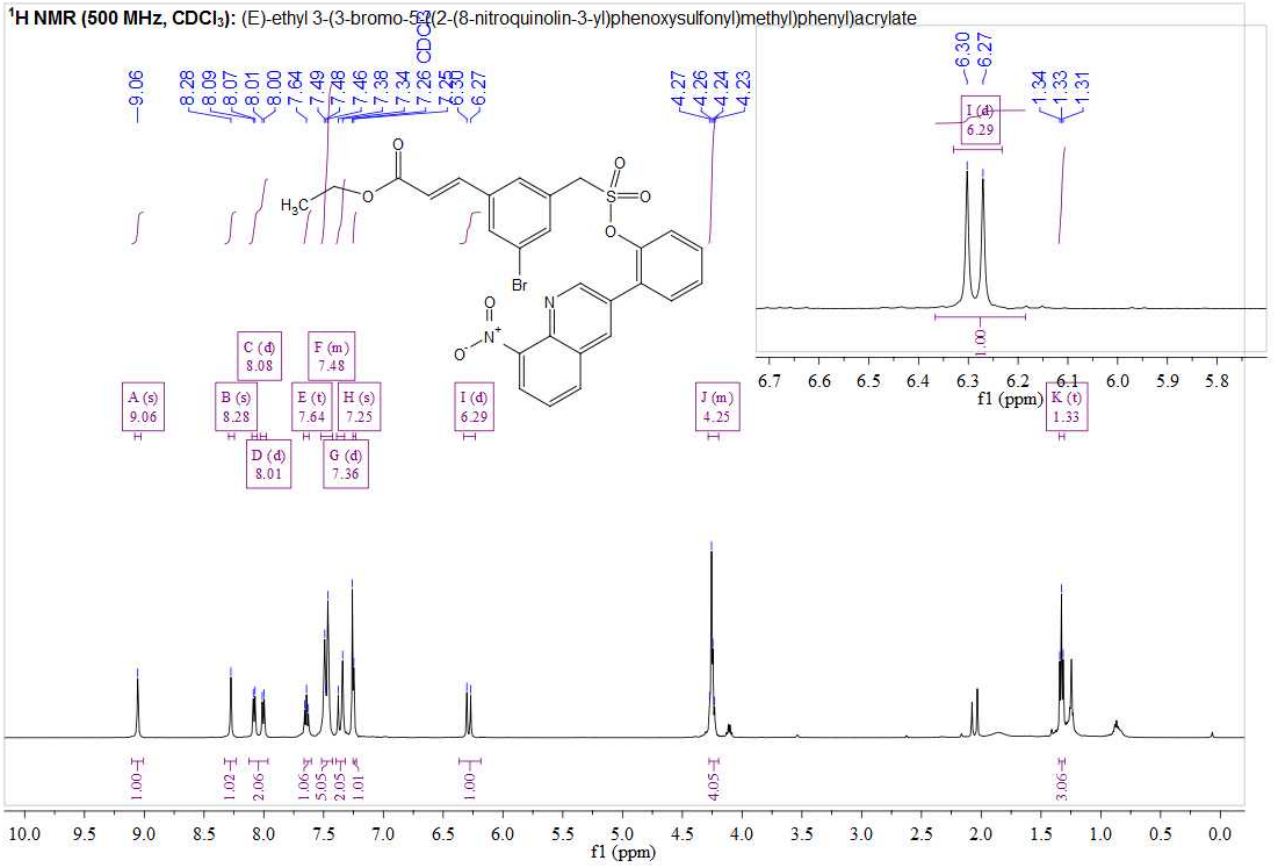


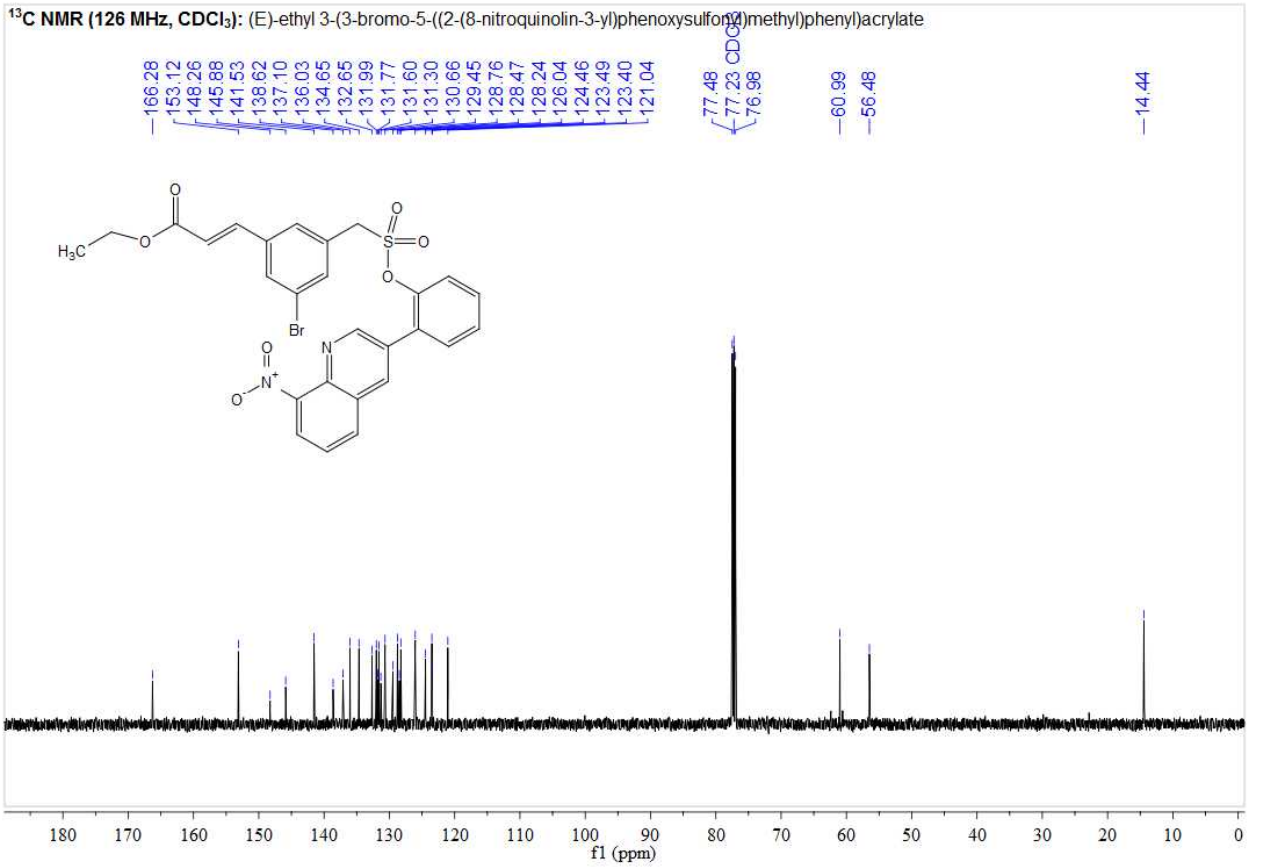
(*E*)-ethyl 3-(3-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)-acrylate (4g):



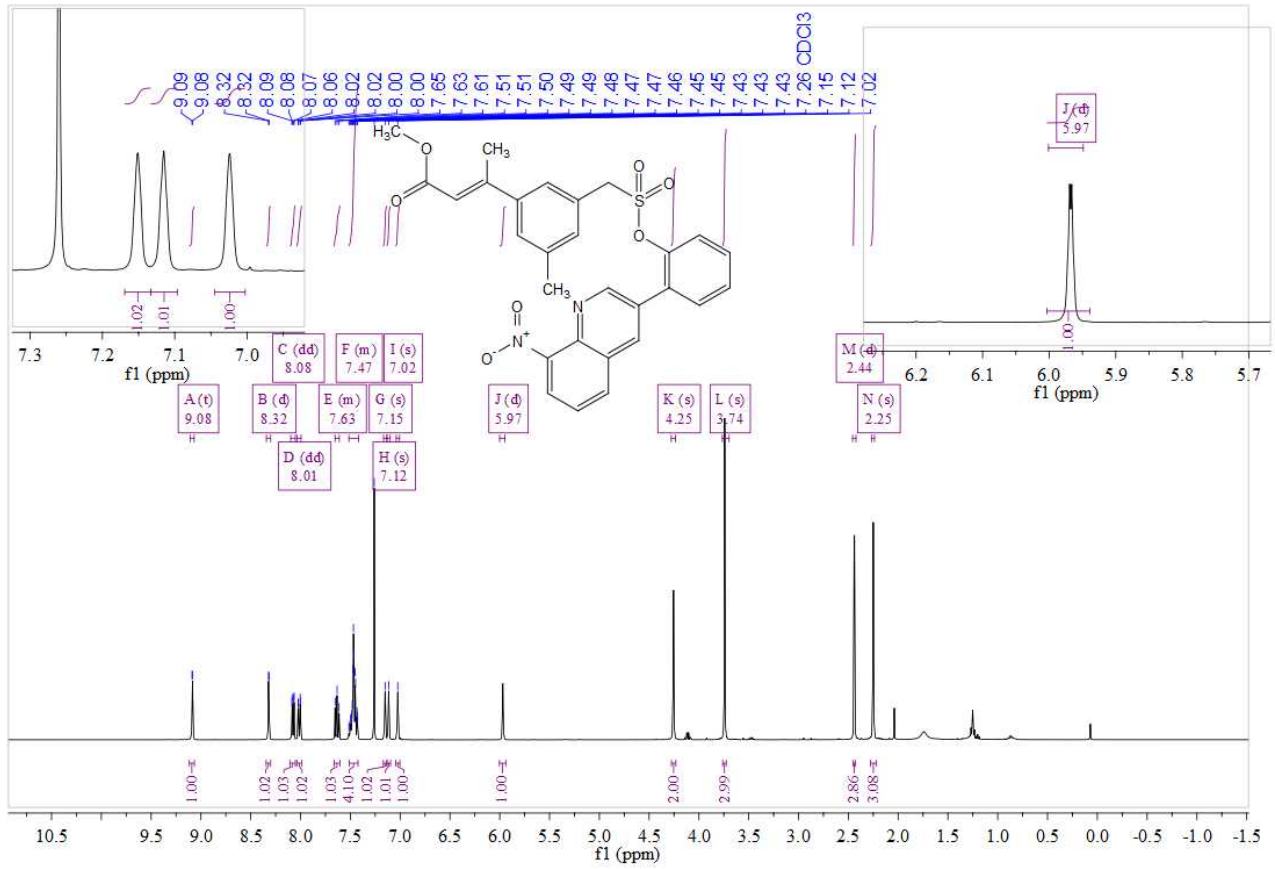


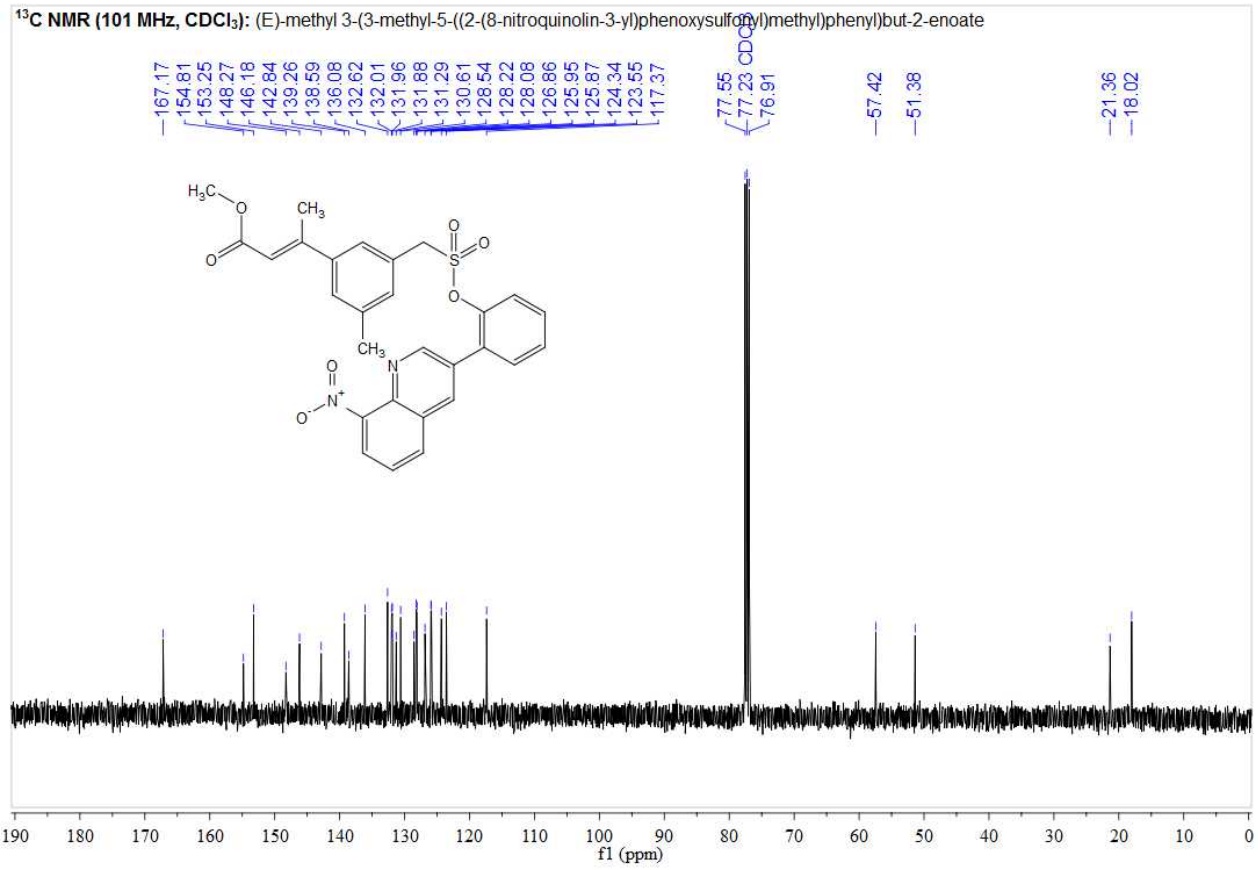
(*E*)-ethyl 3-(3-bromo-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acr-ylate (4h):



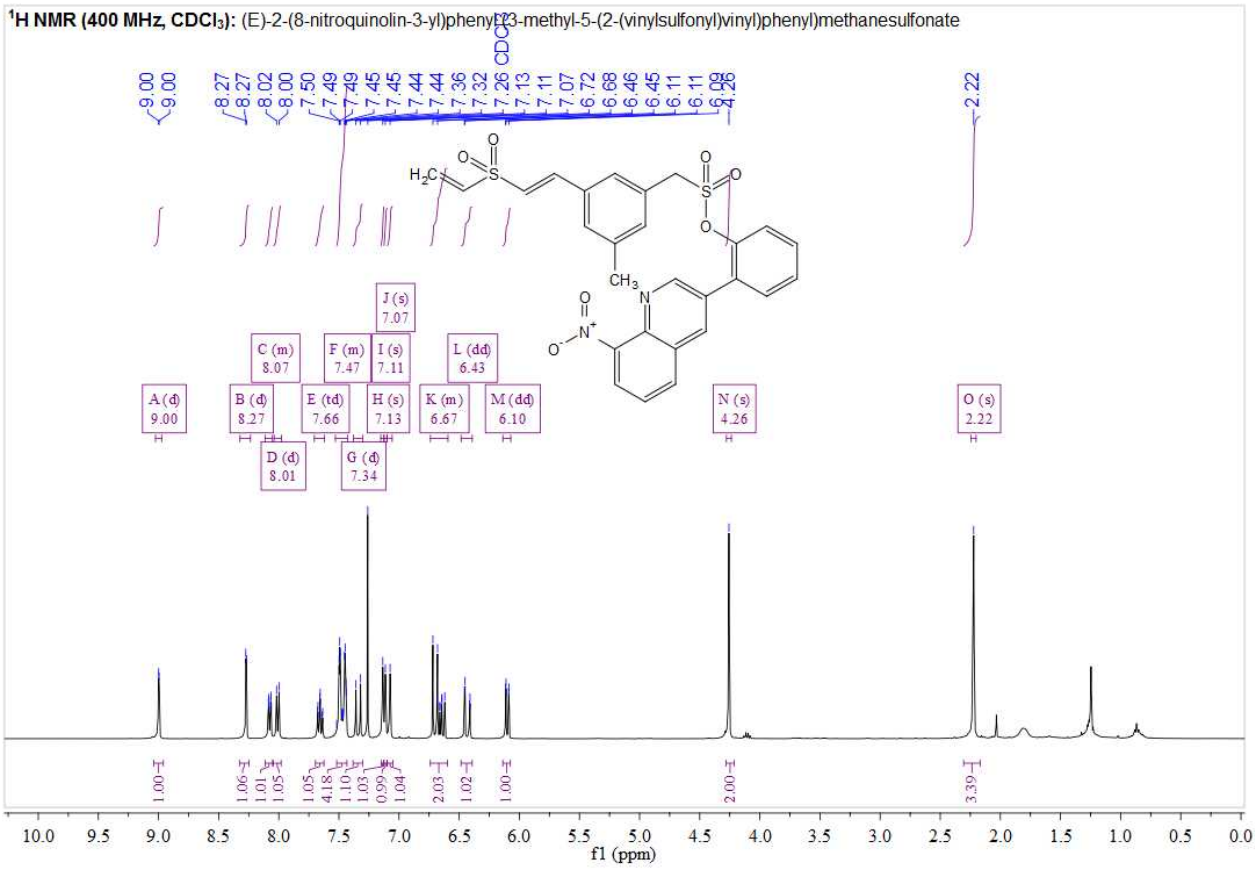


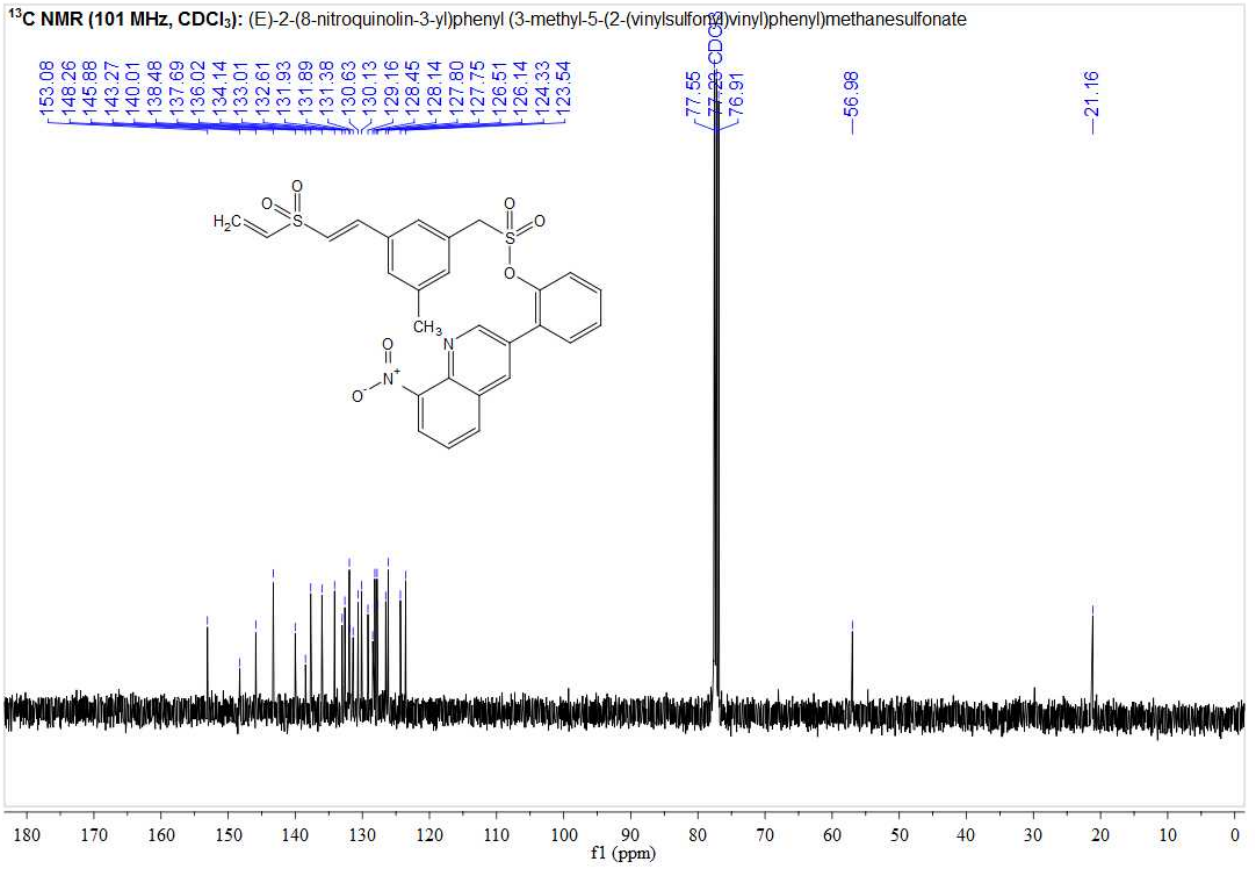
(*E*)-methyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)but-2-enoate (4i):



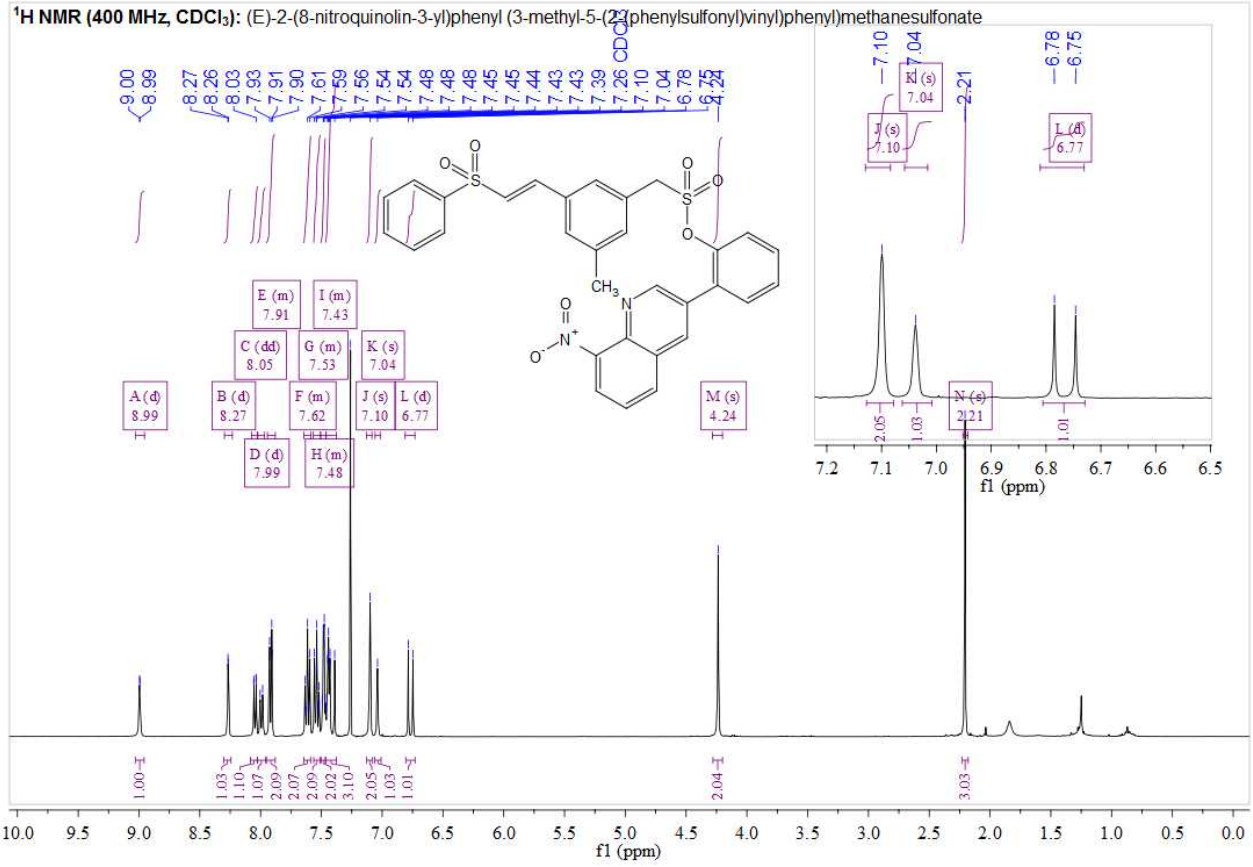


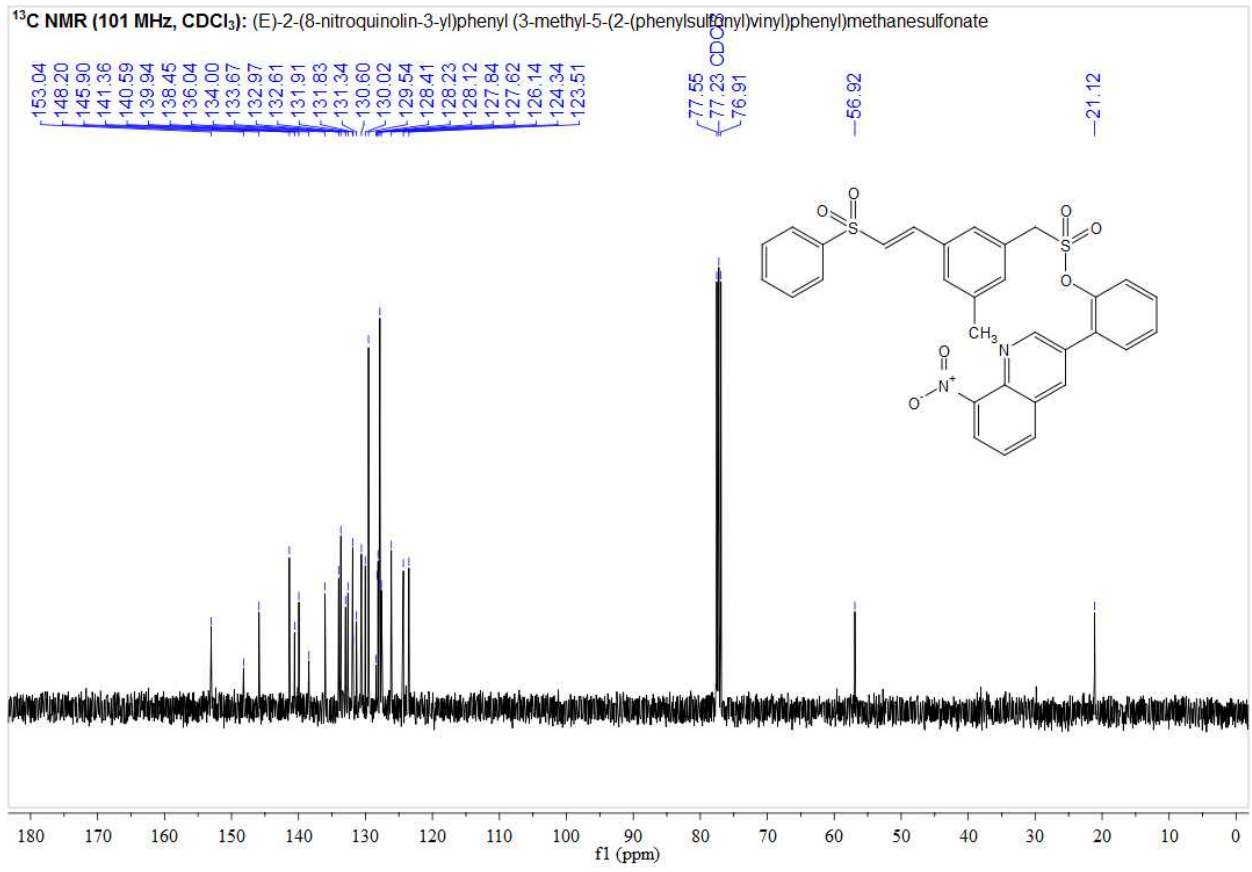
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-methyl-5-(2-(vinylsulfonyl)vinyl)phenyl)methanesulfonate (4j):



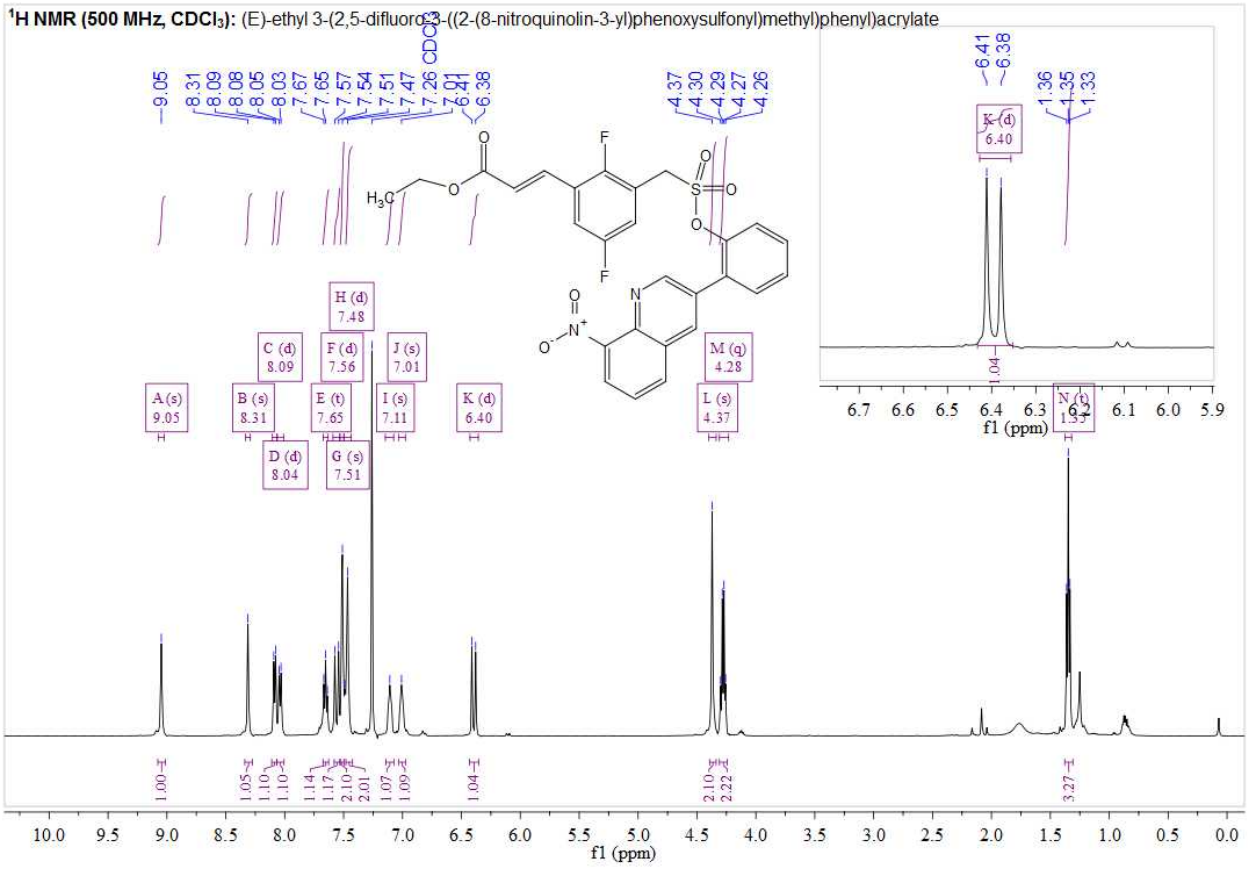


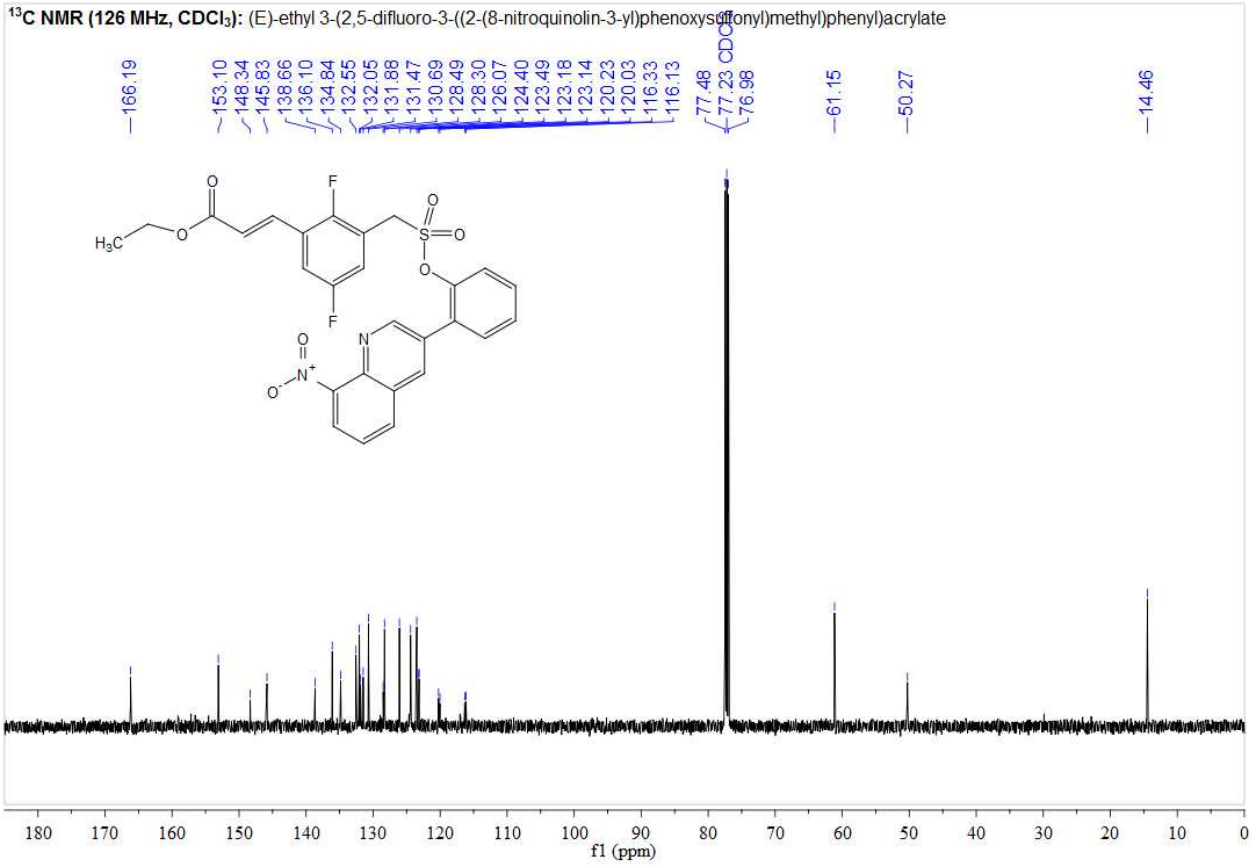
(*E*)-2-(8-nitroquinolin-3-yl)phenyl (3-methyl-5-(2-(phenylsulfonyl)vinyl)phenyl)methanesulfonate (4k):



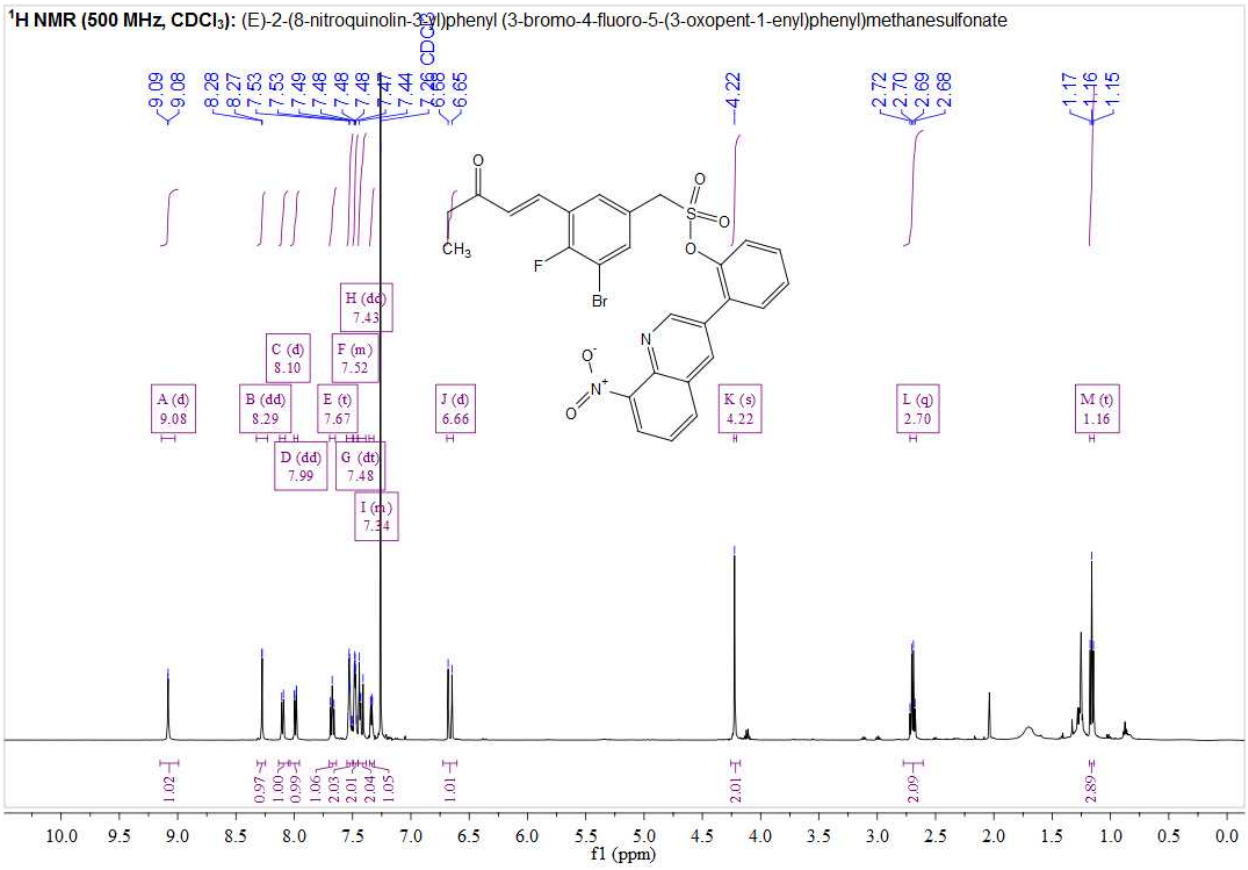


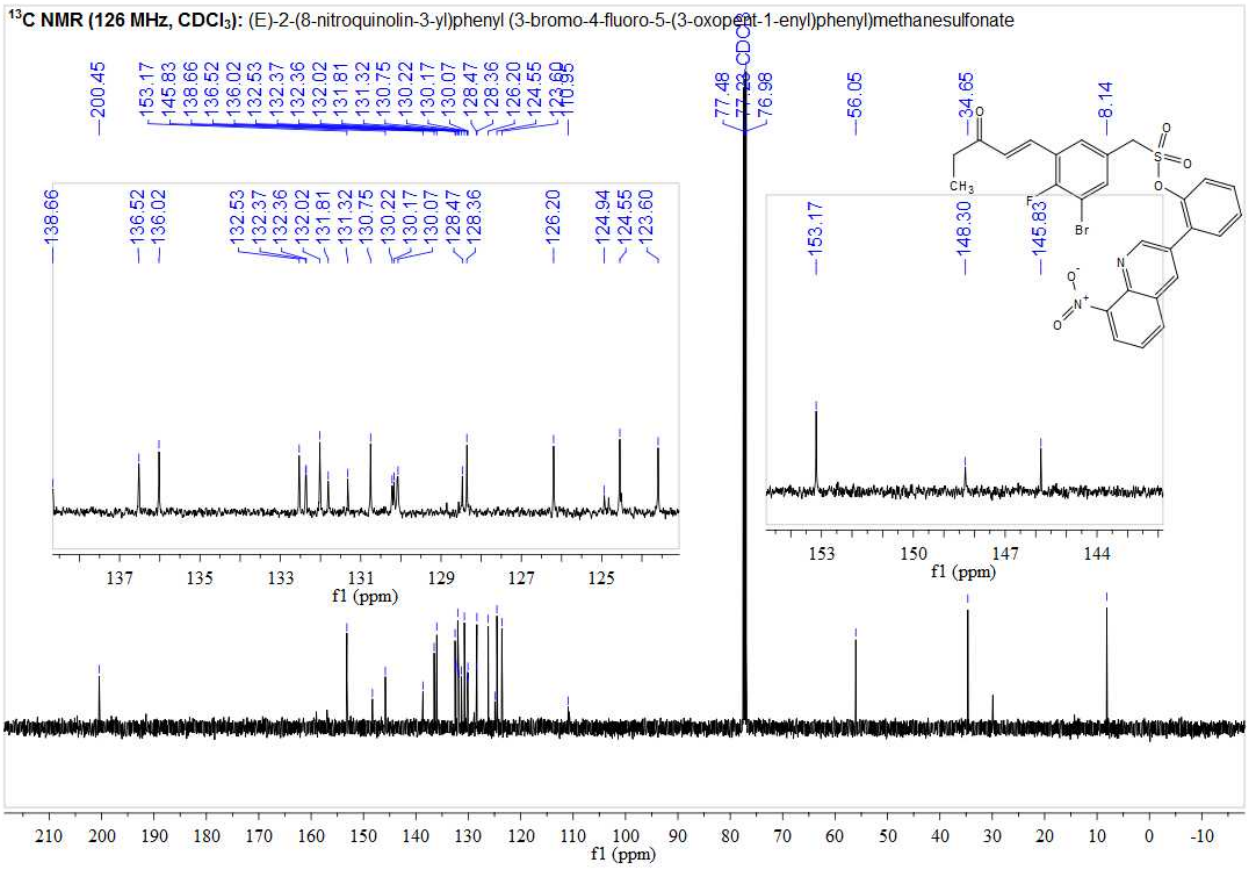
(*E*)-ethyl 3-(2,5-difluoro-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)-acrylate(4l):



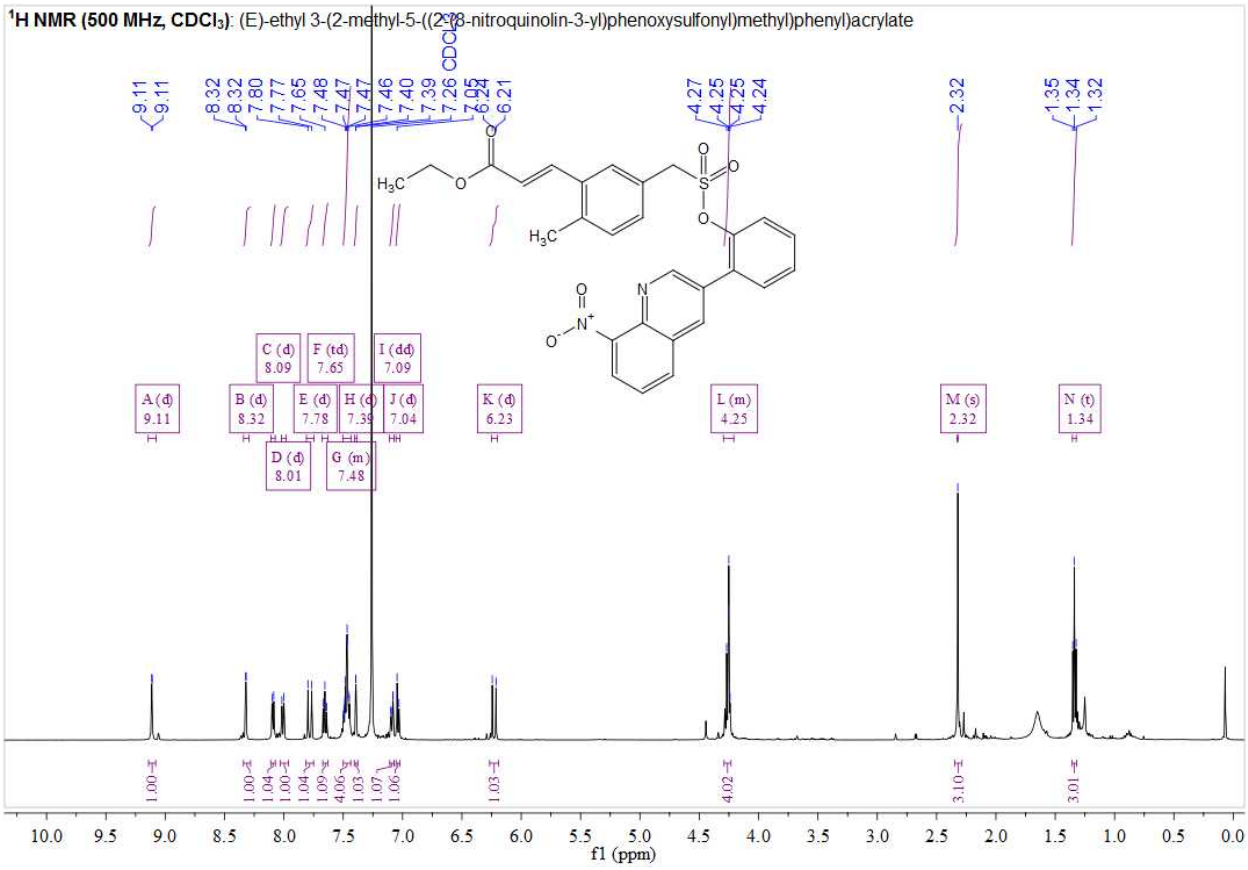


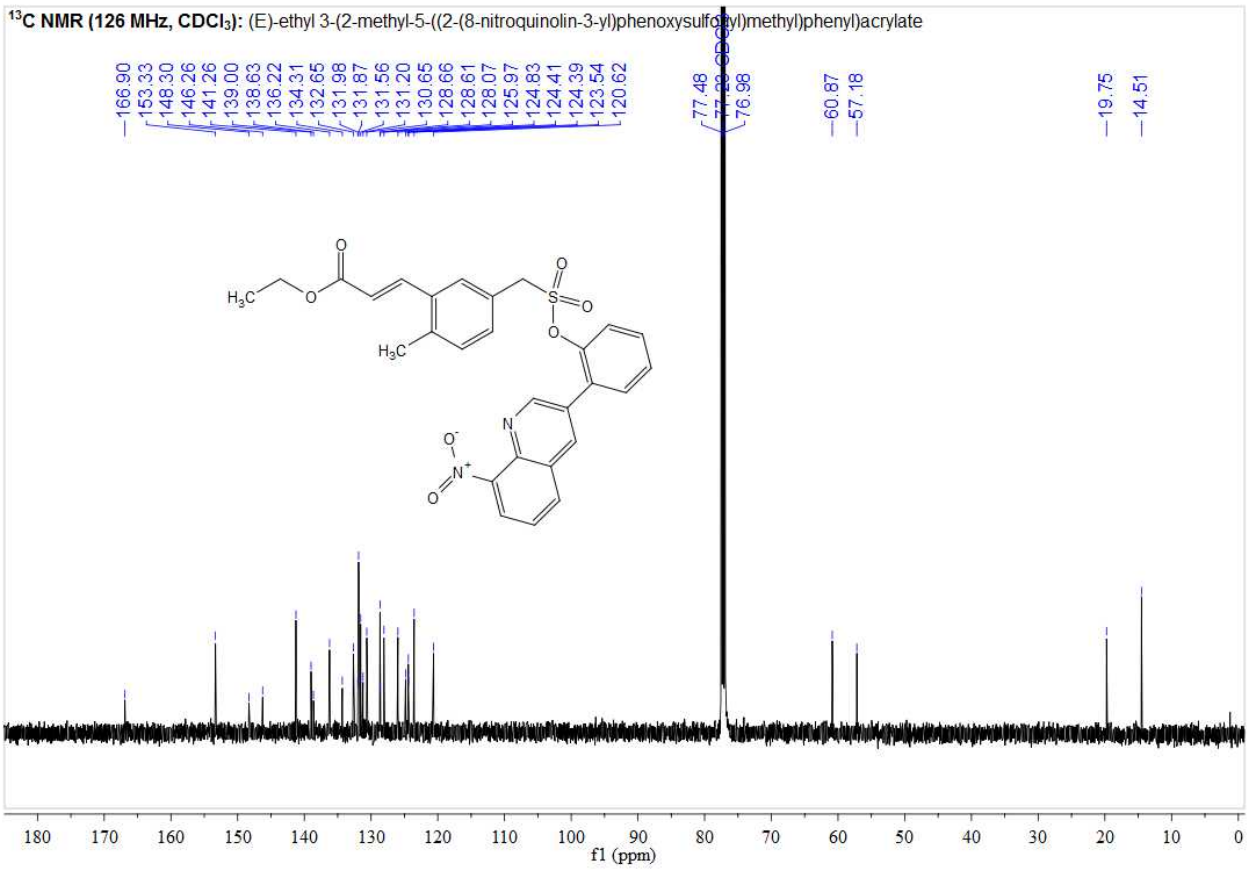
(*E*)-ethyl 3-(3-bromo-2-fluoro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-phenyl)acrylate (4m):



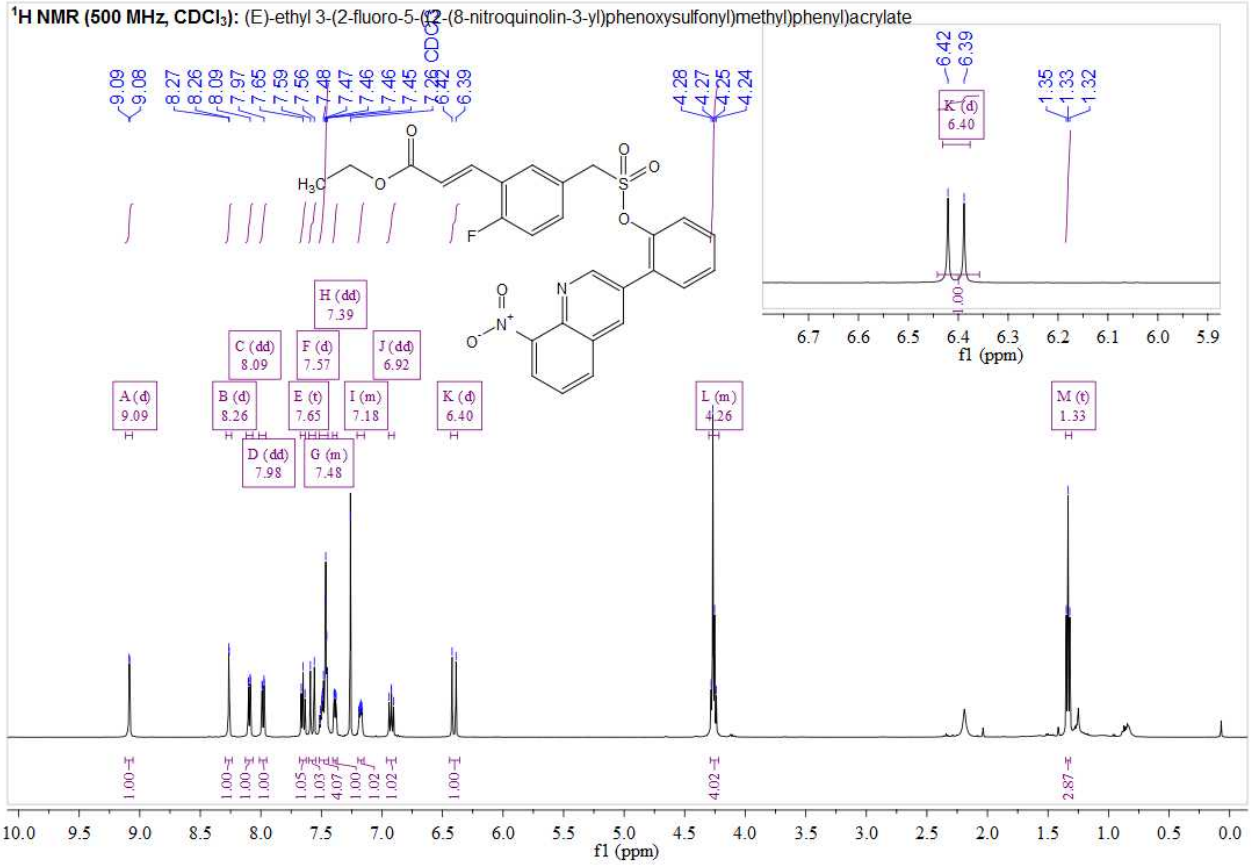


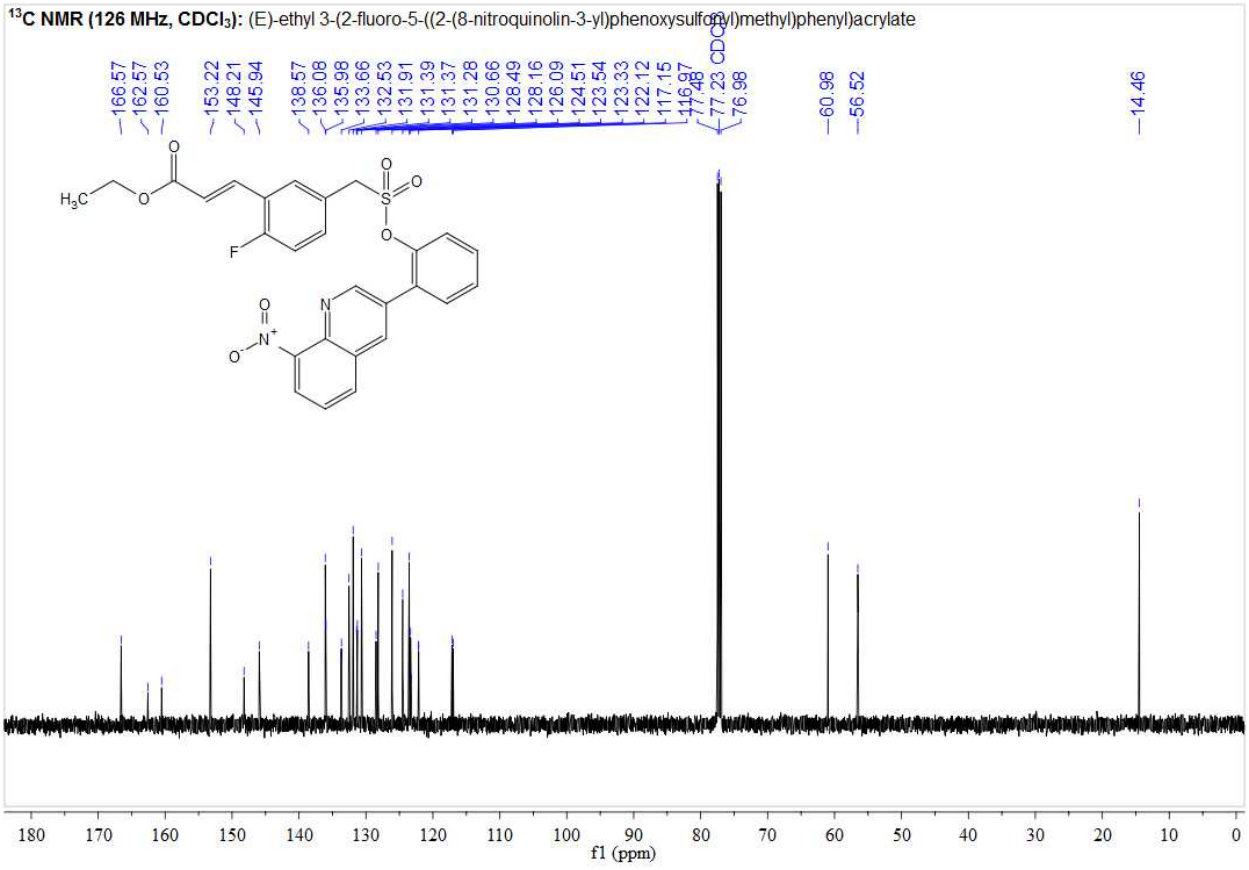
(*E*)-ethyl 3-(2-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4n):



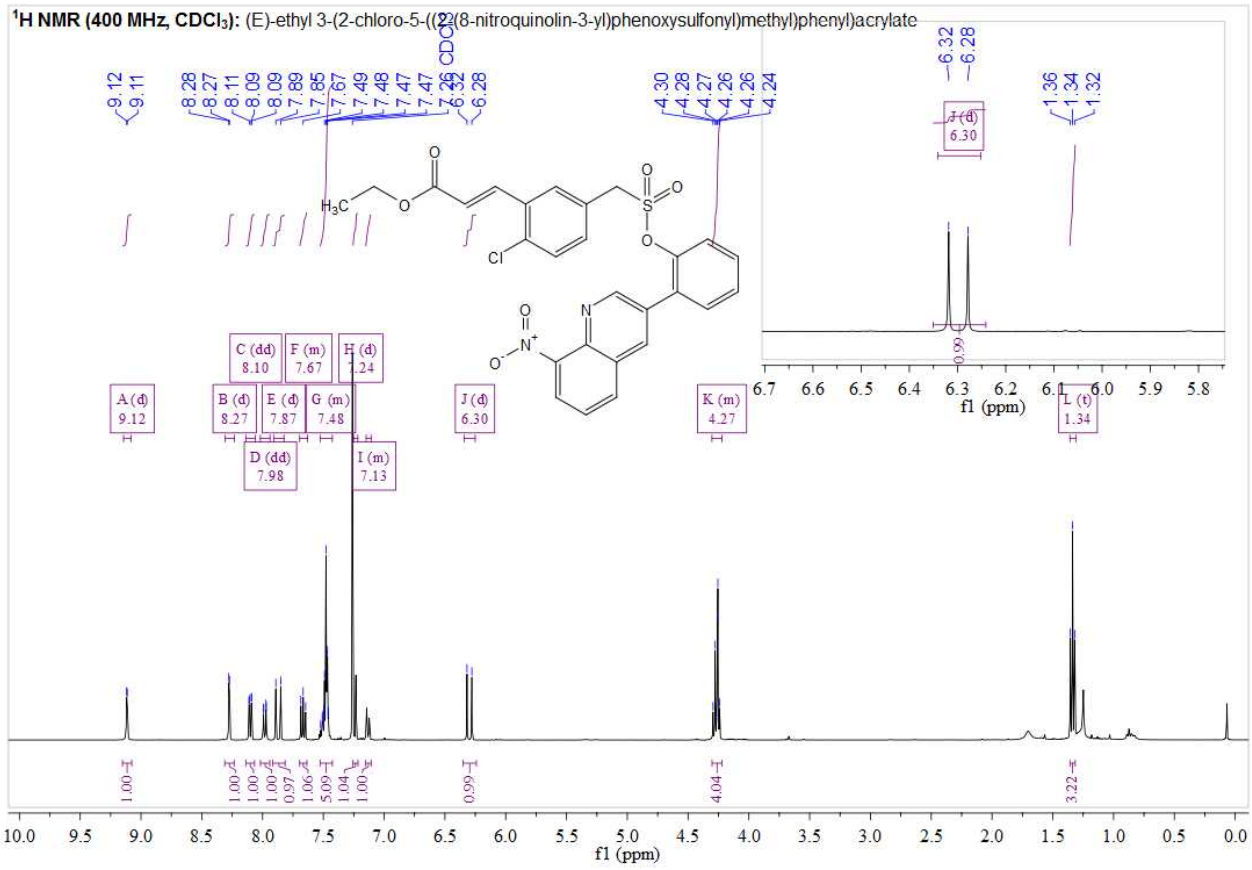


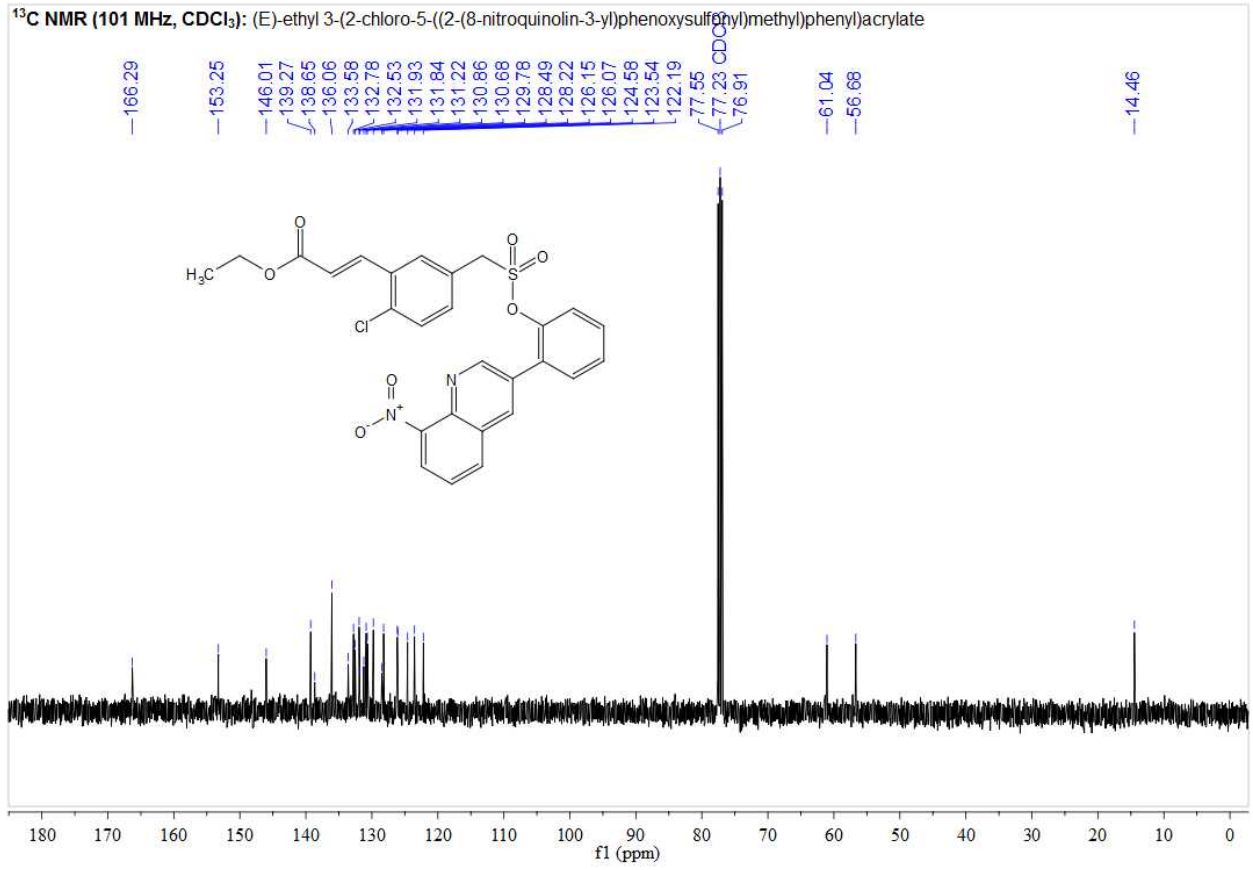
(*E*)-ethyl 3-(2-fluoro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4o):



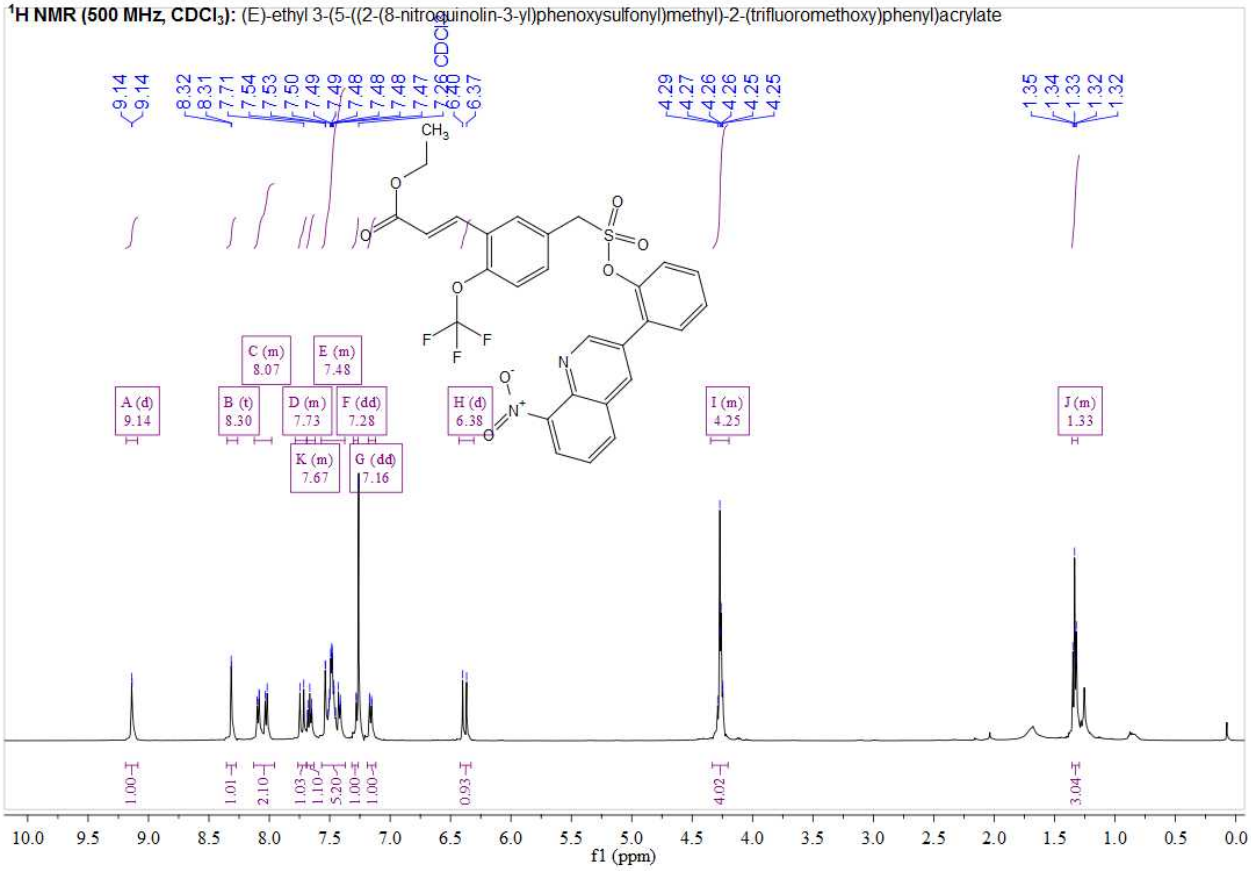


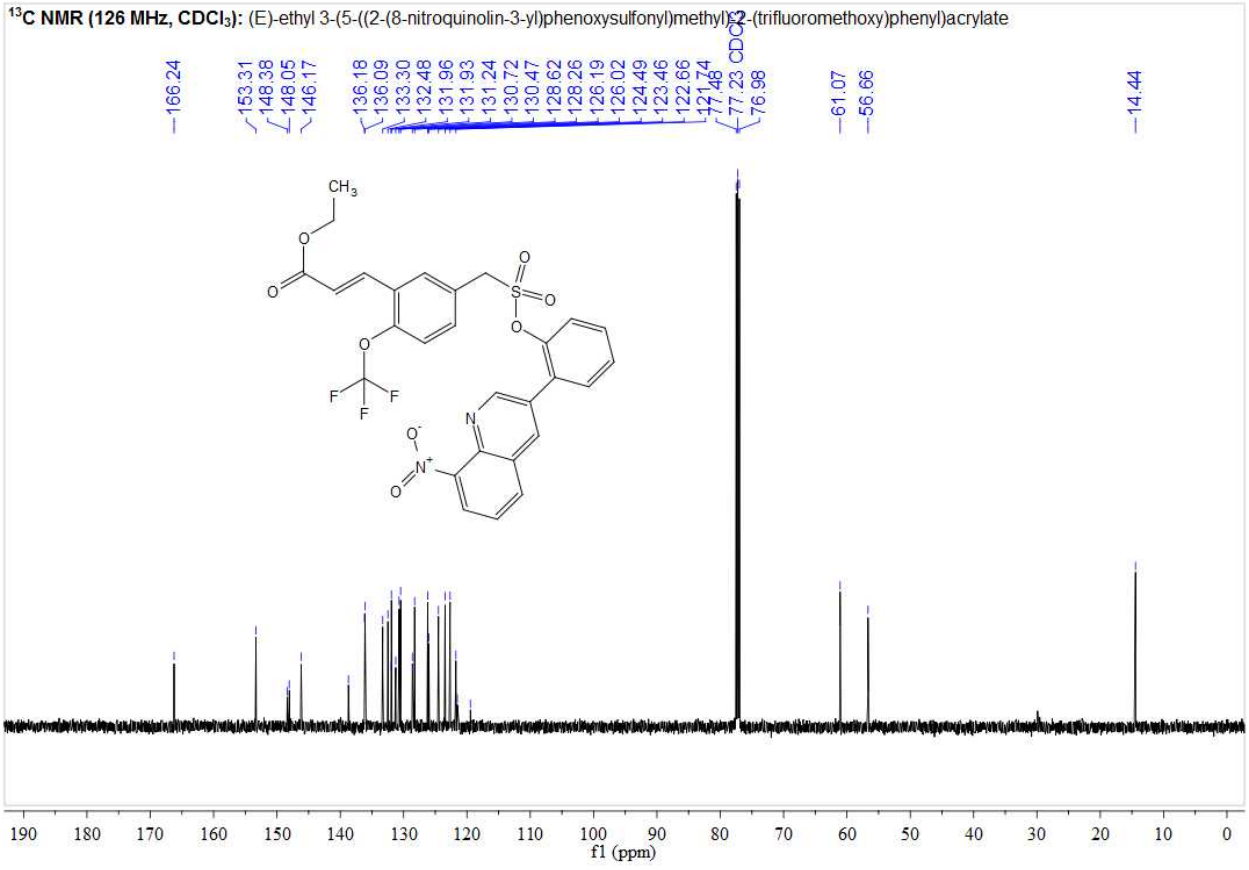
(*E*)-ethyl 3-(2-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (4p):



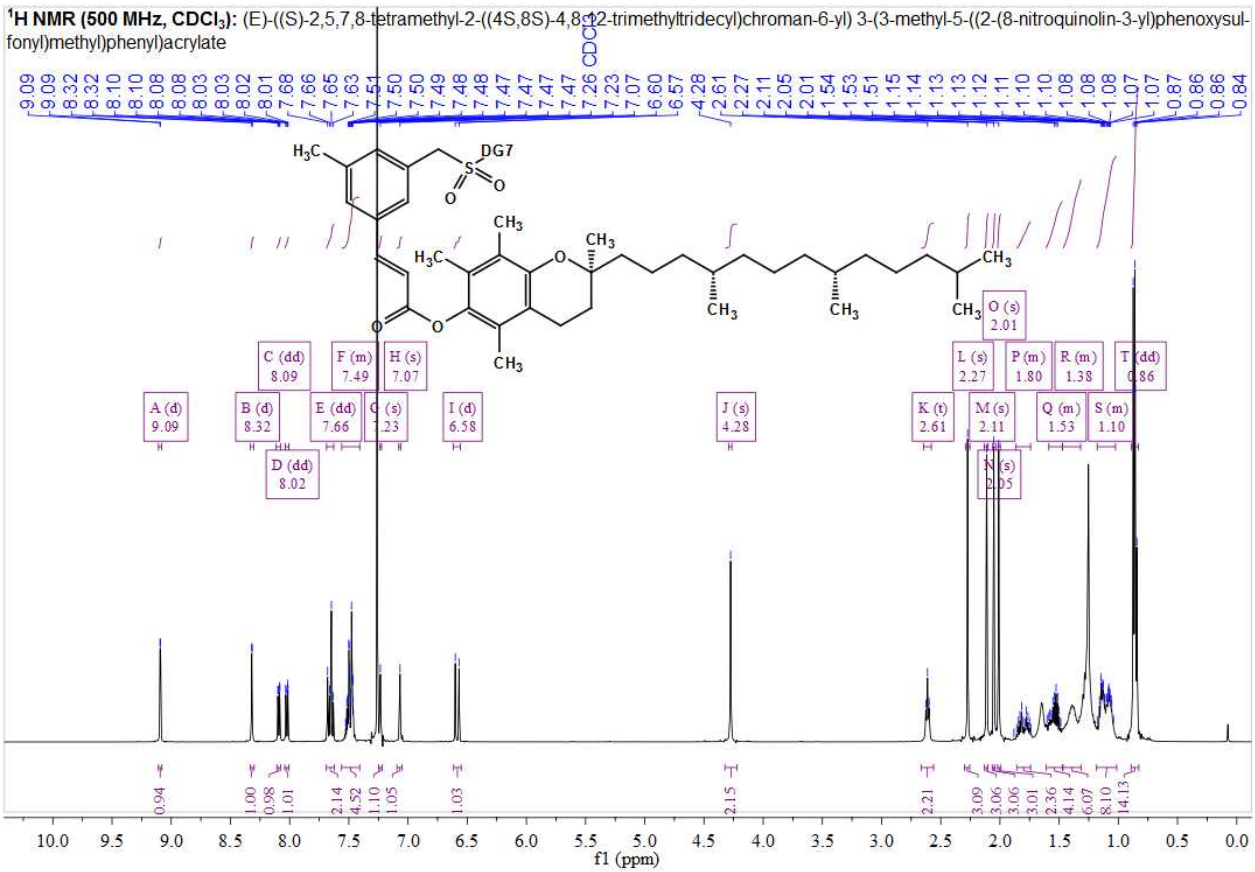


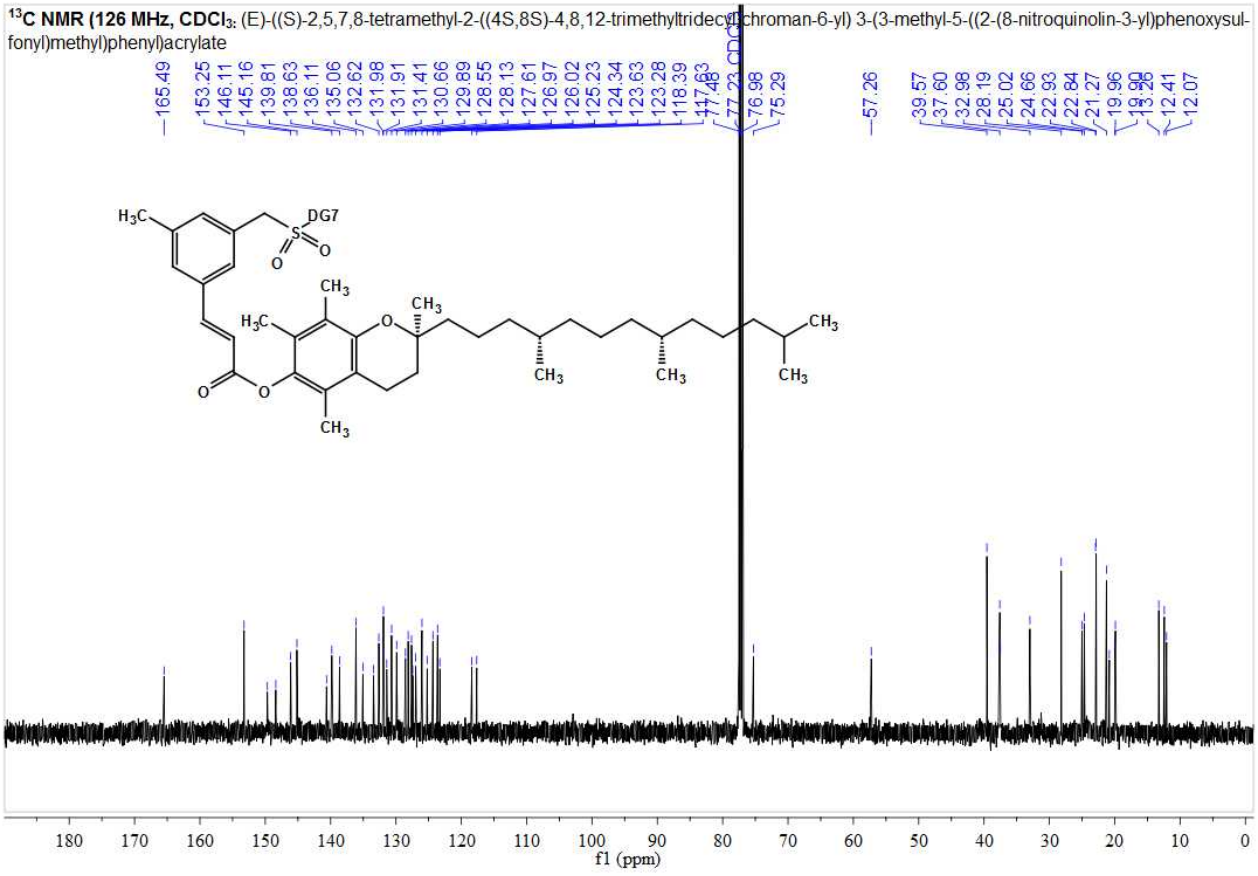
(*E*)-ethyl 3-(5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-2-(trifluoromethoxy)-phenyl)acrylate (4q):

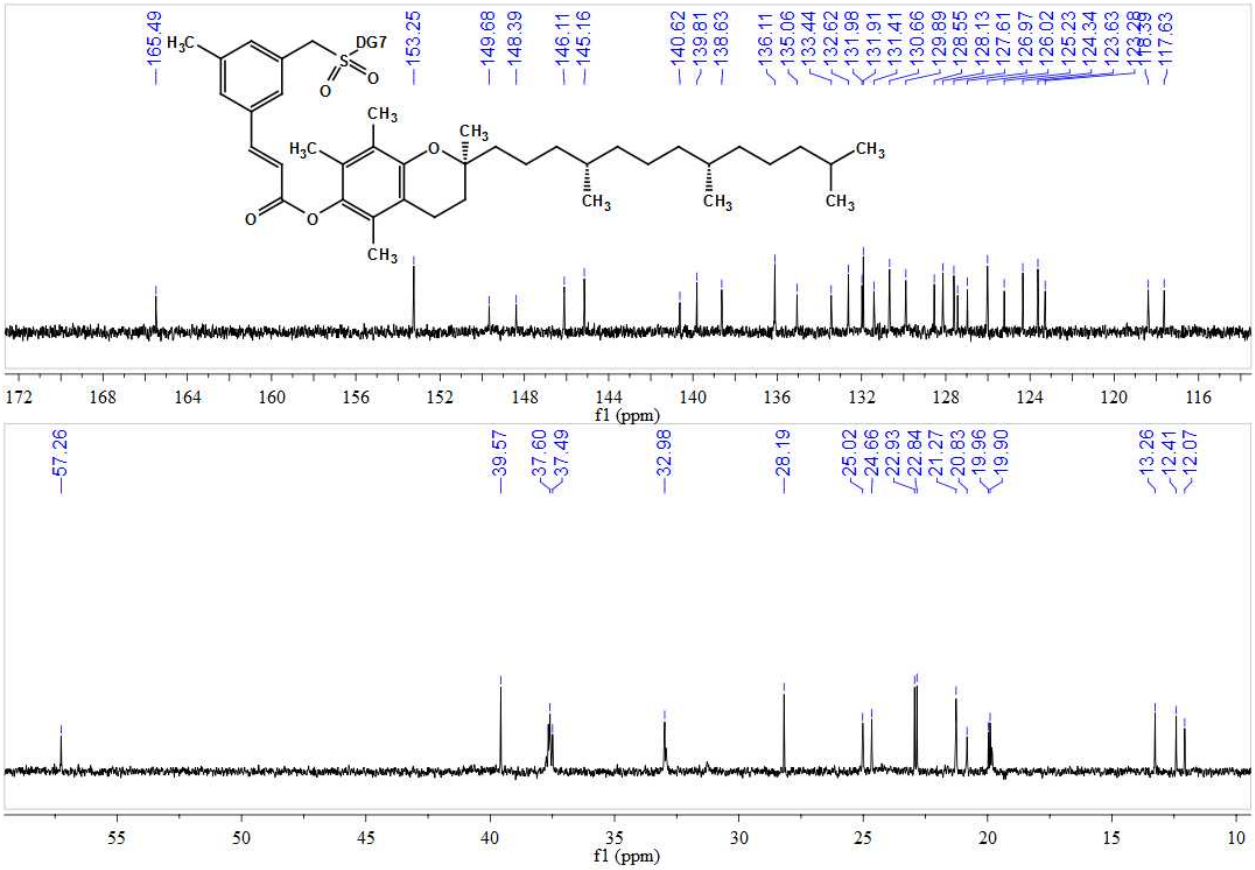




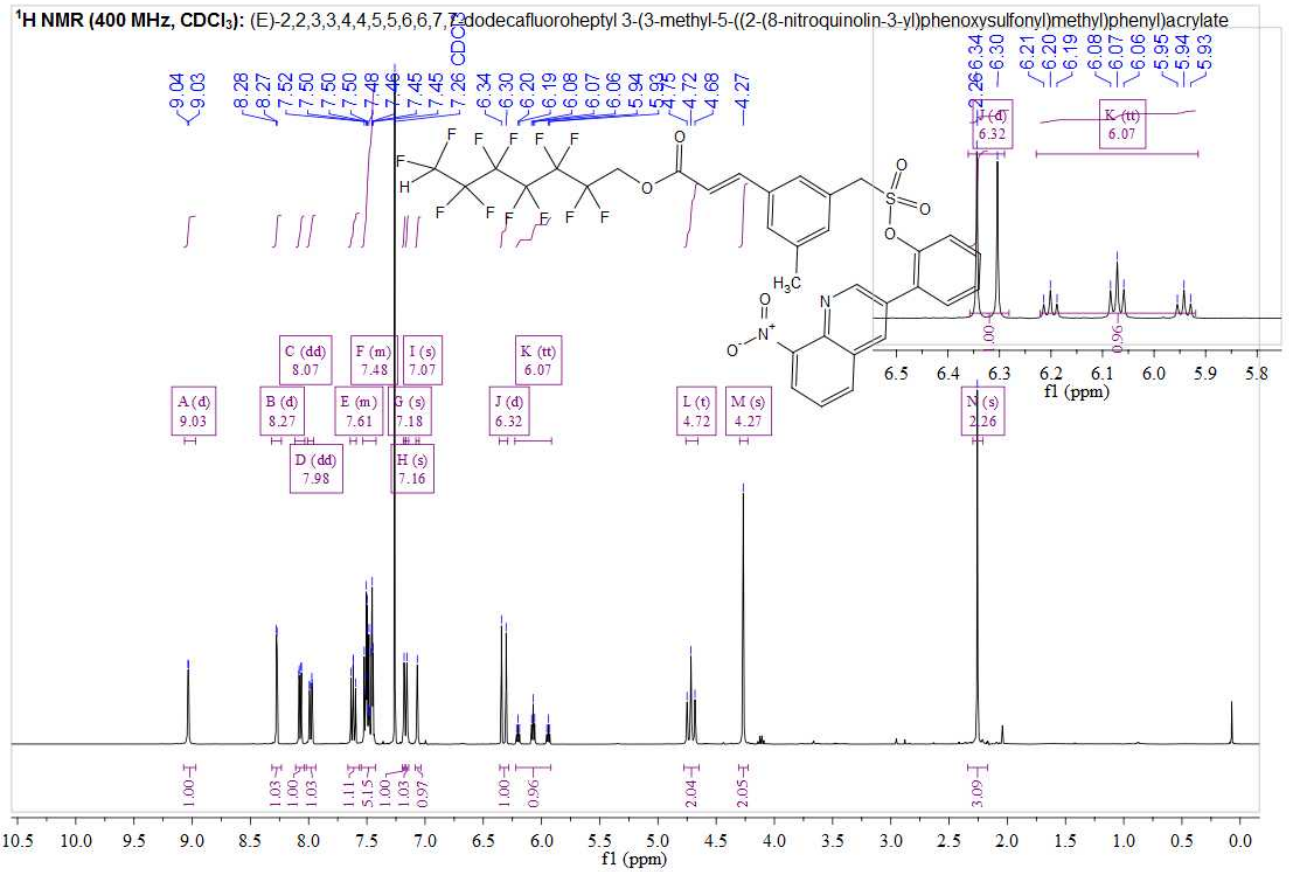
(*E*)-((S)-2,5,7,8-tetramethyl-2-((4S,8S)-4,8,12-trimethyltridecyl)chroman-6-yl) 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (5a):

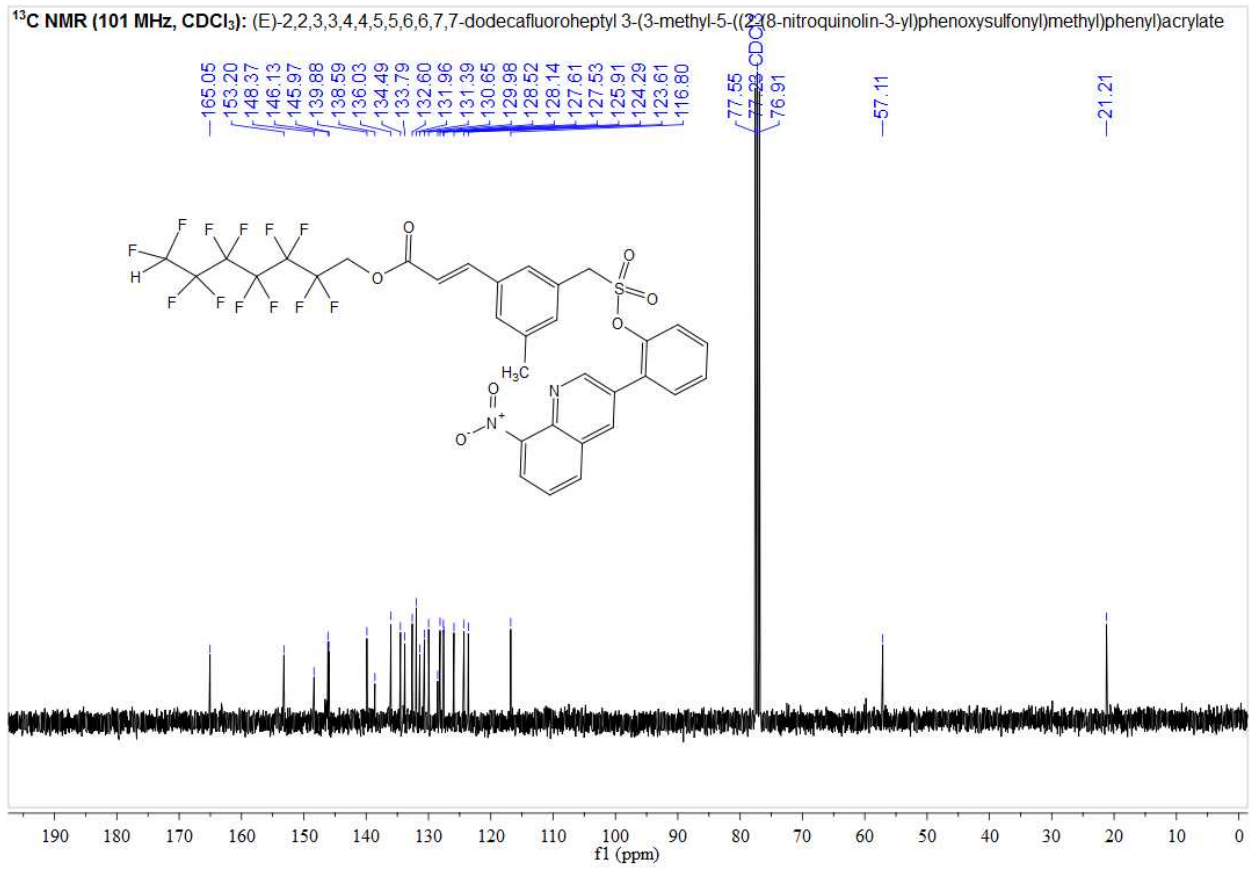




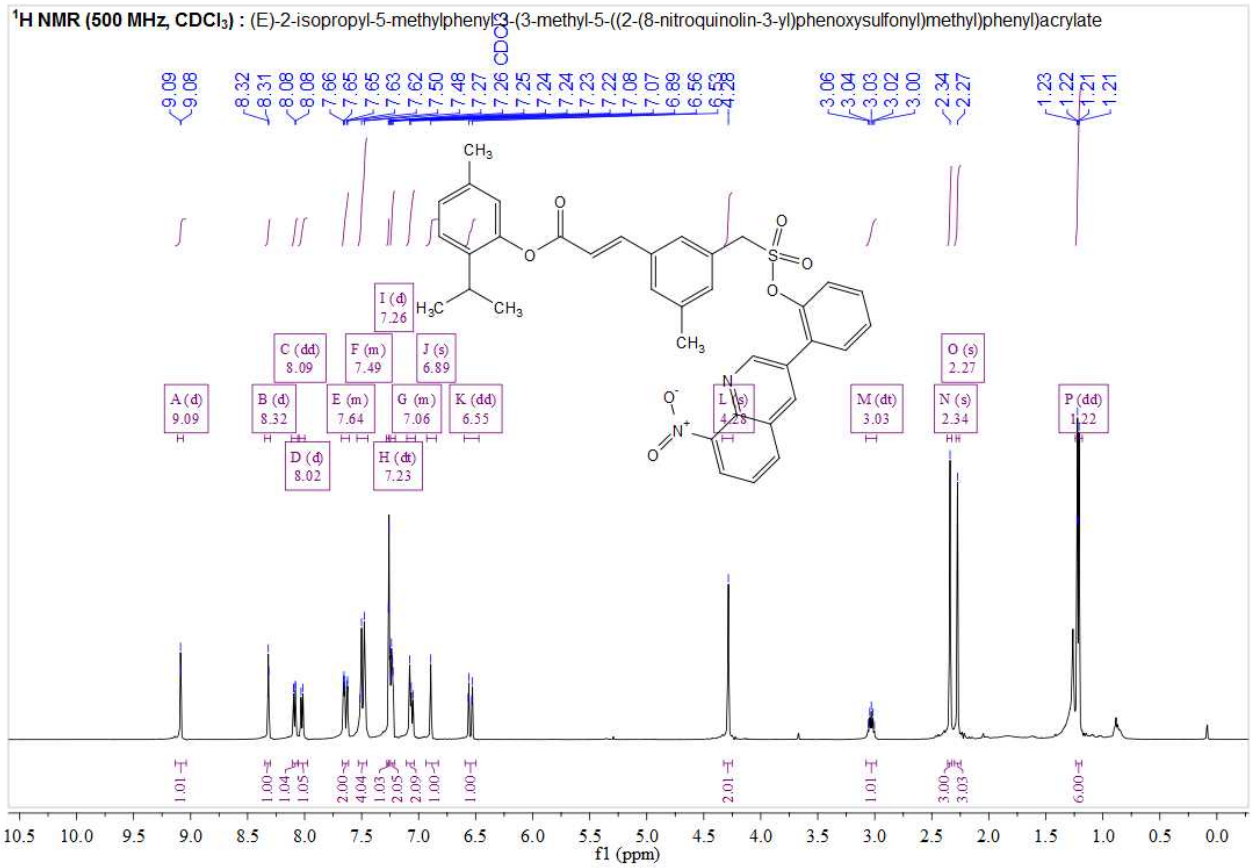

165.49
153.25
149.68
148.39
146.11
145.16
140.62
139.81
138.63
136.11
135.06
133.44
132.62
131.98
131.91
131.41
130.66
129.89
128.55
128.13
127.61
126.97
126.02
125.23
124.34
123.63
117.63
DG7
f1 (ppm)
57.26
39.57
37.60
37.49
32.98
28.19
25.02
24.66
22.93
22.84
21.27
20.83
19.96
19.90
13.26
12.41
12.07
f1 (ppm)

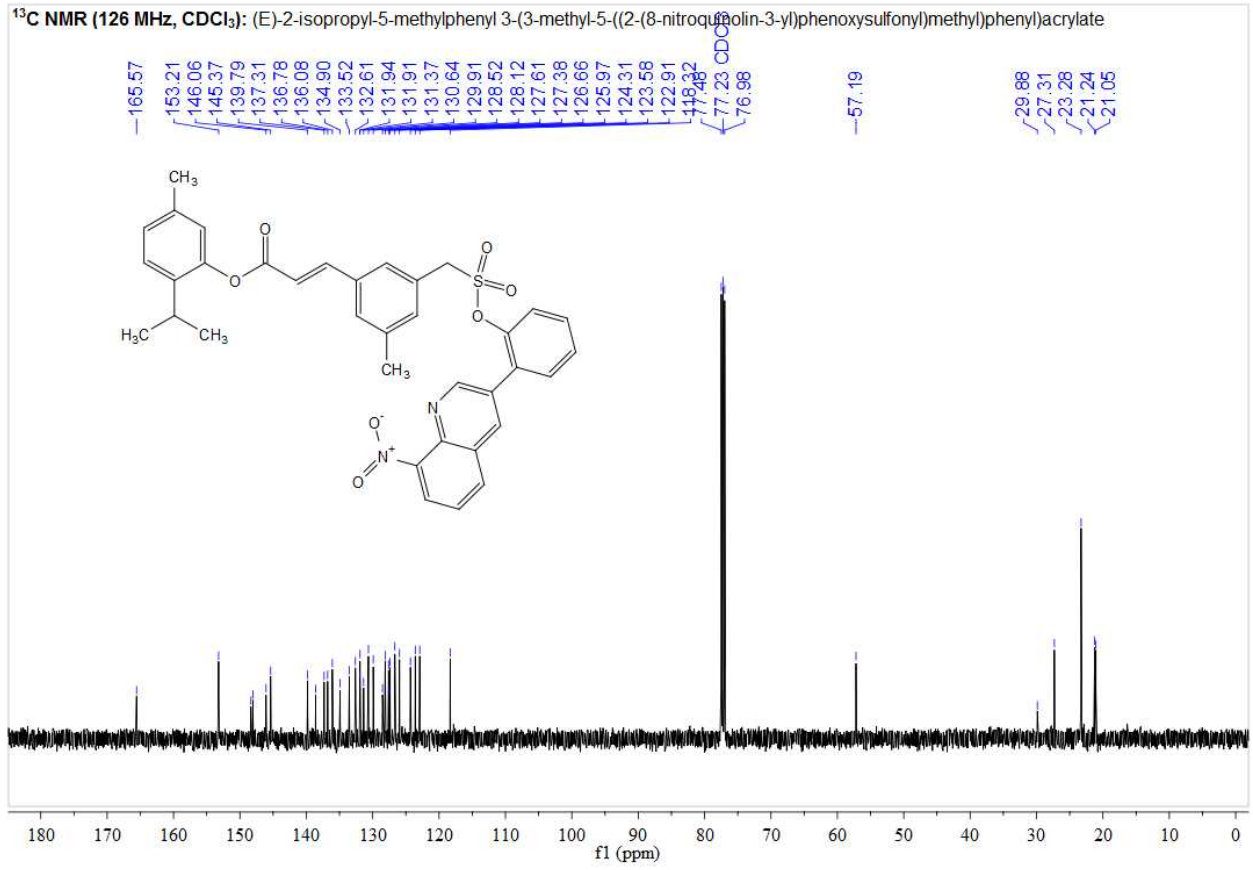
(*E*)-2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)-phenoxysulfonyl)methyl)phenyl)acrylate (5b):



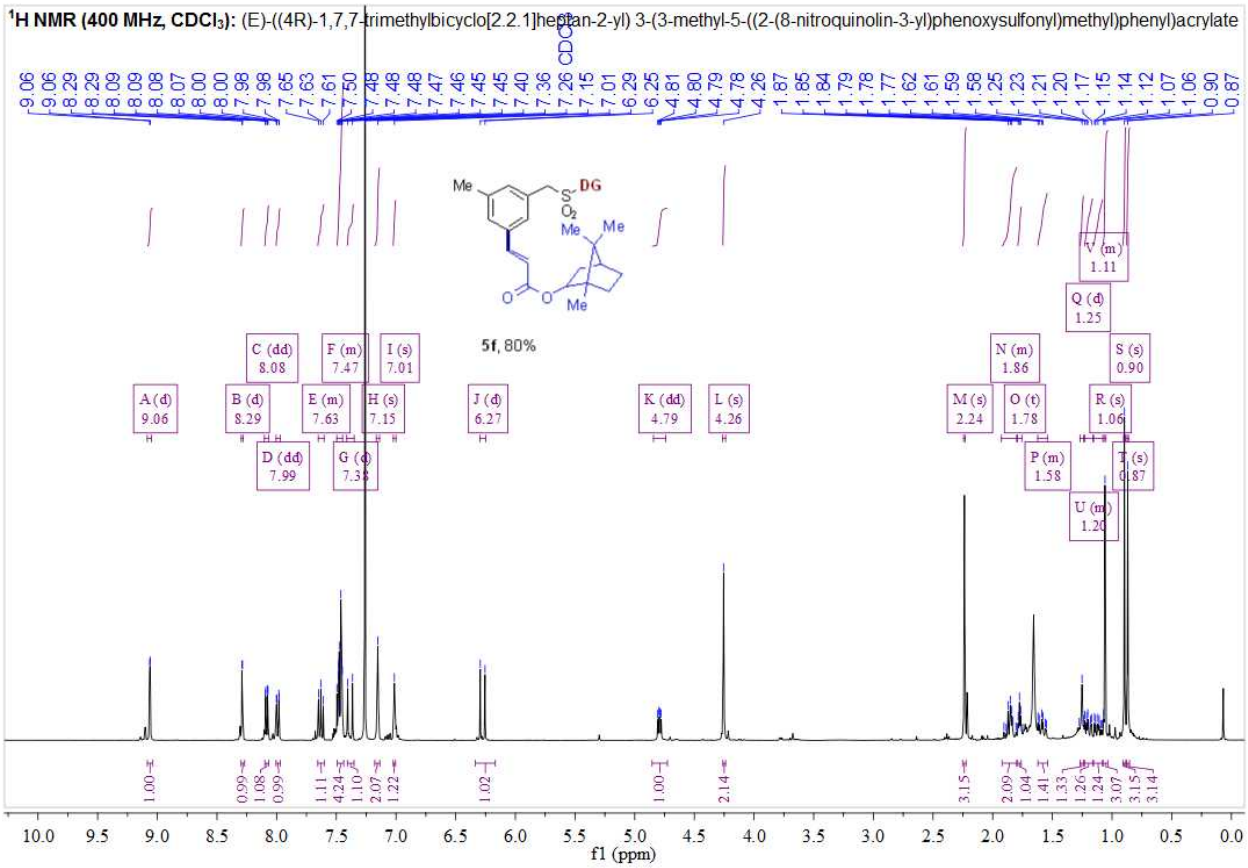


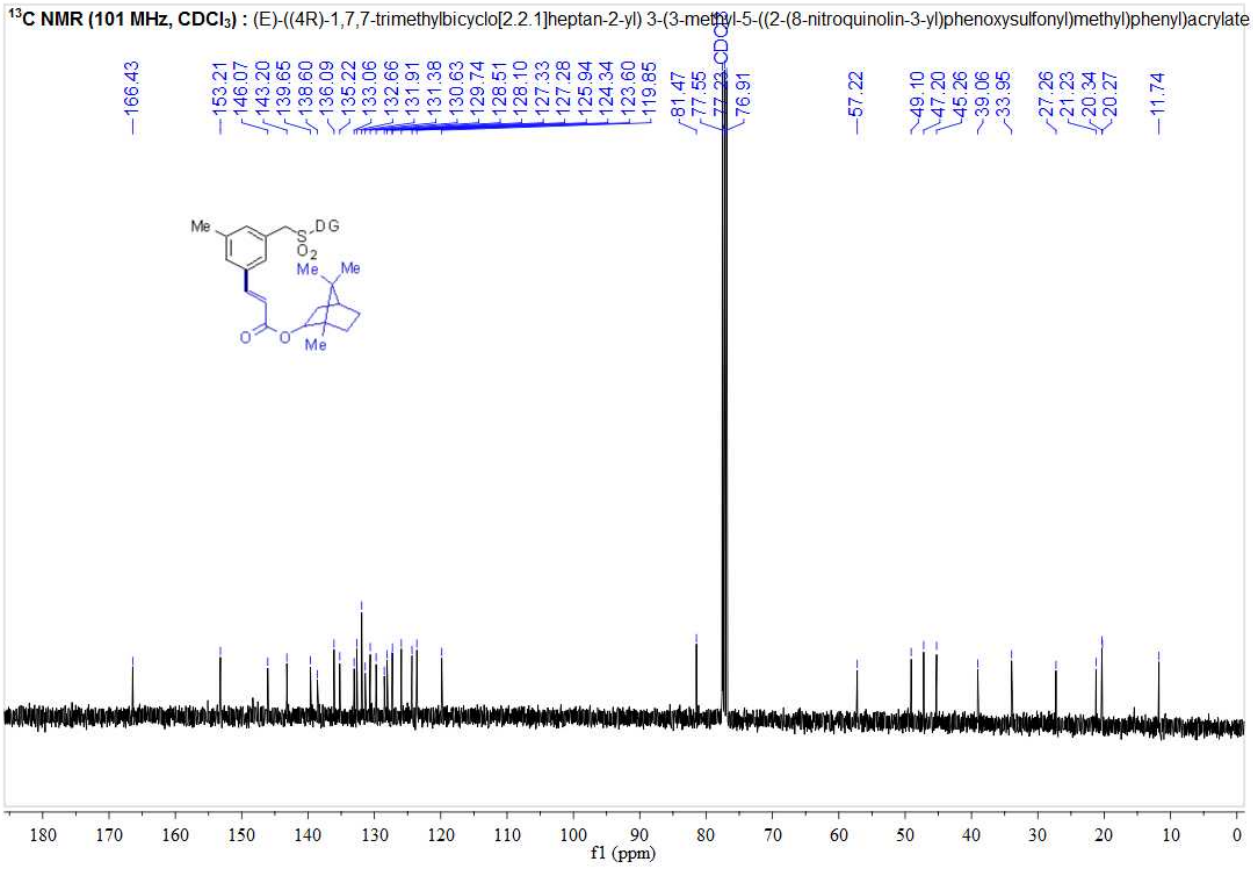
(*E*)-2-isopropyl-5-methylphenyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (5c):



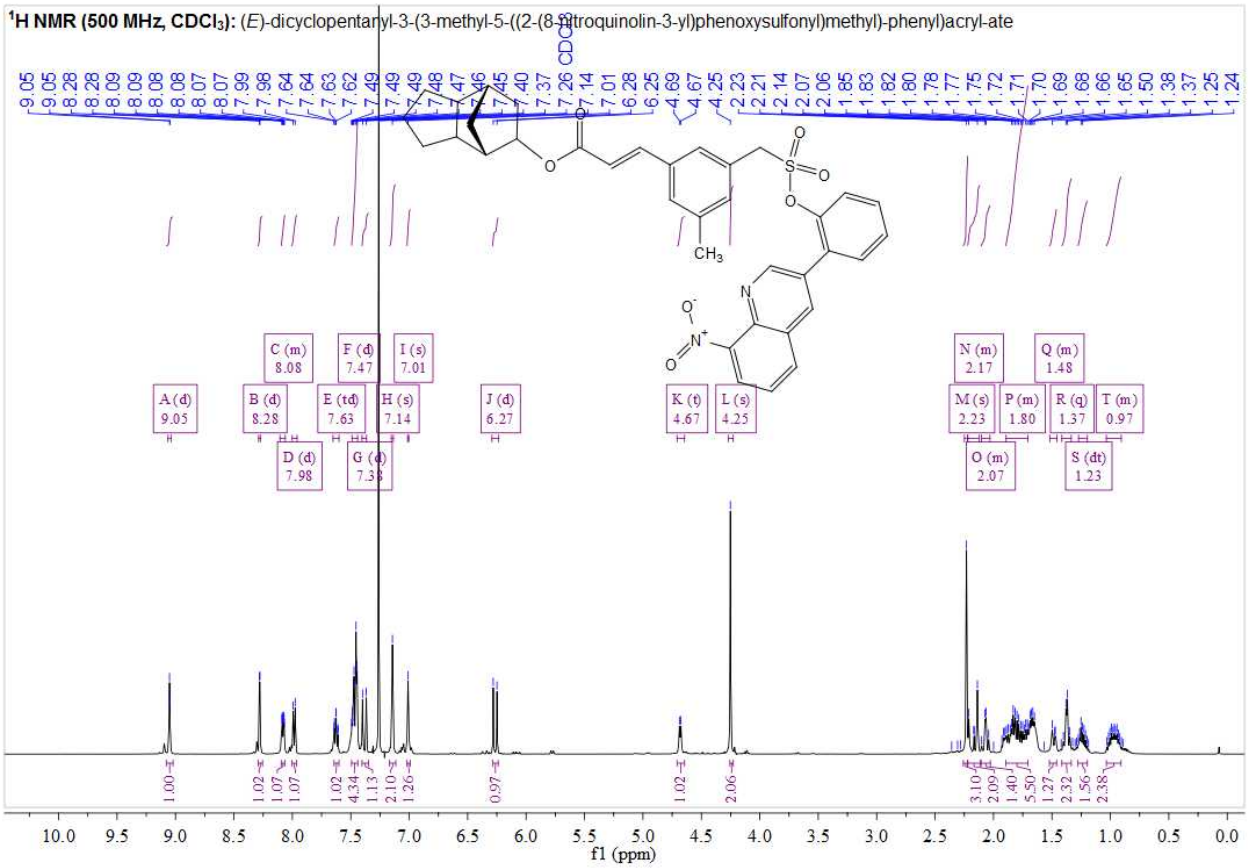


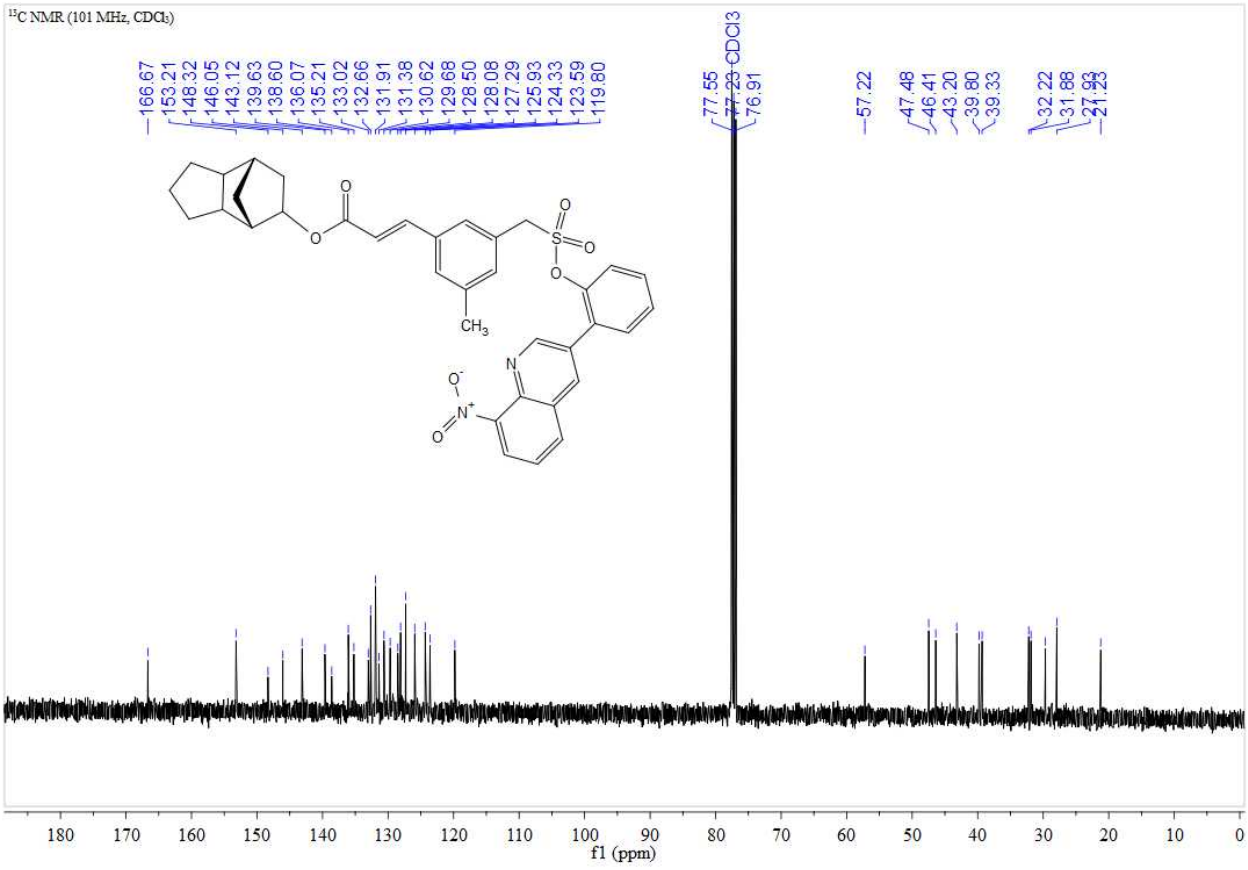
(*E*)-2-isopropyl-5-methylphenyl 3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)acrylate (5d):



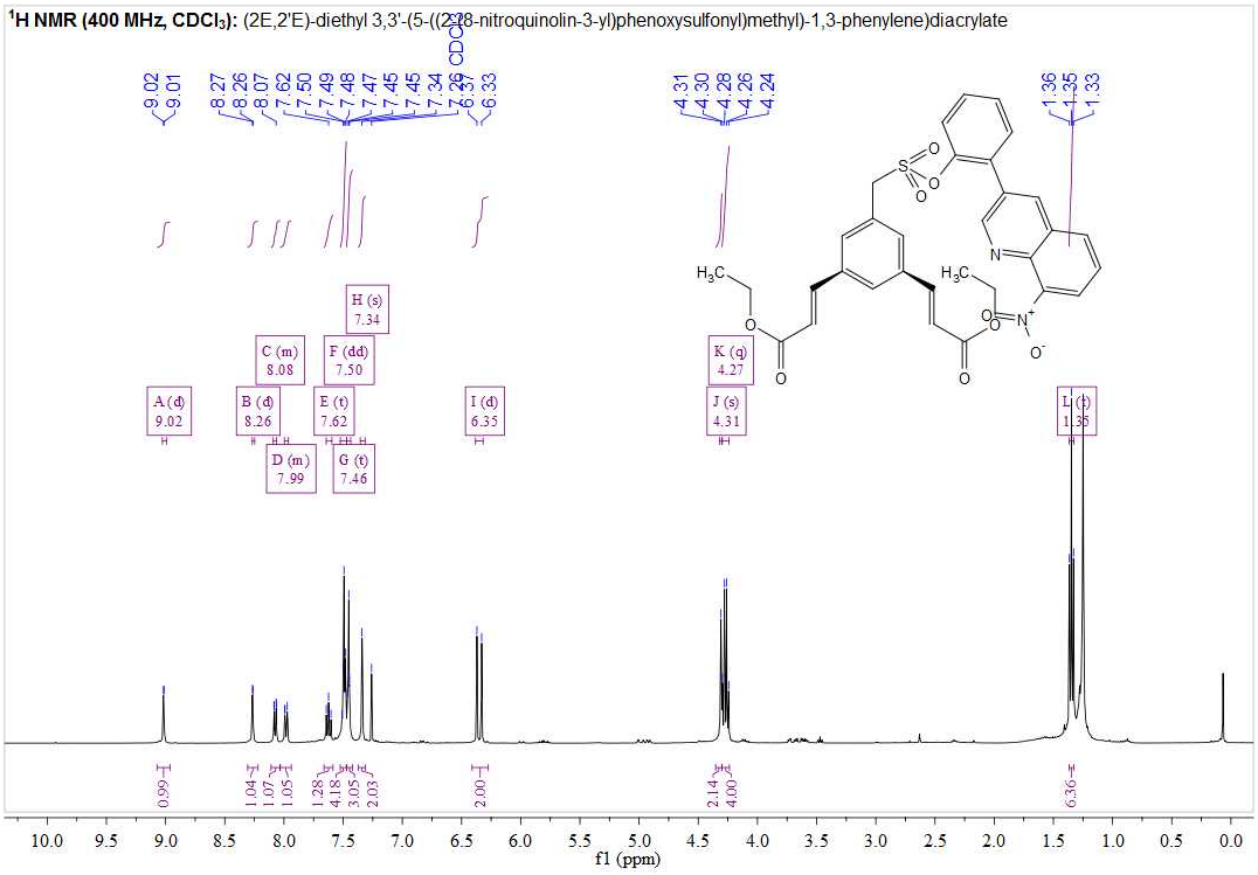


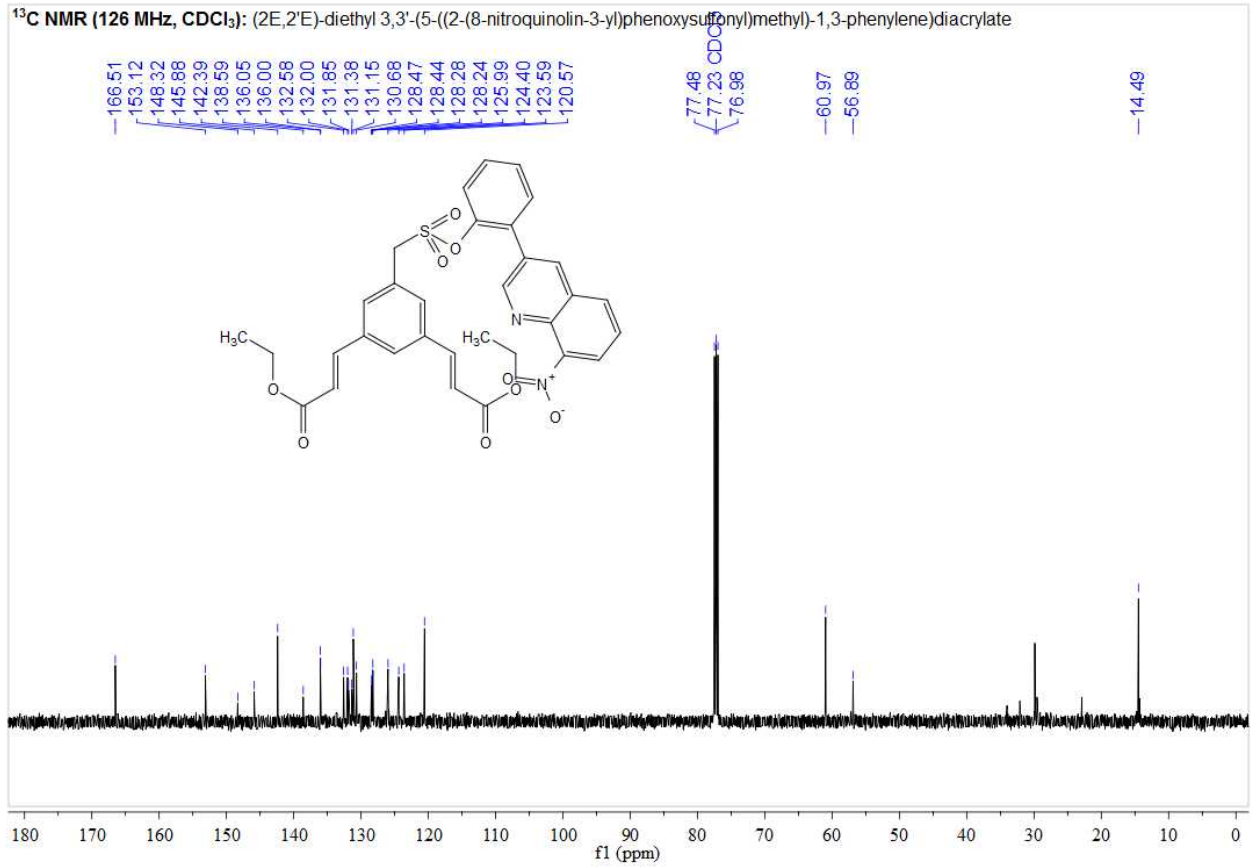
(*E*)-dicyclopentanyl-3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-phenyl)acryl-ate (5e):



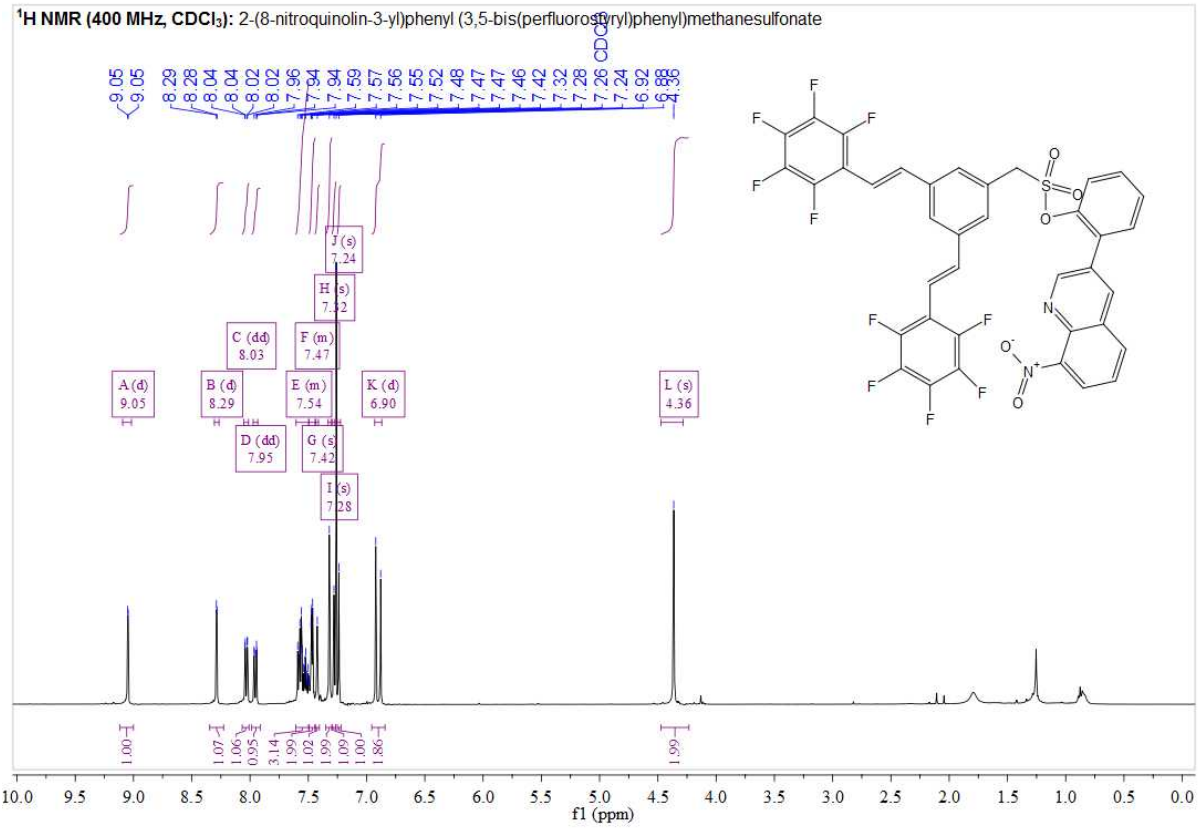


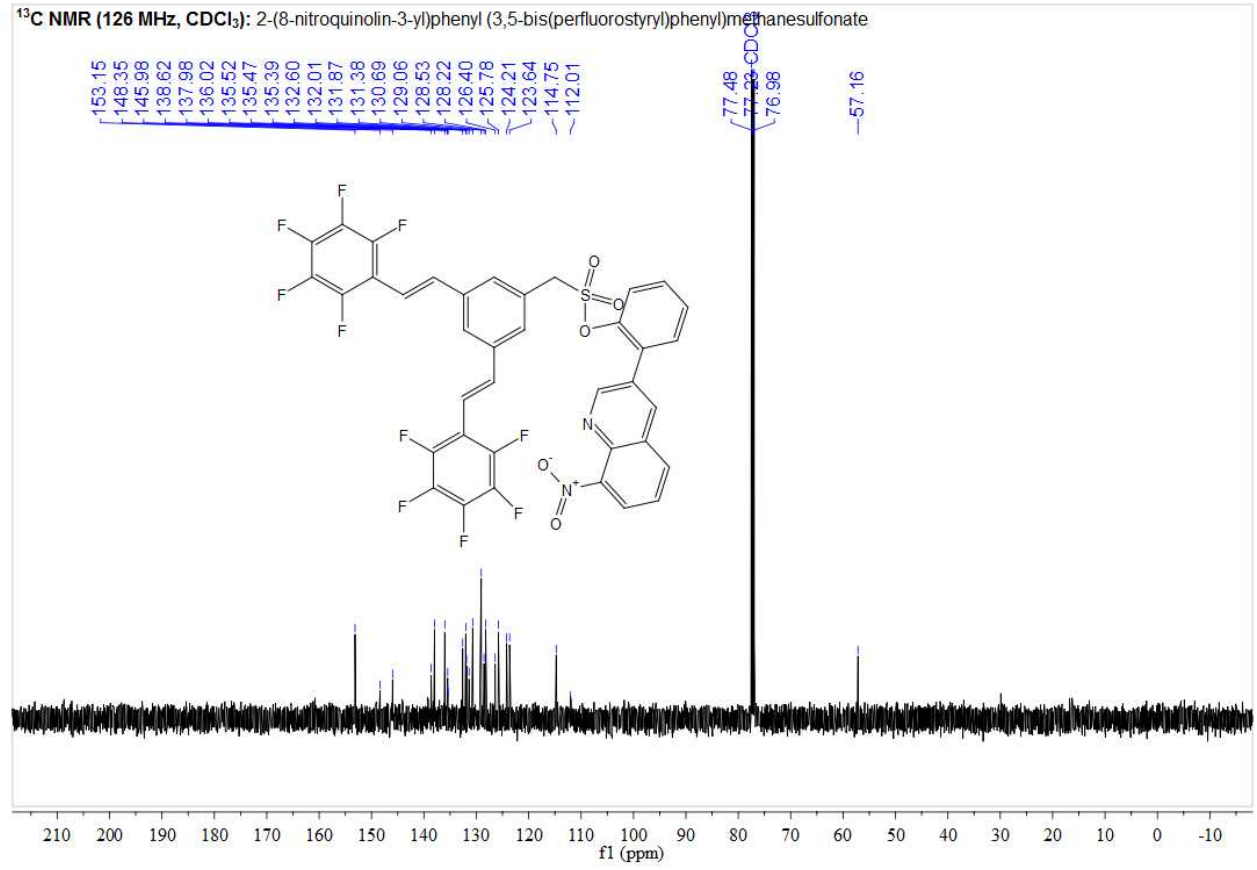
(2*E*,2'*E*)-diethyl 3,3'-(5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-1,3-phenylene)diacrylate (7a):



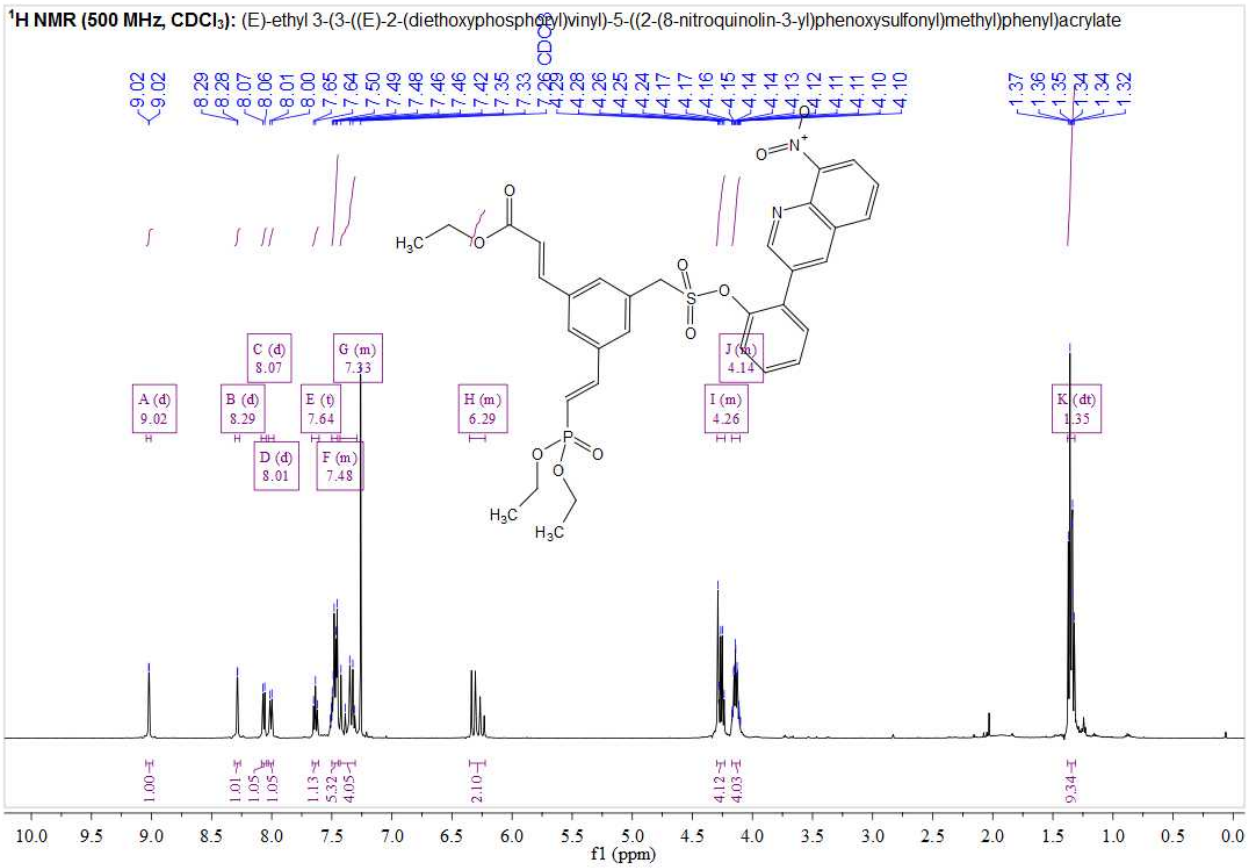


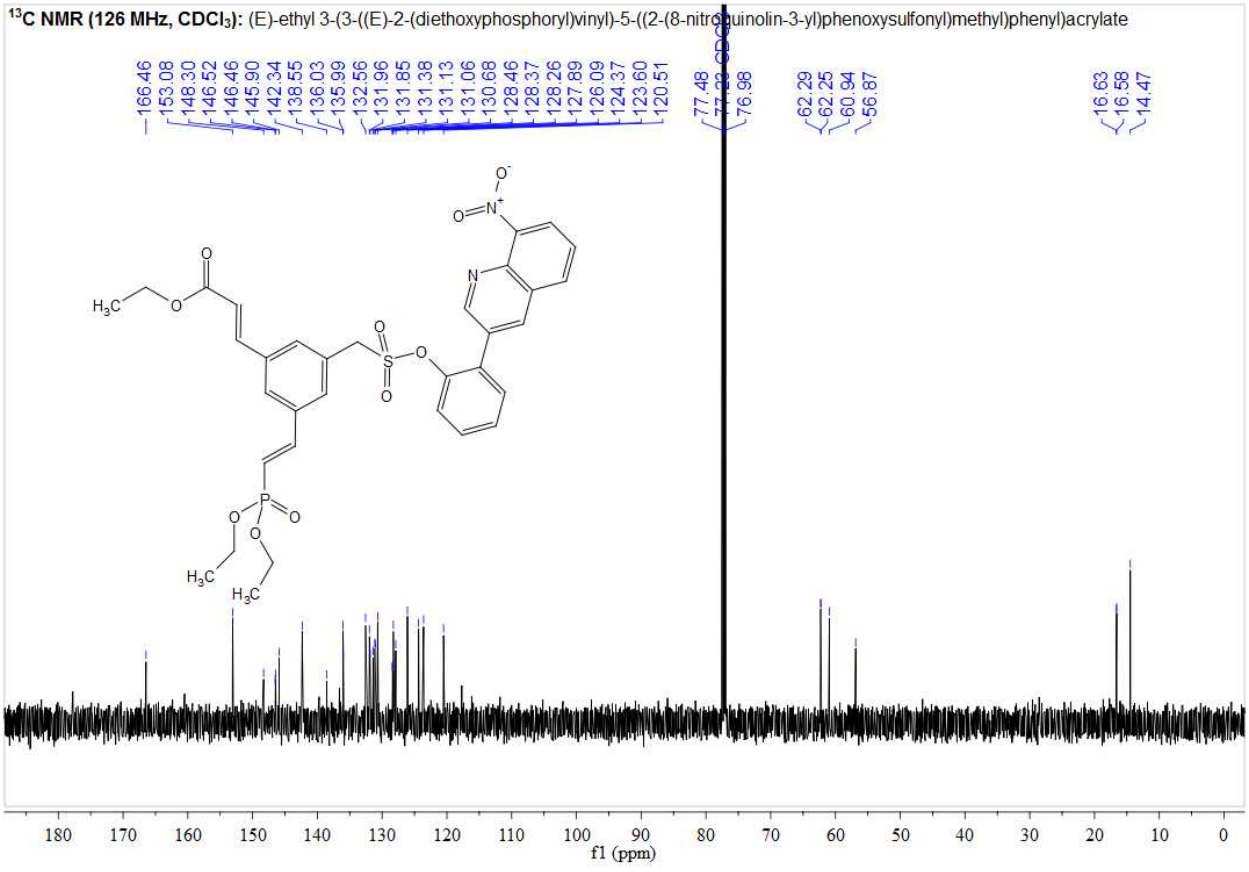
2-(8-nitroquinolin-3-yl)phenyl (3,5-bis(perfluorostyryl)phenyl)methanesulfonate (7b):



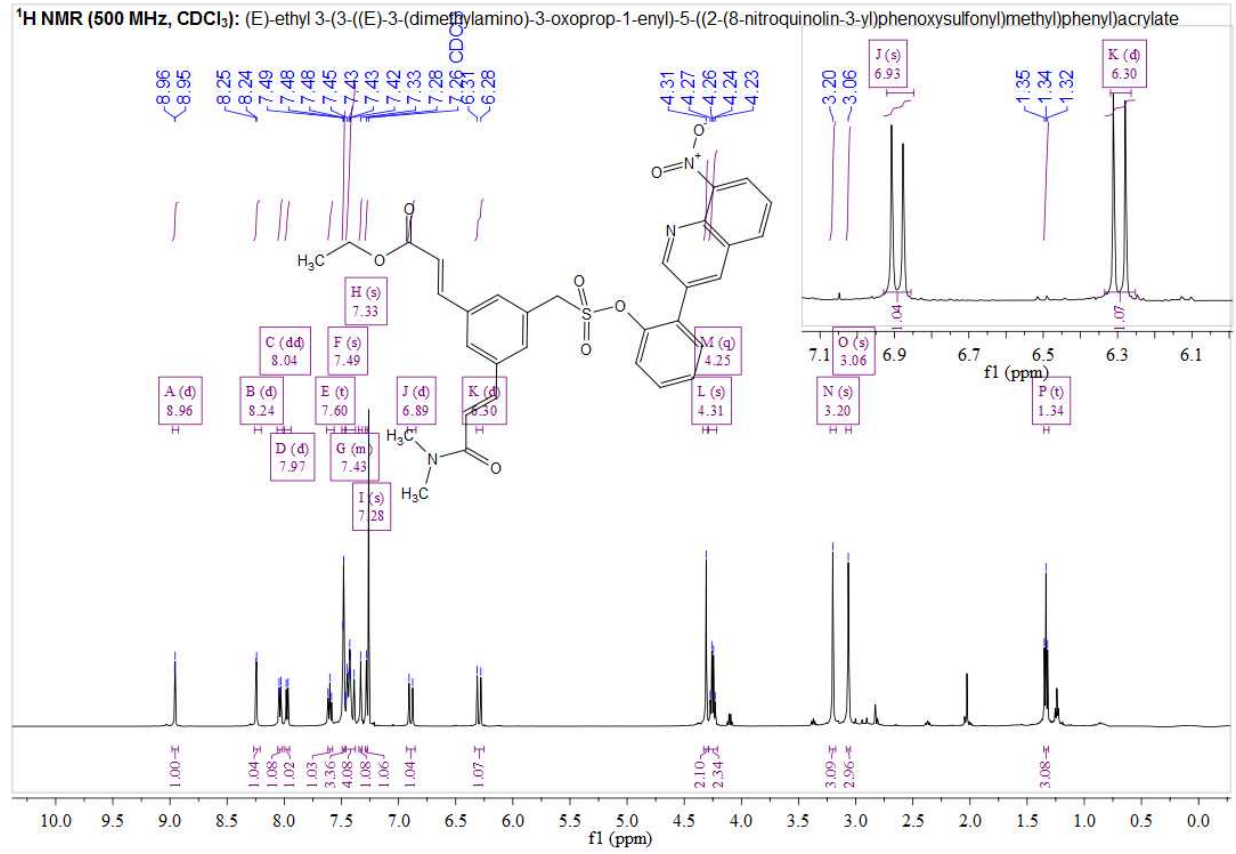


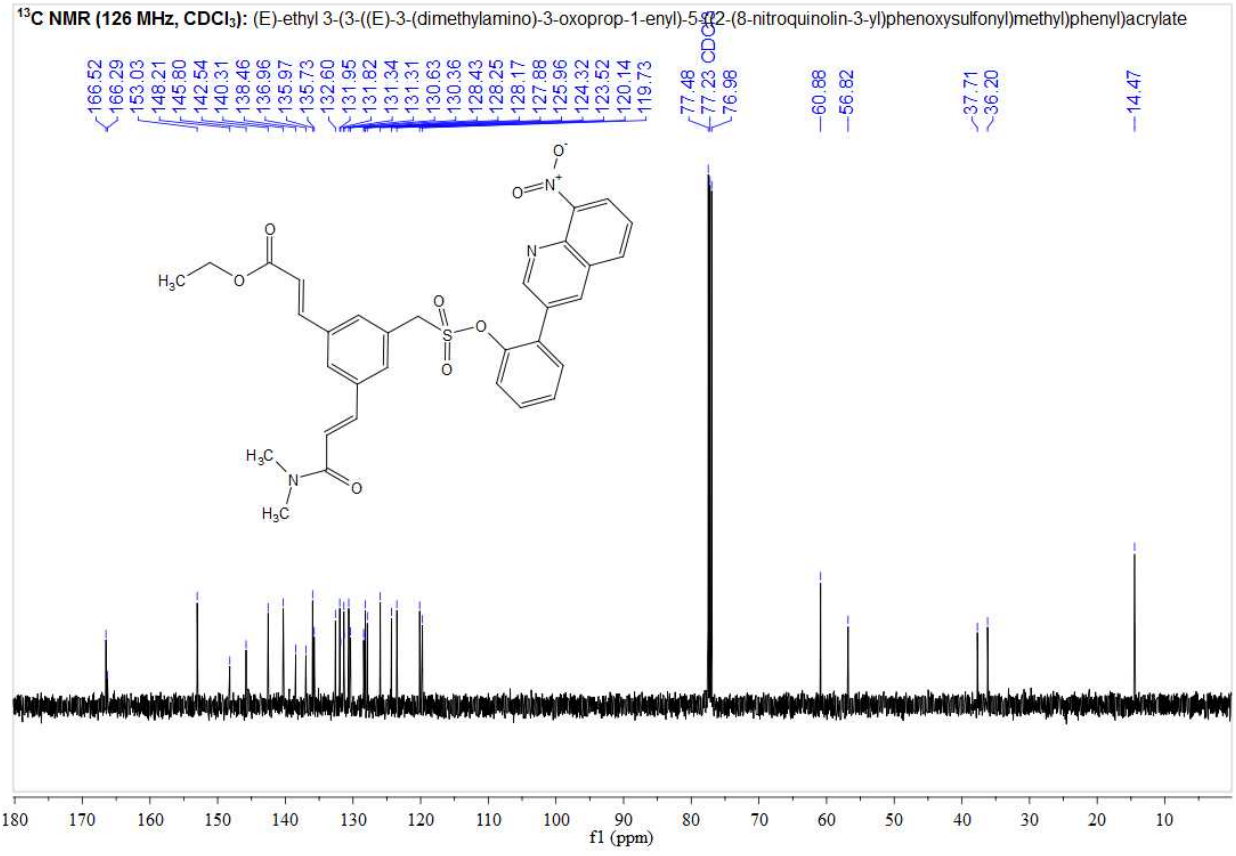
(*E*)-ethyl 3-(3-((E)-2-(diethoxyphosphoryl)vinyl)-5-((2-(8-nitroquinolin-3-yl)phenoxy-sulfonyl)meth-yl)phenyl)acrylate (7c):



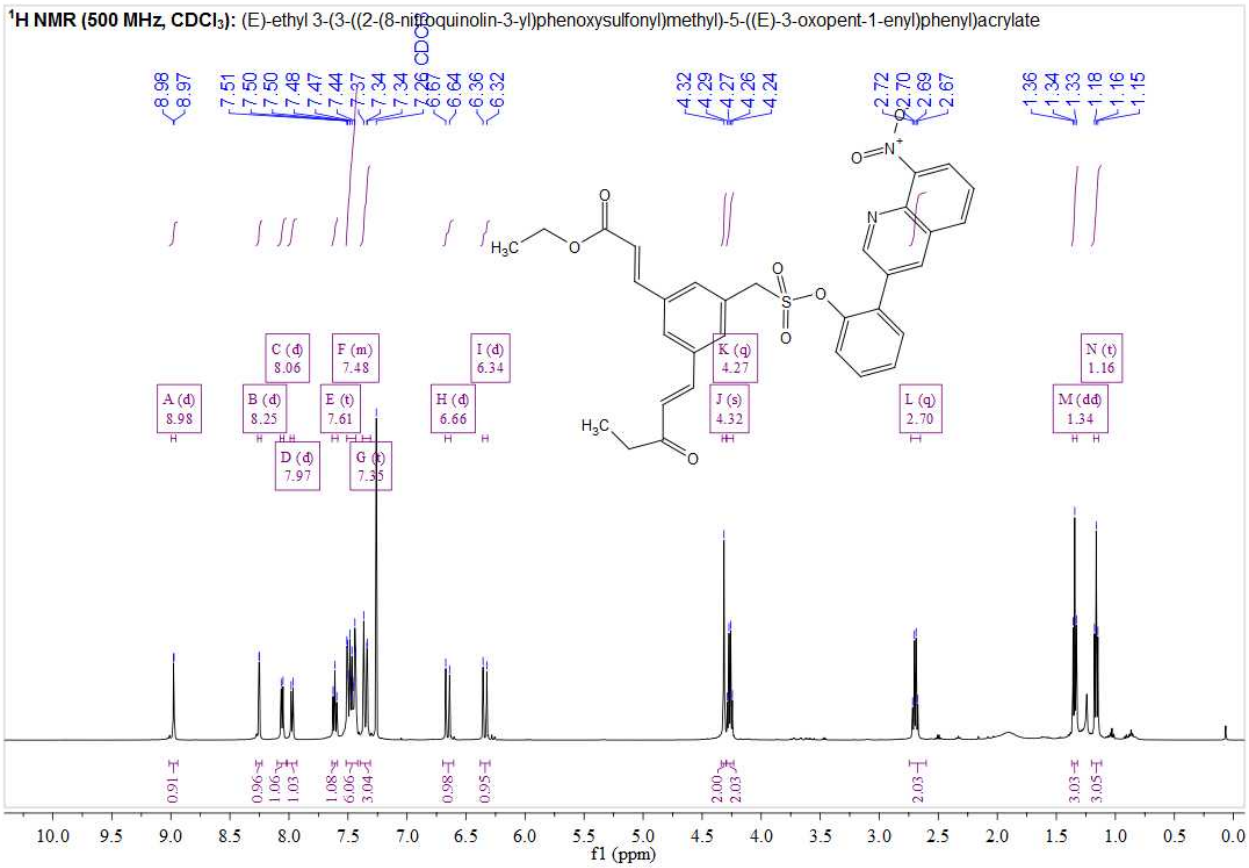


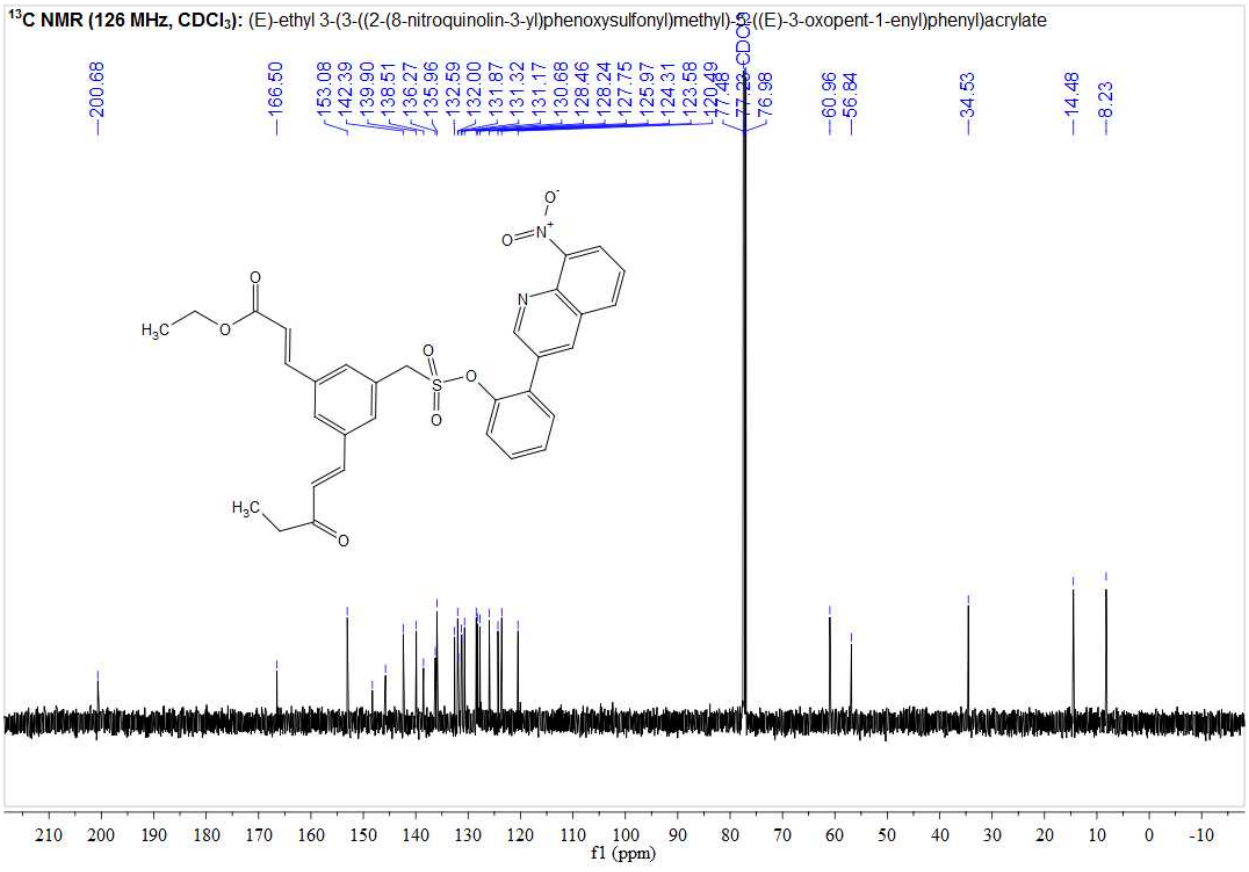
(*E*)-ethyl 3-(3-((E)-3-(dimethylamino)-3-oxoprop-1-enyl)-5-((2-(8-nitroquinolin-3-yl)-phenoxysulfonyl)meth-yl)phenyl)acrylate (7d):



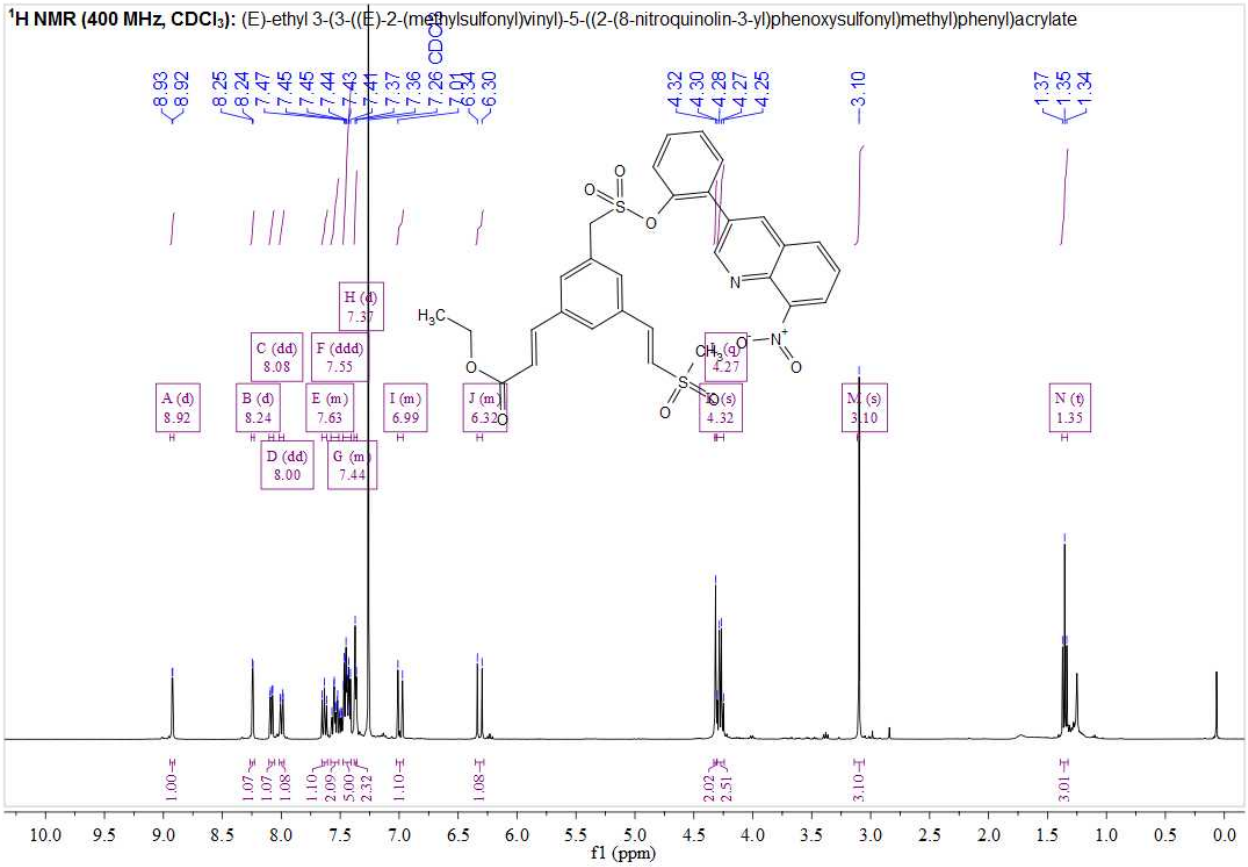


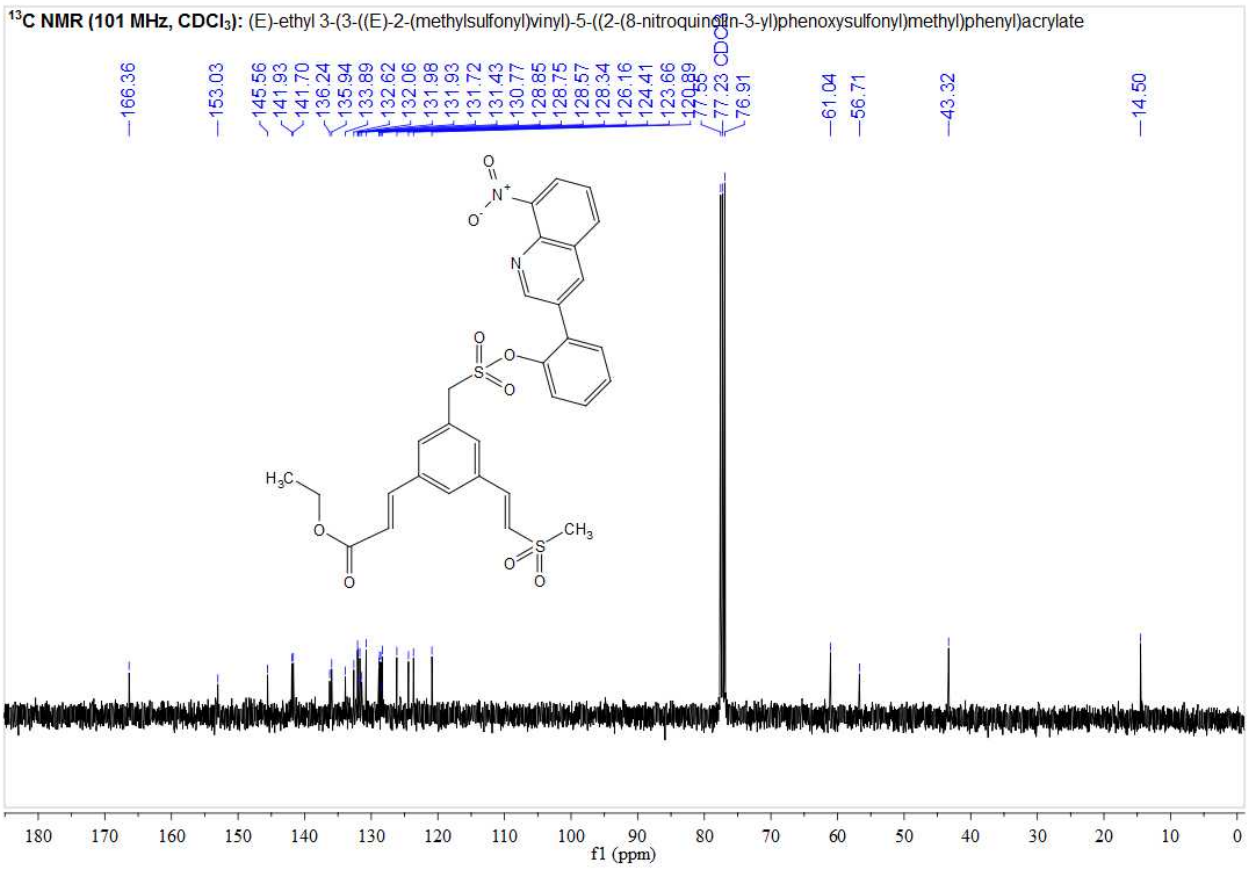
(*E*)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-5-((E)-3-oxopent-1-enyl)phenyl)acrylate (7e):



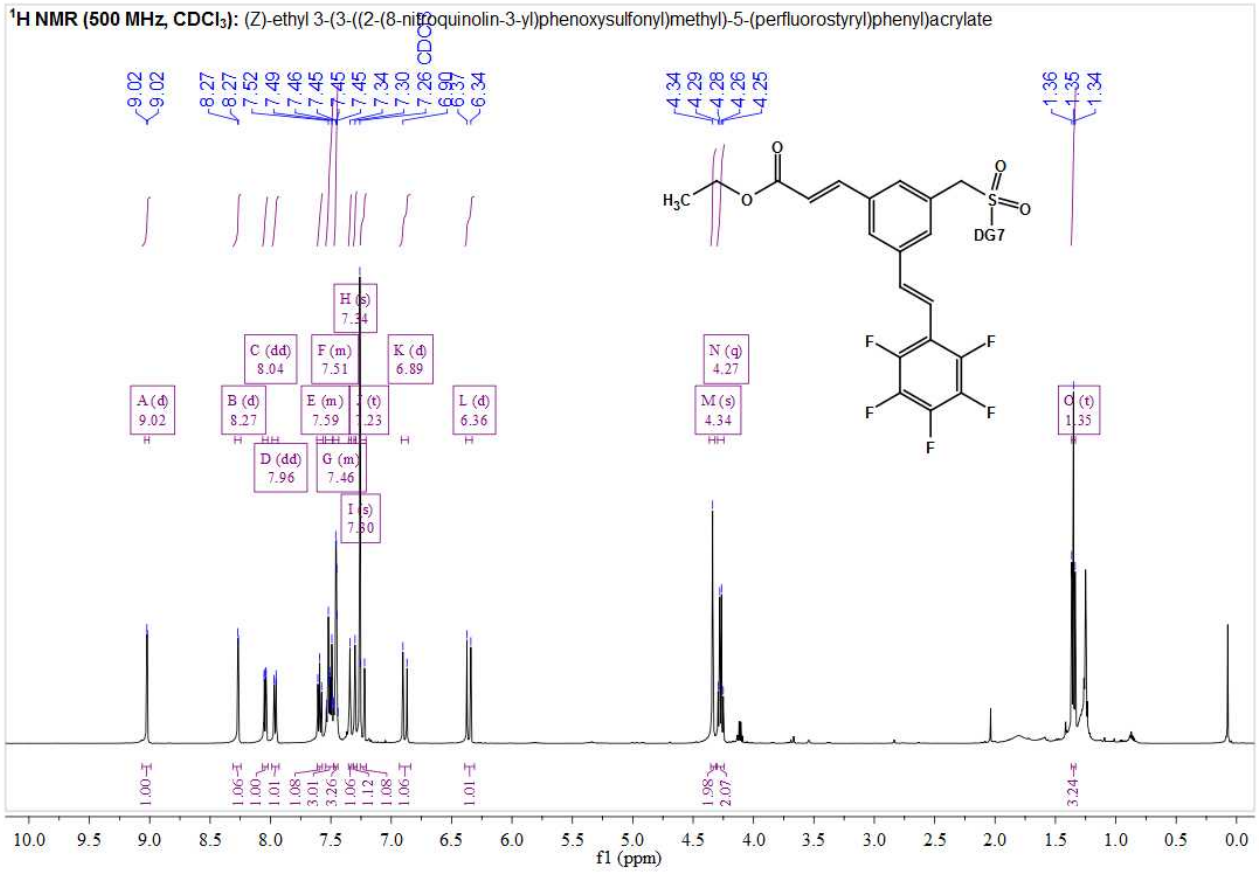


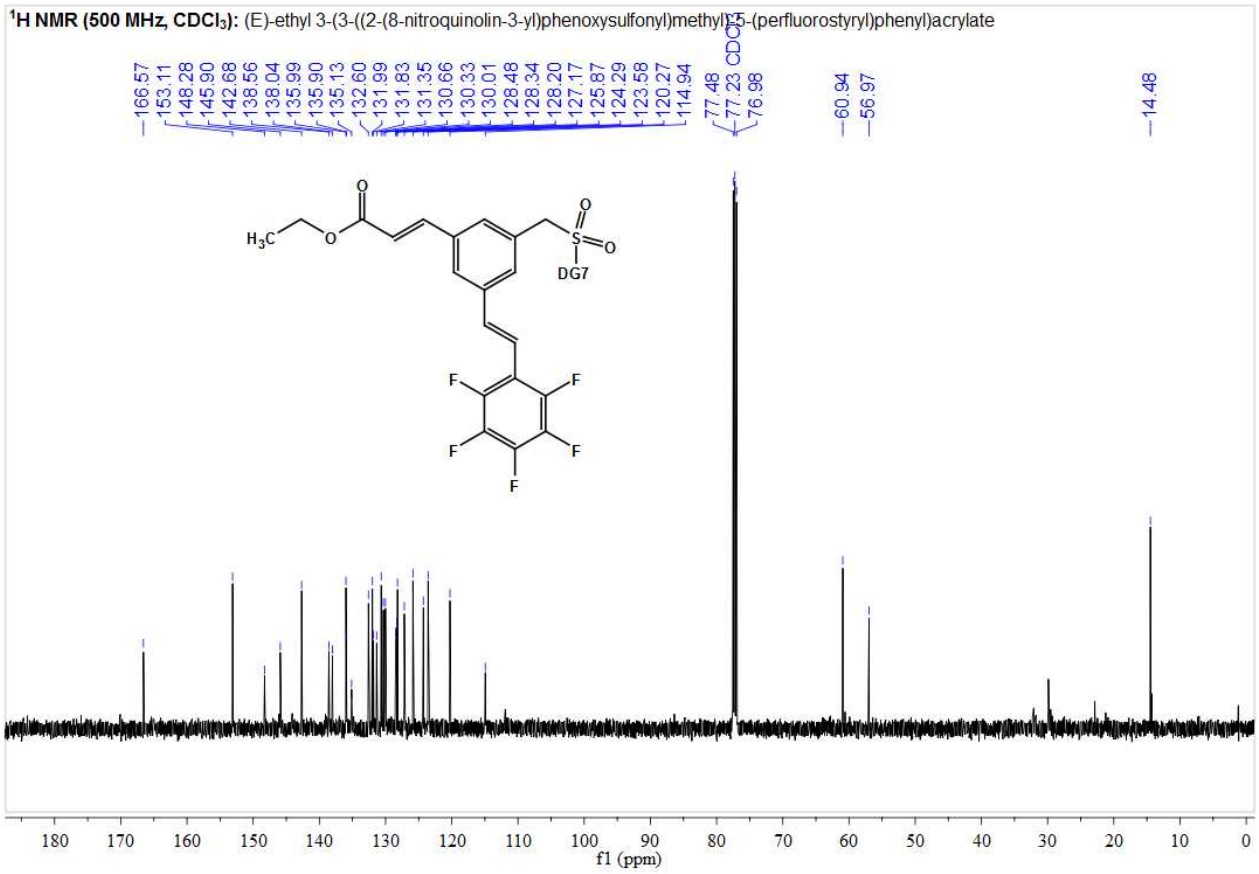
(*E*)-ethyl 3-(3-((E)-2-(methylsulfonyl)vinyl)-5-((2-(8-nitroquinolin-3-yl)phenoxysulfon-yl)methyl)phenyl)-acrylate (7f):



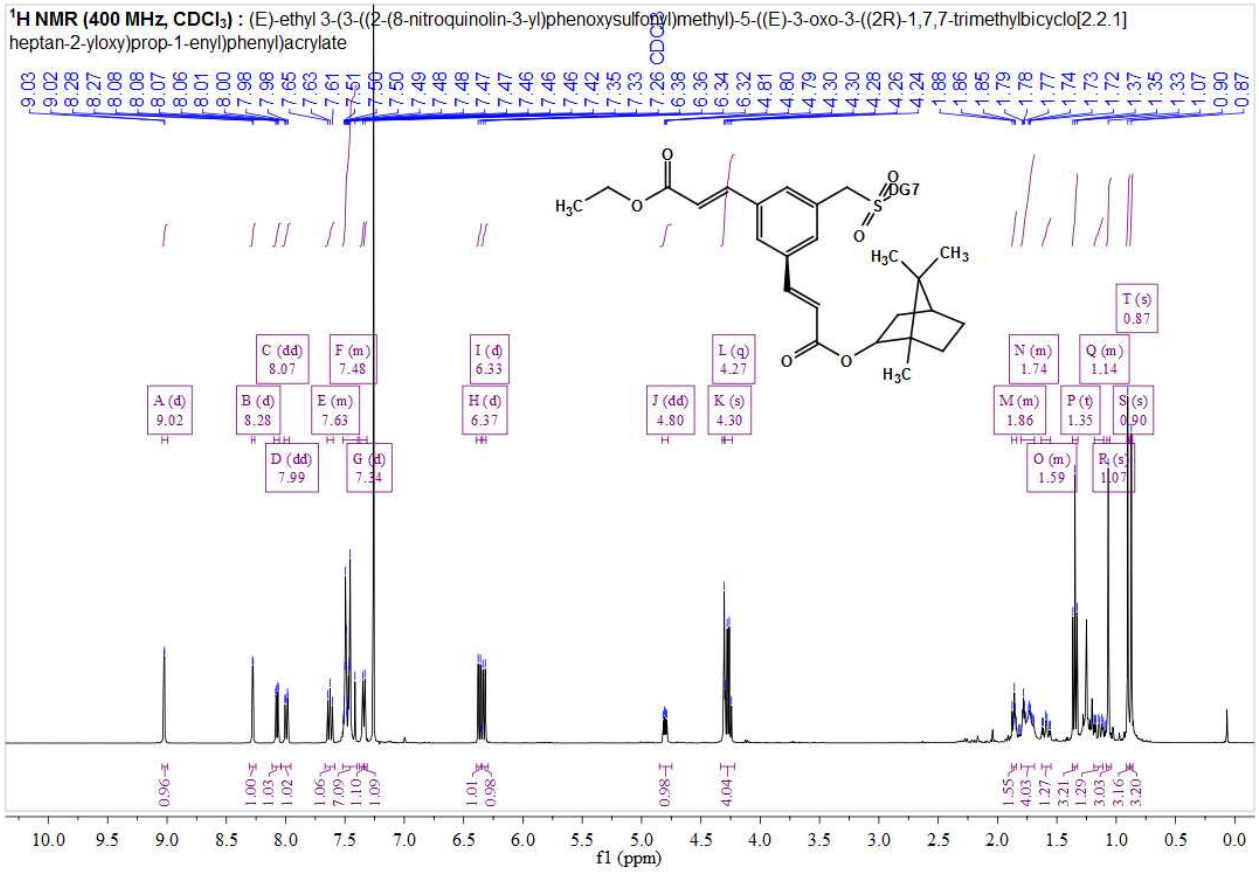


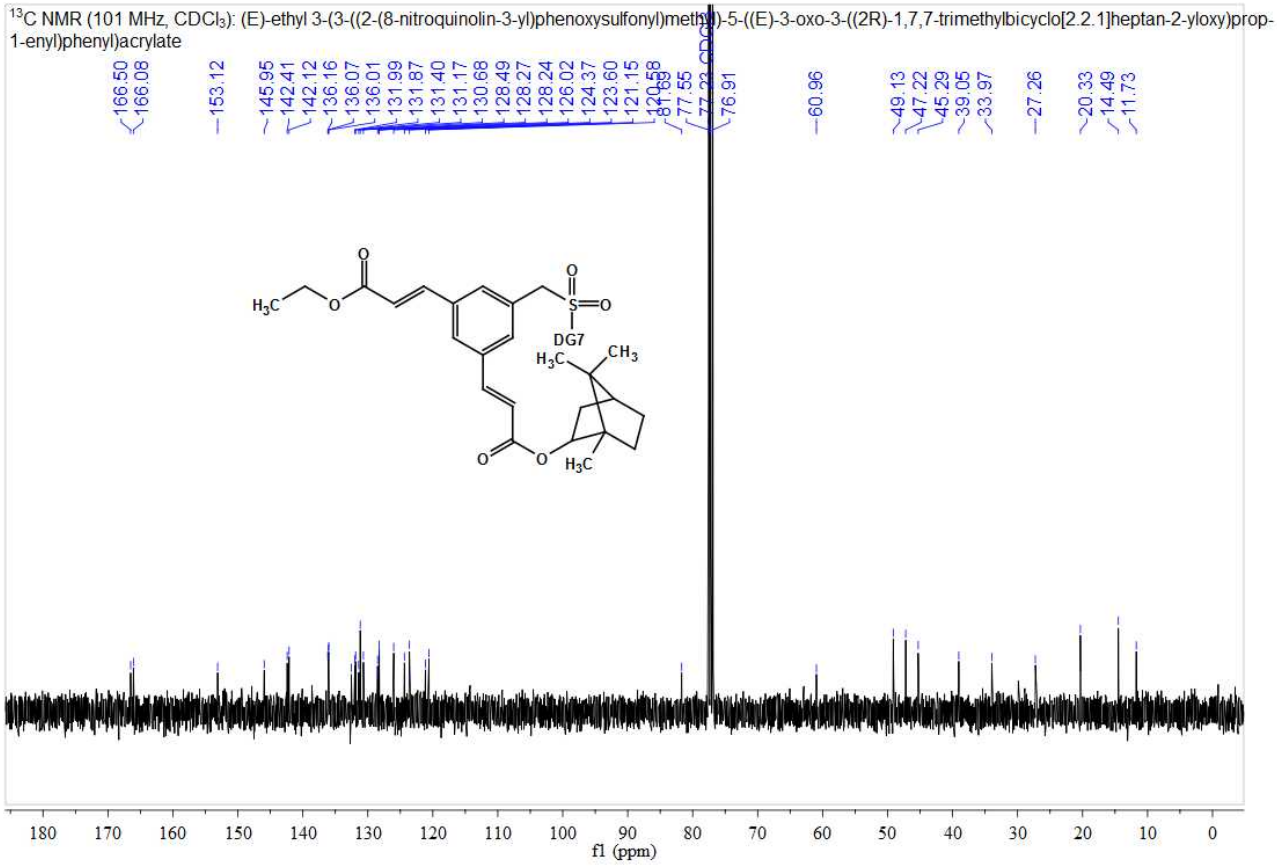
(*E*)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-5-(perfluorostyryl)-phenyl)acrylate(7g):



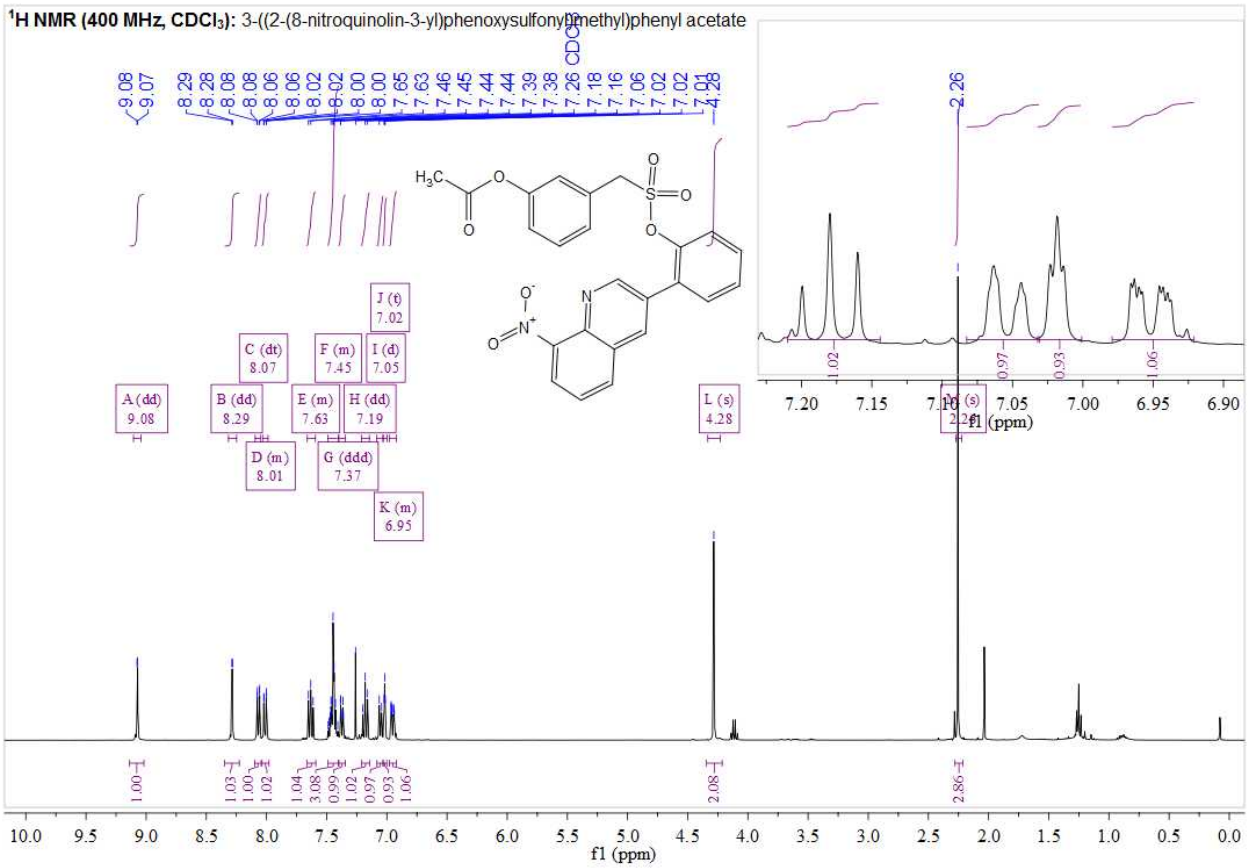


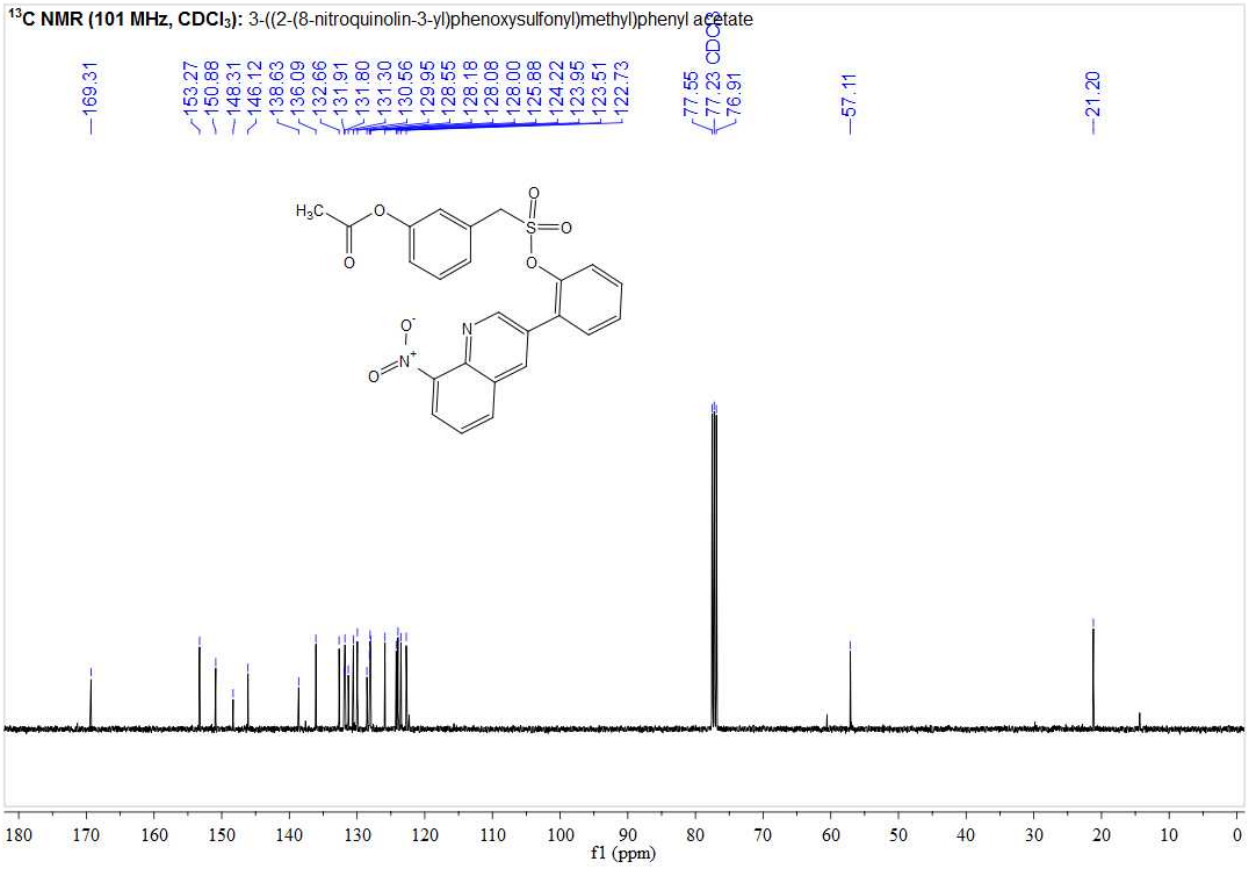
(*E*)-ethyl 3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)-5-((E)-3-oxo-3-((2R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yloxy)prop-1-enyl)phenyl)acrylate (7h):



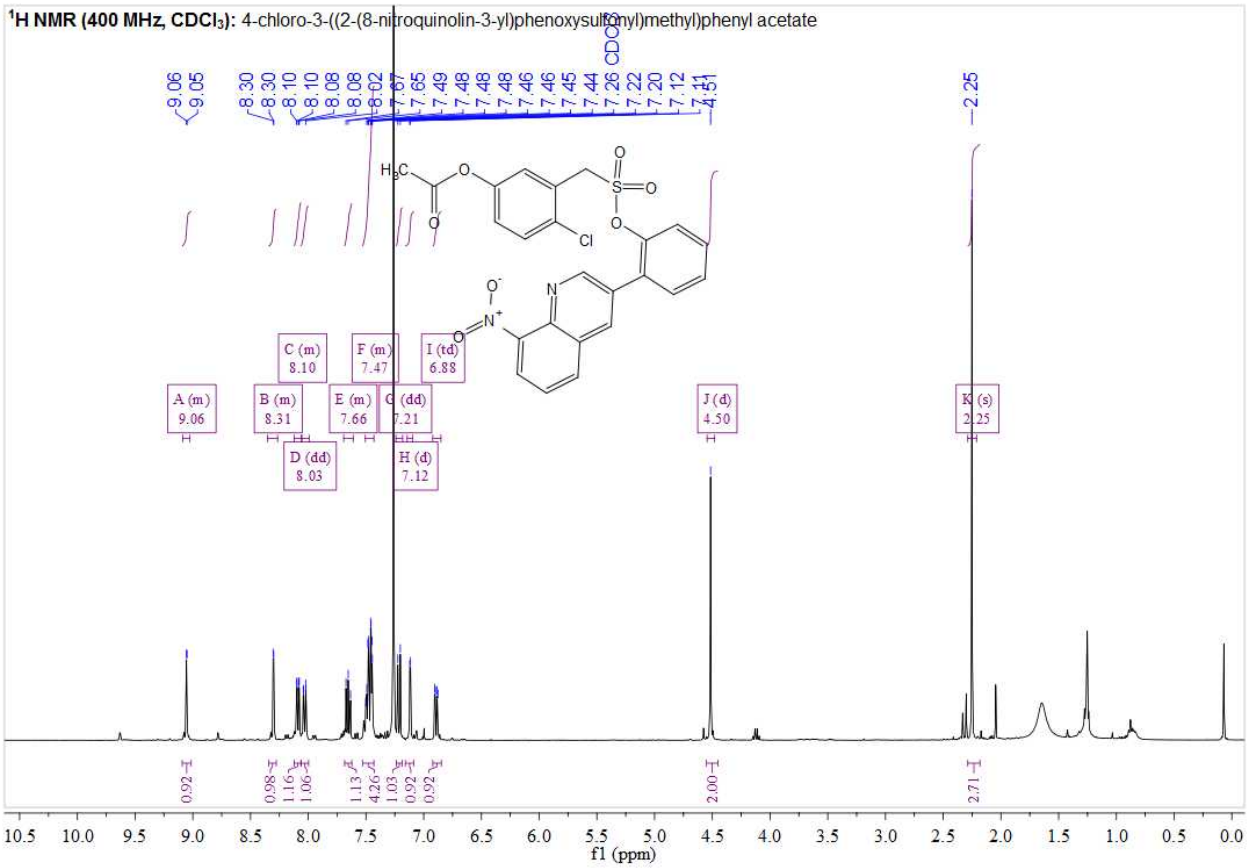


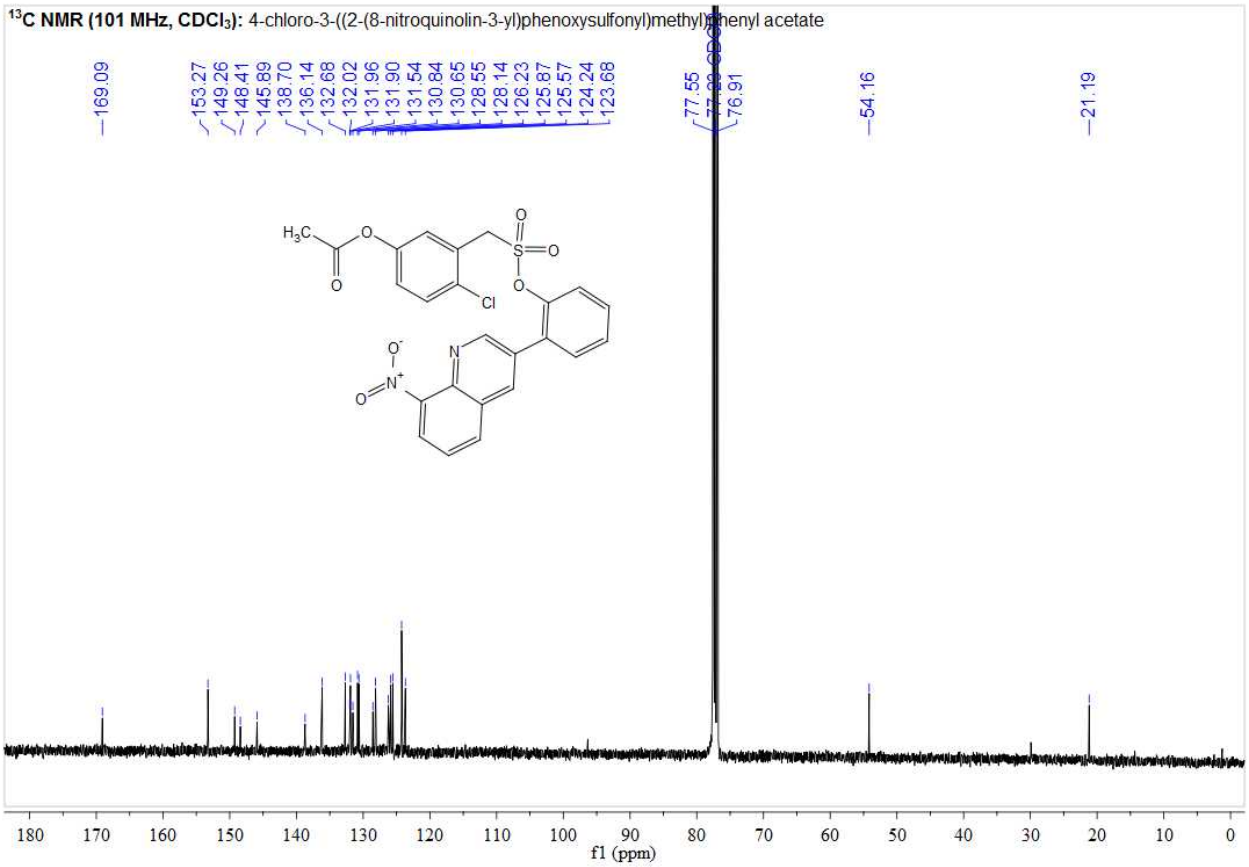
3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9a):



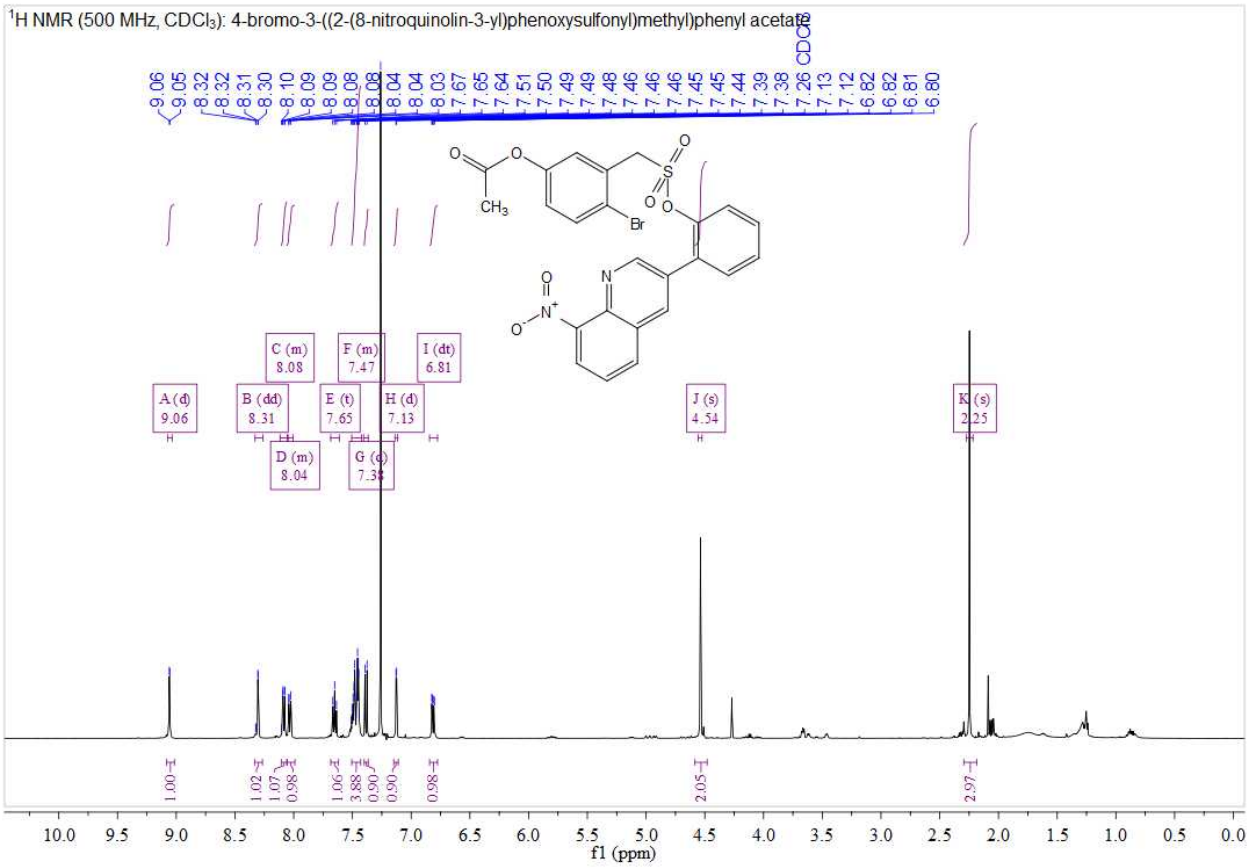


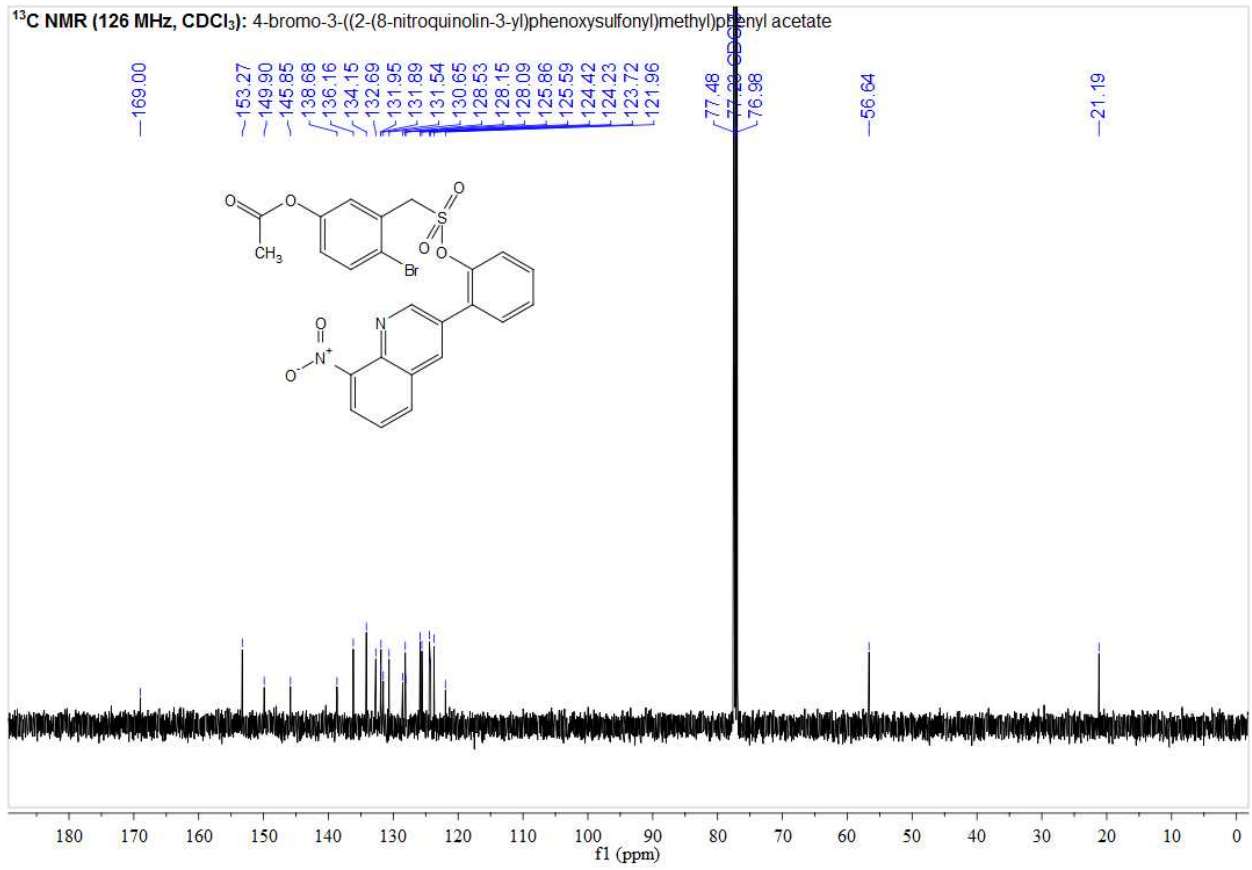
4-chloro-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9b):



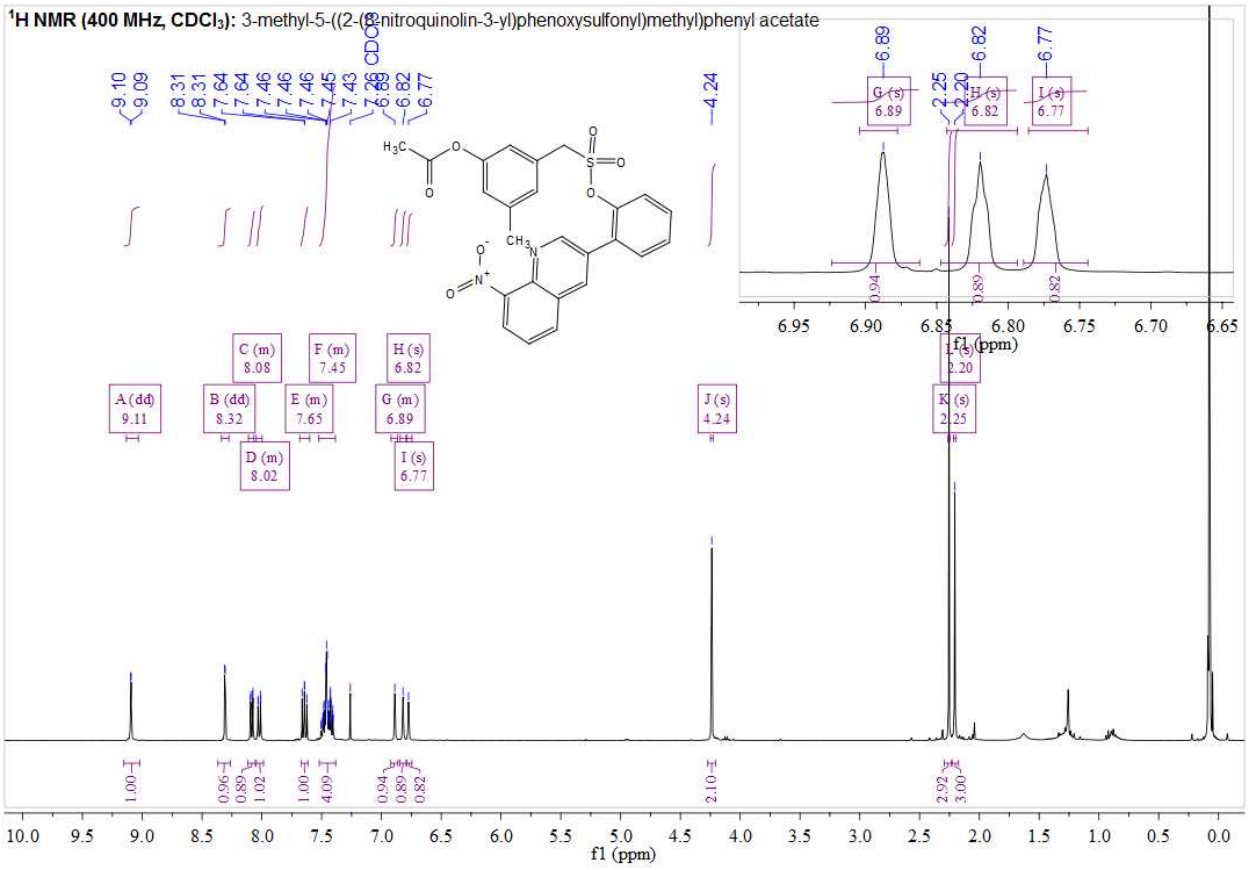


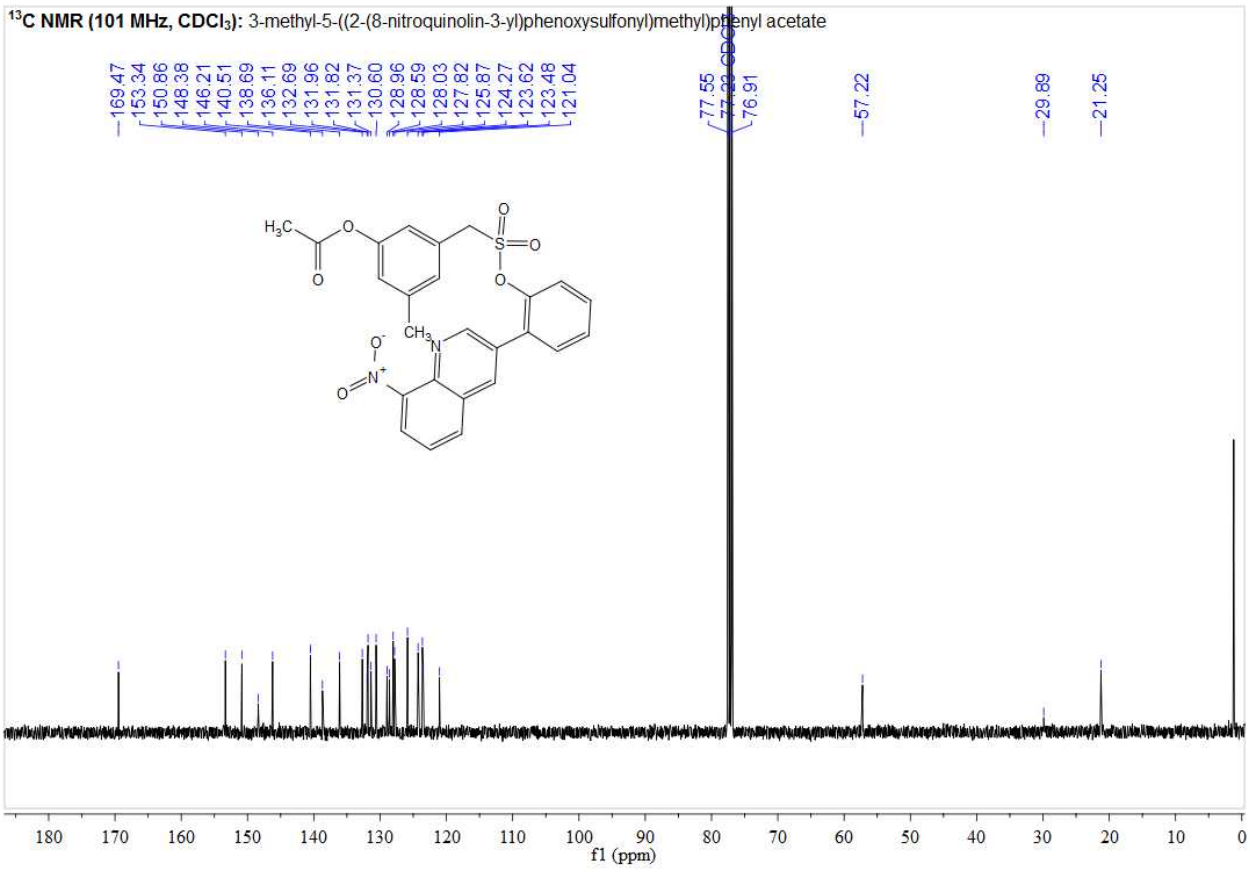
4-bromo-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9c):



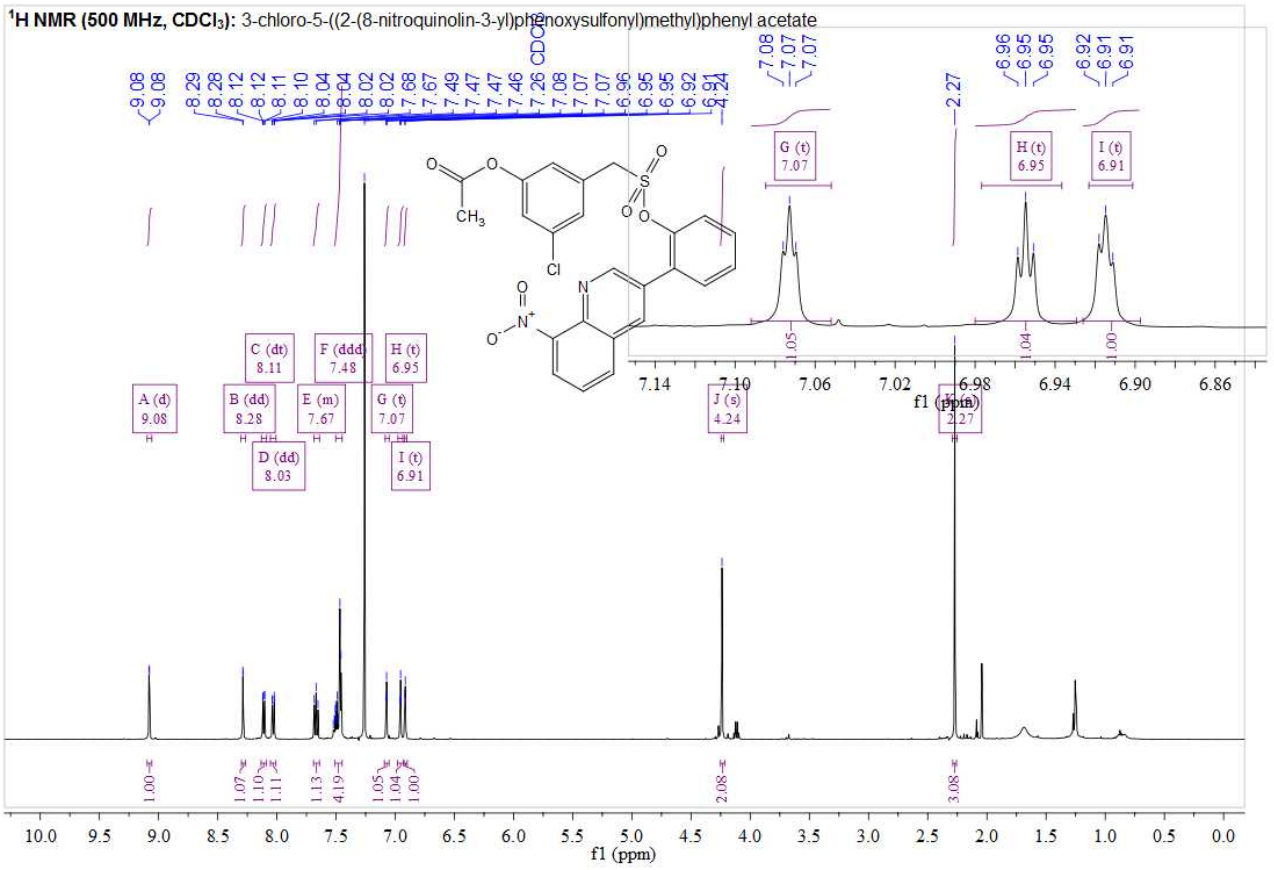


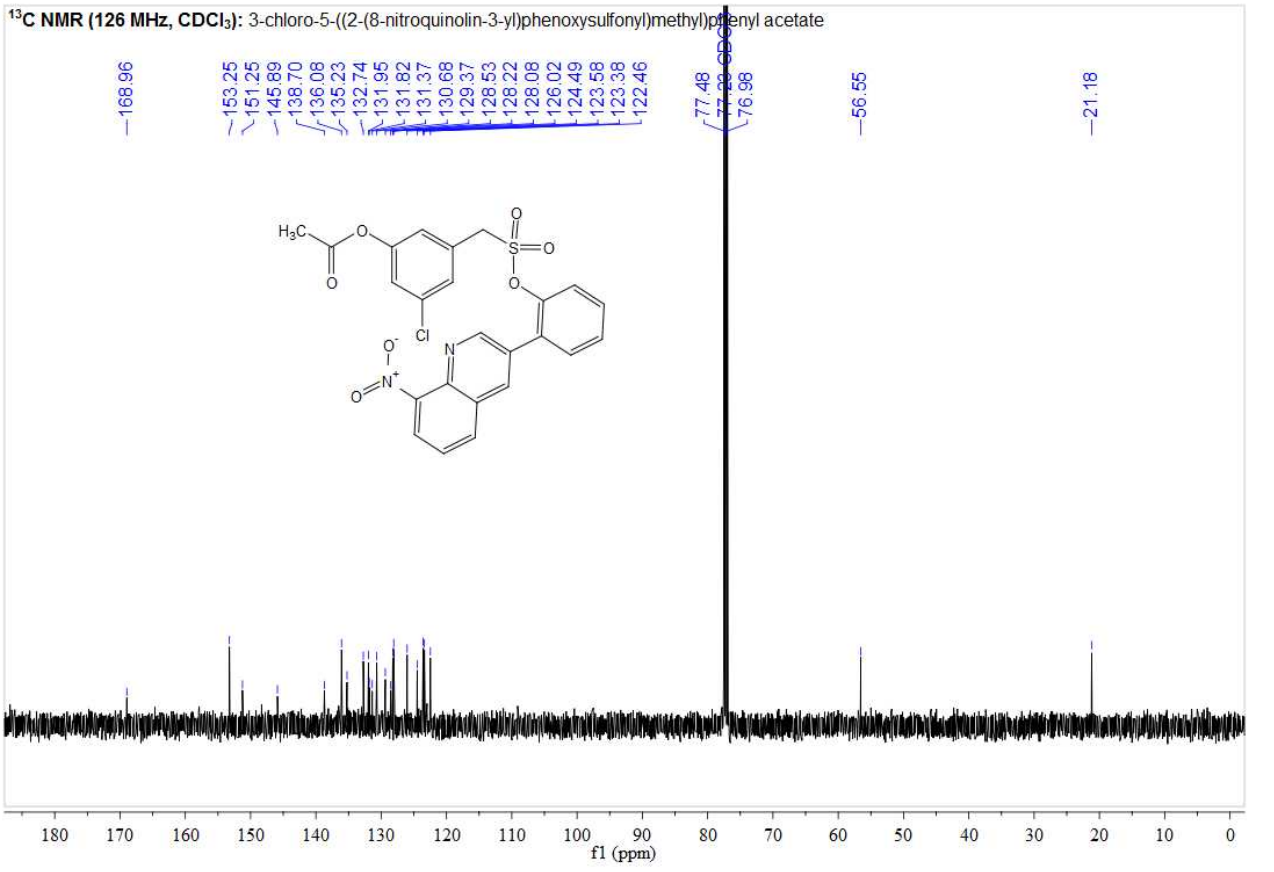
3-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9d):



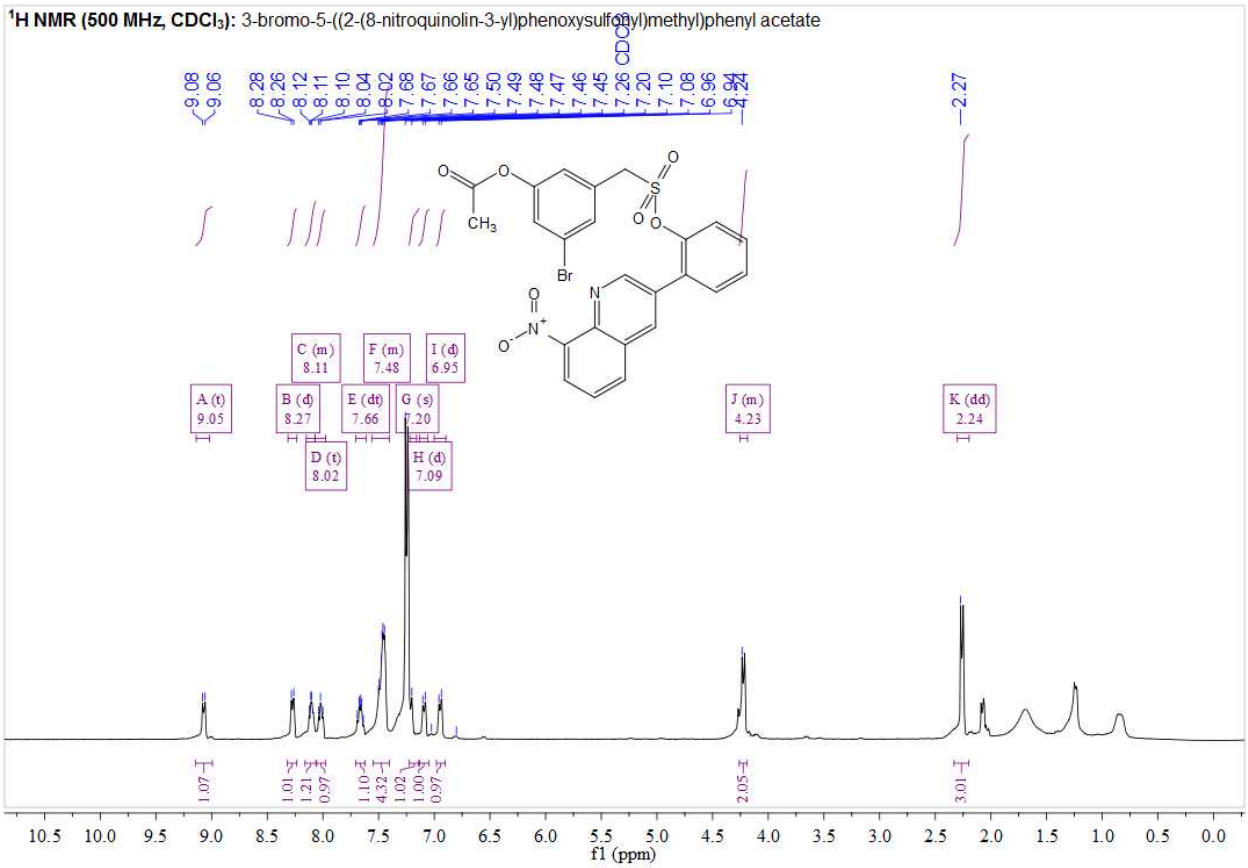


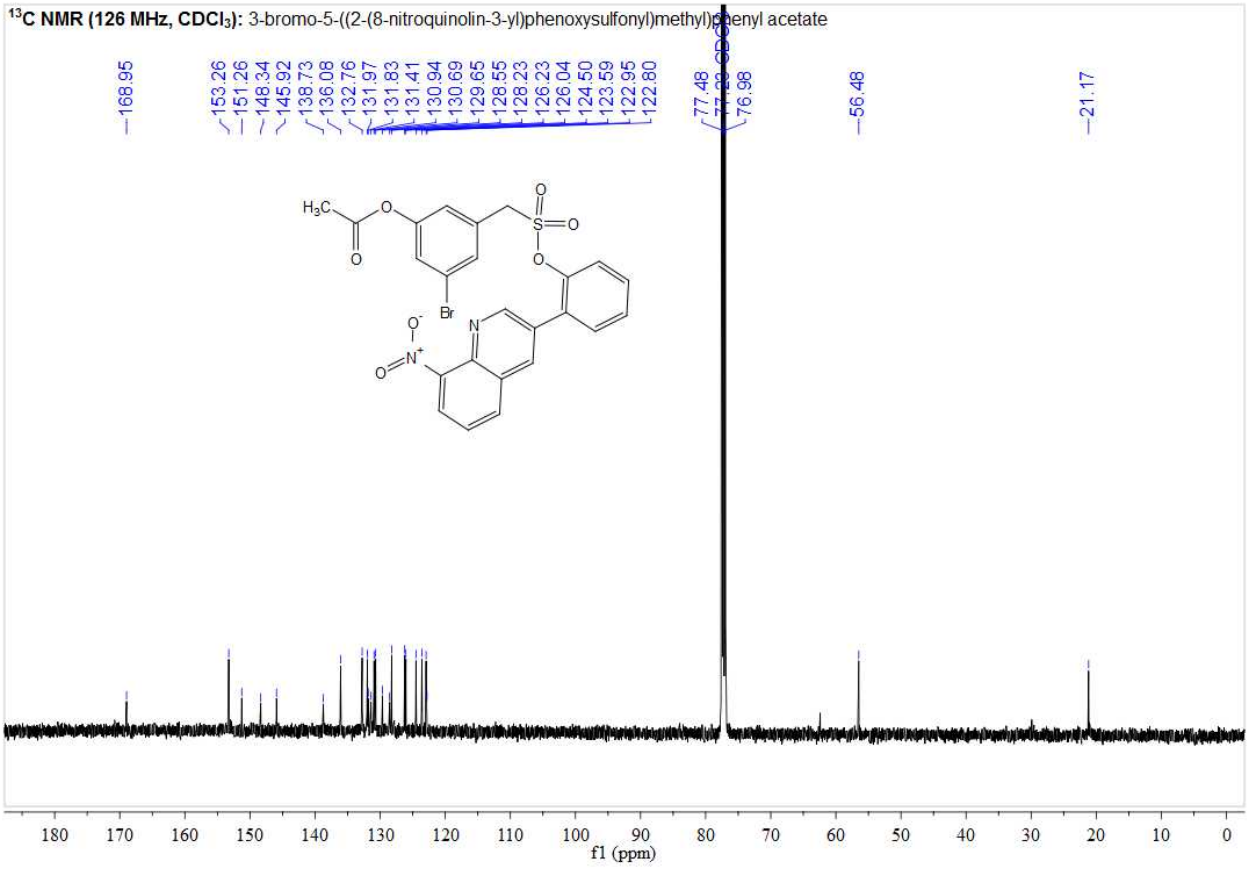
3-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9e):



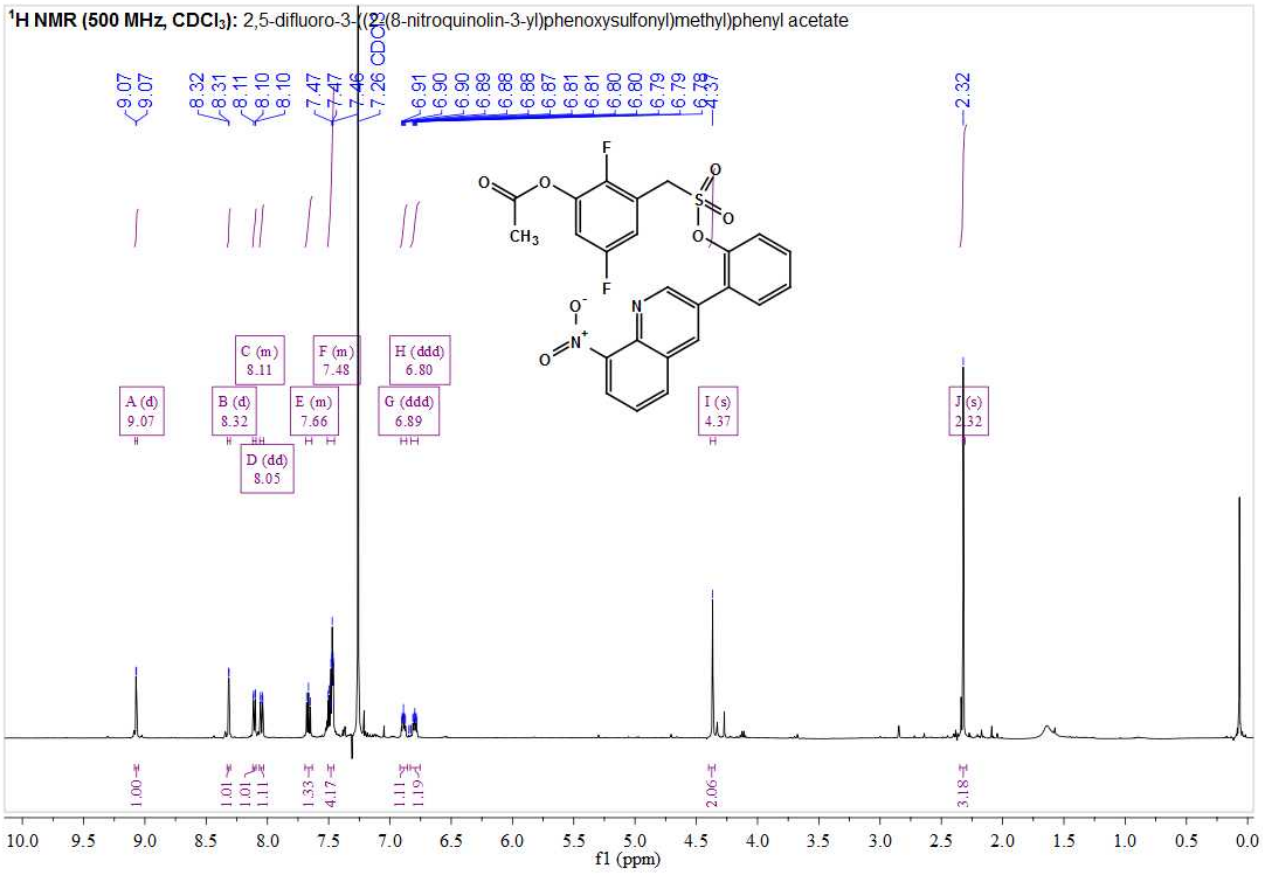


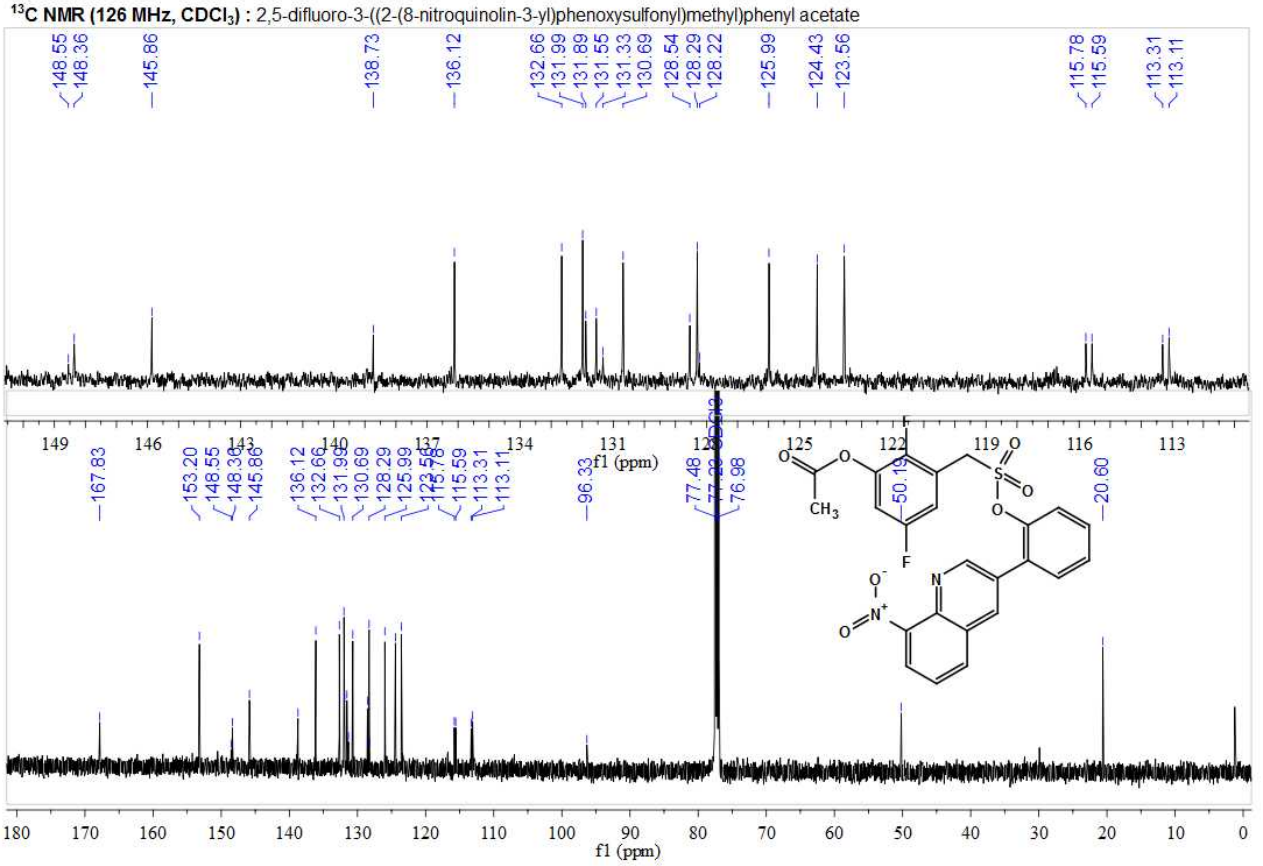
3-bromo-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9f):



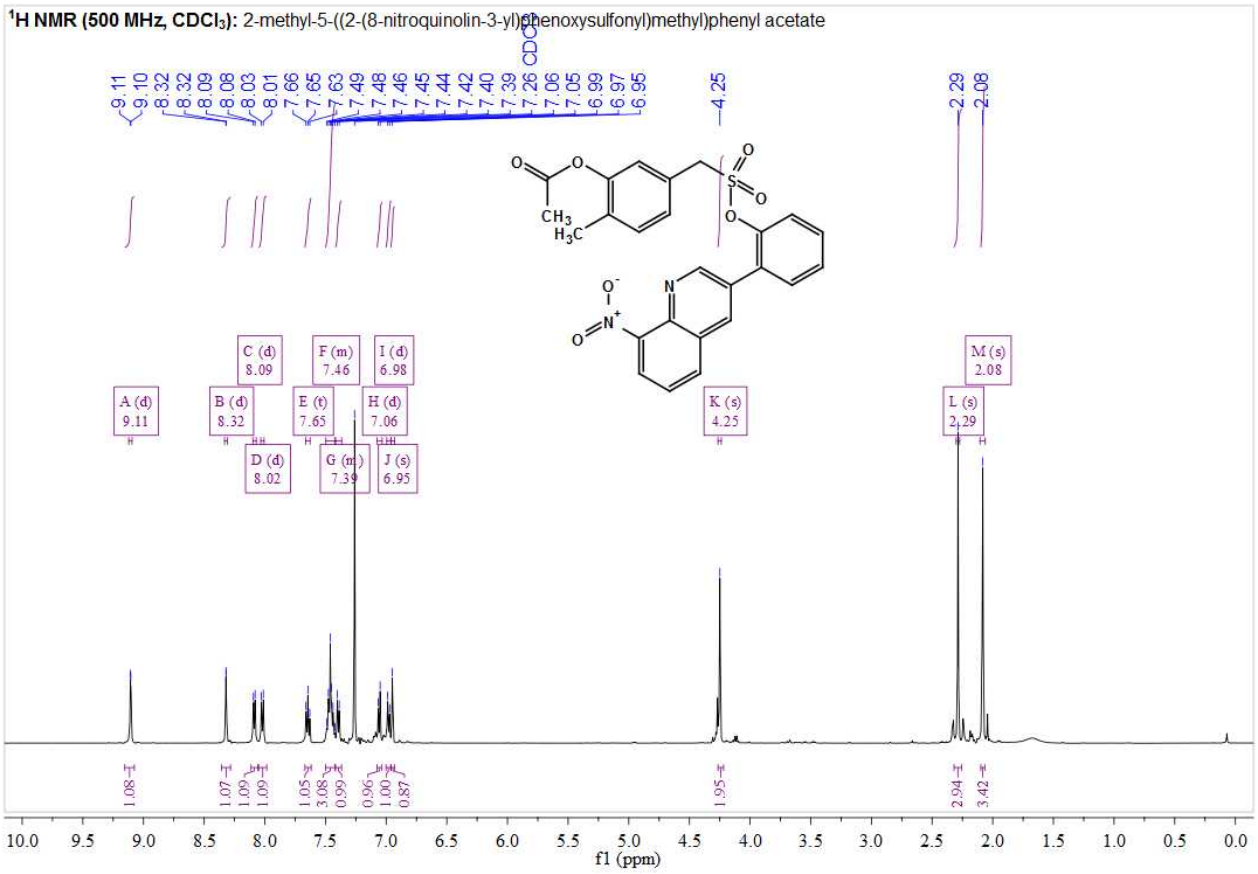


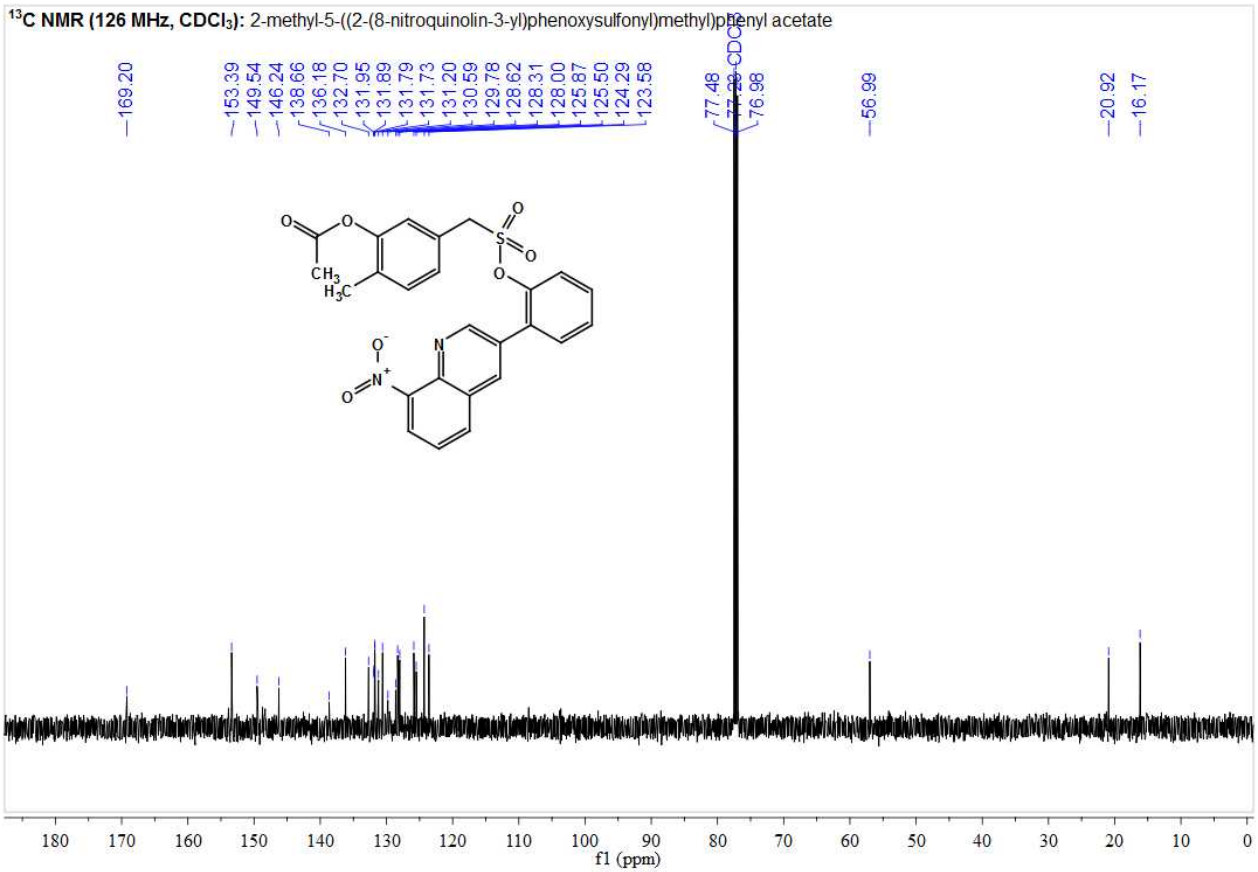
2,5-difluoro-3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9g):



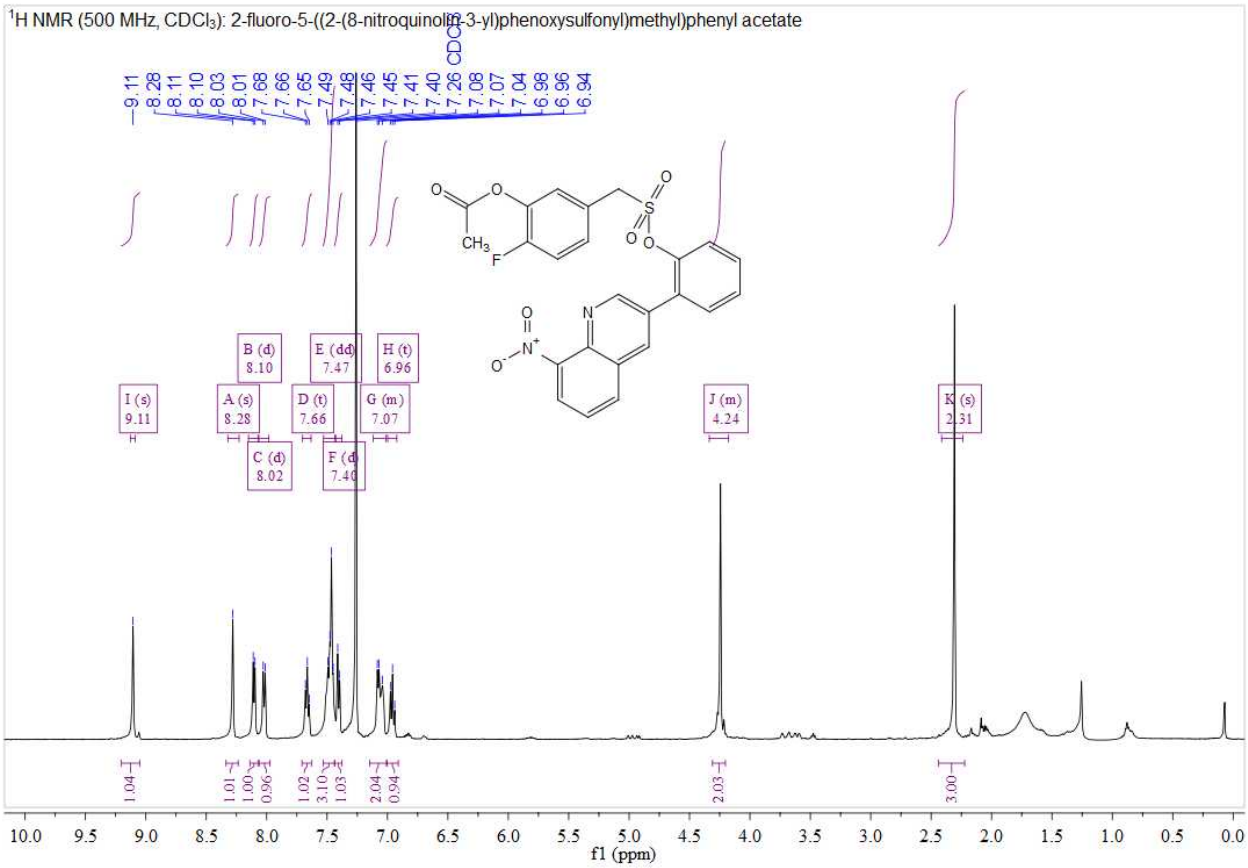


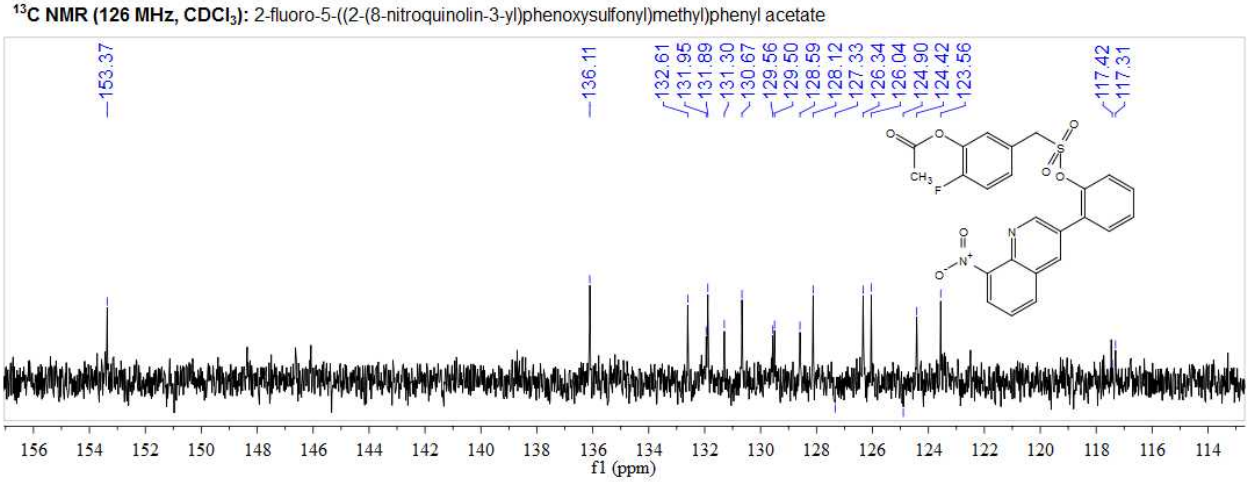
2-methyl-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9h):

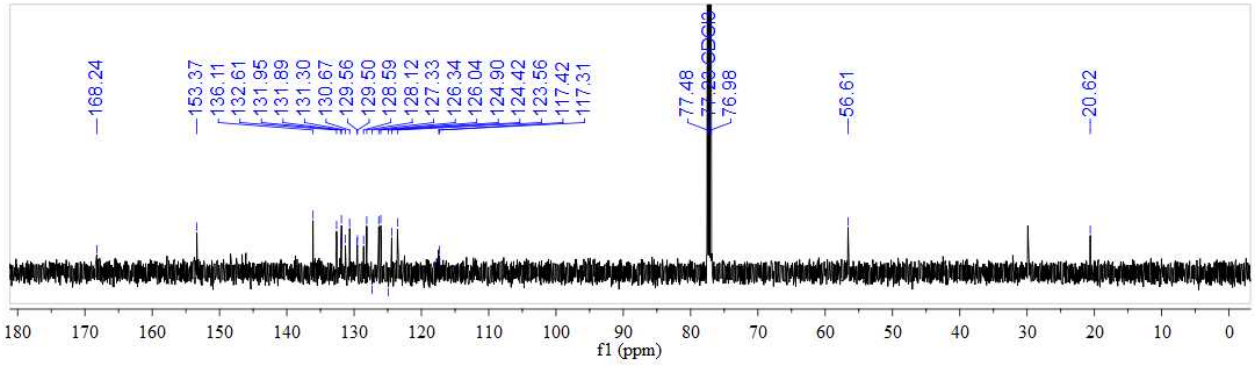




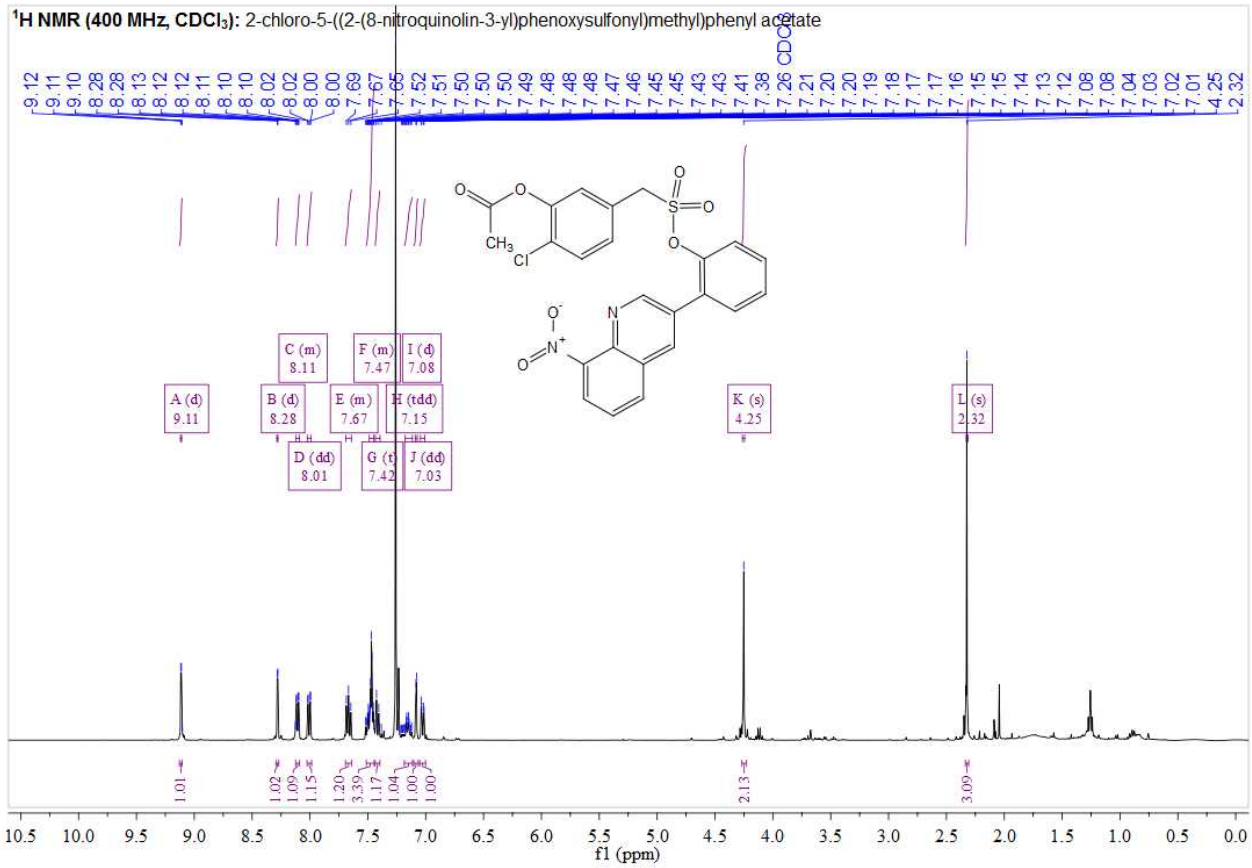
2-fluoro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9i):

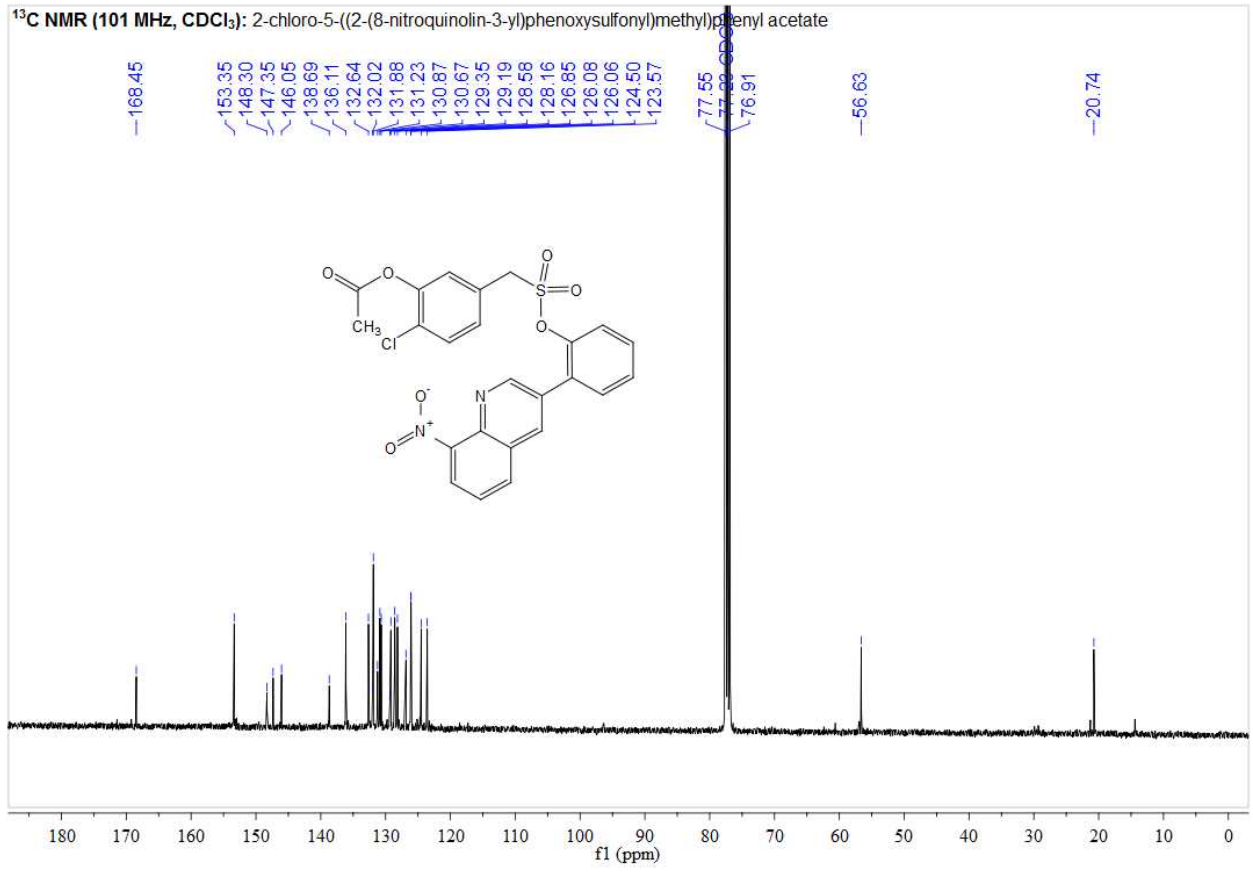




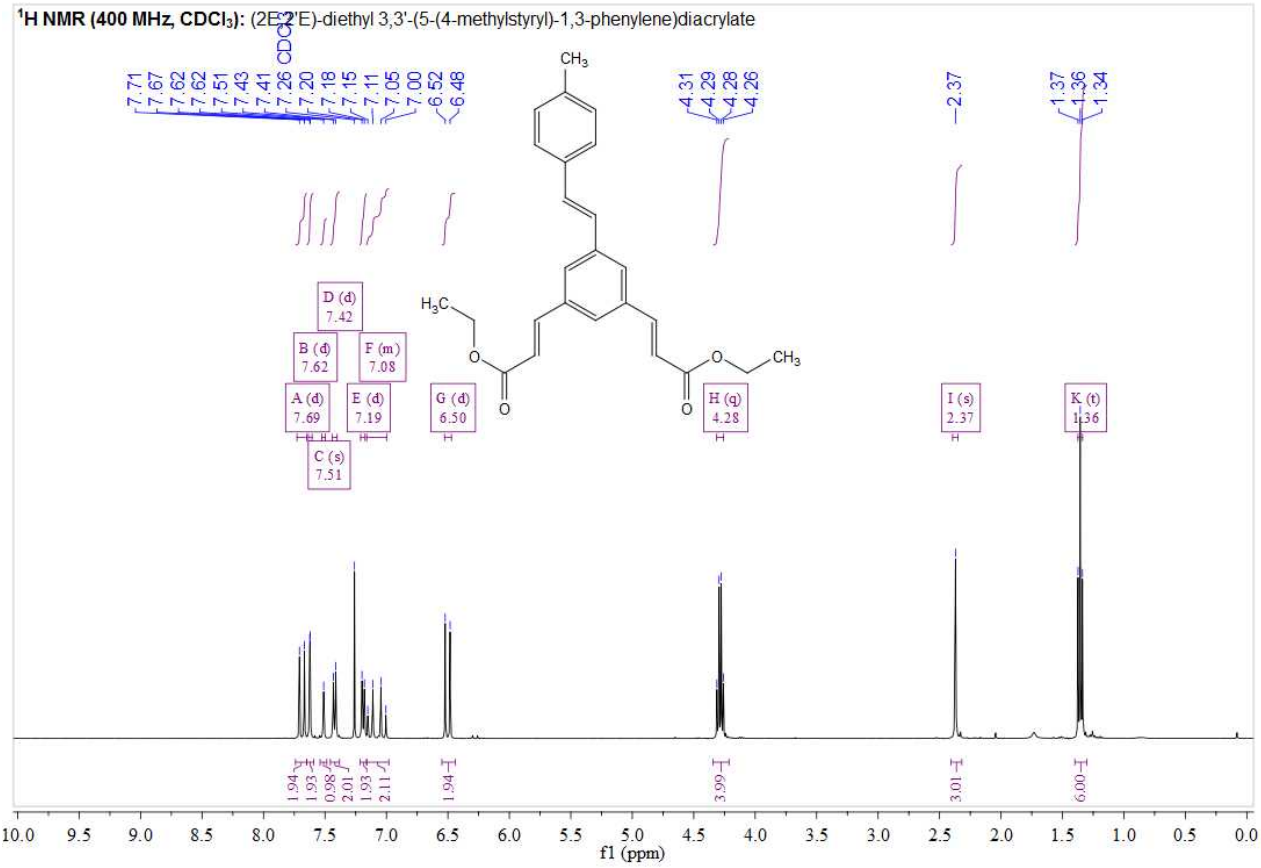


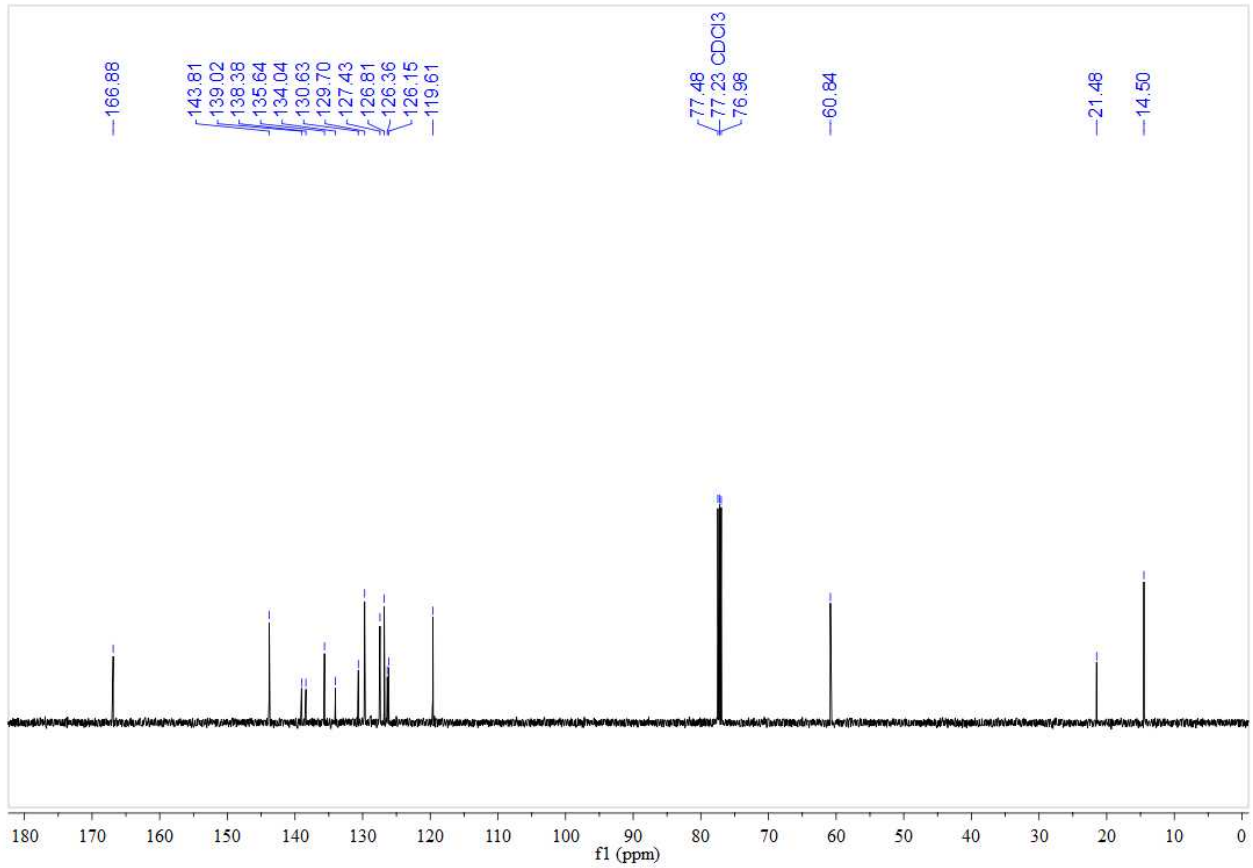
2-chloro-5-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl acetate (9j):



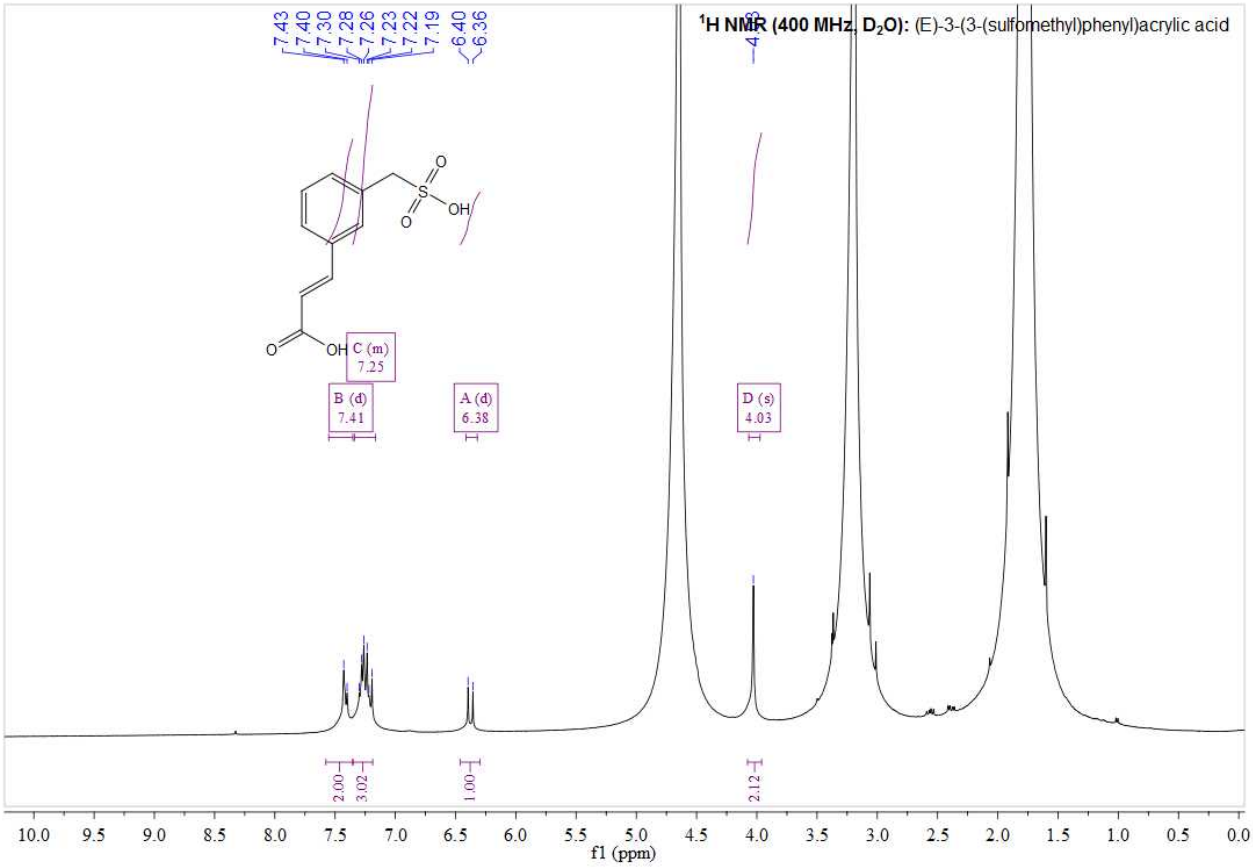


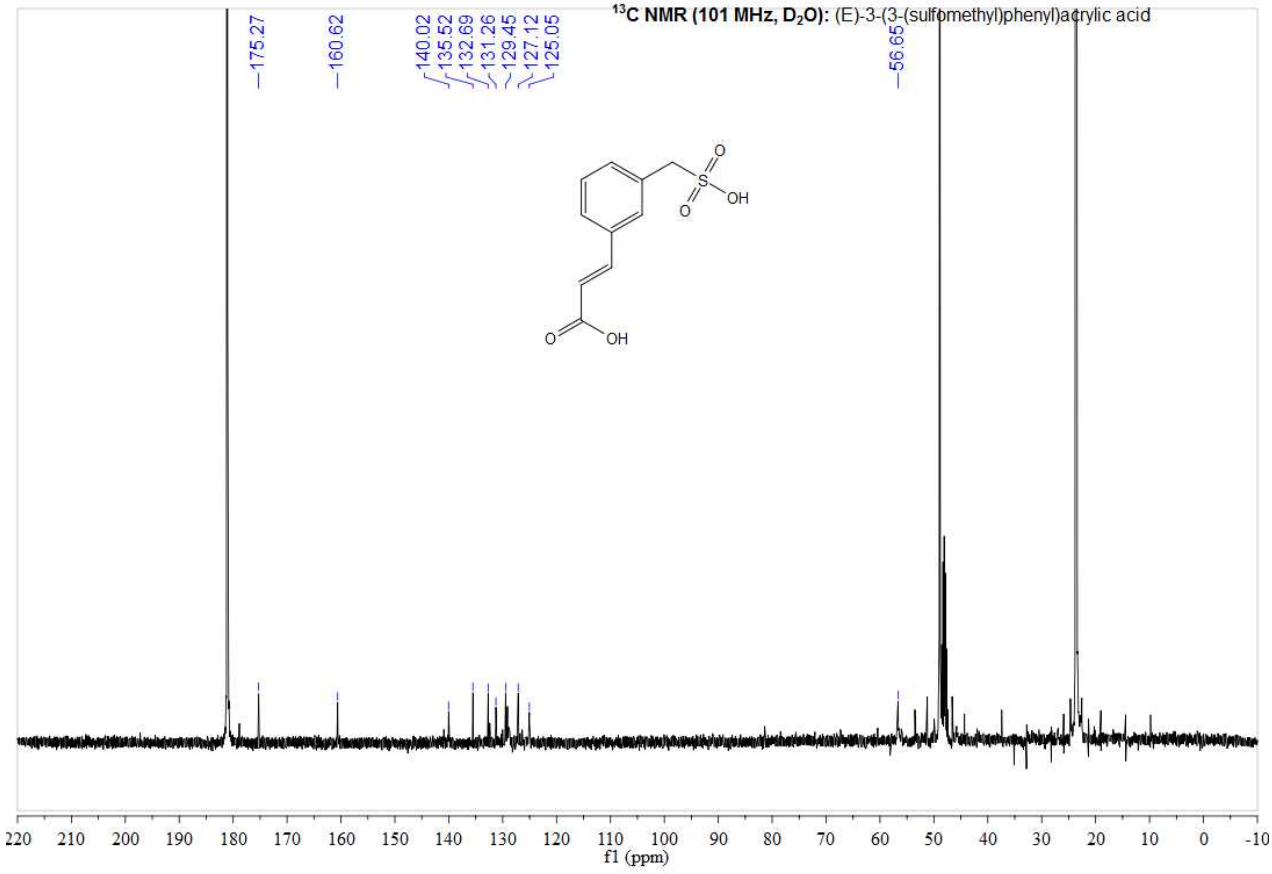
(2*E*,2'*E*)-diethyl 3,3'-(5-(4-methylstyryl)-1,3-phenylene)diacrylate (10):



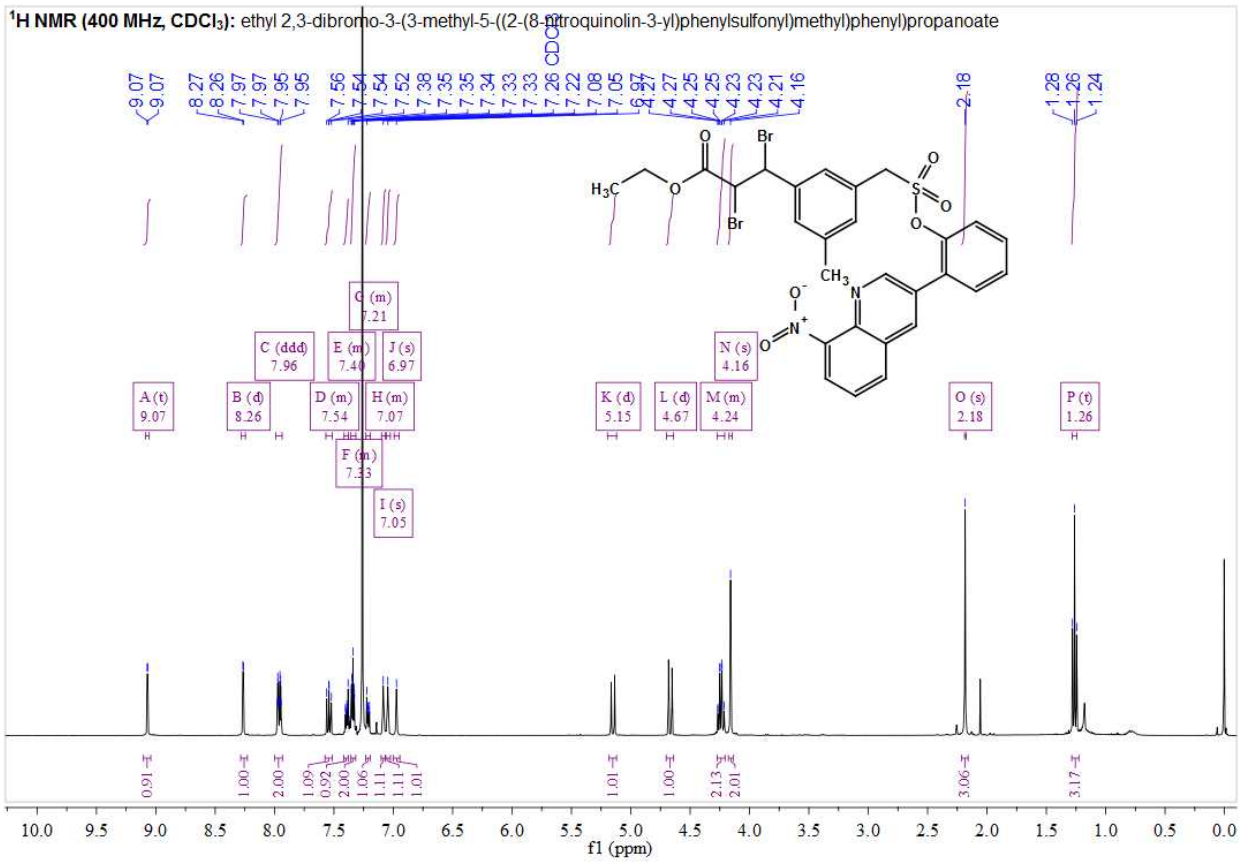


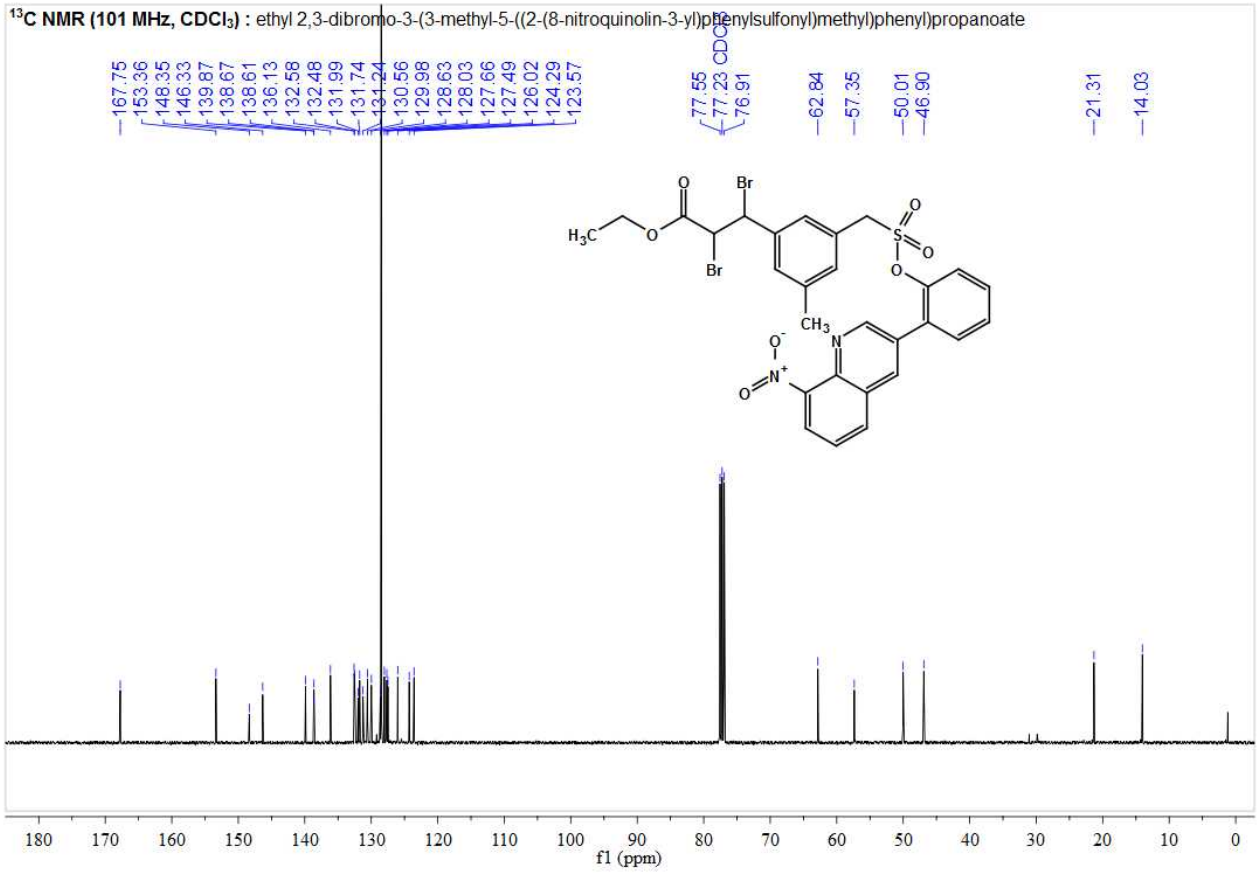
(*E*)-3-(3-(sulfomethyl)phenyl)acrylic acid (12):



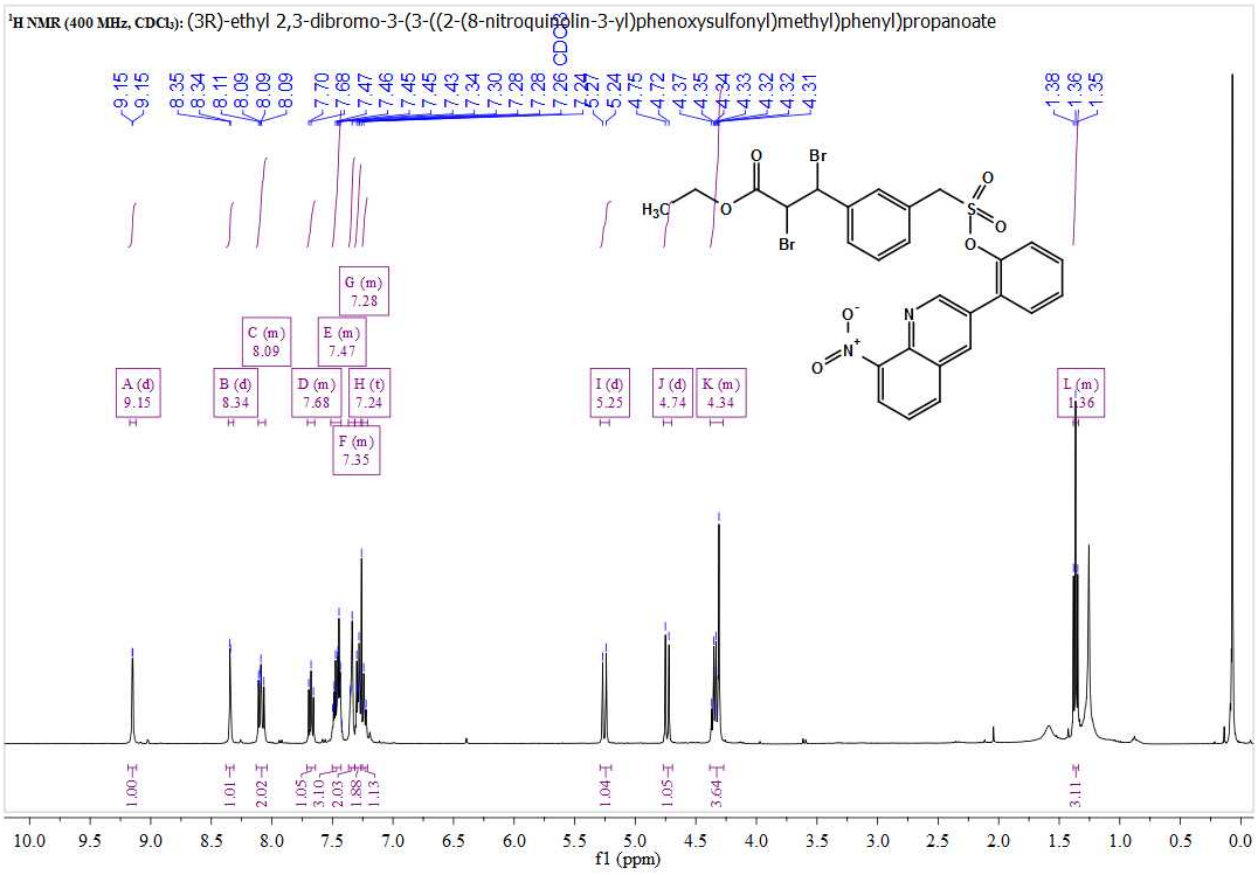


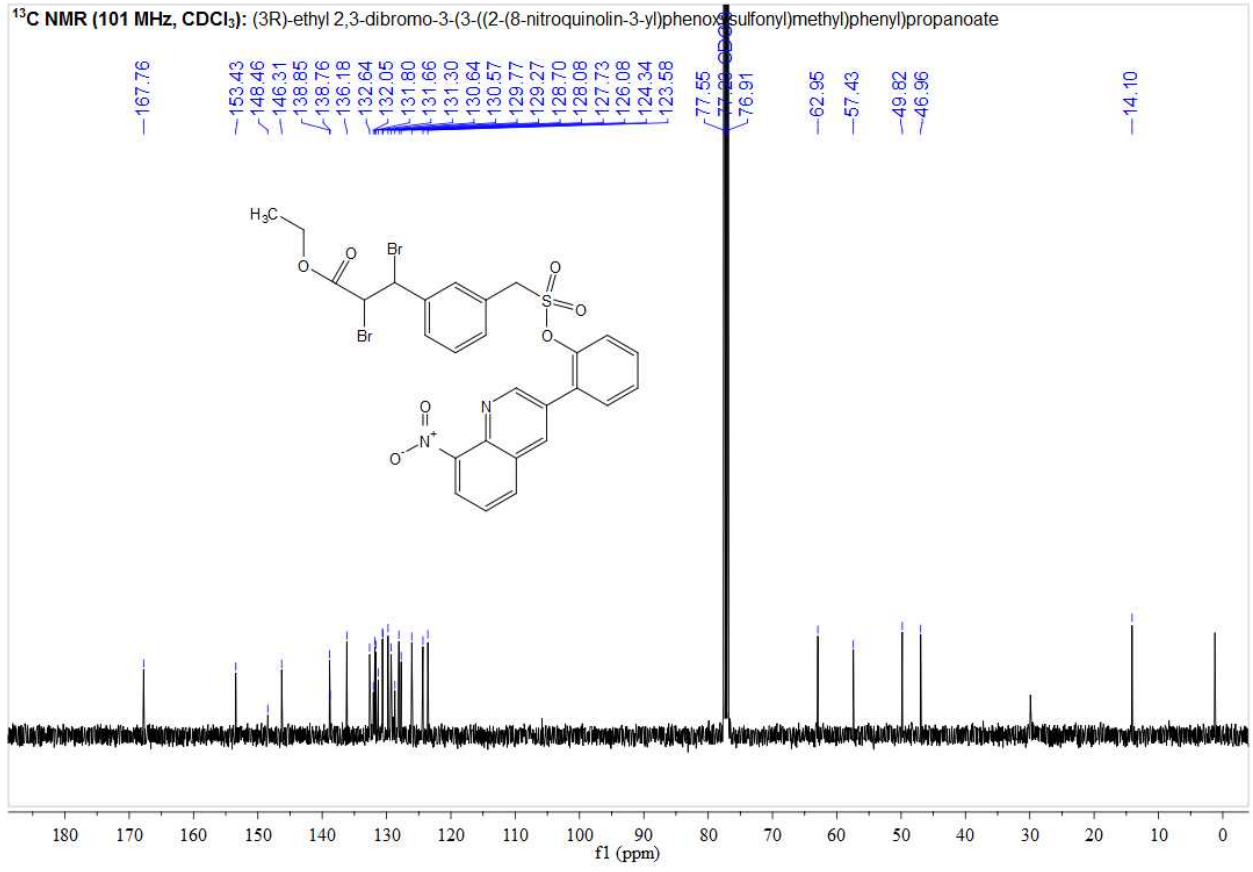
Ethyl 2,3-dibromo-3-(3-methyl-5-((2-(8-nitroquinolin-3-yl)phenylsulfonyl)methyl)phenyl)propane-ate (13):



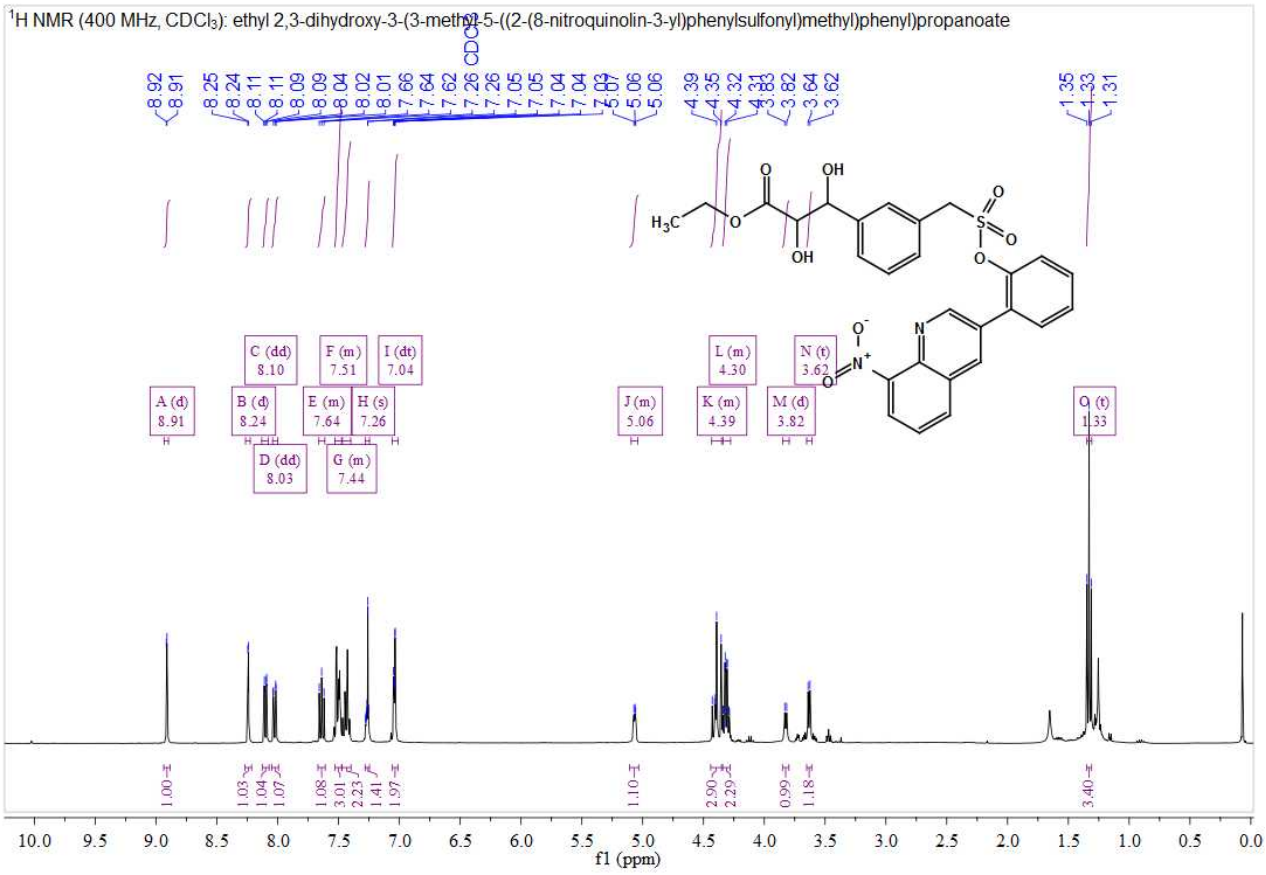


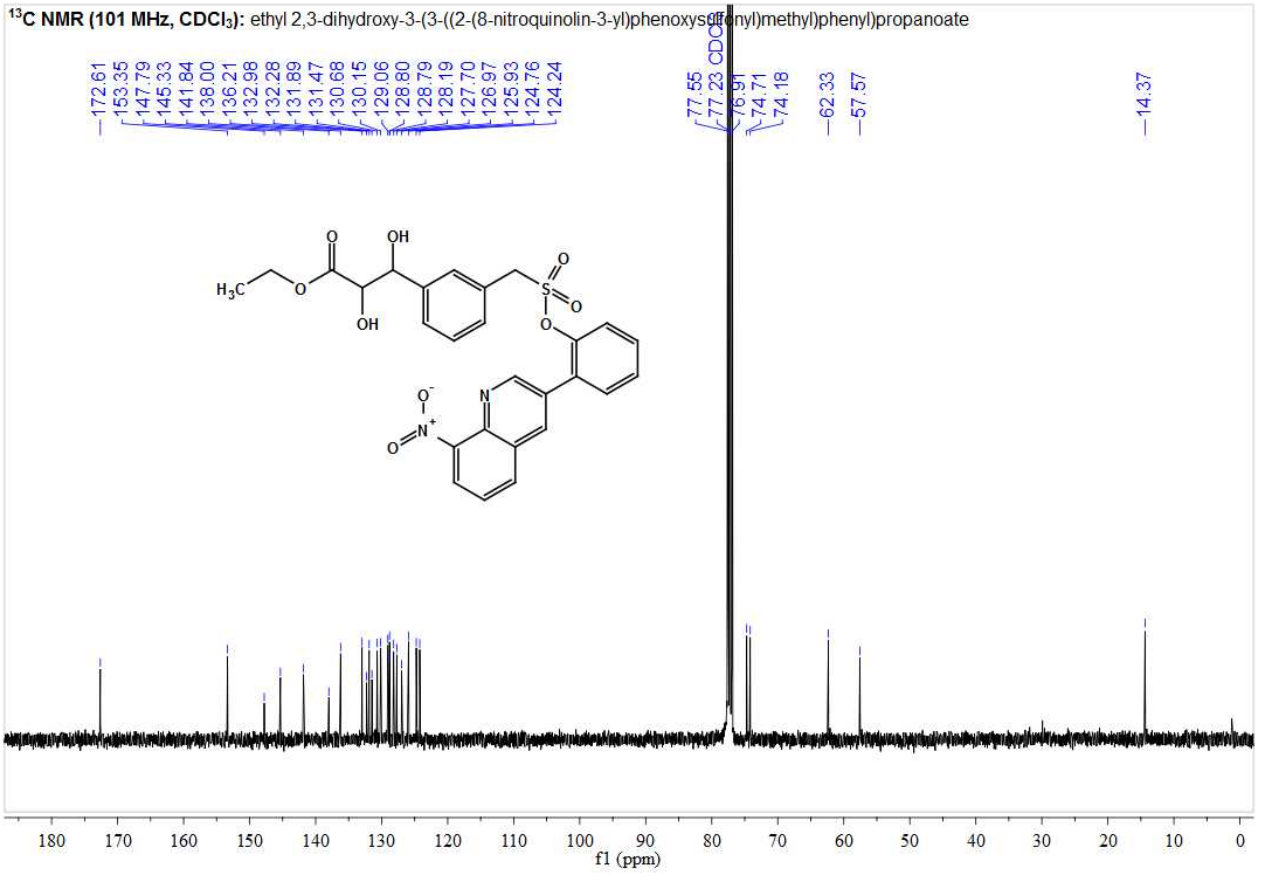
Ethyl2,3-dibromo-3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)propanoate (14):



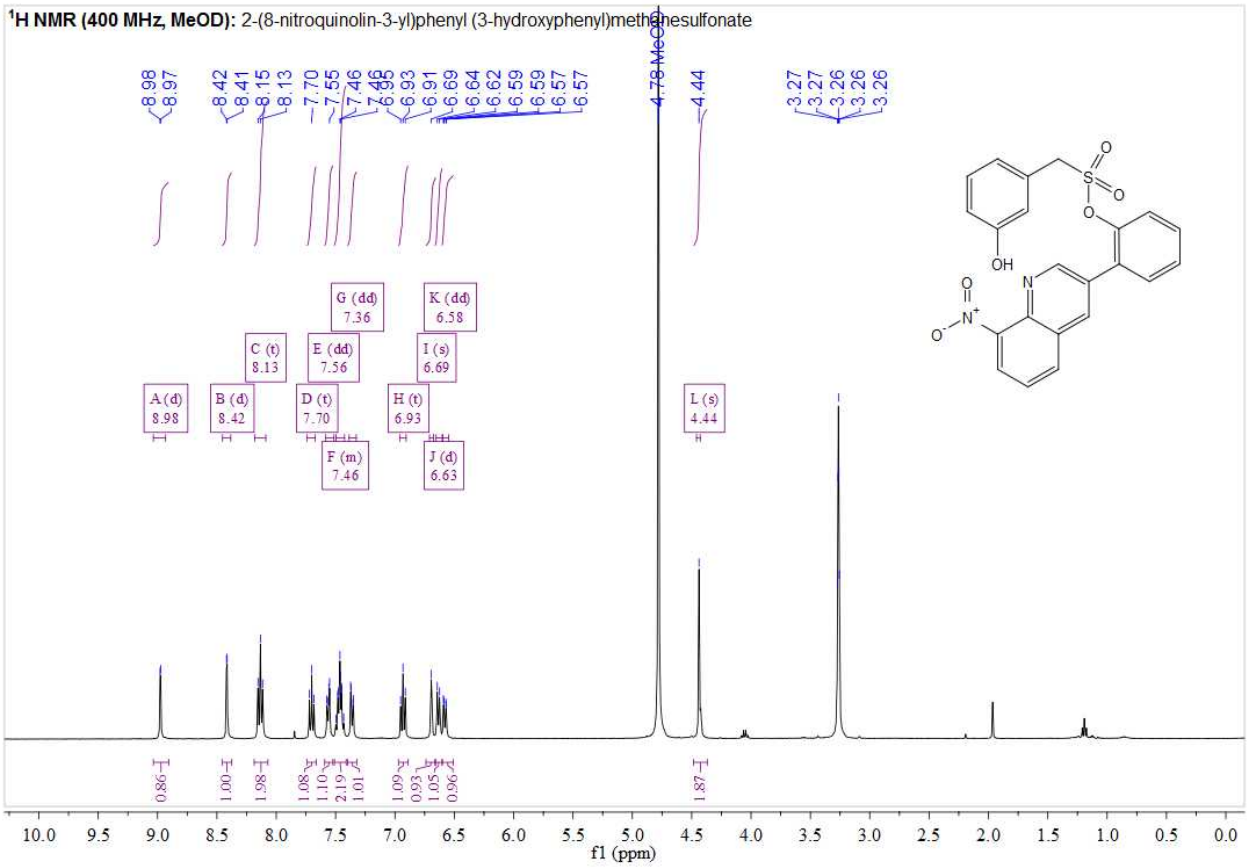


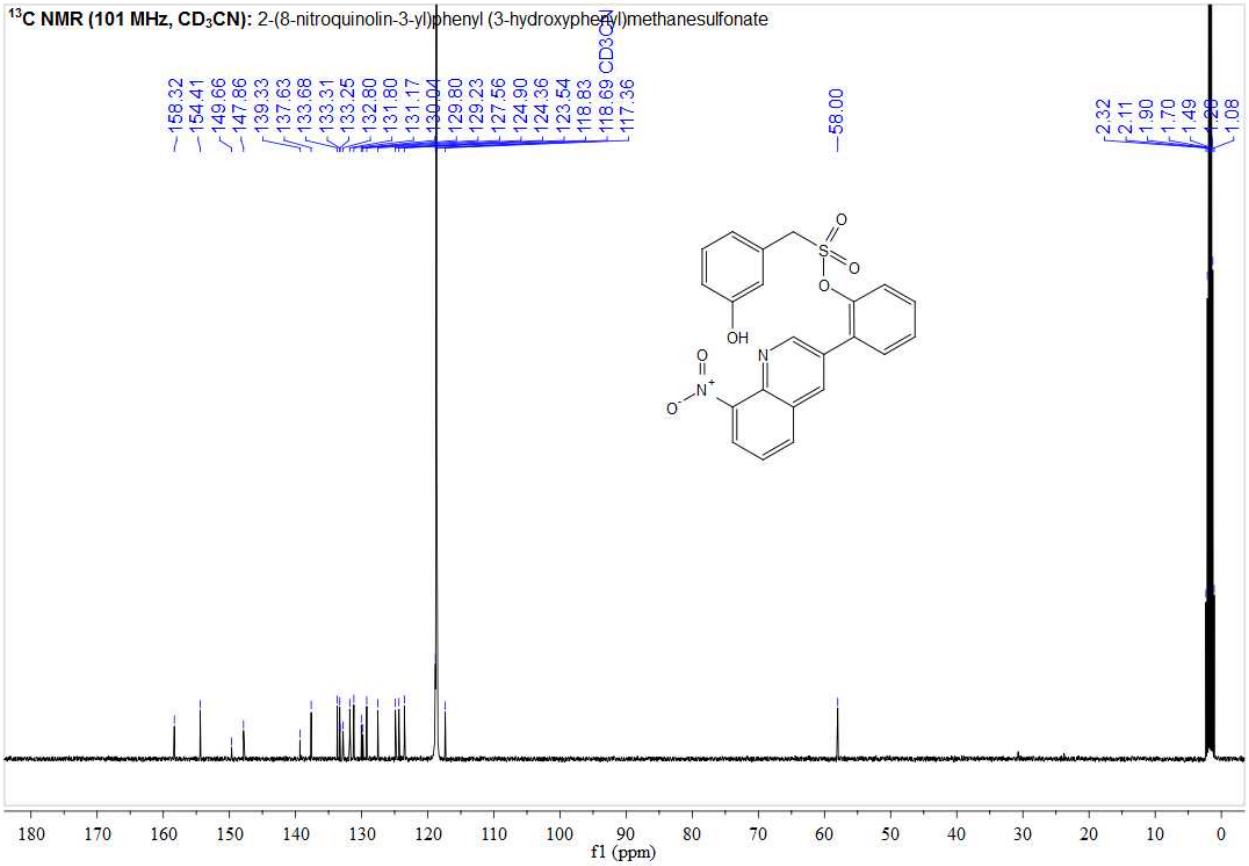
Ethyl 2,3-dihydroxy-3-(3-((2-(8-nitroquinolin-3-yl)phenoxysulfonyl)methyl)phenyl)propaneate (15):



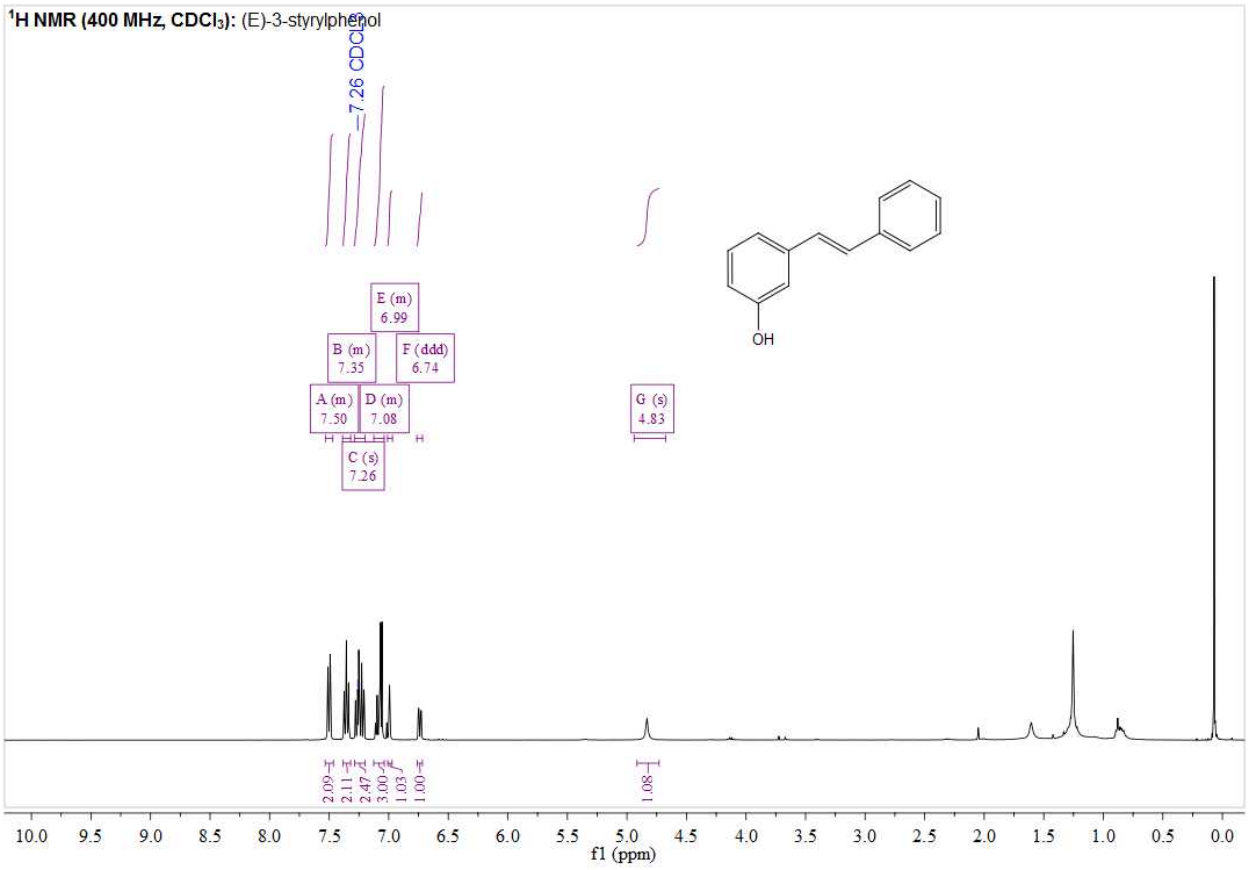


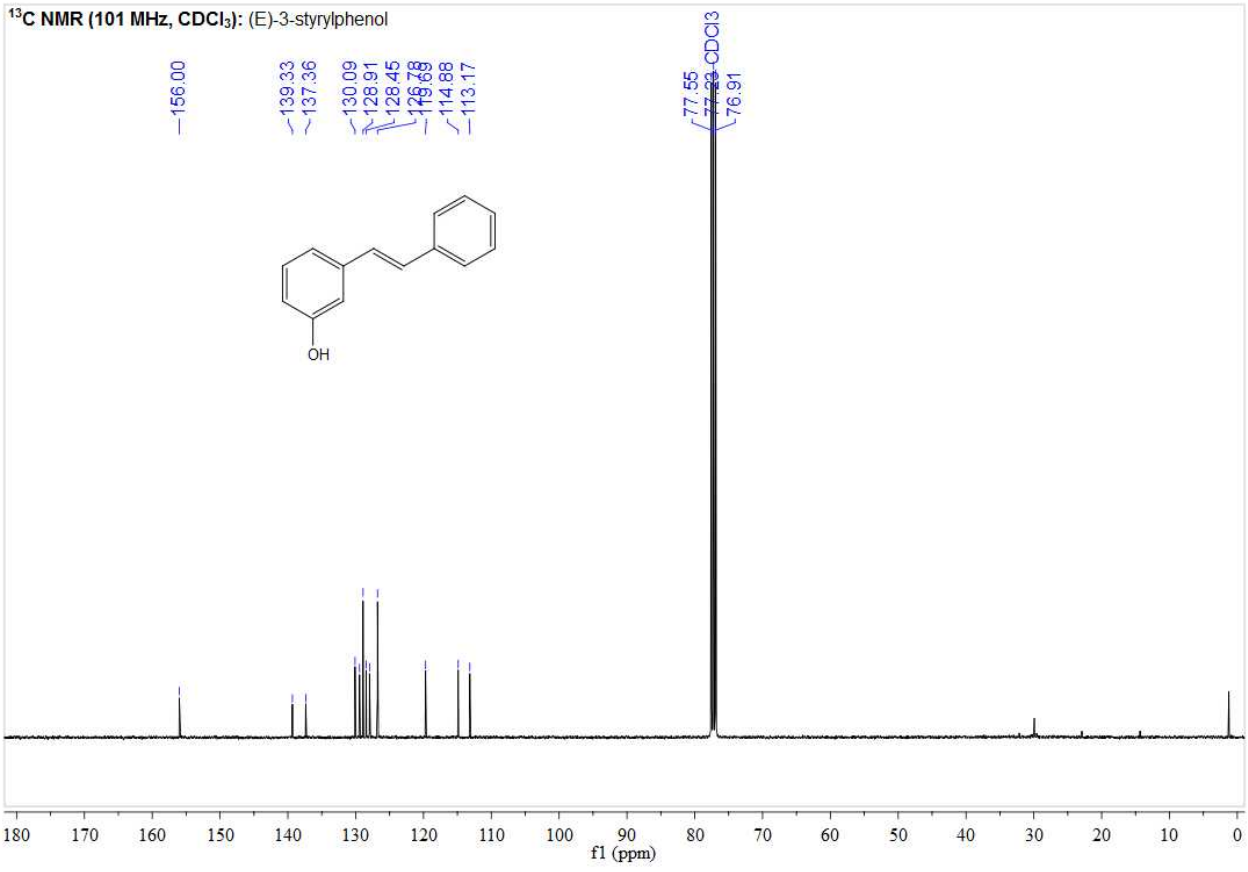
2-(8-nitroquinolin-3-yl)phenyl (3-hydroxyphenyl)methanesulfonate (9a'):



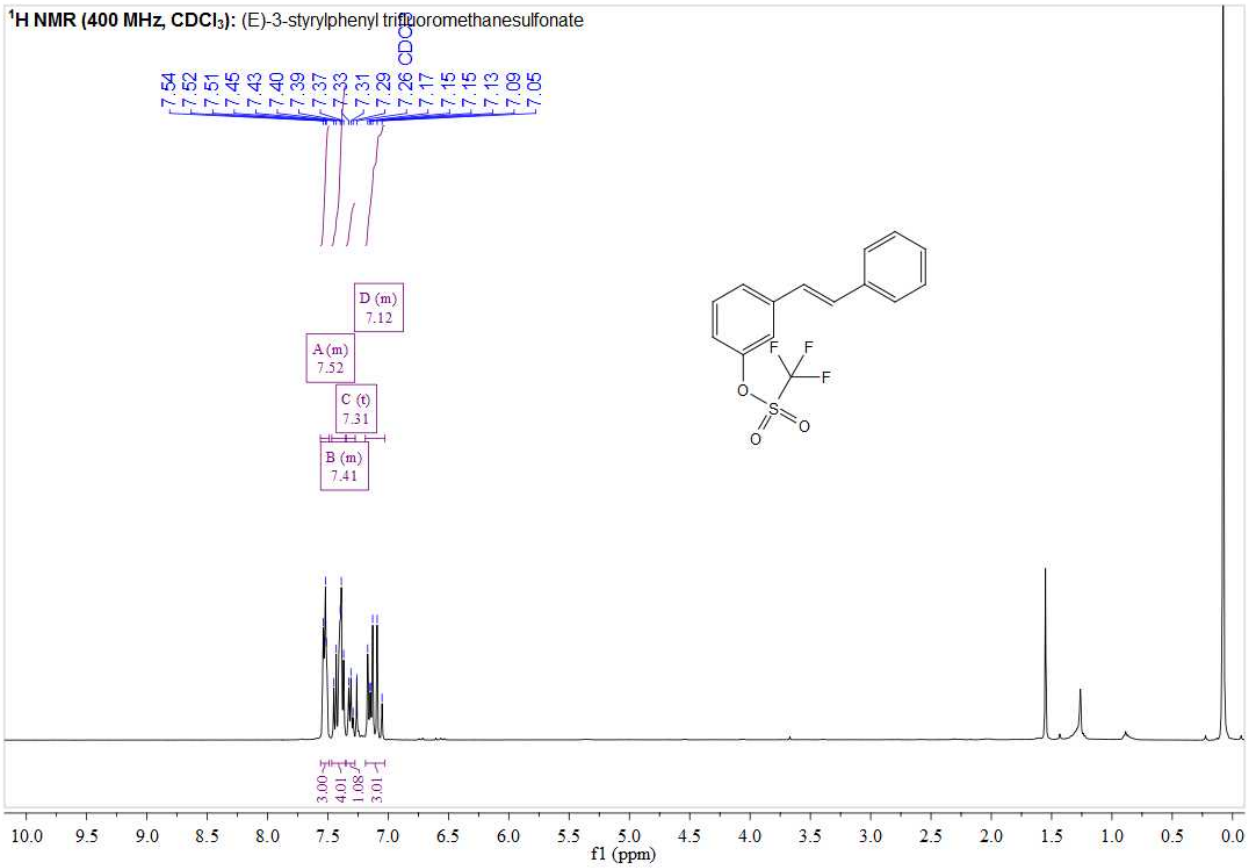


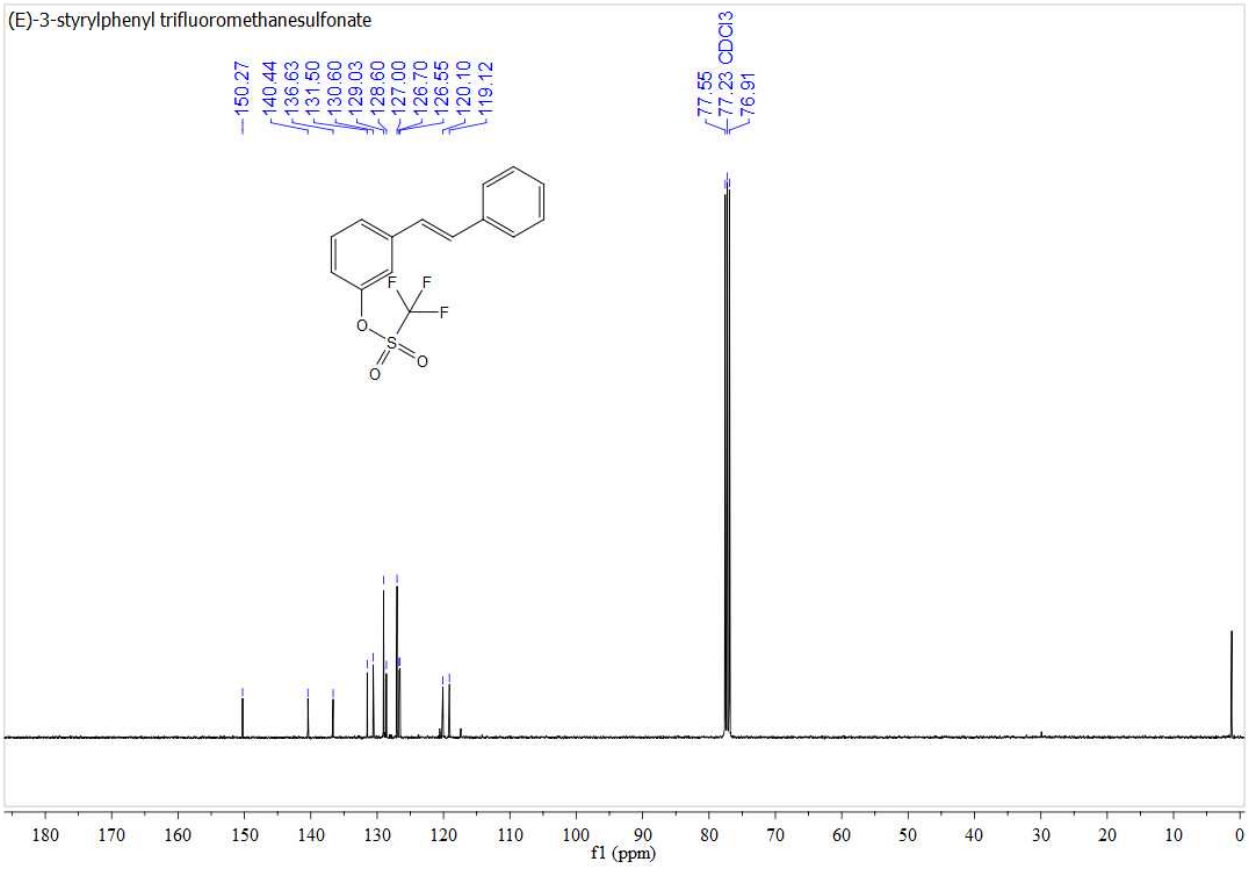
(*E*)-3-styrylphenol (16):



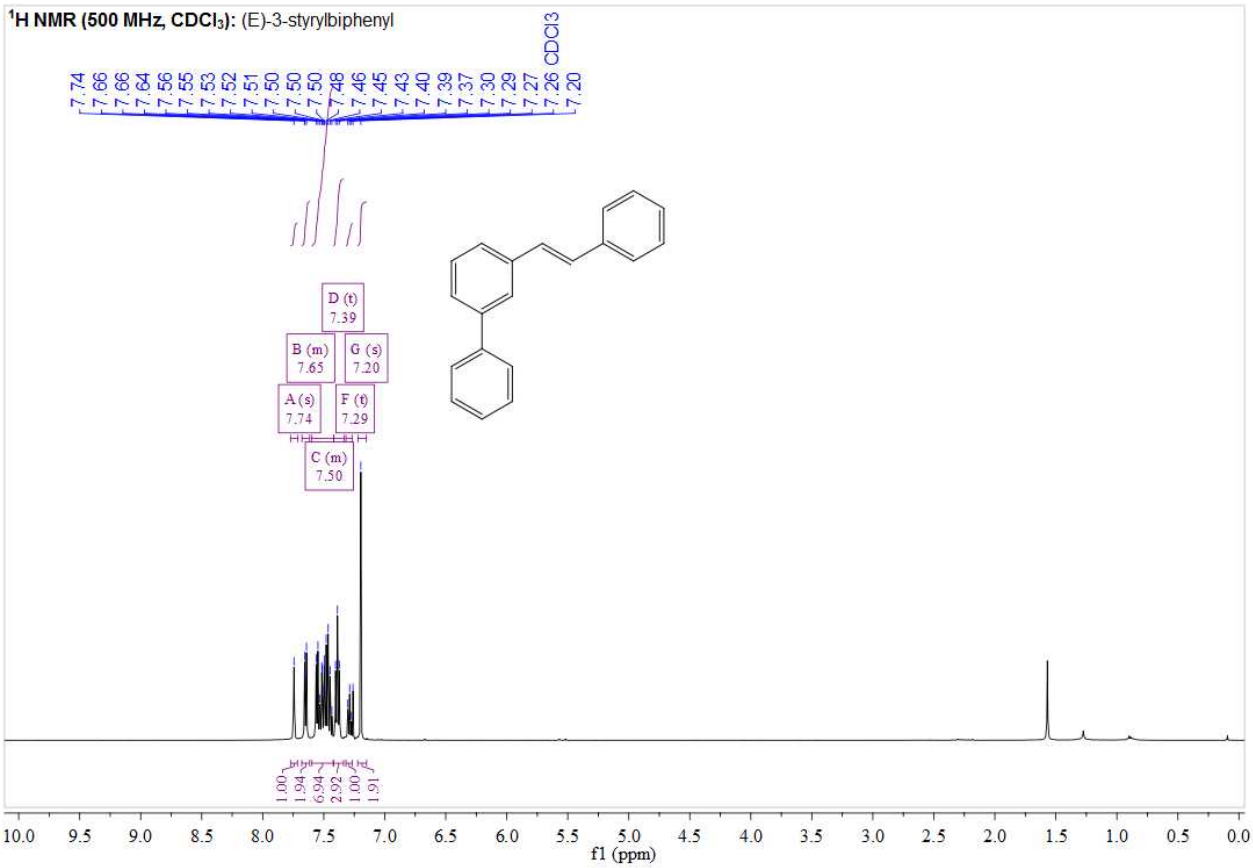


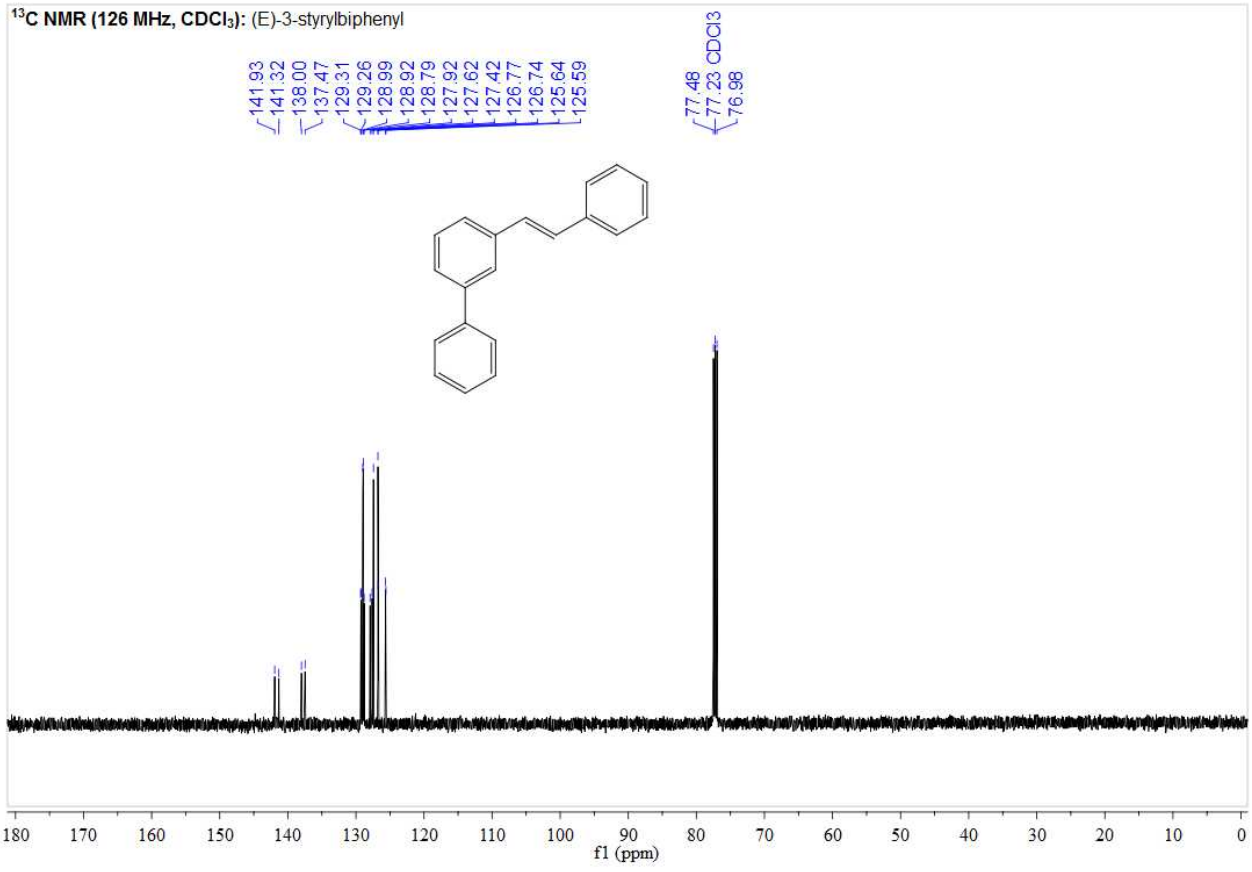
(E)-3-styrylphenyl trifluoromethanesulfonate (17):



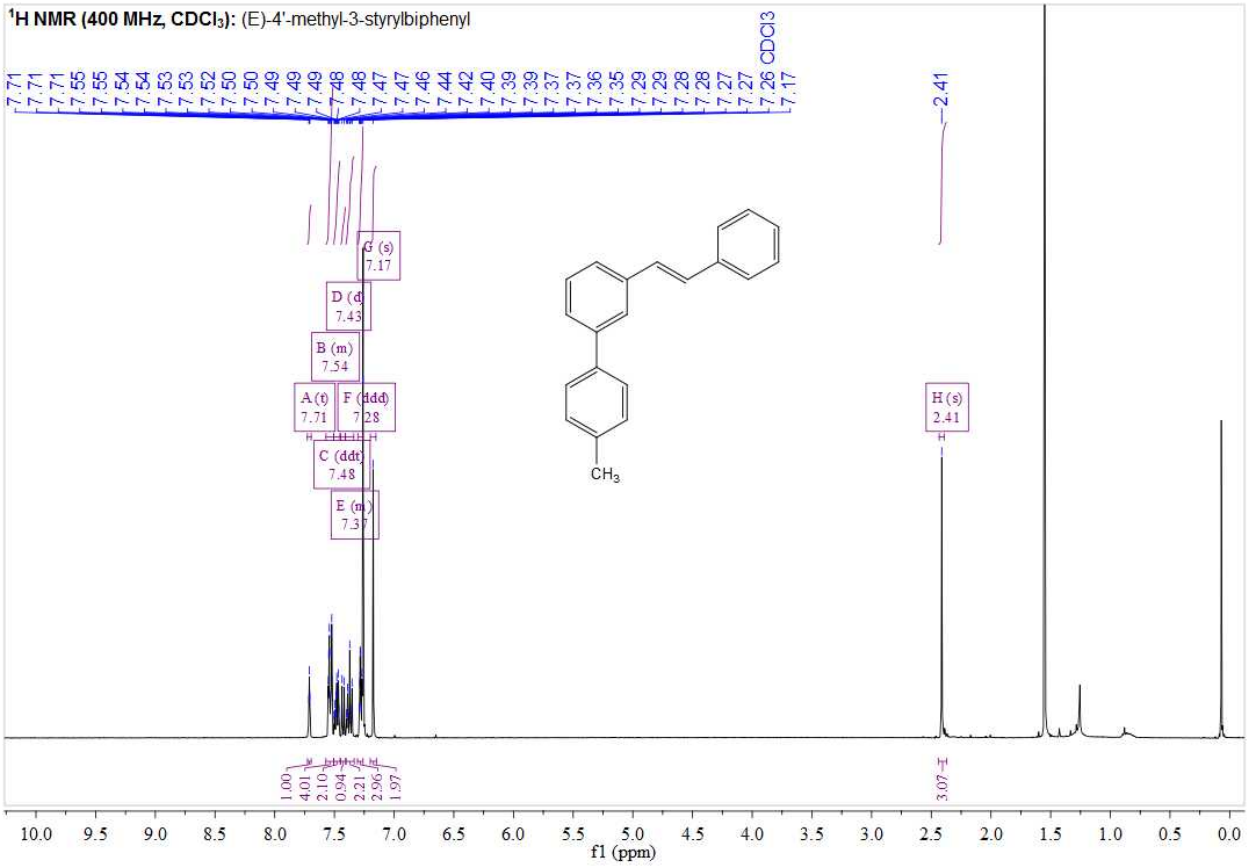


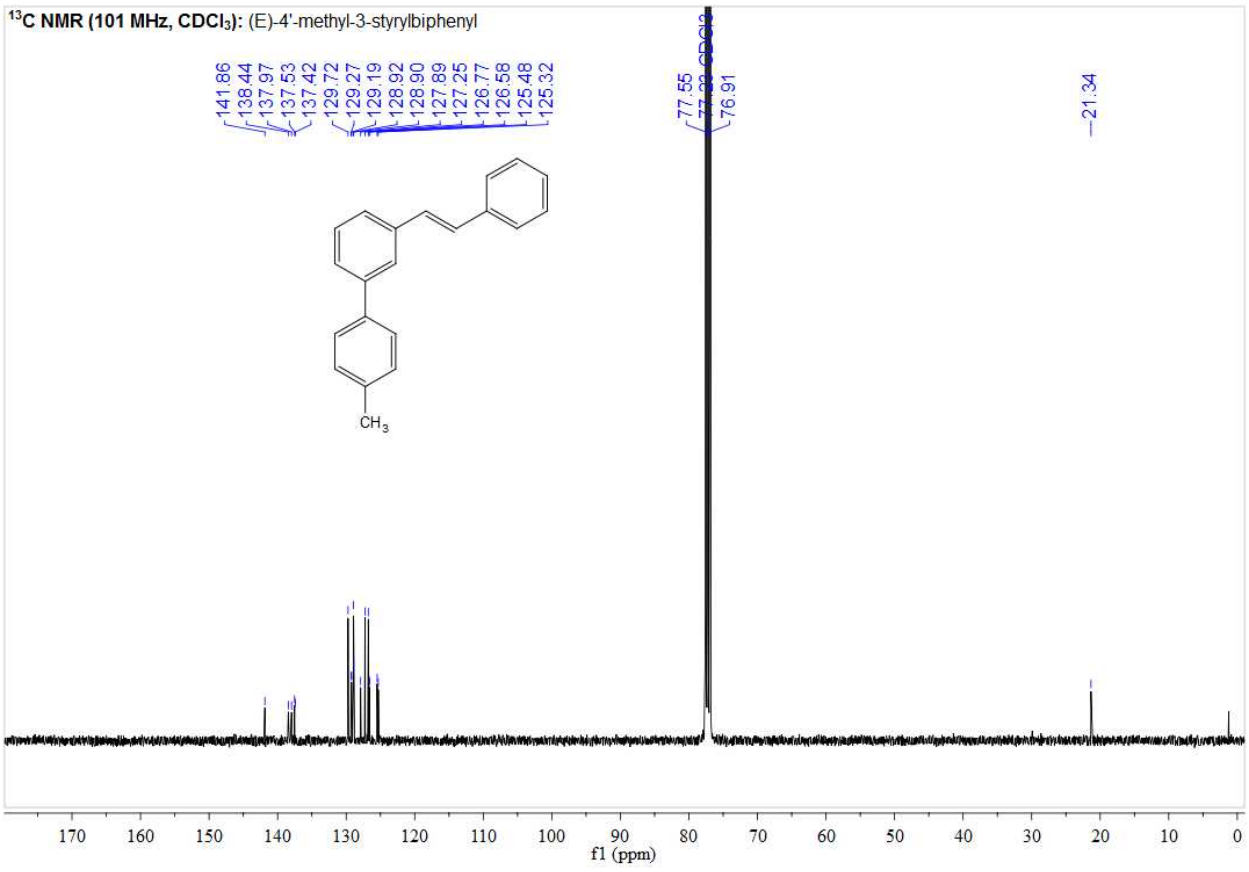
(*E*)-3-styrylbiphenyl (18a):



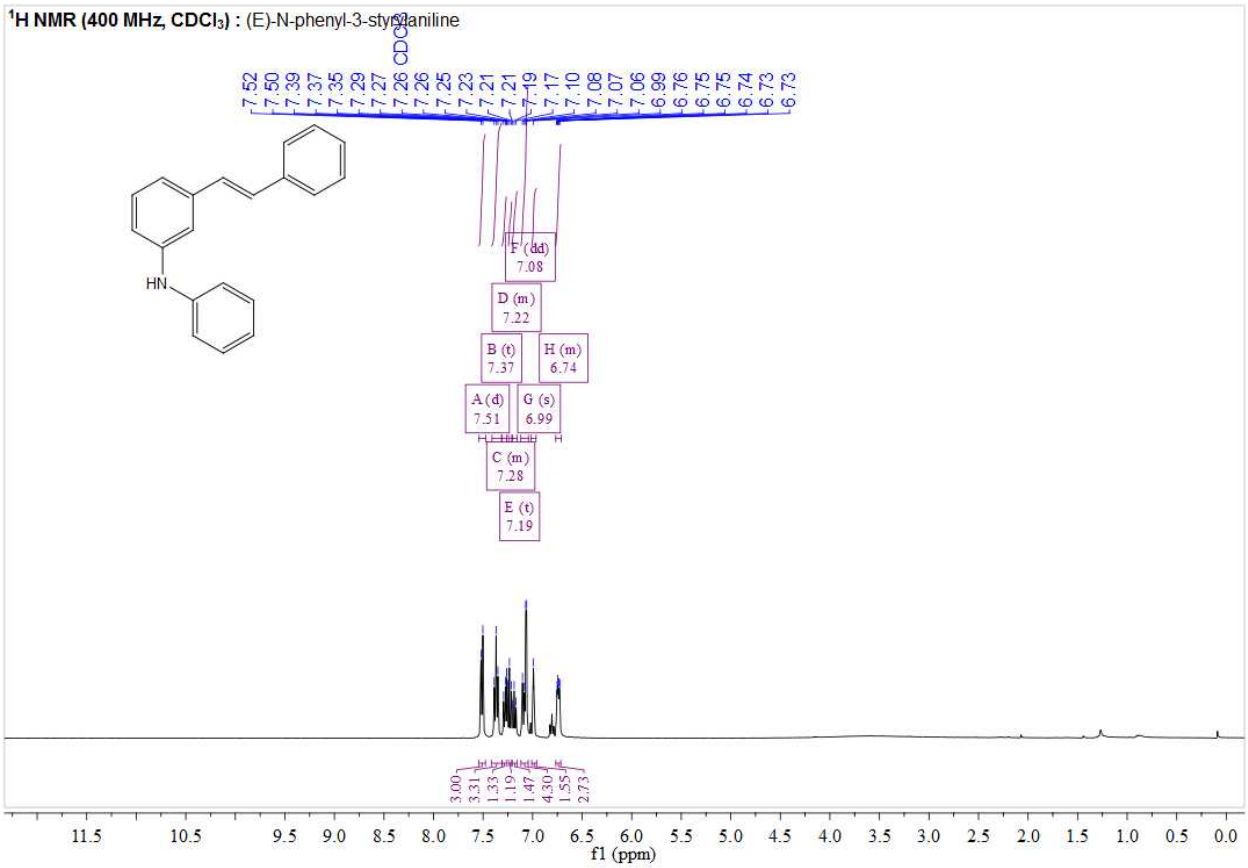


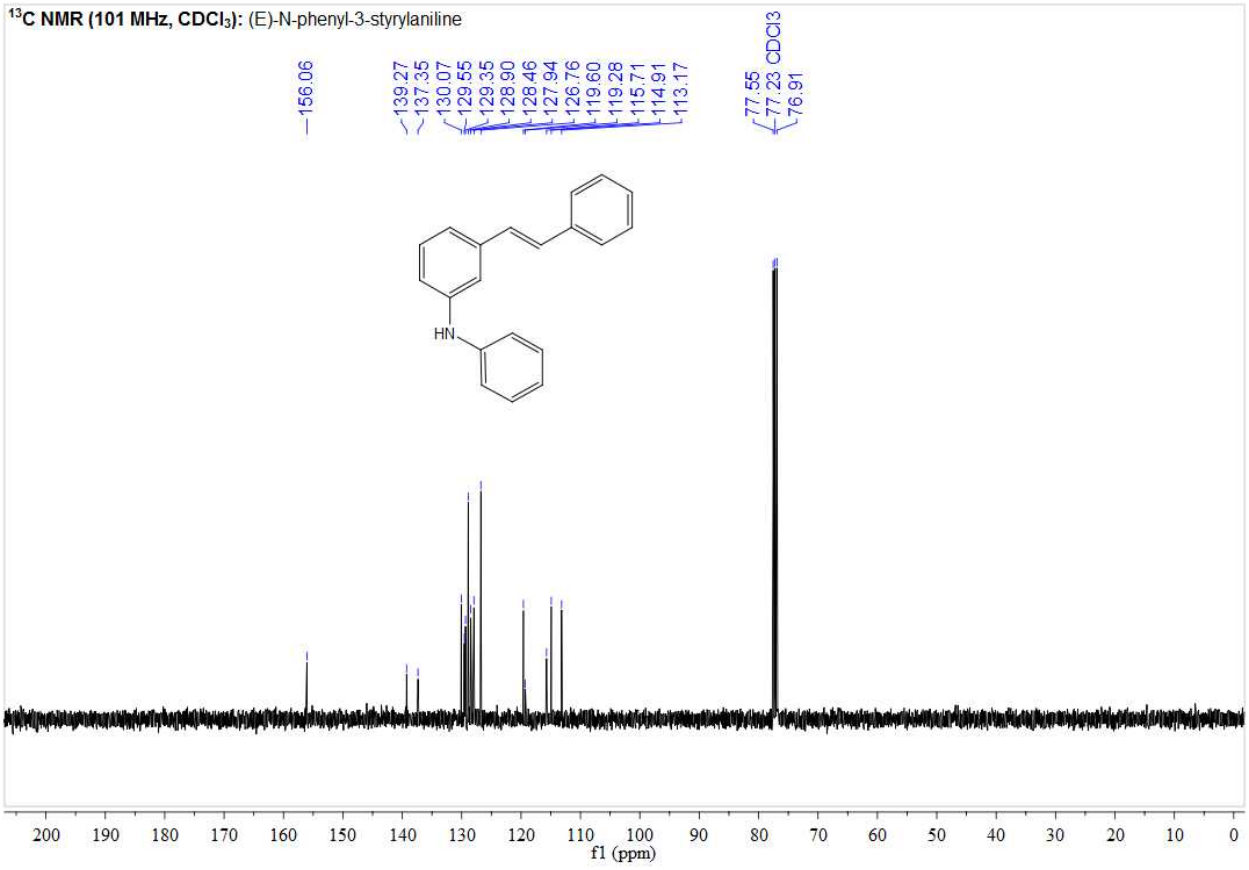
(*E*)-4'-methyl-3-styrylbiphenyl (18b):



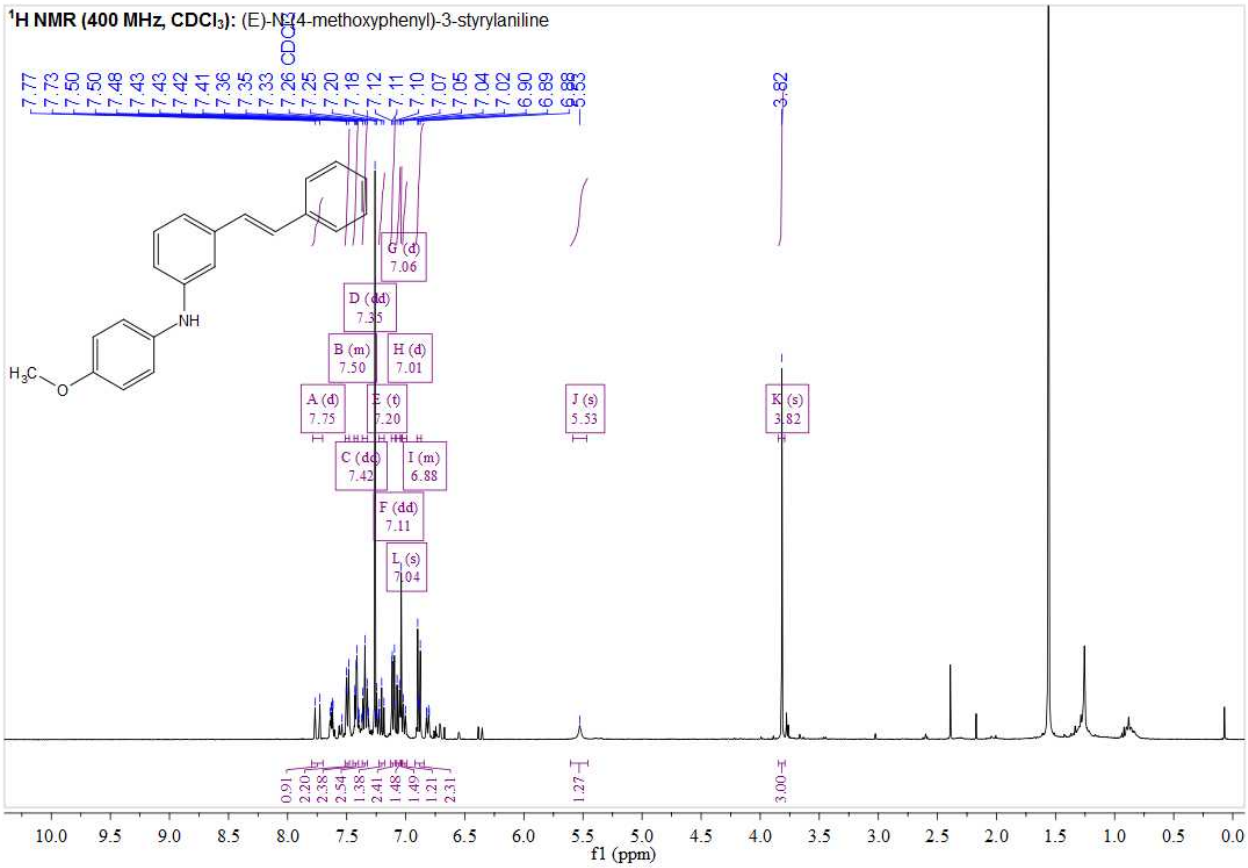


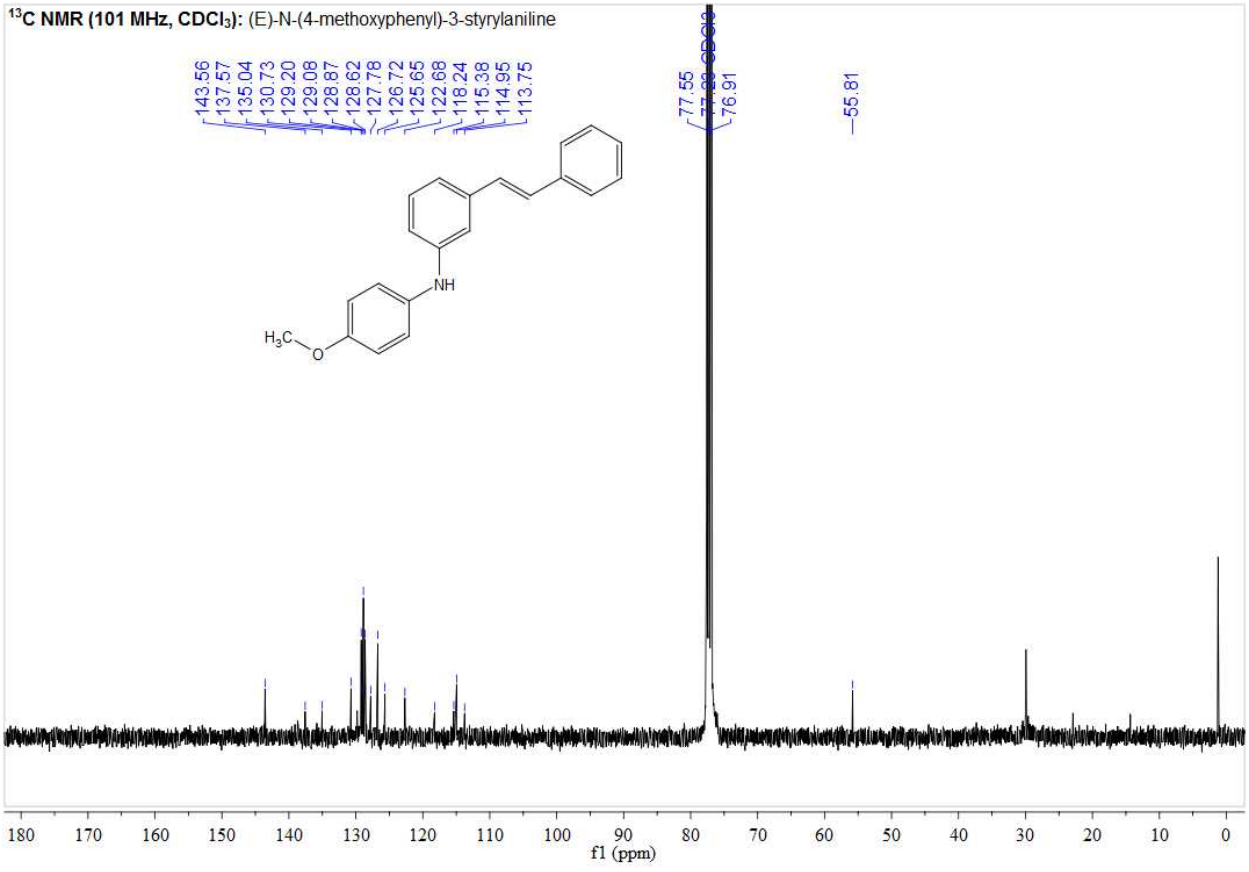
(*E*)-N-phenyl-3-styrylaniline (19a):



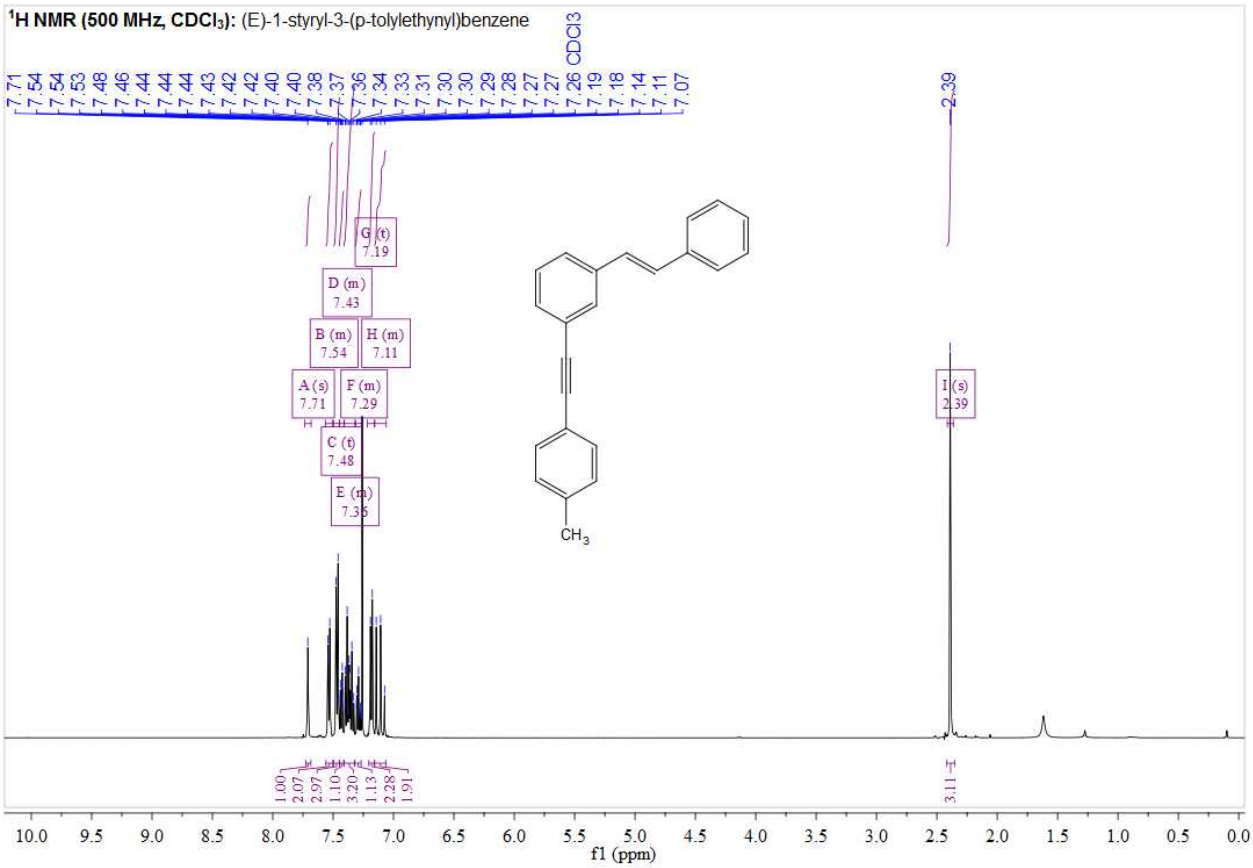


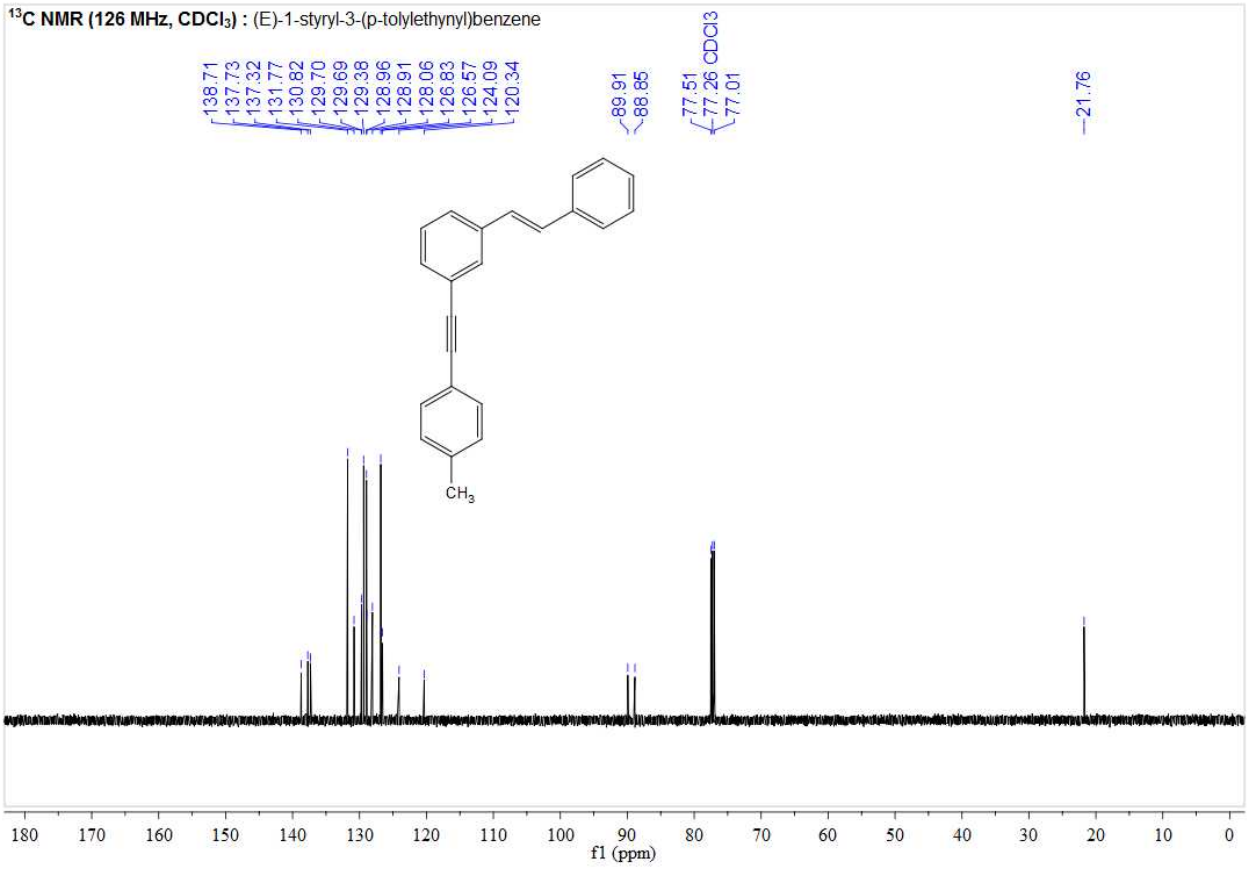
(*E*)-N-(4-methoxyphenyl)-3-styrylaniline (19b):



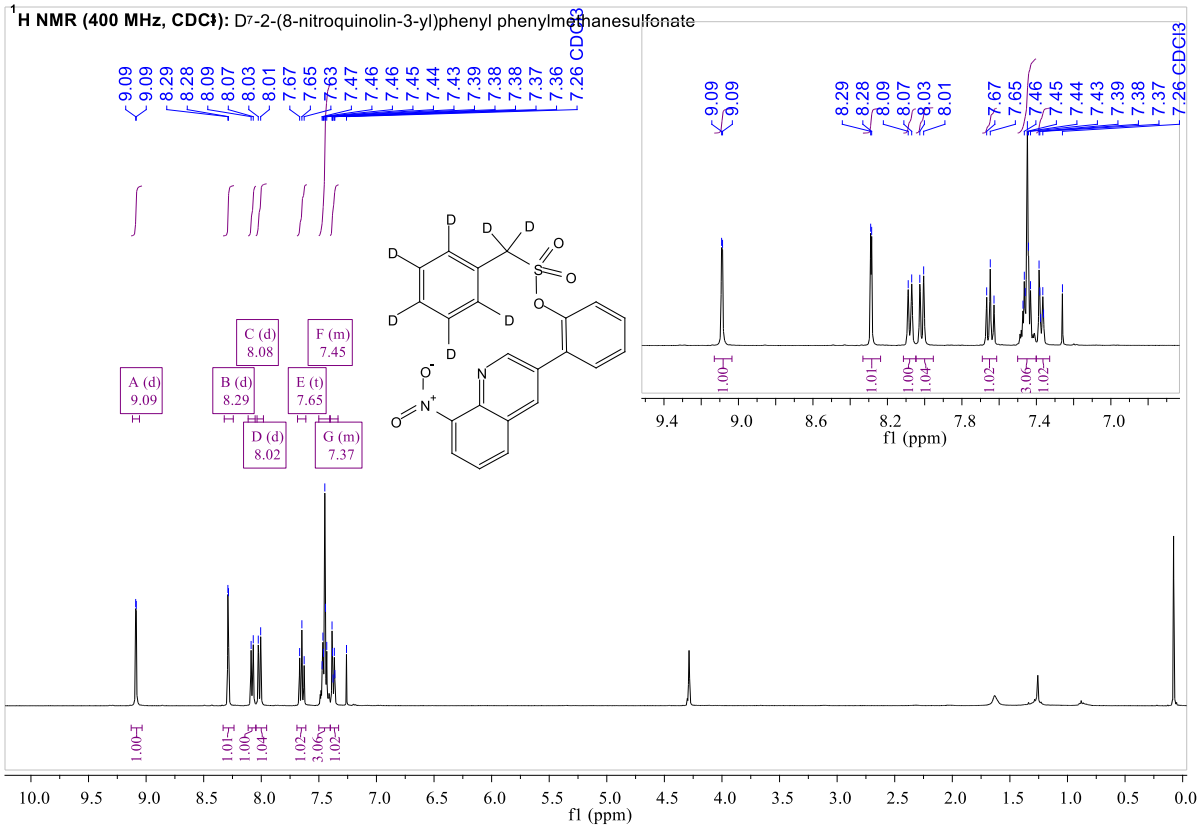


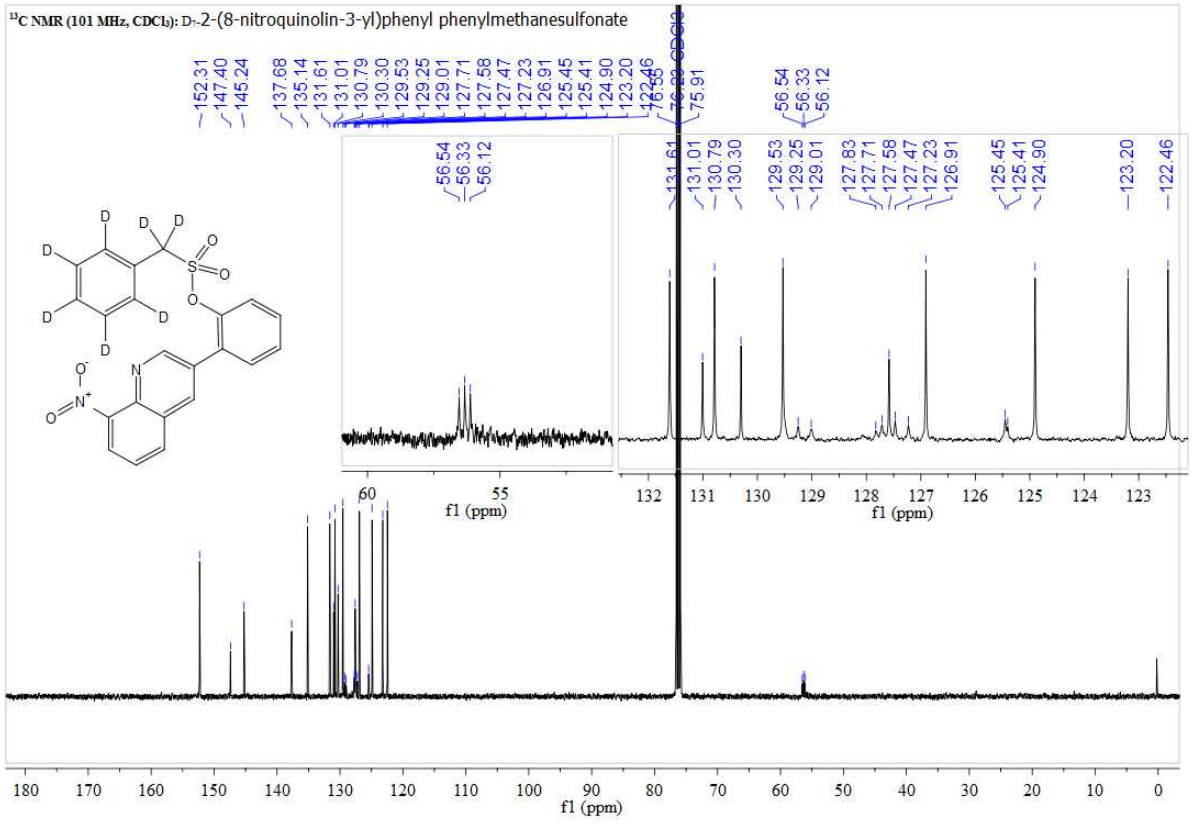
(*E*)-1-styryl-3-(p-tolylethynyl)benzene (20):





2-(8-nitroquinolin-3-yl)phenyl phenylmethanesulfonate (D_7-1):





Cartesian Coordinates of the Optimized Geometries at the M06/6-31G**,SDD(Pd) Level of Theory

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$[Pd(OAc)_2]_3$

Number of imaginary frequencies : 0

Electronic energy : =-1754.0916027
Zero-point correction= 0.315972
Thermal correction to Energy= 0.349810
Thermal correction to Enthalpy= 0.350755
Thermal correction to Gibbs Free Energy= 0.246926
Sum of electronic and zero-point Energies= -1753.775631
Sum of electronic and thermal Energies= -1753.741792
Sum of electronic and thermal Enthalpies= -1753.740848
Sum of electronic and thermal Free Energies= -1753.844676

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Cartesian Coordinates

.....

46	1.539985	-0.981241	-0.002552
8	1.051330	-2.022629	-1.678608
8	0.923281	-2.488570	1.233357
6	-0.163708	-2.587758	1.864606
8	-1.227084	-1.932937	1.670977
46	-1.622140	-0.842778	0.000920
6	-0.065629	-2.579881	-1.877150
8	-1.139747	-2.391083	-1.244603
8	2.289926	-0.103781	1.671800
8	2.645890	0.216109	-1.237609
6	2.272752	1.243469	-1.866804
8	1.227372	1.926579	-1.671702
46	0.079639	1.820792	0.003059
6	2.323470	1.144185	1.869452
8	1.692841	2.037335	1.241374
8	-1.054404	2.025777	1.677153
8	-1.508622	2.181868	-1.233330
6	-2.153149	1.433130	1.874026
6	-2.213948	1.349208	-1.865662
8	-2.614270	0.442686	1.243837
8	-2.293796	0.103739	-1.669052
6	-0.101719	-3.607873	-2.972941
1	0.228167	-4.567075	-2.559914
1	-1.115336	-3.721983	-3.360703
1	0.592480	-3.330353	-3.769070
6	3.191332	1.733023	-2.950665
1	3.911776	2.427404	-2.505158
1	3.741617	0.899358	-3.390597
1	2.625316	2.274286	-3.711340
6	3.248583	1.614785	2.956354
1	2.911219	2.570480	3.361210
1	3.320633	0.859688	3.741976

1	4.246860	1.748798	2.526066
6	-3.023581	1.993318	2.963478
1	-3.605318	1.197526	3.432504
1	-2.416947	2.522411	3.700803
1	-3.720092	2.709920	2.515151
6	-3.084188	1.908704	-2.955899
1	-3.993258	2.314298	-2.499117
1	-2.569977	2.724552	-3.468166
1	-3.370516	1.123621	-3.657954
6	-0.214479	-3.624957	2.951093
1	0.774728	-3.767847	3.389873
1	-0.943748	-3.340275	3.712130
1	-0.538018	-4.573214	2.508624

Substrate-**1**

Number of imaginary frequencies : 0

Electronic energy : =-1730.7331268
Zero-point correction= 0.343243
Thermal correction to Energy= 0.367179
Thermal correction to Enthalpy= 0.368123
Thermal correction to Gibbs Free Energy= 0.288484
Sum of electronic and zero-point Energies= -1730.389884
Sum of electronic and thermal Energies= -1730.365948
Sum of electronic and thermal Enthalpies= -1730.365004
Sum of electronic and thermal Free Energies= -1730.444643

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Cartesian Coordinates

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6	-0.888234	-1.480143	1.394561
1	0.096457	-1.071560	1.134634
1	-0.856963	-1.818108	2.438881
8	-1.294041	1.045694	2.120439
6	-2.274700	1.584264	-0.500177
6	-1.161299	2.368557	-0.823762
6	-3.566861	2.084235	-0.539541
6	-1.393587	3.691882	-1.206725
6	-3.771455	3.403493	-0.927448
1	-4.386403	1.428157	-0.257394
6	-2.684222	4.205046	-1.261857
1	-0.543865	4.316133	-1.478172
1	-4.780694	3.804822	-0.966929
1	-2.841722	5.235413	-1.570312
8	-2.082761	0.256341	-0.137358
16	-1.985393	-0.059214	1.482363
8	-3.305029	-0.456966	1.933255
6	-1.322774	-2.554120	0.445408
6	-0.515752	-2.863567	-0.650943
6	-2.509463	-3.260165	0.654684
6	-0.895597	-3.872868	-1.529345
1	0.420975	-2.325796	-0.804380

6	-2.887337	-4.261617	-0.230826
1	-3.139860	-3.011070	1.506397
6	-2.081543	-4.569575	-1.323599
1	-0.258396	-4.116077	-2.376127
1	-3.813941	-4.806148	-0.064817
1	-2.377318	-5.357862	-2.012181
6	1.198627	2.474229	-0.031198
6	2.450713	1.849718	0.169104
6	0.196358	1.813873	-0.698660
6	3.519824	2.486401	0.841142
6	2.595861	0.513540	-0.299247
6	0.509727	0.530653	-1.230155
6	4.710176	1.832884	1.041328
1	3.379372	3.505962	1.195989
6	3.822167	-0.140529	-0.009148
1	-0.235622	0.014846	-1.838574
6	4.864254	0.502430	0.609241
1	5.532791	2.328125	1.549295
1	5.790672	-0.039171	0.776037
7	1.637569	-0.103316	-1.033675
7	3.999626	-1.563730	-0.317141
8	5.091303	-1.906711	-0.742718
8	3.066447	-2.309126	-0.079032
1	1.023798	3.463496	0.391837

N-Acetylglycine

Number of imaginary frequencies : 0

Electronic energy : =-436.8568818
Zero-point correction= 0.117817
Thermal correction to Energy= 0.126678
Thermal correction to Enthalpy= 0.127622
Thermal correction to Gibbs Free Energy= 0.082579
Sum of electronic and zero-point Energies= -436.739065
Sum of electronic and thermal Energies= -436.730204
Sum of electronic and thermal Enthalpies= -436.729259
Sum of electronic and thermal Free Energies= -436.774303

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Cartesian Coordinates

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6	-1.857377	0.142291	0.002734
8	-1.946766	1.347414	0.016304
8	-2.913670	-0.679120	0.012116
1	-3.703094	-0.116823	0.030914
6	-0.569045	-0.625148	-0.028230
1	-0.564878	-1.283972	-0.908956
1	-0.527492	-1.300069	0.838945
7	0.530805	0.294681	-0.039221
1	0.299243	1.279659	-0.040359
6	1.812412	-0.166552	-0.002702
8	2.064102	-1.359775	0.023368

6	2.883978	0.894167	0.009681
1	2.499515	1.913806	-0.088791
1	3.446780	0.814480	0.944666
1	3.585146	0.693456	-0.805081

HFIP

Number of imaginary frequencies : 0

Electronic energy : =-789.5215432
Zero-point correction= 0.063926
Thermal correction to Energy= 0.072853
Thermal correction to Enthalpy= 0.073798
Thermal correction to Gibbs Free Energy= 0.029122
Sum of electronic and zero-point Energies= -789.457617
Sum of electronic and thermal Energies= -789.448690
Sum of electronic and thermal Enthalpies= -789.447746
Sum of electronic and thermal Free Energies= -789.492421

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Cartesian Coordinates

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6	1.283713	-0.135097	-0.030952
6	0.002827	0.542958	-0.499058
6	-1.262275	-0.164995	-0.025527
1	0.002331	0.474558	-1.600561
9	2.325094	0.424653	-0.642081
9	1.260268	-1.431272	-0.348172
9	1.459475	-0.025078	1.277991
9	-1.448667	-1.315362	-0.664812
9	-1.262854	-0.395704	1.279953
9	-2.307652	0.632927	-0.303789
8	0.045916	1.843754	-0.018262
1	-0.746224	2.306744	-0.311941

AcOH

Number of imaginary frequencies : 0

Electronic energy : =-228.963173
Zero-point correction= 0.062295
Thermal correction to Energy= 0.066778
Thermal correction to Enthalpy= 0.067722
Thermal correction to Gibbs Free Energy= 0.035401
Sum of electronic and zero-point Energies= -228.900878
Sum of electronic and thermal Energies= -228.896395
Sum of electronic and thermal Enthalpies= -228.895451
Sum of electronic and thermal Free Energies= -228.927772

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Cartesian Coordinates

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6	-0.092416	0.124236	0.000363
8	-0.652166	1.192424	-0.000094
8	-0.762605	-1.046342	-0.000050
1	-1.703301	-0.812817	-0.000202
6	1.386716	-0.099499	-0.000074
1	1.676548	-0.681724	0.880034
1	1.675962	-0.682999	-0.879520
1	1.903161	0.860462	-0.000894

Substarate-**2** (olefin)

Number of imaginary frequencies : 0

Electronic energy : =-345.5669177
Zero-point correction= 0.123848
Thermal correction to Energy= 0.131628
Thermal correction to Enthalpy= 0.132572
Thermal correction to Gibbs Free Energy= 0.091621
Sum of electronic and zero-point Energies= -345.443069
Sum of electronic and thermal Energies= -345.435290
Sum of electronic and thermal Enthalpies= -345.434346
Sum of electronic and thermal Free Energies= -345.475297

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Cartesian Coordinates

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6	-2.976719	-0.323139	-0.000018
6	-1.720198	-0.760002	0.000025
1	-3.823727	-1.002692	-0.000092
1	-3.176050	0.746458	0.000043
1	-1.462560	-1.816613	0.000031
6	-0.600963	0.206513	0.000008
8	-0.710578	1.411903	-0.000040
8	0.580011	-0.435719	0.000029
6	1.737250	0.408899	0.000052
6	2.948170	-0.485571	-0.000060
1	1.701139	1.062044	0.881073
1	1.701011	1.062185	-0.880842
1	3.863447	0.114667	0.000546
1	2.957705	-1.128272	0.886115
1	2.958321	-1.127441	-0.886829

$[AgOAc]_2$

Number of imaginary frequencies : 0

Electronic energy : =-750.8299419
Zero-point correction= 0.104041
Thermal correction to Energy= 0.116995

Thermal correction to Enthalpy= 0.117940
Thermal correction to Gibbs Free Energy= 0.061784
Sum of electronic and zero-point Energies= -750.725901
Sum of electronic and thermal Energies= -750.712946
Sum of electronic and thermal Enthalpies= -750.712002
Sum of electronic and thermal Free Energies= -750.768158

Cartesian Coordinates

47	-0.004084	-1.381193	0.001918
8	2.123865	1.122851	0.002249
6	2.682131	-0.012676	0.003384
6	4.188999	-0.000462	-0.012535
1	4.559213	0.679848	0.759186
1	4.595495	-1.001990	0.134411
1	4.528430	0.392574	-0.976341
8	2.119195	-1.144244	0.003647
8	-2.123894	-1.122842	0.002297
6	-2.682132	0.012695	0.003375
6	-4.189002	0.000534	-0.012519
1	-4.559230	-0.679709	0.759254
1	-4.595462	1.002086	0.134360
1	-4.528462	-0.392564	-0.976290
8	-2.119164	1.144253	0.003566
47	0.004085	1.381173	0.001936

AgOAc

Number of imaginary frequencies : 1

Electronic energy : =-375.3640073
Zero-point correction= 0.050347
Thermal correction to Energy= 0.055651
Thermal correction to Enthalpy= 0.056595
Thermal correction to Gibbs Free Energy= 0.019804
Sum of electronic and zero-point Energies= -375.313660
Sum of electronic and thermal Energies= -375.308357
Sum of electronic and thermal Enthalpies= -375.307412
Sum of electronic and thermal Free Energies= -375.344204

Cartesian Coordinates

47	-1.097908	-0.002149	-0.000033
8	0.901291	-1.104269	0.000195
6	1.499613	0.011175	-0.000064
6	3.008025	-0.004801	-0.000228
1	3.361708	-0.555448	-0.876917
1	3.414869	1.007317	-0.005370
1	3.361683	-0.545941	0.882420
8	0.900910	1.123870	0.000200

[AgOAc.HFIP]$_2$

Number of imaginary frequencies : 0

Electronic energy : =-2329.9327226
Zero-point correction= 0.237429
Thermal correction to Energy= 0.270233
Thermal correction to Enthalpy= 0.271177
Thermal correction to Gibbs Free Energy= 0.167851
Sum of electronic and zero-point Energies= -2329.695294
Sum of electronic and thermal Energies= -2329.662490
Sum of electronic and thermal Enthalpies= -2329.661545
Sum of electronic and thermal Free Energies= -2329.764872

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Cartesian Coordinates

.....

1	1.099823	-3.458615	-0.301052
6	0.418032	-3.046296	-1.046892
6	0.146275	-1.588449	-0.804087
1	0.863453	-3.156384	-2.041265
1	-0.521839	-3.603557	-1.051334
8	0.865965	-0.985037	0.041261
8	-0.777749	-1.056958	-1.487191
47	-1.259383	1.081561	-1.420965
47	0.678844	1.116607	0.591889
1	-0.110822	5.721618	0.281927
6	-1.049546	5.160221	0.272483
6	-0.760376	3.707224	-0.005614
1	-1.486010	5.250539	1.272016
1	-1.731865	5.578778	-0.468345
8	0.054522	3.150739	0.785564
8	-1.351242	3.180179	-0.989096
8	-3.482347	-0.910327	-1.280152
8	3.052461	-1.452992	1.566214
6	4.183644	-0.972124	0.942135
1	5.015268	-0.998829	1.659050
1	-2.578001	-1.286206	-1.314139
6	-4.038936	-1.091499	-0.025502
1	-5.110738	-0.861499	-0.084473
6	-3.920236	-2.553513	0.397505
6	-3.458702	-0.127814	1.014734
9	-4.186865	-0.111381	2.124346
9	-3.438213	1.112752	0.520271
9	-2.199894	-0.451873	1.343207
9	-4.353638	-2.755763	1.637008
9	-2.643479	-2.958287	0.330094
9	-4.628492	-3.316931	-0.426843
1	2.292384	-1.457942	0.943830
6	4.582396	-1.877904	-0.222068
6	4.051809	0.493226	0.516830
9	3.474707	1.201987	1.493475
9	5.233558	1.039182	0.259248
9	5.581678	-1.366219	-0.939426

9	4.968668	-3.060017	0.248489
9	3.546603	-2.084306	-1.042642
9	3.282553	0.632517	-0.576074

All the stationary points of the energy profile diagram as shown in Figure 4.

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a

Number of imaginary frequencies : 0

Electronic energy : =-1021.5484806
Zero-point correction= 0.224294
Thermal correction to Energy= 0.243903
Thermal correction to Enthalpy= 0.244847
Thermal correction to Gibbs Free Energy= 0.174248
Sum of electronic and zero-point Energies= -1021.324187
Sum of electronic and thermal Energies= -1021.304577
Sum of electronic and thermal Enthalpies= -1021.303633
Sum of electronic and thermal Free Energies= -1021.374233

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Cartesian Coordinates

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46	-0.164950	-0.214858	0.007257
8	2.621132	-1.155365	-1.150487
6	2.529752	-3.473417	-0.573147
6	2.009440	-2.058438	-0.564509
8	0.901861	-1.928859	0.093044
6	0.826492	2.228513	-1.070110
6	-0.638245	2.488763	-0.732265
8	-1.242138	1.477670	-0.122096
8	-1.190540	3.512164	-1.045473
1	1.395144	3.146712	-0.899176
1	0.886000	1.964397	-2.131434
1	3.561338	-3.493876	-0.928859
1	2.455253	-3.915198	0.424107
1	1.906171	-4.076798	-1.240991
7	1.399563	1.109192	-0.296893
1	2.034750	0.454350	-0.806302
6	1.898033	1.477270	1.011095
8	1.596489	2.541859	1.485238
6	2.766310	0.446865	1.663300
1	3.290306	0.911014	2.500094
1	2.143519	-0.373464	2.038807
1	3.472562	0.010884	0.949060
6	-3.033195	-1.054699	0.281778
6	-4.122177	-2.053405	0.478069
1	-4.789194	-2.034423	-0.389162
1	-3.703904	-3.050787	0.611456
1	-4.719797	-1.770853	1.349944
8	-1.846299	-1.422845	0.274175
8	-3.448436	0.164991	0.128135

1 -2.696380 0.821522 0.001334

[a-I]‡

Number of imaginary frequencies : 1
The smallest frequency is : -910.1520 cm(-1)

Electronic energy : =-1021.5366058
Zero-point correction= 0.219451
Thermal correction to Energy= 0.238680
Thermal correction to Enthalpy= 0.239624
Thermal correction to Gibbs Free Energy= 0.169963
Sum of electronic and zero-point Energies= -1021.317155
Sum of electronic and thermal Energies= -1021.297926
Sum of electronic and thermal Enthalpies= -1021.296981
Sum of electronic and thermal Free Energies= -1021.366643

Cartesian Coordinates

46	-0.222757	-0.250287	0.017313
8	2.462179	-1.315078	-1.110764
6	2.417881	-3.586256	-0.425698
6	1.820588	-2.213602	-0.504960
8	0.698050	-2.060268	0.078177
6	1.075406	1.944840	-1.132061
6	-0.317216	2.465374	-0.775118
8	-1.070850	1.571319	-0.149682
8	-0.685768	3.578817	-1.058071
1	1.789517	2.774935	-1.117554
1	1.032768	1.579054	-2.166134
1	3.012500	-3.788307	-1.319131
1	3.088077	-3.612265	0.440360
1	1.644779	-4.344065	-0.288112
7	1.498732	0.822630	-0.282594
1	2.038618	-0.130054	-0.776270
6	2.081014	1.089997	0.997640
8	2.548363	0.175069	1.635533
6	2.095931	2.514615	1.477314
1	2.434132	2.517500	2.514269
1	2.788298	3.119706	0.880709
1	1.108723	2.985702	1.408975
6	-3.174450	-0.745772	0.257376
6	-4.383735	-1.595920	0.447902
1	-4.887802	-1.299604	1.373229
1	-5.086834	-1.421475	-0.371622
1	-4.104299	-2.648155	0.496063
8	-2.043470	-1.255731	0.260068
8	-3.432238	0.519351	0.103706
1	-2.605433	1.074316	-0.019134

I

Number of imaginary frequencies : 0

Electronic energy : =-1021.5510532
Zero-point correction= 0.223400
Thermal correction to Energy= 0.243142
Thermal correction to Enthalpy= 0.244086
Thermal correction to Gibbs Free Energy= 0.172692
Sum of electronic and zero-point Energies= -1021.327653
Sum of electronic and thermal Energies= -1021.307911
Sum of electronic and thermal Enthalpies= -1021.306967
Sum of electronic and thermal Free Energies= -1021.378361

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Cartesian Coordinates

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46	0.197557	-0.001698	0.164164
8	-0.737909	2.671219	-1.059563
6	0.242808	4.201302	0.495564
6	-0.190206	2.833126	0.044853
8	0.061717	1.890621	0.880889
6	-1.772582	-1.983090	0.598674
6	-0.543036	-2.734716	0.089083
8	0.436790	-1.948429	-0.315236
8	-0.498216	-3.940931	0.088565
1	-1.771612	-2.061959	1.695501
1	-2.658819	-2.510645	0.231626
1	1.318259	4.303612	0.314953
1	-0.285595	4.972479	-0.067721
1	0.078809	4.321606	1.569267
7	-1.735892	-0.581979	0.193674
1	-1.879045	1.654346	-0.903076
6	-2.797969	0.029983	-0.235219
8	-2.791298	1.214642	-0.759047
6	-4.164202	-0.582670	-0.170543
1	-4.905089	0.197290	-0.351034
1	-4.276220	-1.349257	-0.945911
1	-4.352931	-1.051764	0.798895
6	3.162687	-0.411597	-0.194802
6	4.581806	0.043967	-0.234616
1	4.976876	-0.097892	-1.245435
1	4.652633	1.093206	0.051117
1	5.183143	-0.577177	0.435632
8	2.254678	0.390962	0.071137
8	3.002873	-1.673677	-0.459072
1	2.038289	-1.954954	-0.430447

II

Number of imaginary frequencies : 0

Electronic energy : =-1582.1186916
Zero-point correction= 0.225809
Thermal correction to Energy= 0.249905
Thermal correction to Enthalpy= 0.250849
Thermal correction to Gibbs Free Energy= 0.169044
Sum of electronic and zero-point Energies= -1581.892883
Sum of electronic and thermal Energies= -1581.868787
Sum of electronic and thermal Enthalpies= -1581.867842
Sum of electronic and thermal Free Energies= -1581.949648

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Cartesian Coordinates

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46	-0.913041	0.236333	-0.202064
6	-2.995910	-1.764177	0.067830
6	-3.650841	-0.407061	0.301927
8	-2.837720	0.627222	0.207128
8	-4.827557	-0.325112	0.556262
1	-3.572699	-2.263184	-0.722811
1	-3.135767	-2.351443	0.986373
7	-1.584070	-1.661937	-0.283182
6	-0.898166	-2.722087	-0.594035
8	0.356747	-2.678614	-0.921773
8	0.989229	-0.231723	-0.695320
1	0.730377	-1.730625	-0.877381
6	1.970212	0.223578	0.155044
6	3.220102	0.484896	-0.683198
6	2.223328	-0.762244	1.295319
1	1.719762	1.189623	0.626457
9	3.545059	-0.564734	-1.431198
9	2.995312	1.517713	-1.495597
9	4.270265	0.787584	0.085377
9	2.790456	-1.888160	0.862047
9	2.995022	-0.240201	2.246817
9	1.054593	-1.096972	1.864697
8	-0.357060	2.253773	-0.089194
6	-1.112564	3.233082	0.030583
8	-2.398993	3.173791	0.190720
6	-0.563439	4.617676	-0.010420
1	-1.005901	5.150902	-0.857645
1	-0.856543	5.155385	0.896018
1	0.521527	4.596601	-0.109403
1	-2.745470	2.231189	0.227650
6	-1.500824	-4.088311	-0.604129
1	-1.909335	-4.338805	0.380878
1	-2.325417	-4.143319	-1.323256
1	-0.737080	-4.817986	-0.875032

III

Number of imaginary frequencies : 0

Electronic energy : =-3083.9002238
Zero-point correction= 0.509990
Thermal correction to Energy= 0.552768
Thermal correction to Enthalpy= 0.553712
Thermal correction to Gibbs Free Energy= 0.435259
Sum of electronic and zero-point Energies= -3083.390234
Sum of electronic and thermal Energies= -3083.347456
Sum of electronic and thermal Enthalpies= -3083.346512
Sum of electronic and thermal Free Energies= -3083.464965

Cartesian Coordinates

46	-2.341289	0.038113	-0.732209
6	4.191113	-0.540799	1.453620
1	3.559497	-1.357337	1.075939
1	4.733861	-0.932775	2.324945
8	6.096175	-1.693122	0.089825
6	4.050451	-0.993909	-1.892031
6	2.665259	-0.915126	-2.100762
6	4.823911	-1.984876	-2.485621
6	2.083476	-1.897117	-2.914762
6	4.214200	-2.949083	-3.276535
1	5.894364	-1.994761	-2.311359
6	2.840432	-2.907570	-3.488337
1	1.017468	-1.844417	-3.125299
1	4.818959	-3.725919	-3.736432
1	2.358576	-3.650796	-4.117646
6	-5.076651	0.651841	-1.438903
6	-4.213456	1.850393	-1.831764
8	-2.925647	1.733650	-1.606063
8	-4.732578	2.832881	-2.312330
1	-5.714949	0.409458	-2.298591
7	-4.274404	-0.490522	-1.018636
6	-4.797935	-1.663402	-0.858918
8	-4.101209	-2.699129	-0.475721
8	4.659456	0.000872	-1.133224
16	5.499906	-0.381703	0.234758
8	6.310502	0.791521	0.467913
6	3.377813	0.676959	1.789035
6	2.015178	0.494971	2.037622
6	3.936387	1.946694	1.955850
6	1.220008	1.558157	2.450924
1	1.583615	-0.499945	1.930995
6	3.134026	3.013029	2.348693
1	4.996382	2.100201	1.776427
6	1.779399	2.823273	2.601390
1	0.160635	1.400371	2.646963
1	3.578720	3.997997	2.473353
1	1.161301	3.657449	2.926431
1	-3.152119	-2.445527	-0.242138
1	-5.737903	0.982687	-0.624859
6	2.208260	1.482177	-1.451254

6	1.320296	2.453495	-0.948699
6	1.825501	0.161180	-1.543290
6	1.707072	3.814710	-0.889114
6	0.028996	2.048923	-0.504620
6	0.501445	-0.133610	-1.157140
6	0.841339	4.770708	-0.430307
1	2.707959	4.077179	-1.225975
6	-0.792335	3.060923	0.067694
1	0.120548	-1.150762	-1.228311
6	-0.416060	4.381381	0.063069
1	1.127002	5.817960	-0.408340
1	-1.105273	5.106772	0.485087
7	-0.359758	0.749471	-0.678599
7	-2.014643	2.759202	0.818164
8	-2.898064	3.591051	0.830546
8	-2.032387	1.702987	1.442605
1	3.196622	1.799075	-1.777175
6	-6.243682	-1.945662	-1.103810
1	-6.509216	-1.737573	-2.146130
1	-6.453514	-2.992368	-0.880512
1	-6.872094	-1.307076	-0.473514
8	-1.748130	-1.758639	0.072244
6	-1.262310	-1.706393	1.354918
1	-0.786550	-0.739220	1.605045
6	-2.373678	-1.890285	2.390524
6	-0.160935	-2.757276	1.495701
9	-1.951033	-1.618519	3.625146
9	-3.382482	-1.060310	2.112860
9	-2.858441	-3.133950	2.379320
9	0.870272	-2.430517	0.688545
9	0.324935	-2.804802	2.738510
9	-0.562307	-3.972180	1.151693

IV

Number of imaginary frequencies : 0

Electronic energy : =-2294.3142914
Zero-point correction= 0.439776
Thermal correction to Energy= 0.474080
Thermal correction to Enthalpy= 0.475025
Thermal correction to Gibbs Free Energy= 0.373210
Sum of electronic and zero-point Energies= -2293.874515
Sum of electronic and thermal Energies= -2293.840211
Sum of electronic and thermal Enthalpies= -2293.839267
Sum of electronic and thermal Free Energies= -2293.941082

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Cartesian Coordinates

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46	-1.778382	-0.408311	0.418663
6	-1.210337	-2.309208	-1.007197

6	-1.293660	-2.819285	0.296665
6	-0.121496	-3.220634	0.970968
6	1.091660	-3.168887	0.323486
6	1.185652	-2.682320	-0.999786
6	0.048576	-2.227874	-1.640504
1	1.994674	-3.515446	0.823153
6	2.513110	-2.700400	-1.693253
1	2.416168	-2.734013	-2.784753
1	3.144651	-3.537770	-1.376051
8	2.856996	-0.050547	-1.902998
6	4.085030	-0.323284	0.979076
6	3.465298	0.899725	1.265938
6	5.339416	-0.650015	1.472990
6	4.156155	1.783573	2.102167
6	6.003637	0.248830	2.297830
1	5.772700	-1.607739	1.198401
6	5.405263	1.463751	2.617681
1	3.685711	2.729509	2.364014
1	6.984097	-0.002283	2.693233
1	5.911895	2.165785	3.274593
6	-4.037553	-0.041878	2.157447
6	-3.264997	1.267594	2.155379
8	-2.232279	1.313622	1.335486
8	-3.571167	2.195169	2.871862
1	-5.098556	0.220389	2.070625
7	-3.594790	-0.933925	1.101713
6	-4.451550	-1.658365	0.342612
8	-4.107224	-2.283910	-0.662299
8	3.410702	-1.285410	0.232595
8	4.902358	-1.511887	-1.779251
16	3.527189	-1.240216	-1.413532
1	-3.908094	-0.490055	3.156367
6	2.032083	2.551082	0.111483
6	0.858982	2.896802	-0.585971
6	2.189732	1.295694	0.643091
6	0.684662	4.196728	-1.117122
6	-0.142129	1.901771	-0.756499
6	1.088523	0.412740	0.529530
6	-0.461439	4.533092	-1.785415
1	1.479814	4.924484	-0.968895
6	-1.276995	2.279291	-1.522503
1	1.126475	-0.561984	1.014933
6	-1.452923	3.557500	-1.987155
1	-0.605307	5.535518	-2.177023
1	-2.362047	3.785612	-2.535774
1	2.832121	3.286508	0.187707
7	-0.016035	0.686126	-0.136395
7	-2.292401	1.311197	-1.953142
8	-3.458602	1.647827	-1.893051
8	-1.875859	0.255191	-2.407975
1	-2.271205	-3.031696	0.717085
1	-0.189305	-3.623425	1.978265
1	0.111413	-1.835548	-2.654425
1	-2.137763	-2.127175	-1.548151
6	-5.899960	-1.722989	0.796836

1	-6.002839	-1.910280	1.870928
1	-6.416011	-0.782190	0.570806
1	-6.383299	-2.524851	0.236140

[IV-b]‡

Number of imaginary frequencies : 1
The smallest frequency is : -1634.1550 cm(-1)

Electronic energy : =-2294.3008456
Zero-point correction= 0.434972
Thermal correction to Energy= 0.468509
Thermal correction to Enthalpy= 0.469453
Thermal correction to Gibbs Free Energy= 0.370436
Sum of electronic and zero-point Energies= -2293.865873
Sum of electronic and thermal Energies= -2293.832337
Sum of electronic and thermal Enthalpies= -2293.831392
Sum of electronic and thermal Free Energies= -2293.930409

Cartesian Coordinates

46	-1.811817	-0.354608	0.450258
6	-0.888114	-2.212063	-0.229305
6	-0.709079	-3.087256	0.857072
6	0.478619	-3.788432	1.034761
6	1.508047	-3.623840	0.118013
6	1.357261	-2.774101	-0.982883
6	0.160631	-2.082574	-1.155911
1	2.452173	-4.150057	0.256027
6	2.519927	-2.564399	-1.900403
1	2.229592	-2.442867	-2.950971
1	3.265797	-3.363150	-1.828968
8	2.658130	0.110184	-1.960320
6	4.084527	-0.252028	0.852424
6	3.479458	0.948442	1.247788
6	5.370197	-0.593249	1.246532
6	4.218372	1.788612	2.088311
6	6.082391	0.262721	2.076284
1	5.789115	-1.527908	0.884150
6	5.499743	1.452084	2.503616
1	3.761305	2.715048	2.431314
1	7.088682	-0.001022	2.390356
1	6.045035	2.120758	3.164396
6	-4.445832	-0.240542	1.651917
6	-3.773550	1.113531	1.899137
8	-2.586446	1.276327	1.366507
8	-4.343557	1.956716	2.558481
1	-5.421999	-0.028744	1.195339
7	-3.628934	-1.103910	0.817324
6	-4.120709	-2.041476	0.024856
8	-3.405515	-2.667159	-0.809198

8	3.371923	-1.173220	0.093288
8	4.816702	-1.182646	-1.969207
16	3.434424	-1.047435	-1.554288
1	-4.640317	-0.691731	2.636433
6	1.981681	2.661743	0.281123
6	0.777764	3.043584	-0.342318
6	2.168233	1.376235	0.726839
6	0.576969	4.366723	-0.803105
6	-0.223780	2.053053	-0.529259
6	1.057471	0.502470	0.633677
6	-0.585815	4.719477	-1.433464
1	1.367482	5.096059	-0.638457
6	-1.366545	2.443300	-1.278999
1	1.110535	-0.495091	1.068014
6	-1.563378	3.739329	-1.680950
1	-0.749451	5.738324	-1.771296
1	-2.474200	3.978601	-2.221760
1	2.785431	3.393070	0.358007
7	-0.080326	0.818590	0.046021
7	-2.349988	1.471555	-1.772843
8	-3.524206	1.786471	-1.743629
8	-1.904121	0.430663	-2.237839
1	-1.530409	-3.223873	1.560093
1	0.603975	-4.461340	1.879591
1	0.049754	-1.397499	-1.997070
1	-2.119017	-2.240149	-0.622790
6	-5.581204	-2.396865	0.099704
1	-5.938331	-2.454634	1.132414
1	-6.171533	-1.630074	-0.415833
1	-5.739097	-3.352011	-0.403162

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b

Number of imaginary frequencies : 0

Electronic energy : =-2294.3258093
Zero-point correction= 0.441162
Thermal correction to Energy= 0.475054
Thermal correction to Enthalpy= 0.475998
Thermal correction to Gibbs Free Energy= 0.375678
Sum of electronic and zero-point Energies= -2293.884647
Sum of electronic and thermal Energies= -2293.850756
Sum of electronic and thermal Enthalpies= -2293.849811
Sum of electronic and thermal Free Energies= -2293.950131

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Cartesian Coordinates

.....

46	-1.780206	-0.329825	0.438875
6	-0.682037	-1.951152	-0.057501
6	-0.644384	-3.031940	0.835644
6	0.376112	-3.979013	0.775089

6	1.397366	-3.841408	-0.156445
6	1.360908	-2.792638	-1.074925
6	0.298588	-1.886023	-1.054193
1	2.233910	-4.538891	-0.165175
6	2.534540	-2.556925	-1.970486
1	2.263090	-2.358895	-3.015275
1	3.262488	-3.374317	-1.940078
8	2.796348	0.117408	-1.995485
6	4.028071	-0.276023	0.884446
6	3.473646	0.957886	1.257879
6	5.286225	-0.672487	1.315866
6	4.237424	1.773353	2.100757
6	6.022920	0.159553	2.148240
1	5.667378	-1.633160	0.981709
6	5.493606	1.383850	2.544497
1	3.816751	2.722800	2.427115
1	7.006830	-0.151122	2.489300
1	6.058381	2.035543	3.205907
6	-4.295000	-0.510191	1.830622
6	-3.913289	0.986729	1.851757
8	-2.834054	1.301879	1.208989
8	-4.627535	1.738234	2.488000
1	-5.382253	-0.581384	1.717712
7	-3.573405	-1.242059	0.794353
6	-4.148272	-2.092076	0.018123
8	-3.505542	-2.644162	-0.995958
8	3.296495	-1.169623	0.108528
8	4.884998	-1.274527	-1.847757
16	3.482991	-1.076179	-1.534571
1	-4.033534	-0.922710	2.815109
6	1.995969	2.725324	0.323770
6	0.784058	3.127867	-0.273570
6	2.174971	1.430661	0.745196
6	0.591522	4.461195	-0.707903
6	-0.229246	2.149518	-0.472316
6	1.048664	0.579038	0.667212
6	-0.568189	4.833765	-1.332680
1	1.387741	5.181328	-0.530402
6	-1.359680	2.555882	-1.235651
1	1.101586	-0.419907	1.095119
6	-1.543784	3.861493	-1.614228
1	-0.725907	5.860401	-1.649040
1	-2.443158	4.112051	-2.168510
1	2.806458	3.449406	0.399494
7	-0.095874	0.910700	0.097527
7	-2.324283	1.598196	-1.789288
8	-3.484490	1.945159	-1.889233
8	-1.871188	0.525393	-2.172596
1	-1.407225	-3.121579	1.609309
1	0.392923	-4.807368	1.480524
1	0.293892	-1.060232	-1.766187
1	-2.593146	-2.277390	-1.023069
6	-5.563220	-2.550925	0.141848
1	-5.801947	-2.829770	1.171829
1	-6.245568	-1.746406	-0.154663

1	-5.727324	-3.405402	-0.516183

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c

Number of imaginary frequencies : 0

Electronic energy : =-2523.3021371
Zero-point correction= 0.504439
Thermal correction to Energy= 0.544090
Thermal correction to Enthalpy= 0.545034
Thermal correction to Gibbs Free Energy= 0.431331
Sum of electronic and zero-point Energies= -2522.797698
Sum of electronic and thermal Energies= -2522.758047
Sum of electronic and thermal Enthalpies= -2522.757103
Sum of electronic and thermal Free Energies= -2522.870806

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Cartesian Coordinates

.....

46	-1.351213	0.359551	-0.642277
6	-0.562987	-1.322846	-1.302298
6	-1.068235	-2.549412	-0.864958
6	-0.336992	-3.718707	-1.070321
6	0.915786	-3.666134	-1.668655
6	1.412699	-2.446155	-2.125644
6	0.646435	-1.286025	-1.994985
1	1.522567	-4.566182	-1.757727
6	2.834714	-2.346805	-2.575738
1	2.973512	-1.773952	-3.501405
1	3.318477	-3.323464	-2.680860
8	3.618635	-0.009450	-1.500695
6	3.752332	-1.698986	1.204877
6	3.399450	-0.544170	1.920780
6	4.659541	-2.620137	1.709959
6	3.983114	-0.366056	3.180022
6	5.226522	-2.414887	2.960701
1	4.906721	-3.486878	1.103706
6	4.881495	-1.287452	3.699763
1	3.703283	0.508136	3.765432
1	5.933290	-3.138126	3.358692
1	5.309770	-1.127377	4.685766
6	-5.237619	-1.397459	-0.706460
6	-3.967453	-0.705999	-0.220263
8	-3.203474	-0.341521	-1.174493
8	-3.735956	-0.601244	0.998945
1	-4.895391	-2.363319	-1.124160
7	-6.269394	-1.530177	0.281376
6	-6.143953	-2.403971	1.194412
8	-7.097554	-2.485767	2.144071
8	3.142994	-1.982450	-0.010064
8	5.230099	-1.938789	-1.425156
16	3.869767	-1.436612	-1.397143

1	-5.608319	-0.825238	-1.564046
6	2.821822	1.827251	1.468056
6	2.052258	2.797624	0.793918
6	2.520141	0.493873	1.354030
6	2.369247	4.172296	0.906786
6	0.990123	2.358335	-0.047671
6	1.329593	0.173051	0.658883
6	1.670695	5.112966	0.198535
1	3.187640	4.458526	1.564522
6	0.371987	3.362141	-0.849009
1	0.976727	-0.855961	0.661682
6	0.679159	4.693146	-0.704322
1	1.905559	6.169303	0.288912
1	0.156272	5.403547	-1.337139
1	3.694513	2.152000	2.033836
7	0.593202	1.044724	-0.009529
7	-0.516892	3.051767	-1.976724
8	-1.354355	3.880154	-2.281439
8	-0.312038	1.999365	-2.564318
1	-2.014814	-2.596059	-0.328946
1	-0.732646	-4.670581	-0.721577
1	1.054422	-0.337393	-2.342631
1	-7.722806	-1.775415	1.932141
6	-5.059125	-3.408504	1.412230
1	-4.727546	-3.841083	0.461617
1	-4.197848	-2.905074	1.864336
1	-5.402330	-4.207502	2.072634
8	-2.091728	2.261026	0.276883
6	-2.332264	2.377284	1.482581
6	-2.127369	3.693838	2.164470
1	-2.892679	4.393126	1.812614
1	-2.194389	3.602174	3.249448
1	-1.155964	4.103378	1.866563
8	-2.766791	1.421471	2.246693
1	-3.032274	0.594711	1.708254

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d

Number of imaginary frequencies : 0

Electronic energy : =-2523.3216406
Zero-point correction= 0.504618
Thermal correction to Energy= 0.544280
Thermal correction to Enthalpy= 0.545224
Thermal correction to Gibbs Free Energy= 0.429890
Sum of electronic and zero-point Energies= -2522.817022
Sum of electronic and thermal Energies= -2522.777360
Sum of electronic and thermal Enthalpies= -2522.776416
Sum of electronic and thermal Free Energies= -2522.891750

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Cartesian Coordinates

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46	-1.358064	0.480978	-0.140450
6	-0.864852	-1.370186	-0.621502
6	-1.415565	-2.458675	0.057399
6	-0.859160	-3.727899	-0.094105
6	0.268125	-3.910217	-0.884724
6	0.799899	-2.831394	-1.589643
6	0.196951	-1.574822	-1.501850
1	0.747338	-4.886247	-0.945575
6	2.108266	-2.980677	-2.297604
1	2.118346	-2.561664	-3.311782
1	2.454415	-4.018756	-2.334964
8	3.362215	-0.653320	-1.797102
6	3.800676	-1.863342	1.088653
6	3.701985	-0.562231	1.604026
6	4.701631	-2.785748	1.602486
6	4.535129	-0.232646	2.679232
6	5.518495	-2.429913	2.667395
1	4.746582	-3.770988	1.147280
6	5.429208	-1.151915	3.210485
1	4.457420	0.763134	3.112483
1	6.221590	-3.151883	3.074016
1	6.055196	-0.870629	4.053201
6	-5.226121	-0.794568	1.215059
6	-3.868188	-0.118018	1.124811
8	-3.321247	-0.138440	-0.024047
8	-3.423234	0.385372	2.170951
1	-5.973430	0.010352	1.320404
7	-5.482850	-1.651893	0.089347
6	-6.534074	-2.510629	-0.066013
8	-6.692907	-3.154527	-1.088657
8	2.948711	-2.282393	0.075553
8	4.710358	-2.770902	-1.662096
16	3.452178	-2.070737	-1.489778
1	-5.234463	-1.345768	2.164712
6	3.297323	1.730700	0.753742
6	2.511080	2.659377	0.042383
6	2.834412	0.462244	0.994774
6	3.003348	3.960647	-0.217297
6	1.242954	2.240926	-0.455931
6	1.495643	0.198024	0.621172
6	2.278954	4.847286	-0.967669
1	3.976277	4.231609	0.187835
6	0.575805	3.163946	-1.313355
1	1.042518	-0.749471	0.903073
6	1.064591	4.428778	-1.534874
1	2.650705	5.848366	-1.164499
1	0.493055	5.081946	-2.187281
1	4.302990	2.019700	1.056903
7	0.726178	1.031188	-0.062594
7	-0.598095	2.808152	-2.119981
8	-1.380003	3.697683	-2.399249
8	-0.679119	1.647282	-2.495226
1	-2.270000	-2.323772	0.716367
1	-1.292787	-4.571803	0.438110
1	0.623787	-0.738680	-2.054453

6	-7.472899	-2.614386	1.113642
1	-6.945982	-2.944025	2.017009
1	-7.935737	-1.646750	1.341970
1	-8.252227	-3.336912	0.867978
8	-1.750740	2.613441	0.359976
6	-1.757772	3.139495	1.476768
6	-1.315252	4.558454	1.645418
1	-1.886552	5.060495	2.429201
1	-0.259961	4.563854	1.946540
1	-1.408124	5.082653	0.691467
8	-2.102684	2.534965	2.572593
1	-2.514463	1.621204	2.372785
1	-4.871398	-1.540285	-0.711886

VII

Number of imaginary frequencies : 0

Electronic energy : =-2639.9271617
Zero-point correction= 0.569995
Thermal correction to Energy= 0.611326
Thermal correction to Enthalpy= 0.612270
Thermal correction to Gibbs Free Energy= 0.499994
Sum of electronic and zero-point Energies= -2639.357167
Sum of electronic and thermal Energies= -2639.315836
Sum of electronic and thermal Enthalpies= -2639.314892
Sum of electronic and thermal Free Energies= -2639.427168

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Cartesian Coordinates

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46	0.615763	-0.095244	0.772892
6	-2.554387	2.116418	2.608126
6	-1.274737	1.721367	2.217988
6	-1.057597	0.412352	1.790459
6	-2.102357	-0.501400	1.812577
6	-3.398806	-0.083945	2.123866
6	-3.622817	1.229877	2.532754
1	-1.934574	-1.535717	1.503596
1	-0.455111	2.438139	2.209929
1	-4.634215	1.560307	2.761726
6	-4.531152	-1.011137	1.840333
1	-4.230841	-2.063602	1.802964
1	-5.380233	-0.910203	2.527295
1	-2.723255	3.139256	2.938620
6	3.683474	-1.053749	-2.296009
6	2.563197	-0.229315	-1.647759
8	2.297715	-0.598357	-0.440333
8	2.042384	0.679021	-2.286826
1	4.621975	-0.491268	-2.226709
1	3.438520	-1.161472	-3.355869
7	3.860774	-2.362296	-1.708127

1	4.297817	-2.386895	-0.791544
6	2.839598	-3.254330	-1.866728
8	1.952924	-3.098012	-2.699141
6	2.859737	-4.441012	-0.940437
1	2.416696	-5.300353	-1.449949
1	3.862052	-4.686053	-0.578375
1	2.249789	-4.197559	-0.061044
6	0.989084	-0.793663	2.903504
6	1.648557	-1.629437	2.033092
1	0.039925	-1.085892	3.339205
1	1.510192	0.043751	3.363723
1	1.208982	-2.577246	1.718918
6	3.113537	-1.526550	1.768674
8	3.762192	-2.434296	1.293841
8	3.614340	-0.368301	2.185992
6	4.965587	-0.077451	1.800469
6	5.354609	1.213999	2.466966
1	4.985215	0.011373	0.704672
1	5.607542	-0.918139	2.089656
1	6.386479	1.473060	2.209051
1	4.697567	2.021848	2.129014
1	5.283740	1.126775	3.556291
16	-5.284387	-0.644337	0.231068
8	-6.018894	-1.812029	-0.216027
8	-5.904059	0.659009	0.271273
8	-3.981004	-0.393223	-0.745382
6	-2.980227	-1.330064	-0.983150
6	-3.210550	-2.699190	-0.953427
6	-1.700020	-0.811918	-1.256191
6	-2.152130	-3.574312	-1.189287
1	-4.211394	-3.075335	-0.764951
6	-0.670359	-1.717640	-1.533160
6	-0.884963	-3.091322	-1.489093
1	-2.340674	-4.645186	-1.170908
1	0.303965	-1.345350	-1.838872
1	-0.058625	-3.748681	-1.750885
6	0.055266	2.430077	-1.092108
6	-1.421040	0.636960	-1.366909
6	1.285213	3.028785	-0.680677
6	-0.733969	3.235017	-1.965927
6	-2.273676	1.411144	-2.188164
6	1.699582	4.254673	-1.142837
6	-0.322263	4.524649	-2.371628
6	-1.938488	2.698668	-2.468504
1	-3.164823	0.951112	-2.600000
6	0.887741	5.029208	-1.983060
1	2.672117	4.617067	-0.822993
1	-0.982889	5.089720	-3.026097
1	-2.560496	3.315412	-3.114143
1	1.225173	6.006666	-2.313837
7	-0.334355	1.151143	-0.783948
7	2.212603	2.458180	0.302138
8	1.741948	2.145531	1.390852
8	3.395886	2.420074	0.019306

[VII-VIII]‡

Number of imaginary frequencies : 1
The smallest frequency is : -284.7410 cm(-1)

Electronic energy : =-2639.9174577
Zero-point correction= 0.568806
Thermal correction to Energy= 0.609740
Thermal correction to Enthalpy= 0.610684
Thermal correction to Gibbs Free Energy= 0.498813
Sum of electronic and zero-point Energies= -2639.348651
Sum of electronic and thermal Energies= -2639.307718
Sum of electronic and thermal Enthalpies= -2639.306773
Sum of electronic and thermal Free Energies= -2639.418644

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Cartesian Coordinates

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46	0.647348	-0.211669	0.676239
6	-2.383157	1.883671	2.800439
6	-1.095476	1.430985	2.524052
6	-0.907297	0.140078	2.024316
6	-2.006838	-0.704515	1.869866
6	-3.297868	-0.235166	2.104098
6	-3.484573	1.066540	2.575215
1	-1.859057	-1.728509	1.517922
1	-0.240882	2.091366	2.652450
1	-4.493713	1.437604	2.743502
6	-4.463865	-1.099274	1.753648
1	-4.187373	-2.147595	1.600355
1	-5.283473	-1.054863	2.481277
1	-2.528125	2.893828	3.176999
6	3.730667	-0.970226	-2.353685
6	2.570774	-0.186807	-1.725400
8	2.295111	-0.609914	-0.538422
8	2.036949	0.727610	-2.342799
1	4.659685	-0.406664	-2.207060
1	3.543977	-1.037013	-3.428527
7	3.887295	-2.299365	-1.802106
1	4.293216	-2.343049	-0.871312
6	2.844415	-3.164802	-1.988059
8	1.966952	-2.965467	-2.820563
6	2.836722	-4.372074	-1.090122
1	2.315260	-5.191027	-1.591389
1	3.842416	-4.686503	-0.795377
1	2.301250	-4.109508	-0.168877
6	0.701275	-0.844622	2.880601
6	1.452847	-1.645129	1.978928
1	-0.071580	-1.330533	3.467404
1	1.214154	-0.027708	3.387573
1	1.059289	-2.625929	1.699935
6	2.927995	-1.569244	1.818142

8	3.576613	-2.458180	1.306812
8	3.448513	-0.444778	2.310541
6	4.817168	-0.187246	1.960842
6	5.230503	1.073044	2.669326
1	4.866507	-0.078170	0.867094
1	5.426581	-1.053789	2.244471
1	6.269408	1.318375	2.426670
1	4.593169	1.903964	2.352823
1	5.148766	0.955149	3.755068
16	-5.264803	-0.559390	0.223927
8	-6.055028	-1.657717	-0.296155
8	-5.839799	0.752373	0.410391
8	-3.988746	-0.266020	-0.767112
6	-3.001345	-1.204634	-1.056912
6	-3.250264	-2.570605	-1.097499
6	-1.722125	-0.684751	-1.316354
6	-2.204342	-3.443676	-1.391284
1	-4.255285	-2.944727	-0.926031
6	-0.707896	-1.585037	-1.663135
6	-0.936912	-2.957200	-1.685449
1	-2.404088	-4.512107	-1.425970
1	0.264120	-1.211039	-1.974521
1	-0.117938	-3.607228	-1.986777
6	0.079226	2.509708	-1.028901
6	-1.433833	0.767926	-1.354415
6	1.323921	3.057778	-0.596860
6	-0.684262	3.361270	-1.880731
6	-2.274975	1.588097	-2.144377
6	1.782257	4.279640	-1.025116
6	-0.228763	4.646583	-2.251616
6	-1.905305	2.873170	-2.392874
1	-3.180331	1.163866	-2.564309
6	0.997111	5.099891	-1.848022
1	2.764215	4.603049	-0.692369
1	-0.868272	5.251252	-2.891763
1	-2.511537	3.522496	-3.021516
1	1.366564	6.073926	-2.153940
7	-0.336087	1.232721	-0.756654
7	2.211479	2.418353	0.375734
8	1.706522	2.074620	1.438517
8	3.397716	2.345710	0.111985

VIII

Number of imaginary frequencies : 0

Electronic energy : =-2639.9599159
Zero-point correction= 0.570867
Thermal correction to Energy= 0.612305
Thermal correction to Enthalpy= 0.613249
Thermal correction to Gibbs Free Energy= 0.499308

Sum of electronic and zero-point Energies= -2639.389049
Sum of electronic and thermal Energies= -2639.347611
Sum of electronic and thermal Enthalpies= -2639.346667
Sum of electronic and thermal Free Energies= -2639.460608

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Cartesian Coordinates

.....

46	0.659983	-0.322810	0.383047
6	-1.278435	0.483766	2.889962
6	-0.243852	-0.434490	2.631368
6	-0.531175	-1.663526	2.006017
6	-1.865023	-1.939402	1.647275
6	-2.881876	-1.047004	1.940561
6	-2.581278	0.180147	2.560276
1	-2.093158	-2.883558	1.151191
1	0.755440	-0.253882	3.025276
1	-3.385386	0.884008	2.767905
6	-4.294723	-1.402625	1.604727
1	-4.372963	-2.377976	1.116416
1	-4.950191	-1.404355	2.485722
1	-1.038422	1.428762	3.368730
6	3.372442	-0.256773	-2.946985
6	2.255175	0.360056	-2.095493
8	2.282957	-0.084963	-0.883004
8	1.476938	1.168418	-2.589538
1	4.264440	0.376614	-2.889218
1	3.027606	-0.265545	-3.984592
7	3.723292	-1.600160	-2.540243
1	4.280521	-1.677274	-1.694647
6	2.767434	-2.568326	-2.671992
8	1.718335	-2.378804	-3.278320
6	3.129335	-3.900953	-2.066506
1	2.229102	-4.517004	-1.996197
1	3.852996	-4.415192	-2.708769
1	3.581835	-3.773843	-1.076428
6	0.571632	-2.691385	1.836587
6	1.545329	-2.120578	0.819301
1	0.143607	-3.634839	1.476637
1	1.048744	-2.888827	2.804698
1	1.539010	-2.632354	-0.148861
6	2.936828	-1.818843	1.237431
8	3.937588	-2.096800	0.606535
8	2.973639	-1.165967	2.413355
6	4.255650	-0.674585	2.830933
6	4.014226	0.246761	3.996164
1	4.720562	-0.154213	1.985286
1	4.895372	-1.528292	3.090329
1	4.963709	0.642615	4.370820
1	3.386360	1.087620	3.681608
1	3.514303	-0.279599	4.816988
16	-5.144321	-0.222899	0.525813
8	-6.184811	-0.937819	-0.185894
8	-5.437640	0.984155	1.265350
8	-3.982078	0.250876	-0.527725
6	-3.126662	-0.657681	-1.146312

6	-3.518527	-1.940719	-1.507247
6	-1.832011	-0.186500	-1.392858
6	-2.581519	-2.794625	-2.085960
1	-4.547158	-2.258147	-1.357976
6	-0.928674	-1.048995	-2.025877
6	-1.288066	-2.356356	-2.342106
1	-2.885252	-3.801062	-2.364920
1	0.046297	-0.680233	-2.336520
1	-0.544640	-2.987700	-2.823201
6	0.138394	2.777996	-0.471904
6	-1.444864	1.229526	-1.164374
6	1.343875	3.160877	0.185060
6	-0.441450	3.780338	-1.301604
6	-2.148567	2.210375	-1.903057
6	1.964737	4.363837	-0.047786
6	0.175153	5.038944	-1.477187
6	-1.640070	3.470496	-1.979840
1	-3.042550	1.919290	-2.445417
6	1.376342	5.323901	-0.884238
1	2.905731	4.562216	0.457312
1	-0.317616	5.765825	-2.120018
1	-2.116270	4.236670	-2.588505
1	1.866882	6.279919	-1.040441
7	-0.383629	1.514682	-0.416779
7	1.977014	2.350621	1.225210
8	1.239770	1.930634	2.107074
8	3.186003	2.211279	1.199702

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e

Number of imaginary frequencies : 0

Electronic energy : =-2639.931112
Zero-point correction= 0.568918
Thermal correction to Energy= 0.610528
Thermal correction to Enthalpy= 0.611472
Thermal correction to Gibbs Free Energy= 0.494846
Sum of electronic and zero-point Energies= -2639.362194
Sum of electronic and thermal Energies= -2639.320584
Sum of electronic and thermal Enthalpies= -2639.319640
Sum of electronic and thermal Free Energies= -2639.436266

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Cartesian Coordinates

.....

46	1.016098	-1.059422	-0.480479
6	-0.857170	-3.100928	3.430284
6	-0.073025	-3.334285	2.304722
6	-0.586269	-3.089811	1.033698
6	-1.904277	-2.644406	0.913344
6	-2.691351	-2.396102	2.032742
6	-2.152901	-2.617795	3.300964

1	-2.316379	-2.443481	-0.077967
1	0.950244	-3.682957	2.424365
1	-2.751764	-2.411567	4.186346
6	-4.094865	-1.900048	1.884325
1	-4.706167	-2.503951	1.203591
1	-4.615716	-1.851904	2.848002
1	-0.442893	-3.277975	4.419411
6	4.021897	1.854200	-1.202473
6	2.872768	0.860322	-1.315201
8	2.763482	0.050571	-0.313862
8	2.145101	0.897882	-2.303439
1	3.601670	2.866894	-1.183327
1	4.618436	1.775217	-2.121929
7	4.836651	1.701390	-0.021807
1	4.997876	0.750541	0.284778
6	4.902412	2.678945	0.927844
8	4.420931	3.795325	0.776630
6	5.628702	2.297003	2.191837
1	6.355712	3.078268	2.429681
1	4.900744	2.253461	3.008472
1	6.139052	1.331154	2.129833
6	0.227691	-3.183005	-0.229735
6	1.691866	-2.963888	-0.202149
1	-0.213132	-2.340391	-0.931922
1	-0.049753	-4.011279	-0.900544
1	2.241241	-2.979832	0.739842
6	2.444238	-3.342588	-1.413836
8	1.933284	-3.686807	-2.461179
8	3.763371	-3.186449	-1.221560
6	4.566189	-3.102758	-2.409704
6	4.590792	-1.672713	-2.896434
1	4.160510	-3.784686	-3.164386
1	5.558599	-3.452337	-2.109141
1	5.220514	-1.579835	-3.787567
1	3.581717	-1.323768	-3.148917
1	4.989457	-1.012372	-2.116717
16	-4.285403	-0.217001	1.261935
8	-5.682983	0.149852	1.379168
8	-3.242214	0.658553	1.754921
8	-3.985503	-0.538173	-0.342026
6	-4.483390	0.386022	-1.265083
6	-5.761553	0.181143	-1.763812
6	-3.690550	1.464281	-1.684196
6	-6.277384	1.055816	-2.710850
1	-6.337810	-0.659286	-1.387507
6	-4.235218	2.331059	-2.637306
6	-5.511326	2.132733	-3.146972
1	-7.277187	0.897052	-3.105848
1	-3.627336	3.160202	-2.994894
1	-5.906285	2.817695	-3.892709
6	0.959986	4.442242	1.092521
6	-0.190596	4.340301	0.357022
6	-0.684536	3.073229	-0.037705
6	0.028336	1.889400	0.299472
6	1.109104	2.033624	1.219043

6	1.582508	3.274586	1.569340
1	-2.519486	3.825377	-0.892260
1	1.368740	5.409901	1.366273
1	-0.744613	5.227900	0.056979
6	-1.910101	2.937484	-0.725347
1	2.433307	3.339826	2.239203
6	-1.445083	0.628677	-0.952079
6	-2.355103	1.697925	-1.113789
1	-1.669165	-0.329341	-1.419922
7	-0.312391	0.707284	-0.292119
7	1.649426	0.899593	1.980457
8	2.734407	1.038390	2.518677
8	0.942530	-0.092258	2.092821

[e-f]‡

Number of imaginary frequencies : 1
The smallest frequency is : -189.9069 cm(-1)

Electronic energy : =-2639.9200626
Zero-point correction= 0.565857
Thermal correction to Energy= 0.607126
Thermal correction to Enthalpy= 0.608071
Thermal correction to Gibbs Free Energy= 0.492706
Sum of electronic and zero-point Energies= -2639.354206
Sum of electronic and thermal Energies= -2639.312936
Sum of electronic and thermal Enthalpies= -2639.311992
Sum of electronic and thermal Free Energies= -2639.427356

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Cartesian Coordinates

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46	1.015584	-1.082210	-0.557403
6	-0.735297	-2.638237	3.572234
6	0.086764	-2.939980	2.493126
6	-0.428837	-2.938344	1.196957
6	-1.788325	-2.665988	1.009950
6	-2.610120	-2.340520	2.082031
6	-2.071712	-2.319222	3.370674
1	-2.200256	-2.657848	-0.001467
1	1.139380	-3.157571	2.658579
1	-2.705358	-2.055027	4.215660
6	-4.049849	-2.002483	1.866574
1	-4.555354	-2.654498	1.145570
1	-4.622617	-2.023371	2.801287
1	-0.322606	-2.632142	4.577511
6	4.019649	1.782595	-1.226063
6	2.910420	0.744766	-1.219050
8	2.852122	-0.024055	-0.194313
8	2.119967	0.703068	-2.172049
1	3.565474	2.779427	-1.277564
1	4.601042	1.651818	-2.149526

7	4.858925	1.743245	-0.053250
1	5.033572	0.821259	0.327249
6	4.899499	2.789507	0.822574
8	4.391481	3.879573	0.589436
6	5.622177	2.512779	2.115659
1	6.231551	3.382652	2.373242
1	4.874889	2.375210	2.904831
1	6.253938	1.620084	2.079090
6	0.413514	-3.126464	-0.006112
6	1.815770	-2.985455	-0.067478
1	-0.219099	-1.823428	-1.105421
1	-0.029837	-3.701721	-0.822788
1	2.419347	-2.770308	0.814734
6	2.532680	-3.430446	-1.285107
8	1.999753	-3.859856	-2.286091
8	3.851342	-3.236321	-1.138952
6	4.621881	-3.188496	-2.350427
6	4.616160	-1.772025	-2.876739
1	4.202568	-3.897916	-3.071438
1	5.625533	-3.519101	-2.066512
1	5.221553	-1.694157	-3.785889
1	3.595443	-1.443462	-3.110811
1	5.022963	-1.085729	-2.123704
16	-4.372166	-0.332574	1.257301
8	-5.795292	-0.076989	1.364103
8	-3.405960	0.619448	1.765850
8	-4.030097	-0.620188	-0.342596
6	-4.541181	0.303293	-1.259358
6	-5.815036	0.079550	-1.762274
6	-3.766338	1.397947	-1.670494
6	-6.345992	0.951618	-2.703187
1	-6.376229	-0.774819	-1.394889
6	-4.326365	2.259999	-2.619682
6	-5.598485	2.044559	-3.131350
1	-7.342283	0.777348	-3.100497
1	-3.731623	3.100283	-2.973282
1	-6.003822	2.727407	-3.873445
6	0.929963	4.494130	0.892155
6	-0.235531	4.354804	0.187335
6	-0.735588	3.070262	-0.136273
6	-0.013550	1.901046	0.236909
6	1.084491	2.093095	1.127807
6	1.561074	3.350557	1.411332
1	-2.584466	3.790694	-0.988633
1	1.343492	5.473804	1.110257
1	-0.798950	5.226005	-0.142068
6	-1.975801	2.908639	-0.790511
1	2.421254	3.447888	2.064660
6	-1.518418	0.591585	-0.920268
6	-2.429823	1.654208	-1.112757
1	-1.762798	-0.382484	-1.335986
7	-0.367472	0.690542	-0.290945
7	1.641628	1.000037	1.935645
8	2.715975	1.184566	2.481500
8	0.956053	-0.001482	2.076325

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f

Number of imaginary frequencies : 0

Electronic energy : =-2639.9307687
Zero-point correction= 0.566293
Thermal correction to Energy= 0.608684
Thermal correction to Enthalpy= 0.609629
Thermal correction to Gibbs Free Energy= 0.490187
Sum of electronic and zero-point Energies= -2639.364476
Sum of electronic and thermal Energies= -2639.322084
Sum of electronic and thermal Enthalpies= -2639.321140
Sum of electronic and thermal Free Energies= -2639.440582

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Cartesian Coordinates

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46	1.162771	-1.467583	-0.712877
6	-1.110542	-1.143144	3.552106
6	-0.238292	-1.786738	2.687340
6	-0.722100	-2.426984	1.541986
6	-2.100527	-2.428716	1.301264
6	-2.979892	-1.779444	2.163152
6	-2.474559	-1.127682	3.289461
1	-2.484025	-2.915481	0.402873
1	0.827400	-1.760397	2.896081
1	-3.156591	-0.600376	3.954230
6	-4.441865	-1.736112	1.862052
1	-4.782039	-2.564847	1.231961
1	-5.063055	-1.713783	2.765665
1	-0.715056	-0.629777	4.424376
6	3.298893	1.815016	-1.596140
6	2.564489	0.545725	-1.251356
8	2.954927	-0.179359	-0.295507
8	1.549036	0.226845	-1.949547
1	2.630525	2.675886	-1.452360
1	3.537474	1.789217	-2.669065
7	4.467365	1.985180	-0.772891
1	4.815085	1.140847	-0.333674
6	4.754901	3.185094	-0.187881
8	4.149549	4.213649	-0.455918
6	5.866944	3.140735	0.827340
1	6.360859	4.114133	0.856986
1	5.430284	2.938391	1.812443
1	6.602486	2.358374	0.616071
6	0.155457	-3.073577	0.562923
6	1.542230	-3.126461	0.587857
1	0.005800	-2.079099	-1.505883
1	-0.328228	-3.758567	-0.134848
1	2.137081	-2.678753	1.385244
6	2.249040	-4.066961	-0.322803

8	1.708245	-4.850129	-1.071662
8	3.572775	-3.899729	-0.211382
6	4.378087	-4.584241	-1.185873
6	4.404893	-3.800124	-2.475793
1	3.979036	-5.593567	-1.333228
1	5.368394	-4.654101	-0.727096
1	5.087760	-4.265857	-3.193964
1	3.407133	-3.765586	-2.925752
1	4.740573	-2.773722	-2.291519
16	-4.950531	-0.251883	0.981534
8	-6.348181	-0.380712	0.616218
8	-4.470235	0.943722	1.644096
8	-4.019818	-0.523232	-0.349917
6	-4.194783	0.330717	-1.441011
6	-5.284917	0.099614	-2.270519
6	-3.255038	1.338109	-1.700100
6	-5.467020	0.879120	-3.403881
1	-5.979218	-0.691737	-2.004208
6	-3.457792	2.089820	-2.867247
6	-4.543113	1.874757	-3.703556
1	-6.318371	0.699024	-4.054581
1	-2.720665	2.843709	-3.134024
1	-4.657935	2.477762	-4.600523
6	1.259929	4.764623	0.719085
6	0.081718	4.516781	0.068223
6	-0.449778	3.206120	0.009669
6	0.205231	2.118555	0.659397
6	1.412250	2.437833	1.358106
6	1.926556	3.712151	1.367626
1	-2.144891	3.760146	-1.193512
1	1.701031	5.756221	0.730434
1	-0.454576	5.316617	-0.440010
6	-1.622168	2.929051	-0.720961
1	2.864075	3.895135	1.881461
6	-1.343145	0.640054	-0.167681
6	-2.092024	1.641586	-0.842820
1	-1.653871	-0.401005	-0.257913
7	-0.263834	0.852190	0.548838
7	2.167155	1.441591	2.127838
8	3.365993	1.635716	2.277206
8	1.556634	0.507697	2.613392

III (a)

Number of imaginary frequencies : 0

Electronic energy : =-2523.2998982
Zero-point correction= 0.504807
Thermal correction to Energy= 0.544612
Thermal correction to Enthalpy= 0.545556
Thermal correction to Gibbs Free Energy= 0.429721
Sum of electronic and zero-point Energies= -2522.795092

Sum of electronic and thermal Energies= -2522.755286
Sum of electronic and thermal Enthalpies= -2522.754342
Sum of electronic and thermal Free Energies= -2522.870177

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Cartesian Coordinates

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46	-2.775580	0.230467	-0.222075
6	2.987994	-1.228664	-0.922821
1	2.347617	-1.354145	-0.040225
1	2.545165	-1.810981	-1.740712
8	1.276732	0.716480	-1.486009
6	2.866828	2.502700	0.127726
6	1.707401	2.684626	0.888185
6	3.565936	3.566602	-0.417859
6	1.242500	3.987267	1.070402
6	3.102837	4.859066	-0.194142
1	4.449711	3.363511	-1.016600
6	1.941100	5.067249	0.542868
1	0.316212	4.144439	1.619904
1	3.641506	5.703646	-0.615317
1	1.566818	6.075599	0.696465
6	-3.814783	-2.007961	-1.628487
6	-4.738125	-0.822360	-1.936030
8	-4.377227	0.318045	-1.413976
8	-5.733919	-0.999045	-2.604870
1	-3.801902	-2.675098	-2.496991
7	-2.482790	-1.523477	-1.269263
6	-1.426476	-2.183377	-1.568756
8	-0.207047	-1.678270	-1.383244
8	3.325043	1.202329	-0.105316
16	2.712485	0.466552	-1.446684
8	3.536397	0.808848	-2.585356
6	4.422869	-1.554655	-0.665539
6	4.902281	-1.606110	0.643265
6	5.295499	-1.800821	-1.726263
6	6.235277	-1.907134	0.892833
1	4.216440	-1.407370	1.467206
6	6.629967	-2.096887	-1.477301
1	4.926313	-1.752760	-2.749017
6	7.100901	-2.152004	-0.168883
1	6.600399	-1.949393	1.916052
1	7.304566	-2.287371	-2.308127
1	8.144766	-2.387154	0.024215
1	-0.239764	-0.711212	-1.248453
1	-4.239236	-2.558372	-0.775366
6	1.500206	0.506569	2.115198
6	0.764897	-0.673724	2.367554
6	0.954180	1.508084	1.357654
6	1.337802	-1.733777	3.109720
6	-0.543133	-0.796149	1.812313
6	-0.347230	1.311259	0.844945
6	0.668500	-2.916426	3.285623
1	2.331237	-1.586476	3.530652
6	-1.212732	-2.024860	2.065337
1	-0.802784	2.070252	0.195948

6	-0.618692	-3.060475	2.745581
1	1.115767	-3.733646	3.843256
1	-1.182514	-3.979931	2.873708
7	-1.058657	0.209493	1.034949
7	-2.603572	-2.261857	1.669419
8	-2.853395	-3.340349	1.145544
8	-3.410389	-1.382295	1.905073
1	2.515237	0.592591	2.502665
6	-1.413821	-3.563648	-2.132738
1	-1.741186	-3.551817	-3.178662
1	-0.401240	-3.968817	-2.094172
1	-2.093151	-4.213253	-1.572859
8	-3.464963	1.856971	0.766243
6	-3.144456	3.009451	0.261283
6	-4.024574	4.131756	0.756831
1	-3.543324	5.097048	0.584102
1	-4.966970	4.100208	0.199775
1	-4.267515	4.001030	1.814936
8	-2.229707	3.211095	-0.538931

III (b)

Number of imaginary frequencies : 0

Electronic energy : =-2523.3258699
Zero-point correction= 0.504618
Thermal correction to Energy= 0.544280
Thermal correction to Enthalpy= 0.545224
Thermal correction to Gibbs Free Energy= 0.430156
Sum of electronic and zero-point Energies= -2522.821252
Sum of electronic and thermal Energies= -2522.781590
Sum of electronic and thermal Enthalpies= -2522.780646
Sum of electronic and thermal Free Energies= -2522.895714

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Cartesian Coordinates

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46	2.583906	0.286346	0.370259
6	-3.202651	-0.682943	1.779941
1	-2.122280	-0.671033	1.572409
1	-3.349521	-0.915501	2.843913
8	-2.699329	1.867126	2.274353
6	-3.253404	2.468296	-0.389349
6	-2.003160	2.556021	-1.008219
6	-4.051974	3.586416	-0.195306
6	-1.565361	3.816789	-1.422622
6	-3.598324	4.829061	-0.620685
1	-5.012749	3.463981	0.299406
6	-2.353178	4.945229	-1.231251
1	-0.598130	3.902079	-1.916181
1	-4.218217	5.708782	-0.469358
1	-1.996390	5.915840	-1.565559
6	3.163308	-2.047715	1.906885

6	4.267821	-1.048370	2.221674
8	4.081319	0.156676	1.696659
8	5.232702	-1.340171	2.885429
1	2.888856	-2.524433	2.855445
7	2.029562	-1.422087	1.246515
6	0.754856	-1.788910	1.458836
8	-0.217158	-1.179761	0.984643
8	-3.685771	1.226009	0.044279
16	-3.725792	1.022795	1.696262
8	-5.110984	1.166457	2.105670
6	-3.932349	-1.634460	0.879415
6	-3.179373	-2.451279	0.033067
6	-5.323694	-1.756694	0.896261
6	-3.813899	-3.385296	-0.781111
1	-2.092176	-2.353241	0.037279
6	-5.952068	-2.679924	0.069102
1	-5.912040	-1.116031	1.550278
6	-5.199884	-3.498856	-0.768938
1	-3.217646	-4.032331	-1.422926
1	-7.036069	-2.765149	0.083933
1	-5.694857	-4.228088	-1.406365
1	3.615895	-2.828720	1.273855
6	-1.642272	0.211176	-1.817777
6	-0.769219	-0.861184	-2.088211
6	-1.170236	1.361076	-1.227673
6	-1.233954	-2.042655	-2.712479
6	0.591419	-0.745572	-1.695835
6	0.174356	1.352556	-0.799300
6	-0.393286	-3.104573	-2.922292
1	-2.282847	-2.092274	-2.998207
6	1.441727	-1.839927	-2.001516
1	0.558702	2.192977	-0.222048
6	0.961613	-2.997749	-2.562245
1	-0.756208	-4.017915	-3.385097
1	1.659757	-3.808404	-2.749464
7	1.005002	0.345086	-0.989035
7	2.896142	-1.768031	-1.826808
8	3.461404	-2.766735	-1.415714
8	3.443554	-0.724563	-2.146935
1	-2.692849	0.116164	-2.089330
6	0.508382	-3.026186	2.303373
1	0.743047	-2.833386	3.357049
1	-0.551918	-3.280087	2.226430
1	1.112244	-3.881605	1.982188
8	3.311976	2.101779	-0.447833
6	4.431200	2.594644	-0.232409
6	4.881392	3.804441	-0.980392
1	5.204197	4.575227	-0.274804
1	5.751428	3.540556	-1.590025
1	4.081964	4.178742	-1.619674
8	5.301842	2.143143	0.616058
1	4.972679	1.332287	1.121521

III (c)

Number of imaginary frequencies : 0

Electronic energy : =-2294.3079895
Zero-point correction= 0.440241
Thermal correction to Energy= 0.474535
Thermal correction to Enthalpy= 0.475479
Thermal correction to Gibbs Free Energy= 0.372286
Sum of electronic and zero-point Energies= -2293.867748
Sum of electronic and thermal Energies= -2293.833455
Sum of electronic and thermal Enthalpies= -2293.832511
Sum of electronic and thermal Free Energies= -2293.935703

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Cartesian Coordinates

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46	-1.344126	1.060537	0.688065
6	0.355015	-2.149676	-1.852095
1	0.238010	-1.073160	-1.678408
1	0.898987	-2.308249	-2.791351
8	2.006820	-4.028469	-0.886389
6	3.689280	-1.408013	-0.019962
6	3.862587	-0.118665	0.497332
6	4.564607	-2.440079	0.289628
6	4.968150	0.123897	1.314741
6	5.638717	-2.181766	1.133603
1	4.397467	-3.424070	-0.140270
6	5.847841	-0.901736	1.637810
1	5.110371	1.121829	1.726270
1	6.323022	-2.986609	1.388789
1	6.692990	-0.703463	2.291356
6	-2.999343	-0.059410	2.751725
6	-1.551592	-0.352700	3.117535
8	-0.659089	0.007132	2.205736
8	-1.236570	-0.861223	4.168239
1	-3.384163	0.661190	3.491753
7	-3.092927	0.442744	1.395871
6	-4.062764	0.089027	0.523899
8	-3.959523	0.247696	-0.694941
8	2.665355	-1.591520	-0.935909
16	1.483323	-2.712174	-0.574920
8	0.981789	-2.408811	0.749523
6	-0.958438	-2.866080	-1.787256
6	-2.110948	-2.156751	-1.451686
6	-1.042152	-4.229053	-2.082568
6	-3.343949	-2.800766	-1.426902
1	-2.075448	-1.089541	-1.225813
6	-2.272176	-4.872960	-2.035823
1	-0.143151	-4.783592	-2.346507
6	-3.423926	-4.159351	-1.712164
1	-4.228544	-2.209352	-1.200796
1	-2.333186	-5.934811	-2.262323
1	-4.386800	-4.665074	-1.691437
1	-3.559248	-0.991726	2.900932

6	3.262467	2.145910	-0.390528
6	2.280994	3.092227	-0.764722
6	2.900047	0.945033	0.161795
6	2.661071	4.319928	-1.347896
6	0.903481	2.769901	-0.570912
6	1.523971	0.750265	0.420250
6	1.715784	5.224880	-1.755926
1	3.722775	4.526377	-1.468469
6	-0.052746	3.718461	-1.051967
1	1.186549	-0.129987	0.973539
6	0.359639	4.910411	-1.616471
1	2.003088	6.171437	-2.202975
1	-0.401935	5.597281	-1.967819
7	0.580409	1.610732	0.071583
7	-1.516886	3.530509	-1.065526
8	-2.193234	4.453428	-1.468559
8	-2.045275	2.459400	-0.731711
1	4.311065	2.372909	-0.581972
6	-5.321967	-0.523444	1.109432
1	-5.657686	-0.018412	2.021299
1	-6.104374	-0.469312	0.349247
1	-5.151442	-1.579479	1.356053

III (d)

Number of imaginary frequencies : 0

Electronic energy : =-3083.8724255
Zero-point correction= 0.508222
Thermal correction to Energy= 0.551954
Thermal correction to Enthalpy= 0.552899
Thermal correction to Gibbs Free Energy= 0.430001
Sum of electronic and zero-point Energies= -3083.364203
Sum of electronic and thermal Energies= -3083.320471
Sum of electronic and thermal Enthalpies= -3083.319527
Sum of electronic and thermal Free Energies= -3083.442424

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Cartesian Coordinates

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46	1.549145	-0.541848	-0.751275
6	-2.932832	-1.303733	0.798285
1	-1.867873	-1.051278	0.881493
1	-3.256483	-1.731397	1.756416
8	-3.205068	1.153807	1.779616
6	-3.394391	2.113742	-0.992506
6	-2.420989	3.081764	-0.714672
6	-4.622447	2.452763	-1.544360
6	-2.718491	4.411550	-1.033916
6	-4.895035	3.781314	-1.845380
1	-5.347084	1.660986	-1.711962
6	-3.940815	4.761838	-1.591123
1	-1.963074	5.176325	-0.861157

1	-5.854041	4.049656	-2.280588
1	-4.144881	5.800992	-1.835410
6	3.888394	-1.321947	-2.257480
6	3.177473	-2.597579	-1.805362
8	2.061269	-2.428817	-1.142084
8	3.673390	-3.674629	-2.053005
1	4.260394	-1.479764	-3.276669
7	3.009558	-0.160334	-2.163282
6	3.294934	0.931056	-2.774880
8	2.498926	1.991145	-2.687410
8	-3.128778	0.788821	-0.705597
16	-3.754255	0.276901	0.760796
8	-5.192327	0.159505	0.606002
6	-3.214195	-2.183881	-0.379360
6	-2.174489	-2.478361	-1.264195
6	-4.479807	-2.733008	-0.592067
6	-2.401009	-3.316837	-2.350062
1	-1.180687	-2.071166	-1.075839
6	-4.704449	-3.561973	-1.684674
1	-5.289961	-2.502101	0.097367
6	-3.665397	-3.856003	-2.563569
1	-1.580370	-3.556849	-3.022098
1	-5.692562	-3.987135	-1.845564
1	-3.841136	-4.513899	-3.411850
1	1.743966	1.759461	-2.117284
1	4.758004	-1.175932	-1.598829
6	-0.531098	3.564042	0.827368
6	0.787694	3.336692	1.269218
6	-1.114133	2.754239	-0.119511
6	1.395642	4.201067	2.209858
6	1.514032	2.247235	0.710034
6	-0.353950	1.643380	-0.549616
6	2.709964	4.044048	2.559930
1	0.795207	5.003130	2.633362
6	2.875053	2.137378	1.095243
1	-0.790402	0.925600	-1.243070
6	3.463333	3.014788	1.969549
1	3.180076	4.712593	3.274548
1	4.517992	2.893294	2.202439
7	0.898770	1.404154	-0.179587
7	3.770091	1.099819	0.559341
8	4.635763	1.475185	-0.216828
8	3.599902	-0.047406	0.930411
1	-1.085707	4.404353	1.242492
6	4.507851	1.153946	-3.606431
1	4.547255	0.443099	-4.438386
1	4.510210	2.170926	-4.000475
1	5.402094	0.998276	-2.992346
8	0.208914	-1.152079	0.610203
6	0.747558	-1.836995	1.670481
1	1.839101	-1.997360	1.592850
6	0.523659	-1.010902	2.937972
6	0.147151	-3.243425	1.778625
9	0.937245	-1.632715	4.042979
9	1.210638	0.141176	2.847761

9	-0.757779	-0.683178	3.105631
9	0.228542	-3.873905	0.618036
9	0.792186	-3.973324	2.693846
9	-1.147810	-3.209623	2.134673

III (e)

Number of imaginary frequencies : 0

Electronic energy : =-3083.8668801
Zero-point correction= 0.507531
Thermal correction to Energy= 0.551612
Thermal correction to Enthalpy= 0.552556
Thermal correction to Gibbs Free Energy= 0.426653
Sum of electronic and zero-point Energies= -3083.359349
Sum of electronic and thermal Energies= -3083.315268
Sum of electronic and thermal Enthalpies= -3083.314324
Sum of electronic and thermal Free Energies= -3083.440227

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Cartesian Coordinates

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46	-2.365656	-0.708560	-0.340025
6	4.572884	-1.064790	-0.631080
1	3.973070	-1.370376	0.235171
1	4.478864	-1.839042	-1.402653
8	2.274936	-0.057248	-1.475018
6	3.020999	2.460365	-0.050339
6	1.740202	2.398461	0.509554
6	3.518099	3.615694	-0.630570
6	0.945501	3.545713	0.452358
6	2.721331	4.755578	-0.647618
1	4.512321	3.594991	-1.068492
6	1.437810	4.717449	-0.110974
1	-0.068364	3.512125	0.847865
1	3.100387	5.670778	-1.094576
1	0.808008	5.602416	-0.138289
6	-3.442213	-2.998692	-1.679325
6	-4.457270	-1.865326	-1.850065
8	-4.095999	-0.713633	-1.340965
8	-5.511405	-2.075325	-2.407991
1	-3.474179	-3.630124	-2.574025
7	-2.113558	-2.454012	-1.418350
6	-1.051197	-3.041964	-1.828461
8	0.150536	-2.496929	-1.661200
8	3.824853	1.317553	-0.032240
16	3.672755	0.319716	-1.336704
8	4.386156	0.902938	-2.452669
6	5.992675	-0.749219	-0.289631
6	6.340404	-0.407263	1.017321
6	6.976789	-0.772133	-1.278378
6	7.657145	-0.100716	1.336539
1	5.565784	-0.374228	1.783632

6	8.293646	-0.463001	-0.960088
1	6.704080	-1.024278	-2.301797
6	8.635257	-0.128938	0.346891
1	7.920754	0.161926	2.358072
1	9.055580	-0.483744	-1.735100
1	9.666492	0.110207	0.595068
1	0.054995	-1.587844	-1.324806
1	-3.755631	-3.609534	-0.819873
6	1.896141	0.281585	1.865558
6	1.375952	-0.997015	2.161152
6	1.215691	1.123669	1.023925
6	2.099443	-1.896799	2.980238
6	0.129448	-1.383286	1.585348
6	-0.011335	0.664939	0.503983
6	1.642305	-3.167714	3.209826
1	3.037860	-1.554011	3.413055
6	-0.322710	-2.693641	1.895269
1	-0.567564	1.307844	-0.173502
6	0.419004	-3.569434	2.649216
1	2.206533	-3.860520	3.826759
1	0.023015	-4.566344	2.820880
7	-0.533630	-0.527353	0.744855
7	-1.639170	-3.187032	1.480994
8	-1.674935	-4.282190	0.936374
8	-2.600109	-2.481842	1.727576
1	2.858883	0.570830	2.285320
6	-1.011263	-4.371297	-2.499891
1	-1.510651	-4.325568	-3.473898
1	0.024266	-4.679332	-2.650341
1	-1.532341	-5.115386	-1.888590
8	-2.800153	0.968649	0.646865
6	-3.712216	1.818729	0.081005
1	-4.220803	1.413414	-0.813220
6	-4.819723	2.100085	1.091838
6	-2.987726	3.082348	-0.370205
9	-5.714403	2.975375	0.616953
9	-5.464084	0.969343	1.371081
9	-4.341291	2.593481	2.236104
9	-1.996481	2.750558	-1.221874
9	-3.776474	3.946678	-1.004245
9	-2.409739	3.733098	0.651205

III

Number of imaginary frequencies : 0

Electronic energy : =-3083.9008127
Zero-point correction= 0.509265
Thermal correction to Energy= 0.552173
Thermal correction to Enthalpy= 0.553117
Thermal correction to Gibbs Free Energy= 0.434803
Sum of electronic and zero-point Energies= -3083.391548

Sum of electronic and thermal Energies= -3083.348640
Sum of electronic and thermal Enthalpies= -3083.347696
Sum of electronic and thermal Free Energies= -3083.466009

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Cartesian Coordinates

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46	-2.322309	-0.009302	-0.754543
6	3.978914	-0.488229	1.471529
1	3.453293	-1.321196	0.983158
1	4.481663	-0.914047	2.351326
8	6.081075	-1.380029	0.226429
6	4.110748	-0.722809	-1.858392
6	2.740634	-0.689200	-2.156192
6	4.956967	-1.670691	-2.422475
6	2.244428	-1.670659	-3.023738
6	4.432919	-2.633869	-3.274052
1	6.012970	-1.649617	-2.176680
6	3.074418	-2.637617	-3.571419
1	1.191120	-1.651681	-3.295707
1	5.093959	-3.376827	-3.712049
1	2.662234	-3.382601	-4.246545
6	-5.118725	0.478852	-1.309308
6	-4.340493	1.741463	-1.679028
8	-3.039896	1.690752	-1.507898
8	-4.933587	2.711754	-2.094276
1	-5.767603	0.230698	-2.159619
7	-4.239055	-0.629431	-0.957204
6	-4.697979	-1.827500	-0.781883
8	-3.934543	-2.833499	-0.452720
8	4.624558	0.269298	-1.027564
16	5.363745	-0.133718	0.392289
8	6.046158	1.082835	0.769206
6	3.027952	0.612950	1.859260
6	1.785583	0.203747	2.355889
6	3.337012	1.973100	1.847278
6	0.859137	1.130000	2.818724
1	1.556030	-0.860145	2.409535
6	2.407161	2.899912	2.314548
1	4.304372	2.310774	1.484111
6	1.169922	2.487445	2.795464
1	-0.103970	0.788660	3.193808
1	2.661241	3.957794	2.305068
1	0.452718	3.217878	3.164892
1	-2.980025	-2.539721	-0.285183
1	-5.773267	0.739535	-0.465117
6	2.149521	1.675980	-1.508711
6	1.212487	2.593882	-0.994765
6	1.834244	0.339839	-1.617082
6	1.520667	3.974689	-0.930587
6	-0.046663	2.111266	-0.535669
6	0.521160	-0.025109	-1.256732
6	0.614847	4.872119	-0.432614
1	2.492228	4.301254	-1.296389
6	-0.901077	3.063669	0.088281
1	0.188826	-1.054829	-1.375600

6	-0.598787	4.402688	0.099276
1	0.838744	5.934264	-0.405725
1	-1.310095	5.079786	0.562556
7	-0.377100	0.800526	-0.745872
7	-2.068124	2.679536	0.888455
8	-2.985809	3.470024	0.975190
8	-2.001959	1.607971	1.478782
1	3.122016	2.046003	-1.827474
6	-6.141778	-2.170979	-0.946565
1	-6.478211	-1.952709	-1.966066
1	-6.291253	-3.230558	-0.736020
1	-6.758881	-1.574434	-0.265888
8	-1.600320	-1.815627	-0.086876
6	-0.981363	-1.791736	1.136841
1	-0.454838	-0.840239	1.332823
6	-1.957886	-1.962779	2.301903
6	0.101448	-2.872367	1.144579
9	-1.389803	-1.589345	3.453945
9	-3.038525	-1.204578	2.116906
9	-2.370143	-3.225707	2.428763
9	1.101119	-2.507487	0.319216
9	0.642792	-3.031223	2.359995
9	-0.347103	-4.048463	0.733749

III (f)

Number of imaginary frequencies : 0

Electronic energy : =-3083.8821453
Zero-point correction= 0.509582
Thermal correction to Energy= 0.552756
Thermal correction to Enthalpy= 0.553700
Thermal correction to Gibbs Free Energy= 0.434830
Sum of electronic and zero-point Energies= -3083.372563
Sum of electronic and thermal Energies= -3083.329390
Sum of electronic and thermal Enthalpies= -3083.328445
Sum of electronic and thermal Free Energies= -3083.447315

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Cartesian Coordinates

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46	2.343812	0.300407	0.249708
6	-4.284253	0.235104	-1.490757
1	-4.958023	0.478047	-2.323655
1	-4.029401	1.180491	-0.994864
8	-5.671766	-1.957205	-0.768150
6	-3.992549	0.238430	1.752456
6	-2.611413	0.300635	2.008913
6	-4.881077	1.155788	2.302009
6	-2.162923	1.338985	2.837729
6	-4.397006	2.182347	3.102157

1	-5.939967	1.055075	2.090424
6	-3.036365	2.273905	3.371414
1	-1.105588	1.407809	3.083139
1	-5.091792	2.902616	3.525852
1	-2.652983	3.066622	4.007671
6	5.134271	-0.351930	0.354379
6	5.031520	1.114072	-0.074364
8	3.812955	1.597024	-0.125790
8	6.030711	1.736821	-0.354543
1	6.035546	-0.474474	0.965257
7	3.919401	-0.762196	1.048342
6	3.925242	-1.646153	1.975864
8	2.803528	-1.952614	2.622871
8	-4.454586	-0.824112	0.987129
16	-5.398049	-0.601106	-0.351622
8	-6.470846	0.322746	-0.043550
6	-3.072348	-0.526656	-1.930159
6	-3.187091	-1.776624	-2.547084
6	-1.814224	0.065815	-1.805441
6	-2.054434	-2.421690	-3.029941
1	-4.166197	-2.239887	-2.646869
6	-0.683777	-0.573162	-2.308111
1	-1.702331	1.043575	-1.333085
6	-0.803872	-1.819473	-2.915063
1	-2.153080	-3.393048	-3.510053
1	0.282571	-0.082609	-2.209804
1	0.082922	-2.311859	-3.310149
1	2.097137	-1.365013	2.295998
1	5.251447	-0.963260	-0.552670
6	-1.906037	-1.985615	1.167203
6	-0.913092	-2.805317	0.593348
6	-1.645649	-0.659867	1.441514
6	-1.181518	-4.169870	0.329656
6	0.356863	-2.242581	0.279541
6	-0.337398	-0.210335	1.160111
6	-0.222246	-4.986401	-0.208252
1	-2.172244	-4.550278	0.568883
6	1.292828	-3.113407	-0.339836
1	-0.076903	0.826449	1.348330
6	1.030606	-4.446102	-0.544001
1	-0.424945	-6.036013	-0.398014
1	1.801333	-5.060835	-1.000578
7	0.630490	-0.945278	0.626693
7	2.563772	-2.637149	-0.891892
8	3.574807	-3.254304	-0.588734
8	2.519049	-1.673758	-1.638720
1	-2.877504	-2.422648	1.381058
6	5.111964	-2.429293	2.415101
1	5.874838	-1.769614	2.842161
1	4.816253	-3.162002	3.167050
1	5.553773	-2.944025	1.554879
8	0.965531	1.450565	-0.623192
6	1.172946	2.801292	-0.682655
1	2.216473	3.114492	-0.495269
6	0.840255	3.273734	-2.093442

6	0.311668	3.463332	0.387600
9	1.033177	4.586825	-2.241605
9	1.620360	2.641765	-2.967329
9	-0.432186	3.012592	-2.418731
9	0.717321	3.031771	1.600743
9	0.385879	4.790645	0.391470
9	-0.980544	3.122695	0.280320

III (g)

Number of imaginary frequencies : 0

Electronic energy : =-3083.9002238
Zero-point correction= 0.509990
Thermal correction to Energy= 0.552768
Thermal correction to Enthalpy= 0.553712
Thermal correction to Gibbs Free Energy= 0.435259
Sum of electronic and zero-point Energies= -3083.390234
Sum of electronic and thermal Energies= -3083.347456
Sum of electronic and thermal Enthalpies= -3083.346512
Sum of electronic and thermal Free Energies= -3083.464965

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Cartesian Coordinates

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46	-2.341289	0.038113	-0.732209
6	4.191113	-0.540799	1.453620
1	3.559497	-1.357337	1.075939
1	4.733861	-0.932775	2.324945
8	6.096175	-1.693122	0.089825
6	4.050451	-0.993909	-1.892031
6	2.665259	-0.915126	-2.100762
6	4.823911	-1.984876	-2.485621
6	2.083476	-1.897117	-2.914762
6	4.214200	-2.949083	-3.276535
1	5.894364	-1.994760	-2.311359
6	2.840432	-2.907570	-3.488338
1	1.017468	-1.844417	-3.125299
1	4.818959	-3.725919	-3.736432
1	2.358576	-3.650796	-4.117646
6	-5.076651	0.651841	-1.438903
6	-4.213457	1.850393	-1.831764
8	-2.925647	1.733649	-1.606063
8	-4.732578	2.832881	-2.312330
1	-5.714949	0.409458	-2.298591
7	-4.274404	-0.490522	-1.018636
6	-4.797935	-1.663402	-0.858917
8	-4.101209	-2.699129	-0.475720
8	4.659456	0.000872	-1.133224
16	5.499905	-0.381703	0.234758
8	6.310502	0.791521	0.467913
6	3.377813	0.676959	1.789035
6	2.015177	0.494971	2.037622

6	3.936387	1.946693	1.955849
6	1.220008	1.558156	2.450924
1	1.583614	-0.499945	1.930996
6	3.134025	3.013029	2.348693
1	4.996382	2.100201	1.776427
6	1.779398	2.823273	2.601390
1	0.160635	1.400371	2.646963
1	3.578720	3.997997	2.473353
1	1.161300	3.657449	2.926431
1	-3.152118	-2.445527	-0.242138
1	-5.737903	0.982687	-0.624859
6	2.208260	1.482176	-1.451254
6	1.320296	2.453495	-0.948699
6	1.825501	0.161180	-1.543290
6	1.707072	3.814710	-0.889114
6	0.028996	2.048923	-0.504620
6	0.501445	-0.133610	-1.157140
6	0.841339	4.770708	-0.430308
1	2.707959	4.077179	-1.225975
6	-0.792335	3.060923	0.067694
1	0.120548	-1.150762	-1.228311
6	-0.416060	4.381381	0.063069
1	1.127002	5.817960	-0.408340
1	-1.105273	5.106772	0.485087
7	-0.359758	0.749471	-0.678599
7	-2.014643	2.759202	0.818164
8	-2.898064	3.591051	0.830546
8	-2.032387	1.702987	1.442605
1	3.196622	1.799075	-1.777175
6	-6.243682	-1.945662	-1.103810
1	-6.509216	-1.737573	-2.146130
1	-6.453514	-2.992368	-0.880512
1	-6.872094	-1.307076	-0.473514
8	-1.748130	-1.758640	0.072243
6	-1.262310	-1.706393	1.354918
1	-0.786550	-0.739220	1.605045
6	-2.373678	-1.890285	2.390524
6	-0.160935	-2.757276	1.495701
9	-1.951033	-1.618519	3.625146
9	-3.382481	-1.060310	2.112860
9	-2.858441	-3.133950	2.379321
9	0.870272	-2.430517	0.688545
9	0.324935	-2.804802	2.738510
9	-0.562307	-3.972180	1.151693

III (h)

Number of imaginary frequencies : 1

Electronic energy : =-2294.2823009
Zero-point correction= 0.438555
Thermal correction to Energy= 0.472682

Thermal correction to Enthalpy= 0.473626
Thermal correction to Gibbs Free Energy= 0.369315
Sum of electronic and zero-point Energies= -2293.843746
Sum of electronic and thermal Energies= -2293.809619
Sum of electronic and thermal Enthalpies= -2293.808675
Sum of electronic and thermal Free Energies= -2293.912986

Cartesian Coordinates

46	3.983123	-0.586664	0.057397
6	-2.374653	1.421614	-1.772766
1	-1.837063	0.498638	-1.518749
1	-2.395000	1.519905	-2.866660
8	-4.405672	-0.283872	-1.830873
6	-4.834651	0.216349	0.938261
6	-4.448211	-1.092025	1.247011
6	-6.080351	0.716427	1.283040
6	-5.362056	-1.896443	1.930875
6	-6.970698	-0.100718	1.970686
1	-6.328555	1.735833	0.999350
6	-6.611311	-1.405817	2.293483
1	-5.075338	-2.913789	2.192468
1	-7.947806	0.282924	2.251945
1	-7.305087	-2.044378	2.833947
6	6.070302	1.385473	0.360881
6	6.733814	0.024842	0.241025
8	5.896666	-0.995350	0.129090
8	7.932889	-0.123532	0.252030
1	6.455907	2.019035	-0.452924
7	4.632915	1.238528	0.307096
6	3.736149	2.163458	0.722103
8	2.538595	1.909825	0.850452
8	-3.939660	1.035972	0.265034
16	-4.089840	1.061662	-1.385123
8	-4.958101	2.168593	-1.734428
6	-1.796372	2.618668	-1.082357
6	-0.669980	2.461775	-0.273750
6	-2.349859	3.888925	-1.262045
6	-0.095309	3.565370	0.349842
1	-0.219280	1.477186	-0.137519
6	-1.784228	4.985661	-0.624941
1	-3.230473	4.010327	-1.889716
6	-0.658216	4.825346	0.179167
1	0.800689	3.411736	0.947255
1	-2.221949	5.971960	-0.761942
1	-0.214765	5.690098	0.668400
1	6.413830	1.833656	1.305327
6	-2.996752	-2.775276	0.126227
6	-1.721015	-3.198756	-0.309681
6	-3.133255	-1.596930	0.818693
6	-1.524539	-4.409969	-1.010364
6	-0.617072	-2.344332	-0.029638
6	-1.944908	-0.861881	1.088947
6	-0.268886	-4.803875	-1.412636
1	-2.392310	-5.030561	-1.226920

6	0.659013	-2.783179	-0.494835
1	-2.008813	0.056746	1.674578
6	0.838024	-3.987784	-1.146012
1	-0.126998	-5.738614	-1.946219
1	1.836388	-4.273272	-1.463458
7	-0.746147	-1.205509	0.682413
7	1.822660	-1.980032	-0.294526
8	2.945328	-2.527211	-0.237606
8	1.759647	-0.751062	-0.192834
1	-3.872957	-3.374186	-0.120546
6	4.288044	3.542803	1.013442
1	4.838993	3.543014	1.961777
1	4.973924	3.890879	0.233714
1	3.448769	4.236662	1.097846

III (i)

Number of imaginary frequencies : 0

Electronic energy : =-2523.3312742
Zero-point correction= 0.506352
Thermal correction to Energy= 0.545429
Thermal correction to Enthalpy= 0.546373
Thermal correction to Gibbs Free Energy= 0.434577
Sum of electronic and zero-point Energies= -2522.824922
Sum of electronic and thermal Energies= -2522.785845
Sum of electronic and thermal Enthalpies= -2522.784901
Sum of electronic and thermal Free Energies= -2522.896697

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Cartesian Coordinates

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46	-2.451179	-0.524157	-0.194933
6	4.398384	-0.178366	1.742009
1	4.183883	-1.247857	1.623619
1	5.088156	-0.078409	2.590908
8	6.561072	-0.711834	0.361156
6	4.036189	-1.290738	-1.287256
6	2.653005	-1.438389	-1.486080
6	4.923633	-2.341902	-1.486277
6	2.197955	-2.706425	-1.872951
6	4.434577	-3.587092	-1.860013
1	5.985086	-2.171906	-1.341502
6	3.069960	-3.770128	-2.051839
1	1.136379	-2.853324	-2.057283
1	5.128176	-4.409508	-2.013791
1	2.681489	-4.738159	-2.355973
6	-5.128717	-0.674269	-1.300880
6	-4.234001	0.039151	-2.313356
8	-2.986722	0.231153	-1.958054
8	-4.699911	0.385128	-3.376334
1	-5.493766	-1.594746	-1.778156

7	-4.434725	-0.975320	-0.052859
6	-5.100610	-1.270240	1.016067
8	-4.526687	-1.483155	2.173458
8	4.503008	-0.023051	-0.953128
16	5.468014	0.239739	0.353979
8	5.713391	1.661906	0.286336
6	3.157212	0.642473	1.905993
6	1.917206	0.003178	1.983178
6	3.223093	2.029888	2.061184
6	0.759591	0.737854	2.223675
1	1.852354	-1.080014	1.855404
6	2.063698	2.763978	2.284139
1	4.186126	2.532104	2.001640
6	0.832477	2.120277	2.369406
1	-0.209167	0.241926	2.275263
1	2.125340	3.843926	2.398089
1	-0.079181	2.687451	2.546354
1	-3.532092	-1.378326	2.111086
1	-5.998205	-0.024942	-1.135747
6	1.946382	0.992493	-1.554572
6	0.963818	1.972405	-1.302435
6	1.691068	-0.336111	-1.298066
6	1.226383	3.336628	-1.572455
6	-0.289007	1.571347	-0.760818
6	0.395245	-0.650374	-0.828120
6	0.275136	4.294577	-1.342306
1	2.202837	3.600479	-1.973169
6	-1.217263	2.608838	-0.475778
1	0.124065	-1.677703	-0.588360
6	-0.962002	3.920230	-0.790102
1	0.470910	5.339119	-1.565135
1	-1.725995	4.662082	-0.575262
7	-0.545237	0.241199	-0.573659
7	-2.456310	2.383781	0.280526
8	-3.485320	2.860934	-0.157251
8	-2.348670	1.776295	1.338169
1	2.905677	1.314770	-1.950152
6	-6.588765	-1.388752	1.046730
1	-6.956028	-1.992636	0.211648
1	-6.898813	-1.836924	1.991709
1	-7.046101	-0.395926	0.962337
8	-1.987098	-1.299864	1.672375
6	-1.166825	-2.309373	1.832513
6	-1.068809	-2.752428	3.272919
1	-2.065581	-2.911617	3.698122
1	-0.479300	-3.667797	3.348648
1	-0.592163	-1.960747	3.862874
8	-0.509096	-2.835760	0.945147

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meta-C-H-activation –OMe substituted quinoline -**PRC** (Pre reacting Complex)

Number of imaginary frequencies : 0

Electronic energy : =-2204.3835631
Zero-point correction= 0.470828
Thermal correction to Energy= 0.504605
Thermal correction to Enthalpy= 0.505549
Thermal correction to Gibbs Free Energy= 0.406582
Sum of electronic and zero-point Energies= -2203.912735
Sum of electronic and thermal Energies= -2203.878958
Sum of electronic and thermal Enthalpies= -2203.878014
Sum of electronic and thermal Free Energies= -2203.976981

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Cartesian Coordinates

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46	1.800512	-0.393504	-0.411269
6	1.240575	-2.088016	1.283599
6	1.469300	-2.713007	0.047176
6	0.379442	-3.226120	-0.689858
6	-0.890612	-3.178423	-0.163050
6	-1.121218	-2.606506	1.106784
6	-0.070232	-2.033193	1.800618
1	-1.728991	-3.605935	-0.710738
6	-2.496987	-2.674524	1.694419
1	-2.482978	-2.718644	2.789936
1	-3.069478	-3.531392	1.322874
8	-2.920011	-0.046591	1.891746
6	-4.033668	-0.323751	-1.026527
6	-3.441881	0.922074	-1.270437
6	-5.270486	-0.671434	-1.548618
6	-4.147999	1.815108	-2.082467
6	-5.947989	0.234668	-2.355011
1	-5.682452	-1.647340	-1.307330
6	-5.382388	1.477586	-2.622826
1	-3.701031	2.782889	-2.302461
1	-6.915493	-0.030877	-2.772434
1	-5.903376	2.187864	-3.259530
6	3.887838	-0.284925	-2.327130
6	3.272905	1.113087	-2.313481
8	2.300270	1.272432	-1.439073
8	3.639600	1.988120	-3.068592
1	4.959268	-0.192235	-2.535525
7	3.603785	-0.976892	-1.083469
6	4.542771	-1.341871	-0.186977
8	4.265732	-1.658361	0.979506
8	-3.350459	-1.281956	-0.275030
8	-4.916303	-1.563219	1.670745
16	-3.536125	-1.247234	1.362007
1	3.443374	-0.824222	-3.178686
6	-2.041986	2.523047	0.003486
6	-0.879297	2.832226	0.736318
6	-2.173381	1.311408	-0.630587
6	-0.718710	4.071214	1.398609
6	0.136188	1.842827	0.815322
6	-1.061705	0.437857	-0.594250
6	0.423177	4.314861	2.114031
1	-1.507716	4.815502	1.319260

6	1.278681	2.099134	1.632293
1	-1.080421	-0.495726	-1.155610
6	1.421630	3.329334	2.237714
1	0.563312	5.270757	2.612352
1	2.303978	3.535318	2.836141
1	-2.862714	3.239820	-0.008775
7	0.032894	0.682331	0.095779
1	2.486102	-2.937985	-0.257214
1	0.558553	-3.706178	-1.648580
1	-0.247522	-1.567112	2.769374
1	2.099084	-1.778039	1.875661
6	5.986560	-1.405583	-0.650497
1	6.098964	-1.922204	-1.609310
1	6.403097	-0.397604	-0.765817
1	6.557647	-1.932001	0.116321
8	2.146378	1.082421	1.784732
6	3.498646	1.377995	2.099044
1	3.600648	1.736956	3.131539
1	4.038773	0.434268	1.979534
1	3.890358	2.129768	1.400656

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meta-C-H-activation –OMe substituted quinoline -**TS**

Number of imaginary frequencies : 1
The smallest frequency is : -1662.1547 cm(-1)

Electronic energy : =-2204.3628419
Zero-point correction= 0.464588
Thermal correction to Energy= 0.498251
Thermal correction to Enthalpy= 0.499195
Thermal correction to Gibbs Free Energy= 0.399815
Sum of electronic and zero-point Energies= -2203.898254
Sum of electronic and thermal Energies= -2203.864591
Sum of electronic and thermal Enthalpies= -2203.863646
Sum of electronic and thermal Free Energies= -2203.963027

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Cartesian Coordinates

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46	1.853701	-0.318029	-0.391081
6	0.919784	-2.145144	0.334267
6	0.771729	-3.060556	-0.723431
6	-0.399707	-3.789890	-0.893382
6	-1.444645	-3.613423	0.002897
6	-1.326268	-2.725329	1.077066
6	-0.144754	-2.006479	1.241772
1	-2.377372	-4.160584	-0.130847
6	-2.508390	-2.508732	1.967385
1	-2.240226	-2.352640	3.019252
1	-3.238266	-3.322814	1.905601
8	-2.686554	0.158402	1.959570
6	-4.044590	-0.287528	-0.875169
6	-3.442617	0.911732	-1.276940

6	-5.314867	-0.653731	-1.295566
6	-4.172436	1.729459	-2.146691
6	-6.016559	0.178696	-2.157885
1	-5.731529	-1.587224	-0.927287
6	-5.439112	1.369553	-2.587814
1	-3.718668	2.657494	-2.489719
1	-7.010852	-0.103808	-2.493360
1	-5.977086	2.021557	-3.271069
6	4.440399	-0.361923	-1.686906
6	3.921383	1.078942	-1.786965
8	2.725684	1.287713	-1.302943
8	4.612814	1.933130	-2.305507
1	5.500173	-0.315520	-1.407500
7	3.649278	-1.134507	-0.747502
6	4.139037	-2.027661	0.090528
8	3.427802	-2.554424	0.999200
8	-3.341170	-1.185810	-0.077085
8	-4.826684	-1.165446	1.953678
16	-3.438975	-1.016824	1.561101
1	4.390580	-0.795942	-2.697418
6	-2.003520	2.638127	-0.251610
6	-0.818741	3.041335	0.393446
6	-2.145737	1.360137	-0.736074
6	-0.657923	4.348042	0.908707
6	0.212800	2.076600	0.547245
6	-1.018417	0.508761	-0.651186
6	0.494987	4.679676	1.568590
1	-1.458922	5.070287	0.768749
6	1.358664	2.427823	1.322723
1	-1.046964	-0.483853	-1.099145
6	1.499778	3.717892	1.786726
1	0.634765	5.685026	1.957588
1	2.386260	3.987151	2.353883
1	-2.833755	3.341357	-0.311064
7	0.106372	0.847685	-0.050018
1	1.603499	-3.202744	-1.412510
1	-0.501598	-4.491938	-1.717447
1	-0.058907	-1.293309	2.063417
1	2.149751	-2.148931	0.763047
6	5.578719	-2.458074	-0.006998
1	5.856860	-2.708744	-1.035555
1	6.240581	-1.649784	0.326199
1	5.733103	-3.324097	0.637777
8	2.230535	1.440590	1.598978
6	3.591658	1.779566	1.785253
1	3.763946	2.232450	2.770564
1	4.144539	0.837080	1.725340
1	3.930516	2.455309	0.989191

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meta-C-H-activation –OMe substituted quinoline -**Product**

Number of imaginary frequencies : 0

Electronic energy : =-2204.3874156
Zero-point correction= 0.471356
Thermal correction to Energy= 0.505071
Thermal correction to Enthalpy= 0.506015
Thermal correction to Gibbs Free Energy= 0.405931
Sum of electronic and zero-point Energies= -2203.916060
Sum of electronic and thermal Energies= -2203.882345
Sum of electronic and thermal Enthalpies= -2203.881401
Sum of electronic and thermal Free Energies= -2203.981484

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Cartesian Coordinates

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46	1.828943	-0.280624	-0.352219
6	0.710283	-1.883460	0.153502
6	0.699238	-2.985760	-0.715224
6	-0.305659	-3.948114	-0.646522
6	-1.339798	-3.807154	0.269531
6	-1.335741	-2.735255	1.161602
6	-0.289345	-1.810384	1.131746
1	-2.163831	-4.519217	0.284906
6	-2.528837	-2.503660	2.032398
1	-2.279319	-2.275021	3.076306
1	-3.235237	-3.339913	2.010787
8	-2.860413	0.158330	2.008306
6	-3.988475	-0.311172	-0.905354
6	-3.431420	0.916349	-1.292421
6	-5.231358	-0.728956	-1.360535
6	-4.180770	1.708222	-2.169748
6	-5.952528	0.079114	-2.229578
1	-5.614104	-1.685411	-1.015997
6	-5.422929	1.299701	-2.636385
1	-3.759016	2.655460	-2.501041
1	-6.924752	-0.247082	-2.589420
1	-5.976440	1.934055	-3.323863
6	4.328842	-0.556409	-1.760609
6	4.091517	0.968495	-1.666561
8	2.964787	1.314037	-1.140671
8	4.952643	1.709321	-2.108904
1	5.406245	-0.750220	-1.730531
7	3.596613	-1.259158	-0.711750
6	4.146949	-2.150630	0.033579
8	3.495810	-2.689037	1.052839
8	-3.270021	-1.179908	-0.087013
8	-4.907741	-1.289726	1.826386
16	-3.504077	-1.057019	1.543967
1	3.952190	-0.886164	-2.739315
6	-2.024006	2.700432	-0.298360
6	-0.834137	3.136188	0.317126
6	-2.149142	1.411280	-0.757181
6	-0.686501	4.458476	0.794946
6	0.213583	2.189929	0.487030
6	-1.003297	0.587568	-0.678966
6	0.467313	4.822189	1.436098
1	-1.497878	5.166199	0.641335

6	1.351747	2.570331	1.261414
1	-1.024665	-0.409132	-1.114399
6	1.481138	3.877402	1.682481
1	0.599071	5.840521	1.792920
1	2.363653	4.174024	2.241457
1	-2.866179	3.389372	-0.357504
7	0.123006	0.948831	-0.088727
1	1.473445	-3.079537	-1.477064
1	-0.299867	-4.791947	-1.333550
1	-0.315610	-0.962870	1.818210
1	2.586809	-2.311371	1.067320
6	5.533344	-2.681447	-0.131237
1	5.687262	-3.062841	-1.145253
1	6.271927	-1.890705	0.038798
1	5.703549	-3.484667	0.586877
8	2.219569	1.596581	1.584933
6	3.564024	1.959160	1.835958
1	3.671239	2.456189	2.809560
1	4.131294	1.024173	1.852278
1	3.945464	2.597987	1.029746

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meta-C-H-activation quinoline -**PRC**

Number of imaginary frequencies : 0

Electronic energy : =-2089.9179663
Zero-point correction= 0.437437
Thermal correction to Energy= 0.469141
Thermal correction to Enthalpy= 0.470085
Thermal correction to Gibbs Free Energy= 0.373433
Sum of electronic and zero-point Energies= -2089.480529
Sum of electronic and thermal Energies= -2089.448825
Sum of electronic and thermal Enthalpies= -2089.447881
Sum of electronic and thermal Free Energies= -2089.544534

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Cartesian Coordinates

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46	-1.996074	-0.220151	0.365609
6	-1.341891	-2.007398	-1.345042
6	-1.770079	-2.527424	-0.112782
6	-0.819409	-3.040587	0.795600
6	0.510845	-3.099981	0.441097
6	0.933127	-2.657023	-0.827670
6	0.018746	-2.077090	-1.693535
1	1.243697	-3.523913	1.126052
6	2.356302	-2.882159	-1.236211
1	2.450007	-3.133664	-2.299759
1	2.839216	-3.673999	-0.653736
8	2.900816	-0.341917	-1.824174
6	3.851816	-0.174300	1.149695
6	3.297609	1.111002	1.164033
6	5.069259	-0.461371	1.748197

6	4.015237	2.112603	1.822925
6	5.760818	0.552773	2.399628
1	5.457788	-1.473780	1.681535
6	5.230865	1.838690	2.438476
1	3.595547	3.116278	1.858888
1	6.714622	0.337684	2.873941
1	5.765240	2.633518	2.952313
6	-4.260162	0.039216	2.067028
6	-3.511377	1.367586	2.156230
8	-2.450003	1.457046	1.376582
8	-3.853720	2.253107	2.908952
1	-5.335099	0.243289	2.126222
7	-3.884153	-0.686485	0.868325
6	-4.715130	-0.871725	-0.185437
8	-4.293313	-1.144379	-1.316270
8	3.152092	-1.218888	0.538742
8	4.813223	-1.867881	-1.233138
16	3.433056	-1.458579	-1.068026
1	-3.999220	-0.538621	2.967122
6	2.001920	2.410873	-0.504179
6	0.855262	2.585438	-1.303496
6	2.053234	1.406625	0.431986
6	0.772297	3.579187	-2.306634
6	-0.238645	1.699108	-1.113262
6	0.898369	0.607695	0.599474
6	-0.349586	3.683971	-3.087539
1	1.617382	4.250779	-2.445439
6	-1.384158	1.822213	-1.931261
1	0.873568	-0.164065	1.367435
6	-1.431384	2.797378	-2.897292
1	-0.410634	4.448903	-3.857266
1	-2.316957	2.889059	-3.520665
1	2.871936	3.044252	-0.676202
7	-0.185811	0.739846	-0.133867
1	-2.829904	-2.673095	0.068845
1	-1.152150	-3.431989	1.753641
1	0.351247	-1.708455	-2.663080
1	-2.096067	-1.662185	-2.049979
6	-6.208803	-0.790045	0.058873
1	-6.516396	-1.297257	0.979056
1	-6.528209	0.256550	0.131419
1	-6.711543	-1.245307	-0.796367
1	-2.227090	1.148443	-1.773711

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meta-C-H-activation quinoline -**TS**

Number of imaginary frequencies : 1
The smallest frequency is : -1643.3572 cm(-1)

Electronic energy : =-2089.9016341
Zero-point correction= 0.431804
Thermal correction to Energy= 0.462982

Thermal correction to Enthalpy= 0.463926
Thermal correction to Gibbs Free Energy= 0.369684
Sum of electronic and zero-point Energies= -2089.469831
Sum of electronic and thermal Energies= -2089.438652
Sum of electronic and thermal Enthalpies= -2089.437708
Sum of electronic and thermal Free Energies= -2089.531950

Cartesian Coordinates

46	-2.053558	-0.070521	0.235549
6	-1.162450	-1.974554	-0.344898
6	-1.138565	-2.810230	0.787414
6	-0.031129	-3.594769	1.086542
6	1.070947	-3.563350	0.242898
6	1.072072	-2.764040	-0.904501
6	-0.042429	-1.980014	-1.192917
1	1.952667	-4.159934	0.474769
6	2.307273	-2.712516	-1.746183
1	2.100221	-2.644596	-2.820885
1	2.975389	-3.561137	-1.566792
8	2.658933	-0.075988	-1.984590
6	3.845279	-0.327790	0.955170
6	3.308050	0.938344	1.217171
6	5.069932	-0.731533	1.466400
6	4.056617	1.791384	2.035033
6	5.790439	0.135376	2.278010
1	5.438894	-1.720600	1.209728
6	5.278926	1.397380	2.564344
1	3.652098	2.774974	2.267137
1	6.748664	-0.175863	2.685254
1	5.833086	2.078124	3.205327
6	-4.738892	0.031315	1.330383
6	-4.090471	1.396307	1.587751
8	-2.890588	1.567974	1.091643
8	-4.695614	2.236713	2.219600
1	-5.727502	0.222769	0.892384
7	-3.908127	-0.795925	0.475467
6	-4.375024	-1.719992	-0.344280
8	-3.628497	-2.327586	-1.167095
8	3.114502	-1.247359	0.206809
8	4.705248	-1.517334	-1.724746
16	3.311498	-1.247378	-1.430736
1	-4.908252	-0.439826	2.310428
6	2.018561	2.612414	-0.062820
6	0.859355	3.024995	-0.744456
6	2.053691	1.406209	0.596605
6	0.802337	4.234629	-1.476383
6	-0.275854	2.170467	-0.719998
6	0.869498	0.630801	0.602055
6	-0.332365	4.575201	-2.164683
1	1.680328	4.877855	-1.486180
6	-1.431413	2.541218	-1.441504
1	0.845001	-0.322424	1.130012
6	-1.453244	3.717581	-2.147764
1	-0.372205	5.503563	-2.728586

1	-2.348873	3.994838	-2.697570
1	2.911207	3.236242	-0.106128
7	-0.241353	0.993919	-0.011041
1	-2.017894	-2.844611	1.429970
1	-0.024789	-4.230867	1.968377
1	-0.035944	-1.345657	-2.080487
1	-2.348193	-1.948188	-0.860284
6	-5.835411	-2.083562	-0.320850
1	-6.207014	-2.211673	0.700642
1	-6.426966	-1.288887	-0.790619
1	-5.980200	-3.005407	-0.885753
1	-2.299918	1.888343	-1.409411

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meta-C-H-activation quinoline -**Product**

Number of imaginary frequencies : 0

Electronic energy : =-2089.9276526
Zero-point correction= 0.438326
Thermal correction to Energy= 0.469720
Thermal correction to Enthalpy= 0.470664
Thermal correction to Gibbs Free Energy= 0.375735
Sum of electronic and zero-point Energies= -2089.489326
Sum of electronic and thermal Energies= -2089.457932
Sum of electronic and thermal Enthalpies= -2089.456988
Sum of electronic and thermal Free Energies= -2089.551918

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Cartesian Coordinates

.....

46	-2.030367	0.000703	0.252490
6	-0.960164	-1.671668	-0.117559
6	-1.071753	-2.731878	0.796024
6	-0.149367	-3.775065	0.805166
6	0.919894	-3.763742	-0.081543
6	1.037003	-2.735416	-1.015179
6	0.078077	-1.719815	-1.054667
1	1.677413	-4.545243	-0.041171
6	2.267794	-2.654338	-1.861561
1	2.064931	-2.474637	-2.924877
1	2.903299	-3.540473	-1.765659
8	2.783995	-0.030117	-1.979915
6	3.801064	-0.400072	0.981664
6	3.312728	0.881942	1.266072
6	5.005324	-0.858367	1.496982
6	4.086885	1.690517	2.104538
6	5.751886	-0.034907	2.329924
1	5.339367	-1.855292	1.223148
6	5.289074	1.241084	2.635664
1	3.718978	2.685600	2.348596
1	6.694445	-0.390823	2.737421
1	5.865311	1.888759	3.291333
6	-4.680530	-0.143644	1.389590

6	-4.301910	1.352163	1.417334
8	-3.164200	1.651200	0.880226
8	-5.080904	2.116643	1.955803
1	-5.754529	-0.219107	1.188020
7	-3.873637	-0.889126	0.428268
6	-4.379314	-1.798141	-0.327972
8	-3.655900	-2.409252	-1.251519
8	3.049258	-1.273327	0.198875
8	4.722666	-1.598109	-1.656365
16	3.331549	-1.256522	-1.428440
1	-4.502232	-0.542665	2.398322
6	2.102240	2.602255	-0.037963
6	0.949161	3.070253	-0.693822
6	2.078907	1.415055	0.654608
6	0.950258	4.265184	-1.451533
6	-0.238048	2.289331	-0.621383
6	0.851850	0.716928	0.710690
6	-0.178924	4.666322	-2.115275
1	1.868245	4.848083	-1.498971
6	-1.389477	2.724492	-1.314126
1	0.791754	-0.217244	1.265752
6	-1.353137	3.887136	-2.043301
1	-0.174666	5.583516	-2.698599
1	-2.247648	4.215771	-2.566067
1	3.031084	3.165618	-0.126122
7	-0.253155	1.122187	0.106935
1	-1.880466	-2.731240	1.527036
1	-0.249072	-4.583483	1.526653
1	0.201153	-0.907826	-1.772982
1	-2.733199	-2.074585	-1.190790
6	-5.795711	-2.268457	-0.279994
1	-6.083444	-2.543273	0.738999
1	-6.473237	-1.474456	-0.612822
1	-5.915941	-3.130742	-0.937111
1	-2.304115	2.145094	-1.227121

Mode of C-H Activation

***meta* C-H activation**

A

Number of imaginary frequencies : 1
The smallest frequency is : -1593.1595 cm(-1)

Electronic energy : =-2315.3862971
Zero-point correction= 0.443437
Thermal correction to Energy= 0.478512
Thermal correction to Enthalpy= 0.479457
Thermal correction to Gibbs Free Energy= 0.377340
Sum of electronic and zero-point Energies= -2314.942860

Sum of electronic and thermal Energies= -2314.907785
Sum of electronic and thermal Enthalpies= -2314.906840
Sum of electronic and thermal Free Energies= -2315.008957

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Cartesian Coordinates

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46	1.743349	-0.554976	-0.656214
6	0.802611	-2.328038	0.183187
6	0.564360	-3.229780	-0.869359
6	-0.652388	-3.891729	-0.995603
6	-1.656894	-3.652974	-0.067797
6	-1.444140	-2.779127	1.003013
6	-0.215487	-2.134782	1.131144
1	-2.627188	-4.137183	-0.174950
6	-2.579575	-2.483463	1.931549
1	-2.269034	-2.371582	2.977604
1	-3.377068	-3.232078	1.877399
8	-2.552810	0.197412	1.987996
6	-4.033141	-0.065546	-0.801293
6	-3.364649	1.100352	-1.198674
6	-5.344941	-0.323115	-1.172675
6	-4.065526	1.993282	-2.016416
6	-6.018283	0.583124	-1.981462
1	-5.814271	-1.233456	-0.810346
6	-5.372786	1.739277	-2.409586
1	-3.558366	2.893586	-2.358768
1	-7.044344	0.383913	-2.278691
1	-5.888706	2.446139	-3.054026
8	2.303361	0.980715	-1.887814
8	-3.363607	-1.034591	-0.061098
8	-4.784233	-0.962215	2.017414
16	-3.400111	-0.911890	1.588808
6	-1.720020	2.691120	-0.241673
6	-0.490268	2.957402	0.393936
6	-2.019039	1.432828	-0.700318
6	-0.199667	4.254307	0.878094
6	0.425998	1.883837	0.584926
6	-0.973560	0.482029	-0.648803
6	0.961183	4.498781	1.560634
1	-0.925006	5.045386	0.698304
6	1.554777	2.155234	1.414592
1	-1.097574	-0.489706	-1.125308
6	1.821455	3.428887	1.854509
1	1.197887	5.494906	1.922342
1	2.703984	3.569879	2.469833
1	-2.457595	3.490511	-0.305854
7	0.186428	0.694180	-0.057576
7	2.400314	1.104910	2.011969
8	3.442471	1.438107	2.533603
8	1.943233	-0.030798	2.023773
1	1.352589	-3.406057	-1.600890
1	-0.822751	-4.582743	-1.817750
1	-0.057358	-1.432026	1.949035
1	2.076925	-2.329683	0.544666
6	3.332572	1.647502	-1.458354

6	3.906241	2.583762	-2.498756
1	3.108951	3.112914	-3.028632
1	4.592544	3.292692	-2.030829
1	4.453159	1.993290	-3.241398
8	3.821443	1.549133	-0.336539
8	3.399913	-1.587887	-1.274744
6	3.928296	-2.329672	-0.385458
6	5.345220	-2.755270	-0.630771
1	5.583177	-3.654680	-0.060531
1	5.519771	-2.906519	-1.698162
1	5.998811	-1.942315	-0.296711
8	3.352464	-2.703513	0.669447

B

Number of imaginary frequencies : 1
The smallest frequency is : -1625.0778 cm(-1)

Electronic energy : =-2523.2903564
Zero-point correction= 0.499783
Thermal correction to Energy= 0.538796
Thermal correction to Enthalpy= 0.539740
Thermal correction to Gibbs Free Energy= 0.429287
Sum of electronic and zero-point Energies= -2522.790573
Sum of electronic and thermal Energies= -2522.751560
Sum of electronic and thermal Enthalpies= -2522.750616
Sum of electronic and thermal Free Energies= -2522.861070

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Cartesian Coordinates

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46	-1.098092	1.507974	-0.545124
6	0.559143	2.796566	-0.032593
6	1.087416	3.364088	-1.205863
6	2.460477	3.461180	-1.402963
6	3.322617	2.978161	-0.427980
6	2.828677	2.418398	0.755744
6	1.453143	2.344659	0.954029
1	4.399909	3.016462	-0.586426
6	3.789147	1.808777	1.727550
1	3.501584	1.955237	2.775649
1	4.815958	2.163069	1.588560
8	2.685529	-0.605782	2.102009
6	4.028011	-1.257079	-0.708552
6	2.929021	-2.078952	-0.990890
6	5.315882	-1.587905	-1.103380
6	3.174498	-3.244384	-1.724463
6	5.531580	-2.755895	-1.823261
1	6.128245	-0.920515	-0.829384
6	4.455769	-3.578967	-2.142275
1	2.332143	-3.883487	-1.982360
1	6.537828	-3.018948	-2.138052
1	4.614613	-4.486055	-2.719421

6	-3.512472	-1.715548	-2.004405
6	-2.351200	-0.725163	-1.875964
8	-2.630788	0.245706	-1.068816
8	-1.310276	-0.907491	-2.492983
1	-3.098819	-2.665500	-2.352902
7	-4.201491	-1.884796	-0.743563
6	-4.602994	-3.037550	-0.145931
8	-5.073800	-3.041744	0.985928
8	3.834883	-0.034615	-0.070786
8	5.196033	-0.459225	2.003158
16	3.891670	0.009416	1.578672
1	-4.190337	-1.343866	-2.789000
6	0.852572	-2.795296	0.148581
6	-0.355826	-2.503400	0.809511
6	1.588759	-1.800568	-0.445534
6	-1.117957	-3.527561	1.425755
6	-0.776363	-1.148342	0.878025
6	1.010314	-0.512479	-0.472998
6	-2.279982	-3.237323	2.085904
1	-0.756414	-4.551383	1.349526
6	-1.940543	-0.888369	1.653673
1	1.485101	0.279812	-1.048412
6	-2.690197	-1.896805	2.203121
1	-2.898638	-4.017799	2.517101
1	-3.610103	-1.645515	2.721419
1	1.222542	-3.819881	0.163094
7	-0.112166	-0.197684	0.147243
7	-2.381119	0.473203	1.967960
8	-3.578336	0.692119	1.976828
8	-1.510123	1.287070	2.245710
1	0.400871	3.731212	-1.968066
1	2.859072	3.898468	-2.315077
1	1.059665	1.893737	1.865575
1	-0.535178	3.396229	0.346670
6	-4.406894	-4.315980	-0.924375
1	-4.824672	-4.260226	-1.935217
1	-3.337801	-4.545312	-1.018312
1	-4.891902	-5.122986	-0.373033
1	-4.330414	-1.040835	-0.193437
8	-2.216335	3.061274	-1.269434
6	-2.283972	4.091760	-0.523754
8	-1.524976	4.317761	0.452604
6	-3.367947	5.076073	-0.852758
1	-3.147029	6.052196	-0.418198
1	-3.500170	5.147315	-1.934591
1	-4.305674	4.702927	-0.427745

D

Number of imaginary frequencies : 1
The smallest frequency is : -1551.7513 cm(-1)

Electronic energy : =-2315.3680329
Zero-point correction= 0.442064
Thermal correction to Energy= 0.478058
Thermal correction to Enthalpy= 0.479002
Thermal correction to Gibbs Free Energy= 0.369439
Sum of electronic and zero-point Energies= -2314.925969
Sum of electronic and thermal Energies= -2314.889975
Sum of electronic and thermal Enthalpies= -2314.889031
Sum of electronic and thermal Free Energies= -2314.998594

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Cartesian Coordinates

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46	4.241675	-0.312983	0.521360
6	2.884662	0.774279	-0.689570
6	2.557238	2.023421	-0.128105
6	1.249400	2.491355	-0.142591
6	0.250248	1.722647	-0.729409
6	0.556321	0.491990	-1.321148
6	1.860652	0.014782	-1.282570
1	-0.777595	2.088215	-0.753975
6	-0.536416	-0.309242	-1.954673
1	-0.240628	-0.793137	-2.892029
1	-1.437187	0.292482	-2.121312
8	-1.424645	-1.120653	0.432407
6	-3.388696	-2.772397	-1.070675
6	-4.381814	-2.132531	-0.315500
6	-3.361905	-4.149672	-1.232889
6	-5.366783	-2.937376	0.263770
6	-4.355473	-4.925571	-0.647649
1	-2.558055	-4.589490	-1.817197
6	-5.360083	-4.316922	0.098254
1	-6.157782	-2.460444	0.840143
1	-4.343570	-6.004706	-0.775591
1	-6.143479	-4.918300	0.552239
8	4.969380	-1.738016	1.943933
8	-2.415273	-2.014736	-1.713450
8	-0.130949	-2.768733	-0.967718
16	-1.039299	-1.644765	-0.862700
6	-4.464329	-0.164293	1.192839
6	-4.260846	1.213852	1.422368
6	-4.334227	-0.680933	-0.072280
6	-4.385647	1.792456	2.706275
6	-3.880844	2.014349	0.307685
6	-4.073255	0.243505	-1.122061
6	-4.163924	3.133439	2.895864
1	-4.664056	1.152302	3.541603
6	-3.619294	3.386789	0.565869
1	-4.063010	-0.121082	-2.151040
6	-3.786251	3.942906	1.809412
1	-4.269609	3.577151	3.881716
1	-3.607459	5.006745	1.935670
1	-4.667576	-0.818786	2.040088
7	-3.835084	1.520166	-0.954350
7	-3.141979	4.277843	-0.496365
8	-3.622324	5.398973	-0.532330

8	-2.270001	3.863252	-1.241211
1	3.349237	2.629961	0.310471
1	1.001778	3.456750	0.291749
1	2.087389	-0.960542	-1.715098
1	4.005510	0.807608	-1.327169
6	3.821920	-2.274606	1.920484
6	3.489969	-3.464542	2.750526
1	2.633242	-3.233115	3.390499
1	3.192975	-4.290876	2.097520
1	4.347389	-3.757414	3.359462
8	2.931645	-1.767542	1.154461
8	5.825247	0.922094	0.157992
6	5.996828	1.337116	-1.033536
6	7.312372	2.002791	-1.317607
1	7.247215	2.612018	-2.220319
1	7.623713	2.603633	-0.460266
1	8.068451	1.225184	-1.468308
8	5.157588	1.210073	-1.959294

E

Number of imaginary frequencies : 1
The smallest frequency is : -1525.6145 cm(-1)

Electronic energy : =-2523.2789563
Zero-point correction= 0.498533
Thermal correction to Energy= 0.538331
Thermal correction to Enthalpy= 0.539275
Thermal correction to Gibbs Free Energy= 0.424042
Sum of electronic and zero-point Energies= -2522.780423
Sum of electronic and thermal Energies= -2522.740625
Sum of electronic and thermal Enthalpies= -2522.739681
Sum of electronic and thermal Free Energies= -2522.854915

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Cartesian Coordinates

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46	-1.332180	0.009109	0.211629
6	-0.706842	-1.961049	-0.421287
6	-0.795710	-2.832743	0.678274
6	0.203779	-3.761904	0.944934
6	1.314412	-3.822629	0.114108
6	1.426068	-2.980497	-0.997564
6	0.410964	-2.065741	-1.267368
1	2.120519	-4.522352	0.332475
6	2.686665	-3.006829	-1.803901
1	2.519800	-2.882409	-2.880716
1	3.276701	-3.914318	-1.638596
8	3.262565	-0.396062	-1.916887
6	4.369445	-0.881659	1.033082
6	3.944505	0.412415	1.361043
6	5.542945	-1.420759	1.539857
6	4.738427	1.140954	2.252843

6	6.316226	-0.671626	2.417133
1	5.830061	-2.421110	1.227873
6	5.906768	0.607609	2.780633
1	4.411532	2.136964	2.545526
1	7.235080	-1.089611	2.819590
1	6.498673	1.192896	3.479331
6	-5.301002	-1.444377	-0.343393
6	-3.800338	-1.280274	-0.353504
8	-3.274546	-0.595417	0.570466
8	-3.176482	-1.838141	-1.293848
1	-5.503832	-2.523748	-0.398613
7	-5.903981	-0.830088	0.804686
6	-7.228965	-0.864043	1.145328
8	-7.653842	-0.265385	2.116608
8	3.573009	-1.690289	0.226744
8	5.175568	-2.014763	-1.687373
16	3.802598	-1.643539	-1.407480
1	-5.652703	-1.019175	-1.297886
6	2.849835	2.311095	0.214855
6	1.788725	2.853809	-0.538369
6	2.776637	1.035461	0.714596
6	1.854051	4.166616	-1.062311
6	0.663053	2.028873	-0.801138
6	1.546531	0.355989	0.552473
6	0.832962	4.671120	-1.824038
1	2.734896	4.765587	-0.840044
6	-0.324972	2.562431	-1.670004
1	1.379663	-0.592997	1.058282
6	-0.265867	3.851743	-2.135090
1	0.876412	5.683937	-2.212988
1	-1.073091	4.206323	-2.769061
1	3.754115	2.903393	0.349387
7	0.545599	0.819456	-0.169861
7	-1.421124	1.743598	-2.198795
8	-2.513752	2.264585	-2.309828
8	-1.139567	0.602191	-2.540901
1	-1.664742	-2.770491	1.333271
1	0.126892	-4.426965	1.801526
1	0.500067	-1.389313	-2.118758
1	-1.896995	-1.733662	-0.971548
6	-8.113268	-1.697040	0.247817
1	-8.068298	-1.356350	-0.793437
1	-7.812405	-2.751576	0.260273
1	-9.139098	-1.615096	0.609373
1	-5.308261	-0.246886	1.381613
8	-1.845685	1.846438	0.936577
6	-1.133171	2.267408	1.942732
8	-0.234105	1.643828	2.497706
6	-1.489078	3.682746	2.343471
1	-1.050155	3.921451	3.314448
1	-1.088469	4.372503	1.589528
1	-2.573111	3.821420	2.366295

F

Number of imaginary frequencies : 1
The smallest frequency is : -1225.7352 cm(-1)

Electronic energy : =-2294.2524701
Zero-point correction= 0.434632
Thermal correction to Energy= 0.468054
Thermal correction to Enthalpy= 0.468998
Thermal correction to Gibbs Free Energy= 0.370915
Sum of electronic and zero-point Energies= -2293.817838
Sum of electronic and thermal Energies= -2293.784416
Sum of electronic and thermal Enthalpies= -2293.783472
Sum of electronic and thermal Free Energies= -2293.881555

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Cartesian Coordinates

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46	1.616785	-0.908476	-0.586517
6	0.355047	-2.610584	-0.150896
6	-0.107443	-3.387129	-1.225799
6	-1.390408	-3.928213	-1.226090
6	-2.254097	-3.626558	-0.182495
6	-1.832001	-2.834644	0.889981
6	-0.518042	-2.370979	0.921925
1	-3.282945	-3.985010	-0.205277
6	-2.834869	-2.390679	1.906423
1	-2.440944	-2.364017	2.929757
1	-3.750127	-2.991700	1.891955
8	-2.361157	0.242890	2.067778
6	-4.009530	0.313570	-0.693173
6	-3.239120	1.409226	-1.108156
6	-5.356451	0.202925	-1.007145
6	-3.876911	2.382115	-1.885826
6	-5.965085	1.187295	-1.774583
1	-5.904896	-0.657820	-0.634823
6	-5.219645	2.273955	-2.221812
1	-3.292187	3.227989	-2.242899
1	-7.018762	1.102443	-2.026353
1	-5.685001	3.040428	-2.835927
6	4.438216	-0.670739	-0.688557
6	4.058614	-2.100027	-0.286420
8	2.846709	-2.513363	-0.793442
8	4.764859	-2.829436	0.345775
1	5.118793	-0.781597	-1.550530
7	3.297737	0.171632	-0.971246
6	3.386361	1.415612	-1.488109
8	2.398359	2.104778	-1.752059
8	-3.412718	-0.737845	-0.004185
8	-4.755471	-0.528515	2.117800
16	-3.393003	-0.687930	1.648707
1	5.045475	-0.294320	0.151146
6	-1.409707	2.812166	-0.196043
6	-0.134987	2.943209	0.388417
6	-1.846294	1.598363	-0.665222

6	0.311124	4.194049	0.873653
6	0.674406	1.781988	0.519530
6	-0.898426	0.549249	-0.672080
6	1.524901	4.312447	1.495364
1	-0.336168	5.058131	0.738602
6	1.862624	1.928562	1.290171
1	-1.141708	-0.393604	-1.159419
6	2.292322	3.159284	1.722925
1	1.878483	5.274272	1.854075
1	3.222572	3.206217	2.280508
1	-2.067807	3.680118	-0.213250
7	0.299516	0.632216	-0.123318
7	2.656671	0.793305	1.766159
8	3.853414	0.964586	1.929402
8	2.057347	-0.240355	2.031667
1	0.555321	-3.571531	-2.071811
1	-1.728816	-4.550661	-2.051229
1	-0.190691	-1.743608	1.753001
1	1.861850	-2.831106	-0.197691
6	4.783673	1.976353	-1.681914
1	5.306048	2.044921	-0.718671
1	5.394813	1.347270	-2.339743
1	4.698783	2.973073	-2.118428

G

Number of imaginary frequencies : 1
The smallest frequency is : -1406.7498 cm(-1)

Electronic energy : =-3083.853044
Zero-point correction= 0.502996
Thermal correction to Energy= 0.545782
Thermal correction to Enthalpy= 0.546726
Thermal correction to Gibbs Free Energy= 0.428251
Sum of electronic and zero-point Energies= -3083.350048
Sum of electronic and thermal Energies= -3083.307262
Sum of electronic and thermal Enthalpies= -3083.306318
Sum of electronic and thermal Free Energies= -3083.424793

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Cartesian Coordinates

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46	1.119465	-0.918918	-0.067094
6	-0.120659	-2.690155	-0.175854
6	-0.173428	-3.082953	-1.525570
6	-1.375085	-3.459457	-2.116347
6	-2.538511	-3.452395	-1.359406
6	-2.513831	-3.089646	-0.007945
6	-1.307459	-2.716807	0.577747
1	-3.488694	-3.724250	-1.818086
6	-3.801672	-3.031115	0.751771
1	-3.711173	-3.375791	1.789010
1	-4.607384	-3.589305	0.263388

8	-3.603914	-0.598235	1.849385
6	-4.535980	0.392305	-1.011247
6	-3.735137	1.520610	-0.785045
6	-5.746089	0.475148	-1.684189
6	-4.194370	2.743636	-1.285496
6	-6.178846	1.703079	-2.167801
1	-6.329871	-0.431783	-1.813470
6	-5.397439	2.837792	-1.972140
1	-3.577847	3.629460	-1.143822
1	-7.124073	1.771695	-2.699391
1	-5.724328	3.799441	-2.358521
6	3.793836	-1.378022	-1.479575
6	5.021115	-0.825819	-0.752277
8	4.786671	0.097202	0.170315
8	6.133491	-1.229396	-0.996137
1	4.156477	-2.109700	-2.212014
7	2.783008	-1.961813	-0.609575
6	3.021914	-3.089116	0.067351
8	2.139061	-3.637873	0.779926
8	-4.100132	-0.866409	-0.608919
8	-5.879099	-1.371486	1.101244
16	-4.440021	-1.354008	0.934265
1	3.324293	-0.566508	-2.042232
6	-2.245962	2.398816	0.991895
6	-1.136959	2.266204	1.852014
6	-2.503580	1.458480	0.022556
6	-0.858207	3.225529	2.855612
6	-0.308023	1.121767	1.701753
6	-1.545097	0.430385	-0.142039
6	0.216968	3.073165	3.689673
1	-1.515011	4.088657	2.940699
6	0.741996	0.967596	2.643461
1	-1.642604	-0.280159	-0.962595
6	1.022365	1.924141	3.583967
1	0.440781	3.817382	4.447848
1	1.860600	1.760930	4.255105
1	-2.929410	3.233748	1.141781
7	-0.493465	0.273609	0.641130
7	1.521315	-0.273130	2.736663
8	2.725988	-0.177618	2.859952
8	0.878641	-1.314379	2.742226
1	0.746232	-3.089750	-2.108184
1	-1.407094	-3.754565	-3.162128
1	-1.279859	-2.414787	1.624935
1	0.949735	-2.997404	0.430495
6	4.372447	-3.748326	0.020350
1	4.882419	-3.642081	-0.940082
1	5.016638	-3.278405	0.772782
1	4.251635	-4.801508	0.278632
8	2.217372	0.831032	-0.168446
1	3.850433	0.412001	0.140738
6	1.716667	1.924137	-0.807419
1	0.669859	2.179467	-0.534989
6	2.539726	3.140016	-0.378476
6	1.688404	1.754826	-2.329520

9	0.998670	0.643842	-2.647142
9	2.911551	1.624246	-2.844726
9	1.082730	2.772140	-2.942443
9	2.149952	4.256189	-1.002975
9	3.835158	2.967316	-0.610515
9	2.372821	3.336407	0.933075

H

Number of imaginary frequencies : 1
The smallest frequency is : -1675.6873 cm(-1)

Electronic energy : =-2898.7265958
Zero-point correction= 0.552159
Thermal correction to Energy= 0.598185
Thermal correction to Enthalpy= 0.599129
Thermal correction to Gibbs Free Energy= 0.472137
Sum of electronic and zero-point Energies= -2898.174437
Sum of electronic and thermal Energies= -2898.128411
Sum of electronic and thermal Enthalpies= -2898.127467
Sum of electronic and thermal Free Energies= -2898.254459

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Cartesian Coordinates

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46	1.848021	-1.000018	-0.129117
6	1.122080	-3.006624	-0.401416
6	0.938111	-3.242871	-1.776506
6	-0.215571	-3.853167	-2.256125
6	-1.210731	-4.220760	-1.361927
6	-1.060015	-4.003188	0.013120
6	0.109178	-3.414456	0.486911
1	-2.135373	-4.665610	-1.728711
6	-2.205735	-4.313429	0.924224
1	-1.892026	-4.679840	1.909165
1	-2.913960	-5.027410	0.490416
8	-2.438609	-1.961689	2.179108
6	-4.008042	-1.120217	-0.474637
6	-3.490279	0.168971	-0.283349
6	-5.266932	-1.332450	-1.018013
6	-4.291176	1.246102	-0.681181
6	-6.039812	-0.245387	-1.404717
1	-5.618486	-2.354731	-1.127438
6	-5.545690	1.045156	-1.241058
1	-3.896861	2.255811	-0.573699
1	-7.023494	-0.407524	-1.837346
1	-6.137734	1.901321	-1.553721
6	4.351201	-0.100413	-1.311899
6	3.477273	1.116540	-1.043425
8	2.517804	0.950240	-0.176390
8	3.670156	2.187386	-1.603610
1	5.303280	0.065321	-0.784576
7	3.683111	-1.312092	-0.870317

6	4.308124	-2.448380	-0.611675
8	3.706016	-3.451204	-0.132822
8	-3.231305	-2.243314	-0.201486
8	-4.546178	-3.248854	1.694400
16	-3.199021	-2.859523	1.328420
1	4.572432	-0.117943	-2.388016
6	-2.042155	1.427067	1.285098
6	-0.843869	1.568256	2.016267
6	-2.194959	0.411403	0.374962
6	-0.667316	2.609897	2.956759
6	0.181977	0.608956	1.808737
6	-1.053422	-0.387119	0.112951
6	0.491502	2.715572	3.680460
1	-1.473064	3.330698	3.086122
6	1.323490	0.703568	2.648526
1	-1.066463	-1.101157	-0.706542
6	1.494332	1.743102	3.528322
1	0.632004	3.524793	4.390533
1	2.404467	1.775966	4.119867
1	-2.862880	2.114871	1.487612
7	0.074071	-0.296623	0.786995
7	2.350301	-0.345170	2.683185
8	3.514183	0.004026	2.763315
8	1.957727	-1.503801	2.673076
1	1.718889	-2.937277	-2.471731
1	-0.346455	-4.028294	-3.320976
1	0.223469	-3.220773	1.554008
1	2.377132	-3.134140	-0.082332
47	1.192318	2.764432	-0.915208
8	-0.724343	2.493013	-2.169587
6	-0.753146	1.267474	-2.567961
6	-1.968399	0.851665	-3.373347
1	-1.688186	0.813189	-4.431836
1	-2.287283	-0.156529	-3.084408
1	-2.800307	1.552466	-3.259305
8	0.144060	0.444318	-2.349525
8	-0.137856	4.397137	0.266794
6	-1.343006	4.595548	0.168898
6	-2.061321	5.571987	1.053056
1	-3.001718	5.144175	1.415864
1	-1.421262	5.867476	1.886268
1	-2.321270	6.460831	0.468381
8	-2.142760	4.005600	-0.690003
1	-1.631574	3.389753	-1.322848
6	5.781034	-2.570802	-0.889036
1	6.063857	-3.623798	-0.863316
1	6.051081	-2.135708	-1.856227
1	6.344317	-2.038727	-0.113064

I

Number of imaginary frequencies : 1

The smallest frequency is : -405.3770 cm(-1)

Electronic energy : =-2106.1052534
Zero-point correction= 0.389902
Thermal correction to Energy= 0.421153
Thermal correction to Enthalpy= 0.422097
Thermal correction to Gibbs Free Energy= 0.323841
Sum of electronic and zero-point Energies= -2105.715352
Sum of electronic and thermal Energies= -2105.684100
Sum of electronic and thermal Enthalpies= -2105.683156
Sum of electronic and thermal Free Energies= -2105.781412

Cartesian Coordinates

6	1.520783	-2.533623	0.128283
6	1.257204	-3.224367	-1.071291
6	0.047392	-3.870133	-1.321692
6	-0.972519	-3.796664	-0.382378
6	-0.770860	-3.102478	0.812255
6	0.466831	-2.503894	1.061832
1	-1.938883	-4.262492	-0.576429
6	-1.905065	-2.948966	1.773397
1	-1.592268	-2.974083	2.824972
1	-2.701347	-3.686447	1.623317
8	-1.869272	-0.277234	2.075906
6	-3.733641	-0.463428	-0.606018
6	-3.369072	0.844233	-0.956846
6	-4.990402	-0.977710	-0.896258
6	-4.321972	1.599731	-1.654911
6	-5.917629	-0.199327	-1.573743
1	-5.216539	-1.991055	-0.577049
6	-5.575996	1.092564	-1.961507
1	-4.054626	2.601174	-1.986282
1	-6.899442	-0.603586	-1.804920
1	-6.284865	1.705371	-2.512097
8	-2.814084	-1.312585	-0.012668
8	-4.094193	-1.449723	2.152550
16	-2.739118	-1.355659	1.643215
6	-2.015055	2.790116	-0.251940
6	-0.785765	3.407198	0.056291
6	-2.076261	1.461475	-0.599514
6	-0.711753	4.786755	0.359749
6	0.385988	2.600968	0.047082
6	-0.841239	0.758080	-0.623920
6	0.494551	5.385709	0.613912
1	-1.634824	5.363205	0.372830
6	1.605018	3.260146	0.368460
1	-0.828005	-0.294897	-0.909209
6	1.666591	4.611166	0.606841
1	0.553805	6.447953	0.831155
1	2.635899	5.057018	0.810355
1	-2.923126	3.388842	-0.195588
7	0.325454	1.288421	-0.312976
7	2.871261	2.535452	0.509528
8	3.863928	3.033939	0.016051

8	2.848096	1.497808	1.163453
1	2.044112	-3.270773	-1.829055
1	-0.108538	-4.418724	-2.249144
1	0.599229	-1.980684	2.012492
1	3.068477	-2.427437	0.237088
47	1.998988	-0.360887	-0.261918
8	4.178420	-0.659882	-1.063959
6	4.750593	-1.649608	-0.578977
6	6.225452	-1.851874	-0.793193
1	6.739564	-1.778911	0.170805
1	6.410955	-2.857987	-1.180748
1	6.620506	-1.099377	-1.477533
8	4.188017	-2.568374	0.133965

***ortho* C-H activation**

A

Number of imaginary frequencies : 1
The smallest frequency is : -1623.4187 cm(-1)

Electronic energy : =-2315.3767705
Zero-point correction= 0.443761
Thermal correction to Energy= 0.478780
Thermal correction to Enthalpy= 0.479724
Thermal correction to Gibbs Free Energy= 0.377605
Sum of electronic and zero-point Energies= -2314.933009
Sum of electronic and thermal Energies= -2314.897991
Sum of electronic and thermal Enthalpies= -2314.897047
Sum of electronic and thermal Free Energies= -2314.999165

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Cartesian Coordinates

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46	1.725079	-0.421336	-0.561796
6	0.932061	-3.169956	-1.267197
6	0.052028	-4.176203	-1.636362
6	-1.077909	-4.412221	-0.859597
6	-1.338527	-3.615505	0.247032
6	-0.494086	-2.555629	0.580986
6	0.690538	-2.331218	-0.158770
1	-2.226442	-3.799562	0.850405
6	-0.849925	-1.678441	1.747851
1	-0.220581	-0.783788	1.799642
1	-0.783641	-2.207837	2.707629
8	-2.603419	0.289874	2.235908
6	-3.836189	-0.264421	-0.400772
6	-3.472360	0.982271	-0.931765
6	-5.136680	-0.739509	-0.465246
6	-4.464745	1.734069	-1.563350
6	-6.107549	0.030534	-1.095514
1	-5.359788	-1.708001	-0.025348

6	-5.768240	1.260617	-1.652318
1	-4.200788	2.694343	-2.002928
1	-7.128693	-0.335743	-1.159369
1	-6.523545	1.855024	-2.159624
6	2.845114	3.110196	-2.623403
6	2.131539	1.838179	-2.218819
8	2.686358	1.264714	-1.189062
8	1.117932	1.454851	-2.793257
1	2.566398	3.388493	-3.642073
6	3.822566	-2.173268	0.108730
8	3.042345	-2.530597	1.025845
8	-2.848930	-1.079792	0.133643
8	-3.436872	-2.086424	2.343889
16	-2.563804	-1.082236	1.765386
6	-1.878284	2.764480	-0.224995
6	-0.624506	3.101006	0.333027
6	-2.120142	1.490387	-0.667403
6	-0.354948	4.407983	0.802375
6	0.326716	2.061385	0.515070
6	-1.007793	0.615200	-0.716617
6	0.818526	4.694229	1.450137
1	-1.107364	5.177621	0.642389
6	1.468916	2.377146	1.296275
1	-1.069163	-0.316937	-1.270948
6	1.728982	3.657980	1.716803
1	1.030740	5.700342	1.799041
1	2.635050	3.834802	2.288646
1	-2.672086	3.510569	-0.217882
7	0.134721	0.854762	-0.111520
7	2.362490	1.343976	1.827052
8	3.541683	1.610790	1.941143
8	1.834685	0.296643	2.182407
1	0.260997	-4.792420	-2.507433
1	-1.758782	-5.221674	-1.112347
1	1.778179	-2.181036	0.538305
6	5.257961	-2.607299	0.153676
1	5.661890	-2.708610	-0.855644
1	5.829027	-1.827336	0.668557
1	5.358207	-3.538236	0.714611
1	1.849827	-3.029472	-1.835243
8	3.483726	-1.436489	-0.877015
1	2.540196	3.916329	-1.944174
1	3.928698	2.998660	-2.535494

B

Number of imaginary frequencies : 2
The smallest frequency is : -1606.6926 cm(-1)

Electronic energy : =-2523.2777793
Zero-point correction= 0.500019
Thermal correction to Energy= 0.538170

Thermal correction to Enthalpy= 0.539114
Thermal correction to Gibbs Free Energy= 0.430936
Sum of electronic and zero-point Energies= -2522.777761
Sum of electronic and thermal Energies= -2522.739609
Sum of electronic and thermal Enthalpies= -2522.738665
Sum of electronic and thermal Free Energies= -2522.846844

Cartesian Coordinates

46	1.808477	-0.423086	-0.502707
6	1.402397	-3.020402	-1.785981
6	0.655988	-4.026570	-2.379652
6	-0.414011	-4.581329	-1.684705
6	-0.750984	-4.097473	-0.428136
6	-0.046849	-3.038395	0.146820
6	1.081188	-2.496193	-0.515138
1	-1.593491	-4.529283	0.110526
6	-0.499328	-2.515365	1.480544
1	0.016368	-1.594315	1.769400
1	-0.364138	-3.253333	2.282425
8	-2.480029	-0.954206	2.390369
6	-3.702175	-1.038160	-0.308503
6	-3.528925	0.338319	-0.521673
6	-4.927958	-1.659254	-0.486858
6	-4.633219	1.077572	-0.946897
6	-6.013891	-0.900508	-0.909838
1	-5.007080	-2.725850	-0.293632
6	-5.863632	0.463009	-1.147501
1	-4.513539	2.144428	-1.128930
1	-6.978799	-1.377960	-1.058994
1	-6.710931	1.052113	-1.488432
6	4.175044	-1.930991	-0.258244
8	3.499336	-2.616052	0.547326
8	-2.594744	-1.811324	0.021571
8	-3.001653	-3.375880	1.926735
16	-2.276904	-2.159525	1.608764
6	-2.159007	2.069194	0.641756
6	-0.947214	2.387617	1.292425
6	-2.248106	0.943380	-0.136206
6	-0.832925	3.549563	2.092253
6	0.136420	1.479492	1.178265
6	-1.039900	0.263085	-0.414157
6	0.318197	3.808309	2.790816
1	-1.674100	4.236605	2.112867
6	1.262580	1.732005	2.005681
1	-1.002873	-0.490081	-1.196108
6	1.369733	2.875759	2.757794
1	0.412033	4.705649	3.394867
1	2.269923	3.018935	3.348327
1	-3.031469	2.691811	0.830669
7	0.083596	0.477485	0.237549
7	2.312981	0.735187	2.209072
8	3.461485	1.119184	2.312474
8	1.942348	-0.427915	2.323411
1	0.923652	-4.395655	-3.366641

1	-0.988443	-5.395815	-2.119708
1	2.166476	-2.357604	0.185691
6	5.662794	-2.116521	-0.314011
1	6.041741	-1.903286	-1.315464
1	6.114544	-1.398291	0.378878
1	5.934593	-3.124131	0.005431
1	2.276277	-2.629581	-2.303935
8	3.686500	-1.048381	-1.042786
6	1.803785	3.568506	-1.875232
6	1.708076	2.042332	-1.803617
8	2.379529	1.534972	-0.823494
8	0.963387	1.438071	-2.572663
1	1.697249	3.889915	-2.916102
7	0.752045	4.158109	-1.062209
6	-0.564478	4.324485	-1.400107
8	-1.382184	4.689054	-0.562682
1	2.769937	3.916047	-1.498554
6	-0.937715	4.047679	-2.830511
1	-0.411333	4.727999	-3.510710
1	-0.664118	3.023962	-3.111189
1	-2.012550	4.202639	-2.937051
1	0.943130	4.308898	-0.078648

C

Number of imaginary frequencies : 1
The smallest frequency is : -1509.6559 cm(-1)

Electronic energy : =-2294.2865697
Zero-point correction= 0.434951
Thermal correction to Energy= 0.468454
Thermal correction to Enthalpy= 0.469398
Thermal correction to Gibbs Free Energy= 0.370762
Sum of electronic and zero-point Energies= -2293.851619
Sum of electronic and thermal Energies= -2293.818116
Sum of electronic and thermal Enthalpies= -2293.817172
Sum of electronic and thermal Free Energies= -2293.915808

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Cartesian Coordinates

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46	1.620462	-0.344434	-0.539162
6	0.900559	-3.152981	-1.156146
6	0.029223	-4.162727	-1.536871
6	-1.143998	-4.356320	-0.814058
6	-1.453320	-3.518971	0.249798
6	-0.616439	-2.454618	0.587027
6	0.605455	-2.265607	-0.100149
1	-2.368812	-3.682077	0.816473
6	-1.000077	-1.531388	1.710205
1	-0.398011	-0.615532	1.708702

1	-0.902216	-2.006450	2.695749
8	-2.819174	0.393318	2.138005
6	-4.033387	-0.281715	-0.464035
6	-3.688716	0.940510	-1.060596
6	-5.330675	-0.769828	-0.487164
6	-4.698924	1.650382	-1.713443
6	-6.318460	-0.040846	-1.139163
1	-5.538142	-1.717726	0.002475
6	-5.999208	1.163681	-1.760022
1	-4.451482	2.590681	-2.203187
1	-7.336781	-0.419062	-1.169120
1	-6.767269	1.726611	-2.283740
6	4.420772	-0.351638	-1.284519
6	3.860407	1.029970	-1.635302
8	2.608117	1.247725	-1.302510
8	4.561287	1.845797	-2.193623
1	5.342551	-0.180548	-0.714196
7	3.457161	-1.151979	-0.550414
6	3.770086	-1.940850	0.470352
8	2.888420	-2.449986	1.215638
8	-3.033615	-1.062838	0.094947
8	-3.561752	-2.007213	2.346126
16	-2.732326	-0.993576	1.722344
1	4.710163	-0.834516	-2.229517
6	-2.118105	2.800535	-0.532653
6	-0.858340	3.219685	-0.054651
6	-2.339339	1.485214	-0.856867
6	-0.606543	4.572617	0.276967
6	0.131440	2.226311	0.175869
6	-1.206355	0.635398	-0.857273
6	0.586740	4.945091	0.836107
1	-1.384710	5.306655	0.078146
6	1.288930	2.638929	0.889881
1	-1.269241	-0.361704	-1.286227
6	1.533538	3.959293	1.168324
1	0.790406	5.985310	1.071554
1	2.452810	4.214158	1.687013
1	-2.932464	3.523635	-0.566117
7	-0.044434	0.963053	-0.332314
7	2.201549	1.678311	1.518406
8	3.387339	1.939998	1.547327
8	1.680224	0.697068	2.037223
1	0.278381	-4.817938	-2.368101
1	-1.818388	-5.169904	-1.070967
1	1.650577	-2.095891	0.622777
6	5.211400	-2.259742	0.763151
1	5.781273	-2.472770	-0.146188
1	5.680986	-1.403449	1.262087
1	5.251315	-3.116968	1.436572
1	1.858314	-3.050270	-1.663660

D

Number of imaginary frequencies : 1

The smallest frequency is : -1558.5451 cm(-1)

Electronic energy : =-2315.3774657
Zero-point correction= 0.441958
Thermal correction to Energy= 0.477719
Thermal correction to Enthalpy= 0.478663
Thermal correction to Gibbs Free Energy= 0.372434
Sum of electronic and zero-point Energies= -2314.935508
Sum of electronic and thermal Energies= -2314.899747
Sum of electronic and thermal Enthalpies= -2314.898802
Sum of electronic and thermal Free Energies= -2315.005031

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Cartesian Coordinates

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46	-2.423578	-0.440726	0.835748
6	-2.883407	-3.201135	0.170508
6	-2.398522	-4.489378	0.360814
6	-1.082460	-4.770500	0.015318
6	-0.253069	-3.790126	-0.532914
6	-0.724712	-2.495279	-0.700474
6	-2.058307	-2.182950	-0.335687
1	0.755698	-4.053740	-0.838233
6	0.056776	-1.380641	-1.345170
1	-0.011790	-0.446206	-0.769205
1	-0.342338	-1.158389	-2.346193
8	2.315414	-0.355323	-2.208647
6	3.611489	-1.391909	0.219198
6	3.972446	-0.080013	0.560654
6	4.536599	-2.424278	0.187246
6	5.310002	0.151198	0.892768
6	5.860868	-2.165534	0.521580
1	4.197344	-3.414270	-0.106103
6	6.244802	-0.876915	0.878918
1	5.610896	1.157578	1.179319
1	6.590328	-2.970855	0.502914
1	7.277244	-0.670178	1.148973
6	-0.372985	0.965234	3.883131
6	-1.193496	0.429737	2.762144
8	-2.266961	0.996395	2.408791
8	-0.814660	-0.616593	2.126003
1	0.201230	1.819830	3.508415
6	-4.134629	0.014900	-1.404384
8	-3.308933	-0.648308	-2.084642
8	2.281619	-1.691331	-0.069395
8	2.114402	-2.857590	-2.285170
16	1.805249	-1.591135	-1.647914
6	3.272639	2.210013	-0.128217
6	2.239046	3.142830	-0.374565
6	2.988790	1.011230	0.479519
6	2.461257	4.392211	-0.999754
6	0.917688	2.750396	-0.026876
6	1.660097	0.824595	0.953568
6	1.411729	5.231087	-1.282058
1	3.481044	4.673583	-1.256766
6	-0.138735	3.607124	-0.425526

1	1.414594	-0.053788	1.553778
6	0.091073	4.830888	-1.000380
1	1.587333	6.194155	-1.752988
1	-0.756314	5.459157	-1.259572
1	4.277838	2.425091	-0.490557
7	0.663132	1.634192	0.698266
7	-1.532467	3.157317	-0.331920
8	-2.359180	3.964243	0.053726
8	-1.771218	2.026114	-0.726082
1	-3.038863	-5.267188	0.769214
1	-0.688985	-5.775255	0.153561
1	-2.619672	-1.362302	-1.158694
6	-5.191331	0.813506	-2.106955
1	-4.837170	1.849287	-2.157023
1	-5.352669	0.439749	-3.119213
1	-6.118729	0.808646	-1.530447
1	-3.918144	-2.962361	0.415875
8	-4.132888	0.084149	-0.135267
1	-1.023658	1.321542	4.685790
1	0.318065	0.205107	4.255981

E

Number of imaginary frequencies : 1
The smallest frequency is : -1625.0002 cm(-1)

Electronic energy : =-2523.2654961
Zero-point correction= 0.498597
Thermal correction to Energy= 0.538170
Thermal correction to Enthalpy= 0.539115
Thermal correction to Gibbs Free Energy= 0.424964
Sum of electronic and zero-point Energies= -2522.766899
Sum of electronic and thermal Energies= -2522.727326
Sum of electronic and thermal Enthalpies= -2522.726382
Sum of electronic and thermal Free Energies= -2522.840532

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Cartesian Coordinates

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46	1.135366	0.035332	-0.413495
6	1.017616	-2.820117	-1.098243
6	0.419689	-4.009957	-1.485808
6	-0.666489	-4.492782	-0.762521
6	-1.168985	-3.764126	0.307008
6	-0.615656	-2.531521	0.656555
6	0.526160	-2.046069	-0.025209
1	-2.022208	-4.142677	0.868653
6	-1.237040	-1.752948	1.781776
1	-0.828043	-0.741288	1.868774
1	-1.124946	-2.257315	2.750761
8	-3.409639	-0.217196	2.108124
6	-4.313813	-1.043364	-0.578725
6	-4.199813	0.250708	-1.108316

6	-5.474526	-1.790042	-0.706606
6	-5.293409	0.766295	-1.806370
6	-6.551792	-1.251238	-1.401146
1	-5.509057	-2.781384	-0.262760
6	-6.455761	0.020589	-1.959144
1	-5.218692	1.759669	-2.245334
1	-7.464661	-1.830080	-1.512990
1	-7.292177	0.434975	-2.515694
6	5.012487	-1.327170	0.627163
6	3.519608	-1.199455	0.437637
8	3.108232	-0.569096	-0.583716
8	2.782162	-1.725179	1.307421
1	5.227575	-2.398604	0.749782
7	5.745923	-0.740413	-0.458351
6	7.104233	-0.747728	-0.625148
8	7.635232	-0.169762	-1.555980
8	-3.206021	-1.621498	0.027276
8	-3.703616	-2.719127	2.216377
16	-3.038212	-1.550351	1.672597
1	5.229780	-0.858800	1.601247
6	-3.079933	2.346249	-0.349098
6	-1.964327	2.956848	0.265933
6	-3.011076	1.045924	-0.775736
6	-2.013922	4.300037	0.706452
6	-0.819186	2.155921	0.524399
6	-1.733928	0.436975	-0.742903
6	-0.964969	4.853883	1.392861
1	-2.907362	4.880709	0.486125
6	0.187139	2.734450	1.343389
1	-1.560580	-0.491210	-1.278856
6	0.136972	4.050888	1.731264
1	-0.995568	5.890038	1.715783
1	0.953852	4.437111	2.333430
1	-4.016426	2.900167	-0.403443
7	-0.708665	0.928093	-0.082095
7	1.265227	1.941615	1.941922
8	2.336621	2.481143	2.129703
8	0.984729	0.793784	2.269333
1	0.815204	-4.572362	-2.327938
1	-1.124218	-5.442810	-1.028207
1	1.521568	-1.673111	0.743942
6	7.885721	-1.520387	0.410719
1	7.735092	-1.106609	1.415055
1	7.581803	-2.573486	0.441045
1	8.944183	-1.460640	0.154176
1	1.907949	-2.477375	-1.623184
1	5.217240	-0.189952	-1.125615
8	1.753679	1.893295	-0.973823
6	1.138762	2.383486	-2.015601
6	1.580365	3.796228	-2.325161
1	2.670249	3.877592	-2.299492
1	1.194849	4.107092	-3.298186
1	1.186755	4.465705	-1.549665
8	0.263646	1.817445	-2.660343

F

Number of imaginary frequencies : 1
The smallest frequency is : -1347.9962 cm(-1)

Electronic energy : =-2294.2437088
Zero-point correction= 0.434141
Thermal correction to Energy= 0.467510
Thermal correction to Enthalpy= 0.468454
Thermal correction to Gibbs Free Energy= 0.370414
Sum of electronic and zero-point Energies= -2293.809568
Sum of electronic and thermal Energies= -2293.776199
Sum of electronic and thermal Enthalpies= -2293.775255
Sum of electronic and thermal Free Energies= -2293.873294

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Cartesian Coordinates

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46	1.392475	-0.894690	-0.532842
6	-0.142044	-3.481887	-1.290649
6	-1.190435	-4.387114	-1.410080
6	-2.185697	-4.404382	-0.440985
6	-2.147156	-3.495877	0.610909
6	-1.115426	-2.563469	0.711804
6	-0.054594	-2.562097	-0.225725
1	-2.948986	-3.484525	1.348664
6	-1.197164	-1.528223	1.795633
1	-0.364625	-0.817471	1.765102
1	-1.252526	-1.967059	2.800362
8	-2.408405	0.850627	2.103603
6	-3.859140	0.350846	-0.451118
6	-3.314714	1.490902	-1.065178
6	-5.221715	0.094236	-0.461752
6	-4.192072	2.357499	-1.719958
6	-6.073863	0.976722	-1.115900
1	-5.589055	-0.797430	0.038887
6	-5.557335	2.101398	-1.752587
1	-3.788815	3.237175	-2.218842
1	-7.142380	0.779512	-1.134225
1	-6.221345	2.783575	-2.276872
6	4.223986	-0.894301	-0.357623
6	3.706369	-2.271056	0.064894
8	2.491560	-2.597750	-0.473553
8	4.330348	-3.035221	0.743902
1	5.001022	-1.091815	-1.114136
7	3.187018	-0.004877	-0.830633
6	3.418925	1.113010	-1.554886
8	2.514883	1.830384	-1.986331
8	-3.005444	-0.585054	0.120717
8	-3.793564	-1.231625	2.409286
16	-2.710771	-0.524314	1.750937
1	4.741112	-0.494041	0.531424
6	-1.428043	3.033353	-0.512213

6	-0.121512	3.184749	0.001254
6	-1.890981	1.793822	-0.868669
6	0.362570	4.459176	0.375308
6	0.654956	2.015603	0.237690
6	-0.937456	0.750759	-0.882243
6	1.575461	4.594529	0.996340
1	-0.257428	5.327389	0.161419
6	1.827551	2.191244	1.023638
1	-1.180980	-0.198279	-1.351003
6	2.294683	3.442489	1.348438
1	1.957397	5.573214	1.270193
1	3.211663	3.507990	1.925804
1	-2.085252	3.902117	-0.533287
7	0.252971	0.829867	-0.324193
7	2.544714	1.082868	1.656284
8	3.734504	1.227301	1.881525
8	1.885628	0.107431	1.996877
1	-1.217534	-5.086984	-2.241843
1	-3.001113	-5.121247	-0.503979
1	1.347672	-2.760671	0.012593
6	4.872265	1.490731	-1.778727
1	5.403917	1.602457	-0.825638
1	5.402438	0.727802	-2.361378
1	4.900590	2.435532	-2.324297
1	0.669201	-3.512153	-2.017291

G

Number of imaginary frequencies : 1
The smallest frequency is : -1234.1205 cm(-1)

Electronic energy : =-3083.8379585
Zero-point correction= 0.502472
Thermal correction to Energy= 0.545710
Thermal correction to Enthalpy= 0.546654
Thermal correction to Gibbs Free Energy= 0.427010
Sum of electronic and zero-point Energies= -3083.335486
Sum of electronic and thermal Energies= -3083.292249
Sum of electronic and thermal Enthalpies= -3083.291304
Sum of electronic and thermal Free Energies= -3083.410949

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Cartesian Coordinates

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46	-0.937036	0.816505	0.021262
6	0.034830	3.152219	-1.464171
6	0.936562	3.871059	-2.234744
6	2.232999	4.064521	-1.768051
6	2.626984	3.500829	-0.562936
6	1.748940	2.711818	0.181551
6	0.408477	2.551016	-0.242025
1	3.641524	3.656613	-0.198588
6	2.238145	2.078794	1.452652

1	1.521500	1.360214	1.865538
1	2.467558	2.822678	2.227036
8	3.771300	-0.047793	2.050291
6	4.504236	-0.217372	-0.822767
6	3.899524	-1.470630	-1.000106
6	5.812906	0.027298	-1.208888
6	4.650802	-2.476982	-1.609372
6	6.541071	-0.992483	-1.811589
1	6.234249	1.013751	-1.033718
6	5.956950	-2.238897	-2.019715
1	4.195924	-3.453092	-1.770285
1	7.565517	-0.809970	-2.124777
1	6.522304	-3.031147	-2.503123
6	-3.674459	1.846766	-0.968419
6	-4.881186	1.235371	-0.251281
8	-4.676809	0.077896	0.355415
8	-5.952207	1.796919	-0.233778
1	-4.022473	2.777244	-1.435157
7	-2.522984	2.090529	-0.111641
6	-2.505190	3.115770	0.747438
8	-1.474105	3.397744	1.411483
8	3.743082	0.823781	-0.312728
8	4.922458	2.119064	1.470524
16	3.818408	1.193881	1.301469
1	-3.363658	1.177293	-1.777997
6	2.308643	-2.801760	0.378331
6	1.186278	-2.815966	1.235081
6	2.581805	-1.700497	-0.393151
6	0.901554	-3.930212	2.059452
6	0.406984	-1.630853	1.333194
6	1.586410	-0.693192	-0.435650
6	-0.113711	-3.880493	2.978260
1	1.514777	-4.822301	1.951632
6	-0.555185	-1.589726	2.374326
1	1.643220	0.102015	-1.176660
6	-0.834347	-2.686097	3.150491
1	-0.341401	-4.739355	3.602134
1	-1.605117	-2.596230	3.910343
1	3.005249	-3.638795	0.413256
7	0.570349	-0.632629	0.401007
7	-1.214301	-0.341724	2.768999
8	-2.382816	-0.389560	3.090215
8	-0.502519	0.655641	2.803060
1	0.620346	4.305497	-3.179858
1	2.939344	4.660864	-2.340631
1	-0.437519	2.697883	0.684946
6	-3.703608	4.016088	0.885725
1	-3.759936	4.674659	0.009693
1	-4.648861	3.470139	0.942760
1	-3.567523	4.634369	1.773740
1	-0.997138	3.062078	-1.796600
8	-2.217018	-0.797774	-0.174241
1	-3.775236	-0.285473	0.167537
6	-1.899495	-1.778365	-1.068898
1	-0.853606	-2.146005	-0.996273

6	-2.760727	-3.006366	-0.764712
6	-2.051481	-1.304135	-2.516230
9	-2.516951	-4.006285	-1.616924
9	-4.057374	-2.726978	-0.811057
9	-2.471422	-3.452194	0.461619
9	-3.299754	-0.916715	-2.780953
9	-1.703879	-2.233305	-3.403905
9	-1.248457	-0.242295	-2.727644

***para* C-H activation**

A

Number of imaginary frequencies : 1
The smallest frequency is : -1480.5125 cm(-1)

Electronic energy : =-2315.3898191
Zero-point correction= 0.443137
Thermal correction to Energy= 0.478603
Thermal correction to Enthalpy= 0.479547
Thermal correction to Gibbs Free Energy= 0.374618
Sum of electronic and zero-point Energies= -2314.946682
Sum of electronic and thermal Energies= -2314.911216
Sum of electronic and thermal Enthalpies= -2314.910272
Sum of electronic and thermal Free Energies= -2315.015201

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Cartesian Coordinates

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46	-1.942789	-0.495802	0.505825
6	-0.575689	-2.064646	-1.742307
6	-1.106427	-2.254850	-0.455099
6	-0.303143	-2.894259	0.506651
6	1.017209	-3.220597	0.229996
6	1.550174	-2.941393	-1.030369
6	0.735095	-2.410468	-2.033051
1	1.658641	-3.646156	1.000875
6	3.017066	-3.081064	-1.260673
1	3.276960	-3.405666	-2.275743
1	3.515013	-3.737488	-0.539415
8	3.343156	-0.525169	-2.050270
6	3.789980	0.034320	0.972417
6	3.086871	1.240196	0.877636
6	4.988146	-0.071229	1.665426
6	3.635888	2.345471	1.541090
6	5.513381	1.045015	2.301701
1	5.493001	-1.032777	1.680794
6	4.830366	2.255281	2.241278
1	3.087510	3.285012	1.528689
1	6.449557	0.966539	2.847757
1	5.221960	3.131141	2.751888

6	-2.350223	2.849161	3.087608
6	-1.778367	1.668437	2.331917
8	-2.587473	1.221711	1.417778
8	-0.670675	1.208361	2.599145
1	-1.563312	3.349613	3.656213
6	-3.991875	-2.469931	0.923162
8	-3.588223	-3.008223	-0.143591
8	3.268717	-1.117370	0.388374
8	5.291115	-1.724346	-0.998956
16	3.863203	-1.495597	-1.105639
1	-3.116261	2.487116	3.781393
6	1.609397	2.548773	-0.612228
6	0.362987	2.793320	-1.220879
6	1.827882	1.413127	0.127091
6	0.140670	3.997830	-1.928547
6	-0.672335	1.826210	-1.072531
6	0.748103	0.504186	0.221497
6	-1.090974	4.288981	-2.450131
1	0.971071	4.693818	-2.028994
6	-1.924533	2.160022	-1.663225
1	0.858818	-0.396755	0.819416
6	-2.132385	3.360455	-2.298856
1	-1.270014	5.220460	-2.978536
1	-3.122711	3.559672	-2.697568
1	2.399790	3.288824	-0.730380
7	-0.435239	0.693024	-0.341577
7	-3.074005	1.249187	-1.701228
8	-4.174728	1.726374	-1.505990
8	-2.846757	0.078166	-1.975577
1	-0.714472	-3.089850	1.497509
1	1.155173	-2.212254	-3.018026
1	-2.404032	-2.512496	-0.370381
1	-1.189126	-1.586221	-2.502868
6	-5.251513	-2.984714	1.555691
1	-5.204272	-2.874522	2.640892
1	-6.087572	-2.377709	1.192556
1	-5.427014	-4.023848	1.272086
8	-3.420584	-1.499678	1.506324
1	-2.837860	3.550116	2.404248

B

Number of imaginary frequencies : 1
The smallest frequency is : -1493.5533 cm(-1)

Electronic energy : =-2523.2984439
Zero-point correction= 0.500647
Thermal correction to Energy= 0.539506
Thermal correction to Enthalpy= 0.540450
Thermal correction to Gibbs Free Energy= 0.430249
Sum of electronic and zero-point Energies= -2522.797797
Sum of electronic and thermal Energies= -2522.758938

Sum of electronic and thermal Enthalpies= -2522.757994
Sum of electronic and thermal Free Energies= -2522.868195

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Cartesian Coordinates

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46	2.026657	-0.531386	-0.563893
6	0.984241	-2.896139	1.069898
6	1.440563	-2.583723	-0.222487
6	0.625659	-2.931683	-1.316427
6	-0.643412	-3.458900	-1.122467
6	-1.111064	-3.680520	0.175540
6	-0.271882	-3.449779	1.268272
1	-1.299335	-3.654858	-1.969791
6	-2.541677	-4.044631	0.396557
1	-2.696584	-4.732547	1.236568
1	-3.029486	-4.456150	-0.493262
8	-3.038041	-1.989758	2.062478
6	-3.716100	-0.447952	-0.592514
6	-3.087590	0.728436	-0.167218
6	-4.944445	-0.436172	-1.240254
6	-3.736536	1.936558	-0.459914
6	-5.575090	0.774184	-1.495455
1	-5.385774	-1.385087	-1.530950
6	-4.961570	1.962438	-1.112079
1	-3.229730	2.865500	-0.199496
1	-6.535134	0.786554	-2.004725
1	-5.432502	2.918164	-1.331044
6	1.415352	3.619712	-1.250224
6	1.311032	2.096738	-1.387215
8	2.328506	1.490753	-0.875566
8	0.314398	1.591434	-1.896490
1	1.379609	3.866341	-0.182216
6	4.220519	-1.991592	-1.704155
8	3.954561	-2.899221	-0.870644
8	-3.076409	-1.677237	-0.431082
8	-4.941278	-2.937462	0.715086
16	-3.535607	-2.607706	0.848628
6	-1.585919	1.756084	1.504878
6	-0.316185	1.935720	2.084241
6	-1.802816	0.789717	0.554123
6	-0.091430	3.003045	2.983666
6	0.745715	1.078640	1.687569
6	-0.691480	-0.005589	0.203099
6	1.160646	3.253836	3.478026
1	-0.936504	3.636257	3.244967
6	2.017199	1.344755	2.270013
1	-0.792679	-0.750982	-0.581671
6	2.222700	2.413866	3.108832
1	1.339758	4.085847	4.152152
1	3.225888	2.577690	3.490355
1	-2.385837	2.430332	1.802669
7	0.517868	0.129345	0.725849
7	3.189168	0.488388	2.060787
8	4.274642	1.030804	1.971860
8	3.001468	-0.721020	2.031899

1	0.982130	-2.736674	-2.328356
1	-0.640290	-3.638094	2.275679
1	2.746605	-2.657708	-0.438822
1	1.604929	-2.644834	1.926416
6	5.479603	-2.107334	-2.512472
1	5.356563	-1.621875	-3.482541
1	6.278864	-1.588077	-1.972964
1	5.765155	-3.154399	-2.628130
8	3.509895	-0.960180	-1.906576
1	2.379968	3.969321	-1.630881
7	0.328793	4.289630	-1.922255
1	0.353744	4.229403	-2.931571
6	-0.924686	4.243877	-1.377880
8	-1.129886	4.030067	-0.189545
6	-2.044190	4.475333	-2.358628
1	-1.742454	5.081846	-3.218417
1	-2.375217	3.495660	-2.726420
1	-2.884797	4.954861	-1.850482

C

Number of imaginary frequencies : 1
The smallest frequency is : -1609.9168 cm(-1)

Electronic energy : =-2294.3018992
Zero-point correction= 0.436051
Thermal correction to Energy= 0.469297
Thermal correction to Enthalpy= 0.470241
Thermal correction to Gibbs Free Energy= 0.372299
Sum of electronic and zero-point Energies= -2293.865848
Sum of electronic and thermal Energies= -2293.832603
Sum of electronic and thermal Enthalpies= -2293.831658
Sum of electronic and thermal Free Energies= -2293.929600

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Cartesian Coordinates

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46	-1.855994	-0.434615	0.372784
6	-0.419317	-1.947920	-1.830680
6	-0.975006	-2.203188	-0.565467
6	-0.169885	-2.852351	0.389715
6	1.162092	-3.141751	0.128808
6	1.714781	-2.800410	-1.108259
6	0.910189	-2.237674	-2.100924
1	1.793673	-3.596650	0.891141
6	3.184604	-2.931644	-1.328327
1	3.452883	-3.191894	-2.359522
1	3.670813	-3.637589	-0.646812
8	3.514085	-0.320682	-1.912254
6	3.969756	-0.032347	1.162532
6	3.273686	1.182479	1.176506
6	5.153539	-0.215094	1.864875
6	3.812502	2.207662	1.966595

6	5.670404	0.825563	2.624016
1	5.652215	-1.177479	1.796462
6	4.991575	2.038454	2.678189
1	3.271610	3.148629	2.042126
1	6.594988	0.685024	3.177257
1	5.374112	2.853840	3.286359
6	-4.309073	-0.343741	1.912664
6	-3.628017	1.017391	2.064448
8	-2.506119	1.180170	1.405926
8	-4.132451	1.868376	2.765919
1	-5.316611	-0.151019	1.516546
7	-3.554081	-1.238874	1.052833
6	-4.048488	-2.361967	0.569373
8	-3.414459	-3.092689	-0.247999
8	3.450365	-1.119030	0.467088
8	5.466147	-1.605313	-0.975005
16	4.038359	-1.367647	-1.056942
1	-4.435032	-0.758365	2.923997
6	1.838902	2.668992	-0.182551
6	0.618040	2.988923	-0.806016
6	2.034859	1.446476	0.415613
6	0.407886	4.274516	-1.360333
6	-0.410627	2.006168	-0.827801
6	0.955255	0.532004	0.348983
6	-0.805810	4.619176	-1.889243
1	1.229916	4.986848	-1.332277
6	-1.632946	2.394969	-1.445728
1	1.048631	-0.451385	0.809371
6	-1.837844	3.665186	-1.920853
1	-0.977516	5.612189	-2.293413
1	-2.808462	3.904162	-2.345539
1	2.630013	3.417506	-0.177113
7	-0.207666	0.792658	-0.225806
7	-2.734053	1.459155	-1.707407
8	-3.864467	1.829343	-1.459692
8	-2.432277	0.390125	-2.220099
1	-0.603438	-3.111958	1.356014
1	1.346978	-1.984423	-3.065963
1	-2.235849	-2.521730	-0.463403
1	-1.028899	-1.467957	-2.591997
6	-5.421603	-2.810834	0.988697
1	-5.532099	-2.798395	2.077853
1	-6.178478	-2.134292	0.574900
1	-5.600184	-3.817607	0.609610

D

Number of imaginary frequencies : 1
The smallest frequency is : -1555.1570 cm(-1)

Electronic energy : =-2315.3738871
Zero-point correction= 0.442897

Thermal correction to Energy= 0.478239
Thermal correction to Enthalpy= 0.479184
Thermal correction to Gibbs Free Energy= 0.374522
Sum of electronic and zero-point Energies= -2314.930990
Sum of electronic and thermal Energies= -2314.895648
Sum of electronic and thermal Enthalpies= -2314.894703
Sum of electronic and thermal Free Energies= -2314.999366

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Cartesian Coordinates

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46	-3.085436	-0.381983	0.670139
6	-1.343870	-0.864525	-1.738380
6	-1.943670	-1.560524	-0.676939
6	-1.246324	-2.640651	-0.099003
6	-0.010130	-3.027176	-0.588101
6	0.566513	-2.337626	-1.661955
6	-0.102052	-1.250590	-2.227913
1	0.520712	-3.867520	-0.142945
6	1.894130	-2.786102	-2.188952
1	1.977921	-2.673388	-3.276701
1	2.119269	-3.825690	-1.928381
8	3.209791	-0.458090	-1.970512
6	3.795700	-1.499610	0.973797
6	3.662237	-0.194695	1.473292
6	4.752324	-2.383462	1.454644
6	4.526415	0.164569	2.517329
6	5.602923	-1.988798	2.477735
1	4.810454	-3.373242	1.010522
6	5.480177	-0.711610	3.015041
1	4.423261	1.152307	2.962021
1	6.349165	-2.680091	2.859973
1	6.125014	-0.397434	3.831774
6	-2.862087	3.443936	1.568619
6	-3.000391	1.999787	1.235373
8	-3.777055	1.232821	1.881724
8	-2.299551	1.490846	0.296638
1	-2.668996	4.018430	0.657004
6	-4.676624	-2.713556	0.389823
8	-4.359328	-2.637795	-0.822687
8	2.906542	-1.985717	0.016638
8	4.522889	-2.598361	-1.811758
16	3.304567	-1.848970	-1.575157
1	-2.005958	3.569378	2.241422
6	3.052188	2.123534	0.830779
6	2.162662	3.053440	0.248927
6	2.716048	0.792724	0.919811
6	2.444838	4.437936	0.191588
6	0.957636	2.540876	-0.309264
6	1.423678	0.431146	0.436669
6	1.553942	5.310108	-0.381965
1	3.379023	4.799168	0.618924
6	0.103184	3.475787	-0.955344
1	1.071496	-0.592163	0.569806
6	0.367595	4.822686	-0.960942
1	1.765069	6.375274	-0.412326

1	-0.338239	5.492847	-1.443015
1	4.021421	2.478781	1.179908
7	0.604021	1.242947	-0.176836
7	-1.072900	3.037168	-1.712782
8	-2.081169	3.722991	-1.627519
8	-0.942730	2.065865	-2.432560
1	-1.703269	-3.190036	0.722849
1	0.361475	-0.688593	-3.037464
1	-3.194652	-1.868449	-0.808239
1	-1.846954	-0.006206	-2.177793
6	-5.734431	-3.688205	0.819236
1	-5.840144	-4.487481	0.084015
1	-5.502598	-4.090701	1.807675
1	-6.686159	-3.151670	0.894274
8	-4.166236	-1.994930	1.311131
1	-3.759087	3.802954	2.077966

E

Number of imaginary frequencies : 1
The smallest frequency is : -1495.9395 cm(-1)

Electronic energy : =-2523.2839673
Zero-point correction= 0.500866
Thermal correction to Energy= 0.539601
Thermal correction to Enthalpy= 0.540545
Thermal correction to Gibbs Free Energy= 0.428990
Sum of electronic and zero-point Energies= -2522.783101
Sum of electronic and thermal Energies= -2522.744366
Sum of electronic and thermal Enthalpies= -2522.743422
Sum of electronic and thermal Free Energies= -2522.854977

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Cartesian Coordinates

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46	-1.318209	-0.312663	-0.017051
6	0.346533	-1.410409	-2.355812
6	-0.449062	-1.852547	-1.284576
6	0.105441	-2.788710	-0.391929
6	1.436219	-3.173458	-0.495809
6	2.230268	-2.653421	-1.520704
6	1.665520	-1.814241	-2.484241
1	1.879155	-3.844432	0.239331
6	3.703277	-2.888212	-1.515293
1	4.139003	-2.985001	-2.517387
1	4.011019	-3.748444	-0.911343
8	4.293386	-0.257199	-1.525692
6	4.218052	-0.530484	1.559506
6	3.629366	0.737610	1.643015
6	5.235266	-0.927152	2.417537
6	4.104576	1.593392	2.645570
6	5.689284	-0.054208	3.396728
1	5.659413	-1.919405	2.293873

6	5.119964	1.209568	3.510210
1	3.640485	2.571087	2.759520
1	6.483194	-0.363922	4.070855
1	5.458937	1.895891	4.281606
6	-5.056781	-2.118622	-0.457276
6	-3.565577	-1.902456	-0.606071
8	-2.957358	-1.441277	0.405905
8	-3.024975	-2.164514	-1.713848
1	-5.501255	-2.092974	-1.458109
6	-3.120001	1.487220	1.365965
8	-3.947284	1.263520	0.485068
8	3.763780	-1.449698	0.618525
8	5.965676	-1.865823	-0.550267
16	4.592131	-1.484647	-0.812929
6	2.589232	2.504656	0.253343
6	1.519332	3.017433	-0.504323
6	2.559229	1.224211	0.749167
6	1.562952	4.355753	-0.961545
6	0.393537	2.180665	-0.768866
6	1.408144	0.463950	0.445748
6	0.507414	4.898451	-1.640348
1	2.452885	4.942526	-0.743023
6	-0.661969	2.778618	-1.522459
1	1.320994	-0.552368	0.827077
6	-0.610773	4.095668	-1.913583
1	0.528021	5.929513	-1.979675
1	-1.458824	4.491179	-2.463680
1	3.447685	3.147352	0.444033
7	0.376521	0.909430	-0.257860
7	-1.840833	2.055931	-2.033888
8	-2.873973	2.684098	-2.144227
8	-1.677805	0.893459	-2.376110
1	-0.511385	-3.184382	0.415192
1	2.283784	-1.432691	-3.295365
1	-1.753634	-1.934707	-1.533228
1	-0.071468	-0.705408	-3.069611
6	-3.478508	2.295019	2.596030
1	-2.668350	2.978482	2.864784
1	-4.404805	2.849453	2.427179
1	-3.620297	1.610340	3.439896
8	-1.885924	1.082344	1.380403
1	-5.239050	-3.110331	-0.021676
7	-5.632549	-1.146863	0.429067
1	-5.296968	-0.190375	0.318240
6	-5.990482	-1.526029	1.695086
8	-6.089989	-2.691869	2.042520
6	-6.304158	-0.376807	2.620309
1	-6.011147	0.594830	2.209479
1	-7.378442	-0.369140	2.831027
1	-5.789463	-0.546803	3.570493

F

Number of imaginary frequencies : 1
The smallest frequency is : -1156.1567 cm(-1)

Electronic energy : =-2294.251112
Zero-point correction= 0.435328
Thermal correction to Energy= 0.468740
Thermal correction to Enthalpy= 0.469684
Thermal correction to Gibbs Free Energy= 0.370939
Sum of electronic and zero-point Energies= -2293.815784
Sum of electronic and thermal Energies= -2293.782372
Sum of electronic and thermal Enthalpies= -2293.781428
Sum of electronic and thermal Free Energies= -2293.880173

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Cartesian Coordinates

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46	1.643221	-0.937001	-0.571804
6	0.046893	-2.553150	1.343647
6	0.464776	-2.642182	0.006671
6	-0.489373	-2.997025	-0.963001
6	-1.826639	-3.158428	-0.628503
6	-2.237538	-2.946509	0.690287
6	-1.290893	-2.703839	1.686910
1	-2.571810	-3.364302	-1.396488
6	-3.690986	-2.803361	0.992968
1	-3.978009	-3.175079	1.984325
1	-4.344870	-3.255754	0.240073
8	-3.469607	-0.354789	2.094950
6	-3.910489	0.602480	-0.930319
6	-3.019318	1.683686	-0.880346
6	-5.148615	0.698274	-1.553602
6	-3.428064	2.866914	-1.512424
6	-5.531844	1.891359	-2.149369
1	-5.797693	-0.172004	-1.552843
6	-4.663767	2.977944	-2.132372
1	-2.738155	3.707588	-1.539600
1	-6.500783	1.965930	-2.635658
1	-4.941763	3.910281	-2.616670
6	4.384176	-0.720321	-1.260208
6	4.043655	-2.159701	-0.859586
8	2.755634	-2.516974	-1.209349
8	4.806194	-2.929698	-0.355978
1	4.824136	-0.790871	-2.271271
7	3.240979	0.164564	-1.200951
6	3.282590	1.469726	-1.538343
8	2.300005	2.213386	-1.472808
8	-3.533992	-0.629647	-0.405256
8	-5.630633	-0.979227	0.965706
16	-4.185709	-1.065712	1.053858
1	5.194391	-0.420502	-0.577556
6	-1.235303	2.768452	0.453778
6	0.051677	2.791414	1.021826
6	-1.701474	1.659640	-0.212636
6	0.531345	3.965096	1.650259
6	0.865366	1.629829	0.922508

6	-0.806113	0.570028	-0.311500
6	1.798283	4.018512	2.162468
1	-0.129529	4.828257	1.697270
6	2.140696	1.704857	1.552638
1	-1.101230	-0.320520	-0.864119
6	2.603682	2.869528	2.112918
1	2.178285	4.924749	2.624076
1	3.599923	2.867452	2.544442
1	-1.861240	3.653401	0.558315
7	0.414142	0.556814	0.204395
7	3.030181	0.553060	1.719281
8	4.230527	0.748400	1.638304
8	2.510153	-0.523207	1.980370
1	-0.183197	-3.087409	-2.006237
1	-1.619233	-2.548314	2.713631
1	1.953055	-2.947803	-0.506183
6	4.630923	2.019832	-1.966862
1	5.336578	1.988769	-1.126400
1	5.073323	1.441994	-2.786769
1	4.499001	3.055343	-2.285409
1	0.766770	-2.273115	2.110896

G

Number of imaginary frequencies : 1
The smallest frequency is : -1470.7899 cm(-1)

Electronic energy : =-3083.8517483
Zero-point correction= 0.502336
Thermal correction to Energy= 0.545277
Thermal correction to Enthalpy= 0.546221
Thermal correction to Gibbs Free Energy= 0.427331
Sum of electronic and zero-point Energies= -3083.349412
Sum of electronic and thermal Energies= -3083.306472
Sum of electronic and thermal Enthalpies= -3083.305528
Sum of electronic and thermal Free Energies= -3083.424417

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Cartesian Coordinates

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46	1.190837	-1.037419	-0.036896
6	-0.820294	-2.724858	1.532459
6	-0.076141	-2.750928	0.338516
6	-0.748253	-3.044824	-0.862599
6	-2.127784	-3.200055	-0.881931
6	-2.855725	-3.102370	0.306122
6	-2.192324	-2.912091	1.521383
1	-2.654254	-3.361324	-1.821757
6	-4.347155	-3.079178	0.261722
1	-4.821428	-3.602873	1.100842
1	-4.761183	-3.463238	-0.676453
8	-4.613537	-0.796793	1.666198
6	-4.286160	0.563737	-1.145479

6	-3.457067	1.588309	-0.672260
6	-5.332749	0.808212	-2.024685
6	-3.711306	2.880569	-1.152263
6	-5.573461	2.103130	-2.462988
1	-5.946499	-0.027316	-2.347539
6	-4.754973	3.140549	-2.029253
1	-3.048212	3.688516	-0.849085
1	-6.390398	2.296507	-3.152833
1	-4.918522	4.153706	-2.386604
6	3.448401	-1.579123	-2.000335
6	4.817330	-1.053793	-1.560363
8	5.823086	-1.369188	-2.150123
8	4.832631	-0.258701	-0.499474
1	3.640061	-2.312898	-2.793281
7	2.637469	-2.148115	-0.936642
6	2.997461	-3.298884	-0.365137
8	2.299067	-3.847655	0.529169
8	-4.029365	-0.753941	-0.776908
8	-6.367960	-1.374568	-0.043327
16	-4.988973	-1.399866	0.402679
1	2.877092	-0.768112	-2.465638
6	-2.073610	2.322519	1.249012
6	-0.914772	2.232360	2.043798
6	-2.338137	1.393709	0.270952
6	-0.621484	3.237136	2.996460
6	-0.026967	1.137594	1.838462
6	-1.394430	0.352173	0.123528
6	0.537704	3.198789	3.721977
1	-1.335159	4.048839	3.121965
6	1.132813	1.109722	2.664494
1	-1.538753	-0.391970	-0.658606
6	1.421832	2.121571	3.545740
1	0.775386	3.980085	4.437330
1	2.344389	2.056765	4.114661
1	-2.753652	3.157179	1.413814
7	-0.291913	0.231656	0.845368
7	2.081259	-0.009574	2.685099
8	3.262508	0.253052	2.787912
8	1.607241	-1.138057	2.643779
1	-0.178494	-3.119967	-1.788050
1	-2.765285	-2.858471	2.445611
1	1.107652	-3.183259	0.493278
1	-0.305659	-2.521906	2.468541
6	4.269940	-3.990198	-0.773002
1	4.375257	-4.063626	-1.859851
1	5.136164	-3.424886	-0.410151
1	4.282190	-4.986080	-0.329243
8	2.356735	0.686491	-0.226809
1	3.918209	0.018792	-0.225725
6	2.388595	1.657930	-1.180069
1	3.145021	1.482658	-1.978820
6	2.845307	2.956190	-0.500741
6	1.080678	1.856882	-1.951690
9	4.051089	2.771950	0.024849
9	2.022675	3.327499	0.485206

9	2.921557	3.972943	-1.365613
9	0.628774	0.678108	-2.412446
9	0.102921	2.384268	-1.202404
9	1.249270	2.648615	-3.008381