Supporting information

Heterohelicenes Through 1,3-Dipolar-Cycloaddition of Sydnones with Arynes: Synthesis, Origins of Selectivity and Application to pH Triggered Chiroptical Switch with CPL-sign Reversal

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I. General Information

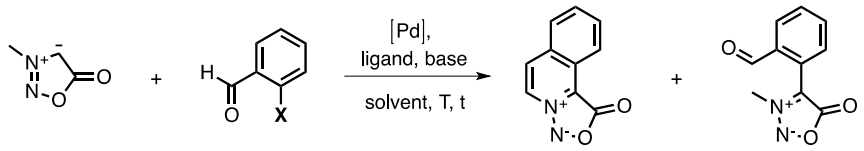
All reactants or reagents including dry solvents were obtained from commercial suppliers and used as received. Unless otherwise noted, all reactions were performed with dry solvents under an atmosphere of argon in oven-dried glassware using standard vacuum-line techniques. All work-up and purification procedures were carried out with reagent-grade solvents in air. Organic solvents (Aldrich) were used without further purification. THF was distilled over Na/benzophenone. Methylene chloride (DCM) was distillated over calcium chloride. Unless otherwise noted, all other commercially available reagents and solvents were used without further purification. Purifications of reactions products were carried out by flash chromatography using Merck silica gel (40-63 µm). Reactions were monitored via thin-layer chromatography (TLC) using EMD Millipore® TLC silica gel glass plates.

FT-ATR-IR spectra were recorded on a Perkin-Elmer UAR Two Spectrum spectrometer and are reported as wavelength numbers (cm^{-1}). Melting points were measured on a Büchi B-545 and are reported in °C. ^{1}H NMR (400 MHz), ^{13}C NMR (100 MHz) were measured on a Brucker Avance 400 MHz spectrometer. Chemical shifts are reported in parts per million (ppm, δ) downfield from residual solvents peaks and coupling constants are reported as Hertz (Hz). Splitting patterns are designated as singlet (s), broad singlet (br. s), doublet (d), triplet (t), quartet (q) and quintet (quin). Splitting patterns that could not be interpreted or easily visualized are designated as multiplet (m). Electrospray mass spectra were obtained using an ESI-Quadripole autopurify, Waters (pump: 2545, mass: ZQ2000) mass Spectrometer. LC-MS spectra were recorded on a Waters Acquity UPLC® equipped PDA eλ Detector and SQ Detector 2, mobile phase A: H_2O + 0.1% formic acid, mobile phase B: acetonitrile + 0.1% formic acid. Automatic chromatographies were performed with a COMBIFLASH RF 200i instrument equipped with UV detector and using flash cartridges Interchim silica 15 or 30 µm. High-resolution mass spectra (HRMS) were performed on a Bruker maXis mass spectrometer by the "Fédération de Recherche ICOA/CBM (FR2708) platform", University of Orléans. Absorbances were measured on a Molecular Device SpectraMax® M5e. Absorbance analysis was performed on Cary® 50 UV-Vis Spectrophotometer. Fluorescence analysis was performed on Fluoromax-4 from Horiba Jobin Yvon. A right-angle configuration was used. Optical density of samples was checked to be less than 0.1 in order to avoid reabsorption artifacts. The relative fluorescence quantum yields Φ_F were determined using Coumarin 102 (Φ_F = 0.764 in ethanol) or 4-(Dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran (DCM, Φ_F = 0.435 in ethanol) as a references.
Chiral SFC chromatograms were recorded using a JASCO SFC apparatus with CHIRALCEL IA chiral column (250 mm × 4.6 mm x 5 µm), mobile phase: CO_2/alcohol, flow rate 1.0 $ml.min^{-1}$ at 25 °C, UV detection (300 nm).

Specific rotation ([α]) spectra were recorded on a Jasco (model P-2000) polarimeter. Electronic circular dichroism spectra (ECD, in M^{-1} cm^{-1}) were recorded on a Jasco J-815 Circular Dichroism Spectrometer equipped with a Peltier thermostatted cell holder and Xe laser. Unless otherwise noted, CD analysis were performed at 20 °C with 1 mm x 1 cm cell. Circularly polarized luminescence (CPL) measurements were performed using JASCO CPL-300 in 1 cm x 1 cm cell. Parameters of the apparatus were adapted for every compounds.

II. Synthesis and Analytical Data of compounds

Sydnone preparation: optimisation

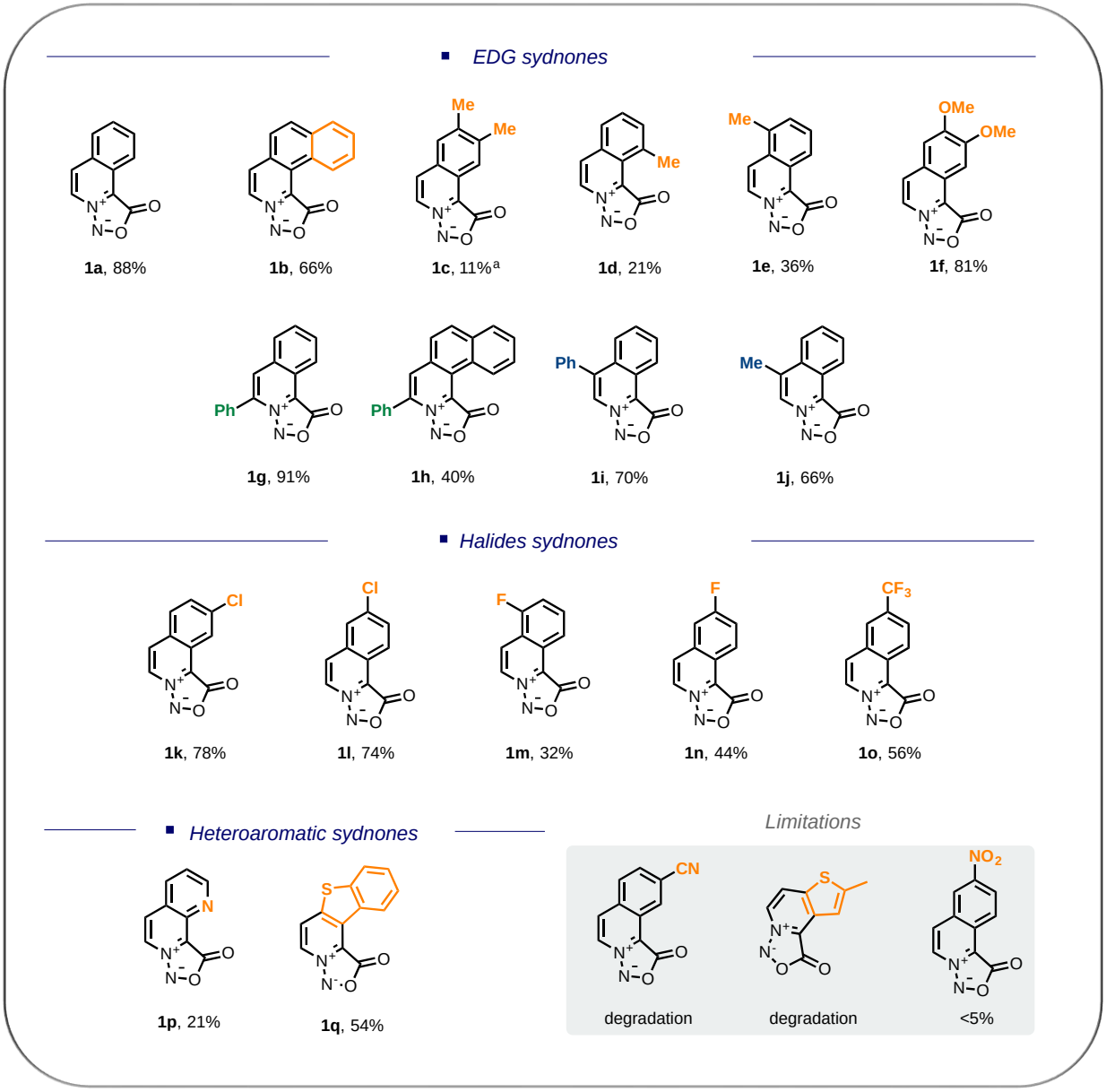


1a **1a'**

Entry	X	[Pd][1]	Ligand[2]	Base	Solvent[3]	T (°C)	t (h)	SM:1a:1a'[4]	Yield[5]
1	I	$Pd(OAc)_2$	PPh_3	**K_2CO_3 (2 equiv)**	DMF	80	16	0 : 5.9 : 1	59%
2	I	$Pd(OAc)_2$	PPh_3	**Cs_2CO_3 (2 equiv)**	DMF	80	16	1.7 : 1 : 0	6%
3	I	$Pd(OAc)_2$	PPh_3	**Et_3N (2 equiv)**	DMF	80	16	46 : 1 : 21	1%
4	I	$Pd(OAc)_2$	PPh_3	**KOH (2 equiv)**	DMF	80	16	1 : 0 : 0	7%
5	I	$Pd(OAc)_2$	PPh_3	***t*BuOK (2 equiv)**	DMF	80	16	10 : 1 : 1	1%
6	**I**	$Pd(OAc)_2$	PPh_3	**K_2CO_3 (4 equiv)**	DMF	80	16	0 : 1 : 0	61%
7	**Br**	**$Pd(OAc)_2$**	**PPh_3**	**K_2CO_3 (4 equiv)**	**DMF**	**80**	**16**	**0 : 1 : 0**	**88%[6]**
8	Br	$Pd(OAc)_2$	PPh_3	K_2CO_3 (4 equiv)	DMF **(anh.)**	80	**16**	0 : 1 : 0	73%
9	**OTf**	$Pd(OAc)_2$	PPh_3	K_2CO_3 (4 equiv)	DMF	80	16	22 : 1 : 0	2%
10	Br	$Pd(OAc)_2$	PPh_3	K_2CO_3 (4 equiv)	DMF	**60**	16	1 : 1,8 : 0	22%
11	Br	$Pd(OAc)_2$	PPh_3	K_2CO_3 (4 equiv)	**Toluene**	80	16	1 : 0 : 5	0%
12	Br	$Pd(OAc)_2$	PPh_3	K_2CO_3 (4 equiv)	**Dioxane**	80	16	3 : 0 :1	0%
13	Br	$Pd(OAc)_2$	PPh_3	K_2CO_3 (4 equiv)	DMF	80	**5**	0 : 20 :1	61%
14	Br	**$Pd(PPh_3)_4$**	-	K_2CO_3 (4 equiv)	DMF	80	16	1 : 4.1 :0	33%
15	Br	**$Pd(PPh_3)_4$**	-	K_2CO_3 (4 equiv)	DMF (anh.)	80	16	1 : 2.5 : 0	28%
16	Br	$Pd(OAc)_2$	**XPhos**	K_2CO_3 (4 equiv)	DMF	80	16	1 : 4.4 : 0	35%
17	Br	-	-	K_2CO_3 (4 equiv)	DMF	80	16	1 : 0 : 0	0%
18	Br	$Pd(OAc)_2$	PPh_3	-	DMF	80	16	4.7 : 0 : 1	0%

Table S1. *[1] 5 mol%. [2] 10 mol%. [3] All the reactions were performed under air atmosphere unless mentioned. « Anh. » means that the reaction was performed in anhydrous conditions. [4] Ratio were determined by proton NMR of the crude mixture. [5] NMR yield were determined using 1,3,5-trimethoxybenzene as an internal standard. [6]isolated yield*

Sydnone preparation: Scope



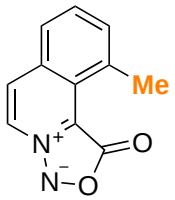
Scheme S1. Sydnone scope

General procedure for the preparation of sydnones

To a solution of *N*-methylsydnone or *N*-benzylsydnone (1.0 equiv) in anhydrous DMF (5.0 mL for 1 mmol of sydnone) were added $Pd(OAc)_2$ (10-20 mol%), triphenylphosphine (20 mol%) and potassium carbonate (4.0 equiv). Argon was bubbled into the solution and corresponding 2-halobenzaldehyde (1.5 equiv) was added. The mixture was stirred at 80 °C until completion. The mixture was evaporated and the crude product was purified by flash chromatography.

Compounds **1a**, **1b**, **1c**, **1f**, **1g**, **1h**, **1i**, **1j**, **1k**, **1n** and **1o** were prepared according to a procedure that we reported previously.[1]

***10-methyl-1-oxo-1H-[1,2,3]oxadiazolo[4,3-a]isoquinolin-4-ium-3-ide* 1d**

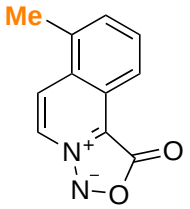


$C_{11}H_8N_2O_2$
MW: 200.19 g.mol^{-1}
Yellow solid
Yield: 21%

Following the general procedure, compound **1d** (13 mg, 0.06 mmol, 21 % yield) was obtained starting from *N*-methylsydnone (30 mg, 0.30 mmol), DMF (1.5 mL), $Pd(OAc)_2$ (16 mg, 0.07 mmol), triphenylphosphine (19 mg, 0.07 mmol), potassium carbonate (200 mg, 1.44 mmol) and 2-bromo-3-methylbenzaldehyde (80 mg, 0.39 mmol), reaction time: 6 hours. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc 100:0 to 8:2).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.90 (d, *J* = 7.3 Hz, 1H), 7.53 – 7.36 (m, 4H), 3.06 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 164.9(C), 134.9(C), 134.5(CH), 127.7(CH), 127.5(C), 127.1(CH), 126.3(CH), 125.9(C), 119.2(2C), 23.9(CH_3).
IR (neat, cm^{-1}): 3098, 1740, 1720, 1413, 1292, 1218, 987, 810, 761.
LCMS (ESI): *m/z*: 219 $[M+H_2O+H]^+$.

***7-methyl-1-oxo-1H-[1,2,3]oxadiazolo[4,3-a]isoquinolin-4-ium-3-ide* 1e**

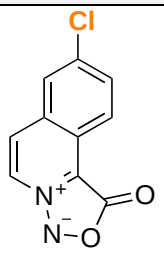


$C_{11}H_8N_2O_2$
MW: 200.19 g.mol^{-1}
Yellow solid
Yield: 36%

Following the general procedure, compound **1e** (44 mg, 0.22 mmol, 36% yield) was obtained starting from *N*-methylsydnone (62 mg, 0.62 mmol), DMF (3 mL), $Pd(OAc)_2$ (30 mg, 0.13 mmol), triphenylphosphine (38 mg, 0.14 mmol), potassium carbonate (400 mg, 2.89 mmol) and 2-bromo-6-methylbenzaldehyde (164 mg, 0.82 mmol), reaction time: 24 hours. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc 100:0 to 8:2).

^{1}H NMR (400 MHz, Methylene Chloride-d_2, δ ppm): 8.35 (d, *J* = 8.1 Hz, 1H), 8.03 (d, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.42 (dt, *J* = 7.4, 1.0 Hz, 1H), 2.65 (s, 3H).
^{13}C NMR (100 MHz, Methylene Chloride-d_2, δ ppm): 165.1(C), 136.1(C), 131.6(CH), 129.6(CH), 126.7(C), 125.6(C), 123.4(CH), 119.4(CH), 119.2(CH), 19.3(CH_3).
IR (neat, cm^{-1}): 3096, 1741, 1720, 1410, 1292, 1222, 981, 810, 760.
LCMS (ESI): *m/z*: 223 $[M+Na]^+$.

***8-chloro-[1,2,3]oxadiazolo[4,3-a]isoquinolin-4-ium-1-olate* 1l**

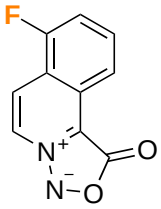


$C_{10}H_5ClN_2O_2$
MW: 220.61 g.mol^{-1}
Yellow solid
Yield: 74%

Following the general procedure, the title compound **1l** was obtained in (164 mg, 0.74 mmol, 74% yield) was obtained starting from *N*-methylsydnone (118 mg, 1.00 mmol) and 2-bromo-5-chlorobenzaldehyde (329 mg, 1.50 mmol). The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc 9/1 to 7/3).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.45 (d, *J* = 8.7 Hz, 1H), 8.02 (d, *J* = 7.4 Hz, 1H), 7.74 (d, *J* = 1.8 Hz, 1H), 7.68 (dd, *J* = 8.7 Hz, *J* = 1.8 Hz, 1H), 7.52 (d, *J* = 7.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 164.4, 134.1 (2C), 132.1, 127.1, 125.2, 124.4, 122.7, 120.4, 105.3.
IR (cm^{-1}): 1742, 976.
LCMS (ESI): *m/z*: 221 [M(^{35}Cl)+H]$^+$, 223 [M(^{37}Cl)+H]$^+$.

***7-fluoro-1-oxo-1H-[1,2,3]oxadiazolo[4,3-a]isoquinolin-4-ium-3-ide* 1m**

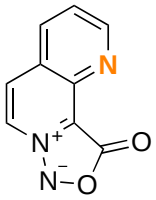


$C_{10}H_5FN_2O_2$
MW: 204.16 g.mol^{-1}
Yellow solid
Yield: 32%

Following the general procedure, compound **1m** (20 mg, 0.09 mmol, 32 % yield) was obtained starting from *N*-methylsydnone (30 mg, 0.30 mmol), DMF (1.5 mL), $Pd(OAc)_2$ (16 mg, 0.07 mmol), triphenylphosphine (19 mg, 0.07 mmol), potassium carbonate (200 mg, 1.44 mmol) and 2-bromo-6-fluorobenzaldehyde (80 mg, 0.39 mmol), reaction time : 5.5 hours. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc 100:0 to 8:2).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.28 (d, *J* = 8.1 Hz, 1H), 8.02 (d, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.69 (td, *J* = 8.1, 5.4 Hz, 1H), 7.27 – 7.20 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 164.4(C), 158.2 (d, *J* = 254 Hz, C), 132.8(d, *J* = 9 Hz, CH), 127.2(d, *J* = 4 Hz, C), 119.7 (2xCH), 119.3 (d, *J* = 5 Hz, CH), 117.2 (d, *J* = 4 Hz, CH), 115.4 (d, *J* = 17 Hz, C), 113. 1 (d, *J* = 19 Hz, CH), 104.9 (C).
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): -119.29.
IR (neat, cm^{-1}): 3096, 1745, 1721, 1607, 1471, 1245, 1031, 910, 791.
LCMS (ESI): *m/z*: 223.1 [M+H_2O+H]$^+$.

***10-oxo-10H-[1,2,3]oxadiazolo[3,4-h][1,7]naphthyridin-7-ium-8-ide* 1p**

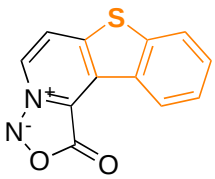


$C_9H_5N_3O_2$
MW: 187.15 g.mol^{-1}
Yellow solid
Yield: 21%

Following the general procedure, compound **1p** (21 mg, 0.11 mmol, 21% yield) was obtained starting from N-methylsydnone (53 mg, 0.52 mmol), DMF (2.5 mL), $Pd(OAc)_2$ (26 mg, 0.11 mmol), triphenylphosphine (30 mg, 0.11 mmol), potassium carbonate (300 mg, 2.17 mmol) and 2-bromopyridinecarboxaldehyde (100 mg, 0.53 mmol), reaction time: 24 hours. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc 100:0 to 0:100).

^{1}H NMR (400 MHz, DMSO-*d*$_6$, δ ppm): 8.93 (dd, *J* = 4.6, 1.7 Hz, 1H), 8.65 (d, *J* = 7.3 Hz, 1H), 8.34 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.99 (d, *J* = 7.4 Hz, 1H), 7.60 (dd, *J* = 8.1, 4.6 Hz, 2H).
^{13}C NMR (100 MHz, DMSO-*d*$_6$, δ ppm): 162.5 (C), 152.7(CH), 142.9(C), 135.7(CH), 125.5(CH), 122.6(CH), 122.4(2C), 121.6(CH).
IR (neat, cm^{-1}): 3045, 1737, 1433, 1232, 1142, 988, 830, 784.
LCMS (ESI) *m/z*: $C_9H_6N_3O_2$ $[M+H]^+$ 188.3.

***1-oxo-1H-benzo[4,5]thieno[3,2-c][1,2,3]oxadiazolo[3,4-a]pyridin-4-ium-3-ide* 1q**



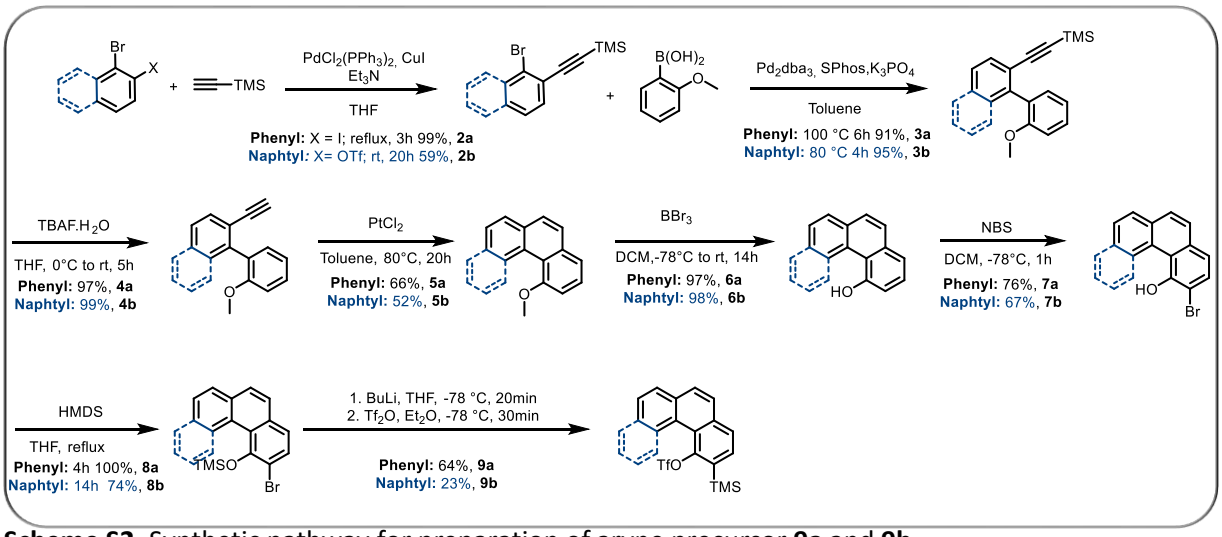
$C_{12}H_6N_2O_2S$
MW: 242.25 g.mol^{-1}
Orange solid
Yield: 54%

Following the general procedure, compound **1q** (82 mg, 0.39 mmol, 54% yield) was obtained starting from N-methylsydnone (60 mg, 0.6 mmol), DMF (2.5 mL), $Pd(OAc)_2$ (13.5 mg, 0.06 mmol), triphenylphosphine (31.5 mg, 0.12 mmol), potassium carbonate (348 mg, 2.5 mmol) and 3-bromobenzo[*b*]thiophene-2-carbaldehyde (180.9 mg, 0.75 mmol), reaction time: 16 hours. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc 100:0 to 8:2).

^{1}H NMR (400 MHz, DMSO-*d*$_6$, δ ppm): 9.40 – 9.34 (m, 1H), 8.74 (d, *J* = 7.3 Hz, 1H), 8.31 (d, *J* = 7.3 Hz, 1H), 8.22 – 8.17 (m, 1H), 7.67 – 7.59 (m, 2H).
^{13}C NMR (100 MHz, DMSO-*d*$_6$, δ ppm): 163.7(C), 140.7(C), 132.3(C), 131.1(C), 128.1(CH), 127.8(C), 126.4(CH), 125.4(CH), 123.3(CH), 121.6(CH), 112.0(CH), 108.3(C).
IR (neat, cm^{-1}): 2924, 1726, 1510, 1443, 1335, 1227, 1157, 1050, 910, 768, 751, 693.
LCMS (ESI) *m/z*: $C_{12}H_7N_2O_2S$ $[M+H]^+$ 243.6.

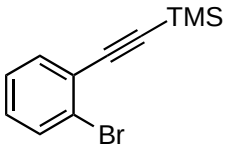
Aryne preparation

Preparation of phenanthryne and benzophenanthryne



Scheme S2. Synthetic pathway for preparation of aryne precursor **9a** and **9b**

((2-bromophenyl)ethynyl)trimethylsilane 2a

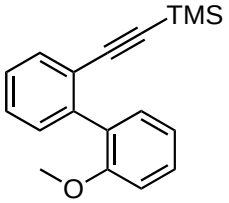


$C_{11}H_{13}BrSi$
MW: 253.21 g.mol^{-1}
Yellow oil
Yield: quantitative

Under argon atmosphere, a solution of trimethylsilylacetylene (1.66 mL, 11.74 mmol, 1.5 equiv) in distilled THF (2 mL) is added to a solution containing 1-bromo-2-iodobenzene (1.02 mL, 7.9 mmol, 1.0 equiv), $PdCl_2(PPh_3)_2$ (112 mg, 0.15 mmol, 0.02 equiv), CuI (61 mg, 0.32 mmol, 0.04 equiv) and NEt_3 (2.2 mL, 15.7 mmol, 2 equiv) in distilled THF (12 mL). The mixture was heated at reflux for 3 hours and allowed to cool to room temperature. It was then filtered through a celite pad and rinsed with EtOAc. The filtrate was evaporated. The crude was partitioned between Et_2O and brine solution. The organic layer was then dried over $MgSO_4$, filtered and concentrated to dryness. Purification by silica gel column chromatography (Heptane 100%) afforded the desired compound as a yellow oil (2 g, 7.9 mmol, quantitative). The spectroscopic data were in accordance with the one reported in the literature. [2]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.57 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.50 – 7.47 (m, 1H), 7.23 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.15 (ddd, *J* = 8.0, 7.4, 1.8 Hz, 1H), 0.28 (s, 9H).

((2'-methoxy-[1,1'-biphenyl]-2-yl)ethynyl)trimethylsilane 3a

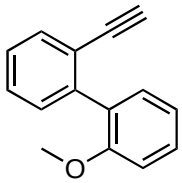


$C_{18}H_{20}OSi$
MW: 280.21 g.mol^{-1}
Orange oil
Yield: 95%

Under argon atmosphere, to a solution of (2-methoxyphenyl)boronic acid (750 mg, 4.93 mmol, 2.0 equiv) in toluene (3 mL) were added Pd_2dba_3 (11 mg, 0.012 mmol, 0.5 mol%) and SPhos (20 mg, 0.048 mmol, 2 mol%). The solution was purged with argon and K_3PO_4 (1.59 g, 6.9 mmol, 3 equiv) was added followed by a solution of ((1-bromophenyl)ethynyl)trimethylsilane (635 mg, 2.50 mmol, 1.0 equiv) in toluene (2 mL). The mixture was heated at 100 °C for 6 hours, cooled down to room temperature and filtered through a pad of celite. The filtrate was concentrated *in vacuo* and purification by column chromatography (heptane/EtOAc, 100:0 to 98:2) to afford the compound as an orange oil (669 mg, 2.38 mmol, 95% yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.54 (dt, *J* = 7.7, 1.0 Hz, 1H), 7.38 – 7.27 (m, 5H), 7.01 – 6.93 (m, 2H), 3.78 (s, 3H), 0.04 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 156.7, 141.9, 132.1, 131.2, 130.0, 129.7, 128.9, 128.2, 126.8, 123.0, 120.1, 110.7, 104.8, 96.4, 55.4, -0.2.
IR (NaCl, cm^{-1}): 3061, 2957, 2158, 1603, 1499, 1463, 1249, 1181, 1004, 865, 841, 796, 753.
LCMS (ESI) : m/z : 281 $[M+H]^+$.

***2-ethynyl-2'-methoxy-1,1'-biphenyl* 4a**

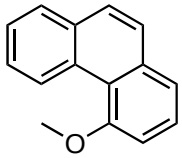


$C_{15}H_{11}O$
MW: 208.26 g.mol^{-1}
Orange oil
Yield: 97%

At 0°C, TBAF.H_2O (5.82 g, 20.8 mmol, 1.5 equiv) was added to ((1-(2-methoxyphenyl)phenyl)ethynyl)trimethylsilane (4.174 g, 14.9 mmol, 1 equiv) in THF (40 mL). The mixture was stirred at room temperature for 5 hours. The solution was diluted with EtOAc and washed with a NH_4Cl solution. The organic layer was dried over Na_2SO_4, filtered and concentrated *in vacuo*. The crude was purified by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 98:2) to afford the desired compound as a yellow solid (3.01 g, 14.4 mmol, 97% yield). The spectroscopic data were in accordance with the one reported in the literature.[3]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.60 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.42 – 7.27 (m, 5H), 7.04 – 6.97 (m, 2H), 3.79 (s, 3H), 2.93 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 157.0, 141.9, 133.2, 131.4, 130.5, 129.8, 129.3, 128.6, 127.1, 122.2, 120.5, 111.3, 83.3, 79.3, 55.8.

***4-methoxyphenanthrene* 5a**



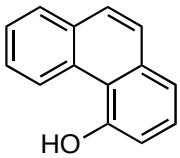
$C_{15}H_{12}O$
MW: 208.26 g.mol^{-1}
White solid
Yield: 66%

Under inert atmosphere, $PtCl_2$ (79 mg, 0.29 mmol, 0.1 equiv) was added to a solution of 2-ethynyl-2'-methoxy-1,1'-biphenyl (618 mg, 2.97 mmol, 1 equiv) in anhydrous toluene (13 mL). The solution was heated at 80 °C for 20 hours. The solvent was removed *in vacuo*. The crude was purified by column

chromatography (SiO_2, heptane 100%) to afford the desired compound as a white solid (413 mg, 1.98 mmol, 66% yield). The spectroscopic data were in accordance with the literature.[4]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.68 (d, *J* = 8.5 Hz, 1H), 7.89 (dt, *J* = 7.8, 1.8 Hz, 1H), 7.77 – 7.69 (m, 2H), 7.68 – 7.61 (m, 1H), 7.59 (ddd, *J* = 9.1, 6.9, 1.9 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.17 (dd, *J* = 5.9, 3.3 Hz, 1H), 4.15 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 158.8, 134.6, 132.7, 130.3, 128.6, 128.2, 127.9, 127.0, 126.4, 126.3, 125.8, 121.4, 120.8, 108.3, 55.6.

***4-hydroxyphenanthrene* 6a**

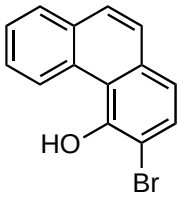


$C_{14}H_{10}O$
MW: 194.23 g.mol^{-1}
White solid
Yield: 97%

Under inert atmosphere, at -78°C, BBr_3 (10 mL, 10 mmol, 1M in DCM, 1.2 equiv) was slowly added to a solution of 4-methoxyphenanthrene (1.736 g, 8.33 mmol, 1 equiv) in dry DCM (20 mL). The solution was allowed to reach room temperature and stirring was maintained for 14 hours. The mixture was cooled at 0°C and a saturated aqueous solution of $NaHCO_3$ was slowly added until bubbling stopped. The organic layer was then separated, dried over $MgSO_4$, filtered and the solvent was removed *in vacuo*. The crude was purified by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 9:1) to afford the desired compound as an off-white solid (1.55 g, 7.98 mmol, 97% yield). The spectroscopic data were in accordance with the literature. [4]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.67 – 9.62 (m, 1H), 7.88 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.71 (q, *J* = 8.8 Hz, 2H), 7.68 – 7.63 (m, 1H), 7.61 – 7.57 (m, 1H), 7.51 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 6.99 (dd, *J* = 7.6, 1.3 Hz, 1H), 5.64 (s, 1H).
LCMS (ESI): *m/z*: 195 $[M+H]^+$.

***3-bromophenanthren-4-ol* 7a**

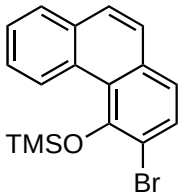


$C_{14}H_9BrO$
MW: 273.13 g.mol^{-1}
White solid
Yield: 76%

At -78°C, under argon, to a solution of 4-hydroxyphenanthrene (1.55 g, 7.98 mmol, 1 equiv) in DCM (33 mL) was added a solution of NBS (1.5 g, 8.42 mmol, 1.2 equiv) in DCM (7 mL). The solution was allowed to warm at room temperature and stirred for 1 hour. A solution of 1M HCl was added to reach pH 4. The mixture was partitioned between DCM and water. The organic layer was separated, dried over $MgSO_4$ and filtered off. Solvent was removed *in vacuo* and the crude was purified by flash chromatography (SiO_2, eluent gradient: Heptane/EtOAc 100:0 to 200:1). The desired compound was obtained as a white solid (1.67 g, 6.11 mmol, 76% yield). Spectroscopic data in accordance with the literature.[7]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.66 (d, *J* = 8.6 Hz, 1H), 7.90 (dd, *J* = 7.7 Hz, *J* = 1.5 Hz, 1H), 7.77 (d, *J* = 8.6 Hz, 1H), 7.71–7.59 (m, 4H), 7.39 (d, *J* = 8.5 Hz, 1H), 6.71 (s, 1H).
LCMS (ESI): *m/z*: 273 $[M(^{79}Br)+H]^+$, 275 $[M(^{81}Br)+H]^+$.

***((3-bromophenanthren-4-yl)oxy)trimethylsilane* 8a**

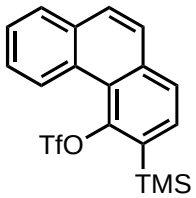


$C_{17}H_{17}BrOSi$
MW: 345.31 g.mol^{-1}
Pink solid
Yield: quantitative

A solution of 3-bromophenanthren-4-ol (1.67 g, 6.11 mmol, 1 equiv) and HMDS (1.6 mL, 7.15 mmol, 1.2 equiv) in distilled THF (18 mL) was heated at reflux for 4 hours. The mixture was then cooled down and the solvent was removed *in vacuo* to afford the desired compound as pink solid (2.11 g, 6.11 mmol, quantitative). Spectroscopic data in accordance with the literature. [4]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.48–9.43 (m, 1H), 9.86–9.82 (m, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.62 (d, *J* = 8.9 Hz, 1H), 7.52 (m, 2H), 7.40 (d, *J* = 8.4 Hz, 1H), 0.21 (s, 9H).
LCMS (ESI): *m/z*: 345 $[M(^{79}Br)+H]^+$, 347 $[M(^{81}Br)+H]^+$.

***3-(trimethylsilyl)phenanthren-4-yl trifluoromethanesulfonate* 9a**

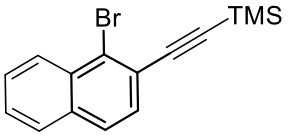


$C_{18}H_{17}F_3O_3SSi$
MW: 398.47 g.mol^{-1}
White solid
Yield: 64%

Under inert atmosphere, at -78 °C, *n*BuLi (0.8 mL, 1.84 mmol, 2.3 M in hexanes, 1.05 equiv) was added dropwise to a solution of ((3-bromophenanthren-4-yl)oxy)trimethylsilane (600 mg, 1.73 mmol, 1 equiv) in freshly distilled THF (8 mL). The mixture was then stirred at this temperature for 20 minutes. Then, Tf_2O (0.4 mL, 2.43 mmol, 1.4 equiv) followed by dry Et_2O (8 mL) were added and the stirring was maintained for 30 minutes. The mixture was quenched by addition of a cold saturated solution of $NaHCO_3$. Et_2O was added and the organic layer was separated, dried over $MgSO_4$ and filtered. The solvent was removed *in vacuo*. Purification by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 99:1) to afford the desired compound as a colorless oil (442 mg, 1.1 mmol, 64% yield). Spectroscopic data in accordance with the literature. [4]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.00 – 8.93 (m, 1H), 7.92 – 7.87 (m, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.71 – 7.61 (m, 4H), 0.53 (s, 9H).
LCMS (ESI): *m/z*: 400 $[M+H]^+$.

***((1-bromonaphthalen-2-yl)ethynyl)trimethylsilane* 2b**

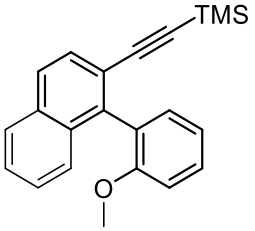


$C_{15}H_{15}BrSi$
MW: 303.27 g.mol^{-1}
Yellow oil
Yield: 59%

Under argon atmosphere, to 1-bromonaphthalen-2-yl trifluoromethanesulfonate (2 g, 5.63 mmol, 1.0 equiv) in DMF (50 mL) were added $PdCl_2(PPh_3)_2$ (147 mg, 0.02 mmol, 0.3 mol%) and CuI (80 mg, 0.04 mmol, 0.6 mol%). After 3 cycles of argon/vacuum, *i*Pr_2NH (7 mL, 49 mmol) and TMS-acetylene (1.1 mL, 7.78 mmol, 1.4 equiv) were added and the mixture was allowed to stir at room temperature for 20 hours. The mixture was then slowly quenched at 0°C with a 1M solution of HCl and DCM was added. The organic layer was separated, dried over Na_2SO_4 and filtered. Solvent was removed *in vacuo* and purification on silica gel chromatography (heptane, 100%) afforded the desired compound as a yellow oil (1.01 g, 3.3 mmol, 59%). The spectroscopic data were in accordance with the literature. [5]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.38 (d, *J* = 8.7 Hz, 1H), 7.91 – 7.89 (m, 2H), 7.71 (ddd, *J* = 8.3, 6.7, 1.8 Hz, 1H), 7.63 (ddd, *J* = 8.0, 7.0, 1.2 Hz, 1H), 7.45 (d, *J* = 9.1 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 133.8(C), 132.2(C), 129.3(CH), 128.3(CH), 128.0(CH), 127.9(CH), 127.5(CH), 127.3(CH), 126.9(C), 123.4(C), 104.4(C), 100.6(CH_3).

***((1-(2-methoxyphenyl)naphthalen-2-yl)ethynyl)trimethylsilane* 3b**

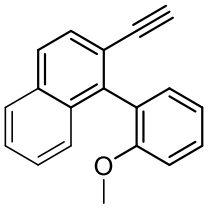


$C_{22}H_{22}OSi$
MW: 330.50 g.mol^{-1}
Pale orange oil
Yield: 95%

Under argon atmosphere, to a solution of (2-methoxyphenyl)boronic acid (221 mg, 1.45 mmol, 2.0 equiv) in toluene (1.5 mL) were added Pd_2dba_3 (4 mg, 0.004 mmol, 0.5 mol%) and SPhos (8 mg, 0.02 mmol, 2 mol%). The solution was purged with argon and K_3PO_4 (505 mg, 2.19 mmol, 3 equiv) was added followed by a solution of ((1-bromonaphthalen-2-yl)ethynyl)trimethylsilane (225 mg, 0.74 mmol, 1.0 equiv) in toluene (1 mL). The mixture was heated at 80 °C for 4 hours, cooled down to room temperature and filtered through a pad of celite. The filtrate was concentrated *in vacuo* and purification by column chromatography (heptane/EtOAc, 100:0 to 99:1) to afford the compound as an orange oil (233 mg, 0.7 mmol, 95% yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.83 (d, *J* = 7.9 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.58 (d, *J* = 8.5 Hz, 1H), 7.51 (d, *J* = 8.6 Hz, 1H), 7.41 – 7.34 (m, 3H), 7.22 – 7.20 (m, 1H), 7.09 – 7.03 (m, 2H), 3.69 (s, 3H), 1.54 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 157.6, 141.3, 133.2, 132.4, 132.0, 129.3, 128.3, 128.1, 128.0, 127.4, 126.8, 126.5, 126.4, 120.7, 111.3, 105.5, 97.6, 55.9, 0.01.
IR (neat, cm^{-1}): 2959, 2145, 1600, 1580, 1492, 1451, 1433, 1247, 1028, 839, 748.
LCMS (ESI) *m/z*: 331 $[M+H]^+$.

***2-ethynyl-1-(2-methoxyphenyl)naphthalene* 4b**

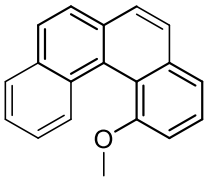


$C_{19}H_{14}O$
MW: 258.32 g.mol^{-1}
Yellow solid
Yield: 88%

At 0°C, TBAF.H_2O (1.366 g, 4.97 mmol, 1.5 equiv) was added to ((1-(2-methoxyphenyl)naphthalen-2-yl)ethynyl)trimethylsilane (1.078 g, 3.26 mmol, 1 equiv) in THF (22 mL). The mixture was stirred at room temperature for 5 hours. The solution was diluted with EtOAc and washed with a saturated NH_4Cl solution. The organic layer was dried over Na_2SO_4, filtered and concentrated *in vacuo*. The crude was purified by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 9:1) to afford the desired compound as a yellow solid (742 mg, 2.87 mmol, 88% yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.87 – 7.85 (m, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.45 (m, 3H), 7.41 – 7.37 (m, 1H), 7.28 – 7.26 (m, 1H), 7.14 – 7.08 (m, 2H), 3.71 (s, 3H), 2.98 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 157.6, 140.9, 133.4, 132.4, 132.0, 129.5, 129.0, 128.2, 127.7, 127.6, 126.9, 126.7, 126.6, 126.5, 126.4, 120.7, 119.7, 111.5, 83.8, 80.1, 56.0.
IR (neat, cm^{-1}): 2956, 2145, 1600, 1580, 1492, 1451, 1433, 1247, 1028, 839, 818, 748.
LCMS (ESI) *m/z*: 259 $[M+H]^+$.

***1-methoxybenzo[c]phenanthrene* 5b**

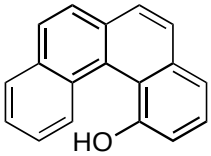


$C_{19}H_{14}O$
MW: 258.32 g.mol^{-1}
Blue solid
Yield: 52%

Under inert atmosphere, $PtCl_2$ (6 mg, 0.02 mmol, 0.2 equiv) was added to a solution of 2-ethynyl-1-(2-methoxyphenyl)naphthalene (34 mg, 0.13 mmol, 1 equiv) in anhydrous toluene (0.5 mL). The solution was heated at 80 °C for 20 hours. The solvent was removed *in vacuo*. The crude was purified by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 98:2) to afford the desired compound as a blue solid (18 mg, 0.07 mmol, 52% yield). The spectroscopic data were in accordance with the literature.[6]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.16 (d, *J* = 8.0 Hz, 1H), 7.98 – 7.93 (m, 2H), 7.87 – 7.77 (m, 3H), 7.67 – 7.50 (m, 4H), 7.16 (dd, *J* = 7.0, 1.9Hz, 1H), 3.89 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 156.7(C), 135.3(C), 132.5(C), 131.7(C), 131.1(CH), 130.2(C), 127.8(CH), 127.2(CH), 127.2(CH), 127.1(CH), 126.7(CH), 126.0(C), 125.9(CH), 125.5(CH), 123.5(CH), 120.9(CH), 120.2(C), 107.5(CH), 54.7(CH_3).

***benzo[c]phenanthren-1-ol* 6b**

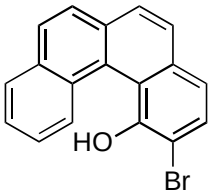


$C_{18}H_{12}O$
MW: 244.29 g.mol^{-1}
Off white solid
Yield: 99%

Under inert atmosphere, at -78°C, BBr_3 (0.4 mL, 0.4 mmol, 1M in DCM, 2.05 equiv) was slowly added to a solution of 1-methoxybenzo[c]phenanthrene (51 mg, 0.19 mmol, 1 equiv) in dry DCM (4 mL). The solution was allowed to reach room temperature and stirring was maintained for 14 hours. The mixture was cooled at 0°C and a saturated aqueous solution of $NaHCO_3$ was slowly added until bubbling stopped. The organic layer was then separated, dried over $MgSO_4$, filtered and the solvent was removed *in vacuo*. The crude was purified by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 8:2) to afford the desired compound as an off-white solid (48 mg, 0.19 mmol, 99% yield). The spectroscopic data were in accordance with the literature. [6]

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.20 (d, *J* = 8.4 Hz, 1H), 8.07 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.92 – 7.87 (m, 2H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.71 (ddd, *J* = 8.4, 6.9, 1.6 Hz, 1H), 7.68 – 7.60 (m, 3H), 7.25 (dd, *J* = 6.8, 2.3 Hz, 1H), 5.54 (s, 1H).
LCMS (ESI) *m/z*: 243 $[M-H]^-$.

***2-bromobenzo[c]phenanthren-1-ol* 7b**

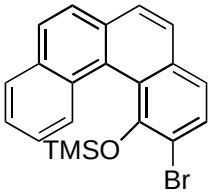


$C_{18}H_{11}BrO$
MW: 323.19 g.mol^{-1}
Off white solid
Yield: 67%

Under inert atmosphere, at -0°C, NBS (22 mg, 0.12 mmol, 1 equiv) in solution in DCM (1.75 mL) was slowly added to a solution of benzo[c]phenanthrene-1-ol (30 mg, 0.12 mmol, 1 equiv) in DCM (2 mL). The solution was stirred 1 hour at this temperature. The solvent was removed *in vacuo*. The crude was purified by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 98:2) to afford the desired compound as an off-white solid (31.2 mg, 0.09 mmol, 75% crude yield). The purity was evaluated at 90% by NMR spectroscopy

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.24 – 8.18 (m, 1H), 8.04 – 7.95 (m, 2H), 7.86 – 7.76 (m, 4H), 7.66 – 7.60 (m, 2H), 7.51 (d, *J* = 8.5 Hz, 1H), 6.25 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 148.9 (C), 134.4(C), 132.8(C), 132.1(C), 129.9(CH), 129.7(CH), 128.9 (C), 128.3(CH), 127.8(CH), 127.3(CH), 127.1(CH), 126.1(CH), 126.0(CH), 125.1(CH), 124.8(C), 121.3(CH), 119.0(C), 107.8(C).
IR (neat, cm^{-1}): 3482, 3046, 1587, 1488, 1343, 1282, 1231, 1065, 835, 756, 617.
LCMS (ESI) *m/z*: 323.7 [M].

***((2-bromobenzo[c]phenanthren-1-yl)oxy)trimethylsilane* 8b**

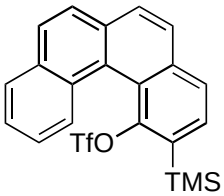


$C_{21}H_{19}BrOSi$
MW: 395.37 g.mol^{-1}
yellow oil
Yield: 74%

Under inert atmosphere, a solution containing 2-bromobenzo[c]phenanthren-1-ol (197 mg, 0.61 mmol, 1 equiv) and HMDS (1 mL, 4.77 mmol, 7.8 equiv) in dry THF (7.5 mL) was heated at reflux overnight. The solvent was removed *in vacuo* afford the desired compound as a yellow oil (210 mg, 0.53 mmol, 87% crude yield). The purity was evaluated at 85% by NMR spectroscopy, the compound was used as obtained.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.20 – 8.16 (m, 1H), 7.91 – 7.86 (m, 2H), 7.78 – 7.70 (m, 4H), 7.54 – 7.50 (m, 2H), 7.48 (d, *J* = 8.5 Hz, 1H), -0.69 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.47(C), 134.14(C), 132.67(C), 131.85(C), 131.73(CH), 130.70(CH), 129.71(C), 128.22(CH), 127.06(CH), 126.99(CH), 126.86(CH), 125.95(CH), 125.90(C), 125.77(CH), 124.57(CH), 124.05(C), 122.44(CH), 114.00(C), -0.19(3xCH_3).

***2-(trimethylsilyl)benzo[c]phenanthren-1-yl trifluoromethanesulfonate* 9b**

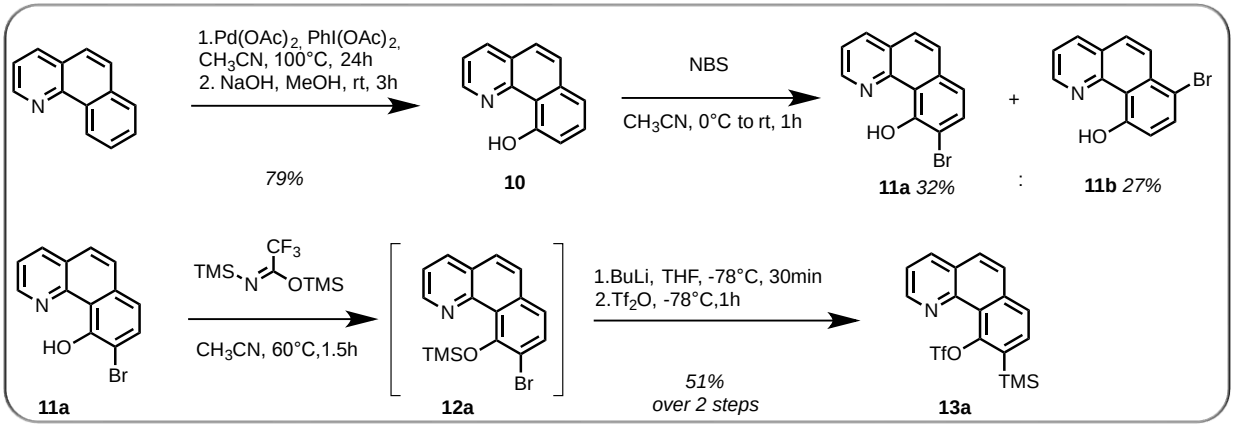


$C_{22}H_{19}F_3O_3SSi$
MW: 448.53 g.mol^{-1}
colorless oil
Yield: 23%

Under inert atmosphere, at -78 °C, BuLi (0.13 mL, 0.25 mmol, 1.9 M in cyclohexane, 1.25 equiv) was added dropwise to a solution of ((2-bromobenzo[c]phenanthren-1-yl)oxy)trimethylsilane (78 mg, 0.20 mmol, 1 equiv) in freshly distilled THF (2 mL). The mixture was then stirred at this temperature for 40 minutes. Then, Tf_2O (60 µL, 0.35 mmol, 1.75 equiv) followed by dry Et_2O (1 mL) were added and the stirring was maintained for 30 minutes. The mixture was quenched by addition of a cold saturated solution of $NaHCO_3$. Et_2O was added and the organic layer was separated, dried over $MgSO_4$ and filtered. The solvent was removed *in vacuo*. Purification by column chromatography (SiO_2, heptane/EtOAc 100:0 -> 99:1) to afford the desired compound as a colorless oil (20 mg, 0.04 mmol, 23% yield).

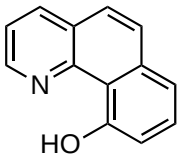
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.22 – 8.18 (m, 1H), 7.92 (dd, *J* = 9.1, 7.3 Hz, 3H), 7.80 – 7.75 (m, 3H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.56 – 7.52 (m, 2H), 0.51 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 148.6(C), 136.1(C), 133.1(C), 132.8(C), 132.1(CH), 132.0(C), 129.5(C), 129.0(CH), 128.6(CH), 128.5(CH), 127.7(CH), 127.5(CH), 126.4(CH), 126.1(CH), 125.8(CH), 125.6(CH), 124.4(C), 121.8(C), 119.8 (q, *J* = 131 Hz), 115.9(C), 0.3(3xCH_3).
IR (neat, cm^{-1}): 1590, 1422, 1203, 1131, 1052, 933, 840, 821, 597.
LCMS (ESI) *m/z*: 447.8[M-H]$^-$.

Preparation of benzoquinolyne



Scheme S3. Synthetic pathway for the preparation of **13a**

***benzo[h]quinolin-10-ol* 10**

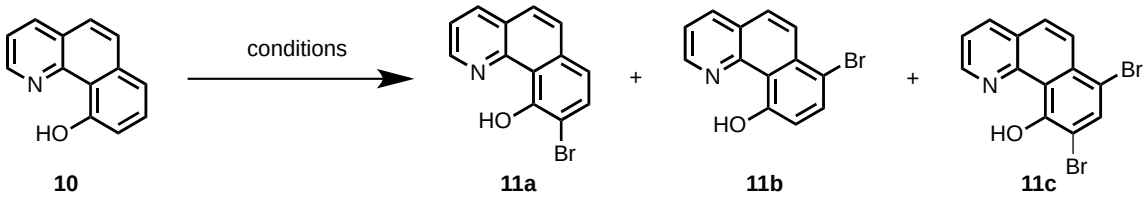


$C_{13}H_9NO$
MW: 195.22 g.mol^{-1}
Yellow solid
Yield: 79%

Following a procedure from the literature[7]: in a sealable tube, were added benzo[*h*]quinoline (720 mg, 4.0 mmol, 1 equiv), $Pd(OAc)_2$ (50 mg, 0.22 mmol, 0.05 equiv), $PhI(OAc)_2$ (1.7 g, 5.2 mmol, 1.3 equiv) in ACN (10 mL). The mixture was heated at 100 °C for 24 hours. After cooling at room temperature, solvents were removed under evaporation. MeOH (10 mL) was added followed by NaOH (400 mg, 10 mmol, 2.5 equiv). Stirring at room temperature was maintained for 3 hours. The mixture was slowly quenched by addition of a 1M solution of HCl until pH 5-6 is reached. The mixture was then concentrated *in vacuo* and the crude was partitioned between EtOAc and water. The organic layer was separated, dried over $MgSO_4$, filtered and concentrated. Purification by silica gel chromatography (Heptane/EtOAc 9:1) afforded the desired compound as a yellow solid (620 mg, 3.17 mmol, 79% yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 14.93 (s, 1H), 8.84 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.27 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.65 – 7.55 (m, 3H), 7.42 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.25 (d, *J* = 7.6 Hz, 1H).
LCMS (ESI) *m/z*: 196 $[M+H]^+$.

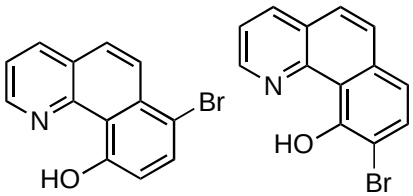
Bromination optimisation



Conditions	^{1}H NMR ratio			
	10	**11a**	**11b**	**11c**
NBS , Toluene/ACN (1:1), rt, 1h*	2.8	1	3.4	0.1
DBDMH, ACN, rt, 1h	1.6	1	2.4	0.5
BDMS, DCM, rt, 1h	17	1	4	0
NBS, DCM, 0°C, 1h*	0.8	1	1.4	0.2
NBS, iPr_2NH, DCM, -78°C, 3h	4.4	1	2.3	0.07
NBS, ACN, 0°C, 1h*	0.1	1	1.7	0.35
NBS, ACN, 0°C then rt, 1h *	**0.2**	**1**	**0.7**	**0.05**
NBS, ACN, 0°C then rt, 1h **	0	1	1.1	0.8
NBS, ACN, 40°C, 1h*	0.3	1	1.1	0.2
NBS, ACN(wet), rt, 1h *	0.9	1	1.3	0.1
NBS, Ag_2SO_4, EtOH, rt, 4h	1.9	1	2.2	0.4
NBS, BArF, ACN, rt, 1h	0.6	1	1.4	0.2
NBS, ACN, rt, 1h*	0.3	1	2	0.6

Table S2. *NBS was solubilized in a 1/3 of the amount of solvent and slowly added with a syringe pump (14 mL/h speed rate) ** syringe pump speed rate: 7 mL/h

9-bromobenzo[h]quinolin-10-ol 11a *& 7-bromobenzo[h]quinolin-10-ol* 11b



$C_{13}H_8BrNO$
MW: 274.12 g.mol^{-1}
Yellow solid
Yield: 59%

Using a syringe pump (14 mL/h speed rate), NBS (550 mg, 3.06 mmol, 1 equiv) in ACN (10 mL) was added to a cold solution (0 °C) of benzo[h]quinolin-10-ol **10** (600 mg, 3.08 mmol, 1 equiv) in ACN (20 mL) with a vigorous stirring. The mixture was stirred at this temperature 1 hour and solvent was removed by evaporation. Purification by silica gel chromatography (Heptane/EtOAc 100:0 -> 99:1) afforded 7-bromobenzo[h]quinolin-10-ol **11b** as a yellow solid (230 mg, 0.84 mmol, 27% yield) and a mixture of 9-bromobenzo[h]quinolin-10-ol **11a** and 7,9-dibromobenzo[h]quinolin-10-ol. Purification

by reverse phase chromatography (H_2O+0.1%TFA/ACN+0.1%TFA 95:5 to 0:100) followed by basic treatment afforded 9-bromobenzo[h]quinolin-10-ol **11a** as a pure pale-yellow powder (264 mg, 0.96 mmol, 32% yield).

Spectroscopic data for 9-bromobenzo[h]quinolin-10-ol **11a**

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 15.95 (s, 1H), 8.83 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.28 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.9 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 1H), 7.60 (dd, *J* = 8.1, 4.7 Hz, 1H), 7.29 (d, *J* = 8.5 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 156.0(C), 147.5(C), 145.1(CH), 136.6(CH), 134.1(C), 133.4(CH), 128.9(CH), 126.5(C), 125.1(CH), 121.5(CH), 118.8(CH), 116.5(C), 107.9(C).

IR (cm^{-1}): 1622, 1584, 1519, 1459, 1427, 1335, 1311, 1128, 829, 724.

LCMS (ESI) *m/z*: $C_{24}H_{17}N_2$ $[M+H]^+$ 333.4.

Spectroscopic data for 7-bromobenzo[h]quinolin-10-ol **11b**

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 15.27 (s, 1H), 8.87 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.33 (dd, *J* = 8.1, 1.8 Hz, 1H), 8.26 (d, *J* = 9.2 Hz, 1H), 7.87 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 9.2 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.14 (d, *J* = 8.5 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.4 (C), 147.8 (C), 145.4 (CH), 136.7 (CH), 133.8 (CH), 132.8 (C), 128.1 (CH), 126.3 (C), 126.1(CH) 121.6 (CH), 117.3 (C), 115.2 (CH), 110.6 (C).

IR (cm^{-1}): 1619, 1575, 1466, 1400, 1329, 1272, 1110, 1032, 817, 715.

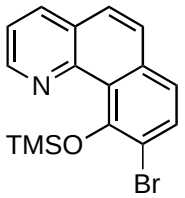
LCMS (ESI) *m/z*: $C_{13}H_9BrNO$ $[M]^+$ 274.2.

Spectroscopic data for 7,9-dibromobenzo[h]quinolin-10-ol **11c**

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 16.37 (s, 1H), 8.88 (dd, *J* = 4.7, 1.8 Hz, 1H), 8.36 (dd, *J* = 8.1, 1.8 Hz, 1H), 8.22 (d, *J* = 9.2 Hz, 1H), 8.14 (s, 1H), 7.79 (d, *J* = 9.2 Hz, 1H), 7.68 (dd, *J* = 8.1, 4.7 Hz, 1H).

The spectroscopic data were in accordance with the literature. [8]

***9-bromo-10-((trimethylsilyl)oxy)benzo[h]quinoline* 12a**

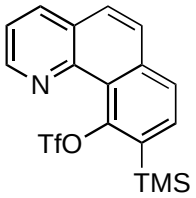


$C_{16}H_{16}BrNOSi$
MW: 346.30 g.mol^{-1}
White solid
Yield: 99%

In a sealable tube, were added 9-bromobenzo[h]quinolin-10-ol **11a** (120 mg, 0.45 mmol, 1 equiv), BSTFA (250 μL, 0.94 mmol, 2.1 equiv) in dry ACN (800 μL). The mixture was heated at 60 °C for 2 hours. The solvent was removed *in vacuo* to give a white solid (153 mg, 0.45 mmol, 99% yield). Due to instability and fast deprotection the compound **12a** was used quickly after in the next step.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.02 (dd, *J* = 4.4, 1.9 Hz, 1H), 8.15 (dd, *J* = 8.0, 1.9 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.53 (dd, *J* = 8.0, 4.3 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 0.30 (s, 9H).

***9-(trimethylsilyl)benzo[h]quinolin-10-yl trifluoromethanesulfonate* 13a**

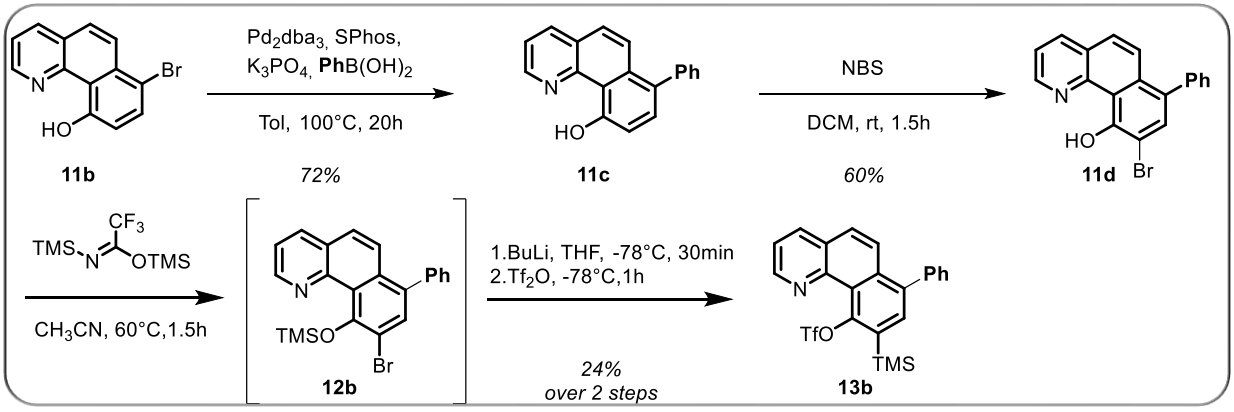


$C_{17}H_{16}F_3NO_3SSi$
MW: 399.46 g.mol^{-1}
Colorless oil
Yield: 51%

At -78°C, under inert atmosphere, *n*BuLi (0.6 mL, 1.05 mmol, 1.2 equiv) was added dropwise to a solution of 9-bromo-10-((trimethylsilyl)oxy)benzo[h]quinoline **12a** (302 mg, 0.85 mmol, 1 equiv) in freshly distilled THF (3 mL). Stirring was maintained at this temperature for 30 minutes then Tf_2O (200 µL, 1.22 mmol, 1.4 equiv) was slowly added. After 1 hour of stirring at this temperature, the solution was allowed to warm to room temperature. A cold saturated solution of $NaHCO_3$ was added to quench the mixture. The crude was then extracted with Et_2O. The organic layer was dried over $MgSO_4$, filtered and concentrated. Purification by silica gel column chromatography (Heptane/EtOAc 100:0 to 98:2) afforded the desired compound as a colorless oil (180.3 mg, 0.45 mmol, 51% yield).

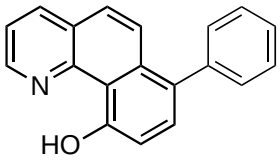
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.02 (dd, *J* = 4.3, 1.9 Hz, 1H), 8.19 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.81 – 7.72 (m, 3H), 7.56 (dd, *J* = 8.0, 4.3 Hz, 1H), 0.51 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.7(C), 148.3(CH), 145.7(C), 137.1(C), 135.9(CH), 134.9(C), 134.2(CH), 128.1(CH), 127.6(CH), 127.5(C), 127.1(CH), 124.3(C), 122.2(CH), 119.0 (q, *J* = 323 Hz).
IR (neat, cm^{-1}): 2925, 1591, 1418, 1390, 1196, 1131, 984, 841, 731, 681.
HRMS (ESI-TOF) *m/z* calcd for $C_{14}H_{17}F_3NO_3SSi$ $[M+H]^+$: 400.0645; found: 400.0641.

Preparation of 7-phenylbenzoquinolyne precursor



Scheme S4. Synthetic pathway for the preparation of **13b**

***7-phenylbenzo[h]quinolin-10-ol* 11c**

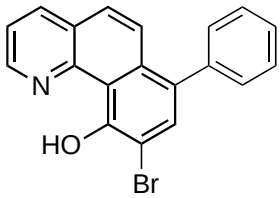


$C_{19}H_{13}NO$
MW: 271.32 g.mol^{-1}
Yellow solid
Yield: 72%

Under inert atmosphere, 7-bromobenzo[h]quinolin-10-ol **11b** (197 mg, 0.72 mmol, 1 equiv), Pd_2dba_3 (8 mg, 8 μmol, 0.01 equiv), SPhos (16 mg, 40 μmol, 0.05 equiv), K_3PO_4 .$3H_2O$ (500 mg, 2.17 mmol, 3 equiv) were suspended in anhydrous toluene (2 mL). The solution was degassed before the addition of phenylboronic acid (176 mg, 1.44 mmol, 2 equiv). The mixture was heated at 100 °C for 20 hours. After cooling at room temperature and filtration through a celite pad, the reaction mixture was concentrated *in vacuo*. Purification by silica gel chromatography (Heptane/EtOAc 100: 0 -> 99:1) afforded the desired compound as a yellow solid (141 mg, 0.52 mmol, 72% yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 15.32 (s, 1H), 8.83 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.22 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.92 (d, *J* = 9.2 Hz, 1H), 7.63 – 7.43 (m, 8H), 7.32 (d, *J* = 8.1 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.2(C), 148.5(C), 144.9(CH), 140.9(C), 136.2(CH), 132.5(C), 131.4(CH), 130.9(C), 130.6(2xCH), 128.4(2xCH), 127.2(CH), 127.0(CH), 126.2(C), 124.6(CH), 121.1(CH), 115.9(C), 113.8(CH).
IR (NaCl, cm^{-1}): 3040, 2617, 2494, 1622, 1532, 1472, 1410, 1336, 1290, 1232, 1130, 824, 716, 632.
LCMS (ESI) *m/z*: $C_{19}H_{14}NO$ $[M+H]^+$ 272.4.

***9-bromo-7-phenylbenzo[h]quinolin-10-ol* 11d**

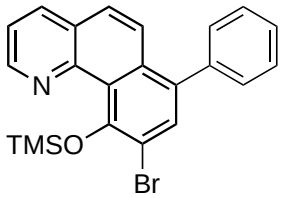


$C_{19}H_{12}BrNO$
MW: 350.21 g.mol^{-1}
Orange solid
Yield: 60% (corrected)

NBS (101 mg, 0.57 mmol, 1.1 equiv) was added by portion to a solution of 7-phenylbenzo[h]quinolin-10-ol **11c** (141 mg, 0.52 mmol, 1 equiv) in anhydrous DCM (10 mL). The solution was stirred at room temperature for 1.5 hour and the solvent was removed *in vacuo.* Purification by silica gel chromatography (Heptane/EtOAc 100: 0 -> 95:5) afforded the desired compound as an orange solid (120.4 mg, 0.34 mmol, 66% crude yield). The product was obtained as an inseparable mixture of regioisomers with 88% of the desired isomer. The corrected yield of the desired isomer is 60%.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 16.33 (s, 1H), 8.82 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.25 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.85 (d, *J* = 8.9 Hz, 2H), 7.62 – 7.55 (m, 2H), 7.53 – 7.41 (m, 5H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 155.6(C), 147.5(C), 144.9(CH), 139.6(C), 136.5(CH), 134.4(CH), 131.7(C), 131.6(C), 130.5(2xCH), 128.6(2xCH), 127.5(CH), 127.0(CH), 126.4(C), 124.9(CH), 121.6(CH), 116.3(C), 107.6(C).
IR (neat, cm^{-1}): 3054, 1618, 1581, 1459, 1442, 1395, 1301, 1127, 880, 830, 725, 703.
LCMS (ESI) *m/z*: $C_{19}H_{13}BrNO$ $[M+H]^+$ 351.4.

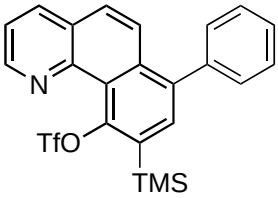
***9-bromo-7-phenyl-10-((trimethylsilyl)oxy)benzo[h]quinoline* 12a**



$C_{22}H_{20}BrNOSi$
MW: 422.39 g.mol^{-1}
white solid
Yield: quantitative

In a sealable tube, were added 9-bromo-7-phenylbenzo[h]quinolin-10-ol (120 mg, 0.34 mmol, 1 equiv), BSTFA (180 µL, 0.68 mmol, 2.1 equiv) in dry ACN (600 µL). The mixture was heated at 60 °C for 2 hours. The solvent was removed *in vacuo* to give a white solid (132 mg, 0.14 mmol, quantitative yield). Due to instability and fast deprotection the compound was used quickly after in the next step.
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.04 (dd, *J* = 4.3, 1.9 Hz, 1H), 8.13 (dd, *J* = 8.0, 1.9 Hz, 1H), 7.84 (s, 1H), 7.78 (d, *J* = 9.1 Hz, 1H), 7.59 – 7.43 (m, 7H), 0.32 (s, 9H).

***7-phenyl-9-(trimethylsilyl)benzo[h]quinolin-10-yl trifluoromethanesulfonate* 13b**

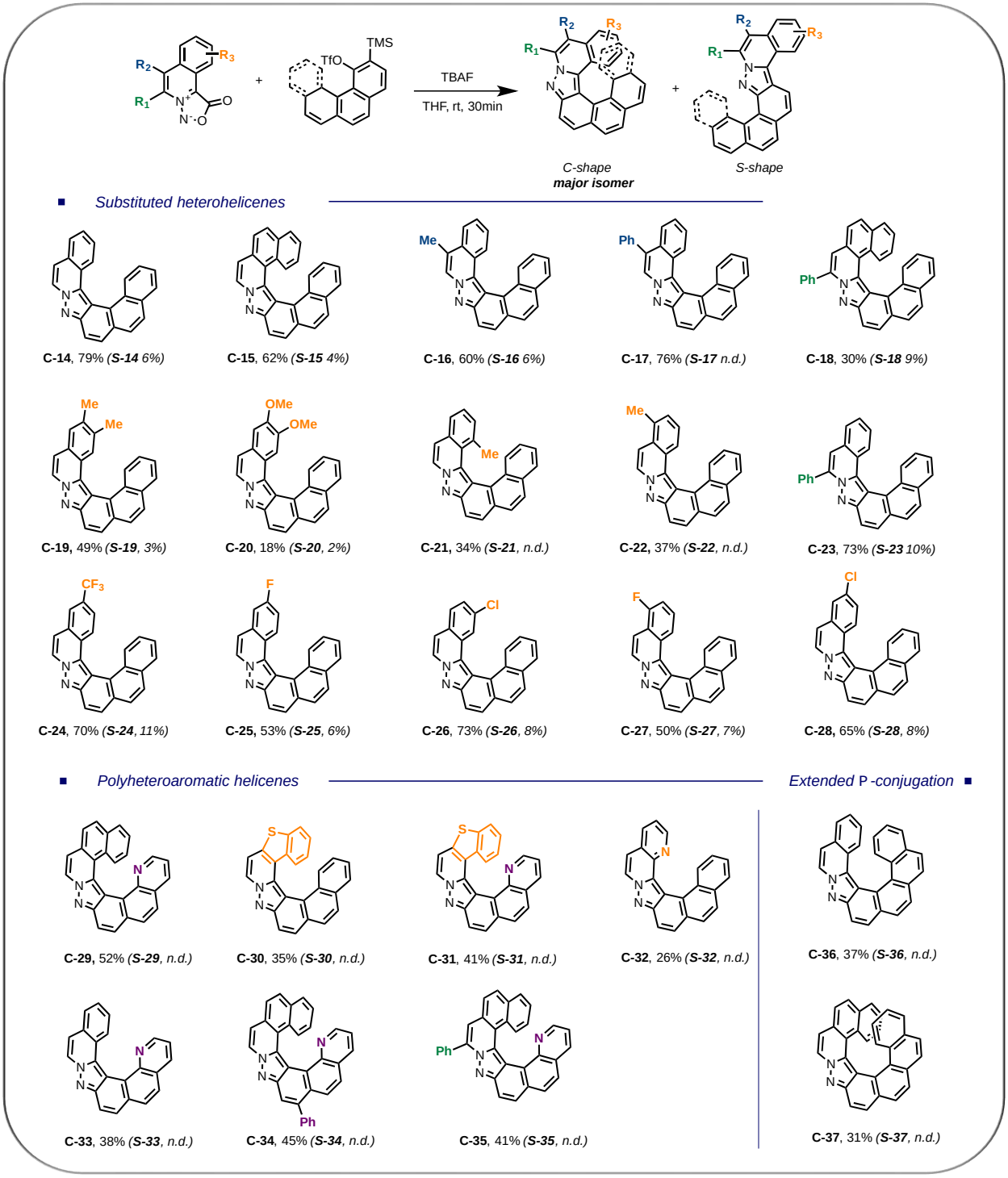


$C_{23}H_{20}F_3NO_3SSi$
MW: 472.55 g.mol^{-1}
Colorless oil
Yield: 24%

At -78°C, under inert atmosphere, *n*BuLi (220 µL, 0.37 mmol, 1.2 equiv) was added dropwise to a solution of 9-bromo-10-((trimethylsilyl)oxy)benzo[h]quinoline **12b** (132 mg, 0.31 mmol, 1 equiv) in freshly distilled THF (2.2 mL). Stirring was maintained at this temperature for 30 minutes then Tf_2O (100 µL, 0.61 mmol, 1.4 equiv) was slowly added. After 1 hour of stirring at this temperature, the solution was allowed to warm to room temperature. A cold saturated solution of $NaHCO_3$ was added to quench the mixture. The crude was then extracted with Et_2O. The organic layer was dried over $MgSO_4$, filtered and concentrated. Purification by silica gel column chromatography (Heptane/EtOAc 100:0 to 99:1) afforded the desired compound as a colorless oil (36 mg, 0.07 mmol, 24% yield).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.05 (dd, *J* = 4.3, 1.9 Hz, 1H), 8.16 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.80 (d, *J* = 9.1 Hz, 1H), 7.72 (s, 1H), 7.66 (d, *J* = 9.1 Hz, 1H), 7.59 – 7.47 (m, 6H), 0.53 (s, 9H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.15(C), 148.3(CH), 145.8(C), 140.2(C), 139.9(C), 135.7(CH), 135.3(CH), 134.9(C), 134.3(C), 130.3(2xCH), 128.8(2xCH), 127.9(2xCH), 127.4(CH), 127.1(C), 125.2(CH), 124.4(C), 122.4(CH), 118.9 (q, *J* = 318 Hz).
IR (neat, cm^{-1}): 1583, 1419, 1379, 1237, 1197, 1131, 984, 859, 834, 733, 702.
HRMS (ESI-TOF) *m/z* calcd for $C_{23}H_{21}F_3NO_3SSi$ $[M+H]^+$: 476.0958; found: 476.0953.

Helicenes scope

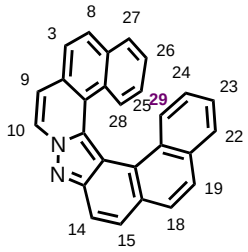


Scheme S5. Helicene scope

General procedure for the preparation of helicenes

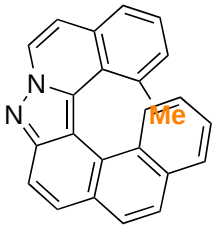
To a solution of the sydnone (1 equiv) and aryne precursor (1.25 equiv) in dry THF (0.4 M) was added dropwise TBAF (1.25 equiv, 1M in THF) over a period of 5 min. The mixture was stirred at room temperature during 15 or 30 min and was then concentrated to dryness *in vacuo*. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc) to afford the desired compound.

Note: Assignment of the C-shape vs the S-shape products has been done by analogy with our precedent report after extensive 2D NMR study and X-ray structures resolution[1]. We noticed by ^{1}H NMR that in the case of the S-shape the proton 29 is deshielded (between 10.6 – 10 ppm) because it is not subjected to the magnetic anisotropy induced by the other terminal benzene.



Example

***16-methylnaphtho[1',2':4,5]indazolo[3,2-a]isoquinoline* C-21**

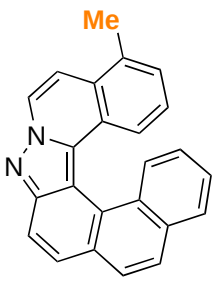


$C_{24}H_{16}N_2$
MW: 332.40 g.mol^{-1}
Yellow solid
Yield: 34%

Compound **C-21** was obtained in 34% yield (8.5 mg, 0.025 mmol) from compound **1d** (15 mg, 0.075 mmol) and compound **9a** (35 mg, 0.09 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 95/5).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.54 (d, *J* = 7.2 Hz, 1H), 8.04 – 7.89 (m, 5H), 7.83 – 7.79 (m, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.61 – 7.49 (m, 2H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.26 (t, *J* = 3.6 Hz, 1H), 7.14 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 1H), 1.56 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.42(C), 137.71(C), 132.81(C), 131.53(C), 130.93(C), 130.34(C), 130.30(CH), 129.88(CH), 129.00(C), 128.03(CH), 127.66(CH), 126.97(CH), 126.95(CH), 126.72(C), 126.62(C), 126.12(CH), 126.04(CH), 125.85(CH), 125.10(CH), 123.77(CH), 117.42(CH), 115.91(CH), 112.37(C), 21.85(CH_3).
IR (cm^{-1}): 3048, 2925, 1531, 1480, 1331, 1202, 907, 828, 805, 749, 731.
LCMS (ESI) *m/z*: $C_{24}H_{17}N_2$ $[M+H]^+$ 333.4.
HRMS (ESI-TOF) *m/z* calcd for $C_{24}H_{17}N_2$ $[M+H]^+$: 333.1386; found: 333.1384.

***13-methylnaphtho[1',2':4,5]indazolo[3,2-a]isoquinoline* C-22**

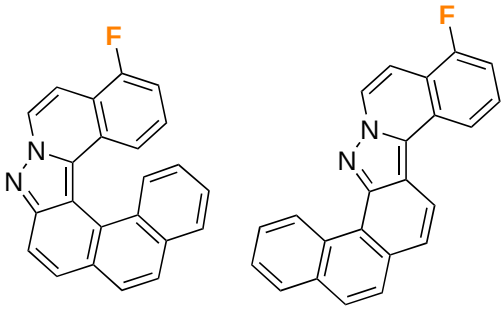


$C_{24}H_{16}N_2$
MW: 332.40 g.mol^{-1}
Yellow solid
Yield: 37%

Compound **C-22** was obtained in 37% yield (12.5 mg, 0.037 mmol) from compound **1e** (20 mg, 0.1 mmol) and compound **9a** (50 mg, 0.125 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 95/5).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.71 (d, *J* = 7.5 Hz, 1H), 8.07 – 8.02 (m, 3H), 7.99 – 7.94 (m, 3H), 7.66 – 7.54 (m, 3H), 7.42 (dt, *J* = 7.3, 1.0 Hz, 1H), 7.34 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.22 (dd, *J* = 8.2, 7.2 Hz, 1H), 2.79 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.98(C), 133.73(C), 133.63(C), 132.80(C), 130.29(CH), 130.27(CH), 129.38(C), 128.89(CH), 128.67(C), 128.13(C), 127.85(CH), 127.27(CH), 127.08(CH), 126.37(CH), 126.31(CH), 125.99(CH), 125.79(C), 125.75(CH), 125.36(C), 124.74(CH), 117.33(CH), 112.40(CH), 110.28(C), 19.94(CH_3).
IR (cm^{-1}): 3048, 1617, 1601, 1532, 1484, 1333, 1218, 905, 828, 784, 730.
LCMS (ESI) *m/z*: $C_{24}H_{17}N_2$ $[M+H]^+$ 333.3.
HRMS (ESI-TOF) *m/z* calcd for $C_{24}H_{17}N_2$ $[M+H]^+$: 333.1386; found: 333.1384.

***13-fluoronaphtho[1',2':4,5]indazolo[3,2-a]isoquinoline* C-27 *and 12-fluoronaphtho[2',1':6,7]indazolo[3,2-a]isoquinoline* S-27**



$C_{23}H_{13}FN_2$
MW: 336.36 g.mol^{-1}
Yellow solids
Yield: 57%

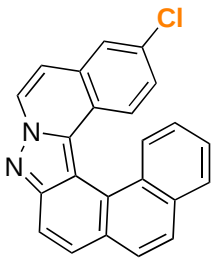
Compounds **C-27** and **S-27** was obtained in 50% (12 mg, 0.035 mmol) and 7% (1.8 mg, 0.005 mmol) yields respectively from compound **1m** (15 mg, 0.073 mmol) and compound **9a** (35 mg, 0.087 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 97/3).

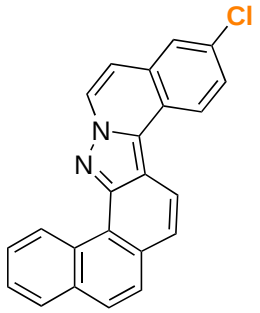
Data for compound **C-27**.
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.72 (d, *J* = 7.5 Hz, 1H), 8.06 (dd, *J* = 8.9, 7.5 Hz, 2H), 8.01 – 7.95 (m, 4H), 7.75 (dd, *J* = 7.5, 0.7 Hz, 1H), 7.62 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.45 (dd, *J* = 6.6, 2.7 Hz, 1H), 7.37 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.32 – 7.26 (m, 2H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 157.95 (d, *J* = 250.7 Hz), 149.87, 132.86, 132.59 (d, *J* = 2.4 Hz), 130.57, 130.11, 129.73, 128.63, 128.02, 127.28, 126.70 (d, *J* = 8.4 Hz), 126.61 (d, *J* = 4.1 Hz), 126.54, 126.39, 125.42, 124.94, 124.65 (d, *J* = 4.0 Hz), 118.75 (d, *J* = 16.9 Hz), 117.40, 112.58 (d, *J* = 19.8 Hz), 110.47, 108.37 (d, *J* = 7.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): -120.97.
IR (cm^{-1}): 3051, 1594, 1533, 1489, 1462, 1333, 1240, 955, 829, 782, 753
LCMS (ESI) *m/z*: $C_{23}H_{14}FN_2$ $[M+H]^+$ 337.
HRMS (ESI-TOF) *m/z* calcd for $C_{23}H_{14}FN_2$ $[M+H]^+$: 337.1136; found: 337.1131.

Data for compound **S-27**.

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm) : 10.53 (dt, *J* = 8.6, 0.6 Hz, 1H), 8.79 (d, *J* = 7.4 Hz, 1H), 8.67 (d, *J* = 8.8 Hz, 1H), 8.44 (d, *J* = 8.8 Hz, 1H), 8.07 – 7.94 (m, 3H), 7.92 – 7.85 (m, 2H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.72 – 7.67 (m, 2H), 7.30 (d, *J* = 7.4 Hz, 1H).
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): -119.58.
IR (cm^{-1}) : 3045, 2922, 1539, 1358, 1260, 1082, 829.
LCMS (ESI) *m/z*: $C_{23}H_{14}FN_2$ $[M+H]^+$ 337.
HRMS (ESI-TOF) *m/z* calcd for $C_{23}H_{14}FN_2$ $[M+H]^+$: 337.1136; found: 337.1130.

***14-chloronaphtho[1',2':4,5]indazolo[3,2-a]isoquinoline* C-28 *and 11-chloronaphtho[2',1':6,7]indazolo[3,2-a]isoquinoline* S-28**





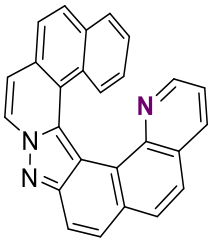
$C_{23}H_{13}ClN_2$
MW: 352.82 $g.mol^{-1}$
Yellow solid
Yield: 73%

Compounds **C-28** and **S-28** was obtained in 65% (23 mg, 0.065 mmol) and 8% (3 mg, 0.008 mmol) yields respectively from compound **1l** (22 mg, 0.1 mmol) and compound **9a** (60 mg, 0.15 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 95/5).

Data for compound **C-28**.
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.65 (d, *J* = 7.3 Hz, 1H), 8.08 – 8.04 (m, 1H), 8.03 (d, *J* = 8.8 Hz, 1H), 7.98 – 7.91 (m, 4H), 7.84 (d, *J* = 2.2 Hz, 1H), 7.61 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.38 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.33 (d, *J* = 7.3 Hz, 1H), 7.26 (dd, *J* = 8.8, 2.2 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 150.1(C), 133.3(C), 132.83(C), 132.81(C), 130.4(CH), 130.38(C), 129.9(CH), 129.8(CH), 129.6(C), 128.5(C), 128.1(CH), 127.8(CH), 127.3(CH), 126.5(CH), 126.3(CH), 126.2(CH), 125.8(CH), 125.4(C), 125.0(CH), 123.5(C), 117.5(CH), 114.8(CH), 110.3(C).
IR (cm^{-1}) : 2917, 1526, 1357, 1331, 1260, 1084, 878, 838, 814, 791, 745.
LCMS (ESI) *m/z*: $C_{23}H_{14}ClN_2$ $[M+H]^+$ 353.4.
HRMS (ESI-TOF) *m/z* calcd for $C_{23}H_{14}ClN_2$ $[M+H]^+$: 353.0840; found: 353.0837.

Data for compound **S-28**.
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 10.53 (dt, *J* = 8.6, 0.6 Hz, 1H), 8.79 (d, *J* = 7.4 Hz, 1H), 8.67 (d, *J* = 8.8 Hz, 1H), 8.44 (d, *J* = 8.8 Hz, 1H), 8.07 – 7.94 (m, 3H), 7.92 – 7.85 (m, 2H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.72 – 7.67 (m, 2H), 7.30 (d, *J* = 7.4 Hz, 1H).
IR (cm^{-1}): 3045, 2922, 1539, 1358, 1260, 1082, 829.
LCMS (ESI) *m/z*: $C_{23}H_{14}ClN_2$ $[M+H]^+$ 353.4.
HRMS (ESI-TOF) *m/z* calcd for $C_{23}H_{14}ClN_2$ $[M+H]^+$: 353.0840; found: 353.0839.

***benzo[7',8']isoquinolino[2',1':2,3]indazolo[5,4-h]quinoline* C-29**

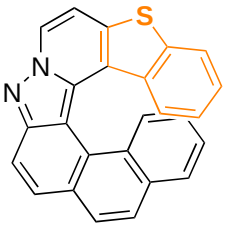


$C_{26}H_{15}N_3$
MW: 369.47 g.mol^{-1}
Yellow solid
Yield: 52%

Compound **C-29** was obtained in 52% yield (21 mg, 0.056 mmol) from compound **1b** (27 mg, 0.11 mmol) and compound **13a** (57 mg, 0.14 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 95/5).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.91 (d, *J* = 7.0 Hz, 1H), 8.26 (d, *J* = 8.9 Hz, 1H), 8.17 – 8.11 (m, 3H), 8.08 (d, *J* = 0.9 Hz, 1H), 7.95 – 7.87 (m, 3H), 7.65 (d, *J* = 7.1 Hz, 1H), 7.41 (dd, *J* = 4.3, 1.8 Hz, 1H), 7.33 (dt, *J* = 8.5, 0.9 Hz, 1H), 7.27 – 7.22 (m, 2H), 7.02 (dd, *J* = 8.1, 4.2 Hz, 1H), 6.30 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 150.2(C), 146.2(CH), 145.0(C), 134.7(CH), 133.9(C), 131.1(C), 130.9(C), 130.2(C), 129.9(CH), 128.6(CH), 128.3(C), 127.7(CH), 127.3(C), 127.1(CH), 127.0(CH), 126.8(C), 126.6(CH), 126.2(CH), 125.1(C), 124.2(CH), 124.1(CH), 123.4(CH), 120.7(CH), 118.9(CH), 116.1(CH), 111.2(C).
IR (cm^{-1}): 3052, 1711, 1517, 1321, 1122, 964, 826, 731.
LCMS (ESI) *m/z*: $C_{26}H_{16}N_3$ $[M+H]^+$ 370.3.
HRMS (ESI-TOF) *m/z* calcd for $C_{26}H_{16}N_3$ $[M+H]^+$: 370.1339; found: 370.1338.
m.p.: 258 - 260 °C.

***benzo[4',5']thieno[3',2':3,4]pyrido[1,2-b]naphtho[1,2-e]indazole* C-30**



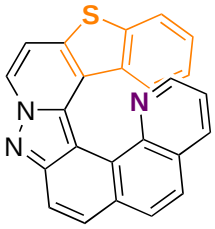
$C_{25}H_{14}N_2S$
MW: 374.46 g.mol^{-1}
Yellow solid
Yield: 35%

Compound **C-30** was obtained in 35% yield (8.5 mg, 0.025 mmol) from compound **1q** (15 mg, 0.075 mmol) and compound **9a** (35 mg, 0.09 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 95/5).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.92 (d, *J* = 7.2 Hz, 1H), 8.06 – 7.93 (m, 5H), 7.92 – 7.86 (m, 2H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.31 (ddd, *J* = 8.0, 6.8, 1.2 Hz, 1H), 7.27 – 7.20 (m, 1H), 6.90 (dt, *J* = 8.2, 0.9 Hz, 1H), 6.67 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 6.59 (ddd, *J* = 8.3, 7.1, 1.1 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 150.9(C), 138.8(C), 135.32(C), 135.29(C), 132.9(C), 132.2(C), 131.0(CH), 130.7(C), 128.5(C), 127.8(CH), 127.7(CH), 127.5(CH), 126.9(CH), 126.6(CH), 126.3(C), 126.2(CH), 126.0(C), 125.8(CH), 125.5(CH), 124.3(CH), 122.6(CH), 121.9(CH), 116.8(CH), 110.1(CH), 108.3(C).
IR (cm^{-1}): 3049, 1925, 1621, 1530, 1382, 1218, 1137, 907, 828, 739, 730.
LCMS (ESI) *m/z*: $C_{25}H_{15}N_2S$ $[M+H]^+$ 375.4.

HRMS (ESI-TOF) ***m/z*** calcd for $C_{25}H_{15}N_2S$ $[M+H]^+$: 375.0950; found: 375.0952.
m.p.: 215 - 217 °C.

benzo[4'',5'']thieno[3'',2'':3',4']pyrido[1',2':2,3]indazolo[5,4-h]quinoline **C-31**

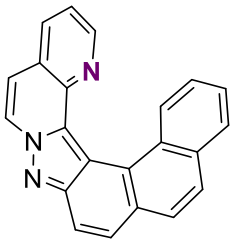


$C_{25}H_{13}N_3S$
MW: 375.45 g.mol^{-1}
Yellow solid
Yield: 41%

Compound **C-31** was obtained in 41% yield (11.6 mg, 0.031 mmol) from compound **1q** (18 mg, 0.076 mmol) and compound **13a** (38 mg, 0.095 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 9/1).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.87 (d, *J* = 7.2 Hz, 1H), 8.25 (dd, *J* = 8.1, 1.8 Hz, 1H), 8.16 – 8.05 (m, 3H), 7.94 (dd, *J* = 4.3, 1.8 Hz, 1H), 7.89 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.22 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.17 (dd, *J* = 8.1, 4.3 Hz, 1H), 6.92 (dt, *J* = 8.2, 0.9 Hz, 1H), 6.54 (ddd, *J* = 8.2, 7.1, 1.1 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 150.9(C), 138.8(C), 135.32(C), 135.29(C), 132.9(C), 132.2(C), 131.0(CH), 130.7(C), 128.5(C), 127.8(CH), 127.7(CH), 127.5(CH), 126.9(CH), 126.6(CH), 126.3(C), 126.2(CH), 126.0(C), 125.8(CH), 125.5(CH), 124.3(CH), 122.6(CH), 121.9(CH), 116.8(CH), 110.1(CH), 108.3(C).
IR (cm^{-1}): 2954, 2923, 2853, 1727, 1621, 1528, 1489, 1389, 1205, 908, 834, 768, 732.
LCMS (ESI) ***m/z*****:** $C_{25}H_{15}N_2S$ $[M+H]^+$ 376.3.
HRMS (ESI-TOF) ***m/z*** calcd for $C_{24}H_{14}N_3S$ $[M+H]^+$: 376.0903; found: 376.0907.

naphtho[1',2':4,5]indazolo[2,3-h][1,7]naphthyridine **C-32**



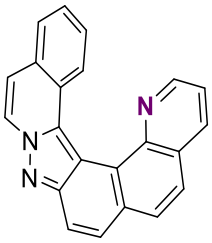
$C_{22}H_{13}N_3$
MW: 319.36 g.mol^{-1}
Yellow solid
Yield: 26%

Compound **C-32** was obtained in 26% yield (5.3 mg, 0.016 mmol) from compound **1p** (12 mg, 0.064 mmol) and compound **9a** (33 mg, 0.082 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 8/2).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.76 – 8.69 (m, 2H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.17 (dd, *J* = 8.0, 1.8 Hz, 1H), 8.06 – 7.91 (m, 5H), 7.59 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.45 (dd, *J* = 8.0, 4.5 Hz, 1H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.32 – 7.26 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 150.2(C), 148.6(CH), 143.3(C), 134.1(CH), 133.91(C), 132.92(C), 132.1(CH), 130.9(CH), 129.8(C), 129.8(C), 127.9(CH), 126.9(CH), 126.9(CH), 126.8(CH), 126.2(CH), 126.1(C), 125.1(C), 123.1(CH), 121.8(CH), 117.0(CH), 114.0(CH), 111.4(C).

IR (cm^{-1}): 3048, 2924, 2853, 1729, 1601, 1480, 1355, 1258, 1109, 828, 729.
LCMS (ESI) *m/z*: $C_{22}H_{14}N_3$ $[M+H]^+$ 320.1.
HRMS (ESI-TOF) *m/z* calcd for $C_{22}H_{14}N_3$ $[M+H]^+$: 320.1182; found: 320.1182.

***isoquinolino[2',1':2,3]indazolo[5,4-h]quinoline* C-33**

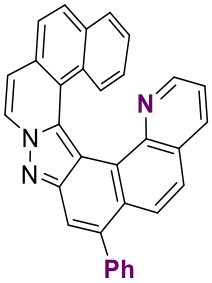


$C_{22}H_{13}N_3$
MW: 319.36 g.mol^{-1}
Yellow solid
Yield: 43%

Compound **C-33** was obtained in 43% yield (8 mg, 0.025 mmol) from compound **1a** (11 mg, 0.058 mmol) and compound **13a** (28 mg, 0.07 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 8/2).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.75 (dd, *J* = 4.3, 1.8 Hz, 1H), 8.63 (d, *J* = 7.3 Hz, 1H), 8.36 (dd, *J* = 8.1, 1.8 Hz, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.98 (d, *J* = 8.9 Hz, 1H), 7.91 (d, *J* = 8.5 Hz, 1H), 7.86 – 7.83 (m, 1H), 7.71 – 7.67 (m, 1H), 7.59 – 7.50 (m, 2H), 7.46 (d, *J* = 7.2 Hz, 1H), 7.32 (ddd, *J* = 8.4, 7.1, 1.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.9(C), 147.8(CH), 145.3(C), 135.8(CH), 134.9(C), 131.5(CH), 130.4(C), 129.6(C), 129.5(CH), 128.4(CH), 127.7(C), 127.35(C), 127.31(CH), 126.7(C), 126.5(C), 126.0(CH), 124.7(CH), 124.5(CH), 121.3(CH), 119.3(CH), 116.6(CH), 109.9(C).
IR (cm^{-1}) : 2917, 2849, 1735, 1529, 1490, 1334, 1248, 958, 836, 793, 731.
LCMS (ESI) *m/z*: $C_{22}H_{14}N_3$ $[M+H]^+$ 320.4.
HRMS (ESI-TOF) *m/z* calcd for $C_{22}H_{14}N_3$ $[M+H]^+$: 320.1182; found: 320.1184.

***7-phenylbenzo[7',8']isoquinolino[2',1':2,3]indazolo[5,4-h]quinoline* C-34**



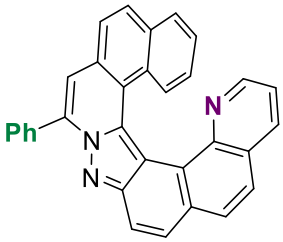
$C_{32}H_{19}N_3$
MW: 445.52 g.mol^{-1}
Yellow solid
Yield: 45%

Compound **C-34** was obtained in 45% yield (11 mg, 0.024 mmol) from compound **1b** (13 mg, 0.055 mmol) and compound **13b** (30 mg, 0.063 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 95/5).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.94 (d, *J* = 7.1 Hz, 1H), 8.19 (s, 1H), 8.17 – 8.05 (m, 3H), 7.94 (d, *J* = 8.6 Hz, 2H), 7.82 – 7.52 (m, 8H), 7.42 (dd, *J* = 4.3, 1.8 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.26 (dd, *J* = 14.9, 1.2 Hz, 1H), 7.02 (dd, *J* = 8.1, 4.2 Hz, 1H), 6.34 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.6 (C), 146.2 (C), 142.0 (C), 141.1 (C), 134.8 (C), 134.1 (C), 131.0 (C), 130.9 (C), 130.4 (3CH), 129.34 (C), 128.7(CH), 128.6 (2CH), 128.5(C), 127.7 (CH), 127.2 (CH), 127.1

(CH), 126.7 (CH), 126.5 (CH), 126.2 (CH), 126.0 (CH), 125.1(C), 124.2 (CH), 123.7(CH), 123.6 (CH), 121.0 (CH), 119.5 (C), 116.2 (CH), 110.8(C).
IR (cm^{-1}): 3052, 1713, 1587, 1499, 1323, 1218, 1122, 965, 907, 826, 730, 702.
LCMS (ESI) *m/z*: $C_{32}H_{20}N_2$ $[M+H]^+$ 446.9.
HRMS (ESI-TOF) *m/z* calcd for $C_{32}H_{20}N_3$ $[M+H]^+$: 446.1652; found: 446.1648.

***11-phenylbenzo[7',8']isoquinolino[2',1':2,3]indazolo[5,4-h]quinoline* C-35**

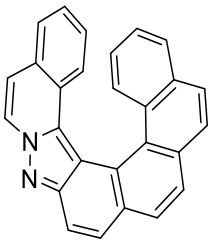


$C_{32}H_{19}N_3$
MW: 445.52 $g.mol^{-1}$
Yellow solid
Yield: 41%

Compound **C-35** was obtained in 41% yield (14 mg, 0.031 mmol) from compound **1h** (24 mg, 0.077 mmol) and compound **13a** (40 mg, 0.10 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 95/5).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.28 (d, *J* = 8.8 Hz, 1H), 8.20 – 8.06 (m, 6H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.93 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.71 (s, 1H), 7.67 – 7.57 (m, 3H), 7.50 – 7.46 (m, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.05 (dd, *J* = 8.1, 4.3 Hz, 1H), 6.33 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.9 (C), 146.1 (C), 138.3 (C), 134.7 (C), 134.4 (C), 130.9 (C), 130.7 (CH), 130.4 (C), 130.1 (2CH), 129.65 (CH), 129.64 (CH), 128.76 (C), 128.71 (2CH), 128.6 (C), 127.9 (C), 127.3 (CH), 126.8 (CH), 126.1 (CH), 124.3 (CH), 124.1 (CH), 124.0 (C), 123.7 (CH), 120.6 (CH), 119.9 (C), 117.0 (CH), 111.2 (C).
IR (cm^{-1}): 3051, 2924, 2852, 1721, 1598, 1526, 1489, 1353, 1205, 908, 835, 731
LCMS (ESI) *m/z*: $C_{32}H_{20}N_2$ $[M+H]^+$ 446.9.
HRMS (ESI-TOF) *m/z* calcd for $C_{32}H_{20}N_3$ $[M+H]^+$: 446.1652; found: 446.1655.
m.p.: 160 - 162 °C.

***phenanthro[4',3':4,5]indazolo[3,2-a]isoquinoline* C-36**

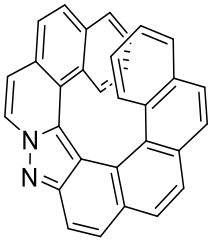


$C_{27}H_{16}N_2$
MW: 368.44 $g.mol^{-1}$
Yellow solid
Yield: 37%

Compound **C-36** was obtained in 37% yield (4.8 mg, 0.013 mmol) from compound **1a** (7.7 mg, 0.041 mmol) and compound **9b** (21.2 mg, 0.047 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 20/1).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.67 (d, *J* = 7.3 Hz, 1H), 8.17 – 8.06 (m, 3H), 8.03 – 7.96 (m, 3H), 7.90 (ddd, *J* = 16.6, 8.2, 1.2 Hz, 2H), 7.70 – 7.66 (m, 1H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.29 – 7.26 (m, 1H), 7.13 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 6.64 – 6.60 (m, 1H), 6.55 (ddd, *J* = 8.3, 7.0, 1.3 Hz, 1H), 6.42 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 133.3, 132.9, 131.7, 131.5, 130.9, 130.7, 128.1, 128.0, 127.8, 127.7, 127.2, 126.5, 126.3, 126.2, 126.0, 125.9, 125.8, 125.4, 125.38, 125.3, 125.0, 124.7, 123.4, 117.2, 116.0, 112.5. One C is missing
IR (cm^{-1}): 3047, 2959, 2925, 2854, 1723, 1609, 1537, 1503, 1260, 1249, 1079, 1016, 907, 838, 791, 729.
LCMS (ESI) *m/z*: $C_{27}H_{17}N_2$ $[M+H]^+$ 369.3.
HRMS (ESI-TOF) *m/z* calcd for $C_{27}H_{17}N_2$ $[M+H]^+$: 369.1386; found: 369.1385.
m.p.: 209 - 211 °C.

***benzo[h]phenanthro[4',3':4,5]indazolo[3,2-a]isoquinoline* C-37**

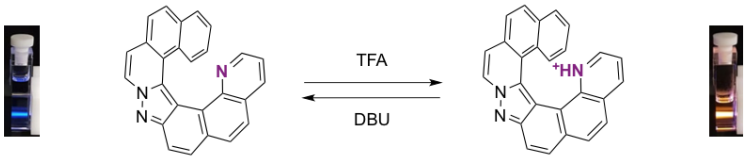


$C_{31}H_{18}N_2$
MW: 418.49 g.mol^{-1}
Yellow solid
Yield: 31%

Compounds **C-37** was obtained in 31% yield (2.8 mg, 0.0067 mmol) respectively from compound **1b** (5 mg, 0.02 mmol) and compound **9b** (15 mg, 0.033 mmol) according to the general procedure. The crude product was purified by flash chromatography (SiO_2, heptane/EtOAc, 100/0 -> 9/1).

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 9.08 (d, *J* = 7.0 Hz, 1H), 8.34 (s, 2H), 8.29 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.84 – 7.76 (m, 2H), 7.69 (d, *J* = 6.9 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 2H), 7.22 – 7.12 (m, 2H), 6.73 (ddd, *J* = 8.0, 6.9, 1.2 Hz, 1H), 6.40 (d, *J* = 8.4 Hz, 1H), 6.00 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 5.91 (d, *J* = 8.6 Hz, 1H), 5.78 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 131.39, 131.29, 130.46, 130.10, 129.86, 129.62, 128.80, 127.92, 127.73, 127.66, 127.32, 126.48, 126.35, 126.19, 125.96, 125.90, 125.80, 125.27, 124.24, 124.04, 123.72, 123.64, 123.17, 122.98, 116.77, 115.17. 5 C missing
IR (cm^{-1}): 2959, 2854, 1723, 1609, 1502, 1260, 1015, 907, 838, 791, 728.
LCMS (ESI) *m/z*: $C_{31}H_{19}N_2$ $[M+H]^+$ 419.5.
HRMS (ESI-TOF) *m/z* calcd for $C_{31}H_{19}N_2$ $[M+H]^+$: 419.1543; found: 419.1541.

III. Optical properties of compound C-29



Scheme S6. Structure and picture of compound **C-29** in its neutral or protonated state upon addition of TFA of DBU.

Chiral SFC analysis

Preparative separation: SFC chromatograms were recorded using a CHIRALPAK IC (250 mm x 20 mm x 5µm), mobile phase: EtOH/CO_2 (3:7), flow rate 33 ml.min^{-1} at 40 °C, detection (220 - 400 nm).
Analysis postpreparative SFC: SFC chromatograms were recorded using a CHIRALPAK IC (250 mm x 4.6 mm x 5µm), mobile phase: EtOH/CO_2 (1:1), flow rate 4 ml.min^{-1} at 40 °C, detection (220 - 400 nm).

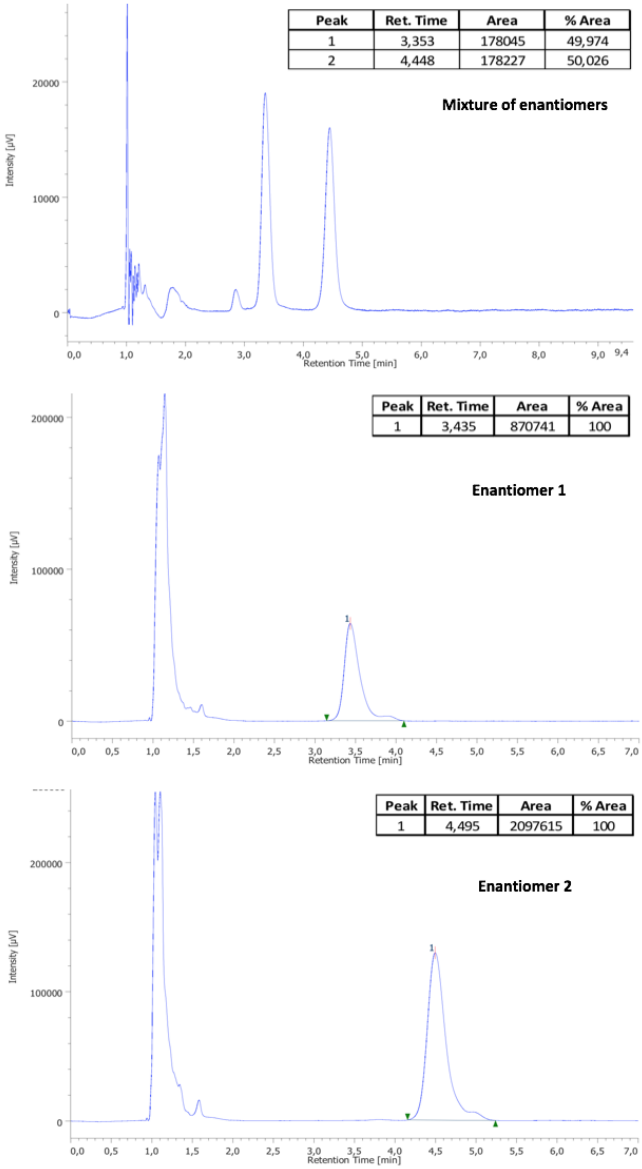


Figure S1. Chiral SFC spectra of the racemic mixture and after separation of each isomer (ee >99 %)

Optical study absorbance and emission neutral form

Absorbance & fluorescence spectra

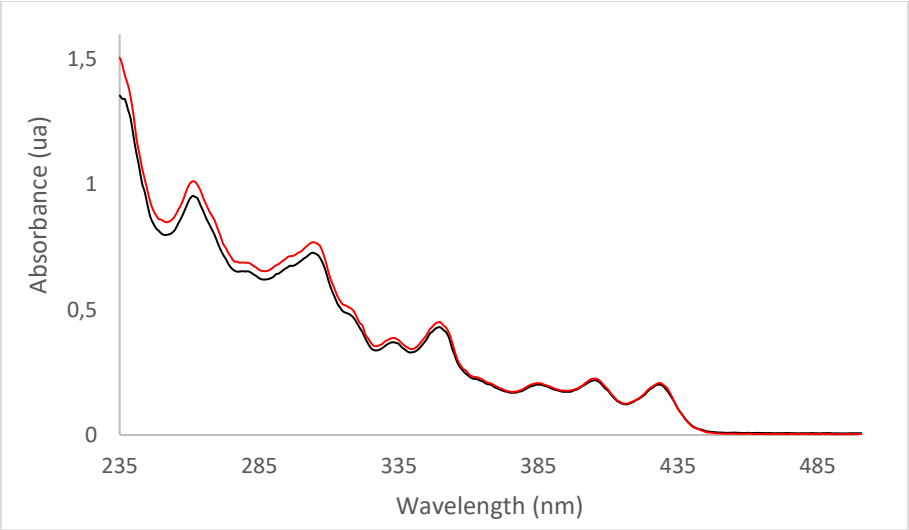


Figure S2. Absorbance spectra for both enantiomers measured in dichloromethane at 50 µM.

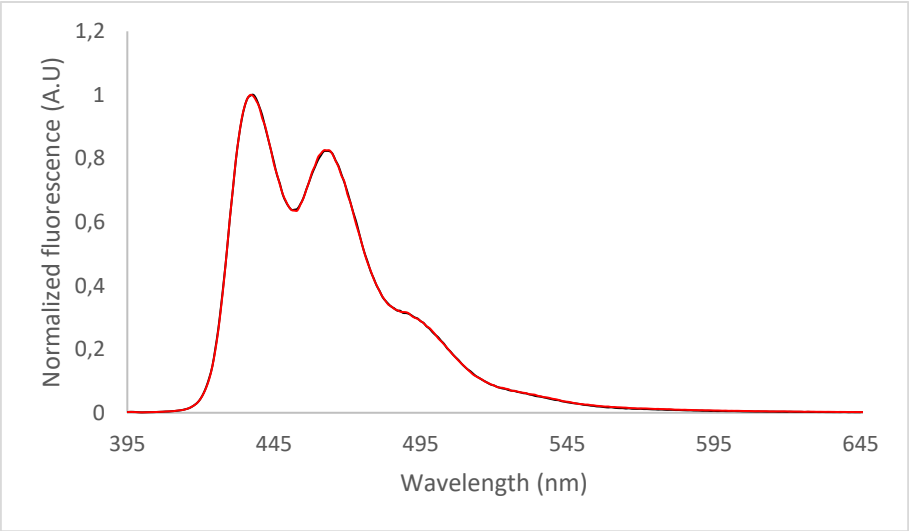


Figure S3. Normalized fluorescence of the basic form both enantiomers (20 µM in dichloromethane) after excitation at 385 nm.

Specific rotation α_D

α_D^{20} (isomer 1): + 1208 (c 5.10^{-5}, $CHCl_3$)

α_D^{20} (isomer 2): - 1130 (c 1.10^{-4}, $CHCl_3$)

Circular dichroism (CD) analysis

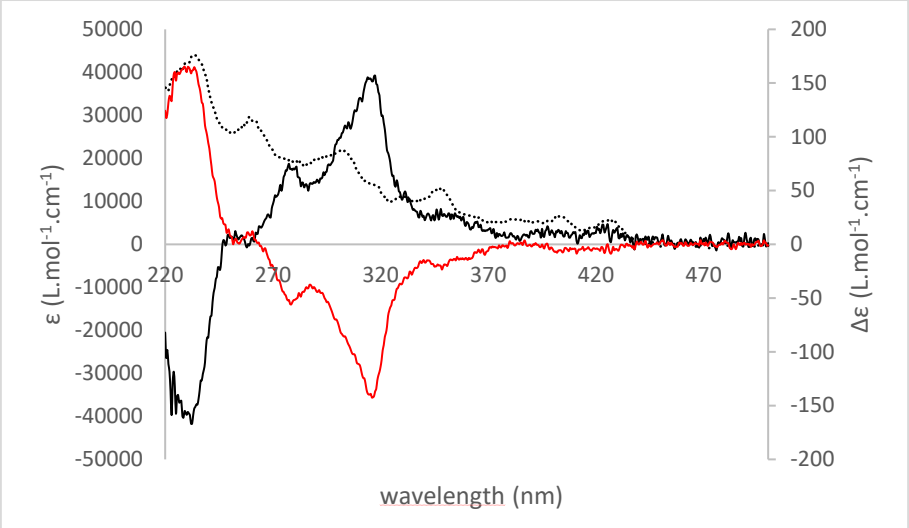
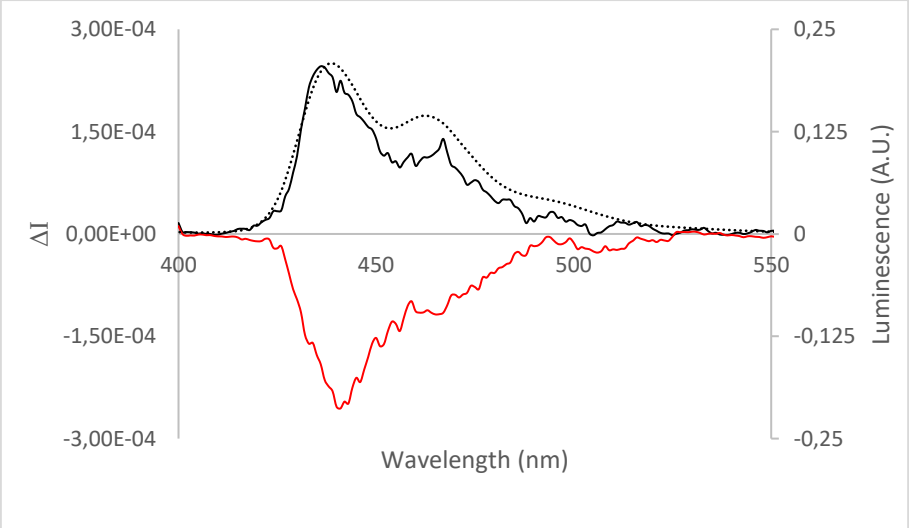


Figure S4. CD spectra were obtained from 50 µM in DCM. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: molecular attenuation coefficient.

Circularly Polarized Luminescence (CPL) study



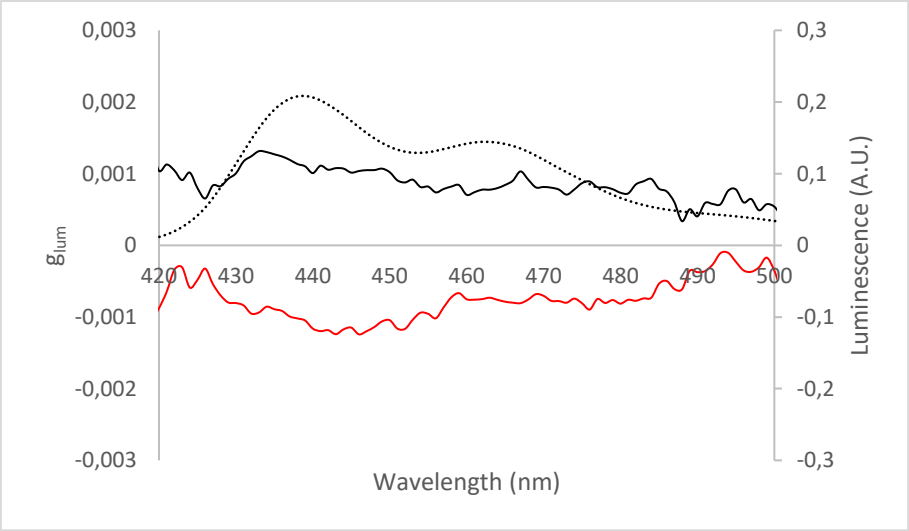


Figure S5. Superimposition of ΔI and luminescence spectra (first graph) and g_{lum} values and luminescence spectra (second graph) depending on wavelength for both enantiomers measured at 50 µM in DCM after excitation at 385 nm. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: fluorescence.

Optical study absorbance and emission acidic form

Absorbance & fluorescence spectra

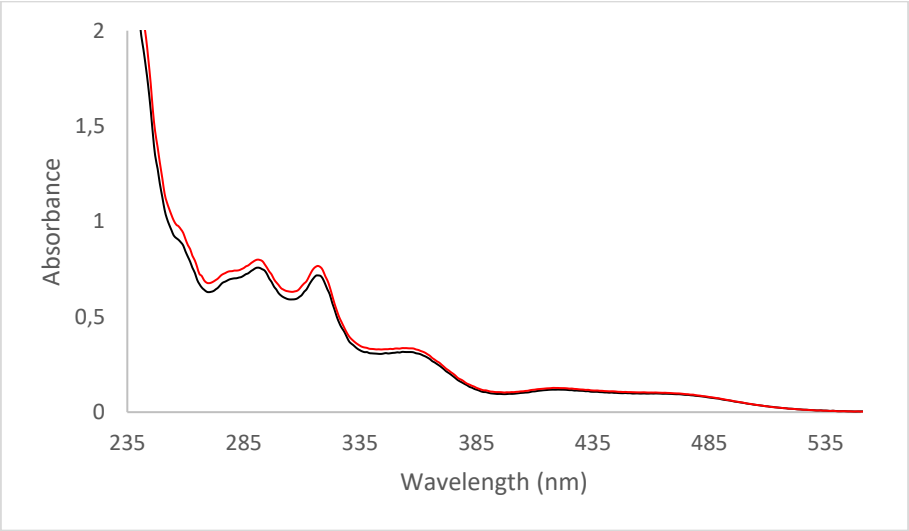


Figure S6. Absorbance spectra for both enantiomers measured in a 10^{-1}M solution of TFA in dichloromethane at 50 µM.

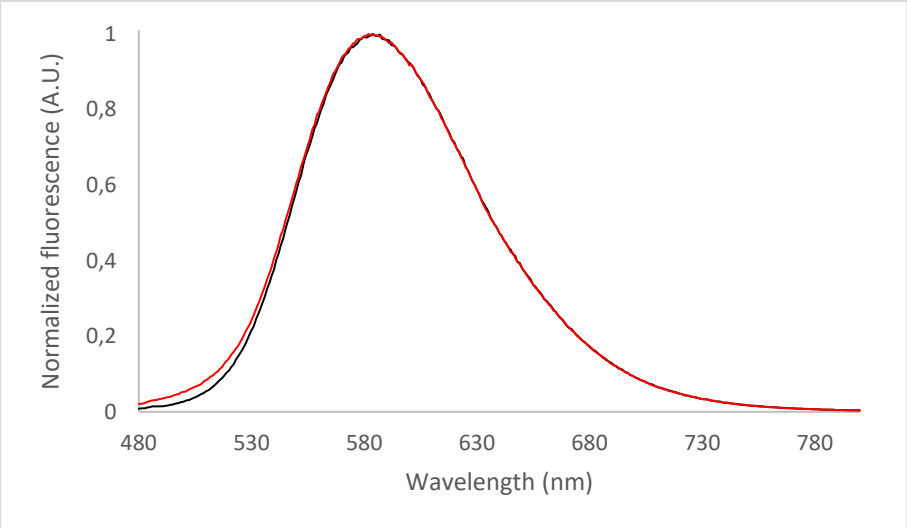


Figure S7. Normalized fluorescence of the acidic form both enantiomers (20 µM in 10^{-1}M solution of TFA in dichloromethane) after excitation at 470 nm.

Circular dichroism (CD) analysis

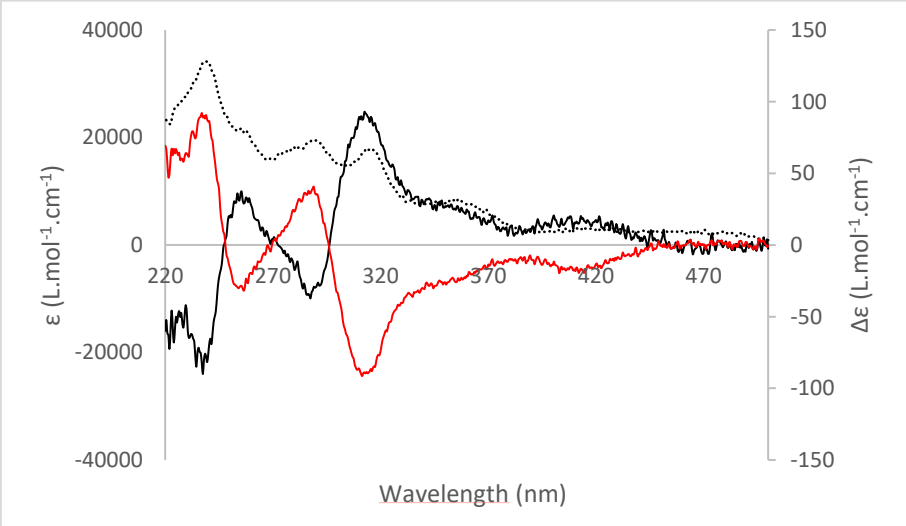


Figure S8. CD spectra were obtained from 50 µM in DCM. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: molecular attenuation coefficient.

Circularly Polarized Luminescence (CPL) study

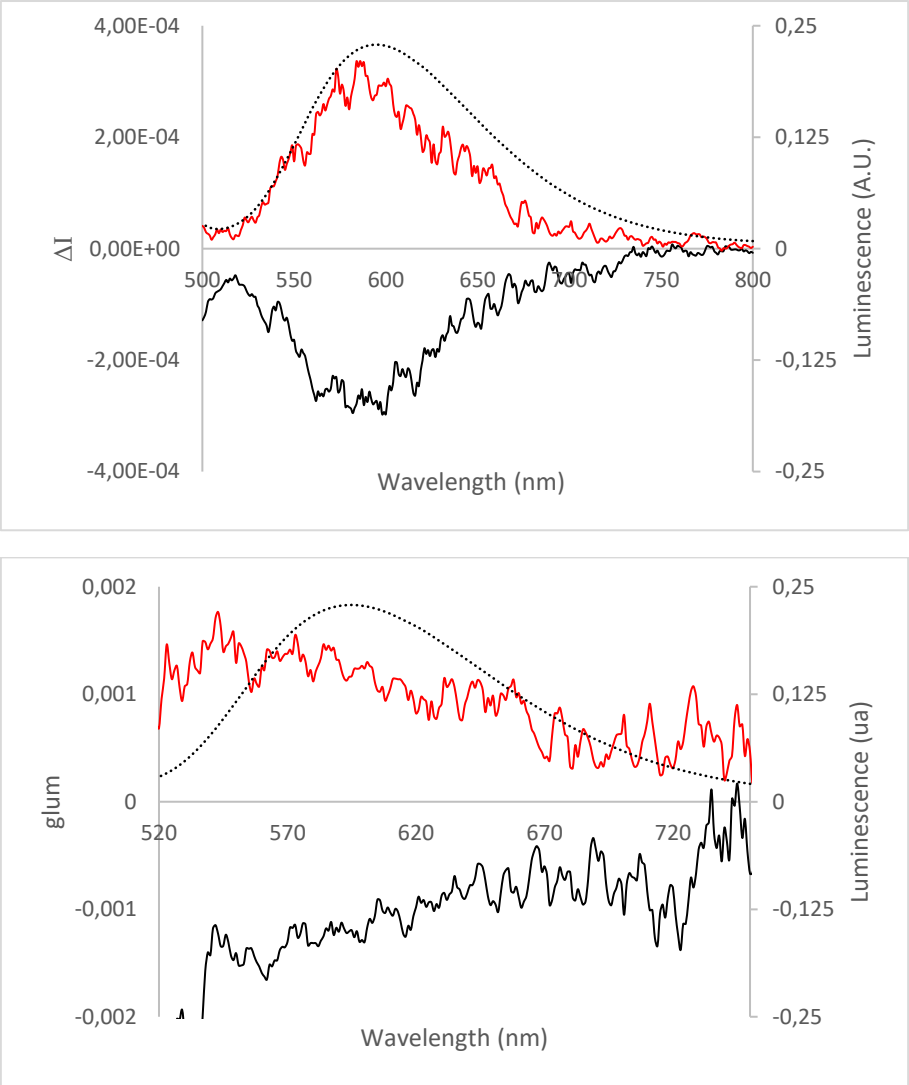


Figure S9. Superimposition of ΔI and luminescence spectra (first graph) and g_{lum} values and luminescence spectra (second graph) depending on wavelength for both enantiomers measured at 50 µM in DCM with 10 M^{-1} of TFA after excitation at 470 nm. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: fluorescence.

Comparison of the chiroptical study responses of both enantiomers in neutral and protonated state

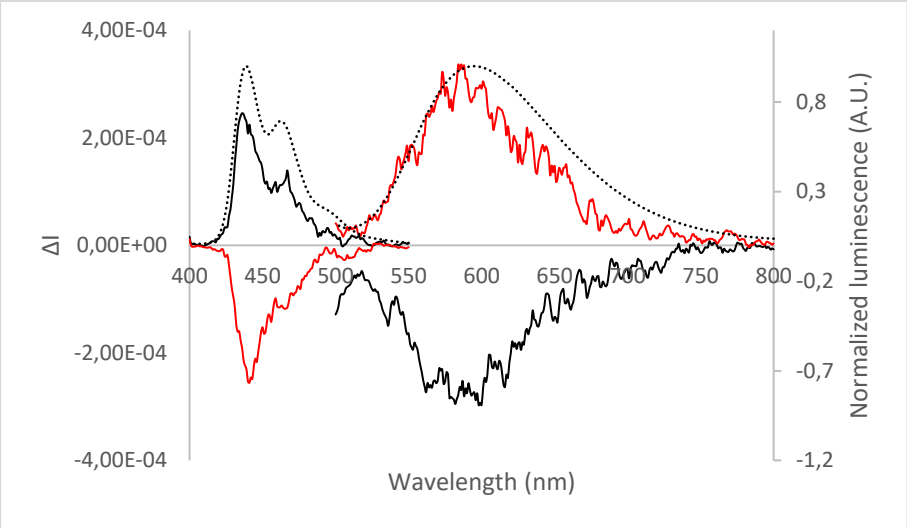


Figure S10. Black solid lines: first enantiomer eluted; red solid lines: second enantiomer eluted; black dotted lines: luminescences

pH-triggered switch by CPL

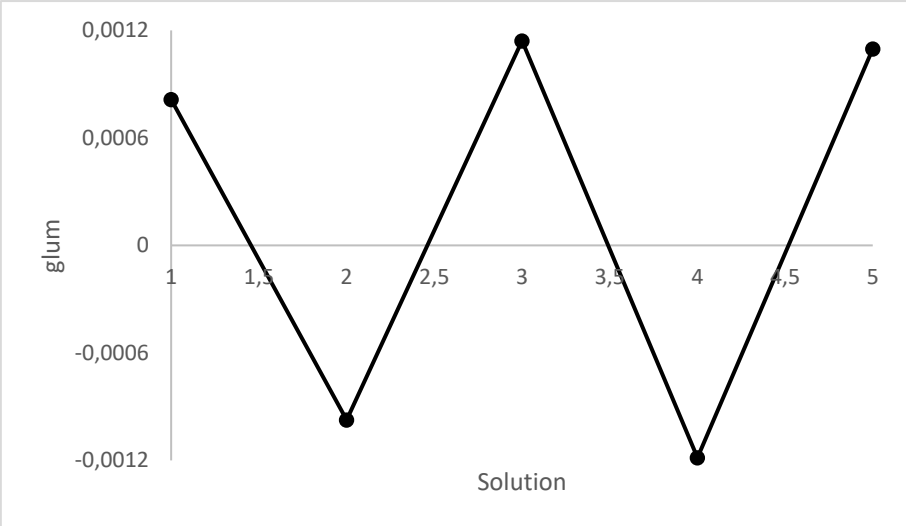
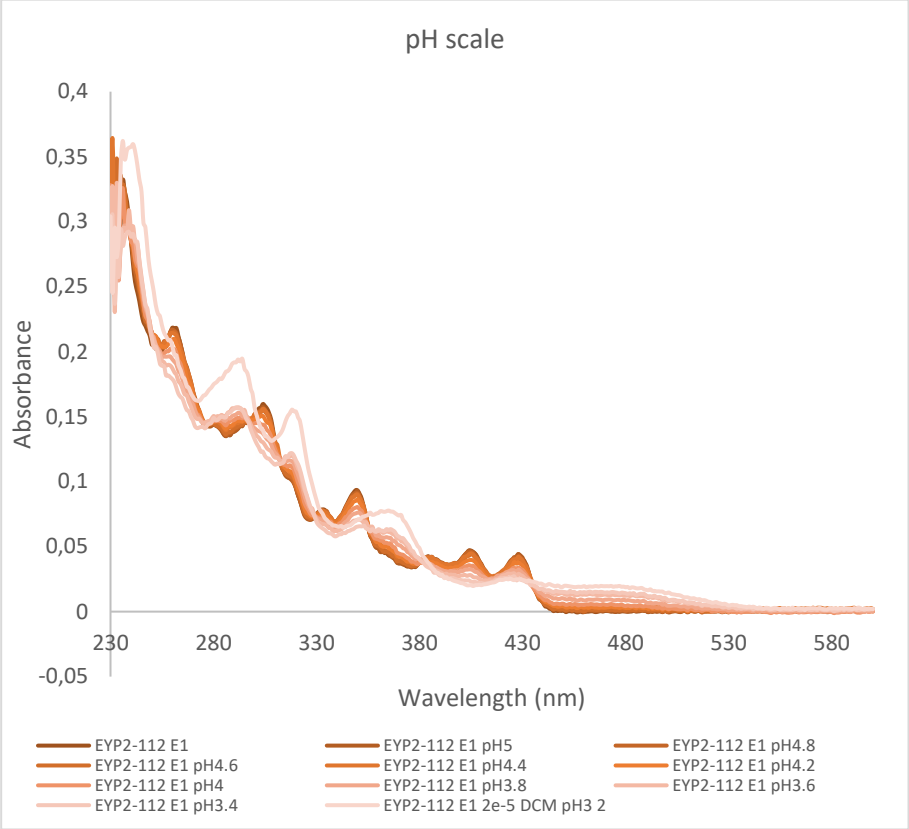


Figure S11. Measurement of the g_{lum} upon protonation/deprotonation

To evaluate the robustness of the compound upon protonation, a series of acidification and basification was realized. To a solution of E1 (50 µM in DCM) was successively added $1{,}98.10^{-5}$ mol of TFA and $1{,}98.10^{-5}$ mol DBU. The CPL response was measured upon every protonation state changes. This procedure was repeated 3 times and demonstrated the efficiency of the pH-triggered switch with no significant decrease of the g_{lum} values.

pKa determination

The pKa was determined by slow acidification of the solution by addition of TFA aliquots and measurement of the absorbance and fluorescence.



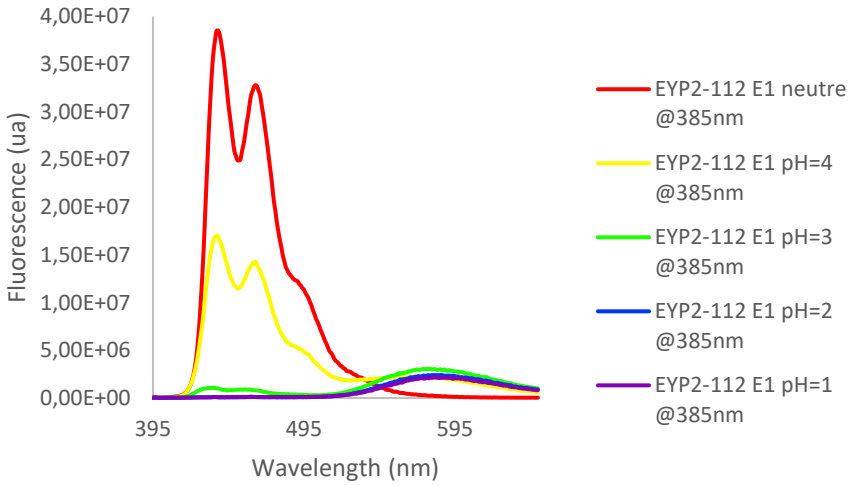


Figure S.12. Absorbance and fluorescence spectra (@385 nm) depending on the pH.

Optical properties of compound C-31

Scheme S7. Structure and picture of compound C-31 in its neutral or protonated state upon addition of TFA.

Chiral SFC *analysis*

Preparative separation: SFC chromatograms were recorded using a CHIRALPAK IC (250 mm x 20 mm x 5µm), mobile phase : EtOH /CO_2 (1:1), flow rate 33 ml.min^{-1} at 40 °C, detection (220 - 400 nm).
Analysis postpreparative SFC: SFC chromatograms were recorded using a CHIRALPAK IC (250 mm x 4.6 mm x 5µm), mobile phase : EtOH /CO_2 (1:1), flow rate 4 ml.min^{-1} at 40 °C, detection (220 - 400 nm).

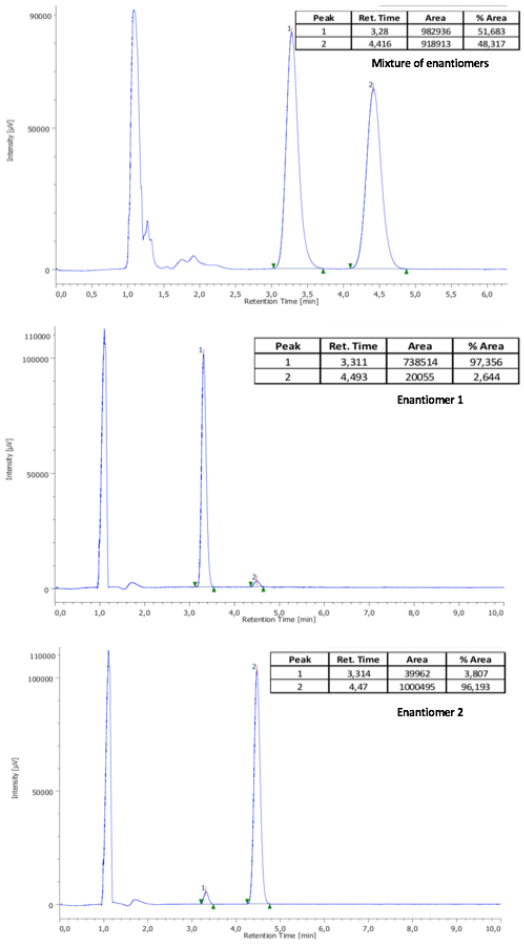


Figure S13. Chiral SFC spectra of the racemic mixture and after separation of each isomer

Optical study absorbance and emission basic form

Absorbance & fluorescence spectra

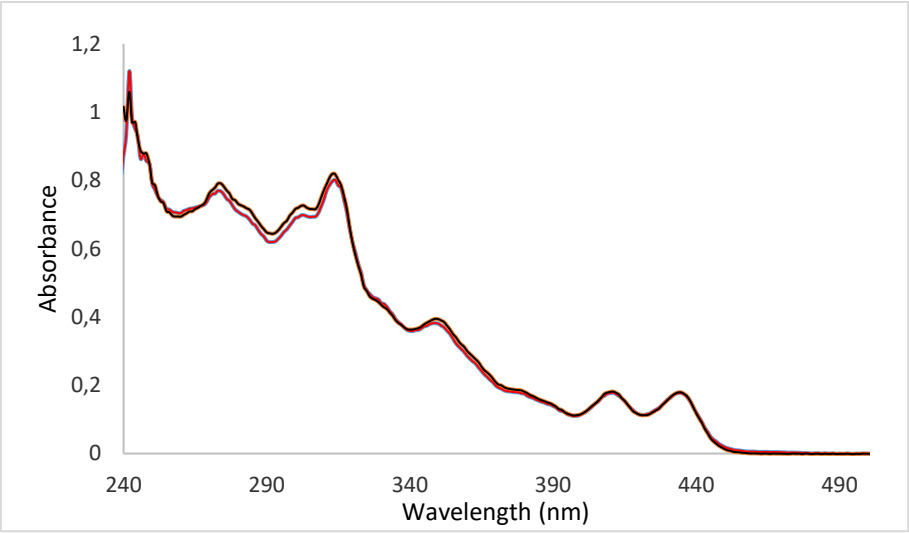


Figure S14. Absorbance spectra for both enantiomers measured in chloroform at 50 µM.

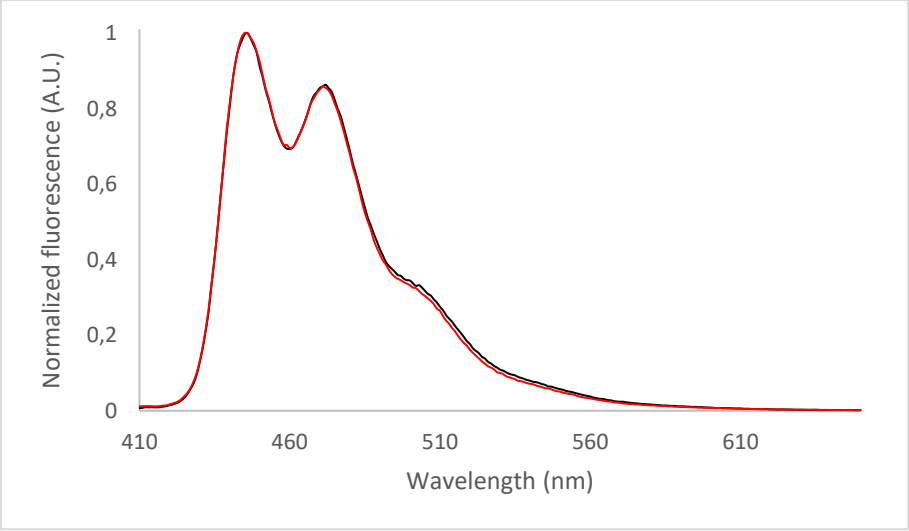


Figure S15. Normalized fluorescence of the basic form both enantiomers (50 µM in chloroform) after excitation at 400 nm.

Circular dichroism (CD) analysis

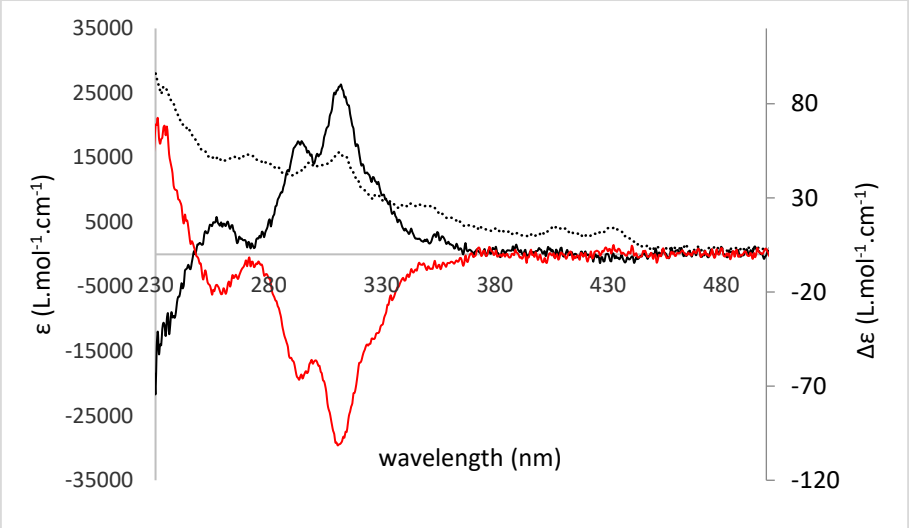
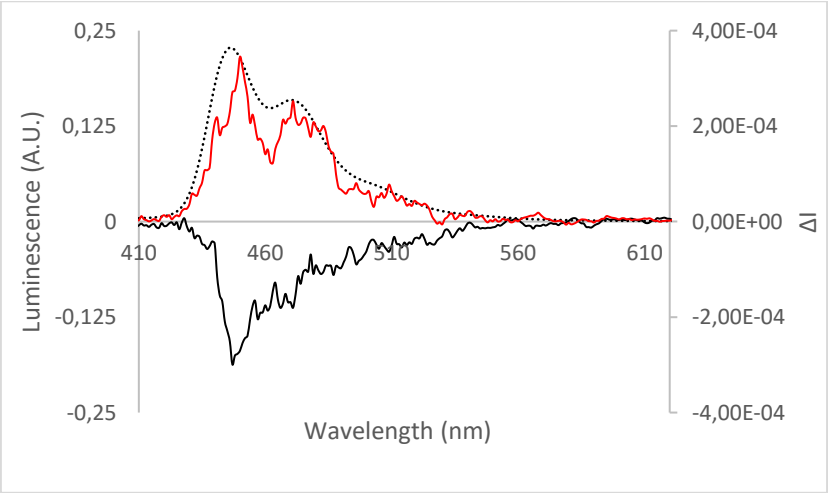


Figure S16. CD spectra were obtained from 50 µM solution in chloroform. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: molecular attenuation coefficient.

Circularly Polarized Luminescence (CPL) study



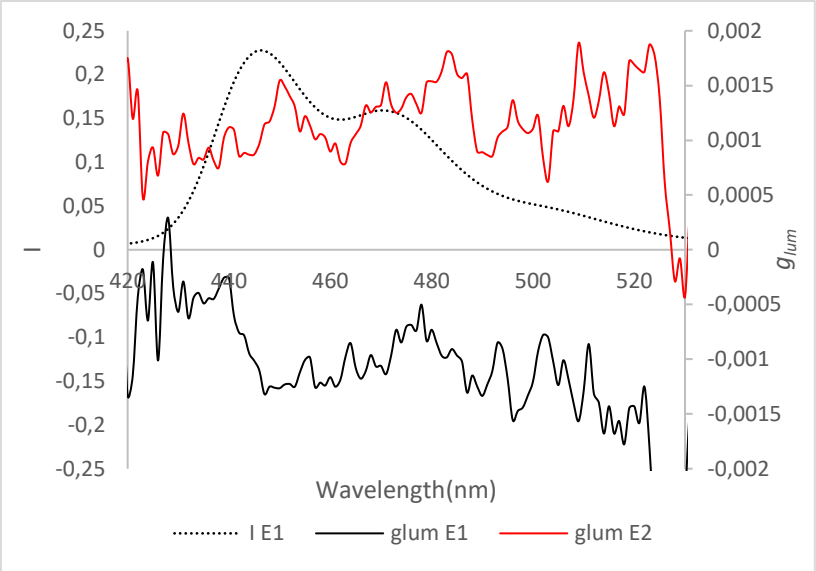


Figure S17. Superimposition of ΔI and luminescence spectra (first graph) and g_{lum} values and luminescence spectra (second graph) depending on wavelength for both enantiomers measured at 50 µM in chloroform after excitation at 350 nm. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: fluorescence.

Optical study absorbance and emission acidic form

Absorbance & fluorescence spectra

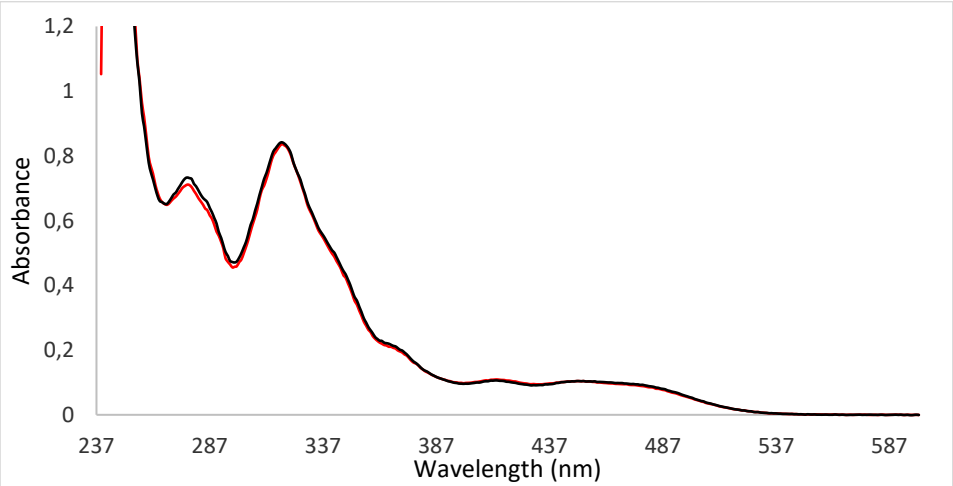


Figure S18. Absorbance spectrum of both enantiomers measured of solutions at 50 µM chloroform with 50 equivalents of TFA.

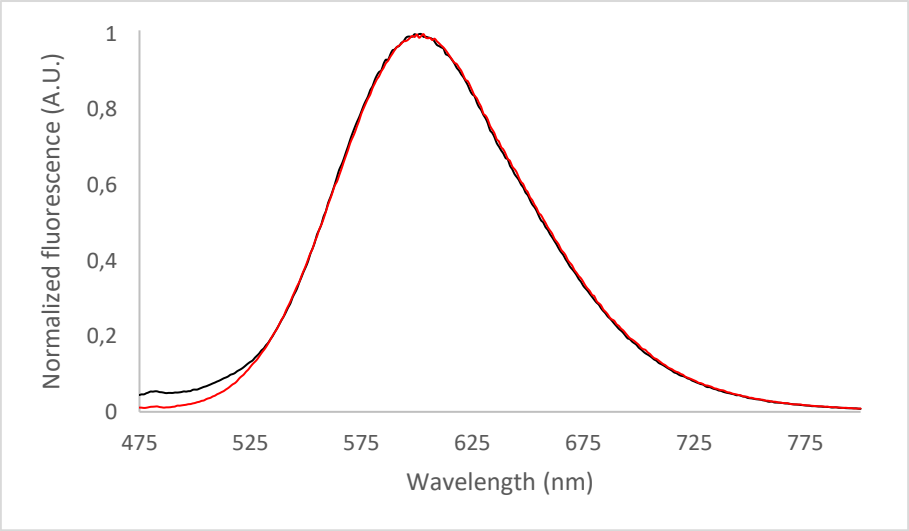


Figure S19. Fluorescence spectra measured after excitation at 465 nm of a solution at 50 µM chloroform with 50 equivalents of TFA.

Circular dichroism analysis

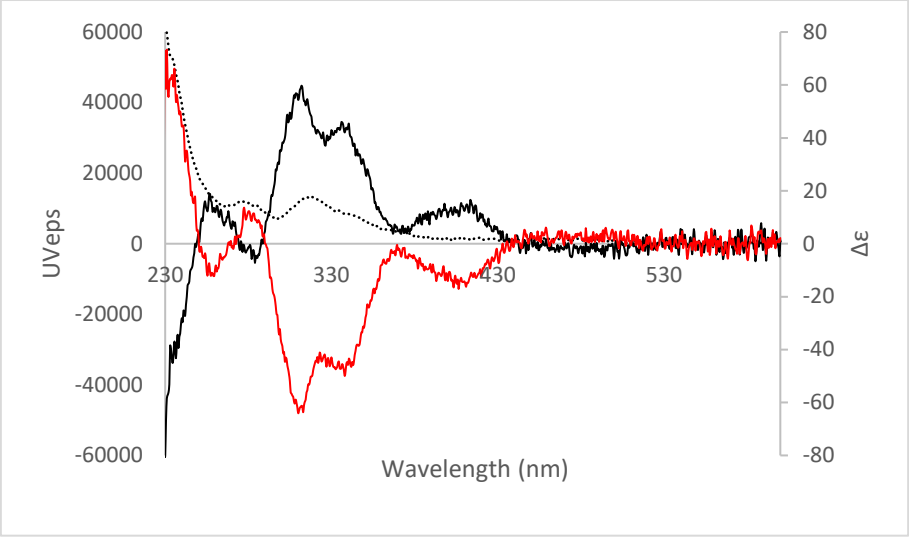
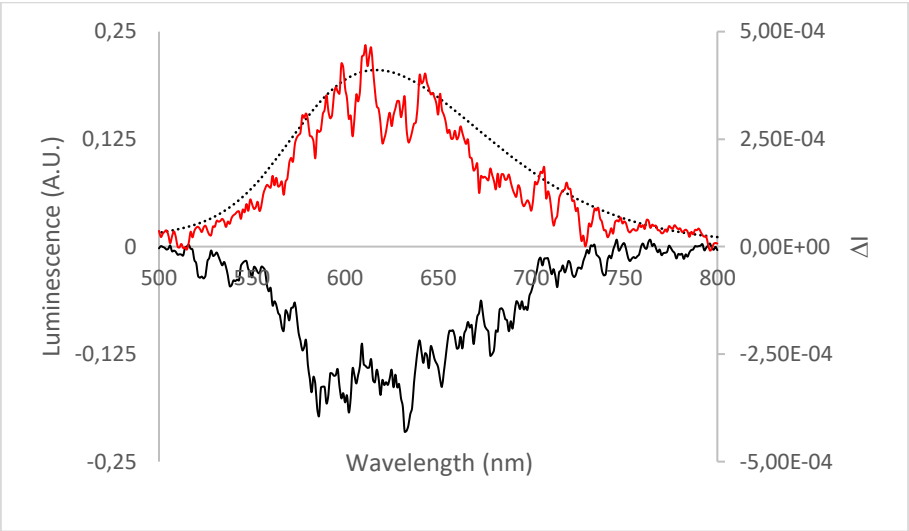


Figure S20. CD spectra were obtained from 50 µM solution in chloroform with 50 eq of TFA. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: molecular attenuation coefficient.

Circularly Polarized Luminescence (CPL) study



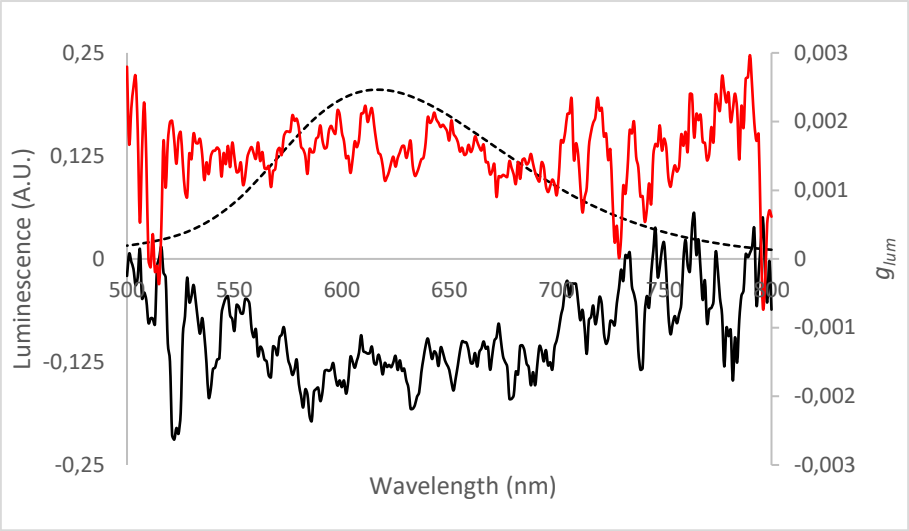


Figure S21. Superimposition of ΔI and luminescence spectra (first graph) and g_{lum} values and luminescence spectra (second graph) depending on wavelength for both enantiomers measured at 50 µM in chloroform with 50 eq of TFA after excitation at 380 nm. Black line: First enantiomer eluted. Red line: second enantiomer eluted. Black dotted line: fluorescence.

IV. Crystallographic data

The data were collected at 100(2) K either on a Nonius Kappa-CCD area detector diffractometer[9] using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) (**C-29**), or on a Bruker D8 Quest diffractometer equipped with an Incoatec Microfocus Source (IμS 3.0 Mo) and a PHOTON III area detector, and operated through the APEX3 software[10] (**C-30**·0.5CH_2Cl_2, **C-35** and **C-36**). The crystals were mounted into glass capillaries or on Mitegen micromounts with a protective coating of Paratone-N oil (Hampton Research). The data were processed with HKL2000[11] (**C-29**) or SAINT[12] (**C-30.**0.5CH_2Cl_2, **C-35** and **C-36**), and absorption effects for **C-30**·0.5CH_2Cl_2, **C-35** and **C-36** were corrected empirically with the program SADABS.[13,14]All structures were solved by intrinsic phasing with SHELXT,[15] expanded by subsequent difference Fourier synthesis and refined by full-matrix least-squares on F^2 with SHELXL[16] using the ShelXle interface.[17] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were introduced at calculated positions and were treated as riding atoms with an isotropic displacement parameter equal to 1.2 times that of the parent atom. In compound **C-29**, atoms N2 and N3 are partly disordered over the positions occupied by C5 and C25, respectively, and the two sets of positions were refined with occupancy parameters constrained to sum to unity and constraints (EXYZ and EADP) for nitrogen and carbon atoms occupying the same sites. Crystal data and structure refinement parameters are given in Table S3. The molecular plots were drawn with ORTEP-3/POV-Ray.[18]

Dihedral angles, for **C-29** (°): N3–C10–C9–C4 = 9.7(2), C10–C9–C4–C3 = 13.2(3), C9–C4–C3–C17 = 18.4(3), C4–C3–C17–C21 = 17.8(3), C3–C17–C21–C25 = 15.6(2). For **C-30** (°): C15–C10–C6–C3 = 6.9(3), C10–C6–C3–C4 = 8.9(4), C6–C3–C4–C16 = 21.5(4), C3–C4–C16–C20 = 23.0(3), C4–C16–C20–C27 = 9.1(3). For **C-35** (°): N3–C8–C7–C2 = 10.8(2), C8–C7–C2–C1 = 13.1(2), C7–C2–C1–C18 = 16.5(3), C2–C1–C18–C19 = 20.7(2), C1–C18–C19–C23 = 17.7(2). For **C-36** (°): C18–C14–C10–C9 = 16.6(2), C14–C10–C9–C4 = 24.5(2), C10–C9–C4–C3 = 20.3(3), C9–C4–C3–C25 = 7.4(3), C4–C3–C25–C26 = 10.3(3).

Comments:
Crystals of **C-30** and **C-36** suitable for crystallographic analysis were obtained by slow evaporation of a dichloromethane and chloroform solution, respectively. Crystals of **C-29** and **C-35** were obtained by slow diffusion of hexanes in dichloromethane at room temperature.
In all four cases, the sequence of torsion angles reflects the asymmetry of the molecule. For **C-29**, the central torsion angle is the largest, and one of the terminal angles is the smallest (not necessarily that involving N3 due to the disorder affecting the nitrogen atoms, see Experimental Section); the sum of the five angles amounts to 74.7°.
The central angle and one of the adjoining angles in both **C-30** and **C-36** are larger than any angle in **C-29**; the other three angles are much smaller in **C-30**, the sum being 69.4°, while one larger terminal angle in **C-36** results in a larger sum of 79.1°. The angles in **C-35** follow the same trend as those in **C-36**, with a slightly smaller sum of 78.8°.

Table S3. Crystal Data and Structure Refinement Details

	C-29	**C-30**·0.5CH_2Cl_2	**C-35**	**C-36**
chemical formula	$C_{26}H_{15}N_3$	$C_{25.5}H_{15}ClN_2S$	$C_{32}H_{19}N_3$	$C_{27}H_{16}N_2$
M (g mol^{-1})	369.41	416.90	445.50	368.42
cryst syst	orthorhombic	orthorhombic	monoclinic	monoclinic
space group	$Pbca$	$Pccn$	$P2_1/c$	$P2_1/c$
a (Å)	14.9185(8)	11.2768(5)	11.0041(9)	7.8038(2)
b (Å)	12.3307(5)	12.0743(4)	15.3437(9)	17.4799(5)
c (Å)	18.6931(11)	27.7032(12)	12.9414(9)	13.0285(3)
β (deg)			103.077(3)	96.2329(12)
V (Å^3)	3438.7(3)	3772.1(3)	2128.4(3)	1766.71(8)
Z	8	8	4	4
reflns collcd	100228	104632	68551	37573
indep reflns	3257	3586	4036	3337
obsd reflns [$I > 2\sigma(I)$]	2554	3269	3451	2878
R_{int}	0.028	0.051	0.056	0.054
params refined	263	267	316	262
R_1	0.046	0.039	0.038	0.040
wR_2	0.106	0.094	0.093	0.098
S	1.047	1.063	1.032	1.049
$\Delta\rho_{min}$ (e Å^{-3})	–0.21	–0.45	–0.21	–0.18
$\Delta\rho_{max}$ (e Å^{-3})	0.15	0.58	0.43	0.42

V. Full computation details

Density functional theory (DFT) calculations were performed using Gaussian 16.[19] Geometry optimizations were carried out for the gas-phase with the M06-2X functional,[20] using the 6-31+G(d,p) basis set, and a tight convergence factor (opt=tight), method which was successfully used in our last work on 1,3-dipolar cycloadditions between sydnones and arynes.[1] Normal mode vibrational analysis on the stationary points allowed us to confirm they are minima (zero imaginary frequencies) or transition structures (TS, one imaginary frequency). TSs were followed along their reaction coordinates to verify that they connect the expected minima. ZPE, enthalpy and free energy corrections were obtained using a standard state of 1 atm pressure and 298 K temperature using Goodvibes v2.0.3.[21] Free energies were computed using Truhlar's quasiharmonic oscillator approximation, setting all frequencies below 100 cm^{-1} to 100 cm^{-1}.[22,23] To obtain accurate energies, single-point energy refinements were then performed at the M06-2X/6-311+G(2d,2p) level of theory, for the gas-phase or using the SMD solvation model[24] for THF. The free energies presented in the manuscript were then obtained by adding the free energy corrections obtained from the frequency analysis to the single-point electronic energies. Visualizations of the computed structures were prepared using CYLview.[25] Frontier molecular orbitals (FMOs) and their energies, as well as natural bond orbitals (NBO), were computed at the HF/6-311+G(2d,2p) level, using the M06-2X optimized geometries. Non-covalent interactions (NCI) and the molecular orbitals composition analyses were carried out using Multiwfn software,[26] and atoms contributions to MOs were calculated by Hirshfeld method.[27]

Time-dependent DFT calculations (TD-DFT) were performed using the B3LYP functional, the 6-311+G(2d,2p) basis set, Grimme's D3 correction with Becke-Johnson (BJ) damping,[28] and the IEF-PCM solvation model[29] for dichloromethane. The ground state (S_0) and first excited state (S_1) were optimized for the two helicenes **C-29** and **C-29·H$^+$** and the oscillator and rotatory strengths of their first 100 vertical transitions were obtained. Vibrational analysis of both states confirmed their geometries are minima on their respective potential energy surfaces. Oscillator and rotatory strengths were fitted to Gaussian functions with a half-width at half-height of 0.2 eV to obtain the predicted spectra, which were normalized to 1 for UV-Vis spectra, or to -100 for CD spectra. For the emission spectra from the S_1 optimized geometry, only the $S_1 \rightarrow S_0$ transition is considered. Frontier molecular orbitals (FMOs) and their energies were obtained using the NBO formalism (pop=(full,NBO) keyword in Gaussian 16). Natural Transition Orbitals (NTOs) were computed using the above methods, using the pop=(Orbitals,NTO,SaveNTO) keywords. Density maps were generated by subtracting the computed density at the S_0 from the density at the S_1 state.

XYZ coordinates of all computed structures are listed in this document and provided in a .zip archive as a separate Supporting Information file. The Gaussian output files for all optimization and frequency analysis, both for the DFT and TD-DFT sections of this work, have been archived and are available for download on Zenodo (DOI 10.5281/zenodo.4268325).

Additional figures, tables and discussion

- Potential energy surfaces for the 5 computed systems

	TS1	ΔΔG‡1	int1	TS2	int2	TS3	products
C-14	10.6	1.7	-34.4	-24.0	-34.4	-35.1	-131.6
S-14	12.3		-40.5	-36.9	-44.8	-45.5	-140.8
C-29	10.4	2.6	-36.3	-34.0	-38.4	-38.9	-136.0
S-29	13.0		-41.0	-39.1	-44.0	-44.7	-138.2
C-33	10.9	2.2	-38.6	-32.2	-36.5	-37.1	-133.9
S-33	13.1		-40.4	-37.0	-44.8	-45.6	-140.2
C-32	11.3	1.4	-36.5	-29.6	-36.6	-37.4	-134.0
S-32	12.7		-41.5	-38.8	-48.0	-48.8	-143.9
C-37	11.5	4.4	-30.3	-29.9	-36.0	-36.7	-132.4
S-37	15.9		-33.5	-31.7	-36.7	-37.3	-131.4
C-36	12.2	4.0	-27.2	-26.3	-33.2	-33.9	-129.3
S-36	16.2		-33.1	-30.0	-38.5	-39.3	-132.6

Table S4: Stationary points of the computed system potential energy surfaces Free energy values (in kcal/mol) calculated at the M06-2X/6-311+G(2d,2p)/SMD(THF)// M06-2X/6-31+G(d,p) level of theory

Noteworthy, in addition of providing an important stabilization of the TS leading to **C-37**, the large aromatic backbones also make this final pyrazole helicene product the only one calculated lower in energy than the less sterically hindered S-shape isomer **S-37**.

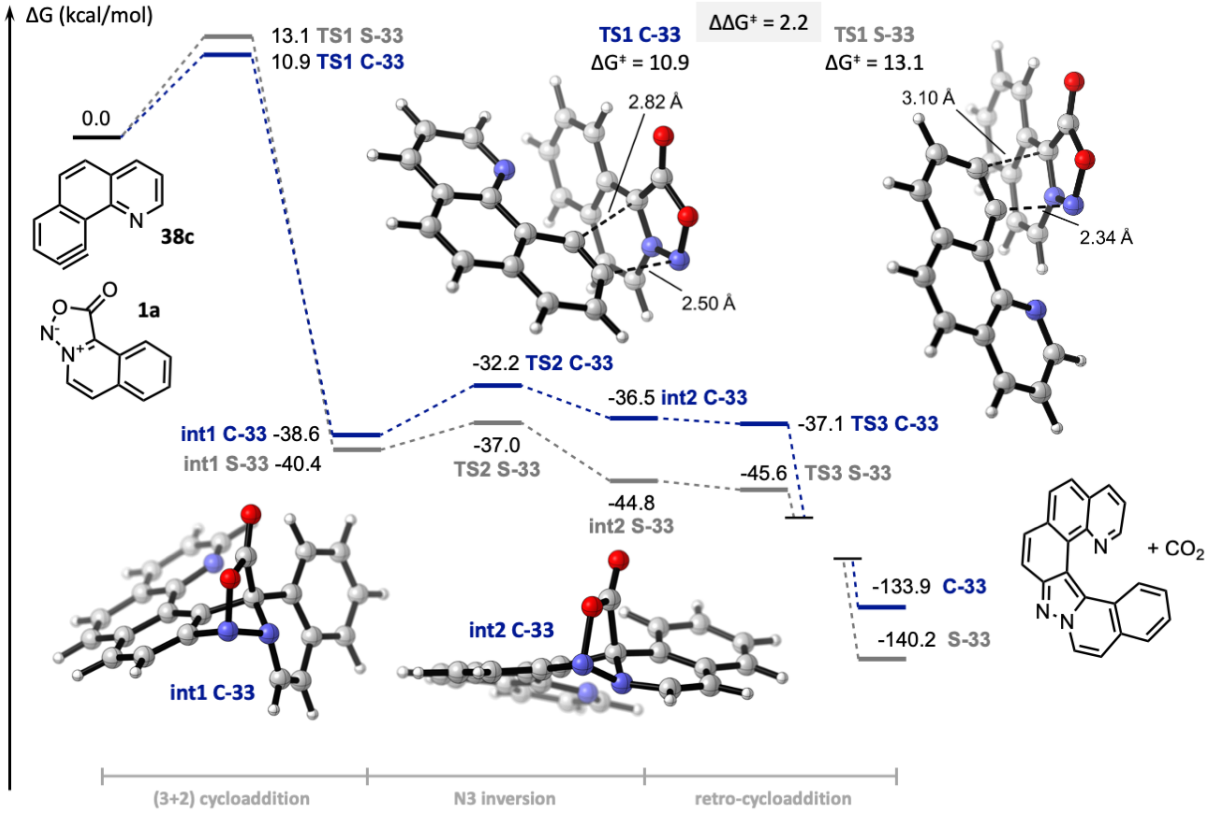


Figure S22: Potential energy surface for the reaction between **1a** and **38c**

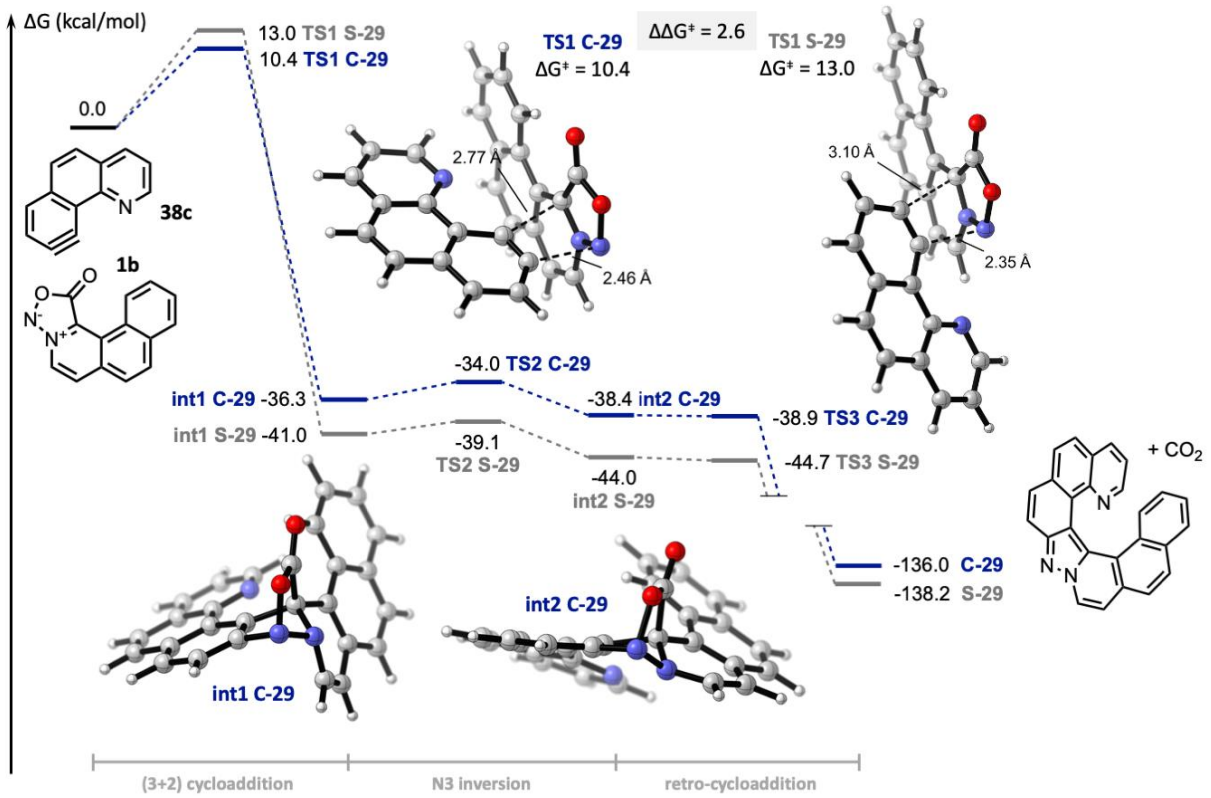


Figure S23: Potential energy surface for the reaction between **1b** and **38c**

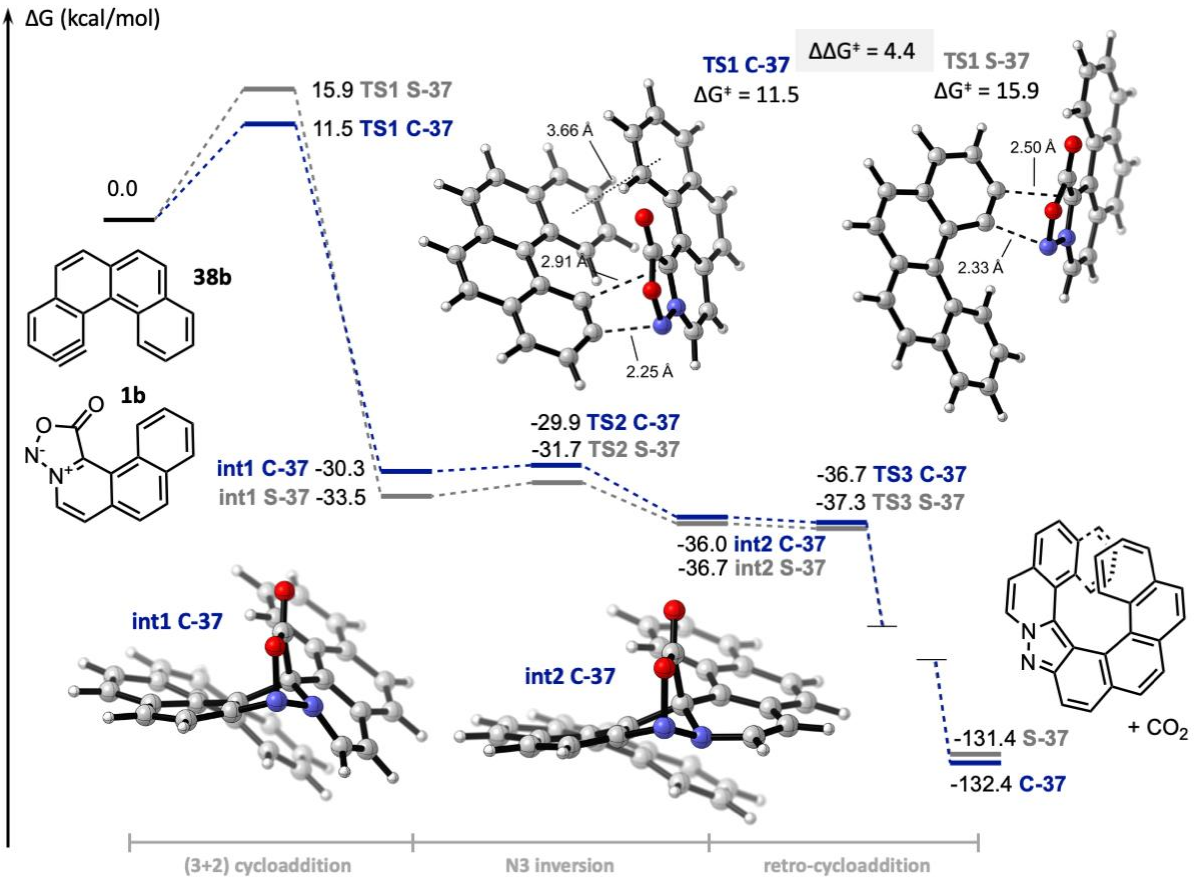


Figure S24: Potential energy surface for the reaction between **1b** and **38b**

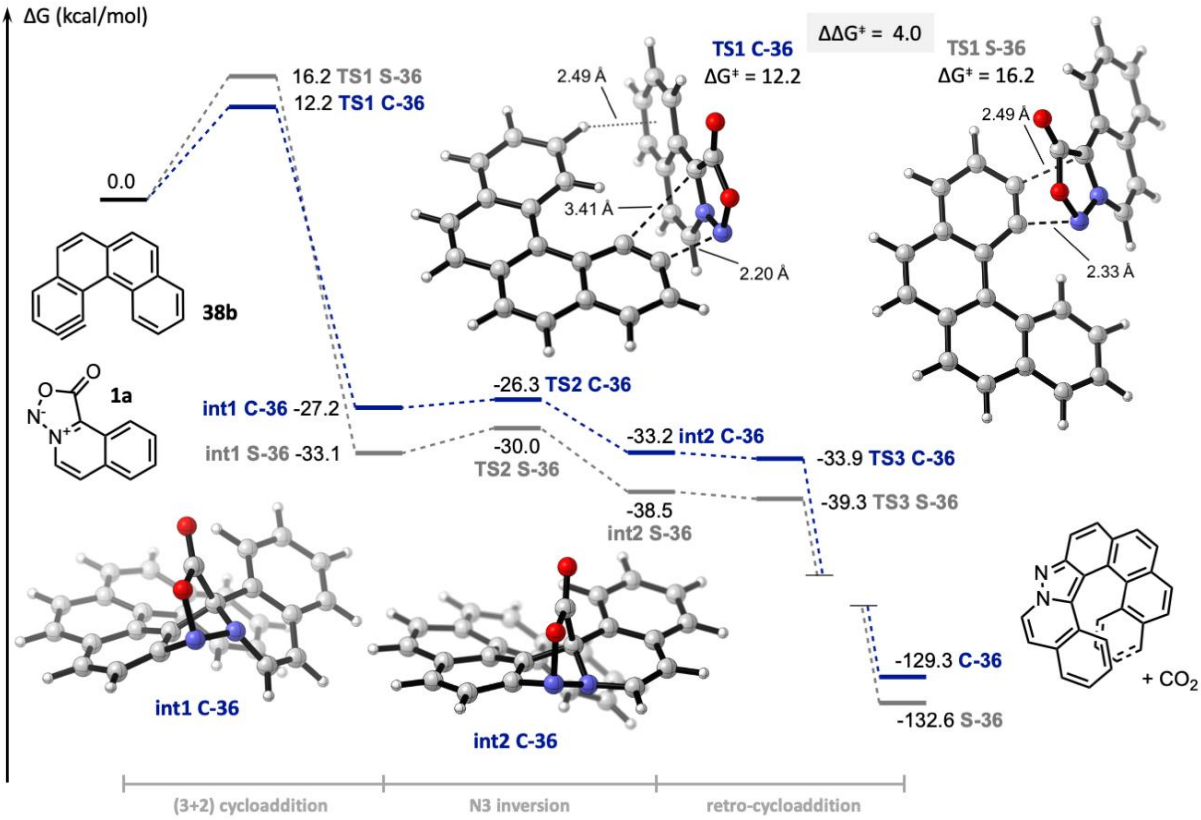


Figure S25: Potential energy surface for the reaction between **1a** and **38b**

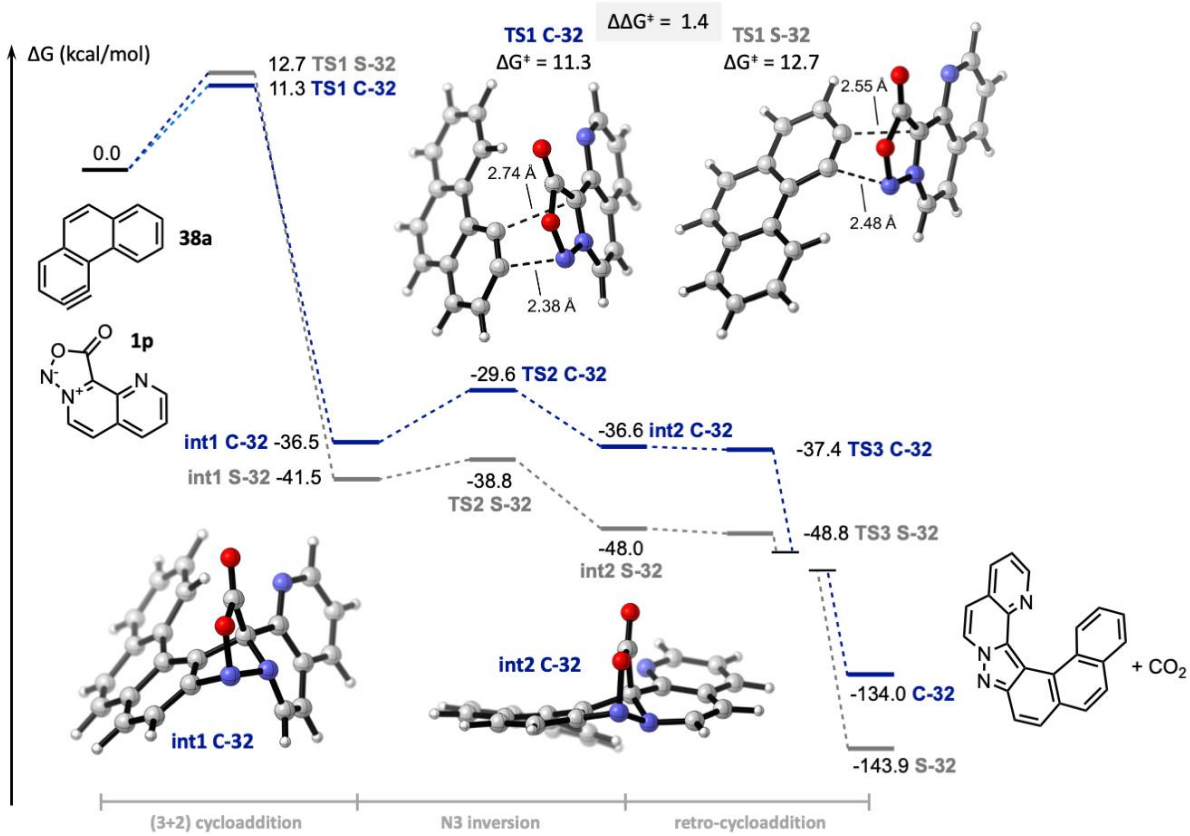


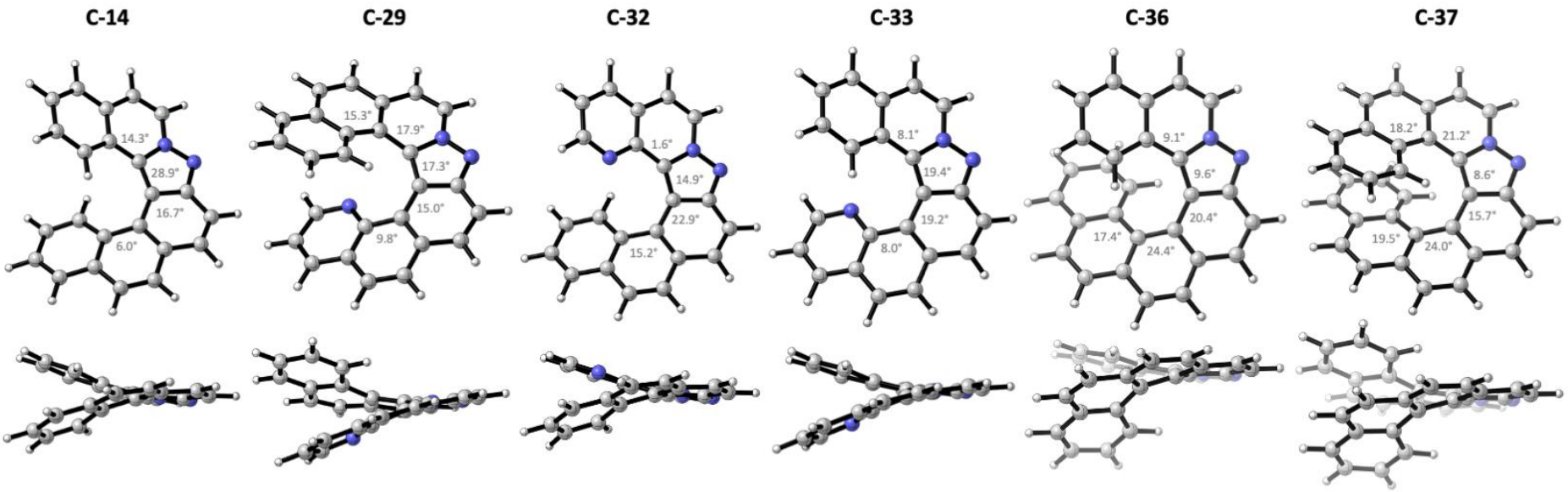
Figure S26: Potential energy surface for the reaction between **1p** and **38a**

- Transition structures geometries

products	ΔΔG‡1	D (°)	distances	
			from N2	from C4
C-14	1.7	-2.7	C_{ext} 2.48	C_{int} 2.95
S-14		-10.9	C_{int} 2.41	C_{ext} 2.65
C-29	2.6	-4.5	C_{ext} 2.45	C_{int} 2.77
S-29		-34.1	C_{int} 2.35	C_{ext} 3.10
C-32	1.4	-13.4	C_{ext} 2.38	Cint 2.74
S-32		-9.3	C_{int} 2.48	C_{ext} 2.55
C-33	2.2	-1.3	C_{ext} 2.50	C_{int} 2.82
S-33		-34.1	C_{int} 2.34	C_{ext} 3.10
C-36	4.0	14.6	C_{ext} 2.20	C_{int} 3.41
S-36		-8.5	C_{int} 2.32	C_{ext} 2.49
C-37	4.4	-3.8	C_{ext} 2.25	C_{int} 2.91
S-37		-9.7	C_{int} 2.32	C_{ext} 2.50

Table S5: TS geometries

- C-shape products computed structures



dihedral angle	X-ray	DFT
N3–C10–C9–C4	9.7	9.8
C10–C9–C4–C3	13.2	15.0
C9–C4–C3–C17	18.4	17.3
C4–C3–C17–C21	17.8	17.9
C3–C17–C21–C25	15.6	15.3

dihedral angle	X-ray	DFT
C18–C14–C10–C9	16.6	17.4
C14–C10–C9–C4	24.5	24.4
C10–C9–C4–C3	20.3	20.4
C9–C4–C3–C25	7.4	9.6
C4–C3–C25–C26	10.3	9.1

Figure S27: Computed structure of the helical products (M06-2X/6-31+G(d,p)) and dihedral angles along the helicene backbone

- Aromatic interactions

Optimized TS1 structures leading to the C-shaped products **C-29**, **C-32**, **C-33**, **C-36** and **C-37** were stripped of the reacting sydnone and aryne functional groups (which were replaced by hydrogen atoms), so that their polycyclic backbones remained in the same orientation and distance. Single-point energy calculations at the M06-2X/6-311+G(2d,2p)/SMD(THF) level of theory were done on these aromatic dimers.

The energies of the two parts of the dimers were then computed independently. The interaction energy was then obtained from $\mathbf{\Delta E_{int,ar} = \Delta E_{dimer} - (\Delta E_{part1} + \Delta E_{part2})}$

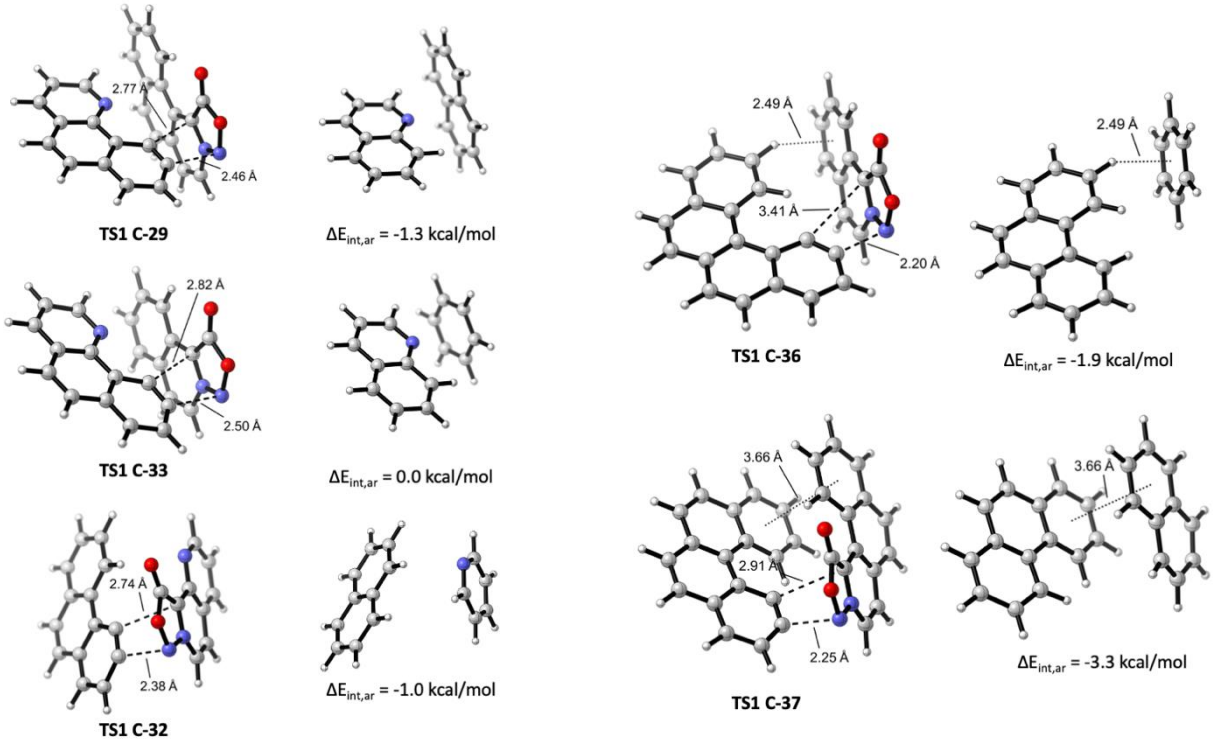


Figure S28: Aromatic dimers (right) vs. TS (left) geometries
Energy values obtained from single point energy calculation at the M06-2X/6-311+G(2d,2p)/SMD(THF) level.

- Distortion/interaction, angles and aromatic dimer energies

<u>Distortion/interaction analysis:</u>[30]

Distortion/interaction analysis was performed by splitting the transition structures optimized at the M06-2X/6-31+G(d,p) level in two fragments: the sydnone (*syd*) and the aryne (*a*). Single-point energies of these fragments were taken at the M06-2X/6-311+G(2d,2p) level. The difference in energy between the distorted fragments and their ground states is called distortion energy ($\mathbf{\Delta E^{\ddagger}_{dist}}$), and the interaction energy ($\mathbf{\Delta E^{\ddagger}_{int}}$) is calculated using the activation energy ($\mathbf{E_a}$) such as

$$E_a = \Delta E^{\ddagger} = \Delta E^{\ddagger}_{dist,syd} + \Delta E^{\ddagger}_{dist,a} + \Delta E^{\ddagger}_{int} = \Delta E^{\ddagger}_{dist,tot} + \Delta E^{\ddagger}_{int}$$

$\Delta E^{\ddagger}_{dist,syd}$ = distortion energy of the sydnone
$\Delta E^{\ddagger}_{dist,a}$ = distortion energy of the aryne
$\Delta E^{\ddagger}_{dist,tot}$ = total distortion energy (sydnone + aryne)

Whereas the distortion energies do not allow to explain the calculated differences in activation energy between the C- and S- regioisomers, we observed a good correlation with the interaction energies, in accordance with the involvement of stabilizing π-stacking forces in the selectivity (**Table S6**).

Houk/Garg aryne distortion model for [4+2] cycloadditions:[31]

The Houk/Garg model on aryne distortion to explain the regioselectivity of 1,3-dipolar cycloaddition between substituted arynes and azides rely on the modification of the aryne angles between the ground-state and the transition structure. An unsymmetrical substitution of the aryne induces a difference in the values of the aryne angles compared with a symmetrical aryne like benzyne. A transition structure will be favored if the modification of those angles in route to the TS goes in the same direction than the deformation induced by the substitution, and in the contrary will be disfavored if both substitution and cycloaddition have opposite effects on the aryne distortion. However, for the studied systems, the modification of the aryne angles in the course of the (3+2) cycloaddition does not correlate with the difference in activation energy observed between the regioisomers.

			distortion interaction				angles modification	aromatic interactions
transition structures	ΔE_a	E_a	$\Delta E^{\ddagger}_{int}$	$\Delta E^{\ddagger}_{dist,tot}$[a]	$\Delta E^{\ddagger}_{dist,syd}$[b]	$\Delta E^{\ddagger}_{dist,a}$[c]	aryne angles *int./ext.*[d]	$\Delta E^{\ddagger}_{int,ar}$
TS1 S-14	1.1	-6.4	-9.7	3.3	2.7	0.6	+1.7/-3.9	
TS1 C-14		-7.5	-9.0	1.5	1.1	0.4	-5.4/+3.4	-0.8
							38a[e] -1.0/+1.5	
TS1 S-33	2.2	-2.8	-5.7	2.8	1.2	1.5	+3.8/-5.6	
TS1 C-33		-5.1	-6.8	1.7	1.2	0.5	-4.0/+2.6	-0.0
							38c[e] -0.1/+0.1	
TS1 S-29	2.9	-3.0	-5.8	2.7	1.2	1.6	+3.6/-5.3	
TS1 C-29		-5.9	-8.2	2.3	1.6	0.6	-3.9/+2.2	-1.3
							38c[e] -0.1/+0.1	
TS1 S-32	1.7	-3.4	-7.2	3.9	3.0	0.8	+0.4/-2.3	
TS1 C-32		-5.0	-8.2	3.1	2.2	0.9	-3.2/+1.3	-1.0
							38a[e] -1.0/+1.5	
TS1 S-37	4.3	-0.8	-8.5	7.7	4.7	3.0	-1.9/-1.1	
TS1 C-37		-5.1	-10.6	5.5	2.7	2.9	-7.8/+5.0	-3.3
							38b[e] +3.6/-1.9	
TS1 S-36	3.7	-0.4	-8.3	7.9	5.0	2.9	-2.1/-0.9	
TS1 C-36		-4.1	-7.3	3.2	1.2	2.0	-9.5/+7.4	-1.9
							38b[e] +3.6/-1.9	

Table S6 Distortion/interaction analysis.
Energy values (in kcal/mol) calculated at the M06-2X/6-311+G(2d,2p)/SMD(THF)// M06-2X/6-31+G(d,p) level of theory; **[a]** total distortion energy (aryne + sydnone); **[b]** sydone distortion energy; **[c]** aryne distortion energy; **[d]** modification of the aryne angles between the TS and the ground state; **[e]** distortion of the aryne vs. benzyne

- Frontier molecular orbitals

FMOs and their energies were computed at the HF/6-311+G(2d,2p) level, using the M06-2X optimized geometries. In all cases, the smallest FMO gap was with the HOMO of the sydnone and the LUMO of the aryne (**Table S7**). The proper HOMO/LUMO symmetries for arynes were HOMO-3/LUMO for **38a**, HOMO-2/LUMO for **38b** and HOMO-4/LUMO+1 for **38c**

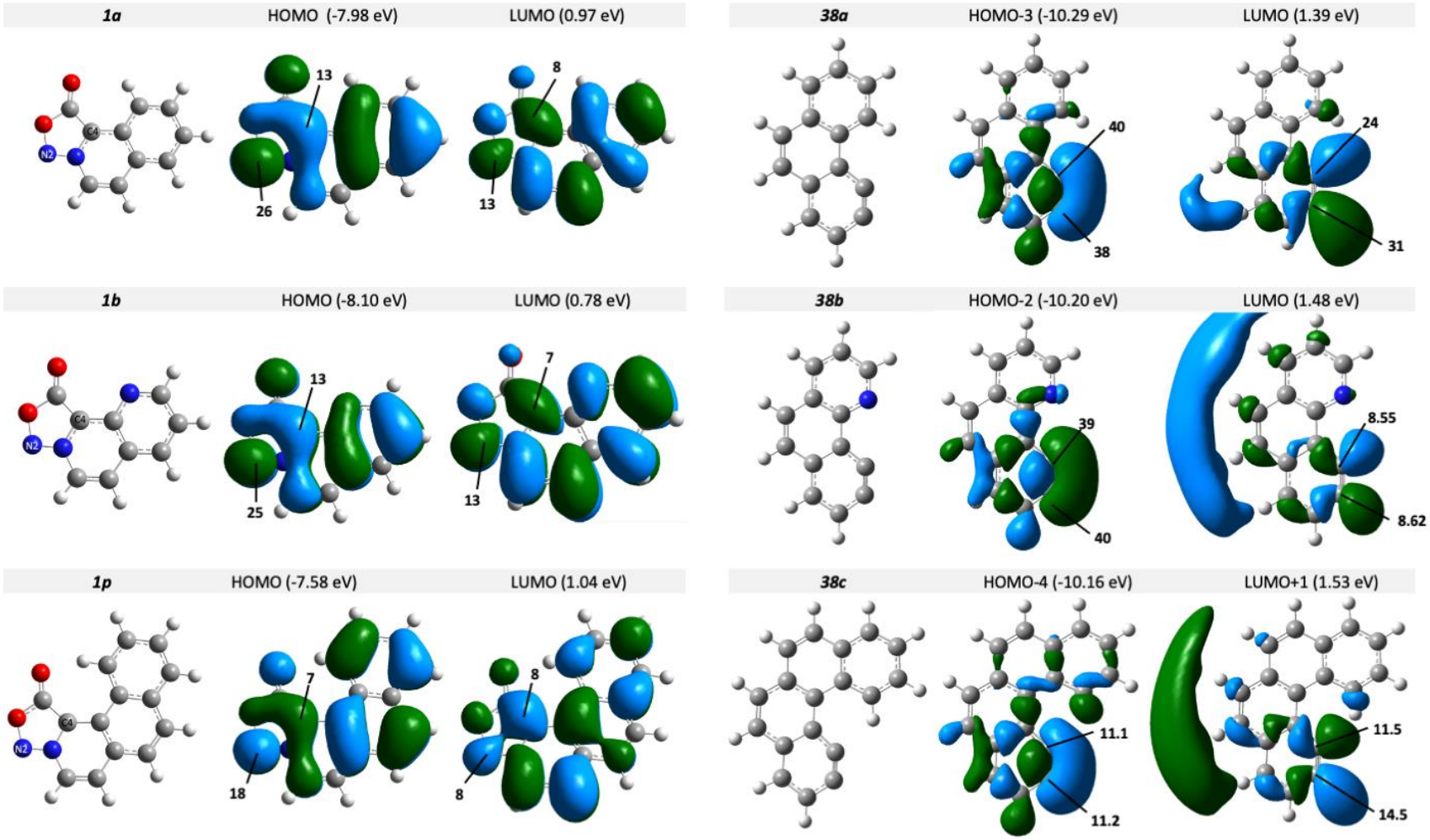


Figure S29: FMOs for sydnones **1a**, **1b**, **1p** and arynes **38a**, **38b**, **38c.** Orbitals were computed at the HF/6-311+G(2d,2p) level of theory on the M06-2X-optimized geometries. Orbital coefficients were calculated by Hirshfeld method using the Multiwfn software.

reaction	$LUMO_{aryne}$ – $HOMO_{sydnone}$ (eV)	$LUMO_{sydnone}$ - $HOMO_{aryne}$ (eV)
38c + **1b**	9.1	11.0
38c + **1a**	9.5	11.2
38b + **1b**	9.1	11.2
38b + **1a**	9.5	11.1
38a + **1p**	9.5	11.1

Table S7: FMOs gaps for each studied system

- Non-covalent interactions analysis

We also performed an NCI analysis in order to understand the kind of interactions involved in TS1 **C-32**. This analysis highlights weak interactions between the aromatic backbone of the aryne and the pyridine-like nitrogen on the sydnone. However, similar forces are found in TS1 **C-33**, for which we calculated a binding aromatic energy of 0 kcal/mol. These results suggest that, even though those weak interactions are indeed present, they do not influence the aromatic interactions we calculated as shown above.

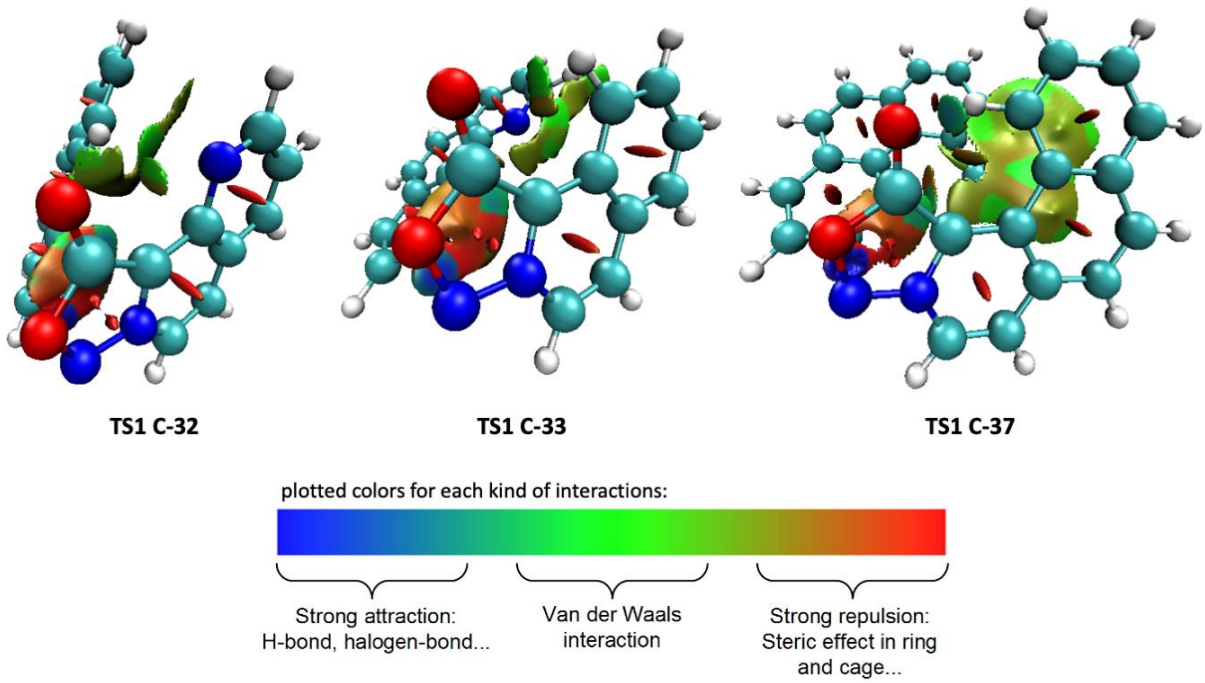


Figure S30: Non-covalent interaction analysis

- Natural Bond Orbital (NBO) analysis of TS1 C-32

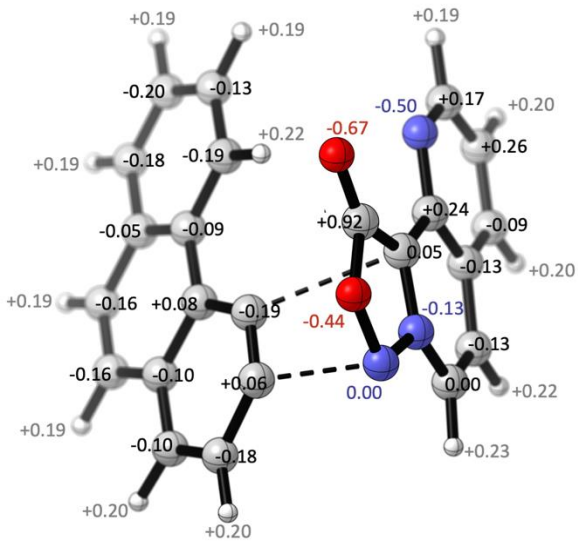


Figure S31: Charges distribution from NBO analysis on **TS1 C-32**, calculated at the HF/6-311+G(2d,2p) level on the M06-2X-optimized geometries

- Racemization barriers and transition structures

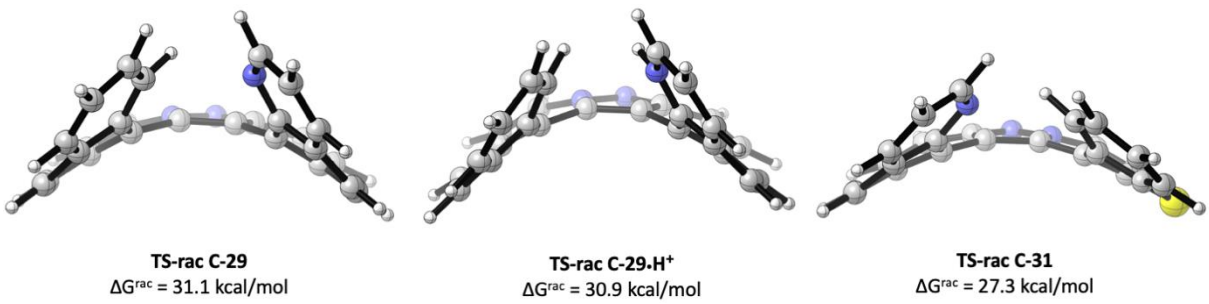


Figure S32: Transition structures and free energy barriers for the racemization of helicenes C-29, C-29.H+ and C-31, computed at the M06-2X/6-311+G(2d,2p)/SMD(THF)//M06-2X/6-31+G(d,p) level of theory.

- Energies, corrections and single-point energies for all computed structure

1b + 38c → C-29							
	M06-2X/6-31+G(d,p)					M06-2X/6-311+G(2d,2p)	
	optimization energies and corrections					SPE	SPE THF
structure	**E**	**ZPE**	**H**	**G(T)**	**qh-G(T)**	**E**	**E**
38c	-554.037619	0.159126	-553.868251	-553.913116	-553.913102	-554.171416	-554.188540
1b	-797.913914	0.193570	-797.707478	-797.759230	-797.757859	-798.118646	-798.139638
TS1 C-29	-1351.966543	0.353957	-1351.589535	-1351.664644	-1351.659982	-1352.303439	-1352.337552
TS1 S-29	-1351.961237	0.353711	-1351.584316	-1351.661065	-1351.655076	-1352.298222	-1352.333007
int1 C-29	-1352.051678	0.357785	-1351.671960	-1351.743073	-1351.740056	-1352.386297	-1352.417055
int1 S-29	-1352.054757	0.357540	-1351.675071	-1351.747127	-1351.743887	-1352.389701	-1352.423853
TS2 C-29	-1352.046462	0.356638	-1351.668386	-1351.737856	-1351.735606	-1352.380333	-1352.412673
TS2 S-29	-1352.051908	0.356867	-1351.673477	-1351.743866	-1351.741176	-1352.386232	-1352.420688
int2 C-29	-1352.051862	0.356728	-1351.673004	-1351.743742	-1351.741626	-1352.386420	-1352.418974
int2 S-29	-1352.058205	0.357088	-1351.678840	-1351.750752	-1351.747994	-1352.393182	-1352.427996
TS3 C-29	-1352.051242	0.355881	-1351.673525	-1351.743716	-1351.741688	-1352.385522	-1352.419167
TS3 S-29	-1352.057476	0.356208	-1351.679267	-1351.750704	-1351.747994	-1352.392219	-1352.428293
C-29	-1163.668713	0.343602	-1163.305381	-1163.371082	-1163.369414	-1163.945286	-1163.974341
S-29	-1163.667919	0.343825	-1163.304207	-1163.371130	-1163.368796	-1163.945091	-1163.977763
carbone dioxide	-188.515916	0.010339	-188.501668	-188.525358	-188.525358	-188.578482	-188.579811

1p + 38a → C-32							
	M06-2X/6-31+G(d,p)					M06-2X/6-311+G(2d,2p)	
	optimization energies and corrections					SPE	SPE THF
structure	**E**	**ZPE**	**H**	**G(T)**	**qh-G(T)**	**E**	**E**
38a	-538.003841	0.170800	-537.822637	-537.867745	-537.867740	-538.132560	-538.148012
1p	-660.356720	0.134032	-660.212534	-660.257636	-660.257636	-660.531482	-660.554216
TS1 C-32	-1198.373457	0.306157	-1198.046788	-1198.116936	-1198.112331	-1198.675029	-1198.710235
TS1 S-32	-1198.370548	0.306122	-1198.043791	-1198.115254	-1198.109738	-1198.672118	-1198.707590
int1 C-32	-1198.463082	0.310539	-1198.133267	-1198.198498	-1198.196447	-1198.762458	-1198.791895
int1 S-32	-1198.469982	0.310418	-1198.140059	-1198.206414	-1198.203767	-1198.769217	-1198.799457
TS2 C-32	-1198.452601	0.309381	-1198.124358	-1198.188709	-1198.186730	-1198.751107	-1198.780162
TS2 S-32	-1198.466541	0.309769	-1198.137844	-1198.202624	-1198.200474	-1198.764973	-1198.794956
int2 C-32	-1198.461144	0.309845	-1198.131829	-1198.197211	-1198.195509	-1198.760486	-1198.790925
int2 S-32	-1198.480817	0.310180	-1198.151037	-1198.217272	-1198.215134	-1198.779985	-1198.809220
TS3 C-32	-1198.460427	0.308909	-1198.132320	-1198.197226	-1198.195594	-1198.759521	-1198.791419
TS3 S-32	-1198.480059	0.309201	-1198.151510	-1198.217380	-1198.215247	-1198.778946	-1198.809701
C-32	-1010.077245	0.296560	-1009.763566	-1009.823859	-1009.822587	-1010.318620	-1010.345983
S-32	-1010.093409	0.296737	-1009.779381	-1009.840632	-1009.839019	-1010.334699	-1010.361456
carbone dioxide	-188.515916	0.010339	-188.501668	-188.525358	-188.525358	-188.578482	-188.579811

1a + 38c → C-33							
	M06-2X/6-31+G(d,p)					M06-2X/6-311+G(2d,2p)	
	optimization energies and corrections					SPE	SPE THF
structure	**E**	**ZPE**	**H**	**G(T)**	**qh-G(T)**	**E**	**E**
38c	-554.037619	0.159126	-553.868251	-553.913116	-553.913102	-554.171416	-554.188540
1a	-644.329539	0.146126	-644.173188	-644.218305	-644.218305	-644.498904	-644.517541
TS1 C-33	-1198.379445	0.306303	-1198.052571	-1198.122902	-1198.118312	-1198.681235	-1198.714136
TS1 S-33	-1198.376694	0.306398	-1198.049770	-1198.119871	-1198.115614	-1198.678313	-1198.710594
int1 C-33	-1198.470733	0.310448	-1198.140991	-1198.206437	-1198.204189	-1198.770031	-1198.798430
int1 S-33	-1198.471105	0.310422	-1198.141242	-1198.207402	-1198.204832	-1198.770607	-1198.801045
TS2 C-33	-1198.460044	0.309493	-1198.131723	-1198.195913	-1198.193952	-1198.758573	-1198.787657
TS2 S-33	-1198.464571	0.309428	-1198.136165	-1198.201061	-1198.198887	-1198.763361	-1198.794924
int2 C-33	-1198.464429	0.309564	-1198.135279	-1198.201087	-1198.199118	-1198.763632	-1198.793821
int2 S-33	-1198.474329	0.309804	-1198.144833	-1198.211392	-1198.209074	-1198.773951	-1198.807023
TS3 C-33	-1198.464188	0.308770	-1198.136177	-1198.201363	-1198.199471	-1198.763183	-1198.794196
TS3 S-33	-1198.473873	0.308918	-1198.145557	-1198.211642	-1198.209354	-1198.773230	-1198.807474
C-33	-1010.081360	0.296528	-1009.767701	-1009.828070	-1009.826739	-1010.322592	-1010.349081
S-33	-1010.086361	0.296238	-1009.772721	-1009.834424	-1009.832558	-1010.328071	-1010.358274
carbone dioxide	-188.515916	0.010339	-188.501668	-188.525358	-188.525358	-188.578482	-188.579811

1a + 38b → C-36							
	M06-2X/6-31+G(d,p)					**M06-2X/6-311+G(2d,2p)**	
	optimization energies and corrections					SPE	SPE THF
structure	**E**	**ZPE**	**H**	**G(T)**	**qh-G(T)**	**E**	**E**
38b	-691.592096	0.218103	-691.360921	-691.412325	-691.411604	-691.756346	-691.775400
1a	-644.329539	0.146126	-644.173188	-644.218305	-644.218305	-644.498904	-644.517541
TS1 C-36	-1335.932046	0.365365	-1335.543418	-1335.619067	-1335.614346	-1336.263874	-1336.299451
TS1 S-36	-1335.925808	0.365601	-1335.537040	-1335.612585	-1335.607679	-1336.257637	-1336.293589
int1 C-36	-1336.006726	0.368928	-1335.615723	-1335.686252	-1335.684157	-1336.336318	-1336.367150
int1 S-36	-1336.014109	0.369501	-1335.622476	-1335.693907	-1335.691144	-1336.344196	-1336.376997
TS2 C-36	-1336.005534	0.368330	-1335.615713	-1335.684745	-1335.682963	-1336.334589	-1336.365750
TS2 S-36	-1336.008375	0.368482	-1335.618222	-1335.688519	-1335.685970	-1336.337663	-1336.371484
int2 C-36	-1336.014855	0.368681	-1335.623955	-1335.694590	-1335.692733	-1336.344384	-1336.376170
int2 S-36	-1336.019608	0.368988	-1335.628282	-1335.700123	-1335.697419	-1336.349747	-1336.384732
TS3 C-36	-1336.014567	0.367839	-1335.624832	-1335.694930	-1335.693106	-1336.343861	-1336.376632
TS3 S-36	-1336.018644	0.367924	-1335.628607	-1335.700122	-1335.697394	-1336.348485	-1336.385138
C-36	-1147.629264	0.355561	-1147.253793	-1147.320045	-1147.318082	-1147.900866	-1147.929167
S-36	-1147.630562	0.355453	-1147.254998	-1147.322298	-1147.319893	-1147.902650	-1147.933864
carbone dioxide	-188.515916	0.010339	-188.501668	-188.525358	-188.525358	-188.578482	-188.579811

1b + 38b → C-37							
	M06-2X/6-31+G(d,p)					**M06-2X/6-311+G(2d,2p)**	
	optimization energies and corrections					SPE	SPE THF
structure	**E**	**ZPE**	**H**	**G(T)**	**qh-G(T)**	**E**	**E**
38b	-691.592096	0.218103	-691.360921	-691.412325	-691.411604	-691.756346	-691.775400
1b	-797.913914	0.193570	-797.707478	-797.759230	-797.757859	-798.118646	-798.139638
TS1 C-37	-1489.518708	0.412722	-1489.080316	-1489.159968	-1489.155665	-1489.885730	-1489.923140
TS1 S-37	-1489.510506	0.412916	-1489.071765	-1489.153418	-1489.147346	-1489.877753	-1489.916313
int1 C-37	-1489.596427	0.416200	-1489.155567	-1489.231035	-1489.228863	-1489.960967	-1489.994328
int1 S-37	-1489.597825	0.416683	-1489.156318	-1489.233576	-1489.230015	-1489.963378	-1489.999700
TS2 C-37	-1489.596360	0.415853	-1489.156578	-1489.230041	-1489.228396	-1489.960655	-1489.994030
TS2 S-37	-1489.595119	0.415903	-1489.154956	-1489.230763	-1489.227552	-1489.959986	-1489.996619
int2 C-37	-1489.604744	0.415795	-1489.164194	-1489.239468	-1489.237743	-1489.969327	-1490.002892
int2 S-37	-1489.601877	0.416210	-1489.160734	-1489.237972	-1489.234763	-1489.967276	-1490.004047
TS3 C-37	-1489.604231	0.414950	-1489.164840	-1489.239538	-1489.237904	-1489.968575	-1490.003234
TS3 S-37	-1489.600698	0.415220	-1489.160786	-1489.237604	-1489.234440	-1489.965814	-1490.004236
C-37	-1301.219331	0.402742	-1300.794281	-1300.864368	-1300.863128	-1301.526040	-1301.556368
S-37	-1301.213242	0.402989	-1300.787639	-1300.860184	-1300.857298	-1301.520810	-1301.554644
carbone dioxide	-188.515916	0.010339	-188.501668	-188.525358	-188.525358	-188.578482	-188.579811

- Full computational spectra showing all transitions

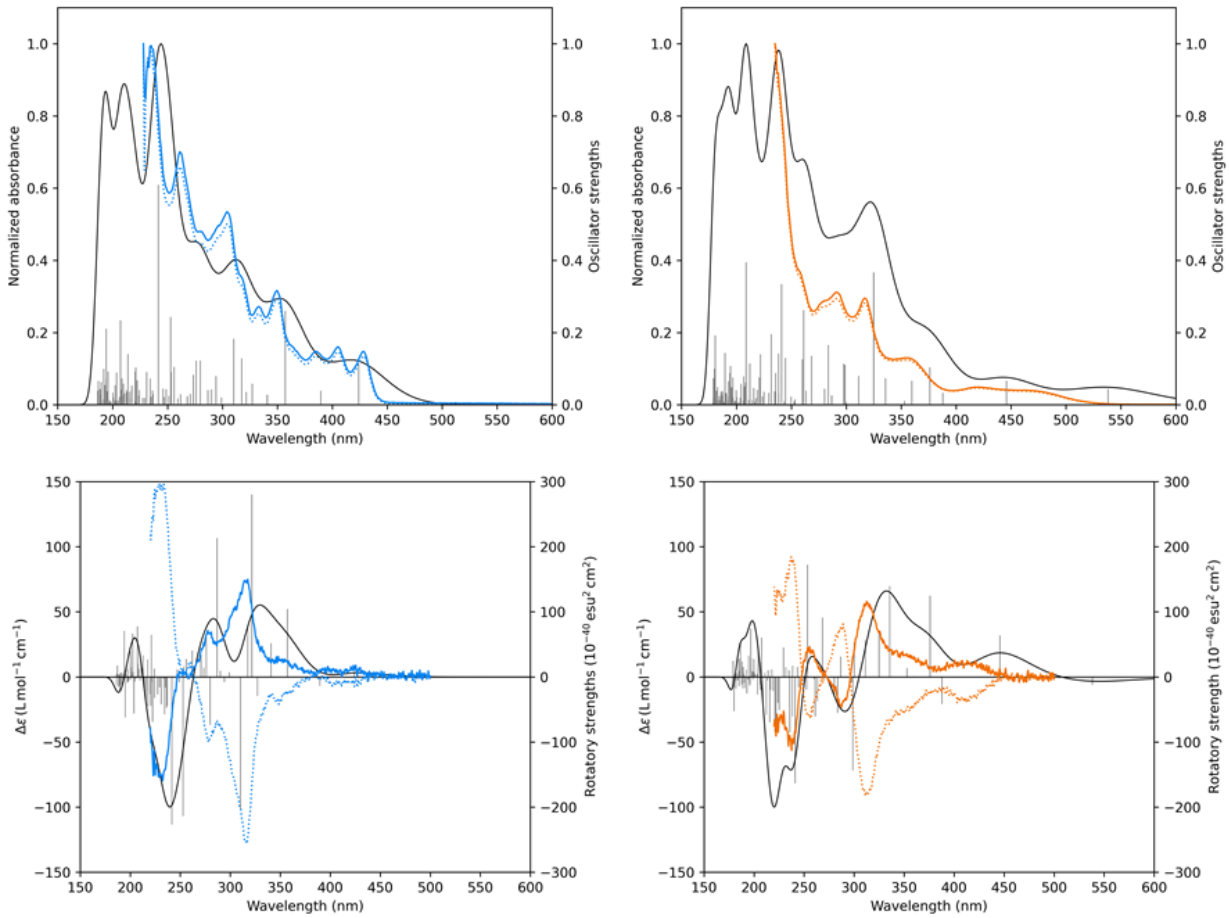


Figure S33: Experimental and computational spectra of **C-29** (blue) and **C-29•H+** (orange). Top: Experimental absorption spectra (color), along with oscillator strengths for all transitions (grey bars) and full predicted spectra (black curves) from TD-DFT calculations. Bottom: Experimental circular dichroism (CD) spectra for the (+)-enantiomer (full color) and (–)-enantiomer (dashed color), along with rotatory strengths for all transitions (grey bars) and full predicted spectra (black curves) from TD-DFT calculations.

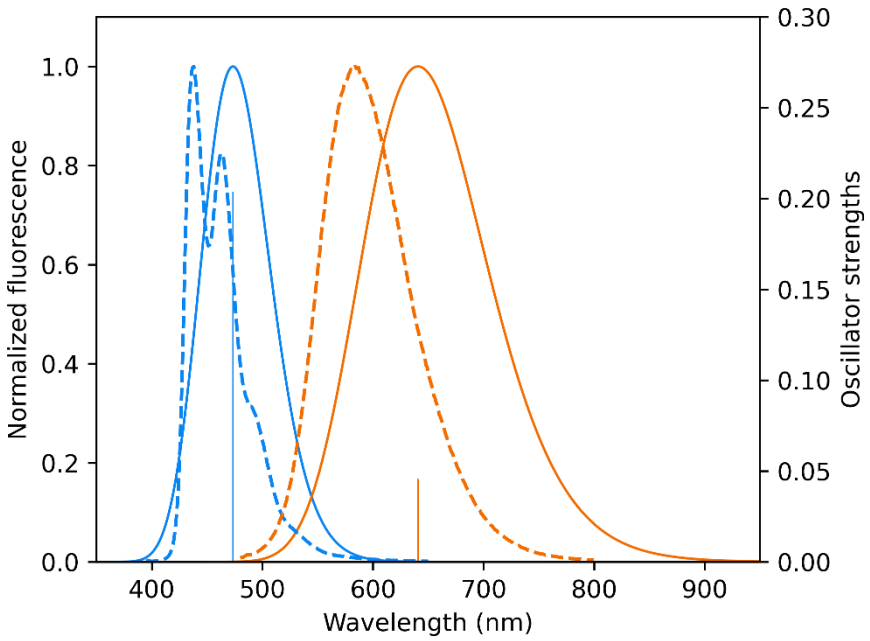


Figure S34. Experimental emission spectra (dashed curves) recorded in CH_2Cl_2 (C = 5 × 10^{-5} M), along oscillator strength for S1 → S0 transition (bars) and predicted spectra (full curves) from TD-DFT calculations.

- Comparison of HOMO and LUMO with NTOs

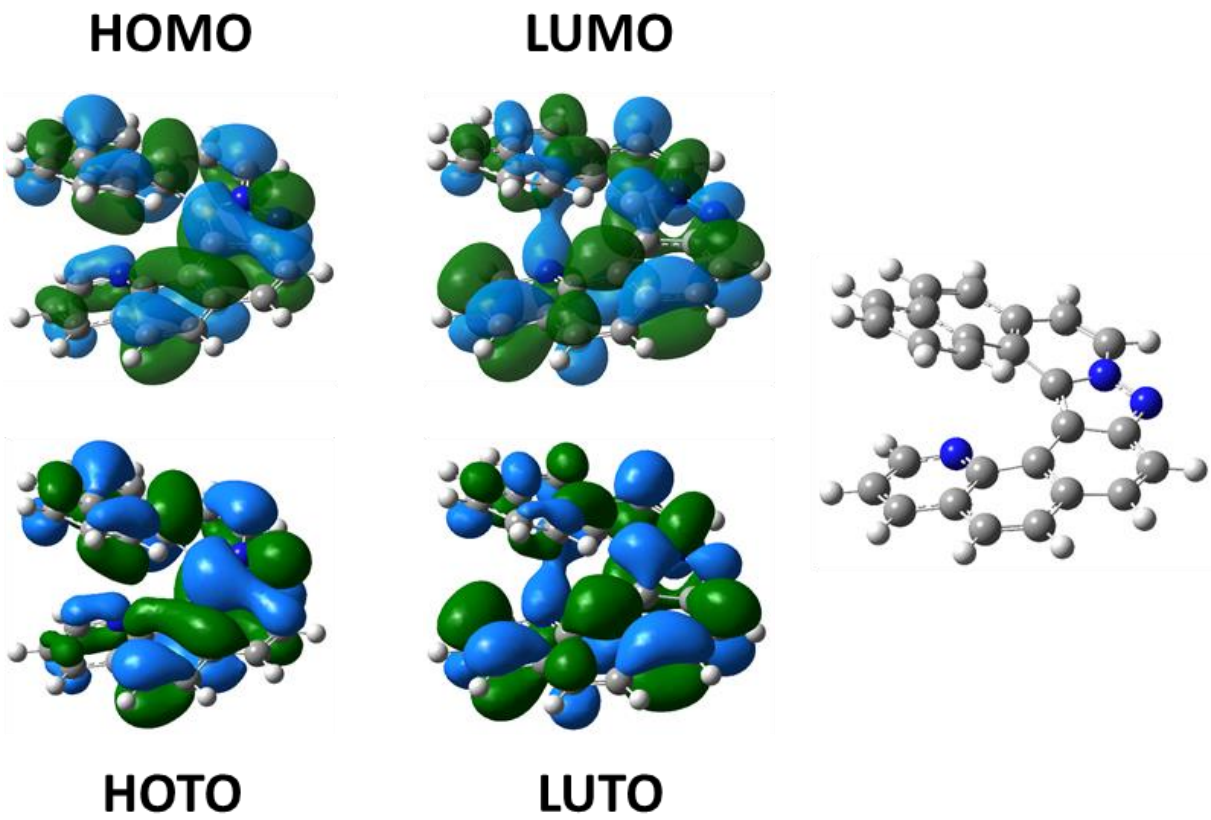


Figure S35: Comparison of the HOMO and LUMO orbitals of the S0 (ground) state of **C-29**, with the Natural Transition Orbitals (NTOs) for the S0 → S1 transition.

Orbital contributions for the S_0 → S_1 transition of **C-29**:

HOMO → LUMO (0.69)

HOMO-1 → LUMO+1 (-0.12)

Natural transition orbital contributions for the S_0 → S_1 transition of **C-29**:

HOTO → LUTO (0.96)

Orbital contributions for the S_1 → S_0 transition from the 1st excited state of **C-29**:

LUMO → HOMO (0.70)

NTO contributions for the S_1 → S_0 transition from the 1st excited state of **C-29**:

LUTO → HOTO (0.98)

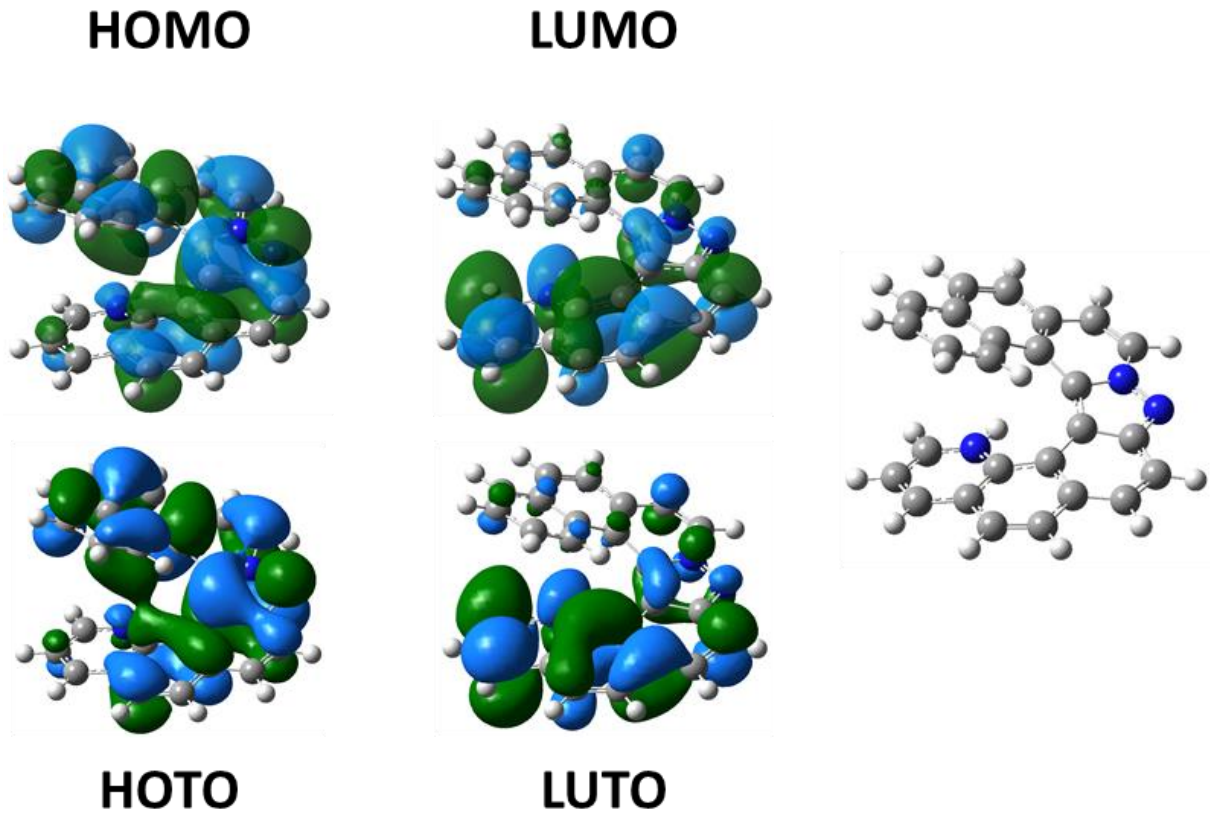


Figure S36: Comparison of the HOMO and LUMO orbitals of the S0 (ground) state of **C-29·H⁺**, with the Natural Transition Orbitals (NTOs) for the S0 → S1 transition.

Orbital contributions for the S_0 → S_1 transition of **C-29·H⁺**:

HOMO → LUMO (0.70)

Natural transition orbital contributions for the S_0 → S_1 transition of **C-29·H⁺**:

HOTO → LUTO (0.99)

Orbital contributions for the S_1 → S_0 transition from the 1st excited state of **C-29·H⁺**:

LUMO → HOMO (0.71)

NTO contributions for the S_1 → S_0 transition from the 1st excited state of **C-29·H⁺**:

LUTO → HOTO (1.00)

- Frontier Molecular Orbitals energies

Orbital	**C-29** (S_0)	**C-29·H$^+$** (S_0)
LUMO+4	-0.02183	-0.0539
LUMO+3	-0.04135	-0.07496
LUMO+2	-0.04818	-0.08545
LUMO+1	-0.06693	-0.09483
LUMO	-0.0783	-0.12863
HOMO	-0.20602	-0.23407
HOMO-1	-0.22477	-0.25071
HOMO-2	-0.24163	-0.27029
HOMO-3	-0.24937	-0.28149
HOMO-4	-0.26117	-0.30329

Table S8: Natural Bond Orbitals (NBOs) energies (in eV) for **C-29** and **C-29·H$^+$** in their S_0 states.

Protonation of **C-29** lowers the LUMO energy more than the HOMO energy, reducing the HOMO-LUMO gap from 0.12772 eV for **C-29** to 0.10544 for **C-29·H$^+$**.

- Electronic density changes during $S_0 – S_1$ transitions

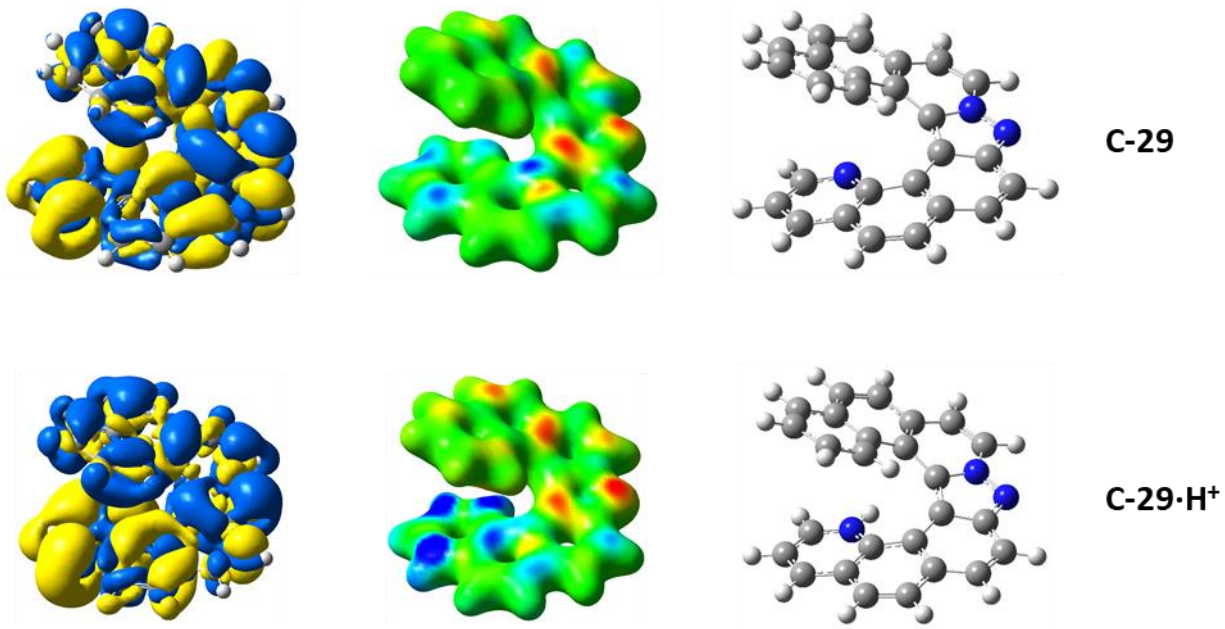


Figure S37: Difference between the S_1 and S_0 densities ($S_1 – S_0$) for the $S_0 \rightarrow S_1$ transition of both compounds. Left: Isosurface of $S_1 – S_0$ with an isovalue of 0.0004. Right: $S_1 – S_0$ mapped on the S_0 density, using an isovalue of 0.04. The mapped density is color-coded between -2.5 x 10^{-3} (red) and 2.5 x 10^{-3} (blue). A blue region indicates an area where the difference between the S_1 and S_0 densities is positive, so that more electronic density is found at that position in the S_1 state than the S0 state. The opposite is true for red regions, indicating more electronic density at the S_0 state than the S_1 state.

For both compounds, there is significant intramolecular charge-transfer character, from the pyrazole ring and the polyaromatic section from the sydnone partner in the S_0 state, to the pyridine ring in the S_1 state.

- Calculation of the g_{lum} values

The luminescence dissymmetry factor g_{lum} of a given transition (e.g. S_1 to S_0) is given by the equation $g_{lum} = 4R_{1\text{-}0}/D_{1\text{-}0}$, where $R = \|\mu_e\| \cdot \|\mu_m\| \cos\theta$ is the transition rotatory strength, $D = \|\mu_e\|^2$ is the transition dipole strength, μ_e and μ_m are the electric and magnetic transition dipole moments, respectively, and θ the angle between the two. To compute g_{lum}, the rotatory and dipole strength for the $S_1 \rightarrow S_0$ transition from the S_1 state of **C-29** and **C-29·H$^+$** were extracted from the Gaussian output. The rotatory strength is given directly from the velocity gauge in units of 10^{-40} esu^2 cm^2. The dipole strength is the square of the electric dipole moment as the length gauge, in au. Considering 1 au = 2.541746 D = 10^{-18} esu cm, that value is obtained in units of 10^{-40} esu^2 cm^2. From there, the g_{lum} value can be computed at the wavelength of the transition.

Parameter	C-29	C-29·H$^+$
Transition wavelength	473.44	640.82
Rotatory strength (10^{-40} esu^2 cm^2)	33.7965	-12.097
Dipole strength (au^2)	3.1738	0.9626
Dipole strength (10^{-40} esu^2 cm^2)	205035.0619	62186.25956
g_{lum}	0.000659331	-0.000778114

- Visualizations of the magnetic and electric dipole vectors

The electric (obtained from the velocity gauge) and magnetic dipole vectors corresponding to the $S_1 \rightarrow S_0$ transition from the S_1 state of **C-29** and **C-29·H$^+$** were extracted from the Gaussian output and visualized on top of the molecules using Vesta 3.5.2.

Parameter	C-29	C-29·H$^+$
	Electric dipole moment (au)	
X	-1.7291	-0.9492
Y	-0.4084	-0.2469
Z	0.1311	0.0273
Norm	1.7815	0.9812
	Magnetic dipole moment (au)	
X	-0.0607	0.0091
Y	0.2647	0.2179
Z	1.1046	0.3551
Norm	1.1375	0.4167
θ (between electric and magnetic dipoles)	85.92°	97.22°

DFT-optimized geometries and vibrational frequencies (TS)

sydnones

1a

N	-1.42054	0.99689	0.00009
N	-2.72321	0.94650	0.00009
O	-3.00204	-0.38817	-0.00003
C	-1.85158	-1.17490	-0.00009
C	-0.79437	-0.20620	-0.00000
O	-1.87826	-2.38204	-0.00020
C	0.62523	-0.30135	-0.00002
C	1.29631	-1.53992	-0.00013
C	1.35983	0.91004	0.00007
C	2.67811	-1.55652	-0.00014
C	2.76617	0.86004	0.00006
C	3.41770	-0.35844	-0.00005
H	3.33024	1.78857	0.00013
H	4.50185	-0.39397	-0.00006
C	0.63047	2.15418	0.00018
C	-0.71860	2.20361	0.00019
H	-1.33344	3.09309	0.00027
H	1.18020	3.08982	0.00026
H	3.20093	-2.50748	-0.00022
H	0.71325	-2.45535	-0.00020

1b

N	2.52409	0.37674	-0.00005
N	3.60761	-0.34274	-0.00013
O	3.15483	-1.61950	-0.00020
C	1.77479	-1.70284	-0.00016
C	1.33684	-0.31509	-0.00006
O	1.23990	-2.78766	-0.00021
C	0.09052	0.41205	0.00003
C	-1.23315	-0.18465	0.00002
C	0.18712	1.82106	0.00012
C	-2.37196	0.67460	0.00011
C	-1.46307	-1.58349	-0.00007
C	-0.97639	2.64517	0.00021
C	-3.67357	0.11917	0.00011
C	-2.21618	2.09322	0.00021
C	-2.74239	-2.09475	-0.00007
H	-0.62622	-2.26755	-0.00014
H	-0.84461	3.72317	0.00028
C	-3.86288	-1.24184	0.00002
H	-4.52285	0.79679	0.00018
H	-3.10525	2.71677	0.00027
H	-2.88117	-3.17100	-0.00014
H	-4.86593	-1.65647	0.00002
C	1.46897	2.46047	0.00012
C	2.61853	1.76058	0.00004
H	3.62643	2.15148	0.00004
H	1.51676	3.54419	0.00020

1p

N	-1.38208	0.99903	0.00009
N	-2.68053	0.97619	0.00009
O	-2.99466	-0.34295	-0.00002
C	-1.85663	-1.17446	-0.00010
C	-0.77684	-0.22081	-0.00002
O	-1.94581	-2.37013	-0.00020
C	0.64619	-0.31628	-0.00003
C	1.38697	0.89390	0.00007
C	2.54140	-1.57840	-0.00014
C	2.78749	0.80361	0.00006
C	3.37605	-0.44479	-0.00005
H	3.38723	1.70986	0.00014
H	4.45336	-0.56287	-0.00006
C	0.67540	2.14675	0.00018
C	-0.67121	2.20205	0.00019
H	-1.28321	3.09356	0.00026
H	1.23461	3.07671	0.00026
H	2.97995	-2.57352	-0.00022
N	1.21960	-1.53357	-0.00013

arynes

38a

C	1.50698	0.72527	0.00001
C	0.81672	1.98832	0.00001
C	-0.54055	2.05295	0.00001
C	0.71178	-0.46666	-0.00000
H	1.40598	2.90079	0.00002
H	-1.04188	3.01692	0.00001
C	3.65449	-0.51906	0.00001
C	2.93269	0.67142	0.00001
C	1.53743	-1.59937	-0.00001
C	2.77616	-1.60436	-0.00000
H	4.73664	-0.55255	0.00001
H	3.47653	1.61284	0.00002

C	-0.72461	-0.40349	-0.00000
C	-1.51611	-1.57149	-0.00001
C	-1.35046	0.86616	-0.00000
C	-2.89137	-1.48323	-0.00002
H	-1.01936	-2.53808	-0.00002
C	-2.76266	0.93071	-0.00000
C	-3.52009	-0.22071	-0.00001
H	-3.49369	-2.38595	-0.00002
H	-3.24288	1.90554	-0.00000
H	-4.60364	-0.15832	-0.00001

38b

C	-2.51995	0.38001	-0.00003
C	-2.48683	1.80834	-0.00004
C	-1.30004	2.47460	-0.00003
C	-1.25968	-0.32212	-0.00001
H	-3.42493	2.35546	-0.00005
H	-1.28301	3.56086	-0.00003
C	-3.88813	-1.69479	-0.00004
C	-3.77193	-0.31122	-0.00005
C	-1.54112	-1.69132	-0.00002
C	-2.62027	-2.29627	-0.00003
H	-4.84469	-2.20300	-0.00005
H	-4.67598	0.29277	-0.00006
C	-0.00684	0.37635	-0.00000
C	-0.04910	1.78365	-0.00001
C	1.16683	2.53997	0.00001
C	2.37398	1.92012	0.00003
H	1.09940	3.62420	0.00000
H	3.29463	2.49718	0.00003
C	1.28025	-0.29636	0.00002
C	2.46428	0.49137	0.00003
C	1.42810	-1.70486	0.00002
C	3.73082	-0.13770	0.00005
H	0.55457	-2.34587	0.00002
H	4.61943	0.48794	0.00006
C	3.84127	-1.50889	0.00005
C	2.67364	-2.29574	0.00004
H	4.81789	-1.98206	0.00006
H	2.75102	-3.37830	0.00004

38c

C	1.48411	0.73026	0.00001
C	0.79160	1.99246	0.00001
C	-0.56593	2.05573	0.00001
C	0.69469	-0.46477	0.00000
H	1.37905	2.90601	0.00002
H	-1.07188	3.01725	0.00001
C	3.62596	-0.51804	0.00001
C	2.90994	0.67564	0.00001
C	1.51879	-1.59098	-0.00001
C	2.75701	-1.61356	-0.00001
H	4.70876	-0.54913	0.00001
H	3.45527	1.61610	0.00002
C	-0.74228	-0.40459	0.00000
C	-1.36736	0.86449	0.00000
C	-2.74517	-1.50409	-0.00003
C	-2.77812	0.89175	-0.00000
C	-3.47383	-0.29489	-0.00001
H	-3.27289	-2.45524	-0.00001
H	-3.29550	1.84764	0.00000
H	-4.55805	-0.31577	-0.00001
N	-1.42874	-1.56905	-0.00001

1b + 38c → C-29

TS1 C-29

C	3.70920	0.50551	0.17035
C	4.36707	1.77606	0.33209
C	3.66431	2.93976	0.34673
C	2.28926	0.49763	0.01625
H	5.44765	1.79160	0.44356
H	4.17624	3.89053	0.46862
C	3.84939	-1.95946	0.01603
C	4.45061	-0.71306	0.16481
C	1.76594	-0.79071	-0.14403
C	2.46937	-1.82606	-0.12360
H	4.41232	-2.88542	0.01295
H	5.52987	-0.65699	0.28423
C	1.54050	1.72721	0.04212
C	2.23491	2.94818	0.20634
C	-0.48996	2.77614	-0.05984
C	1.46684	4.13175	0.22826
C	0.09964	4.04995	0.09481
H	-1.57017	2.68358	-0.16857
H	1.96370	5.09094	0.35036
H	-0.52431	4.93692	0.10616
C	-3.29484	1.32546	-2.06298
C	-0.96115	-2.38158	2.32992
C	-2.47633	0.32594	-1.58362
C	-0.12303	-3.14737	1.60513
C	-1.77771	-1.37386	1.72243
C	-4.19553	1.99569	-1.21149

C	-1.68936	-1.11672	0.33857
C	-2.51764	-0.06592	-0.22260
C	-0.75045	-1.93054	-0.39568
C	-2.67481	-0.64173	2.55525
C	-3.41343	0.63112	0.63955
C	-4.24461	1.65307	0.11881
C	-3.47369	0.32213	2.03186
C	-0.33758	-2.10674	-1.79516
N	-0.07929	-2.93017	0.24351
N	0.79607	-3.58762	-0.48490
O	0.55621	-3.14971	-1.75452
O	-0.63162	-1.60157	-2.85008
H	-3.23525	1.59923	-3.11143
H	-1.78838	-0.15844	-2.26107
H	-1.02449	-2.53782	3.40128
H	0.52907	-3.92970	1.96838
H	-4.83821	2.77884	-1.60135
H	-2.70506	-0.87859	3.61465
H	-4.16400	0.87706	2.66060
H	-4.92240	2.16250	0.79844
N	0.19682	1.65132	-0.08602

One imaginary frequency: -106.39 cm^{-1}

TS1 S-29

C	-3.18159	1.97089	-0.98660
C	-4.56332	2.12382	-1.35807
C	-5.48350	1.16485	-1.07646
C	-2.80164	0.77943	-0.29022
H	-4.86329	3.03427	-1.86909
H	-6.52523	1.30032	-1.35367
C	-0.87339	2.85098	-0.97507
C	-2.21776	2.97008	-1.30695
C	-1.45160	0.83567	0.03735
C	-0.57606	1.68855	-0.24210
H	-0.15085	3.60982	-1.25596
H	-2.55915	3.85234	-1.84296
C	-3.75610	-0.27338	-0.05490
C	-5.10491	-0.05982	-0.42934
C	-4.21238	-2.37998	0.71854
C	-6.02617	-1.09411	-0.16448
C	-5.58521	-2.25812	0.42207
H	-3.83490	-3.30067	1.15960
H	-7.07123	-0.96029	-0.43180
H	-6.26313	-3.07501	0.64314
C	5.47721	1.67969	0.42810
C	0.99095	-2.47319	-0.63361
C	4.23276	1.11771	0.61358
C	0.02643	-2.03198	0.19735
C	2.27732	-1.84576	-0.69802
C	6.41466	1.09276	-0.44340
C	2.56082	-0.70419	0.08386
C	3.85687	-0.06748	-0.06628
C	1.50853	-0.26360	0.96501
C	3.25262	-2.39392	-1.58266
C	4.80441	-0.64916	-0.95896
C	6.07683	-0.05255	-1.12375
C	4.47818	-1.82318	-1.70253
C	1.30923	0.77570	1.98209
N	0.34039	-0.95894	1.00737
N	-0.59291	-0.46561	1.79760
O	0.03771	0.54351	2.45227
O	1.99157	1.64329	2.47182
H	5.73216	2.58751	0.96527
H	3.53953	1.59084	1.29460
H	0.78433	-3.31993	-1.27909
H	-0.99229	-2.38663	0.30037
H	7.39273	1.54343	-0.57860
H	2.98923	-3.27767	-2.15615
H	5.22445	-2.24052	-2.37232
H	6.78073	-0.51942	-1.80723
N	-3.32126	-1.43418	0.48989

One imaginary frequency: -105.33 cm^{-1}

int1 C-29

C	-3.31110	0.94536	-0.01115
C	-3.81310	2.28609	-0.18087
C	-2.98315	3.34974	-0.28855
C	-1.90172	0.71291	0.04788
H	-4.89007	2.42044	-0.22565
H	-3.37487	4.35412	-0.42285
C	-3.80483	-1.42135	0.21260
C	-4.23457	-0.11596	0.08090
C	-1.46752	-0.62886	0.15407
C	-2.43220	-1.61939	0.23308
H	-4.48643	-2.26145	0.28485
H	-5.29541	0.11203	0.03736
C	-1.02428	1.86963	-0.03497
C	-1.56154	3.16551	-0.21721
C	1.12615	2.67442	-0.01918
C	-0.65528	4.24036	-0.31269

C	0.69791	4.00034	-0.22141
H	2.18638	2.44013	0.07877
H	-1.03858	5.24746	-0.45522
H	1.42283	4.80358	-0.29217
C	3.33934	0.67214	2.14319
C	0.19432	-2.05042	-2.49338
C	2.25812	0.04696	1.57367
C	-0.70369	-2.74923	-1.78946
C	1.26136	-1.33761	-1.78879
C	4.51787	0.91092	1.39721
C	1.18418	-1.05581	-0.42661
C	2.28275	-0.39987	0.22247
C	-0.12692	-1.47339	0.23057
C	2.42315	-0.98979	-2.53288
C	3.45369	-0.10414	-0.53786
C	4.56213	0.53733	0.07907
C	3.49576	-0.41048	-1.92396
C	-0.19529	-2.07766	1.67413
N	-0.58983	-2.73406	-0.40060
N	-1.79887	-2.93717	0.32189
O	-1.24917	-2.95810	1.65997
O	0.44958	-1.91977	2.66404
H	3.28027	0.99816	3.17684
H	1.36483	-0.08810	2.16222
H	0.20940	-2.09812	-3.57552
H	-1.47130	-3.39647	-2.19789
H	5.36886	1.39925	1.86143
H	2.44686	-1.22153	-3.59377
H	4.39139	-0.16584	-2.48868
H	5.44440	0.73264	-0.52490
N	0.29569	1.65410	0.07353

int1 S-29

C	-2.20539	1.84162	-0.82396
C	-3.36571	2.59806	-1.21944
C	-4.61820	2.12070	-1.02644
C	-2.37901	0.55422	-0.23299
H	-3.20961	3.56974	-1.67909
H	-5.48693	2.69879	-1.32907
C	0.22974	1.69360	-0.66361
C	-0.91622	2.38138	-1.02709
C	-1.19541	-0.12639	0.07803
C	0.05485	0.42357	-0.12139
H	1.22066	2.11230	-0.81185
H	-0.83713	3.36409	-1.48313
C	-3.72536	0.05603	0.00349
C	-4.82928	0.84272	-0.40339
C	-5.09526	-1.58243	0.83243
C	-6.12084	0.33324	-0.16239
C	-6.26171	-0.88774	0.45701
H	-5.17105	-2.54464	1.33402
H	-6.98807	0.91433	-0.46516
H	-7.23878	-1.31105	0.66214
C	4.30016	2.06503	1.51134
C	1.46806	-2.33738	-1.82147
C	3.27538	1.21061	1.18765
C	0.32123	-2.45169	-1.13268
C	2.57648	-1.53455	-1.29696
C	5.55697	1.96589	0.86791
C	2.40759	-0.68894	-0.20329
C	3.44466	0.20937	0.18891
C	1.02783	-0.64785	0.39168
C	3.83980	-1.58737	-1.94751
C	4.70198	0.13832	-0.48270
C	5.74822	1.02145	-0.10828
C	4.87488	-0.79311	-1.54040
C	0.72725	-0.69805	1.91817
N	0.25408	-1.87073	0.12299
N	-1.00515	-1.47785	0.65693
O	-0.55424	-1.18049	2.01701
O	1.38108	-0.41994	2.87665
H	4.14573	2.81929	2.27625
H	2.33204	1.29487	1.71212
H	1.59879	-2.86693	-2.75727
H	-0.53629	-3.04618	-1.42670
H	6.36112	2.64018	1.14429
H	3.96657	-2.27237	-2.78090
H	5.83857	-0.84372	-2.03999
H	6.70247	0.94057	-0.62205
N	-3.87309	-1.13540	0.61739

TS2 C-29

C	-3.29533	0.74837	-0.03416
C	-3.84020	2.08261	0.00459
C	-3.05281	3.17510	-0.13967
C	-1.88760	0.56731	-0.18639
H	-4.90861	2.18981	0.16874
H	-3.47152	4.17615	-0.08552
C	-3.68188	-1.65188	0.05709
C	-4.16439	-0.35762	0.08533
C	-1.39079	-0.75103	-0.08256
C	-2.30325	-1.79443	-0.02460

H	-4.32794	-2.51998	0.12371
H	-5.22986	-0.17259	0.18434
C	-1.08459	1.73487	-0.51560
C	-1.65493	3.02677	-0.43611
C	0.92128	2.57576	-1.24240
C	-0.82337	4.12635	-0.72772
C	0.47935	3.90647	-1.11744
H	1.93239	2.35882	-1.58312
H	-1.22674	5.13317	-0.65680
H	1.14851	4.72754	-1.34948
C	0.23797	-3.35445	-1.59055
H	-0.27066	-4.20811	-2.02232
N	-1.59727	-3.07888	0.05272
C	1.41816	-2.84404	-1.98987
N	-0.38710	-2.75973	-0.53524
H	1.95132	-3.28626	-2.82108
O	-1.17790	-3.08401	1.48807
C	2.02005	-1.73540	-1.25302
C	-0.03264	-1.51930	0.13082
C	-0.22638	-2.10904	1.58929
C	3.34305	-1.33136	-1.60044
C	1.36726	-1.08190	-0.21040
H	3.84056	-1.84645	-2.41728
O	0.33342	-1.85785	2.61290
C	3.97898	-0.32971	-0.92706
C	2.01756	-0.04008	0.51946
C	3.33500	0.34511	0.14653
H	4.98712	-0.03189	-1.20345
C	1.38315	0.68623	1.56547
C	3.97487	1.41656	0.82447
C	2.01891	1.72391	2.19816
H	1.50754	2.26459	2.98825
C	3.33401	2.09730	1.82859
H	3.82894	2.91690	2.33982
H	0.37333	0.42907	1.86351
H	4.98388	1.68934	0.52576
N	0.16850	1.53001	-0.95942

One imaginary frequency: -105.46 cm^{-1}

TS2 S-29

C	-2.25929	1.88277	-0.79471
C	-3.43811	2.63396	-1.14316
C	-4.67886	2.12362	-0.95995
C	-2.40207	0.56566	-0.26476
H	-3.30536	3.62869	-1.55868
H	-5.56182	2.69773	-1.22680
C	0.18042	1.77537	-0.65593
C	-0.98285	2.45387	-0.98322
C	-1.20364	-0.10828	-0.00655
C	0.04154	0.47608	-0.17536
H	1.15766	2.22684	-0.79166
H	-0.92462	3.45671	-1.39657
C	-3.73586	0.03184	-0.03400
C	-4.85879	0.81492	-0.39259
C	-5.06514	-1.66405	0.74374
C	-6.13757	0.27192	-0.15782
C	-6.24845	-0.97645	0.41133
H	-5.11714	-2.64688	1.20686
H	-7.01901	0.84924	-0.42457
H	-7.21502	-1.42583	0.61055
C	4.01221	2.37965	1.28334
C	1.83971	-2.78253	-1.44040
C	3.07622	1.41566	1.00046
C	0.58643	-2.77975	-0.94282
C	2.78649	-1.73809	-1.05431
C	5.31284	2.30985	0.72948
C	2.43938	-0.68872	-0.20374
C	3.38419	0.32584	0.13721
C	1.02247	-0.61764	0.28556
C	4.11313	-1.78904	-1.57214
C	4.69816	0.25586	-0.41031
C	5.64469	1.26504	-0.09573
C	5.03371	-0.82800	-1.26584
C	0.69122	-0.72482	1.81616
N	0.24002	-1.78309	-0.08380
N	-0.99641	-1.49508	0.47220
O	-0.56368	-1.26096	1.88651
O	1.34045	-0.44046	2.77792
H	3.75489	3.19641	1.95021
H	2.09925	1.47532	1.46660
H	2.15832	-3.56998	-2.11039
H	-0.18427	-3.51288	-1.14962
H	6.04337	3.07686	0.96527
H	4.37850	-2.61318	-2.22811
H	6.03913	-0.87842	-1.67525
H	6.64112	1.19206	-0.52349
N	-3.85394	-1.18591	0.53253

One imaginary frequency: -106.46 cm^{-1}

int2 C-29

C	-3.25034	-0.84252	0.04170
C	-4.33498	0.09994	0.16637

C	-4.13946	1.43100	0.00819
C	-1.92947	-0.35742	-0.19461
H	-5.32037	-0.28910	0.40634
H	-4.95923	2.13359	0.12937
C	-2.49440	-3.15517	0.02153
C	-3.50924	-2.22538	0.15434
C	-0.88159	-1.29917	-0.13587
C	-1.21039	-2.64917	-0.12332
H	-2.67076	-4.22430	0.05251
H	-4.53214	-2.55094	0.31805
C	-1.77424	1.03853	-0.57154
C	-2.85670	1.93200	-0.40454
C	-0.44890	2.67765	-1.47050
C	-2.64125	3.28486	-0.73436
C	-1.42397	3.66954	-1.25186
H	0.50651	2.93535	-1.92373
H	-3.44505	4.00301	-0.59424
H	-1.22085	4.70109	-1.51733
C	0.59565	2.50743	2.02131
C	3.06218	-2.01707	-1.39774
C	0.64625	1.27147	1.43067
C	2.11125	-2.95230	-1.26391
C	2.84257	-0.64424	-0.93587
C	1.55808	3.49800	1.70256
C	1.71171	-0.29773	-0.20632
C	1.65786	0.94996	0.48279
C	0.66467	-1.35867	-0.00970
C	3.85368	0.33198	-1.16090
C	2.66172	1.92281	0.21885
C	2.57377	3.20319	0.82938
C	3.74786	1.58813	-0.63446
C	0.85330	-2.06473	1.40312
N	0.84421	-2.55418	-0.85320
N	0.00585	-3.45284	-0.19565
O	0.50406	-3.35635	1.24618
O	1.26006	-1.59014	2.42341
H	-0.18607	2.72784	2.74142
H	-0.09341	0.52477	1.69868
H	4.02345	-2.27756	-1.82427
H	2.20119	-3.99347	-1.54998
H	1.50135	4.47694	2.16795
H	4.71494	0.05711	-1.76314
H	4.51245	2.33560	-0.82857
H	3.33929	3.94007	0.60023
N	-0.61548	1.40908	-1.14857

int2 S-29

C	-2.33140	1.97741	-0.58694
C	-3.53054	2.74447	-0.80740
C	-4.75697	2.18615	-0.67588
C	-2.43653	0.59894	-0.23966
H	-3.42505	3.78922	-1.08517
H	-5.65633	2.77129	-0.84679
C	0.11384	1.89874	-0.52223
C	-1.06923	2.58857	-0.73276
C	-1.22069	-0.07818	-0.10192
C	0.01735	0.54731	-0.19434
H	1.07229	2.39061	-0.63855
H	-1.03496	3.63573	-1.01944
C	-3.75473	0.00870	-0.05979
C	-4.89949	0.80844	-0.29012
C	-5.03594	-1.80250	0.51071
C	-6.16276	0.21152	-0.10866
C	-6.23859	-1.10350	0.29063
H	-5.06011	-2.83826	0.84205
H	-7.06004	0.80035	-0.28069
H	-7.19226	-1.59638	0.44382
C	3.85776	2.57295	1.12420
C	2.10228	-2.99225	-0.92641
C	2.97047	1.56087	0.85517
C	0.77837	-2.91323	-0.72276
C	2.94963	-1.80190	-0.81599
C	5.17586	2.53352	0.60784
C	2.46140	-0.62085	-0.26604
C	3.34905	0.44906	0.05058
C	1.00511	-0.58762	0.09150
C	4.31056	-1.86843	-1.22364
C	4.70061	0.37403	-0.39635
C	5.58719	1.44928	-0.12495
C	5.14771	-0.80022	-1.05879
C	0.67908	-0.94446	1.58958
N	0.21818	-1.65272	-0.55047
N	-0.99305	-1.51208	0.12505
O	-0.53563	-1.52640	1.58705
O	1.35269	-0.75574	2.56204
H	3.55244	3.40103	1.75605
H	1.98514	1.58156	1.30783
H	2.56110	-3.94195	-1.17362
H	0.07547	-3.73570	-0.78150
H	5.86363	3.34597	0.81876
H	4.67225	-2.78625	-1.67815
H	6.17969	-0.85077	-1.39513
H	6.60771	1.38475	-0.49290
N	-3.83853	-1.27452	0.34501

TS3 C-29

C	-3.20871	-0.94619	0.03720
C	-4.31956	-0.03832	0.17783
C	-4.16487	1.29961	0.02736
C	-1.90667	-0.41937	-0.20652
H	-5.29078	-0.45787	0.42399
H	-5.00404	1.97645	0.16173
C	-2.38520	-3.23572	-0.01355
C	-3.42428	-2.33937	0.14033
C	-0.82906	-1.32949	-0.16487
C	-1.11647	-2.68904	-0.17116
H	-2.52810	-4.30997	0.01106
H	-4.43518	-2.69682	0.31165
C	-1.79639	0.98099	-0.57961
C	-2.90259	1.84129	-0.39543
C	-0.53209	2.66126	-1.48984
C	-2.73062	3.20189	-0.72007
C	-1.53210	3.62390	-1.25138
H	0.40819	2.94919	-1.95624
H	-3.55285	3.89580	-0.56544
H	-1.36200	4.66222	-1.51363
C	0.48128	2.53706	1.98594
C	3.14423	-1.93086	-1.36137
C	0.58326	1.29620	1.41281
C	2.22753	-2.90066	-1.23578
C	2.87493	-0.56601	-0.90682
C	1.41209	3.55696	1.66623
C	1.72205	-0.25430	-0.19490
C	1.61636	0.99897	0.48031
C	0.70581	-1.34375	-0.01545
C	3.85718	0.44048	-1.12610
C	2.58970	2.00252	0.21805
C	2.44946	3.28670	0.81095
C	3.70012	1.69715	-0.61511
C	0.88860	-2.04887	1.43764
N	0.94811	-2.54395	-0.82693
N	0.10950	-3.45058	-0.26352
O	0.57909	-3.32242	1.32163
O	1.27322	-1.48643	2.42908
H	-0.31625	2.73807	2.69429
H	-0.12862	0.52545	1.68570
H	4.12011	-2.16076	-1.77244
H	2.35430	-3.93983	-1.51341
H	1.31507	4.53914	2.11799
H	4.73608	0.18872	-1.71274
H	4.44115	2.46880	-0.80570
H	3.19261	4.04642	0.58288
N	-0.65648	1.38707	-1.17177

One imaginary frequency: -359.56 cm^{-1}

TS3 S-29

C	-2.33291	1.97531	-0.57444
C	-3.53087	2.74913	-0.77348
C	-4.75795	2.19215	-0.64061
C	-2.43770	0.59276	-0.24939
H	-3.42442	3.79832	-1.03351
H	-5.65718	2.78273	-0.79230
C	0.11369	1.89753	-0.51959
C	-1.06980	2.58835	-0.71650
C	-1.21880	-0.08750	-0.12667
C	0.01984	0.54009	-0.21197
H	1.07061	2.39304	-0.63033
H	-1.03703	3.63953	-0.98833
C	-3.75529	0.00002	-0.07965
C	-4.90012	0.80762	-0.28241
C	-5.03718	-1.82455	0.44559
C	-6.16372	0.20894	-0.10695
C	-6.23995	-1.11586	0.25740
H	-5.06170	-2.87018	0.74438
H	-7.06067	0.80422	-0.25702
H	-7.19365	-1.61037	0.40503
C	3.86696	2.58520	1.06558
C	2.09252	-3.01319	-0.87436
C	2.97684	1.56870	0.82400
C	0.76992	-2.93598	-0.66392
C	2.94124	-1.82376	-0.78398
C	5.18049	2.53482	0.53891
C	2.45472	-0.63216	-0.25480
C	3.34730	0.44239	0.03643
C	0.99903	-0.58496	0.09482
C	4.30075	-1.90250	-1.19488
C	4.69552	0.35628	-0.41786
C	5.58549	1.43555	-0.17461
C	5.13915	-0.83205	-1.05785
C	0.66580	-0.89776	1.63467
N	0.21440	-1.67325	-0.49583
N	-0.99944	-1.51072	0.08723
O	-0.52331	-1.45566	1.68589
O	1.40128	-0.64607	2.55542
H	3.56837	3.42424	1.68605
H	1.99882	1.59289	1.29134
H	2.55082	-3.96739	-1.10536
H	0.06507	-3.75742	-0.70277

H	5.87082	3.35035	0.72865
H	4.65879	-2.83071	-1.63083
H	6.16940	-0.89023	-1.39808
H	6.60344	1.36182	-0.54784
N	-3.83998	-1.29522	0.28568

One imaginary frequency: -350.26 cm^{-1}

C-29

C	3.14779	0.83070	0.34658
C	4.16823	-0.16988	0.39646
C	3.91931	-1.46170	0.04174
C	1.83497	0.47551	-0.02265
H	5.15893	0.12598	0.73094
H	4.69498	-2.21978	0.10393
C	2.58422	3.20682	0.48868
C	3.49011	2.20308	0.62063
C	0.82107	1.49202	0.06869
C	1.23219	2.85282	0.19793
H	2.84685	4.25043	0.62308
H	4.52102	2.42532	0.88197
C	1.61678	-0.84085	-0.57020
C	2.64146	-1.81900	-0.48236
C	0.22514	-2.28847	-1.68501
C	2.35483	-3.11261	-0.97498
C	1.13874	-3.35987	-1.56389
H	3.11033	-3.89030	-0.89488
H	0.88408	-4.33912	-1.95415
C	-2.07496	3.45653	-0.43954
H	-2.09797	4.53501	-0.52016
N	0.22147	3.71715	0.06034
C	-3.10820	2.61504	-0.66745
N	-0.85004	2.93128	-0.10511
H	-4.06769	3.01408	-0.97613
C	-2.96765	1.20946	-0.41989
C	-0.59101	1.57106	-0.02458
C	-4.08805	0.33670	-0.58130
C	-1.73807	0.69774	0.03084
H	-5.00863	0.74821	-0.98529
C	-3.99929	-0.98043	-0.25177
C	-1.71131	-0.63157	0.59197
C	-2.82352	-1.48883	0.38285
H	-4.84057	-1.65016	-0.40744
C	-2.77465	-2.82134	0.86162
H	-0.72754	-2.43865	-2.19023
C	-0.65772	-1.09367	1.41836
C	-0.64763	-2.38054	1.90427
H	0.14969	-0.41802	1.67532
C	-1.69869	-3.26991	1.59165
H	-3.61939	-3.47590	0.66322
H	-1.67334	-4.29112	1.95854
H	0.17365	-2.71165	2.53212
N	0.44731	-1.08230	-1.21133

S-29

C	2.31579	-1.83523	-0.42447
C	3.50586	-2.62235	-0.54710
C	4.73737	-2.07449	-0.37137
C	2.40644	-0.46516	-0.12079
H	3.40119	-3.67639	-0.78882
H	5.63692	-2.67631	-0.46927
C	-0.13216	-1.79508	-0.50541
C	1.04357	-2.46801	-0.63843
C	1.16202	0.26419	-0.04173
C	-0.09457	-0.41343	-0.15774
H	-1.07083	-2.29723	-0.70557
H	1.03918	-3.51643	-0.92165
C	3.70865	0.12391	0.08301
C	4.86719	-0.68998	-0.04907
C	4.98651	1.96281	0.59016
C	6.12814	-0.08741	0.15213
C	6.19775	1.24658	0.47054
H	5.00753	3.01934	0.85172
H	7.02634	-0.69193	0.05312
H	7.14667	1.74594	0.63278
C	-0.86129	3.02719	-0.01749
H	-0.14036	3.83048	0.05486
N	1.00335	1.58909	0.08233
C	-2.19051	3.15962	-0.22223
N	-0.32197	1.76552	0.05548
H	-2.62074	4.14877	-0.32973
C	-3.04448	2.00680	-0.25546
C	-1.06689	0.60420	-0.03336
C	-4.44628	2.16191	-0.48466
C	-2.50283	0.72629	-0.04480
H	-4.82766	3.15828	-0.68895
C	-5.28062	1.08749	-0.47241
C	-3.40722	-0.37965	0.17303
C	-4.79096	-0.20359	-0.10308
H	-6.33999	1.20372	-0.68275
C	-2.99807	-1.60049	0.76327
C	-5.68082	-1.29087	0.07144
C	-3.88944	-2.63199	0.95869
C	-5.23956	-2.49223	0.57507

H	-5.93259	-3.31549	0.71508
H	-3.55329	-3.55061	1.42913
H	-6.72976	-1.14683	-0.17322
H	-1.97925	-1.70086	1.11587
N	3.79505	1.43675	0.40805

1p + 38a → C-32

TS1 C-32

C	-2.10862	2.16271	0.52349
C	-3.45520	1.92957	0.97665
C	-4.08017	0.74365	0.75280
C	-1.44562	1.10824	-0.17814
H	-3.96902	2.72461	1.51010
H	-5.09505	0.58481	1.10761
C	-0.14348	3.66070	0.37928
C	-1.45307	3.40312	0.77592
C	-0.12525	1.43726	-0.52551
C	0.39272	2.55086	-0.26844
H	0.35337	4.60625	0.56150
H	-2.00716	4.17707	1.30171
C	-2.11531	-0.14013	-0.44027
C	-3.43367	-0.32527	0.04077
C	-2.13633	-2.36640	-1.38819
C	-4.08164	-1.55792	-0.20115
C	-3.44422	-2.56272	-0.89855
H	-1.64313	-3.15164	-1.95299
H	-5.09389	-1.70043	0.16815
H	-3.95349	-3.50402	-1.08072
C	2.59862	1.06791	1.60285
H	2.87578	2.02198	2.03057
N	2.72417	2.12471	-0.50066
C	2.26714	-0.05077	2.27972
N	2.57999	1.02707	0.21429
H	2.27697	-0.03094	3.36428
O	2.63437	1.69273	-1.79407
C	1.90654	-1.26682	1.59635
C	2.17302	-0.04949	-0.48916
C	2.22287	0.36223	-1.88241
C	1.57213	-2.45731	2.26225
C	1.87561	-1.27753	0.18073
H	1.57894	-2.48960	3.34824
O	2.03146	-0.19039	-2.92785
C	1.23314	-3.56604	1.51467
C	1.24351	-3.46135	0.11089
H	0.96191	-4.50357	1.98616
H	0.98284	-4.32320	-0.49874
N	1.55512	-2.35950	-0.55034
C	-1.48377	-1.17211	-1.16657
H	-0.48348	-1.01036	-1.56138

One imaginary frequency: -140.35 cm^{-1}

TS1 S-32

C	-2.03600	2.05915	0.33219
C	-3.29648	2.71730	0.11027
C	-4.41716	2.01364	-0.19795
C	-1.99660	0.63342	0.21774
H	-3.33738	3.79970	0.19472
H	-5.35963	2.52908	-0.36219
C	0.37218	2.21651	0.87317
C	-0.86663	2.80783	0.65552
C	-0.70384	0.14748	0.44470
C	0.31409	0.82643	0.72781
H	1.25533	2.79020	1.13146
H	-0.96122	3.88792	0.73797
C	-3.18436	-0.11722	-0.09941
C	-4.39731	0.58102	-0.31104
C	-4.31355	-2.21954	-0.50502
C	-5.56295	-0.15427	-0.62543
C	-5.52363	-1.52876	-0.72221
H	-4.29118	-3.30250	-0.57448
H	-6.49390	0.38270	-0.78729
H	-6.42576	-2.08279	-0.96189
C	1.33678	-1.45734	-1.66251
H	0.52147	-1.96656	-2.15896
N	0.33059	-2.10202	0.36639
C	2.32519	-0.75626	-2.25242
N	1.33651	-1.55541	-0.27585
H	2.34241	-0.67999	-3.33433
O	0.68965	-2.02925	1.68139
C	3.35968	-0.11265	-1.47913
C	2.19864	-0.87767	0.51684
C	1.82990	-1.24387	1.87672
C	4.42639	0.59381	-2.05569
C	3.30621	-0.17797	-0.06577
H	4.50434	0.66777	-3.13691
O	2.29042	-1.03625	2.96088
C	5.35863	1.18763	-1.22802
C	5.19897	1.06248	0.16388
H	6.19781	1.74346	-1.63026
H	5.91714	1.52397	0.83723
C	-3.16233	-1.52532	-0.19809
H	-2.22487	-2.04482	-0.01927

N	4.20718	0.40326	0.74221

One imaginary frequency: -139.90 cm^{-1}

int1 C-32

C	1.82098	-2.19762	-0.47965
C	3.19207	-2.10569	-0.91565
C	3.87494	-0.93883	-0.84956
C	1.16391	-1.02133	-0.00039
H	3.65848	-2.99877	-1.32183
H	4.89758	-0.87422	-1.21088
C	-0.19406	-3.54617	-0.22107
C	1.14339	-3.43033	-0.56429
C	-0.22730	-1.12501	0.17973
C	-0.83702	-2.36696	0.11935
H	-0.72964	-4.48803	-0.25577
H	1.69428	-4.30015	-0.91020
C	1.96353	0.16641	0.25609
C	3.29376	0.22286	-0.22843
C	2.25930	2.35307	1.26314
C	4.05755	1.38926	-0.01837
C	3.54293	2.45029	0.70011
H	1.87185	3.15498	1.88380
H	5.07050	1.42836	-0.40994
H	4.14238	3.34055	0.86201
C	-2.54804	-0.89435	-1.63522
H	-2.95487	-1.77021	-2.12827
N	-2.27999	-2.21705	0.35633
C	-2.16499	0.23169	-2.25853
N	-2.52217	-0.93953	-0.24042
H	-2.25812	0.32517	-3.33382
O	-2.37636	-1.82192	1.75365
C	-1.77145	1.39344	-1.45995
C	-1.44861	-0.17390	0.42229
C	-1.85646	-0.54446	1.85618
C	-1.74192	2.69178	-1.97466
C	-1.49364	1.24656	-0.08431
H	-1.93499	2.85754	-3.03099
O	-1.75523	0.03347	2.89095
C	-1.49456	3.75794	-1.11941
C	-1.30222	3.49517	0.23567
H	-1.46988	4.77784	-1.48722
H	-1.14395	4.30449	0.94317
N	-1.29105	2.26152	0.74485
C	1.48996	1.22417	1.05484
H	0.52948	1.14762	1.55041

int1 S-32

C	-1.74773	1.98439	0.16492
C	-2.97268	2.72751	0.03062
C	-4.15406	2.09870	-0.16818
C	-1.78296	0.55767	0.07479
H	-2.92394	3.81085	0.09226
H	-5.07327	2.66864	-0.27186
C	0.67691	2.02510	0.50911
C	-0.53745	2.67948	0.38121
C	-0.52540	-0.05333	0.16948
C	0.64901	0.64250	0.37330
H	1.60408	2.55817	0.69256
H	-0.57729	3.76310	0.44677
C	-3.06020	-0.12280	-0.10404
C	-4.23334	0.66367	-0.23413
C	-4.42300	-2.12453	-0.31589
C	-5.48234	0.03229	-0.41594
C	-5.58124	-1.34178	-0.45988
H	-4.49564	-3.20716	-0.33660
H	-6.36897	0.65262	-0.51560
H	-6.54724	-1.81709	-0.59700
C	1.32709	-1.31497	-1.80543
H	0.57303	-1.76820	-2.43922
N	-0.17741	-1.49270	0.10113
C	2.45275	-0.72984	-2.25061
N	1.14664	-1.47263	-0.43546
H	2.66303	-0.69163	-3.31275
O	0.16809	-1.81682	1.48319
C	3.44110	-0.20274	-1.30515
C	1.72279	-0.44923	0.44855
C	1.37426	-1.18887	1.75511
C	4.71770	0.21562	-1.68566
C	3.12052	-0.08069	0.06396
H	5.02384	0.14131	-2.72563
O	1.92377	-1.27444	2.80482
C	5.58246	0.72597	-0.72325
C	5.14060	0.82063	0.59472
H	6.58123	1.05551	-0.98795
H	5.78348	1.22755	1.37006
C	-3.18861	-1.53026	-0.14033
H	-2.31074	-2.15206	-0.02645
N	3.92170	0.43410	0.98627

TS2 C-32

C	-2.21623	-1.91154	-0.65572

C	-3.52547	-1.63186	-1.19261
C	-4.04820	-0.38426	-1.16123
C	-1.42809	-0.83066	-0.14499
H	-4.07530	-2.45345	-1.64295
H	-5.02178	-0.17910	-1.59771
C	-0.45869	-3.53671	-0.21090
C	-1.73196	-3.23370	-0.66394
C	-0.06870	-1.12182	0.08573
C	0.33687	-2.45237	0.11734
H	-0.07416	-4.54893	-0.16494
H	-2.38439	-4.02197	-1.02799
C	-2.09788	0.43712	0.11255
C	-3.37467	0.67496	-0.45557
C	-2.23954	2.56691	1.26199
C	-4.01636	1.90850	-0.22589
C	-3.44886	2.85250	0.60781
H	-1.82339	3.27366	1.97306
H	-4.98425	2.08857	-0.68585
H	-3.95748	3.79407	0.78997
C	3.21875	-1.25851	-1.07888
H	3.73438	-2.17998	-1.32229
N	1.76508	-2.52833	0.44641
C	3.48915	-0.04251	-1.59014
N	2.19688	-1.38343	-0.18960
H	4.28381	0.09073	-2.31193
O	1.81464	-2.06165	1.87175
C	2.74442	1.11010	-1.10444
C	1.29310	-0.37330	0.34564
C	1.51864	-0.72447	1.84662
C	3.06831	2.40692	-1.52683
C	1.70675	0.99977	-0.14432
H	3.85069	2.53872	-2.26926
O	1.45130	-0.03732	2.81990
C	2.40998	3.50161	-0.99109
C	1.44128	3.27405	-0.01487
H	2.64825	4.51154	-1.30649
H	0.91281	4.09882	0.45619
N	1.10734	2.05321	0.39529
C	-1.58126	1.37454	1.02483
H	-0.66984	1.15735	1.56579

One imaginary frequency: -102.97 cm^{-1}

TS2 S-32

C	-1.87538	2.00068	-0.18532
C	-3.13203	2.66421	-0.41277
C	-4.28741	1.96542	-0.49677
C	-1.85078	0.57618	-0.06093
H	-3.12835	3.74544	-0.51638
H	-5.23068	2.47523	-0.67217
C	0.54711	2.19609	0.12707
C	-0.69565	2.77051	-0.08637
C	-0.56655	0.03966	0.09743
C	0.58101	0.80859	0.18708
H	1.45134	2.78572	0.23161
H	-0.78307	3.84932	-0.17939
C	-3.10006	-0.17432	-0.11199
C	-4.30658	0.53526	-0.34127
C	-4.38084	-2.23720	0.01100
C	-5.52985	-0.16579	-0.40303
C	-5.57210	-1.53298	-0.23306
H	-4.40833	-3.31192	0.15946
H	-6.44248	0.39626	-0.58198
H	-6.51881	-2.06158	-0.27939
C	1.64073	-1.99198	-1.36845
H	1.00105	-2.73541	-1.82962
N	-0.16164	-1.38055	0.24221
C	2.89472	-1.68609	-1.76458
N	1.12645	-1.35812	-0.27726
H	3.34059	-2.20196	-2.60484
O	0.18238	-1.45468	1.69458
C	3.66502	-0.67111	-1.04785
C	1.69178	-0.21740	0.41880
C	1.35240	-0.74123	1.84666
C	4.98480	-0.34905	-1.38682
C	3.10527	0.06336	0.02172
H	5.47466	-0.88210	-2.19714
O	1.91856	-0.62002	2.88654
C	5.65206	0.64950	-0.69035
C	4.97935	1.32461	0.32786
H	6.67547	0.91244	-0.93500
H	5.46307	2.12280	0.88356
C	-3.17071	-1.57413	0.07199
H	-2.26786	-2.13658	0.26751
N	3.72204	1.04199	0.67567

One imaginary frequency: -107.13 cm^{-1}

int2 C-32

C	-2.49224	-1.80639	0.00546
C	-3.85773	-1.50896	0.35699
C	-4.28736	-0.23281	0.49389
C	-1.56101	-0.73275	-0.14178
H	-4.53014	-2.34357	0.53392

H	-5.30909	-0.01993	0.79568
C	-0.79284	-3.48954	-0.45646
C	-2.09968	-3.15207	-0.16078
C	-0.20127	-1.10642	-0.24815
C	0.11546	-2.44090	-0.47765
H	-0.46979	-4.51178	-0.61581
H	-2.85542	-3.92592	-0.06356
C	-2.09112	0.61874	-0.24346
C	-3.43174	0.86871	0.14122
C	-1.89854	2.93353	-0.95565
C	-3.94533	2.18046	0.06486
C	-3.18508	3.20563	-0.45947
H	-1.32346	3.71916	-1.43568
H	-4.96595	2.36145	0.39082
H	-3.59456	4.20844	-0.52900
C	3.29244	-1.07976	-1.20670
H	3.84948	-1.91139	-1.62221
N	1.56260	-2.60458	-0.55772
C	3.79046	0.14779	-0.99297
N	1.93526	-1.32654	-0.99743
H	4.82021	0.36730	-1.24936
O	1.93597	-2.54127	0.92528
C	2.96551	1.20129	-0.40097
C	1.20213	-0.50889	-0.01763
C	1.66626	-1.27316	1.29568
C	3.43002	2.50455	-0.20437
C	1.67283	0.91140	0.07979
H	4.41567	2.78488	-0.56578
O	1.80241	-0.83258	2.39755
C	2.63407	3.41868	0.47472
C	1.39837	2.99495	0.96188
H	2.97050	4.43518	0.64694
H	0.75872	3.66767	1.52680
N	0.92926	1.76021	0.77595
C	-1.36782	1.66326	-0.85158
H	-0.39769	1.45166	-1.28246

int2 S-32

C	-2.03263	2.00637	-0.08253
C	-3.33189	2.61784	-0.17398
C	-4.45467	1.86732	-0.25016
C	-1.92890	0.58090	-0.08262
H	-3.38715	3.70261	-0.18092
H	-5.43135	2.33792	-0.32138
C	0.39353	2.31423	0.09574
C	-0.88867	2.82961	0.00761
C	-0.61160	0.10568	-0.03556
C	0.50252	0.92840	0.05241
H	1.27334	2.93989	0.18365
H	-1.03705	3.90581	0.01080
C	-3.14011	-0.23002	-0.13868
C	-4.39239	0.43035	-0.22861
C	-4.30810	-2.36263	-0.15298
C	-5.58132	-0.32772	-0.28832
C	-5.54593	-1.70498	-0.25326
H	-4.27316	-3.44674	-0.11583
H	-6.52969	0.19811	-0.35893
H	-6.46655	-2.27802	-0.29753
C	1.90522	-2.27718	-0.78350
H	1.37854	-3.20675	-0.96464
N	-0.13773	-1.28812	-0.00960
C	3.24196	-2.14244	-0.77156
N	1.09794	-1.13866	-0.65640
H	3.87328	-3.00321	-0.95887
O	0.30212	-1.44568	1.44968
C	3.86445	-0.82942	-0.57874
C	1.65186	-0.04421	0.15719
C	1.41439	-0.68449	1.57198
C	5.21847	-0.57559	-0.79983
C	3.07618	0.26047	-0.15970
H	5.87636	-1.37792	-1.12233
O	2.05507	-0.55531	2.57265
C	5.70671	0.71214	-0.60470
C	4.82589	1.71189	-0.19762
H	6.75390	0.94307	-0.76570
H	5.17471	2.72865	-0.04117
C	-3.13056	-1.64310	-0.09655
H	-2.18961	-2.17001	-0.01659
N	3.52556	1.49451	0.02811

TS3 C-32

C	-2.48071	-1.80540	0.00912
C	-3.84267	-1.51318	0.37413
C	-4.27650	-0.23770	0.51037
C	-1.55697	-0.72927	-0.15335
H	-4.50979	-2.34973	0.56144
H	-5.29596	-0.02837	0.82222
C	-0.78420	-3.48619	-0.47286
C	-2.08487	-3.15269	-0.15830
C	-0.19580	-1.09787	-0.28000
C	0.12187	-2.43196	-0.51632
H	-0.45859	-4.50777	-0.63093

H	-2.83713	-3.92810	-0.04799
C	-2.09201	0.61954	-0.25180
C	-3.42980	0.86570	0.14541
C	-1.91514	2.93298	-0.97189
C	-3.94952	2.17546	0.07022
C	-3.19852	3.20158	-0.46462
H	-1.34780	3.71977	-1.45921
H	-4.96750	2.35340	0.40592
H	-3.61243	4.20261	-0.53344
C	3.31467	-1.10320	-1.18030
H	3.87168	-1.94253	-1.57886
N	1.55233	-2.59550	-0.61378
C	3.81107	0.12453	-0.96601
N	1.95625	-1.34334	-0.97361
H	4.84704	0.33657	-1.20345
O	1.89500	-2.52925	1.01707
C	2.98378	1.18342	-0.39056
C	1.19751	-0.50827	-0.03808
C	1.63652	-1.27704	1.32521
C	3.45856	2.48187	-0.18459
C	1.67805	0.90495	0.06145
H	4.45561	2.75045	-0.52296
O	1.73015	-0.74881	2.39981
C	2.65698	3.40498	0.47392
C	1.40380	2.99495	0.92872
H	3.00002	4.41780	0.65426
H	0.75704	3.67632	1.47509
N	0.92561	1.76602	0.73380
C	-1.37812	1.66561	-0.86904
H	-0.41051	1.45686	-1.30695

One imaginary frequency: -358.63 cm^{-1}

TS3 S-32

C	-2.03720	2.00079	-0.09393
C	-3.33715	2.61058	-0.17864
C	-4.45913	1.85792	-0.25197
C	-1.93092	0.57730	-0.10069
H	-3.39436	3.69524	-0.18362
H	-5.43691	2.32673	-0.31949
C	0.39022	2.31572	0.07754
C	-0.89305	2.82672	-0.00340
C	-0.60903	0.10403	-0.07870
C	0.50415	0.93009	0.01530
H	1.26806	2.94284	0.17349
H	-1.04490	3.90243	0.00796
C	-3.13942	-0.23586	-0.14233
C	-4.39386	0.42170	-0.22752
C	-4.30324	-2.37064	-0.12939
C	-5.58170	-0.33940	-0.27550
C	-5.54301	-1.71602	-0.23043
H	-4.26647	-3.45418	-0.08012
H	-6.53160	0.18396	-0.34358
H	-6.46260	-2.29136	-0.26517
C	1.89752	-2.29456	-0.76489
H	1.36698	-3.22415	-0.93158
N	-0.14332	-1.27534	-0.07540
C	3.23380	-2.15636	-0.75566
N	1.09472	-1.15464	-0.63523
H	3.86450	-3.02069	-0.92856
O	0.31220	-1.39741	1.53132
C	3.85817	-0.84462	-0.57047
C	1.64441	-0.03700	0.13548
C	1.39947	-0.65346	1.59544
C	5.21684	-0.60163	-0.77855
C	3.07017	0.25357	-0.17344
H	5.87387	-1.41201	-1.08218
O	2.09932	-0.45094	2.55196
C	5.70948	0.68503	-0.59386
C	4.82791	1.69499	-0.21144
H	6.75980	0.90867	-0.74408
H	5.18081	2.71191	-0.06499
C	-3.12694	-1.64887	-0.08553
H	-2.18549	-2.17383	0.00050
N	3.52449	1.48869	0.00071

One imaginary frequency: -358.43 cm^{-1}

C-32

C	2.38968	1.66877	0.40398
C	3.70094	1.21321	0.74547
C	4.03367	-0.10427	0.66852
C	1.39623	0.73454	0.04874
H	4.43000	1.94812	1.07612
H	5.02424	-0.44652	0.95496
C	0.92562	3.59406	0.00547
C	2.12880	3.08651	0.37674
C	0.05675	1.25545	-0.09392
C	-0.13769	2.66676	-0.20759
H	0.73654	4.65874	-0.07350
H	2.95327	3.75281	0.61573
C	1.80466	-0.61940	-0.24380

C	3.11107	-1.04621	0.11917
C	1.42917	-2.78425	-1.29010
C	3.51098	-2.37880	-0.14868
C	2.68314	-3.24002	-0.82944
H	4.50231	-2.69605	0.16406
H	3.00594	-4.25368	-1.04568
C	-3.43465	1.76890	-0.54343
H	-3.90173	2.71163	-0.79584
N	-1.41823	3.00285	-0.41213
C	-4.06963	0.59025	-0.37690
N	-2.06714	1.83813	-0.37101
H	-5.14332	0.53158	-0.51369
C	-3.33354	-0.57179	0.04742
C	-1.25701	0.74367	-0.12687
C	-3.95845	-1.78749	0.37556
C	-1.92731	-0.49184	0.21223
H	-5.03328	-1.88647	0.24925
C	-3.19961	-2.82766	0.87115
C	-1.82031	-2.62022	1.04834
H	-3.64789	-3.77775	1.13926
H	-1.19593	-3.40641	1.46711
H	0.80129	-3.43947	-1.88608
C	1.00303	-1.50870	-0.99997
H	0.05417	-1.16075	-1.38879
N	-1.20018	-1.49593	0.73523

S-32

C	-1.87755	1.89413	-0.00001
C	-3.16741	2.51375	-0.00001
C	-4.30576	1.77197	-0.00000
C	-1.78015	0.48853	0.00000
H	-3.21611	3.59915	-0.00001
H	-5.28090	2.25163	-0.00000
C	0.55217	2.24497	-0.00001
C	-0.71364	2.74336	-0.00001
C	-0.43645	-0.04174	0.00000
C	0.69322	0.83107	-0.00001
H	1.43097	2.87885	-0.00002
H	-0.87749	3.81716	-0.00002
C	-2.98393	-0.31322	0.00001
C	-4.24633	0.34439	0.00001
C	-4.15304	-2.44905	0.00002
C	-5.43883	-0.41763	0.00001
C	-5.40003	-1.79207	0.00002
H	-4.11722	-3.53421	0.00003
H	-6.38970	0.10893	0.00001
H	-6.32024	-2.36774	0.00003
C	2.05647	-2.43346	0.00001
H	1.50097	-3.36190	0.00002
N	-0.05772	-1.33462	0.00001
C	3.40322	-2.32017	0.00001
N	1.27905	-1.29405	0.00000
H	4.01515	-3.21497	0.00001
C	4.03267	-1.02357	-0.00000
C	1.79964	-0.02261	-0.00000
C	5.42673	-0.84180	-0.00001
C	3.22575	0.14006	-0.00001
H	6.08214	-1.70864	-0.00000
C	5.93868	0.43935	-0.00002
C	5.04128	1.52338	-0.00002
H	7.00761	0.62024	-0.00002
H	5.42038	2.54256	-0.00003
N	3.72527	1.39214	-0.00002
C	-2.97548	-1.73299	0.00002
H	-2.02912	-2.25523	0.00002

1p + 38c → C-33

TS1 C-33

C	-2.92805	-1.49933	-0.37512
C	-4.25144	-0.93554	-0.42982
C	-4.46198	0.39375	-0.24040
C	-1.83173	-0.62302	-0.10633
H	-5.09063	-1.59689	-0.62629
H	-5.46722	0.80415	-0.28292
C	-1.45437	-3.47997	-0.53990
C	-2.71638	-2.89479	-0.58243
C	-0.60229	-1.29232	-0.06284
C	-0.48299	-2.51936	-0.26928
H	-1.29129	-4.53932	-0.69826
H	-3.58304	-3.52015	-0.78231
C	-2.04905	0.78808	0.08221
C	-3.37014	1.29053	0.01609
C	-1.17544	2.86418	0.47573
C	-3.54821	2.67730	0.20514
C	-2.44902	3.47157	0.43691
H	-0.28801	3.46972	0.65201
H	-4.54909	3.09948	0.16454
H	-2.54447	4.54137	0.58704
C	2.45002	-1.49209	-1.70924
H	2.46672	-2.38435	-2.32008
N	1.95932	-2.89651	0.13263
C	2.61800	-0.22085	-2.13594

N	2.23068	-1.70438	-0.35406
H	2.79363	-0.04811	-3.19265
O	1.79355	-2.67095	1.47731
C	2.57724	0.90352	-1.23541
C	2.09161	-0.68937	0.52043
C	1.82077	-1.32299	1.79139
C	2.78345	2.22760	-1.66747
C	2.31482	0.66103	0.13290
H	2.98133	2.41935	-2.71831
O	1.67779	-0.89876	2.90998
C	2.73754	3.26720	-0.75918
C	2.26045	1.72485	1.05295
C	2.47957	3.01160	0.60223
H	2.90240	4.28608	-1.09413
H	2.04057	1.51032	2.09382
H	2.44965	3.83842	1.30547
N	-0.97078	1.57347	0.30686

One imaginary frequency: -74.49 cm^{-1}

TS1 S-33

C	-2.64378	1.88725	-0.83527
C	-4.04748	1.92017	-1.15024
C	-4.85635	0.85889	-0.89500
C	-2.12104	0.70296	-0.22457
H	-4.45636	2.82297	-1.59499
H	-5.91675	0.90416	-1.12715
C	-0.43487	2.99291	-0.84483
C	-1.79612	2.99484	-1.12586
C	-0.77296	0.87868	0.06428
C	0.00547	1.82832	-0.19084
H	0.19748	3.83560	-1.10359
H	-2.24307	3.86717	-1.59658
C	-2.95528	-0.45390	-0.02435
C	-4.33276	-0.35640	-0.33717
C	-3.16788	-2.63782	0.63049
C	-5.13563	-1.49188	-0.10347
C	-4.55766	-2.63746	0.39370
H	-2.68294	-3.54018	0.99818
H	-6.19916	-1.44889	-0.32385
H	-5.14203	-3.52970	0.58904
C	1.00392	-1.80560	-0.03606
H	0.03389	-2.28471	0.02581
N	0.24392	-0.41846	1.72379
C	2.00031	-2.05622	-0.91354
N	1.19784	-0.78163	0.88392
H	1.86552	-2.85171	-1.63895
O	0.80546	0.60906	2.42966
C	3.22625	-1.29607	-0.92209
C	2.28165	0.01230	0.88426
C	2.04818	0.97444	1.93744
C	4.27767	-1.56720	-1.81790
C	3.36909	-0.22938	-0.00083
H	4.17346	-2.38400	-2.52653
O	2.71690	1.86268	2.40388
C	5.42596	-0.79901	-1.79447
C	4.54118	0.55130	0.01624
C	5.55468	0.26104	-0.87634
H	6.23327	-1.01155	-2.48743
H	4.62162	1.36454	0.73053
H	6.46157	0.85690	-0.87046
N	-2.38470	-1.59524	0.42889

One imaginary frequency: -103.95 cm^{-1}

int1 C-33

C	-2.45185	-1.60702	-0.43459
C	-3.79449	-1.15381	-0.69936
C	-4.14257	0.14854	-0.57238
C	-1.44992	-0.66127	-0.05898
H	-4.52817	-1.89289	-1.00834
H	-5.15646	0.47835	-0.78099
C	-0.87306	-3.45423	-0.31632
C	-2.15003	-2.97954	-0.55388
C	-0.13398	-1.14140	0.08558
C	0.09038	-2.50351	-0.01273
H	-0.61766	-4.50622	-0.37686
H	-2.94593	-3.66432	-0.83138
C	-1.85327	0.71799	0.15344
C	-3.18070	1.11761	-0.12538
C	-1.27140	2.82844	0.83363
C	-3.51265	2.47081	0.08439
C	-2.55447	3.33902	0.55861
H	-0.49005	3.47903	1.22345
H	-4.52390	2.81006	-0.12453
H	-2.77382	4.38669	0.73176
C	2.20152	-1.47813	-1.68899
H	2.33780	-2.39842	-2.24576
N	1.51127	-2.78840	0.21873
C	2.19768	-0.24481	-2.22020
N	2.12815	-1.60671	-0.29727
H	2.34339	-0.10951	-3.28557
O	1.68398	-2.51378	1.64214
C	2.16296	0.92698	-1.33744

C	1.30736	-0.59529	0.39324
C	1.55776	-1.15164	1.80370
C	2.57285	2.19118	-1.78150
C	1.80099	0.76987	0.01315
H	2.84427	2.32430	-2.82517
O	1.63381	-0.61356	2.86550
C	2.66847	3.25431	-0.89147
C	1.92585	1.82584	0.91033
C	2.36774	3.06651	0.45969
H	2.99811	4.22630	-1.24521
H	1.65674	1.67237	1.94990
H	2.47227	3.88919	1.16040
N	-0.93514	1.56727	0.64738

int1 S-33

C	-1.76980	1.97208	0.22995
C	-3.00129	2.71397	0.13872
C	-4.18593	2.09177	-0.06970
C	-1.79720	0.55284	0.07915
H	-2.95595	3.79408	0.24412
H	-5.10902	2.66083	-0.13719
C	0.65187	1.98673	0.56420
C	-0.55725	2.65604	0.46714
C	-0.54993	-0.07997	0.14080
C	0.62221	0.60930	0.37750
H	1.58388	2.50998	0.75476
H	-0.58973	3.73661	0.57339
C	-3.07386	-0.11748	-0.11426
C	-4.25283	0.66119	-0.19338
C	-4.24765	-2.06800	-0.37014
C	-5.47379	-0.01658	-0.38206
C	-5.47794	-1.38986	-0.47386
H	-4.21665	-3.15375	-0.42799
H	-6.39605	0.55487	-0.44796
H	-6.39759	-1.94668	-0.61563
C	1.30573	-1.16418	-1.88445
H	0.56201	-1.57713	-2.55679
N	-0.20312	-1.51479	-0.00839
C	2.41065	-0.50292	-2.27213
N	1.13172	-1.45565	-0.53120
H	2.60984	-0.35800	-3.32752
O	0.13835	-1.90203	1.36456
C	3.41148	-0.06556	-1.28982
C	1.69821	-0.48578	0.41190
C	1.32213	-1.27937	1.67273
C	4.68321	0.37309	-1.66999
C	3.10396	-0.11017	0.08625
H	4.94011	0.40761	-2.72518
O	1.86577	-1.37761	2.73137
C	5.61859	0.75396	-0.70962
C	4.03395	0.26845	1.04697
C	5.30019	0.69939	0.64600
H	6.60233	1.09007	-1.02200
H	3.76963	0.21158	2.09856
H	6.03358	0.98880	1.39132
N	-3.08825	-1.46318	-0.19768

TS2 C-33

C	-2.75204	-1.44386	-0.26178
C	-4.10185	-0.94115	-0.31753
C	-4.37288	0.38280	-0.24979
C	-1.65783	-0.53597	-0.11068
H	-4.90635	-1.66428	-0.41631
H	-5.39511	0.74810	-0.29131
C	-1.27257	-3.36899	-0.33390
C	-2.54527	-2.83485	-0.36233
C	-0.35722	-1.08772	-0.06190
C	-0.22898	-2.46688	-0.19518
H	-1.07862	-4.43270	-0.41230
H	-3.40987	-3.48236	-0.47282
C	-1.96157	0.88654	-0.07631
C	-3.30268	1.33322	-0.14145
C	-1.16755	3.03907	0.00245
C	-3.53147	2.72342	-0.11922
C	-2.46241	3.58863	-0.04798
H	-0.29077	3.68324	0.05701
H	-4.55209	3.09444	-0.16482
H	-2.60192	4.66385	-0.03372
C	2.77359	-1.58267	-1.51079
H	3.06614	-2.49886	-2.00968
N	1.18076	-2.85860	-0.11616
C	3.26908	-0.35537	-1.75278
N	1.77999	-1.71207	-0.58087
H	4.03363	-0.21481	-2.50577
O	1.43447	-2.71125	1.37015
C	2.86082	0.77116	-0.91530
C	1.14502	-0.67783	0.21340
C	1.35597	-1.37460	1.60923
C	3.53714	1.99952	-1.02039
C	1.87007	0.63496	0.08054
H	4.28717	2.11568	-1.79787
O	1.44802	-0.88179	2.69421
C	3.29054	3.03285	-0.13047

C	1.66968	1.65880	1.00781
C	2.37068	2.85366	0.90703
H	3.83373	3.96836	-0.22354
H	0.95407	1.51210	1.80807
H	2.20589	3.64005	1.63688
N	-0.92866	1.74255	-0.01223

One imaginary frequency: -101.29 cm^{-1}

TS2 S-33

C	-1.93328	1.99265	-0.25578
C	-3.20635	2.63125	-0.47298
C	-4.35593	1.91697	-0.51402
C	-1.88119	0.57409	-0.10307
H	-3.22121	3.70974	-0.60113
H	-5.31095	2.40849	-0.67759
C	0.48636	2.20967	0.02214
C	-0.76049	2.77538	-0.19341
C	-0.59917	0.03689	0.05413
C	0.53946	0.82442	0.12286
H	1.38444	2.81606	0.08327
H	-0.85360	3.85048	-0.31739
C	-3.11993	-0.18907	-0.11607
C	-4.34246	0.49155	-0.32748
C	-4.18436	-2.20777	0.08234
C	-5.52531	-0.27398	-0.33406
C	-5.45261	-1.63328	-0.13010
H	-4.09249	-3.27745	0.25689
H	-6.47955	0.22081	-0.49523
H	-6.34104	-2.25501	-0.12467
C	1.67303	-2.03481	-1.32917
H	1.05835	-2.81460	-1.76310
N	-0.18147	-1.37880	0.20316
C	2.93155	-1.72397	-1.70437
N	1.10171	-1.32716	-0.31264
H	3.41008	-2.27888	-2.50080
O	0.15956	-1.42063	1.67534
C	3.67761	-0.67261	-1.00970
C	1.66174	-0.18827	0.37882
C	1.29478	-0.67880	1.81552
C	5.00988	-0.38835	-1.34259
C	3.08889	0.07516	0.03480
H	5.48202	-0.95253	-2.14217
O	1.84660	-0.47561	2.85624
C	5.72840	0.59056	-0.66496
C	3.81336	1.04579	0.72194
C	5.13614	1.30933	0.37371
H	6.75893	0.78880	-0.94269
H	3.34301	1.57727	1.54507
H	5.70104	2.06222	0.91288
N	-3.05867	-1.52009	0.08991

One imaginary frequency: -117.58 cm^{-1}

int2 C-33

C	-2.68532	-1.59494	-0.01429
C	-4.05037	-1.17701	0.18701
C	-4.39295	0.13133	0.24340
C	-1.64983	-0.61423	-0.08677
H	-4.80520	-1.95041	0.29644
H	-5.42349	0.43361	0.40671
C	-1.11545	-3.41673	-0.36555
C	-2.40366	-2.97153	-0.14447
C	-0.32065	-1.08784	-0.16172
C	-0.12137	-2.44891	-0.36906
H	-0.87072	-4.46324	-0.50682
H	-3.22724	-3.67727	-0.09367
C	-2.04944	0.78174	-0.18583
C	-3.40283	1.14614	0.01381
C	-1.45993	2.94551	-0.67377
C	-3.73711	2.50967	-0.09866
C	-2.76197	3.42280	-0.43578
H	-0.66639	3.62861	-0.97143
H	-4.76601	2.82040	0.06298
H	-2.98487	4.47889	-0.53972
C	3.10155	-1.37304	-1.30300
H	3.55516	-2.25909	-1.73106
N	1.30313	-2.73403	-0.47892
C	3.68630	-0.17193	-1.20145
N	1.75773	-1.50998	-0.95635
H	4.69699	-0.03094	-1.56623
O	1.71381	-2.66976	1.00722
C	3.00317	0.95219	-0.55700
C	1.14137	-0.59823	0.02102
C	1.54235	-1.38074	1.34638
C	3.63844	2.19754	-0.44893
C	1.75257	0.77118	0.06471
H	4.59199	2.34524	-0.94832
O	1.68351	-0.92959	2.44594
C	3.08421	3.21511	0.31597
C	1.24903	1.76402	0.90124
C	1.89941	2.98778	1.01815
H	3.59207	4.17115	0.39616
H	0.34368	1.57529	1.46650

H	1.48950	3.75645	1.66543
N	-1.11648	1.67641	-0.55824

int2 S-33

C	-2.08802	2.00622	-0.15716
C	-3.40068	2.59047	-0.25808
C	-4.51271	1.81948	-0.29766
C	-1.95297	0.58738	-0.11527
H	-3.47615	3.67316	-0.30047
H	-5.49919	2.26830	-0.37402
C	0.33083	2.33372	0.00163
C	-0.95329	2.84182	-0.10276
C	-0.63792	0.11241	-0.06143
C	0.47089	0.94777	0.01194
H	1.18300	3.00036	0.04912
H	-1.10450	3.91672	-0.14134
C	-3.15060	-0.24065	-0.13010
C	-4.41563	0.38699	-0.22684
C	-4.10247	-2.32282	-0.04485
C	-5.55777	-0.43815	-0.23835
C	-5.40728	-1.80321	-0.14889
H	-3.94826	-3.39646	0.03736
H	-6.54233	0.01617	-0.31320
H	-6.26217	-2.47036	-0.15162
C	1.86829	-2.25265	-0.84086
H	1.32682	-3.17139	-1.03276
N	-0.16333	-1.27739	-0.03270
C	3.20339	-2.11990	-0.85977
N	1.07259	-1.11506	-0.66667
H	3.82791	-2.97620	-1.08625
O	0.26510	-1.41430	1.44034
C	3.83969	-0.82133	-0.61676
C	1.63247	-0.02323	0.14405
C	1.36002	-0.64166	1.56726
C	5.20845	-0.62896	-0.82810
C	3.07098	0.25898	-0.13504
H	5.80591	-1.45442	-1.20506
O	1.97729	-0.46859	2.57845
C	5.80601	0.59762	-0.55282
C	3.67805	1.47100	0.17241
C	5.04439	1.64739	-0.04433
H	6.86993	0.72968	-0.72172
H	3.09526	2.27457	0.60891
H	5.51138	2.59682	0.19519
N	-3.01377	-1.57838	-0.03544

TS3 C-33

C	-2.67662	-1.59469	-0.01768
C	-4.04030	-1.17880	0.19321
C	-4.38391	0.12952	0.25239
C	-1.64407	-0.61282	-0.09825
H	-4.79355	-1.95291	0.30820
H	-5.41360	0.43038	0.42357
C	-1.10794	-3.41563	-0.38107
C	-2.39345	-2.97236	-0.14917
C	-0.31409	-1.08432	-0.18545
C	-0.11426	-2.44484	-0.39762
H	-0.86217	-4.46210	-0.52071
H	-3.21572	-3.67900	-0.09057
C	-2.04509	0.78222	-0.19534
C	-3.39721	1.14545	0.01518
C	-1.46218	2.94579	-0.69130
C	-3.73393	2.50867	-0.09550
C	-2.76260	3.42220	-0.44189
H	-0.67234	3.62963	-0.99697
H	-4.76168	2.81855	0.07476
H	-2.98720	4.47803	-0.54477
C	3.11989	-1.38521	-1.28547
H	3.57616	-2.27445	-1.70310
N	1.30007	-2.72910	-0.51657
C	3.69838	-0.18072	-1.18816
N	1.77811	-1.52264	-0.93400
H	4.71153	-0.04004	-1.54638
O	1.68477	-2.66254	1.07391
C	3.01107	0.94387	-0.55138
C	1.13979	-0.60024	0.01208
C	1.51357	-1.38666	1.37158
C	3.64834	2.18833	-0.44050
C	1.75488	0.76455	0.05975
H	4.60674	2.33288	-0.93144
O	1.61705	-0.87671	2.45467
C	3.08883	3.20801	0.31678
C	1.24497	1.76129	0.88877
C	1.89683	2.98346	1.00834
H	3.59742	4.16335	0.40024
H	0.33637	1.57415	1.44872
H	1.48302	3.75388	1.65106
N	-1.11604	1.67735	-0.57757

One imaginary frequency: -301.31 cm^{-1}

TS3 S-33

C	-2.09217	1.99725	-0.17292
C	-3.40620	2.58025	-0.25477
C	-4.51804	1.80791	-0.27739
C	-1.95415	0.57991	-0.13280
H	-3.48351	3.66291	-0.29414
H	-5.50626	2.25550	-0.33633
C	0.32810	2.33275	-0.03909
C	-0.95761	2.83612	-0.13094
C	-0.63517	0.10727	-0.09031
C	0.47286	0.94630	-0.02996
H	1.17826	3.00205	0.00414
H	-1.11260	3.91057	-0.16753
C	-3.14942	-0.25008	-0.14290
C	-4.41714	0.37585	-0.21555
C	-4.09584	-2.33553	-0.07475
C	-5.55797	-0.45164	-0.21851
C	-5.40357	-1.81709	-0.14771
H	-3.93838	-3.41009	-0.01334
H	-6.54436	0.00157	-0.27333
H	-6.25710	-2.48597	-0.14466
C	1.86030	-2.28872	-0.77023
H	1.31532	-3.21192	-0.92517
N	-0.16664	-1.27184	-0.04616
C	3.19449	-2.15191	-0.80582
N	1.06862	-1.14718	-0.61310
H	3.81819	-3.01517	-1.00709
O	0.27621	-1.33275	1.55216
C	3.83210	-0.84860	-0.60237
C	1.62768	-0.01596	0.13083
C	1.35138	-0.57256	1.60807
C	5.20266	-0.66903	-0.81715
C	3.06574	0.24816	-0.15557
H	5.79710	-1.50870	-1.16647
O	2.01678	-0.30741	2.57500
C	5.80437	0.56244	-0.57916
C	3.67818	1.46706	0.11457
C	5.04500	1.63035	-0.10461
H	6.86914	0.68528	-0.74929
H	3.09861	2.28564	0.52622
H	5.51562	2.58453	0.10745
N	-3.00874	-1.58926	-0.07266

One imaginary frequency: -321.44 cm^{-1}

C-33

C	-2.55587	1.48804	-0.41556
C	-3.85708	0.93702	-0.63677
C	-4.10611	-0.39272	-0.48194
C	-1.47235	0.63775	-0.11478
H	-4.65616	1.61441	-0.92566
H	-5.09615	-0.80326	-0.65889
C	-1.21245	3.50819	-0.10533
C	-2.39252	2.91964	-0.42980
C	-0.16961	1.24167	-0.00575
C	-0.08337	2.66274	0.11102
H	-1.09504	4.58455	-0.04301
H	-3.26703	3.52620	-0.64802
C	-1.76774	-0.73629	0.21493
C	-3.07308	-1.25296	-0.00505
C	-1.06424	-2.72020	1.13939
C	-3.31049	-2.60432	0.33179
C	-2.30572	-3.34950	0.90020
H	-4.29564	-3.02895	0.15570
H	-2.45515	-4.38588	1.18230
C	3.23665	1.98879	0.64560
H	3.61905	2.96123	0.92561
N	1.15791	3.08907	0.36657
C	3.94994	0.84771	0.55975
N	1.88690	1.96705	0.35708
H	5.00758	0.85645	0.79768
C	3.33600	-0.35953	0.06886
C	1.17617	0.81758	0.07442
C	4.11077	-1.50622	-0.20195
C	1.95035	-0.36487	-0.23139
H	5.16615	-1.49686	0.05610
C	3.54885	-2.60590	-0.81706
C	1.41458	-1.47029	-0.92276
C	2.19841	-2.57093	-1.20745
H	4.15481	-3.48050	-1.03087
H	1.76902	-3.40939	-1.74656
H	-0.25747	-3.27009	1.62087
H	0.38584	-1.43786	-1.25584
N	-0.80002	-1.47359	0.81182

S-33

C	-1.94220	1.89105	0.00001
C	-3.24460	2.48699	0.00001
C	-4.37130	1.72676	-0.00000
C	-1.80957	0.49007	-0.00000

H	-3.31232	3.57135	0.00001
H	-5.35627	2.18584	-0.00000
C	0.47830	2.26507	0.00001
C	-0.79224	2.75368	0.00001
C	-0.46343	-0.03274	-0.00000
C	0.66147	0.85451	0.00001
H	1.31903	2.94829	0.00002
H	-0.96328	3.82608	0.00002
C	-3.00026	-0.32672	-0.00001
C	-4.27524	0.30256	-0.00001
C	-3.96321	-2.41094	-0.00002
C	-5.42197	-0.52130	-0.00001
C	-5.27443	-1.88657	-0.00002
H	-3.81282	-3.48911	-0.00003
H	-6.40630	-0.05966	-0.00001
H	-6.12998	-2.55307	-0.00003
C	2.02399	-2.40760	-0.00001
H	1.45408	-3.32719	-0.00002
N	-0.07956	-1.31828	-0.00001
C	3.36954	-2.30486	-0.00001
N	1.25708	-1.26078	-0.00001
H	3.97436	-3.20455	-0.00001
C	4.01215	-1.01453	0.00000
C	1.78337	0.00913	0.00000
C	5.41618	-0.89521	0.00001
C	3.21575	0.15902	0.00001
H	6.01773	-1.80002	0.00000
C	6.02041	0.34605	0.00002
C	3.85129	1.41664	0.00002
C	5.22968	1.50817	0.00002
H	7.10250	0.42584	0.00002
H	3.25490	2.32029	0.00002
H	5.70327	2.48453	0.00003
N	-2.87280	-1.67580	-0.00002

1a + 38b → C-36

TS1 C-36

N	2.14760	-1.83838	-0.71635
N	1.72470	-3.03916	-0.36163
O	2.05006	-3.12105	0.97477
C	2.56886	-1.93618	1.46091
C	2.61068	-1.08066	0.29341
O	2.90641	-1.77322	2.60483
C	3.08351	0.23845	0.07156
C	3.67256	1.01247	1.09414
C	2.94866	0.75930	-1.24067
C	4.13758	2.27645	0.79283
C	3.42541	2.05780	-1.51240
C	4.01769	2.80094	-0.51152
H	3.31840	2.46303	-2.51428
H	4.38750	3.79828	-0.72506
C	2.32928	-0.06317	-2.24305
C	1.93487	-1.33341	-1.98819
H	1.46025	-2.01115	-2.68465
H	2.16939	0.33980	-3.23743
C	-0.75699	-1.39924	-0.10133
C	-0.43133	-2.60653	-0.20894
C	-1.17101	-3.78024	-0.28158
C	-2.11619	-1.00365	-0.03386
H	-0.78080	-4.78742	-0.36648
C	-2.52032	-3.47135	-0.22164
C	-3.00742	-2.13226	-0.10937
H	-3.25274	-4.27354	-0.26439
C	-2.64369	0.33827	0.06832
C	-4.41728	-1.90889	-0.08509
C	-4.04639	0.49051	0.05841
C	-4.91037	-0.64485	-0.01127
C	-1.81852	1.53627	0.16959
C	-4.64375	1.79071	0.11196
C	-2.45339	2.81088	0.20992
C	-3.87987	2.90860	0.17331
C	-0.40214	1.52022	0.25323
C	-1.68003	3.99198	0.30198
C	0.32953	2.68474	0.35361
C	-0.30803	3.93919	0.37163
H	-5.08792	-2.76202	-0.13558
H	-5.98303	-0.47199	-0.00390
H	-5.72800	1.85854	0.09644
H	-4.33447	3.89500	0.20659
H	-2.19888	4.94678	0.32611
H	0.12191	0.57379	0.25222
H	1.41070	2.62780	0.43142
H	0.27670	4.85050	0.45003
H	4.59861	2.87692	1.57020
H	3.75305	0.59453	2.09247

One imaginary frequency: - 89.10cm^{-1}

TS1 S-36

N	-1.51618	1.07318	0.76119
N	-0.36006	0.78590	1.33865
O	-0.65993	-0.28565	2.15182

C	-1.90024	-0.82014	1.85764
C	-2.42262	0.07716	0.84164
O	-2.35620	-1.79157	2.40213
C	-3.70439	0.19958	0.22116
C	-4.72241	-0.75162	0.40640
C	-3.89942	1.31189	-0.63080
C	-5.92532	-0.58638	-0.25656
C	-5.13364	1.45446	-1.28980
C	-6.13268	0.51595	-1.10492
H	-5.29149	2.30711	-1.94412
H	-7.08246	0.62988	-1.61684
C	-2.82350	2.26390	-0.78478
C	-1.66303	2.14805	-0.10338
H	-0.82390	2.83058	-0.13651
H	-2.95602	3.11103	-1.44927
C	-0.87342	-1.24124	-0.58949
C	0.22842	-0.66592	-0.37960
C	1.52617	-1.18792	-0.48353
C	-1.00867	-2.58877	-0.96308
C	1.45548	-2.59604	-0.76362
C	0.20796	-3.24688	-1.01381
C	2.79321	-0.53544	-0.29376
C	2.66785	-3.35160	-0.73869
C	3.84973	-2.75556	-0.42089
C	3.93757	-1.34848	-0.18880
C	5.20124	-0.76789	0.15425
C	2.94889	0.90510	-0.21969
C	4.21273	1.44392	0.14418
C	5.32588	0.56886	0.35601
C	4.37956	2.84561	0.24074
C	1.92439	1.81559	-0.57709
C	3.35045	3.70454	-0.06731
C	2.11981	3.17759	-0.50670
H	-1.94827	-3.09422	-1.15892
H	0.23140	-4.31076	-1.23683
H	2.62522	-4.41792	-0.94104
H	4.76095	-3.34358	-0.35469
H	6.05742	-1.42757	0.26486
H	6.28063	1.00225	0.64086
H	5.34915	3.23249	0.54287
H	3.49196	4.77850	-0.00125
H	1.32743	3.85568	-0.81211
H	0.98233	1.42997	-0.94837
H	-6.71819	-1.31442	-0.11971
H	-4.54351	-1.59484	1.06625

One imaginary frequency: -218.47 cm^{-1}

int1 C-36

N	1.61410	2.44840	-0.25635
N	2.92501	1.93360	-0.22747
O	3.03909	1.76285	1.23735
C	1.79499	1.36534	1.66419
C	0.89249	1.36626	0.39930
O	1.54290	1.09337	2.79794
C	-0.54619	1.74025	0.57788
C	-1.33568	1.18435	1.58009
C	-1.08312	2.67618	-0.33105
C	-2.67216	1.55855	1.69708
C	-2.42187	3.05574	-0.18158
C	-3.20960	2.50238	0.82107
H	-2.84533	3.78129	-0.87127
H	-4.24947	2.79969	0.91601
C	-0.25941	3.20319	-1.42197
C	1.07782	3.06090	-1.37598
H	1.78324	3.47186	-2.08903
H	-0.72443	3.76138	-2.22566
C	1.47577	0.09884	-0.34170
C	2.74934	0.53885	-0.64889
C	3.81915	-0.27276	-1.01994
C	1.20043	-1.30036	-0.37024
H	4.78850	0.15423	-1.25084
C	3.59637	-1.62833	-0.95070
C	2.33728	-2.15004	-0.56402
H	4.40688	-2.32751	-1.13464
C	-0.08373	-1.93842	-0.12926
C	2.24397	-3.54329	-0.24525
C	-0.08291	-3.25917	0.35723
C	1.11087	-4.04612	0.30648
C	-1.36169	-1.35337	-0.47669
C	-1.29708	-3.85595	0.82332
C	-2.55808	-1.98128	-0.03254
C	-2.48611	-3.21172	0.69140
C	-1.48031	-0.27052	-1.38142
C	-3.81340	-1.43806	-0.39498
C	-2.71324	0.20479	-1.76519
C	-3.89486	-0.36066	-1.24497
H	3.12609	-4.16310	-0.37570
H	1.06641	-5.07651	0.64759
H	-1.24475	-4.84234	1.27542
H	-3.40678	-3.65955	1.05510
H	-4.71409	-1.91646	-0.01952
H	-0.58461	0.17673	-1.80168
H	-2.77169	1.02832	-2.47038
H	-4.86175	0.03846	-1.53501

H	-3.29047	1.11666	2.47137
H	-0.90186	0.45970	2.26260

int1 S-36

N	-1.34646	-1.29495	0.47576
N	-0.05122	-0.79669	0.83828
O	-0.40719	-0.25903	2.15459
C	-1.69044	0.22334	2.05522
C	-2.10232	-0.04392	0.59870
O	-2.27328	0.74249	2.95813
C	-3.52705	-0.17231	0.17993
C	-4.54721	0.60891	0.70950
C	-3.76906	-1.07589	-0.87520
C	-5.83838	0.49818	0.18974
C	-5.06771	-1.16888	-1.38401
C	-6.09304	-0.38605	-0.85686
H	-5.27351	-1.86498	-2.19249
H	-7.09637	-0.47122	-1.26210
C	-2.67301	-1.91295	-1.37960
C	-1.50521	-1.99832	-0.71828
H	-0.69993	-2.67375	-0.98391
H	-2.84533	-2.53859	-2.24766
C	-1.19788	0.94069	-0.15421
C	0.07141	0.43491	0.01328
C	1.23989	1.12919	-0.36157
C	-1.43150	2.20285	-0.69971
C	0.99952	2.46996	-0.80516
C	-0.31558	2.95475	-1.01069
C	2.60719	0.66188	-0.22814
C	2.10617	3.36976	-0.93452
C	3.35072	2.98644	-0.55084
C	3.62589	1.62959	-0.18394
C	4.95494	1.25466	0.19259
C	2.99125	-0.73341	-0.18576
C	4.31038	-1.07704	0.21549
C	5.26865	-0.04208	0.45213
C	4.68873	-2.43926	0.28720
C	2.15757	-1.77309	-0.66270
C	3.82482	-3.43329	-0.10880
C	2.55947	-3.08835	-0.62721
H	-2.43894	2.58706	-0.82585
H	-0.43038	3.96826	-1.38470
H	1.91336	4.38420	-1.27092
H	4.17509	3.69396	-0.55870
H	5.70439	2.03615	0.28072
H	6.26896	-0.31981	0.77238
H	5.69076	-2.68245	0.63001
H	4.12812	-4.47419	-0.06282
H	1.90661	-3.86476	-1.01451
H	1.20753	-1.51363	-1.11314
H	-6.64080	1.09988	0.60348
H	-4.33129	1.28592	1.53052

TS2 C-36

N	-1.61008	-2.33076	-0.44693
N	-2.91527	-1.87704	-0.37949
O	-3.05898	-1.82371	1.12107
C	-1.83480	-1.42745	1.57936
C	-0.90182	-1.33319	0.32063
O	-1.58431	-1.22216	2.72858
C	0.52388	-1.72542	0.55364
C	1.29345	-1.07123	1.51346
C	1.06542	-2.77978	-0.21296
C	2.62177	-1.43319	1.70918
C	2.40302	-3.13701	0.01135
C	3.17388	-2.47016	0.95413
H	2.83429	-3.94654	-0.57164
H	4.21031	-2.75722	1.10343
C	0.26373	-3.47880	-1.21664
C	-1.06272	-3.25093	-1.29699
H	-1.75608	-3.76007	-1.95601
H	0.72724	-4.22286	-1.85176
C	-1.48506	-0.02273	-0.32984
C	-2.75993	-0.44509	-0.66570
C	-3.82925	0.39197	-0.97443
C	-1.19256	1.36942	-0.32206
H	-4.80342	-0.01456	-1.22108
C	-3.59469	1.74192	-0.83986
C	-2.32189	2.23853	-0.46618
H	-4.40236	2.45450	-0.97932
C	0.11216	1.97721	-0.12412
C	-2.19181	3.62416	-0.12789
C	0.15720	3.29598	0.36509
C	-1.02534	4.10220	0.37500
C	1.36181	1.35863	-0.51493
C	1.40189	3.86856	0.77687
C	2.58722	1.95815	-0.11252
C	2.57012	3.19694	0.60039
C	1.42745	0.25523	-1.40152
C	3.81637	1.36905	-0.49293
C	2.63532	-0.27233	-1.79665
C	3.84513	0.26724	-1.31460
H	-3.06731	4.26113	-0.21270
H	-0.94811	5.12871	0.72198

H	1.39003	4.85723	1.22690
H	3.51398	3.62514	0.92642
H	4.73984	1.82704	-0.14862
H	0.51015	-0.17113	-1.79542
H	2.65124	-1.11653	-2.47916
H	4.79224	-0.17183	-1.61195
H	3.22306	-0.90887	2.44436
H	0.84888	-0.26967	2.09672

One imaginary frequency: -99.31 cm^{-1}

TS2 S-36

N	-1.30838	1.11418	0.31269
N	-0.06673	0.70608	0.76975
O	-0.47653	0.14892	2.10563
C	-1.73030	-0.36600	1.92921
C	-2.08205	-0.10320	0.43205
O	-2.36448	-0.90516	2.78584
C	-3.50836	0.05977	0.02636
C	-4.42347	-0.96985	0.23002
C	-3.90075	1.27501	-0.57892
C	-5.74568	-0.82340	-0.18324
C	-5.23640	1.39808	-0.98743
C	-6.14568	0.36332	-0.79772
H	-5.55842	2.32503	-1.45389
H	-7.17413	0.48595	-1.12266
C	-2.95524	2.38109	-0.74785
C	-1.69295	2.28084	-0.28254
H	-0.93979	3.05963	-0.32259
H	-3.28928	3.30124	-1.20937
C	-1.12020	-1.09339	-0.23747
C	0.12588	-0.53810	-0.01791
C	1.33477	-1.17887	-0.34106
C	-1.26692	-2.37923	-0.75803
C	1.17778	-2.53885	-0.75857
C	-0.10478	-3.08841	-0.99882
C	2.66642	-0.62376	-0.19906
C	2.33671	-3.37764	-0.83127
C	3.54777	-2.91013	-0.43287
C	3.73895	-1.52722	-0.10823
C	5.03802	-1.05960	0.26742
C	2.96141	0.79426	-0.20860
C	4.25507	1.22955	0.18799
C	5.26971	0.26346	0.47601
C	4.55640	2.61286	0.20568
C	2.07266	1.76660	-0.73239
C	3.64362	3.53933	-0.23992
C	2.40401	3.10198	-0.75111
H	-2.24597	-2.81482	-0.92886
H	-0.16012	-4.11411	-1.35245
H	2.21160	-4.41092	-1.14130
H	4.41141	-3.56845	-0.40152
H	5.83221	-1.78990	0.39406
H	6.24791	0.61373	0.79341
H	5.53989	2.92546	0.54589
H	3.88902	4.59639	-0.23831
H	1.71464	3.82248	-1.18081
H	1.13589	1.44706	-1.17512
H	-6.45828	-1.62477	-0.02000
H	-4.10109	-1.87695	0.73420

One imaginary frequency: -122.04 cm^{-1}

int2 C-36

N	2.42093	-0.82773	-0.93644
N	2.49367	-2.20819	-0.73678
O	2.82998	-2.29101	0.76643
C	2.14512	-1.27498	1.31972
C	1.47271	-0.46835	0.12940
O	2.08323	-1.03496	2.49022
C	1.43411	0.98810	0.47050
C	0.46452	1.51688	1.31652
C	2.51783	1.78140	0.04953
C	0.48389	2.86904	1.64395
C	2.52336	3.14091	0.38480
C	1.50377	3.68674	1.15608
H	3.34686	3.76400	0.04662
H	1.51788	4.74402	1.40132
C	3.64722	1.17308	-0.65999
C	3.61176	-0.10596	-1.06016
H	4.41355	-0.62623	-1.57065
H	4.53152	1.77149	-0.84634
C	0.34259	-1.44026	-0.28099
C	1.07382	-2.54105	-0.70228
C	0.55368	-3.81909	-0.87908
C	-1.06700	-1.54215	-0.17745
H	1.18760	-4.64285	-1.18615
C	-0.77996	-3.97728	-0.56331
C	-1.58744	-2.87612	-0.19136
H	-1.23647	-4.96219	-0.59297
C	-2.00718	-0.44323	-0.06352
C	-2.93530	-3.09889	0.24241
C	-3.27128	-0.71026	0.49076

C	-3.70564	-2.06405	0.66643
C	-1.75826	0.87919	-0.59673
C	-4.15430	0.36938	0.80885
C	-2.64537	1.93650	-0.25457
C	-3.82447	1.65289	0.50300
C	-0.71994	1.15856	-1.52085
C	-2.38213	3.24810	-0.71601
C	-0.50354	2.43670	-1.98405
C	-1.31839	3.50223	-1.55039
H	-3.30432	-4.11984	0.27572
H	-4.69862	-2.24003	1.07029
H	-5.09439	0.13891	1.30208
H	-4.48354	2.47481	0.76886
H	-3.05296	4.04867	-0.41557
H	-0.08678	0.35305	-1.87886
H	0.30443	2.62242	-2.68470
H	-1.12450	4.51114	-1.90022
H	-0.29454	3.28085	2.27782
H	-0.31876	0.87287	1.70481

int2 S-36

N	-1.27462	-1.04913	-0.12464
N	-0.07821	-0.71920	0.52654
O	-0.57275	-0.33540	1.91596
C	-1.79471	0.21122	1.72990
C	-2.05589	0.16528	0.18070
O	-2.49581	0.64794	2.59458
C	-3.49589	0.05443	-0.19986
C	-4.30267	1.15417	-0.46597
C	-4.05054	-1.24247	-0.16613
C	-5.65920	0.98142	-0.74059
C	-5.41205	-1.39937	-0.44116
C	-6.21096	-0.29730	-0.73229
H	-5.84357	-2.39626	-0.42149
H	-7.26654	-0.43586	-0.94281
C	-3.20178	-2.39173	0.16494
C	-1.86681	-2.27452	0.21504
H	-1.17276	-3.08054	0.42415
H	-3.66634	-3.35600	0.33556
C	-1.05322	1.20711	-0.29395
C	0.17198	0.59378	-0.08390
C	1.41533	1.22137	-0.26562
C	-1.11997	2.55420	-0.66091
C	1.32604	2.62622	-0.51617
C	0.07540	3.24336	-0.74843
C	2.71878	0.59842	-0.13323
C	2.51261	3.42360	-0.42936
C	3.68575	2.86221	-0.04018
C	3.81446	1.44288	0.11608
C	5.07937	0.88541	0.48452
C	2.96723	-0.81928	-0.30134
C	4.22720	-1.34632	0.09402
C	5.25884	-0.46088	0.53735
C	4.48296	-2.73273	-0.03796
C	2.06948	-1.69200	-0.96718
C	3.55990	-3.56730	-0.62214
C	2.35733	-3.02844	-1.12501
H	-2.05909	3.06507	-0.83130
H	0.06599	4.30678	-0.96998
H	2.43662	4.49141	-0.61212
H	4.56892	3.47634	0.11189
H	5.88985	1.56485	0.73265
H	6.21012	-0.88352	0.84858
H	5.44048	-3.11815	0.30177
H	3.77020	-4.62623	-0.73297
H	1.65877	-3.66771	-1.65589
H	1.15842	-1.29726	-1.40127
H	-6.28154	1.84494	-0.95005
H	-3.88505	2.15377	-0.44145

TS3 C-36

N	2.45056	-0.82820	-0.91041
N	2.50145	-2.18758	-0.76767
O	2.80821	-2.29511	0.84247
C	2.12283	-1.28495	1.34610
C	1.47405	-0.46317	0.12072
O	1.99500	-0.99892	2.50606
C	1.43486	0.99073	0.46113
C	0.46113	1.51761	1.30495
C	2.51763	1.78801	0.04483
C	0.47646	2.86909	1.63234
C	2.51841	3.14836	0.37953
C	1.49512	3.69083	1.14696
H	3.34191	3.77323	0.04469
H	1.50521	4.74800	1.39280
C	3.65329	1.18444	-0.65601
C	3.63398	-0.09900	-1.04354
H	4.44244	-0.62093	-1.54093
H	4.53510	1.78744	-0.83959
C	0.35492	-1.43013	-0.30354
C	1.09376	-2.52558	-0.72764
C	0.58274	-3.81089	-0.89511
C	-1.05411	-1.54388	-0.19156
H	1.22297	-4.63069	-1.19958

C	-0.74683	-3.97822	-0.57444
C	-1.56309	-2.88150	-0.20179
H	-1.19632	-4.96643	-0.60069
C	-2.00082	-0.45203	-0.07199
C	-2.90739	-3.11508	0.23429
C	-3.26162	-0.72925	0.48568
C	-3.68516	-2.08589	0.66012
C	-1.76225	0.87458	-0.60011
C	-4.15081	0.34343	0.81084
C	-2.65483	1.92460	-0.25000
C	-3.83007	1.63016	0.50981
C	-0.72898	1.16547	-1.52629
C	-2.40119	3.24004	-0.70545
C	-0.52194	2.44722	-1.98397
C	-1.34179	3.50532	-1.54202
H	-3.26846	-4.13879	0.26875
H	-4.67563	-2.26999	1.06654
H	-5.08764	0.10475	1.30635
H	-4.49330	2.44679	0.78151
H	-3.07603	4.03484	-0.39877
H	-0.09331	0.36515	-1.89118
H	0.28199	2.64154	-2.68690
H	-1.15546	4.51721	-1.88727
H	-0.30385	3.27831	2.26560
H	-0.31891	0.87049	1.69391

One imaginary frequency: -305.07 cm^{-1}

TS3 S-36

N	1.27277	-1.05981	-0.08232
N	0.07212	-0.72952	0.46387
O	0.59750	-0.23149	1.97666
C	1.78615	0.27632	1.73601
C	2.05226	0.16057	0.15464
O	2.55597	0.77004	2.51844
C	3.49168	0.03166	-0.20931
C	4.30604	1.12195	-0.49474
C	4.04270	-1.26536	-0.14007
C	5.66365	0.93767	-0.75086
C	5.40703	-1.43411	-0.39776
C	6.21201	-0.34268	-0.70687
H	5.83447	-2.43175	-0.34906
H	7.26929	-0.48895	-0.90288
C	3.19058	-2.40433	0.20988
C	1.85601	-2.28454	0.26652
H	1.15707	-3.07945	0.49819
H	3.65250	-3.36579	0.40257
C	1.05958	1.18448	-0.34597
C	-0.16726	0.57181	-0.13520
C	-1.41281	1.21036	-0.29283
C	1.12743	2.53613	-0.70154
C	-1.31860	2.61437	-0.53571
C	-0.06540	3.22766	-0.77670
C	-2.71659	0.59515	-0.14203
C	-2.49781	3.41919	-0.43358
C	-3.66953	2.86414	-0.02998
C	-3.80339	1.44635	0.12672
C	-5.06450	0.89669	0.52031
C	-2.97898	-0.82167	-0.30520
C	-4.23337	-1.34035	0.11694
C	-5.25070	-0.44804	0.58007
C	-4.50106	-2.72504	-0.00866
C	-2.10365	-1.70059	-0.99188
C	-3.59700	-3.56635	-0.61265
C	-2.40304	-3.03534	-1.14315
H	2.06730	3.04671	-0.86813
H	-0.05464	4.29222	-0.99290
H	-2.41721	4.48696	-0.61446
H	-4.54657	3.48329	0.13633
H	-5.86553	1.58160	0.78353
H	-6.19776	-0.86456	0.91166
H	-5.45346	-3.10380	0.35227
H	-3.81672	-4.62390	-0.71797
H	-1.72125	-3.67888	-1.69038
H	-1.20173	-1.31066	-1.44843
H	6.29148	1.79396	-0.97334
H	3.89215	2.12323	-0.49720

One imaginary frequency: -356.84 cm^{-1}

C-36

C	-2.66752	1.85251	-0.18950
C	-3.91837	1.32297	-0.60272
C	-4.06102	-0.01184	-0.85614
C	-1.55445	0.98822	-0.02594
H	-4.74590	2.00921	-0.76011
H	-4.98973	-0.40938	-1.25524
C	-1.38880	3.85448	0.41800
C	-2.55929	3.26921	0.06255
C	-0.26756	1.64873	0.07208
C	-0.21498	3.04230	0.38408
H	-1.30733	4.90976	0.65336
H	-3.46891	3.85913	-0.00950

C	-1.80720	-0.42970	0.02937
C	-3.01699	-0.91359	-0.52176
C	-1.12500	-2.78273	0.42951
C	-3.20066	-2.32267	-0.72528
C	-2.26150	-3.21773	-0.32882
H	-4.11011	-2.65257	-1.22000
C	3.17097	2.48715	0.34731
H	3.56009	3.43959	0.68178
N	1.03398	3.49899	0.52627
C	3.89968	1.39377	0.04048
N	1.79590	2.43488	0.24818
H	4.97930	1.42580	0.13367
C	3.26117	0.20977	-0.47402
C	1.09092	1.30163	-0.10136
C	4.01800	-0.89881	-0.90480
C	1.84999	0.18385	-0.61110
H	5.09677	-0.87700	-0.77691
C	3.40409	-1.98323	-1.49798
C	1.25338	-0.89650	-1.29198
C	2.01518	-1.96659	-1.71668
H	3.99501	-2.83339	-1.82309
C	-0.93262	-1.39722	0.67794
H	-2.38842	-4.28066	-0.51515
C	0.05934	-1.03189	1.61836
C	-0.23261	-3.72649	0.98685
C	0.78105	-3.33074	1.83110
C	0.89821	-1.97170	2.17873
H	0.15412	0.00578	1.91394
H	1.65074	-1.65859	2.89568
H	1.45962	-4.06338	2.25617
H	-0.37977	-4.77850	0.75627
H	0.18997	-0.87655	-1.49492
H	1.53505	-2.79534	-2.22698

S-36

C	-1.08293	2.59587	0.22914
C	-2.21629	3.43111	0.02396
C	-3.40704	2.89112	-0.36104
C	-1.21589	1.19205	0.11988
H	-2.09438	4.50712	0.10976
H	-4.25105	3.52759	-0.61230
C	1.35423	2.51620	0.51388
C	0.19129	3.21898	0.48052
C	0.03952	0.47170	0.02334
C	1.29576	1.12006	0.23482
H	2.29226	3.02473	0.69999
H	0.20110	4.29491	0.62881
C	-2.53084	0.61641	-0.02490
C	-2.86928	-0.77874	0.22873
C	-3.58468	1.48055	-0.39975
C	-4.12028	-1.28134	-0.21957
C	-4.84854	0.94487	-0.81544
C	-5.08244	-0.39066	-0.79773
H	-5.60874	1.63932	-1.16260
H	-6.02804	-0.79775	-1.14514
C	2.09100	-2.18589	-0.74596
H	1.37627	-2.95537	-1.00656
N	0.20411	-0.80015	-0.36849
C	3.43460	-2.31225	-0.75305
N	1.52781	-0.98005	-0.38176
H	3.88080	-3.25782	-1.03940
C	4.28295	-1.20737	-0.38170
C	2.25747	0.12819	-0.02083
C	5.68662	-1.33026	-0.37846
C	3.69403	0.02749	-0.00817
H	6.12915	-2.27963	-0.66718
C	6.48844	-0.26700	-0.01442
C	4.52877	1.09908	0.36601
C	5.90262	0.95412	0.36173
H	7.56824	-0.37325	-0.01555
C	-2.07782	-1.63053	1.03627
C	-4.45676	-2.63797	0.00056
C	-2.44441	-2.93598	1.27939
C	-3.62752	-3.46257	0.72505
H	-1.17911	-1.24221	1.49474
H	-1.82072	-3.55805	1.91383
H	-3.90107	-4.49780	0.90336
H	-5.40541	-3.00518	-0.38214
H	4.08994	2.04264	0.66543
H	6.53193	1.78870	0.65317

1b + 38b → C-37

TS1 C-37

N	0.45235	-3.11077	-0.11085
N	-0.62232	-3.71899	0.36440
O	-0.79534	-3.14614	1.60159
C	0.01655	-2.05339	1.78960
C	0.84111	-2.00606	0.57466
O	-0.00573	-1.42202	2.81388
C	1.99297	-1.26820	0.15236
C	2.45085	-0.03763	0.75948
C	2.69194	-1.78379	-0.95934
C	3.70745	0.48983	0.35063

C	1.66013	0.72498	1.65201
C	3.93466	-1.20852	-1.36375
C	4.17902	1.69474	0.92172
C	4.44867	-0.14155	-0.69632
C	2.12627	1.91800	2.15922
H	0.67344	0.38137	1.93000
H	4.46353	-1.65216	-2.20221
C	3.40541	2.39816	1.81486
H	5.15085	2.07052	0.61307
H	5.40617	0.28326	-0.98443
H	1.49320	2.49413	2.82609
H	3.76594	3.33242	2.23365
C	2.14938	-2.88634	-1.69327
C	1.02376	-3.52021	-1.29459
H	0.54204	-4.35856	-1.77907
H	2.65299	-3.22433	-2.59254
C	-1.71694	-1.16386	-0.52942
C	-2.15767	-2.34007	-0.53725
C	-3.45830	-2.81992	-0.38324
C	-2.55059	-0.02748	-0.42736
H	-3.76493	-3.85910	-0.38081
C	-4.33776	-1.76408	-0.20991
C	-3.92064	-0.39644	-0.19858
H	-5.39386	-1.97168	-0.05615
C	-2.15812	1.35724	-0.42854
C	-4.86426	0.63133	0.10840
C	-3.10833	2.31150	-0.01752
C	-4.46093	1.92560	0.23184
C	-0.83474	1.81056	-0.81792
C	-2.72030	3.67790	0.17099
C	-0.47301	3.16501	-0.57686
C	-1.44270	4.07901	-0.05230
C	0.10265	0.99100	-1.49380
C	0.82591	3.61669	-0.90626
C	1.34858	1.46699	-1.84288
C	1.73225	2.78166	-1.51915
H	-5.90128	0.35867	0.28271
H	-5.17040	2.69760	0.51698
H	-3.47011	4.38231	0.52055
H	-1.14401	5.10920	0.12226
H	1.08836	4.64769	-0.68259
H	-0.16509	-0.02476	-1.75862
H	2.04473	0.81396	-2.36275
H	2.72717	3.13702	-1.76986

One imaginary frequency: -172.00 cm^{-1}

TS1 S-37

N	-0.67820	1.36362	0.81155
N	0.43103	0.90567	1.36494
O	-0.00422	-0.13572	2.14392
C	-1.30351	-0.48330	1.86357
C	-1.72371	0.49073	0.84101
O	-1.84727	-1.38254	2.45126
C	-2.95899	0.84154	0.18318
C	-4.11822	-0.01880	0.10014
C	-2.98351	2.08551	-0.47491
C	-5.29153	0.48145	-0.53524
C	-4.13228	-1.35773	0.56573
C	-4.17436	2.55051	-1.10750
C	-6.44192	-0.33742	-0.62974
C	-5.29829	1.78684	-1.11332
C	-5.26094	-2.13756	0.44237
H	-3.25365	-1.77490	1.03707
H	-4.16087	3.52726	-1.58187
C	-6.43340	-1.62458	-0.14782
H	-7.32898	0.06980	-1.10697
H	-6.20910	2.14223	-1.58648
H	-5.24260	-3.15870	0.80911
H	-7.31895	-2.24653	-0.23037
C	-1.80238	2.89950	-0.53407
C	-0.65919	2.53147	0.07893
H	0.27541	3.07601	0.10670
H	-1.83160	3.83505	-1.08163
C	-0.34474	-1.00391	-0.61046
C	0.81672	-0.56411	-0.39484
C	2.04681	-1.22643	-0.51409
C	-0.63052	-2.32004	-1.01435
C	1.81664	-2.61241	-0.81760
C	0.50333	-3.11178	-1.07828
C	3.37977	-0.72343	-0.32222
C	2.93594	-3.50035	-0.80909
C	4.17812	-3.04658	-0.48624
C	4.42525	-1.66190	-0.23453
C	5.74779	-1.23239	0.10870
C	3.69748	0.68938	-0.23336
C	5.01647	1.07728	0.12717
C	6.02394	0.07931	0.32415
C	5.34301	2.44989	0.23370
C	2.78140	1.71400	-0.57649
C	4.41786	3.42333	-0.06309
C	3.13277	3.04404	-0.49892
H	-1.62067	-2.70909	-1.22696
H	0.40567	-4.16650	-1.32365
H	2.77294	-4.55161	-1.02840
H	5.01727	-3.73464	-0.43277

H	6.52431	-1.98596	0.20694
H	7.02295	0.39851	0.60806
H	6.35195	2.72090	0.53308
H	4.68214	4.47348	0.00859
H	2.42246	3.81019	-0.79818
H	1.79853	1.44326	-0.94417

One imaginary frequency: -214.22 cm^{-1}

int1 C-37

N	2.08340	-2.31812	-0.25009
N	3.34596	-1.74978	-0.04061
O	3.27451	-1.63747	1.43175
C	1.96498	-1.34315	1.71851
C	1.21571	-1.30373	0.33511
O	1.56911	-1.20285	2.83423
C	-0.22281	-1.74268	0.29946
C	-1.23168	-1.08430	1.06487
C	-0.55520	-2.76403	-0.58932
C	-2.58261	-1.51887	0.93471
C	-0.96856	0.04504	1.89000
C	-1.90279	-3.21341	-0.65685
C	-3.61223	-0.82856	1.62567
C	-2.88238	-2.61574	0.08378
C	-1.98761	0.70609	2.52919
H	0.04717	0.39981	2.01330
H	-2.14387	-4.02902	-1.33306
C	-3.32669	0.26629	2.40171
H	-4.63535	-1.17808	1.51355
H	-3.91342	-2.95173	0.00893
H	-1.76146	1.57619	3.13742
H	-4.12148	0.79597	2.91758
C	0.42494	-3.33396	-1.51232
C	1.73422	-3.07247	-1.34350
H	2.54889	-3.47517	-1.93402
H	0.09316	-3.99455	-2.30355
C	1.82427	0.00857	-0.30115
C	3.15262	-0.34809	-0.42968
C	4.20984	0.53790	-0.62784
C	1.46174	1.38129	-0.42096
H	5.22914	0.17908	-0.71474
C	3.88954	1.87623	-0.58747
C	2.55078	2.31049	-0.42696
H	4.67111	2.62875	-0.63801
C	0.11413	1.92043	-0.46368
C	2.29446	3.69518	-0.16095
C	-0.08131	3.24027	-0.01933
C	1.04043	4.11439	0.14766
C	-1.01663	1.22632	-1.04151
C	-1.40726	3.73578	0.18932
C	-2.32320	1.75187	-0.84702
C	-2.49124	2.98790	-0.14885
C	-0.86871	0.11920	-1.91152
C	-3.43670	1.09253	-1.41785
C	-1.96367	-0.47269	-2.50056
C	-3.26454	-0.00410	-2.23059
H	3.13641	4.38067	-0.13456
H	0.85538	5.14169	0.44879
H	-1.52566	4.72621	0.62002
H	-3.49893	3.35372	0.02905
H	-4.42968	1.49112	-1.22741
H	0.12437	-0.25614	-2.13928
H	-1.81893	-1.31526	-3.17031
H	-4.12254	-0.49520	-2.67912

int1 S-37

N	-0.51445	-1.54833	0.50649
N	0.68145	-0.86011	0.85205
O	0.21106	-0.27104	2.10507
C	-1.12983	-0.01211	1.94784
C	-1.44729	-0.40893	0.47567
O	-1.80402	0.41742	2.83281
C	-2.81556	-0.78363	-0.02287
C	-3.96206	0.04494	0.16910
C	-2.88221	-1.90790	-0.84185
C	-5.20353	-0.36060	-0.40687
C	-3.92568	1.28274	0.87313
C	-4.13154	-2.29059	-1.40229
C	-6.35747	0.44660	-0.22888
C	-5.25897	-1.55193	-1.17719
C	-5.05518	2.05093	1.01077
H	-3.00042	1.62163	1.32110
H	-4.17276	-3.18426	-2.01827
C	-6.29058	1.62796	0.46463
H	-7.29494	0.11210	-0.66502
H	-6.21084	-1.85347	-1.60583
H	-4.99996	2.98948	1.55292
H	-7.17710	2.24069	0.59223
C	-1.68731	-2.69111	-1.16681
C	-0.52889	-2.47306	-0.52449
H	0.37934	-3.04887	-0.66055
H	-1.76270	-3.48580	-1.89898
C	-0.63880	0.62712	-0.31791
C	0.67646	0.30249	-0.07269

C	1.76513	1.10079	-0.47872
C	-1.00008	1.79587	-0.99191
C	1.38236	2.35817	-1.04641
C	0.02727	2.65226	-1.33583
C	3.17259	0.81605	-0.27180
C	2.37649	3.37359	-1.22346
C	3.64292	3.17945	-0.77394
C	4.06581	1.90138	-0.28480
C	5.41607	1.72302	0.15541
C	3.71876	-0.51413	-0.10426
C	5.05484	-0.66085	0.35652
C	5.87322	0.49915	0.53047
C	5.59137	-1.95661	0.54939
C	3.03282	-1.68224	-0.51556
C	4.86770	-3.07689	0.21413
C	3.58911	-2.93126	-0.36299
H	-2.03953	2.03738	-1.19076
H	-0.19627	3.60502	-1.80757
H	2.07596	4.32479	-1.65279
H	4.37594	3.97989	-0.82102
H	6.06330	2.59456	0.19620
H	6.88774	0.37215	0.89779
H	6.60273	-2.04764	0.93615
H	5.29219	-4.06595	0.35247
H	3.04976	-3.80997	-0.70382
H	2.07468	-1.57773	-1.01025

TS2 C-37

N	-2.09907	-2.25966	-0.32416
N	-3.35529	-1.70824	-0.09601
O	-3.29334	-1.64204	1.38969
C	-1.98765	-1.35422	1.68806
C	-1.22564	-1.28638	0.30739
O	-1.59126	-1.23962	2.80709
C	0.20652	-1.74690	0.29423
C	1.21006	-1.07876	1.05925
C	0.53812	-2.80820	-0.54782
C	2.56098	-1.51772	0.95086
C	0.93990	0.05846	1.87093
C	1.88715	-3.25906	-0.59231
C	3.58522	-0.81718	1.63918
C	2.86462	-2.63583	0.12914
C	1.95313	0.72671	2.51215
H	-0.07763	0.41134	1.98617
H	2.13015	-4.09968	-1.23641
C	3.29359	0.28778	2.39870
H	4.60897	-1.16914	1.54118
H	3.89591	-2.97390	0.06796
H	1.72098	1.60135	3.11159
H	4.08409	0.82429	2.91409
C	-0.43842	-3.43592	-1.43419
C	-1.74615	-3.13678	-1.31047
H	-2.55972	-3.57345	-1.87771
H	-0.10999	-4.16882	-2.15989
C	-1.82018	0.04753	-0.29573
C	-3.15275	-0.29439	-0.43405
C	-4.20031	0.60601	-0.61425
C	-1.44212	1.41521	-0.40894
H	-5.22368	0.26019	-0.70566
C	-3.86435	1.94046	-0.55795
C	-2.51981	2.35784	-0.40393
H	-4.63750	2.70226	-0.59713
C	-0.08801	1.93529	-0.46681
C	-2.24220	3.73880	-0.13990
C	0.12995	3.25380	-0.02955
C	-0.97862	4.14227	0.15041
C	1.02715	1.21999	-1.04925
C	1.46462	3.73191	0.16239
C	2.34292	1.72682	-0.86708
C	2.53446	2.96598	-0.18064
C	0.85809	0.10511	-1.90583
C	3.44308	1.04280	-1.43459
C	1.94095	-0.51325	-2.49024
C	3.25018	-0.06234	-2.23103
H	-3.07470	4.43529	-0.10308
H	-0.77651	5.16765	0.44712
H	1.60155	4.72300	0.58602
H	3.54888	3.31806	-0.01362
H	4.44311	1.42778	-1.25322
H	-0.14173	-0.25587	-2.12708
H	1.77976	-1.36288	-3.14709
H	4.09842	-0.57388	-2.67522

One imaginary frequency: -60.47 cm^{-1}

TS2 S-37

N	0.47761	-1.46014	0.33974
N	-0.68062	-0.84559	0.78699
O	-0.18319	-0.32928	2.09542
C	1.14301	-0.04246	1.91489
C	1.44172	-0.37365	0.41035
O	1.85046	0.36156	2.78777
C	2.81477	-0.79116	-0.03381
C	3.92379	0.10413	0.06064

C	2.96288	-2.05804	-0.59900
C	5.18792	-0.30766	-0.45339
C	3.83270	1.39716	0.65015
C	4.24379	-2.44668	-1.08735
C	6.29632	0.57551	-0.38566
C	5.31486	-1.60240	-1.02447
C	4.92294	2.23050	0.70086
H	2.90030	1.72175	1.09689
H	4.35062	-3.43661	-1.52144
C	6.17114	1.82209	0.17364
H	7.24982	0.24090	-0.78562
H	6.28295	-1.91118	-1.40967
H	4.82843	3.20755	1.16400
H	7.02459	2.49051	0.22256
C	1.85615	-3.00692	-0.70995
C	0.63872	-2.68673	-0.22873
H	-0.23821	-3.32425	-0.22958
H	2.03031	-3.97979	-1.15007
C	0.62824	0.73106	-0.29343
C	-0.68572	0.38084	-0.04556
C	-1.79208	1.17016	-0.40439
C	0.94900	1.94288	-0.91045
C	-1.44521	2.46618	-0.90057
C	-0.10041	2.79962	-1.18796
C	-3.18933	0.82355	-0.23021
C	-2.46934	3.46161	-1.01188
C	-3.72949	3.19952	-0.57896
C	-4.11677	1.87800	-0.18062
C	-5.46545	1.62492	0.22496
C	-3.68990	-0.53398	-0.17146
C	-5.02816	-0.75555	0.25290
C	-5.88598	0.36180	0.50028
C	-5.52872	-2.07742	0.33653
C	-2.96112	-1.64836	-0.65783
C	-4.76787	-3.14690	-0.07267
C	-3.48499	-2.91985	-0.61338
H	1.97555	2.21659	-1.12796
H	0.10143	3.77895	-1.61279
H	-2.19851	4.44683	-1.37989
H	-4.48679	3.97844	-0.57704
H	-6.14259	2.46914	0.31923
H	-6.90080	0.17492	0.84015
H	-6.54263	-2.22661	0.69769
H	-5.16551	-4.15526	-0.02084
H	-2.91578	-3.75236	-1.01598
H	-1.99479	-1.48830	-1.12305

One imaginary frequency: -111.53 cm^{-1}

int2 C-37

N	2.32811	-1.68710	-0.81260
N	3.52404	-1.08630	-0.42128
O	3.52805	-1.34957	1.09089
C	2.23643	-1.25597	1.45658
C	1.39364	-1.04260	0.12806
O	1.83294	-1.35557	2.57890
C	0.05651	-1.72417	0.22997
C	-1.02354	-1.16626	0.97546
C	-0.05392	-2.99707	-0.31909
C	-2.29006	-1.81599	0.93188
C	-0.89727	0.00772	1.76910
C	-1.31547	-3.65071	-0.31110
C	-3.40027	-1.22812	1.59416
C	-2.41109	-3.05615	0.25149
C	-1.98268	0.54148	2.41692
H	0.07418	0.47480	1.88529
H	-1.39675	-4.62934	-0.77577
C	-3.25624	-0.06872	2.31302
H	-4.36447	-1.72579	1.53013
H	-3.38157	-3.54445	0.22148
H	-1.86207	1.43877	3.01578
H	-4.10920	0.37259	2.81913
C	1.11382	-3.69585	-0.86032
C	2.28581	-3.06423	-1.01466
H	3.20148	-3.50743	-1.38758
H	1.02296	-4.74413	-1.11905
C	1.75751	0.42232	-0.24953
C	3.12623	0.31618	-0.45229
C	4.00735	1.38922	-0.52246
C	1.15395	1.70391	-0.30191
H	5.07100	1.23025	-0.65707
C	3.45282	2.63919	-0.33657
C	2.05569	2.81289	-0.20229
H	4.08753	3.51918	-0.29065
C	-0.26276	1.98588	-0.43095
C	1.52768	4.11004	0.10552
C	-0.73150	3.23048	0.02242
C	0.19689	4.28259	0.31346
C	-1.19813	1.09557	-1.08339
C	-2.13789	3.46210	0.13783
C	-2.59118	1.34559	-0.94802
C	-3.03405	2.52256	-0.26833
C	-0.79293	0.03549	-1.93174
C	-3.52238	0.46046	-1.53911
C	-1.71995	-0.79048	-2.52959
C	-3.09789	-0.59965	-2.30728

H	2.22404	4.93478	0.22584
H	-0.19552	5.24539	0.62872
H	-2.47313	4.40330	0.56483
H	-4.10213	2.68330	-0.14838
H	-4.58266	0.64901	-1.39251
H	0.26241	-0.12148	-2.13183
H	-1.38109	-1.59822	-3.17103
H	-3.81887	-1.27190	-2.76177

int2 S-37

N	-0.44633	-1.43469	-0.05949
N	0.68514	-0.91508	0.56902
O	0.16654	-0.61180	1.96372
C	-1.13029	-0.26929	1.80530
C	-1.42514	-0.37837	0.26637
O	-1.86961	0.04945	2.69083
C	-2.83635	-0.75120	-0.08742
C	-3.90568	0.19256	-0.07108
C	-3.09558	-2.09925	-0.31651
C	-5.19400	-0.22211	-0.51915
C	-3.77093	1.51157	0.44662
C	-4.39784	-2.49873	-0.72532
C	-6.25877	0.71652	-0.55119
C	-5.40229	-1.58281	-0.86901
C	-4.82669	2.38863	0.43111
H	-2.83985	1.80660	0.91712
H	-4.57762	-3.54997	-0.93113
C	-6.08019	1.99975	-0.10051
H	-7.22726	0.38863	-0.91923
H	-6.38721	-1.89167	-1.20825
H	-4.70571	3.38219	0.85110
H	-6.90294	2.70706	-0.11848
C	-2.07046	-3.11980	-0.07959
C	-0.79158	-2.77096	0.12277
H	0.03364	-3.44774	0.31276
H	-2.36331	-4.16262	-0.06030
C	-0.61023	0.80381	-0.27642
C	0.70342	0.41215	-0.06216
C	1.82508	1.21715	-0.31656
C	-0.89419	2.07342	-0.78732
C	1.50487	2.56557	-0.66762
C	0.17216	2.93962	-0.95087
C	3.21620	0.82941	-0.17039
C	2.54195	3.55371	-0.64648
C	3.79028	3.22410	-0.22703
C	4.15462	1.85851	0.01713
C	5.49483	1.54246	0.40514
C	3.70082	-0.53198	-0.26942
C	5.03131	-0.81834	0.14148
C	5.89800	0.25031	0.53096
C	5.51801	-2.14637	0.07291
C	2.96612	-1.57290	-0.89219
C	4.75152	-3.15075	-0.46886
C	3.47706	-2.84673	-0.99170
H	-1.90403	2.38671	-1.02070
H	-0.01196	3.95790	-1.28171
H	2.28943	4.57845	-0.90259
H	4.55799	3.98565	-0.12225
H	6.17972	2.36106	0.60757
H	6.90648	0.01128	0.85688
H	6.52602	-2.34835	0.42491
H	5.13869	-4.16261	-0.53282
H	2.90063	-3.61817	-1.49294
H	2.00400	-1.35492	-1.34101

TS3 C-37

N	2.34769	-1.69621	-0.78818
N	3.51890	-1.07559	-0.47718
O	3.53182	-1.30491	1.16013
C	2.25738	-1.22671	1.48280
C	1.40146	-1.03659	0.12245
O	1.78349	-1.30929	2.58521
C	0.07053	-1.72323	0.23220
C	-1.01477	-1.16529	0.97247
C	-0.03721	-2.99939	-0.31168
C	-2.27872	-1.81951	0.92728
C	-0.89531	0.01117	1.76327
C	-1.29680	-3.65746	-0.30431
C	-3.39298	-1.23460	1.58536
C	-2.39520	-3.06308	0.25162
C	-1.98441	0.54212	2.40721
H	0.07488	0.47853	1.88467
H	-1.37346	-4.63861	-0.76443
C	-3.25523	-0.07308	2.30190
H	-4.35478	-1.73674	1.52053
H	-3.36440	-3.55384	0.22149
H	-1.86817	1.44049	3.00532
H	-4.11102	0.36558	2.80559
C	1.13063	-3.69743	-0.84932
C	2.30587	-3.07060	-0.99989
H	3.22444	-3.51328	-1.36516
H	1.04087	-4.74702	-1.10354
C	1.75352	0.41763	-0.26837
C	3.12064	0.31379	-0.48635

C	4.00225	1.39045	-0.54619
C	1.14813	1.69986	-0.30786
H	5.06544	1.23323	-0.68609
C	3.44793	2.63604	-0.34528
C	2.04913	2.80808	-0.20449
H	4.08133	3.51673	-0.29562
C	-0.26864	1.97968	-0.43355
C	1.52145	4.10303	0.10762
C	-0.73800	3.22386	0.02191
C	0.18977	4.27467	0.31528
C	-1.20478	1.08905	-1.08531
C	-2.14459	3.45468	0.13884
C	-2.59768	1.33817	-0.94732
C	-3.04047	2.51496	-0.26680
C	-0.80137	0.02855	-1.93404
C	-3.52950	0.45182	-1.53532
C	-1.72902	-0.79925	-2.52852
C	-3.10641	-0.60927	-2.30301
H	2.21714	4.92792	0.23047
H	-0.20262	5.23656	0.63334
H	-2.47981	4.39522	0.56728
H	-4.10850	2.67474	-0.14526
H	-4.58954	0.63976	-1.38625
H	0.25341	-0.12627	-2.13807
H	-1.39120	-1.60702	-3.17046
H	-3.82812	-1.28259	-2.75471

One imaginary frequency: -341.60 cm^{-1}

TS3 S-37

N	-0.44703	-1.44232	-0.00962
N	0.69427	-0.92864	0.49953
O	0.14321	-0.52035	2.03539
C	-1.11556	-0.21195	1.83392
C	-1.42035	-0.37631	0.26095
O	-1.93104	0.14398	2.64685
C	-2.83181	-0.75965	-0.06919
C	-3.90491	0.18204	-0.07741
C	-3.09147	-2.11290	-0.26836
C	-5.19028	-0.24614	-0.52048
C	-3.77625	1.51205	0.41196
C	-4.39305	-2.52610	-0.66670
C	-6.25685	0.68908	-0.58071
C	-5.39748	-1.61571	-0.83643
C	-4.83327	2.38672	0.36881
H	-2.85181	1.81450	0.88977
H	-4.57038	-3.58267	-0.84557
C	-6.08267	1.98337	-0.16123
H	-7.22304	0.34991	-0.94448
H	-6.38145	-1.93352	-1.16993
H	-4.71729	3.38915	0.76863
H	-6.90673	2.68833	-0.20051
C	-2.06507	-3.12637	-0.01836
C	-0.78546	-2.77820	0.17969
H	0.04189	-3.44787	0.38227
H	-2.35763	-4.16888	0.02141
C	-0.61440	0.78636	-0.30697
C	0.70104	0.39074	-0.10505
C	1.82495	1.20684	-0.33576
C	-0.89775	2.06569	-0.79837
C	1.50257	2.55743	-0.66798
C	0.16787	2.93200	-0.95111
C	3.21500	0.82298	-0.18044
C	2.53399	3.54956	-0.63042
C	3.78062	3.22047	-0.20437
C	4.14694	1.85470	0.02961
C	5.48282	1.54121	0.43544
C	3.70990	-0.53535	-0.28588
C	5.03443	-0.81898	0.14477
C	5.88969	0.25031	0.55810
C	5.52945	-2.14362	0.07187
C	2.99410	-1.57359	-0.93398
C	4.77864	-3.14695	-0.49336
C	3.51291	-2.84401	-1.03715
H	-1.90706	2.38399	-1.02561
H	-0.01603	3.95345	-1.27231
H	2.27877	4.57597	-0.87690
H	4.54411	3.98387	-0.08379
H	6.16022	2.36138	0.65577
H	6.89358	0.01303	0.89906
H	6.53209	-2.34353	0.43998
H	5.17229	-4.15611	-0.55978
H	2.95015	-3.61289	-1.55748
H	2.04063	-1.35491	-1.40021

One imaginary frequency: -375.40 cm^{-1}

C-37

C	3.39908	-0.73504	0.11012
C	3.76187	-2.09346	0.30406
C	2.81020	-3.07450	0.30919
C	2.03929	-0.39146	-0.10753
H	4.80399	-2.32984	0.50068
H	3.06868	-4.10254	0.54674

C	4.15324	1.59523	0.00705
C	4.42905	0.27397	0.14247
C	1.72346	1.01527	0.03355
C	2.77846	1.97797	-0.02538
H	4.92452	2.35677	-0.02107
H	5.45634	-0.06473	0.24582
C	1.11495	-1.45169	-0.42041
C	1.47493	-2.77387	-0.06628
C	-1.11673	-2.30533	-1.08997
C	0.48685	-3.81397	-0.08593
C	-0.78040	-3.57024	-0.50603
H	0.77615	-4.80011	0.26752
C	0.16813	4.18834	-0.11271
H	0.66959	5.13664	-0.25274
N	2.33614	3.23943	-0.04494
C	-1.16878	3.97965	-0.13954
N	1.00661	3.11394	0.05589
H	-1.83769	4.81216	-0.32595
C	-1.70890	2.68284	0.14661
C	0.56299	1.80960	0.20500
C	-3.11959	2.46137	0.13336
C	-0.84103	1.62278	0.46627
H	-3.76813	3.27566	-0.17722
C	-3.63815	1.24941	0.47670
C	-1.39198	0.43151	1.06303
C	-2.79520	0.22198	1.00205
H	-4.70841	1.06935	0.42381
C	-3.34172	-0.97288	1.52842
C	-0.14872	-1.26587	-1.11993
C	-0.60205	-0.49743	1.78355
C	-1.16322	-1.63344	2.32236
H	0.45308	-0.29694	1.92904
C	-2.54061	-1.89370	2.16383
H	-4.41286	-1.13644	1.44333
H	-2.96970	-2.80438	2.57003
H	-0.53875	-2.33342	2.86856
H	-1.53870	-4.34826	-0.47684
C	-0.43376	-0.12910	-1.91150
C	-2.37769	-2.10921	-1.69582
C	-2.65963	-0.95081	-2.38647
C	-1.65969	0.02920	-2.52535
H	0.33060	0.62601	-2.05098
H	-1.84933	0.91685	-3.12120
H	-3.63093	-0.80872	-2.84981
H	-3.11562	-2.90429	-1.62478

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C	-1.45225	2.52332	-0.27945
C	-2.49240	3.45681	-0.54561
C	-3.77018	3.02449	-0.74111
C	-1.76144	1.15208	-0.13473
H	-2.23619	4.50650	-0.65755
H	-4.55302	3.71879	-1.03394
C	0.97240	2.15928	-0.12877
C	-0.09279	2.99599	-0.24463
C	-0.61471	0.26586	-0.18808
C	0.72509	0.75313	-0.10111
H	1.98077	2.55451	-0.14157
H	0.06818	4.06603	-0.33856
C	-3.14100	0.73533	-0.09349
C	-3.61299	-0.55002	0.40738
C	-4.11683	1.66172	-0.52640
C	-4.95233	-0.94557	0.14641
C	-5.46933	1.23985	-0.74826
C	-5.85582	-0.03424	-0.49103
H	-6.17295	1.96612	-1.14589
H	-6.87231	-0.36176	-0.69114
C	0.99961	-2.66518	-0.94490
H	0.17302	-3.34061	-1.12138
N	-0.64783	-1.04476	-0.46398
C	2.30869	-2.93068	-1.15125
N	0.63589	-1.41000	-0.51993
H	2.60519	-3.90276	-1.52829
C	3.31286	-1.95481	-0.83713
C	1.53652	-0.39393	-0.25724
C	4.69165	-2.24719	-1.07137
C	2.93998	-0.71672	-0.28423
H	4.94544	-3.19390	-1.53955
C	5.66234	-1.35369	-0.73970
C	3.97120	0.14444	0.24783
C	5.33209	-0.15360	-0.03695
H	6.70686	-1.56408	-0.95129
C	3.69654	1.21254	1.13671
C	6.34984	0.70264	0.44811
C	4.70700	2.01079	1.62513
C	6.04656	1.77810	1.25001
H	6.83565	2.42203	1.62458
H	4.47085	2.81236	2.31783
H	7.38229	0.47547	0.19650
H	2.68075	1.36879	1.47768
C	-2.84872	-1.37219	1.27040
C	-5.42169	-2.19906	0.60577
C	-3.33903	-2.56866	1.74535
C	-4.62615	-3.01041	1.38094
H	-1.86842	-1.04391	1.58700

H	-2.73078	-3.16839	2.41522
H	-4.99957	-3.96348	1.74221
H	-6.44035	-2.49087	0.36405

CO_2

O	-0.00000	-1.16293	0.00587
O	-0.00000	1.16293	0.00587
C	-0.00000	-0.00000	-0.01565

Racemizations

TS racemization C-29

C	2.82220	-1.42650	0.66493
C	3.82598	-0.76215	1.43926
C	3.88891	0.59346	1.51701
C	1.76749	-0.69575	0.07245
H	4.54394	-1.38067	1.97084
H	4.63430	1.09562	2.12663
C	2.08104	-3.52610	-0.30340
C	2.97532	-2.84130	0.44333
C	0.61765	-1.46271	-0.40122
C	0.85986	-2.85692	-0.62774
H	2.18175	-4.58045	-0.53493
H	3.86070	-3.32647	0.84396
C	2.05222	0.71210	-0.12647
C	3.05786	1.35889	0.64926
C	1.82318	2.57906	-1.44836
C	3.31319	2.72411	0.40161
C	2.69334	3.34943	-0.65326
H	4.04637	3.24350	1.01341
H	2.89369	4.38541	-0.90305
C	-2.49596	-3.17552	-0.58171
H	-2.61421	-4.19972	-0.90754
N	-0.23901	-3.55236	-0.90399
C	-3.39645	-2.43775	0.08991
N	-1.22542	-2.66730	-0.75544
H	-4.37019	-2.84742	0.33232
C	-3.08368	-1.08308	0.43949
C	-0.81947	-1.36515	-0.46893
C	-4.01324	-0.34885	1.23988
C	-1.90371	-0.47676	-0.03596
H	-4.85698	-0.88755	1.66154
C	-3.83077	0.97361	1.49140
C	-1.91478	0.97224	-0.06306
C	-2.82861	1.68582	0.76665
H	-4.50771	1.52264	2.13953
C	-2.85330	3.09873	0.73116
H	1.38559	3.01227	-2.34608
C	-1.22734	1.70102	-1.05544
C	-1.33737	3.07416	-1.13261
H	-0.64081	1.15543	-1.78112
C	-2.11198	3.78896	-0.20016
H	-3.52453	3.62330	1.40571
H	-2.16637	4.87177	-0.25192
H	-0.83561	3.61057	-1.93109
N	1.49308	1.33159	-1.18721

One imaginary frequency: -41.31 cm^{-1}

TS racemization C-29.H^+

C	2.60521	-1.66012	0.77846
C	3.62914	-1.04268	1.56759
C	3.82273	0.30477	1.58310
C	1.63290	-0.86773	0.11854
H	4.25910	-1.69233	2.16781
H	4.57450	0.76893	2.21193
C	1.70335	-3.70349	-0.16782
C	2.62645	-3.08708	0.60948
C	0.44580	-1.52360	-0.40442
C	0.56550	-2.94089	-0.58194
H	1.71845	-4.77006	-0.36297
H	3.43278	-3.64695	1.07210
C	2.08368	0.46601	-0.12634
C	3.11559	1.09098	0.62887
C	2.08551	2.32680	-1.62729
C	3.48780	2.40373	0.29447
C	2.96765	3.03595	-0.82527
H	4.24213	2.90128	0.89758
H	3.27838	4.03118	-1.11559
C	-2.81308	-2.91981	-0.67235
H	-3.03211	-3.92635	-1.00161
N	-0.58385	-3.53148	-0.88075
C	-3.64965	-2.08440	-0.02940
N	-1.48673	-2.55112	-0.79502
H	-4.66721	-2.39084	0.18351
C	-3.20156	-0.77815	0.35372
C	-0.97464	-1.29052	-0.51855
C	-4.03001	0.03326	1.19186
C	-1.95795	-0.29762	-0.09843
H	-4.94156	-0.40457	1.58662
C	-3.65779	1.29601	1.52986
C	-1.78419	1.13855	-0.06156
C	-2.56774	1.91223	0.84012
H	-4.24654	1.88746	2.22421

C	-2.38161	3.31257	0.90178
H	1.70710	2.69409	-2.57357
C	-1.06054	1.83921	-1.04910
C	-0.96286	3.21499	-1.03430
H	-0.70928	1.27729	-1.90884
C	-1.57160	3.95840	-0.00512
H	-2.94984	3.88043	1.63272
H	-1.47087	5.03802	0.02039
H	-0.46324	3.73872	-1.84394
N	1.67959	1.11146	-1.25356
H	1.05661	0.58761	-1.86097

One imaginary frequency: -34.73 cm^{-1}

TS racemization C-31

N	-1.39542	1.52210	-1.08402
C	-1.55511	2.80898	-1.31728
C	-2.44234	3.63681	-0.60569
C	-3.24128	3.04329	0.34121
C	-3.14765	1.65361	0.56321
C	-2.13876	0.92341	-0.13259
C	-4.11887	0.96488	1.34270
C	-4.16263	-0.39017	1.26339
C	-3.16327	-1.13976	0.56611
C	-2.00936	-0.51023	0.04209
C	-3.42420	-2.54056	0.36411
C	-2.53990	-3.31922	-0.29353
C	-1.25345	-2.75847	-0.56131
C	-0.90449	-1.37872	-0.37179
N	-0.21516	-3.55406	-0.78013
N	0.84209	-2.74961	-0.64496
C	0.53881	-1.39817	-0.42675
C	2.05707	-3.36379	-0.46403
C	3.07459	-2.66968	0.08601
C	2.86868	-1.28310	0.29259
C	1.72027	-0.59510	-0.11118
S	4.11610	-0.28221	0.97933
C	3.21524	1.14838	0.56329
C	2.00323	0.84203	-0.09519
C	3.68738	2.45468	0.70054
C	2.98418	3.47839	0.08375
C	1.86912	3.17820	-0.71020
C	1.39642	1.87862	-0.81382
H	-0.94455	3.23000	-2.11586
H	-2.50633	4.69574	-0.82951
H	-3.98400	3.61511	0.89155
H	-4.86512	1.52995	1.89316
H	-4.96817	-0.94539	1.73591
H	-4.37290	-2.93784	0.71302
H	-2.70756	-4.36976	-0.50226
H	2.05714	-4.41896	-0.69990
H	4.01899	-3.14761	0.31368
H	4.60970	2.65252	1.23718
H	3.33655	4.50142	0.16691
H	1.38379	3.97005	-1.27253
H	0.58226	1.62523	-1.47060

One imaginary frequency: -46.15 cm^{-1}

TD-DFT-optimized geometries and transition data

C-29 (S_0 state)

C	3.12744	0.85400	0.35236
C	4.14327	-0.14283	0.41908
C	3.89953	-1.43426	0.06400
C	1.81333	0.49567	-0.03324
H	5.12513	0.15189	0.76392
H	4.67144	-2.18752	0.14198
C	2.55103	3.22340	0.48934
C	3.45998	2.22079	0.62595
C	0.80314	1.50640	0.06061
C	1.20846	2.87125	0.19519
H	2.81938	4.26081	0.62579
H	4.48230	2.44745	0.89584
C	1.60881	-0.81538	-0.58864
C	2.63677	-1.79360	-0.48097
C	0.25493	-2.27571	-1.73985
C	2.36618	-3.08487	-0.97691
C	1.16633	-3.33713	-1.59376
H	3.11794	-3.85683	-0.88069
H	0.92785	-4.31427	-1.98715
C	-2.12173	3.42949	-0.44503
H	-2.18016	4.50119	-0.53133
N	0.18618	3.73087	0.05437
C	-3.14012	2.56754	-0.66225
N	-0.89057	2.93067	-0.11493
H	-4.10189	2.94899	-0.96881
C	-2.97890	1.17167	-0.41214
C	-0.61180	1.56909	-0.02714
C	-4.07788	0.28023	-0.57101
C	-1.73440	0.67997	0.03880
H	-5.00271	0.67084	-0.97233
C	-3.96617	-1.03314	-0.23695
C	-1.68457	-0.64384	0.60156
C	-2.78792	-1.52053	0.39723
H	-4.79297	-1.71282	-0.39160
C	-2.71941	-2.84473	0.88340
H	-0.67746	-2.43238	-2.26963
C	-0.62792	-1.09005	1.42406
C	-0.60216	-2.37126	1.91964
H	0.16971	-0.41129	1.67357
C	-1.63855	-3.27270	1.61649
H	-3.54979	-3.51069	0.69061
H	-1.59904	-4.28692	1.98805
H	0.22104	-2.68736	2.54460
N	0.45913	-1.06694	-1.25969

Excited state information

Excited State 1: Singlet-A 2.9250 eV 423.88 nm f=0.1147 <S**2>=0.000

95 -> 98 -0.12235

96 -> 97 0.68551

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1164.41777513

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1829 eV 389.53 nm f=0.0388 <S**2>=0.000

95 -> 97 0.30105

96 -> 98 0.62592

Excited State 3: Singlet-A 3.4720 eV 357.09 nm f=0.2599 <S**2>=0.000

95 -> 97 0.58938

95 -> 98 0.10769

96 -> 98 -0.29853

96 -> 99 -0.15641

Excited State 4: Singlet-A 3.6383 eV 340.77 nm f=0.0278 <S**2>=0.000

95 -> 98 0.48110

96 -> 99 0.44295

96 ->100 -0.17902

Excited State 5: Singlet-A 3.7899 eV 327.14 nm f=0.0583 <S**2>=0.000

93 -> 97 0.30258

94 -> 97 -0.29599

95 -> 97 0.18289

95 -> 98 -0.21130

96 -> 99 0.31073

96 ->100 0.35697

Excited State 6: Singlet-A 3.8557 eV 321.56 nm f=0.0354 <S**2>=0.000

92 -> 97 -0.12916

93 -> 98 -0.10703

94 -> 97 0.54147

95 -> 98 0.11205

95 -> 99 -0.11516

96 -> 99 0.16700

96 ->100 0.31230

Excited State 7: Singlet-A 3.9059 eV 317.43 nm f=0.1288 <S**2>=0.000

93 -> 97 -0.25951

94 -> 97 -0.26088

95 -> 98 0.31454

96 -> 99 -0.21331

96 ->100 0.43964

Excited State 8: Singlet-A 3.9971 eV 310.18 nm f=0.1825 <S**2>=0.000

91 -> 97 -0.15104

92 -> 97 0.34968

93 -> 97 0.40723

94 -> 98 0.12929

95 -> 98 0.25178

96 -> 99 -0.23691

Excited State 9: Singlet-A 4.1463 eV 299.02 nm f=0.0201 <S**2>=0.000

91 -> 97 0.11230

92 -> 97 -0.31374

93 -> 97 0.13121

93 -> 98 0.11964

94 -> 98 0.54524

Excited State 10: Singlet-A 4.2152 eV 294.13 nm f=0.0796 <S**2>=0.000

91 -> 97 -0.11509

92 -> 97 0.32388

93 -> 97 -0.30063

93 -> 98 -0.13648

94 -> 98 0.29967

95 ->100 0.17775

96 ->101 -0.31036

Excited State 11: Singlet-A 4.2748 eV 290.03 nm f=0.0425 <S**2>=0.000

91 -> 97 0.12159

93 -> 98 -0.43509

95 -> 99 0.48845

Excited State 12: Singlet-A 4.3236 eV 286.76 nm f=0.0406 <S**2>=0.000

92 -> 97 0.17123

93 -> 97 -0.10607

93 -> 98 0.23010

94 -> 97 0.11319

94 -> 98 0.13641

95 -> 99 0.37391

95 ->100 0.25213

96 ->100 0.10672

96 ->101 0.36527

Excited State 13: Singlet-A 4.4313 eV 279.79 nm f=0.1227 <S**2>=0.000

91 -> 97 -0.19514

92 -> 97 -0.11856

92 -> 98 -0.28398

93 -> 98 -0.31214

94 -> 99 -0.17517

95 -> 99 -0.15694

95 ->100 0.25911

96 ->101 0.31328

Excited State 14: Singlet-A 4.4916 eV 276.03 nm f=0.1221 <S**2>=0.000

91 -> 97 0.38696

92 -> 98 -0.12112

93 -> 97 0.10403

94 -> 98 -0.15902

94 ->100 -0.11413

95 ->100 0.43273

96 ->101 -0.17629

96 ->102 -0.10197

Excited State 15: Singlet-A 4.5335 eV 273.49 nm f=0.0829 <S**2>=0.000

90 -> 97 0.19121

91 -> 97 0.34248

92 -> 97 0.21995

93 -> 99 -0.13985

94 -> 99 0.24749

95 -> 99 -0.17846

95 ->100 -0.16723

96 ->101 0.29337

Excited State 16: Singlet-A 4.5792 eV 270.75 nm f=0.0300 <S**2>=0.000

90 -> 97 0.20652

91 -> 97 -0.10016

91 -> 98 -0.18185

92 -> 98 0.49226

92 -> 99 -0.11055

93 -> 98 -0.14138

94 -> 99 0.10273

94 ->100 0.14978

95 ->100 0.22255

Excited State 17: Singlet-A 4.6261 eV 268.01 nm f=0.0236 <S**2>=0.000

91 -> 97 -0.23154

92 -> 97 -0.11055

92 -> 98 -0.15020

93 -> 99 0.14829

94 -> 99 0.57590

94 ->100 -0.10249

Excited State 18: Singlet-A 4.7336 eV 261.93 nm f=0.0288 <S**2>=0.000

90 -> 97 0.21322

91 -> 98 0.11758

92 -> 98 -0.12568

93 -> 98 0.11993

94 ->100 -0.14376

95 ->101 -0.13781

96 ->102 0.54399

Excited State 19: Singlet-A 4.7815 eV 259.30 nm f=0.0177 <S**2>=0.000

90 -> 97 0.28145

91 -> 97 0.10088

91 -> 98 0.28359

91 -> 99 -0.12721

92 -> 98 0.22959

92 -> 99 0.22104

92 ->100 0.10202

93 -> 99 0.35591

94 ->100 -0.16374

Excited State 20: Singlet-A 4.8438 eV 255.96 nm f=0.1050 <S**2>=0.000

90 -> 97 0.18199

91 -> 98 0.35713

92 -> 99 -0.12854

93 -> 99 -0.23985

94 ->100 0.19128

96 ->102 -0.25833

96 ->103 0.22733

96 ->104 -0.24154

Excited State 21: Singlet-A 4.8924 eV 253.42 nm f=0.0902 <S**2>=0.000

90 -> 97 0.39791

90 -> 98 -0.10208

91 -> 98 -0.33825

92 -> 98 -0.17527

93 -> 99 0.17375

93 ->100 -0.13172

94 ->101 0.11861

95 ->101 0.16931

96 ->102 -0.10103

Excited State 22: Singlet-A 4.9045 eV 252.80 nm f=0.2430 <S**2>=0.000

90 -> 98 -0.17389

91 -> 99 -0.11390

92 -> 99 0.22635

93 -> 99 0.18263

94 ->100 0.42712

95 ->101 -0.30115

96 ->104 -0.11733

Excited State 23: Singlet-A 4.9387 eV 251.05 nm f=0.0246 <S**2>=0.000

90 -> 98 -0.17945

92 -> 99 0.24391

93 ->100 0.10523

94 ->100 0.12093

95 ->101 0.55343

96 ->102 0.18436

Excited State 24: Singlet-A 4.9837 eV 248.78 nm f=0.0431 <S**2>=0.000

92 -> 99 0.10523

96 ->103 0.58953

96 ->104 0.26337

96 ->106 -0.13597

Excited State 25: Singlet-A 5.0193 eV 247.01 nm f=0.0215 <S**2>=0.000

90 -> 98 0.19456

91 -> 98 -0.23259

91 -> 99 -0.20125

91 ->100 -0.15791

92 -> 99 0.20489

92 ->100 0.14052

93 -> 99 -0.27065

93 ->100 0.32381

96 ->104 -0.14859

Excited State 26: Singlet-A 5.0411 eV 245.95 nm f=0.0446 <S**2>=0.000

90 -> 98 -0.22071

91 -> 99 0.10064

92 -> 99 -0.30266

92 ->100 0.28045

93 -> 99 0.17760

93 ->100 0.40232

95 ->102 -0.14098

96 ->104 0.10232

Excited State 27: Singlet-A 5.1323 eV 241.58 nm f=0.6091 <S**2>=0.000

90 -> 97 0.10430

90 -> 98 0.19594

91 -> 98 0.10045

93 -> 98 0.10164

94 ->100 0.23055

95 ->102 -0.11800

96 ->103 -0.17399

96 ->104 0.48826

Excited State 28: Singlet-A 5.2334 eV 236.91 nm f=0.0294 <S**2>=0.000

90 -> 98 0.40143

91 -> 99 0.26578

93 -> 99 0.14080

93 ->101 -0.13437

94 ->100 0.11227

94 ->101 0.22889

95 ->102 -0.16176

96 ->102 0.13860

96 ->104 -0.16365

96 ->105 -0.15929

Excited State 29: Singlet-A 5.2466 eV 236.32 nm f=0.0393 <S**2>=0.000

91 -> 99 0.17902

91 ->100 -0.20527

92 ->100 0.48833

92 ->101 0.11305

93 ->100 -0.31996

95 ->102 0.10031

Excited State 30: Singlet-A 5.2763 eV 234.99 nm f=0.0222 <S**2>=0.000

91 -> 99 0.10971

96 ->105 0.65869

Excited State 31: Singlet-A 5.2934 eV 234.23 nm f=0.0727 <S**2>=0.000

90 -> 99 0.11075

91 ->100 -0.12163

93 ->100 0.12829

94 ->101 0.34070

95 ->102 0.52312

Excited State 32: Singlet-A 5.3193 eV 233.08 nm f=0.0033 <S**2>=0.000

96 ->103 0.12444

96 ->104 0.10388

96 ->106 0.66522

Excited State 33: Singlet-A 5.3679 eV 230.97 nm f=0.0901 <S**2>=0.000

91 -> 99 -0.24072

91 ->100 0.14124

92 ->100 0.15127

92 ->101 -0.10876

93 ->100 -0.11153

93 ->101 -0.17115

94 ->100 -0.13402

94 ->101 0.38227

94 ->102 0.10075

95 ->103 0.12160

95 ->104 -0.12791

96 ->105 0.10313

96 ->107 0.11561

96 ->108 0.20880

Excited State 34: Singlet-A 5.4077 eV 229.27 nm f=0.0189 <S**2>=0.000

89 -> 97 0.23315

90 -> 98 -0.19409

91 -> 99 0.33010

92 -> 99 0.22533

93 ->101 0.13968

94 ->101 0.23337

95 ->101 -0.11354

95 ->102 -0.11071

95 ->103 -0.15030

95 ->104 0.15856

96 ->108 0.13119

Excited State 35: Singlet-A 5.4532 eV 227.36 nm f=0.0192 <S**2>=0.000

87 -> 97 0.10063

88 -> 97 0.59222

89 -> 97 0.20227

96 ->108 -0.11464

Excited State 36: Singlet-A 5.4858 eV 226.01 nm f=0.0024 <S**2>=0.000

93 ->101 0.10628

95 ->103 0.61209

95 ->104 0.14981

95 ->106 -0.12572

96 ->107 -0.13673

Excited State 37: Singlet-A 5.5285 eV 224.26 nm f=0.0402 <S**2>=0.000

91 ->100 -0.19305

92 ->100 -0.11091

92 ->101 0.12907

93 ->101 0.35168

94 ->101 0.12610

95 ->102 -0.21240

95 ->104 -0.34711

96 ->107 -0.13709

Excited State 38: Singlet-A 5.5367 eV 223.93 nm f=0.0255 <S**2>=0.000

90 -> 98 0.10162

90 -> 99 0.10699

91 ->100 -0.21647

92 ->100 -0.12600

94 ->101 -0.10848

95 ->104 -0.20881

96 ->107 0.46727

96 ->108 0.22084

96 ->109 -0.13610

Excited State 39: Singlet-A 5.5767 eV 222.32 nm f=0.0678 <S**2>=0.000

89 -> 97 -0.13035

90 -> 99 -0.27847

91 -> 99 -0.12156

92 -> 99 -0.13220

92 ->101 0.11917

93 ->101 0.28651

95 ->104 0.34240

96 ->107 0.18215

96 ->108 0.12186

Excited State 40: Singlet-A 5.5877 eV 221.89 nm f=0.0066 <S**2>=0.000

89 -> 97 -0.10355

91 ->100 -0.31300

93 ->101 -0.16539

95 ->104 0.14487

96 ->107 -0.18650

96 ->108 0.38762

96 ->109 0.28527

Excited State 41: Singlet-A 5.6073 eV 221.11 nm f=0.1032 <S**2>=0.000

89 -> 97 0.30974

90 -> 98 0.11112

90 -> 99 0.11961

91 ->100 0.26864

92 ->101 0.19366

93 ->101 0.12433

94 ->102 -0.12177

96 ->108 0.11019

96 ->109 0.35941

Excited State 42: Singlet-A 5.6224 eV 220.52 nm f=0.0919 <S**2>=0.000

89 -> 97 -0.19745

91 ->100 0.20102

93 ->101 0.10448

94 ->102 -0.19952

95 ->104 -0.20933

96 ->107 -0.27761

96 ->108 0.33382

96 ->109 -0.23782

Excited State 43: Singlet-A 5.6353 eV 220.01 nm f=0.0097 <S**2>=0.000

88 -> 97 0.15323

89 -> 97 -0.32989

90 -> 99 -0.15850

91 -> 99 0.12213

92 ->101 -0.10252

94 ->102 -0.19657

95 ->104 -0.13334

96 ->107 0.18295

96 ->108 -0.11497

96 ->109 0.37711

Excited State 44: Singlet-A 5.6987 eV 217.57 nm f=0.0535 <S**2>=0.000

89 -> 97 0.13828

90 -> 99 -0.30610

92 ->101 -0.11544

94 ->102 0.17230

96 ->110 0.49402

Excited State 45: Singlet-A 5.7044 eV 217.35 nm f=0.0418 <S**2>=0.000

89 -> 97 -0.10251

90 -> 99 0.30202

94 ->102 -0.22973

95 ->102 -0.11825

95 ->105 0.14020

96 ->110 0.44883

96 ->111 0.10264

Excited State 46: Singlet-A 5.7453 eV 215.80 nm f=0.0175 <S**2>=0.000

90 -> 99 -0.11766

93 ->103 0.12157

95 ->105 0.58626

95 ->106 0.10483

96 ->111 0.21403

Excited State 47: Singlet-A 5.7503 eV 215.61 nm f=0.0361 <S**2>=0.000

90 -> 99 -0.12453

90 ->100 -0.15647

91 ->100 0.10125

91 ->101 -0.20207

92 ->100 -0.11534

92 ->101 0.47974

93 ->101 -0.22696

94 ->102 0.14141

Excited State 48: Singlet-A 5.7936 eV 214.00 nm f=0.1402 <S**2>=0.000

86 -> 97 0.13331

87 -> 97 -0.18113

89 -> 97 -0.10217

90 -> 99 0.16911

90 ->100 0.32943

91 ->101 -0.10273

93 ->101 0.11127

93 ->102 -0.26144

94 ->102 0.28656

95 ->106 -0.12462

96 ->111 -0.16158

Excited State 49: Singlet-A 5.8036 eV 213.63 nm f=0.0354 <S**2>=0.000

86 -> 97 0.14168

95 ->105 -0.21414

96 ->109 -0.12063

96 ->111 0.58648

Excited State 50: Singlet-A 5.8208 eV 213.00 nm f=0.0041 <S**2>=0.000

86 -> 97 -0.17082

89 -> 98 0.15040

90 ->100 0.21379

94 ->103 -0.18194

95 ->105 -0.11335

95 ->106 0.52778

Excited State 51: Singlet-A 5.8257 eV 212.82 nm f=0.0350 <S**2>=0.000

86 -> 97 -0.26915

88 -> 98 -0.13762

90 ->100 0.35015

92 ->101 0.18395

93 ->101 -0.13235

94 ->102 -0.13734

95 ->106 -0.29332

96 ->111 0.13526

Excited State 52: Singlet-A 5.8351 eV 212.48 nm f=0.0405 <S**2>=0.000

87 -> 97 -0.19175

88 -> 98 0.42148

89 -> 98 0.41324

90 ->100 -0.12921

95 ->106 -0.14117

Excited State 53: Singlet-A 5.8794 eV 210.88 nm f=0.0317 <S**2>=0.000

87 -> 97 0.38536

88 -> 98 0.37910

90 ->100 0.16893

93 ->102 -0.14599

94 ->103 0.23706

94 ->104 -0.15472

Excited State 54: Singlet-A 5.9084 eV 209.84 nm f=0.0581 <S**2>=0.000

86 -> 97 0.39704

87 -> 97 -0.21171

91 ->101 0.11941

93 ->102 -0.11865

94 ->102 -0.20807

94 ->103 0.20480

95 ->108 -0.13268

96 ->112 -0.21905

Excited State 55: Singlet-A 5.9385 eV 208.78 nm f=0.0249 <S**2>=0.000

86 -> 97 -0.14809

87 -> 97 0.11688

88 -> 98 -0.29199

89 -> 98 0.35069

90 ->100 -0.12318

93 ->102 -0.20998

94 ->103 0.29831

96 ->112 -0.12283

Excited State 56: Singlet-A 5.9446 eV 208.56 nm f=0.0732 <S**2>=0.000

87 -> 97 -0.24085

93 ->102 0.21955

94 ->102 0.10139

94 ->103 0.41461

95 ->106 0.13504

96 ->112 0.35495

Excited State 57: Singlet-A 5.9679 eV 207.75 nm f=0.0416 <S**2>=0.000

86 -> 98 0.13605

89 -> 98 0.18802

93 ->102 -0.20505

94 ->103 -0.14822

94 ->104 -0.13430

95 ->107 -0.12717

95 ->108 -0.19446

96 ->112 0.46500

96 ->113 0.11049

Excited State 58: Singlet-A 5.9834 eV 207.21 nm f=0.2341 <S**2>=0.000

90 -> 99 -0.10769

91 ->101 -0.11548

94 ->102 -0.10445

94 ->104 0.54092

96 ->115 0.18697

Excited State 59: Singlet-A 6.0142 eV 206.15 nm f=0.0218 <S**2>=0.000

86 -> 98 -0.11971

87 -> 97 0.10711

87 -> 98 -0.13691

90 ->100 0.16161

90 ->101 -0.14751

92 ->102 0.20033

93 ->102 0.35012

95 ->107 -0.29957

95 ->108 -0.27459

Excited State 60: Singlet-A 6.0488 eV 204.97 nm f=0.0115 <S**2>=0.000

91 ->101 -0.18289

94 ->104 0.11972

95 ->109 -0.29337

96 ->113 0.39239

96 ->114 0.14767

96 ->115 -0.32125

Excited State 61: Singlet-A 6.0646 eV 204.44 nm f=0.0031 <S**2>=0.000

87 -> 98 -0.12925

91 ->101 0.13879

92 ->102 0.10421

93 ->103 0.22769

95 ->107 0.38682

95 ->108 -0.20691

95 ->109 -0.30974

96 ->115 0.19344

Excited State 62: Singlet-A 6.0874 eV 203.67 nm f=0.0891 <S**2>=0.000

86 -> 98 -0.20181

87 -> 97 0.12320

91 ->101 0.48284

92 ->101 0.17089

93 ->103 -0.13953

94 ->104 0.14001

95 ->107 -0.15746

95 ->108 0.11484

95 ->109 -0.11761

Excited State 63: Singlet-A 6.0964 eV 203.37 nm f=0.0023 <S**2>=0.000

86 -> 97 -0.13527

91 ->101 0.10501

93 ->103 0.18417

94 ->105 -0.16120

95 ->107 0.10480

95 ->108 -0.25299

95 ->109 0.35209

96 ->113 0.18895

96 ->114 0.28941

Excited State 64: Singlet-A 6.1140 eV 202.79 nm f=0.0118 <S**2>=0.000

86 -> 98 0.15317

87 -> 98 -0.24350

93 ->103 -0.11992

93 ->104 -0.10774

94 ->104 -0.12319

95 ->107 -0.17119

96 ->112 -0.17260

96 ->113 0.35724

96 ->114 -0.11436

96 ->115 0.29474

96 ->116 0.12174

Excited State 65: Singlet-A 6.1289 eV 202.30 nm f=0.0544 <S**2>=0.000

86 -> 98 0.11865

92 ->102 0.30355

93 ->102 -0.10642

93 ->103 0.27471

93 ->104 -0.27405

95 ->107 -0.12940

95 ->108 0.22601

95 ->110 0.10012

96 ->113 -0.16826

96 ->115 -0.16321

Excited State 66: Singlet-A 6.1403 eV 201.92 nm f=0.0104 <S**2>=0.000

86 -> 97 0.14185

87 -> 98 0.27063

93 ->103 0.29805

95 ->108 0.16367

95 ->109 0.13509

95 ->110 -0.10382

96 ->113 0.28357

96 ->114 -0.13691

96 ->115 0.15906

96 ->116 -0.18390

96 ->117 -0.11501

Excited State 67: Singlet-A 6.1473 eV 201.69 nm f=0.0050 <S**2>=0.000

93 ->103 -0.11177

95 ->109 -0.13102

95 ->110 -0.11209

96 ->114 0.52798

96 ->115 0.31295

Excited State 68: Singlet-A 6.1778 eV 200.69 nm f=0.0204 <S**2>=0.000

91 ->102 -0.14604

92 ->102 0.41342

93 ->103 -0.30836

95 ->107 0.20355

95 ->109 0.15968

95 ->110 -0.13670

96 ->114 -0.10082

96 ->117 -0.10181

Excited State 69: Singlet-A 6.1888 eV 200.34 nm f=0.0023 <S**2>=0.000

93 ->104 0.11200

94 ->105 0.13941

95 ->107 0.11982

95 ->109 0.13327

95 ->110 0.57506

96 ->115 0.10114

Excited State 70: Singlet-A 6.1917 eV 200.24 nm f=0.0336 <S**2>=0.000

87 -> 98 -0.17254

92 ->102 0.19029

92 ->104 0.10646

93 ->103 0.18482

93 ->104 0.47552

95 ->108 0.13443

95 ->110 -0.14962

96 ->116 0.11730

96 ->117 0.10553

Excited State 71: Singlet-A 6.2459 eV 198.51 nm f=0.0081 <S**2>=0.000

86 -> 97 -0.12549

87 -> 98 0.34620

89 -> 99 -0.22735

90 ->101 -0.16757

93 ->104 0.15218

94 ->104 -0.11406

94 ->105 -0.23819

95 ->107 -0.10253

95 ->109 -0.11793

95 ->110 0.11005

95 ->111 -0.13437

96 ->116 0.14901

Excited State 72: Singlet-A 6.2620 eV 197.99 nm f=0.0081 <S**2>=0.000

87 -> 98 0.18973

92 ->102 0.14057

94 ->105 0.43523

95 ->108 -0.12938

95 ->111 0.29154

96 ->117 0.20963

Excited State 73: Singlet-A 6.2836 eV 197.32 nm f=0.0129 <S**2>=0.000

89 -> 98 0.10752

89 -> 99 0.11934

90 ->101 -0.18842

92 ->102 -0.10323

94 ->106 -0.14821

95 ->111 0.19103

96 ->116 0.50904

Excited State 74: Singlet-A 6.2914 eV 197.07 nm f=0.0067 <S**2>=0.000

87 -> 98 0.10126

89 -> 99 0.12807

93 ->104 -0.10951

94 ->106 0.27224

95 ->111 -0.33531

96 ->115 0.10052

96 ->116 0.14918

96 ->117 0.36119

Excited State 75: Singlet-A 6.2975 eV 196.88 nm f=0.0058 <S**2>=0.000

90 ->101 0.16121

94 ->105 -0.34024

94 ->106 -0.15840

95 ->110 0.16957

95 ->111 0.26519

96 ->117 0.37011

Excited State 76: Singlet-A 6.3310 eV 195.84 nm f=0.0923 <S**2>=0.000

86 -> 98 -0.11524

90 ->101 0.38372

91 ->102 -0.13487

94 ->106 0.33204

95 ->108 -0.11197

95 ->111 0.16218

96 ->116 0.16932

96 ->117 -0.23031

Excited State 77: Singlet-A 6.3414 eV 195.52 nm f=0.0208 <S**2>=0.000

86 -> 98 0.17803

90 ->101 -0.28194

92 ->103 -0.10942

94 ->105 -0.16829

94 ->106 0.41670

95 ->111 0.26701

96 ->116 -0.13375

Excited State 78: Singlet-A 6.3592 eV 194.97 nm f=0.0374 <S**2>=0.000

84 -> 97 0.10897

86 -> 98 -0.10038

87 -> 98 -0.12818

87 -> 99 -0.10117

88 -> 99 -0.30549

91 ->104 0.12335

92 ->103 0.33502

92 ->104 -0.23864

95 ->111 0.12242

96 ->118 0.10750

Excited State 79: Singlet-A 6.3864 eV 194.14 nm f=0.2105 <S**2>=0.000

85 -> 97 0.13234

86 -> 98 0.41291

91 ->101 0.11603

91 ->102 -0.11373

92 ->104 -0.22690

93 ->104 0.12727

94 ->102 0.13671

94 ->107 -0.16536

96 ->117 -0.12861

Excited State 80: Singlet-A 6.3923 eV 193.96 nm f=0.0706 <S**2>=0.000

82 -> 97 0.12081

84 -> 97 -0.12883

85 -> 97 0.10639

88 -> 99 0.38808

89 -> 99 0.25621

90 ->101 -0.18196

92 ->103 0.24437

92 ->104 -0.18911

94 ->107 0.11756

Excited State 81: Singlet-A 6.4233 eV 193.02 nm f=0.0548 <S**2>=0.000

84 -> 97 -0.13354

85 -> 97 0.28974

88 -> 99 0.11427

89 -> 99 -0.23986

91 ->102 -0.13434

92 ->103 0.15667

92 ->104 0.21541

94 ->108 -0.10690

96 ->118 0.28123

96 ->119 0.11046

Excited State 82: Singlet-A 6.4333 eV 192.72 nm f=0.0121 <S**2>=0.000

84 -> 97 -0.12368

85 -> 97 0.20998

89 -> 99 -0.20816

90 ->101 0.11252

91 ->102 0.34754

92 ->104 -0.17207

94 ->107 -0.18117

94 ->108 -0.21097

96 ->118 -0.17193

96 ->119 -0.18407

Excited State 83: Singlet-A 6.4398 eV 192.53 nm f=0.0041 <S**2>=0.000

88 -> 99 0.10402

91 ->102 -0.12808

92 ->103 -0.20903

92 ->104 -0.17480

93 ->106 -0.14497

94 ->107 -0.13656

95 ->112 -0.22835

96 ->118 0.36521

96 ->119 -0.29213

Excited State 84: Singlet-A 6.4597 eV 191.94 nm f=0.0994 <S**2>=0.000

84 -> 97 0.16714

85 -> 97 -0.18002

88 -> 99 0.13509

90 ->101 0.11272

91 ->102 0.33530

92 ->102 0.10409

92 ->103 0.11911

94 ->107 -0.12962

95 ->112 0.15965

96 ->118 0.36333

96 ->119 0.11841

Excited State 85: Singlet-A 6.4683 eV 191.68 nm f=0.0156 <S**2>=0.000

84 -> 97 -0.12289

92 ->103 -0.23240

92 ->104 -0.21759

93 ->105 -0.24218

93 ->106 -0.13772

96 ->119 0.45622

Excited State 86: Singlet-A 6.4790 eV 191.36 nm f=0.0018 <S**2>=0.000

89 -> 99 -0.16727

92 ->103 -0.17574

92 ->104 -0.17009

93 ->105 0.48927

94 ->108 0.15682

95 ->111 0.10330

95 ->112 0.19778

Excited State 87: Singlet-A 6.4853 eV 191.18 nm f=0.0014 <S**2>=0.000

85 -> 97 0.13773

88 -> 99 -0.16393

89 -> 99 0.24546

89 ->100 0.16207

93 ->105 0.32845

94 ->108 -0.17145

95 ->112 -0.27881

96 ->119 0.19341

Excited State 88: Singlet-A 6.5138 eV 190.34 nm f=0.0041 <S**2>=0.000

84 -> 97 0.21246

84 -> 98 0.12742

85 -> 97 -0.23062

88 -> 99 0.26525

89 -> 99 -0.19703

89 ->100 0.14506

93 ->106 -0.14291

94 ->108 -0.10807

95 ->112 -0.21834

96 ->118 -0.19530

96 ->119 0.17218

Excited State 89: Singlet-A 6.5235 eV 190.06 nm f=0.0092 <S**2>=0.000

84 -> 97 -0.23781

84 -> 98 -0.10327

85 -> 97 -0.14427

89 ->100 -0.17535

92 ->103 0.16751

92 ->104 0.14018

93 ->106 -0.22540

94 ->107 -0.19689

94 ->109 0.13199

95 ->113 -0.19450

95 ->115 0.28270

Excited State 90: Singlet-A 6.5377 eV 189.64 nm f=0.0628 <S**2>=0.000

83 -> 97 -0.13576

84 -> 97 -0.21530

85 -> 97 -0.10246

87 -> 99 -0.10820

88 ->100 -0.15072

89 -> 99 -0.10176

89 ->100 0.18036

91 ->102 0.21326

93 ->106 -0.17800

94 ->107 0.20229

94 ->108 0.25482

95 ->112 -0.24507

Excited State 91: Singlet-A 6.5429 eV 189.49 nm f=0.0430 <S**2>=0.000

86 -> 98 0.11719

88 ->100 -0.12383

89 ->100 -0.12436

91 ->103 0.11626

92 ->103 -0.10709

93 ->106 0.18530

94 ->107 0.33820

94 ->108 -0.17425

94 ->110 0.13968

95 ->113 -0.27216

95 ->115 0.17876

Excited State 92: Singlet-A 6.5474 eV 189.36 nm f=0.0144 <S**2>=0.000

89 ->100 0.13855

93 ->106 0.45138

94 ->107 -0.22973

94 ->108 0.18896

94 ->109 0.13953

95 ->112 -0.11783

95 ->113 -0.23961

96 ->119 0.10030

Excited State 93: Singlet-A 6.5639 eV 188.89 nm f=0.0152 <S**2>=0.000

83 -> 97 0.10799

84 -> 97 -0.16332

84 -> 98 0.40240

85 -> 98 -0.24564

88 ->100 0.28450

95 ->112 0.16898

95 ->113 -0.17166

Excited State 94: Singlet-A 6.5695 eV 188.73 nm f=0.0272 <S**2>=0.000

84 -> 97 -0.22800

85 -> 97 -0.19838

87 -> 99 -0.10393

89 ->100 -0.13134

91 ->104 0.11933

92 ->103 -0.10401

93 ->106 0.17270

93 ->109 0.10443

94 ->108 -0.28934

95 ->112 -0.11942

95 ->113 0.32532

Excited State 95: Singlet-A 6.5823 eV 188.36 nm f=0.0433 <S**2>=0.000

83 -> 97 0.11332

84 -> 97 -0.24860

84 -> 98 -0.27855

85 -> 97 -0.16615

85 -> 98 0.19793

88 ->100 0.23244

89 ->100 0.29467

94 ->107 0.12865

94 ->109 -0.13175

Excited State 96: Singlet-A 6.5885 eV 188.18 nm f=0.0070 <S**2>=0.000

89 ->100 0.18835

94 ->107 0.10509

94 ->109 0.48168

95 ->114 0.29924

95 ->115 0.10841

Excited State 97: Singlet-A 6.6262 eV 187.11 nm f=0.0659 <S**2>=0.000

83 -> 97 0.10716

91 ->103 0.32817

91 ->104 -0.22552

92 ->104 -0.12117

94 ->109 0.11745

94 ->110 -0.15268

95 ->113 0.18534

95 ->114 -0.20947

95 ->115 0.17651

96 ->122 -0.11793

Excited State 98: Singlet-A 6.6349 eV 186.87 nm f=0.0139 <S**2>=0.000

81 -> 97 -0.10557

82 -> 97 -0.21678

83 -> 98 0.14700

84 -> 98 -0.17003

87 -> 99 -0.23432

88 ->100 0.14278

89 ->100 -0.15475

90 ->104 -0.10275

91 ->103 0.10440

91 ->104 -0.17333

95 ->112 -0.12393

95 ->114 0.28114

95 ->115 -0.14736

Excited State 99: Singlet-A 6.6539 eV 186.33 nm f=0.0388 <S**2>=0.000

87 -> 99 0.11428

88 ->100 -0.24339

90 ->102 0.10292

91 ->104 -0.12545

93 ->108 0.16562

94 ->109 -0.21091

94 ->110 -0.13973

95 ->114 0.36814

95 ->115 0.15100

96 ->122 -0.13945

Excited State 100: Singlet-A 6.6564 eV 186.26 nm f=0.0177 <S**2>=0.000

82 -> 97 0.16282

83 -> 97 -0.12109

84 -> 97 0.11098

85 -> 97 0.11451

88 ->100 0.25778

90 ->102 -0.10782

91 ->103 -0.17338

94 ->108 0.10950

94 ->109 -0.21856

94 ->110 -0.15506

95 ->114 0.12448

95 ->115 0.34539

Transition energies, wavelengths and oscillator strengths

state E(eV) wavelength(nm) oscillator_strength

1 2.9250 423.88 0.1147

2 3.1829 389.53 0.0388

3 3.4720 357.09 0.2599

4 3.6383 340.77 0.0278

5 3.7899 327.14 0.0583

6 3.8557 321.56 0.0354

7 3.9059 317.43 0.1288

8 3.9971 310.18 0.1825

9 4.1463 299.02 0.0201

10 4.2152 294.13 0.0796

11 4.2748 290.03 0.0425

12 4.3236 286.76 0.0406

13 4.4313 279.79 0.1227

14 4.4916 276.03 0.1221

15 4.5335 273.49 0.0829

16 4.5792 270.75 0.0300

17 4.6261 268.01 0.0236

18 4.7336 261.93 0.0288

19	4.7815	259.30	0.0177
20	4.8438	255.96	0.1050
21	4.8924	253.42	0.0902
22	4.9045	252.80	0.2430
23	4.9387	251.05	0.0246
24	4.9837	248.78	0.0431
25	5.0193	247.01	0.0215
26	5.0411	245.95	0.0446
27	5.1323	241.58	0.6091
28	5.2334	236.91	0.0294
29	5.2466	236.32	0.0393
30	5.2763	234.99	0.0222
31	5.2934	234.23	0.0727
32	5.3193	233.08	0.0033
33	5.3679	230.97	0.0901
34	5.4077	229.27	0.0189
35	5.4532	227.36	0.0192
36	5.4858	226.01	0.0024
37	5.5285	224.26	0.0402
38	5.5367	223.93	0.0255
39	5.5767	222.32	0.0678
40	5.5877	221.89	0.0066
41	5.6073	221.11	0.1032
42	5.6224	220.52	0.0919
43	5.6353	220.01	0.0097
44	5.6987	217.57	0.0535
45	5.7044	217.35	0.0418
46	5.7453	215.80	0.0175
47	5.7503	215.61	0.0361
48	5.7936	214.00	0.1402
49	5.8036	213.63	0.0354
50	5.8208	213.00	0.0041
51	5.8257	212.82	0.0350
52	5.8351	212.48	0.0405
53	5.8794	210.88	0.0317
54	5.9084	209.84	0.0581
55	5.9385	208.78	0.0249
56	5.9446	208.56	0.0732
57	5.9679	207.75	0.0416
58	5.9834	207.21	0.2341
59	6.0142	206.15	0.0218
60	6.0488	204.97	0.0115
61	6.0646	204.44	0.0031
62	6.0874	203.67	0.0891
63	6.0964	203.37	0.0023
64	6.1140	202.79	0.0118
65	6.1289	202.30	0.0544
66	6.1403	201.92	0.0104
67	6.1473	201.69	0.0050
68	6.1778	200.69	0.0204
69	6.1888	200.34	0.0023
70	6.1917	200.24	0.0336
71	6.2459	198.51	0.0081
72	6.2620	197.99	0.0081
73	6.2836	197.32	0.0129
74	6.2914	197.07	0.0067
75	6.2975	196.88	0.0058
76	6.3310	195.84	0.0923
77	6.3414	195.52	0.0208
78	6.3592	194.97	0.0374
79	6.3864	194.14	0.2105
80	6.3923	193.96	0.0706

81 6.4233 193.02 0.0548

82 6.4333 192.72 0.0121

83 6.4398 192.53 0.0041

84 6.4597 191.94 0.0994

85 6.4683 191.68 0.0156

86 6.4790 191.36 0.0018

87 6.4853 191.18 0.0014

88 6.5138 190.34 0.0041

89 6.5235 190.06 0.0092

90 6.5377 189.64 0.0628

91 6.5429 189.49 0.0430

92 6.5474 189.36 0.0144

93 6.5639 188.89 0.0152

94 6.5695 188.73 0.0272

95 6.5823 188.36 0.0433

96 6.5885 188.18 0.0070

97 6.6262 187.11 0.0659

98 6.6349 186.87 0.0139

99 6.6539 186.33 0.0388

100 6.6564 186.26 0.0177

Rotatory strengths (velocity)

state XX YY ZZ R(velocity) E-M Angle

1 -5.2897 143.4736 -84.8774 17.7688 86.45

2 -3.5209 -7.4449 -30.0464 -13.6707 111.23

3 60.7966 452.5717 -200.1268 104.4138 83.66

4 77.3235 96.3750 -18.7920 51.6355 69.51

5 -69.8359 6.0562 -24.2665 -29.3487 112.27

6 470.0816 375.1235 -4.1900 280.3384 32.59

7 66.6581 176.4287 -16.3247 75.5874 81.34

8 -365.5878 47.4557 -290.2166 -202.7829 135.85

9 25.4673 -10.2640 6.5796 7.2610 72.68

10 -38.1949 5.9197 8.5364 -7.9129 95.88

11 12.5002 54.3339 -38.4912 9.4477 86.19

12 436.8622 216.3690 -13.4351 213.2654 42.13

13 -72.0073 -102.4195 -46.7687 -73.7318 124.93

14 101.0611 84.5621 -1.4917 61.3772 77.14

15 3.7344 24.4262 14.3553 14.1719 79.09

16 95.9761 1.3456 5.2419 34.1879 66.08

17 4.0111 -15.0655 10.8610 -0.0644 90.00

18 104.5724 33.9910 -16.3281 40.7451 71.15

19 16.4405 -15.9408 -11.5565 -3.6856 97.17

20 1.5554 -1.5120 82.4191 27.4875 72.51

21 199.3788 -160.3920 9.6825 16.2231 79.86

22 -454.8406 2.6014 -188.5315 -213.5902 162.03

23 -29.3341 69.7511 -44.6772 -1.4201 90.66

24 -32.8725 10.7222 -2.2509 -8.1337 126.47

25 44.5584 -24.2968 14.7844 11.6820 73.37

26 -25.5303 18.1041 1.9735 -1.8176 91.87

27 -457.0079 -69.1297 -153.5110 -226.5495 163.23

28 -92.4552 16.9169 -57.0795 -44.2059 116.67

29 -54.5522 -69.8349 -16.9541 -47.1137 121.60

30 -51.8668 9.1393 -6.1275 -16.2850 113.00

31 -128.3287 27.1574 -71.3525 -57.5079 103.65

32 -3.5965 -2.1660 -1.7913 -2.5180 108.38

33 -127.7122 -12.7192 14.6092 -41.9407 113.35

34 3.4897 -29.1761 -21.3853 -15.6906 116.99

35 -67.1962 4.1935 -17.2841 -26.7623 113.90

36 0.7789 2.7941 -3.1035 0.1565 86.56

37 105.6553 -146.8483 -55.6114 -32.2681 114.75

38 38.4504 -32.7776 32.8346 12.8358 65.28

39 -108.7433 -34.0156 -63.8236 -68.8608 117.49

40 -9.8945 -2.0758 -10.6859 -7.5521 107.77

41 201.2782 -63.5969 56.6632 64.7815 49.53

42 -112.1196 -30.4341 8.8479 -44.5686 120.15

43 -49.7716 -14.6357 -15.2359 -26.5477 130.78

44 -64.6990 -22.7025 -47.2518 -44.8844 120.57

45 95.5844 -34.7100 19.8557 26.9101 62.93

46 48.2217 -126.9797 14.3974 -21.4535 148.53

47 -100.4300 29.4310 -55.5104 -42.1698 131.45

48 -8.8280 -73.3929 19.3029 -20.9727 128.39

49 38.4320 -67.0318 10.6750 -5.9749 143.32

50 -20.9849 1.6323 11.8749 -2.4926 142.39

51 40.6452 13.8850 44.8283 33.1195 17.90

52 11.7510 -3.6755 32.6729 13.5828 73.07

53 3.7569 -10.2802 66.8629 20.1132 64.59

54 29.6307 -63.4772 16.9031 -5.6478 94.68

55 -25.8004 5.0556 57.8692 12.3748 39.03

56 7.5868 -41.3935 37.0782 1.0905 85.86

57 61.9920 -14.2555 12.3232 20.0199 74.78

58 131.1012 -87.7410 189.1831 77.5144 49.05

59 -32.9010 26.7274 -0.1967 -2.1234 96.31

60 -1.3518 2.7074 -7.5801 -2.0749 119.12

61 -4.0569 -11.9021 -4.8956 -6.9516 118.71

62 -83.6882 -6.1378 -78.7683 -56.1981 124.07

63 0.2737 -8.9862 9.1337 0.1404 81.99

64 17.9224 11.4575 -5.8260 7.8513 54.52

65 59.6250 86.2592 53.5859 66.4900 44.51

66 -10.5134 10.6635 21.1310 7.0937 60.71

67 1.3945 -9.1742 12.9925 1.7376 77.21

68 53.8290 -28.0959 18.4191 14.7174 71.35

69 16.7806 -31.8743 1.8376 -4.4187 105.69

70 136.4163 -54.5190 35.9202 39.2725 55.85

71 -16.7919 6.9570 -7.6208 -5.8186 113.51

72 -51.2077 32.5932 -4.0113 -7.5420 108.14

73 -2.6900 -1.2683 40.2777 12.1065 69.69

74 -32.7684 0.3861 15.0897 -5.7642 105.11

75 -34.4920 -0.1138 7.6686 -8.9791 133.90

76 14.8971 -50.2915 35.7952 0.1336 89.75

77 3.4506 6.2903 4.4643 4.7351 57.85

78 -33.8955 -109.4928 -42.9697 -62.1193 161.49

79 63.8669 -134.5276 102.2031 10.5141 85.56

80 13.0327 127.6468 71.7206 70.8000 25.69

81 -68.0964 9.6876 42.8855 -5.1745 101.49

82 -24.3431 2.2359 22.0348 -0.0241 90.00

83 9.3392 0.1962 6.5882 5.3746 67.80

84 9.2750 80.5538 -96.8489 -2.3400 93.41

85 -4.9984 -17.7852 -24.3456 -15.7097 165.75

86 -6.1704 8.4982 -0.1001 0.7426 82.31

87 18.8462 1.7676 0.0424 6.8854 47.34

88 -15.6526 4.1147 -24.5455 -12.0278 121.01

89 19.6094 2.5399 -3.2480 6.3004 38.51

90 -14.3452 15.6042 -67.1480 -21.9630 106.40

91 16.5508 -75.2681 -1.9525 -20.2233 119.99

92 4.3949 0.4841 6.0130 3.6307 70.13

93 -14.9370 -8.3885 -0.8553 -8.0603 104.38

94 -31.4067 -52.4420 39.9546 -14.6314 132.61

95 -0.0568 -13.8660 -30.5501 -14.8243 109.00

96 7.3185 12.1731 -7.2548 4.0789 78.23

97 -50.7527 18.5323 85.1030 17.6276 44.22

98 30.3058 -40.5900 7.3071 -0.9924 92.78

99 -21.2222 -12.6971 -5.2850 -13.0681 121.49

100 -8.7372 31.6209 -7.9100 4.9912 53.66

Transition dipoles

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	1.1835	0.4292	-0.1268	1.6009	0.1147
2	-0.7050	0.0134	-0.0276	0.4980	0.0388
3	1.5704	-0.7349	-0.2229	3.0558	0.2599
4	0.5144	0.1258	-0.1782	0.3122	0.0278
5	0.1276	-0.7770	-0.0889	0.6279	0.0583
6	0.2426	-0.2712	-0.4924	0.3749	0.0354
7	0.6232	0.9568	-0.2049	1.3458	0.1288
8	0.6557	1.1909	-0.1254	1.8638	0.1825
9	0.1488	0.3835	0.1678	0.1974	0.0201
10	-0.4474	-0.7521	-0.0677	0.7704	0.0796
11	-0.6211	-0.1222	0.0738	0.4062	0.0425
12	-0.3173	-0.0904	-0.5240	0.3834	0.0406
13	0.8898	-0.4801	0.3293	1.1306	0.1227
14	0.3184	0.9518	0.3200	1.1097	0.1221
15	0.5154	-0.6779	0.1470	0.7468	0.0829
16	0.4502	0.0917	0.2365	0.2670	0.0300
17	-0.2565	0.3767	-0.0220	0.2081	0.0236
18	-0.0826	0.4324	-0.2331	0.2481	0.0288
19	0.3268	-0.2028	0.0548	0.1509	0.0177
20	-0.3823	0.8588	-0.0292	0.8846	0.1050
21	-0.7046	-0.3000	-0.4077	0.7527	0.0902
22	0.4278	1.3551	-0.0515	2.0220	0.2430
23	0.2156	0.3752	-0.1265	0.2032	0.0246
24	0.1369	-0.5316	0.2274	0.3531	0.0431
25	-0.2698	-0.2050	-0.2447	0.1747	0.0215
26	0.3871	0.4579	0.0399	0.3611	0.0446
27	-0.7225	2.0651	-0.2403	4.8444	0.6091

28	0.3106	0.3373	-0.1377	0.2292	0.0294	47	-0.1965	-0.4531	0.1107	0.2562	0.0361
29	-0.5025	-0.1506	-0.1753	0.3059	0.0393	48	-0.9333	0.2598	-0.2216	0.9876	0.1402
30	0.3360	-0.2396	0.0360	0.1716	0.0222	49	-0.3271	-0.0576	-0.3723	0.2489	0.0354
31	-0.0564	0.7460	0.0328	0.5608	0.0727	50	-0.0297	0.1662	-0.0044	0.0285	0.0041
32	-0.0044	0.1269	-0.0973	0.0256	0.0033	51	0.1611	0.4524	0.1195	0.2449	0.0350
33	0.0879	-0.8077	0.1585	0.6852	0.0901	52	-0.1782	-0.4941	0.0849	0.2831	0.0405
34	0.3267	-0.1087	0.1541	0.1423	0.0189	53	-0.1555	0.4376	-0.0657	0.2200	0.0317
35	-0.0297	0.3772	-0.0211	0.1436	0.0192	54	0.4807	-0.2671	0.3145	0.4013	0.0581
36	-0.0438	0.0548	0.1139	0.0179	0.0024	55	-0.3718	-0.0745	-0.1646	0.1709	0.0249
37	-0.0424	0.3356	0.4271	0.2969	0.0402	56	-0.6865	-0.1186	-0.1309	0.5024	0.0732
38	-0.3430	0.1373	-0.2270	0.1880	0.0255	57	0.4876	-0.0037	0.2160	0.2844	0.0416
39	-0.0737	0.6642	0.2230	0.4963	0.0678	58	1.1414	0.1874	0.5087	1.5968	0.2341
40	0.1114	0.1828	0.0452	0.0479	0.0066	59	-0.3308	0.1768	-0.0847	0.1479	0.0218
41	-0.7785	-0.1410	-0.3545	0.7516	0.1032	60	0.0358	0.2753	0.0225	0.0776	0.0115
42	-0.3319	-0.7111	-0.2274	0.6675	0.0919	61	-0.0943	0.0769	-0.0767	0.0207	0.0031
43	-0.0045	-0.2579	-0.0600	0.0702	0.0097	62	-0.5316	-0.5576	0.0599	0.5971	0.0891
44	-0.2882	0.5270	-0.1487	0.3829	0.0535	63	0.1006	0.0372	-0.0607	0.0152	0.0023
45	0.4438	-0.2006	0.2483	0.2988	0.0418	64	0.0889	0.0702	0.2573	0.0790	0.0118
46	-0.2748	-0.0401	-0.2169	0.1242	0.0175	65	0.3814	0.2912	0.3630	0.3620	0.0544

66 0.1034 0.2210 -0.0968 0.0689 0.0104

67 -0.1785 0.0144 -0.0328 0.0332 0.0050

68 0.1086 -0.3508 0.0017 0.1349 0.0204

69 -0.0815 -0.0872 -0.0287 0.0151 0.0023

70 -0.1663 -0.3458 -0.2720 0.2213 0.0336

71 0.1937 -0.0784 -0.0947 0.0526 0.0081

72 0.1603 -0.1589 -0.0458 0.0530 0.0081

73 -0.2614 0.0051 -0.1235 0.0836 0.0129

74 -0.1463 -0.0617 -0.1349 0.0434 0.0067

75 -0.1636 -0.0449 -0.0939 0.0376 0.0058

76 -0.6941 0.2595 -0.2143 0.5951 0.0923

77 0.2351 -0.2764 0.0490 0.1341 0.0208

78 0.4666 -0.0753 0.1280 0.2398 0.0374

79 -1.0351 -0.2807 -0.4419 1.3455 0.2105

80 0.5221 -0.2967 0.3007 0.4511 0.0706

81 0.1706 0.5648 0.0161 0.3483 0.0548

82 0.0683 0.2689 0.0062 0.0770 0.0121

83 0.1180 0.1013 0.0429 0.0260 0.0041

84 -0.7887 -0.0387 -0.0668 0.6280 0.0994

85 0.2650 -0.1416 0.0904 0.0985 0.0156

86 0.0947 0.0459 -0.0042 0.0111 0.0018

87 -0.0616 0.0085 0.0710 0.0089 0.0014

88 0.0555 -0.1500 0.0060 0.0256 0.0041

89 -0.0389 0.1657 0.1694 0.0576 0.0092

90 -0.6147 0.0586 -0.1031 0.3919 0.0628

91 -0.5022 -0.0463 -0.1187 0.2685 0.0430

92 0.2787 -0.0506 0.0970 0.0896 0.0144

93 -0.1714 0.2452 -0.0721 0.0947 0.0152

94 0.2970 -0.2674 -0.0976 0.1693 0.0272

95 -0.1973 -0.4732 -0.0737 0.2683 0.0433

96 0.0387 -0.0752 -0.1899 0.0432 0.0070

97 0.1033 0.5879 -0.2224 0.4058 0.0659

98 0.1205 -0.0293 0.2650 0.0856 0.0139

99 0.1578 0.4589 0.0483 0.2378 0.0388

100 -0.2759 -0.1556 -0.0913 0.1087 0.0177

Ground to excited state transition velocity dipole moments (Au):

state X Y Z Dip. S. Osc.

1 -0.1270 -0.0461 0.0138 0.0185 0.1144

2	0.0823	-0.0015	0.0032	0.0068	0.0387
3	-0.2007	0.0936	0.0284	0.0498	0.2604
4	-0.0692	-0.0163	0.0238	0.0056	0.0280
5	-0.0176	0.1084	0.0128	0.0122	0.0586
6	-0.0338	0.0385	0.0698	0.0075	0.0352
7	-0.0888	-0.1377	0.0294	0.0277	0.1286
8	-0.0968	-0.1754	0.0191	0.0405	0.1838
9	-0.0225	-0.0582	-0.0261	0.0046	0.0200
10	0.0687	0.1169	0.0107	0.0185	0.0796
11	0.0975	0.0193	-0.0119	0.0100	0.0425
12	0.0510	0.0141	0.0834	0.0097	0.0409
13	-0.1451	0.0782	-0.0538	0.0301	0.1231
14	-0.0528	-0.1572	-0.0531	0.0303	0.1224
15	-0.0852	0.1133	-0.0251	0.0207	0.0829
16	-0.0757	-0.0153	-0.0401	0.0076	0.0300
17	0.0441	-0.0645	0.0036	0.0061	0.0240
18	0.0144	-0.0744	0.0402	0.0074	0.0282
19	-0.0575	0.0354	-0.0092	0.0046	0.0176
20	0.0679	-0.1533	0.0052	0.0281	0.1053
21	0.1269	0.0539	0.0736	0.0244	0.0905
22	-0.0773	-0.2443	0.0096	0.0657	0.2431
23	-0.0387	-0.0676	0.0230	0.0066	0.0242
24	-0.0264	0.0973	-0.0406	0.0118	0.0430
25	0.0498	0.0375	0.0450	0.0059	0.0213
26	-0.0716	-0.0842	-0.0080	0.0123	0.0442
27	0.1356	-0.3889	0.0457	0.1717	0.6069
28	-0.0592	-0.0641	0.0263	0.0083	0.0288
29	0.0974	0.0292	0.0338	0.0115	0.0397
30	-0.0649	0.0469	-0.0066	0.0065	0.0222
31	0.0104	-0.1446	-0.0066	0.0211	0.0722
32	0.0011	-0.0244	0.0174	0.0009	0.0031
33	-0.0170	0.1590	-0.0307	0.0265	0.0896
34	-0.0652	0.0222	-0.0304	0.0057	0.0190
35	0.0057	-0.0756	0.0054	0.0058	0.0192
36	0.0086	-0.0112	-0.0227	0.0007	0.0024
37	0.0087	-0.0675	-0.0867	0.0121	0.0399
38	0.0698	-0.0281	0.0458	0.0078	0.0254
39	0.0152	-0.1364	-0.0457	0.0209	0.0681

40	-0.0237	-0.0372	-0.0090	0.0020	0.0066	59	0.0729	-0.0390	0.0186	0.0072	0.0217
41	0.1592	0.0290	0.0729	0.0315	0.1019	60	-0.0092	-0.0611	-0.0051	0.0038	0.0115
42	0.0678	0.1471	0.0465	0.0284	0.0917	61	0.0223	-0.0170	0.0170	0.0011	0.0032
43	0.0006	0.0527	0.0129	0.0029	0.0095	62	0.1177	0.1246	-0.0131	0.0295	0.0880
44	0.0600	-0.1102	0.0316	0.0167	0.0533	63	-0.0220	-0.0083	0.0127	0.0007	0.0021
45	-0.0924	0.0418	-0.0515	0.0129	0.0412	64	-0.0199	-0.0156	-0.0572	0.0039	0.0116
46	0.0582	0.0085	0.0462	0.0056	0.0176	65	-0.0858	-0.0658	-0.0817	0.0184	0.0543
47	0.0416	0.0956	-0.0235	0.0114	0.0360	66	-0.0230	-0.0500	0.0217	0.0035	0.0103
48	0.1986	-0.0549	0.0472	0.0447	0.1399	67	0.0393	-0.0039	0.0071	0.0016	0.0048
49	0.0695	0.0120	0.0792	0.0112	0.0351	68	-0.0249	0.0793	-0.0001	0.0069	0.0203
50	0.0062	-0.0356	0.0009	0.0013	0.0041	69	0.0189	0.0196	0.0070	0.0008	0.0023
51	-0.0341	-0.0968	-0.0254	0.0112	0.0348	70	0.0381	0.0786	0.0613	0.0114	0.0334
52	0.0381	0.1062	-0.0184	0.0131	0.0406	71	-0.0446	0.0181	0.0221	0.0028	0.0082
53	0.0335	-0.0946	0.0143	0.0103	0.0317	72	-0.0357	0.0365	0.0102	0.0027	0.0079
54	-0.1041	0.0586	-0.0681	0.0189	0.0581	73	0.0604	-0.0013	0.0285	0.0045	0.0129
55	0.0809	0.0159	0.0359	0.0081	0.0247	74	0.0344	0.0142	0.0311	0.0024	0.0068
56	0.1485	0.0250	0.0282	0.0235	0.0717	75	0.0388	0.0104	0.0215	0.0021	0.0060
57	-0.1075	0.0007	-0.0478	0.0139	0.0421	76	0.1605	-0.0602	0.0494	0.0318	0.0912
58	-0.2508	-0.0416	-0.1116	0.0771	0.2337	77	-0.0541	0.0639	-0.0117	0.0071	0.0205

78	-0.1089	0.0178	-0.0296	0.0131	0.0372
79	0.2422	0.0657	0.1036	0.0737	0.2094
80	-0.1229	0.0697	-0.0714	0.0251	0.0711
81	-0.0400	-0.1332	-0.0035	0.0194	0.0547
82	-0.0158	-0.0637	-0.0022	0.0043	0.0122
83	-0.0281	-0.0249	-0.0101	0.0015	0.0043
84	0.1869	0.0086	0.0163	0.0353	0.0991
85	-0.0624	0.0339	-0.0207	0.0055	0.0154
86	-0.0219	-0.0108	0.0008	0.0006	0.0017
87	0.0136	-0.0023	-0.0163	0.0005	0.0013
88	-0.0132	0.0360	-0.0013	0.0015	0.0041
89	0.0089	-0.0395	-0.0402	0.0033	0.0090
90	0.1470	-0.0147	0.0249	0.0225	0.0623
91	0.1202	0.0116	0.0284	0.0154	0.0426
92	-0.0672	0.0114	-0.0235	0.0052	0.0144
93	0.0415	-0.0587	0.0176	0.0055	0.0152
94	-0.0713	0.0642	0.0233	0.0098	0.0269
95	0.0479	0.1147	0.0177	0.0158	0.0434
96	-0.0088	0.0183	0.0454	0.0025	0.0068
97	-0.0255	-0.1430	0.0536	0.0240	0.0657
98	-0.0296	0.0071	-0.0636	0.0050	0.0136
99	-0.0386	-0.1123	-0.0115	0.0142	0.0388
100	0.0677	0.0383	0.0228	0.0066	0.0179

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	-0.0554	0.2542	0.9273
2	-0.0733	0.1061	-0.1874
3	-0.1301	-0.3612	2.2585
4	-0.0816	0.1574	1.1020
5	0.0597	-0.1930	0.3610
6	-0.3917	-0.0912	2.2764
7	-0.1345	0.1425	1.8269
8	0.0129	0.7607	0.4327
9	-0.0870	0.0476	-0.2112
10	0.0802	-0.0585	-0.3599
11	-0.0014	-0.2307	-0.9175
12	-0.3245	-0.0713	1.9348
13	0.0427	-0.5006	0.1044
14	0.0917	0.0682	-1.1035
15	-0.1051	-0.0671	-0.3456
16	0.0654	-0.1726	-0.6669
17	-0.1304	-0.1249	-0.6611
18	-0.1350	0.1464	1.0667
19	0.1895	0.1813	-0.1885
20	-0.0218	-0.1320	0.3896
21	-0.1537	0.0142	0.4226

22	0.0472	0.6582	0.1143
23	-0.0975	0.4403	1.0824
24	-0.0609	-0.0750	0.0154
25	0.1123	-0.2652	0.2998
26	-0.0390	0.0128	0.3927
27	-0.0242	0.4468	-0.0922
28	-0.0037	0.7538	0.4574
29	-0.1433	-0.0695	-0.6679
30	-0.0395	-0.2977	0.3033
31	0.2358	0.4045	-1.3042
32	-0.2119	0.0510	-0.0351
33	-0.0465	-0.3114	-0.4434
34	0.2046	-0.2639	-0.1964
35	0.5686	0.3194	-0.3460
36	-0.0766	-0.0225	-0.0238
37	-0.3724	0.4672	-0.0800
38	0.2458	0.1710	-0.0281
39	-0.1115	0.6353	-0.6228
40	0.1123	0.2062	-0.4168
41	0.1435	-0.0167	0.4699
42	0.2514	-0.3866	0.0167
43	0.3261	-0.3327	-0.4642
44	0.3139	0.5141	-0.0654
45	-0.3619	-0.2840	-0.0456
46	-0.1805	0.1183	-0.2104
47	-0.0714	-0.4377	-0.2980
48	-0.0997	0.0586	0.0863
49	-0.0620	0.0010	-0.0140
50	0.0159	0.0672	0.0382
51	-0.0468	-0.2552	-0.1484
52	-0.0965	0.0909	-0.3467
53	0.1624	-0.1894	-0.3429
54	0.1651	-0.2256	-0.3702
55	0.1598	-0.0110	-0.0358
56	0.0284	-0.0700	-0.0515
57	0.0797	0.1917	-0.5657
58	-0.1806	0.1755	-0.3073
59	0.0247	0.1624	0.1370
60	-0.0360	0.0404	-0.0357
61	-0.2378	-0.2020	-0.2767
62	-0.1329	-0.2527	0.4746
63	0.0083	-0.0348	0.0023
64	0.1135	0.0062	-0.1722
65	-0.1579	0.0317	-0.6374
66	-0.0591	-0.1728	-0.1473
67	0.0428	-0.1591	-0.0893
68	0.4229	0.3118	0.0907
69	-0.4078	0.2727	-0.2694
70	-0.3241	0.5223	0.1502
71	0.0541	0.1106	-0.2380
72	-0.2130	-0.3619	-0.1731
73	0.2351	-0.4425	-0.1017
74	-0.0976	0.3643	-0.2395
75	-0.1512	-0.2334	-0.0249
76	-0.0604	-0.0373	0.1535
77	-0.1019	-0.0097	0.0185
78	0.5083	-0.2469	0.0626
79	-0.1561	-0.0103	0.4723
80	-0.2405	0.1910	-0.3876
81	-0.1318	0.0756	0.1088
82	-0.0160	0.0092	-0.1438
83	0.1090	-0.3499	0.0257

84	-0.0242	0.2083	0.0226
85	0.1558	-0.1164	0.1047
86	-0.0486	0.0452	0.2194
87	0.0987	0.2723	-0.3833
88	-0.1097	-0.3621	0.4886
89	-0.0579	-0.1193	-0.0551
90	-0.1392	0.4696	0.2000
91	-0.2247	0.1997	0.1428
92	-0.0007	0.0093	-0.1510
93	-0.0102	0.2456	0.3750
94	0.0571	-0.2001	0.0833
95	-0.0772	-0.1516	0.3310
96	-0.0735	-0.3437	0.2164
97	-0.1320	-0.0886	0.0405
98	0.1571	-0.2413	-0.0838
99	0.2078	0.0445	0.0466
100	0.0937	0.0013	-0.0534

C-29 (S_1 state)

C	3.18532	0.69681	0.34572
C	4.10685	-0.36792	0.42652
C	3.76684	-1.63986	0.04175
C	1.82846	0.40370	-0.07032
H	5.10492	-0.16231	0.78934
H	4.48870	-2.44194	0.12151
C	2.72959	3.09255	0.52089
C	3.58816	2.02736	0.63360
C	0.89226	1.45533	0.06346
C	1.36989	2.80775	0.22575
H	3.04775	4.11119	0.68112
H	4.61914	2.19149	0.91594
C	1.53165	-0.87459	-0.65016
C	2.49489	-1.92485	-0.54250
C	0.07539	-2.26219	-1.78175
C	2.15590	-3.18483	-1.04838
C	0.91449	-3.36067	-1.65953
H	2.85908	-4.00217	-0.96599
H	0.61369	-4.32101	-2.05194
C	-1.92520	3.51513	-0.45939
H	-1.93782	4.58871	-0.54548
N	0.39689	3.70601	0.08041
C	-2.99932	2.69181	-0.69639
N	-0.74705	2.96174	-0.12044
H	-3.93328	3.11833	-1.02531
C	-2.90348	1.30575	-0.43519
C	-0.52645	1.58898	-0.01723
C	-4.01461	0.43954	-0.63194
C	-1.67407	0.75637	0.06196
H	-4.91029	0.84503	-1.08045
C	-3.95433	-0.87108	-0.26399
C	-1.68686	-0.55388	0.64171
C	-2.82062	-1.39246	0.42657
H	-4.79882	-1.52431	-0.43682
C	-2.83139	-2.69429	0.95805
H	-0.88001	-2.35997	-2.28368
C	-0.66230	-1.02747	1.48952
C	-0.70840	-2.29733	2.02021
H	0.16593	-0.38317	1.73277
C	-1.78732	-3.15040	1.73711
H	-3.68765	-3.32690	0.76681
H	-1.80997	-4.15002	2.14667
H	0.09135	-2.63589	2.66339
N	0.36377	-1.04242	-1.30914

Excited state information

Excited State 1: Singlet-A 2.6188 eV 473.44 nm f=0.2036 <S**2>=0.000

96 -> 97 0.69721

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1164.42390243

Copying the excited state density for this state as the 1-particle RhoCI density.

Rotatory strengths (velocity)

state XX YY ZZ R(velocity) E-M Angle

1 2.0219 224.5481 -125.1807 33.7965 85.94

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	1.7291	0.4084	-0.1311	3.1738	0.2036

Ground to excited state transition velocity dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-0.1661	-0.0392	0.0128	0.0293	0.2030

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	-0.0607	0.2647	1.1046

C-29·H$^+$ (S_0 state)

C	3.10700	0.92446	0.36210
C	4.14007	-0.05157	0.44293
C	3.93058	-1.35168	0.09981
C	1.79209	0.53985	-0.00899
H	5.11282	0.26740	0.78934
H	4.71369	-2.08929	0.18999
C	2.48585	3.28035	0.45432
C	3.41448	2.29894	0.61143
C	0.76122	1.52985	0.07263
C	1.14815	2.90327	0.17263
H	2.73607	4.32442	0.56946
H	4.43124	2.54857	0.87758
C	1.64836	-0.76942	-0.54812
C	2.68260	-1.73743	-0.45509
C	0.30592	-2.33936	-1.74615
C	2.44163	-3.02717	-0.95729
C	1.25166	-3.33834	-1.58437
H	3.21475	-3.77587	-0.85907
H	1.05651	-4.32317	-1.97513
C	-2.19548	3.39954	-0.44285
H	-2.27384	4.46921	-0.53646
N	0.11329	3.74118	0.02555
C	-3.20002	2.51754	-0.64615
N	-0.95230	2.92564	-0.12107
H	-4.16957	2.88109	-0.94876
C	-3.01539	1.12659	-0.39147
C	-0.65618	1.57089	-0.00508
C	-4.09379	0.21253	-0.54909
C	-1.76169	0.66022	0.06652
H	-5.02874	0.58353	-0.94411
C	-3.94951	-1.10107	-0.22611
C	-1.68173	-0.66500	0.62688
C	-2.76081	-1.56869	0.40178
H	-4.76022	-1.79790	-0.38661
C	-2.65591	-2.89758	0.86658
H	-0.62767	-2.47861	-2.26629
C	-0.61407	-1.09271	1.44656
C	-0.55194	-2.38371	1.91396
H	0.15554	-0.39226	1.72512
C	-1.56190	-3.30774	1.59049
H	-3.46774	-3.58257	0.66471
H	-1.49403	-4.32636	1.94417
H	0.27435	-2.68665	2.54071
N	0.53014	-1.12399	-1.24718
H	-0.17824	-0.41674	-1.39303

Excited state information

Excited State wavelength (nm) Oscillator strength

Transition wavelengths and oscillator strengths

Excited State 1: Singlet-A 2.3036 eV 538.21 nm f=0.0437 <S**2>=0.000

96 -> 97 0.70268

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1164.88706518

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.7810 eV 445.83 nm f=0.0665 <S**2>=0.000

95 -> 97 0.68763

96 -> 98 0.14726

Excited State 3: Singlet-A 3.1966 eV 387.86 nm f=0.0332 <S**2>=0.000

94 -> 97 0.50931

95 -> 99 0.10201

96 -> 98 0.45362

96 -> 99 0.10267

Excited State 4: Singlet-A 3.2975 eV 375.99 nm f=0.1040 <S**2>=0.000

93 -> 97 0.10550

94 -> 97 -0.45998

95 -> 97 -0.10802

96 -> 98 0.49130

Excited State 5: Singlet-A 3.4475 eV 359.64 nm f=0.0666 <S**2>=0.000

93 -> 97 0.21784

95 -> 98 -0.24592

96 -> 99 0.58671

96 ->100 0.14652

Excited State 6: Singlet-A 3.5130 eV 352.93 nm f=0.0109 <S**2>=0.000

93 -> 97 0.56959

95 -> 98 0.33510

96 ->100 -0.22435

Excited State 7: Singlet-A 3.6944 eV 335.60 nm f=0.0737 <S**2>=0.000

93 -> 97 0.25511

95 -> 99 0.10129

96 -> 99 -0.26592

96 ->100 0.55734

Excited State 8: Singlet-A 3.8155 eV 324.95 nm f=0.3666 <S**2>=0.000

92 -> 97 -0.17774

93 -> 97 -0.17935

95 -> 98 0.52418

96 -> 99 0.19074

96 ->100 0.27492

96 ->101 0.10719

Excited State 9: Singlet-A 3.9839 eV 311.21 nm f=0.0798 <S**2>=0.000

95 -> 99 0.59772

95 ->100 -0.14216

96 ->100 -0.14110

96 ->101 -0.27400

Excited State 10: Singlet-A 4.1310 eV 300.13 nm f=0.0082 <S**2>=0.000

94 -> 98 0.62914

95 ->100 0.25768

96 ->101 -0.12108

Excited State 11: Singlet-A 4.1499 eV 298.77 nm f=0.1108 <S**2>=0.000

92 -> 97 0.64665

95 -> 98 0.13563

96 -> 99 0.10055

96 ->101 -0.10747

Excited State 12: Singlet-A 4.1647 eV 297.70 nm f=0.1137 <S**2>=0.000

92 -> 97 0.12498

93 -> 98 -0.20580

94 -> 98 -0.16842

95 -> 99 0.21975

95 ->100 0.51731

96 ->101 0.21323

Excited State 13: Singlet-A 4.3255 eV 286.64 nm f=0.0259 <S**2>=0.000

91 -> 97 0.44438

93 -> 98 0.34619

94 -> 99 -0.15404

95 -> 99 -0.11776

95 ->100 0.19680

96 ->101 -0.25997

Excited State 14: Singlet-A 4.3726 eV 283.55 nm f=0.1655 <S**2>=0.000

91 -> 97 0.42109

92 -> 98 0.10739

93 -> 98 -0.14636

94 -> 98 0.17253

94 -> 99 -0.12148

94 ->100 0.11139

95 ->100 -0.22999

96 ->101 0.36289

Excited State 15: Singlet-A 4.4253 eV 280.17 nm f=0.0445 <S**2>=0.000

91 -> 97 0.15101

93 -> 98 0.14190

94 -> 99 0.63051

94 ->100 0.10055

95 ->100 0.10527

96 ->101 0.11028

Excited State 16: Singlet-A 4.6186 eV 268.45 nm f=0.1355 <S**2>=0.000

91 -> 97 -0.19089

93 -> 98 0.36510

93 -> 99 -0.21092

94 -> 99 -0.15060

94 ->100 0.36183

96 ->101 0.25374

Excited State 17: Singlet-A 4.7082 eV 263.34 nm f=0.0388 <S**2>=0.000

93 -> 99 0.47042

94 ->100 0.25176

96 ->102 -0.41358

Excited State 18: Singlet-A 4.7484 eV 261.11 nm f=0.2621 <S**2>=0.000

93 -> 98 -0.30780

93 -> 99 -0.12657

93 ->100 0.19794

94 ->100 0.44495

95 ->101 -0.19370

96 ->101 -0.14878

96 ->102 0.12359

96 ->103 -0.17521

Excited State 19: Singlet-A 4.7683 eV 260.02 nm f=0.1261 <S**2>=0.000

90 -> 97 0.10754

93 -> 98 -0.13034

93 -> 99 -0.23768

95 ->101 0.53667

96 ->102 -0.25559

96 ->103 -0.11530

Excited State 20: Singlet-A 4.8945 eV 253.31 nm f=0.0156 <S**2>=0.000

89 -> 97 0.11482

90 -> 97 -0.25755

91 -> 98 -0.13804

92 -> 98 0.13817

93 -> 99 0.28941

95 ->101 0.31831

96 ->102 0.36800

Excited State 21: Singlet-A 4.9121 eV 252.40 nm f=0.0097 <S**2>=0.000

89 -> 97 0.18244

90 -> 97 0.53728

92 -> 98 -0.13583

93 -> 99 0.11670

93 ->100 0.10689

96 ->102 0.11185

96 ->103 0.28958

Excited State 22: Singlet-A 4.9646 eV 249.74 nm f=0.0227 <S**2>=0.000

89 -> 97 -0.38836

90 -> 97 -0.18686

92 -> 98 -0.23867

96 ->103 0.45557

Excited State 23: Singlet-A 5.0686 eV 244.61 nm f=0.1297 <S**2>=0.000

89 -> 97 0.39654

90 -> 97 -0.16953

91 -> 98 0.20004

92 -> 98 -0.20292

93 ->100 -0.31656

94 ->101 0.12809

95 ->102 -0.12732

96 ->101 -0.10206

96 ->103 0.14053

Excited State 24: Singlet-A 5.0925 eV 243.46 nm f=0.0091 <S**2>=0.000

89 -> 97 0.24871

90 -> 97 -0.10500

91 -> 98 0.21703

92 -> 98 0.30427

93 ->100 0.36844

94 ->101 -0.11467

95 ->102 0.13275

96 ->102 -0.14193

96 ->103 0.23602

Excited State 25: Singlet-A 5.1438 eV 241.03 nm f=0.3342 <S**2>=0.000

90 -> 97 -0.10643

91 -> 98 0.13971

92 -> 98 -0.32822

92 -> 99 -0.11318

92 ->100 -0.13541

93 ->100 0.33636

94 ->101 0.13012

95 ->102 0.10646

95 ->103 0.19881

96 ->103 -0.16880

96 ->104 -0.22116

Excited State 26: Singlet-A 5.1996 eV 238.45 nm f=0.0309 <S**2>=0.000

88 -> 97 0.23088

89 -> 97 -0.13849

91 -> 98 0.20800

92 -> 98 0.12577

94 ->101 0.33417

95 ->102 0.23198

96 ->102 0.12287

96 ->104 0.33995

Excited State 27: Singlet-A 5.2026 eV 238.31 nm f=0.1417 <S**2>=0.000

88 -> 97 -0.15470

91 -> 98 -0.16540

92 -> 98 -0.20157

92 -> 99 -0.13338

93 ->100 0.12788

94 ->101 -0.14503

96 ->104 0.53375

Excited State 28: Singlet-A 5.2617 eV 235.64 nm f=0.0882 <S**2>=0.000

88 -> 97 0.29008

91 -> 98 -0.19436

92 -> 98 -0.12873

92 -> 99 0.52405

95 ->102 0.11191

95 ->103 -0.11441

Excited State 29: Singlet-A 5.2801 eV 234.82 nm f=0.0369 <S**2>=0.000

88 -> 97 0.51118

91 -> 98 0.14897

92 -> 99 -0.16284

94 ->101 -0.28228

95 ->102 -0.27535

Excited State 30: Singlet-A 5.3512 eV 231.69 nm f=0.1958 <S**2>=0.000

88 -> 97 0.13768

91 -> 98 -0.23598

92 ->100 -0.10702

93 ->100 -0.14677

94 ->101 -0.30167

94 ->102 -0.13490

95 ->102 0.39907

95 ->103 0.20041

Excited State 31: Singlet-A 5.4041 eV 229.43 nm f=0.0329 <S**2>=0.000

87 -> 97 0.14903

91 -> 98 -0.24028

91 -> 99 0.22593

92 -> 98 0.14337

94 ->101 0.18765

95 ->102 -0.25551

95 ->103 0.41977

Excited State 32: Singlet-A 5.5090 eV 225.06 nm f=0.0358 <S**2>=0.000

87 -> 97 0.10117

88 -> 97 -0.10653

91 -> 99 -0.23764

92 -> 99 0.26432

93 ->101 0.11071

94 ->101 -0.15476

95 ->102 -0.10072

95 ->103 0.30335

96 ->105 0.21139

96 ->106 -0.30071

Excited State 33: Singlet-A 5.5412 eV 223.75 nm f=0.0230 <S**2>=0.000

87 -> 97 -0.16819

91 -> 98 0.15713

91 -> 99 0.50255

92 ->100 0.16668

93 ->101 -0.22806

94 ->101 -0.12549

96 ->105 0.11373

96 ->106 -0.18198

Excited State 34: Singlet-A 5.5892 eV 221.83 nm f=0.1401 <S**2>=0.000

87 -> 97 0.26175

91 -> 99 -0.18005

91 ->100 0.12778

92 ->100 0.47098

93 ->101 -0.22670

94 ->102 -0.18690

95 ->103 -0.10669

Excited State 35: Singlet-A 5.6168 eV 220.74 nm f=0.0757 <S**2>=0.000

87 -> 97 0.36225

91 ->100 0.22399

92 ->100 -0.33055

93 ->101 -0.24337

95 ->103 -0.17490

95 ->104 -0.22162

Excited State 36: Singlet-A 5.6588 eV 219.10 nm f=0.0209 <S**2>=0.000

87 -> 97 -0.27447

91 -> 98 -0.15462

95 ->104 -0.19444

96 ->105 0.47718

96 ->107 0.17538

Excited State 37: Singlet-A 5.6613 eV 219.00 nm f=0.0413 <S**2>=0.000

92 ->100 -0.17829

93 ->101 -0.19157

95 ->103 -0.12248

95 ->104 0.57891

Excited State 38: Singlet-A 5.6961 eV 217.67 nm f=0.0180 <S**2>=0.000

87 -> 97 0.23710

91 -> 98 0.12868

93 ->101 0.10101

94 ->102 0.10136

95 ->104 0.15447

96 ->105 0.33309

96 ->106 0.42597

Excited State 39: Singlet-A 5.7282 eV 216.45 nm f=0.0084 <S**2>=0.000

91 ->100 -0.14147

93 ->101 -0.14732

95 ->104 0.11718

96 ->104 0.10720

96 ->105 -0.16430

96 ->106 0.12422

96 ->107 0.58177

Excited State 40: Singlet-A 5.7481 eV 215.69 nm f=0.0468 <S**2>=0.000

90 -> 98 0.36655

91 -> 99 0.11808

91 ->100 0.16388

93 ->101 0.33544

94 ->103 0.13962

96 ->106 -0.18128

96 ->107 0.25768

Excited State 41: Singlet-A 5.7924 eV 214.05 nm f=0.0129 <S**2>=0.000

86 -> 97 0.13867

89 -> 98 0.31642

90 -> 98 0.43190

91 ->100 -0.31461

93 ->101 -0.15103

94 ->103 -0.12180

Excited State 42: Singlet-A 5.8080 eV 213.47 nm f=0.0032 <S**2>=0.000

86 -> 97 0.29963

87 -> 97 0.11245

89 -> 98 -0.18998

90 -> 98 -0.13398

91 ->100 -0.27742

92 -> 99 -0.12862

93 ->102 -0.10348

94 ->102 0.29479

96 ->106 -0.22722

Excited State 43: Singlet-A 5.8427 eV 212.20 nm f=0.1141 <S**2>=0.000

86 -> 97 0.54161

93 ->101 0.11679

94 ->102 -0.35300

Excited State 44: Singlet-A 5.8789 eV 210.90 nm f=0.0127 <S**2>=0.000

89 -> 98 -0.17556

91 ->100 -0.13517

96 ->108 0.61858

Excited State 45: Singlet-A 5.9391 eV 208.76 nm f=0.3945 <S**2>=0.000

86 -> 97 0.21813

87 -> 97 -0.10034

89 -> 98 0.16775

89 -> 99 -0.15369

90 -> 99 -0.19156

91 ->100 0.28604

93 ->102 0.10918

94 ->102 0.32423

94 ->103 -0.14796

96 ->108 0.20507

Excited State 46: Singlet-A 5.9544 eV 208.22 nm f=0.0616 <S**2>=0.000

85 -> 97 0.44686

89 -> 99 -0.22393

90 -> 99 -0.29651

94 ->102 -0.13936

94 ->103 -0.24719

Excited State 47: Singlet-A 5.9742 eV 207.53 nm f=0.0507 <S**2>=0.000

85 -> 97 0.31044

89 -> 99 0.26481

90 -> 99 0.38951

91 ->100 0.11788

94 ->102 0.10213

94 ->103 -0.27053

96 ->109 0.10995

Excited State 48: Singlet-A 5.9857 eV 207.13 nm f=0.0200 <S**2>=0.000

85 -> 97 0.16778

89 -> 98 0.39730

90 -> 98 -0.20045

92 ->101 -0.21147

93 ->102 -0.11293

94 ->103 0.29076

96 ->108 0.10195

96 ->109 -0.20923

Excited State 49: Singlet-A 6.0023 eV 206.56 nm f=0.0784 <S**2>=0.000

85 -> 97 -0.23050

89 -> 98 0.21323

90 -> 98 -0.16178

93 ->102 -0.17433

96 ->109 0.47850

Excited State 50: Singlet-A 6.0163 eV 206.08 nm f=0.0115 <S**2>=0.000

85 -> 97 0.27522

93 ->101 -0.12456

93 ->102 0.12357

94 ->103 0.35579

96 ->109 0.39505

Excited State 51: Singlet-A 6.0727 eV 204.17 nm f=0.0578 <S**2>=0.000

84 -> 97 -0.15006

88 -> 98 -0.33407

91 ->100 -0.10291

92 ->101 -0.22871

93 ->102 0.41704

95 ->105 0.15212

95 ->106 -0.11796

Excited State 52: Singlet-A 6.0950 eV 203.42 nm f=0.0195 <S**2>=0.000

93 ->102 -0.25904

95 ->105 0.55872

96 ->112 -0.10807

Excited State 53: Singlet-A 6.1090 eV 202.95 nm f=0.0072 <S**2>=0.000

88 -> 98 0.10120

92 ->101 -0.14216

93 ->102 0.12745

94 ->104 -0.22033

95 ->105 0.10962

95 ->106 0.50026

95 ->107 0.18947

96 ->111 0.12643

Excited State 54: Singlet-A 6.1479 eV 201.67 nm f=0.0022 <S**2>=0.000

96 ->110 0.62216

96 ->111 -0.16334

96 ->112 -0.16432

Excited State 55: Singlet-A 6.1671 eV 201.04 nm f=0.0073 <S**2>=0.000

84 -> 97 0.26961

89 -> 99 -0.12460

90 -> 99 0.13150

94 ->104 0.31623

95 ->105 0.18031

95 ->106 0.27175

95 ->107 -0.23722

96 ->110 -0.10091

96 ->111 -0.10300

96 ->113 -0.12527

Excited State 56: Singlet-A 6.1752 eV 200.78 nm f=0.0018 <S**2>=0.000

84 -> 97 0.30295

88 -> 98 -0.20398

89 -> 99 -0.14608

90 -> 99 0.12130

94 ->104 -0.25118

95 ->105 -0.11712

95 ->107 0.35839

96 ->108 0.11622

96 ->111 -0.15527

Excited State 57: Singlet-A 6.1924 eV 200.22 nm f=0.0207 <S**2>=0.000

82 -> 97 0.11939

84 -> 97 0.28018

88 -> 98 -0.17853

89 -> 99 0.17281

90 -> 99 -0.10089

92 ->101 0.10711

95 ->107 -0.11462

96 ->110 0.18824

96 ->111 0.34544

96 ->112 0.29347

Excited State 58: Singlet-A 6.2075 eV 199.73 nm f=0.0404 <S**2>=0.000

84 -> 97 0.11754

89 -> 98 -0.11106

89 -> 99 0.24982

90 -> 99 -0.17088

92 ->101 -0.27569

93 ->102 -0.22073

93 ->103 0.31358

94 ->103 -0.13587

95 ->106 0.11181

95 ->108 -0.11033

96 ->112 -0.16014

Excited State 59: Singlet-A 6.2265 eV 199.12 nm f=0.0048 <S**2>=0.000

82 -> 97 -0.11204

88 -> 98 -0.16101

89 -> 99 0.22332

90 -> 99 -0.16459

91 ->101 -0.10736

92 ->101 0.30531

93 ->103 0.14549

94 ->104 0.25368

95 ->106 0.12042

95 ->107 0.28744

96 ->111 -0.12872

Excited State 60: Singlet-A 6.2406 eV 198.67 nm f=0.0111 <S**2>=0.000

89 -> 99 -0.11581

92 ->101 -0.26434

94 ->104 0.38289

95 ->107 0.33451

96 ->111 0.27830

Excited State 61: Singlet-A 6.2556 eV 198.20 nm f=0.0086 <S**2>=0.000

92 ->101 -0.21210

93 ->103 -0.20949

96 ->111 -0.36127

96 ->112 0.42756

Excited State 62: Singlet-A 6.2950 eV 196.96 nm f=0.0195 <S**2>=0.000

81 -> 97 0.13596

82 -> 97 -0.34629

83 -> 97 -0.18577

88 -> 98 -0.10008

89 -> 99 -0.20968

90 -> 99 0.12578

91 ->101 0.34806

93 ->103 0.19891

96 ->112 0.19067

Excited State 63: Singlet-A 6.3037 eV 196.68 nm f=0.0756 <S**2>=0.000

82 -> 97 0.21951

87 -> 98 -0.12928

88 -> 98 0.23616

93 ->103 0.30248

95 ->108 0.34929

96 ->111 -0.13573

96 ->112 0.11830

96 ->114 0.12294

Excited State 64: Singlet-A 6.3163 eV 196.29 nm f=0.0213 <S**2>=0.000

81 -> 97 -0.28693

82 -> 97 -0.27950

83 -> 97 0.22297

90 -> 99 -0.10908

90 ->100 0.22877

95 ->108 0.36720

95 ->109 -0.10295

Excited State 65: Singlet-A 6.3289 eV 195.90 nm f=0.0170 <S**2>=0.000

81 -> 97 0.26565

83 -> 97 -0.24335

86 -> 98 0.10809

87 -> 98 0.12966

88 -> 98 -0.10584

88 -> 99 0.14861

89 -> 99 0.11510

89 ->100 -0.12781

90 ->100 -0.18433

93 ->103 -0.14324

95 ->108 0.32931

95 ->109 -0.10581

96 ->113 -0.10230

Excited State 66: Singlet-A 6.3401 eV 195.56 nm f=0.0486 <S**2>=0.000

81 -> 97 0.13885

83 -> 97 -0.25123

84 -> 97 0.21755

89 ->100 0.27168

90 ->100 0.41739

91 ->101 -0.14459

93 ->103 -0.10199

95 ->108 -0.11814

96 ->113 -0.12337

Excited State 67: Singlet-A 6.3490 eV 195.28 nm f=0.0172 <S**2>=0.000

82 -> 97 -0.18310

84 -> 97 0.16195

88 -> 99 -0.18359

90 ->100 -0.10009

91 ->101 -0.15007

94 ->104 0.10542

96 ->113 0.51624

Excited State 68: Singlet-A 6.3701 eV 194.63 nm f=0.1075 <S**2>=0.000

81 -> 97 0.14944

82 -> 97 0.29668

84 -> 97 -0.15842

88 -> 98 -0.22557

88 -> 99 -0.14710

90 ->100 0.29580

91 ->101 0.19439

96 ->112 -0.11054

96 ->113 0.18078

Excited State 69: Singlet-A 6.3895 eV 194.04 nm f=0.0878 <S**2>=0.000

87 -> 98 0.18683

88 -> 98 0.19818

88 -> 99 0.11629

89 -> 99 0.12068

89 ->100 0.13156

91 ->101 0.39008

95 ->106 -0.12059

96 ->112 -0.10855

96 ->114 -0.23587

96 ->115 -0.14378

Excited State 70: Singlet-A 6.4317 eV 192.77 nm f=0.0655 <S**2>=0.000

86 -> 98 0.21233

86 -> 99 -0.11638

87 -> 98 0.10299

88 -> 99 0.33382

90 ->100 0.11114

91 ->101 -0.12852

93 ->103 0.13856

93 ->104 0.21779

95 ->109 -0.27258

95 ->113 0.10248

96 ->113 0.20650

Excited State 71: Singlet-A 6.4397 eV 192.53 nm f=0.0235 <S**2>=0.000

86 -> 98 0.28287

86 -> 99 -0.13104

87 -> 98 0.22247

89 ->100 0.13005

95 ->109 0.42835

96 ->114 0.18033

96 ->115 0.17641

Excited State 72: Singlet-A 6.4518 eV 192.17 nm f=0.0116 <S**2>=0.000

81 -> 97 -0.11405

86 -> 98 -0.13559

87 -> 98 -0.17743

88 -> 99 0.25951

89 ->100 -0.17517

90 ->100 0.10663

91 ->101 -0.10974

95 ->108 0.11625

95 ->109 0.35971

96 ->114 -0.30139

Excited State 73: Singlet-A 6.4942 eV 190.91 nm f=0.0326 <S**2>=0.000

81 -> 97 0.14481

83 -> 97 0.15604

86 -> 98 -0.10472

87 -> 98 -0.11639

89 ->100 0.47767

90 ->100 -0.16241

93 ->102 -0.11727

96 ->114 -0.15114

Excited State 74: Singlet-A 6.5142 eV 190.33 nm f=0.0319 <S**2>=0.000

81 -> 97 0.23810

83 -> 97 0.21228

86 -> 98 -0.16575

87 -> 99 0.10230

93 ->104 0.47049

95 ->109 0.12434

Excited State 75: Singlet-A 6.5231 eV 190.07 nm f=0.0098 <S**2>=0.000

81 -> 97 -0.25623

83 -> 97 -0.25649

86 -> 98 0.17326

87 -> 99 -0.13461

88 -> 99 -0.21893

93 ->104 0.38719

96 ->113 -0.10764

Excited State 76: Singlet-A 6.5407 eV 189.56 nm f=0.1437 <S**2>=0.000

81 -> 97 -0.18082

83 -> 97 -0.20551

85 -> 98 0.18530

86 -> 98 -0.20760

88 -> 98 -0.10859

88 -> 99 0.24917

92 ->102 -0.12012

96 ->114 0.33624

Excited State 77: Singlet-A 6.5599 eV 189.00 nm f=0.0071 <S**2>=0.000

94 ->105 0.16836

94 ->106 0.12201

94 ->107 0.10525

95 ->110 0.44172

96 ->115 0.24768

96 ->116 -0.35156

96 ->117 0.10046

Excited State 78: Singlet-A 6.5688 eV 188.75 nm f=0.0062 <S**2>=0.000

94 ->105 -0.12964

94 ->107 -0.15131

95 ->110 -0.35263

96 ->114 -0.26336

96 ->115 0.43359

96 ->116 -0.13085

96 ->117 0.11143

Excited State 79: Singlet-A 6.5940 eV 188.03 nm f=0.0098 <S**2>=0.000

85 -> 98 0.12672

86 -> 98 -0.15269

87 -> 98 0.22856

92 ->102 0.11977

94 ->106 -0.15617

95 ->110 0.10506

95 ->112 -0.15452

96 ->114 -0.10268

96 ->115 0.24431

96 ->116 0.39660

Excited State 80: Singlet-A 6.6097 eV 187.58 nm f=0.0363 <S**2>=0.000

87 -> 98 -0.11690

88 ->100 0.10476

92 ->102 -0.30722

94 ->105 -0.15942

94 ->106 0.26662

95 ->110 0.19640

95 ->111 0.16344

96 ->115 0.10345

96 ->116 0.33039

Excited State 81: Singlet-A 6.6232 eV 187.20 nm f=0.0259 <S**2>=0.000

84 -> 98 0.10953

85 -> 98 0.40664

85 -> 99 -0.19935

87 -> 98 0.16936

88 -> 99 -0.16408

88 ->100 0.10190

94 ->105 -0.21375

94 ->106 0.16194

96 ->115 -0.17217

96 ->116 -0.14283

Excited State 82: Singlet-A 6.6527 eV 186.37 nm f=0.0378 <S**2>=0.000

87 -> 98 0.10952

92 ->102 -0.14036

94 ->105 0.30659

95 ->110 -0.10234

95 ->111 0.25585

96 ->115 -0.18039

96 ->117 0.42956

Excited State 83: Singlet-A 6.6554 eV 186.29 nm f=0.0110 <S**2>=0.000

85 -> 98 0.25771

85 -> 99 -0.11379

87 -> 98 -0.14097

87 -> 99 -0.19150

92 ->102 0.18166

94 ->105 0.16353

94 ->106 -0.15817

95 ->111 0.28745

95 ->112 0.27638

96 ->117 -0.17801

Excited State 84: Singlet-A 6.6722 eV 185.82 nm f=0.0338 <S**2>=0.000

87 -> 98 -0.16375

87 -> 99 -0.14387

88 ->100 0.16236

92 ->102 0.33436

94 ->106 0.12222

95 ->111 -0.24355

96 ->116 0.10433

96 ->117 0.38196

Excited State 85: Singlet-A 6.6847 eV 185.48 nm f=0.0030 <S**2>=0.000

94 ->105 0.31755

94 ->106 0.42578

94 ->107 -0.10285

94 ->108 -0.13285

95 ->110 -0.17210

95 ->112 -0.19537

96 ->117 -0.21482

Excited State 86: Singlet-A 6.6975 eV 185.12 nm f=0.0129 <S**2>=0.000

85 -> 98 -0.17625

86 -> 98 -0.12526

87 -> 98 0.11124

87 -> 99 -0.20753

88 ->100 0.33589

91 ->102 0.13951

92 ->102 0.15488

92 ->103 0.10079

93 ->105 0.10374

94 ->105 -0.11577

95 ->111 0.31128

95 ->112 -0.16007

96 ->118 -0.11310

Excited State 87: Singlet-A 6.7033 eV 184.96 nm f=0.0101 <S**2>=0.000

86 -> 98 -0.11014

87 -> 98 0.17226

87 -> 99 -0.14708

88 ->100 0.15165

92 ->102 -0.13938

94 ->105 0.15256

94 ->106 0.12730

94 ->107 0.27371

95 ->110 -0.12996

95 ->111 -0.18518

95 ->112 0.29974

96 ->118 -0.22754

Excited State 88: Singlet-A 6.7241 eV 184.39 nm f=0.0240 <S**2>=0.000

86 -> 98 -0.11409

87 -> 98 0.10858

91 ->102 0.11043

94 ->107 0.10274

95 ->112 0.10636

96 ->118 0.59960

Excited State 89: Singlet-A 6.7467 eV 183.77 nm f=0.0007 <S**2>=0.000

87 -> 99 0.13643

94 ->105 -0.10041

94 ->107 0.51564

95 ->110 -0.11453

95 ->111 0.19899

95 ->112 -0.18828

96 ->117 0.10361

Excited State 90: Singlet-A 6.7661 eV 183.24 nm f=0.0123 <S**2>=0.000

86 -> 99 0.17200

87 -> 98 0.10347

87 ->100 0.14872

88 ->100 -0.26239

91 ->102 0.11688

91 ->103 -0.15041

92 ->102 0.18877

94 ->105 -0.12714

94 ->106 0.13371

95 ->111 0.13438

95 ->112 0.31721

95 ->113 -0.10944

Excited State 91: Singlet-A 6.7821 eV 182.81 nm f=0.0494 <S**2>=0.000

85 -> 98 0.12651

86 -> 98 0.15282

87 -> 99 0.33341

88 ->100 0.21294

91 ->102 0.39620

95 ->113 -0.19751

Excited State 92: Singlet-A 6.8231 eV 181.71 nm f=0.0388 <S**2>=0.000

90 ->101 -0.17810

91 ->102 0.30691

92 ->103 -0.10677

94 ->108 -0.15793

95 ->113 0.47525

95 ->114 -0.13153

Excited State 93: Singlet-A 6.8324 eV 181.46 nm f=0.0109 <S**2>=0.000

80 -> 97 -0.26001

86 -> 99 -0.16808

87 -> 99 -0.12534

88 ->100 -0.27065

91 ->102 0.30519

92 ->103 0.12111

93 ->106 0.10889

95 ->112 -0.10429

95 ->113 -0.22589

96 ->119 0.10901

Excited State 94: Singlet-A 6.8414 eV 181.23 nm f=0.0034 <S**2>=0.000

80 -> 97 0.13707

96 ->117 -0.12282

96 ->119 0.61683

Excited State 95: Singlet-A 6.8589 eV 180.76 nm f=0.1923 <S**2>=0.000

80 -> 97 0.19501

86 -> 99 0.16578

86 ->100 0.10784

92 ->103 0.50296

95 ->114 -0.22140

96 ->119 -0.13541

Excited State 96: Singlet-A 6.8841 eV 180.10 nm f=0.0412 <S**2>=0.000

80 -> 97 0.28121

87 -> 99 -0.14561

91 ->102 0.12288

92 ->103 -0.17219

94 ->105 0.10168

94 ->108 0.46144

94 ->109 0.12551

95 ->112 -0.10363

96 ->119 -0.10608

Excited State 97: Singlet-A 6.8911 eV 179.92 nm f=0.0997 <S**2>=0.000

80 -> 97 -0.34120

87 -> 99 0.17306

90 ->101 -0.13696

91 ->102 -0.10243

92 ->103 0.19871

93 ->106 -0.14224

94 ->108 0.35084

94 ->109 0.10719

95 ->113 0.15332

Excited State 98: Singlet-A 6.9216 eV 179.13 nm f=0.0736 <S**2>=0.000

87 -> 99 -0.10450

90 ->101 -0.18814

92 ->103 0.19093

93 ->105 -0.22470

95 ->114 0.45322

95 ->115 0.15775

95 ->116 -0.11272

Excited State 99: Singlet-A 6.9316 eV 178.87 nm f=0.0201 <S**2>=0.000

80 -> 97 -0.24473

86 -> 98 0.13710

86 -> 99 0.41666

86 ->100 0.22252

87 -> 99 -0.10054

87 ->100 0.13815

90 ->101 0.13275

91 ->103 0.17321

92 ->103 -0.10820

93 ->105 -0.12091

96 ->120 -0.11801

Excited State 100: Singlet-A 6.9448 eV 178.53 nm f=0.0072 <S**2>=0.000

90 ->101 -0.17023

93 ->105 0.49991

93 ->106 0.29459

95 ->111 -0.11740

95 ->114 0.10325

Rotatory strengths (velocity)

state XX YY ZZ R(velocity) E-M Angle

1 -26.3597 36.4557 -46.4826 -12.1289 98.73

2 66.0800 177.5915 -52.7033 63.6561 77.99

3 -28.1561 -42.4348 -53.9540 -41.5150 150.75

4 156.6506 276.0193 -58.3308 124.7797 71.87

5 8.5387 34.2373 -39.8997 0.9588 89.72

6 22.7565 27.7670 -9.4792 13.6815 80.80

7 262.4370 205.2894 -49.3266 139.4666 69.40

8 -42.6631 454.5357 -204.3882 69.1615 86.38

9 138.1406 62.4543 -28.8495 57.2485 77.22

10 67.2254 88.7260 3.0628 53.0047 57.39

11 -233.8141 -1.4443 -195.6955 -143.6513 143.90

12 -28.5022 30.9398 -26.4342 -7.9989 92.34

13 70.6560 -1.0462 24.2581 31.2893 58.60

14 -96.0169 -28.2025 -41.3036 -55.1743 128.78

15 -59.5585 1.8779 -22.9922 -26.8909 105.26

16 315.0339 -96.5047 54.6208 91.0500 63.70

17 -86.8101 0.3665 -26.2916 -37.5784 114.77

18 -101.5667 -42.7004 -37.3501 -60.5390 106.19

19 40.5386 -39.9954 -10.0154 -3.1574 92.33

20 281.1106 231.2368 4.6347 172.3273 13.11

21 -26.1078 -3.1621 -28.5410 -19.2703 130.24

22 34.3311 -27.4511 -36.2065 -9.7755 97.86

23 -31.3020 -60.2325 44.5654 -15.6564 103.92

24 44.0126 6.2397 -4.2687 15.3279 73.17

25 -349.1172 -27.3658 -113.1675 -163.2168 149.86

26 10.9753 59.4724 -18.5368 17.3036 79.36

27 -143.2987 -4.3735 -34.5799 -60.7507 116.24

28 -137.6419 24.5355 -141.8460 -84.9841 125.27

29 -10.5106 53.5301 -12.9578 10.0206 84.75

30 46.5609 -98.7094 96.7179 14.8565 80.19

31 170.4385 -60.7552 26.4306 45.3713 33.18

32 -120.7956 -9.6372 -22.3720 -50.9349 140.24

33 -106.7758 1.1083 -13.3276 -39.6651 169.22

34 -224.8911 7.9033 -23.8255 -80.2711 129.46

35 -154.9243 40.6988 -140.1886 -84.8047 132.77

36 -37.2665 -39.6174 12.6597 -21.4081 106.34

37 7.5393 -36.2621 -3.3492 -10.6907 105.17

38 64.4631 -68.0591 37.6333 11.3458 57.20

39 -45.0112 -2.6783 -12.2645 -19.9847 151.13

40 -161.6650 -3.0655 -43.7951 -69.5085 147.75

41 62.2982 -18.6544 -13.4772 10.0555 77.66

42 -18.6926 -7.2859 9.2860 -5.5641 147.36

43 -45.0041 -89.7099 -39.2767 -57.9969 130.03

44 12.1485 -4.0454 10.5823 6.2285 66.66

45 111.9065 -442.1310 209.4611 -40.2544 106.46

46 -77.2397 51.7569 19.9676 -1.8384 91.24

47 55.8150 34.3272 90.3319 60.1580 46.47

48 23.1113 0.1439 45.7599 23.0050 37.42

49 -48.8596 -30.4423 20.2737 -19.6761 129.33

50 -4.0624 -22.6655 -8.7631 -11.8304 112.78

51 49.0506 8.3760 79.5351 45.6539 55.34

52 -6.7289 -40.8751 -33.7489 -27.1176 135.56

53 39.3000 -24.1665 -0.9074 4.7420 41.85

54 -3.4787 0.9639 -1.0047 -1.1732 105.17

55 8.8764 -19.4597 21.1641 3.5270 60.25

56 10.8546 -2.9895 3.7174 3.8608 46.98

57 -21.6549 0.6521 44.4958 7.8310 61.26

58 19.3838 9.2099 53.1125 27.2354 74.92

59 21.9524 7.6769 -8.2094 7.1400 63.76

60 -21.7457 14.5338 -5.7159 -4.3093 121.80

61 4.4352 -9.1776 32.2486 9.1687 69.33

62 35.6326 33.7342 18.3579 29.2416 63.98

63 136.4243 7.2046 79.7049 74.4446 52.52

64 15.3984 -37.0681 26.5092 1.6132 81.03

65 -33.2397 -21.7319 22.7499 -10.7406 125.85

66 -12.9755 -28.8407 1.6416 -13.3915 108.51

67 -50.6083 2.5983 17.8848 -10.0418 129.84

68 56.6505 -5.6560 47.0473 32.6806 64.42

69 27.2335 -38.0382 -1.5906 -4.1318 93.24

70 -33.1515 -74.1487 31.5392 -25.2537 149.36

71 -20.3466 -1.0925 10.9884 -3.4835 115.06

72 -12.5746 60.4563 -15.1489 10.9110 60.71

73 -40.2990 -15.3168 3.5833 -17.3442 109.22

74 -48.0941 4.2777 16.7759 -9.0135 106.17

75 16.7580 -12.7117 4.9092 2.9852 78.03

76 75.0042 -11.1606 -46.5561 5.7625 86.62

77 -3.7543 47.2278 2.8778 15.4504 41.65

78 -3.4990 -48.5516 -0.4135 -17.4880 149.88

79 25.2650 30.4919 14.7348 23.4972 11.63

80 41.0172 -121.1926 45.6741 -11.5004 103.12

81 3.0693 -36.6532 33.2378 -0.1154 90.37

82 113.3998 21.2742 28.2128 54.2956 55.32

83 -9.3266 28.7738 9.5338 9.6603 75.58

84 85.6540 -39.8715 41.1532 28.9786 64.37

85 15.9375 6.6575 4.9525 9.1825 17.10

86 1.8537 11.7989 -26.6086 -4.3187 97.77

87 -38.7470 -9.2963 5.9174 -14.0420 132.00

88 24.0847 5.9441 51.0246 27.0178 31.25

89 -4.4317 -7.2692 -3.8823 -5.1944 146.25

90 7.6034 -1.1837 -22.2206 -5.2670 110.77

91 17.3269 25.1992 -25.0825 5.8145 74.23

92 6.4636 -34.9773 -24.5338 -17.6825 147.01

93 28.6733 20.2832 -18.9778 9.9929 58.97

94 -3.2072 13.8794 1.6310 4.1011 53.70

95 -75.5427 -26.9265 116.1655 4.5654 84.38

96 0.6130 35.9182 -38.4483 -0.6390 91.94

97 9.4396 -79.1719 -87.7730 -52.5018 130.50

98 -5.1787 -9.8829 88.4987 24.4790 49.24

99 7.8051 -19.7789 -34.1197 -15.3645 128.01

100 -40.8901 -0.0177 -8.9718 -16.6265 159.19

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	0.8211	0.3112	-0.0535	0.7740	0.0437
2	0.7239	-0.6280	-0.2397	0.9758	0.0665
3	-0.5958	0.2085	-0.1579	0.4233	0.0332
4	-0.8149	0.7016	0.3624	1.2876	0.1040
5	0.8871	0.0410	-0.0160	0.7889	0.0666
6	0.1833	-0.2945	-0.0761	0.1261	0.0109
7	-0.0041	-0.7963	-0.4244	0.8143	0.0737
8	1.4933	1.2748	-0.2591	3.9221	0.3666
9	0.2592	-0.7936	0.3466	0.8172	0.0798
10	0.1968	-0.1541	-0.1378	0.0815	0.0082
11	0.6782	0.7935	0.0221	1.0900	0.1108
12	1.0483	-0.0547	0.1116	1.1145	0.1137
13	-0.0405	0.4491	-0.2022	0.2442	0.0259
14	-0.2504	-1.1858	-0.2765	1.5452	0.1655
15	0.1356	-0.6262	-0.0156	0.4108	0.0445
16	0.9579	-0.1708	0.5009	1.1977	0.1355

17	0.0959	0.5721	0.0104	0.3366	0.0388	36	0.2942	-0.1993	0.1563	0.1507	0.0209
18	-0.5852	1.3358	-0.3558	2.2534	0.2621	37	-0.0328	0.5160	0.1755	0.2981	0.0413
19	-1.0066	0.0721	-0.2472	1.0796	0.1261	38	-0.2037	-0.2211	-0.1958	0.1287	0.0180
20	0.0667	-0.0008	-0.3549	0.1304	0.0156	39	-0.0527	0.1794	-0.1583	0.0600	0.0084
21	0.1397	0.2386	-0.0623	0.0803	0.0097	40	0.2375	-0.5249	0.0172	0.3322	0.0468
22	-0.2897	0.2501	-0.1995	0.1863	0.0227	41	0.0376	0.2212	0.2010	0.0908	0.0129
23	-0.6258	0.7472	-0.3078	1.0447	0.1297	42	0.0221	-0.0959	0.1131	0.0225	0.0032
24	0.0036	-0.2338	0.1360	0.0732	0.0091	43	0.7859	-0.3570	0.2284	0.7973	0.1141
25	-0.1986	-1.6073	-0.1694	2.6517	0.3342	44	0.2487	0.0374	0.1585	0.0883	0.0127
26	0.0681	0.4285	0.2326	0.2424	0.0309	45	-1.4757	0.5242	-0.5088	2.7112	0.3945
27	-0.0904	-1.0475	-0.0781	1.1114	0.1417	46	0.5465	-0.2442	0.2530	0.4223	0.0616
28	-0.3268	-0.7400	0.1727	0.6842	0.0882	47	-0.3921	0.3721	-0.2325	0.3463	0.0507
29	0.4588	0.2738	-0.0144	0.2856	0.0369	48	0.2677	-0.0509	0.2495	0.1365	0.0200
30	-0.4972	1.0607	-0.3481	1.4935	0.1958	49	0.6991	0.0313	0.2078	0.5329	0.0784
31	0.2715	0.3002	0.2913	0.2487	0.0329	50	-0.2590	-0.0962	-0.0427	0.0782	0.0115
32	0.1946	0.4671	0.0975	0.2656	0.0358	51	0.4187	-0.3961	0.2378	0.3887	0.0578
33	0.0115	0.4110	0.0050	0.1691	0.0230	52	-0.0995	0.3417	0.0620	0.1305	0.0195
34	-0.1928	-0.9887	-0.0915	1.0231	0.1401	53	0.0157	-0.2018	-0.0834	0.0479	0.0072
35	-0.1522	0.6966	0.2043	0.5501	0.0757	54	0.0205	0.1181	0.0184	0.0147	0.0022

55	-0.1924	-0.0983	-0.0376	0.0481	0.0073	74	0.2262	-0.3254	0.2068	0.1999	0.0319
56	0.0708	-0.0813	-0.0223	0.0121	0.0018	75	-0.2233	0.0872	0.0623	0.0613	0.0098
57	-0.0839	-0.3575	0.0416	0.1366	0.0207	76	-0.8419	-0.3612	-0.2402	0.8970	0.1437
58	-0.0859	0.5069	0.0341	0.2655	0.0404	77	0.0601	0.0010	0.2017	0.0443	0.0071
59	-0.0744	-0.1346	0.0887	0.0315	0.0048	78	0.1910	-0.0403	0.0228	0.0386	0.0062
60	0.0261	0.2291	-0.1390	0.0725	0.0111	79	0.0260	0.1490	0.1941	0.0605	0.0098
61	-0.2181	-0.0773	0.0488	0.0559	0.0086	80	-0.4213	-0.0513	-0.2104	0.2244	0.0363
62	-0.3180	0.0811	-0.1362	0.1262	0.0195	81	0.3572	0.0780	0.1619	0.1599	0.0259
63	0.5828	0.1955	0.3341	0.4895	0.0756	82	0.4014	0.1373	0.2282	0.2321	0.0378
64	-0.1864	-0.2562	-0.1924	0.1374	0.0213	83	0.0335	-0.2011	0.1617	0.0677	0.0110
65	-0.2531	0.0684	-0.2026	0.1098	0.0170	84	-0.3535	-0.2131	-0.1912	0.2069	0.0338
66	0.0782	-0.5473	-0.0831	0.3126	0.0486	85	-0.0362	0.0587	-0.1165	0.0183	0.0030
67	0.1932	-0.2517	0.0987	0.1104	0.0172	86	-0.2794	-0.0149	-0.0127	0.0785	0.0129
68	-0.7937	-0.0372	-0.2395	0.6886	0.1075	87	0.1575	0.1693	0.0883	0.0613	0.0101
69	-0.6368	-0.3464	-0.1882	0.5609	0.0878	88	0.3250	-0.1329	0.1494	0.1456	0.0240
70	0.5238	0.2012	0.3180	0.4160	0.0655	89	-0.0413	-0.0324	-0.0355	0.0040	0.0007
71	0.1178	0.3664	0.0233	0.1487	0.0235	90	-0.2611	-0.0294	0.0713	0.0741	0.0123
72	0.2496	-0.0915	-0.0497	0.0732	0.0116	91	0.4236	0.3431	0.0180	0.2975	0.0494
73	-0.4255	-0.0675	-0.1383	0.2047	0.0326	92	0.4782	-0.0154	0.0581	0.2323	0.0388

93 0.1652 -0.1724 -0.0903 0.0652 0.0109

94 -0.0909 -0.0952 0.0527 0.0201 0.0034

95 -0.3879 -0.9871 -0.1394 1.1443 0.1923

96 0.4795 0.1186 -0.0178 0.2442 0.0412

97 -0.6950 -0.3169 -0.0839 0.5906 0.0997

98 -0.2459 -0.6065 -0.0752 0.4340 0.0736

99 0.3285 0.0985 0.0279 0.1184 0.0201

100 0.0773 -0.1720 -0.0836 0.0425 0.0072

Ground to excited state transition velocity dipole moments (Au):

state X Y Z Dip. S. Osc.

1 -0.0696 -0.0261 0.0047 0.0055 0.0436

2 -0.0742 0.0642 0.0246 0.0102 0.0667

3 0.0701 -0.0248 0.0185 0.0059 0.0333

4 0.0987 -0.0850 -0.0439 0.0189 0.1040

5 -0.1120 -0.0056 0.0021 0.0126 0.0662

6 -0.0242 0.0381 0.0098 0.0021 0.0110

7 0.0011 0.1082 0.0579 0.0151 0.0739

8 -0.2091 -0.1790 0.0364 0.0771 0.3666

9 -0.0383 0.1163 -0.0507 0.0176 0.0800

10 -0.0301 0.0237 0.0209 0.0019 0.0084

11 -0.1035 -0.1208 -0.0034 0.0253 0.1107

12 -0.1604 0.0083 -0.0172 0.0261 0.1137

13 0.0063 -0.0714 0.0321 0.0062 0.0258

14 0.0405 0.1908 0.0443 0.0400 0.1660

15 -0.0226 0.1019 0.0027 0.0109 0.0447

16 -0.1624 0.0291 -0.0852 0.0345 0.1355

17 -0.0166 -0.0990 -0.0018 0.0101 0.0388

18 0.1022 -0.2329 0.0622 0.0686 0.2620

19 0.1762 -0.0131 0.0436 0.0331 0.1261

20 -0.0111 0.0009 0.0636 0.0042 0.0154

21 -0.0248 -0.0426 0.0119 0.0026 0.0095

22 0.0532 -0.0452 0.0360 0.0062 0.0226

23 0.1162 -0.1392 0.0576 0.0362 0.1296

24 -0.0007 0.0433 -0.0251 0.0025 0.0089

25 0.0381 0.3035 0.0320 0.0946 0.3337

26 -0.0135 -0.0816 -0.0443 0.0088 0.0307

27 0.0168 0.2000 0.0156 0.0405 0.1412

28	0.0630	0.1422	-0.0336	0.0253	0.0873	47	0.0860	-0.0818	0.0517	0.0168	0.0509
29	-0.0888	-0.0533	0.0027	0.0107	0.0368	48	-0.0593	0.0112	-0.0545	0.0066	0.0200
30	0.0971	-0.2087	0.0683	0.0576	0.1954	49	-0.1533	-0.0069	-0.0460	0.0257	0.0776
31	-0.0535	-0.0594	-0.0578	0.0097	0.0327	50	0.0580	0.0210	0.0091	0.0039	0.0117
32	-0.0391	-0.0944	-0.0195	0.0108	0.0356	51	-0.0928	0.0882	-0.0532	0.0192	0.0574
33	-0.0024	-0.0835	-0.0011	0.0070	0.0229	52	0.0224	-0.0763	-0.0137	0.0065	0.0194
34	0.0398	0.2028	0.0189	0.0431	0.1398	53	-0.0034	0.0454	0.0190	0.0024	0.0072
35	0.0316	-0.1432	-0.0422	0.0233	0.0752	54	-0.0049	-0.0269	-0.0037	0.0008	0.0022
36	-0.0606	0.0415	-0.0323	0.0064	0.0206	55	0.0434	0.0221	0.0088	0.0024	0.0072
37	0.0071	-0.1074	-0.0360	0.0129	0.0413	56	-0.0162	0.0183	0.0047	0.0006	0.0018
38	0.0425	0.0463	0.0410	0.0056	0.0179	57	0.0194	0.0819	-0.0091	0.0072	0.0210
39	0.0110	-0.0375	0.0322	0.0026	0.0081	58	0.0193	-0.1161	-0.0077	0.0139	0.0407
40	-0.0497	0.1110	-0.0039	0.0148	0.0467	59	0.0168	0.0308	-0.0199	0.0016	0.0047
41	-0.0083	-0.0469	-0.0424	0.0041	0.0127	60	-0.0062	-0.0527	0.0317	0.0038	0.0111
42	-0.0047	0.0201	-0.0243	0.0010	0.0032	61	0.0499	0.0181	-0.0113	0.0029	0.0085
43	-0.1684	0.0767	-0.0486	0.0366	0.1136	62	0.0737	-0.0185	0.0316	0.0068	0.0195
44	-0.0539	-0.0082	-0.0333	0.0041	0.0126	63	-0.1340	-0.0454	-0.0771	0.0260	0.0747
45	0.3215	-0.1147	0.1105	0.1287	0.3931	64	0.0437	0.0591	0.0449	0.0074	0.0213
46	-0.1193	0.0535	-0.0562	0.0203	0.0617	65	0.0591	-0.0164	0.0469	0.0060	0.0171

66	-0.0184	0.1274	0.0195	0.0169	0.0485
67	-0.0458	0.0589	-0.0232	0.0061	0.0175
68	0.1851	0.0087	0.0559	0.0375	0.1067
69	0.1482	0.0814	0.0439	0.0305	0.0867
70	-0.1239	-0.0474	-0.0750	0.0232	0.0656
71	-0.0272	-0.0866	-0.0053	0.0083	0.0233
72	-0.0587	0.0216	0.0116	0.0040	0.0114
73	0.1015	0.0162	0.0333	0.0117	0.0326
74	-0.0547	0.0777	-0.0493	0.0115	0.0319
75	0.0532	-0.0209	-0.0147	0.0035	0.0097
76	0.2019	0.0868	0.0579	0.0516	0.1432
77	-0.0136	0.0003	-0.0481	0.0025	0.0069
78	-0.0454	0.0104	-0.0054	0.0022	0.0061
79	-0.0060	-0.0361	-0.0467	0.0035	0.0097
80	0.1016	0.0124	0.0509	0.0131	0.0359
81	-0.0865	-0.0188	-0.0394	0.0094	0.0257
82	-0.0973	-0.0332	-0.0559	0.0137	0.0373
83	-0.0092	0.0489	-0.0395	0.0040	0.0110
84	0.0867	0.0522	0.0468	0.0124	0.0338
85	0.0095	-0.0143	0.0284	0.0011	0.0030
86	0.0688	0.0033	0.0032	0.0047	0.0129
87	-0.0390	-0.0417	-0.0218	0.0037	0.0101
88	-0.0806	0.0326	-0.0374	0.0090	0.0242
89	0.0106	0.0075	0.0082	0.0002	0.0006
90	0.0643	0.0072	-0.0175	0.0045	0.0120
91	-0.1051	-0.0855	-0.0045	0.0184	0.0492
92	-0.1199	0.0035	-0.0140	0.0146	0.0387
93	-0.0406	0.0437	0.0225	0.0041	0.0108
94	0.0226	0.0243	-0.0122	0.0013	0.0033
95	0.0979	0.2486	0.0349	0.0726	0.1920
96	-0.1207	-0.0296	0.0045	0.0155	0.0408
97	0.1755	0.0799	0.0213	0.0377	0.0991
98	0.0619	0.1539	0.0192	0.0279	0.0731
99	-0.0834	-0.0249	-0.0069	0.0076	0.0200
100	-0.0192	0.0438	0.0212	0.0027	0.0071

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	-0.0102	0.2469	0.2959

2	-0.1043	-0.1863	1.2946
3	-0.1958	0.2294	-0.0689
4	0.1768	0.2124	-1.4739
5	0.0206	-0.1556	0.9157
6	-0.0291	-0.0812	1.0112
7	-0.1910	-0.2378	1.8350
8	-0.1621	0.4270	2.3019
9	0.2153	-0.1404	-1.1852
10	-0.1254	0.0052	1.4458
11	0.0862	0.7000	-0.1584
12	-0.0598	-0.2227	0.7514
13	-0.0508	-0.0717	0.5083
14	-0.1044	-0.2167	0.1797
15	0.0392	-0.1905	0.6462
16	0.0111	-0.0185	-0.7965
17	0.0528	0.2807	-0.5903
18	-0.1528	0.2671	0.5313
19	-0.0858	0.0365	0.3037
20	-0.3844	0.5013	1.9943
21	0.1183	0.3493	0.2583
22	-0.4488	0.0678	0.5384
23	0.0977	0.2207	0.1216
24	0.0044	-0.1926	-0.8168
25	0.0025	-0.4016	-0.2844
26	-0.0225	0.2498	-0.7702
27	-0.0668	-0.2778	0.4743
28	-0.1857	-0.5289	-0.5113
29	-0.0708	0.0077	0.8677
30	0.2914	0.0559	-0.0618
31	-0.0952	-0.1378	-0.4314
32	-0.1337	0.4669	0.2520
33	-0.0655	0.4119	0.0158
34	0.0314	-0.3848	0.3634
35	-0.0489	0.6151	-0.3642
36	-0.2972	-0.7664	0.1578
37	-0.3113	0.0613	0.0179
38	0.2383	0.0445	-0.0517
39	-0.2170	0.3225	-0.1044
40	-0.0059	-0.5556	0.2403
41	0.0832	0.3167	-0.5807
42	-0.0758	-0.1195	0.1233
43	0.0875	-0.3415	0.2450
44	-0.1511	-0.1302	0.1054
45	-0.0959	-0.2148	-0.2813
46	-0.2807	-0.4158	0.2308
47	0.6038	-0.1262	-0.1198
48	-0.0687	0.1509	-0.2881
49	0.0692	0.0292	0.1651
50	-0.2814	0.3216	-0.1693
51	-0.1314	0.0315	-0.5315
52	-0.3717	0.2029	0.1439
53	0.0317	0.1148	-0.0307
54	0.0797	0.0450	-0.1261
55	0.0316	0.1173	-0.0657
56	0.0196	0.2176	0.0108
57	-0.0667	0.0917	-0.1470
58	0.3058	-0.1235	-0.7932
59	0.2135	-0.0923	-0.3109
60	0.0024	0.1146	0.0586
61	0.1940	0.1944	0.3778
62	-0.0056	-0.4145	0.6785
63	-0.0558	-0.2699	-0.6934

64	0.0852	0.0235	-0.0786
65	-0.1122	0.2053	-0.0128
66	0.2359	-0.0372	-0.2135
67	0.1605	-0.0780	-0.0868
68	0.0752	-0.1411	0.3538
69	-0.2369	0.2617	0.2209
70	0.0778	0.0970	0.1477
71	-0.0403	0.0490	0.0649
72	-0.2542	-0.0548	-0.2386
73	-0.2422	-0.2645	0.3389
74	0.2625	-0.0322	-0.1561
75	-0.0001	-0.2224	0.1098
76	-0.1167	0.0600	0.4186
77	-0.3491	-0.0643	-0.2299
78	0.3583	-0.0239	0.2570
79	-0.0341	-0.1823	-0.3725
80	-0.2897	-0.0268	0.3519
81	-0.0378	-0.1177	0.1424
82	-0.0287	-0.5861	-0.6089
83	0.2325	-0.2001	-0.5547
84	-0.1160	0.5739	0.2185
85	0.1340	-0.0544	0.2654
86	-0.0780	-0.1678	0.4470
87	0.0904	0.3278	-0.1149
88	-0.2841	0.2023	0.0311
89	-0.3919	-0.1716	-0.0039
90	-0.0681	0.1748	0.1397
91	-0.0833	0.0230	0.1427
92	0.1642	0.0749	-0.0440
93	0.1076	0.2737	0.1358
94	0.1851	0.0497	0.0831
95	-0.1174	0.0823	-0.1170
96	-0.0064	0.0713	0.1464
97	-0.4077	0.1831	0.0248
98	-0.0502	0.1714	0.1638
99	0.2434	-0.1716	0.0815
100	0.0267	-0.3563	-0.0888

C-29·H$^+$ (S_1 state)

C	3.12503	0.88779	0.35285
C	4.10153	-0.11794	0.48614
C	3.82804	-1.41775	0.14576
C	1.80915	0.51449	-0.08761
H	5.08009	0.15134	0.85701
H	4.58102	-2.18231	0.27492
C	2.54936	3.26226	0.44385
C	3.45155	2.25852	0.60577
C	0.80643	1.52021	0.02146
C	1.20584	2.88829	0.15704
H	2.80693	4.30234	0.56813
H	4.46888	2.48381	0.89251
C	1.62331	-0.78093	-0.63209
C	2.59536	-1.78471	-0.46296
C	0.21466	-2.36688	-1.79860
C	2.32680	-3.09925	-0.92475
C	1.11177	-3.37156	-1.56488
H	3.06106	-3.87445	-0.77557
H	0.87373	-4.36995	-1.89702
C	-2.14663	3.43155	-0.40142
H	-2.20949	4.50361	-0.48159
N	0.17590	3.72814	0.02780
C	-3.17954	2.56541	-0.58188
N	-0.91353	2.92977	-0.12872
H	-4.15007	2.94518	-0.85731
C	-3.00173	1.17984	-0.35098
C	-0.62534	1.57521	-0.02884
C	-4.07129	0.26890	-0.52384
C	-1.72046	0.68685	0.08352
H	-5.00829	0.63966	-0.91201
C	-3.92100	-1.05027	-0.21187
C	-1.64395	-0.64203	0.63219
C	-2.73316	-1.53129	0.41545
H	-4.73481	-1.74260	-0.37444
C	-2.65661	-2.84832	0.89605
H	-0.72327	-2.49695	-2.30909
C	-0.57840	-1.07578	1.44138
C	-0.53512	-2.36936	1.92488
H	0.20736	-0.38909	1.70719
C	-1.56242	-3.26988	1.63016
H	-3.47906	-3.52293	0.70501
H	-1.51596	-4.28391	1.99867
H	0.29660	-2.67992	2.53958
N	0.49823	-1.08895	-1.36907
H	-0.11793	-0.34656	-1.64660

Excited state information

Excited State 1: Singlet-A 1.9348 eV 640.82 nm f=0.0456 <S**2>=0.000

96 -> 97 0.70517

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1164.89389215

Copying the excited state density for this state as the 1-particle RhoCI density.

Rotatory strengths (velocity)

state XX YY ZZ R(velocity) E-M Angle

1 -19.1639 28.1555 -45.2828 -12.0970 97.21

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	0.9492	0.2469	-0.0273	0.9626	0.0456

Ground to excited state transition velocity dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-0.0675	-0.0172	0.0020	0.0049	0.0456

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	0.0091	0.2179	0.355

VI. REFERENCES

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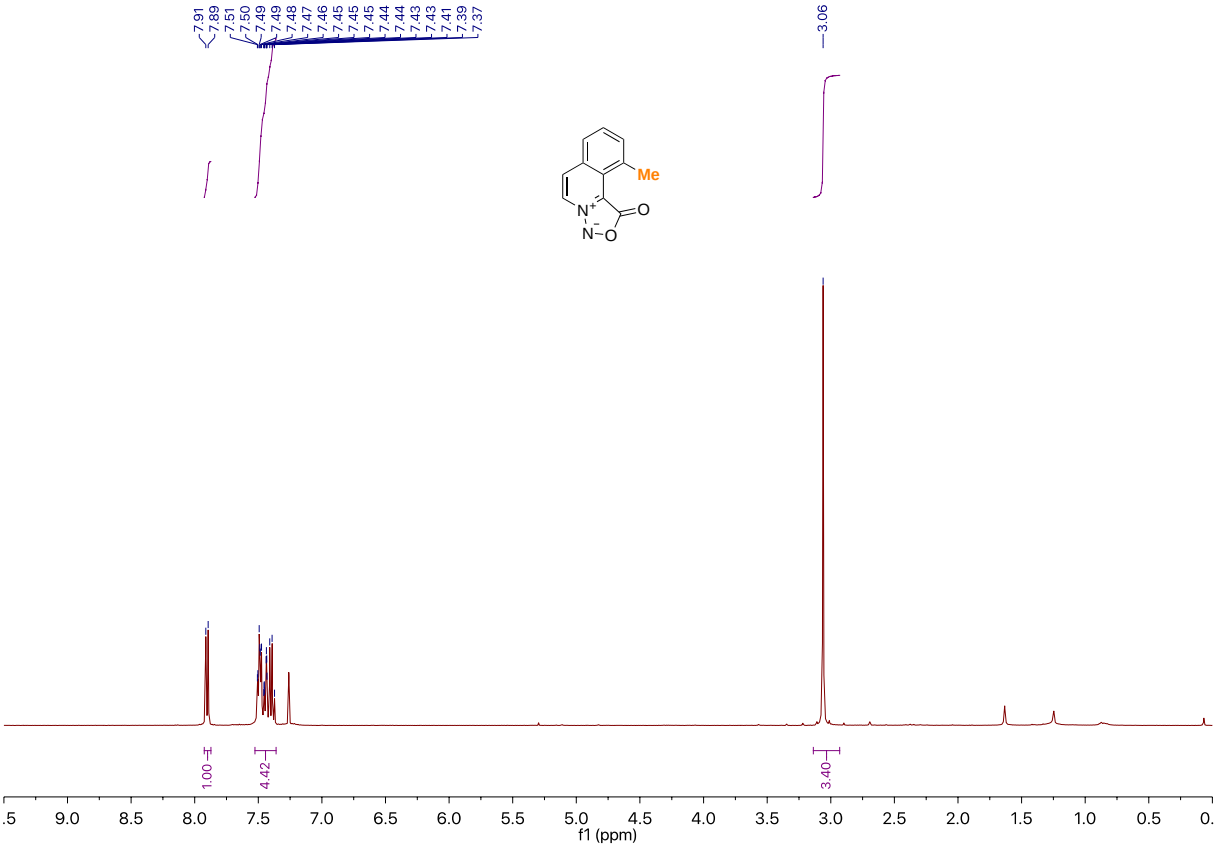
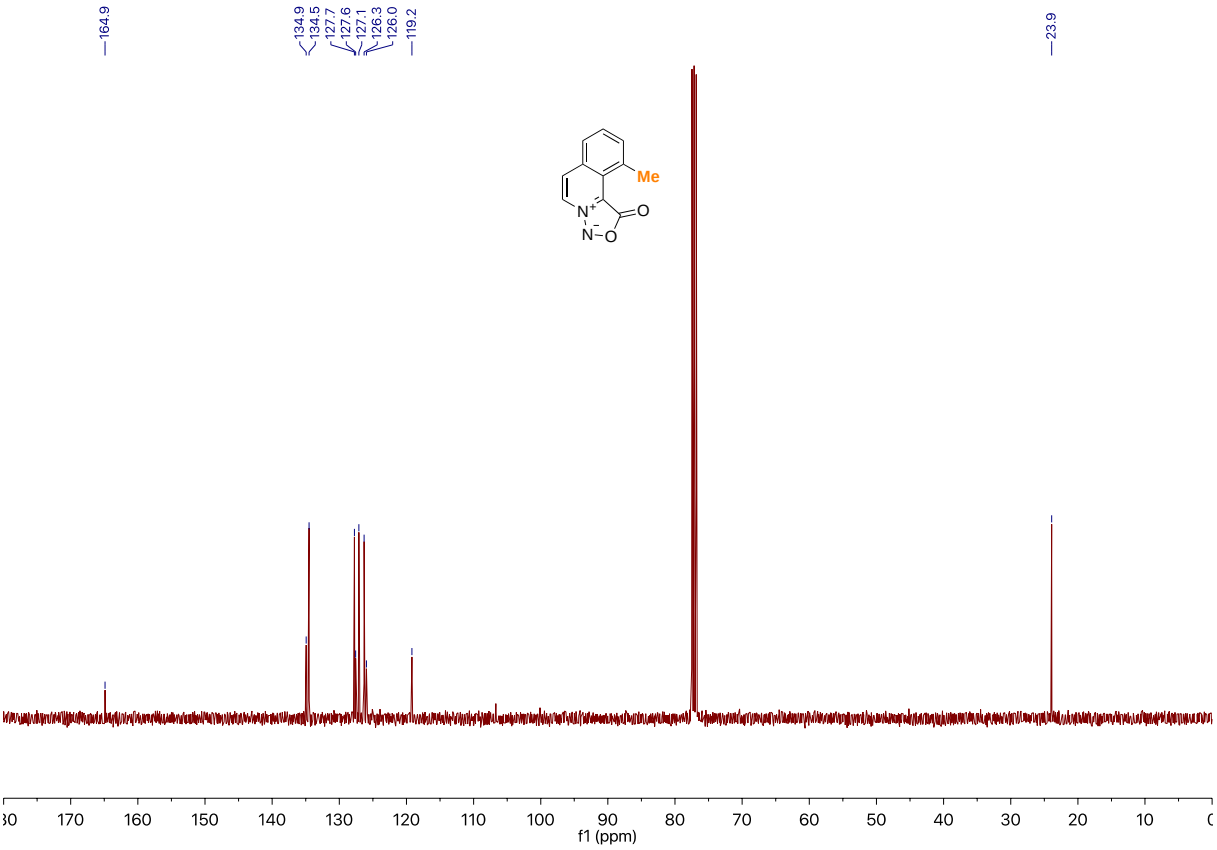
VII. NMR Spectra ^{1}H & ^{13}C

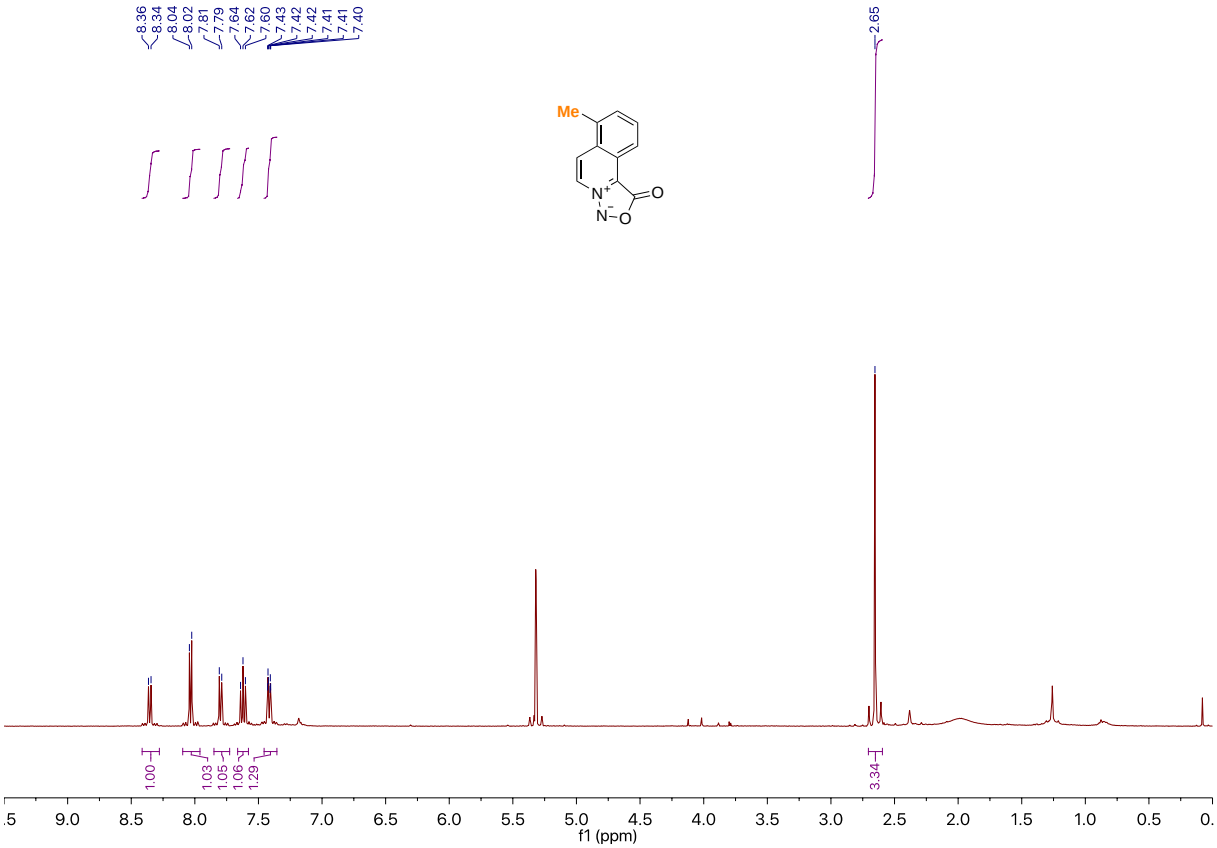
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **1d**



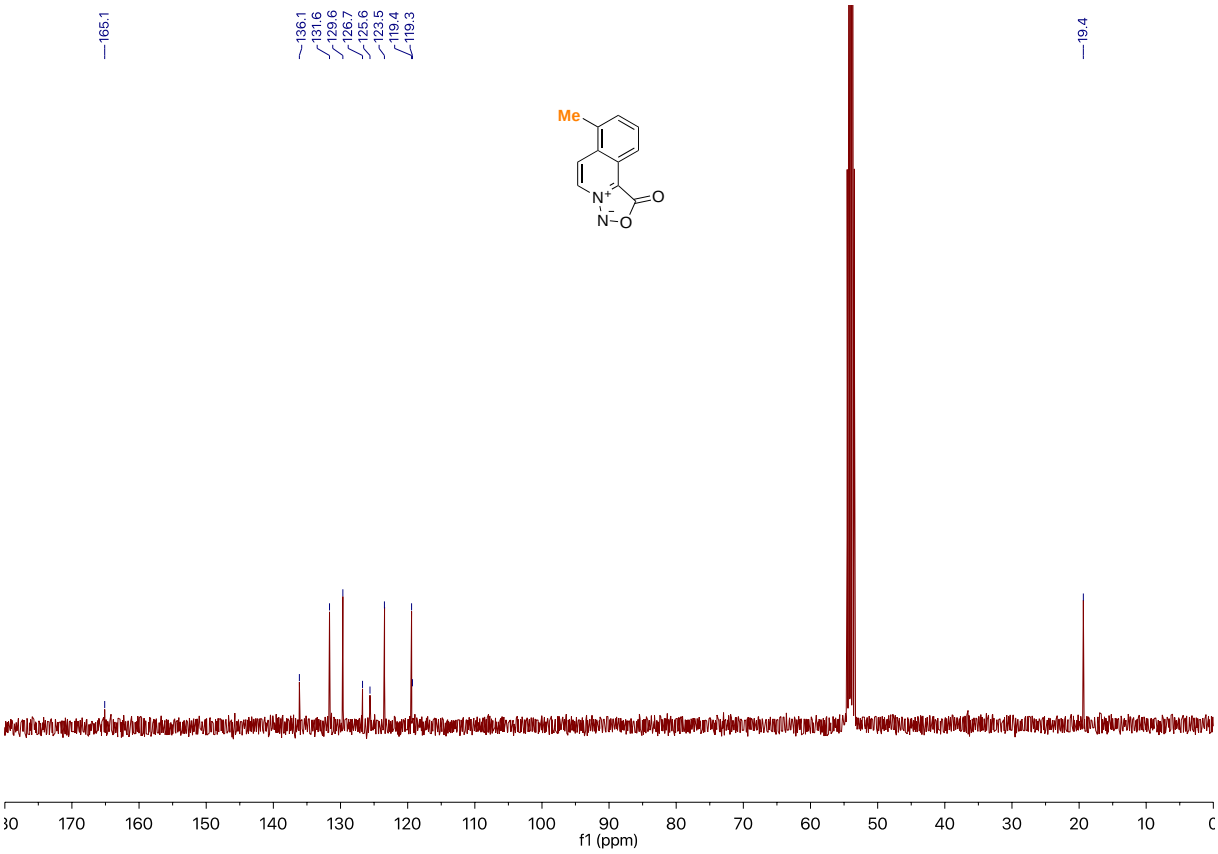
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **1d**



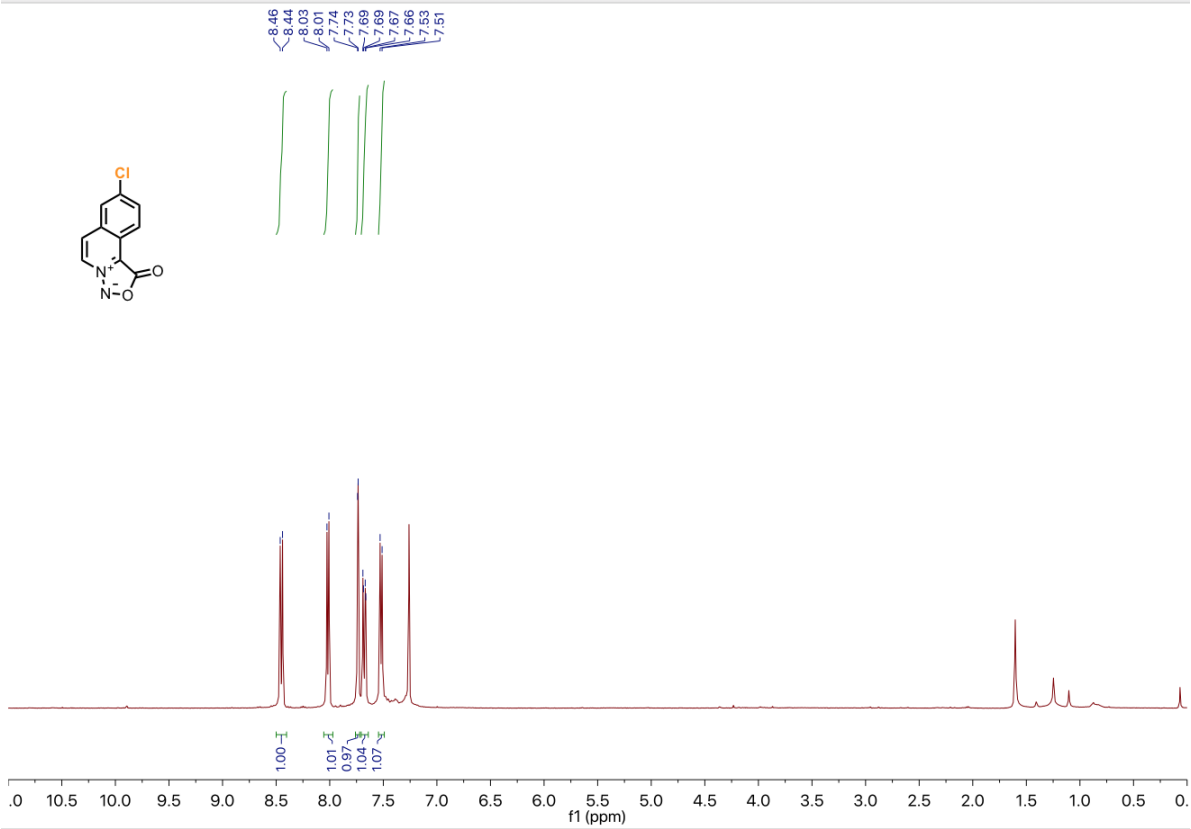
^{1}H NMR Spectrum (400 MHz, CD_2Cl_2) of **1e**



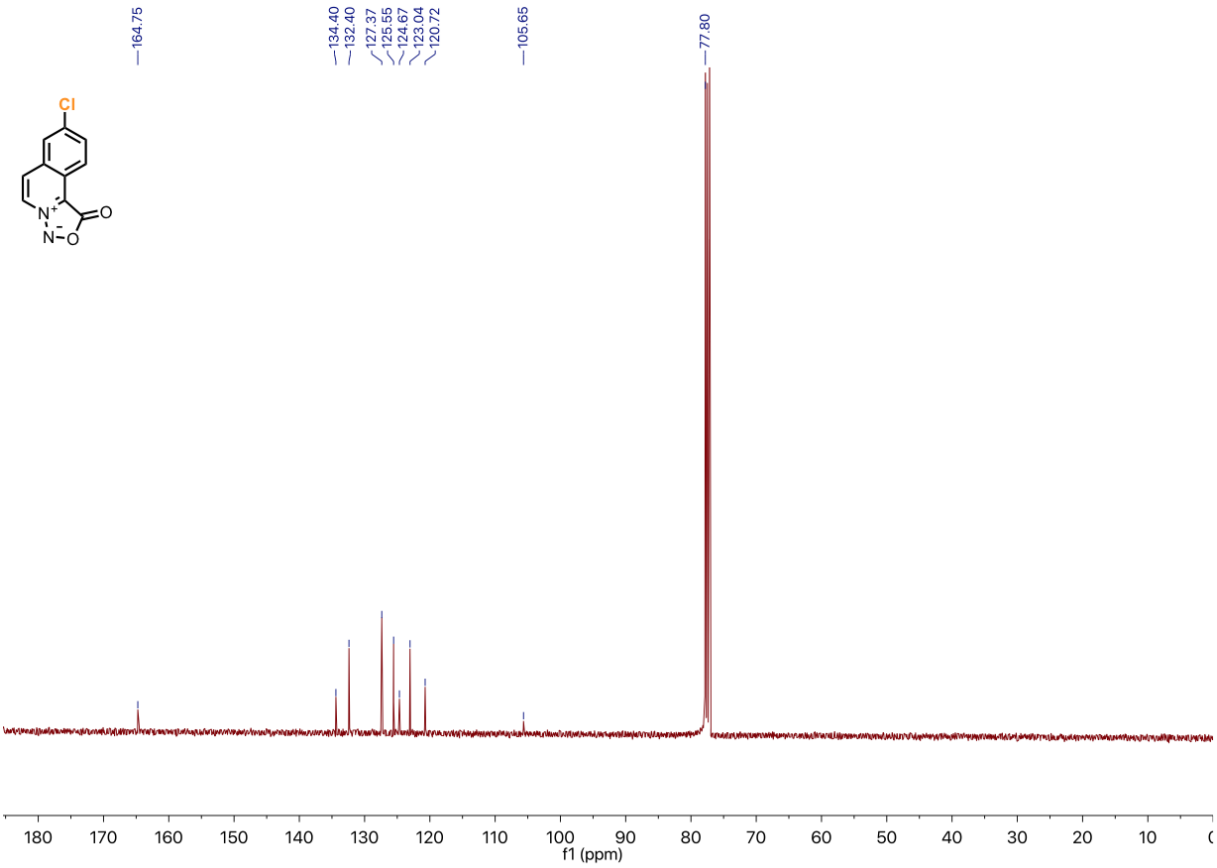
^{13}C NMR Spectrum (100 MHz, CD_2Cl_2) of **1e**



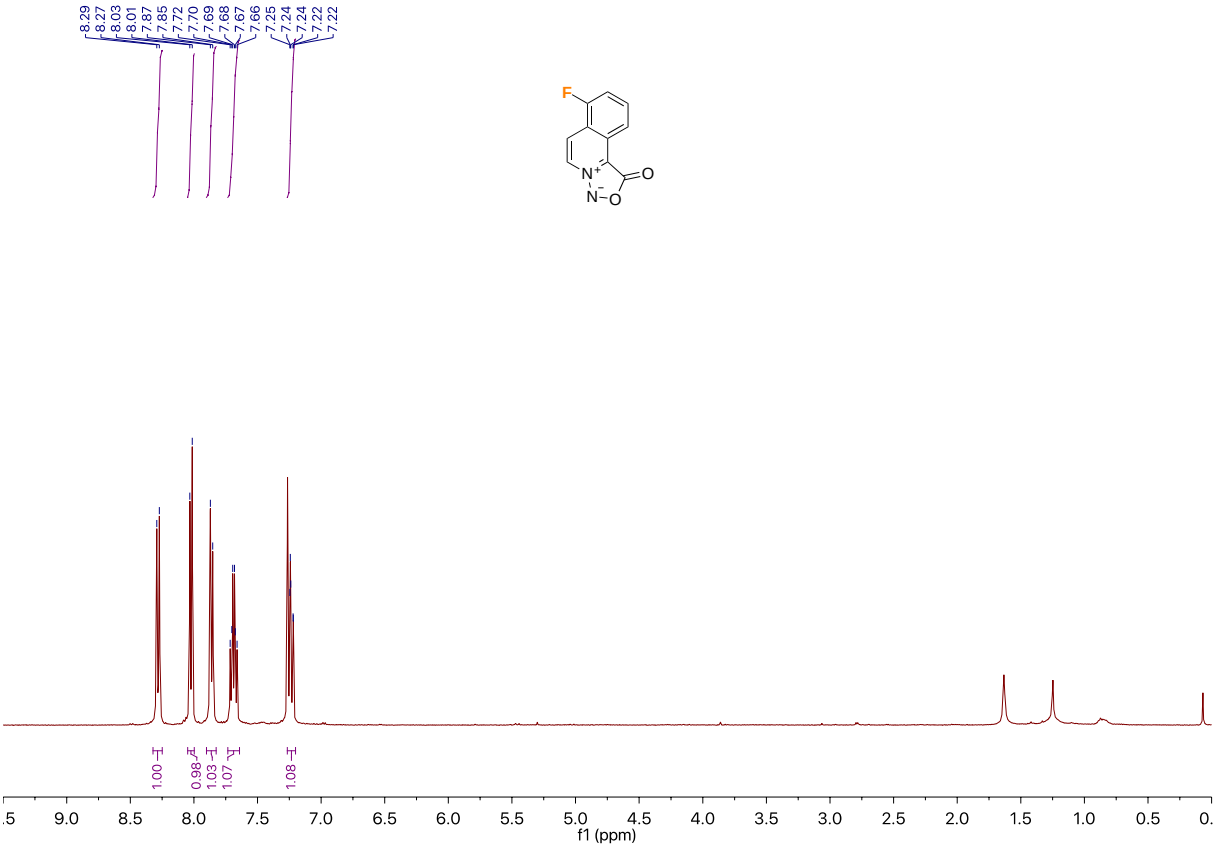
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **1l**



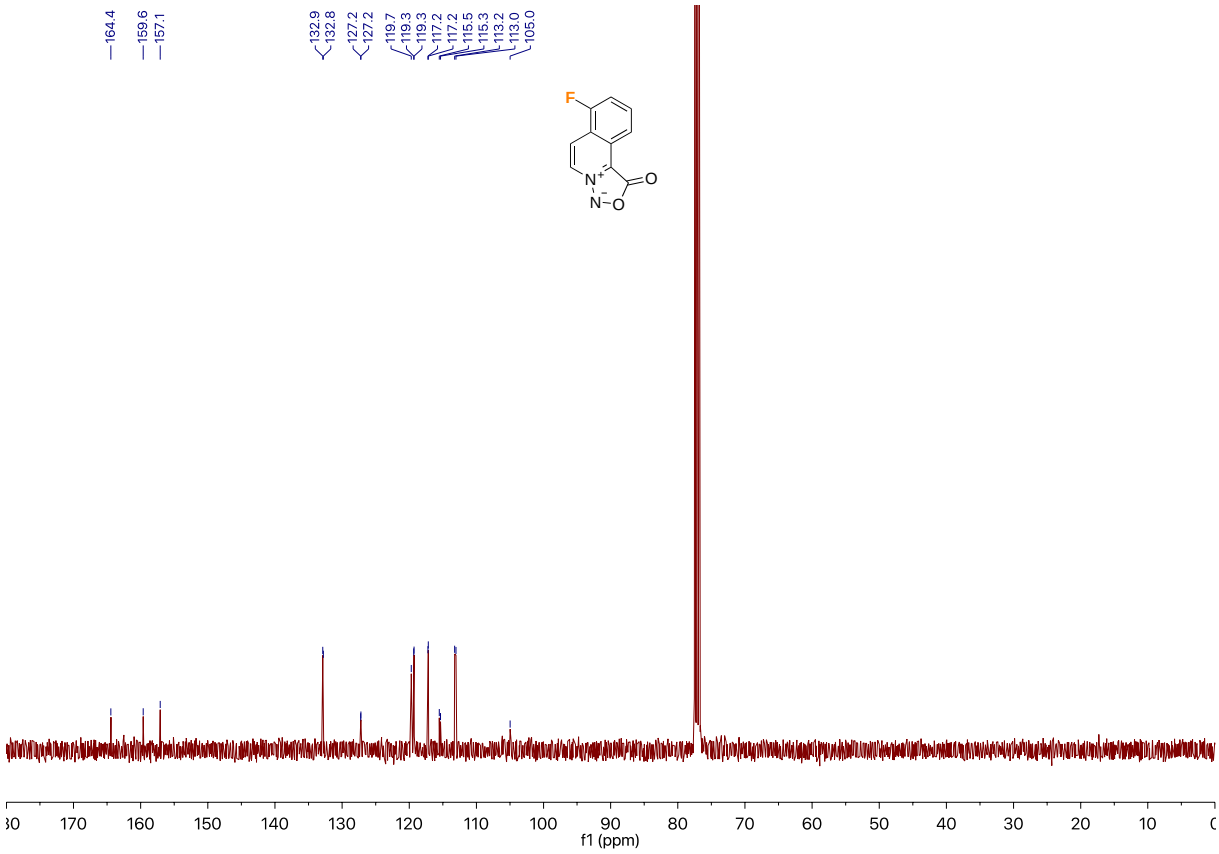
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **1d**



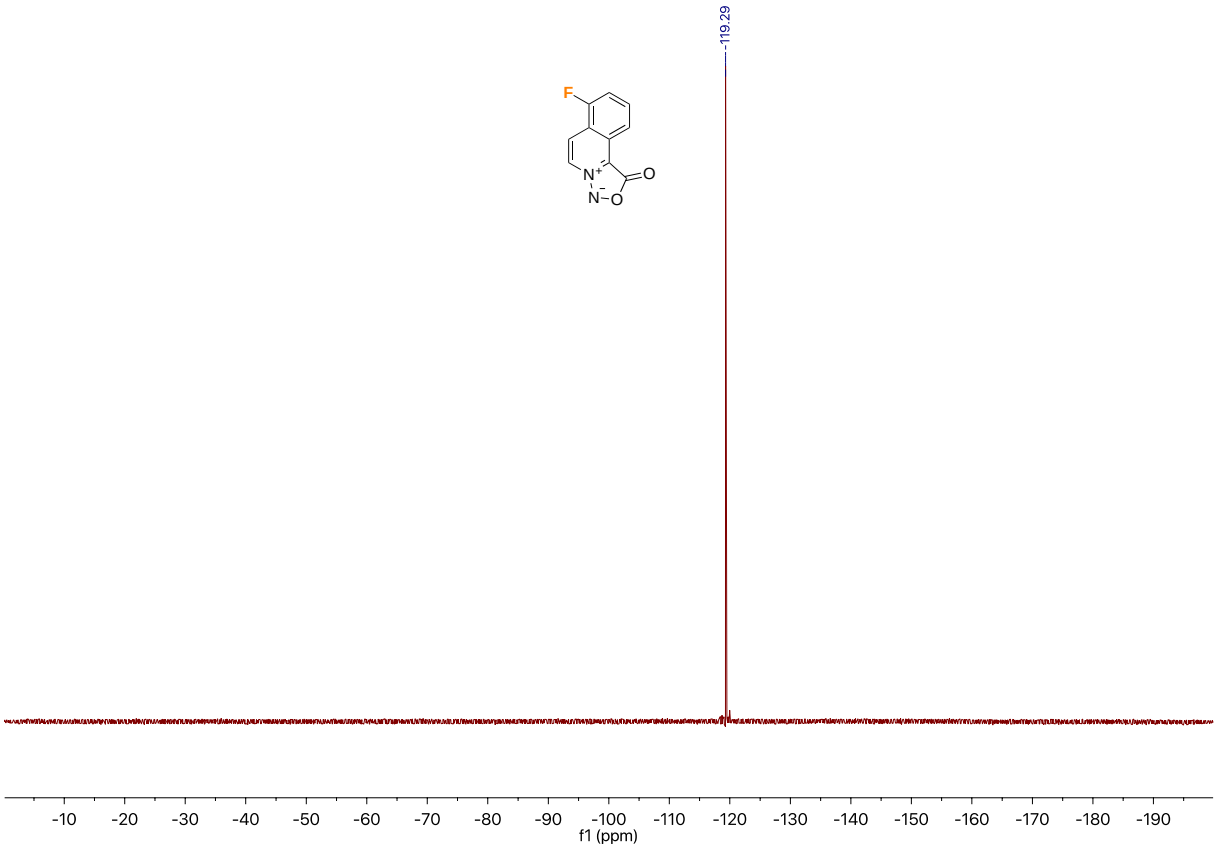
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **1m**



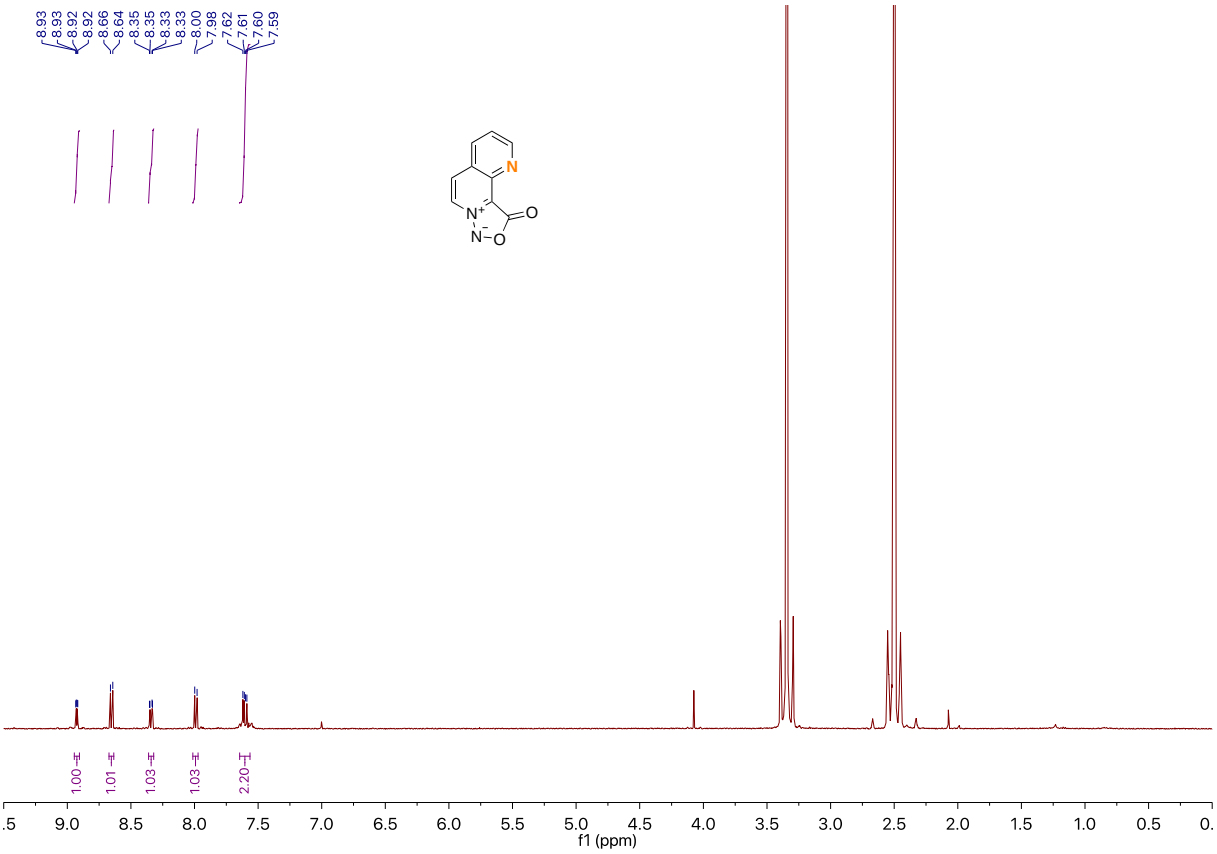
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **1m**



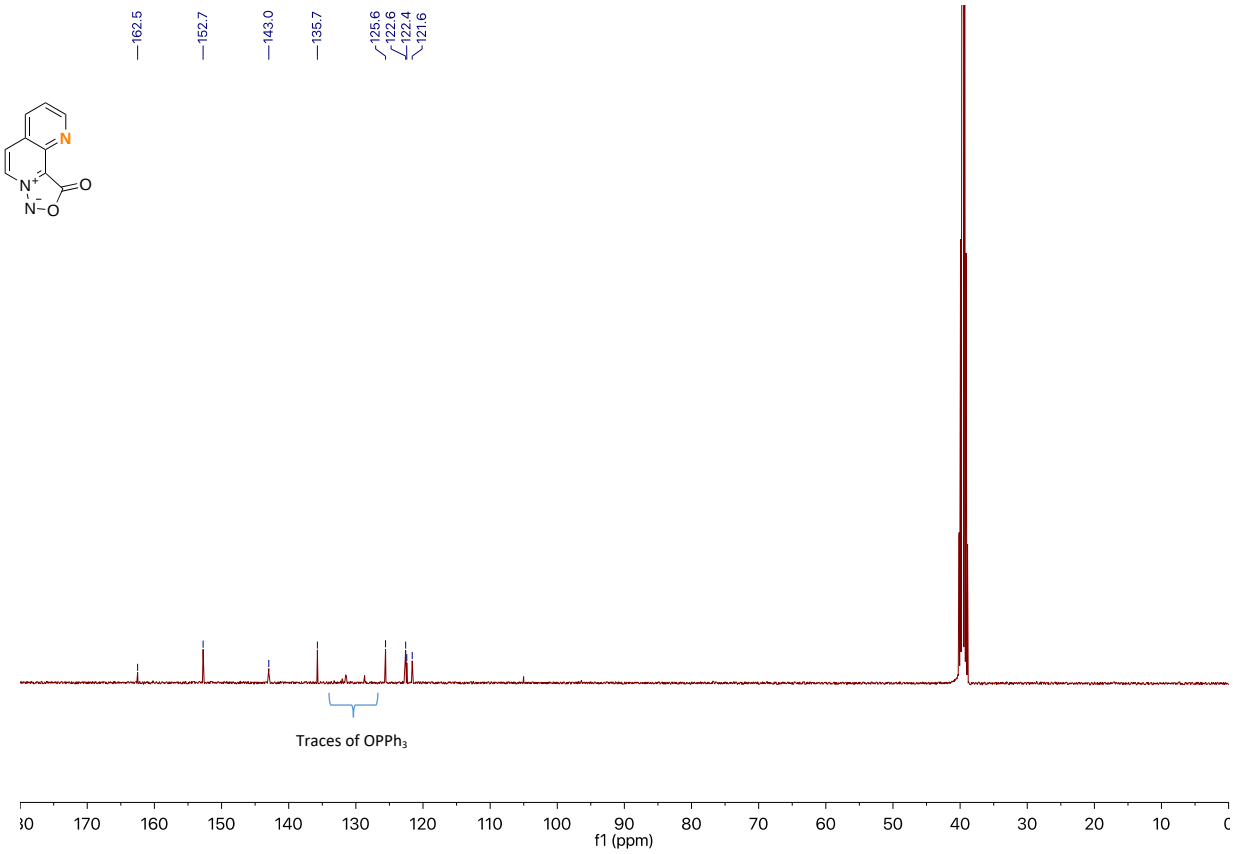
^{19}F NMR Spectrum (376 MHz, $CDCl_3$) of **1m**



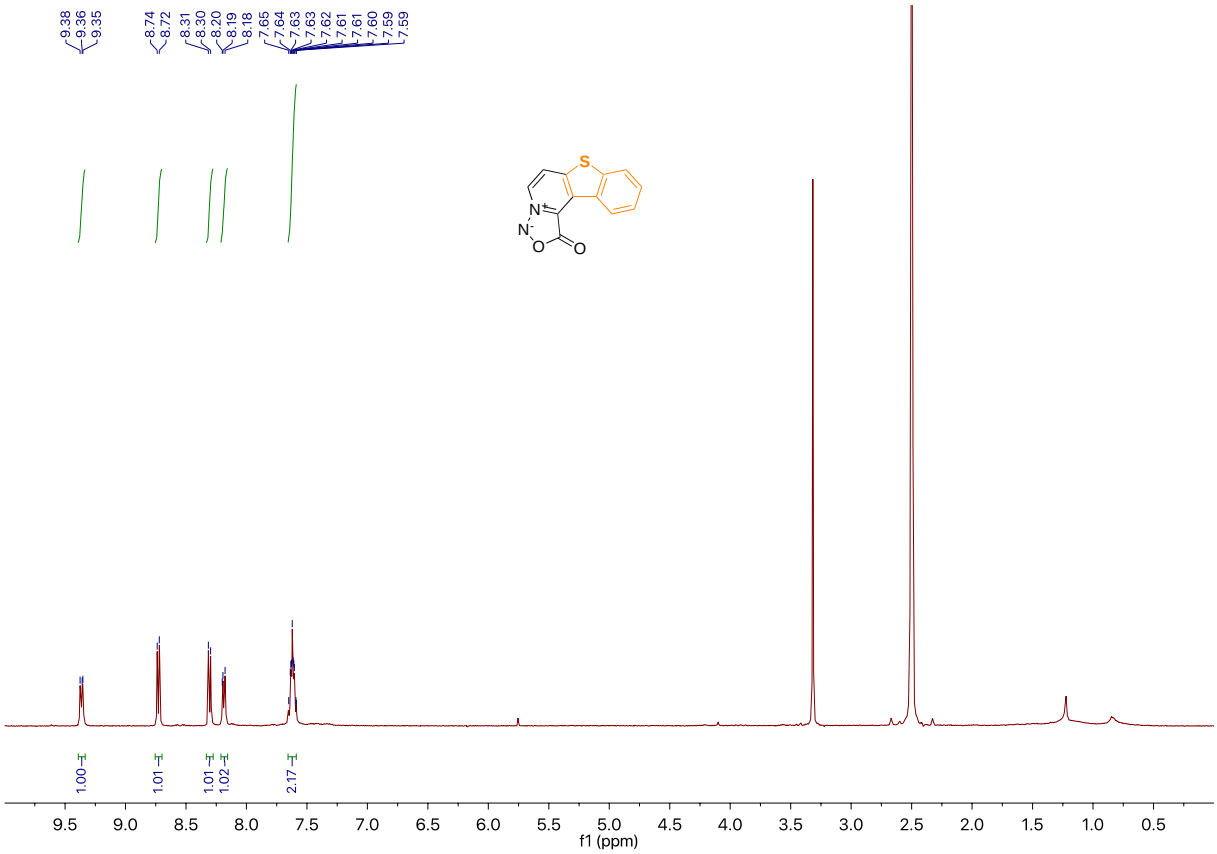
^{1}H NMR Spectrum (400 MHz, DMSO-*d6*) of **1p**



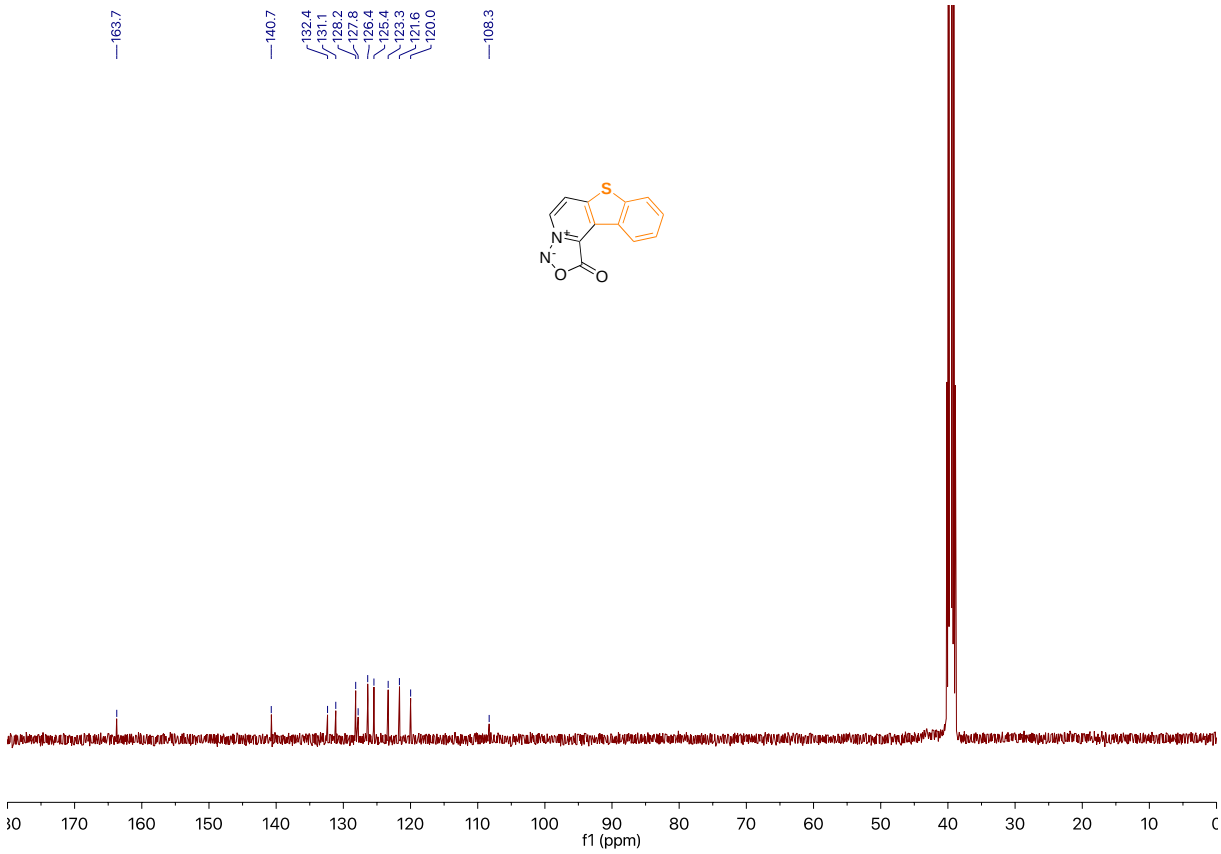
^{13}C NMR Spectrum (100 MHz, DMSO-*d6*) of **1p**



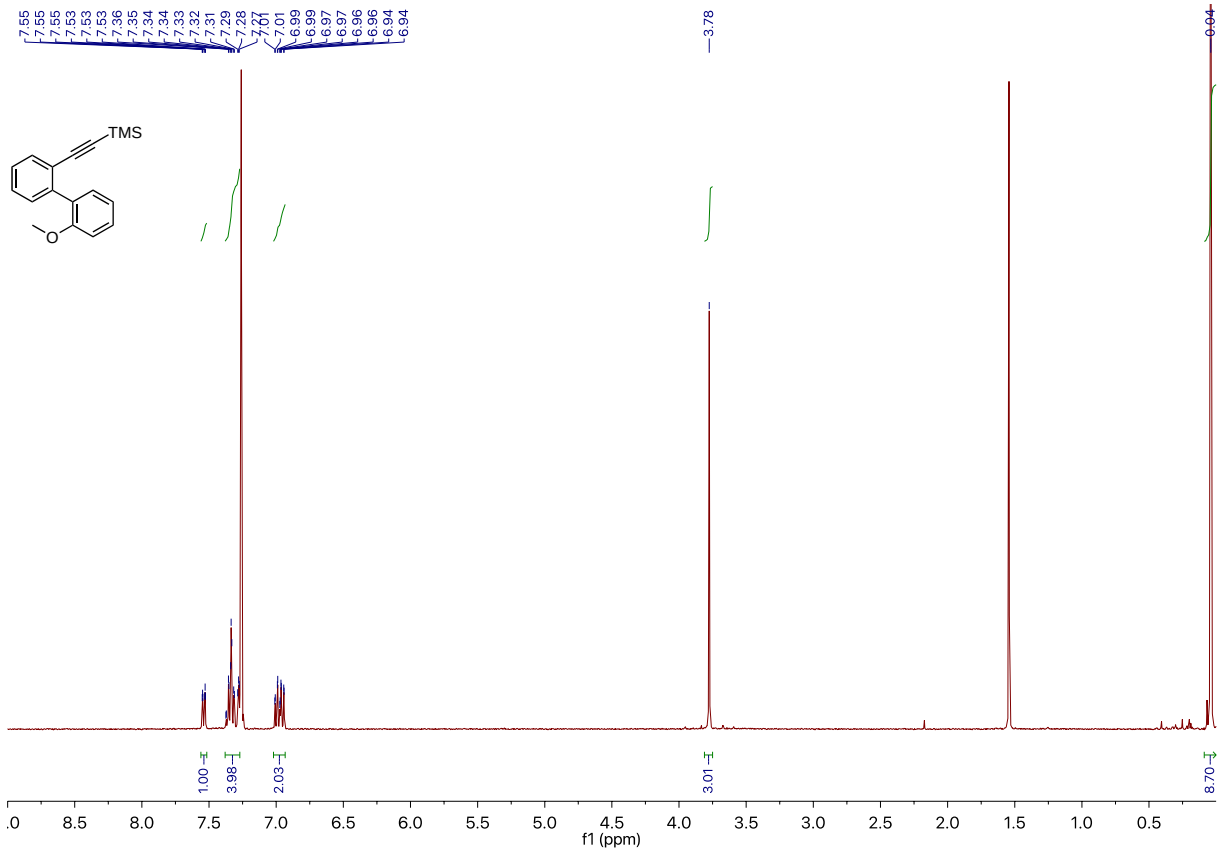
^{1}H NMR Spectrum (400 MHz, DMSO-*d6*) of **1q**



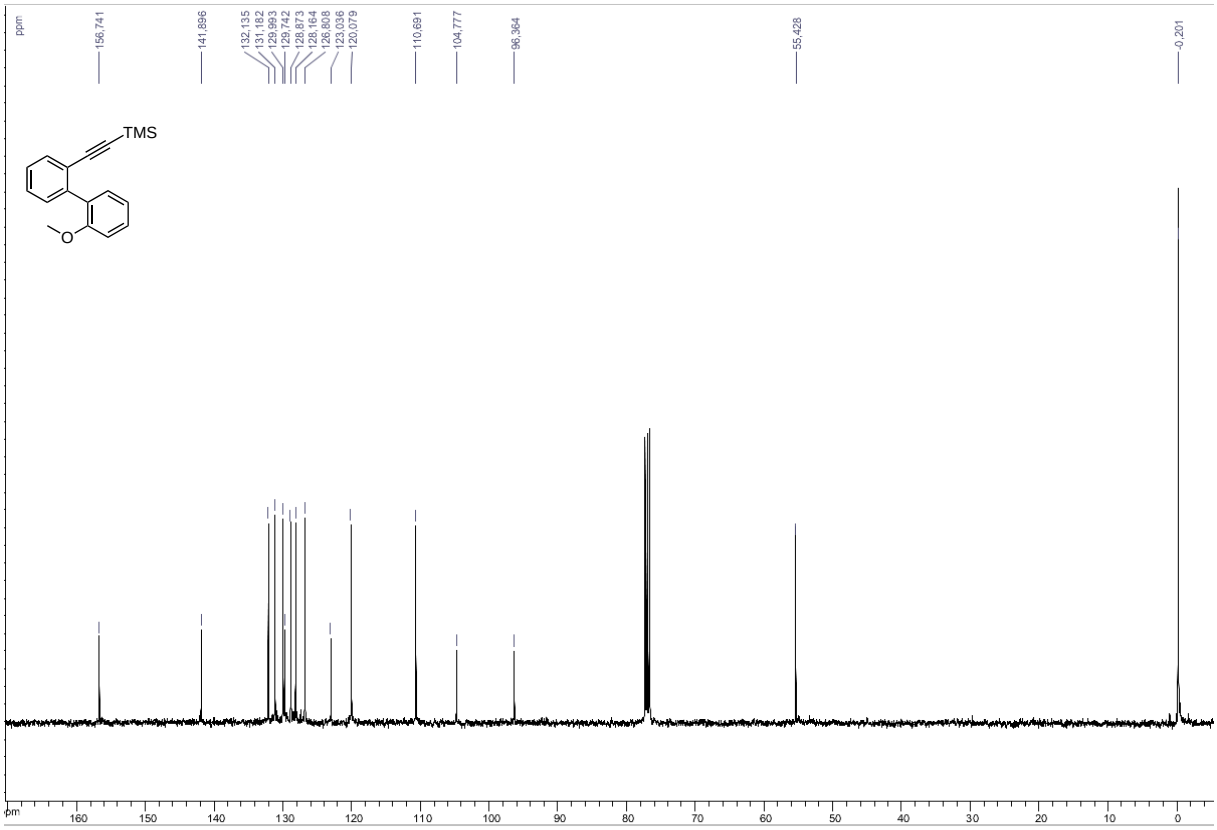
^{13}C NMR Spectrum (100 MHz, DMSO-*d6*) of **1q**



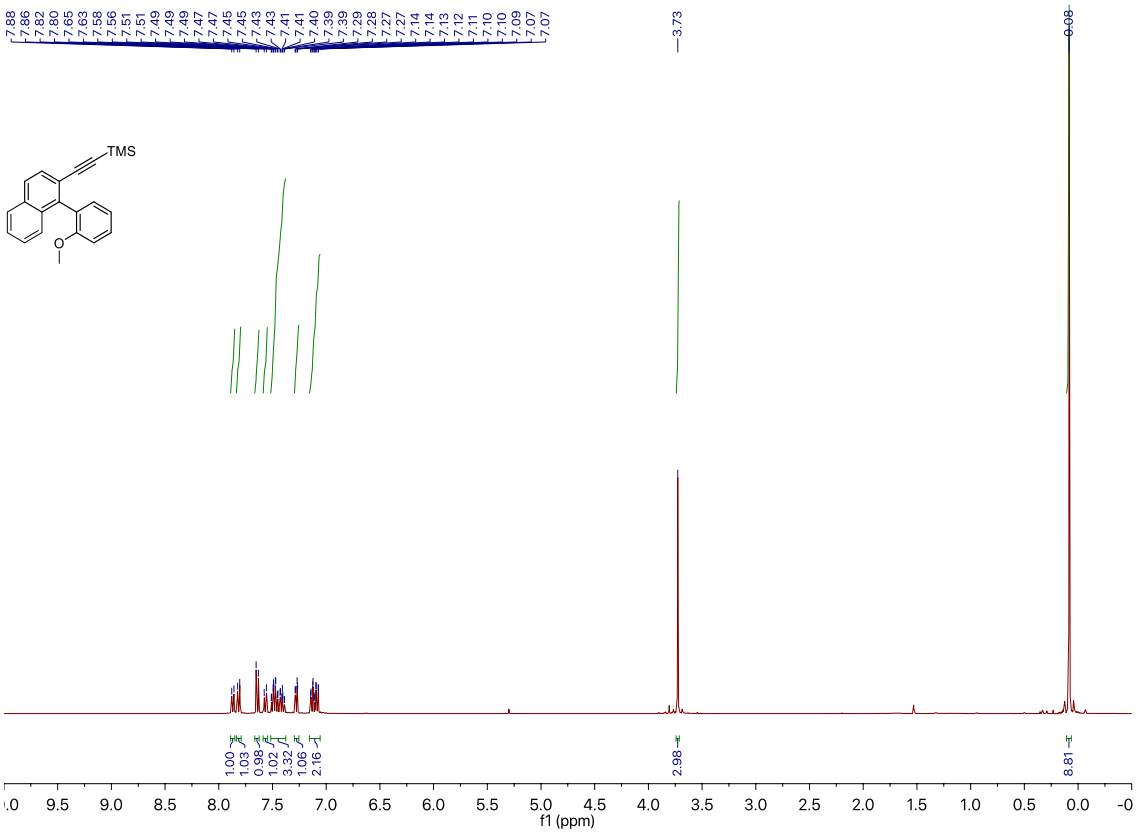
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **3a**



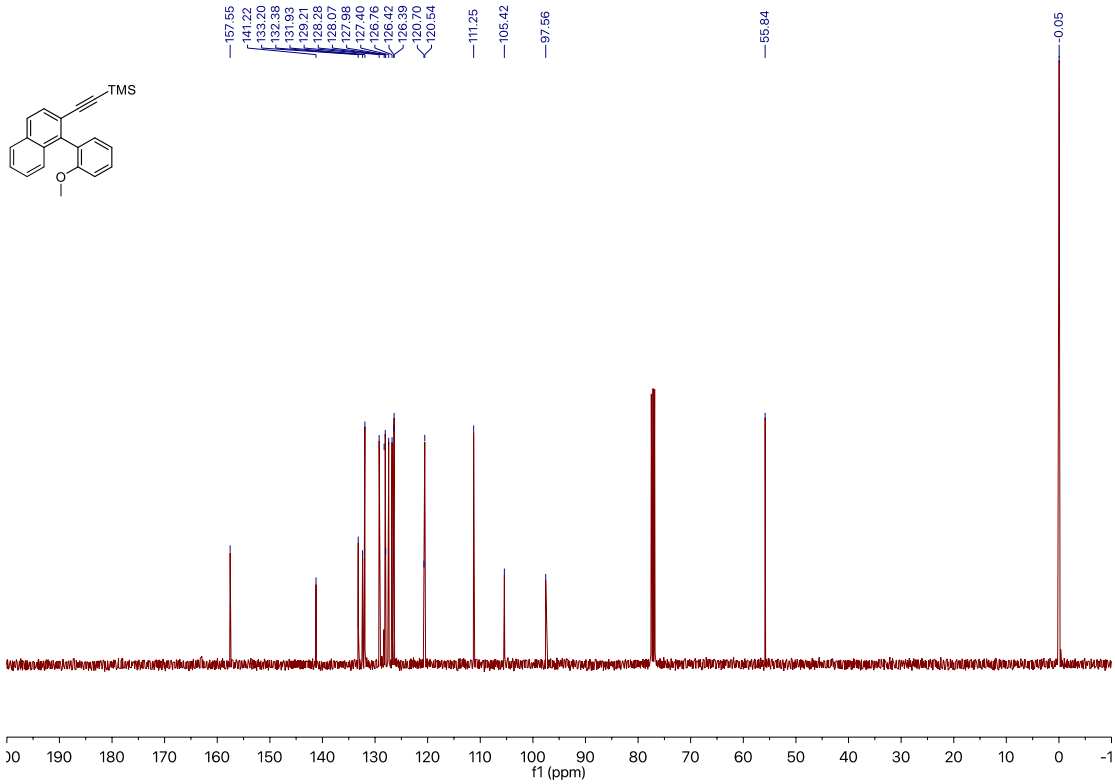
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **3a**



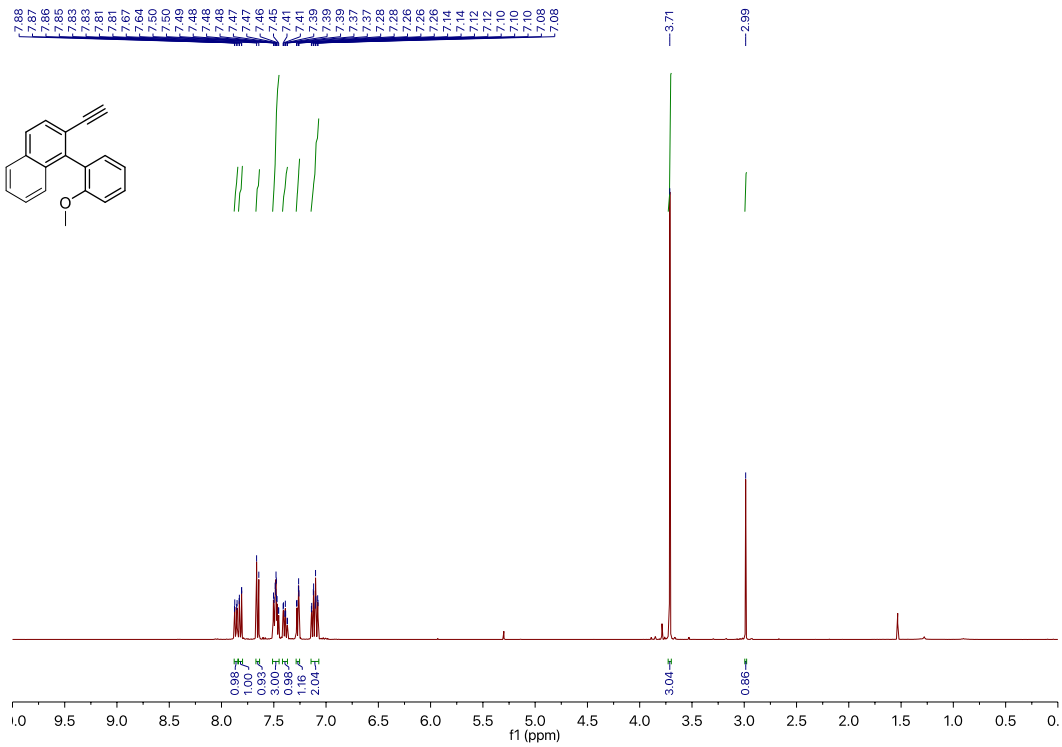
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **3b**



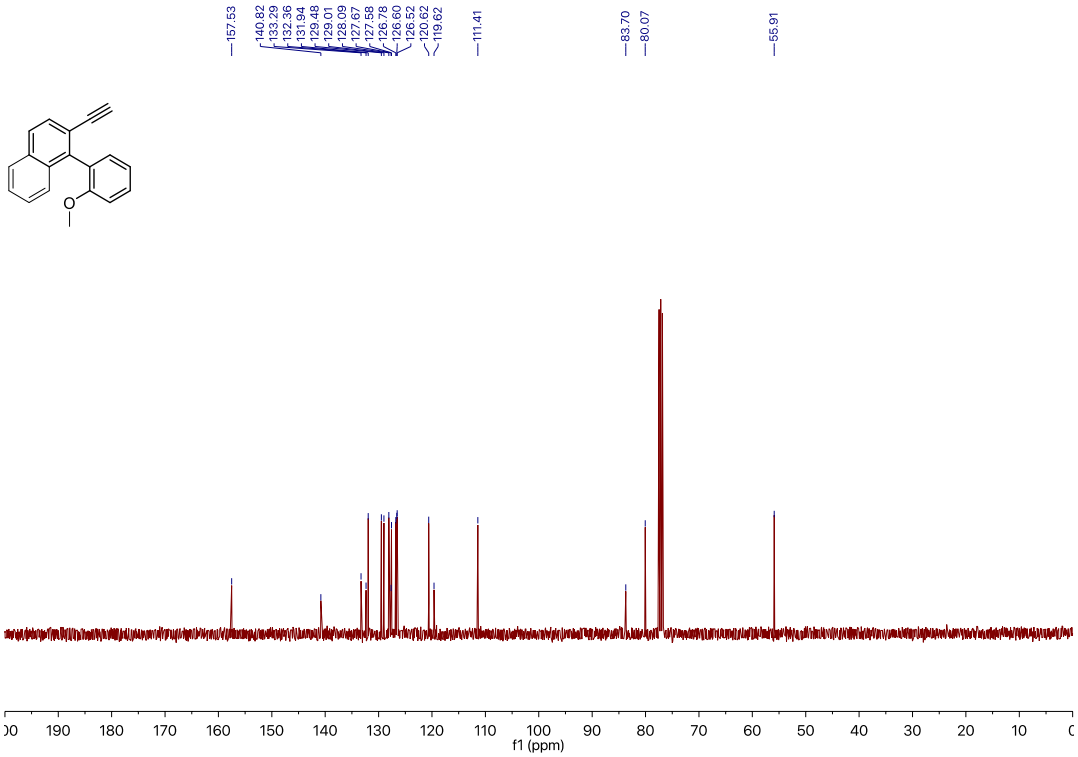
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **3b**



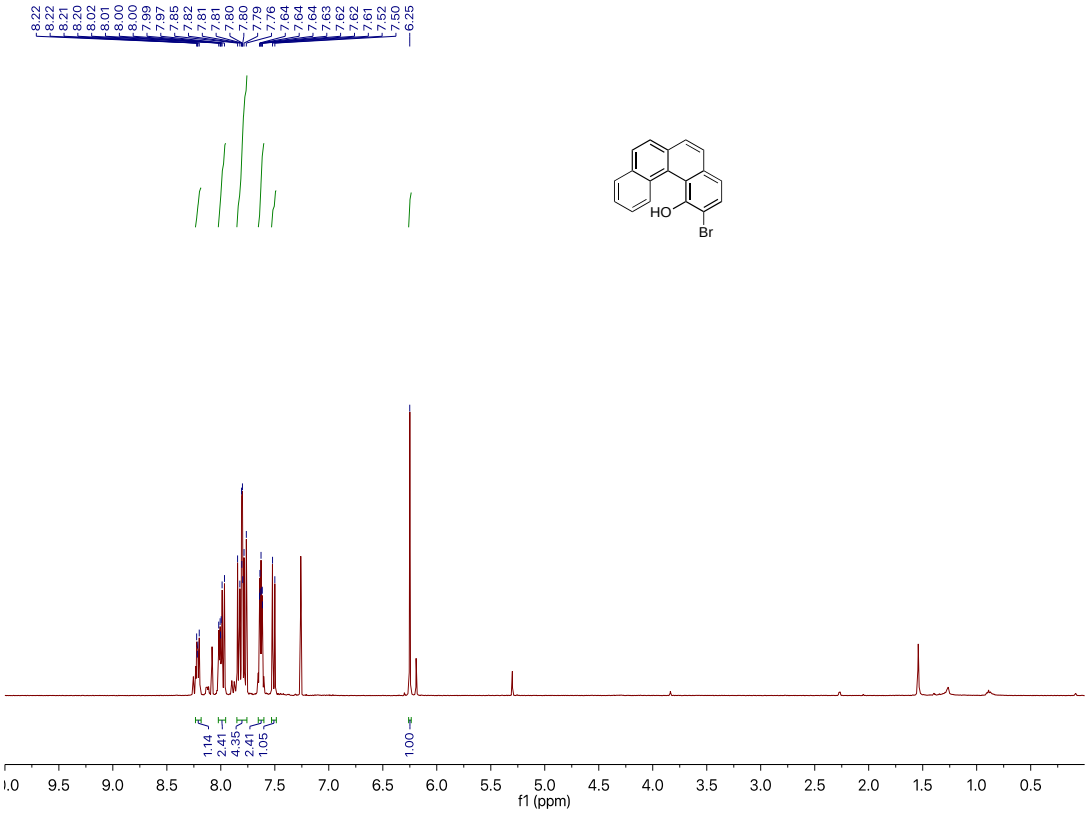
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **4b**



^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **4b**



^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **7b**



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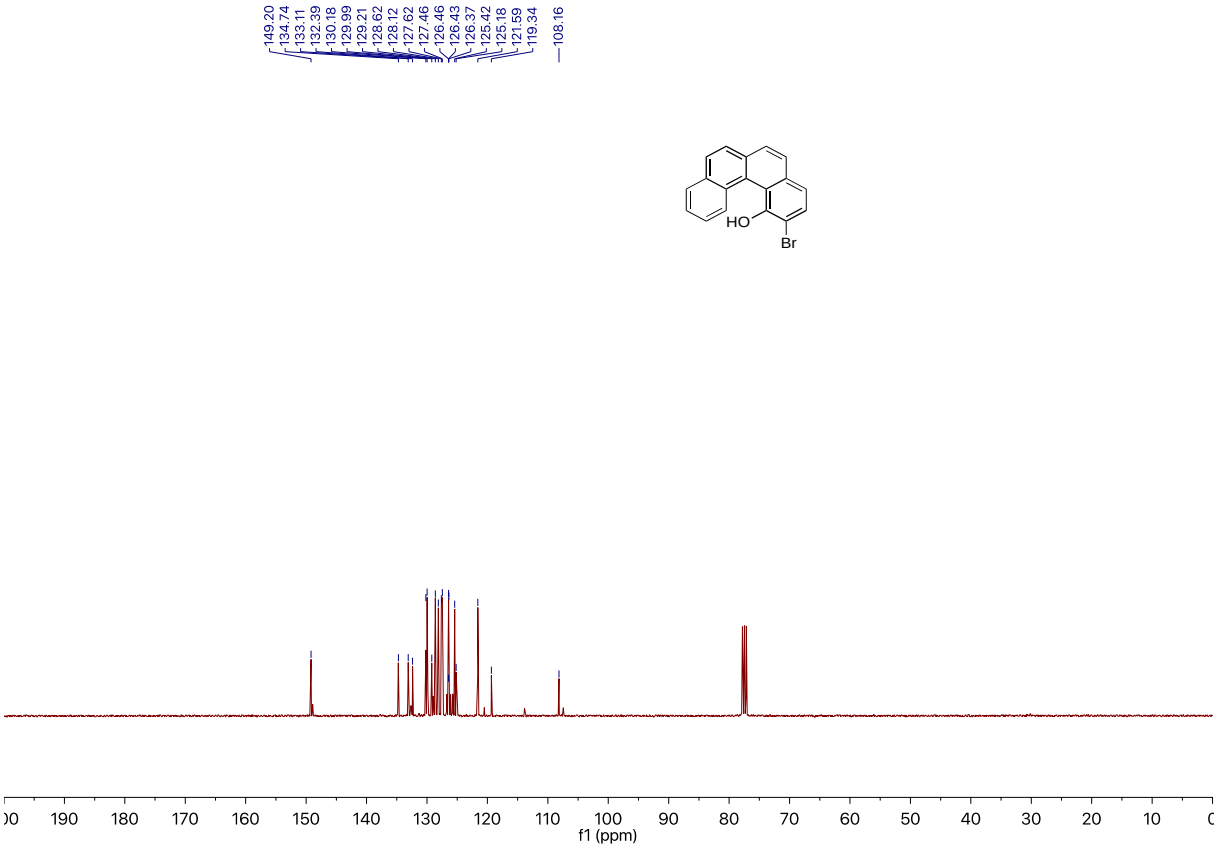

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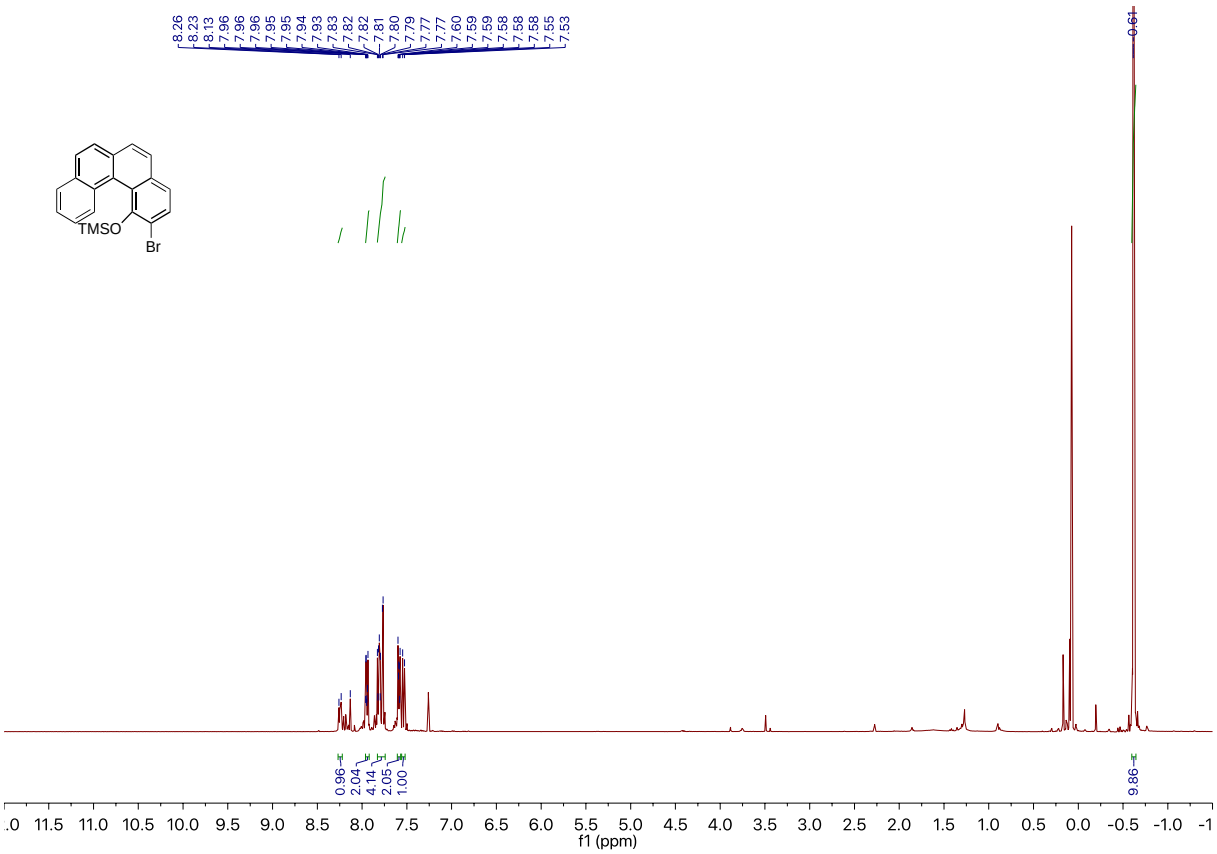
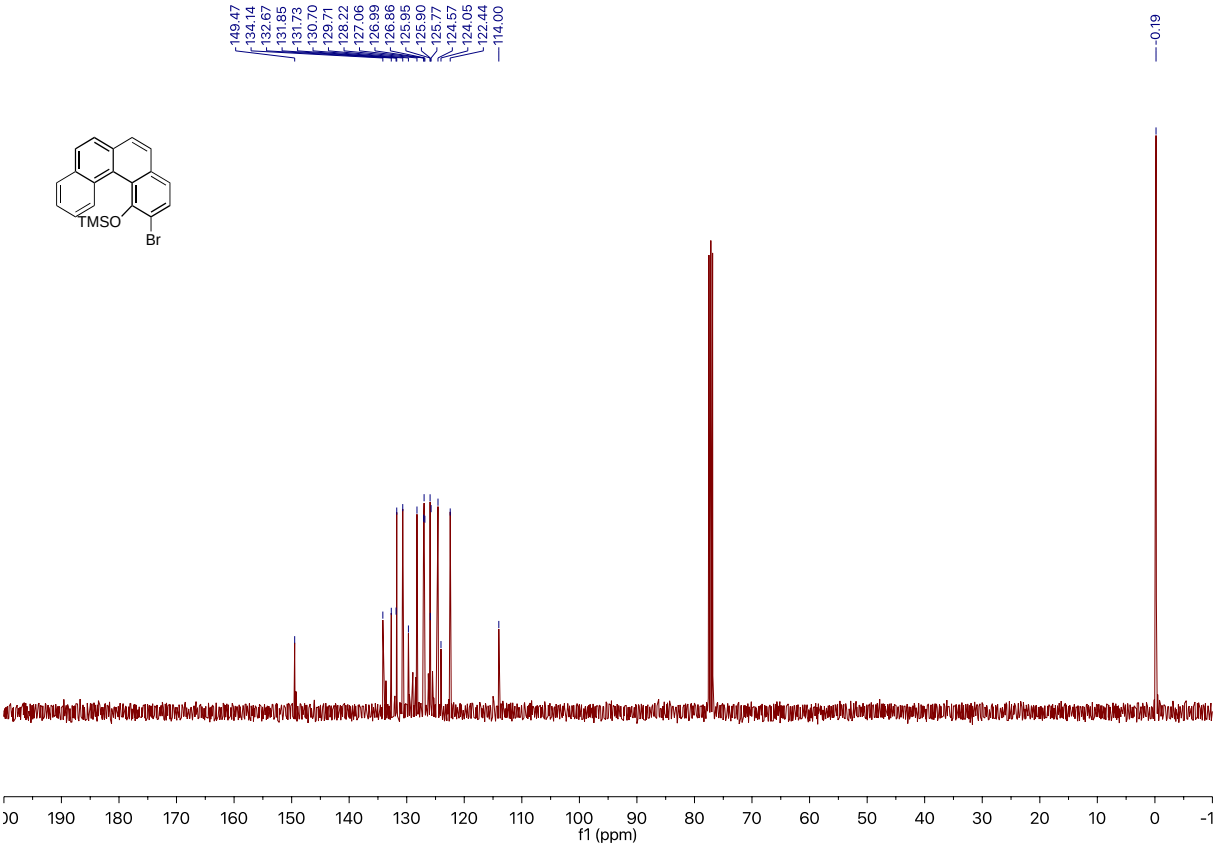
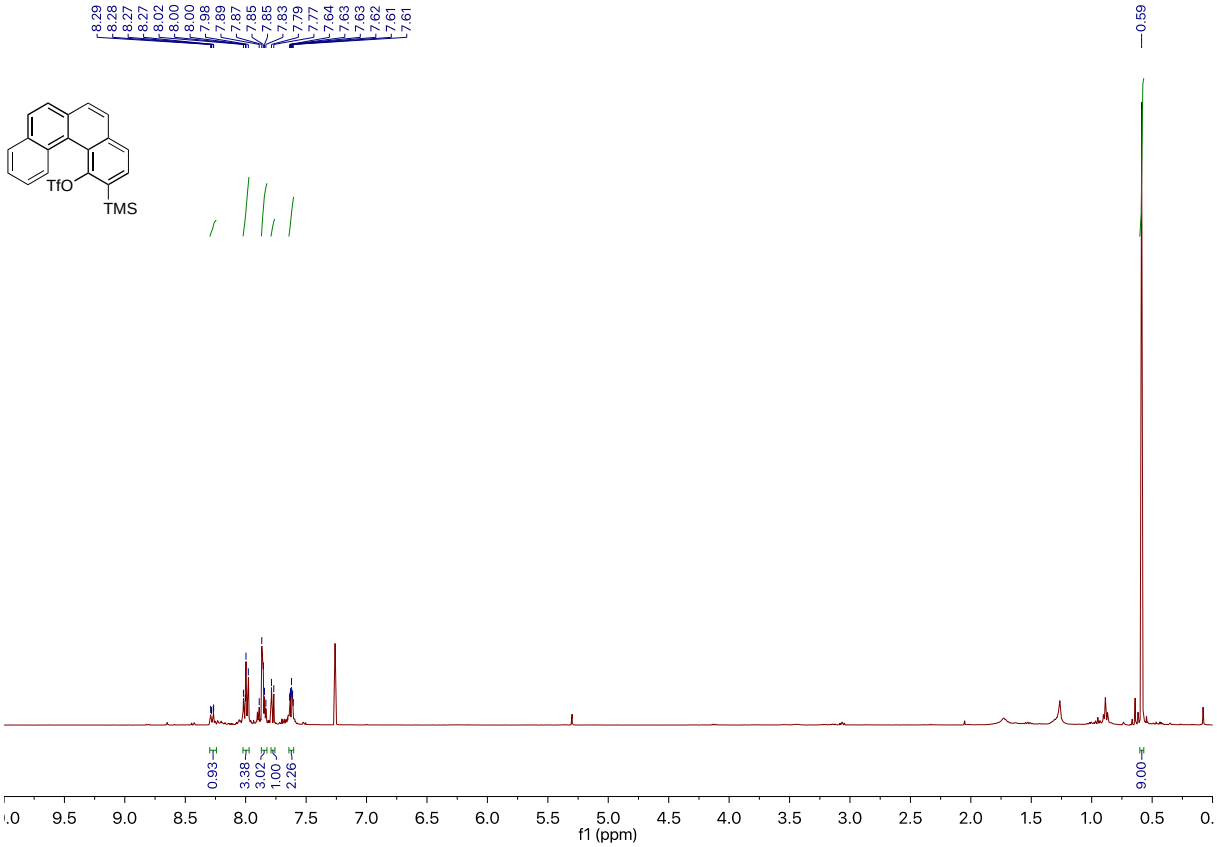


^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **8b**



^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **9b**



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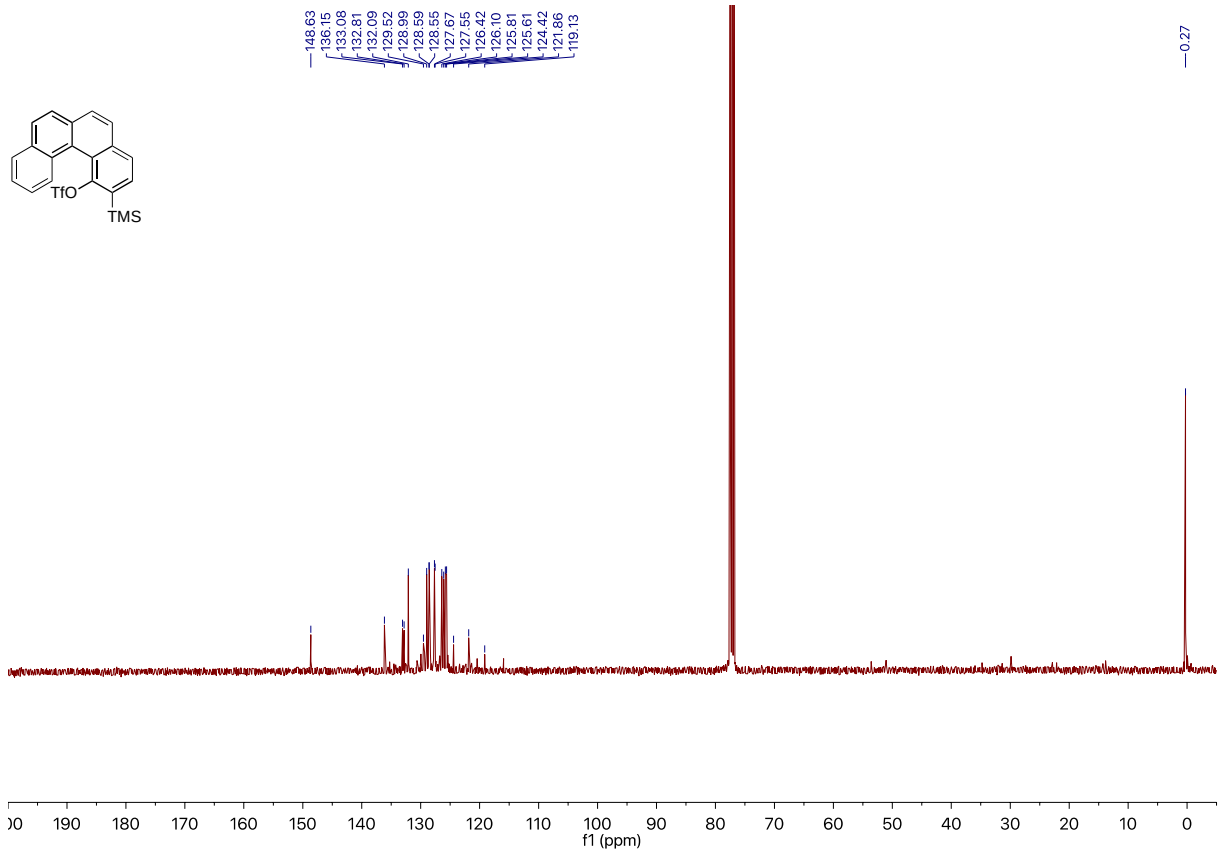

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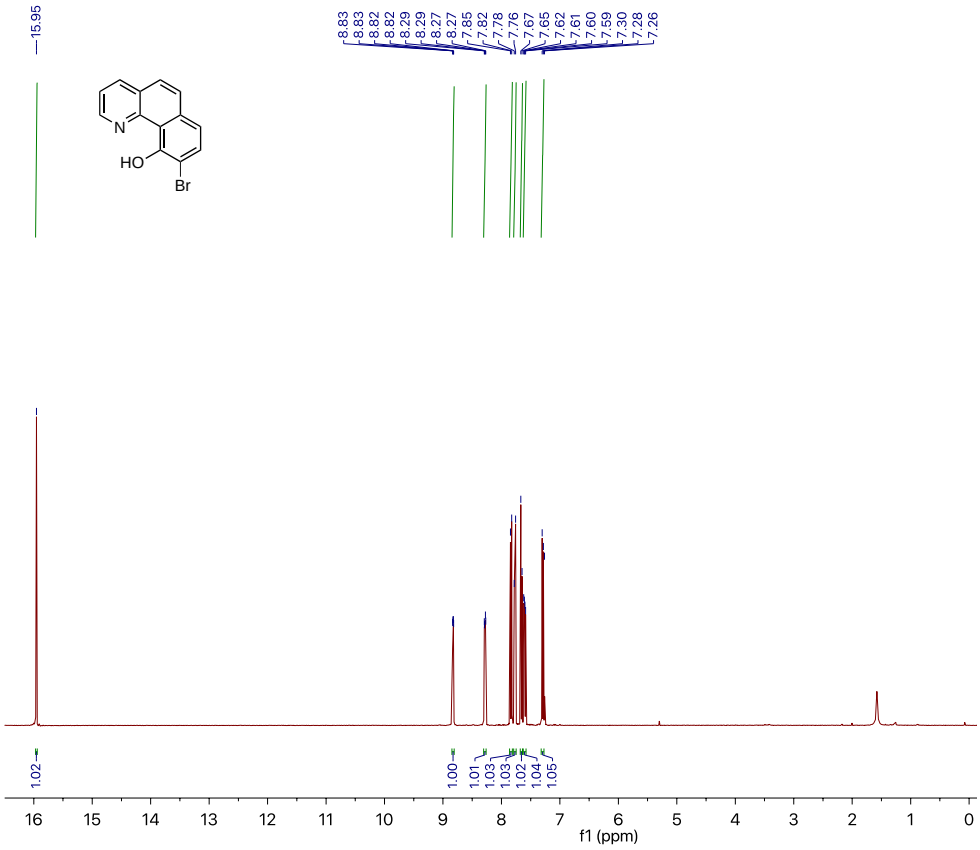

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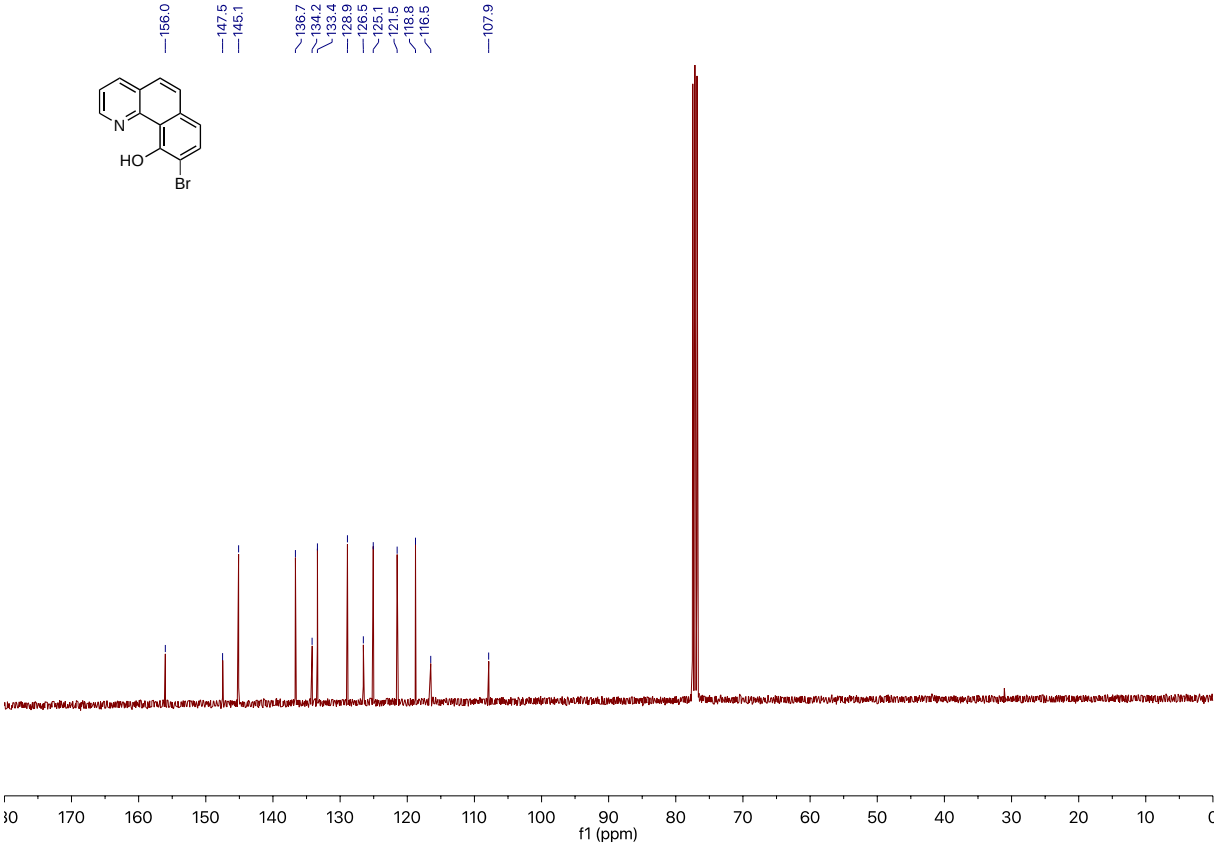

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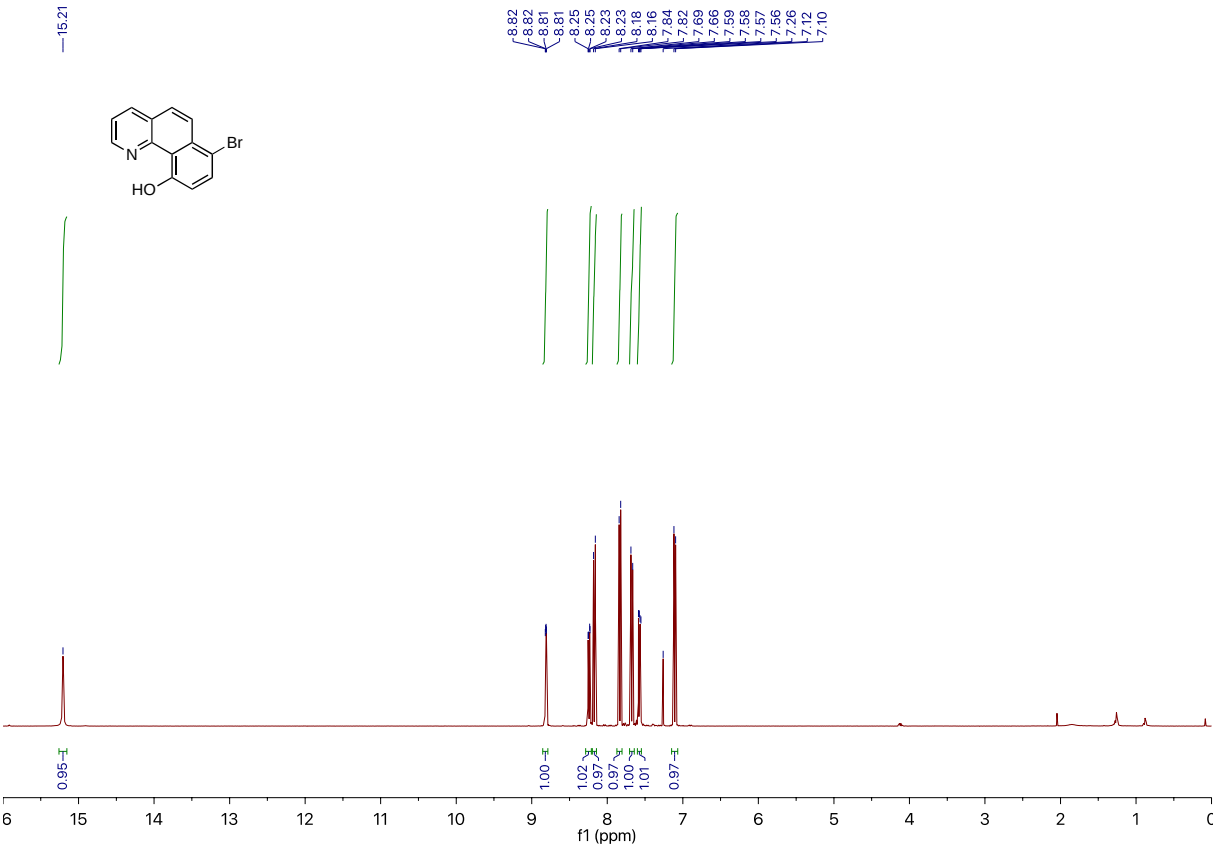

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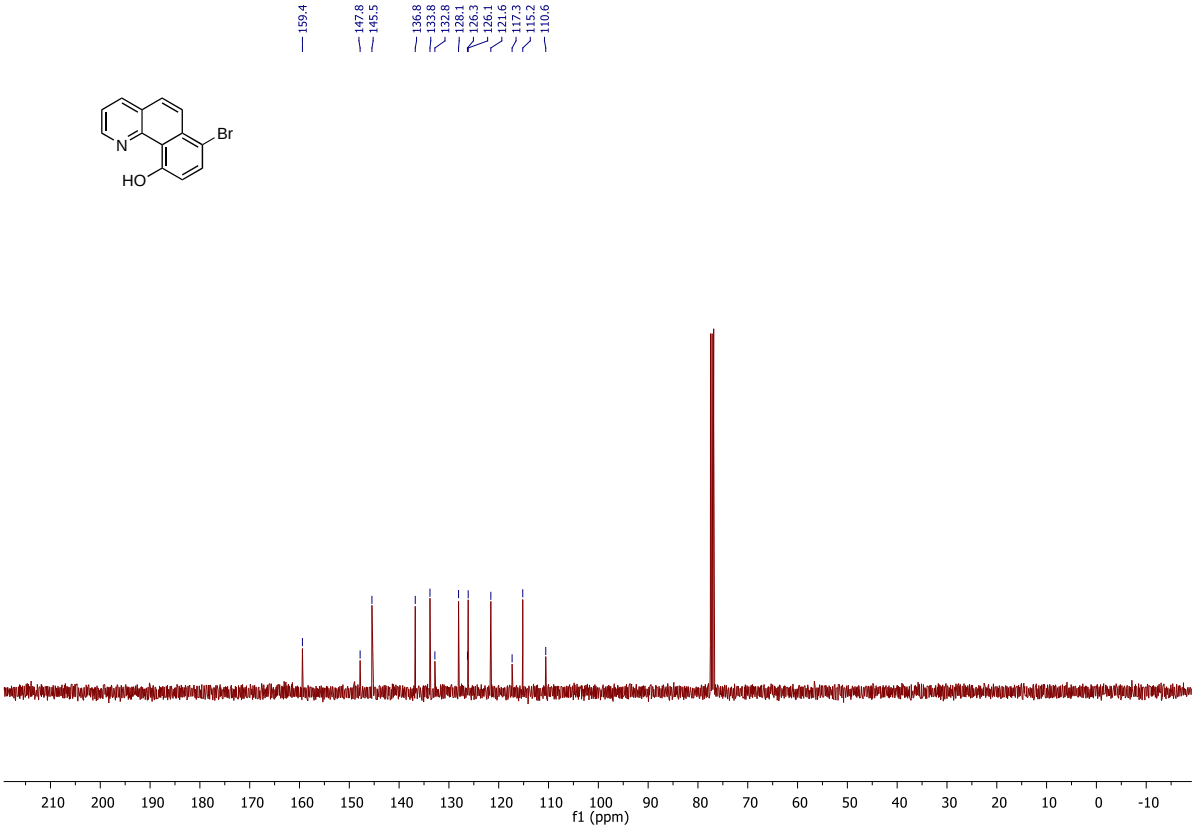

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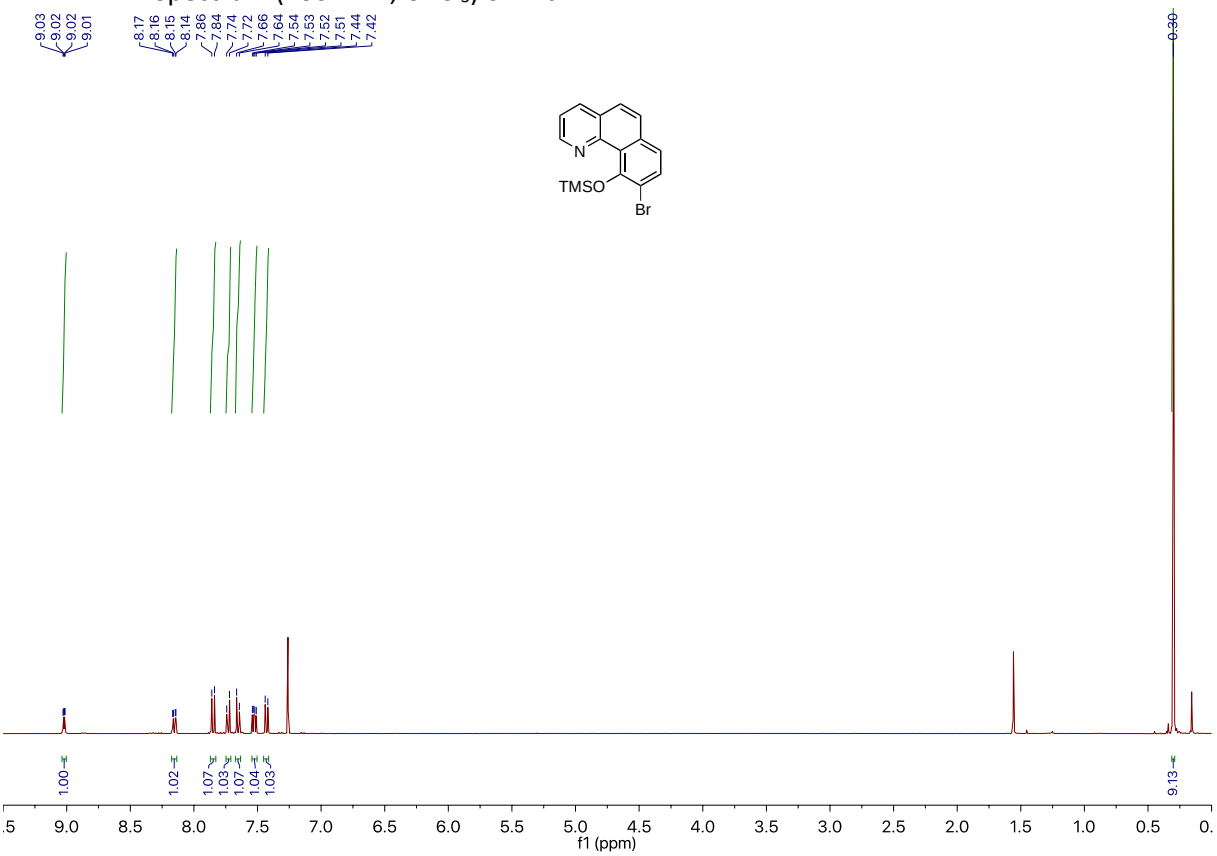

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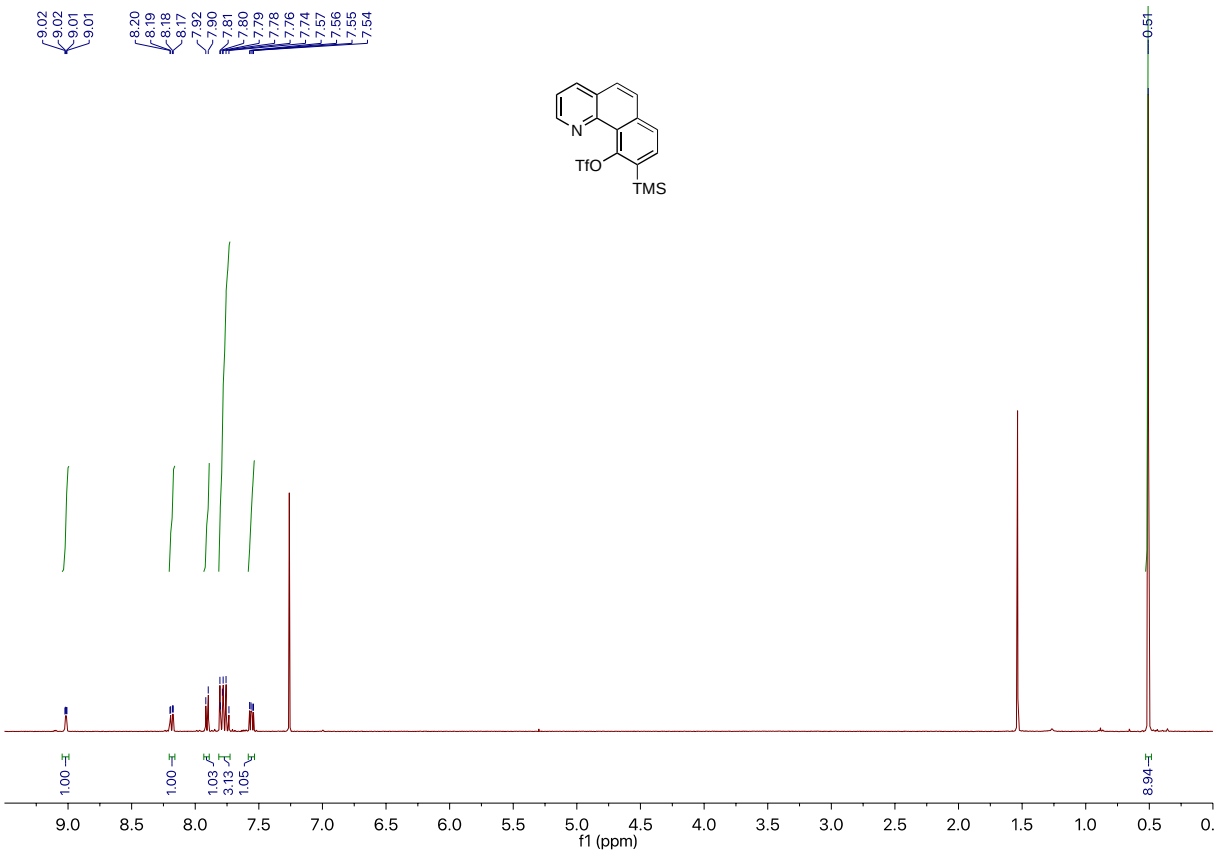

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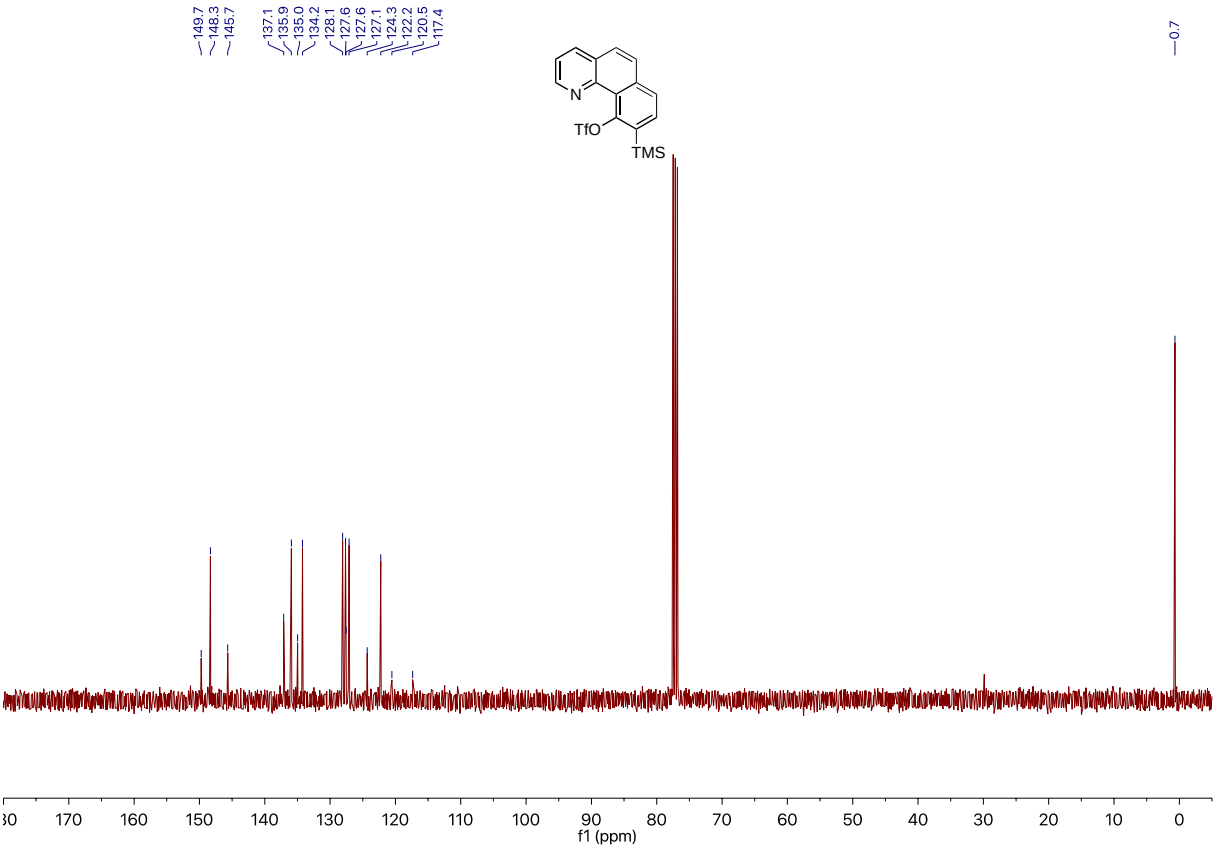
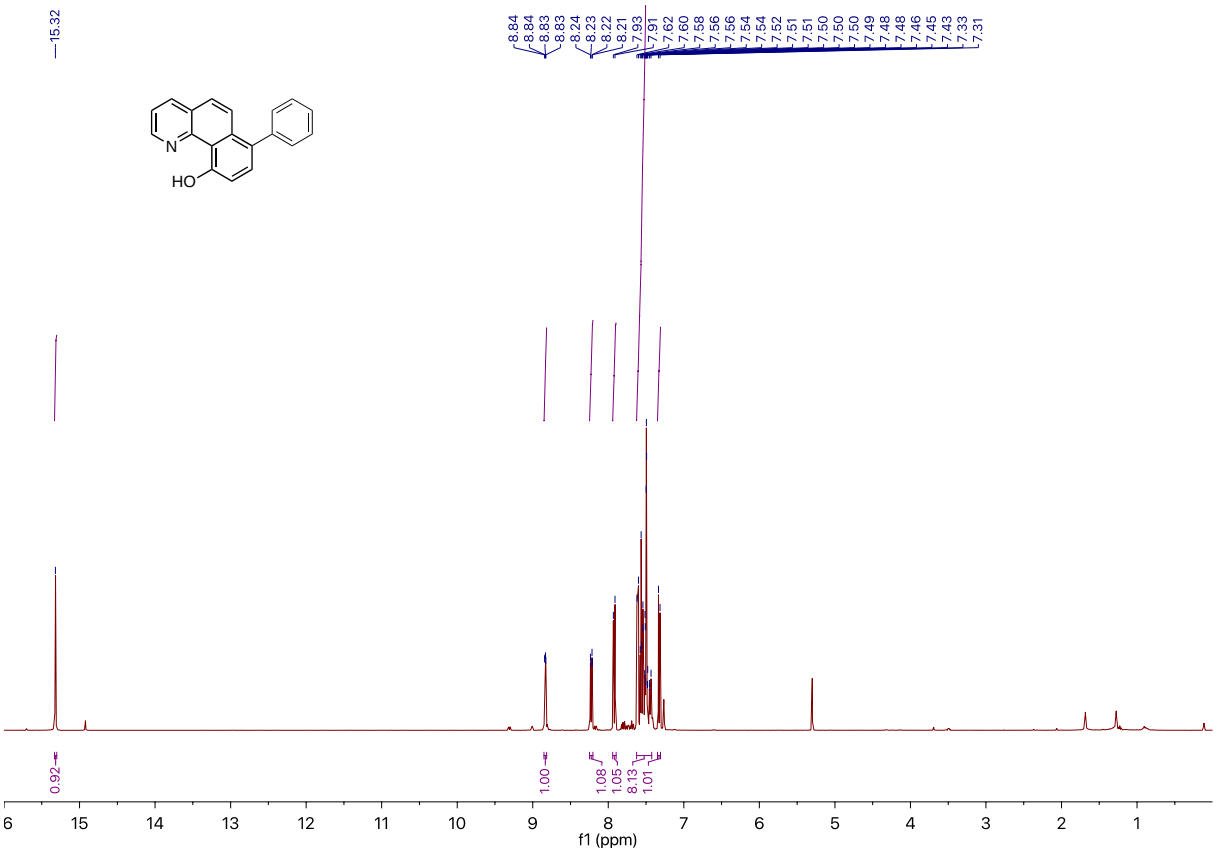


^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **11c**



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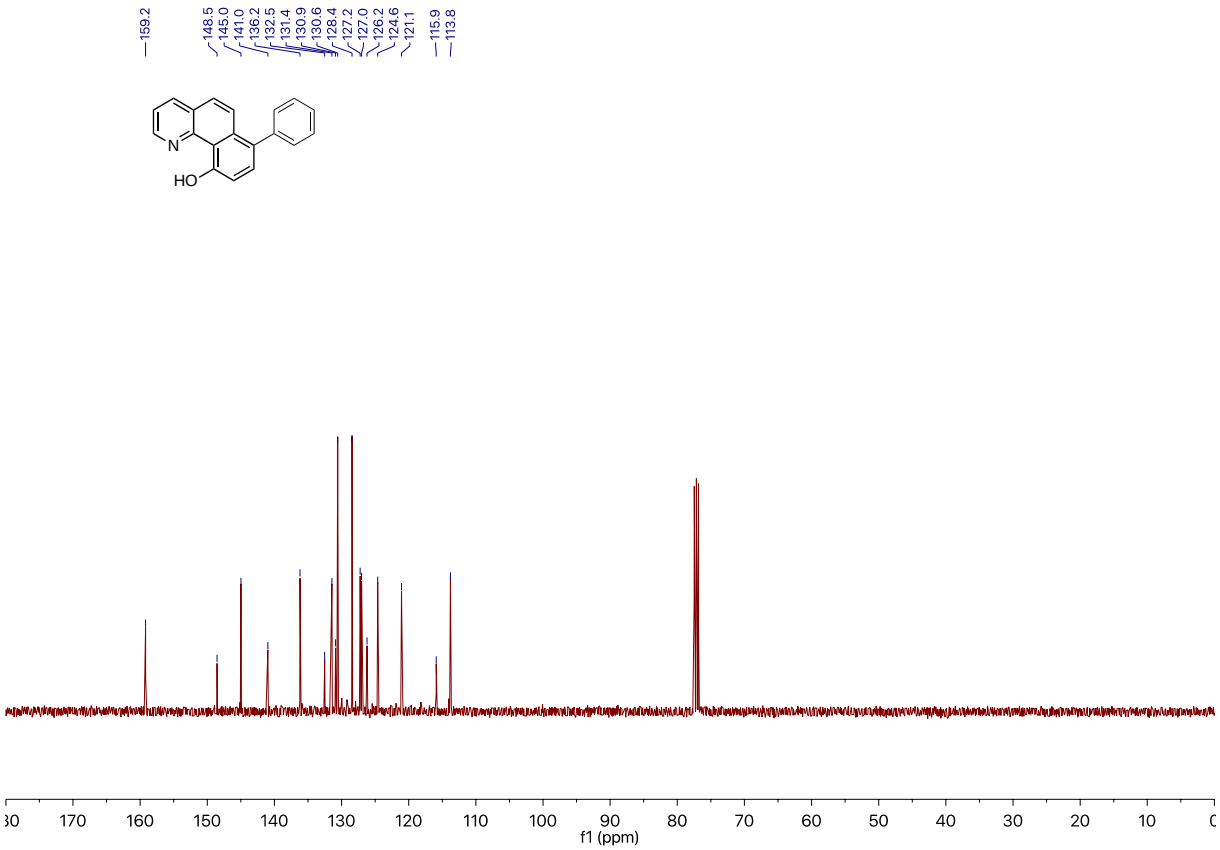

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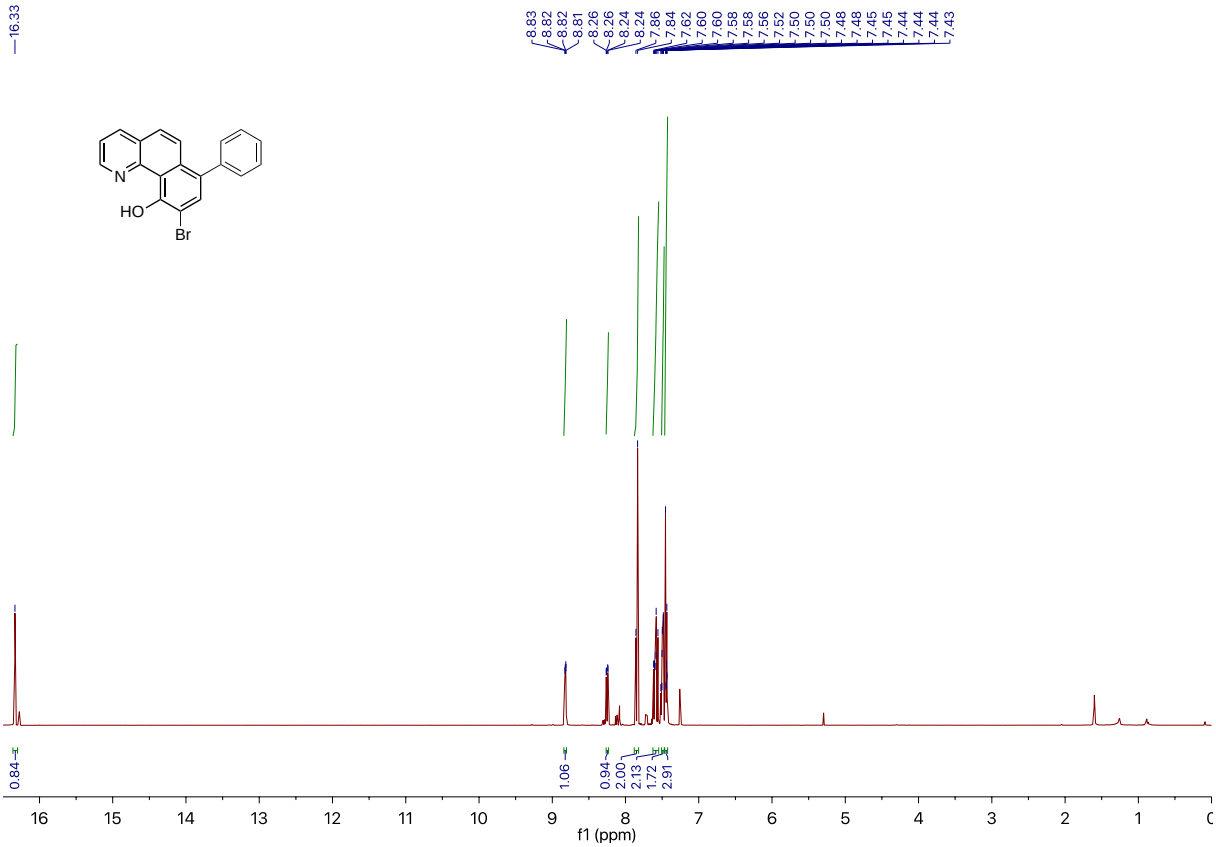
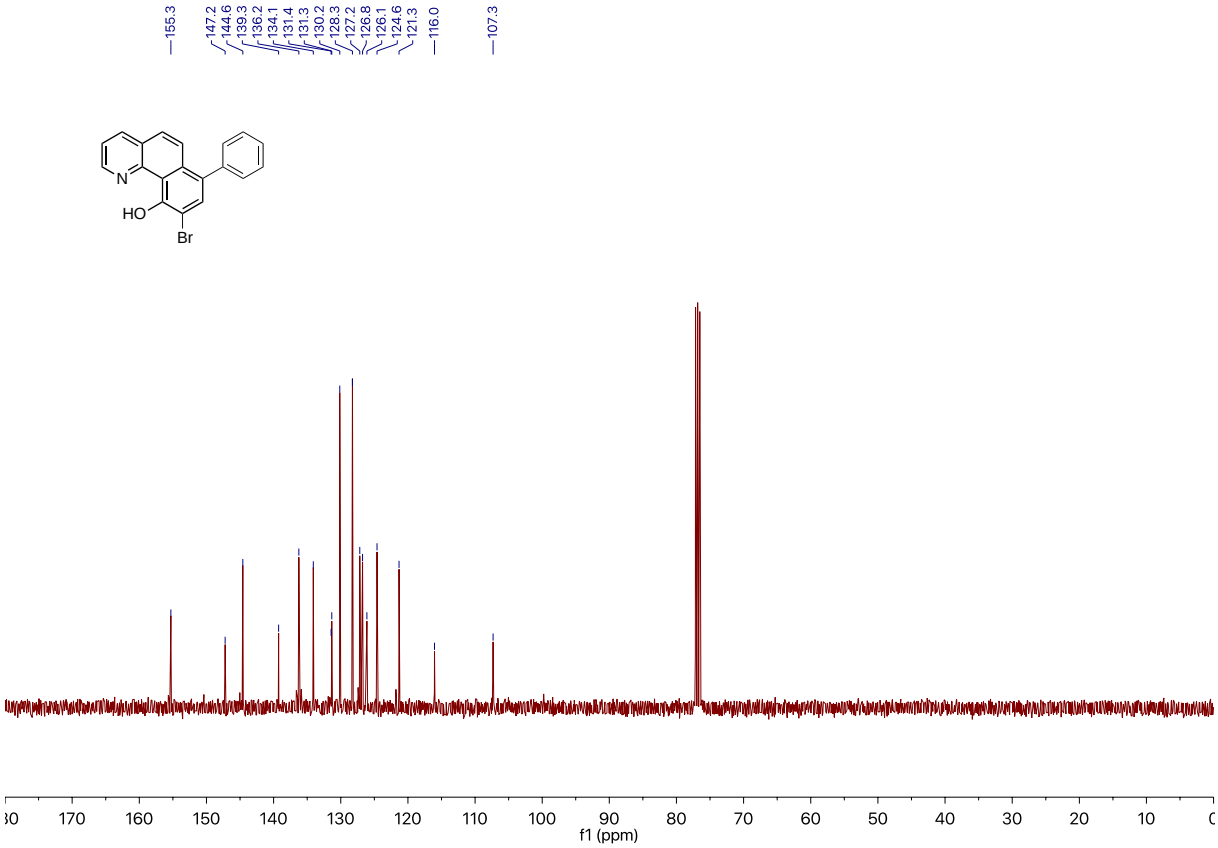
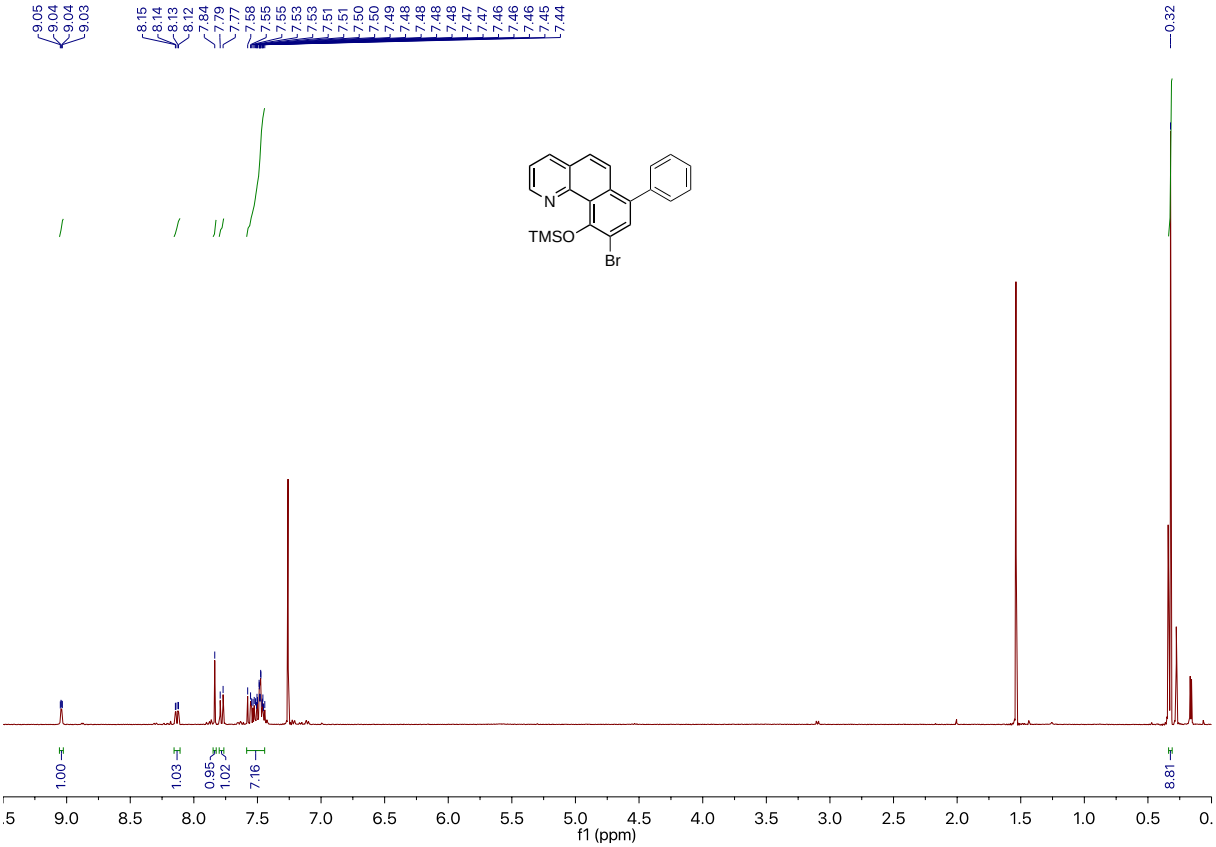


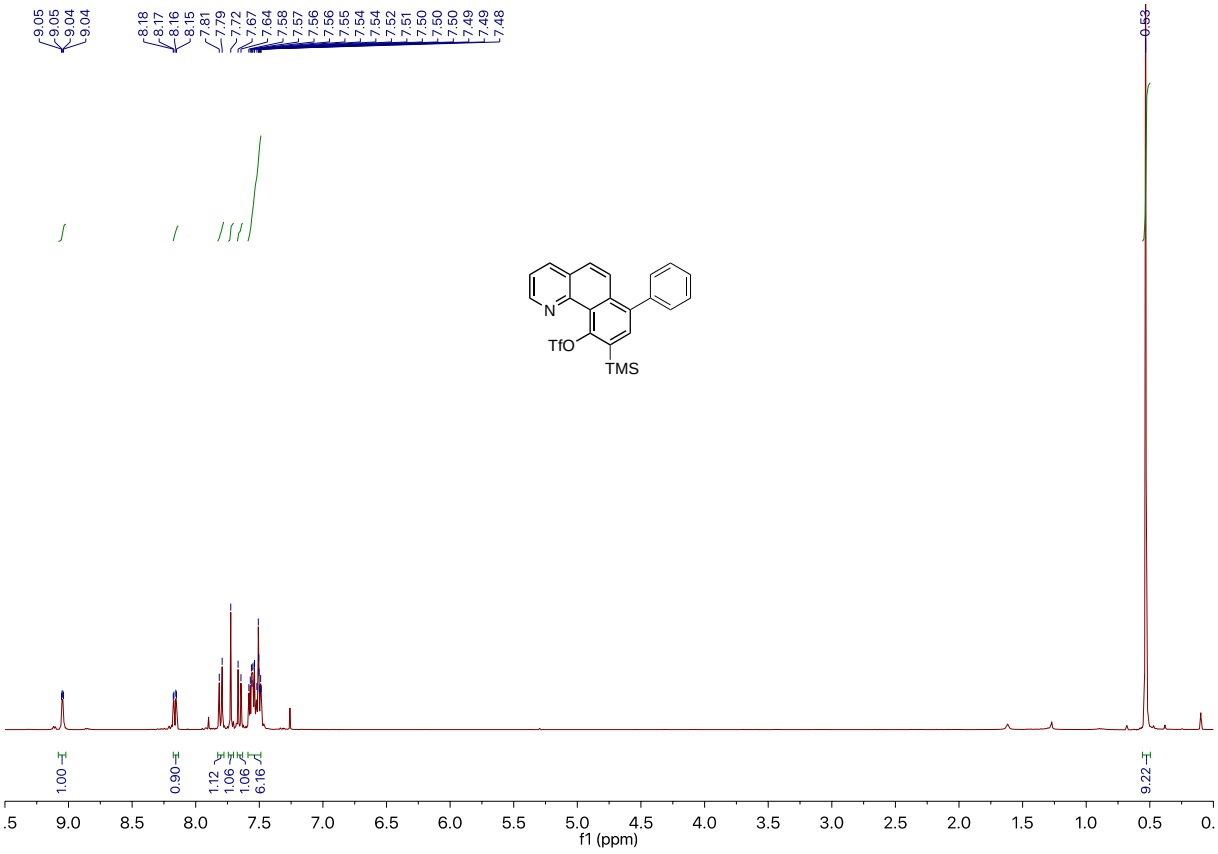
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **11d**



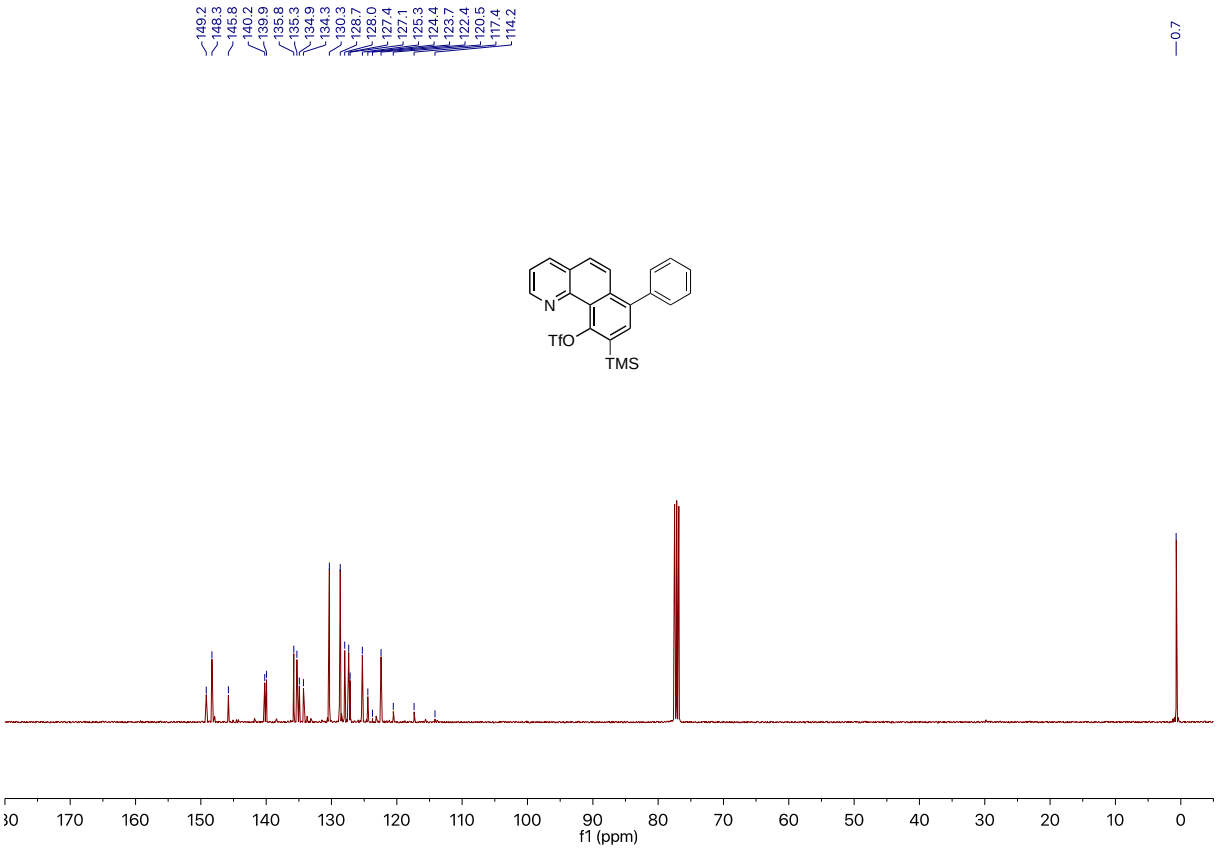
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **12b**



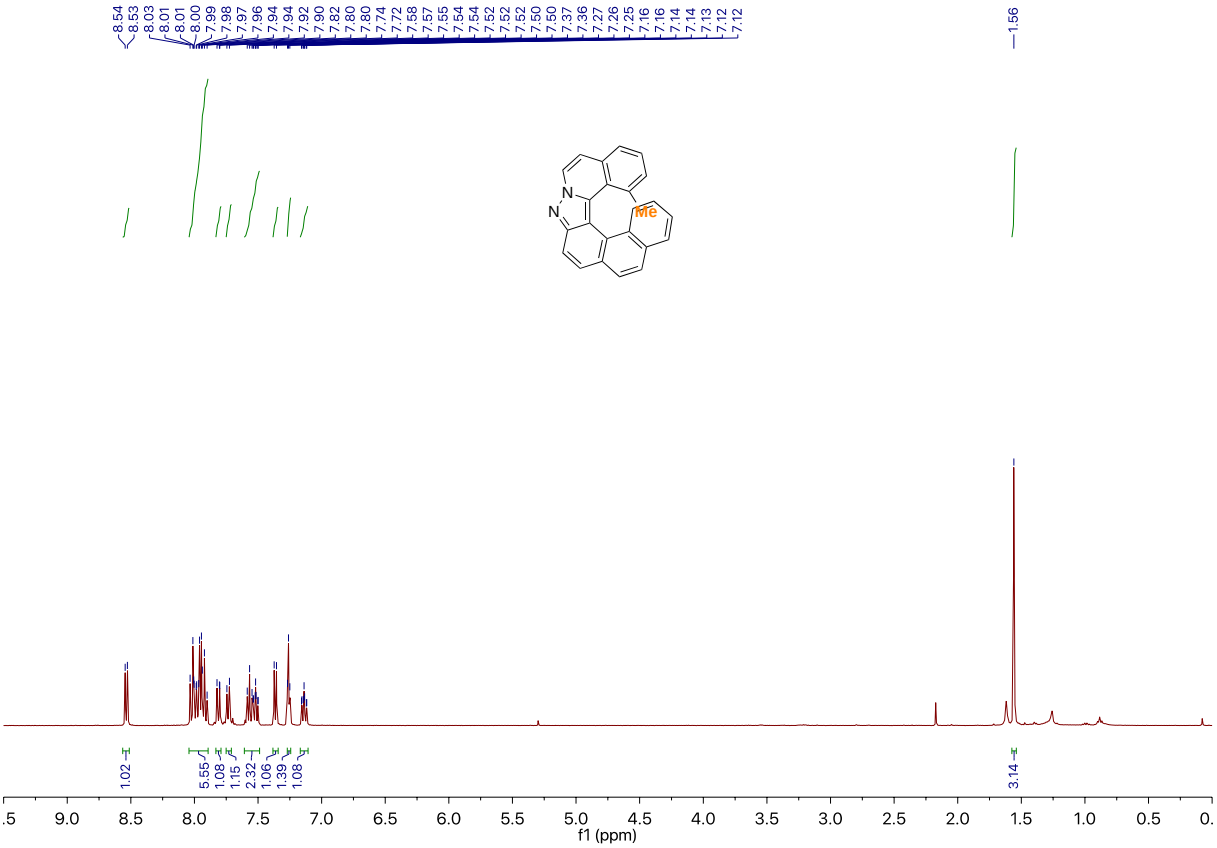
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **13b**



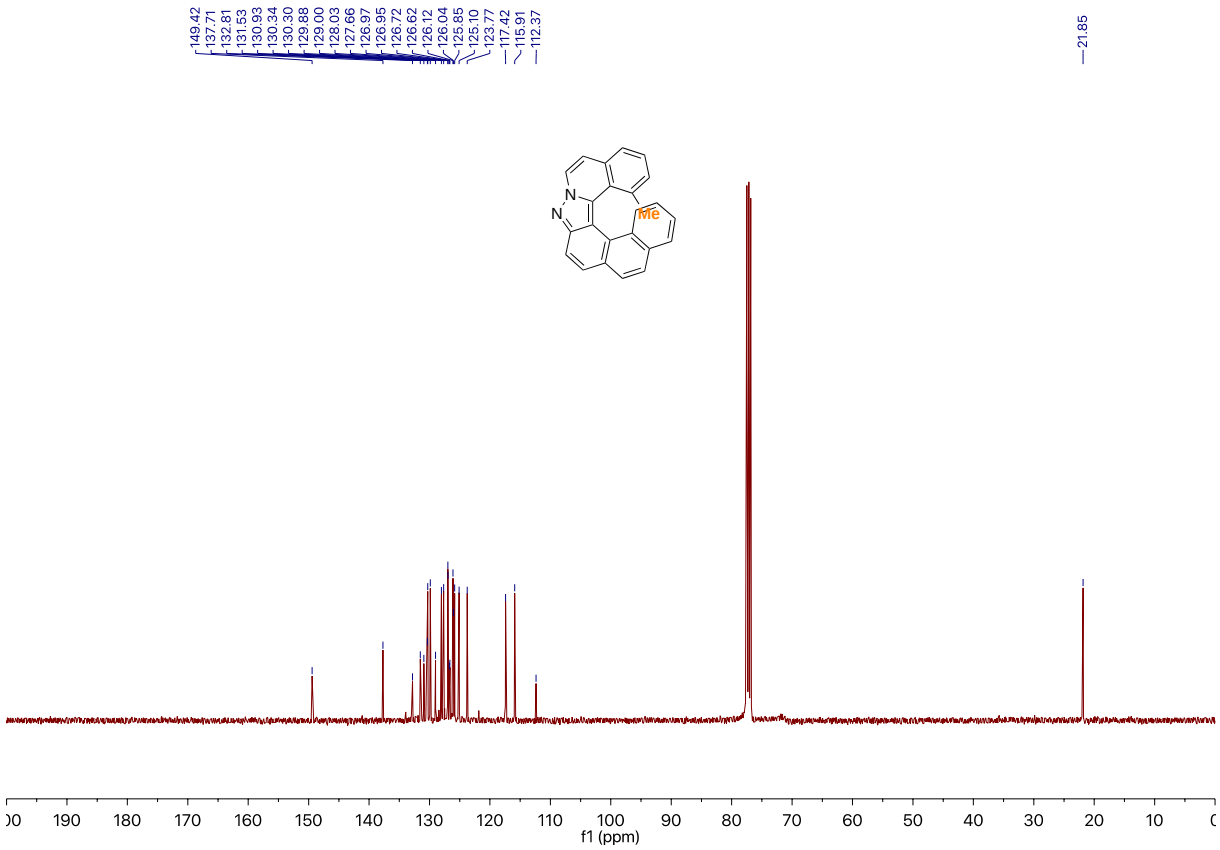
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **13b**



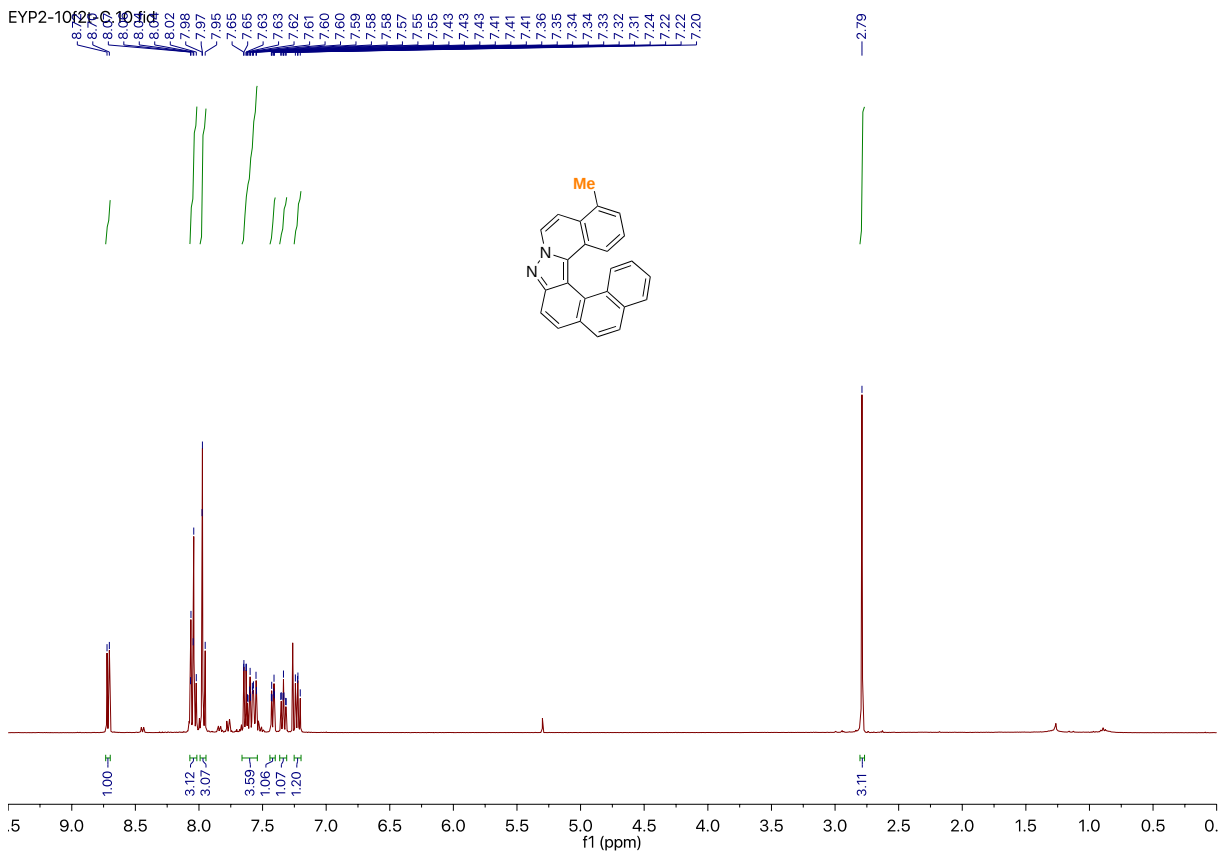
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-21**



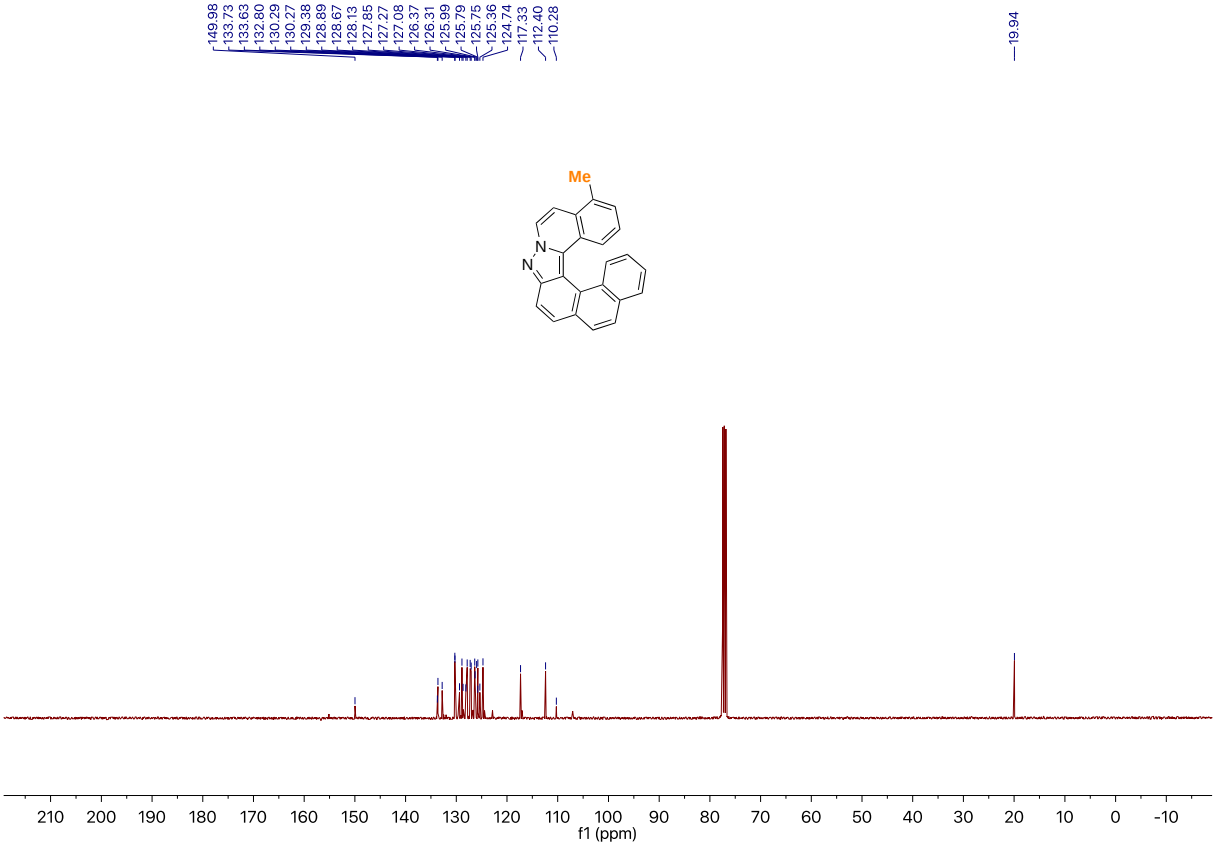
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-21**



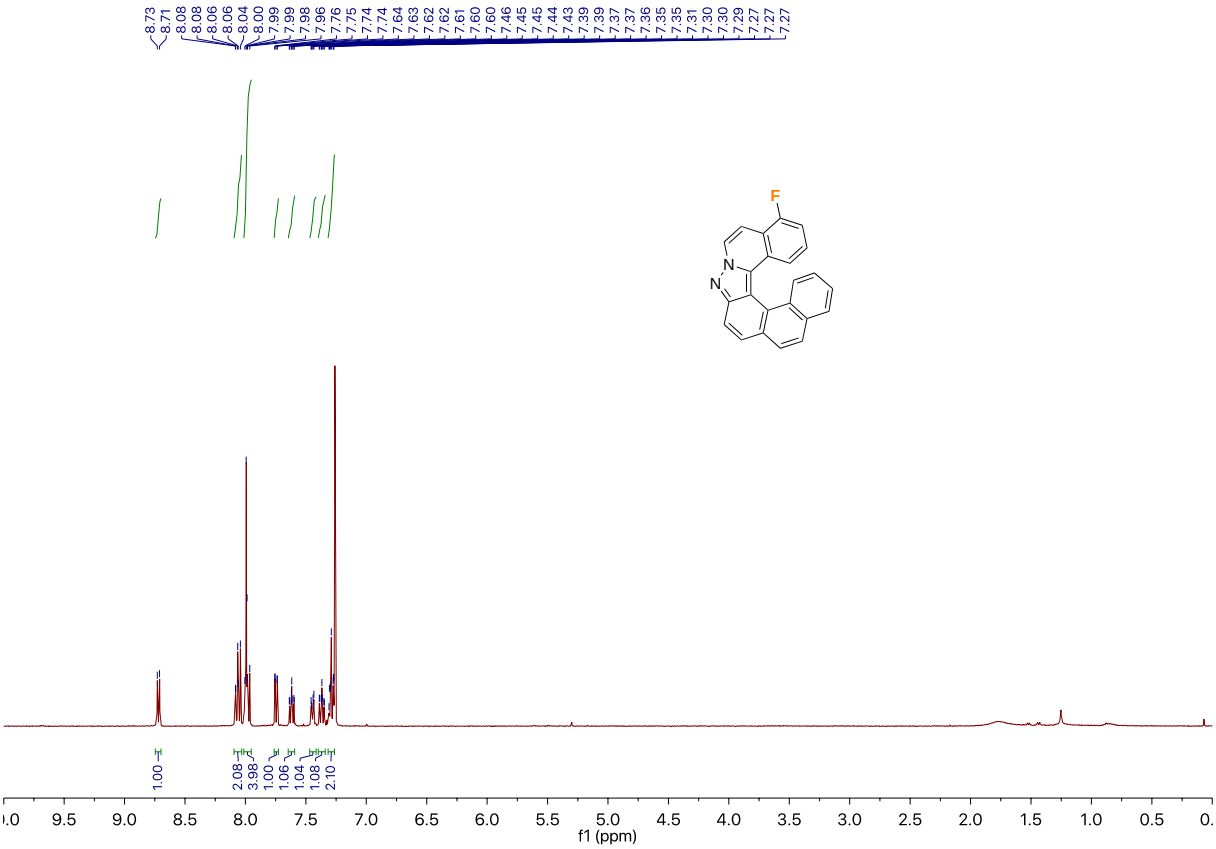
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-22**



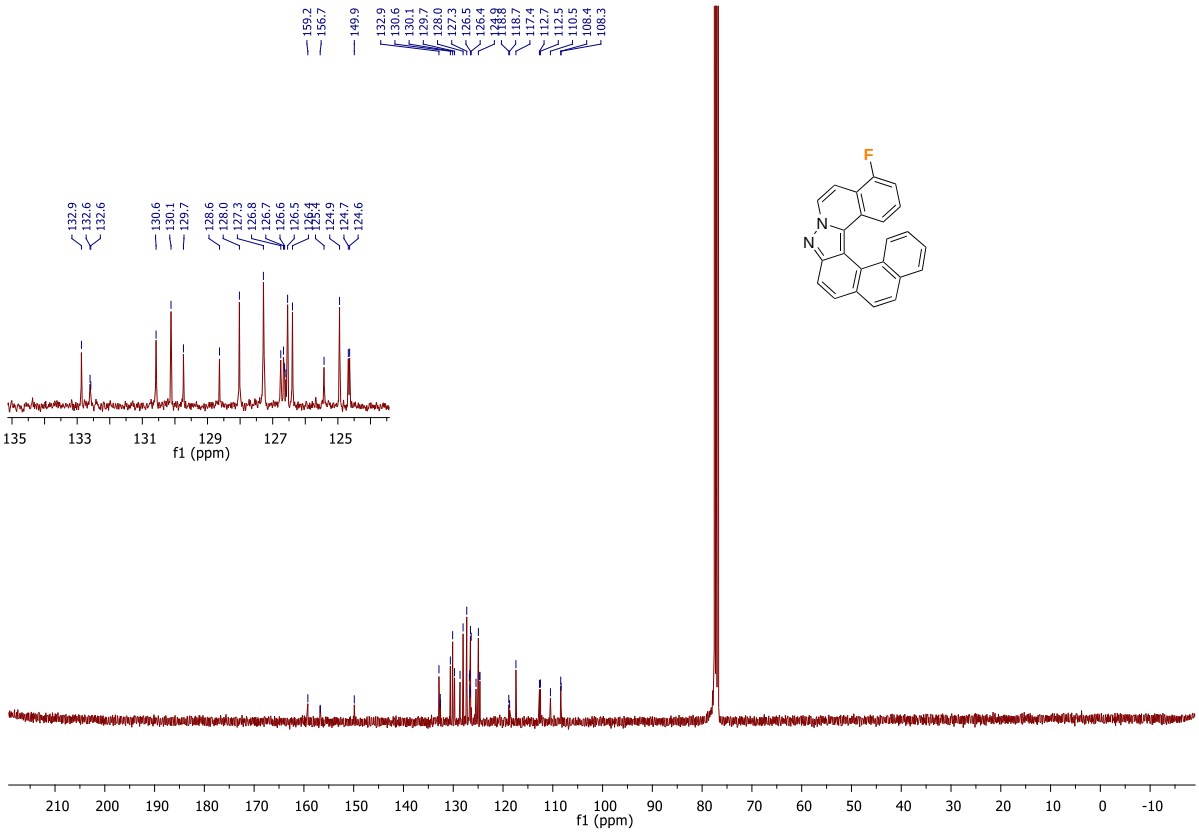
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-22**



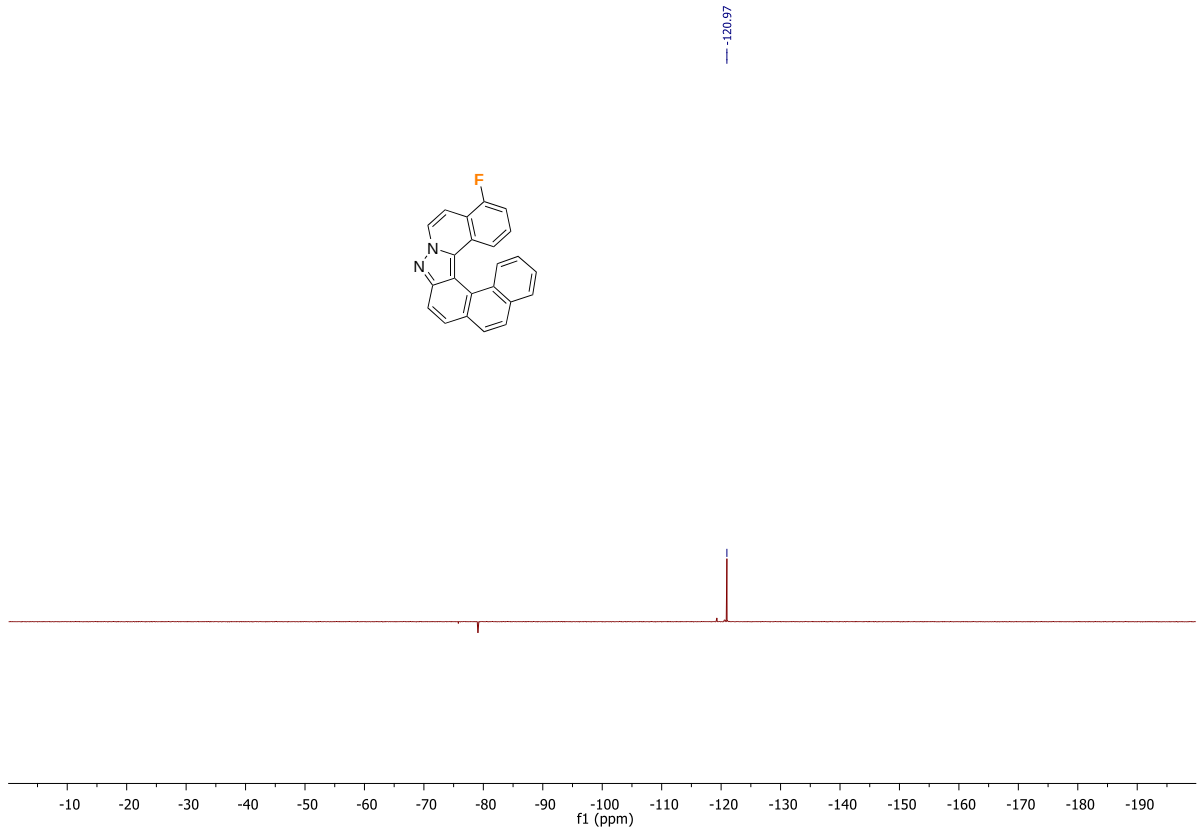
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-27**



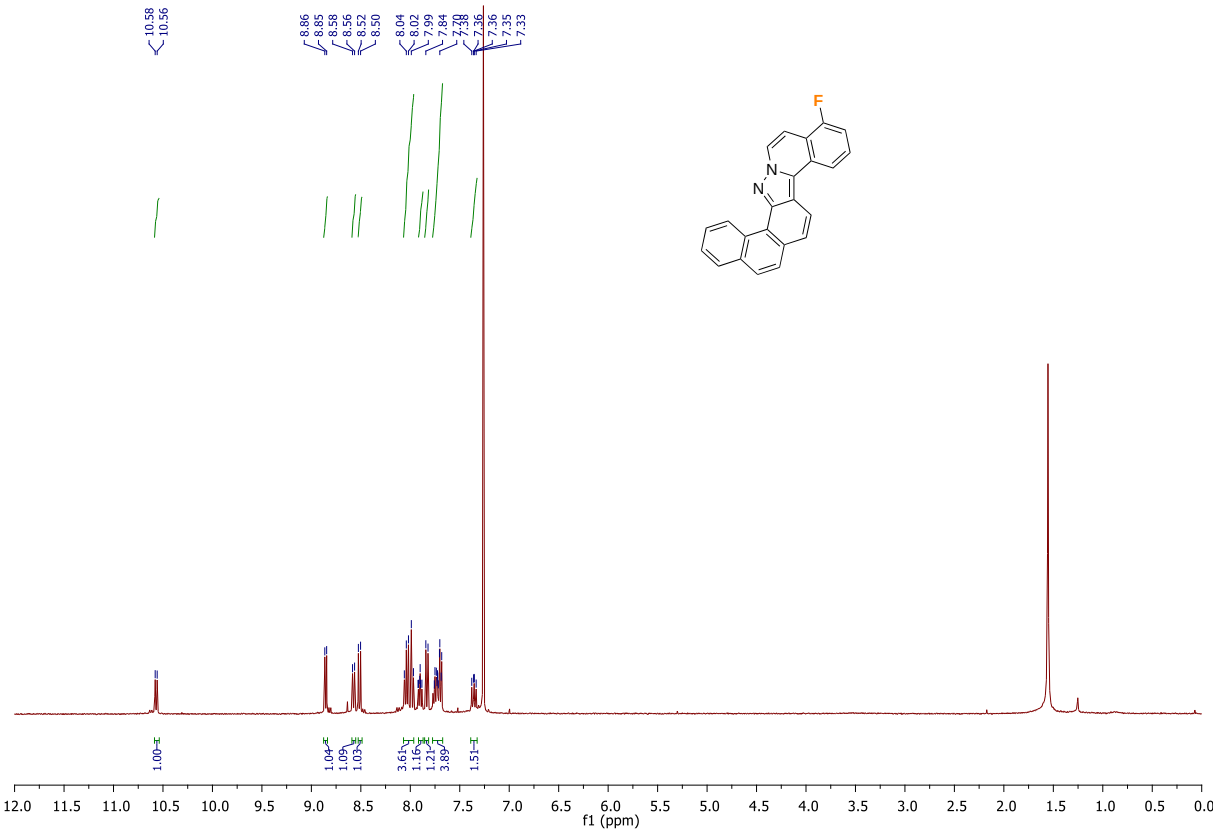
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-27**



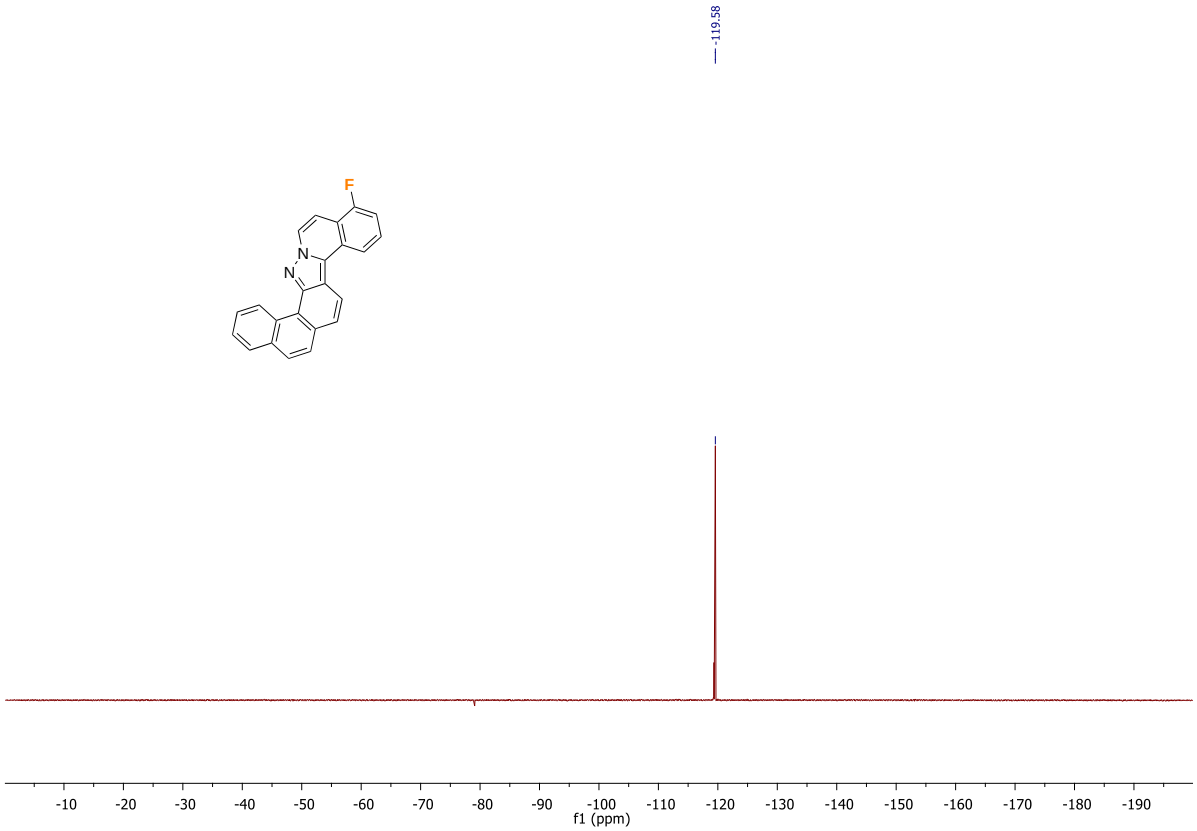
^{19}F NMR Spectrum (376 MHz, $CDCl_3$) of **C-27**



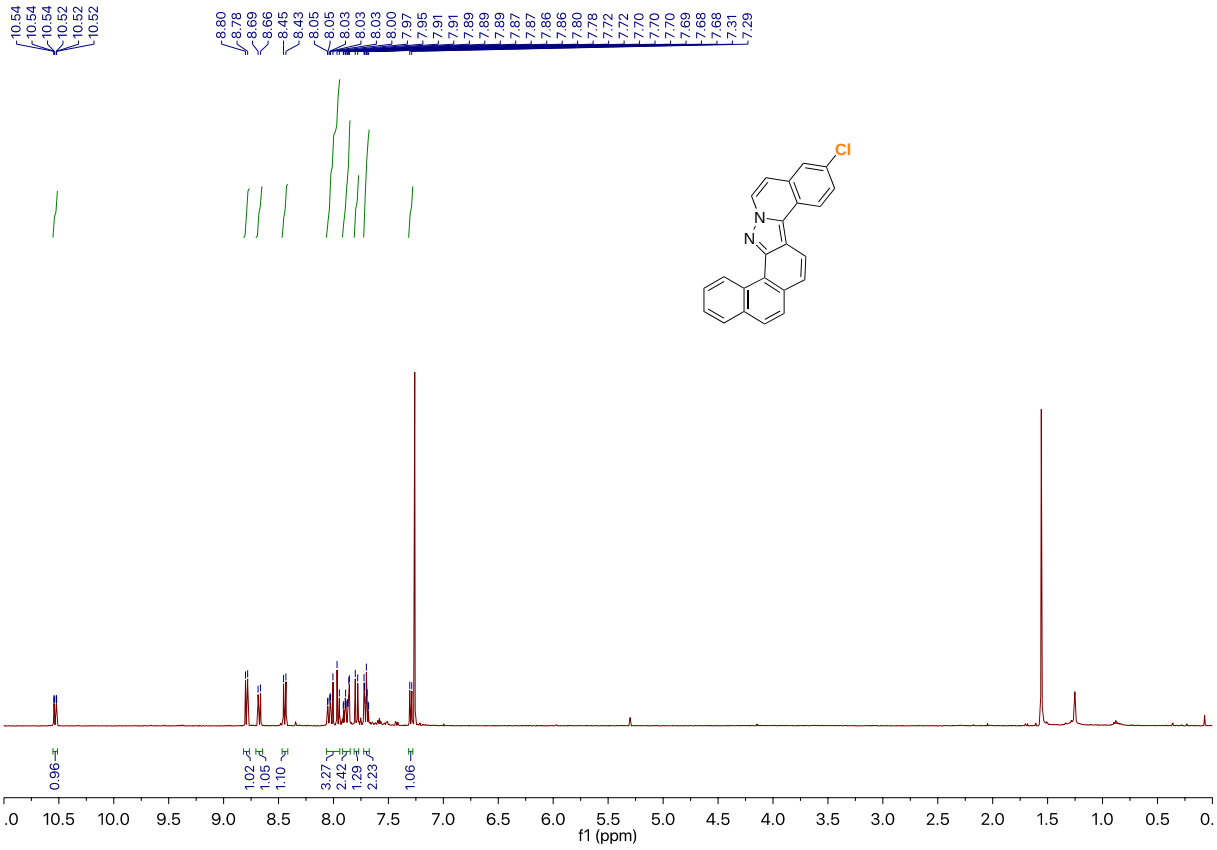
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **S-27**



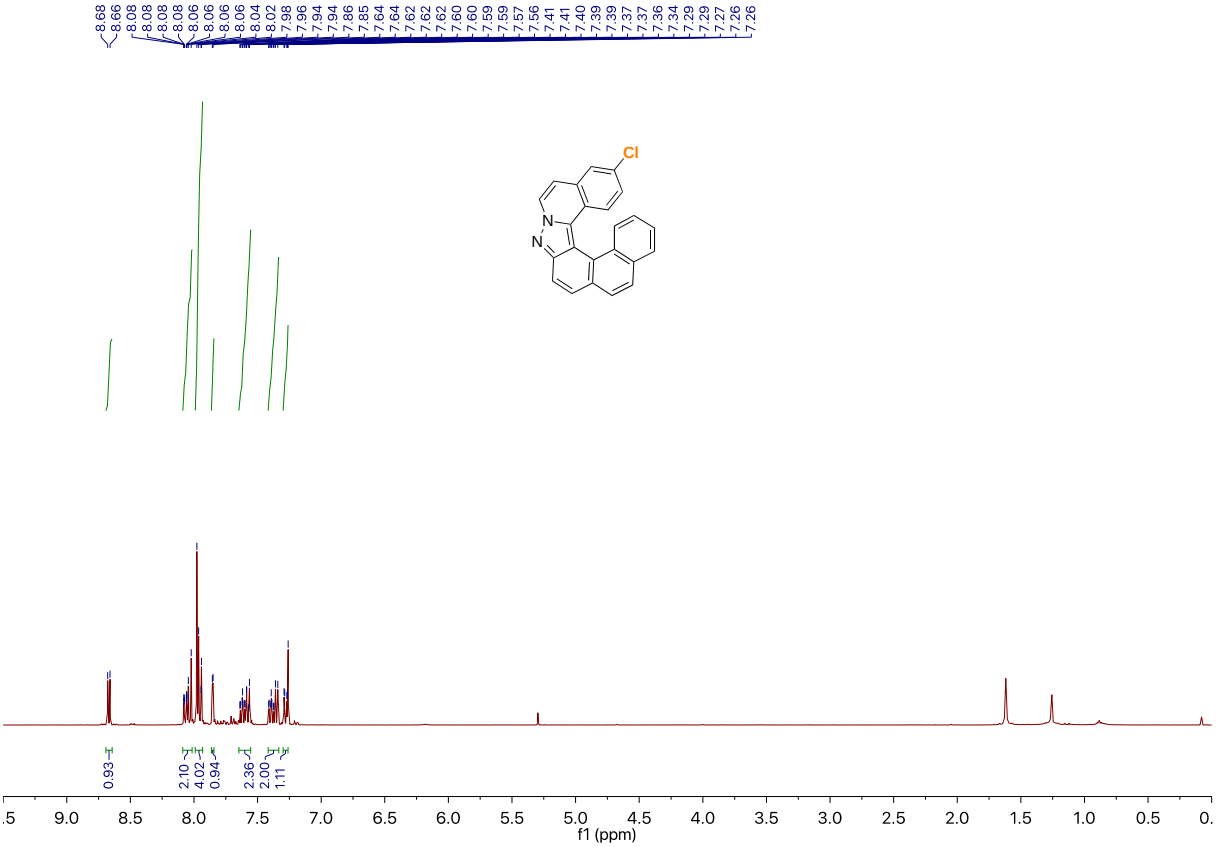
^{19}F NMR Spectrum (376 MHz, $CDCl_3$) of **S-27**



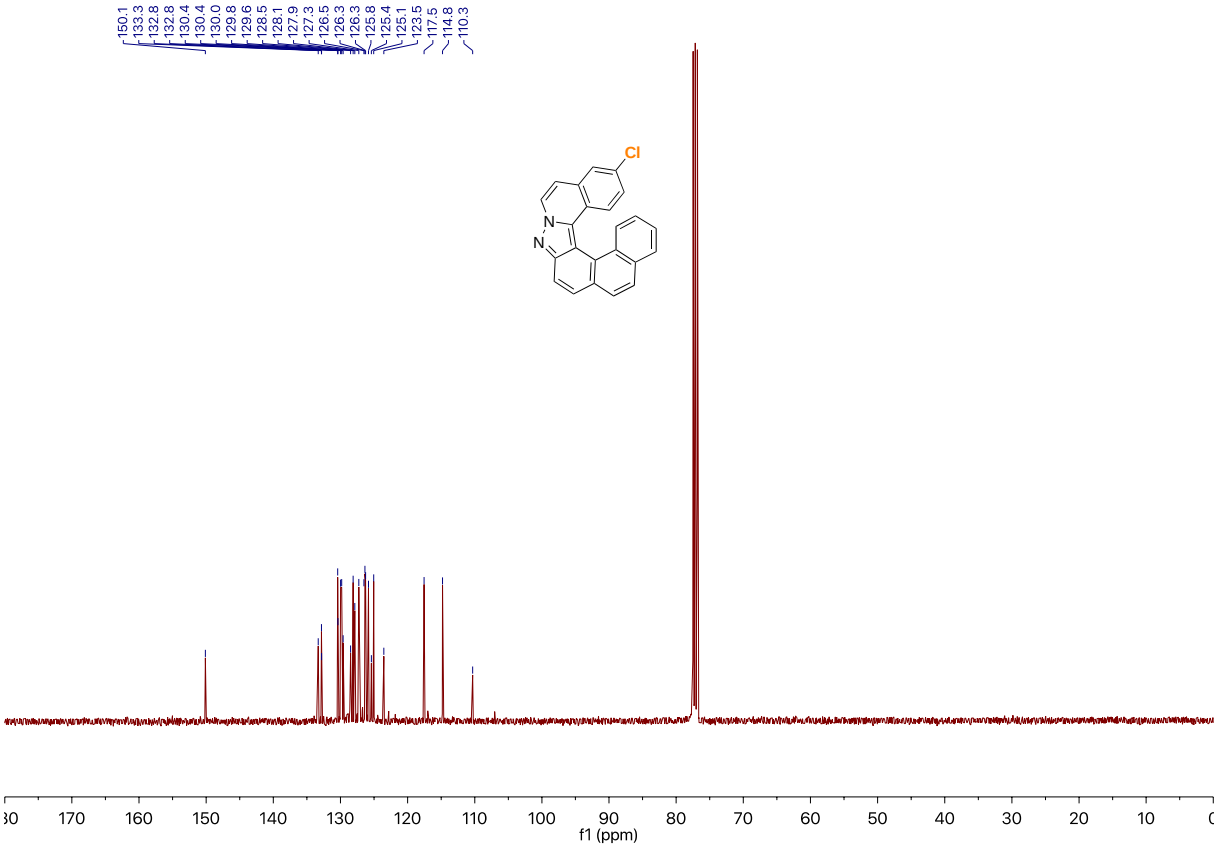
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **S-28**



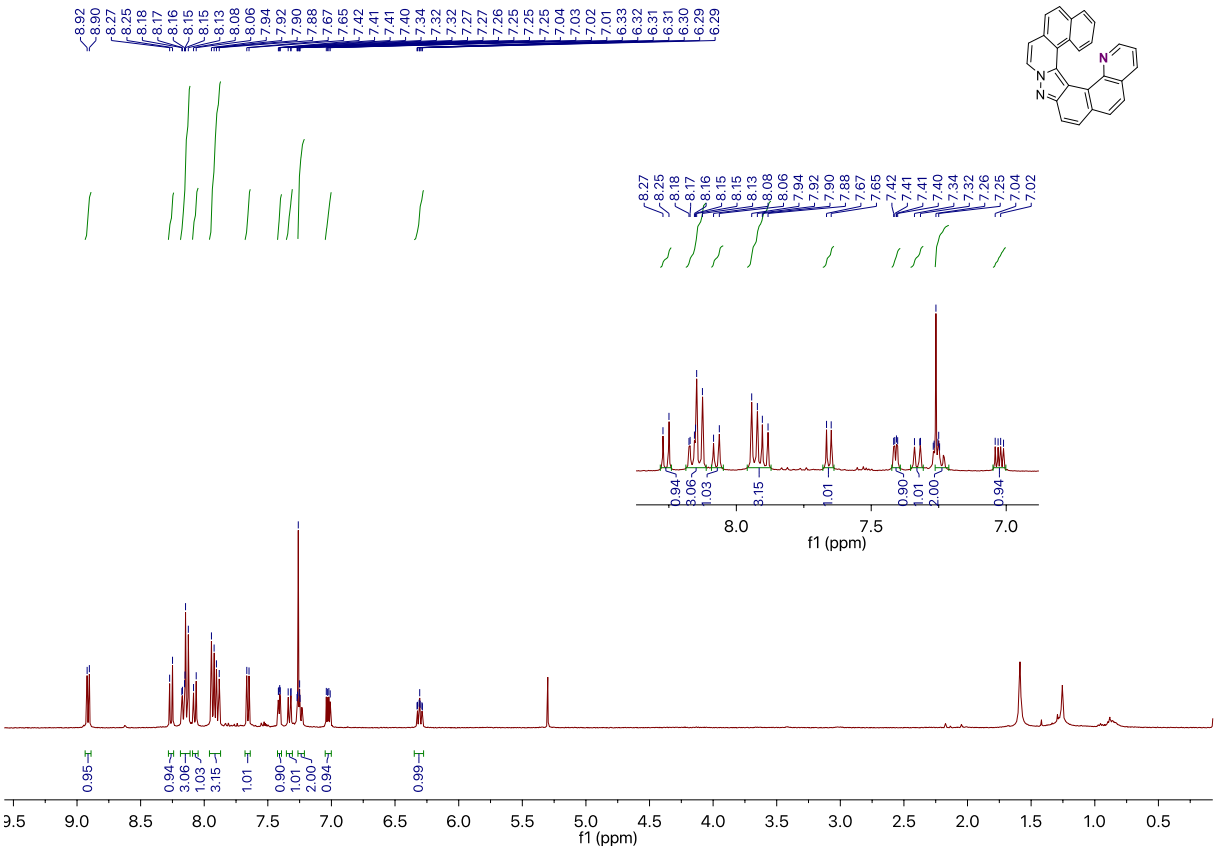
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-28**



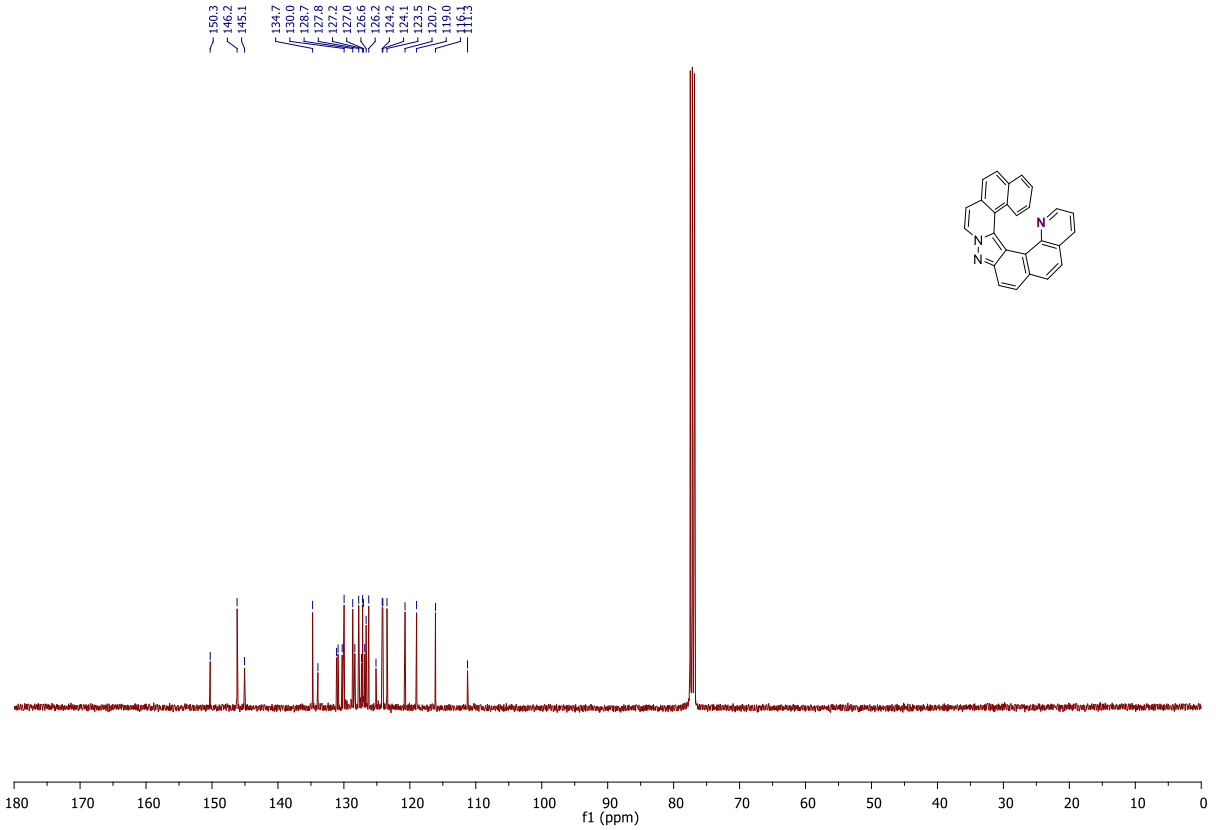
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-28**



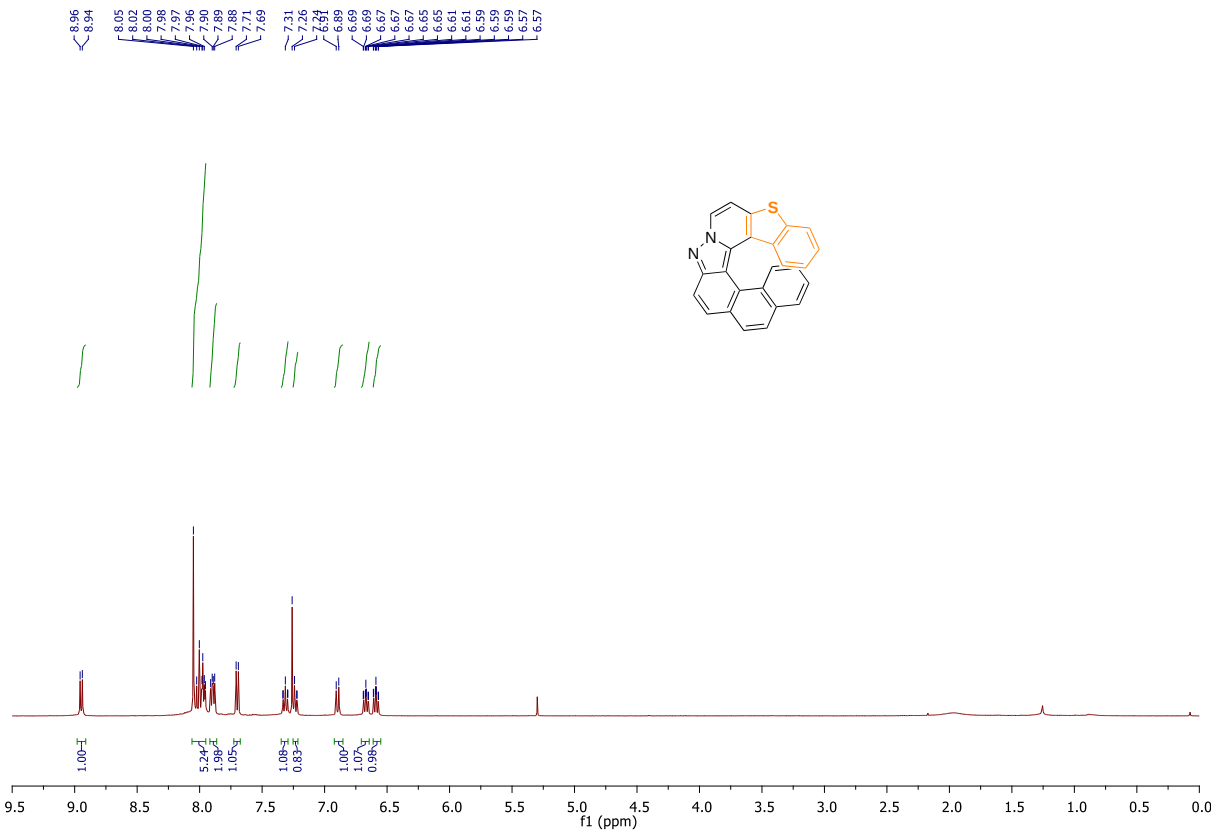
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-29**



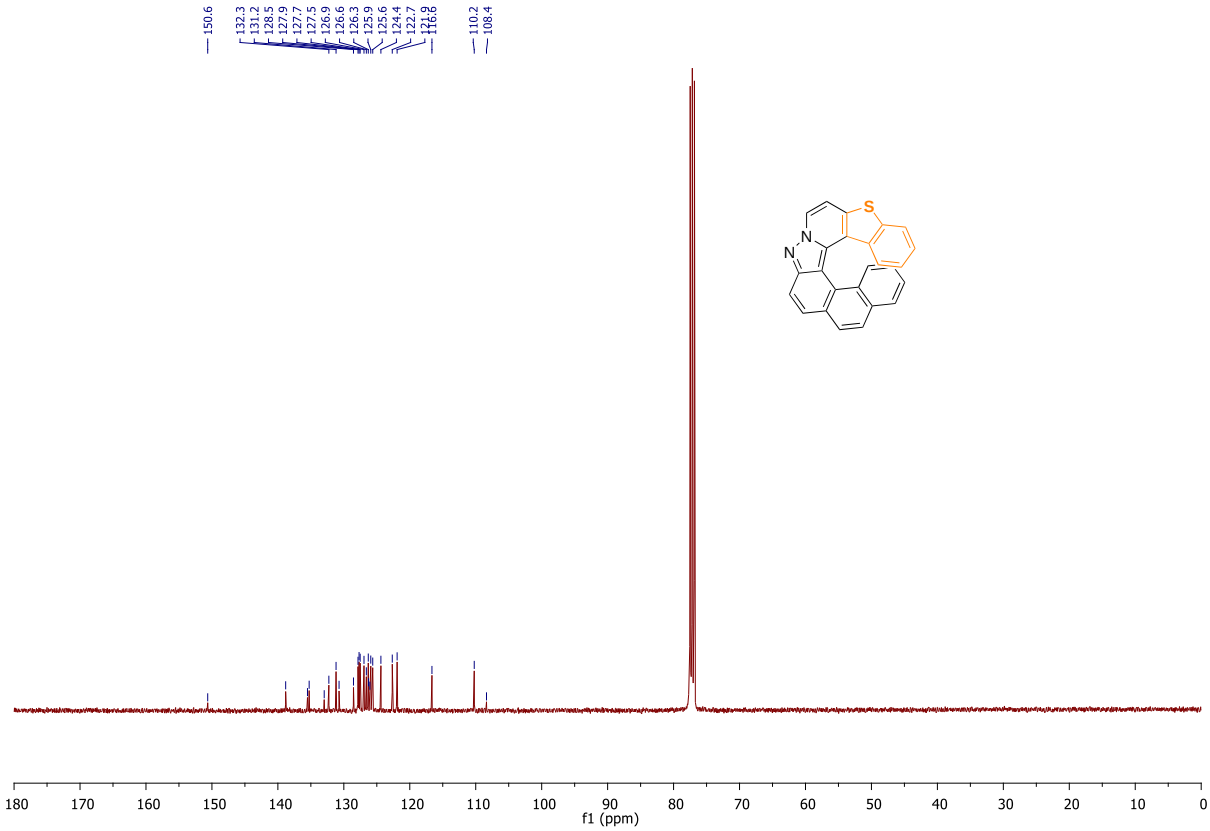
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-29**



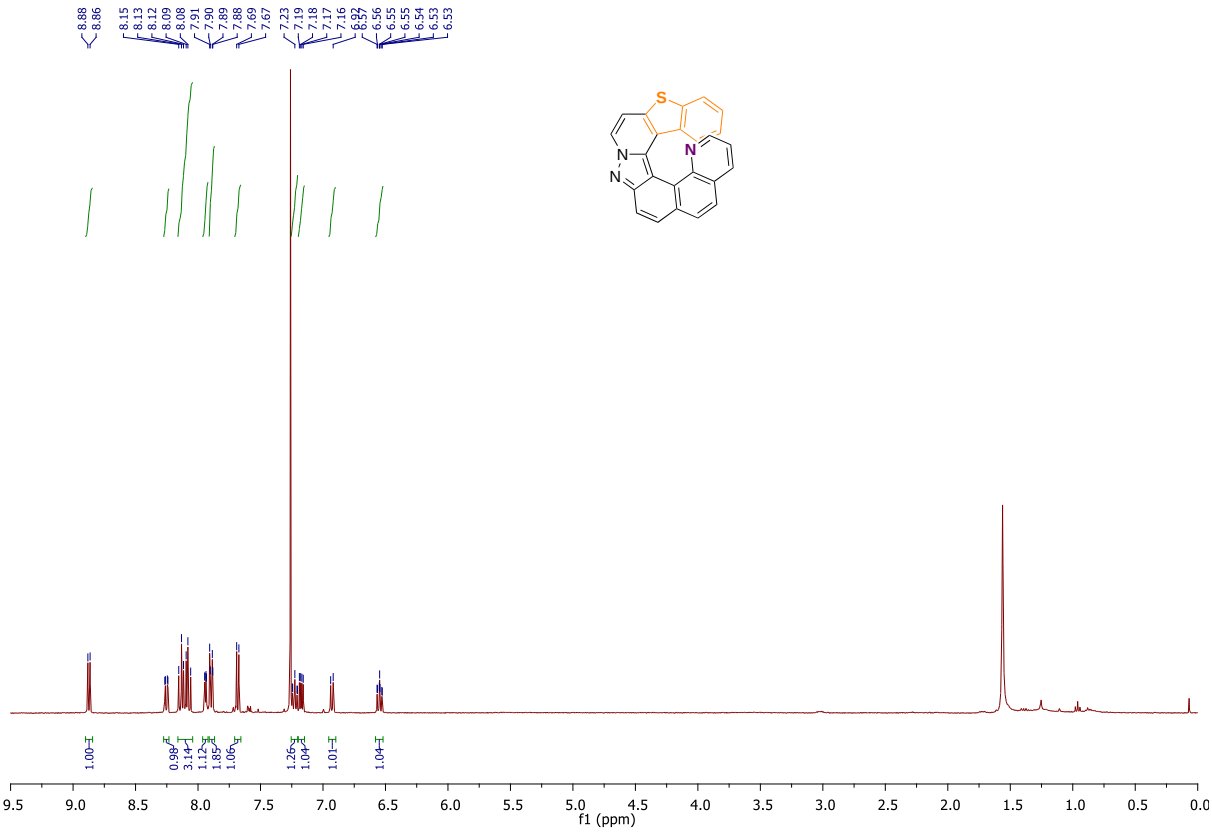
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-30**



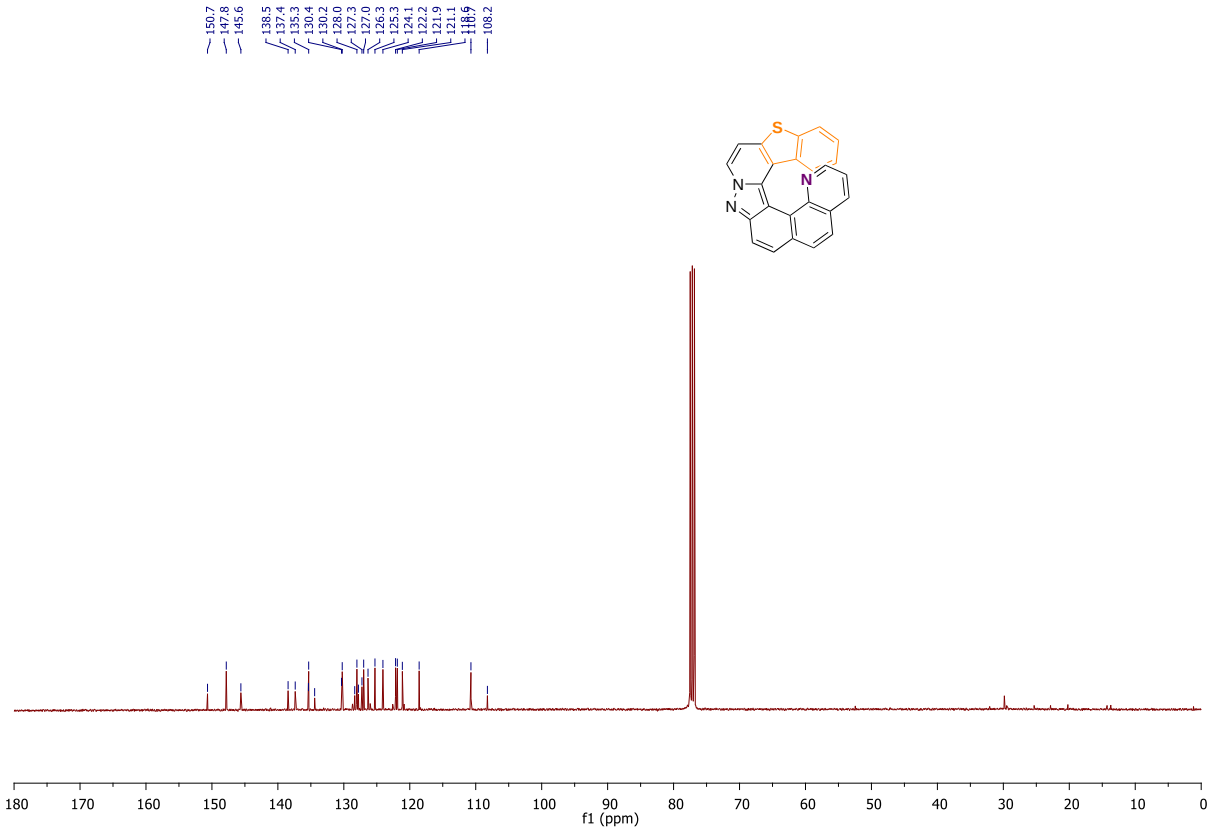
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-30**



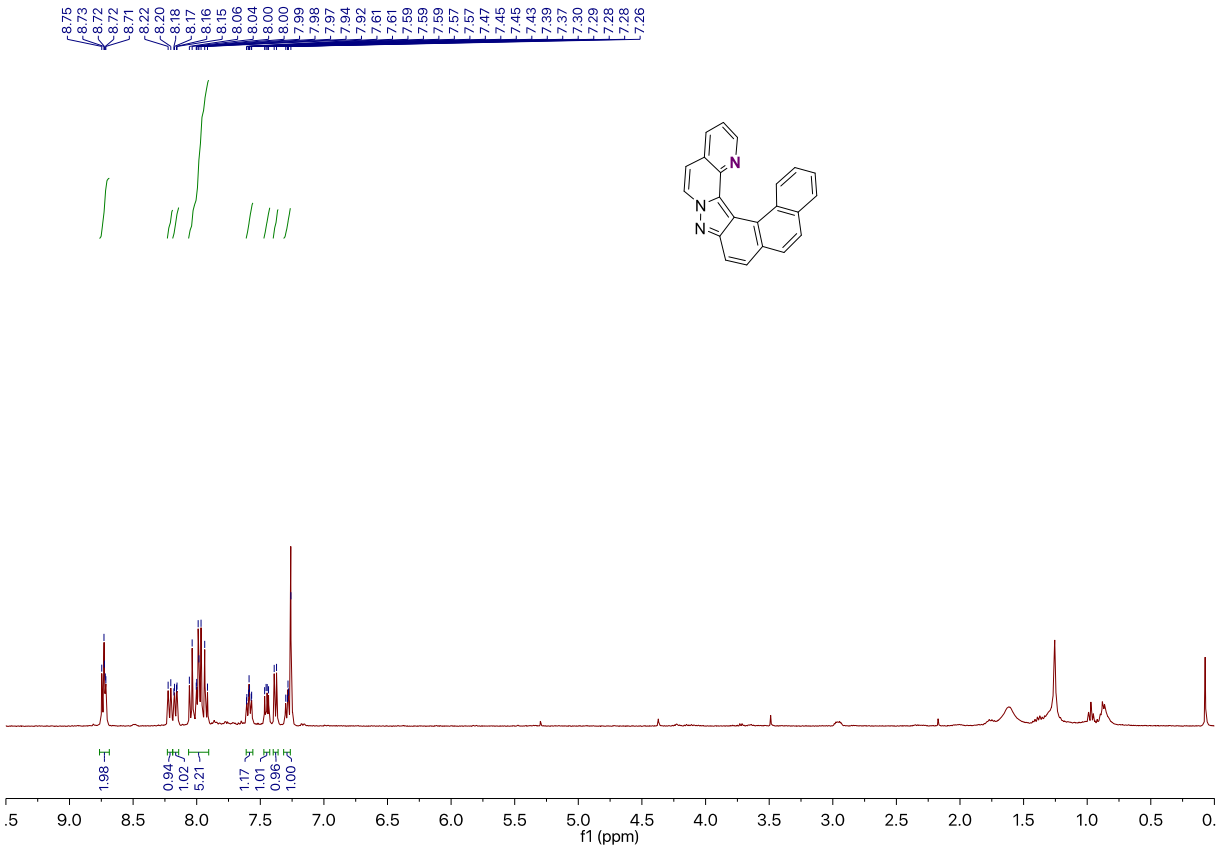
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-31**



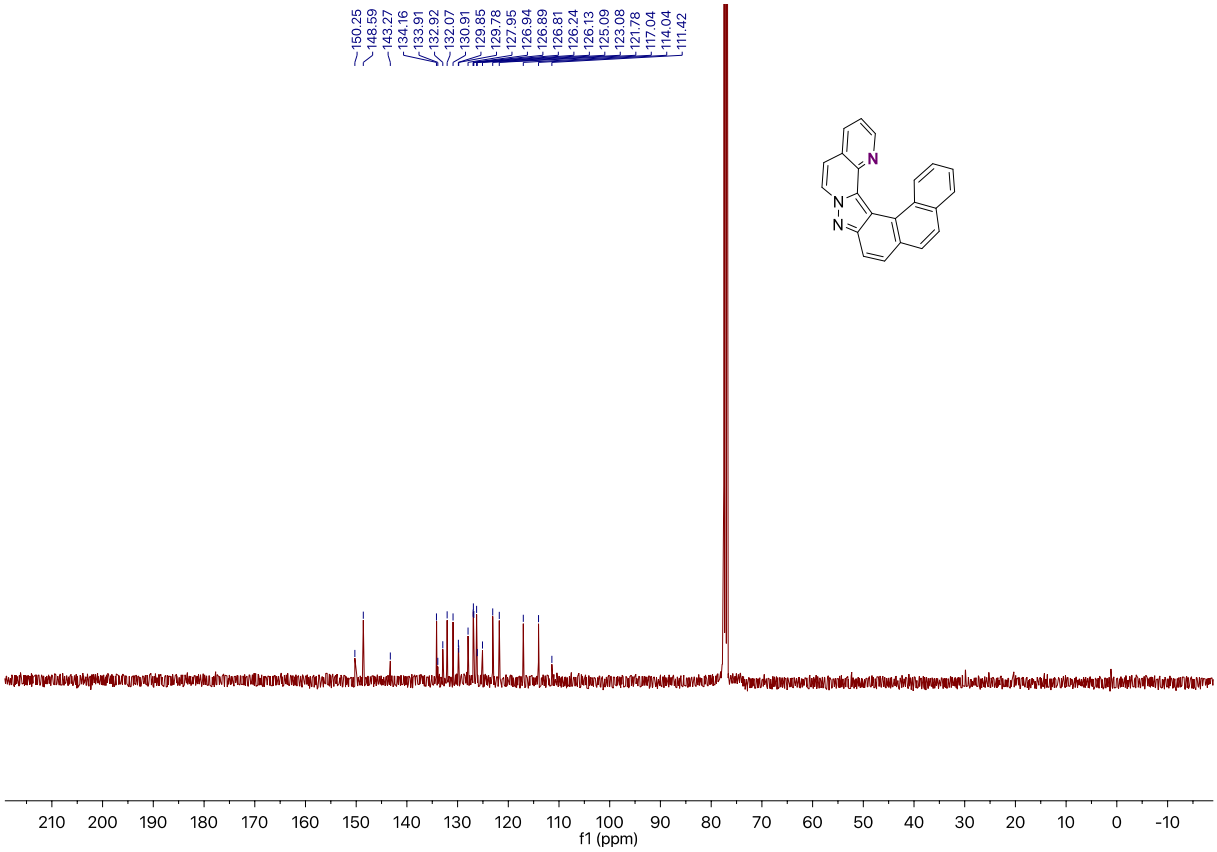
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-31**



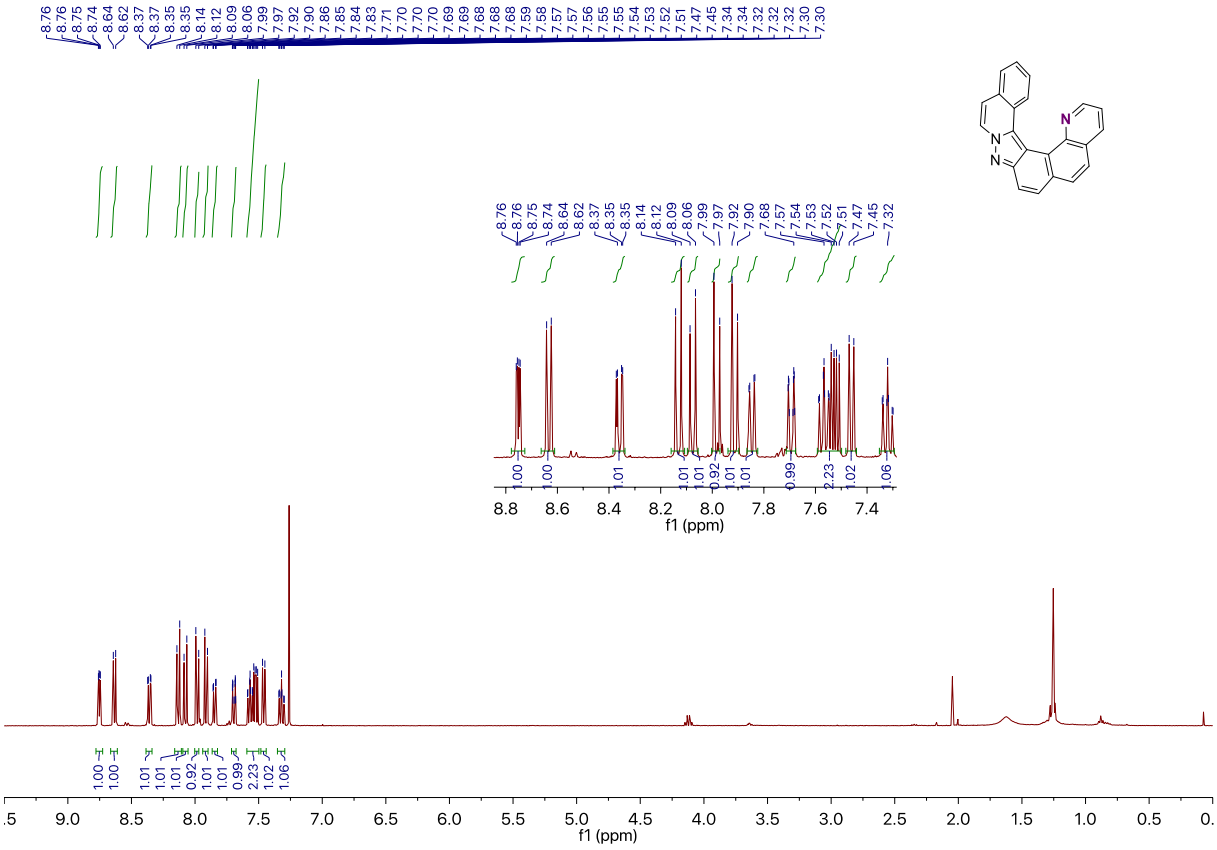
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-32**



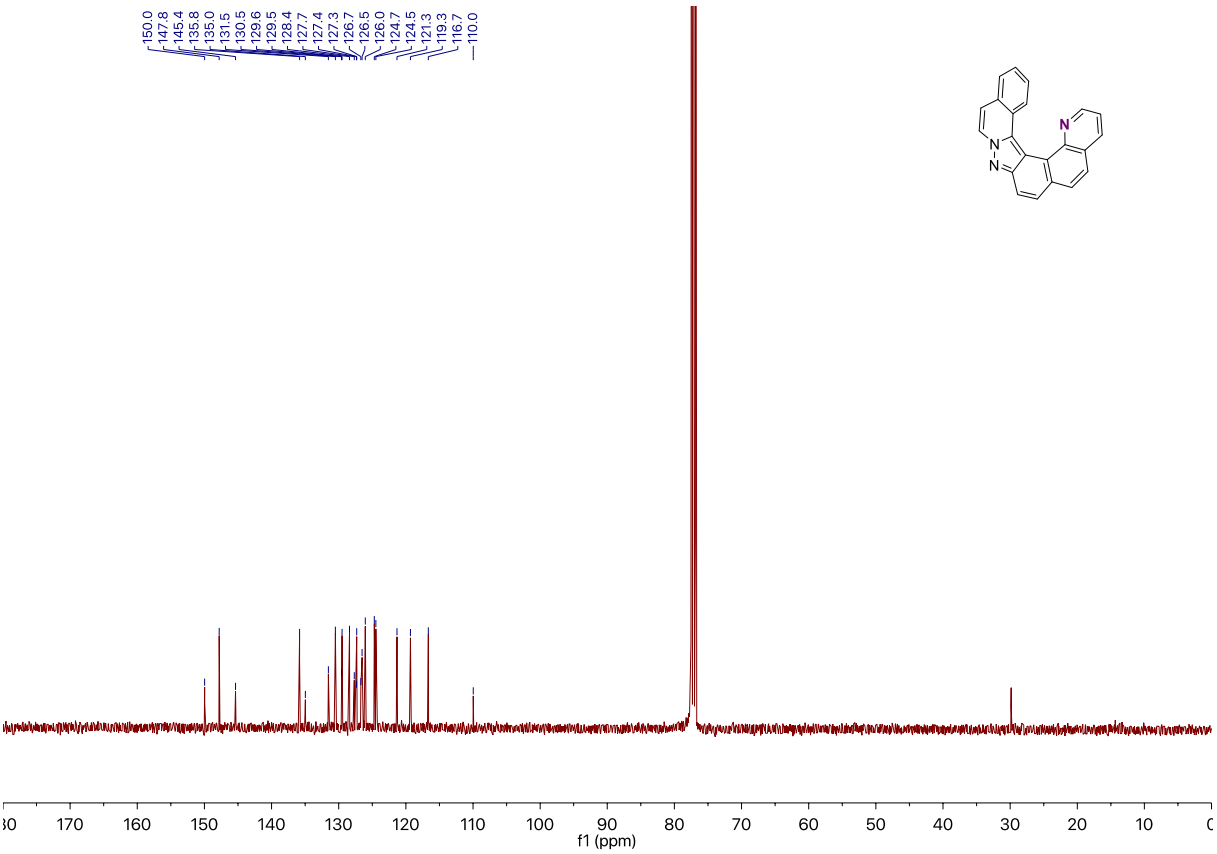
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-32**



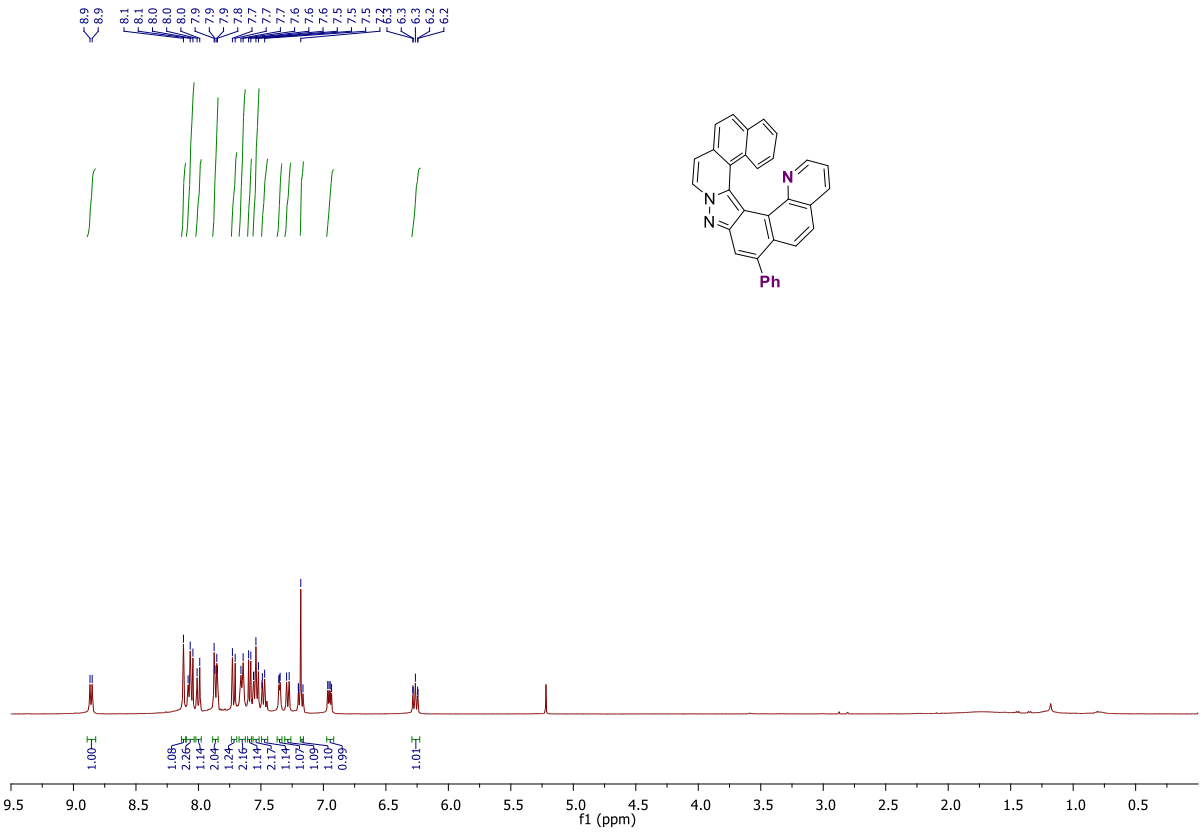
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-33**



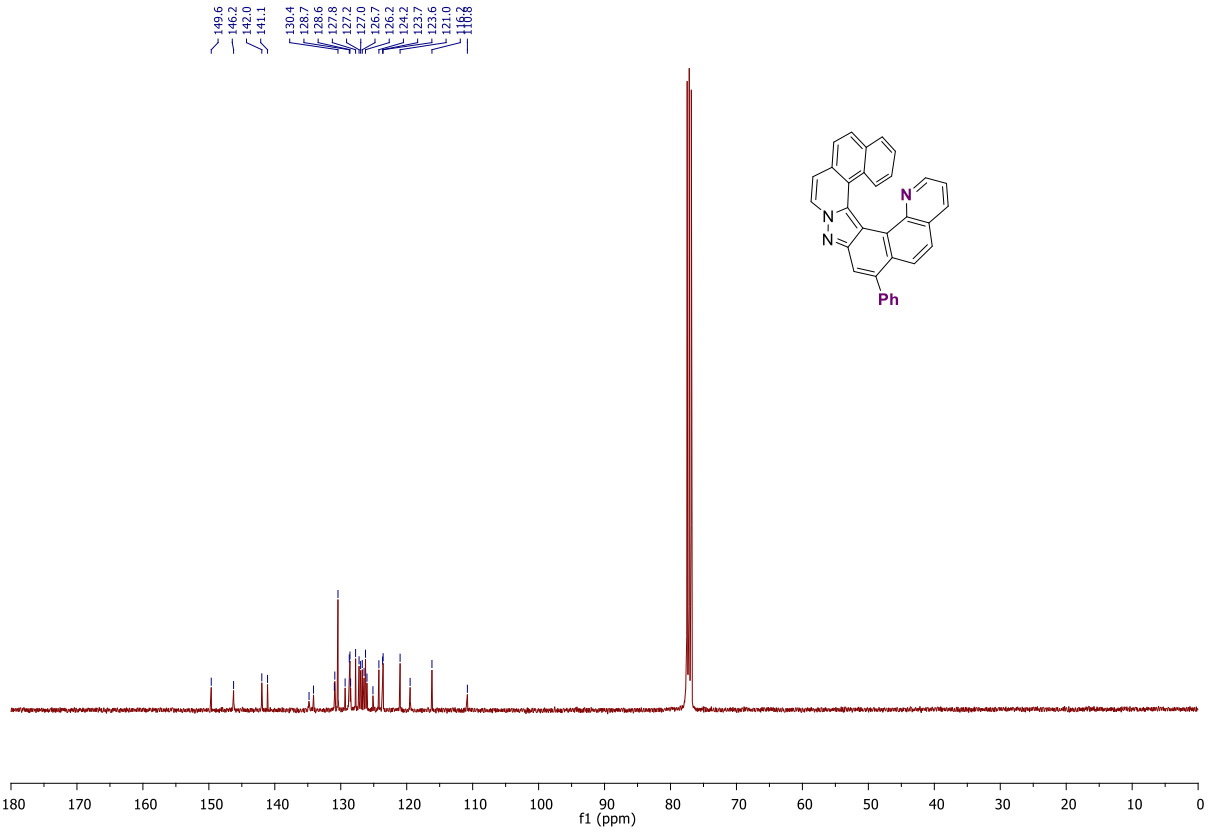
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-33**



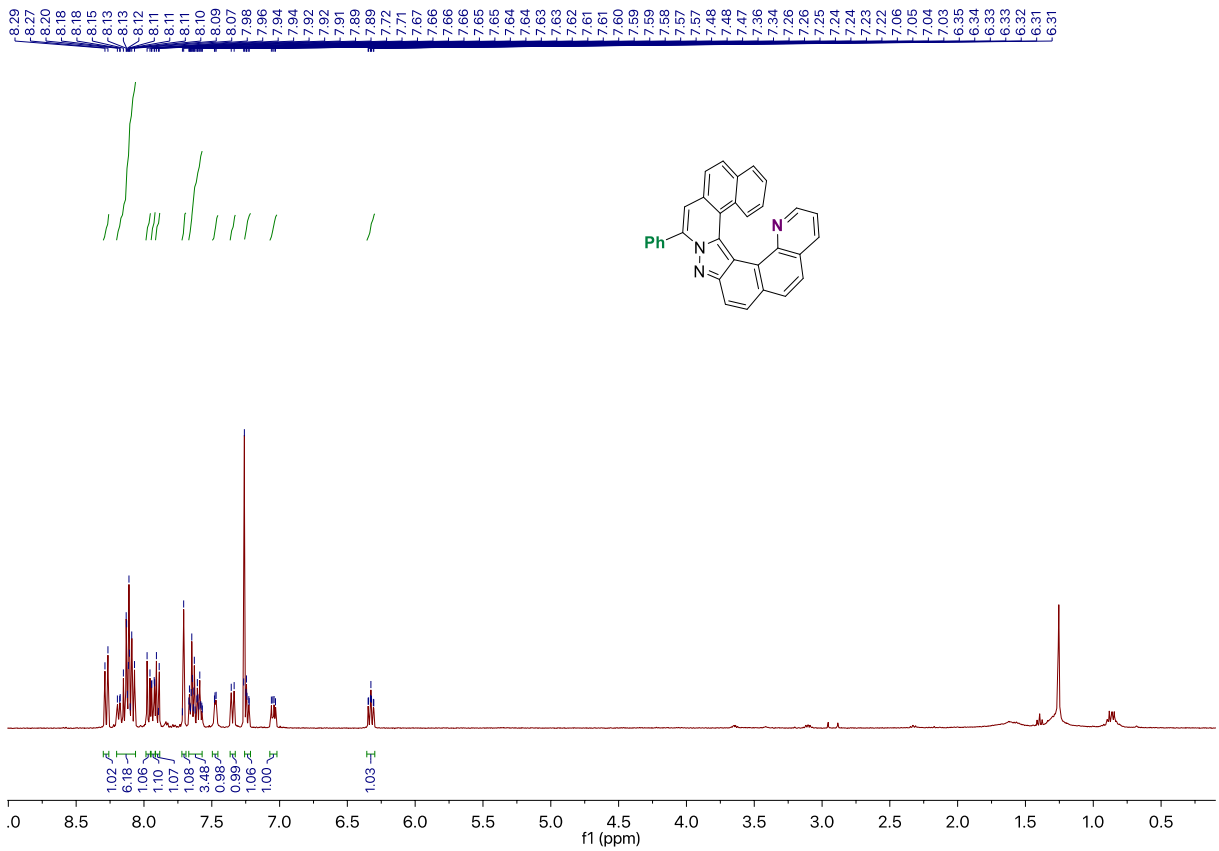
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-34**



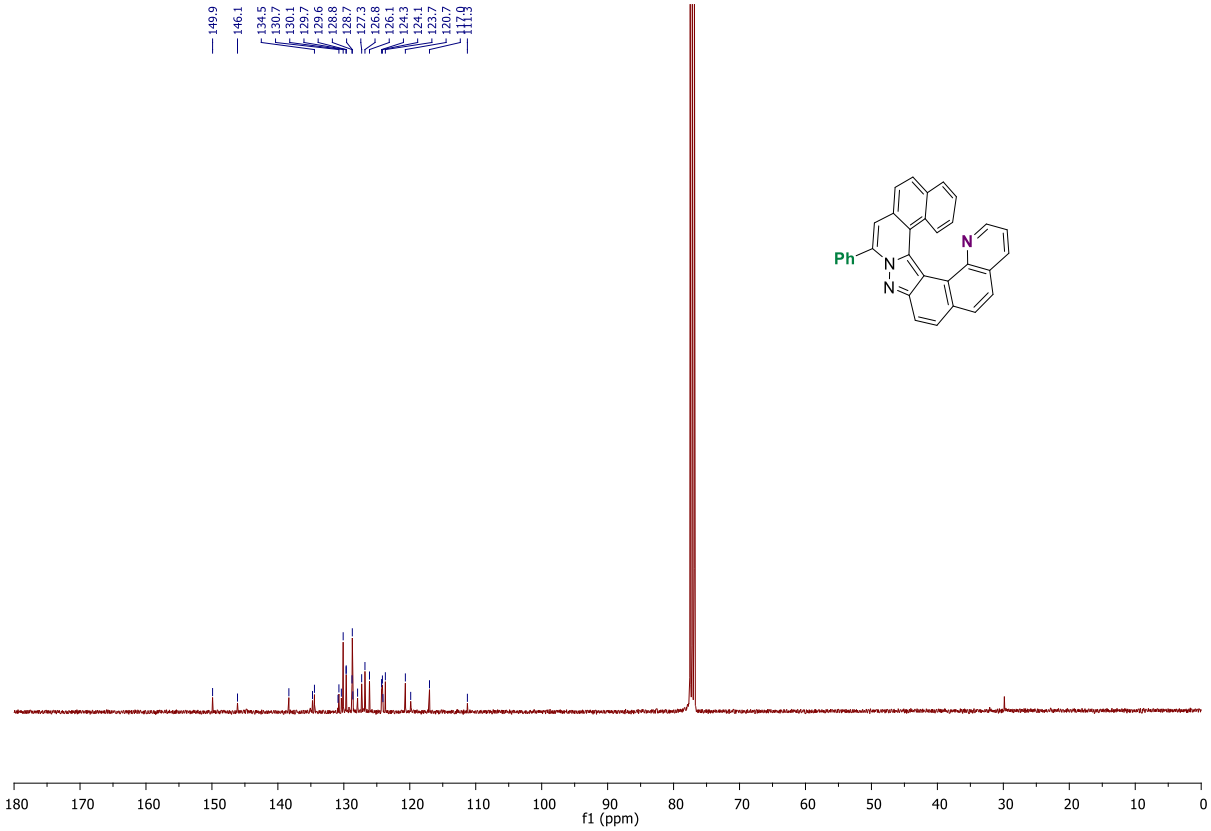
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-34**



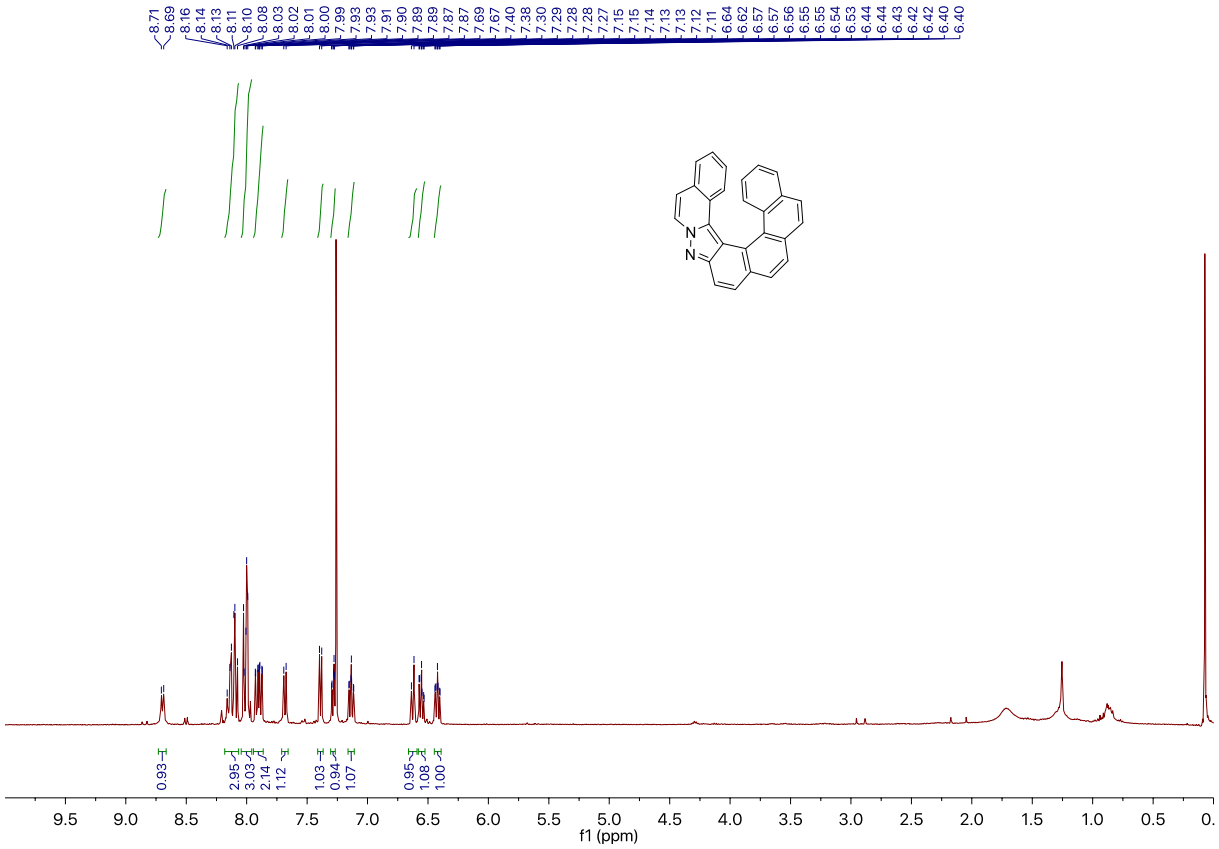
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-35**



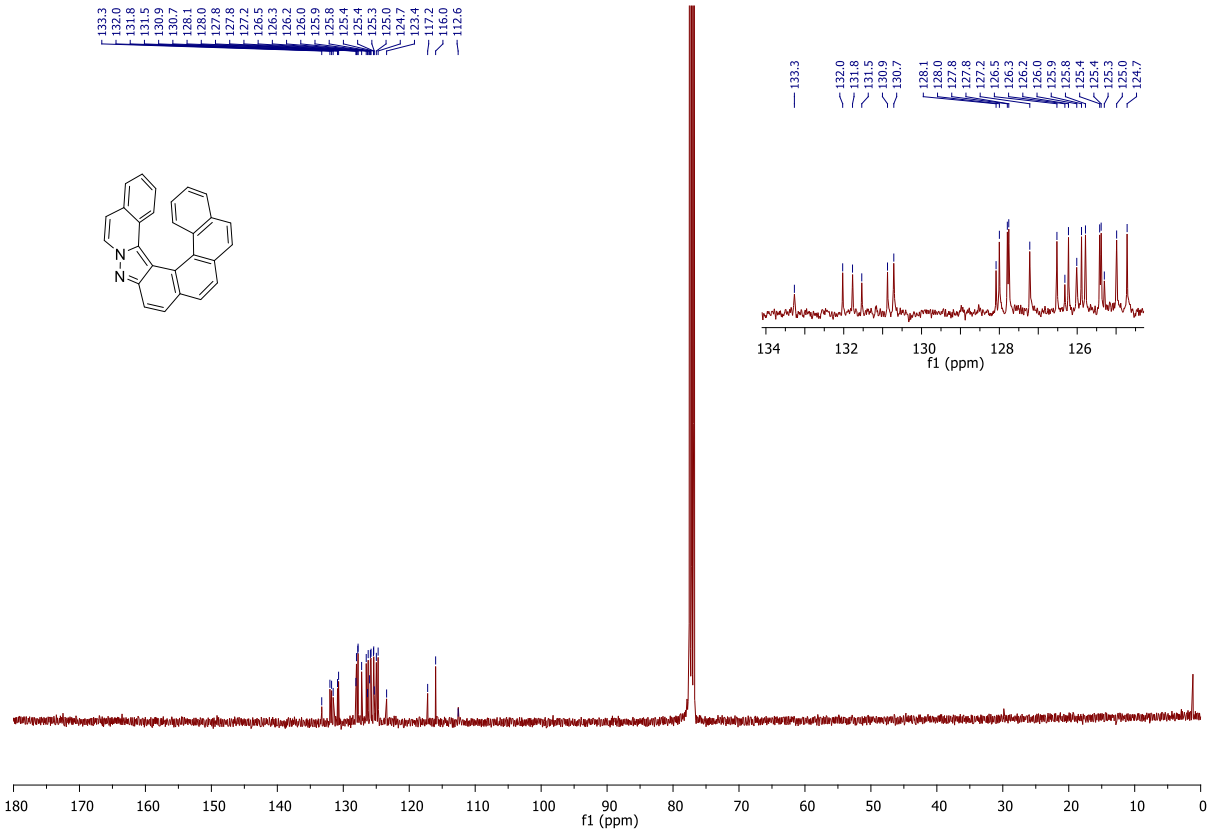
^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-35**



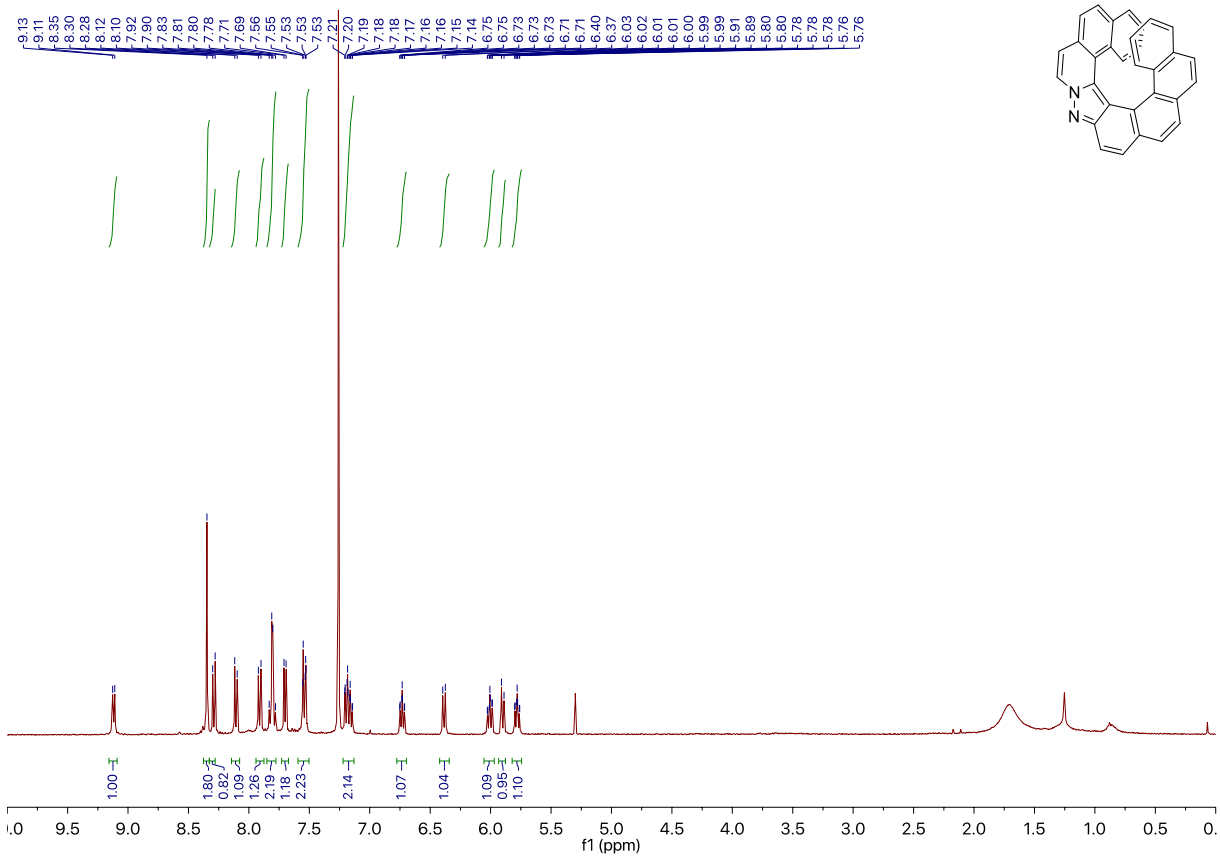
^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-36**



^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-36**



^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of **C-37**



^{13}C NMR Spectrum (100 MHz, $CDCl_3$) of **C-37**