Supporting Information

Visible-Light-Driven Reductive Carboarylation of Styrenes with CO_2 and Aryl Halides

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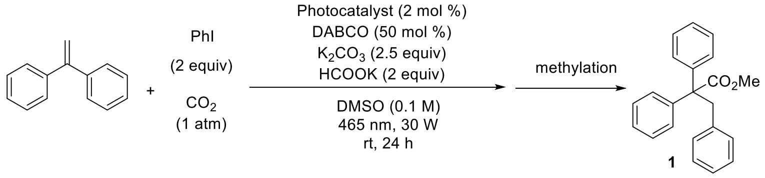
1. General Information

Unless otherwise noted, commercial available reagents were purchased from commercial suppliers (such as Strem, Alfa Aesar, J&K Chemical Co., Energy Chemical, Sinocompound and Adamas) and used as received. Solvents were generally dried over 4 Å molecular sieves. Purification of products was performed by flash chromatography (FC) using silica gel or preparative thin layer chromatography. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE III spectrometer (400 MHz and 101 MHz, respectively). Chemical shifts are reported parts per million (ppm) referenced to $CDCl_3$ (δ 7.26 ppm), tetramethylsilane (TMS, δ 0.00 ppm) for ^{1}H NMR; $CDCl_3$ (δ 77.16 ppm) for ^{13}C NMR. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, td = triplet of doublet and m = multiplet,. To distinguish, some ^{13}C NMR chemical shifts retain two decimal places. High-resolution mass spectra (HRMS) were obtained on an Impact II UHR-TOF mass spectrometry equipped with an ESI source from Bruker at Fujian Institute of Research on the Structure of Matter. The Blue LED strips (1 meter, 30W) were purchased from Prime LED Co., Ltd. (China). CO_2 gas (Purity: 99.995%) was purchased from Linde. $^{13}CO_2$ gas (99% ^{13}C) was purchased from Shanghai Wusheng Biological Technology Co., Ltd., who buys from Sigma-Aldrich, USA.

2. Experimental Section

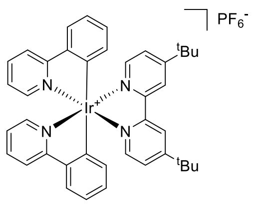
2.1 Optimization of reaction conditions

Table S1. Photocatalyst optimization.[a]

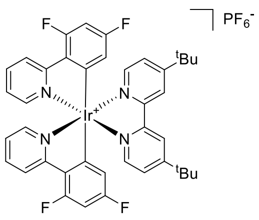


Entry	Photocatalyst	Yield[b] [%]
1	$[Ir(ppy)_2(dtbbpy)]PF_6$ **1a**	82%
2	$[Ir(dF(ppy))_2(dtbbpy)]PF_6$ **1b**	53%
3	$[Ir(dFCF_3(ppy))_2(dtbbpy)]PF_6$ **1c**	50%
4	$[Ir(dM(ppy))_2(dtbbpy)]PF_6$ **1d**	68%
5	$Ir(ppy)_3$ **1e**	7%
6	4-CzIPN (3 mol%) **1f**	47%
7	$[Ir(ppy)_2(dtbbpy)]PF_6$ (1 mol%) **1a**	77%

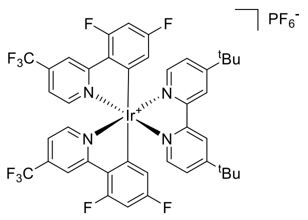
[a] Reaction conditions: 1,1-diphenylethylene (0.2 mmol), iodobenzene (0.4 mmol), photocatalyst (2 mol %), DABCO (0.1 mmol), K_2CO_3 (0.5 mmol), HCOOK (0.4 mmol), 1 atm CO_2, 30 W blue LEDs, rt, 24 h. DABCO = triethylenediamine. [b] Yield was determined by ^{1}H NMR with CH_2Br_2 as internal standard.



1a

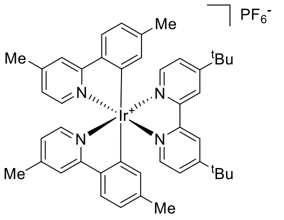


1b



1c

1e



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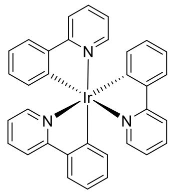

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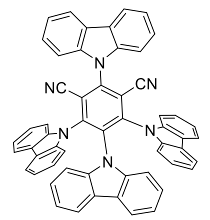
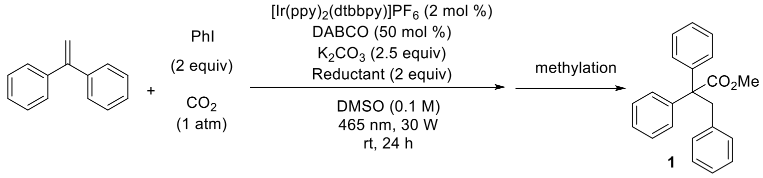


1f

Table S2. Reductant optimization.[a]



Entry	Reductant	Yield[b] [%]
1	HCO_2K	82%
2	HCO_2Cs	82%
3	HCO_2Na	82%
4	$(HCO_2)_2Ca$	11%
5	NaH	9%
6	CaH_2	7%

[a] Reaction conditions: 1,1-diphenylethylene (0.2 mmol), iodobenzene (0.4 mmol), [Ir(ppy)$_2$(dtbbpy)]PF$_6$ (2 mol %), DABCO (0.1 mmol), K_2CO_3 (0.5 mmol), reductant (0.4 mmol), 1 atm CO_2, 30 W blue LEDs, rt, 24 h. DABCO = triethylenediamine. [b] Yield was determined by ^1H NMR with CH_2Br_2 as internal standard.

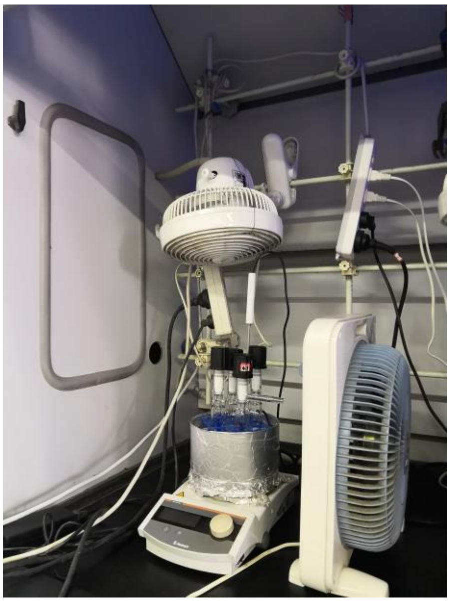
2.2 General procedures for synthesis of products

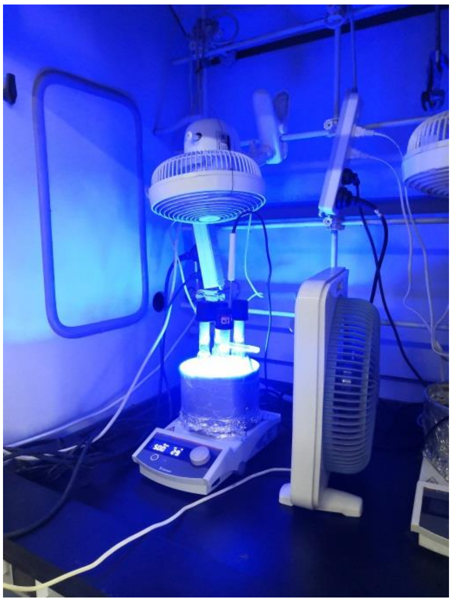
General Procedure A

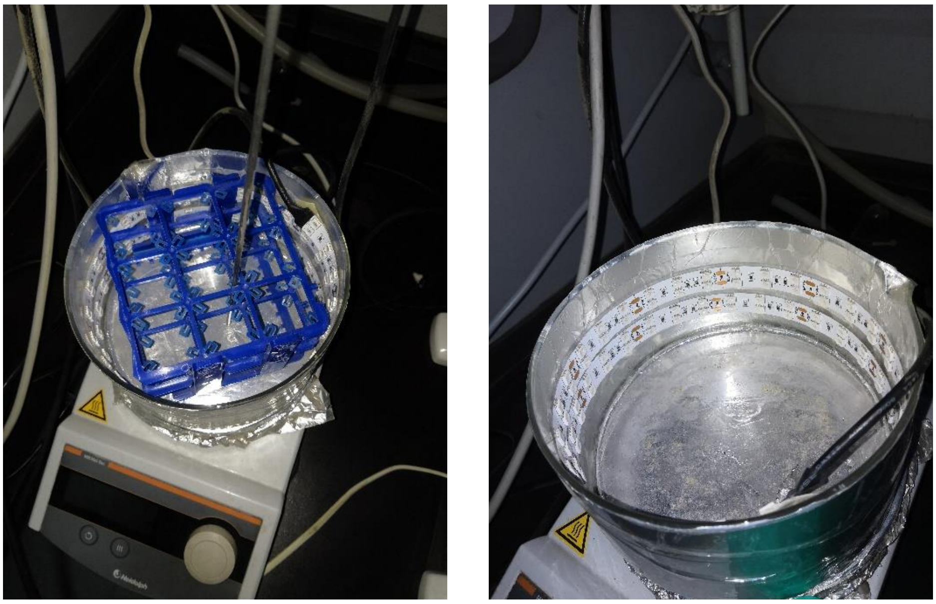
The oven-dried Schlenk tube (38 mL) containing a stirring bar was charged with alkene (0.20 mmol, 1.0 equiv), corresponding halide (2.0 equiv), photocatalyst (2 mol%), DABCO (50 mol%), K_2CO_3 (2.0 equiv), HCOOK (2.0 equiv) and anhydrous DMSO (2 mL) (Note that ahydrous condition is important in order to avoid the alkene reduction reactions with water). N_2 gas in a balloon was bubbled into the mixture under stirring for 30 seconds through a needle and the tube was then evacuated and back-filled with CO_2 for 3 times. The mixture was placed under a 30 W blue LED (λmax=465 nm, 3 cm-4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 ^oC) light source and stirred at ambient temperature for 24 h or 48 h (for some aryl bromides and chlorides). Upon completion of the reaction, all the solvent were removed under reduced pressure at high temperature. (The following procedure is different from **General procedure B**) The crude residue was dissolved in 10 mL acetone, and K_2CO_3 (5 equiv) and CH_3I (10 equiv) were added. The mixture was stirred at 70 °C for 2 h and then cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 25 mL of EtOAc. The filtrate was concentrated in vacuo, and crude ^1H NMR spectrum was taken using CH_2Br_2 as internal standard. The resulting residue was purified by flash silica gel chromatography or preparative thin layer chromatography using petroleum ether/EtOAc (100:1-10:1) as the eluent to give the desired products.

General Procedure B

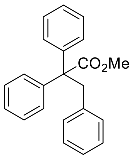
The oven-dried Schlenk tube (38 mL) containing a stirring bar was charged with alkene (0.20 mmol, 1.0 equiv), corresponding halide (2.0 equiv), photocatalyst (2 mol%), DABCO (50 mol%), K_2CO_3 (2.0 equiv), HCOOK (2.0 equiv) and anhydrous DMSO (2 mL) (Note that ahydrous condition is important in order to avoid the alkene reduction reactions with water). N_2 gas in a balloon was bubbled into the mixture under stirring for 30 seconds through a needle and the tube was then evacuated and back-filled with CO_2 for 3 times. The mixture was placed under a 30 W blue LED (λmax=465 nm, 3 cm-4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 °C) light source and stirred at ambient temperature for 24 h or 48 h (for some aryl bromides and chlorides).. Upon completion of the reaction, then AcOH (0.2 mL) was added and the system was stirred for 10 min at room temperature. The solvent along with other volatile matter was removed directly under reduced pressure at high temperature. The residue was re-dissolved in MeOH (4 mL) and then $SOCl_2$ (0.4 mL) was added dropwise carefully. The Schlenk tube was capped and stirred at 100 °C for 6 h. After cooled to room temperature, the mixture was diluted with EtOAc (10 mL) and quenched with saturated aqueous solution of sodium hydrogen carbonate. The reaction was extracted with EtOAc (30 mL ×3) and the organic layers were combined and dried over Na_2SO_4. After concentrated under reduced pressure, crude ^1H NMR spectrum was taken using CH_2Br_2 as internal standard. The resulting residue was purified by flash silica gel chromatography or preparative thin layer chromatography using petroleum ether/EtOAc (100:1-10:1) as the eluent to give the desired products.







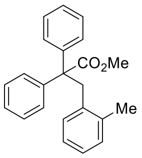
2.2 Characterization of products



1

methyl 2,2,3-triphenylpropanoate

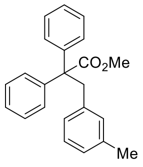
The general procedure **A** was followed. Yield: 49.6 mg (78%) for X = I; 43.1 mg (68%) for X = Br.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.21 (m, 6H), 7.17 – 7.15 (m, 4H), 7.11 –7.08 (m, 1H), 7.03 (t, *J* = 7.3 Hz, 2H, 2H), 6.66 (d, *J* = 6.8 Hz, 2H), 3.71 (s, 2H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 142.8, 137.4, 131.0, 129.4, 127.8, 127.6, 127.0, 126.4, 62.1, 52.4, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{20}O_2Na^+$ [M+Na$^+$] 339.1356, found 339.1353.



2

methyl 2,2-diphenyl-3-(o-tolyl)propanoate

The general procedure **A** was followed. Yield: 47.5 mg (72%) for X = I; 42.1 mg (64%) for X = Br.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.16 (m, 7H), 7.14 – 7.08 (m, 4H), 7.07 – 7.04 (m, 2H), 6.91 – 6.89 (m, 1H), 3.77 (s, 2H), 3.72 (s, 3H), 1.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ174.6, 142.5, 138.9, 136.1, 130.1, 129.9, 129.2, 127.8, 127.0, 126.6, 125.7, 61.9, 52.4, 39.7, 18.9. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1509.

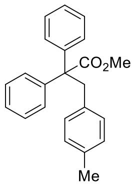


3

methyl 2,2-diphenyl-3-(m-tolyl)propanoate

The general procedure **A** was followed. Yield: 47.1 mg (71%) for X = I; 48.3 mg (73%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.22 (m, 6H), 7.18 – 7.15 (m, 4H), 6.96 – 6.90 (m, 2H), 6.52 (d, *J* = 7.1 Hz, 1H), 6.35 (s, 1H), 3.68 (s, 3H), 3.66 (s, 2H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 142.9, 137.2, 136.9, 132.0, 129.4, 127.9, 127.7, 127.4, 127.0, 126.9, 62.1, 52.3, 44.5, 21.4. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1511.

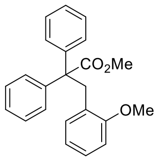


4

methyl 2,2-diphenyl-3-(p-tolyl)propanoate

The general procedure **A** was followed. Yield: 50.2 mg (76%) for X = I; 44.0 mg (67%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.16 (m, 10H), 6.85 (d, *J* = 7.7 Hz, 2H), 6.54 (d, *J* = 7.8 Hz, 2H), 3.67 (s, 5H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 142.9, 135.8, 134.1, 130.8, 129.4, 128.3, 127.7, 126.9, 62.1, 52.3, 44.1, 21.1. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1512.

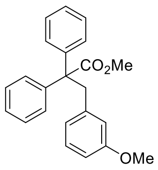


5

methyl 3-(2-methoxyphenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 38.8 mg (56%) for X = I.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.08 (m, 12H), 6.79 (t, *J* = 7.4 Hz, 1H), 6.51 (d, *J* = 8.2 Hz, 1H), 3.83 (s, 2H), 3.69 (s, 3H), 3.15 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 158.0, 143.0, 131.1, 129.3, 127.8, 127.4, 126.7, 126.3, 119.9, 109.7, 61.8, 54.7, 52.3, 36.4. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_3Na^+$ [M+Na$^+$] 369.1461, found 369.1460.

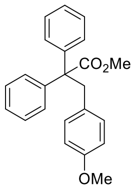


6

methyl 3-(3-methoxyphenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 49.2 mg (71%) for X = I; 47.1 mg (68%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 – 7.21 (m, 6H), 7.20 – 7.16 (m, 4H), 6.97 (t, *J* = 7.9 Hz, 1H), 6.65 (dd, *J* = 8.2, 2.6 Hz, 1H), 6.37 (d, *J* = 7.5 Hz, 1H), 6.10 (s, 1H), 3.69 (s, 5H), 3.53 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.1, 158.8, 142.8, 138.9, 129.4, 128.5, 127.8, 127.0, 123.4, 115.9, 112.6, 62.1, 55.0, 52.4, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_3Na^+$ [M+Na$^+$] 369.1461, found 369.1461.

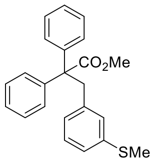


7

methyl 3-(4-methoxyphenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 46.4 mg (67%) for X = I.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.24 – 7.15 (m, 10H), 6.60 – 6.55 (m, 4H), 3.72 (s, 3H), 3.68 (s, 3H), 3.65 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.2, 158.2, 142.9, 132.0, 129.4, 129.3, 127.8, 126.9, 112.9, 62.2, 55.2, 52.3, 43.7. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_3Na^+$ [M+Na$^+$] 369.1461, found 369.1460.

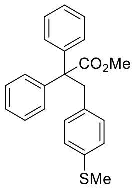


8

methyl 3-(3-(methylthio)phenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 47.8 mg (66%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 – 7.22 (m, 6H), 7.19 – 7.15 (m, 4H), 7.02 – 6.95 (m, 2H), 6.58 (d, *J* = 6.9 Hz, 1H), 6.37 (s, 1H), 3.68 (s, 3H), 3.67 (s, 2H), 2.21 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.9, 142.7, 138.1, 137.2, 129.4, 128.9, 127.9, 127.8, 127.7, 127.0, 124.9, 62.1, 52.4, 44.3, 15.7. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2SNa^+$ [M+Na$^+$] 385.1233, found 385.1233.

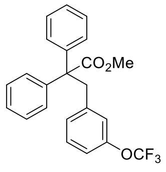


9

methyl 3-(4-(methylthio)phenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 48.0 mg (66%) for X = I.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.24 – 7.21 (m, 6H), 7.18 – 7.14 (m, 4H), 6.93 (d, *J* = 8.3 Hz, 2H), 6.57 (d, *J* = 8.2 Hz, 2H), 3.67 (s, 3H), 3.66 (s, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 142.7, 136.1, 134.2, 131.5, 129.3, 127.8, 127.0, 125.8, 62.1, 52.3, 44.0, 15.9. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2SNa^+$ [M+Na$^+$] 385.1233, found 385.1232.

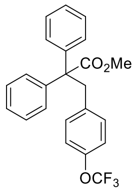


10

methyl 2,2-diphenyl-3-(3-(trifluoromethoxy)phenyl)propanoate

The general procedure **A** was followed. Yield: 53.9 mg (67%) for X = I; 58.8 mg (73%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 – 7.23 (m, 6H), 7.17 – 7.14 (m, 4H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.95 (d, *J* = 8.2 Hz, 1H), 6.61 (d, *J* = 7.6 Hz, 1H), 6.55 (s, 1H), 3.72 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.9, 148.7, 142.5, 139.8, 129.5, 129.2, 128.7, 127.9, 127.2, 123.5, 120.5 (q, *J* = 257.3 Hz), 119.0, 62.1, 52.4, 44.3. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}F_3O_3Na^+$ [M+Na$^+$] 423.1178, found 423.1182.

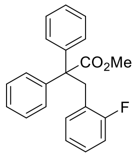


11

methyl 2,2-diphenyl-3-(4-(trifluoromethoxy)phenyl)propanoate

The general procedure **A** was followed. Yield: 51.9 mg (65%) for X = I; 53.8 mg (67%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.23 – 7.21 (m, 6H), 7.17 – 7.14 (m, 4H), 6.87 (d, *J* = 8.2 Hz, 2H), 6.67 (d, *J* = 8.4 Hz, 2H), 3.70 (s, 2H), 3.67 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 147.9, 142.5, 136.3, 132.3, 129.3, 127.9, 127.1, 120.6 (q, *J* = 257.6 Hz), 119.9, 62.2, 52.4, 43.8. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}F_3O_3Na^+$ [M+Na$^+$] 423.1178, found 423.1181.

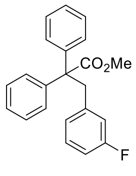


12

methyl 3-(2-fluorophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 38.7 mg (58%) for X = I; 40.2 mg (60%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.24 – 7.16 (m, 10H), 7.11 – 7.02 (m, 2H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.71 (t, *J* = 9.2 Hz, 1H), 3.80 (s, 2H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.3, 161.8 (d, *J* = 246.6 Hz), 142.5, 132.1 (d, *J* = 4.0 Hz), 129.2, 128.3 (d, *J* = 8.4 Hz), 127.8, 127.0, 124.8 (d, *J* = 14.7 Hz), 123.5 (d, *J* = 3.6 Hz), 114.9 (d, *J* = 23.4 Hz), 61.6, 52.5, 36.3. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}FO_2Na^+$ [M+Na$^+$] 357.1261, found 357.1261.

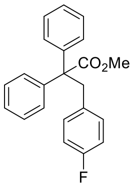


13

methyl 3-(3-fluorophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 45.1 mg (67%) for X = I; 51.4 mg (77%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.27 – 7.22 (m, 6H), 7.18 – 7.15 (m, 4H), 7.00 – 6.94 (m, 1H), 6.78 (td, J = 8.4, 2.6 Hz, 1H), 6.43 (d, J = 7.7 Hz, 1H), 6.39 (d, J = 10.4 Hz, 1H), 3.70 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.9, 162.2 (d, J = 244.2 Hz), 142.5, 140.0 (d, J = 7.5 Hz), 129.3, 128.8 (d, J = 8.3 Hz), 127.9, 127.1, 126.7 (d, J = 2.7 Hz), 117.7 (d, J = 21.5 Hz), 113.2 (d, J = 20.9 Hz), 62.1, 52.5, 44.2 (d, J = 1.8 Hz). HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}FO_2Na^+$ [M+Na$^+$] 357.1261, found 357.1262.

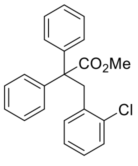


14

methyl 3-(4-fluorophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 46.8 mg (70%) for X = I.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.24 –7.21 (m, 6H), 7.18 – 7.14 (m, 4H), 6.71 (t, J = 8.7 Hz, 2H), 6.62 – 6.59 (m, 2H), 3.68 (s, 5H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 161.7 (d, J = 244.5 Hz), 142.7, 133.0 (d, J = 3.3 Hz), 132.4 (d, J = 7.8 Hz), 129.4, 127.8, 127.1, 114.3 (d, J = 20.9 Hz), 62.2, 52.4, 43.7. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}FO_2Na^+$ [M+Na$^+$] 357.1261, found 357.1261.

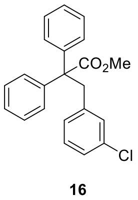


15

methyl 3-(2-chlorophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 39.1 mg (56%) for X = I; 44.9 mg (64%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.26 – 7.05 (m, 14H), 3.99 (s, 2H), 3.71 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.4, 142.1, 136.4, 135.7, 131.3, 129.2, 129.2, 127.8, 127.0, 126.3, 61.6, 52.5, 39.7. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}ClO_2Na^+$ [M+Na$^+$] 373.0966, found 373.0966.

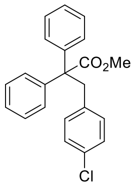


16

methyl 3-(3-chlorophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 45.8 mg (65%) for X = I; 51.5 mg (73%) for X = Br.

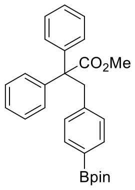
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 – 7.24 (m, 6H), 7.17 – 7.14 (m, 4H), 7.07 (d, J = 8.0 Hz, 1H), 6.95 (t, J = 7.9 Hz, 1H), 6.61 (s, 1H), 6.54 (d, J = 7.6 Hz, 1H), 3.69 (s, 3H), 3.67 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.9, 142.5, 139.5, 133.3, 131.1, 129.3, 129.2, 128.7, 127.9, 127.2, 126.5, 62.1, 52.4, 44.2. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}ClO_2Na^+$ [M+Na$^+$] 373.0966, found 373.0965.



17

methyl 3-(4-chlorophenyl)-2,2-diphenylpropanoate

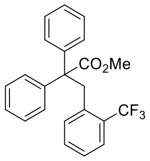
The general procedure **A** was followed. Yield: 47.2 mg (67%) for X = I; 43.5 mg (62%) for X = Br.
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 – 7.22 (m, 6H), 7.18 – 7.14 (m, 4H), 6.99 (d, *J* = 8.4 Hz, 2H), 6.58 (d, *J* = 8.4 Hz, 2H), 3.67 (s, 3H), 3.66 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.9, 142.5, 135.9, 132.4, 132.3, 129.3, 127.9, 127.6, 127.1, 62.1, 52.4, 43.9. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}ClO_2Na^+$ [M+Na$^+$] 373.0966, found 373.0966.



18

methyl 2,2-diphenyl-3-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propanoate

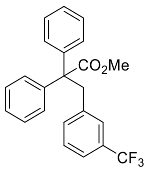
The general procedure **A** was followed. Yield: 48.9 mg (55%) for X = Br.
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.49 (d, *J* = 7.9 Hz, 2H), 7.32 – 7.03 (m, 10H), 6.67 (d, *J* = 7.6 Hz, 2H), 3.72 (s, 2H), 3.67 (s, 3H), 1.32 (s, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 142.8, 140.8, 134.0, 130.5, 129.3, 127.8, 127.0, 83.8, 62.1, 52.3, 44.8, 25.0. HRMS (m/z, ESI-TOF): Calcd for $C_{28}H_{31}BO_4Na^+$ [M+Na$^+$] 465.2208, found 465.2208.



19

methyl 2,2-diphenyl-3-(2-(trifluoromethyl)phenyl)propanoate

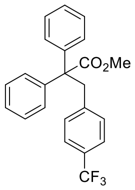
The general procedure **A** was followed. Yield: 53.1 mg (69%) for X = Br; 36.6 mg (48%) for X = Cl.
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.42 (d, *J* = 7.8 Hz, 1H), 7.29 – 7.01 (m, 13H), 4.03 (s, 2H), 3.61 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.77, 142.54, 137.24 (q, *J* = 1.6 Hz), 131.21, 130.59, 129.45 (q, *J* = 29.1 Hz), 128.97, 128.00, 127.05, 126.24, 126.14 (q, *J* = 6.1 Hz), 124.44 (q, *J* = 274.4 Hz), 60.72, 52.65, 39.05 (d, *J* = 2.5 Hz). HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}F_3O_2Na^+$ [M+Na$^+$] 407.1229, found 407.1228.



20

methyl 2,2-diphenyl-3-(3-(trifluoromethyl)phenyl)propanoate

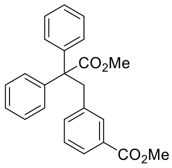
The general procedure **A** was followed. Yield: 47.1 mg (61%) for X = I; 53.9 mg (70%) for X = Br. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.35 (d, *J* = 7.8 Hz, 1H), 7.26 – 7.23 (m, 6H), 7.18 – 7.14 (m, 5H), 6.93 (d, *J* = 7.7 Hz, 1H), 6.77 (s, 1H), 3.74 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.7, 142.3, 138.3, 134.3, 129.7 (q, *J* = 31.9 Hz), 129.2, 127.9, 127.83, 127.78, 127.2, 124.1 (q, *J* = 273.3 Hz), 123.1 (q, *J* = 3.8 Hz), 62.1, 52.3, 44.2. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}F_3O_2Na^+$ [M+Na$^+$] 407.1229, found 407.1229.



21

methyl 2,2-diphenyl-3-(4-(trifluoromethyl)phenyl)propanoate

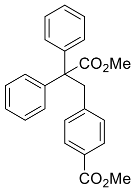
The general procedure **A** was followed. Yield: 52.2 mg (68%) for X = I; 53.8 mg (70%) for X = Br. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.29 – 7.23 (m, 8H), 7.17 – 7.15 (m, 4H), 6.77 (d, *J* = 7.9 Hz, 2H), 3.76 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.9, 142.4, 141.7, 131.3, 129.3, 128.6 (q, *J* = 32.6 Hz), 127.9, 127.2, 124.4 (q, *J* = 272.6 Hz), 124.3 (q, *J* = 3.8 Hz), 62.1, 52.5, 44.3. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}F_3O_2Na^+$ [M+Na$^+$] 407.1229, found 407.1225.



22

methyl 3-(3-methoxy-3-oxo-2,2-diphenylpropyl)benzoate

The general procedure **A** was followed. Yield: 48.1 mg (64%) for X = I; 52.3 mg (70%) for X = Br. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.78 (d, *J* = 7.8 Hz, 1H), 7.42 (s, 1H), 7.25 – 7.22 (m, 6H), 7.18 – 7.14 (m, 4H), 7.08 (t, *J* = 7.7 Hz, 1H), 6.77 (d, *J* = 7.7 Hz, 1H), 3.83 (s, 3H), 3.75 (s, 2H), 3.71 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.8, 167.2, 142.5, 137.7, 135.7, 132.1, 129.4, 129.3, 127.9, 127.7, 127.5, 127.1, 62.1, 52.4, 52.0, 44.3. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{22}O_4Na^+$ [M+Na$^+$] 397.1410, found 397.1409.

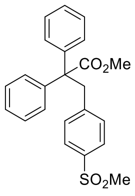


23

methyl 4-(3-methoxy-3-oxo-2,2-diphenylpropyl)benzoate

The general procedure **A** was followed. Yield: 49.6 mg (66%) for X = I; 57.6 mg (77%) for X = Br; 52.1 mg (70%) for X = Cl.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.25 – 7.21 (m, 6H), 7.18 – 7.14 (m, 4H), 6.74 (d, *J* = 8.3 Hz, 2H), 3.86 (s, 3H), 3.75 (s, 2H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 167.3, 143.1, 142.4, 131.0, 129.3, 128.7, 128.2, 127.9, 127.1, 62.1, 52.5, 52.1, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{22}O_4Na^+$ [M+Na$^+$] 397.1410, found 397.1410.

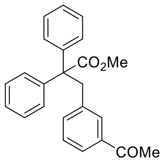


24

methyl 3-(4-(methylsulfonyl)phenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 50.6 mg (64%) for X = Br; 48.7 mg (62%) for X = Cl.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.26 – 7.24 (m, 6H), 7.17 – 7.14 (m, 4H), 6.87 (d, *J* = 8.3 Hz, 2H), 3.79 (s, 2H), 3.69 (s, 3H), 2.99 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 144.3, 142.1, 138.3, 132.0, 129.2, 128.0, 127.3, 126.4, 62.1, 52.6, 44.6, 44.4. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_4SNa^+$ [M+Na$^+$] 417.1131, found 417.1131.

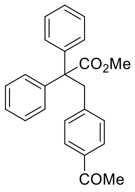


25

methyl 3-(3-acetylphenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 48.8 mg (68%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.8 Hz, 1H), 7.26 –7.23 (m, 6H), 7.19 – 7.14 (m, 5H), 7.07 (s, 1H), 7.01 (d, *J* = 7.6 Hz, 1H), 3.76 (s, 2H), 3.69 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.3, 173.8, 142.5, 137.8, 136.3, 135.8, 131.5, 129.4, 127.9, 127.8, 127.2, 126.1, 62.1, 52.4, 44.3, 26.6. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{22}O_3Na^+$ [M+Na$^+$] 381.1461, found 381.1460.

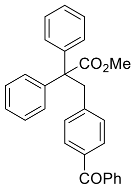


26

methyl 3-(4-acetylphenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 43.1 mg (60%) for X = I; 47.5 mg (66%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.25 – 7.23 (m, 6H), 7.17 – 7.15 (m, 4H), 6.76 (d, *J* = 8.2 Hz, 2H), 3.76 (s, 2H), 3.69 (s, 3H), 2.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.2, 173.9, 143.4, 142.4, 135.3, 131.2, 129.3, 127.9, 127.6, 127.2, 62.1, 52.5, 44.5, 26.7. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{22}O_3Na^+$ [M+Na$^+$] 381.1461, found 381.1461.

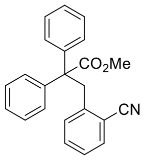


27

methyl 3-(4-benzoylphenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 44.8 mg (53%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.43 (m, 4H), 7.25 – 7.23 (m, 6H), 7.20 – 7.17 (m, 4H), 6.79 (d, *J* = 8.0 Hz, 2H), 3.80 (s, 2H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 173.9, 142.7, 142.5, 137.9, 135.5, 132.3, 130.9, 130.0, 129.4, 129.3, 128.3, 127.9, 127.2, 62.1, 52.5, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{29}H_{24}O_3Na^+$ [M+Na$^+$] 443.1618, found 443.1616.

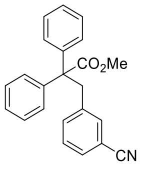


28

methyl 3-(2-cyanophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 41.2 mg (60%) for X = Br; 43.5 mg (64%) for X = Cl.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.33 (m, 2H), 7.25 – 7.21 (m, 7H), 7.19 – 7.15 (m, 5H), 4.05 (s, 2H), 3.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 141.7, 141.6, 132.6, 132.0, 130.7, 129.3, 128.0, 127.3, 127.0, 117.8, 115.0, 62.1, 52.7, 41.9. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}NO_2Na^+$ [M+Na$^+$] 364.1308, found 364.1307.

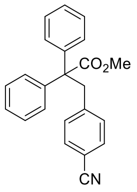


29

methyl 3-(3-cyanophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 39.6 mg (58%) for X = I; 45.8 mg (67%) for X = Br; 37.2 mg (54%) for X = Cl.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.7 Hz, 1H), 7.29 – 7.23 (m, 6H), 7.17 – 7.10 (m, 5H), 6.92 – 6.90 (m, 2H), 3.72 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 142.1, 139.0, 135.6, 134.6, 130.1, 129.3, 128.2, 128.0, 127.4, 119.0, 111.4, 62.1, 52.6, 44.1. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}NO_2Na^+$ [M+Na$^+$] 364.1308, found 364.1311.

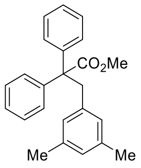


30

methyl 3-(4-cyanophenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 44.4 mg (65%) for X = I; 46.7 mg (68%) for X = Br; 49.2 mg (72%) for X = Cl.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.30 (d, *J* = 8.2 Hz, 2H), 7.27 – 7.22 (m, 6H), 7.17 – 7.13 (m, 4H), 6.77 (d, *J* = 8.1 Hz, 2H), 3.75 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.8, 143.3, 142.1, 131.7, 131.2, 129.2, 128.0, 127.3, 119.2, 110.1, 62.1, 52.6, 44.6. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}NO_2Na^+$ [M+Na$^+$] 364.1308, found 364.1309.

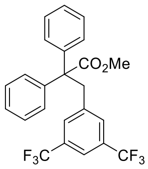


31

methyl 3-(3,5-dimethylphenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 49.7 mg (72%) for X = I.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 – 7.21 (m, 6H), 7.18 – 7.15 (m, 4H), 6.74 (s, 1H), 6.22 (s, 2H), 3.68 (s, 3H), 3.61 (s, 2H), 2.10 (s, 6H).; ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.1, 143.0, 137.0, 136.7, 129.5, 128.9, 127.9, 127.7, 126.9, 62.1, 52.2, 44.4, 21.3. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{24}O_2Na^+$ [M+Na$^+$] 367.1669, found 367.1670.

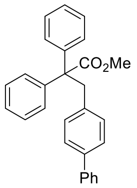


32

methyl 3-(3,5-bis(trifluoromethyl)phenyl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 44.8 mg (50%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.61 (s, 1H), 7.29 – 7.25 (m, 6H), 7.17 – 7.14 (m, 4H), 7.06 (s, 2H), 3.79 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.5, 141.9, 139.9, 131.4 (d, *J* = 4.1 Hz), 130.5 (q, *J* = 33.0 Hz), 129.2, 128.2, 127.6, 123.4 (q, *J* = 273.7 Hz), 120.4 – 120.3 (m), 62.2, 52.6, 44.2. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{18}F_6O_2Na^+$ [M+Na$^+$] 475.1103, found 475.1102.

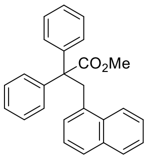


33

methyl 3-([1,1'-biphenyl]-4-yl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 52.4 mg (67%) for X = I.

^{1}H NMR (400 MHz, $CDCl_3$) δ7.53 (d, *J* = 7.4 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.31 – 7.18 (m, 13H), 6.72 (d, *J* = 8.0 Hz, 2H), 3.75 (s, 2H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 142.8, 141.0, 139.1, 136.5, 131.4, 129.4, 128.8, 127.8, 127.2, 127.0, 126.2, 62.2, 52.4, 44.2. HRMS (m/z, ESI-TOF): Calcd for $C_{28}H_{24}O_2Na^+$ [M+Na$^+$] 415.1669, found 415.1669.

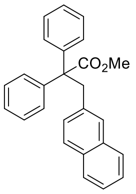


34

methyl 3-(naphthalen-1-yl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 46.2 mg (63%) for X = I.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.64 (m, 2H), 7.32 – 7.02 (m, 15H), 4.24 (s, 2H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 142.7, 134.0, 133.4, 133.3, 129.2, 128.3, 127.9, 127.8, 127.3, 126.9, 125.2, 125.0, 124.9, 123.6, 62.0, 52.4, 39.2. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{22}O_2Na^+$ [M+Na$^+$] 389.1512, found 389.1512.

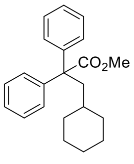


35

methyl 3-(naphthalen-2-yl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 36.5 mg (50%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.70 (m, 1H), 7.57 – 7.54 (m, 1H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.24 – 7.16 (m, 11H), 6.70 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 142.8, 135.0, 133.1, 132.2, 129.9, 129.4, 127.8, 127.5, 127.0, 126.7, 125.6, 125.5, 62.3, 52.4, 44.7. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{22}O_2Na^+$ [M+Na$^+$] 389.1512, found 389.1512.

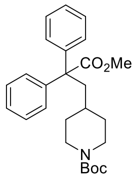


36

methyl 3-cyclohexyl-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 38.3 mg (59%) for X = I; 45.9 mg (71%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.20 (m, 10H), 3.64 (s, 3H), 2.30 (d, *J* = 5.1 Hz, 2H), 1.53 – 1.49 (m, 3H), 1.22 (d, *J* = 12.2 Hz, 2H), 1.11 – 0.96 (m, 4H), 0.90 – 0.81 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.2, 143.8, 129.1, 127.9, 126.8, 59.9, 52.2, 45.5, 34.8, 34.6, 26.5, 26.4. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{26}O_2Na^+$ [M+Na$^+$] 345.1825, found 345.1826.

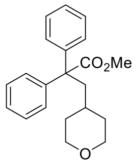


37

tert-butyl 4-(3-methoxy-3-oxo-2,2-diphenylpropyl)piperidine-1-carboxylate

The general procedure **A** was followed. Yield: 54.4 mg (64%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.22 (m, 10H), 3.86 (s, 2H), 3.66 (s, 3H), 2.45 (t, *J* = 13.4 Hz, 2H), 2.34 (s, 2H), 1.41 (s, 9H), 1.26 – 1.04 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.9, 154.9, 143.4, 129.0, 128.0, 127.0, 79.2, 60.0, 52.4, 44.6, 33.4, 33.3, 28.5. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{33}NO_4$ Na^+ [$M+Na^+$] 446.2302, found 446.2301.

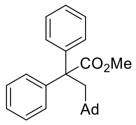


38

methyl 2,2-diphenyl-3-(tetrahydro-2H-pyran-4-yl)propanoate

The general procedure **A** was followed. Yield: 46.5 mg (72%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 6.74 (m, 10H), 3.77 – 3.73 (m, 2H), 3.66 (s, 3H), 3.14 (t, *J* = 11.6 Hz, 2H), 2.35 (d, *J* = 4.9 Hz, 2H), 1.42 – 1.16 (m, 3H), 1.04 (d, *J* = 12.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.9, 143.4, 129.0, 128.0, 127.0, 68.1, 59.9, 52.4, 45.1, 34.4, 32.4. HRMS (m/z, ESI-TOF): Calcd for $C_{21}H_{24}O_3Na^+$ [$M+Na^+$] 347.1618, found 347.1618.

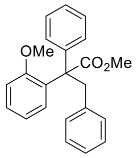


39

methyl 3-((3r,5r,7r)-adamantan-1-yl)-2,2-diphenylpropanoate

The general procedure **A** was followed. Yield: 48.6 mg (65%) for X = Br.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.7 Hz, 4H), 7.25 – 7.15 (m, 6H), 3.61 (s, 3H), 2.44 (s, 2H), 1.75 (s, 3H), 1.56 – 1.53 (m, 3H), 1.47 – 1.44 (m, 3H), 1.23 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 145.5, 129.1, 127.8, 126.5, 56.6, 52.0, 51.9, 42.8, 36.9, 33.8, 28.9. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{30}O_2Na^+$ [$M+Na^+$] 397.2138, found 397.2138.

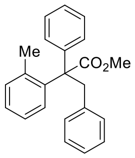


40

methyl 2-(2-methoxyphenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 47.4 mg (68%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.59 (d, *J* = 7.5 Hz, 2H), 7.30 – 7.18 (m, 4H), 7.04 – 6.95 (m, 4H), 6.84 – 6.70 (m, 4H), 4.00 (d, *J* = 13.2 Hz, 1H), 3.59 (s, 3H), 3.47 (d, *J* = 13.1 Hz, 1H), 3.33 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.5, 157.5, 141.6, 137.9, 131.8, 131.0, 129.9, 129.5, 128.3, 127.7, 127.2, 127.0, 126.0, 120.0, 111.2, 58.5, 55.1, 52.0, 42.7. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_3Na^+$ [M+Na$^+$] 369.1461, found 369.1462.

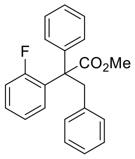


41

methyl 2,3-diphenyl-2-(o-tolyl)propanoate

The general procedure **A** was followed. Yield: 43.4 mg (66%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.44 – 7.41 (m, 1H), 7.30 – 7.27 (m, 2H), 7.21 – 7.11 (m, 6H), 7.08 – 7.04 (m, 3H), 6.60 (d, *J* = 7.1 Hz, 2H), 3.80 (d, *J* = 12.5 Hz, 1H), 3.66 (s, 3H), 3.63 (d, *J* = 12.5 Hz, 1H), 1.73 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.7, 142.3, 141.7, 138.0, 136.8, 132.3, 130.9, 129.2, 128.3, 127.58, 127.56, 127.2, 126.6, 125.6, 60.4, 52.2, 46.0, 21.1. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1515.

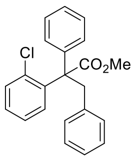


42

methyl 2-(2-fluorophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 47.4 mg (71%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.52 (d, *J* = 7.5 Hz, 2H), 7.34 – 7.16 (m, 4H), 7.11 – 6.94 (m, 5H), 6.85 (dd, *J* = 11.6, 8.2 Hz, 1H), 6.78 (d, *J* = 7.6 Hz, 2H), 4.08 (d, *J* = 13.2 Hz, 1H), 3.65 (s, 3H), 3.48 (d, *J* = 13.2 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.5, 161.1 (d, *J* = 247.9 Hz), 141.3, 137.1, 130.9, 130.8, 130.3 (d, *J* = 11.7 Hz), 128.9 (d, *J* = 8.9 Hz), 128.8, 128.1, 127.5, 127.4, 126.4, 123.4 (d, *J* = 3.2 Hz), 115.9 (d, *J* = 23.5 Hz), 58.8 (d, *J* = 1.9 Hz), 52.5, 42.8. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}FO_2Na^+$ [M+Na$^+$] 357.1261, found 357.1261.

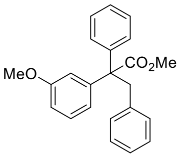


43

methyl 2-(2-chlorophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 47.1 mg (67%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.51 (d, *J* = 7.0 Hz, 2H), 7.31 – 7.23 (m, 4H), 7.17 (t, *J* = 6.8 Hz, 2H), 7.12 – 7.06 (m, 2H), 7.03 (t, *J* = 7.2 Hz, 2H), 6.72 (d, *J* = 7.5 Hz, 2H), 3.92 (d, *J* = 13.4 Hz, 1H), 3.80 (d, *J* = 13.4 Hz, 1H), 3.66 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.5, 140.9, 140.6, 136.8, 134.9, 131.2, 131.1, 130.8, 129.4, 128.4, 127.9, 127.6, 127.1, 126.6, 126.1, 61.1, 52.5, 42.6. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}ClO_2Na^+$ [M+Na$^+$] 373.0966, found 373.0966.

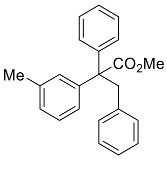


44

methyl 2-(3-methoxyphenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 50.8 mg (73%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.12 (m, 6H), 7.10 (d, *J* = 7.0 Hz, 1H), 7.05 (t, *J* = 7.2 Hz, 2H), 6.77 (t, *J* = 6.4 Hz, 2H), 6.72 (s, 1H), 6.67 (d, *J* = 7.8 Hz, 2H), 3.73 – 3.64 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0, 159.0, 144.4, 142.6, 137.4, 130.9, 129.4, 128.7, 127.7, 127.6, 127.0, 126.4, 121.7, 115.6, 112.3, 62.1, 55.3, 52.3, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_3Na^+$ [M+Na$^+$] 369.1461, found 369.1459.

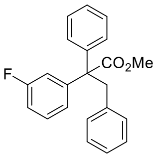


45

methyl 2,3-diphenyl-2-(m-tolyl)propanoate

The general procedure **A** was followed. Yield: 45.8 mg (69%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 6.99 (m, 12H), 6.65 (d, *J* = 7.5 Hz, 2H), 3.76 (d, *J* = 12.8 Hz, 1H), 3.68 (s, 3H), 3.62 (d, *J* = 12.8 Hz, 1H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 142.79, 142.76, 137.5, 137.3, 131.0, 130.0, 129.5, 127.74, 127.70, 127.6, 127.5, 126.8, 126.4, 126.2, 62.1, 52.3, 44.6, 21.7. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1512.

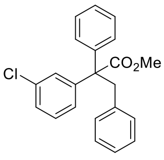


46

methyl 2-(3-fluorophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 44.4 mg (66%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.03 (m, 9H), 6.94 – 6.84 (m, 3H), 6.67 (d, *J* = 7.0 Hz, 2H), 3.77 (d, *J* = 12.8 Hz, 1H), 3.70 (s, 3H), 3.62 (d, *J* = 12.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 162.3 (d, *J* = 244.7 Hz), 145.4 (d, *J* = 7.1 Hz), 142.4, 137.0, 130.8, 129.1, 129.0 (d, *J* = 8.2 Hz), 128.0, 127.7, 127.3, 126.6, 125.2 (d, *J* = 2.8 Hz), 116.8 (d, *J* = 23.0 Hz), 113.9 (d, *J* = 21.0 Hz), 62.0 (d, *J* = 1.7 Hz), 52.5, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}FO_2Na^+$ [M+Na$^+$] 357.1261, found 357.1261.

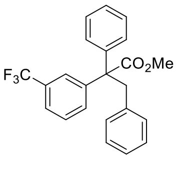


47

methyl 2-(3-chlorophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 49.3 mg (70%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.28 – 7.03 (m, 11H), 6.98 (d, *J* = 7.7 Hz, 1H), 6.65 (d, *J* = 7.7 Hz, 2H), 3.77 (d, *J* = 12.8 Hz, 1H), 3.69 (s, 3H), 3.60 (d, *J* = 12.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.6, 144.9, 142.2, 136.9, 133.6, 130.8, 129.7, 129.1, 128.8, 128.1, 127.8, 127.7, 127.3, 127.1, 126.6, 62.0, 52.5, 44.4. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}ClO_2Na^+$ [M+Na$^+$] 373.0966, found 373.0966.

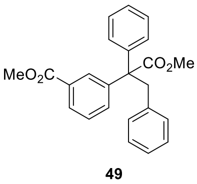


48

methyl 2,3-diphenyl-2-(3-(trifluoromethyl)phenyl)propanoate

The general procedure **A** was followed. Yield: 54.2 mg (70%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.46 (d, *J* = 7.8 Hz, 1H), 7.31 – 7.19 (m, 8H), 7.12 (t, *J* = 7.3 Hz, 1H), 7.05 (t, *J* = 7.3 Hz, 2H), 6.63 (d, *J* = 7.5 Hz, 2H), 3.92 (d, *J* = 12.8 Hz, 1H), 3.71 (s, 3H), 3.52 (d, *J* = 12.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.6, 143.8, 142.2, 136.7, 133.1, 130.8, 129.8 (q, *J* = 32.0 Hz), 128.9, 128.3, 128.0, 127.9, 127.5, 126.7, 126.6 (q, *J* = 3.9 Hz), 124.2 (q, *J* = 273.3 Hz), 123.7 (q, *J* = 3.9 Hz), 62.2, 52.6, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}F_3O_2Na^+$ [M+Na$^+$] 407.1229, found 407.1229.

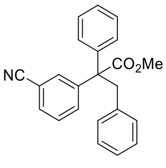


49

methyl 3-(1-methoxy-1-oxo-2,3-diphenylpropan-2-yl)benzoate

The general procedure **A** was followed. Yield: 50.2 mg (67%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.91 (d, *J* = 6.9 Hz, 1H), 7.86 (s, 1H), 7.30 – 7.24 (m, 5H), 7.19 – 7.16 (m, 2H), 7.10 (t, *J* = 7.2 Hz, 1H), 7.03 (t, *J* = 7.3 Hz, 2H), 6.65 (d, *J* = 7.1 Hz, 2H), 3.85 (s, 2H), 3.81 (d, *J* = 12.9 Hz, 1H), 3.70 –3.66 (m, 4H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.8, 167.1, 143.3, 142.3, 137.0, 134.4, 130.8, 130.2, 129.7, 129.1, 128.2, 128.0, 127.73, 127.70, 127.2, 126.5, 62.1, 52.5, 52.2, 44.4. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{22}O_4Na^+$ [M+Na$^+$] 397.1410, found 397.1410.

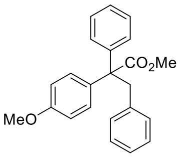


50

methyl 2-(3-cyanophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 45.1 mg (66%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.48 (d, *J* = 7.4 Hz, 1H), 7.35 – 7.19 (m, 8H), 7.16 – 7.12 (m, 1H), 7.07 (t, *J* = 7.4 Hz, 2H), 6.63 (d, *J* = 7.3 Hz, 2H), 3.99 (d, *J* = 12.8 Hz, 1H), 3.72 (s, 3H), 3.41 (d, *J* = 12.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.2, 144.3, 141.8, 136.4, 134.3, 133.5, 130.6, 130.4, 128.6, 128.5, 128.2, 127.9, 127.8, 126.9, 119.0, 111.5, 61.9, 52.7, 44.3. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{19}NO_2Na^+$ [M+Na$^+$] 364.1308, found 364.1309.

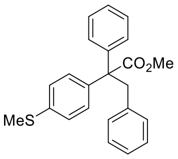


51

methyl 2-(4-methoxyphenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 52.7 mg (76%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.24 – 7.21 (m, 3H), 7.14 – 7.08 (m, 5H), 7.04 (t, *J* = 7.0 Hz, 2H), 6.77 (d, *J* = 8.7 Hz, 2H), 6.67 (d, *J* = 7.5 Hz, 2H), 3.78 (s, 3H), 3.72 (d, *J* = 12.8 Hz, 1H), 3.68 (s, 3H), 3.64 (d, *J* = 12.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.3, 158.4, 143.1, 137.5, 135.0, 131.0, 130.5, 129.3, 127.7, 127.6, 126.9, 126.4, 113.1, 61.5, 55.3, 52.3, 44.7. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_3Na^+$ [M+Na$^+$] 369.1461, found 369.1463.

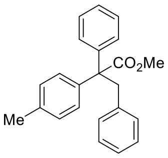


52

methyl 2-(4-(methylthio)phenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 50.7 mg (70%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.23 – 7.02 (m, 12H), 6.67 (d, *J* = 7.1 Hz, 2H), 3.68 (s, 5H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 142.7, 139.6, 137.2, 137.1, 130.9, 129.8, 129.2, 127.8, 127.6, 127.0, 126.4, 125.6, 61.7, 52.3, 44.4, 15.7. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2SNa^+$ [M+Na$^+$] 385.1233, found 385.1233.

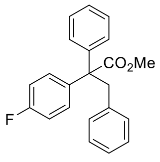


53

methyl 2,3-diphenyl-2-(p-tolyl)propanoate

The general procedure **A** was followed. Yield: 47.2 mg (71%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.21 – 7.01 (m, 12H), 6.67 (d, *J* = 7.4 Hz, 2H), 3.76 (d, *J* = 12.8 Hz, 1H), 3.67 (s, 3H), 3.62 (d, *J* = 12.8 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.2, 142.9, 139.9, 137.5, 136.6, 131.0, 129.4, 129.1, 128.5, 127.7, 127.5, 126.8, 126.3, 61.8, 52.3, 44.5, 21.1. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1510.

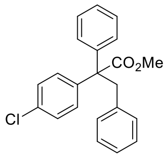


54

methyl 2-(4-fluorophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 48.0 mg (72%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.26 – 7.17 (m, 5H), 7.11 – 7.03 (m, 5H), 6.88 (t, *J* = 8.6 Hz, 2H), 6.66 (d, *J* = 7.7 Hz, 2H), 3.78 (d, *J* = 12.8 Hz, 1H), 3.69 (s, 3H), 3.59 (d, *J* = 12.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 161.7 (d, *J* = 246.3 Hz), 142.8, 138.6 (d, *J* = 3.3 Hz), 137.2, 131.2 (d, *J* = 7.9 Hz), 130.9, 129.0, 128.0, 127.7, 127.2, 126.5, 114.4 (d, *J* = 21.2 Hz), 61.6, 52.4, 44.6. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}FO_2Na^+$ [M+Na$^+$] 357.1261, found 357.1264.

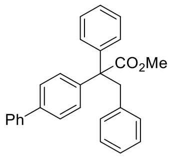


55

methyl 2-(4-chlorophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 50.6 mg (72%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.27 – 7.01 (m, 12H), 6.66 (d, *J* = 7.7 Hz, 2H), 3.78 (d, *J* = 12.8 Hz, 1H), 3.69 (s, 3H), 3.58 (d, *J* = 12.7 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.7, 142.5, 141.3, 137.0, 132.8, 131.0, 130.9, 129.0, 128.0, 127.7, 127.3, 126.6, 61.7, 52.4, 44.4. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{19}ClO_2Na^+$ [M+Na$^+$] 373.0966, found 373.0963.

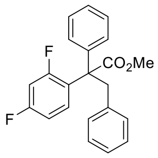


56

methyl 2-([1,1'-biphenyl]-4-yl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 55.8 mg (71%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.59 (d, *J* = 7.1 Hz, 2H), 7.48 – 7.18 (m, 12H), 7.12 – 7.02 (m, 3H), 6.70 (d, *J* = 6.8 Hz, 2H), 3.74 (s, 2H), 3.71 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.1, 142.7, 141.9, 140.6, 139.6, 137.3, 131.0, 129.8, 129.3, 128.8, 127.8, 127.6, 127.4, 127.1, 127.0, 126.4, 126.3, 61.9, 52.4, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{28}H_{24}O_2Na^+$ [M+Na$^+$] 415.1669, found 415.1668.

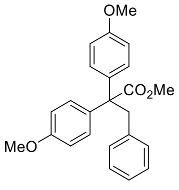


57

methyl 2-(2,4-difluorophenyl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 50.0 mg (71%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.47 – 7.43 (m, 2H), 7.24 – 7.19 (m, 1H), 7.12 – 6.95 (m, 7H), 6.90 – 6.85 (m, 1H), 6.76 (d, *J* = 7.2 Hz, 2H), 3.99 (d, *J* = 13.2 Hz, 1H), 3.66 (s, 3H), 3.48 (d, *J* = 13.1 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.30, 162.0 (d, *J* = 247.8 Hz), 161.0 (d, *J* = 249.1 Hz), , 137.06 (d, *J* = 3.2 Hz), 136.75, 130.80, 130.58 (d, *J* = 8.0 Hz), 130.42 (d, *J* = 3.7 Hz), 130.24 (d, *J* = 11.8 Hz), 129.14 (d, *J* = 8.9 Hz), 127.63, 126.60, 123.59 (d, *J* = 3.2 Hz), 116.00 (d, *J* = 23.3 Hz), 114.86 (d, *J* = 21.2 Hz), 58.18, 52.53, 43.15. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{18}F_2O_2Na^+$ [M+Na$^+$] 375.1167, found 375.1168.

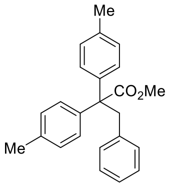


58

methyl 2,2-bis(4-methoxyphenyl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 49.9 mg (66%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.12 – 7.02 (m, 7H), 6.76 (d, *J* = 8.9 Hz, 4H), 6.68 (d, *J* = 7.1 Hz, 2H), 3.79 (s, 6H), 3.68 (s, 3H), 3.65 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.5, 158.4, 137.6, 135.2, 131.1, 130.4, 127.6, 126.3, 113.1, 60.9, 55.3, 52.3, 44.8. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{24}O_4Na^+$ [M+Na$^+$] 399.1567, found 399.1568.

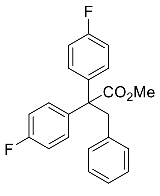


59

methyl 3-phenyl-2,2-di-p-tolylpropanoate

The general procedure **A** was followed. Yield: 46.9 mg (68%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.10 – 7.01 (m, 11H), 6.68 (d, *J* = 8.1 Hz, 2H), 3.67 (s, 2H), 3.66 (s, 3H), 2.31 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.4, 140.0, 137.6, 136.5, 131.0, 129.2, 128.4, 127.5, 126.3, 61.5, 52.3, 44.5, 21.1. HRMS (m/z, ESI-TOF): Calcd for $C_{24}H_{24}O_2Na^+$ [M+Na$^+$] 367.1669, found 367.1667.



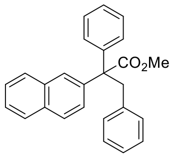
60

methyl 2,2-bis(4-fluorophenyl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 53.1 mg (75%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.14 – 7.04 (m, 7H), 6.91 (t, *J* = 8.7 Hz, 4H), 6.65 (d, *J* = 7.2 Hz, 2H), 3.70 (s, 3H), 3.66 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.8, 161.8 (d, *J* = 246.7 Hz), 138.5 (d, *J* =

3.3 Hz), 136.9, 130.9 (d, *J* = 7.9 Hz), 130.8, 127.8, 126.7, 114.7 (d, *J* = 21.2 Hz), 61.1, 52.5, 44.7. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{18}F_2O_2Na^+$ [M+Na$^+$] 375.1167, found 375.1166.

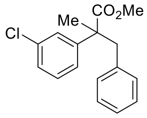


61

methyl 2-(naphthalen-2-yl)-2,3-diphenylpropanoate

The general procedure **A** was followed. Yield: 48.4 mg (66%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.80 – 7.74 (m, 3H), 7.68 (d, *J* = 8.7 Hz, 1H), 7. 49 – 7.43 (m, 2H), 7.25 – 7.07 (m, 7H), 7.01 (t, *J* = 7.4 Hz, 2H), 6.67 (d, *J* = 7.4 Hz, 2H), 3.93 (d, *J* = 12.8 Hz, 1H), 3.74 – 3.70 (m, 4H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 142.6, 140.3, 137.3, 132.9, 132.4, 131.0, 129.5, 128.4, 127.84, 127.80, 127.77, 127.6, 127.5, 127.3, 127.0, 126.5, 126.3, 126.1, 62.2, 52.4, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{22}O_2Na^+$ [M+Na$^+$] 389.1512, found 389.1513.

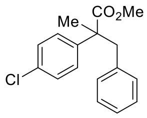


62

methyl 2-(3-chlorophenyl)-2-methyl-3-phenylpropanoate

The general procedure **A** was followed. Yield: 39.4 mg (68%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.27 – 7.23 (m, 3H), 7.20 – 7.15 (m, 4H), 6.91 – 6.89 (m, 2H), 3.69 (s, 3H), 3.41 (d, *J* = 13.3 Hz, 1H), 3.14 (d, *J* = 13.3 Hz, 1H), 1.46 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 175.9, 145.5, 136.9, 134.4, 130.6, 129.7, 128.0, 127.3, 126.80, 126.77, 124.8, 52.4, 51.4, 45.4, 22.1. HRMS (m/z, ESI-TOF): Calcd for $C_{17}H_{17}ClO_2Na^+$ [M+Na$^+$] 311.0809, found 311.0809.

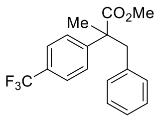


63

methyl 2-(4-chlorophenyl)-2-methyl-3-phenylpropanoate

The general procedure **A** was followed. Yield: 33.9 mg (59%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.29 – 7.27 (m, 2H), 7.21 – 7.16 (m, 5H), 6.89 – 6.86 (m, 2H), 3.67 (s, 3H), 3.38 (d, *J* = 13.3 Hz, 1H), 3.15 (d, *J* = 13.3 Hz, 1H), 1.46 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 176.1, 141.8, 137.0, 132.9, 130.6, 128.6, 128.01, 127.95, 126.7, 52.4, 51.0, 45.5, 22.1. HRMS (m/z, ESI-TOF): Calcd for $C_{17}H_{17}ClO_2Na^+$ [M+Na$^+$] 311.0809, found 311.0809.

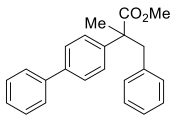


64

methyl 2-methyl-3-phenyl-2-(4-(trifluoromethyl)phenyl)propanoate

The general procedure **A** was followed. Yield: 39.3 mg (61%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.58 (d, *J* = 5.2 Hz, 2H), 7.40 (d, *J* = 4.2 Hz, 2H), 7.20 – 7.17 (m, 3H), 6.90 – 6.88 (m, 2H), 3.69 (s, 3H), 3.44 (d, *J* = 12.5 Hz, 1H), 3.19 (d, *J* = 12.5 Hz, 1H), 1.51 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 175.8, 147.4, 136.8, 130.6, 129.3 (q, *J* = 32.6 Hz), 128.1, 126.9, 126.8, 125.39 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 272.7 Hz), 52.5, 51.6, 45.4, 22.2. HRMS (m/z, ESI-TOF): Calcd for $C_{18}H_{17}F_3O_2Na^+$ [M+Na$^+$] 345.1073, found 345.1071.

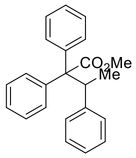


65

methyl 2-([1,1'-biphenyl]-4-yl)-2-methyl-3-phenylpropanoate

The general procedure **A** was followed. Yield: 47.1 mg (71%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.60 (d, *J* = 7.9 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.31 (m, 3H), 7.19 – 7.17 (m, 3H), 6.95 – 6.93 (m, 2H), 3.69 (s, 3H), 3.48 (d, *J* = 13.3 Hz, 1H), 3.20 (d, *J* = 13.2 Hz, 1H), 1.51 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 176.4, 142.5, 140.7, 139.8, 137.4, 130.6, 128.9, 128.0, 127.4, 127.13, 127.11, 126.8, 126.6, 52.3, 51.2, 45.5, 22.3. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1511.

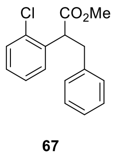


66

methyl 2,2,3-triphenylbutanoate

The general procedure **A** was followed. Yield: 36.8 mg (56%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.46 (d, *J* = 7.8 Hz, 2H), 7.33 – 7.19 (m, 6H), 7.14 – 7.01 (m, 5H), 6.73 (d, *J* = 7.7 Hz, 2H), 4.60 (q, *J* = 7.2 Hz, 1H), 3.51 (s, 3H), 1.22 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.2, 142.1, 141.6, 138.5, 132.2, 130.8, 130.2, 127.9, 127.2, 127.1, 126.9, 126.6, 126.5, 66.4, 52.1, 42.5, 17.4. HRMS (m/z, ESI-TOF): Calcd for $C_{23}H_{22}O_2Na^+$ [M+Na$^+$] 353.1512, found 353.1513.



67

methyl 2-(2-chlorophenyl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 28.6 mg (52%).

^{1}H NMR (400 MHz, CDCl$_3$) δ7.37 (dd, *J* = 15.3, 7.6 Hz, 2H), 7.26 – 7.15 (m, 7H), 4.45 (dd, *J* = 8.7, 6.5 Hz, 1H), 3.61 (s, 3H), 3.36 (dd, *J* = 13.8, 8.8 Hz, 1H), 3.02 (dd, *J* = 13.7, 6.3 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.3, 138.7, 136.4, 133.8, 129.7, 129.0, 128.8, 128.5, 128.3, 127.1, 126.4, 52.1, 49.5, 38.9. HRMS (m/z, ESI-TOF): Calcd for $C_{16}H_{15}ClO_2Na^+$ [M+Na$^+$] 297.0653, found 297.0651

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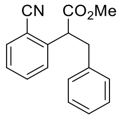
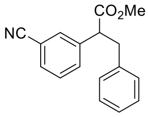


68

methyl 2-(2-cyanophenyl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 27.0 mg (51%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.60 – 7.57 (m, 3H), 7.36 – 7.32 (m, 1H), 7.26 – 7.13 (m, 5H), 4.39 (t, *J* = 7.7 Hz, 1H), 3.64 (s, 3H), 3.44 (dd, *J* = 13.8, 8.2 Hz, 1H), 3.06 (dd, *J* = 13.7, 7.3 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 172.5, 142.2, 137.8, 133.1, 133.1, 129.1, 128.6, 128.1, 127.9, 126.8, 117.6, 113.1, 52.5, 51.2, 39.8. HRMS (m/z, ESI-TOF): Calcd for $C_{17}H_{15}NO_2Na^+$ [M+Na$^+$] 288.0995, found 288.0995.

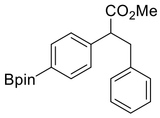


69

methyl 2-(3-cyanophenyl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 25.1 mg (47%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.58 (s, 1H), 7.56 – 7.51 (m, 2H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.26 – 7.17 (m, 3H), 7.06 (d, *J* = 7.0 Hz, 2H), 3.88 (t, *J* = 7.8 Hz, 1H), 3.64 (s, 3H), 3.41 (dd, *J* = 13.8, 8.1 Hz, 1H), 3.01 (dd, *J* = 13.7, 7.5 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.0, 140.0, 138.0, 132.7, 131.9, 131.3, 129.5, 129.0, 128.6, 126.9, 118.7, 112.9, 53.2, 52.5, 39.8. HRMS (m/z, ESI-TOF): Calcd for $C_{17}H_{15}NO_2Na^+$ [M+Na$^+$] 288.0995, found 288.0993.

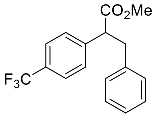


70

methyl 3-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propanoate

The general procedure **A** was followed. Yield: 41.1 mg (56%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 7.7 Hz, 2H), 7.27 – 7.13 (m, 3H), 7.10 (d, *J* = 7.2 Hz, 2H), 3.86 (dd, *J* = 8.5, 6.9 Hz, 1H), 3.58 (s, 3H), 3.42 (dd, *J* = 13.8, 8.6 Hz, 1H), 3.02 (dd, *J* = 13.7, 6.9 Hz, 1H), 1.33 (s, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.7, 141.8, 139.0, 135.3, 129.0, 128.5, 127.5, 126.5, 83.9, 53.9, 52.2, 39.7, 25.0. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{27}BO_4Na^+$ [M+Na$^+$] 389.1895, found 389.1897.

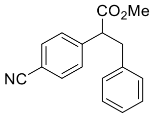


71

methyl 3-phenyl-2-(4-(trifluoromethyl)phenyl)propanoate

The general procedure **A** was followed. Yield: 33.4 mg (54%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.55 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 7.9 Hz, 2H), 7.26 – 7.16 (m, 3H), 7.09 (d, *J* = 7.0 Hz, 2H), 3.92 (t, *J* = 7.7 Hz, 1H), 3.61 (s, 3H), 3.43 (dd, *J* = 13.8, 8.4 Hz, 1H), 3.02 (dd, *J* = 13.7, 7.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.3, 142.6, 138.5, 129.8 (q, *J* = 32.5 Hz), 129.0, 128.59, 128.55, 126.7, 125.7 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 273.1 Hz), 53.5, 52.3, 39.8. HRMS (m/z, ESI-TOF): Calcd for $C_{17}H_{15}F_3O_2Na^+$ [M+Na$^+$] 331.0916, found 331.0918.

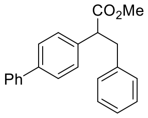


72

methyl 2-(4-cyanophenyl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 29.2 mg (55%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.6 Hz, 2H), 7.39 (d, *J* = 7.5 Hz, 2H), 7.26 – 7.16 (m, 3H), 7.06 (d, *J* = 7.2 Hz, 2H), 3.90 (t, *J* = 7.6 Hz, 1H), 3.63 (s, 3H), 3.42 (dd, *J* = 13.4, 8.2 Hz, 1H), 3.02 (dd, *J* = 13.4, 7.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.8, 143.7, 138.0, 132.4, 129.0, 128.9, 128.5, 126.8, 118.7, 111.4, 53.6, 52.4, 39.6. HRMS (m/z, ESI-TOF): Calcd for $C_{17}H_{15}NO_2Na^+$ [M+Na$^+$] 288.0995, found 288.0995.

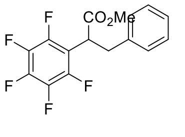


73

methyl 2-([1,1'-biphenyl]-4-yl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 35.1 mg (55%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.52 (m, 4H), 7.44 – 7.30 (m, 5H), 7.26 – 7.13 (m, 5H), 3.90 (dd, *J* = 8.9, 6.6 Hz, 1H), 3.60 (s, 3H), 3.45 (dd, *J* = 13.7, 8.9 Hz, 1H), 3.06 (dd, *J* = 13.7, 6.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 140.7, 140.4, 139.1, 137.8, 129.0, 128.9, 128.49, 128.46, 127.5, 127.4, 127.1, 126.5, 53.4, 52.2, 39.9. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{20}O_2Na^+$ [M+Na$^+$] 339.1356, found 339.1355.

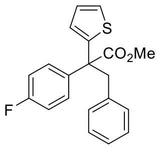


74

methyl 2-(perfluorophenyl)-3-phenylpropanoate

The general procedure **A** was followed. Yield: 32.8 mg (50%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.15 (m, 3H), 7.05 – 7.02 (m, 2H), 4.26 (dd, *J* = 10.5, 5.7 Hz, 1H), 3.74 (s, 3H), 3.61 (dd, *J* = 13.9, 5.7 Hz, 1H), 3.06 (dd, *J* = 14.0, 10.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, the signal of the peaks of the carbons on the pentafluoroarene are very low and not interpreted) δ 170.8, 137.7, 128.73, 128.69, 127.0, 52.9, 42.4, 36.3. HRMS (m/z, ESI-TOF): Calcd for $C_{16}H_{11}F_5O_2Na^+$ [M+Na$^+$] 353.0571, found 353.0567.

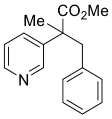


75

methyl 2-(4-fluorophenyl)-3-phenyl-2-(thiophen-2-yl)propanoate

The general procedure **A** was followed. Yield: 38.2 mg (56%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25 – 7.23 (m, 1H), 7.17 – 7.07 (m, 5H), 6.96 – 6.90 (m, 4H), 6.72 (d, *J* = 7.1 Hz, 2H), 3.80 (d, *J* = 12.8 Hz, 1H), 3.73 (s, 3H), 3.66 (d, *J* = 12.8 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.2, 161.9 (d, *J* = 246.5 Hz), 146.3, 138.8, 136.6, 130.7, , 130.1 (d, *J* = 8.0 Hz), 127.8, 127.6, 126.9, 126.3, 125.3, 114.7 (d, *J* = 21.4 Hz), 59.2, 52.7, 46.2. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{17}FO_2SNa^+$ [M+Na$^+$] 363.0825, found 363.0821.

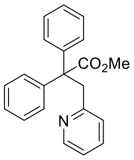


76

methyl 2-methyl-3-phenyl-2-(pyridin-3-yl)propanoate

The general procedure **B** was followed. Yield: 23.0 mg (45%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.56 (s, 1H), 8.51 (d, *J* = 4.2 Hz, 1H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.20 – 7.17 (m, 3H), 6.90 – 6.88 (m, 2H), 3.70 (s, 3H), 3.43 (d, *J* = 13.3 Hz, 1H), 3.20 (d, *J* = 13.3 Hz, 1H), 1.53 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 175.6, 148.2, 148.2, 138.7, 136.5, 134.4, 130.6, 128.1, 126.9, 123.2, 52.5, 50.2, 45.4, 21.9. HRMS (m/z, ESI-TOF): Calcd for $C_{16}H_{17}NO_2Na^+$ [M+Na$^+$] 278.1151, found 278.1152.

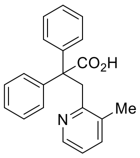


77

methyl 2,2-diphenyl-3-(pyridin-2-yl)propanoate

The general procedure **B** was followed. Yield: 40.5 mg (64%) for X = I; 35.1 mg (55%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.38 (d, *J* = 4.3 Hz, 1H), 7.35 (td, *J* = 7.7, 1.9 Hz, 1H), 7.22 – 7.16 (m, 10H), 7.01 – 6.98 (m, 1H), 6.69 (d, *J* = 7.8 Hz, 1H), 3.96 (s, 2H), 3.73 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.4, 158.1, 148.8, 143.0, 135.6, 129.1, 127.8, 126.8, 124.6, 121.3, 60.6, 52.5, 46.7. HRMS (m/z, ESI-TOF): Calcd for $C_{21}H_{19}NO_2Na^+$ [M+Na$^+$] 340.1308, found 340.1308.

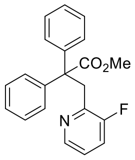


78

3-(3-methylpyridin-2-yl)-2,2-diphenylpropanoic acid

The general procedure **B** was followed. Yield: 37.3 mg (56%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.09 (d, *J* = 5.3 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.16 (m, 6H), 7.11 – 7.07 (m, 5H), 4.05 (s, 2H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 176.1, 155.5, 143.7, 142.4, 140.9, 133.8, 128.4, 128.2, 126.9, 122.5, 62.6, 40.4, 19.2. HRMS (m/z, ESI-TOF): Calcd for $C_{21}H_{19}NO_2Na^+$ [M+Na$^+$] 340.1308, found 340.1308.

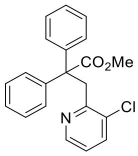


79

methyl 3-(3-fluoropyridin-2-yl)-2,2-diphenylpropanoate

The general procedure **B** was followed. Yield: 58.1 mg (87%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.27 (d, *J* = 4.5 Hz, 1H), 7.27– 7.14 (m, 10H), 7.08 (t, *J* = 8.9 Hz, 1H), 7.04 – 7.00 (m, 1H), 4.03 (s, 2H), 3.71 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.2, 157.9 (d, *J* = 257.1 Hz), 146.7 (d, *J* = 14.1 Hz), 144.4, 143.2, 128.9, 127.7, 126.8, 122.7 (d, *J* = 3.7 Hz), 122.0 (d, *J* = 19.7 Hz), 58.9, 52.3, 38.9 (d, *J* = 2.2 Hz). HRMS (m/z, ESI-TOF): Calcd for $C_{21}H_{18}FNO_2Na^+$ [M+Na$^+$] 358.1214, found 358.1215.

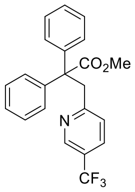


80

methyl 3-(3-chloropyridin-2-yl)-2,2-diphenylpropanoate

The general procedure **B** was followed. Yield: 45.5 mg (65%) for X = Br.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.34 (d, *J* = 4.7, 1.5 Hz, 1H), 7.49 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.28 – 7.14 (m, 10H), 7.00 (dd, *J* = 8.1, 4.7 Hz, 1H), 4.12 (s, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.3, 155.4, 146.4, 143.6, 136.4, 131.7, 129.0, 127.8, 126.7, 122.3, 58.5, 52.2, 42.9. HRMS (m/z, ESI-TOF): Calcd for $C_{21}H_{18}ClNO_2Na^+$ [M+Na$^+$] 374.0918, found 374.0918.

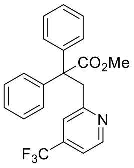


81

methyl 2,2-diphenyl-3-(5-(trifluoromethyl)pyridin-2-yl)propanoate

The general procedure **B** was followed. Yield: 60.3 mg (78%) for X = Br; 52.5 mg (68%) for X = Cl.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.65 (s, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.24 – 7.19 (m, 10H), 6.83 (d, *J* = 8.2 Hz, 1H), 4.05 (s, 2H), 3.72 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.1, 162.4 (d, *J* = 1.6 Hz), 145.6 (q, *J* = 4.1 Hz), 142.6, 132.7 (q, *J* = 3.5 Hz), 129.0, 127.9, 127.1, 124.4, 124.3 (q, *J* = 33.0 Hz), 123.8 (q, *J* = 273.2 Hz), 60.5, 52.6, 46.7. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{18}F_3NO_2Na^+$ [M+Na$^+$] 408.1182, found 408.1182.



82

methyl 2,2-diphenyl-3-(4-(trifluoromethyl)pyridin-2-yl)propanoate

The general procedure **B** was followed. Yield: 43.3 mg (56%) for X = Cl.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.1 Hz, 1H), 7.26 (d, *J* = 2.1 Hz, 11H), 6.82 (s, 1H), 4.09 (s, 2H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 159.9, 149.6, 142.4, 137.8 (q, *J* = 33.9 Hz), 129.1, 128.0, 127.1, 122.8 (q, *J* = 274.1 Hz), 120.5 (q, *J* = 3.6 Hz), 116.9 (q, *J* = 3.3 Hz), 60.8, 52.6, 46.7. HRMS (m/z, ESI-TOF): Calcd for $C_{22}H_{18}F_3NO_2Na^+$ [M+Na$^+$] 408.1182, found 408.1182.

2.3 Mechanistic studies

Stern-Volmer fluorescence quenching experiments

Fluorescence spectra were collected on Edinburgh FS5 spectrofluorimeter. Samples for the quenching experiments were prepared in a 4 mL glass cuvette with a septum screw cap. **1a** was irradiated at 465 nm and the emission intensity at 590 nm was observed. In a typical experiment, the emission spectrum of a 5.0 x 10^{-5} M solution of **1a** in DMSO was collected.

DABCO: A stock solution of DABCO (56.1 mg, 0.5 mmol) in 1 ml of DMSO was prepared. Then, different amounts of this stock solution were added to a solution of the photocatalyst **1a.** in DMSO (5.0 x 10^{-5} M). As shown, a significant decrease of [Ir(ppy)$_2$(dtbbpy)]PF_6 (**1a)** luminescence was observed, suggesting that the mechanism might operate via a canonical photo-redox cycle consisting of a reductive quenching with DABCO.

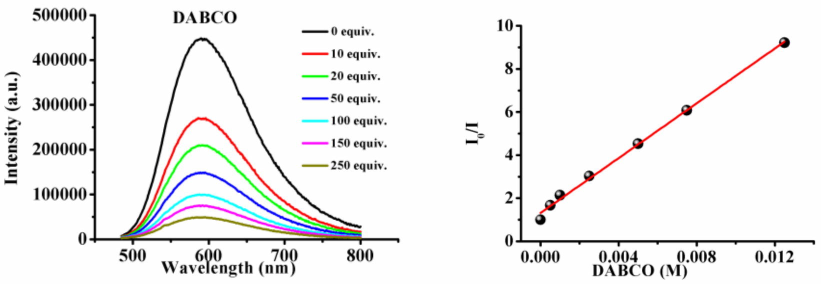


Figure S1. Stern-Volmer quenching by DABCO.

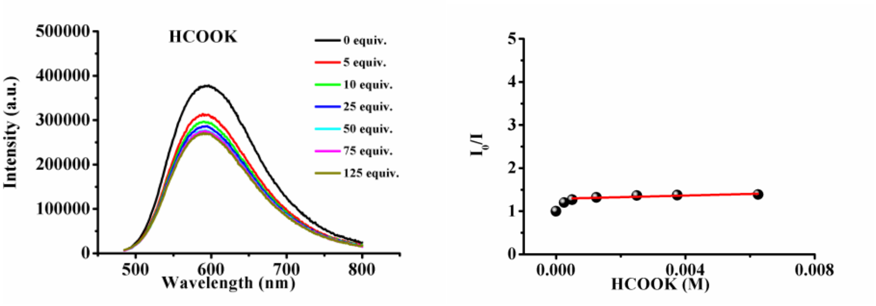


Figure S2. Stern-Volmer quenching by HCOOK.

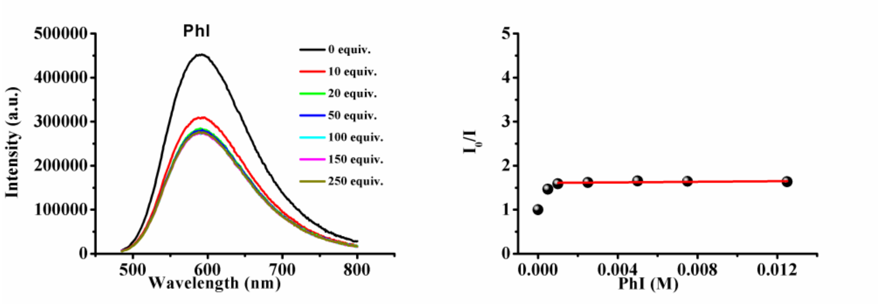


Figure S3. Stern-Volmer quenching by iodobenzene.

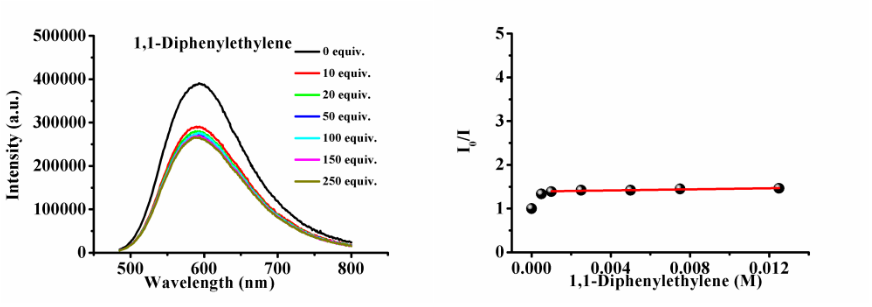
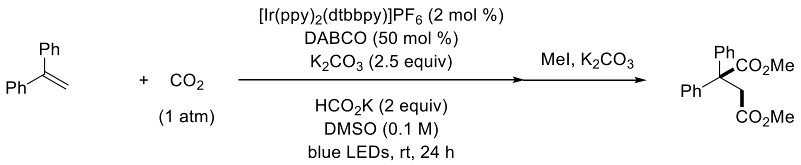


Figure S4. Stern-Volmer quenching by 1,1-diphenylethylene.

Control experiment without using aryl halide:

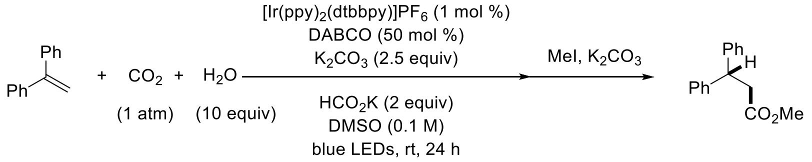


83, 10%

The oven-dried Schlenk tube (38 mL) containing a stirring bar was charged with 1,1 diphenylethylene (36 μL, 0.2 mmol), [Ir(ppy)$_2$(dtbbpy)]PF$_6$ (3.6 mg, 0.004 mmol, 2 mmol%), DABCO (11.2 mg, 0.1 mmol), K_2CO_3 (69.1 mg, 0.5 mmol), HCOOK (33.6 g, 0.4 mmol), and anhydrous DMSO (2 mL) (Note that ahydrous condition is important in order to avoid the alkene reduction reactions with water). N_2 gas in a balloon was bubbled into the mixture under stirring for 30 seconds through a needle and the tube was then evacuated and back-filled with CO_2 for 3 times. The mixture was placed under a

30 W blue LED (λmax=465 nm, 3 cm-4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 ºC) light source and stirred at ambient temperature for 24 h. Upon completion of the reaction, the reaction was quenched with H_2O, then extracted 3 times with EtOAc. The combined aqueous layers were acidized by 1N HCl, then extracted 5 times with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude residue was dissolved in 10 mL acetone, and K_2CO_3 (5 equiv) and CH_3I (10 equiv) were added. The mixture was stirred at 70 ºC for 2 h and then cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 25 mL of EtOAc. The filtrate was concentrated in vacuo. The resulting residue was purified by preparative thin layer chromatography to give the product **83** in10% yield (6.0 mg). ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 – 6.76 (m, 10H), 3.67 (s, 3H), 3.49 (s, 3H), 3.43 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.5, 171.2, 142.5, 128.7, 128.1, 127.2, 57.7, 52.7, 51.8, 43.8. HRMS (m/z, ESI-TOF): Calcd for $C_{18}H_{18}O_4Na^+$ [$M+Na^+$] 321.1097, found 321.1097.

Control experiment without using aryl halide in the presence of water:

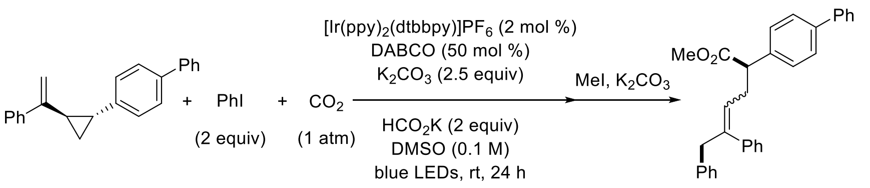


84, 24%

The oven-dried Schlenk tube (38 mL) containing a stirring bar was charged with 1,1 diphenylethylene (36 µL, 0.2 mmol), [Ir(ppy)$_2$(dtbbpy)]PF$_6$ (1.8 mg, 0.002 mmol, 1 mmol%), DABCO (11.2 mg, 0.1 mmol), K_2CO_3 (69.1 mg, 0.5 mmol), HCOOK (33.6 g, 0.4 mmol), H_2O (36 µL, 2 mmol) and anhydrous DMSO (2 mL) (Note that ahydrous condition is important in order to avoid the alkene reduction reactions with water). N_2 gas in a balloon was bubbled into the mixture under stirring for 30 seconds through a needle and the tube was then evacuated and back-filled with CO_2 for 3 times. The mixture was placed under a 30 W blue LED (λmax=465 nm, 3 cm-4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 ºC) light source and stirred at ambient temperature for 24 h. Upon completion of the reaction, all the solvent were removed under reduced pressure at high temperature. The crude residue was dissolved in 10 mL acetone, and K_2CO_3 (5 equiv) and CH_3I (10 equiv) were added. The mixture was stirred at 70 ºC for 2 h and then cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 25 mL of EtOAc. The filtrate was concentrated in vacuo. The resulting residue was purified by preparative thin layer chromatography to the product **84** in 24% yield (11.3 mg). ^1H NMR (400 MHz, $CDCl_3$) δ 7.35 – 6.95 (m, 10H), 4.49 (t, J = 8.0 Hz, 1H), 3.51 (s, 3H), 2.99 (d, J = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4, 143.6, 128.7, 127.8, 126.7, 51.8, 47.1, 40.7. HRMS (m/z, ESI-TOF): Calcd for $C_{16}H_{16}O_2Na^+$ [$M+Na^+$] 263.1043, found 263.1043.

Reaction with radical clock:

4-(2-(1-phenylvinyl)cyclopropyl)-1,1'-biphenyl was synthesized following the literature procedures.^{S1}

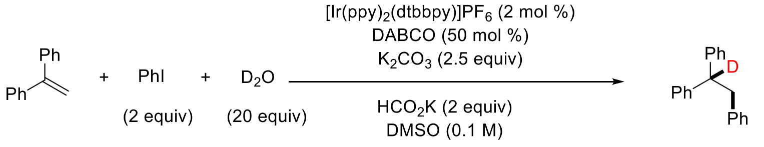


85, 49% (Z/E = 5.9/1)

The general procedure **A** was followed. Yield **85**: 42.6 mg (49%).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.75 – 7.36 (m, 9H), 7.36 – 7.09 (m, 10H), 5.96 (t, *J* = 7.3 Hz, 1H), 3.98 (d, *J* = 16.0 Hz, 1H), 3.89 (d, *J* = 15.9 Hz, 1H), 3.81 (t, *J* = 7.5 Hz, 1H), 3.75 (s, 3H), 3.17 – 3.09 (m, 1H), 2.88 – 2.80 (m, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.0, 140.8, 140.5, 139.9, 139.5, 137.7, 128.9, 128.5, 128.5, 128.3, 128.3, 127.5, 127.4, 127.2, 127.1, 127.0, 126.5, 126.0, 52.3, 51.4, 36.0, 33.2. HRMS (m/z, ESI-TOF): Calcd for $C_{31}H_{28}O_2Na^+$ [M+Na$^+$] 455.1982, found 455.1981.

Isotope-labelling study:

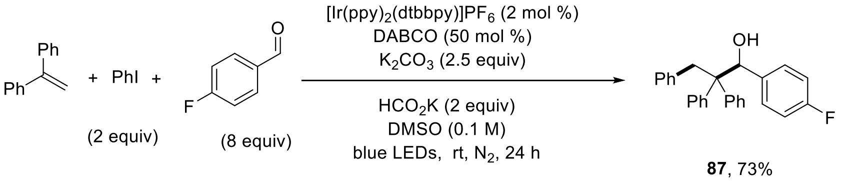


86, 82% (75% D)

The oven-dried Schlenk tube (38 mL) containing a stirring bar was charged with 1,1 diphenylethylene (36 μL, 0.2 mmol), iodobenzene (45 μL, 0.4 mmol), [Ir(ppy)$_2$(dtbbpy)]PF$_6$ (3.6 mg, 0.004 mmol, 2 mmol%), DABCO (11.2 mg, 0.1 mmol), K$_2$CO$_3$ (69.1 mg, 0.5 mmol), HCOOK (33.6 g, 0.4 mmol) D$_2$O (72μL, 4 mmol) and anhydrous DMSO (2 mL) (Note that ahydrous condition is important in order to avoid the alkene reduction reactions with water). N$_2$ gas in a balloon was bubbled into the mixture under stirring for 30 seconds through a needle and the tube was then evacuated and back-filled with N$_2$ for 3 times. The mixture was placed under a 30 W blue LED (λmax=465 nm, 3 cm-4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 °C) light source and stirred at ambient temperature for 24 h. Upon completion of the reaction, the reaction was quenched with H$_2$O, then extracted 3 times with EtOAc. The combined organic layers were dried over anhydrous Na$_2$SO$_4$ and concentrated under reduced pressure. The crude product was purified by prepared TLC to give the product **86** in 82% yield (42.3 mg).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.35 – 7.13 (m, 13H), 7.06 (d, *J* = 6.9 Hz, 2H), 3.41 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 144.5, 140.4, 129.2, 128.5, 128.2, 128.2, 126.3, 126.0, 53.2, 42.1. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{17}D\ Na^+$ [M+Na$^+$] 282.1363, found 282.1368.

Investigation of using aldehyde as the electrophile:

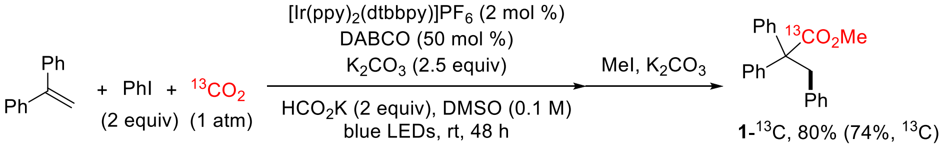


87, 73%

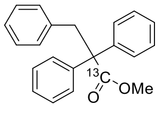
The oven-dried Schlenk tube (38 mL) containing a stirring bar was charged with 1,1 diphenylethylene (36 μL, 0.2 mmol), iodobenzene (45 μL, 0.4 mmol), [Ir(ppy)$_2$(dtbbpy)]PF$_6$ (3.6 mg, 0.004 mmol, 2 mmol%), DABCO (11.2 mg, 0.1 mmol), K$_2$CO$_3$ (69.1 mg, 0.5 mmol), HCOOK (33.6 g, 0.4 mmol), 4-Fluorobenzaldehyde (172 μL, 1.6 mmol) and anhydrous DMSO (2 mL) (Note that ahydrous condition is important in order to avoid the alkene reduction reactions with water). N_2 gas in a balloon was bubbled into the mixture under stirring for 30 seconds through a needle and the tube was then evacuated and back-filled with N_2 for 3 times. The mixture was placed under a 30 W blue LED (λmax=465 nm, 3 cm-4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 °C) light source and stirred at ambient temperature for 24 h. Upon completion of the reaction, the reaction was quenched with H_2O, then extracted 3 times with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by prepared TLC to give the product **87** in 73% yield (55.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.21 (m, 8H), 7.21 – 7.09 (m, 3H), 7.05 (t, *J* = 7.3 Hz, 2H), 6.86 (t, *J* = 8.7 Hz, 2H), 6.74 – 6.71 (m, 2H), 6.62 (d, *J* = 7.3 Hz, 2H), 5.63 (d, *J* = 3.1 Hz, 1H), 3.54 (d, *J* = 13.5 Hz, 1H), 3.12 (d, *J* = 13.6 Hz, 1H), 2.25 (d, *J* = 3.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4 (d, *J* = 246.4 Hz), 143.8, 141.9, 137.6, 136.3 (d, *J* = 3.2 Hz), 131.1, 131.0, 130.6 (d, *J* = 8.0 Hz), 130.3, 127.7, 127.5, 127.1, 126.5, 126.2, 114.2 (d, *J* = 21.1 Hz), 76.2, 58.7, 44.3. HRMS (m/z, ESI-TOF): Calcd for $C_{27}H_{23}FO\,Na^+$ [M+Na$^+$] 405.1625, found 405.1625.

Reaction with ^{13}C labled CO_2:



The general procedure **A** was followed for this reaction to give **1**-^{13}C.

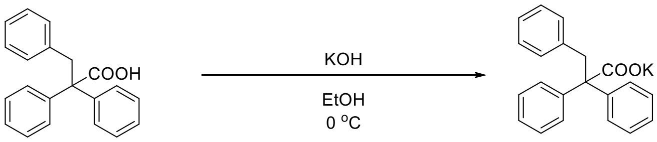


1-^{13}C

methyl 2,2,3-triphenylpropanoate

Yield: 50.8 mg (80%), 74% ^{13}C (calculated from GC-MS)

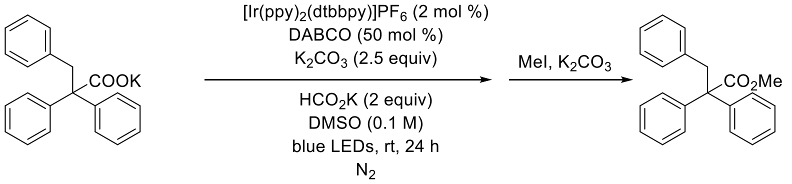
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.12 (m, 10H), 7.11 – 7.07 (m, 1H), 7.03 (t, *J* = 7.8 Hz, 2H), 6.66 (d, *J* = 8.1 Hz, 2H), 3.73 – 3.69 (m, 2H), 3.69 – 3.66 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 142.9, 137.4, 131.0, 129.4, 129.4, 127.8, 127.6, 12.0, 126.4, 62.2, 62.1 (d, *J* = 56.9 Hz), 52.3, 44.5. HRMS (m/z, ESI-TOF): Calcd for $C_{21}{}^{13}CH_{20}O_2Na^+$ [M+Na$^+$] 340.1389, found 340.1389.



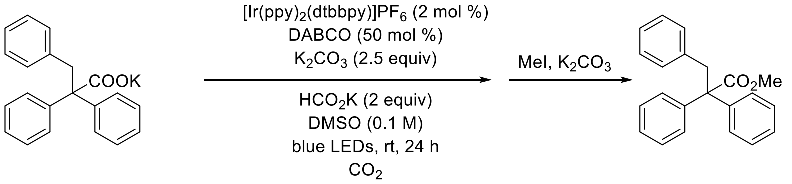
1-K was prepared by treating **1-H (**120.9 mg, 0.4 mmol) with KOH (22.4 mg, 0.4 mmol) and stirred for 5 min at 0 °C. EtOH and H_2O were then removed under high vacuum to afford **1-K** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 – 6.86 (m, 13H), 6.69 (d, *J* = 7.2 Hz, 2H), 3.58 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.7, 145.8, 139.6, 131.0, 129.6, 127.5, 127.4, 126.0, 125.8, 64.5, 45.2.

Stability of potassium salt of product in presence of N_2 or CO_2:



1, 87% (NMR)



1, 87% (NMR)

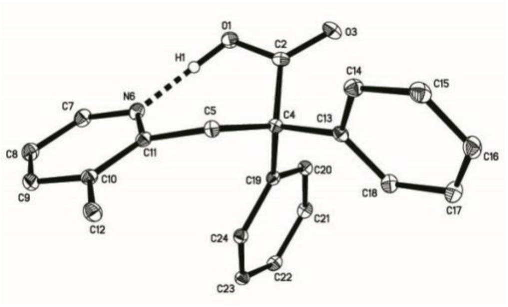
The oven-dried Schlenk tube (38 mL) containing a stirring bar was charged with **1-K** (34.0 mg, 0.10 mmol), $[Ir(ppy)_2(dtbbpy)]PF_6$ (1.8 mg, 0.002 mmol, 2 mol%), DABCO (6.1 mg, 0.05 mmol), K_2CO_3 (34.5 mg, 0.25 mmol), HCOOK (16.8 mg, 0.2 mmol) and anhydrous DMSO (1 mL). N_2 gas in a balloon was bubbled into the mixture under stirring for 30 seconds through a needle and the tube was then evacuated and back-filled with CO_2 or N_2 for 3 times. The mixture was placed under a 30 W blue LED (λmax=465 nm, 3 cm away, with cooling fan to keep the reaction temperature at 25~30 °C) light source and stirred at ambient temperature for 24 h. Upon completion of the reaction, all the solvent were removed under reduced pressure at high temperature. The crude residue was dissolved in 10 mL acetone, and K_2CO_3 (5 equiv) and CH_3I (10 equiv) were added. The mixture was stirred at 70 °C for 2 h and then cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 25 mL of EtOAc. The filtrate was concentrated in vacuo, and crude ^{1}H NMR spectrum was taken using CH_2Br_2 as internal standard, which indicated formation of 87% of **1**.

2.4 Gram-scale experiment

The oven-dried Schlenk tube (250 mL) containing a stirring bar was charged with 1,1 diphenylethylene (0.9 g, 5 mmol), iodobenzene (1.11 ml, 10 mmol), $[Ir(ppy)_2(dtbbpy)]PF_6$ (91.4 mg, 0.1 mmol, 2 mmol%), DABCO (280.4 mg, 2.5 mmol, 50 mol%), K_2CO_3 (1.73 g, 12.5 mmol), HCOOK (0.84 g, 10 mmol) and anhydrous DMSO (50 mL). N_2 gas in a balloon was bubbled into the mixture under stirring for 10 min through a needle and the tube was then evacuated and back-filled with CO_2 for 3 times. The mixture was placed under a 30 W blue LED (λmax=465 nm, 7.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 °C) light source and stirred at ambient temperature for 24 h. Upon completion of the reaction, all the solvent were removed under reduced pressure at high temperature. The crude residue was dissolved in 50 mL acetone, and K_2CO_3 (3.46 g, 25 mmol) and CH_3I (3 mL, 50 mmol) were added. The mixture was stirred at 70 °C for 2 h and then cooled to room temperature. The crude reaction mixture was diluted with EtOAc (25 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional

125 mL of EtOAc. The filtrate was concentrated in vacuo, and crude ^{1}H NMR spectrum was taken using CH_2Br_2 as internal standard. The resulting residue was purified by flash silica gel chromatography or preparative thin layer chromatography using petroleum ether/EtOAc (100:1) as the eluent to give **1** in 69% yield (1.09 g).

3. X-Ray Crystallographic Spectrum of 78



The CCDC number of this compound is **1942129**

Table S3. Crystal data and structure refinement for **78**.

Empirical formula	C21 H19 N O2	
Formula weight	317.37	
Temperature	108(3) K	
Wavelength	1.34050 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 16.6583(2) Å	α= 90°.
	b = 9.92980(10) Å	β= 90°.
	c = 19.3483(2) Å	γ= 90°.
Volume	3200.47(6) Å^3	
Z	8	
Density (calculated)	1.317 Mg/m^3	
Absorption coefficient	0.430 mm^{-1}	
F(000)	1344	
Crystal size	0.1 x 0.1 x 0.1 mm^3	
Theta range for data collection	4.60 to 60.41°.	
Index ranges	-20<=h<=21, -12<=k<=9, -25<=l<=23	
Reflections collected	13499	
Independent reflections	3565 [R(int) = 0.0163]	
Completeness to theta = 60.41°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.90836	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3565 / 1 / 222	
Goodness-of-fit on F^2	1.038	

Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0877
R indices (all data)	R1 = 0.0375, wR2 = 0.0891
Largest diff. peak and hole	0.326 and -0.177 e.Å^{-3}

Table S4. Bond lengths [Å] and angles [°] for **78**.

O(1)-C(2)	1.3073(12)
O(1)-H(1)	0.960(16)
C(2)-O(3)	1.2147(13)
C(2)-C(4)	1.5580(13)
C(4)-C(19)	1.5350(13)
C(4)-C(13)	1.5418(13)
C(4)-C(5)	1.5627(13)
C(5)-C(11)	1.5091(14)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
N(6)-C(11)	1.3406(13)
N(6)-C(7)	1.3422(14)
C(7)-C(8)	1.3740(16)
C(7)-H(7)	0.9300
C(8)-C(9)	1.3832(16)
C(8)-H(8)	0.9300
C(9)-C(10)	1.3897(15)
C(9)-H(9)	0.9300
C(10)-C(11)	1.3999(14)
C(10)-C(12)	1.5009(14)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(18)	1.3879(14)
C(13)-C(14)	1.3983(14)
C(14)-C(15)	1.3856(15)
C(14)-H(14)	0.9300
C(15)-C(16)	1.3869(17)
C(15)-H(15)	0.9300
C(16)-C(17)	1.3804(16)
C(16)-H(16)	0.9300

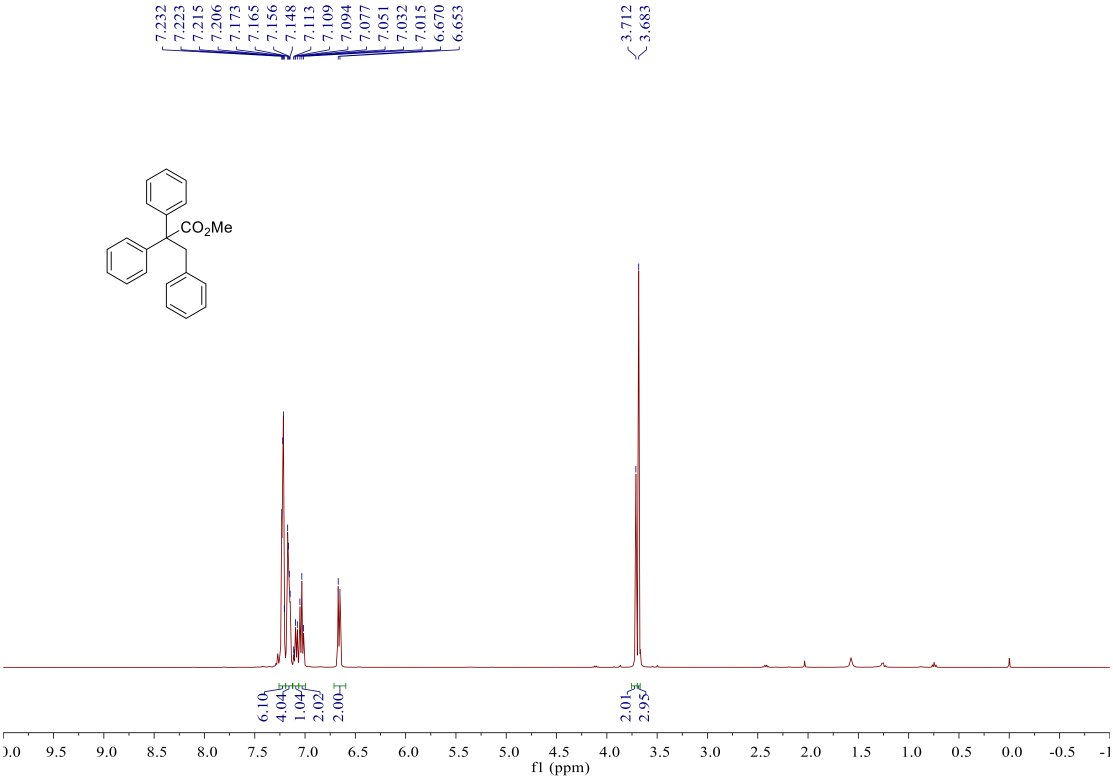
C(17)-C(18)	1.3951(15)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(24)	1.3960(14)
C(19)-C(20)	1.3989(14)
C(20)-C(21)	1.3870(14)
C(20)-H(20)	0.9300
C(21)-C(22)	1.3894(15)
C(21)-H(21)	0.9300
C(22)-C(23)	1.3888(15)
C(22)-H(22)	0.9300
C(23)-C(24)	1.3907(14)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(2)-O(1)-H(1)	111.8(14)
O(3)-C(2)-O(1)	121.59(9)
O(3)-C(2)-C(4)	121.13(9)
O(1)-C(2)-C(4)	117.20(8)
C(19)-C(4)-C(13)	110.87(8)
C(19)-C(4)-C(2)	106.93(8)
C(13)-C(4)-C(2)	107.80(8)
C(19)-C(4)-C(5)	112.45(8)
C(13)-C(4)-C(5)	106.30(8)
C(2)-C(4)-C(5)	112.44(8)
C(11)-C(5)-C(4)	119.70(8)
C(11)-C(5)-H(5A)	107.4
C(4)-C(5)-H(5A)	107.4
C(11)-C(5)-H(5B)	107.4
C(4)-C(5)-H(5B)	107.4
H(5A)-C(5)-H(5B)	106.9
C(11)-N(6)-C(7)	120.70(9)
N(6)-C(7)-C(8)	121.38(10)
N(6)-C(7)-H(7)	119.3
C(8)-C(7)-H(7)	119.3
C(7)-C(8)-C(9)	118.51(10)
C(7)-C(8)-H(8)	120.7
C(9)-C(8)-H(8)	120.7

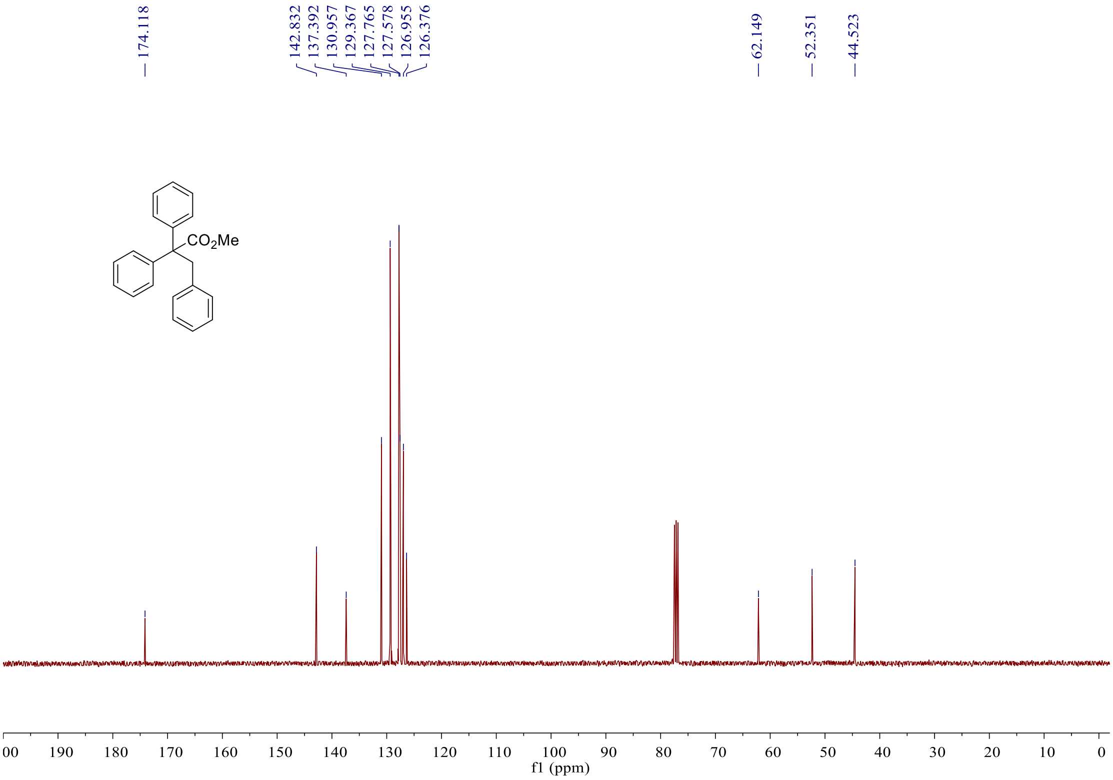
C(8)-C(9)-C(10)	120.85(10)
C(8)-C(9)-H(9)	119.6
C(10)-C(9)-H(9)	119.6
C(9)-C(10)-C(11)	117.32(9)
C(9)-C(10)-C(12)	120.83(9)
C(11)-C(10)-C(12)	121.83(9)
N(6)-C(11)-C(10)	121.22(9)
N(6)-C(11)-C(5)	117.45(9)
C(10)-C(11)-C(5)	121.30(9)
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	118.02(9)
C(18)-C(13)-C(4)	122.54(9)
C(14)-C(13)-C(4)	119.43(9)
C(15)-C(14)-C(13)	120.95(10)
C(15)-C(14)-H(14)	119.5
C(13)-C(14)-H(14)	119.5
C(14)-C(15)-C(16)	120.37(10)
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-H(15)	119.8
C(17)-C(16)-C(15)	119.37(10)
C(17)-C(16)-H(16)	120.3
C(15)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	120.24(10)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(13)-C(18)-C(17)	121.04(10)
C(13)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(24)-C(19)-C(20)	118.01(9)
C(24)-C(19)-C(4)	121.86(9)
C(20)-C(19)-C(4)	120.05(9)
C(21)-C(20)-C(19)	121.14(9)
C(21)-C(20)-H(20)	119.4

C(19)-C(20)-H(20)	119.4
C(20)-C(21)-C(22)	120.18(9)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	119.44(9)
C(23)-C(22)-H(22)	120.3
C(21)-C(22)-H(22)	120.3
C(22)-C(23)-C(24)	120.24(9)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(23)-C(24)-C(19)	120.99(9)
C(23)-C(24)-H(24)	119.5
C(19)-C(24)-H(24)	119.5

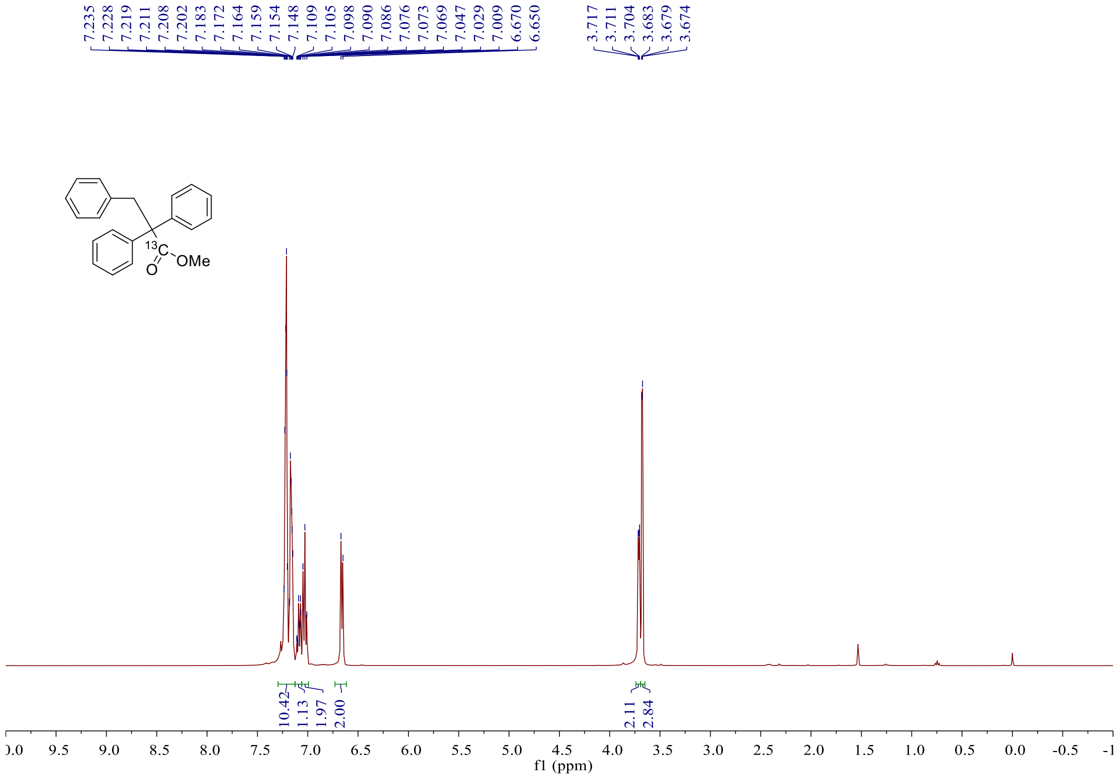
4. NMR Spectra of Compounds

1





1-^{13}C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3.711
3.704
3.683
3.679
3.674
13C
OMe
O
10.42
1.13
1.97
2.00
2.11
2.84
10.0
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8.5
8.0
7.5
7.0
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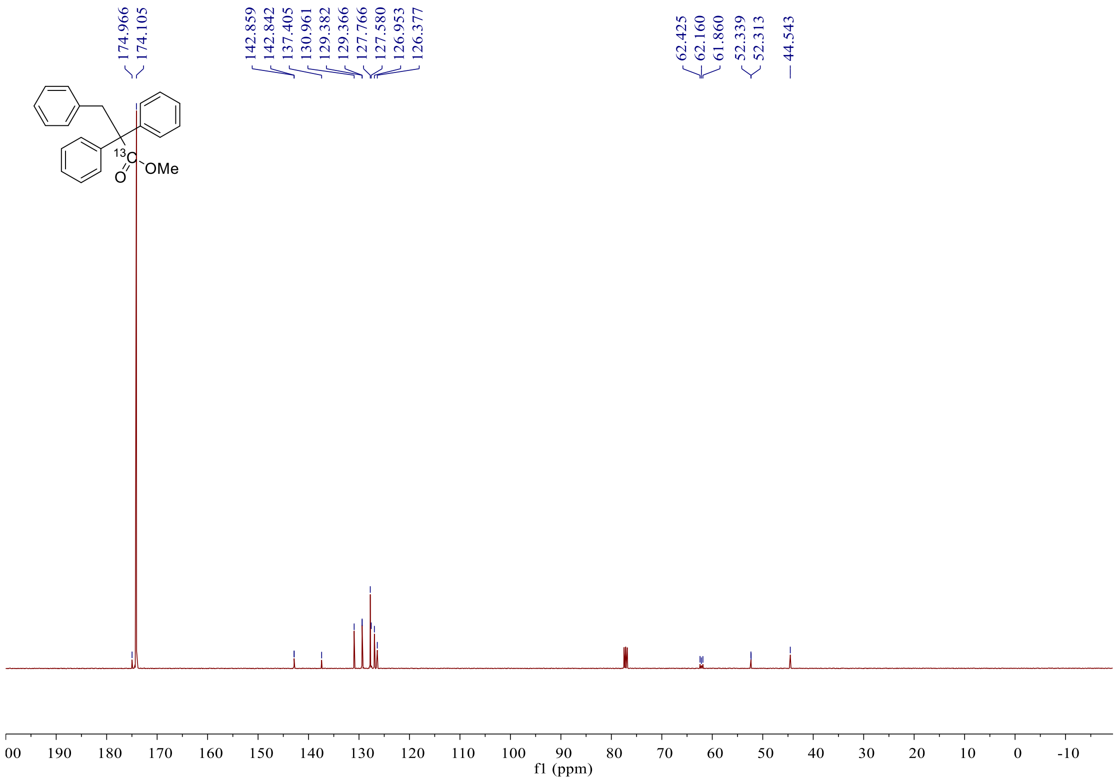
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44.543
13C
OMe
O
200
190
180
170
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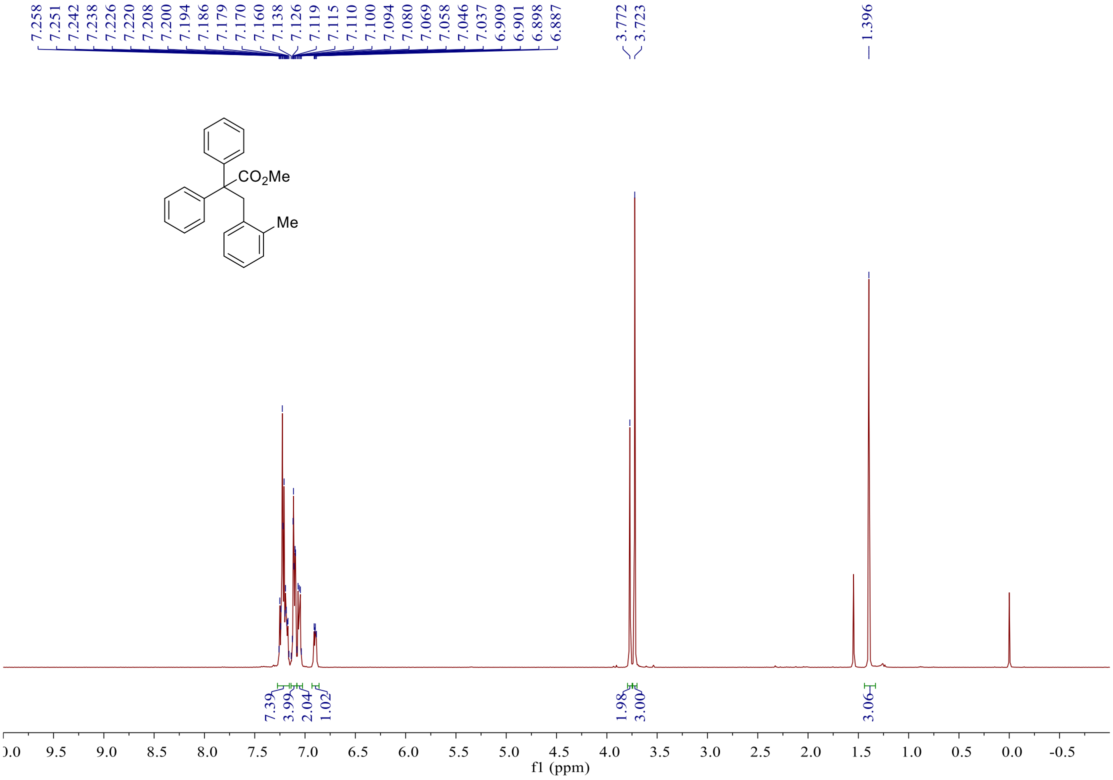
2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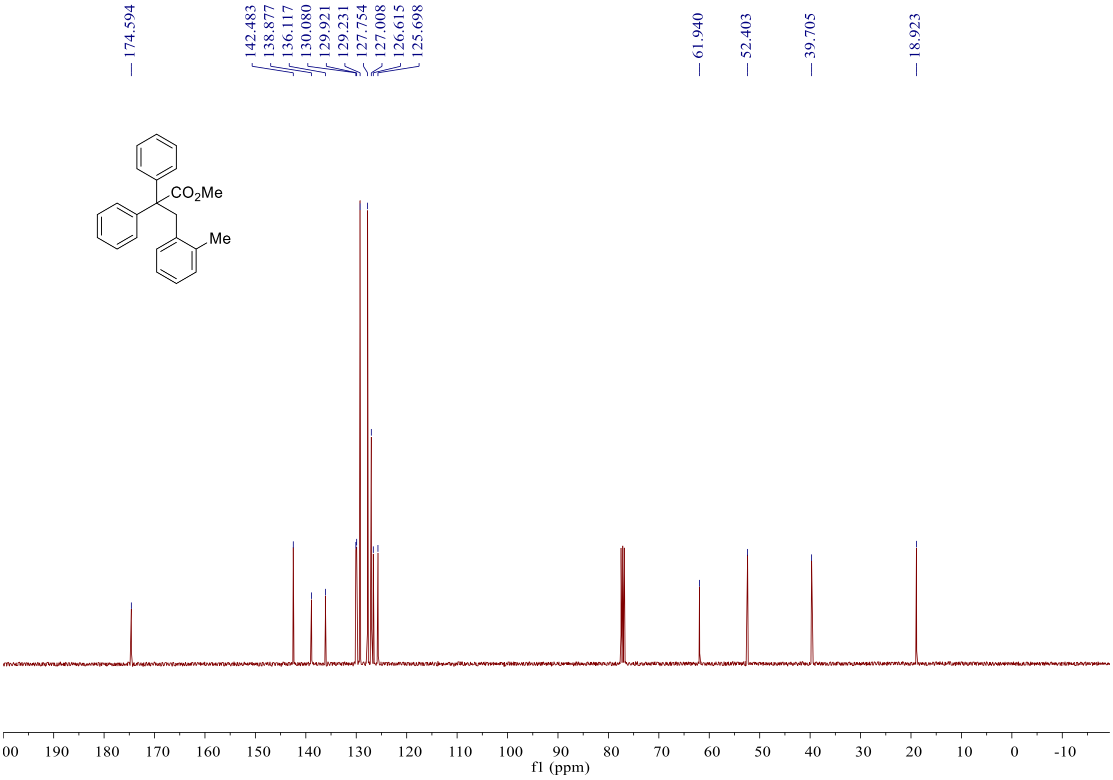
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CO2Me
Me
00
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180
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20
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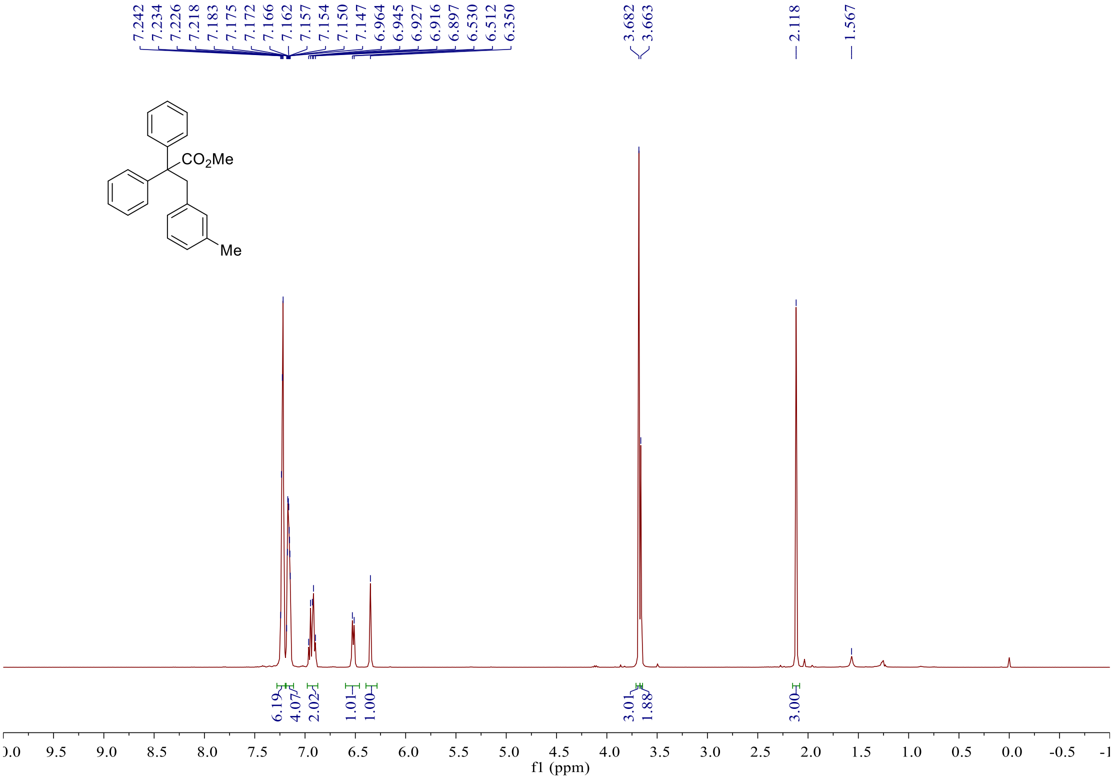
f1 (ppm)

3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Me
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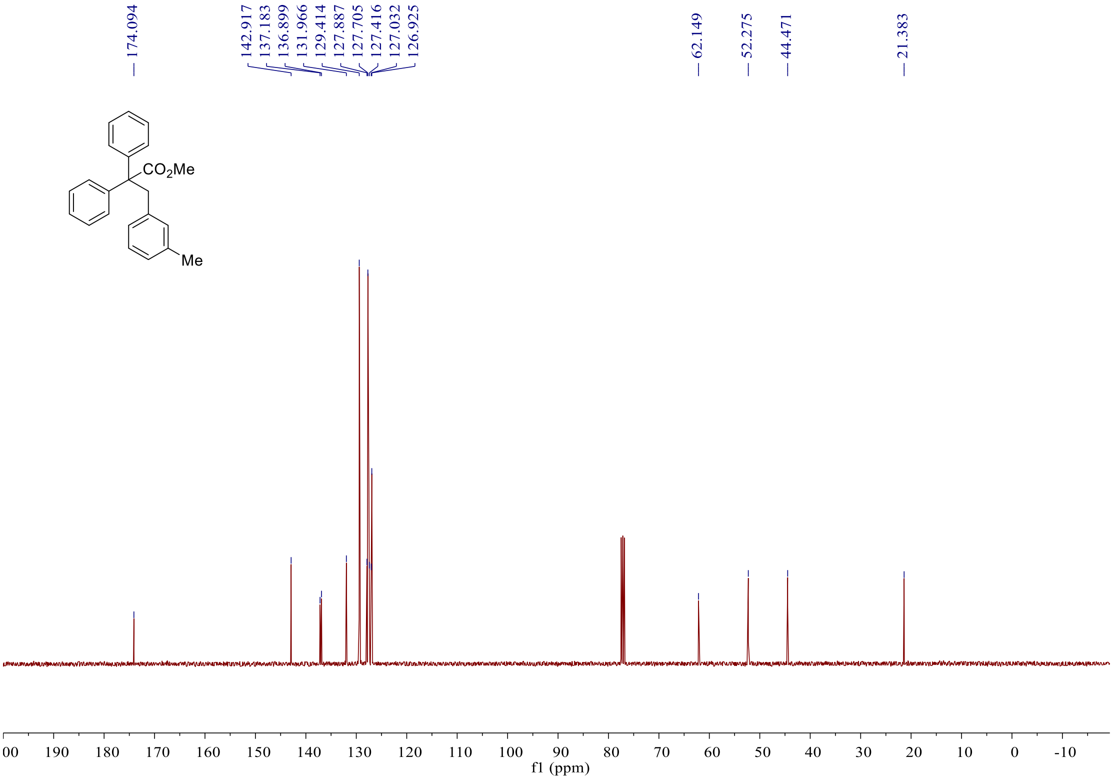
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Me
00
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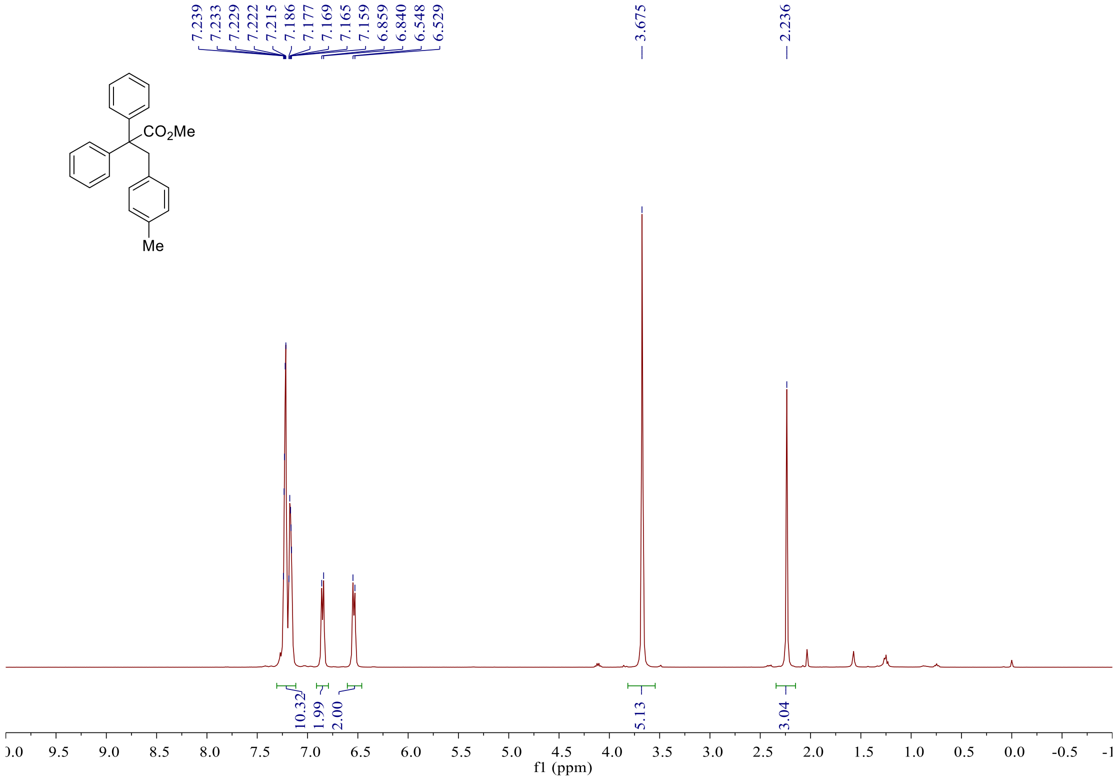
4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CO$_2$Me
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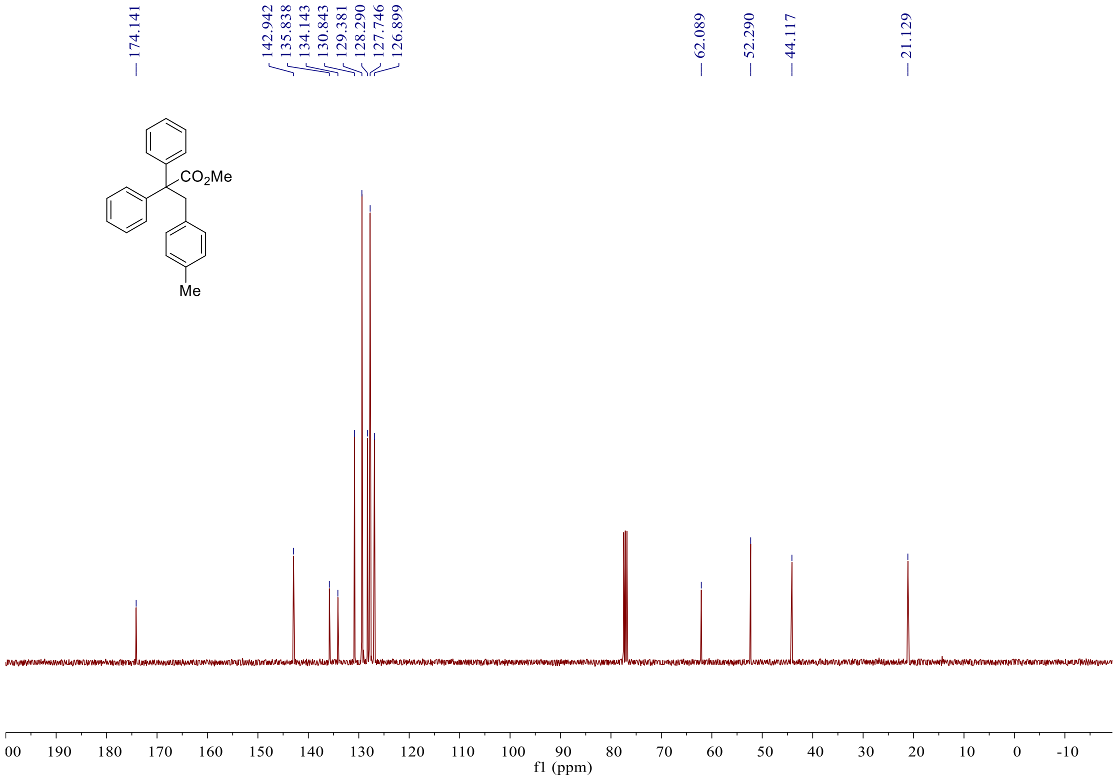
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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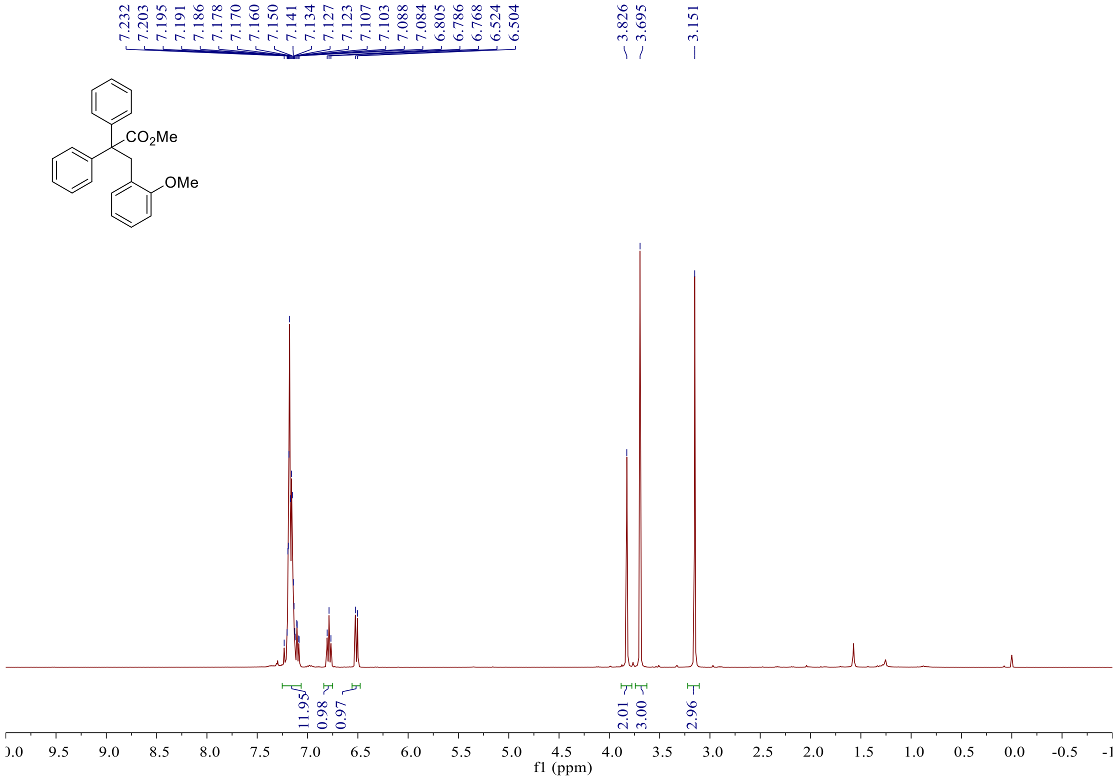
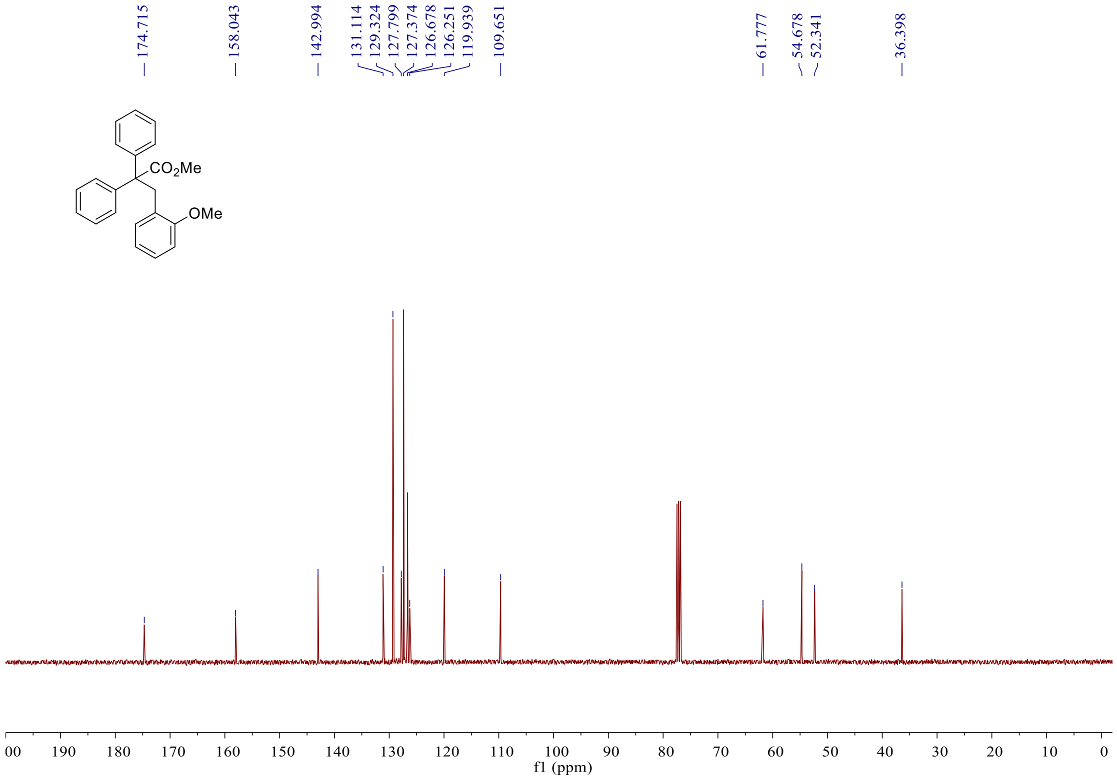
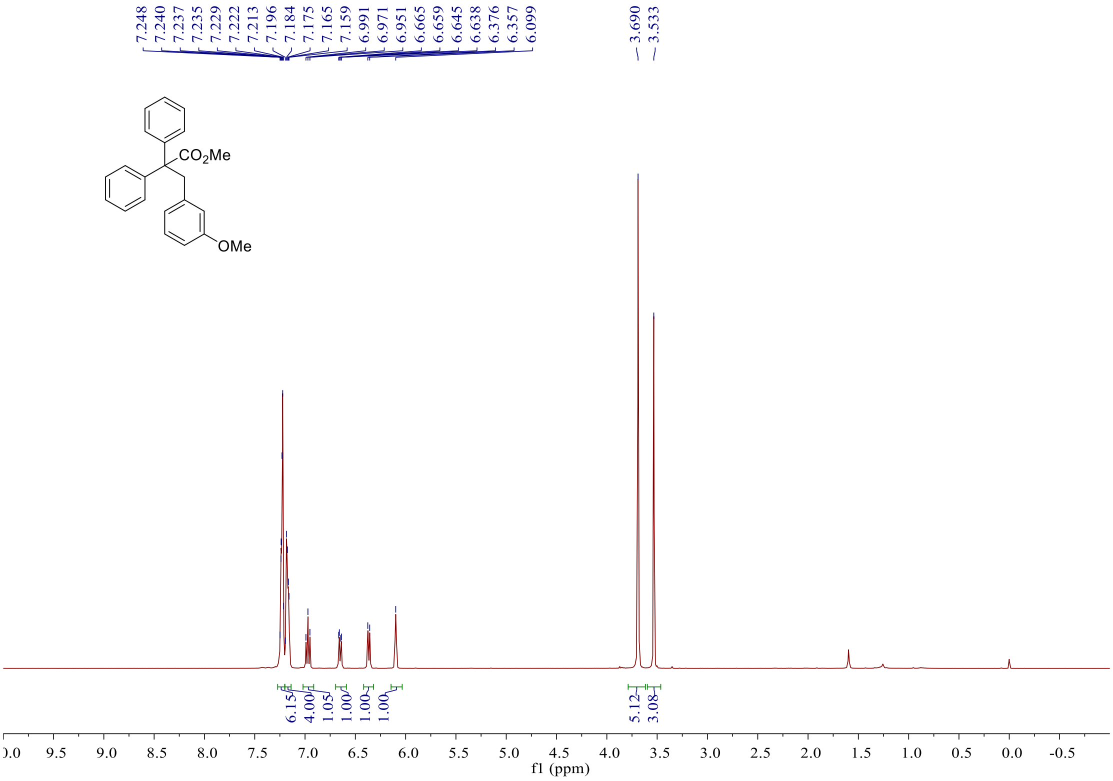
142.942
135.838
134.143
130.843
129.381
128.290
127.746
126.899
62.089
52.290
44.117
21.129
CO$_2$Me
Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

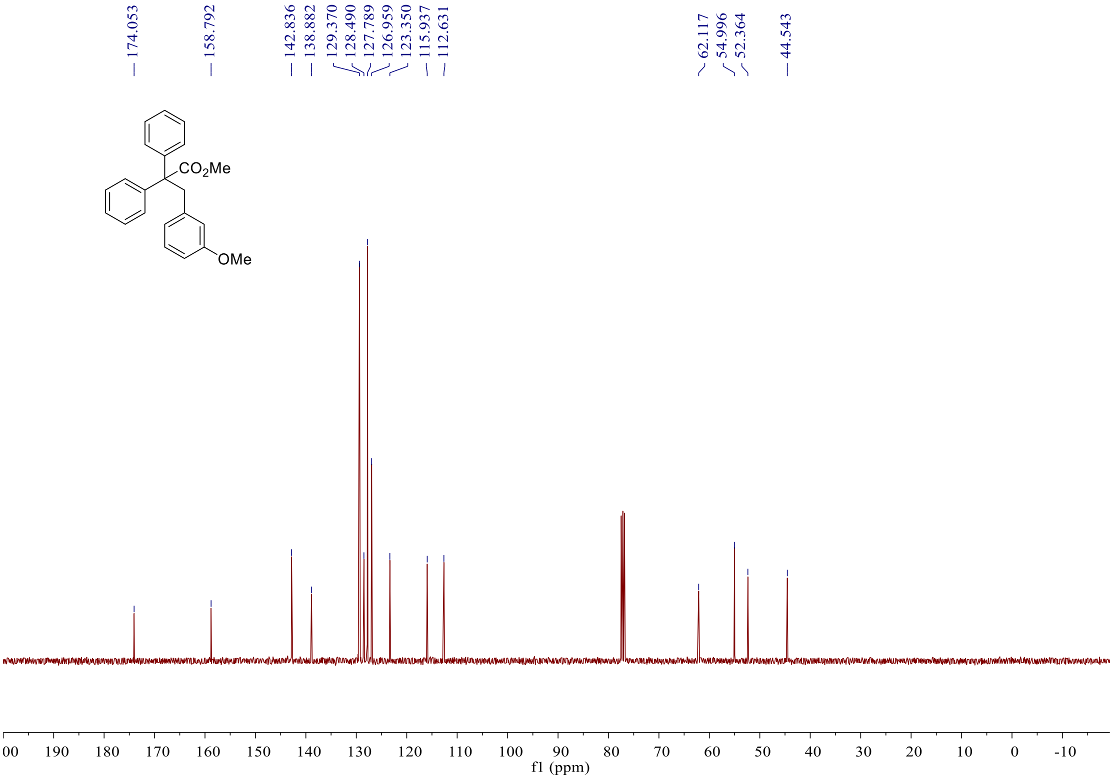
5


7.232
7.203
7.195
7.191
7.186
7.178
7.170
7.160
7.150
7.141
7.134
7.127
7.123
7.107
7.103
7.088
7.084
6.805
6.786
6.768
6.524
6.504
3.826
3.695
3.151
CO2Me
OMe
11.95
0.98
0.97
2.01
3.00
2.96
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

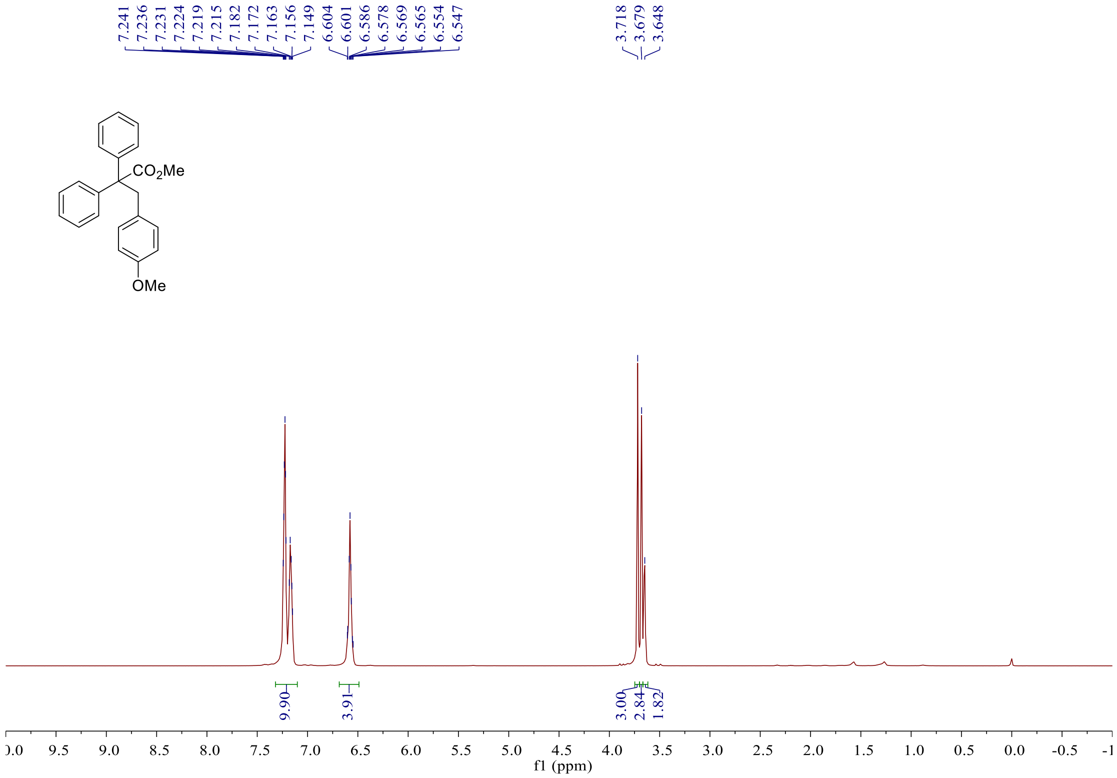

174.715
158.043
142.994
131.114
129.324
127.799
127.374
126.678
126.251
119.939
109.651
61.777
54.678
52.341
36.398
CO2Me
OMe
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

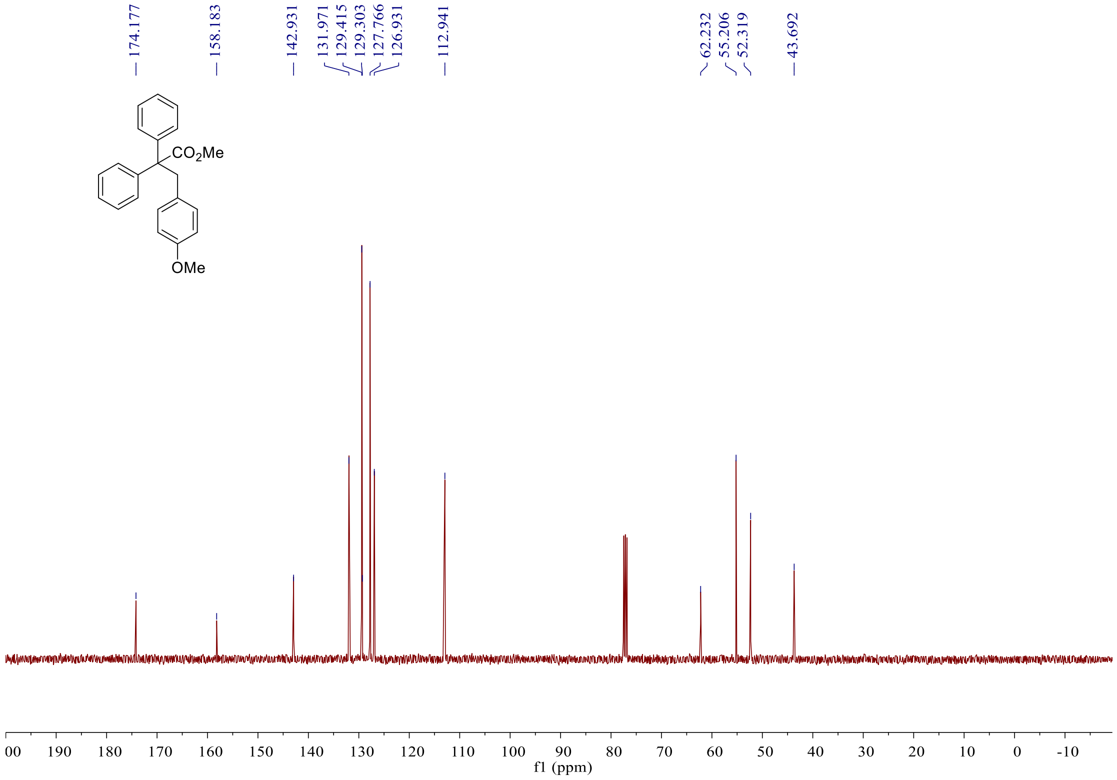
6


7.248
7.240
7.237
7.235
7.229
7.222
7.213
7.196
7.184
7.175
7.165
7.159
6.991
6.971
6.951
6.665
6.659
6.645
6.638
6.376
6.357
6.099
3.690
3.533
CO2Me
OMe
6.15
4.00
1.05
1.00
1.00
1.00
5.12
3.08
).0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

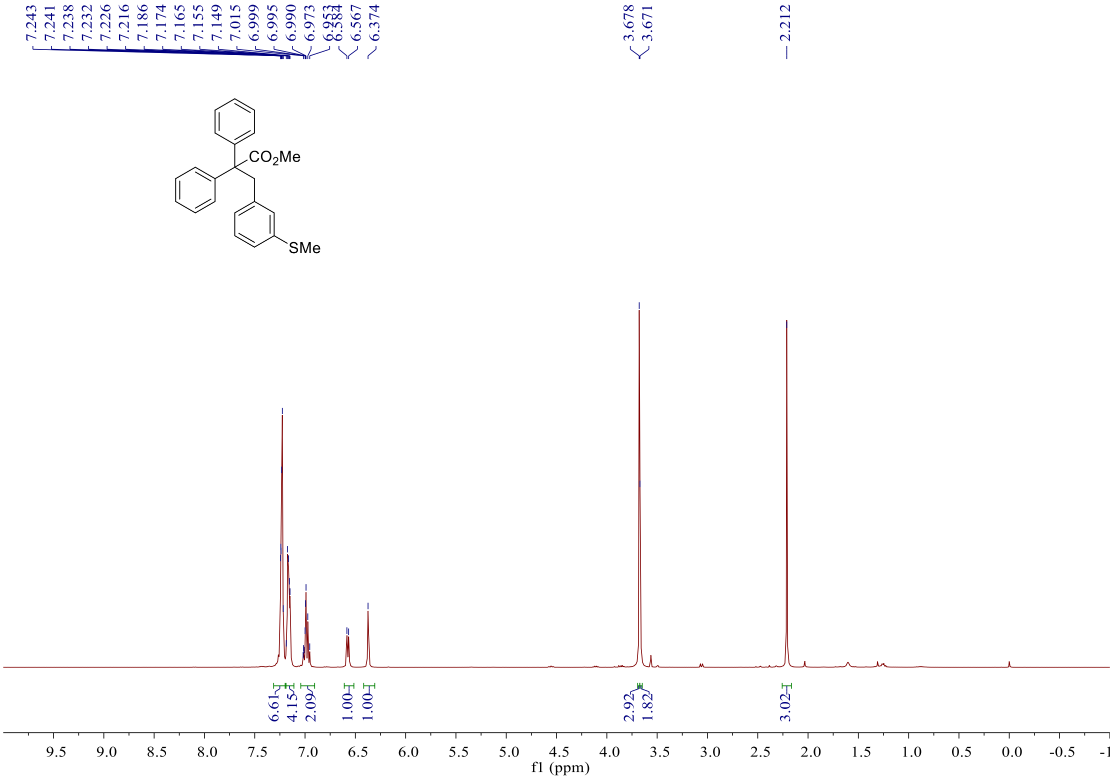

174.053
158.792
142.836
138.882
129.370
128.490
127.789
126.959
123.350
115.937
112.631
62.117
54.996
52.364
44.543
CO2Me
OMe
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

7

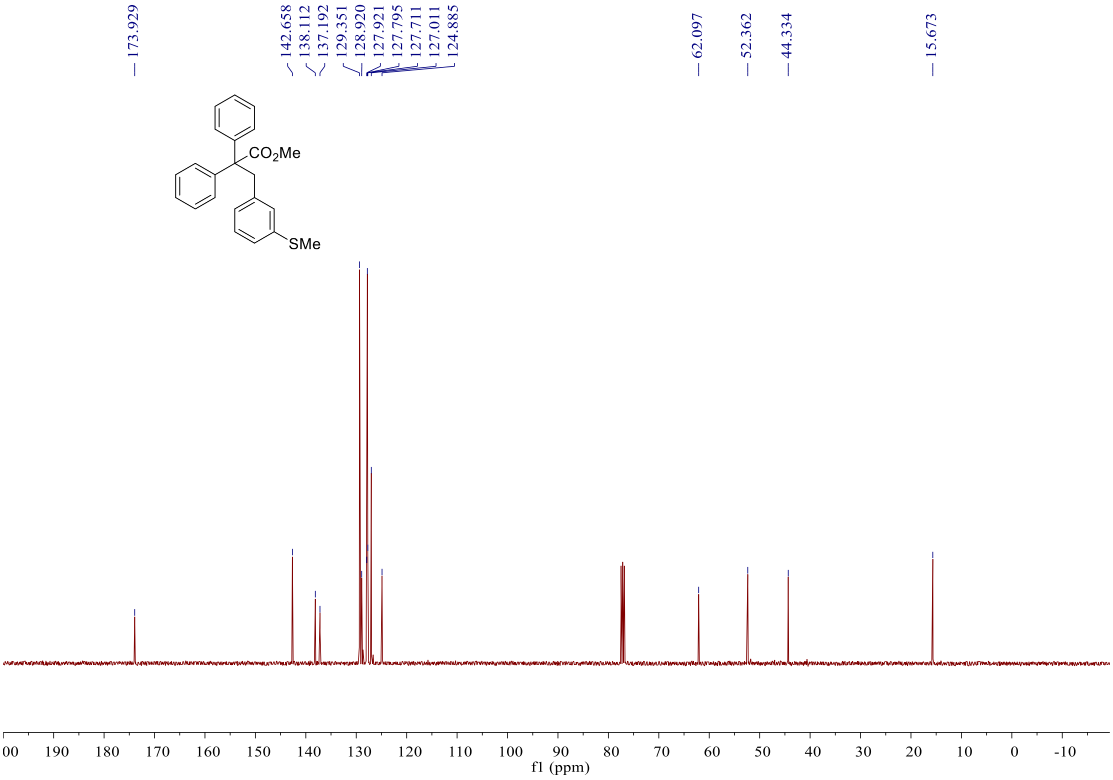

7.241
7.236
7.231
7.224
7.219
7.215
7.182
7.172
7.163
7.156
7.149
6.604
6.601
6.586
6.578
6.569
6.565
6.554
6.547
3.718
3.679
3.648
CO$_2$Me
OMe
9.90
3.91
3.00
2.84
1.82
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


174.177
158.183
142.931
131.971
129.415
129.303
127.766
126.931
112.941
62.232
55.206
52.319
43.692
CO$_2$Me
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

8

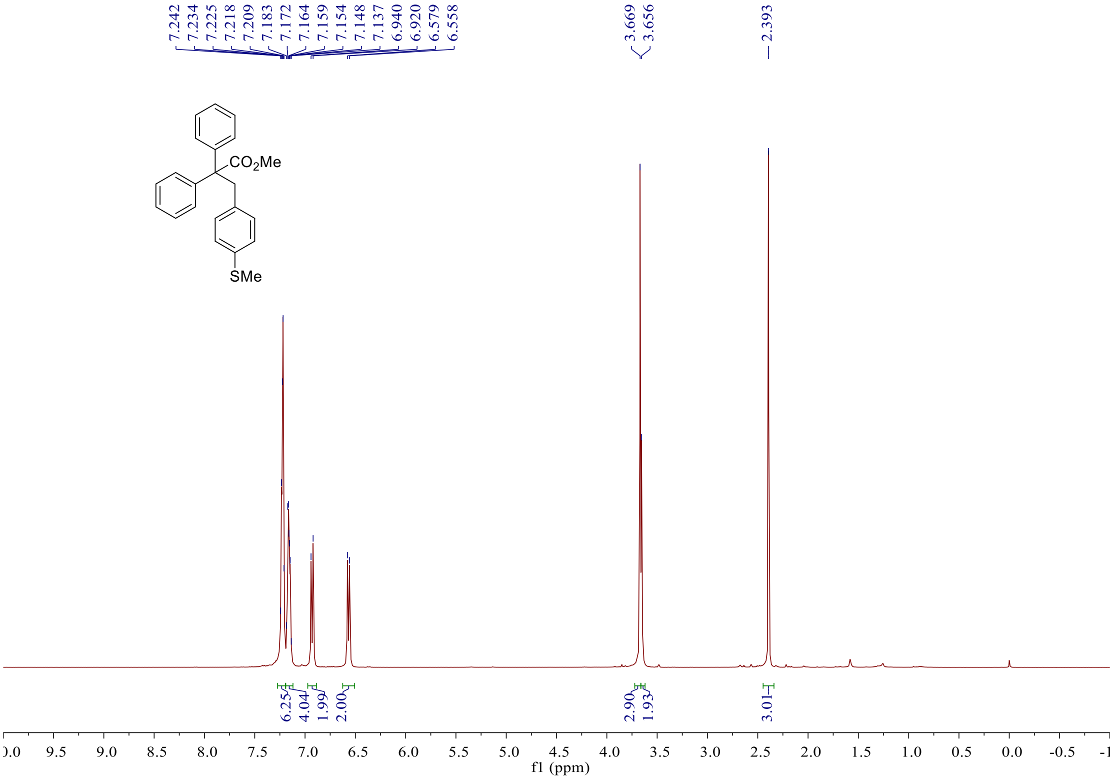


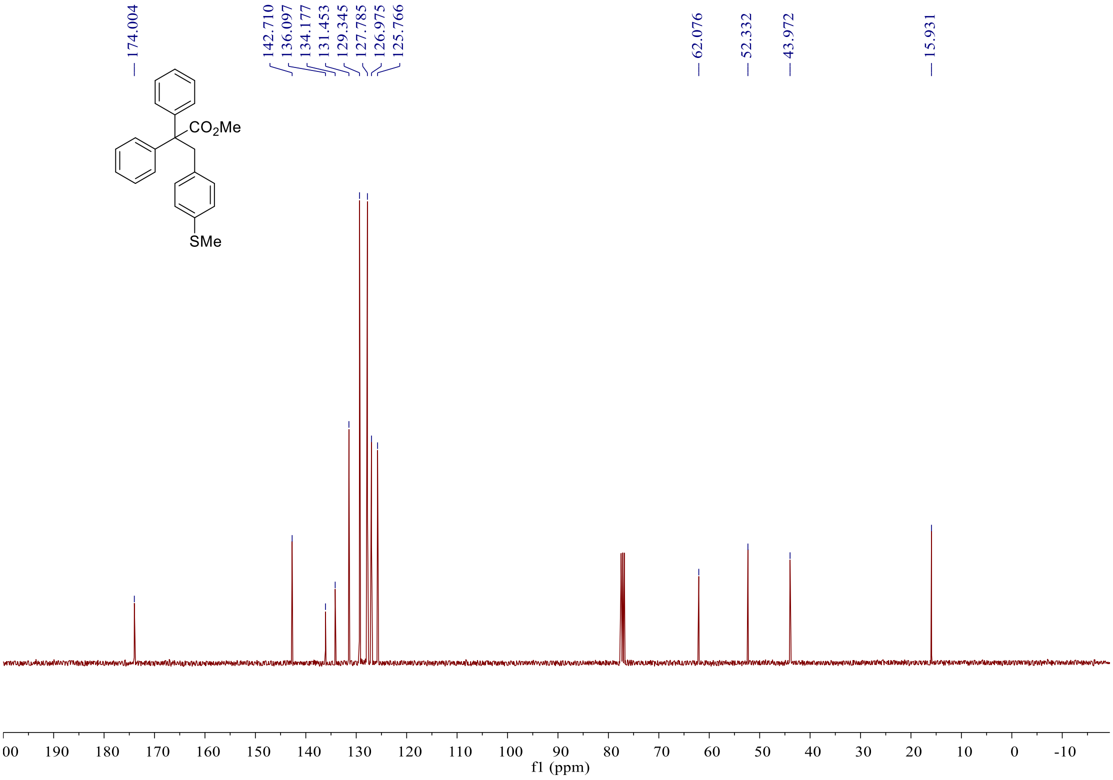
7.243
7.241
7.238
7.232
7.226
7.216
7.186
7.174
7.165
7.155
7.149
7.015
6.999
6.995
6.990
6.973
6.953
6.584
6.567
6.374
3.678
3.671
2.212
CO2Me
SMe
6.61
4.15
2.09
1.00
1.00
2.92
1.82
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)



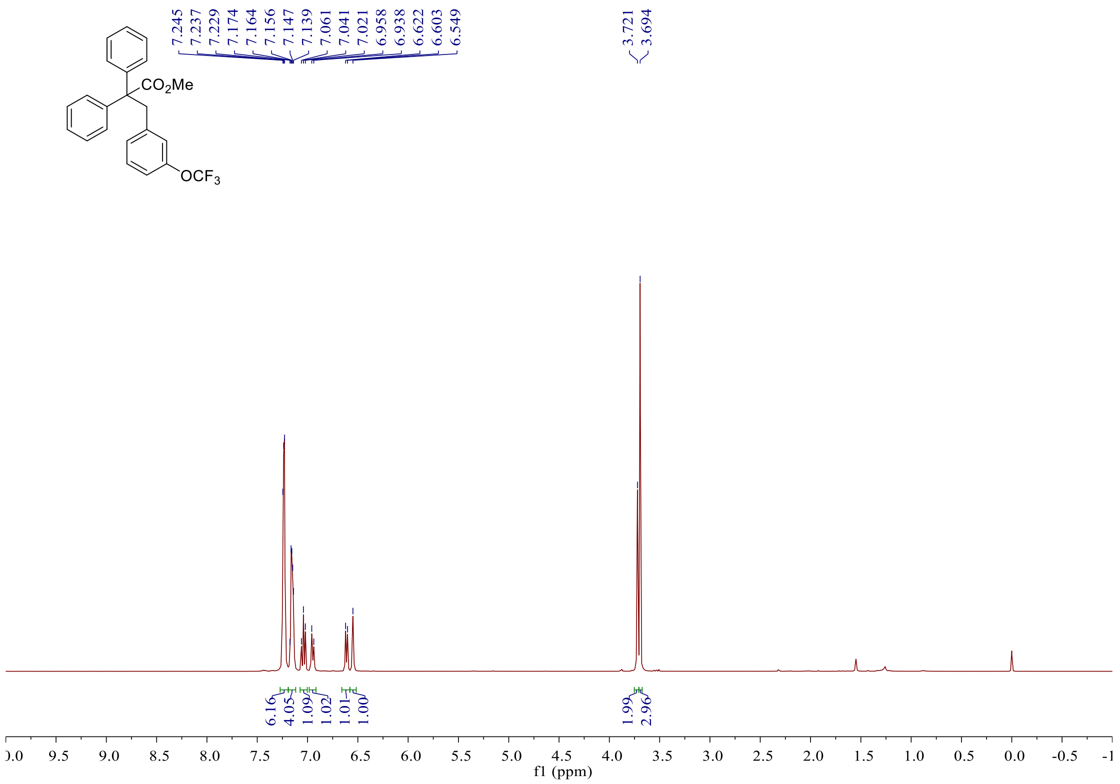
173.929
142.658
138.112
137.192
129.351
128.920
127.921
127.795
127.711
127.011
124.885
62.097
52.362
44.334
15.673
CO2Me
SMe
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

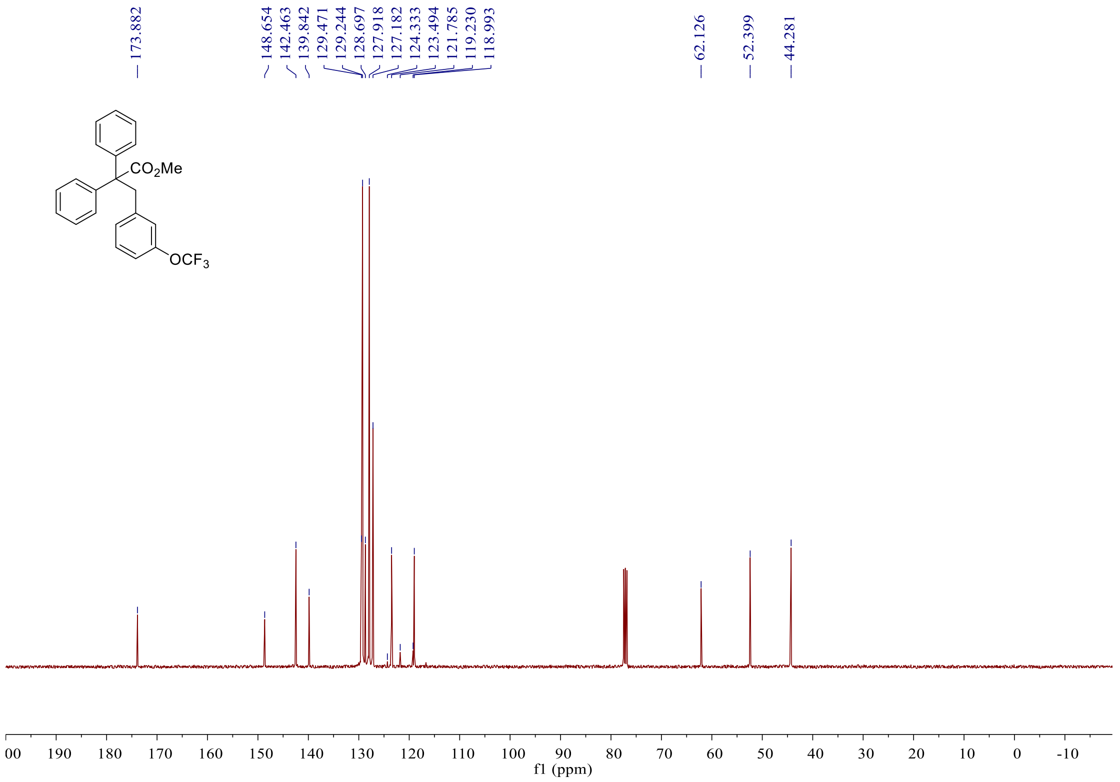
9


7.242
7.234
7.225
7.218
7.209
7.183
7.172
7.164
7.159
7.154
7.148
7.137
6.940
6.920
6.579
6.558
3.669
3.656
2.393
CO2Me
SMe
6.25
4.04
1.99
2.00
2.90
1.93
3.01
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

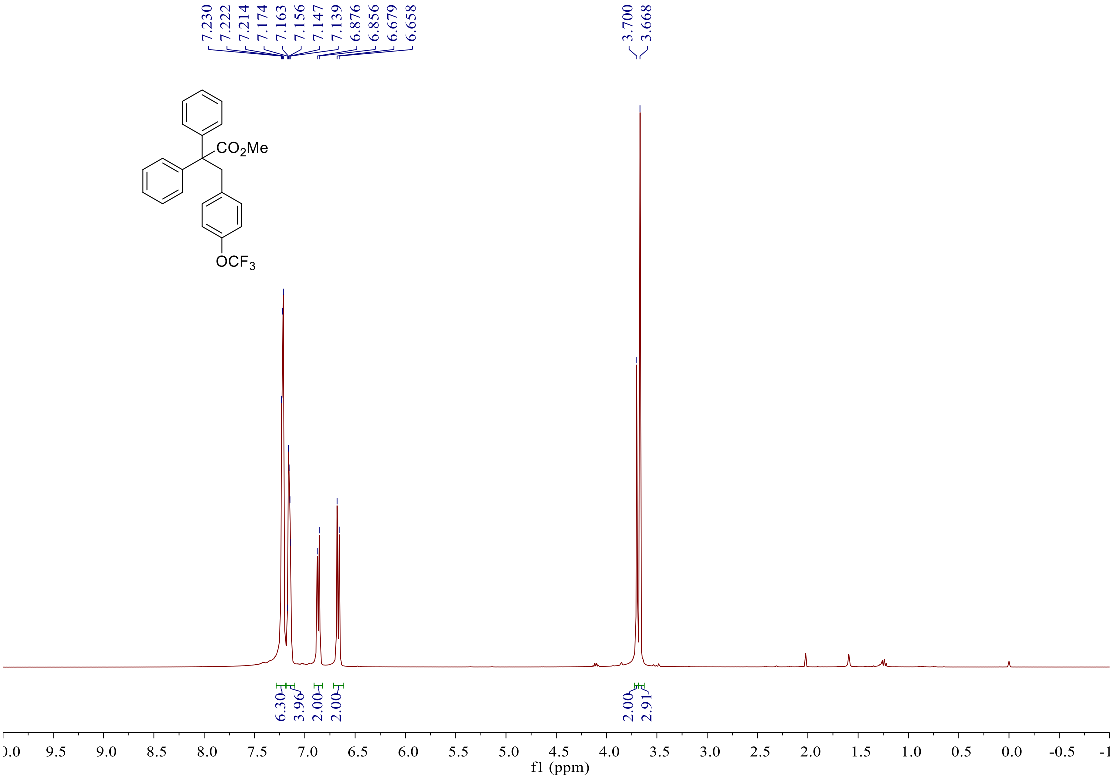

174.004
142.710
136.097
134.177
131.453
129.345
127.785
126.975
125.766
62.076
52.332
43.972
15.931
CO2Me
SMe
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

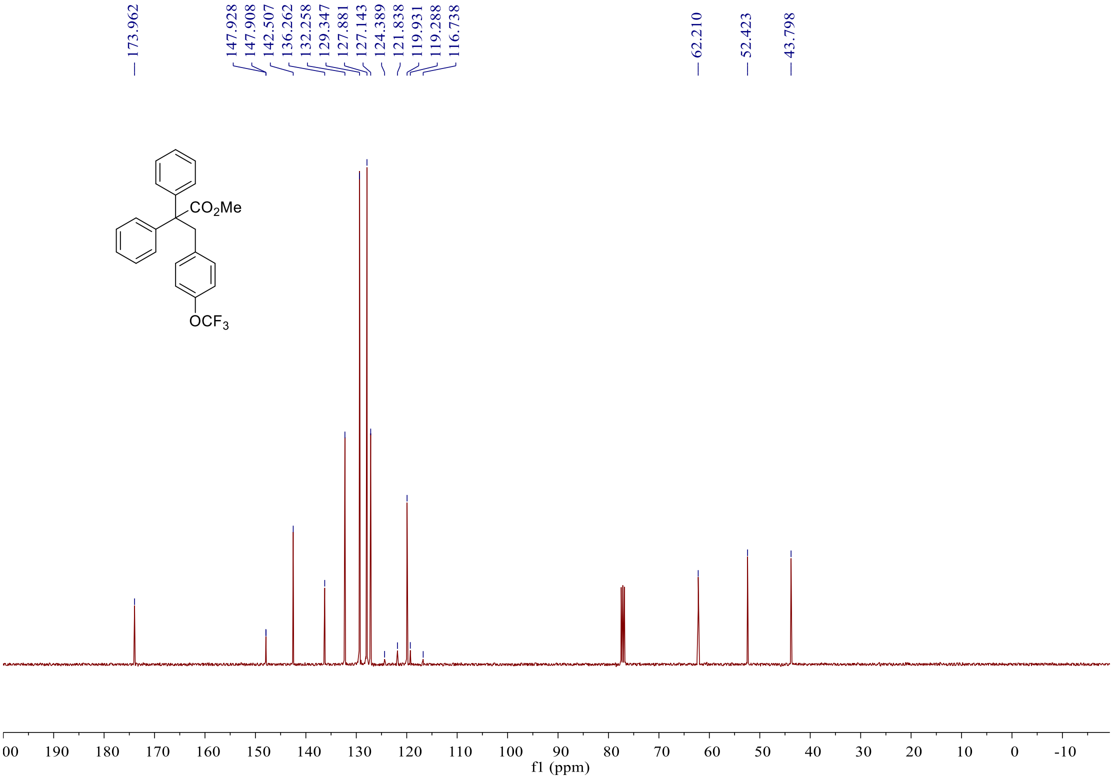
10


7.245
7.237
7.229
7.174
7.164
7.156
7.147
7.139
7.061
7.041
7.021
6.958
6.938
6.622
6.603
6.549
3.721
3.694
CO2Me
OCF3
6.16
4.05
1.09
1.02
1.01
1.00
1.99
2.96
).0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

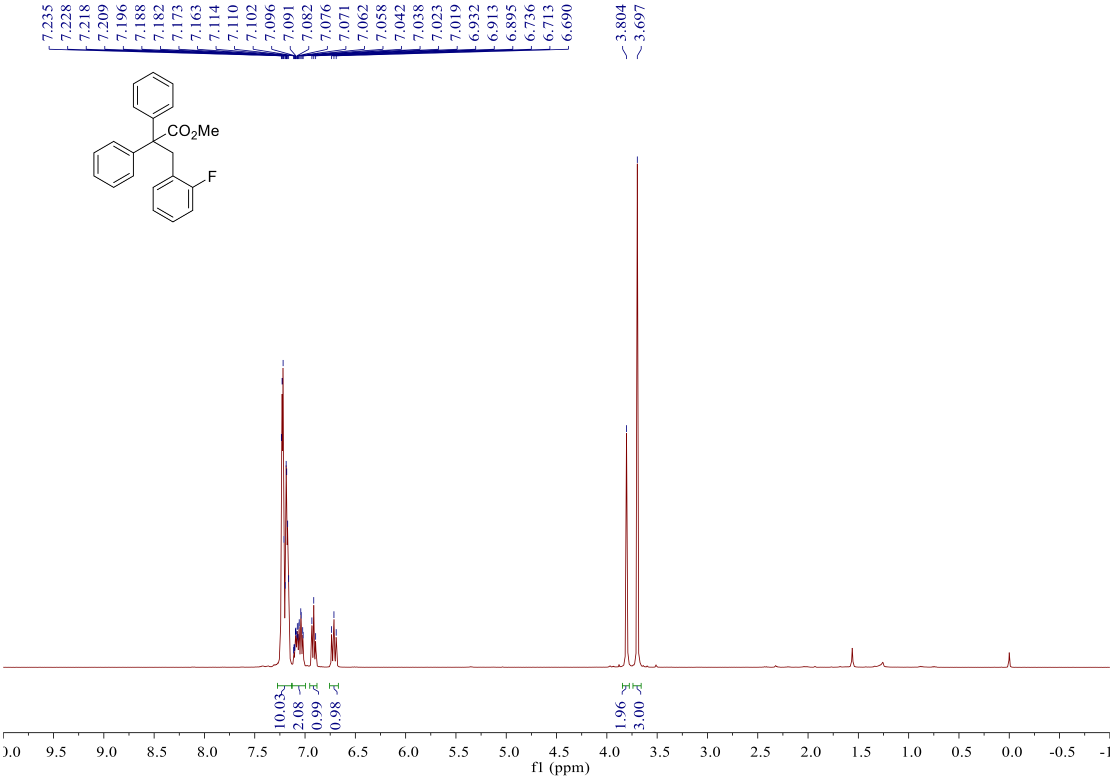

173.882
148.654
142.463
139.842
129.471
129.244
128.697
127.918
127.182
124.333
123.494
121.785
119.230
118.993
62.126
52.399
44.281
CO2Me
OCF3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

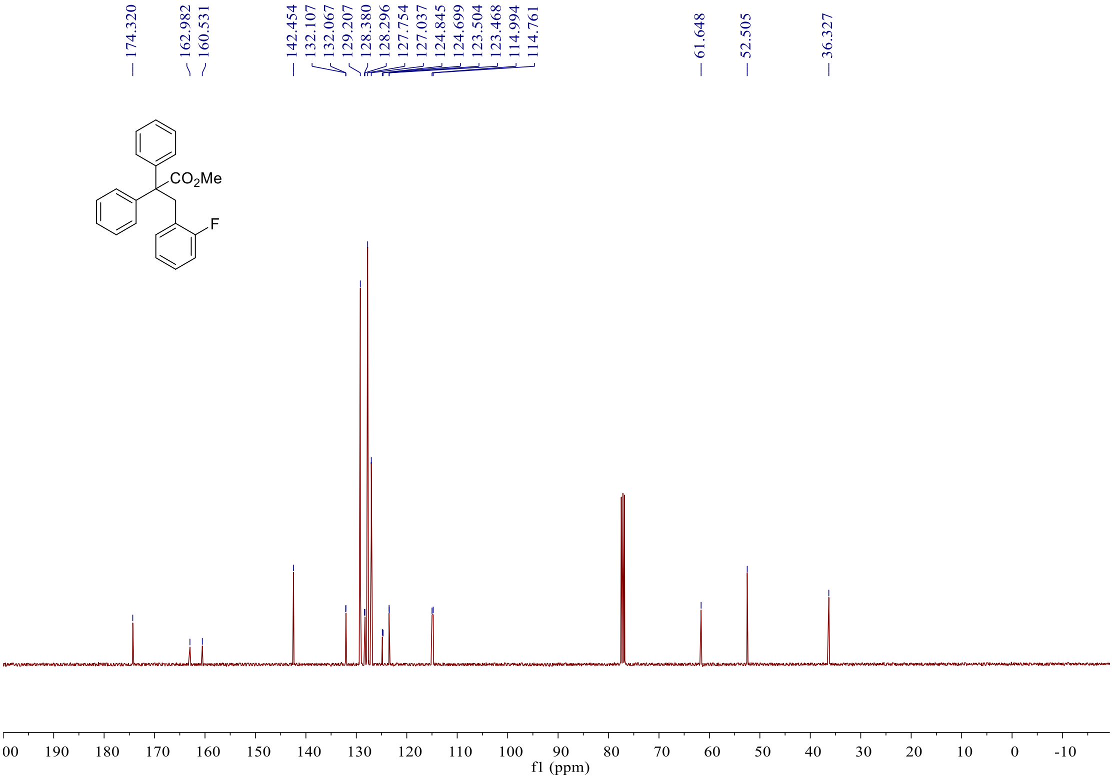
11


7.230
7.222
7.214
7.174
7.163
7.156
7.147
7.139
6.876
6.856
6.679
6.658
3.700
3.668
CO2Me
OCF3
6.30
3.96
2.00
2.00
2.00
2.91
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

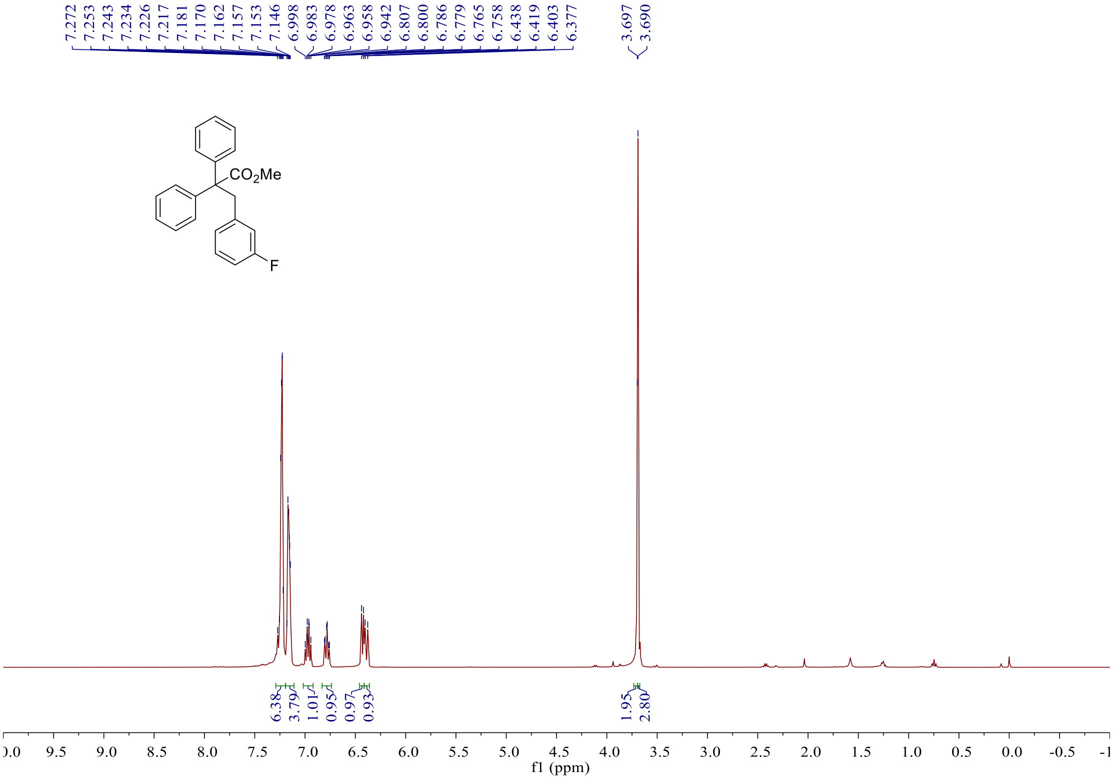

173.962
147.928
147.908
142.507
136.262
132.258
129.347
127.881
127.143
124.389
121.838
119.931
119.288
116.738
62.210
52.423
43.798
CO2Me
OCF3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

12

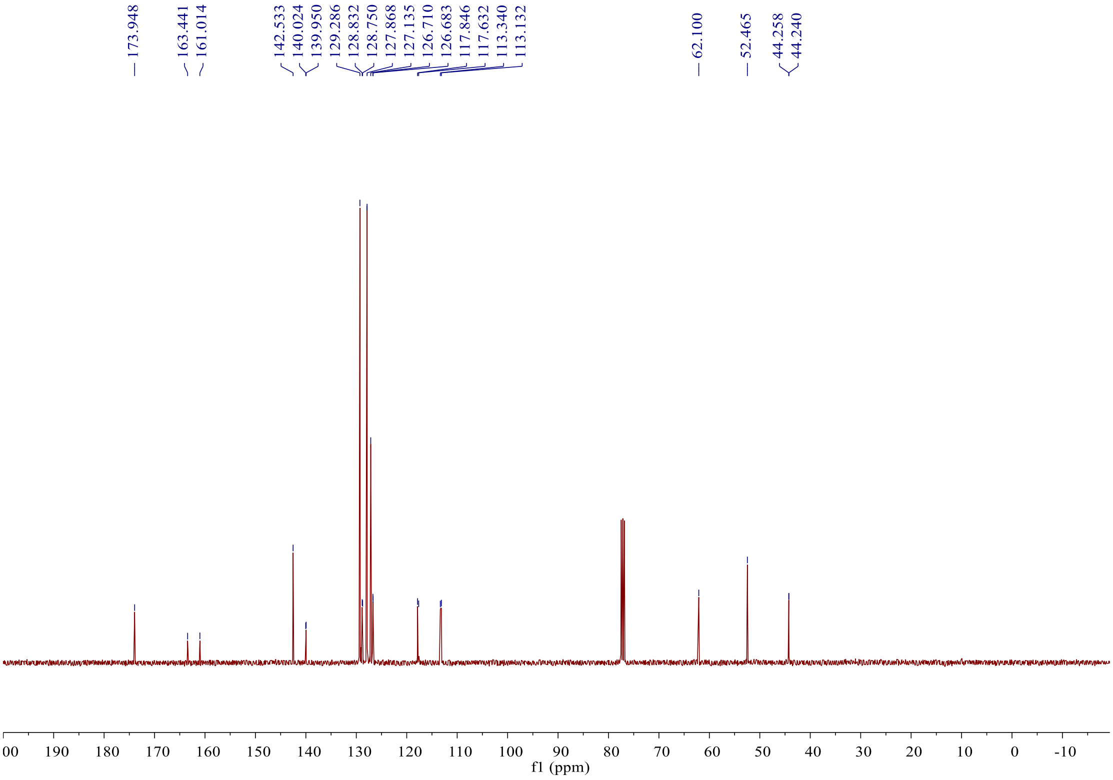

7.235
7.228
7.218
7.209
7.196
7.188
7.182
7.173
7.163
7.114
7.110
7.102
7.096
7.091
7.082
7.076
7.071
7.062
7.058
7.042
7.038
7.023
7.019
6.932
6.913
6.895
6.736
6.713
6.690
3.804
3.697
CO2Me
F
10.03
2.08
0.99
0.98
1.96
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


174.320
162.982
160.531
142.454
132.107
132.067
129.207
128.380
128.296
127.754
127.037
124.845
124.699
123.504
123.468
114.994
114.761
61.648
52.505
36.327
CO2Me
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

13

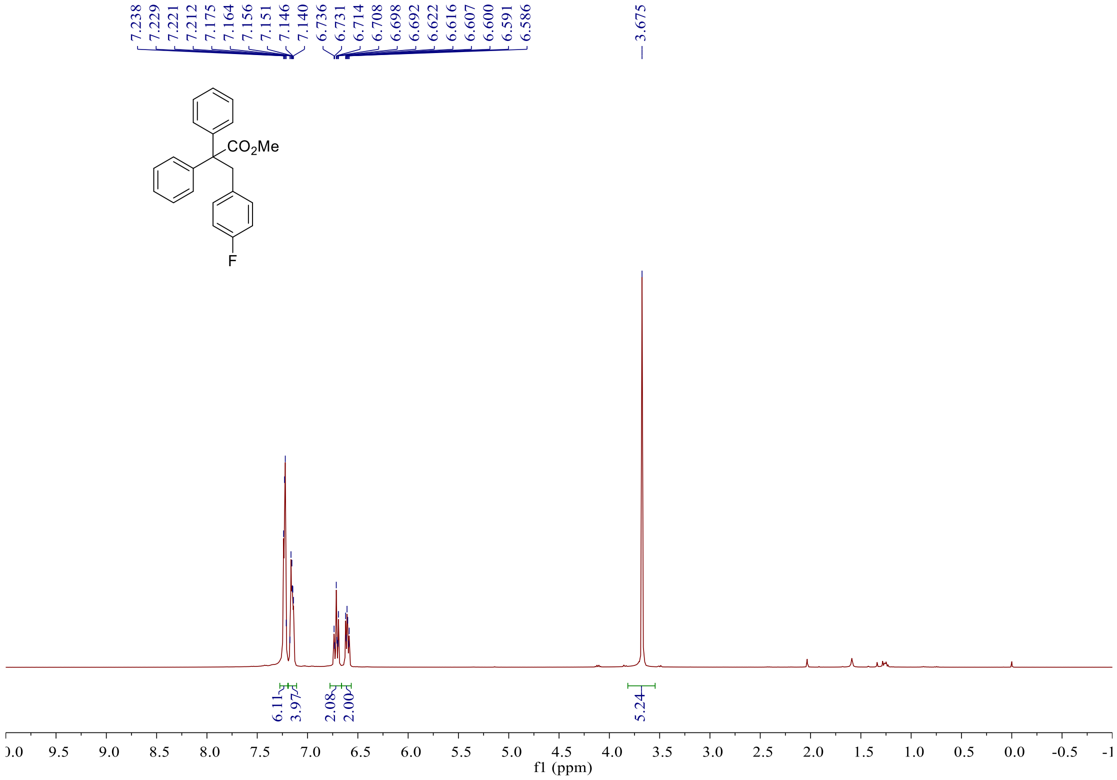


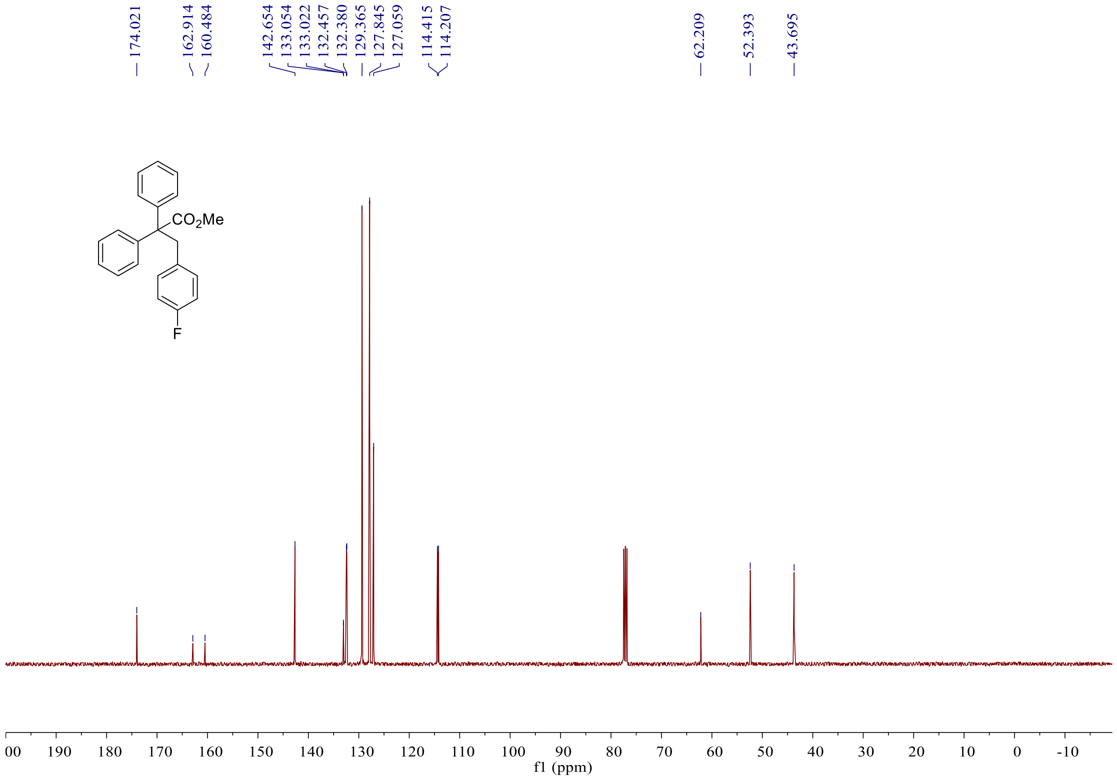
7.272
7.253
7.243
7.234
7.226
7.217
7.181
7.170
7.162
7.157
7.153
7.146
6.998
6.983
6.978
6.963
6.958
6.942
6.807
6.800
6.786
6.779
6.765
6.758
6.438
6.419
6.403
6.377
3.697
3.690
CO2Me
F
6.38
3.79
1.01
0.95
0.97
0.93
1.95
2.80
f1 (ppm)



173.948
163.441
161.014
142.533
140.024
139.950
129.286
128.832
128.750
127.868
127.135
126.710
126.683
117.846
117.632
113.340
113.132
62.100
52.465
44.258
44.240
f1 (ppm)

14


7.238
7.229
7.221
7.212
7.175
7.164
7.156
7.151
7.146
7.140
6.736
6.731
6.714
6.708
6.698
6.692
6.622
6.616
6.607
6.600
6.591
6.586
3.675
CO2Me
F
6.11
3.97
2.08
2.00
5.24
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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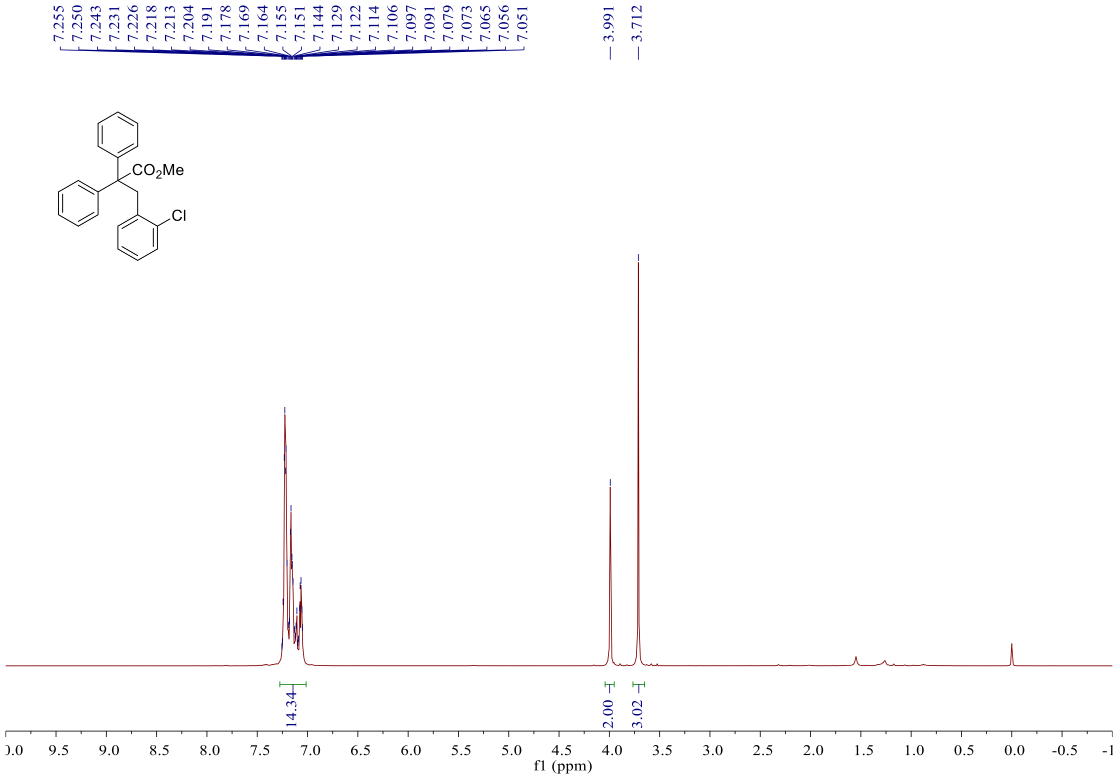
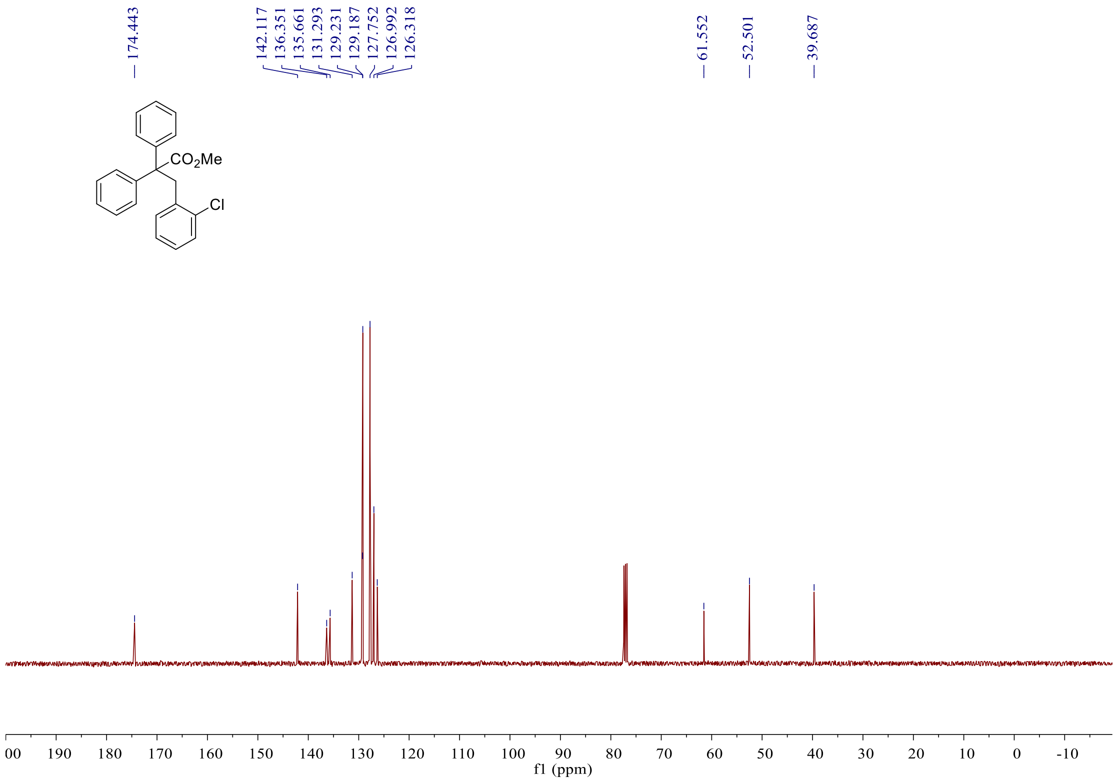
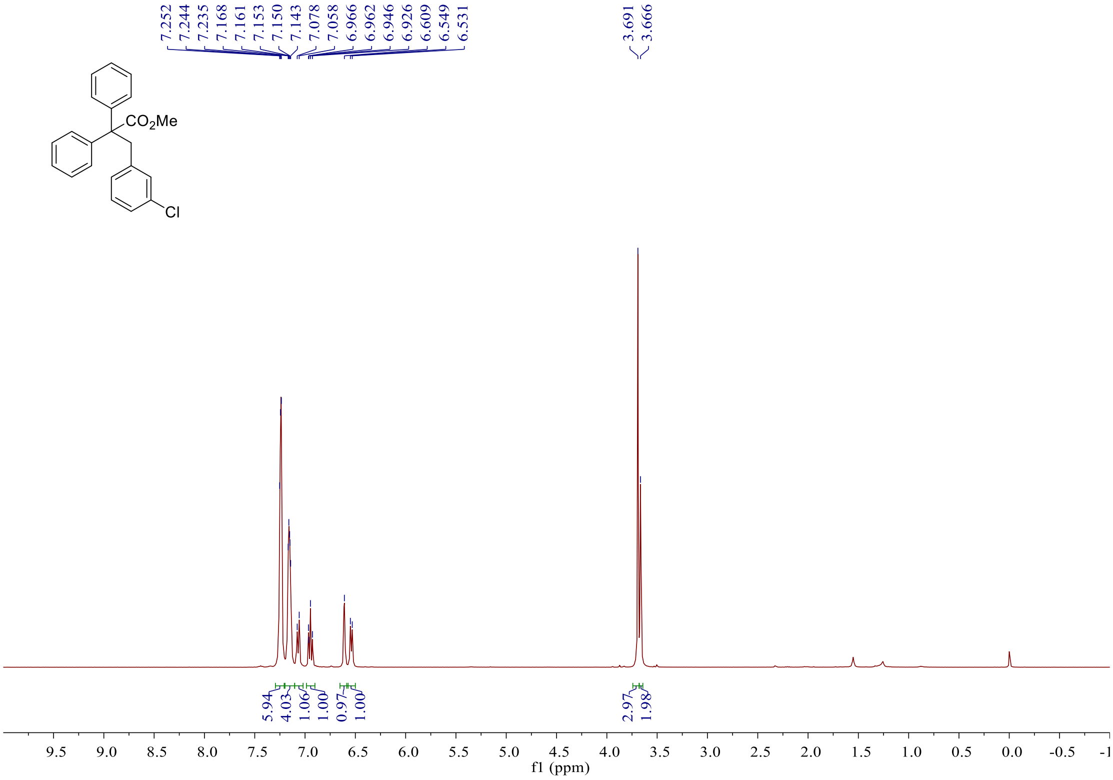
162.914
160.484
142.654
133.054
133.022
132.457
132.380
129.365
127.845
127.059
114.415
114.207
62.209
52.393
43.695
CO2Me
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

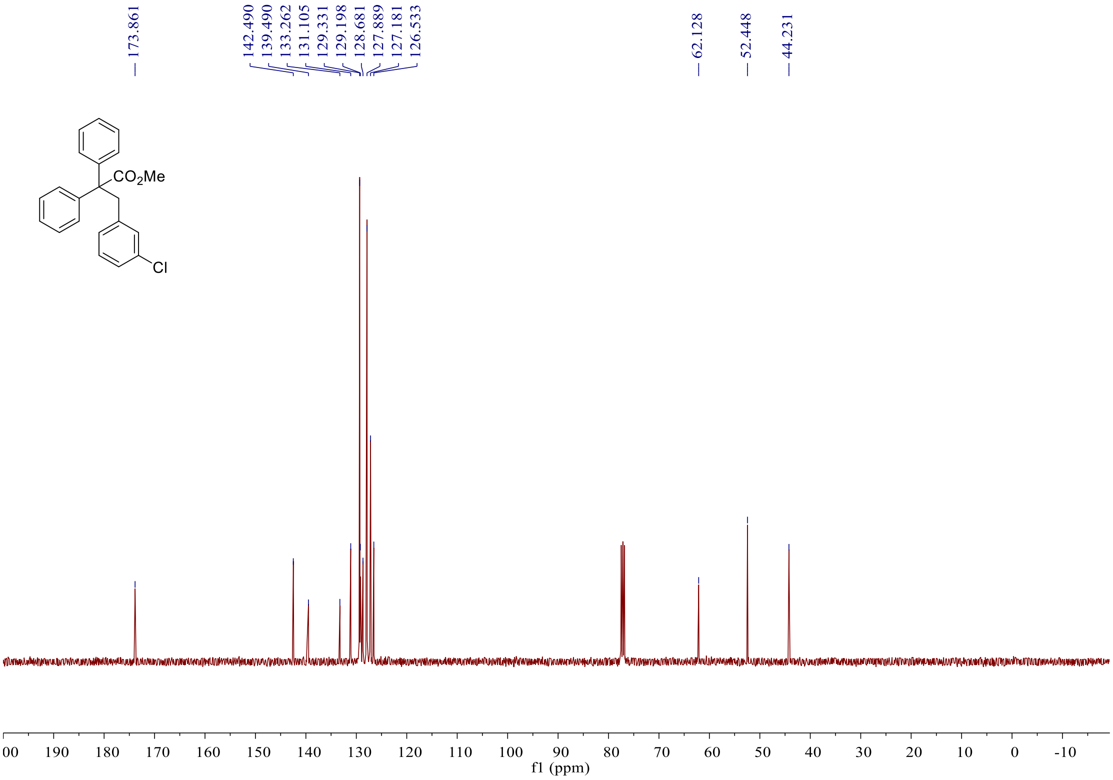
15


7.255
7.250
7.243
7.231
7.226
7.218
7.213
7.204
7.191
7.178
7.169
7.164
7.155
7.151
7.144
7.129
7.122
7.114
7.106
7.097
7.091
7.079
7.073
7.065
7.056
7.051
3.991
3.712
CO2Me
Cl
14.34
2.00
3.02
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

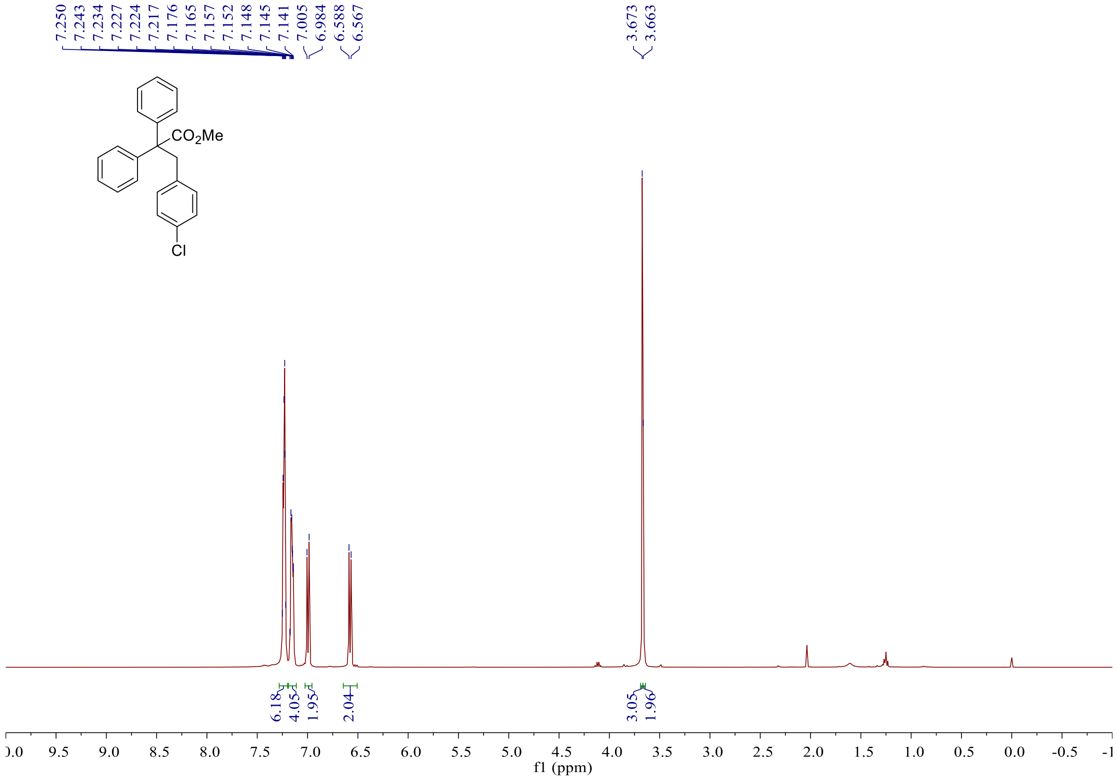

174.443
142.117
136.351
135.661
131.293
129.231
129.187
127.752
126.992
126.318
61.552
52.501
39.687
CO2Me
Cl
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

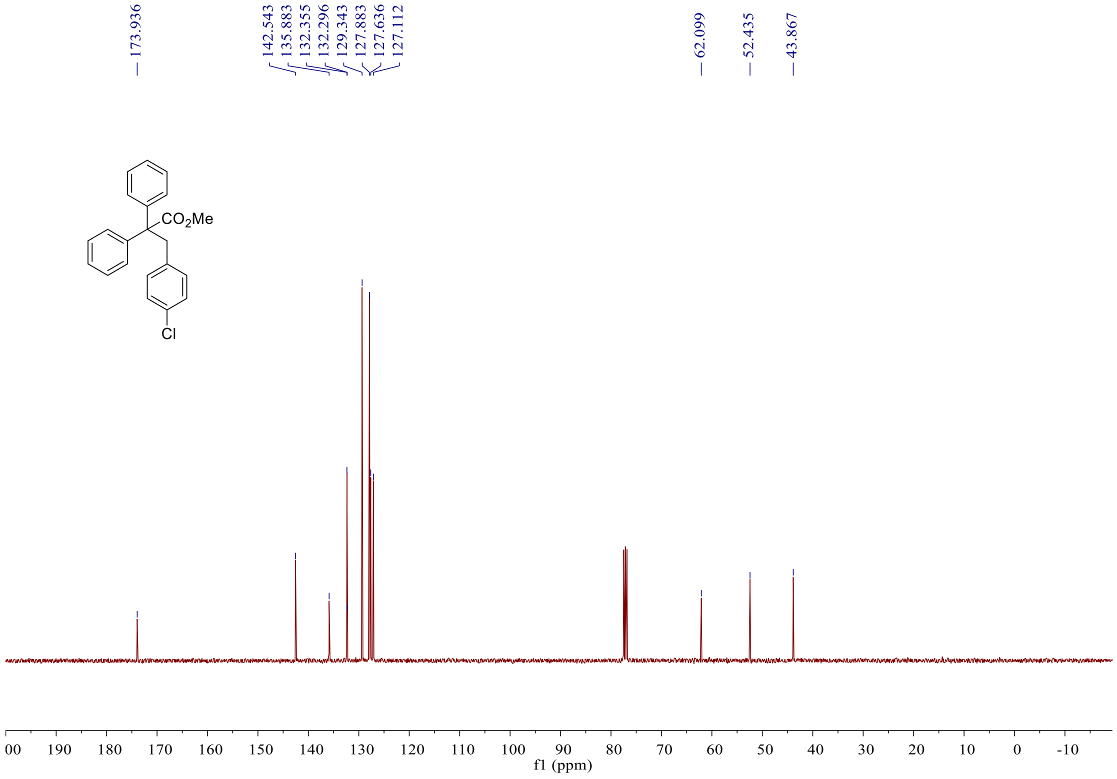
16


7.252
7.244
7.235
7.168
7.161
7.153
7.150
7.143
7.078
7.058
6.966
6.962
6.946
6.926
6.609
6.549
6.531
3.691
3.666
CO$_2$Me
Cl
5.94
4.03
1.06
1.00
0.97
1.00
2.97
1.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

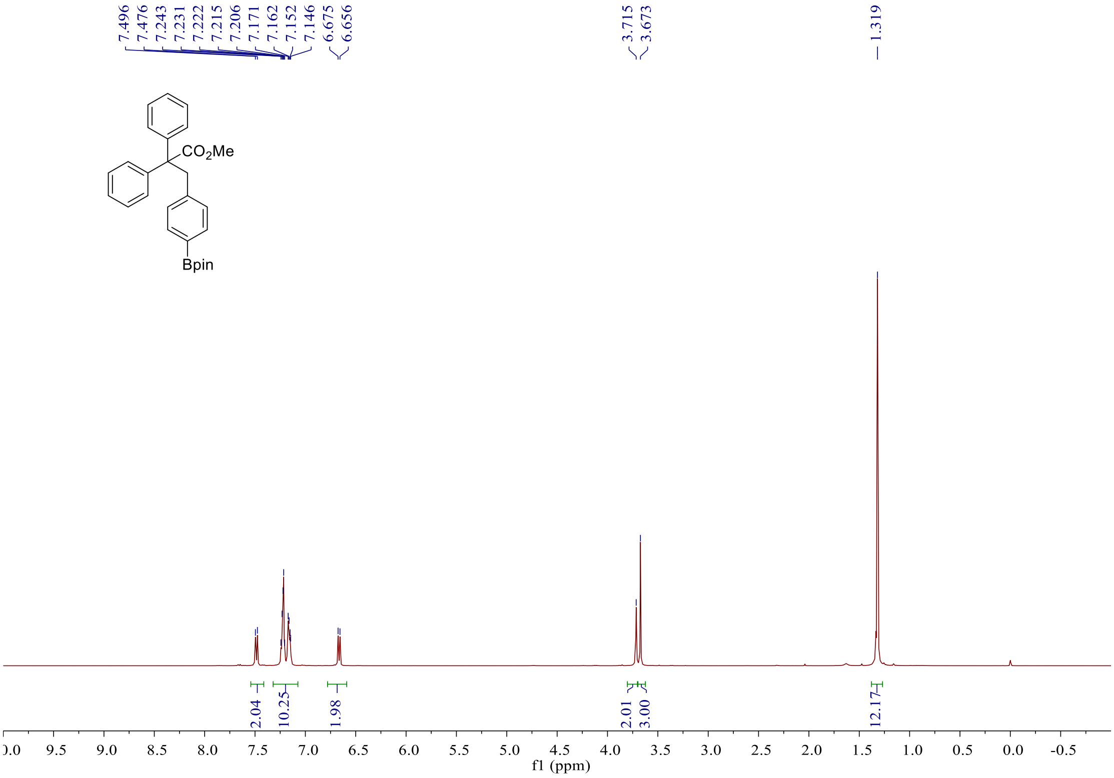

173.861
142.490
139.490
133.262
131.105
129.331
129.198
128.681
127.889
127.181
126.533
62.128
52.448
44.231
CO$_2$Me
Cl
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

17


7.250
7.243
7.234
7.227
7.224
7.217
7.176
7.165
7.157
7.152
7.148
7.145
7.141
7.005
6.984
6.588
6.567
3.673
3.663
CO2Me
Cl
6.18
4.05
1.95
2.04
3.05
1.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


173.936
142.543
135.883
132.355
132.296
129.343
127.883
127.636
127.112
62.099
52.435
43.867
CO2Me
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

18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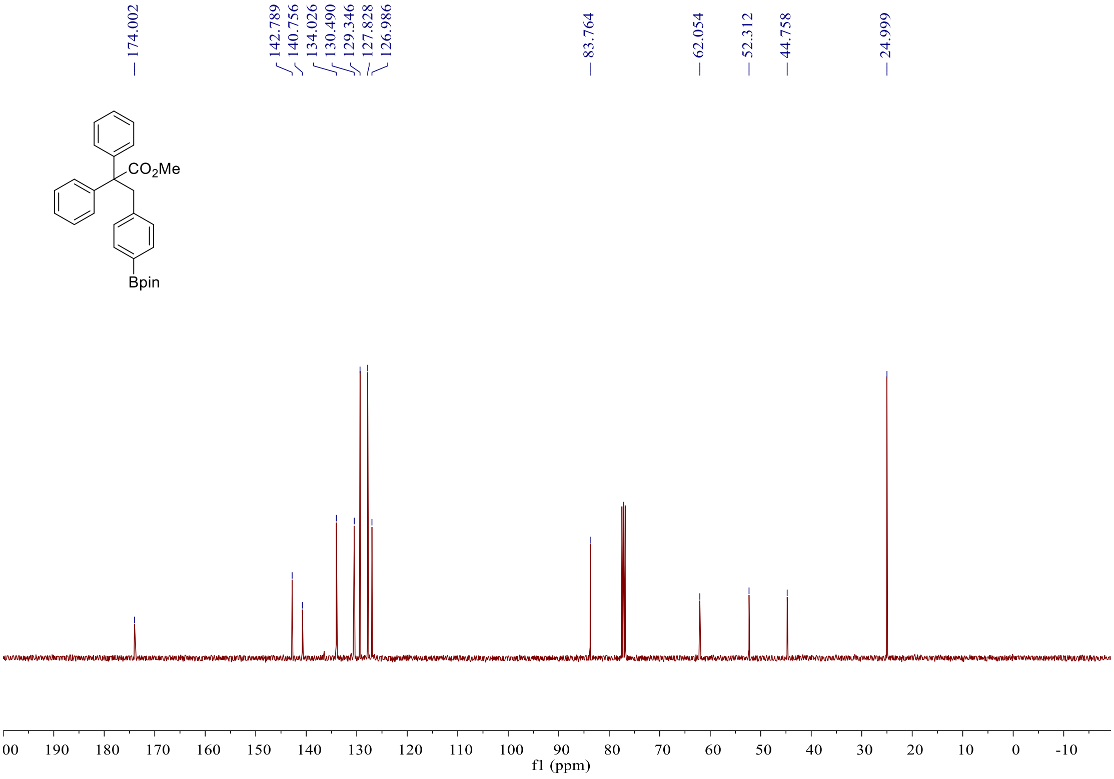
7.476
7.243
7.231
7.222
7.215
7.206
7.171
7.162
7.152
7.146
6.675
6.656
3.715
3.673
1.319
CO2Me
Bpin
2.04
10.25
1.98
2.01
3.00
12.17
).0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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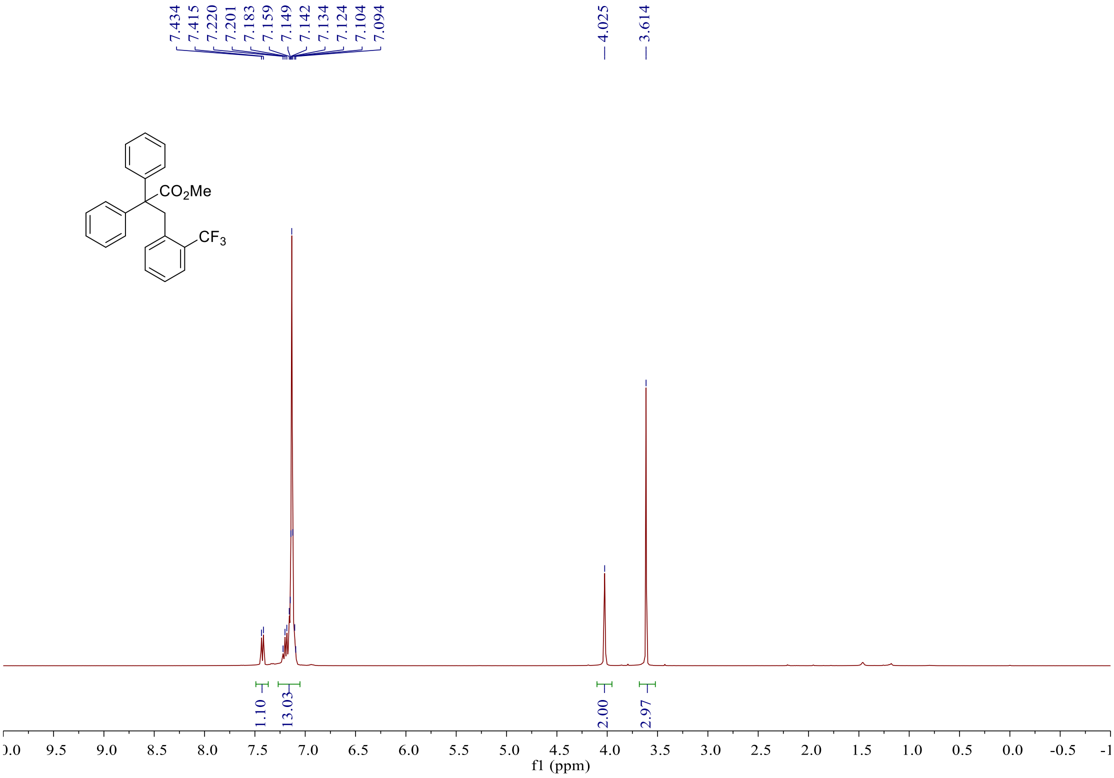
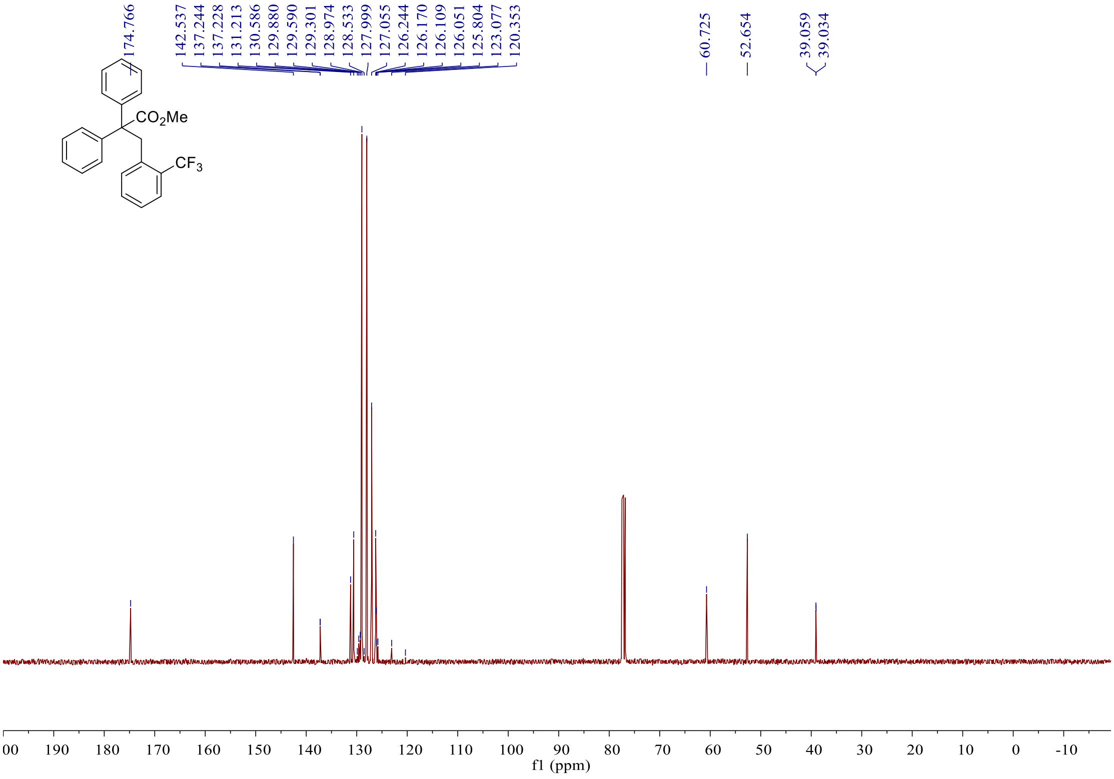
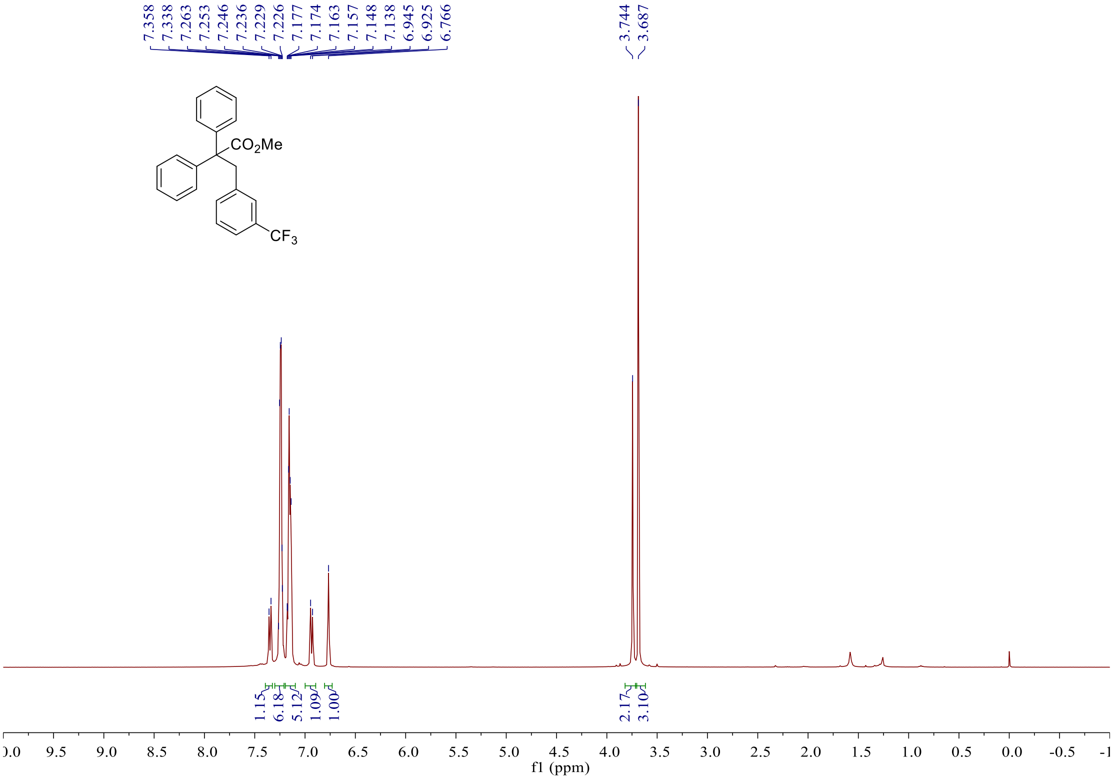
142.789
140.756
134.026
130.490
129.346
127.828
126.986
83.764
62.054
52.312
44.758
24.999
CO2Me
Bpin
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

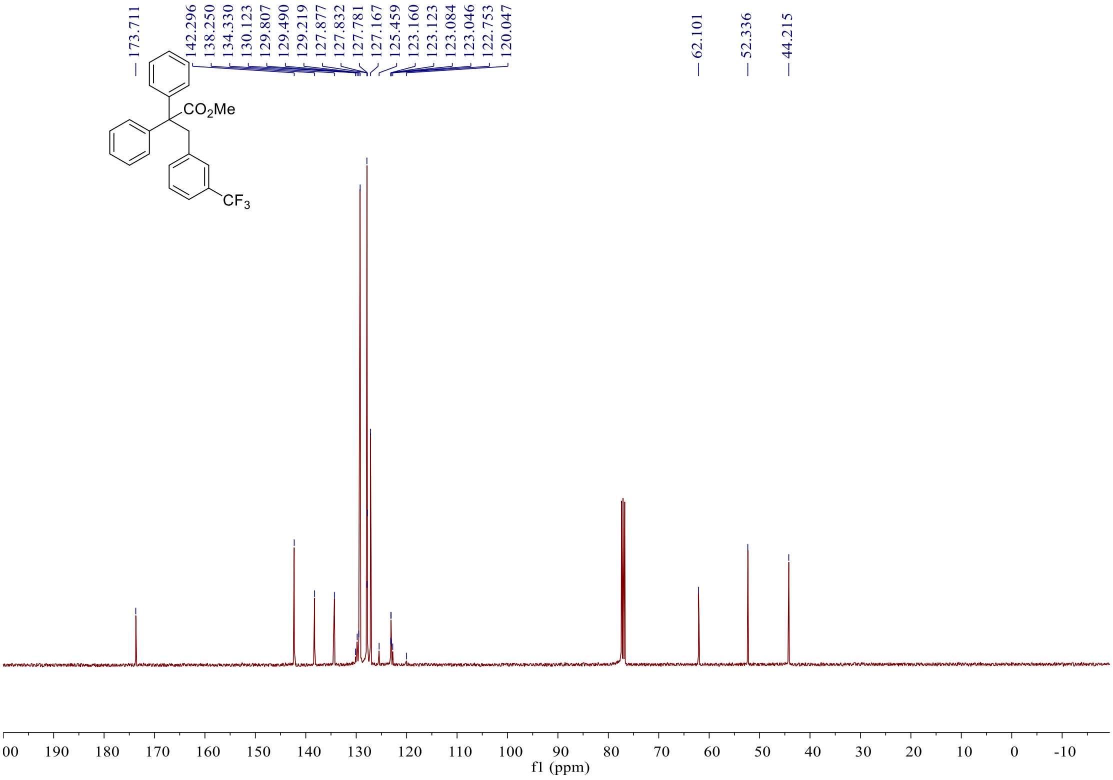
19


7.434
7.415
7.220
7.201
7.183
7.159
7.149
7.142
7.134
7.124
7.104
7.094
4.025
3.614
CO$_2$Me
CF$_3$
1.10
13.03
2.00
2.97
f1 (ppm)


174.766
142.537
137.244
137.228
131.213
130.586
129.880
129.590
129.301
128.974
128.533
127.999
127.055
126.244
126.170
126.109
126.051
125.804
123.077
120.353
60.725
52.654
39.059
39.034
CO$_2$Me
CF$_3$
f1 (ppm)

20


7.358
7.338
7.263
7.253
7.246
7.236
7.229
7.226
7.177
7.174
7.163
7.157
7.148
7.138
6.945
6.925
6.766
3.744
3.687
CO2Me
CF3
1.15
6.18
5.12
1.09
1.00
2.17
3.10
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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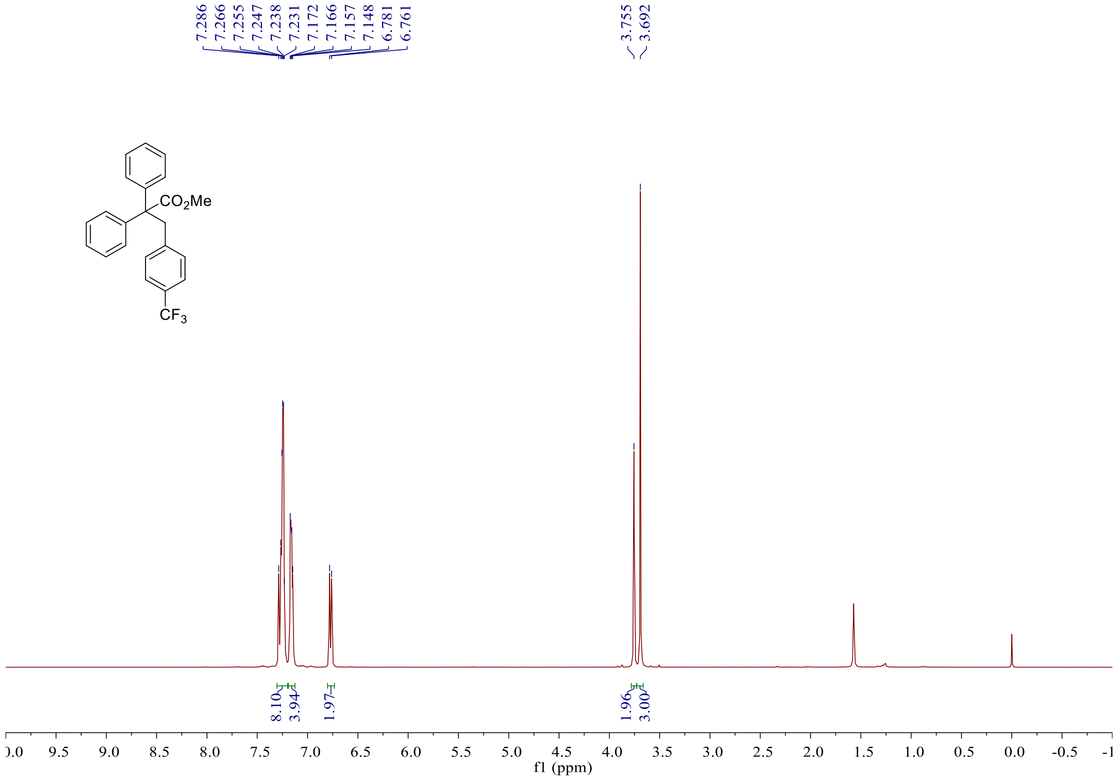
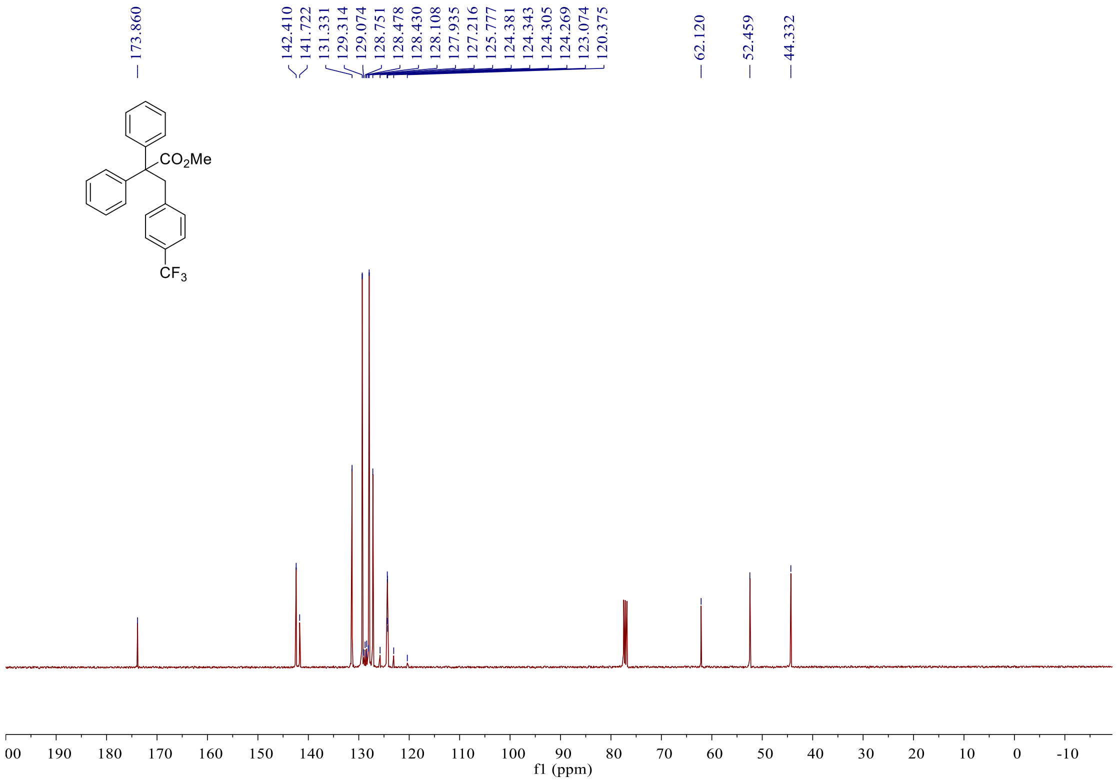
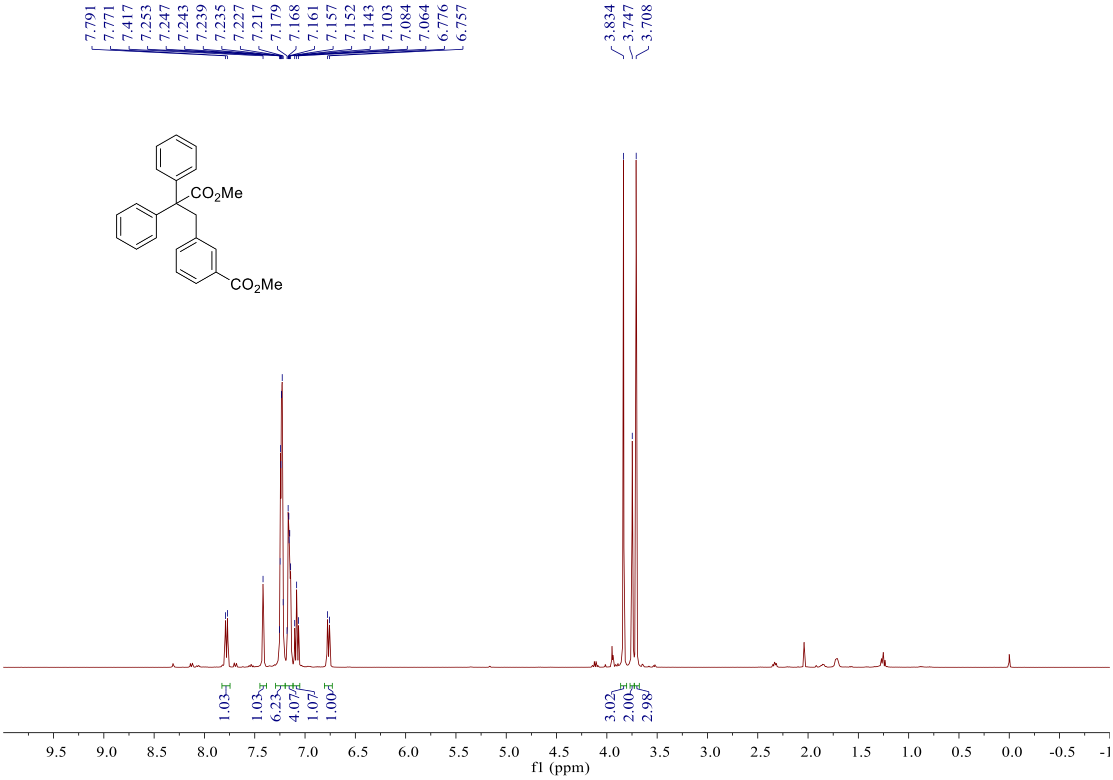
142.296
138.250
134.330
130.123
129.807
129.490
129.219
127.877
127.832
127.781
127.167
125.459
123.160
123.123
123.084
123.046
122.753
120.047
62.101
52.336
44.215
CO2Me
CF3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

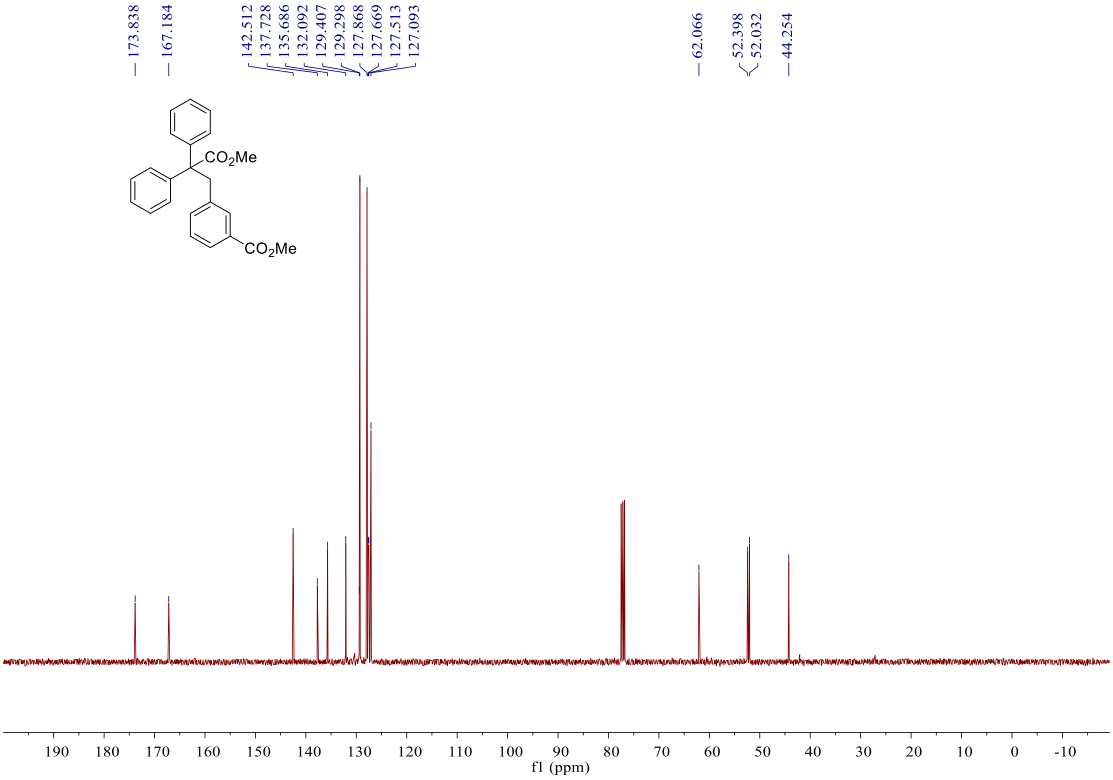
21


7.286
7.266
7.255
7.247
7.238
7.231
7.172
7.166
7.157
7.148
6.781
6.761
3.755
3.692
CO_2Me
CF_3
8.10
3.94
1.97
1.96
3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

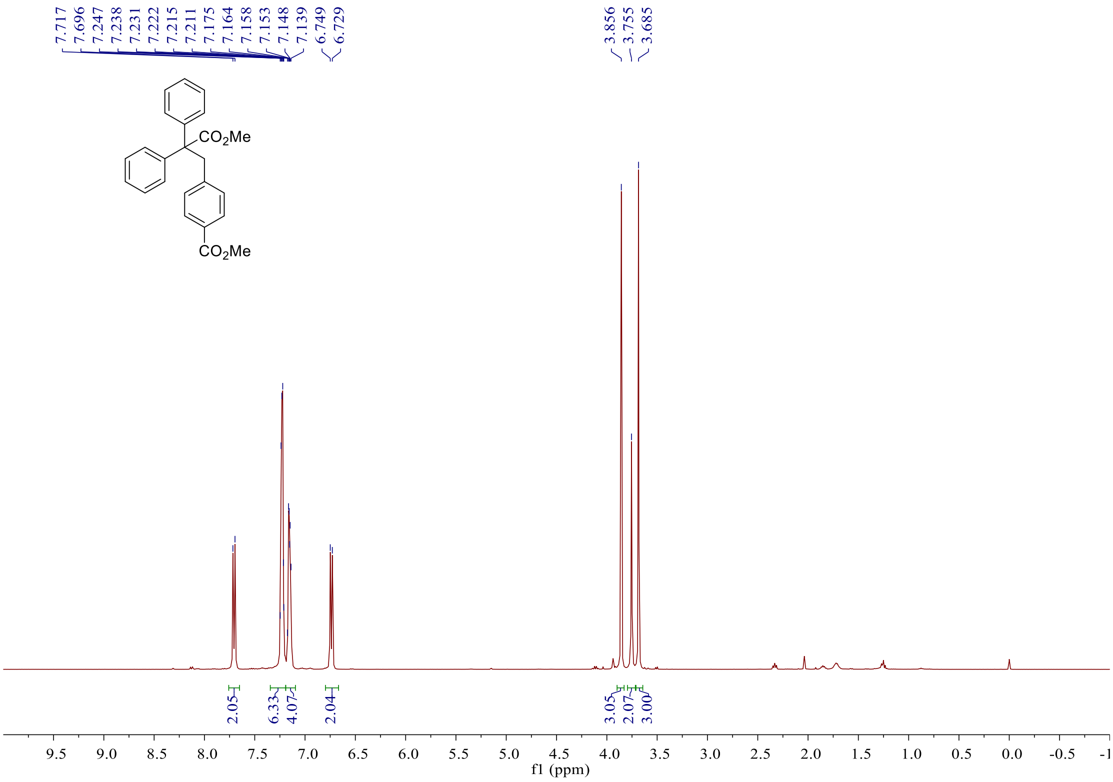

173.860
142.410
141.722
131.331
129.314
129.074
128.751
128.478
128.430
128.108
127.935
127.216
125.777
124.381
124.343
124.305
124.269
123.074
120.375
62.120
52.459
44.332
CO_2Me
CF_3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

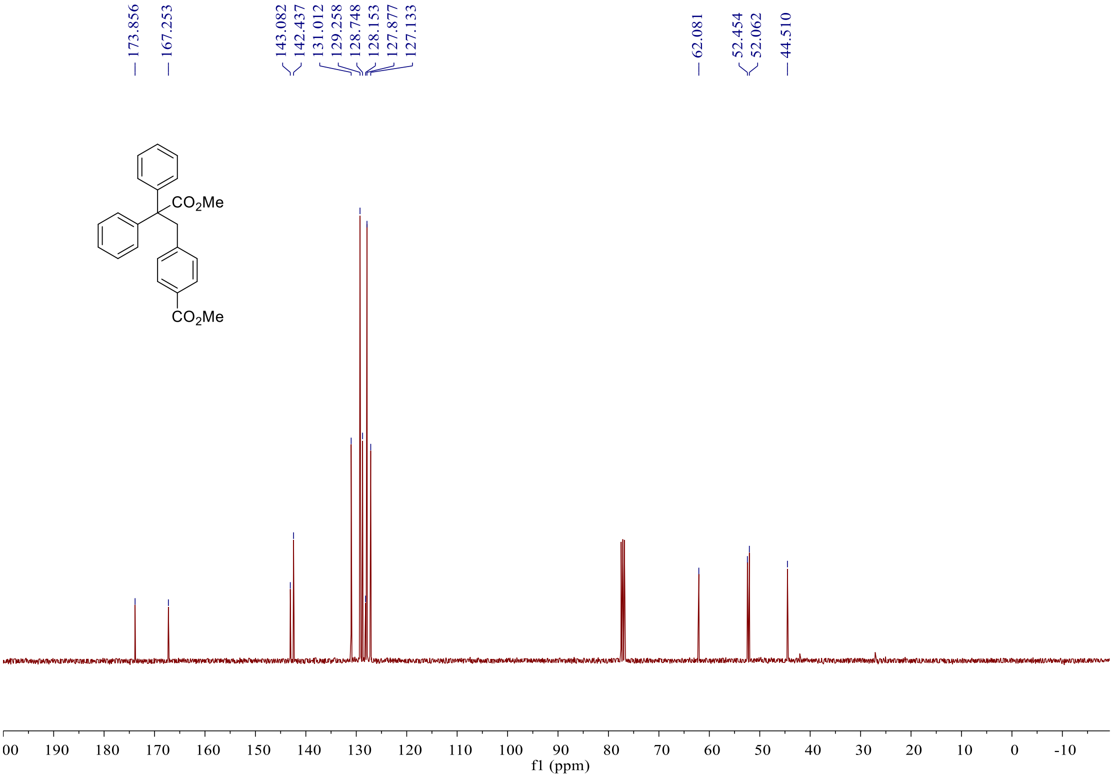
22


7.791
7.771
7.417
7.253
7.247
7.243
7.239
7.235
7.227
7.217
7.179
7.168
7.161
7.157
7.152
7.143
7.103
7.084
7.064
6.776
6.757
3.834
3.747
3.708
CO$_2$Me
CO$_2$Me
1.03
1.03
6.23
4.07
1.07
1.00
3.02
2.00
2.98
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

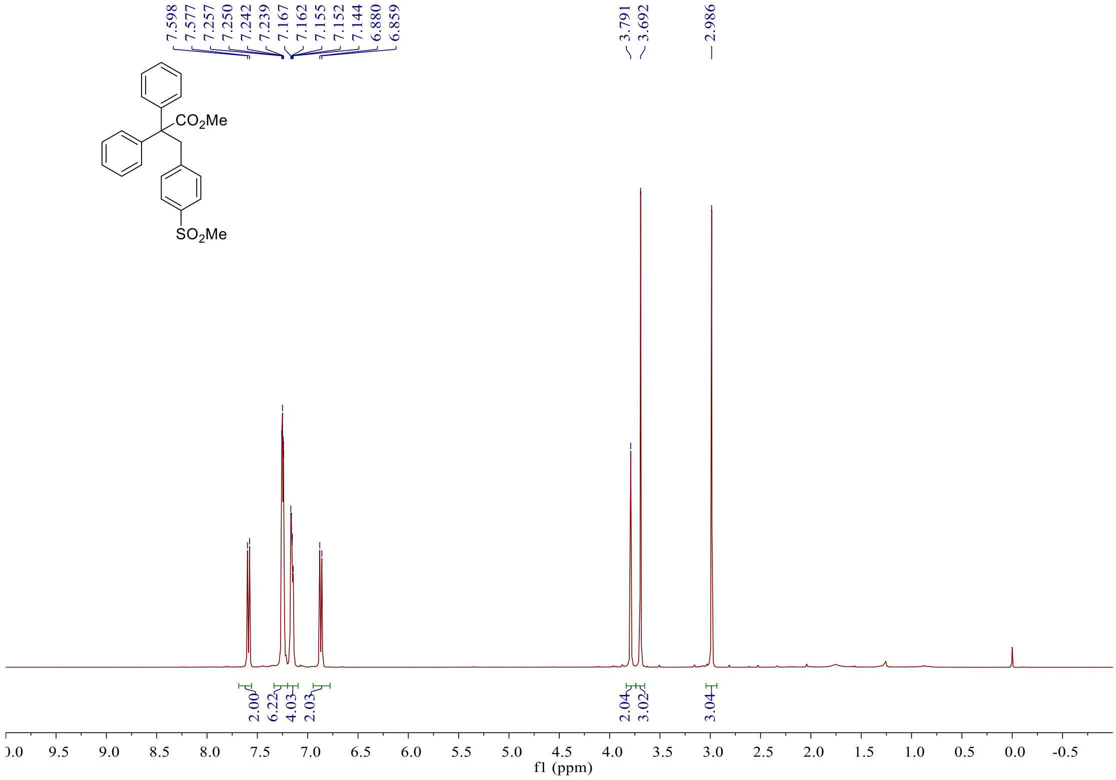

173.838
167.184
142.512
137.728
135.686
132.092
129.407
129.298
127.868
127.669
127.513
127.093
62.066
52.398
52.032
44.254
CO$_2$Me
CO$_2$Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

23

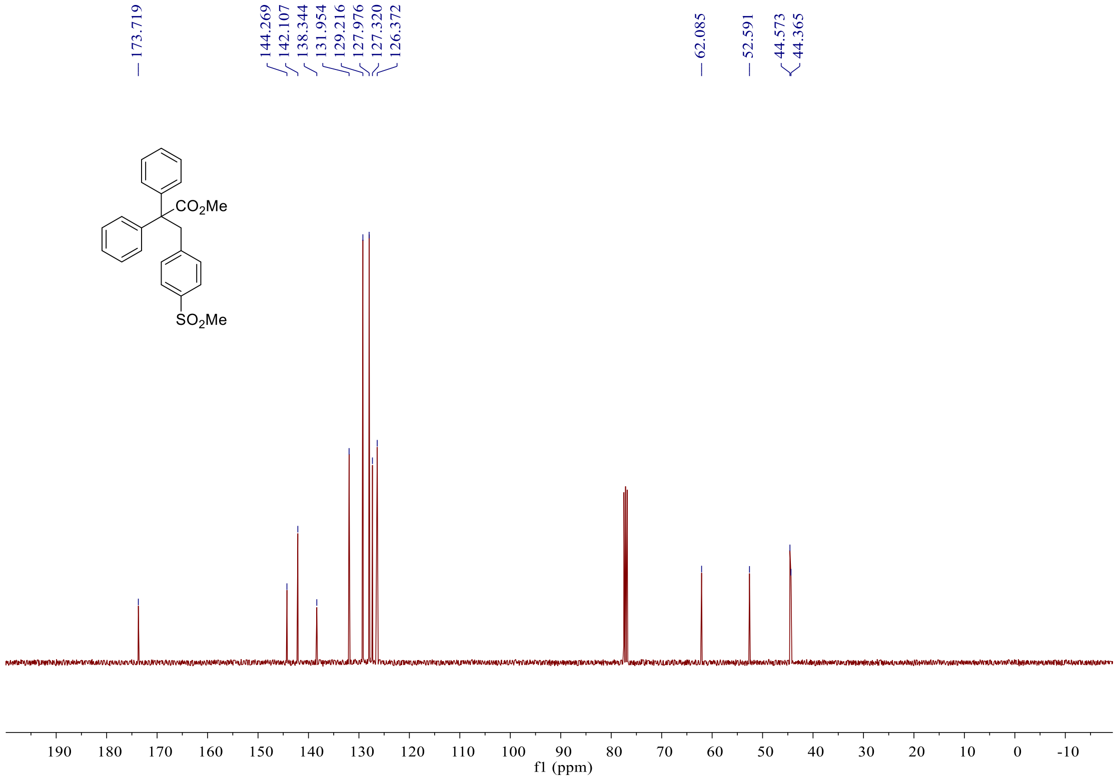

7.717
7.696
7.247
7.238
7.231
7.222
7.215
7.211
7.175
7.164
7.158
7.153
7.148
7.139
6.749
6.729
3.856
3.755
3.685
CO2Me
CO2Me
2.05
6.33
4.07
2.04
3.05
2.07
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


173.856
167.253
143.082
142.437
131.012
129.258
128.748
128.153
127.877
127.133
62.081
52.454
52.062
44.510
CO2Me
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

24

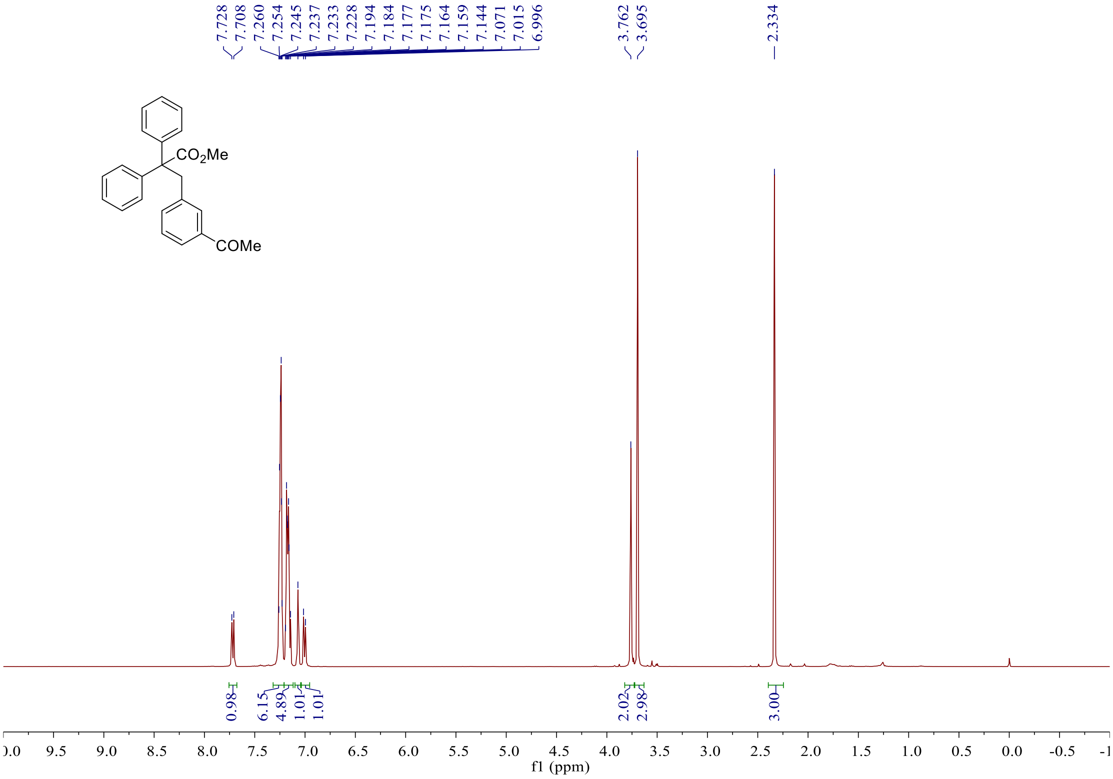


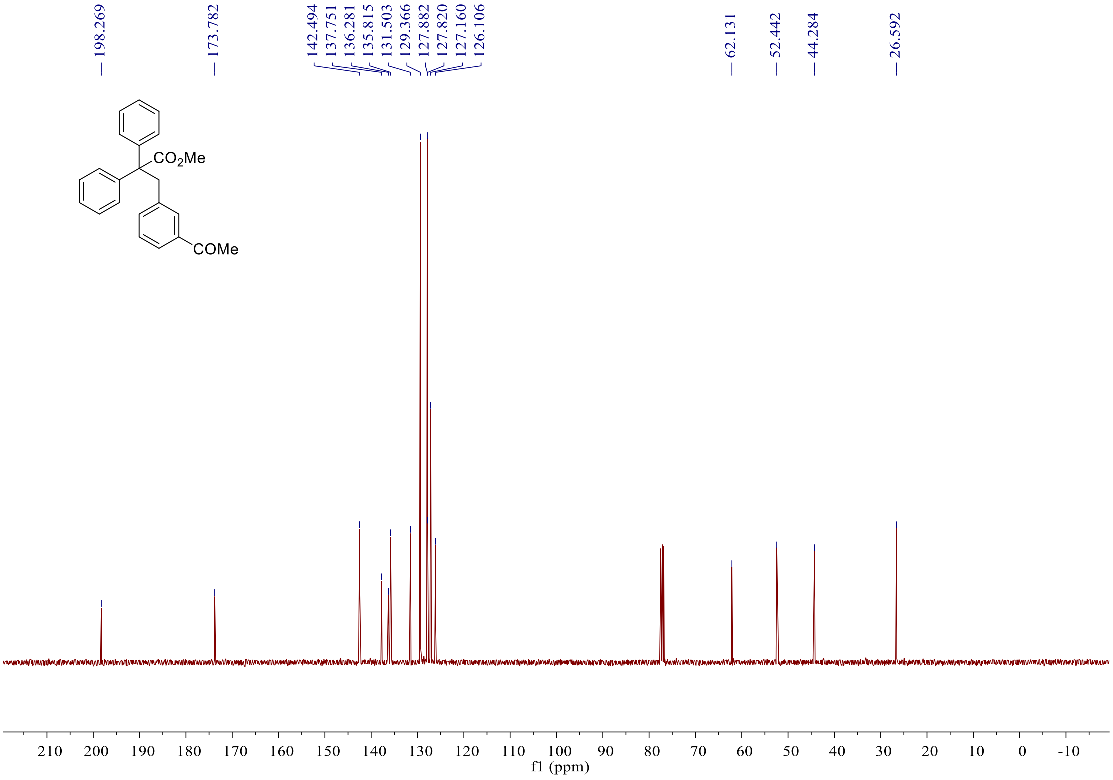
7.598
7.577
7.257
7.250
7.242
7.239
7.167
7.162
7.155
7.152
7.144
6.880
6.859
3.791
3.692
2.986
CO2Me
SO2Me
2.00
6.22
4.03
2.03
2.04
3.02
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



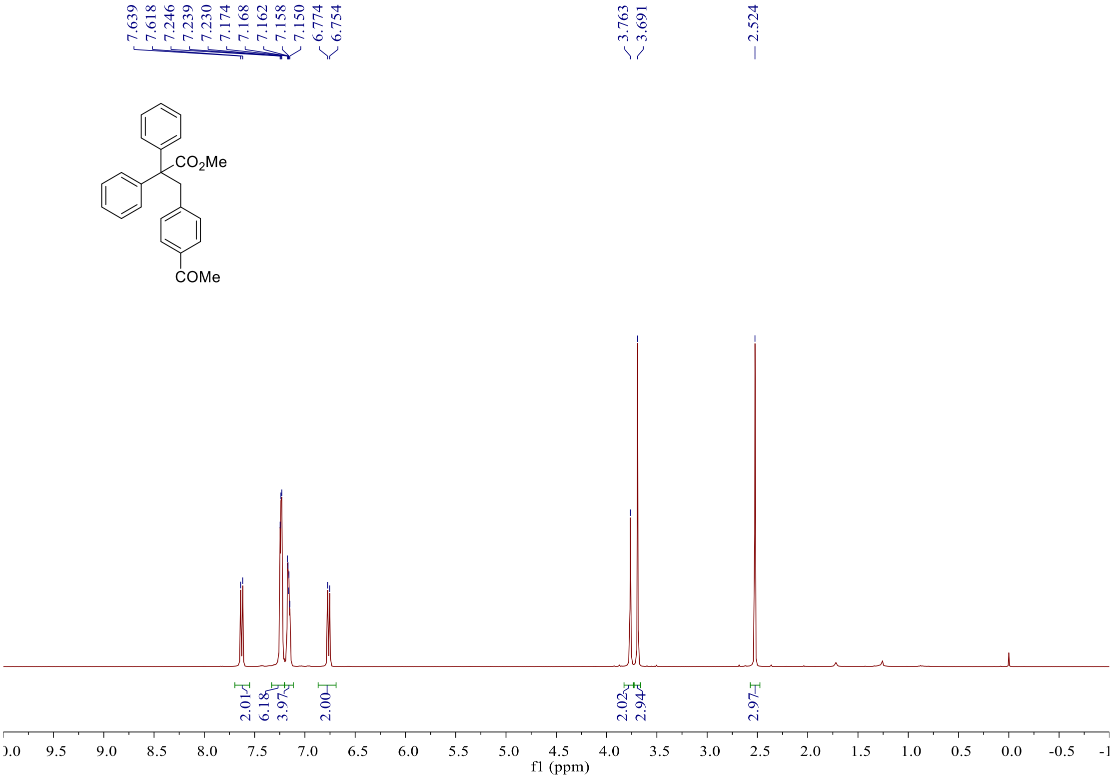
173.719
144.269
142.107
138.344
131.954
129.216
127.976
127.320
126.372
62.085
52.591
44.573
44.365
CO2Me
SO2Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

25


7.728
7.708
7.260
7.254
7.245
7.237
7.233
7.228
7.194
7.184
7.177
7.175
7.164
7.159
7.144
7.071
7.015
6.996
3.762
3.695
2.334
CO_2Me
COMe
0.98
6.15
4.89
1.01
1.01
2.02
2.98
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


198.269
173.782
142.494
137.751
136.281
135.815
131.503
129.366
127.882
127.820
127.160
126.106
62.131
52.442
44.284
26.592
CO_2Me
COMe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

26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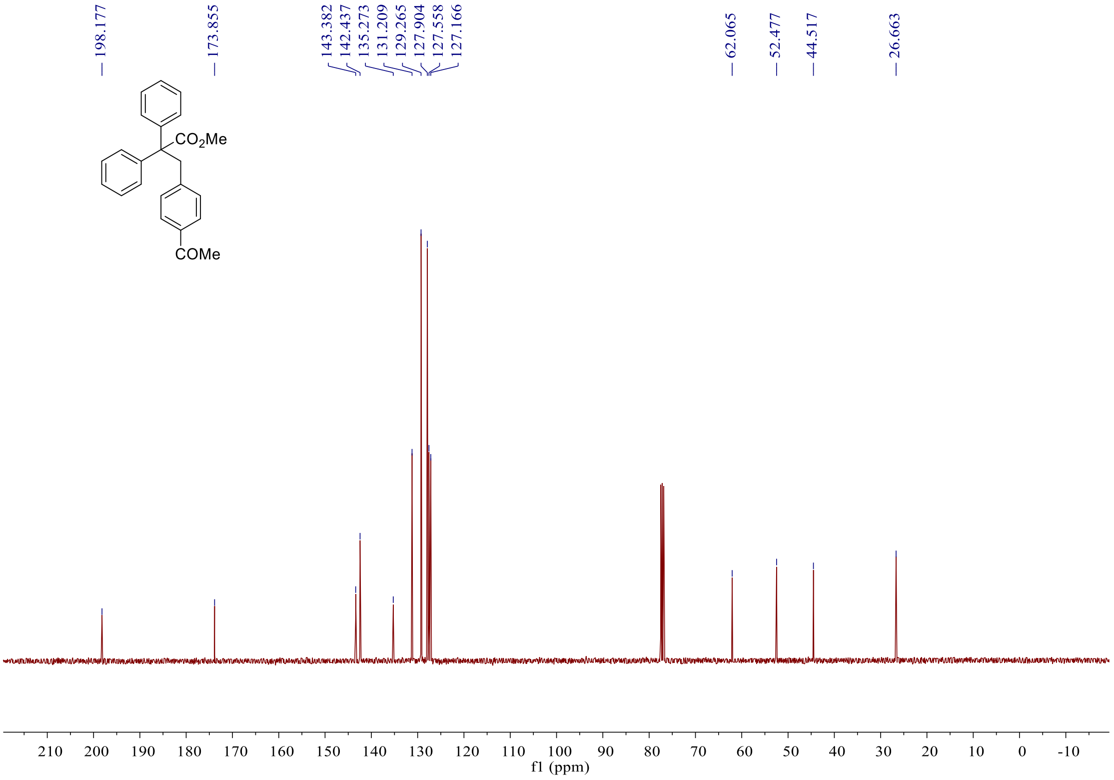
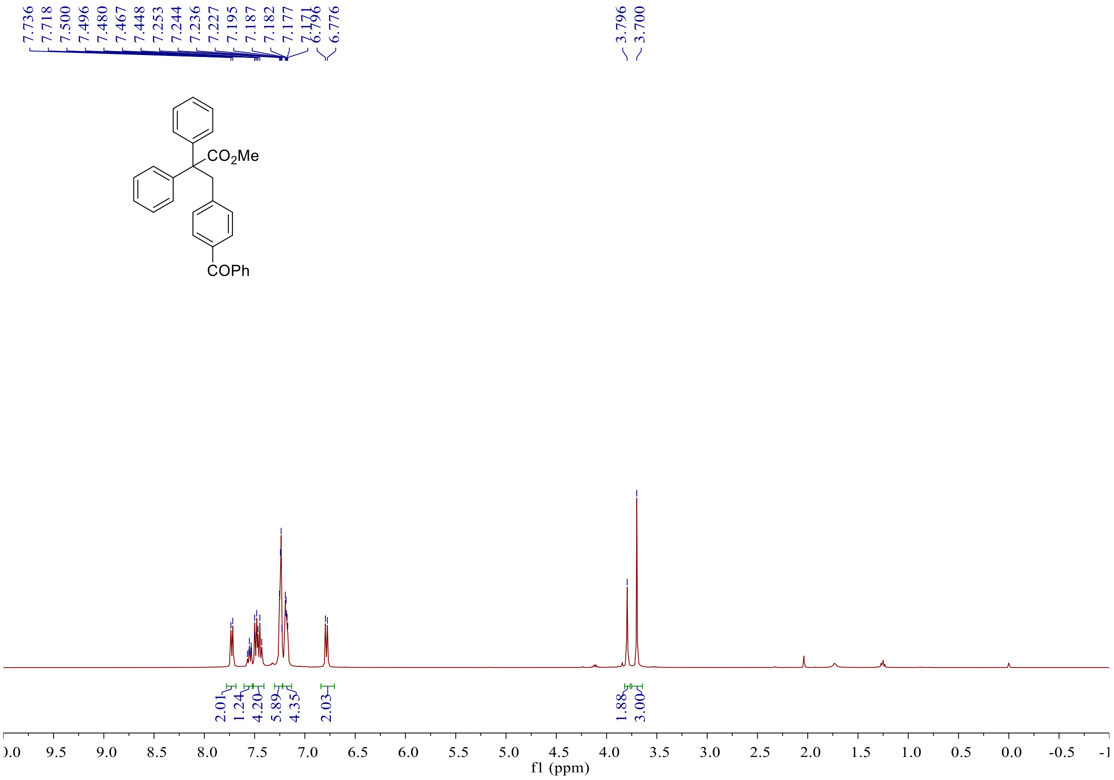
7.618
7.246
7.239
7.230
7.174
7.168
7.162
7.158
7.150
6.774
6.754
3.763
3.691
2.524
CO2Me
COMe
2.01
6.18
3.97
2.00
2.02
2.94
2.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


198.177
173.855
143.382
142.437
135.273
131.209
129.265
127.904
127.558
127.166
62.065
52.477
44.517
26.663
CO2Me
COMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

27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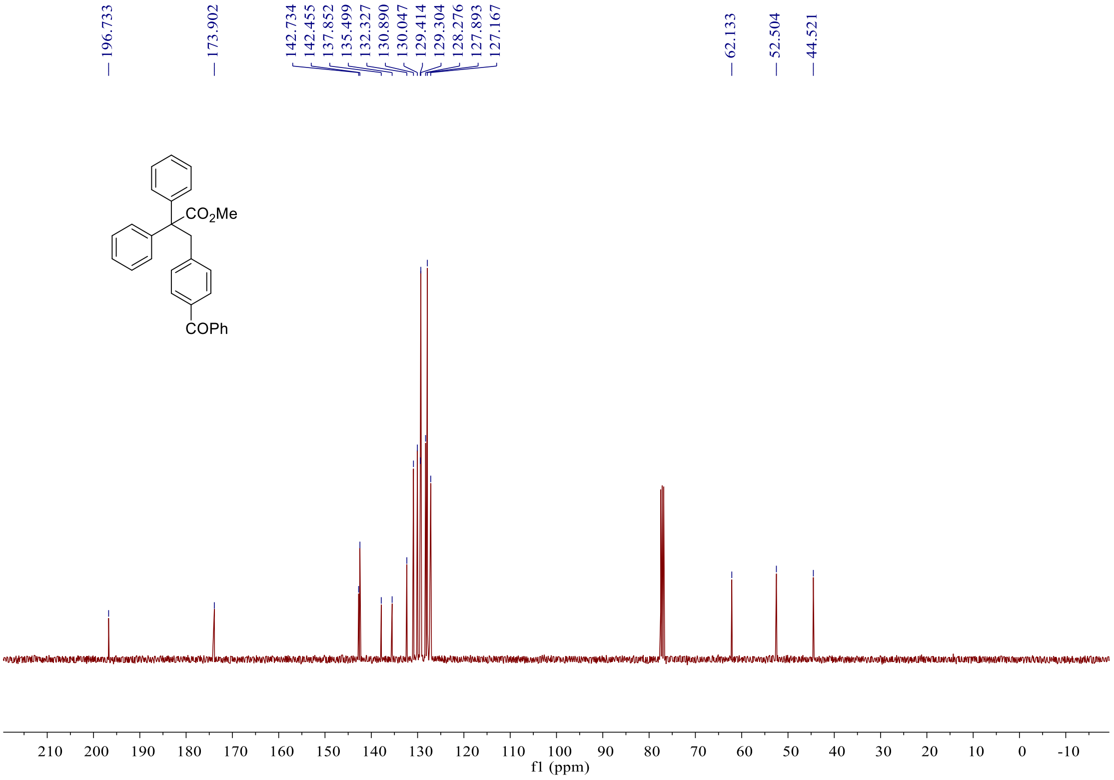
7.718
7.500
7.496
7.480
7.467
7.448
7.253
7.244
7.236
7.227
7.195
7.187
7.182
7.177
7.171
6.796
6.776
3.796
3.700
CO2Me
COPh
2.01
1.24
4.20
5.89
4.35
2.03
1.88
3.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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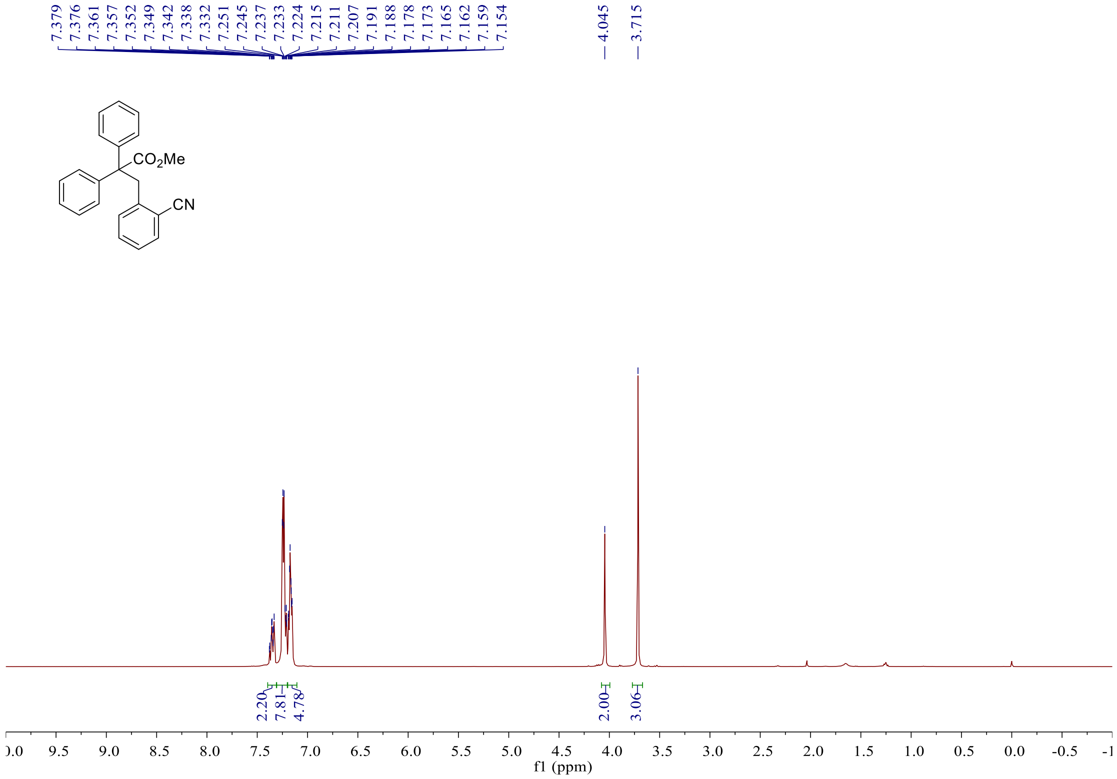
173.902
142.734
142.455
137.852
135.499
132.327
130.890
130.047
129.414
129.304
128.276
127.893
127.167
62.133
52.504
44.521
CO2Me
COPh
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

28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7.361
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7.352
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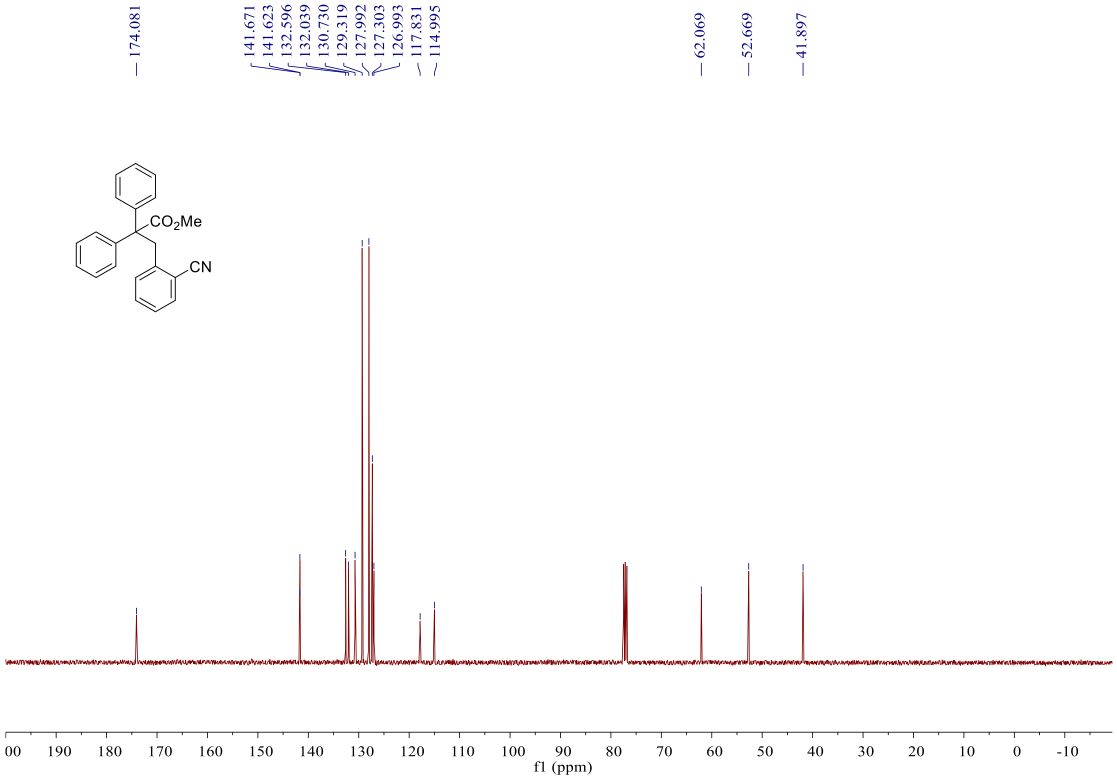
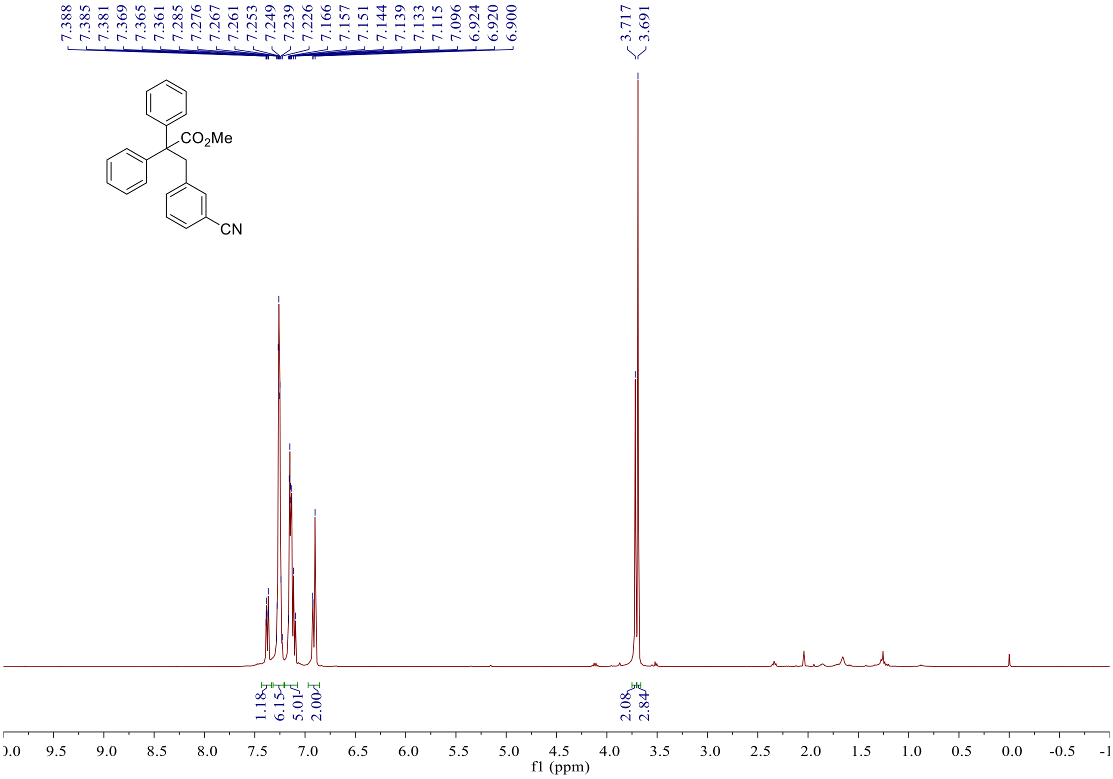
7.342
7.338
7.332
7.251
7.245
7.237
7.233
7.224
7.215
7.211
7.207
7.191
7.188
7.178
7.173
7.165
7.162
7.159
7.154
4.045
3.715
CO2Me
CN
2.20
7.81
4.78
2.00
3.06
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


174.081
141.671
141.623
132.596
132.039
130.730
129.319
127.992
127.303
126.993
117.831
114.995
62.069
52.669
41.897
CO2Me
CN
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

29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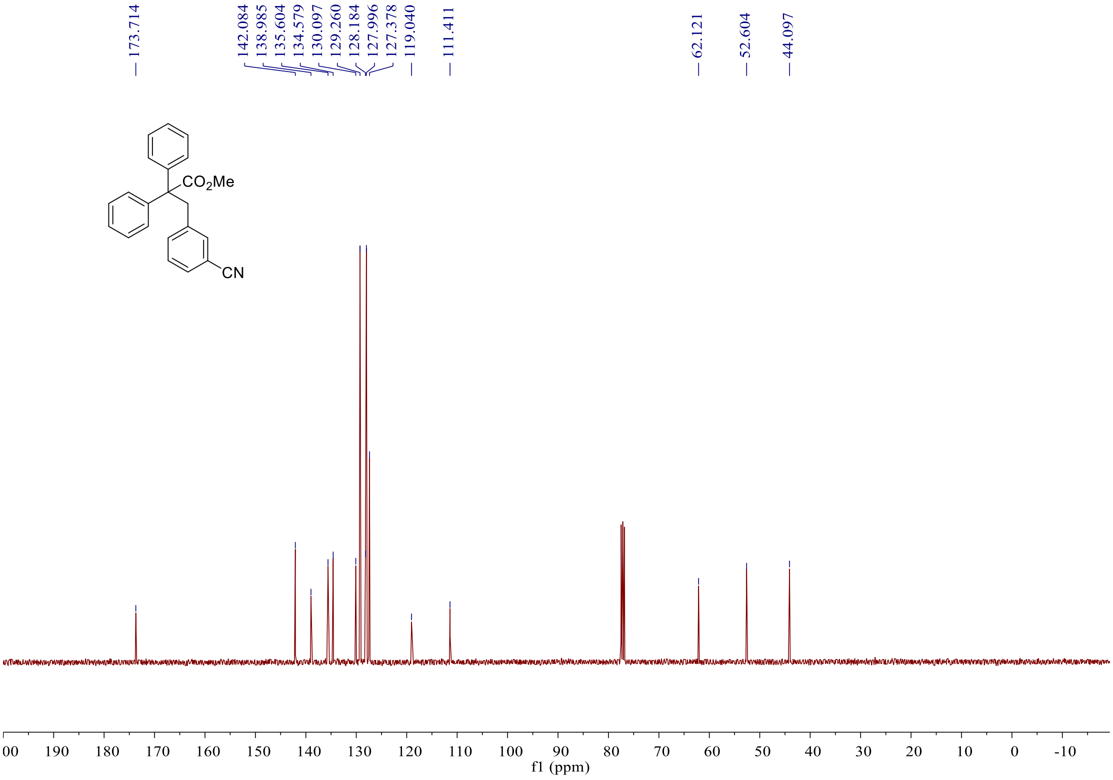
7.365
7.361
7.285
7.276
7.267
7.261
7.253
7.249
7.239
7.226
7.166
7.157
7.151
7.144
7.139
7.133
7.115
7.096
6.924
6.920
6.900
3.717
3.691
CO2Me
CN
1.18
6.15
5.01
2.00
2.08
2.84
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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135.604
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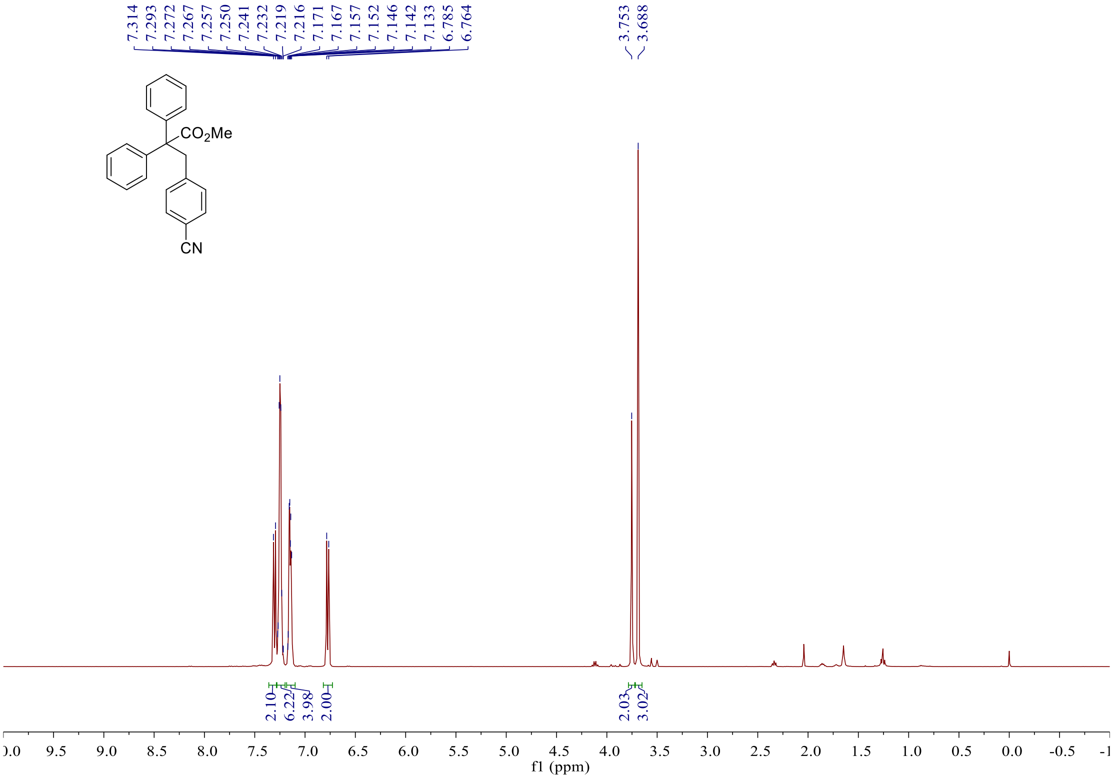
129.260
128.184
127.996
127.378
119.040
111.411
62.121
52.604
44.097
CO2Me
CN
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

30


7.314
7.293
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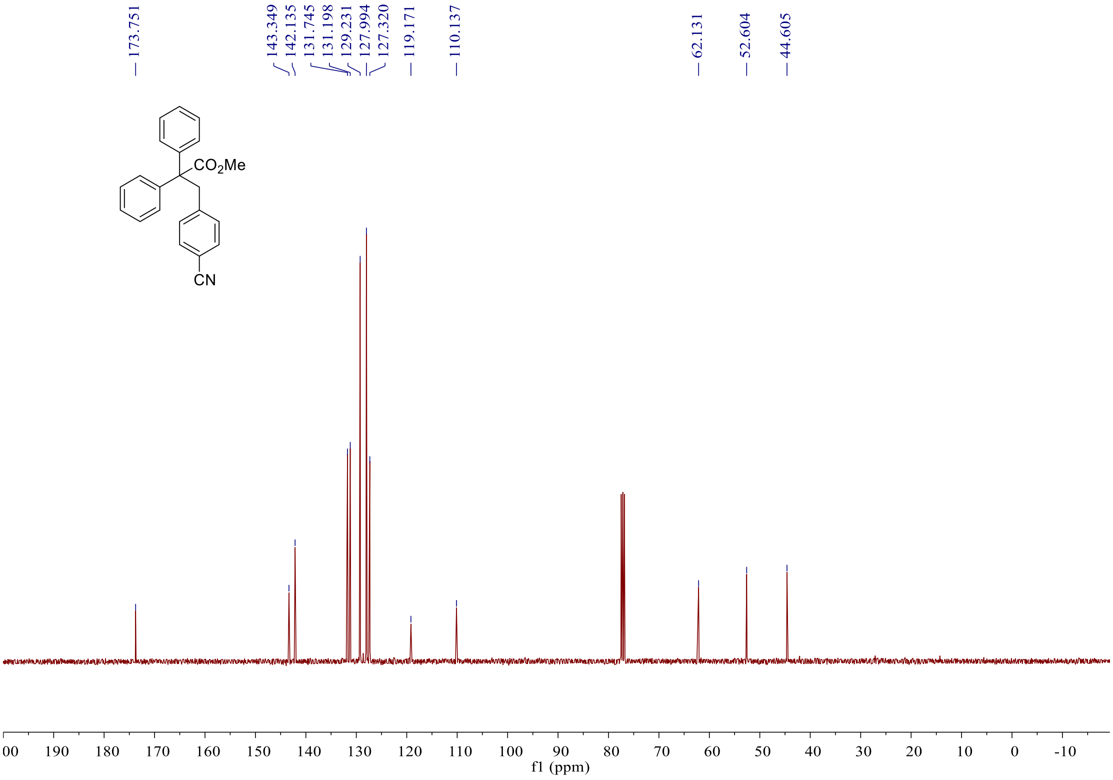
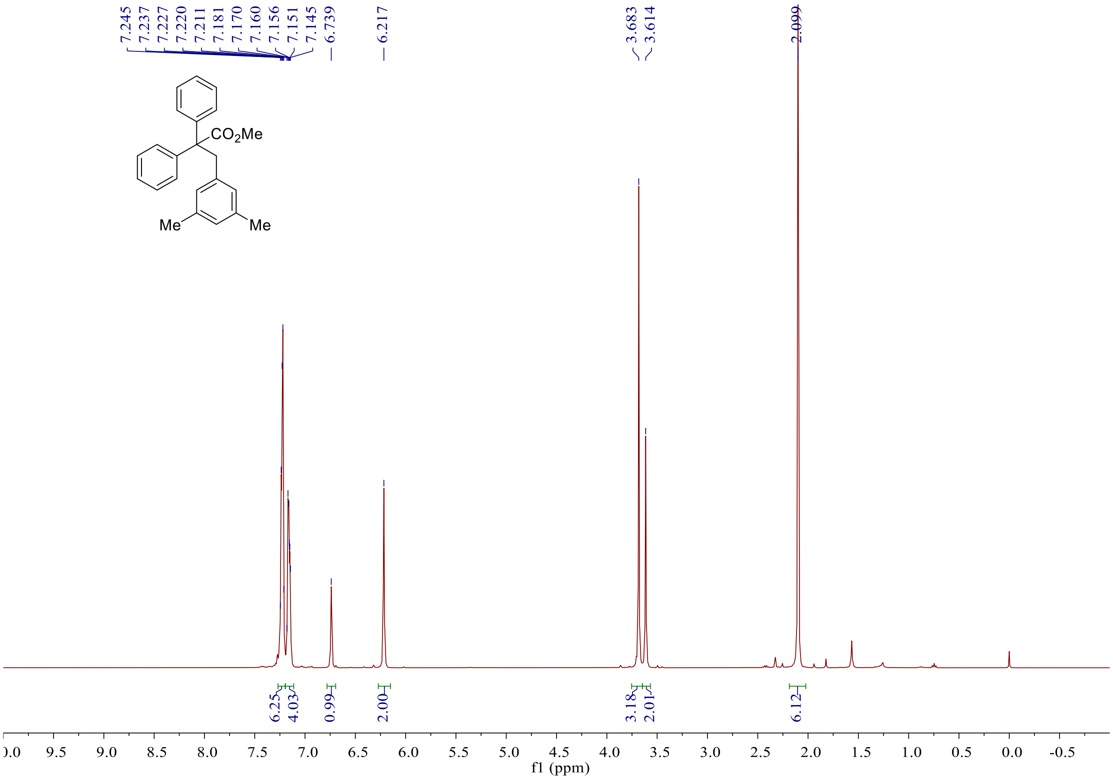
7.267
7.257
7.250
7.241
7.232
7.219
7.216
7.171
7.167
7.157
7.152
7.146
7.142
7.133
6.785
6.764
3.753
3.688
CO2Me
CN
2.10
6.22
3.98
2.00
2.03
3.02
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


173.751
143.349
142.135
131.745
131.198
129.231
127.994
127.320
119.171
110.137
62.131
52.604
44.605
CO2Me
CN
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

31


7.245
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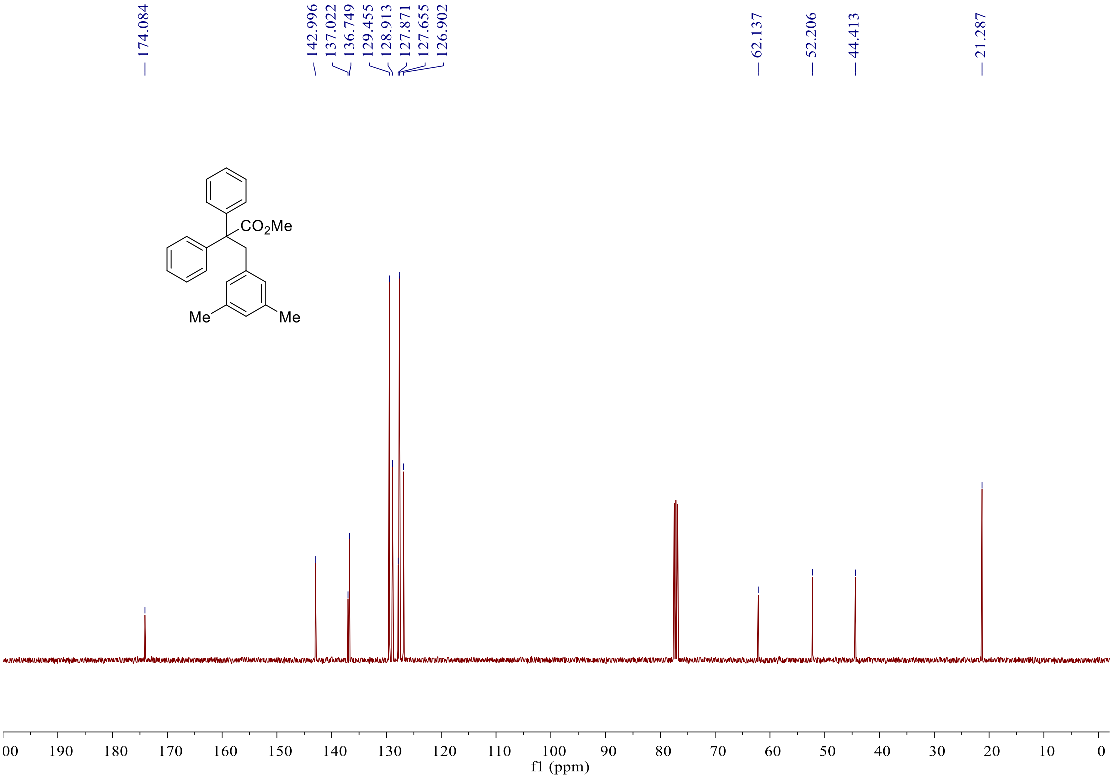
7.220
7.211
7.181
7.170
7.160
7.156
7.151
7.145
6.739
6.217
3.683
3.614
2.099
CO2Me
Me
Me
6.25
4.03
0.99
2.00
3.18
2.01
6.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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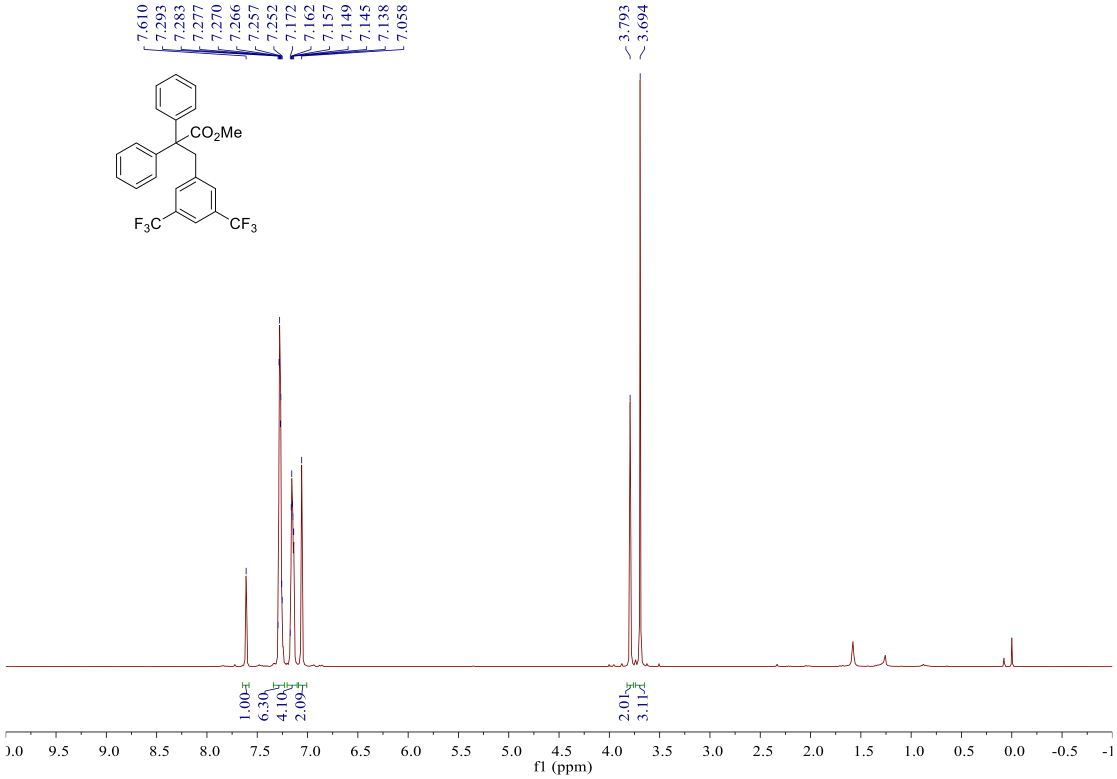
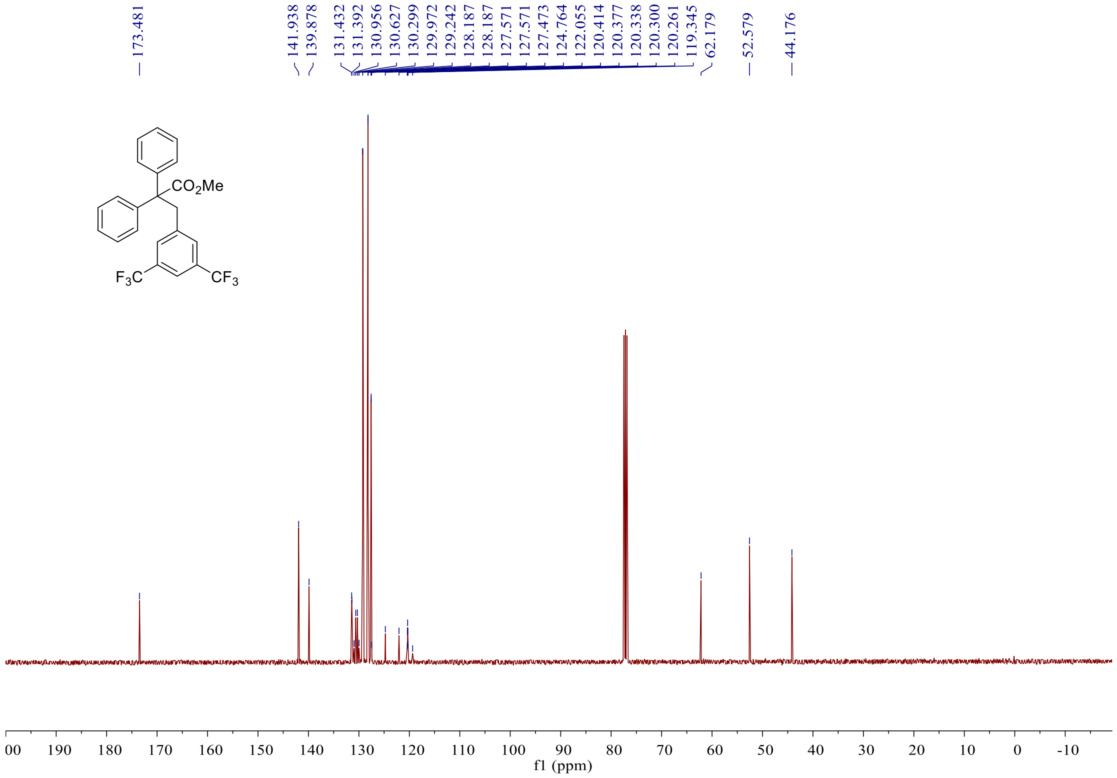
142.996
137.022
136.749
129.455
128.913
127.871
127.655
126.902
62.137
52.206
44.413
21.287
CO2Me
Me
Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

32


7.610
7.293
7.283
7.277
7.270
7.266
7.257
7.252
7.172
7.162
7.157
7.149
7.145
7.138
7.058
3.793
3.694
CO$_2$Me
F$_3$C
CF$_3$
1.00
6.30
4.10
2.09
2.01
3.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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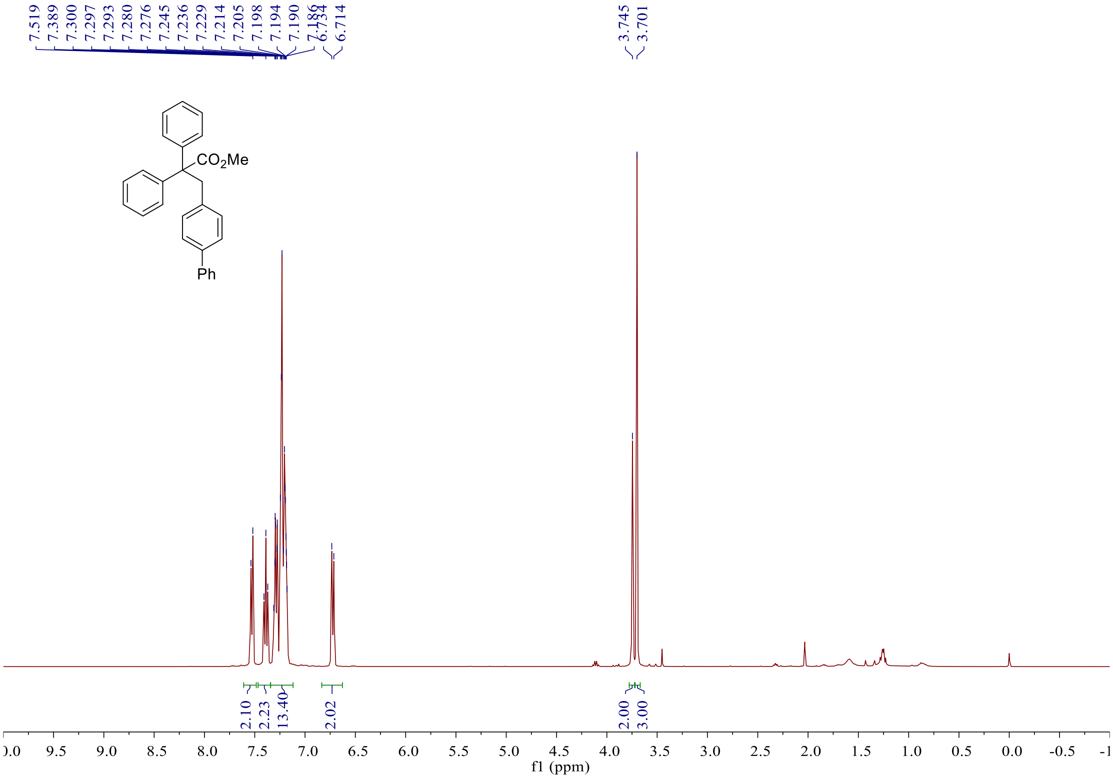
141.938
139.878
131.432
131.392
130.956
130.627
130.299
129.972
129.242
128.187
128.187
127.571
127.571
127.473
124.764
122.055
120.414
120.377
120.338
120.300
120.261
119.345
62.179
52.579
44.176
CO$_2$Me
F$_3$C
CF$_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

33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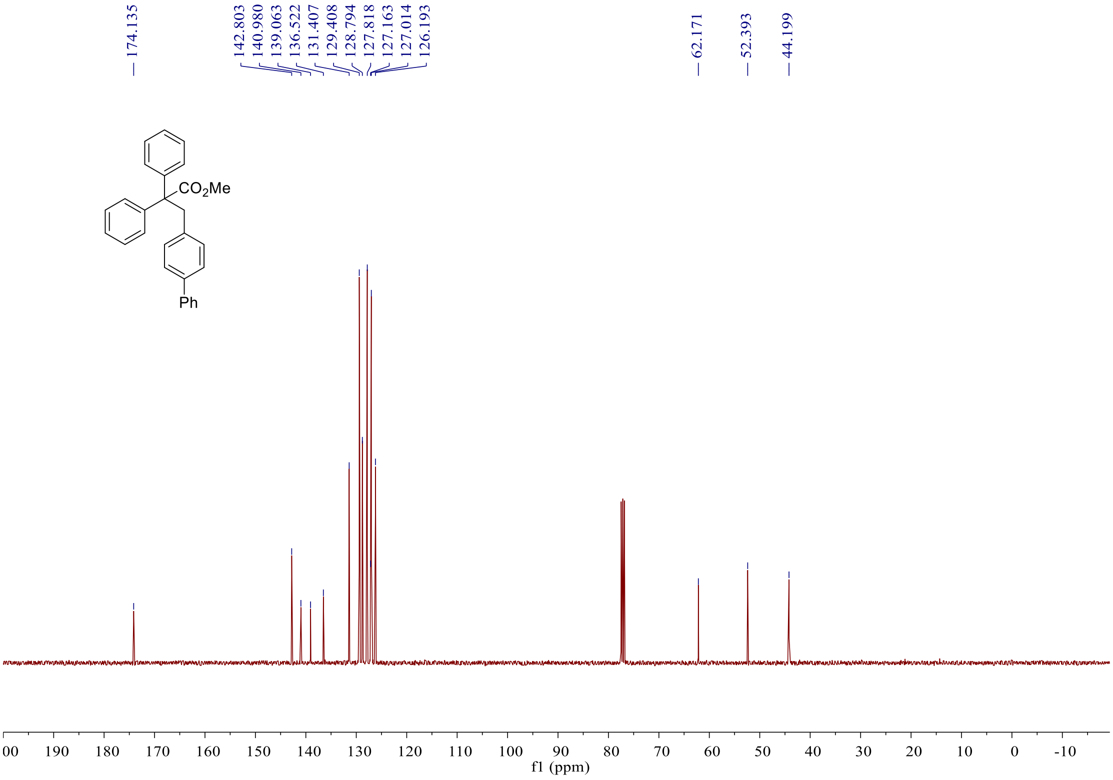
7.300
7.297
7.293
7.280
7.276
7.245
7.236
7.229
7.214
7.205
7.198
7.194
7.190
7.186
6.734
6.714
3.745
3.701
CO$_2$Me
Ph
2.10
2.23
13.40
2.02
2.00
3.00
).0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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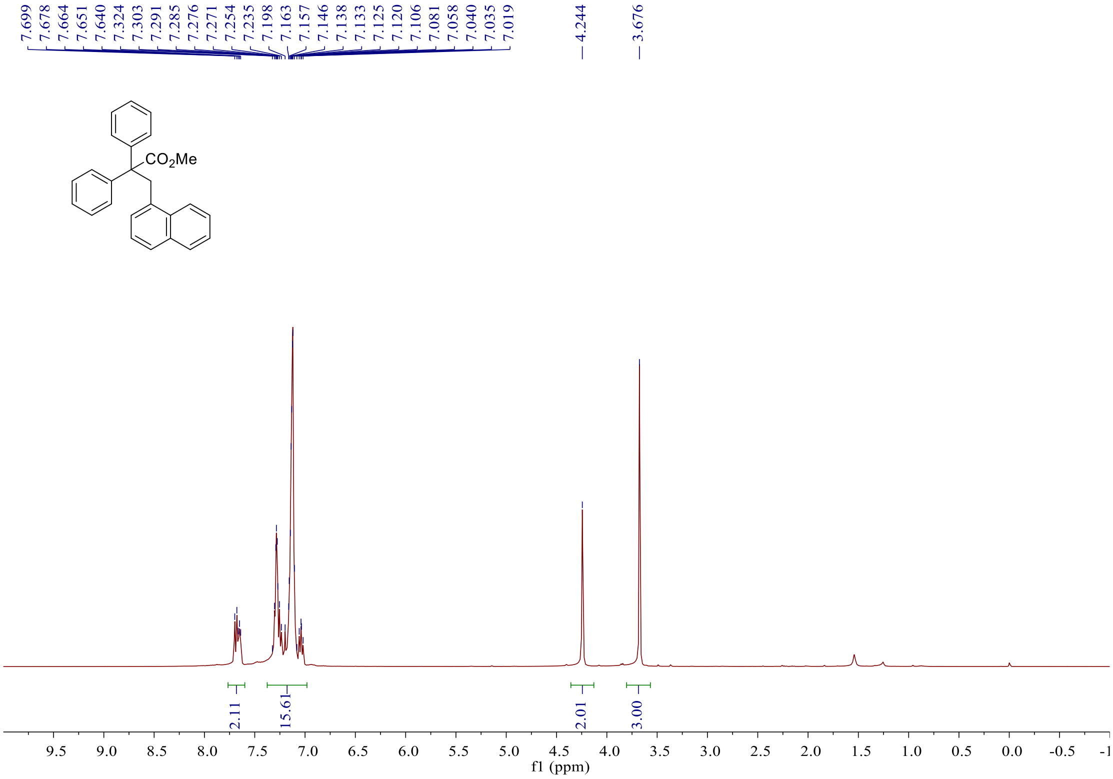
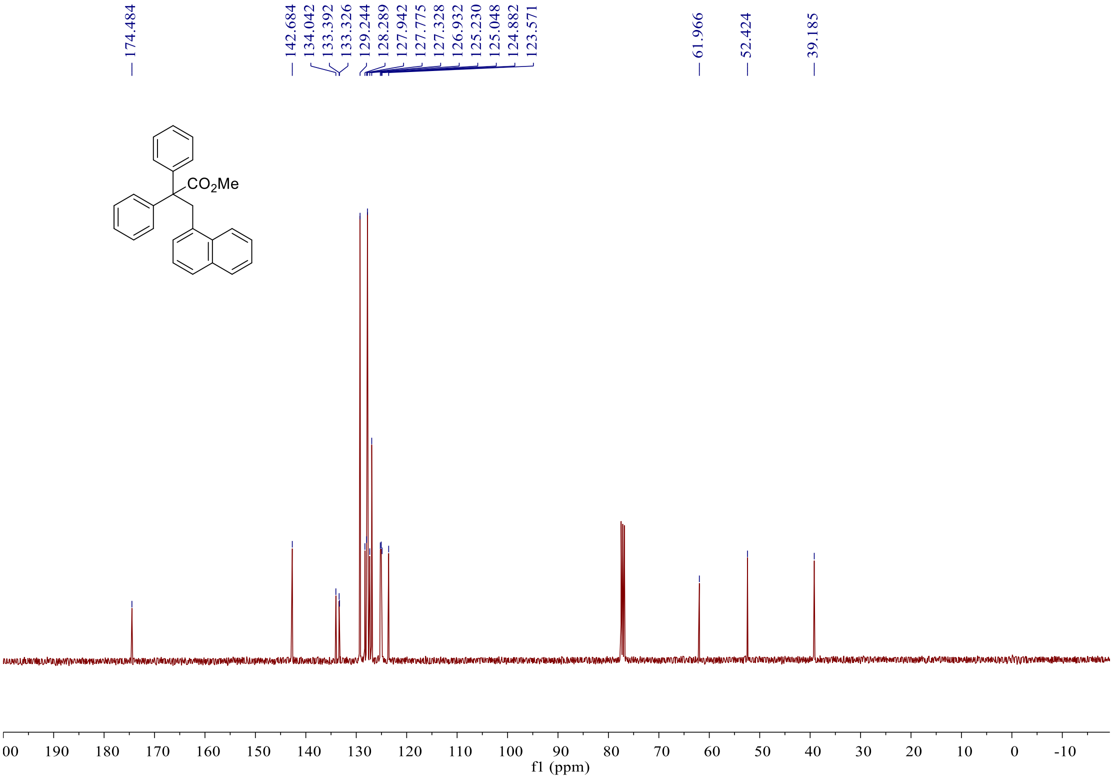
142.803
140.980
139.063
136.522
131.407
129.408
128.794
127.818
127.163
127.014
126.193
62.171
52.393
44.199
CO$_2$Me
Ph
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

34


7.699
7.678
7.664
7.651
7.640
7.324
7.303
7.291
7.285
7.276
7.271
7.254
7.235
7.198
7.163
7.157
7.146
7.138
7.133
7.125
7.120
7.106
7.081
7.058
7.040
7.035
7.019
4.244
3.676
CO2Me
2.11
15.61
2.01
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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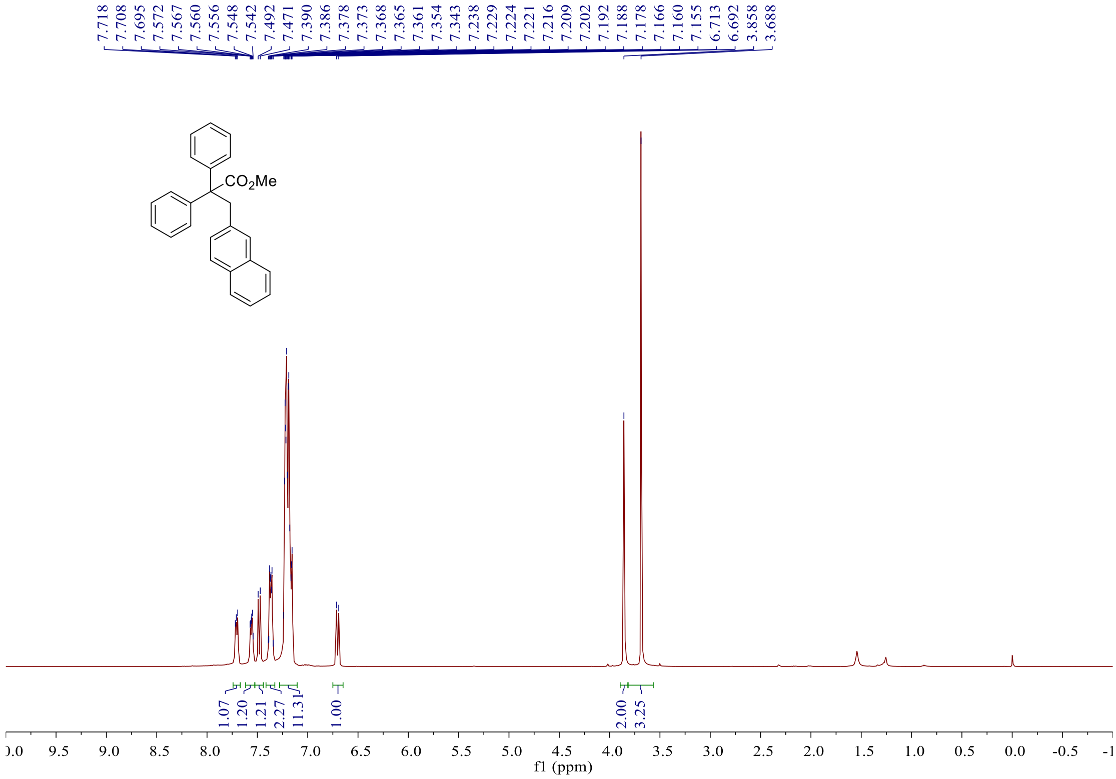
133.392
133.326
129.244
128.289
127.942
127.775
127.328
126.932
125.230
125.048
124.882
123.571
61.966
52.424
39.185
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

35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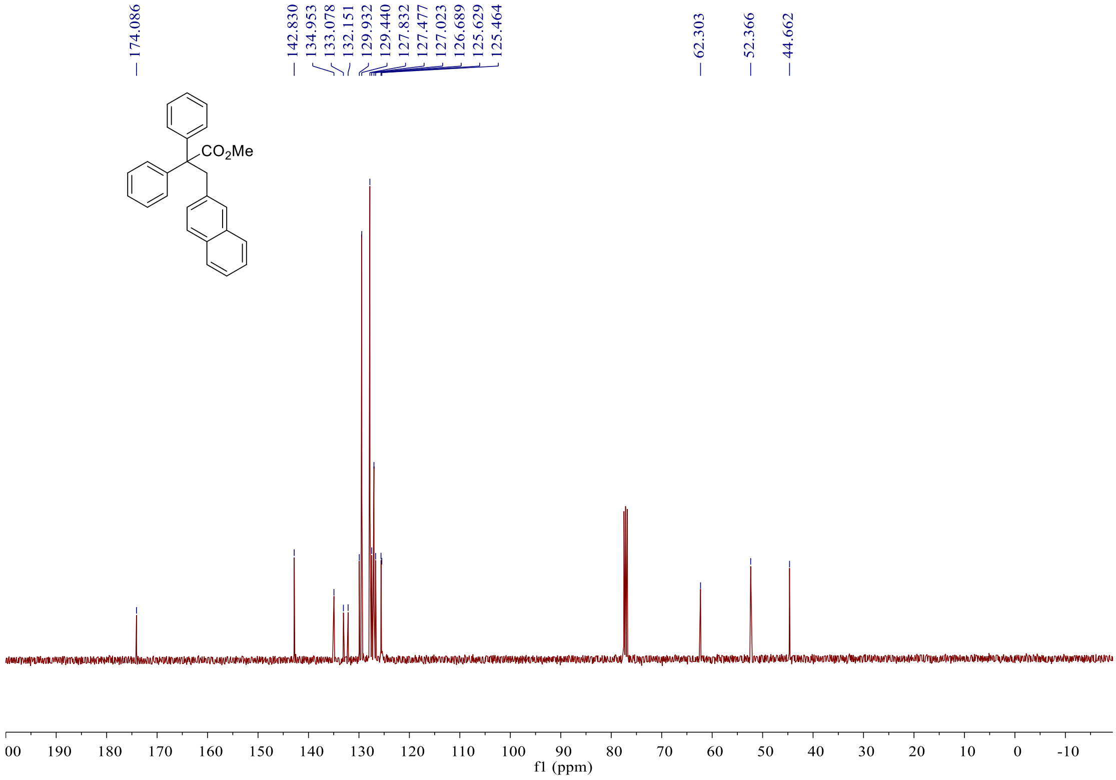
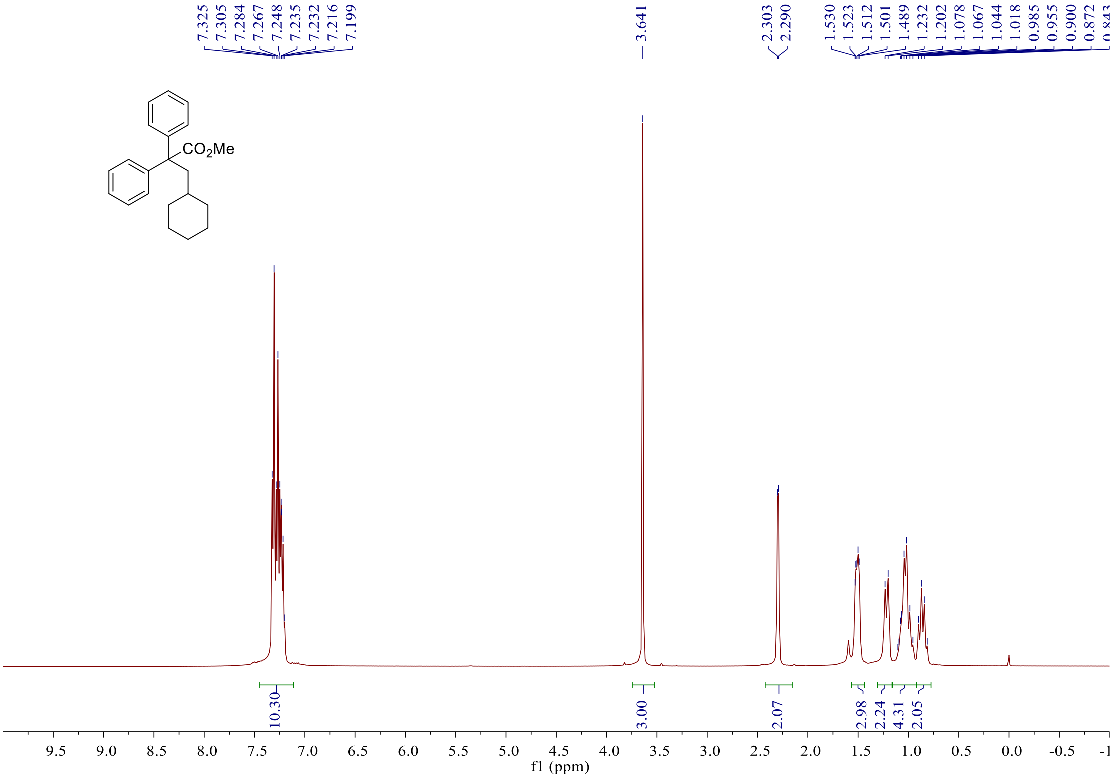
7.708
7.695
7.572
7.567
7.560
7.556
7.548
7.542
7.492
7.471
7.390
7.386
7.378
7.373
7.368
7.365
7.361
7.354
7.343
7.238
7.229
7.224
7.221
7.216
7.209
7.202
7.192
7.188
7.178
7.166
7.160
7.155
6.713
6.692
3.858
3.688
CO_2Me
1.07
1.20
1.21
2.27
11.31
1.00
2.00
3.25
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


174.086
142.830
134.953
133.078
132.151
129.932
129.440
127.832
127.477
127.023
126.689
125.629
125.464
62.303
52.366
44.662
CO_2Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

36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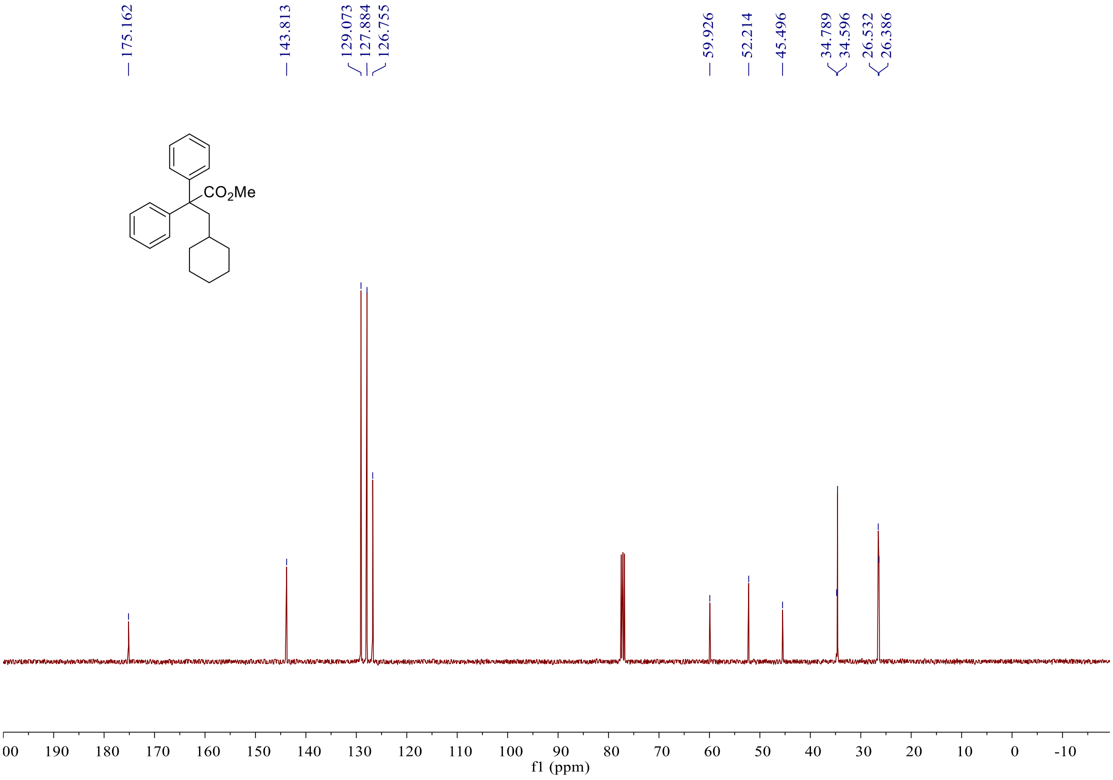
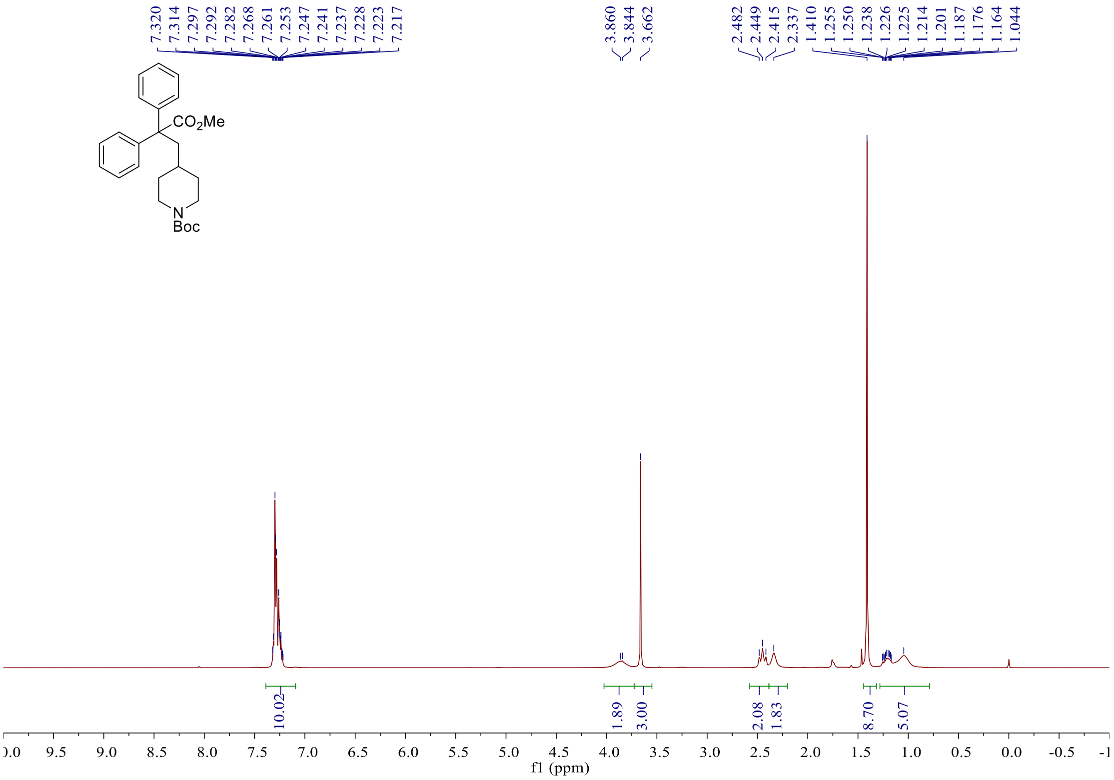
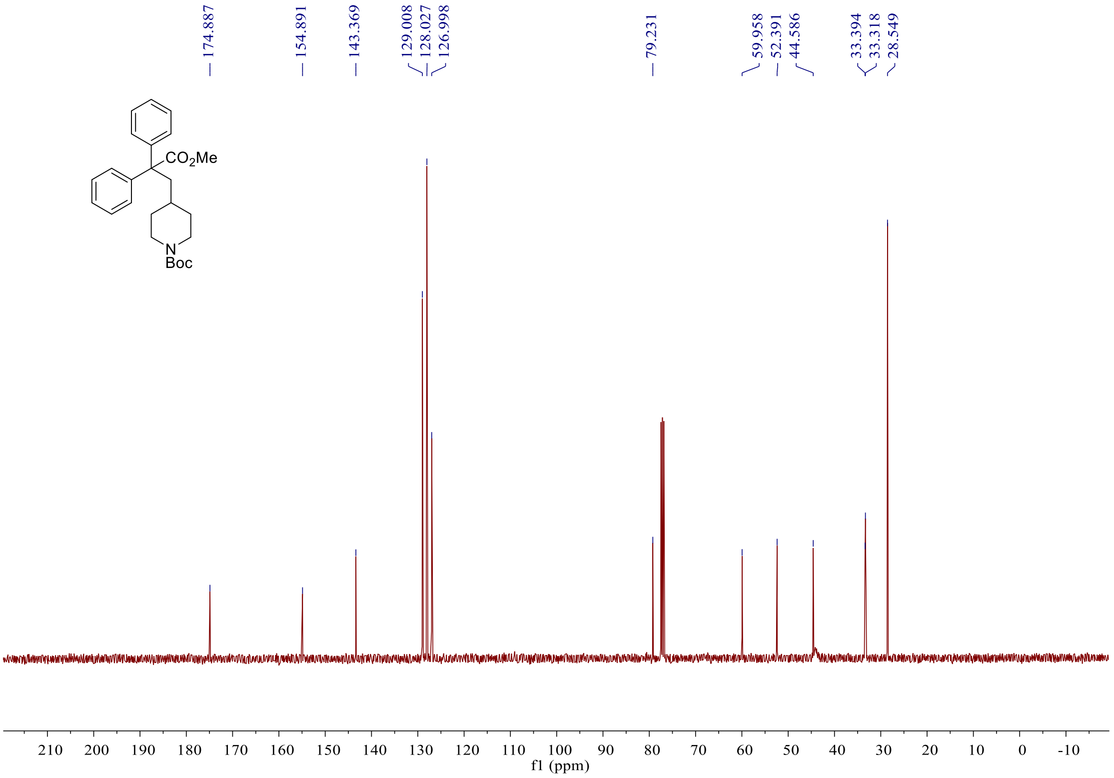
7.305
7.284
7.267
7.248
7.235
7.232
7.216
7.199
3.641
2.303
2.290
1.530
1.523
1.512
1.501
1.489
1.232
1.202
1.078
1.067
1.044
1.018
0.985
0.955
0.900
0.872
0.843
CO2Me
10.30
3.00
2.07
2.98
2.24
4.31
2.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


175.162
143.813
129.073
127.884
126.755
59.926
52.214
45.496
34.789
34.596
26.532
26.386
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

37


7.320
7.314
7.297
7.292
7.282
7.268
7.261
7.253
7.247
7.241
7.237
7.228
7.223
7.217
3.860
3.844
3.662
2.482
2.449
2.415
2.337
1.410
1.255
1.250
1.238
1.226
1.225
1.214
1.201
1.187
1.176
1.164
1.044
CO_2Me
N
Boc
10.02
1.89
3.00
2.08
1.83
8.70
5.07
).0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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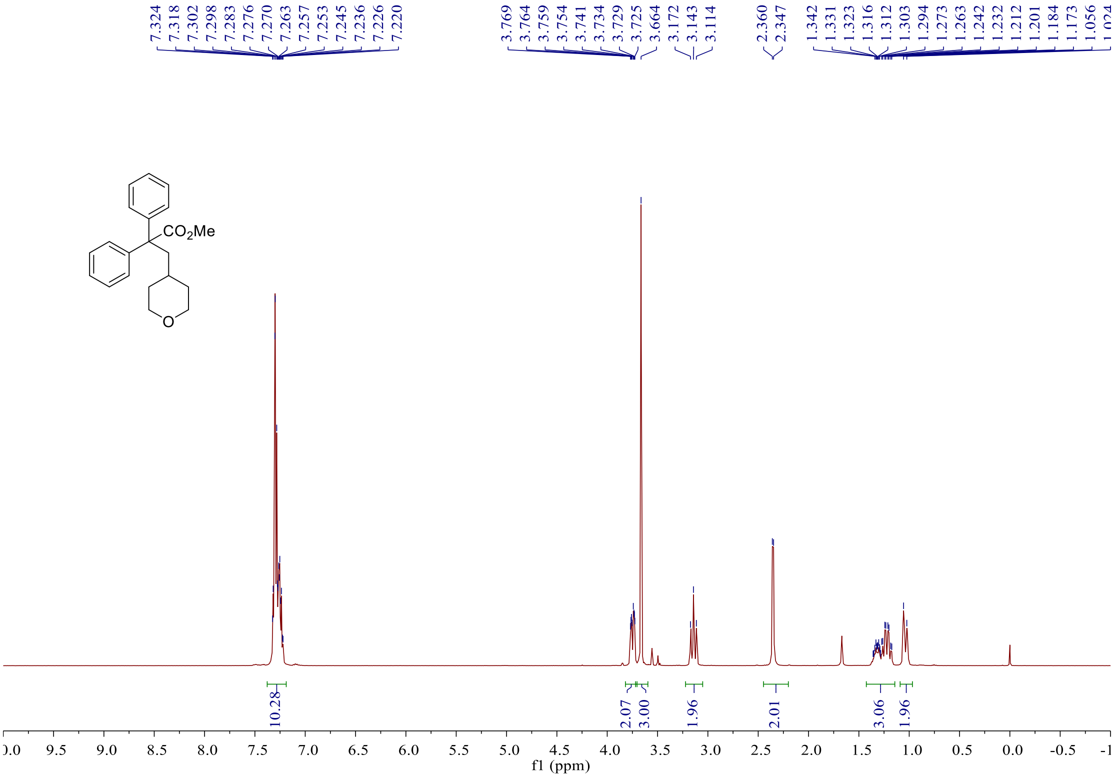
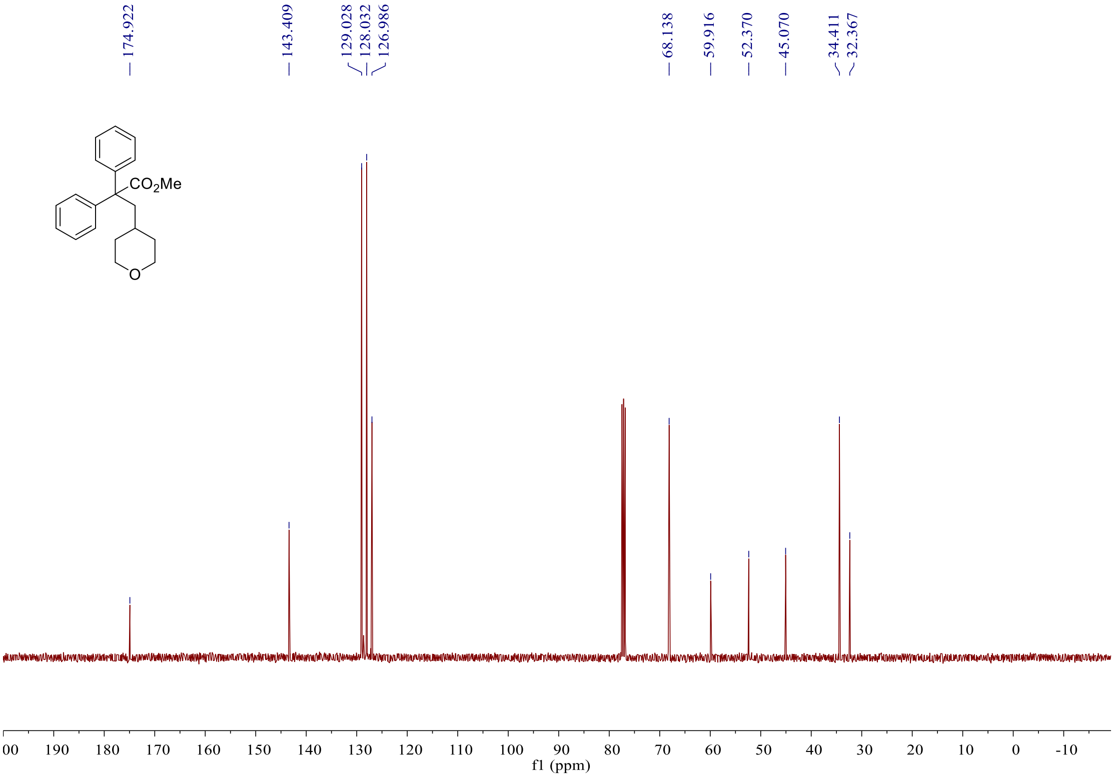
154.891
143.369
129.008
128.027
126.998
79.231
59.958
52.391
44.586
33.394
33.318
28.549
CO_2Me
N
Boc
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

38


7.324
7.318
7.302
7.298
7.283
7.276
7.270
7.263
7.257
7.253
7.245
7.236
7.226
7.220
3.769
3.764
3.759
3.754
3.741
3.734
3.729
3.725
3.664
3.172
3.143
3.114
2.360
2.347
1.342
1.331
1.323
1.316
1.312
1.303
1.294
1.273
1.263
1.242
1.232
1.212
1.201
1.184
1.173
1.056
1.024
CO2Me
O
10.28
2.07
3.00
1.96
2.01
3.06
1.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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143.409
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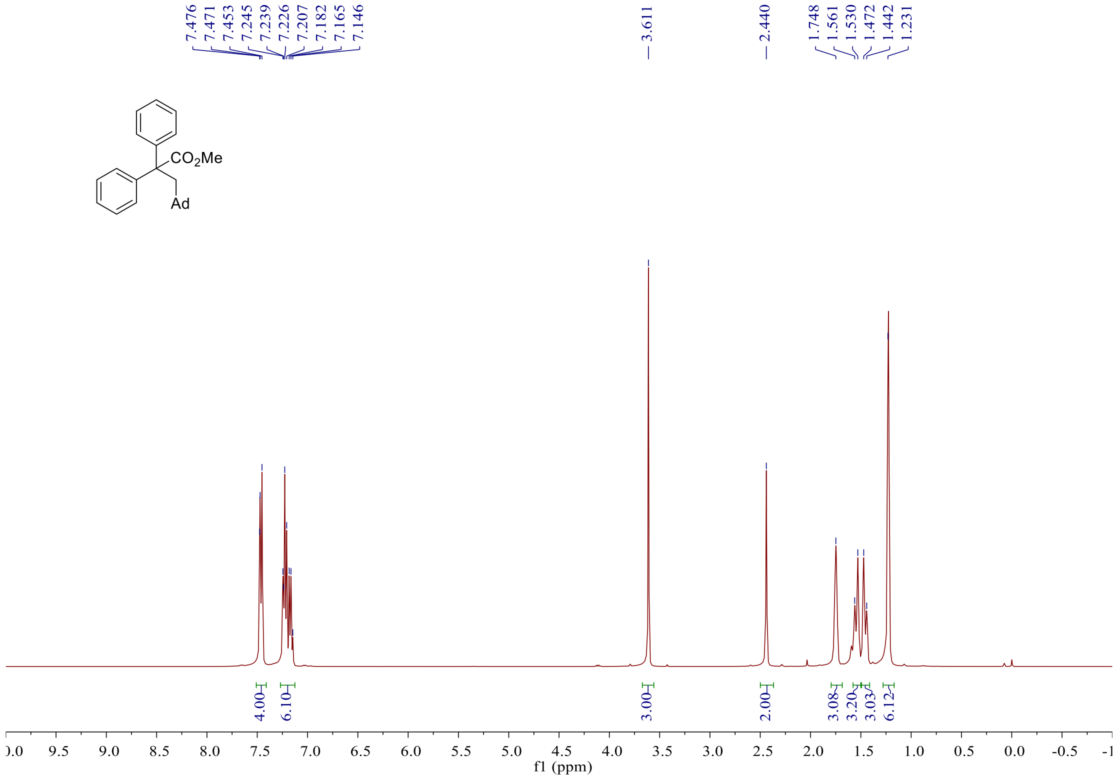
128.032
126.986
68.138
59.916
52.370
45.070
34.411
32.367
CO2Me
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

39


7.476
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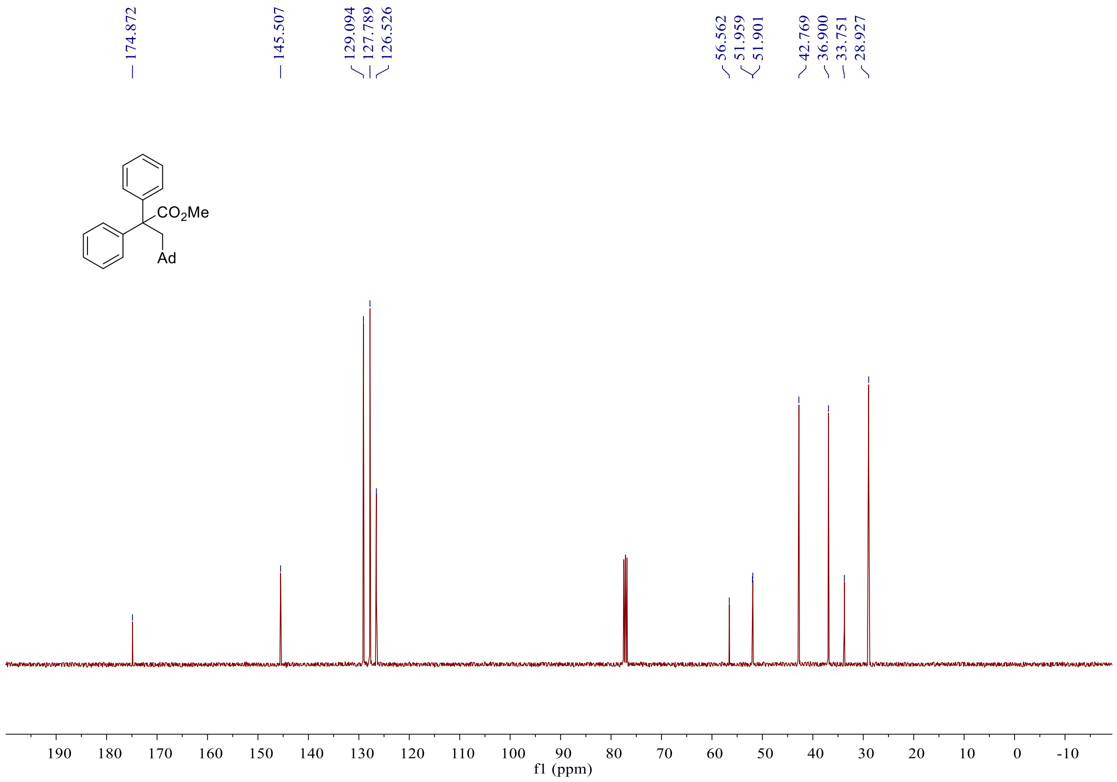
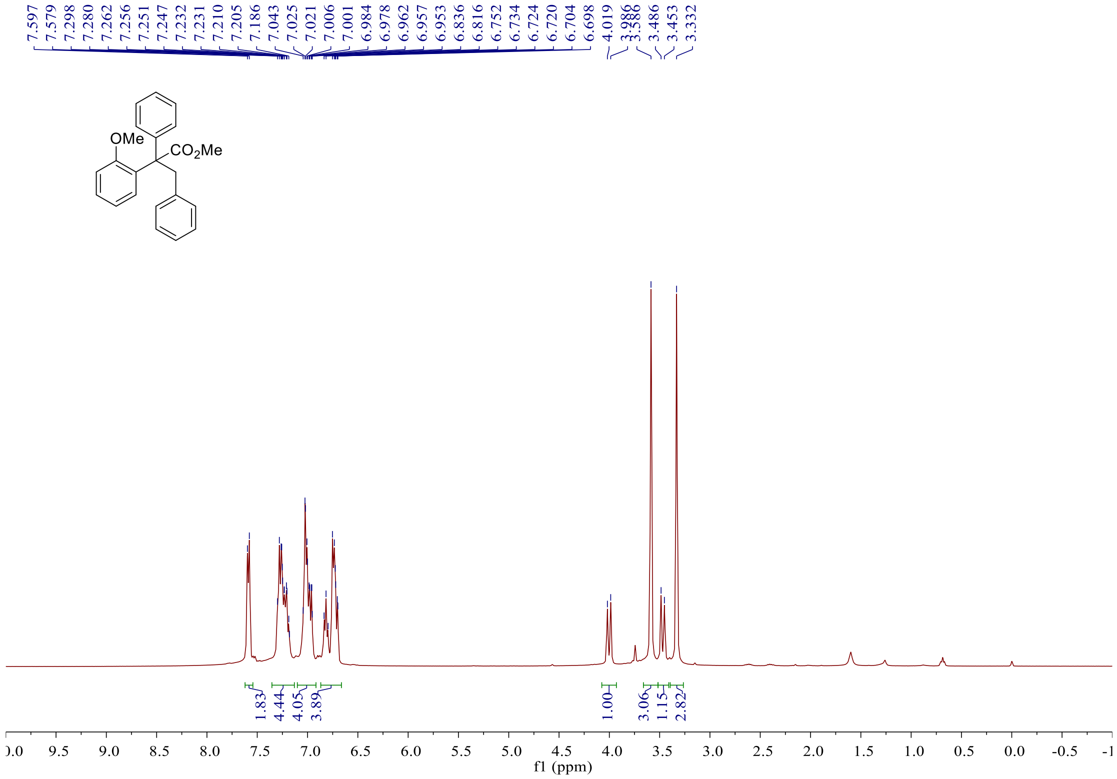
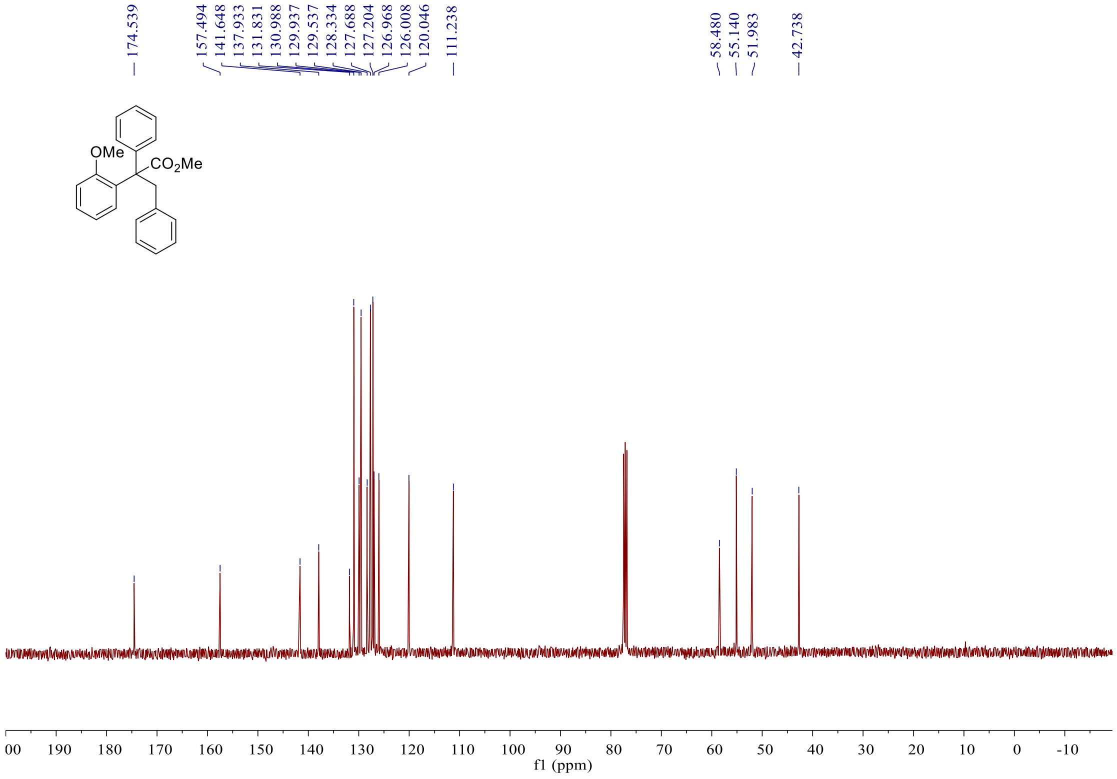
7.239
7.226
7.207
7.182
7.165
7.146
3.611
2.440
1.748
1.561
1.530
1.472
1.442
1.231
CO2Me
Ad
4.00
6.10
3.00
2.00
3.08
3.20
3.03
6.12
f1 (ppm)

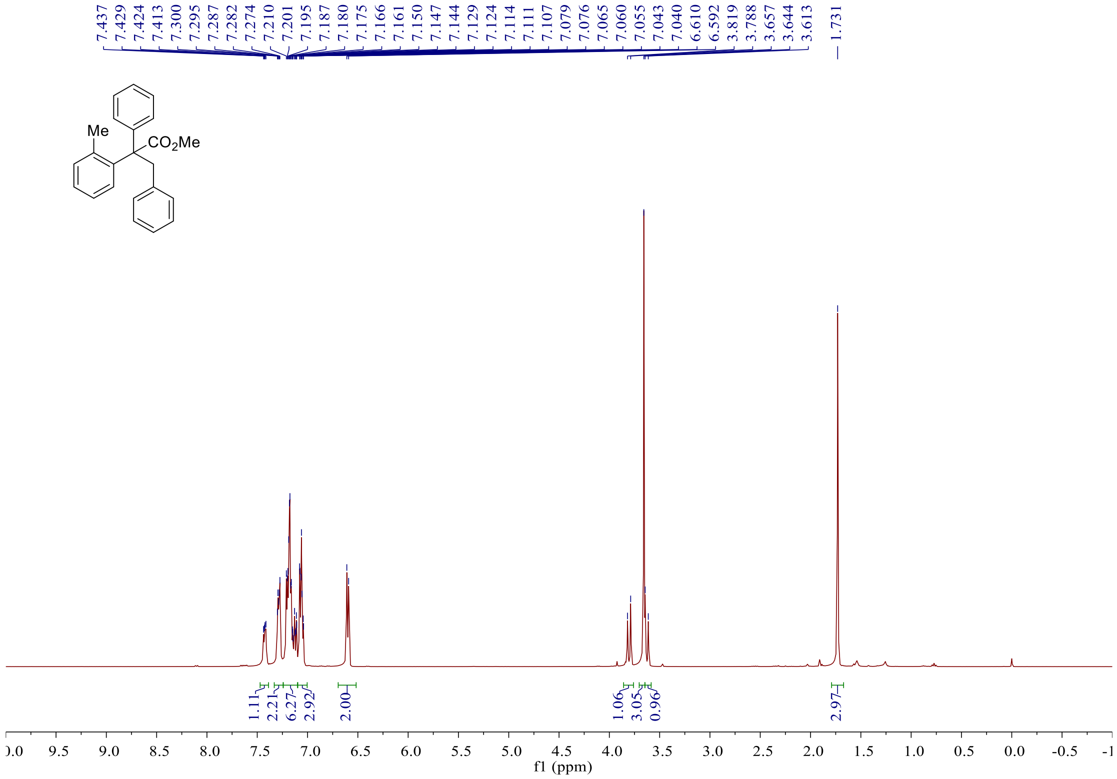

174.872
145.507
129.094
127.789
126.526
56.562
51.959
51.901
42.769
36.900
33.751
28.927
CO2Me
Ad
f1 (ppm)

40


7.597
7.579
7.298
7.280
7.262
7.256
7.251
7.247
7.232
7.231
7.210
7.205
7.186
7.043
7.025
7.021
7.006
7.001
6.984
6.978
6.962
6.957
6.953
6.836
6.816
6.752
6.734
6.724
6.720
6.704
6.698
4.019
3.986
3.586
3.486
3.453
3.332
OMe
CO2Me
1.83
4.44
4.05
3.89
1.00
3.06
1.15
2.82
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


174.539
157.494
141.648
137.933
131.831
130.988
129.937
129.537
128.334
127.688
127.204
126.968
126.008
120.046
111.238
58.480
55.140
51.983
42.738
OMe
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

41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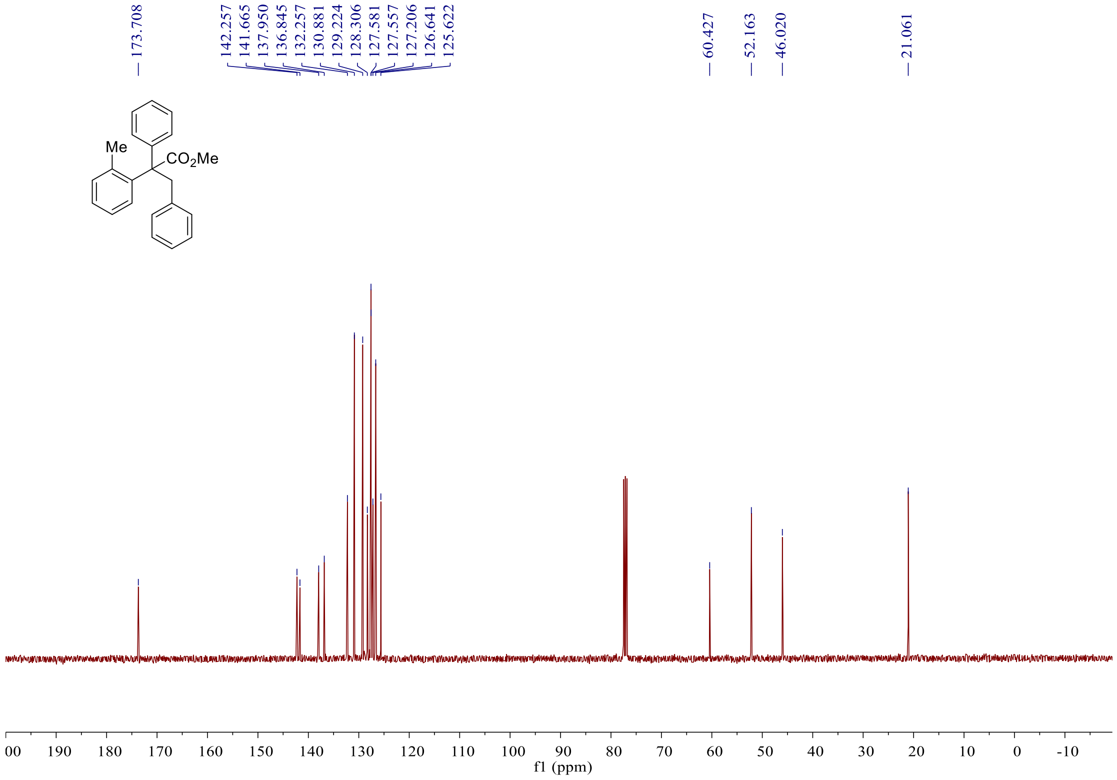
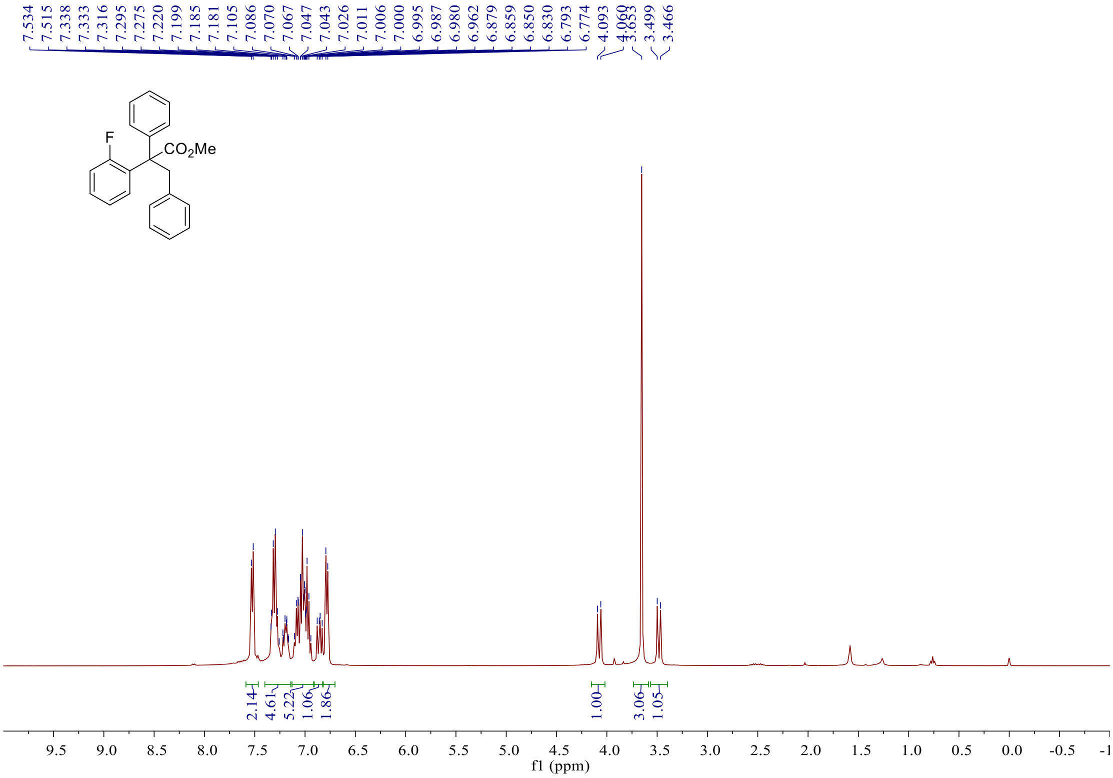
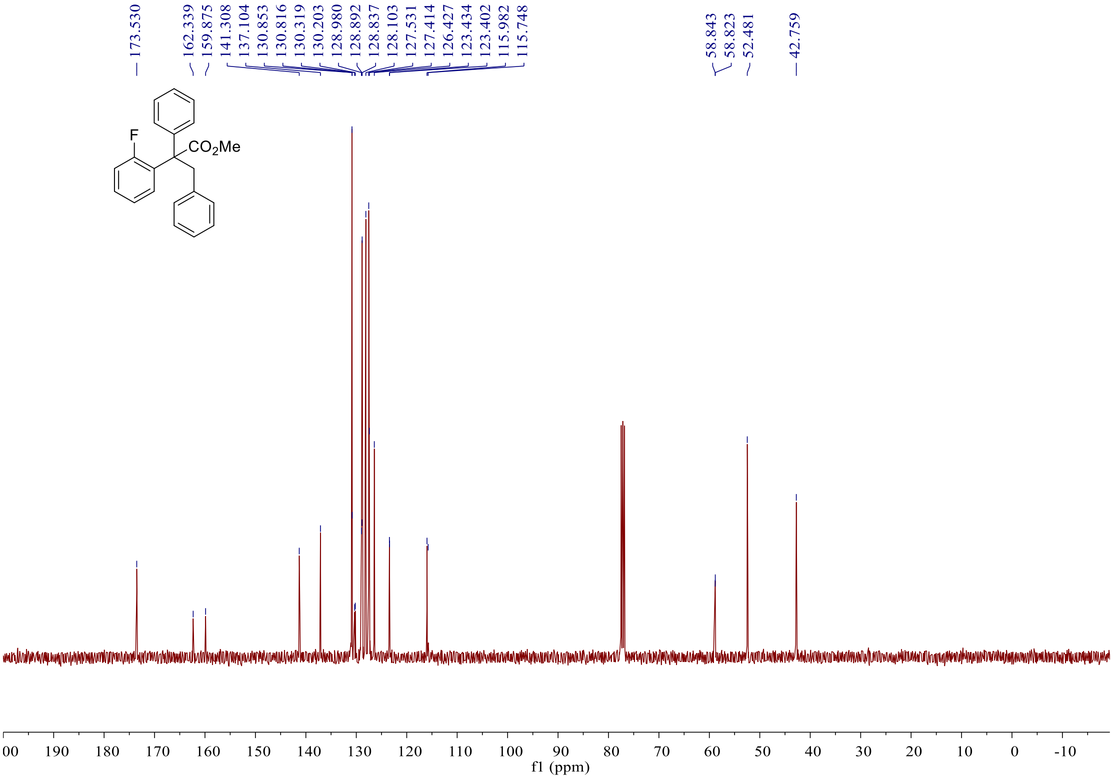
7.282
7.274
7.210
7.201
7.195
7.187
7.180
7.175
7.166
7.161
7.150
7.147
7.144
7.129
7.124
7.114
7.111
7.107
7.079
7.076
7.065
7.060
7.055
7.043
7.040
6.610
6.592
3.819
3.788
3.657
3.644
3.613
1.731
Me
CO2Me
1.11
2.21
6.27
2.92
2.00
1.06
3.05
0.96
2.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


173.708
142.257
141.665
137.950
136.845
132.257
130.881
129.224
128.306
127.581
127.557
127.206
126.641
125.622
60.427
52.163
46.020
21.061
Me
CO2Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

42


7.534
7.515
7.338
7.333
7.316
7.295
7.275
7.220
7.199
7.185
7.181
7.105
7.086
7.070
7.067
7.047
7.043
7.026
7.011
7.006
7.000
6.995
6.987
6.980
6.962
6.879
6.859
6.850
6.830
6.793
6.774
4.093
4.060
3.653
3.499
3.466
F
CO2Me
2.14
4.61
5.22
1.06
1.86
1.00
3.06
1.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


173.530
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130.853
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130.319
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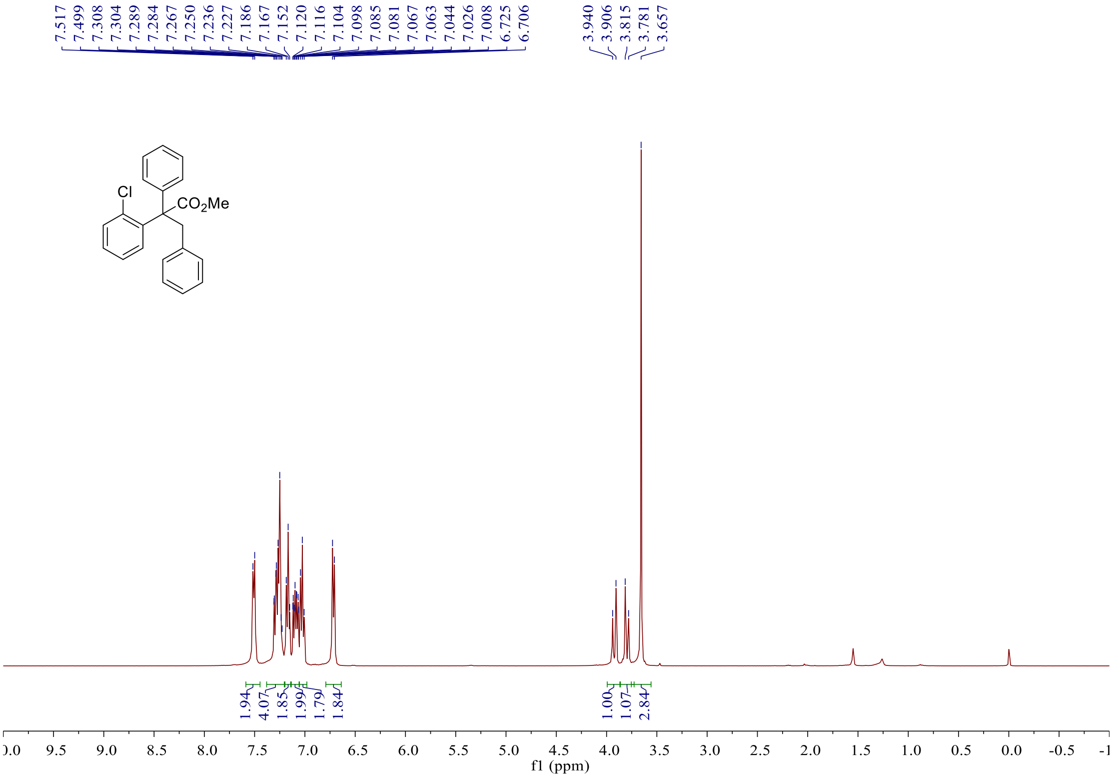
128.980
128.892
128.837
128.103
127.531
127.414
126.427
123.434
123.402
115.982
115.748
58.843
58.823
52.481
42.759
F
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

43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7.304
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7.284
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7.250
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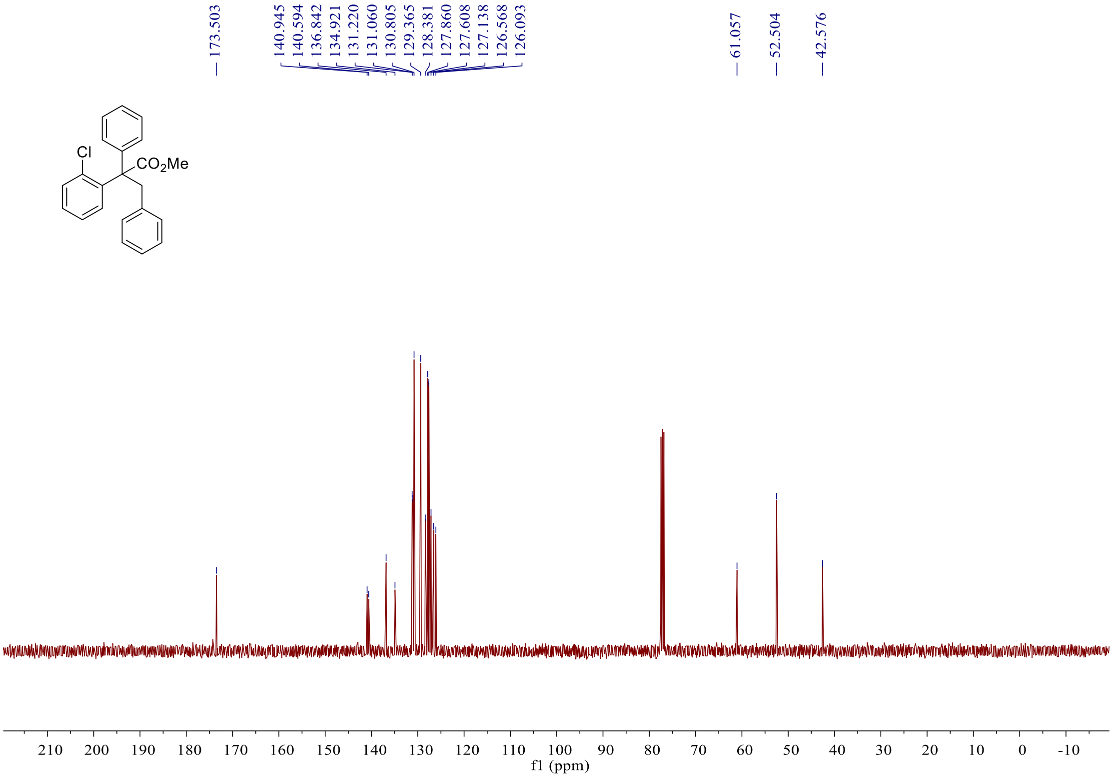
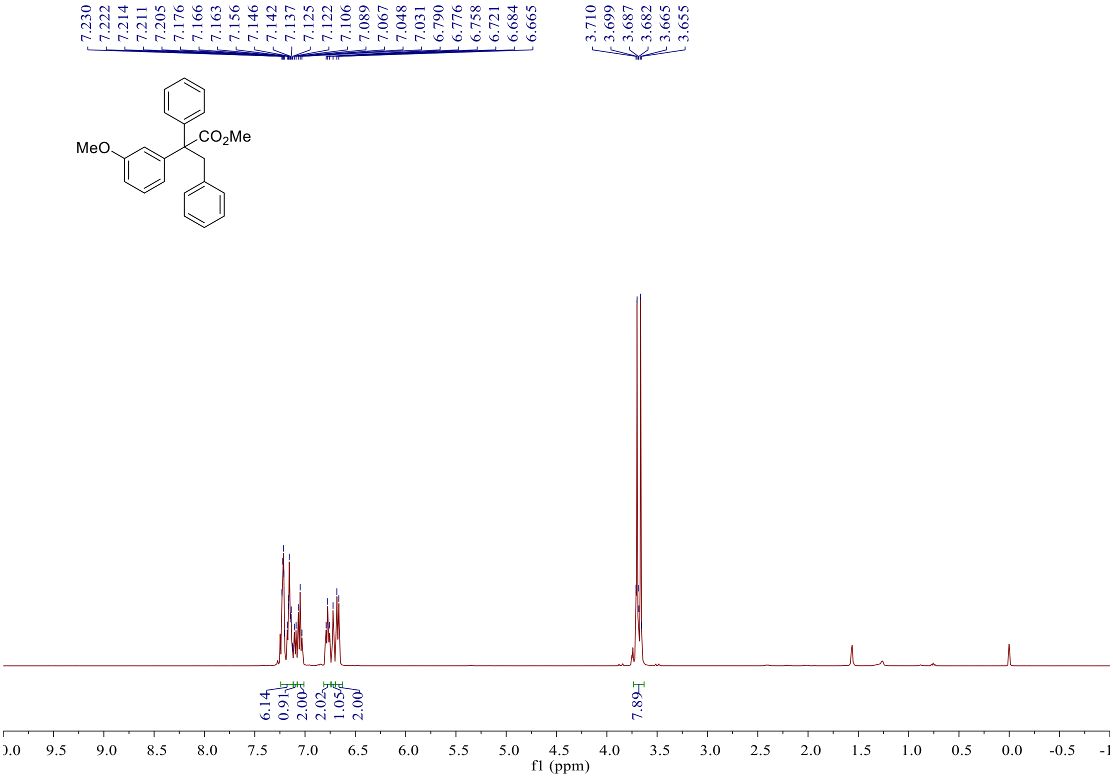
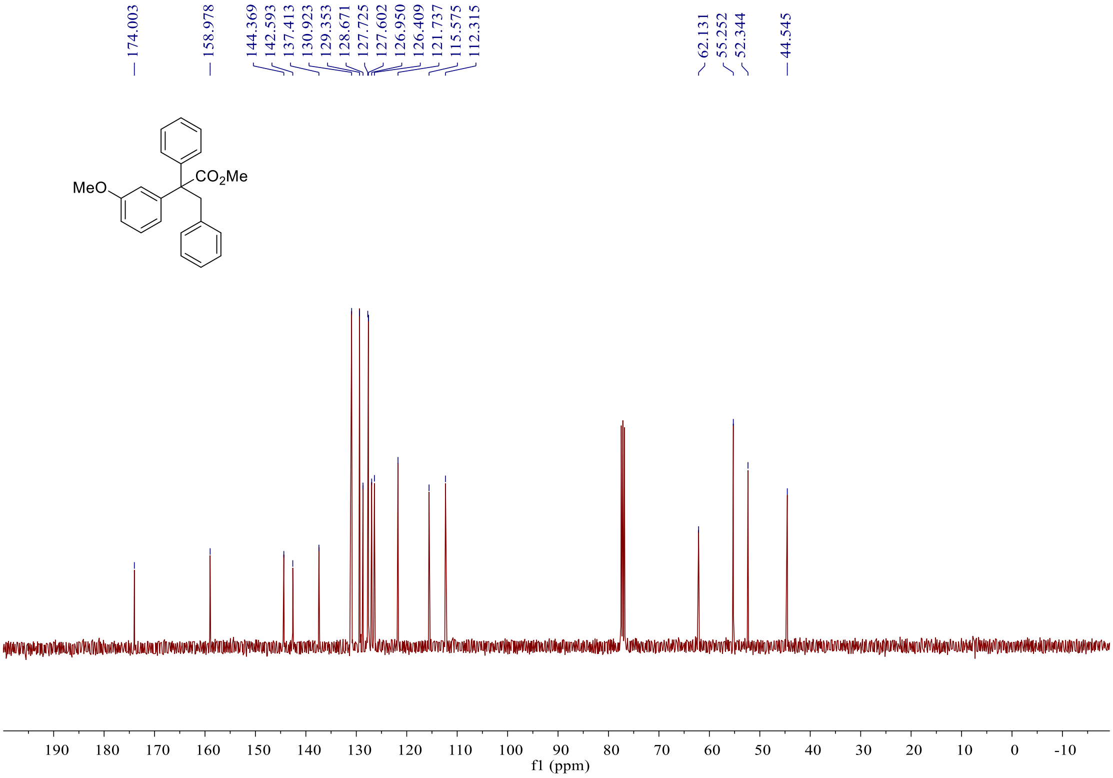
7.227
7.186
7.167
7.152
7.120
7.116
7.104
7.098
7.085
7.081
7.067
7.063
7.044
7.026
7.008
6.725
6.706
3.940
3.906
3.815
3.781
3.657
Cl
CO2Me
1.94
4.07
1.85
1.99
1.79
1.84
1.00
1.07
2.84
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

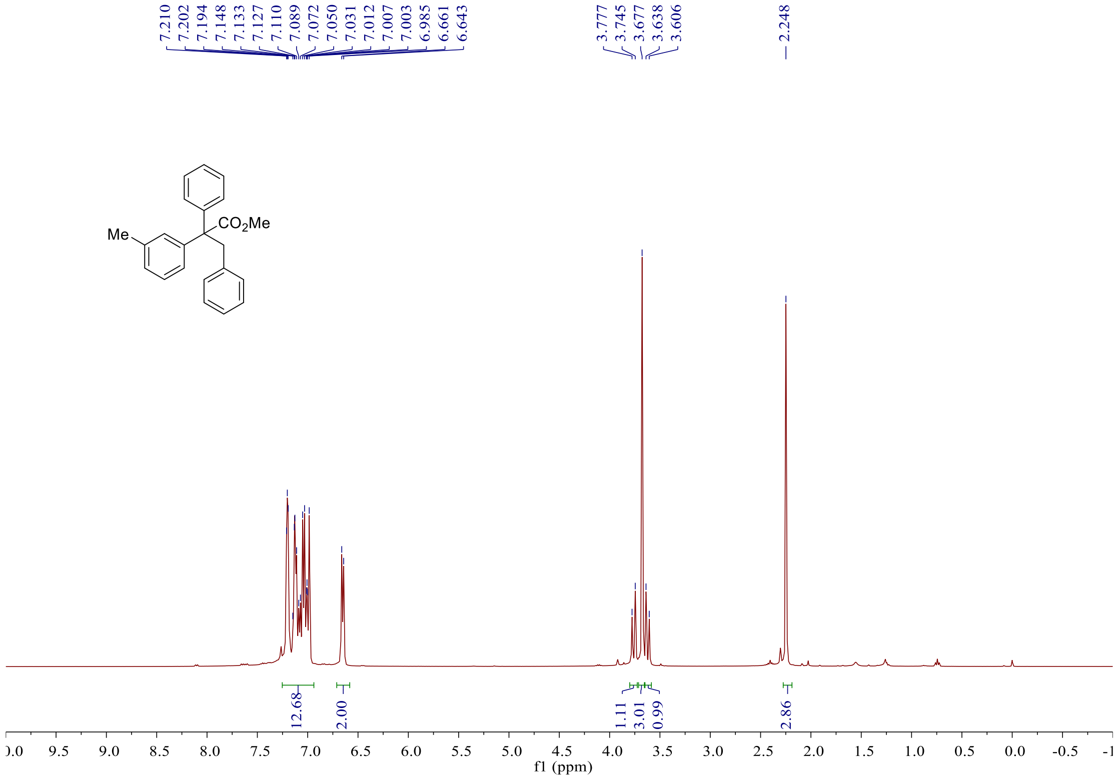

173.503
140.945
140.594
136.842
134.921
131.220
131.060
130.805
129.365
128.381
127.860
127.608
127.138
126.568
126.093
61.057
52.504
42.576
Cl
CO2Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

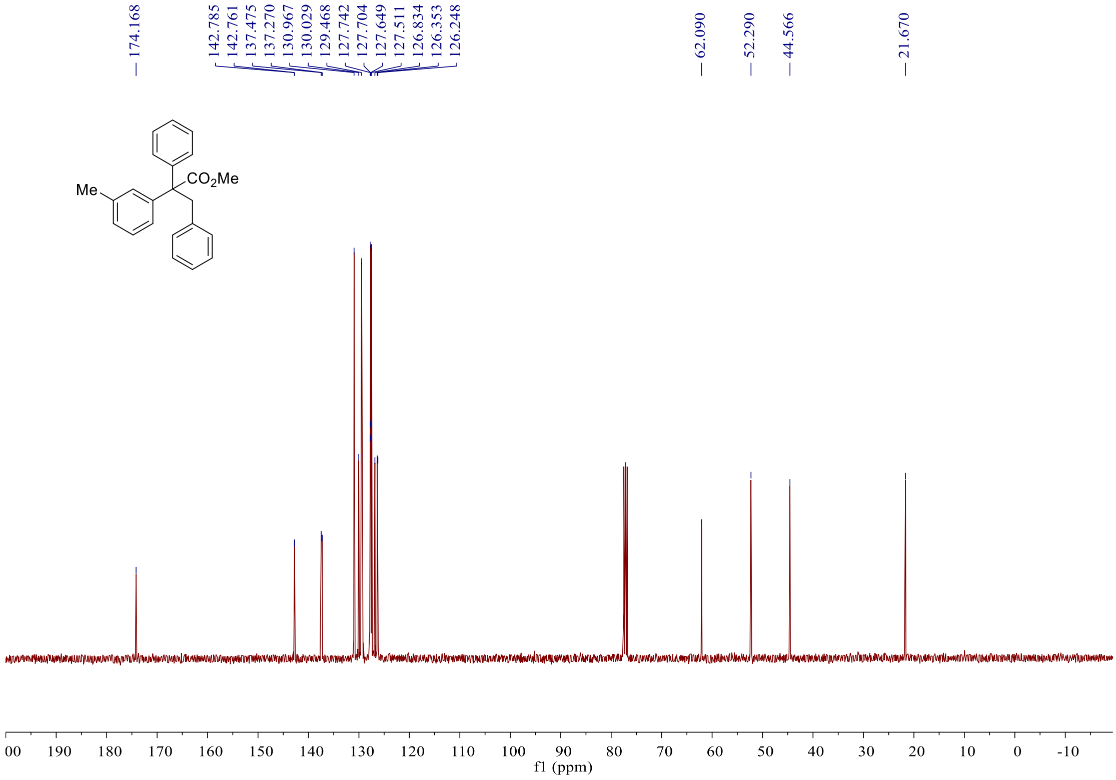
44


7.230
7.222
7.214
7.211
7.205
7.176
7.166
7.163
7.156
7.146
7.142
7.137
7.125
7.122
7.106
7.089
7.067
7.048
7.031
6.790
6.776
6.758
6.721
6.684
6.665
3.710
3.699
3.687
3.682
3.665
3.655
MeO
CO2Me
6.14
0.91
2.00
2.02
1.05
2.00
7.89
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


174.003
158.978
144.369
142.593
137.413
130.923
129.353
128.671
127.725
127.602
126.950
126.409
121.737
115.575
112.315
62.131
55.252
52.344
44.545
MeO
CO2Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

45


7.210
7.202
7.194
7.148
7.133
7.127
7.110
7.089
7.072
7.050
7.031
7.012
7.007
7.003
6.985
6.661
6.643
3.777
3.745
3.677
3.638
3.606
2.248
Me
CO$_2$Me
12.68
2.00
1.11
3.01
0.99
2.86
f1 (ppm)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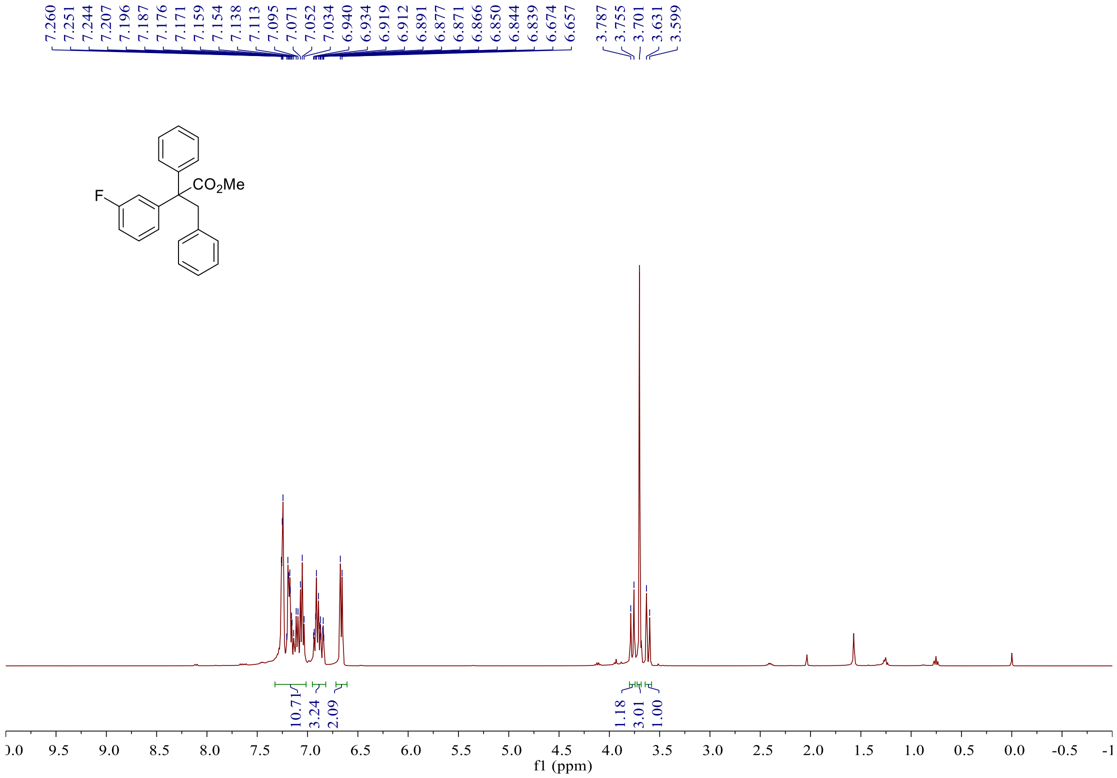
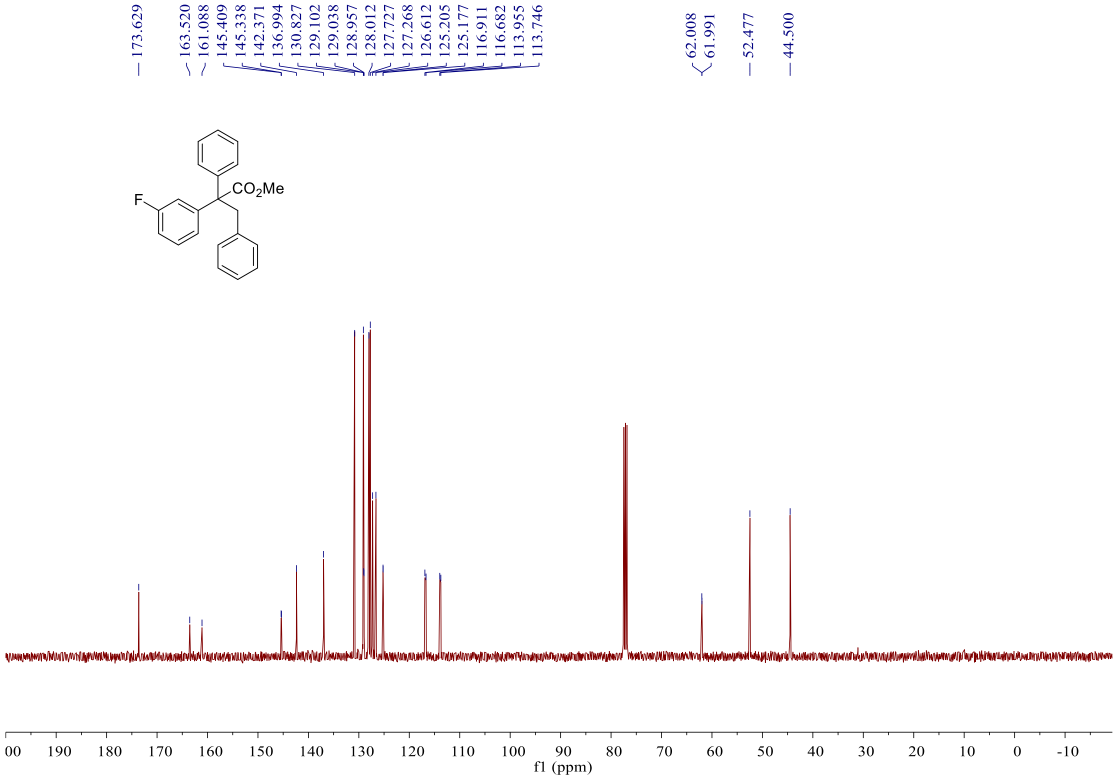
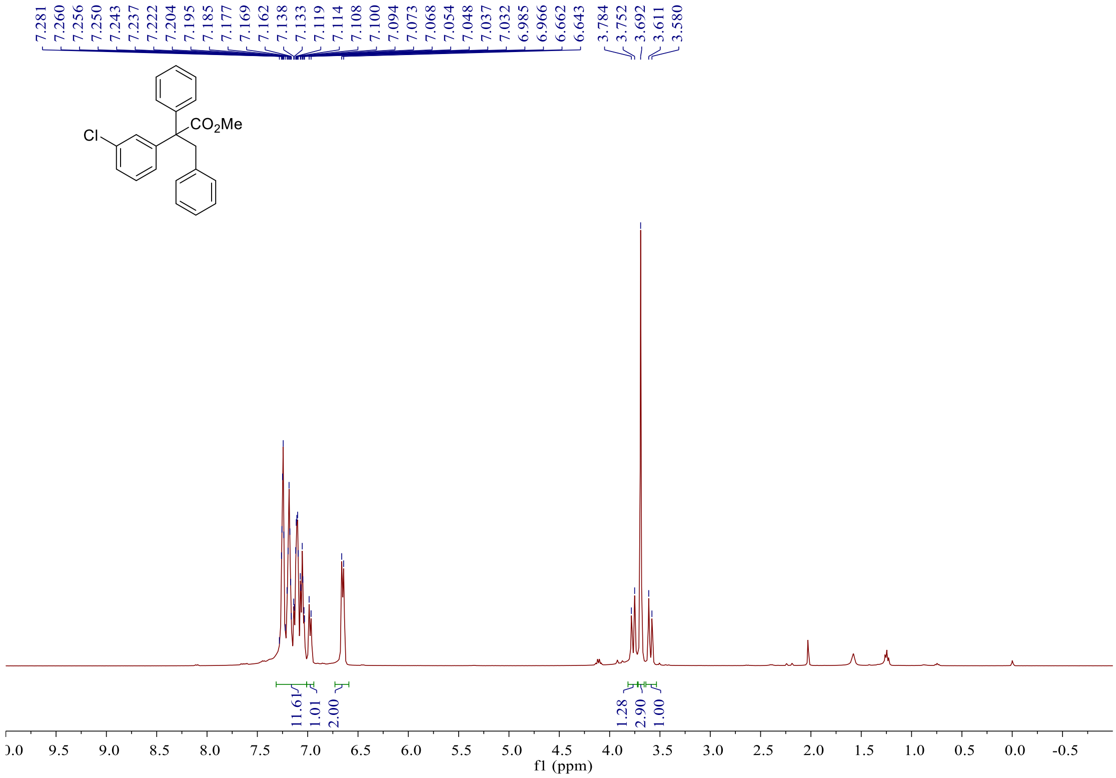
142.785
142.761
137.475
137.270
130.967
130.029
129.468
127.742
127.704
127.649
127.511
126.834
126.353
126.248
62.090
52.290
44.566
21.670
Me
CO$_2$Me
f1 (ppm)

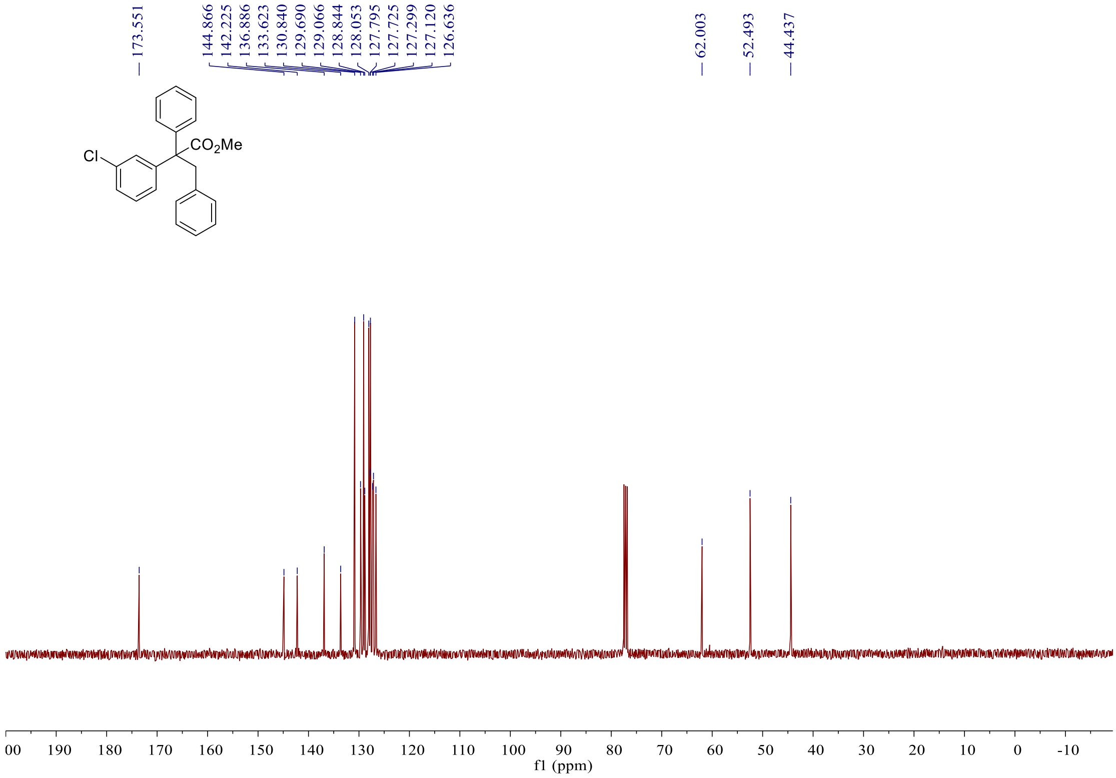
46


7.260
7.251
7.244
7.207
7.196
7.187
7.176
7.171
7.159
7.154
7.138
7.113
7.095
7.071
7.052
7.034
6.940
6.934
6.919
6.912
6.891
6.877
6.871
6.866
6.850
6.844
6.839
6.674
6.657
3.787
3.755
3.701
3.631
3.599
F
CO2Me
10.71
3.24
2.09
1.18
3.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

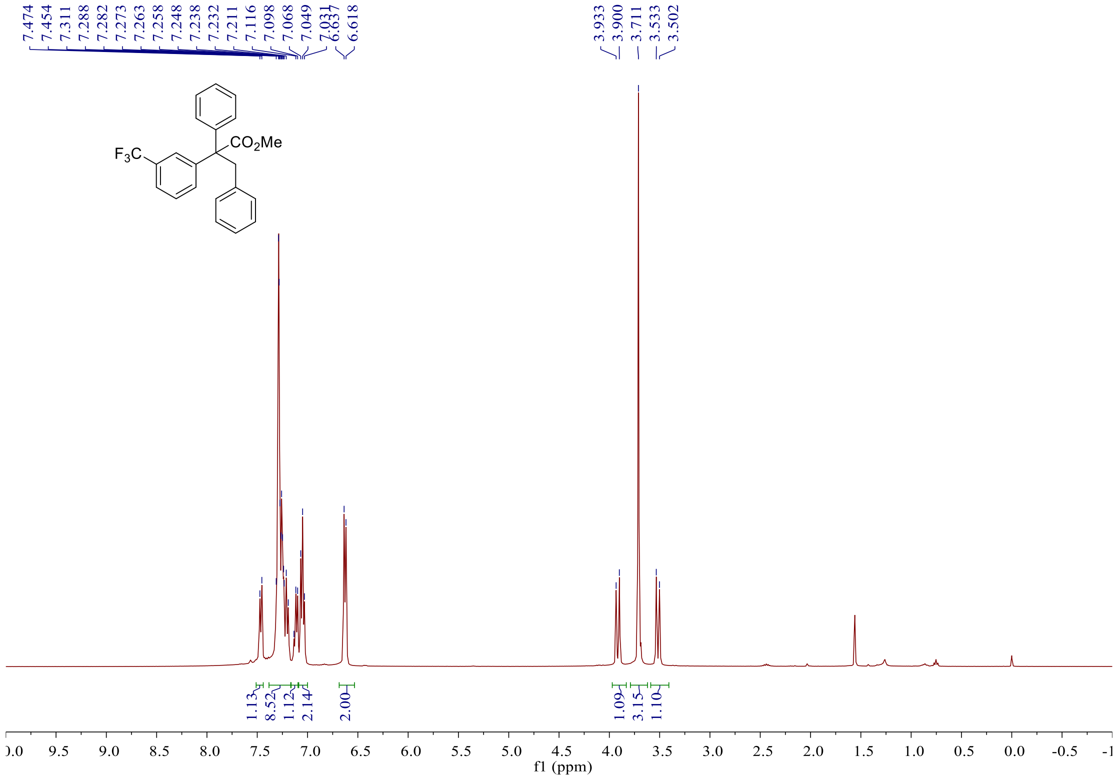

173.629
163.520
161.088
145.409
145.338
142.371
136.994
130.827
129.102
129.038
128.957
128.012
127.727
127.268
126.612
125.205
125.177
116.911
116.682
113.955
113.746
62.008
61.991
52.477
44.500
F
CO2Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

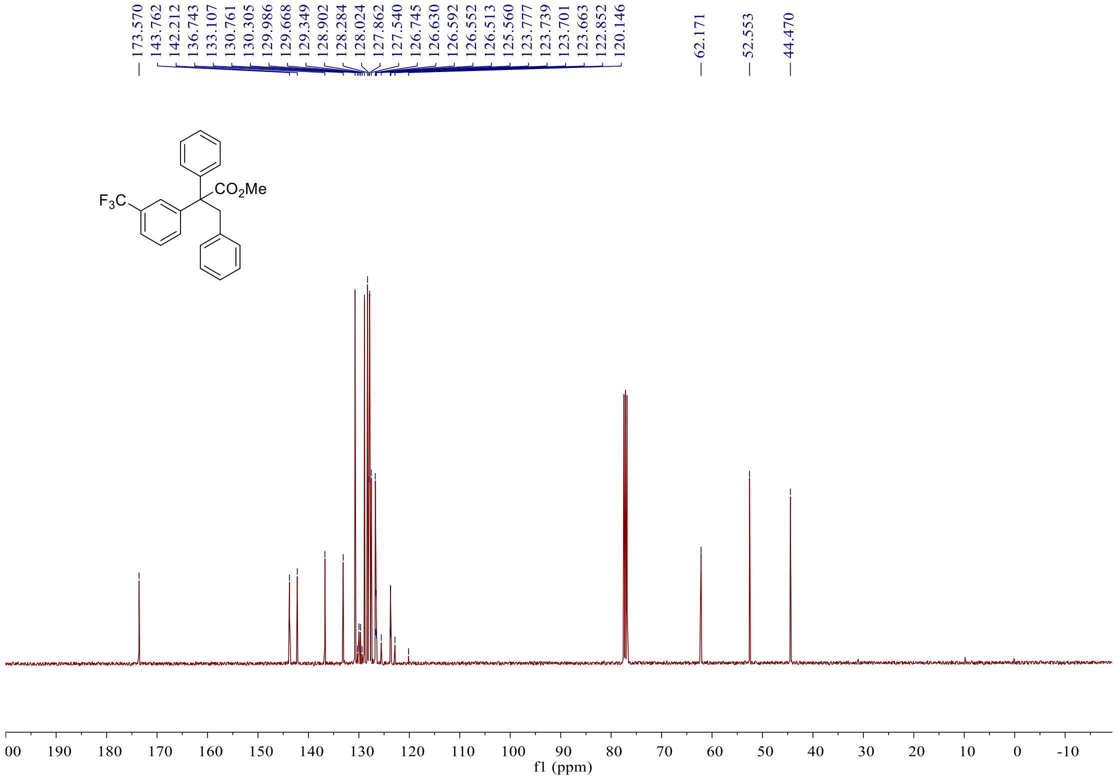
47


7.281
7.260
7.256
7.250
7.243
7.237
7.222
7.204
7.195
7.185
7.177
7.169
7.162
7.138
7.133
7.119
7.114
7.108
7.100
7.094
7.073
7.068
7.054
7.048
7.037
7.032
6.985
6.966
6.662
6.643
3.784
3.752
3.692
3.611
3.580
Cl
CO2Me
11.61
1.01
2.00
1.28
2.90
1.00
).0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


173.551
144.866
142.225
136.886
133.623
130.840
129.690
129.066
128.844
128.053
127.795
127.725
127.299
127.120
126.636
62.003
52.493
44.437
Cl
CO2Me
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

48


7.474
7.454
7.311
7.288
7.282
7.273
7.263
7.258
7.248
7.238
7.232
7.211
7.116
7.098
7.068
7.049
7.031
6.637
6.618
3.933
3.900
3.711
3.533
3.502
F3C
CO2Me
1.13
8.52
1.12
2.14
2.00
1.09
3.15
1.10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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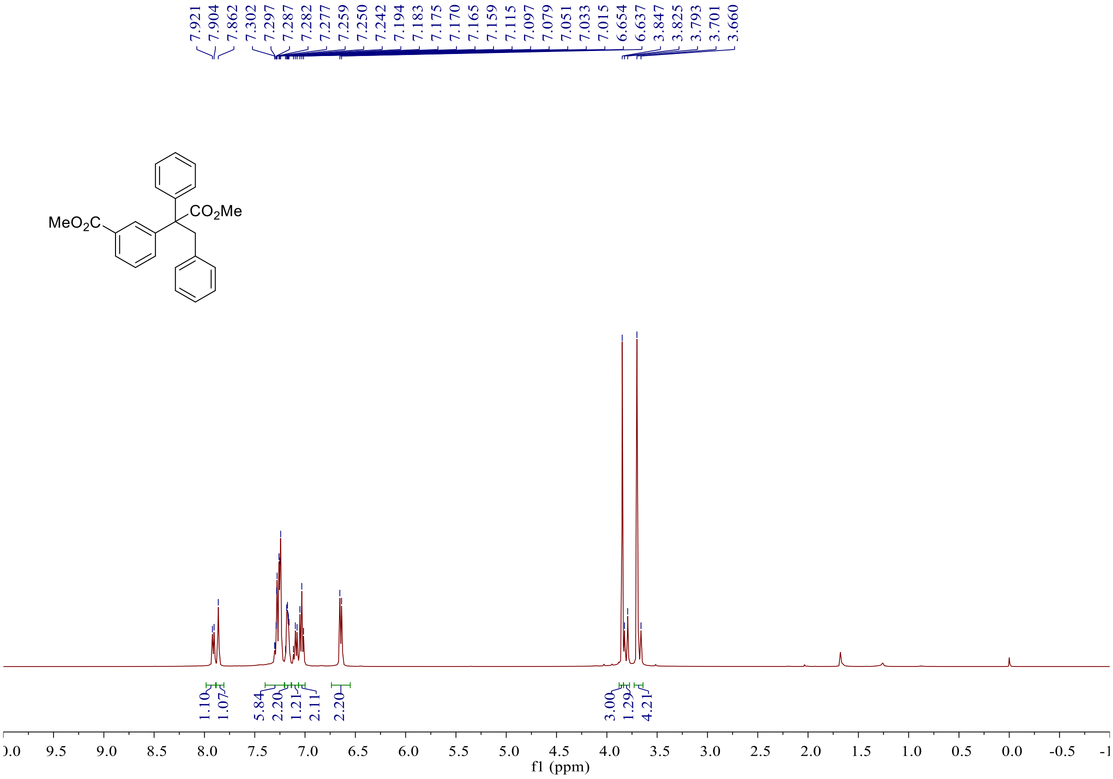
143.762
142.212
136.743
133.107
130.761
130.305
129.986
129.668
129.349
128.902
128.284
128.024
127.862
127.540
126.745
126.630
126.592
126.552
126.513
125.560
123.777
123.739
123.701
123.663
122.852
120.146
62.171
52.553
44.470
F3C
CO2Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

49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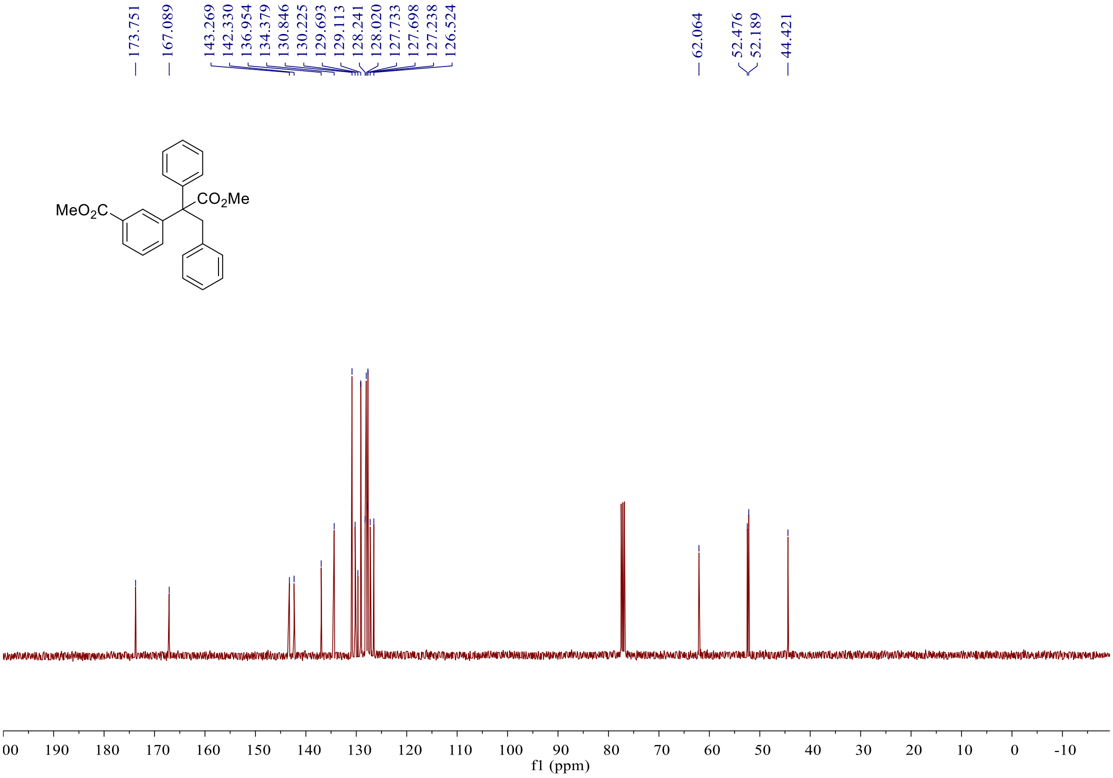
7.904
7.862
7.302
7.297
7.287
7.282
7.277
7.259
7.250
7.242
7.194
7.183
7.175
7.170
7.165
7.159
7.115
7.097
7.079
7.051
7.033
7.015
6.654
6.637
3.847
3.825
3.793
3.701
3.660
MeO2C
CO2Me
1.10
1.07
5.84
2.20
1.21
2.11
2.20
3.00
1.29
4.21
f1 (ppm)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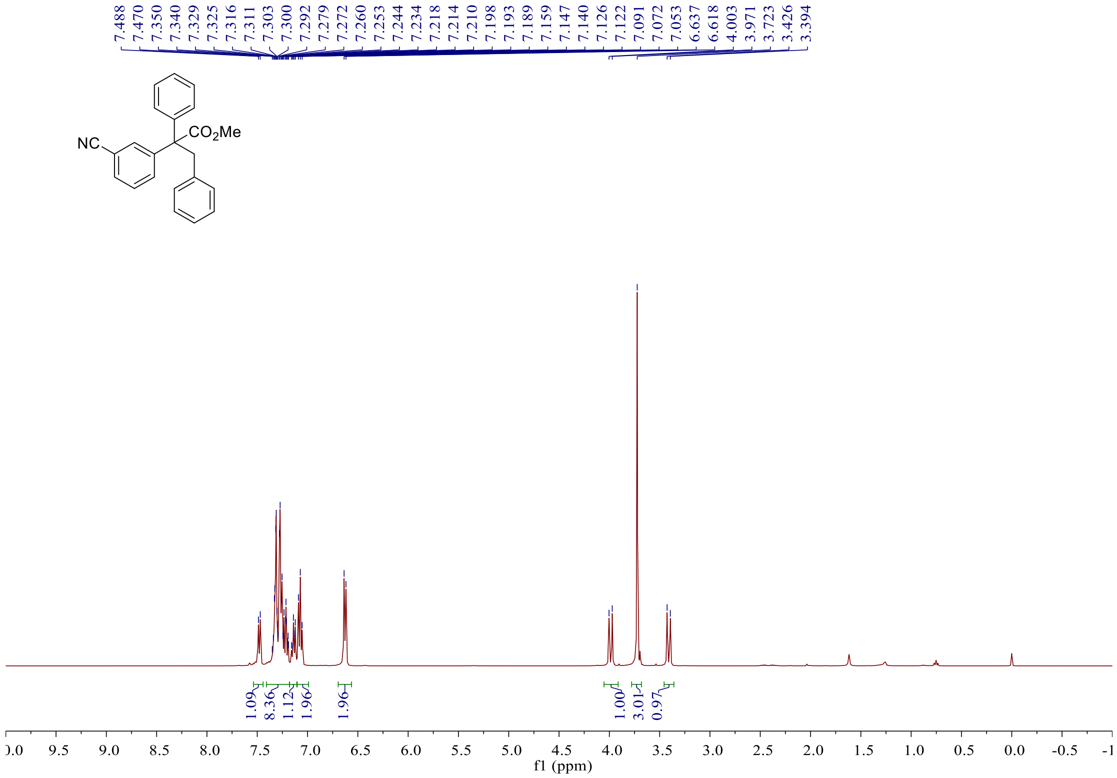
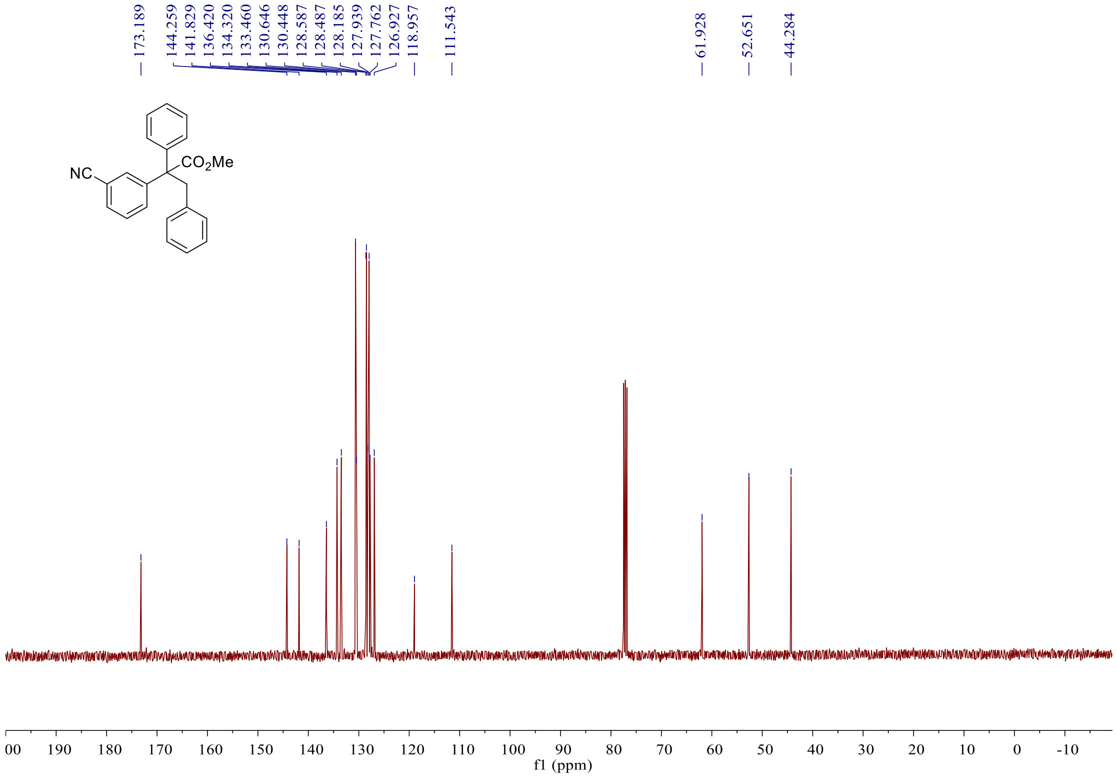
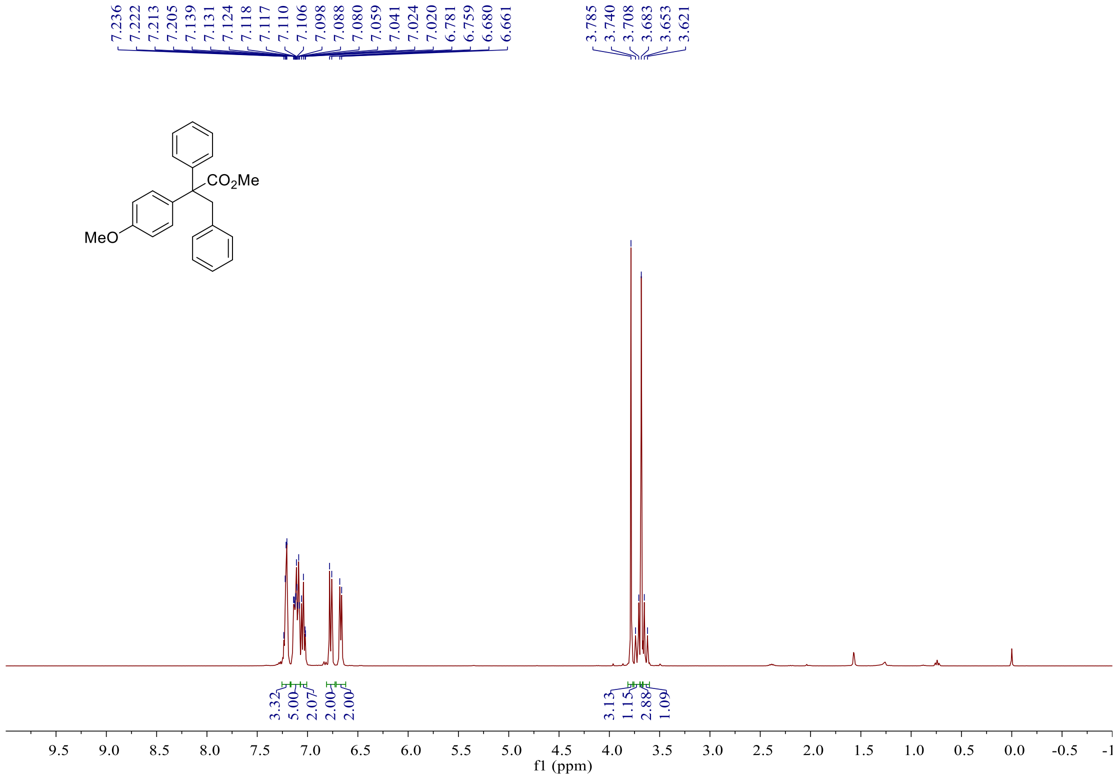
143.269
142.330
136.954
134.379
130.846
130.225
129.693
129.113
128.241
128.020
127.733
127.698
127.238
126.524
62.064
52.476
52.189
44.421
MeO2C
CO2Me
f1 (ppm)

50


7.488
7.470
7.350
7.340
7.329
7.325
7.316
7.311
7.303
7.300
7.292
7.279
7.272
7.260
7.253
7.244
7.234
7.218
7.214
7.210
7.198
7.193
7.189
7.159
7.147
7.140
7.126
7.122
7.091
7.072
7.053
6.637
6.618
4.003
3.971
3.723
3.426
3.394
NC
CO2Me
1.09
8.36
1.12
1.96
1.96
1.00
3.01
0.97
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


173.189
144.259
141.829
136.420
134.320
133.460
130.646
130.448
128.587
128.487
128.185
127.939
127.762
126.927
118.957
111.543
61.928
52.651
44.284
NC
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

51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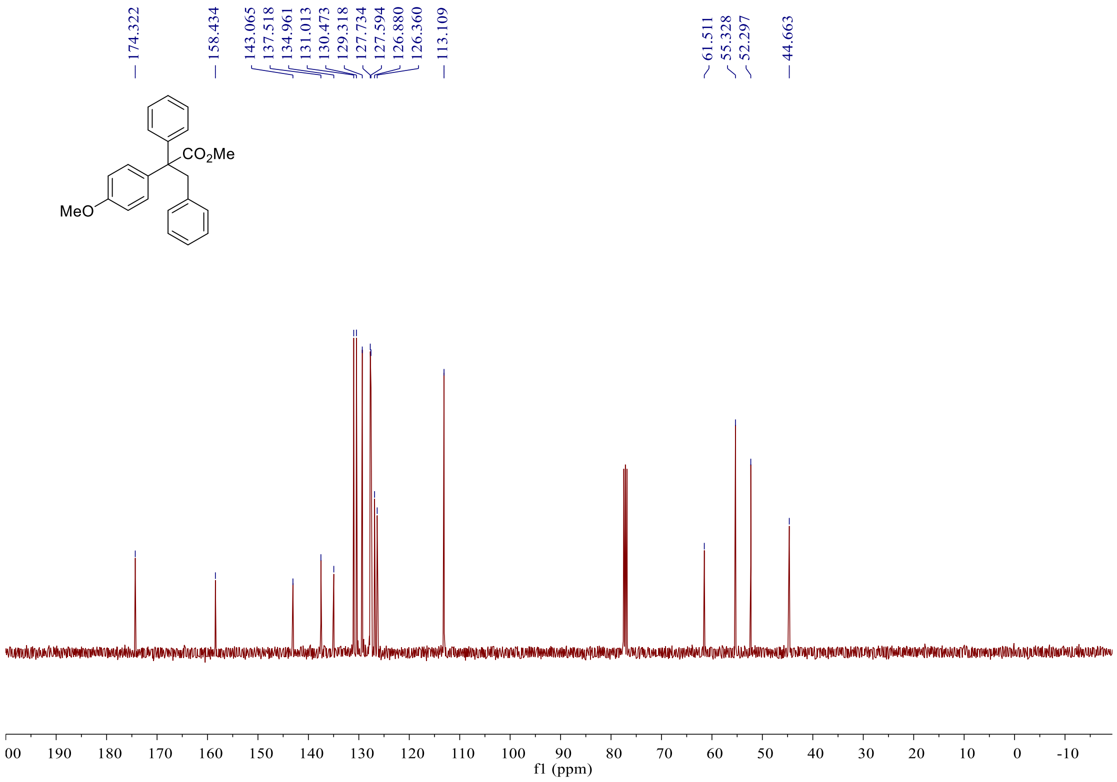
7.222
7.213
7.205
7.139
7.131
7.124
7.118
7.117
7.110
7.106
7.098
7.088
7.080
7.059
7.041
7.024
7.020
6.781
6.759
6.680
6.661
3.785
3.740
3.708
3.683
3.653
3.621
CO$_2$Me
MeO
3.32
5.00
2.07
2.00
2.00
3.13
1.15
2.88
1.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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158.434
143.065
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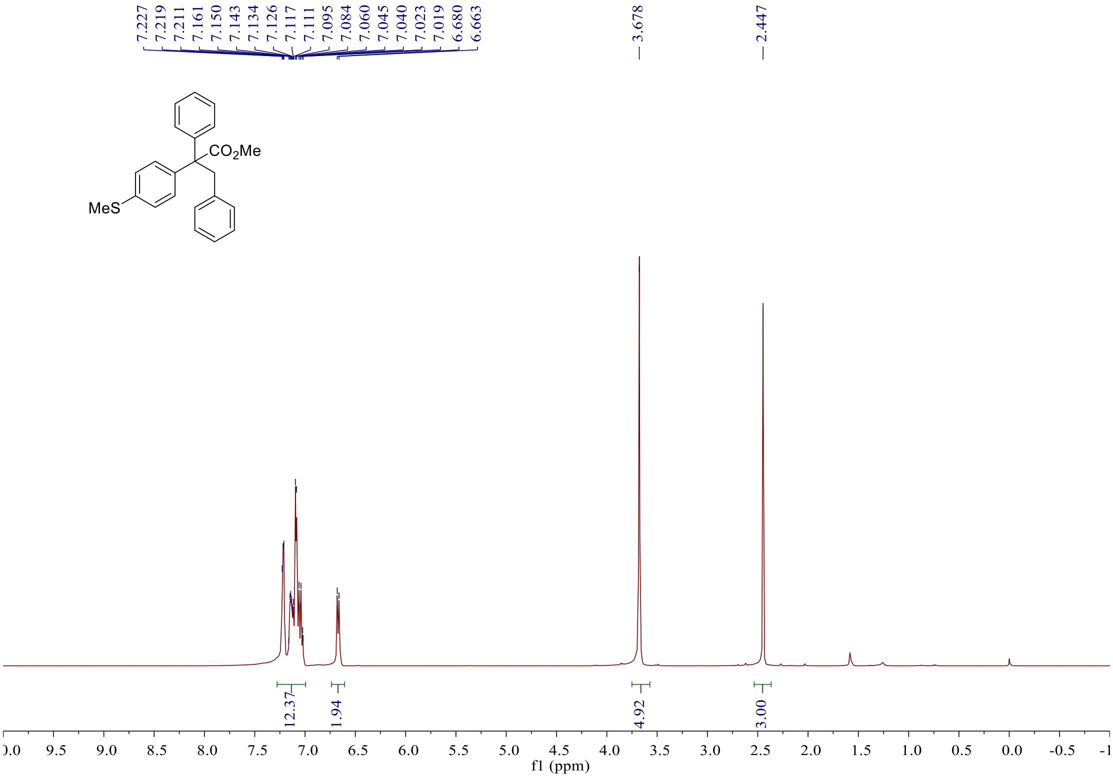
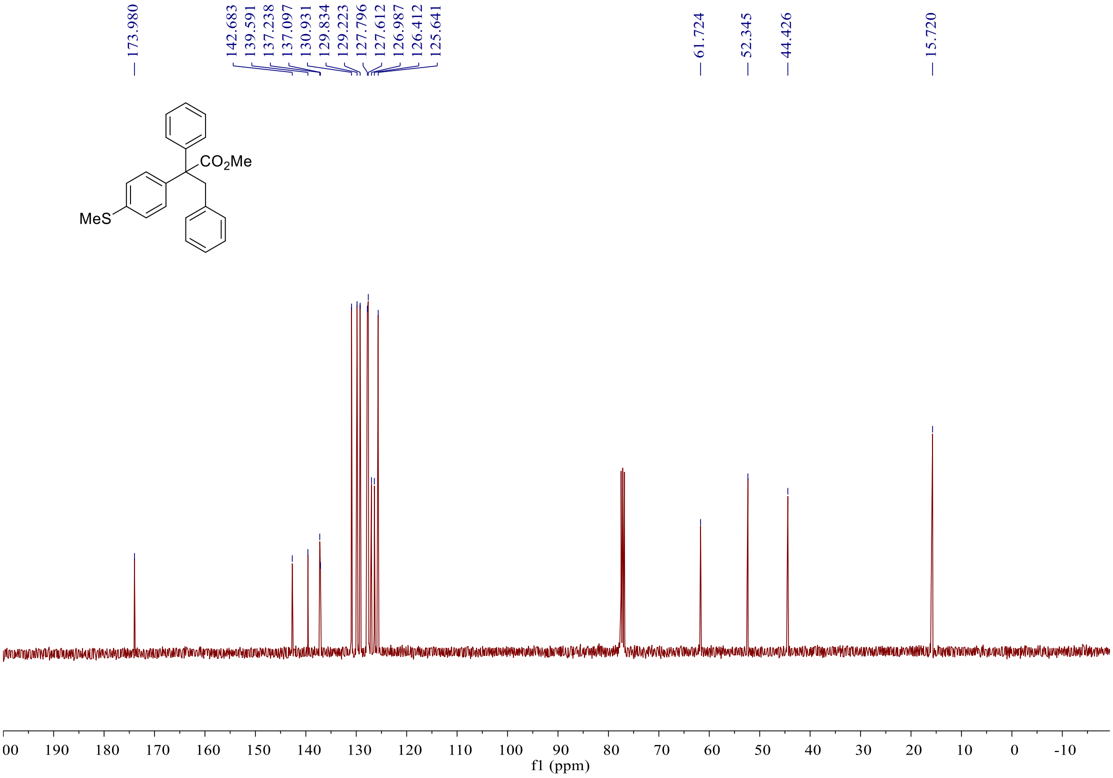
134.961
131.013
130.473
129.318
127.734
127.594
126.880
126.360
113.109
61.511
55.328
52.297
44.663
CO$_2$Me
MeO
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

52


7.227
7.219
7.211
7.161
7.150
7.143
7.134
7.126
7.117
7.111
7.095
7.084
7.060
7.045
7.040
7.023
7.019
6.680
6.663
3.678
2.447
CO2Me
MeS
12.37
1.94
4.92
3.00
).0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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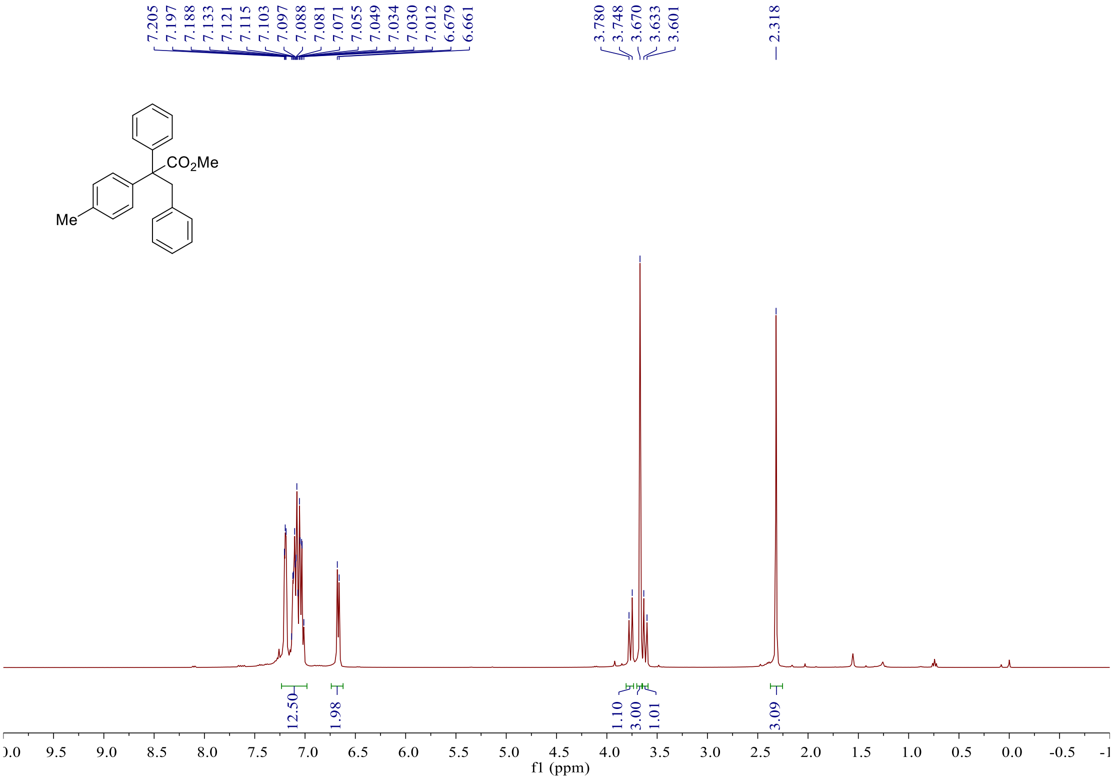
137.238
137.097
130.931
129.834
129.223
127.796
127.612
126.987
126.412
125.641
61.724
52.345
44.426
15.720
CO2Me
MeS
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

53


7.205
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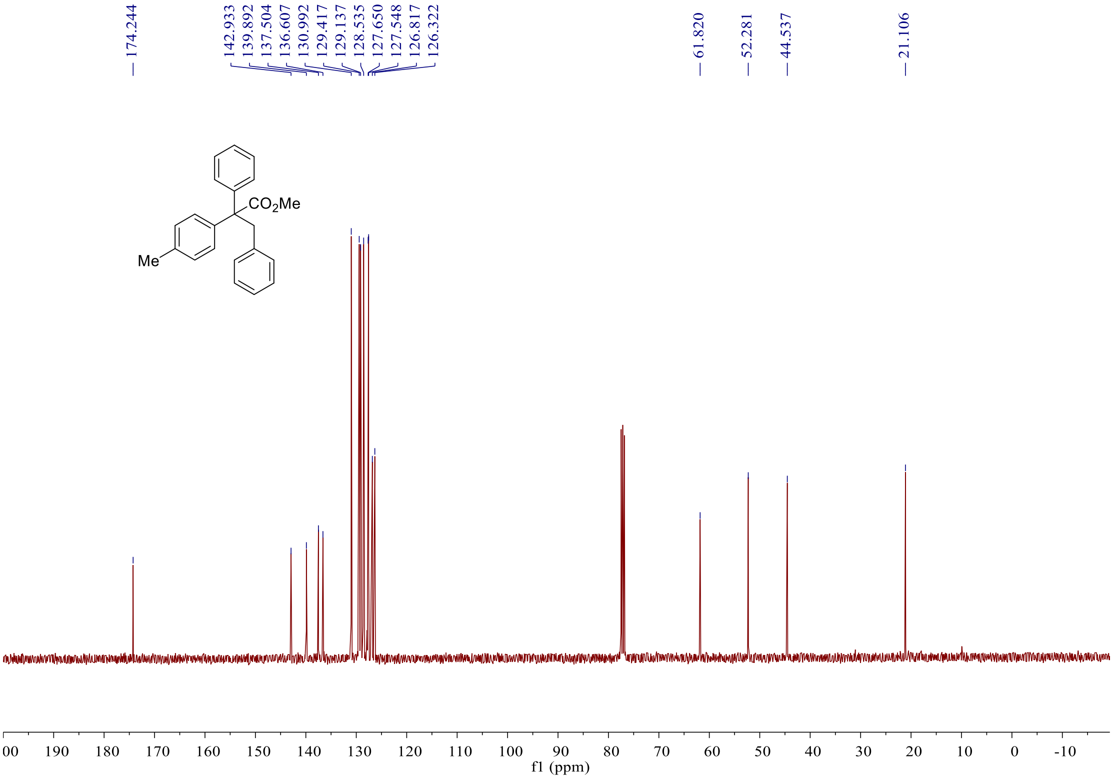
7.121
7.115
7.103
7.097
7.088
7.081
7.071
7.055
7.049
7.034
7.030
7.012
6.679
6.661
3.780
3.748
3.670
3.633
3.601
2.318
CO2Me
Me
12.50
1.98
1.10
3.00
1.01
3.09
f1 (ppm)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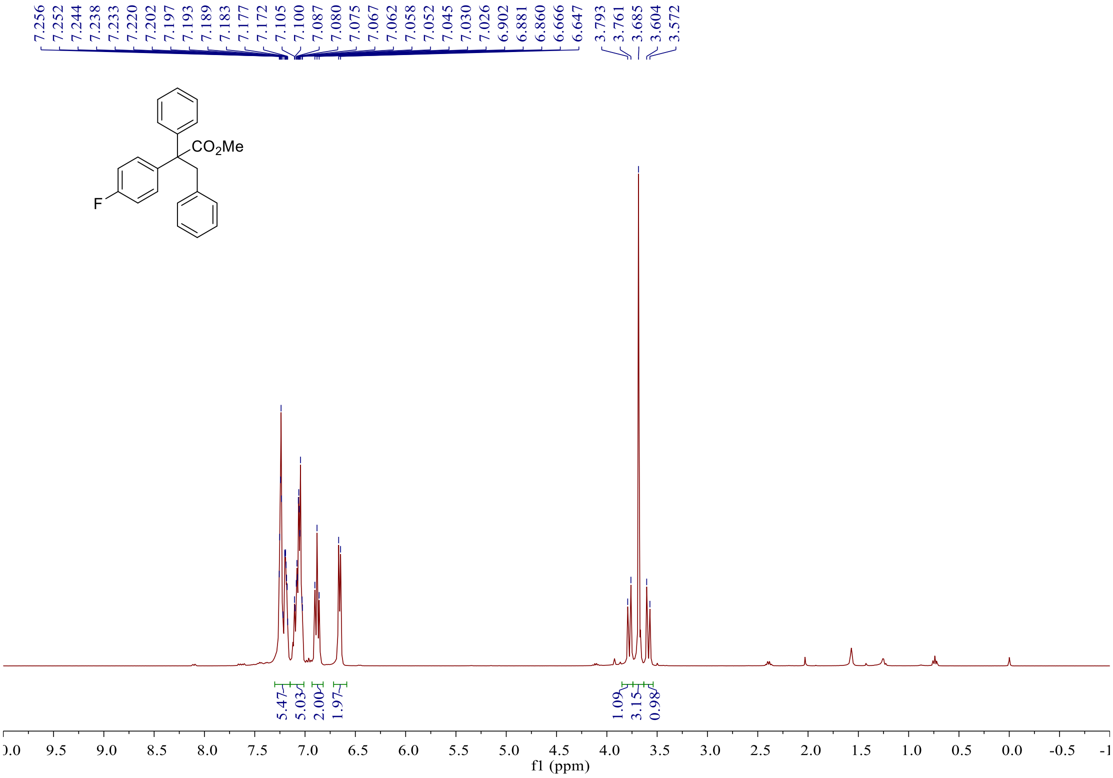
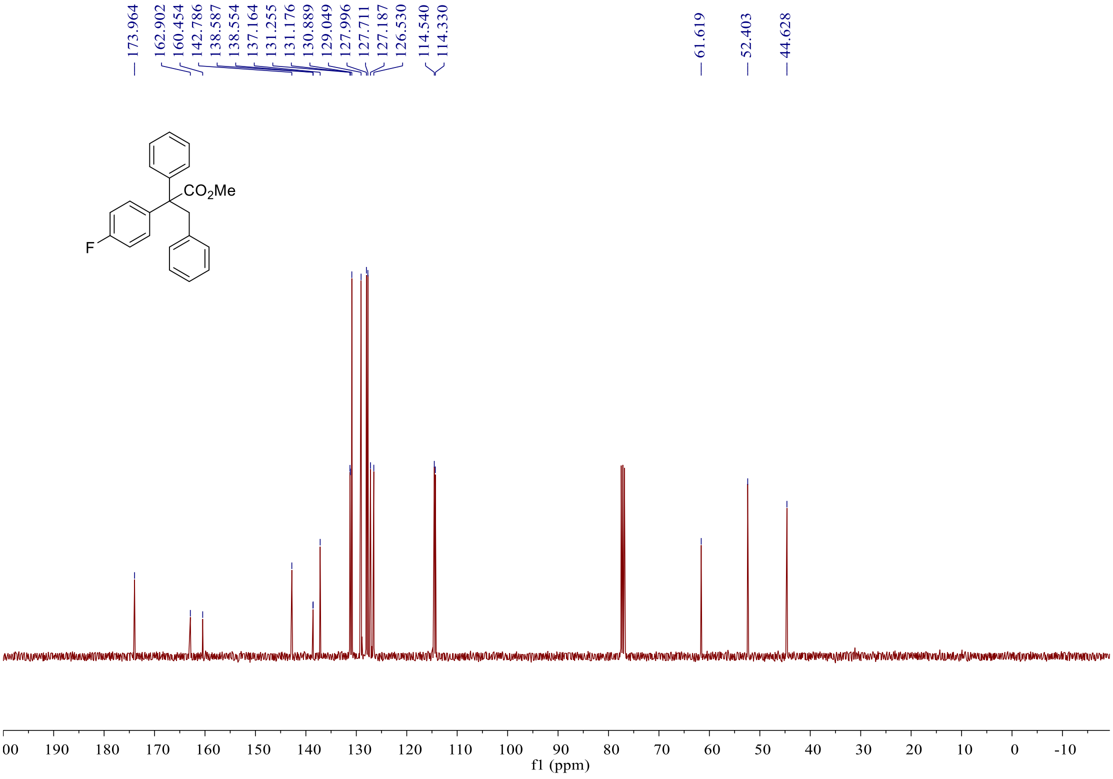
137.504
136.607
130.992
129.417
129.137
128.535
127.650
127.548
126.817
126.322
61.820
52.281
44.537
21.106
CO2Me
Me
f1 (ppm)

54


7.256
7.252
7.244
7.238
7.233
7.220
7.202
7.197
7.193
7.189
7.183
7.177
7.172
7.105
7.100
7.087
7.080
7.075
7.067
7.062
7.058
7.052
7.045
7.030
7.026
6.902
6.881
6.860
6.666
6.647
3.793
3.761
3.685
3.604
3.572
CO2Me
F
5.47
5.03
2.00
1.97
1.09
3.15
0.98
f1 (ppm)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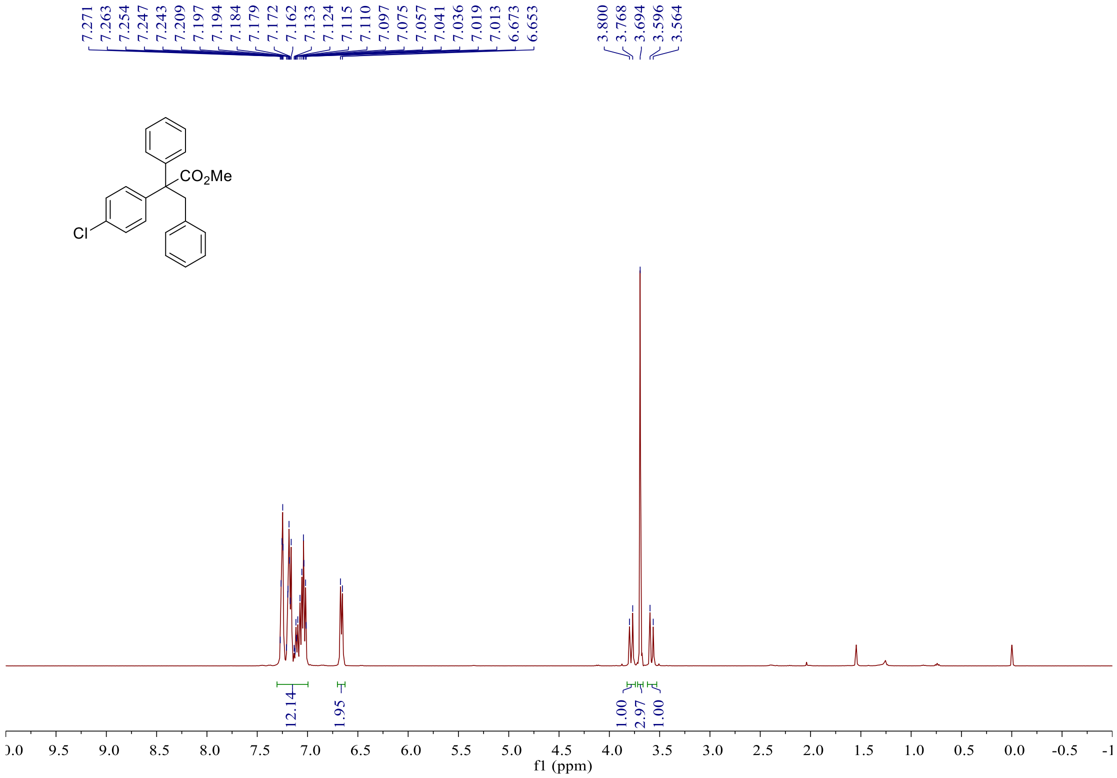
127.711
127.187
126.530
114.540
114.330
61.619
52.403
44.628
CO2Me
F
f1 (ppm)

55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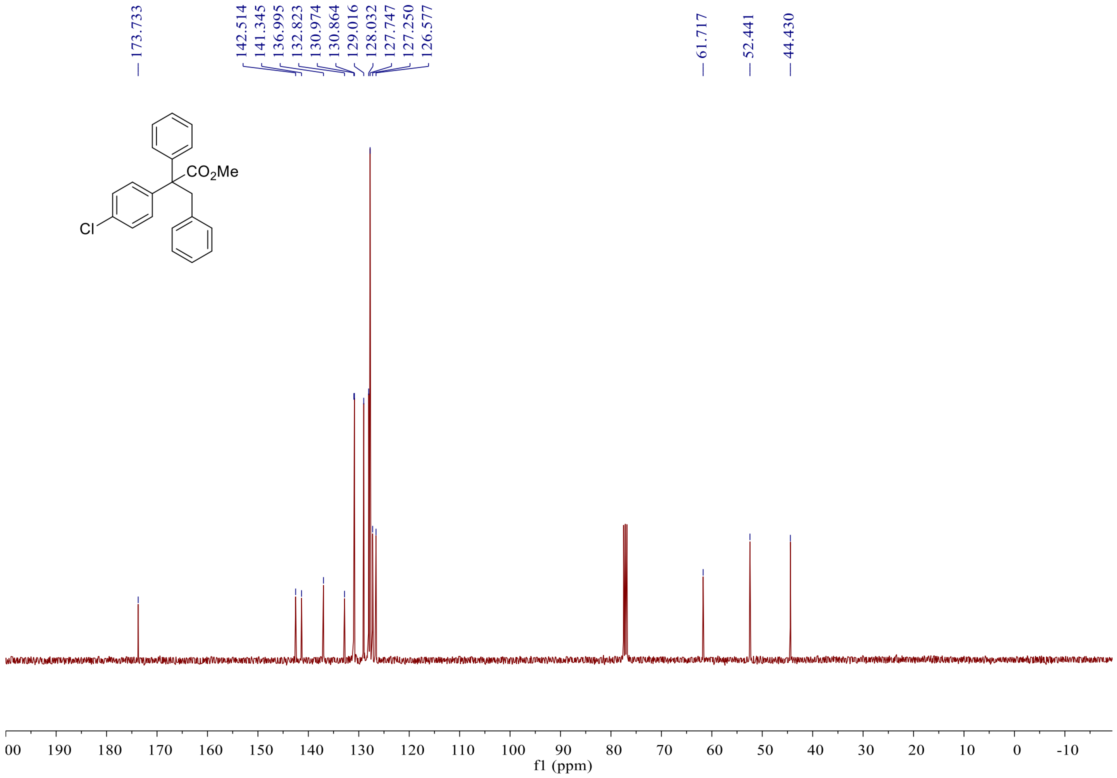
7.243
7.209
7.197
7.194
7.184
7.179
7.172
7.162
7.133
7.124
7.115
7.110
7.097
7.075
7.057
7.041
7.036
7.019
7.013
6.673
6.653
3.800
3.768
3.694
3.596
3.564
CO2Me
Cl
12.14
1.95
1.00
2.97
1.00
f1 (ppm)


173.733
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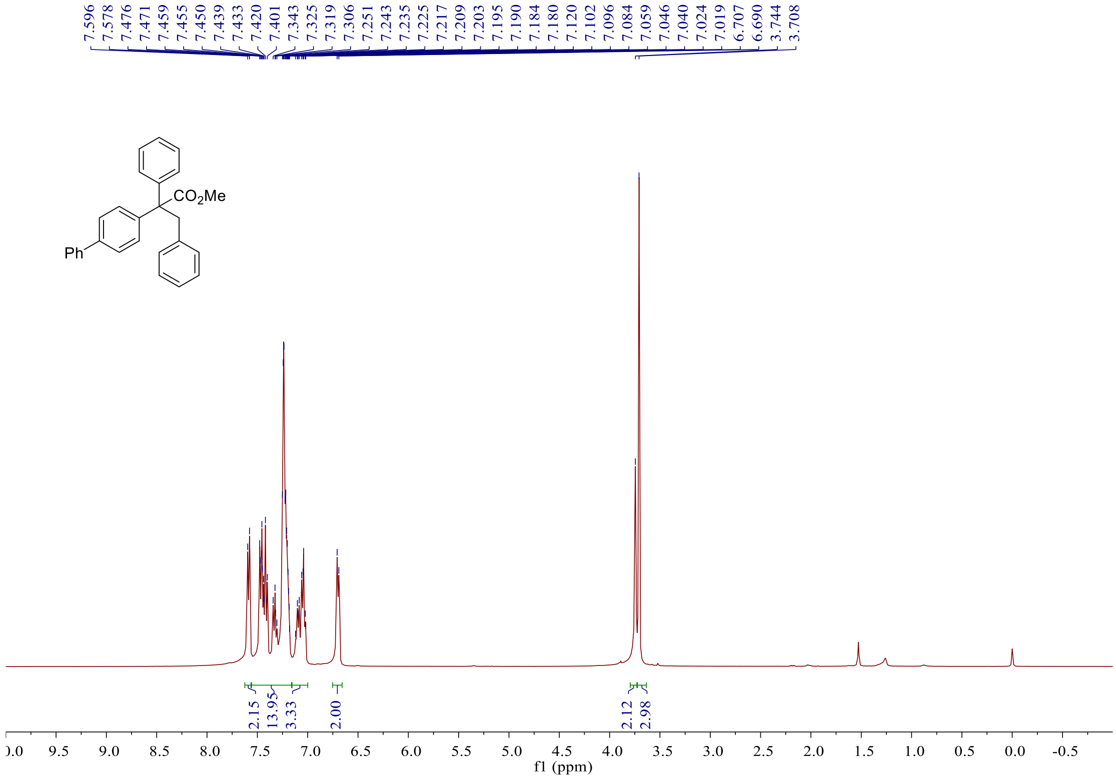
141.345
136.995
132.823
130.974
130.864
129.016
128.032
127.747
127.250
126.577
61.717
52.441
44.430
CO2Me
Cl
f1 (ppm)

56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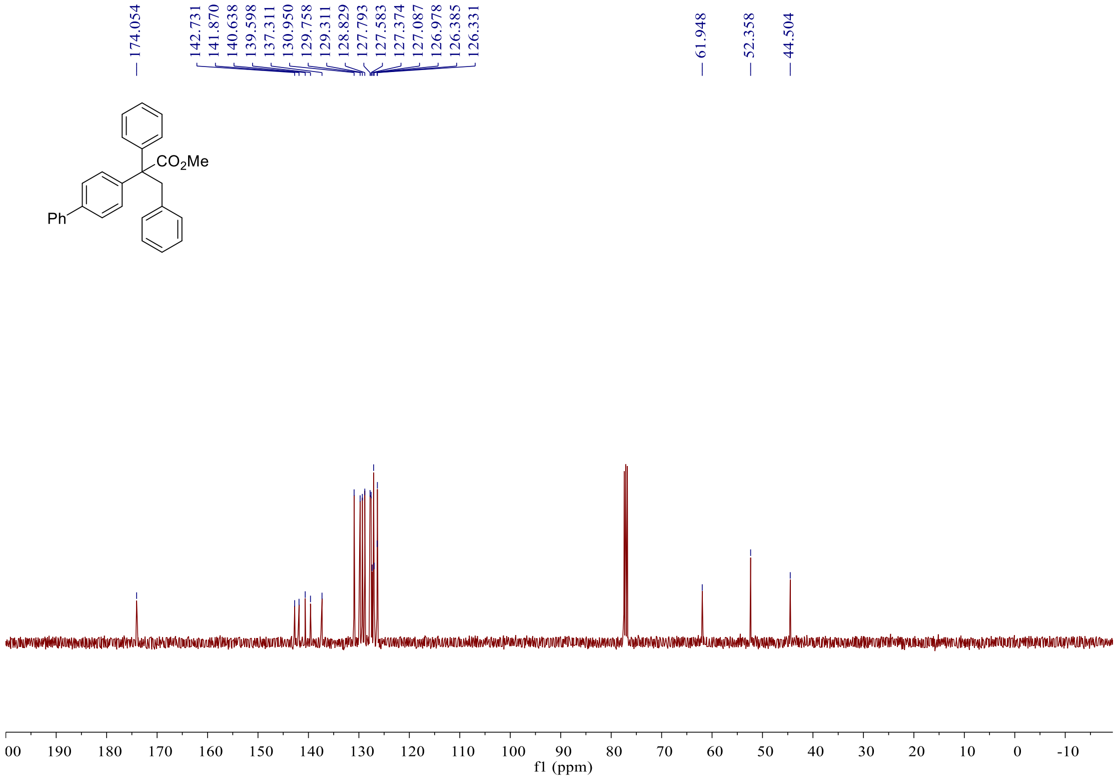
7.439
7.433
7.420
7.401
7.343
7.325
7.319
7.306
7.251
7.243
7.235
7.225
7.217
7.209
7.203
7.195
7.190
7.184
7.180
7.120
7.102
7.096
7.084
7.059
7.046
7.040
7.024
7.019
6.707
6.690
3.744
3.708
CO2Me
Ph
2.15
13.95
3.33
2.00
2.12
2.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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139.598
137.311
130.950
129.758
129.311
128.829
127.793
127.583
127.374
127.087
126.978
126.385
126.331
61.948
52.358
44.504
CO2Me
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
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20
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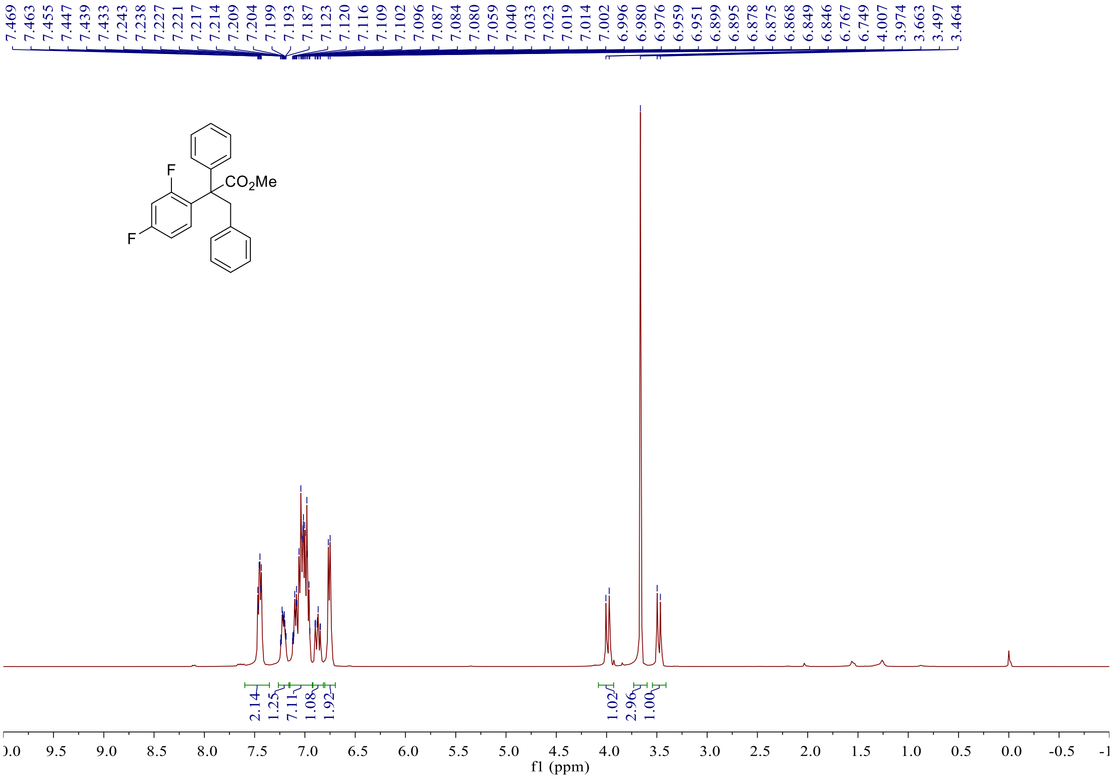
0
-10
f1 (ppm)

57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7.217
7.214
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7.204
7.199
7.193
7.187
7.123
7.120
7.116
7.109
7.102
7.096
7.087
7.084
7.080
7.059
7.040
7.033
7.023
7.019
7.014
7.002
6.996
6.980
6.976
6.959
6.951
6.899
6.895
6.878
6.875
6.868
6.849
6.846
6.767
6.749
4.007
3.974
3.663
3.497
3.464
F
F
CO2Me
2.14
1.25
7.11
1.08
1.92
1.02
2.96
1.00
).0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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1.5
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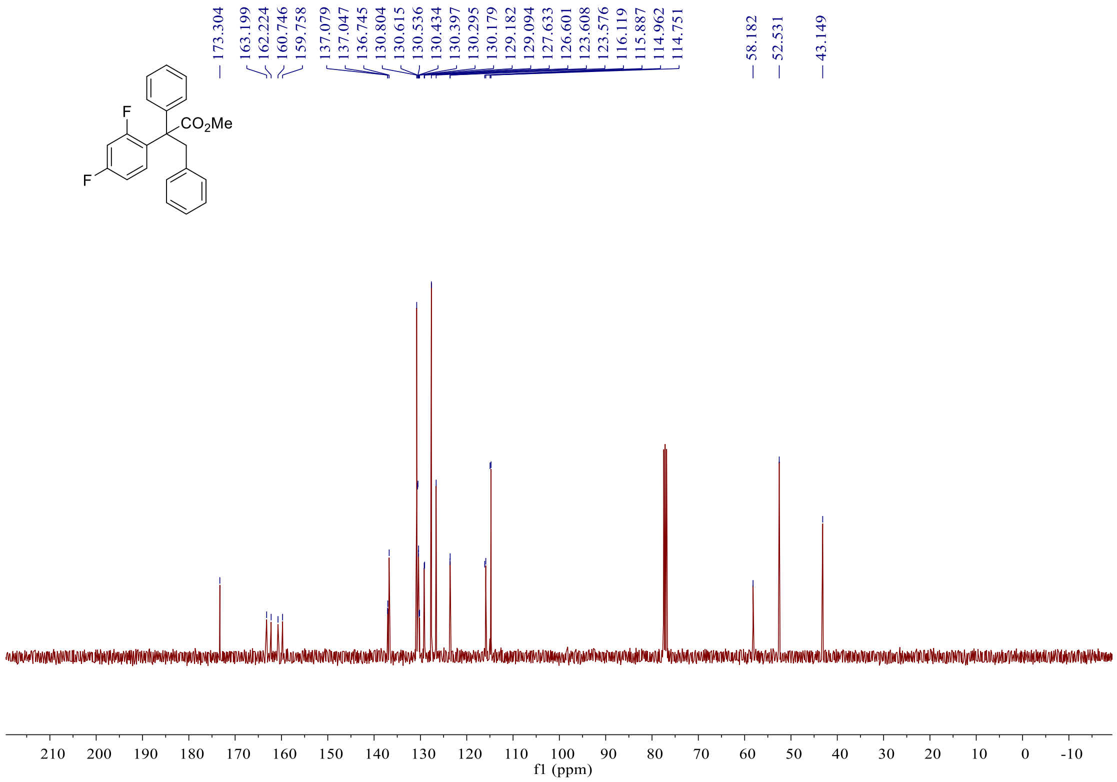
-0.5
-1
f1 (ppm)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162.224
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137.047
136.745
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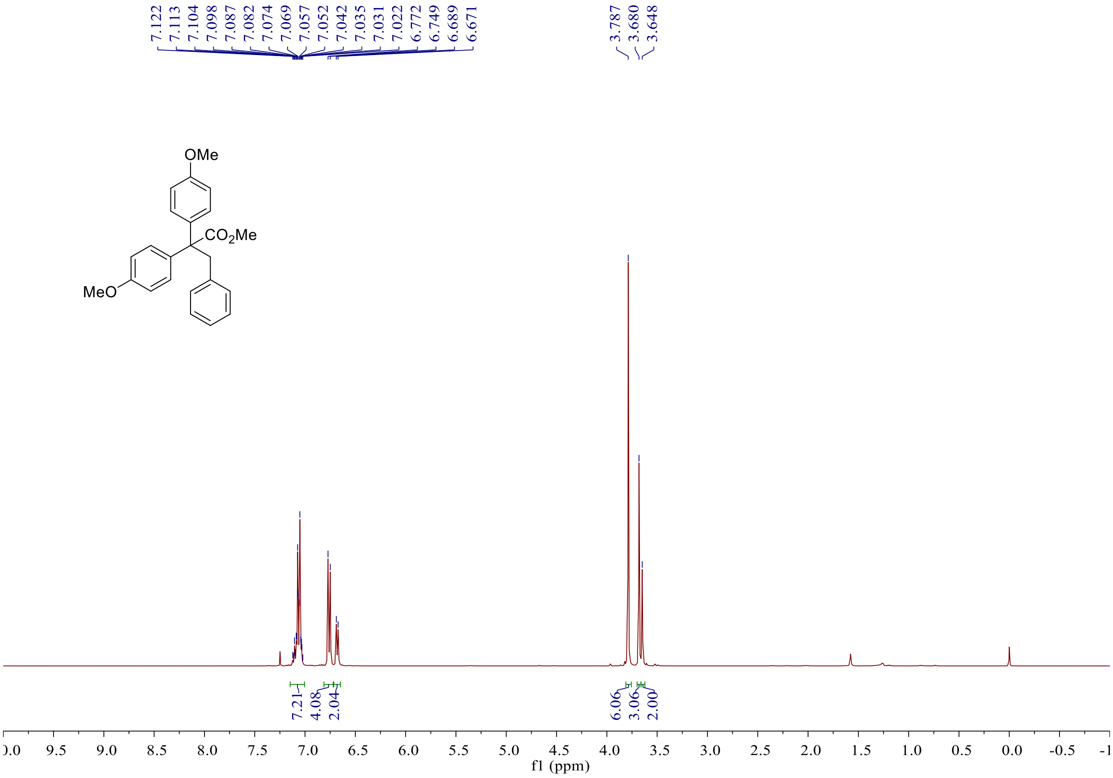
130.536
130.434
130.397
130.295
130.179
129.182
129.094
127.633
126.601
123.608
123.576
116.119
115.887
114.962
114.751
58.182
52.531
43.149
F
F
CO2Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

58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7.087
7.082
7.074
7.069
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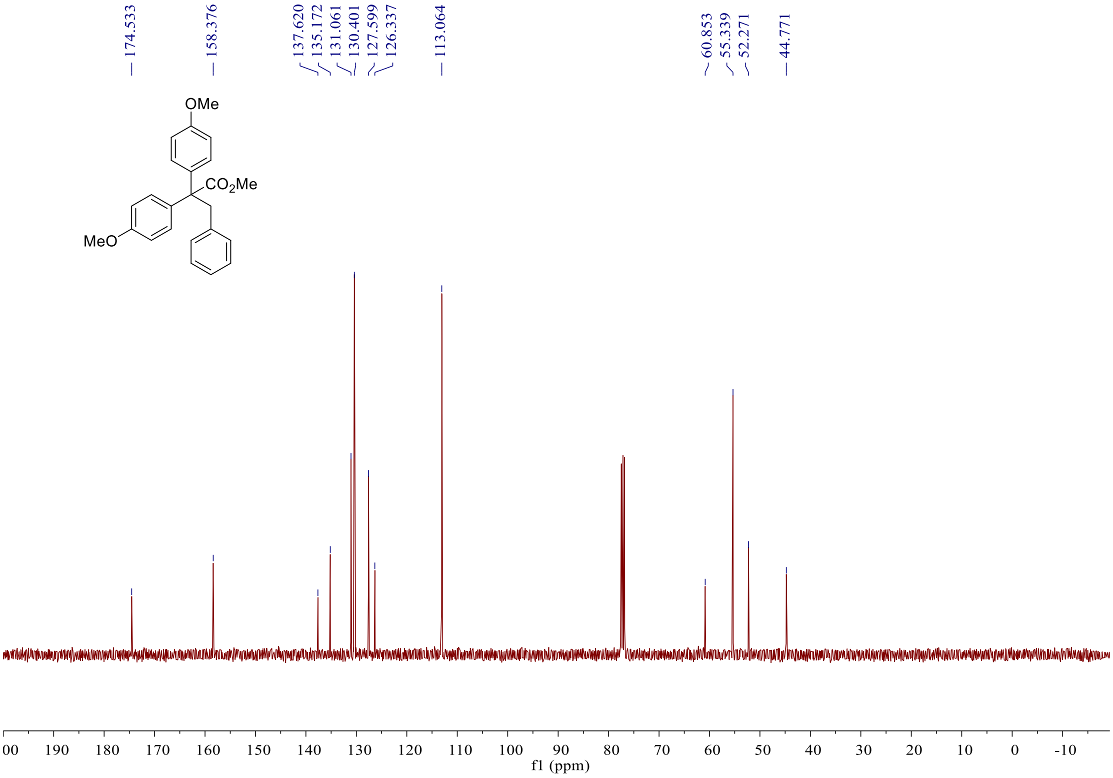
7.052
7.042
7.035
7.031
7.022
6.772
6.749
6.689
6.671
3.787
3.680
3.648
OMe
CO2Me
MeO
7.21
4.08
2.04
6.06
3.06
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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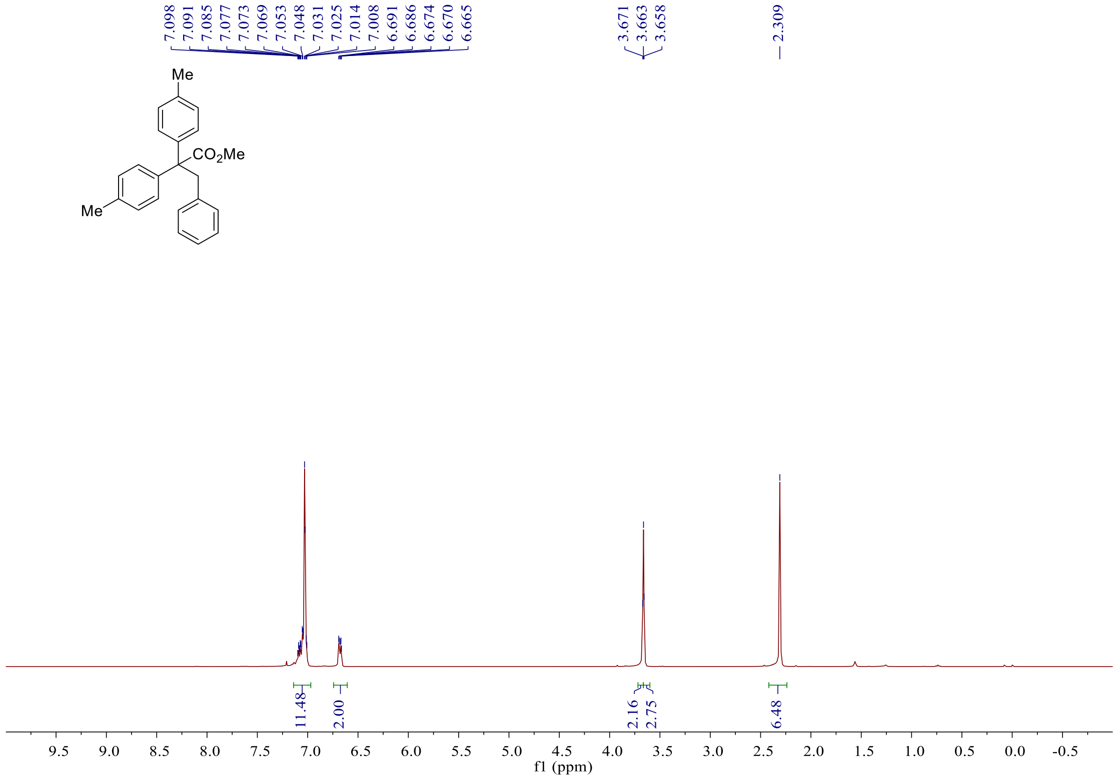
135.172
131.061
130.401
127.599
126.337
113.064
60.853
55.339
52.271
44.771
OMe
CO2Me
MeO
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

59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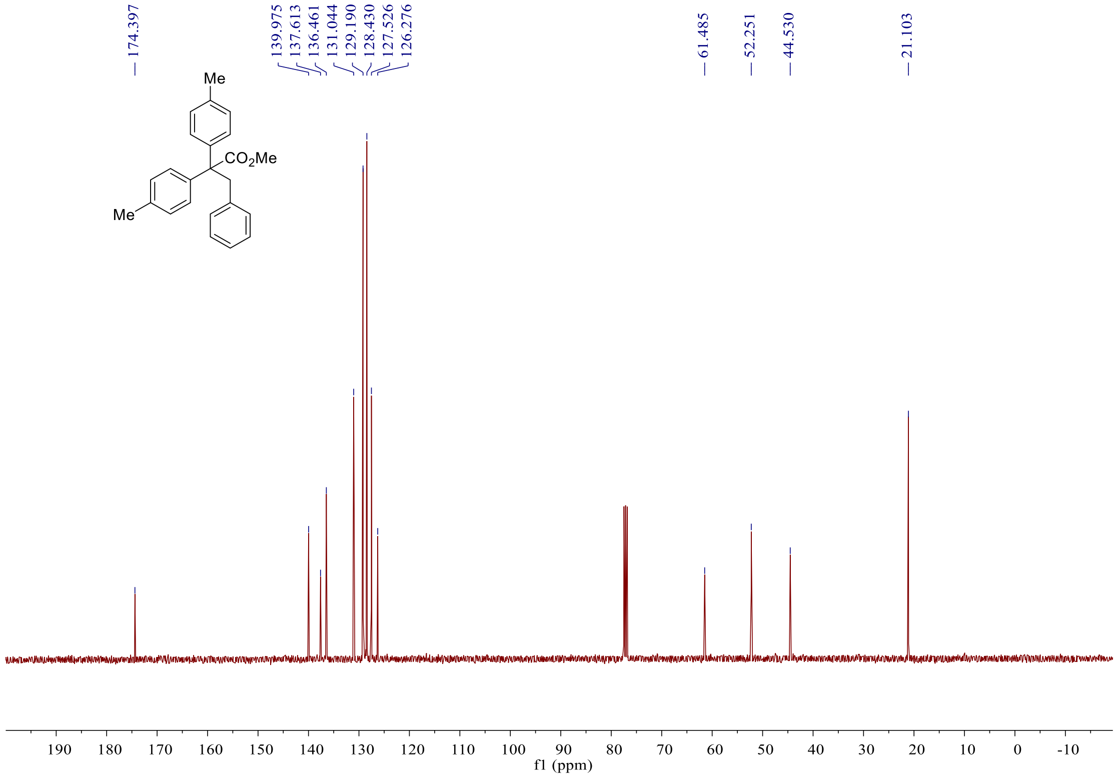
7.073
7.069
7.053
7.048
7.031
7.025
7.014
7.008
6.691
6.686
6.674
6.670
6.665
3.671
3.663
3.658
2.309
Me
CO2Me
Me
11.48
2.00
2.16
2.75
6.48
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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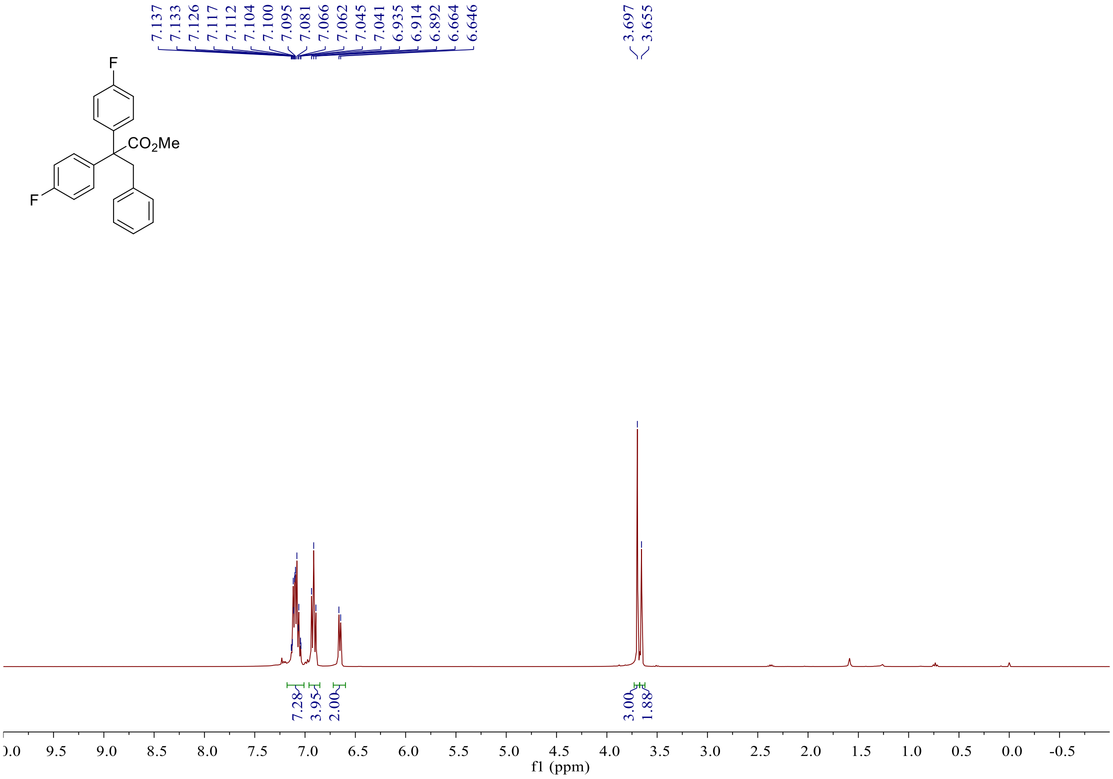
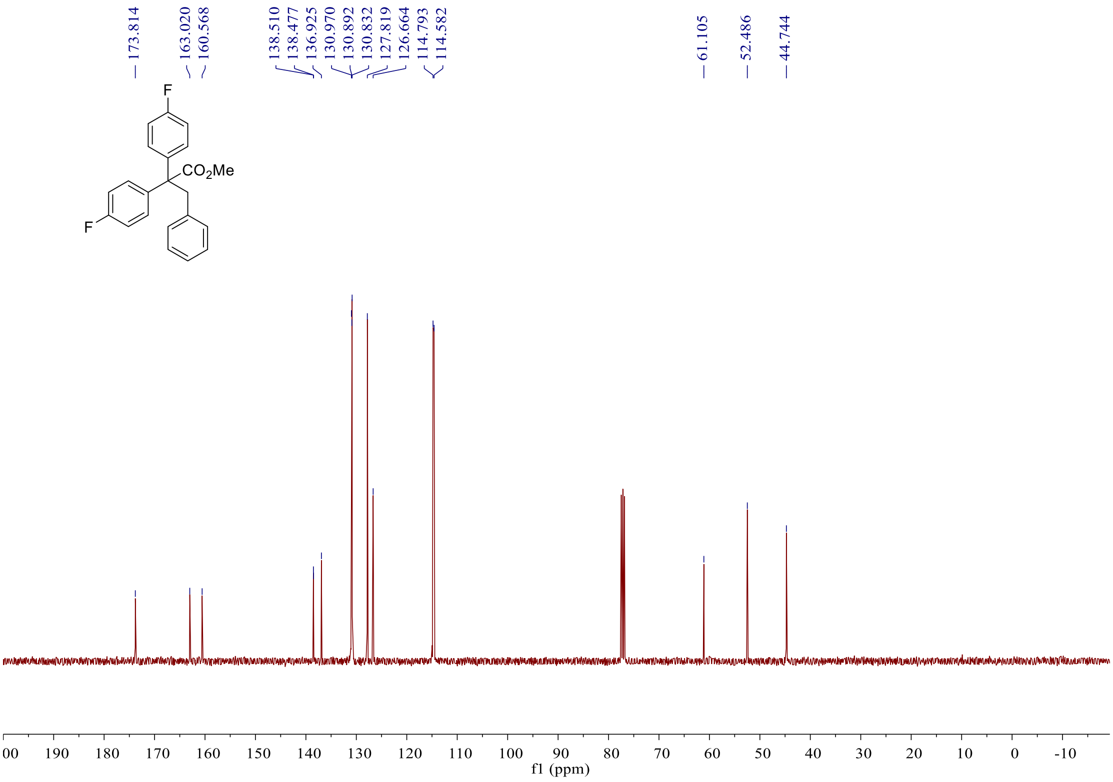
137.613
136.461
131.044
129.190
128.430
127.526
126.276
61.485
52.251
44.530
21.103
Me
CO2Me
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

60


7.137
7.133
7.126
7.117
7.112
7.104
7.100
7.095
7.081
7.066
7.062
7.045
7.041
6.935
6.914
6.892
6.664
6.646
3.697
3.655
F
CO2Me
F
7.28
3.95
2.00
3.00
1.88
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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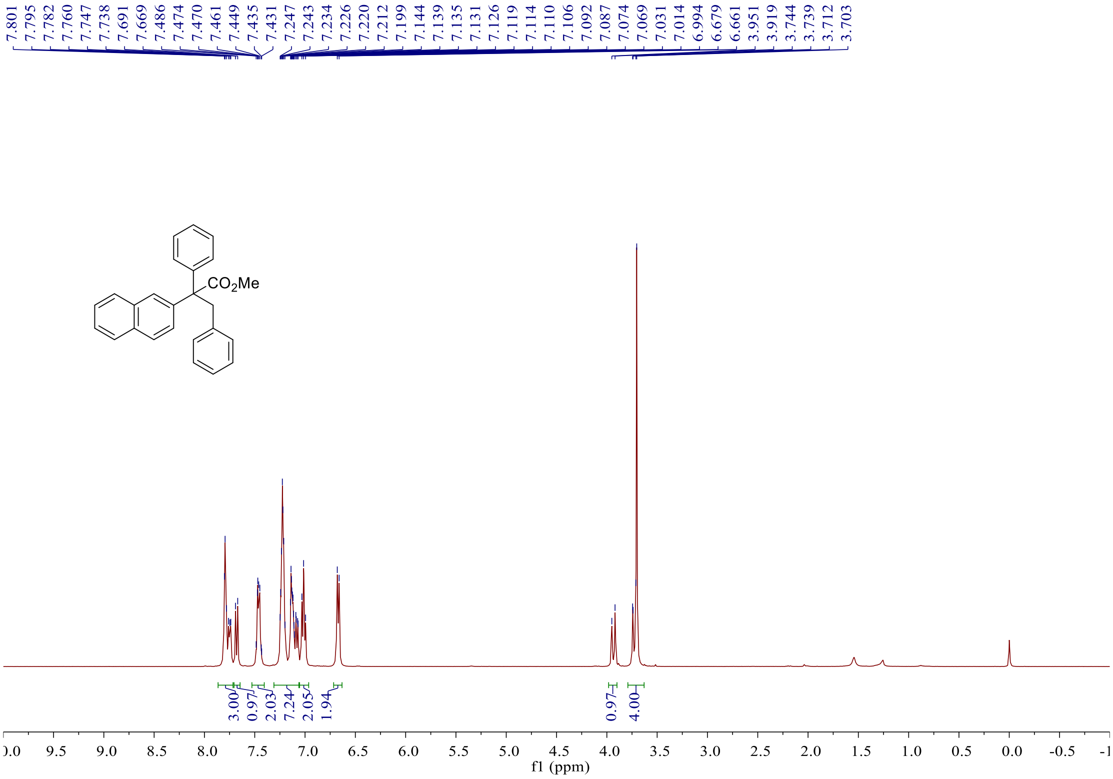
163.020
160.568
138.510
138.477
136.925
130.970
130.892
130.832
127.819
126.664
114.793
114.582
61.105
52.486
44.744
F
CO2Me
F
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

61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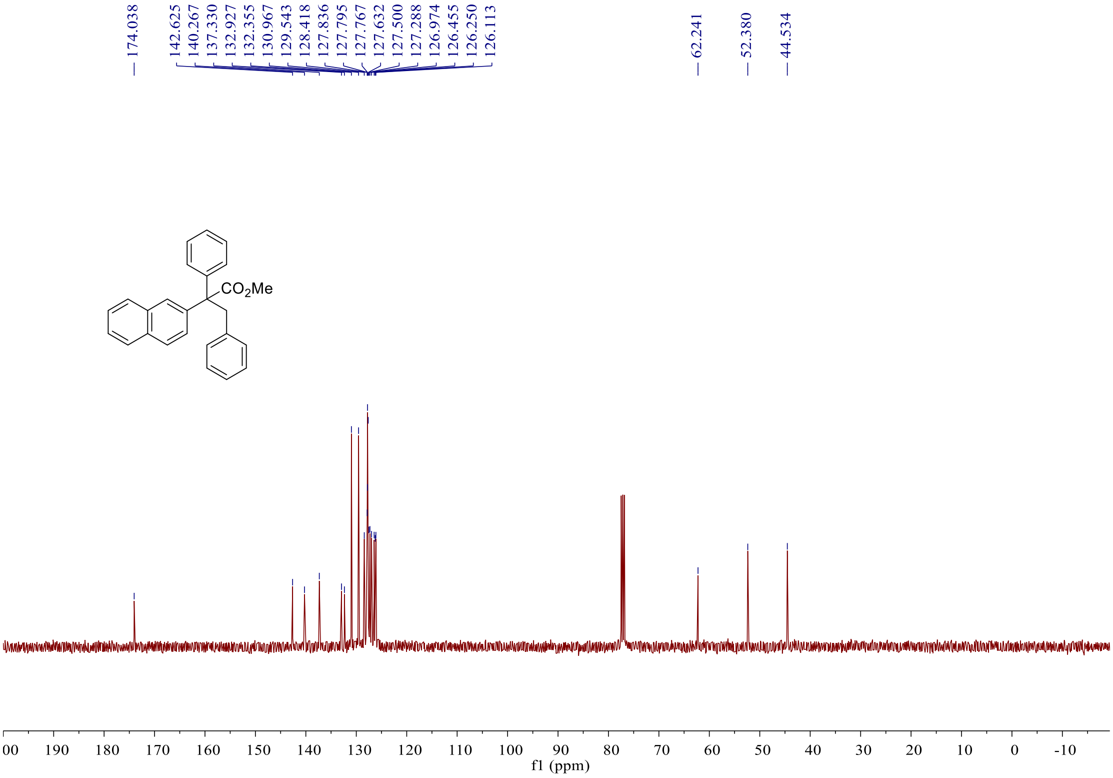
7.795
7.782
7.760
7.747
7.738
7.691
7.669
7.486
7.474
7.470
7.461
7.449
7.435
7.431
7.247
7.243
7.234
7.226
7.220
7.212
7.199
7.144
7.139
7.135
7.131
7.126
7.119
7.114
7.110
7.106
7.092
7.087
7.074
7.069
7.031
7.014
6.994
6.679
6.661
3.951
3.919
3.744
3.739
3.712
3.703
CO_2Me
3.00
0.97
2.03
7.24
2.05
1.94
0.97
4.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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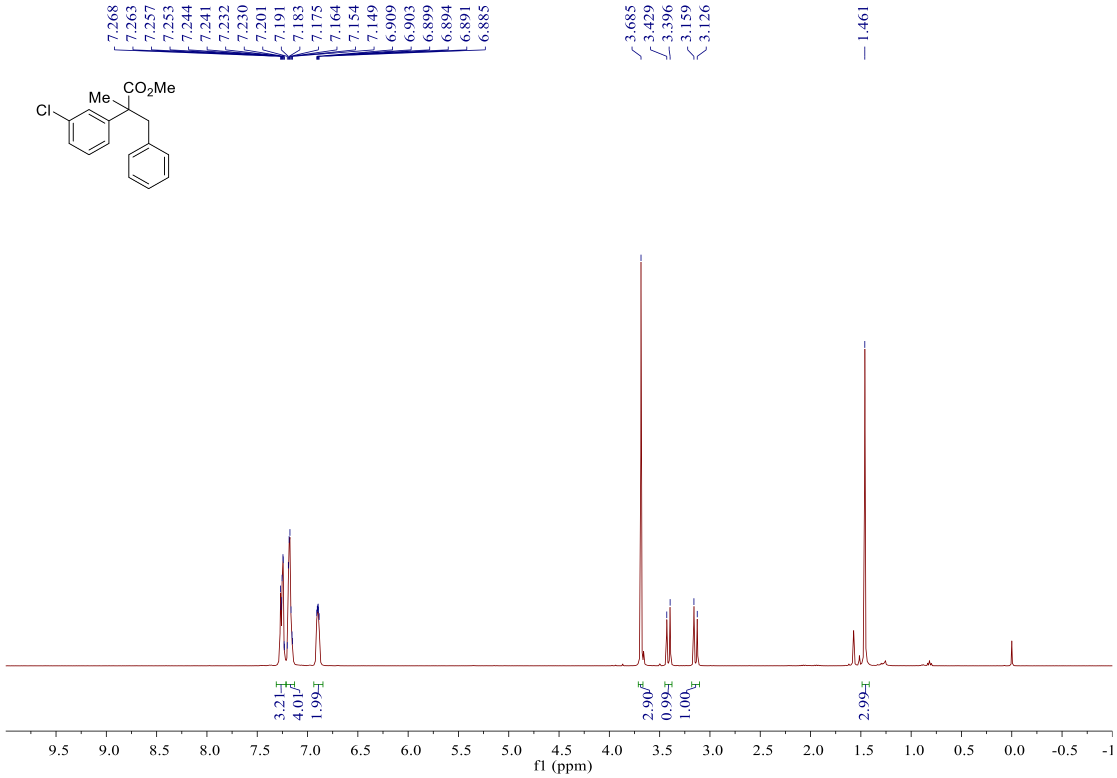
140.267
137.330
132.927
132.355
130.967
129.543
128.418
127.836
127.795
127.767
127.632
127.500
127.288
126.974
126.455
126.250
126.113
62.241
52.380
44.534
CO_2Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

62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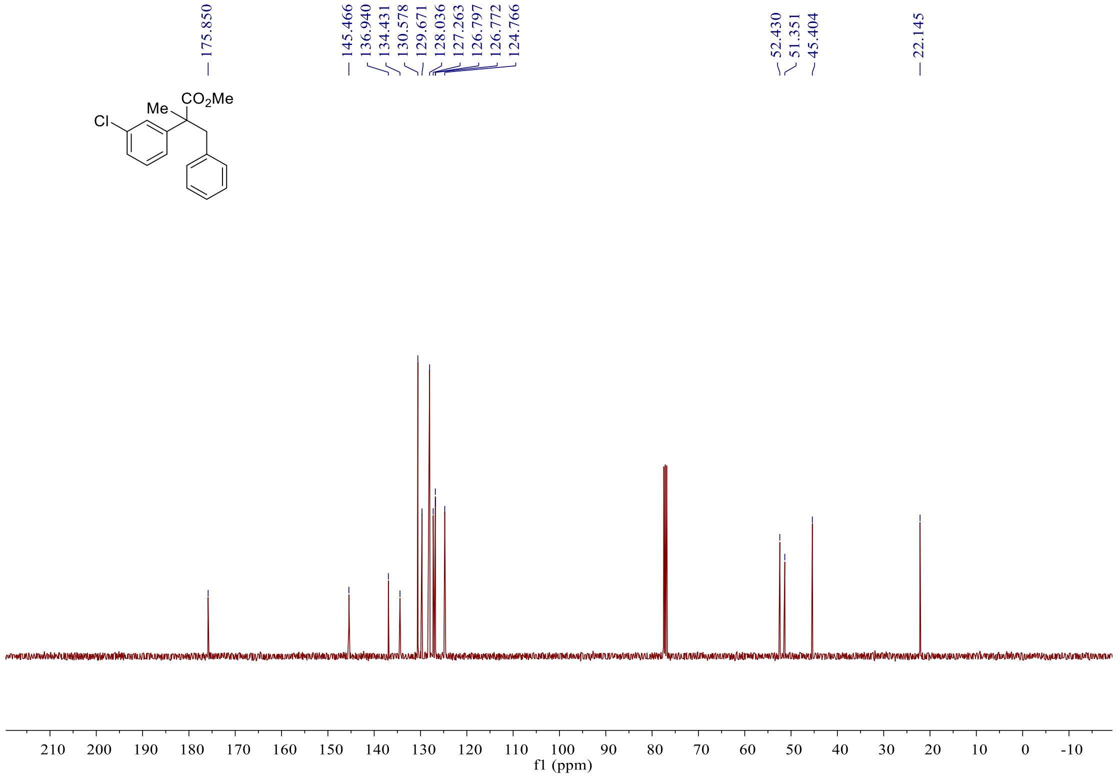
7.257
7.253
7.244
7.241
7.232
7.230
7.201
7.191
7.183
7.175
7.164
7.154
7.149
6.909
6.903
6.899
6.894
6.891
6.885
3.685
3.429
3.396
3.159
3.126
1.461
CO2Me
Me
Cl
3.21
4.01
1.99
2.90
0.99
1.00
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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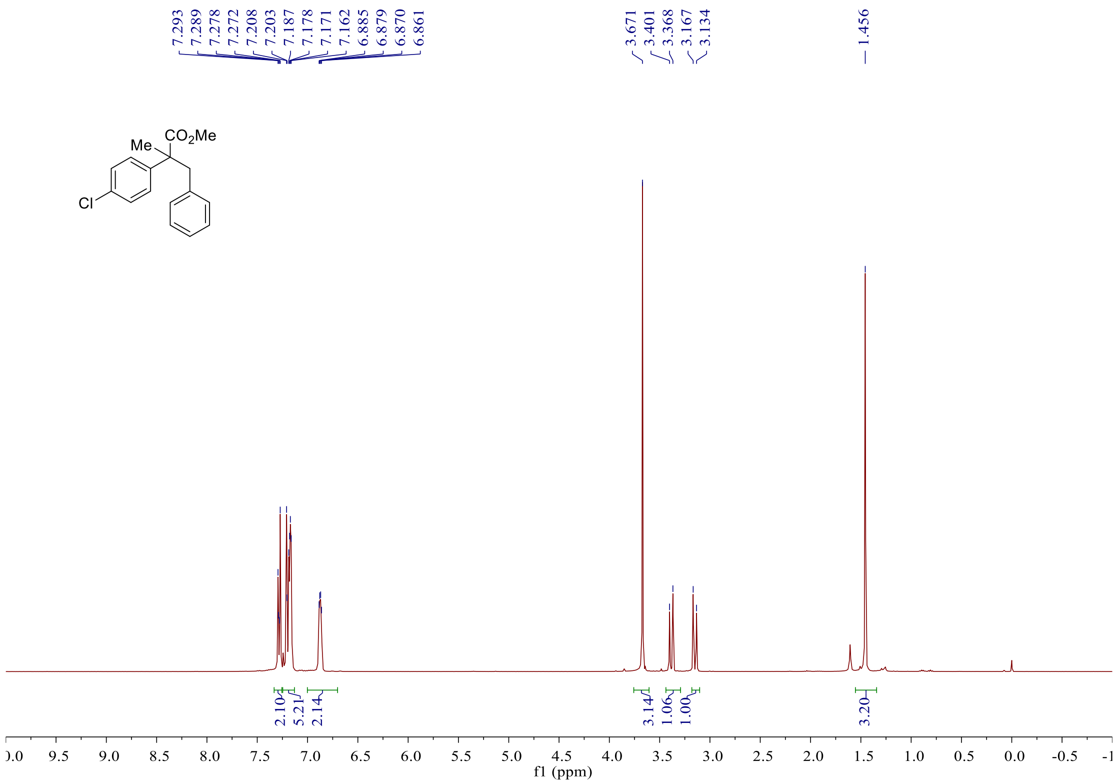
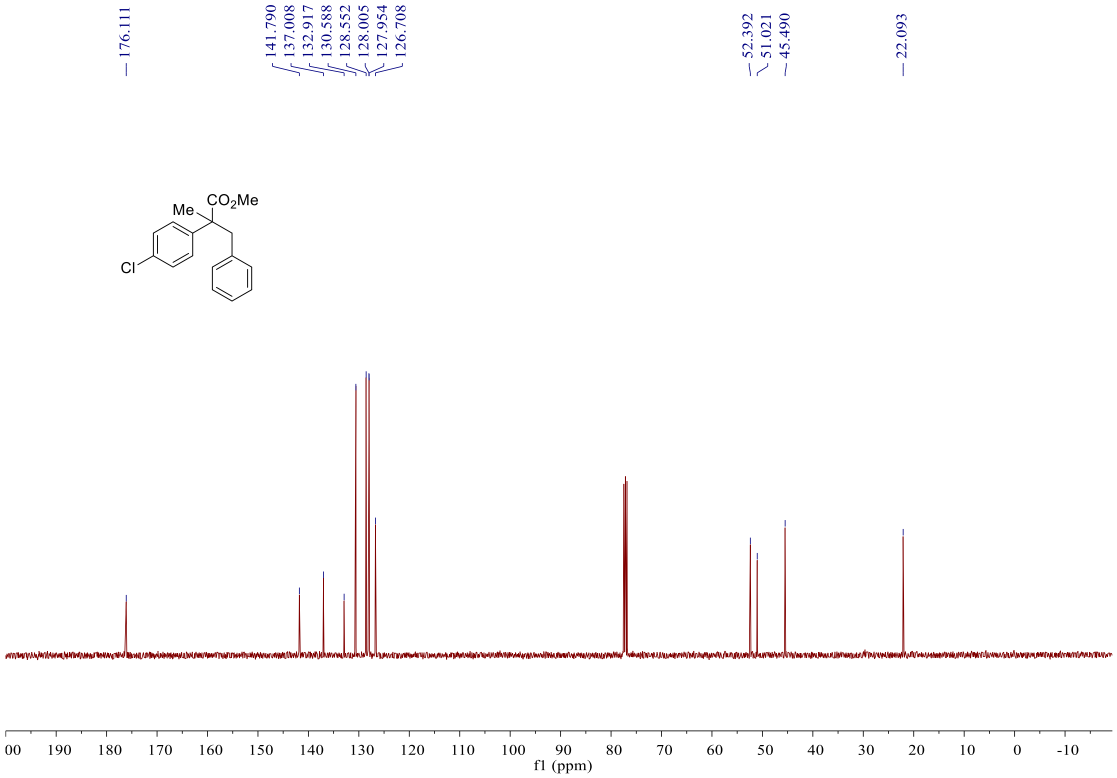
130.578
129.671
128.036
127.263
126.797
126.772
124.766
52.430
51.351
45.404
22.145
CO2Me
Me
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

63


7.293
7.289
7.278
7.272
7.208
7.203
7.187
7.178
7.171
7.162
6.885
6.879
6.870
6.861
3.671
3.401
3.368
3.167
3.134
1.456
Me
CO_2Me
Cl
2.10
5.21
2.14
3.14
1.06
1.00
3.20
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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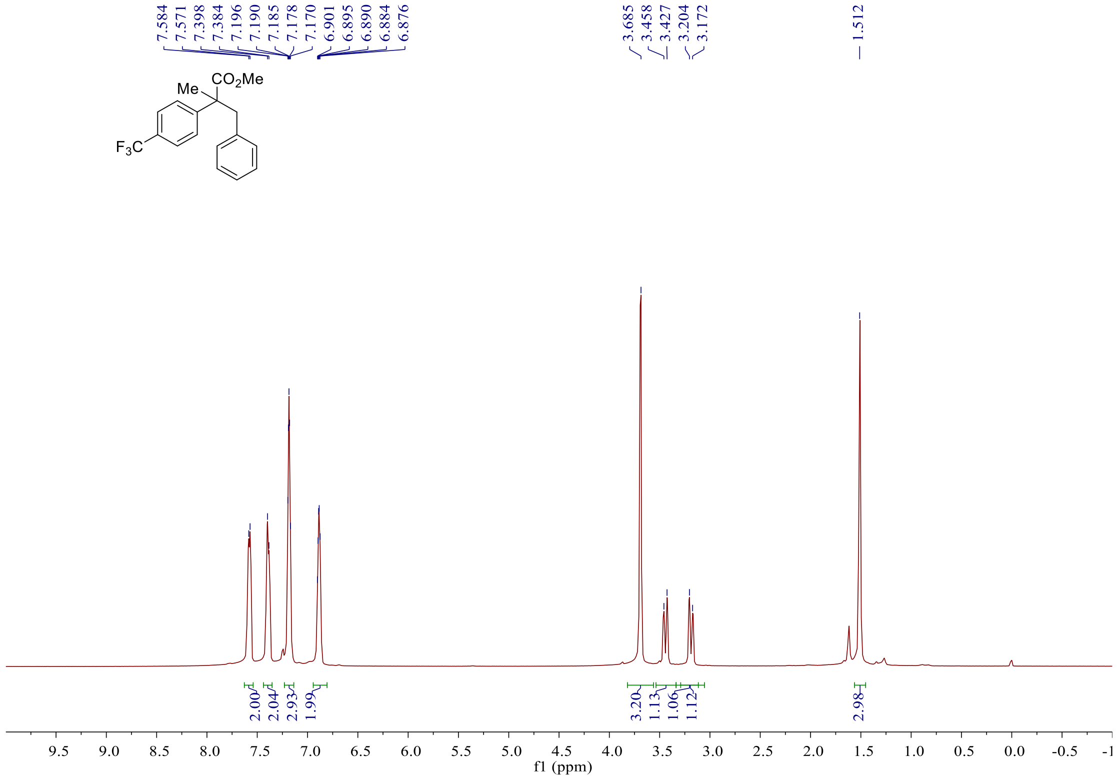
130.588
128.552
128.005
127.954
126.708
52.392
51.021
45.490
22.093
Me
CO_2Me
Cl
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

64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7.178
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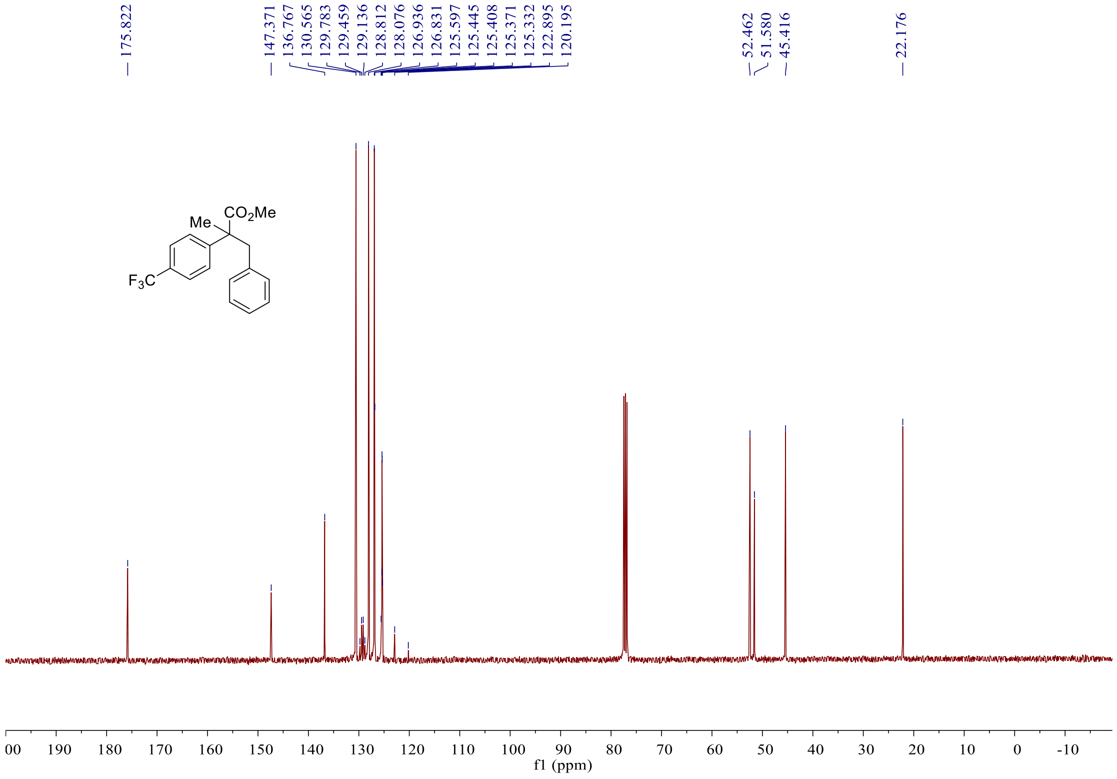
6.895
6.890
6.884
6.876
3.685
3.458
3.427
3.204
3.172
1.512
Me
CO2Me
F3C
2.00
2.04
2.93
1.99
3.20
1.13
1.06
1.12
2.98
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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129.136
128.812
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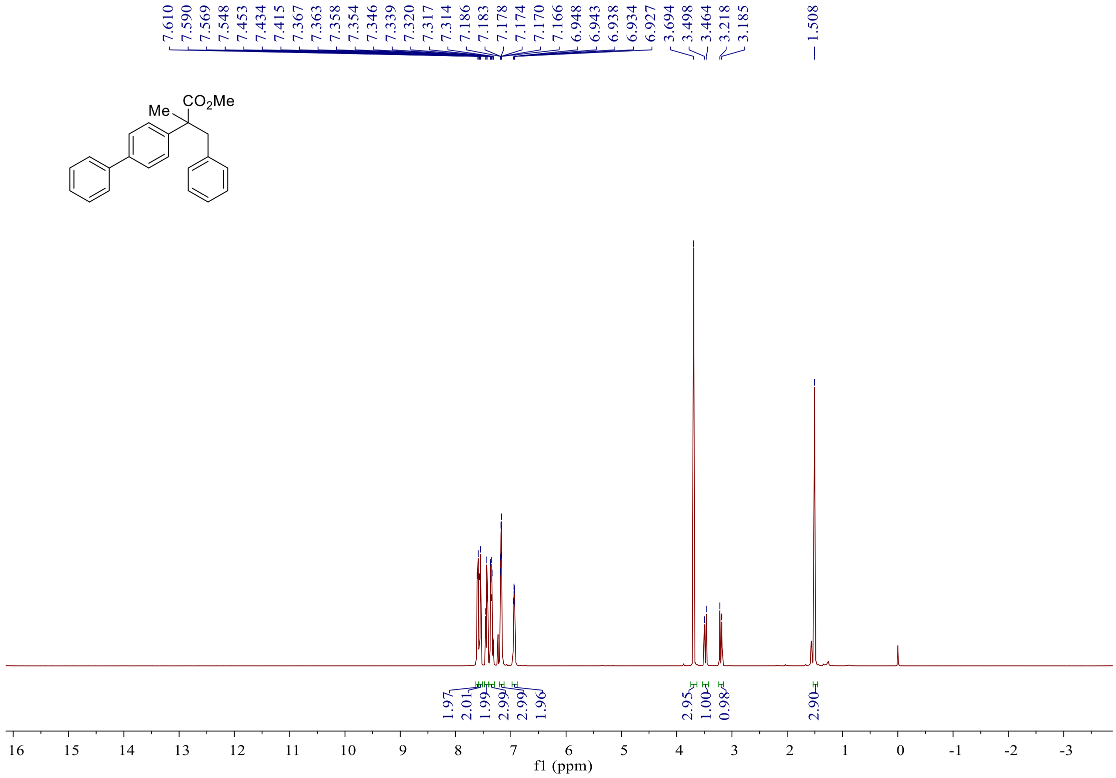
126.936
126.831
125.597
125.445
125.408
125.371
125.332
122.895
120.195
52.462
51.580
45.416
22.176
Me
CO2Me
F3C
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

65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7.358
7.354
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7.339
7.320
7.317
7.314
7.186
7.183
7.178
7.174
7.170
7.166
6.948
6.943
6.938
6.934
6.927
3.694
3.498
3.464
3.218
3.185
1.508
Me
CO2Me
1.97
2.01
1.99
2.99
2.99
1.96
2.95
1.00
0.98
2.90
16
15
14
13
12
11
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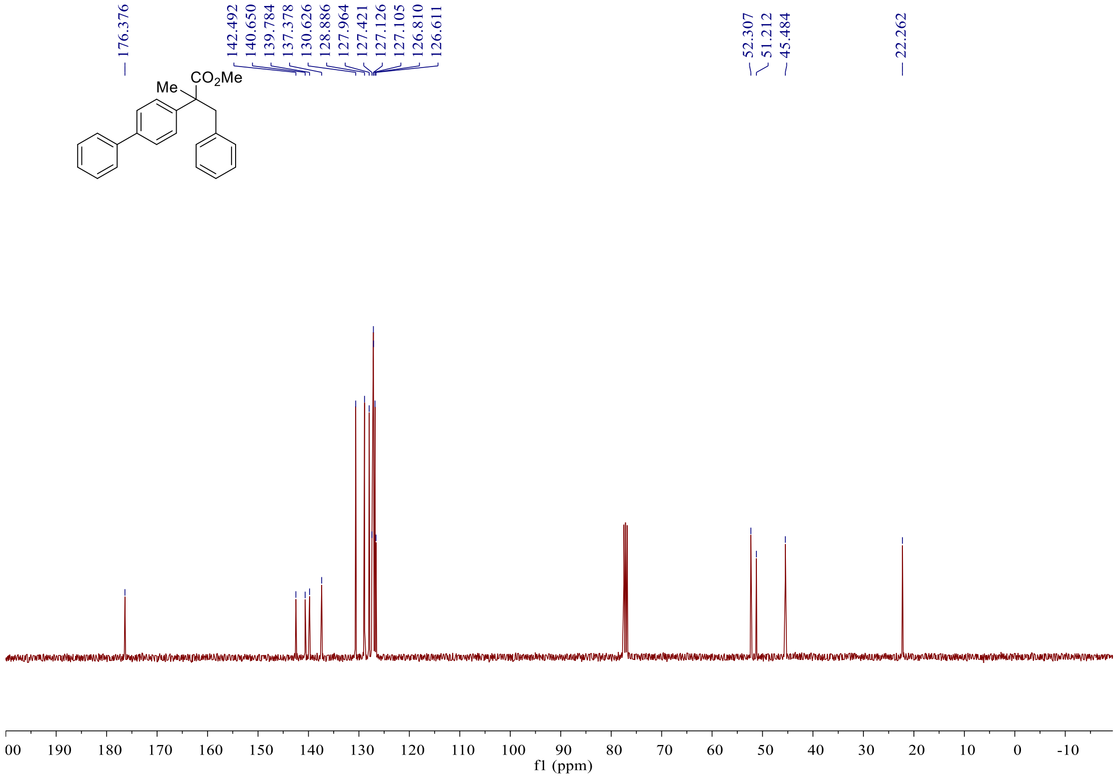
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)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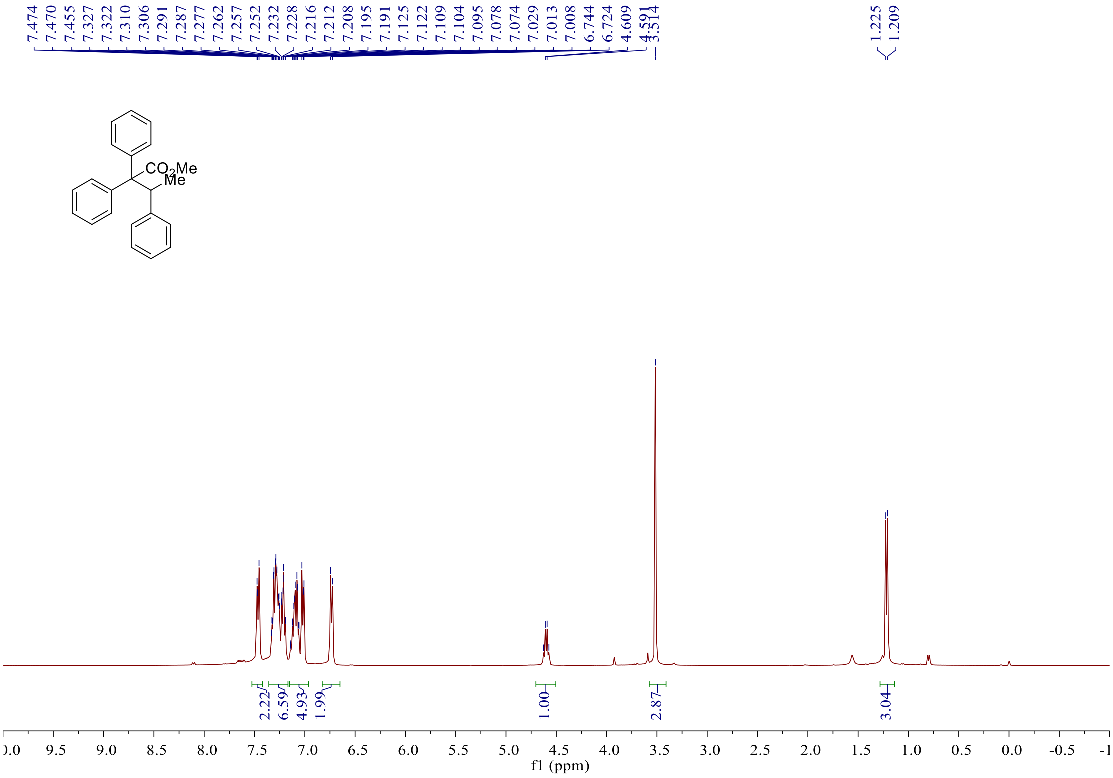
127.964
127.421
127.126
127.105
126.810
126.611
52.307
51.212
45.484
22.262
Me
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

66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7.277
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7.257
7.252
7.232
7.228
7.216
7.212
7.208
7.195
7.191
7.125
7.122
7.109
7.104
7.095
7.078
7.074
7.029
7.013
7.008
6.744
6.724
4.609
4.591
3.514
1.225
1.209
CO2Me
Me
2.22
6.59
4.93
1.99
1.00
2.87
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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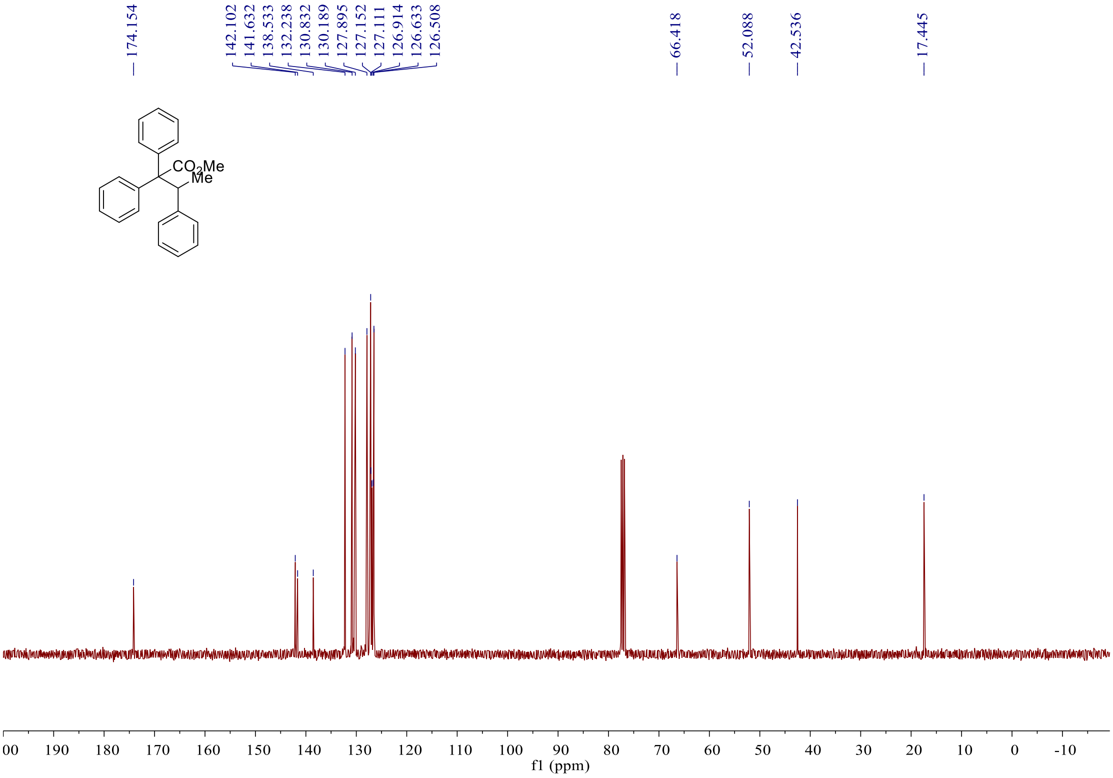
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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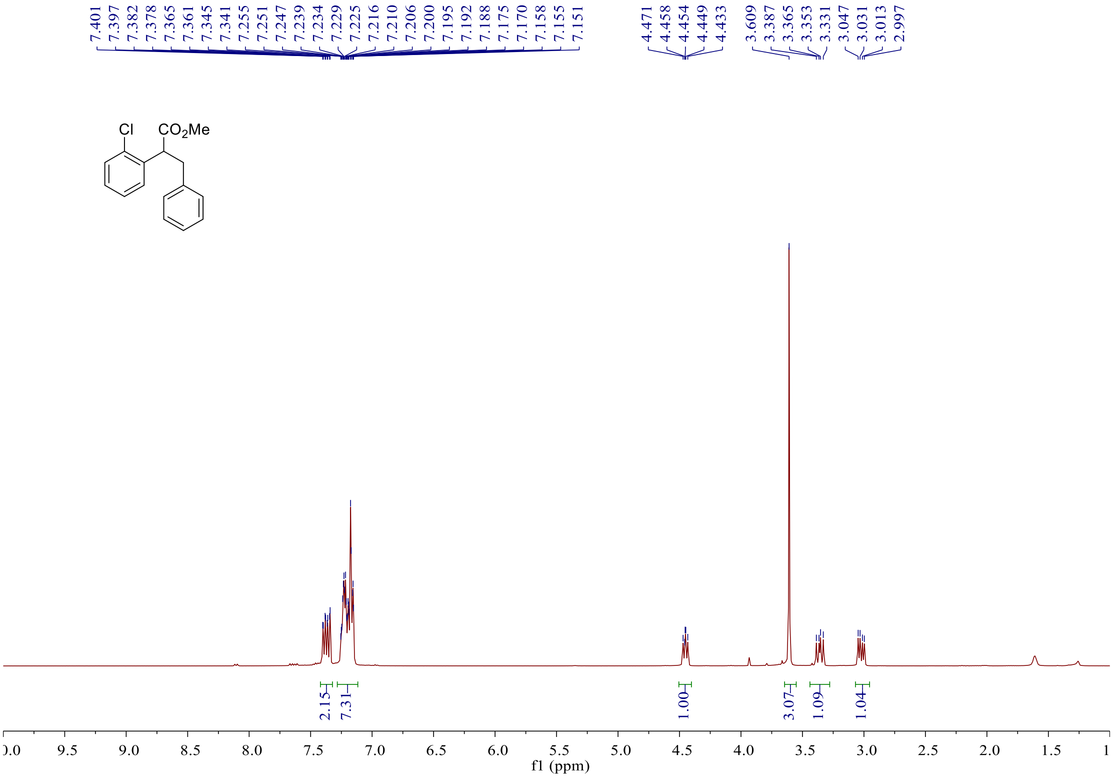
130.189
127.895
127.152
127.111
126.914
126.633
126.508
66.418
52.088
42.536
17.445
CO2Me
Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

67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7.234
7.229
7.225
7.216
7.210
7.206
7.200
7.195
7.192
7.188
7.175
7.170
7.158
7.155
7.151
4.471
4.458
4.454
4.449
4.433
3.609
3.387
3.365
3.353
3.331
3.047
3.031
3.013
2.997
Cl
CO2Me
2.15
7.31
1.00
3.07
1.09
1.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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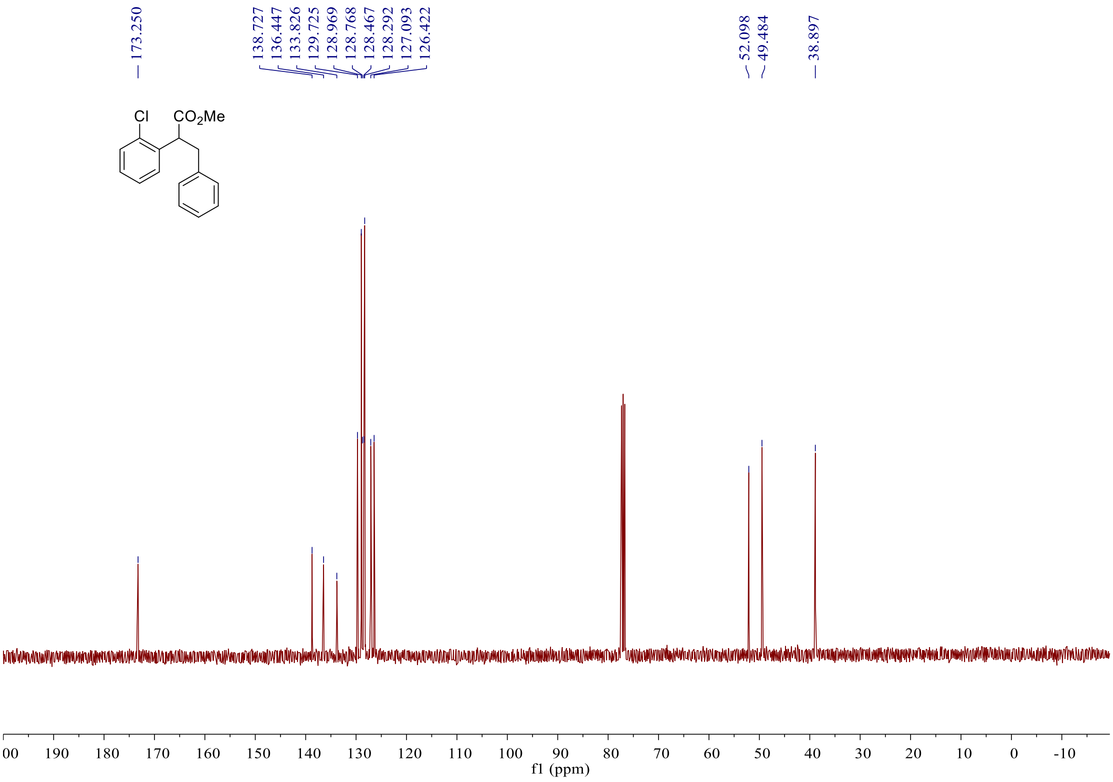
2.0
1.5
1
f1 (ppm)


173.250
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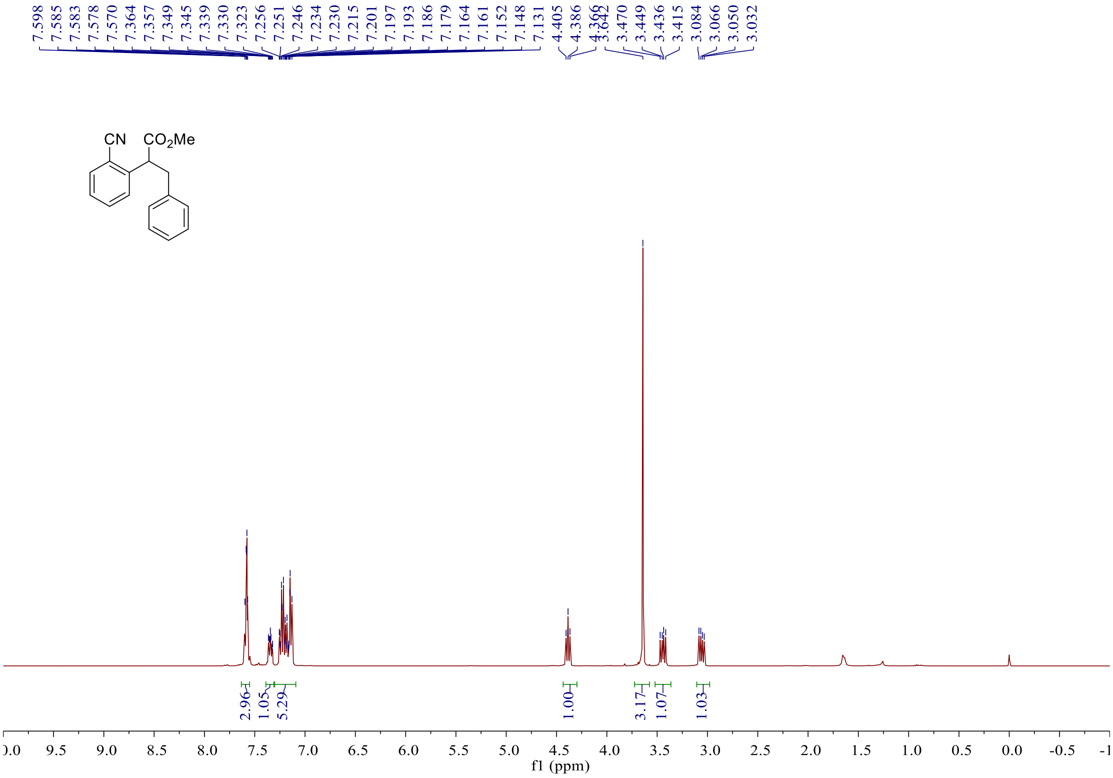
136.447
133.826
129.725
128.969
128.768
128.467
128.292
127.093
126.422
52.098
49.484
38.897
Cl
CO2Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

68


7.598
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7.339
7.330
7.323
7.256
7.251
7.246
7.234
7.230
7.215
7.201
7.197
7.193
7.186
7.179
7.164
7.161
7.152
7.148
7.131
4.405
4.386
4.366
3.642
3.470
3.449
3.436
3.415
3.084
3.066
3.050
3.032
CN
CO2Me
2.96
1.05
5.29
1.00
3.17
1.07
1.03
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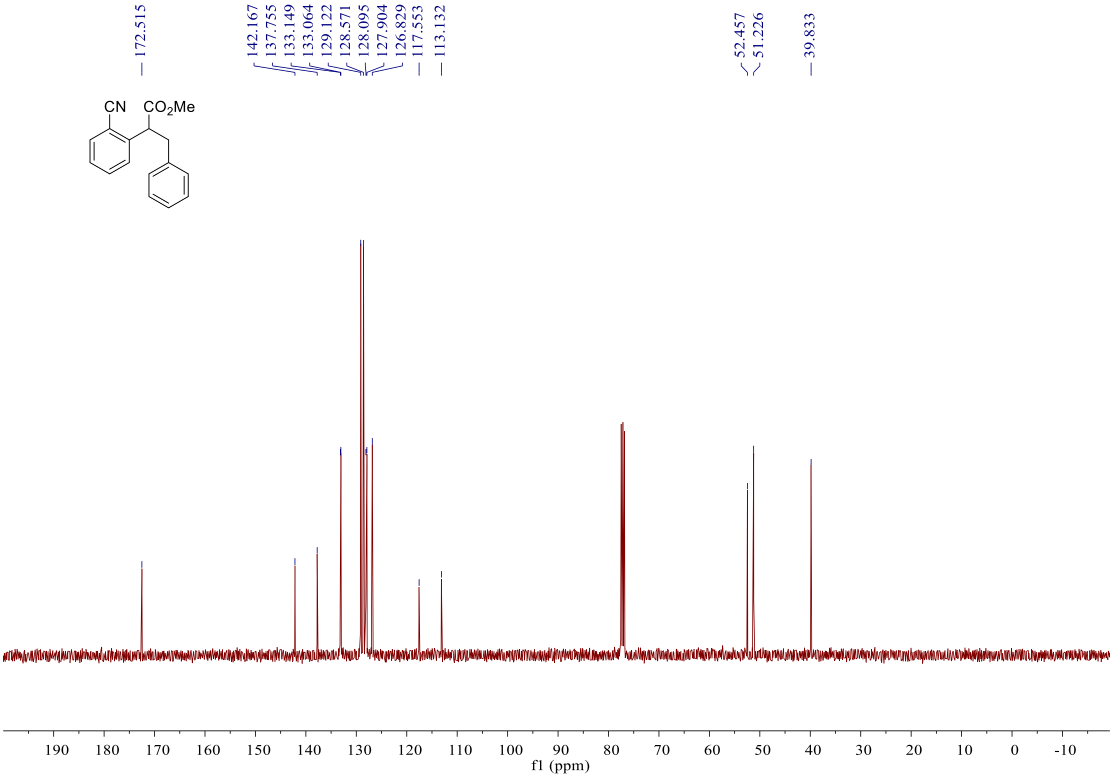
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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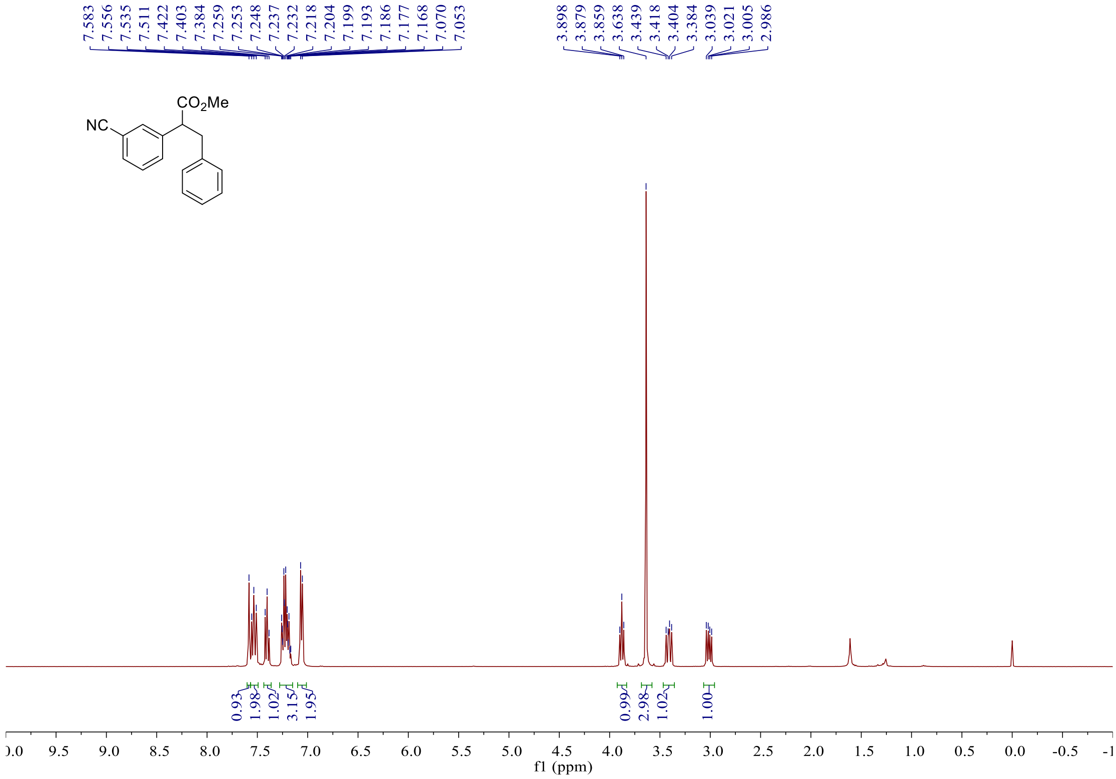
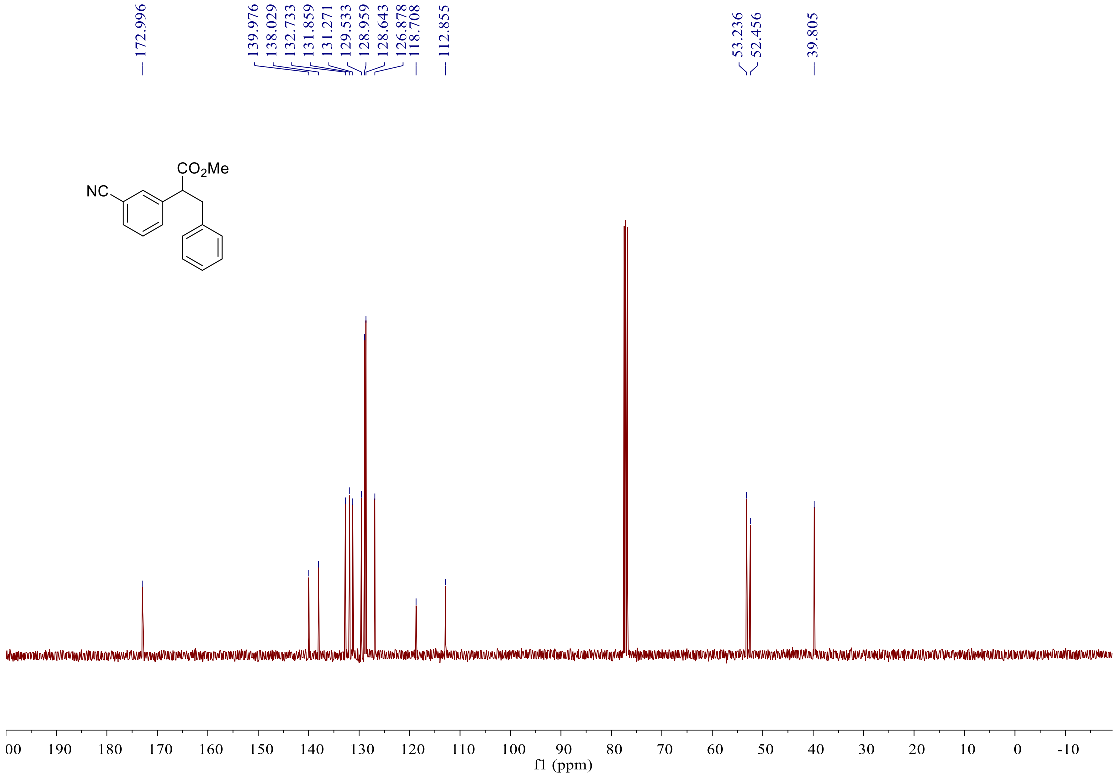
142.167
137.755
133.149
133.064
129.122
128.571
128.095
127.904
126.829
117.553
113.132
52.457
51.226
39.833
CN
CO2Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

69


7.583
7.556
7.535
7.511
7.422
7.403
7.384
7.259
7.253
7.248
7.237
7.232
7.218
7.204
7.199
7.193
7.186
7.177
7.168
7.070
7.053
3.898
3.879
3.859
3.638
3.439
3.418
3.404
3.384
3.039
3.021
3.005
2.986
CO2Me
NC
0.93
1.98
1.02
3.15
1.95
0.99
2.98
1.02
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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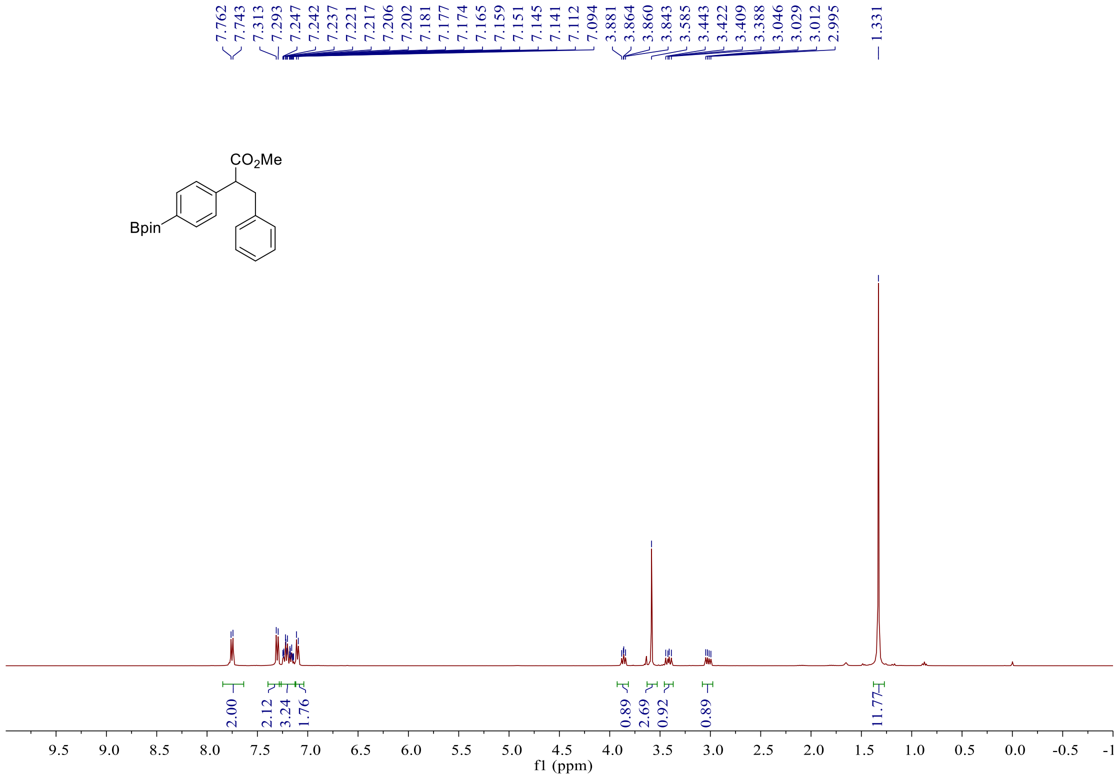
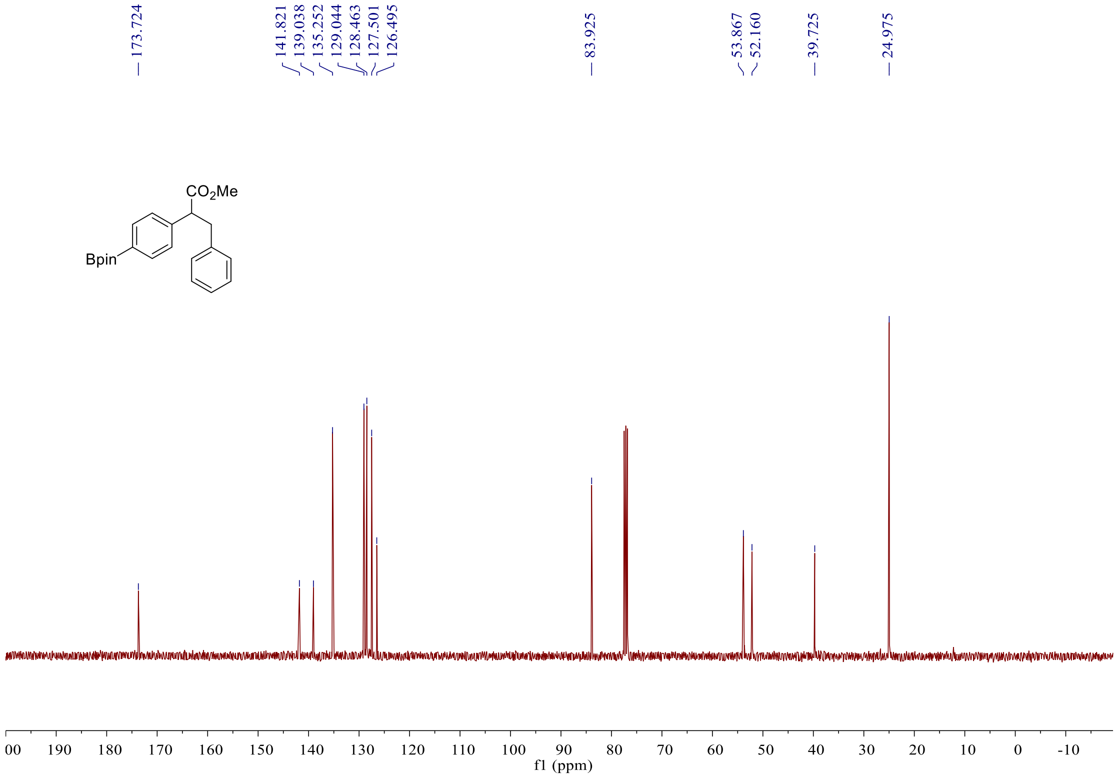
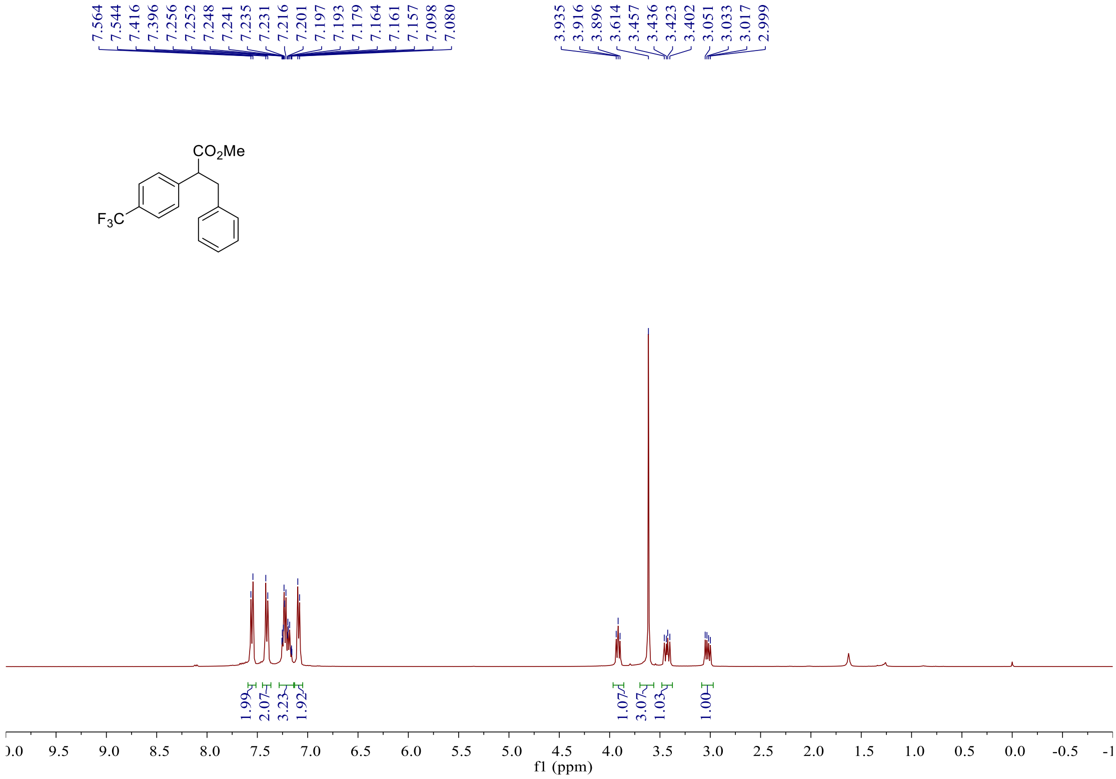
139.976
138.029
132.733
131.859
131.271
129.533
128.959
128.643
126.878
118.708
112.855
53.236
52.456
39.805
CO2Me
NC
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

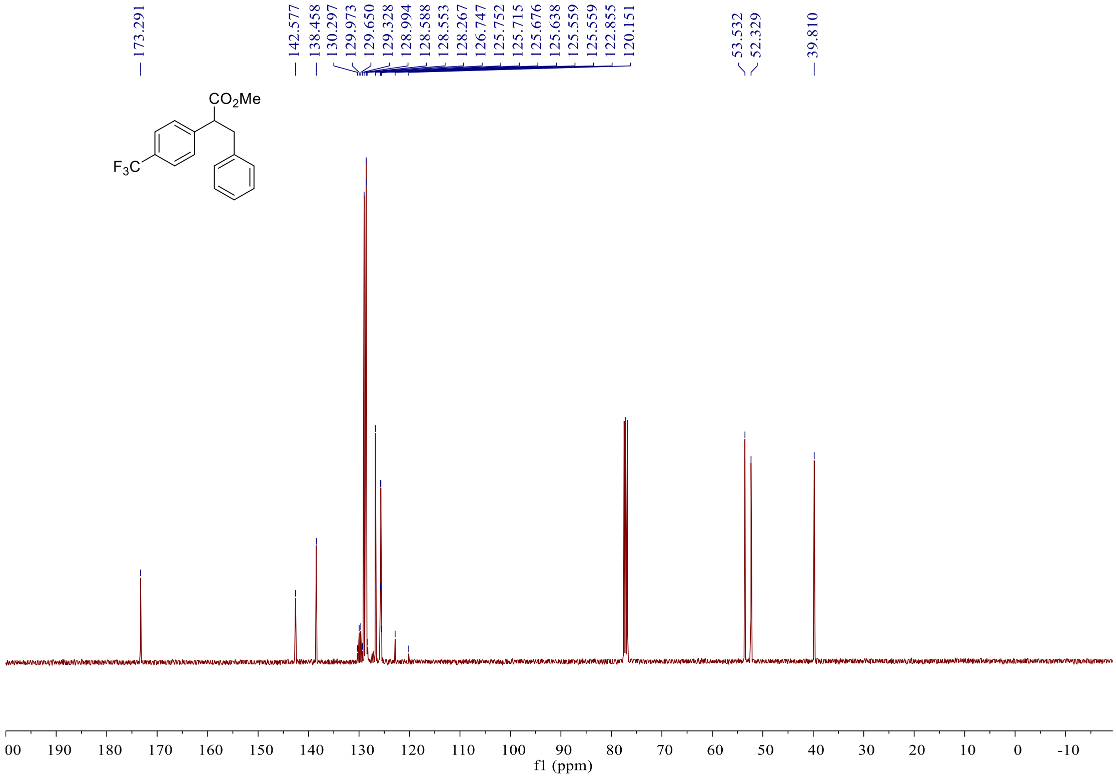
70


7.762
7.743
7.313
7.293
7.247
7.242
7.237
7.221
7.217
7.206
7.202
7.181
7.177
7.174
7.165
7.159
7.151
7.145
7.141
7.112
7.094
3.881
3.864
3.860
3.843
3.585
3.443
3.422
3.409
3.388
3.046
3.029
3.012
2.995
1.331
CO2Me
Bpin
2.00
2.12
3.24
1.76
0.89
2.69
0.92
0.89
11.77
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

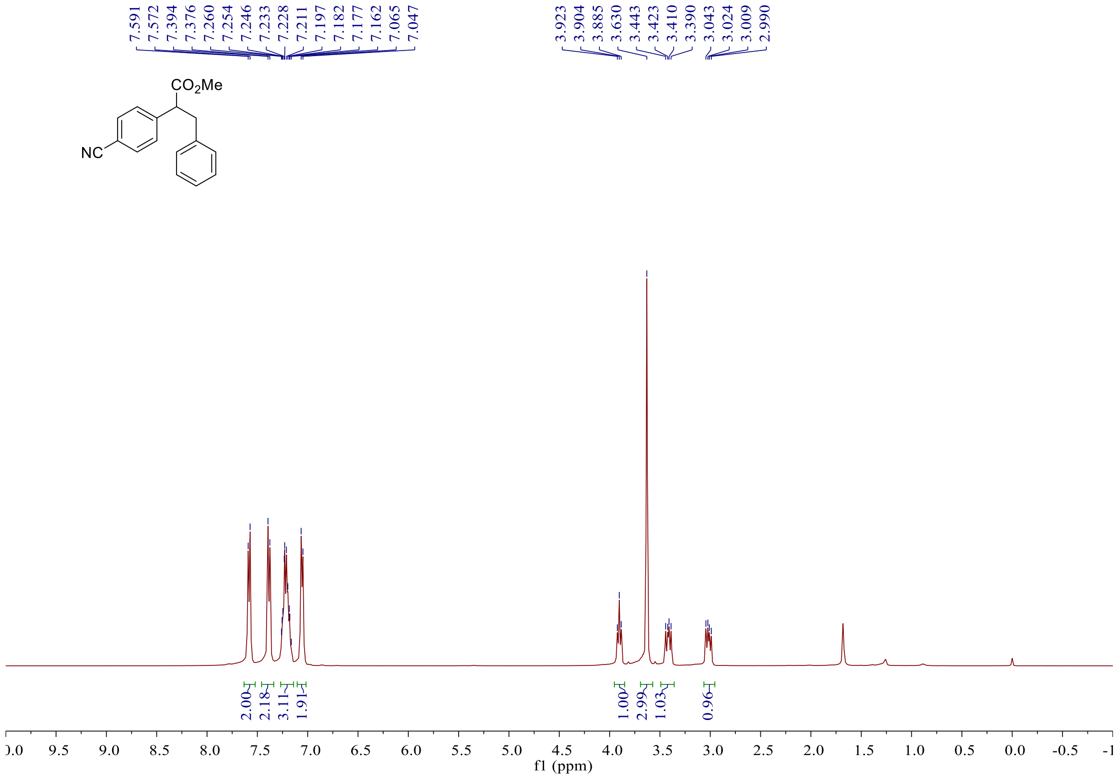

173.724
141.821
139.038
135.252
129.044
128.463
127.501
126.495
83.925
53.867
52.160
39.725
24.975
CO2Me
Bpin
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

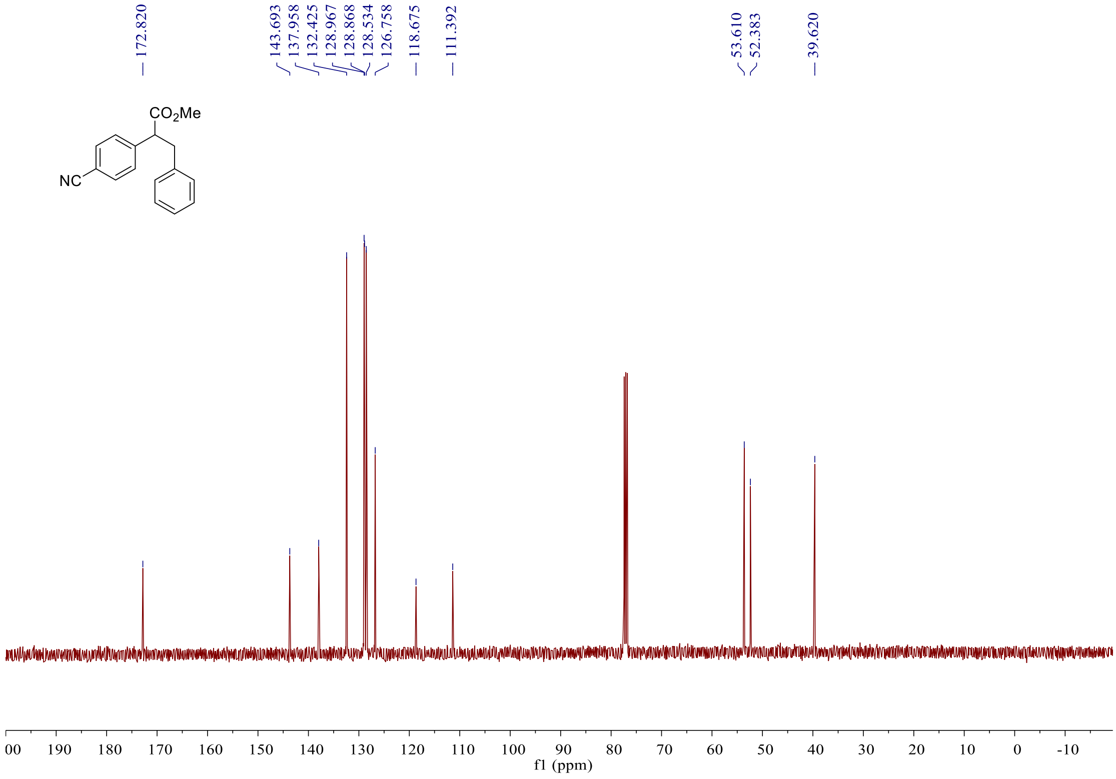
71


7.564
7.544
7.416
7.396
7.256
7.252
7.248
7.241
7.235
7.231
7.216
7.201
7.197
7.193
7.179
7.164
7.161
7.157
7.098
7.080
3.935
3.916
3.896
3.614
3.457
3.436
3.423
3.402
3.051
3.033
3.017
2.999
CO2Me
F3C
1.99
2.07
3.23
1.92
1.07
3.07
1.03
1.00
).0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

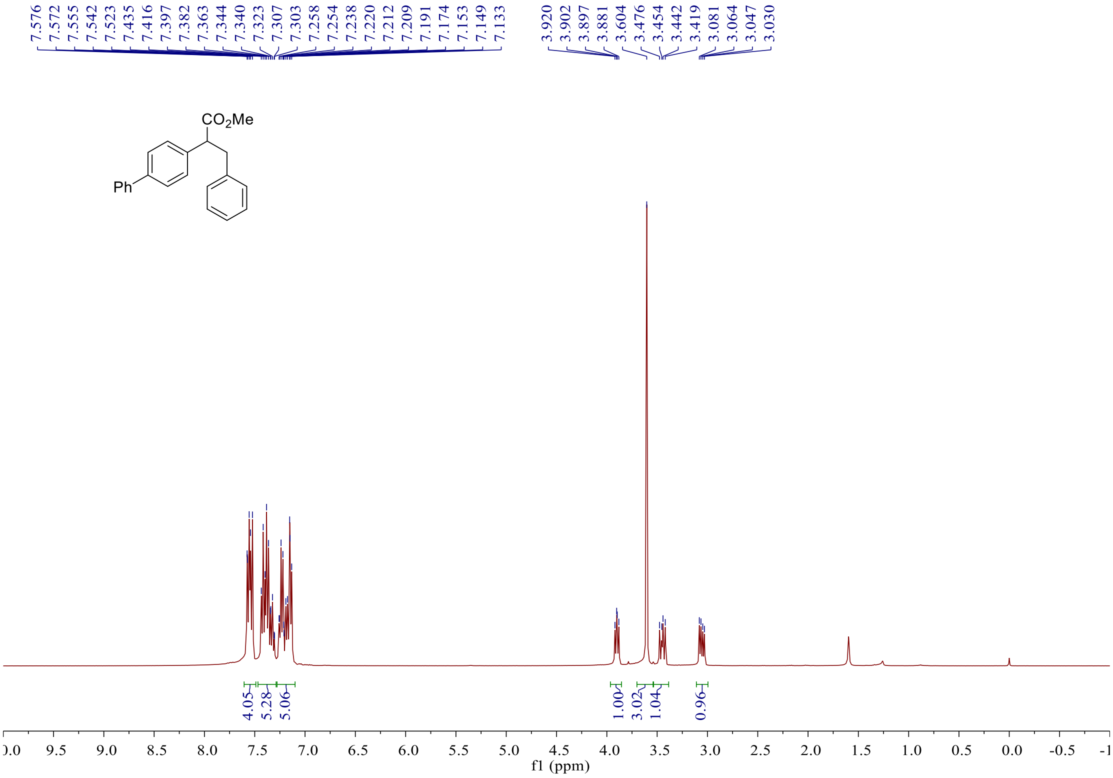

173.291
142.577
138.458
130.297
129.973
129.650
129.328
128.994
128.588
128.553
128.267
126.747
125.752
125.715
125.676
125.638
125.559
125.559
122.855
120.151
53.532
52.329
39.810
CO2Me
F3C
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

72


7.591
7.572
7.394
7.376
7.260
7.254
7.246
7.233
7.228
7.211
7.197
7.182
7.177
7.162
7.065
7.047
3.923
3.904
3.885
3.630
3.443
3.423
3.410
3.390
3.043
3.024
3.009
2.990
CO2Me
NC
2.00
2.18
3.11
1.91
1.00
2.99
1.03
0.96
f1 (ppm)


172.820
143.693
137.958
132.425
128.967
128.868
128.534
126.758
118.675
111.392
53.610
52.383
39.620
CO2Me
NC
f1 (ppm)

73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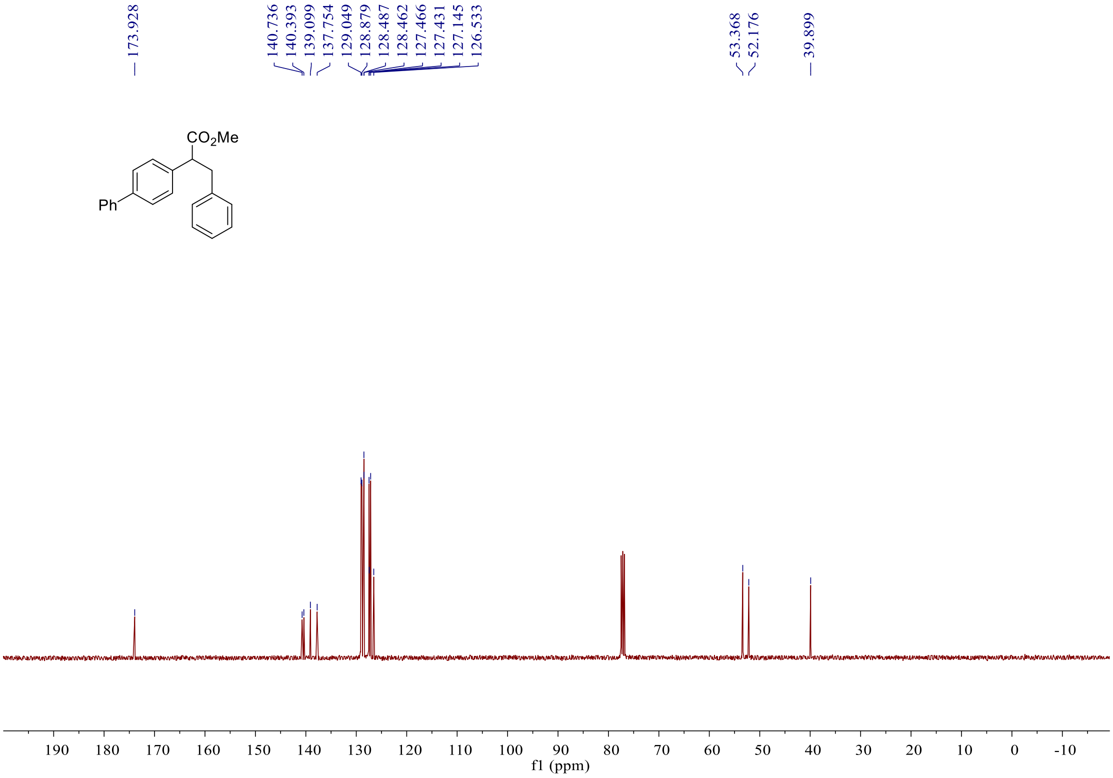
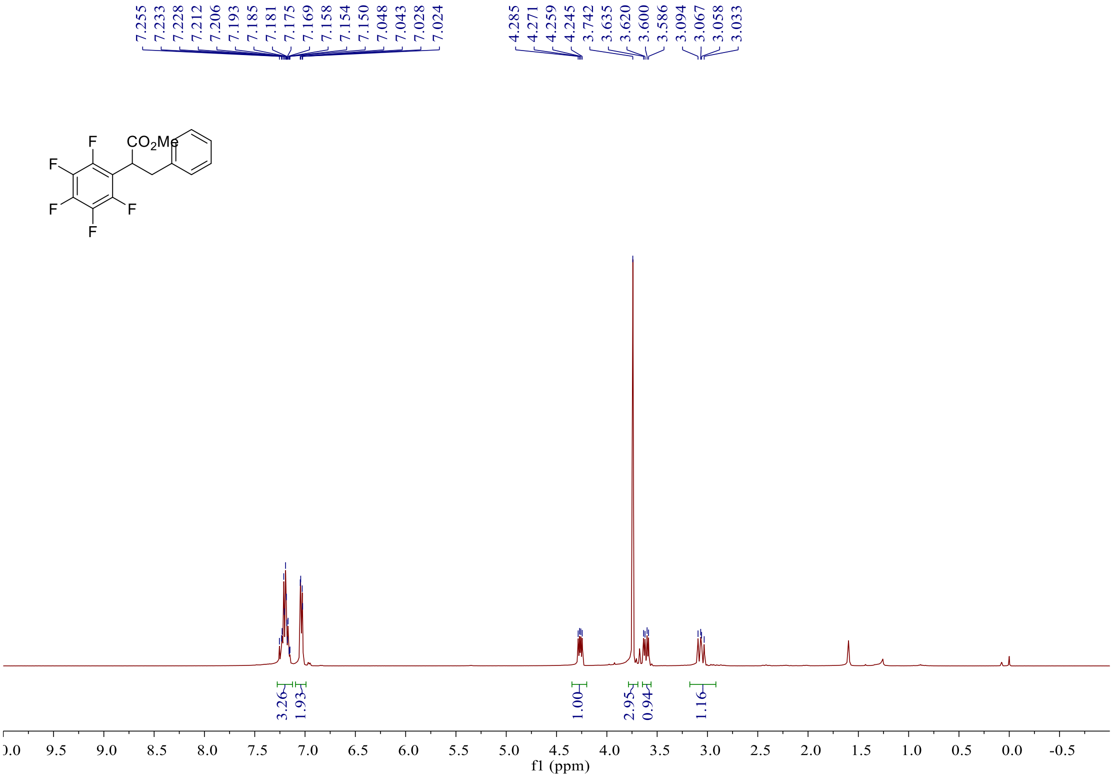
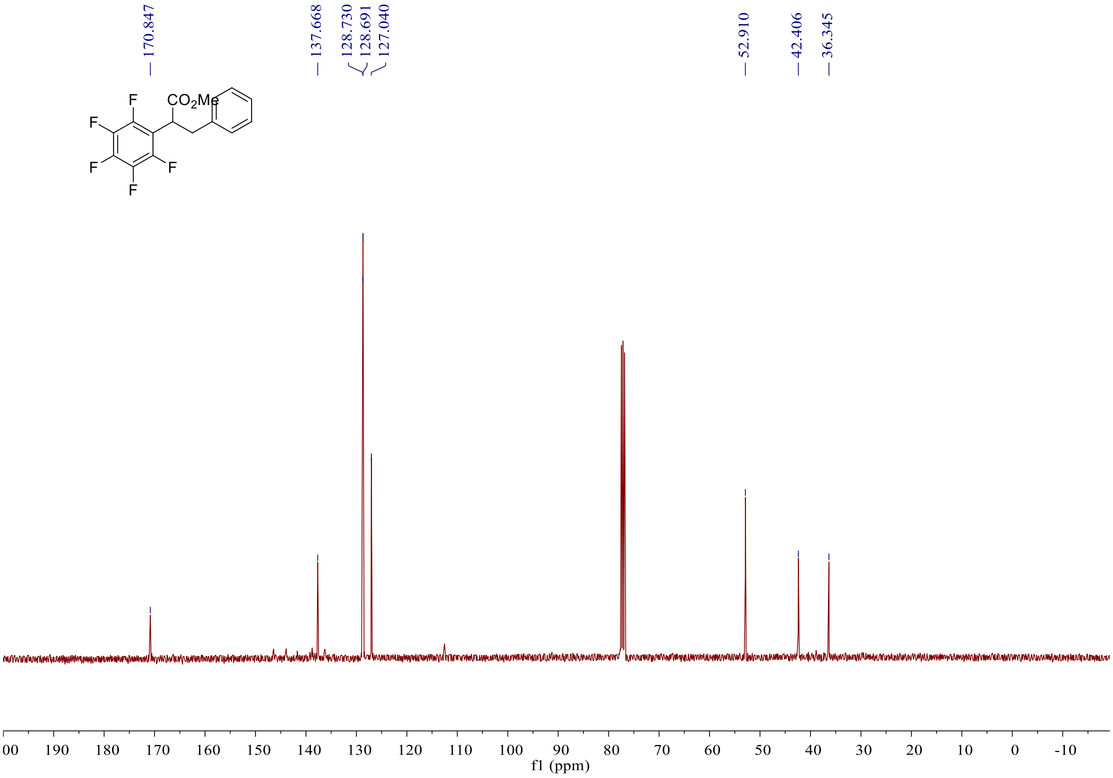
7.523
7.435
7.416
7.397
7.382
7.363
7.344
7.340
7.323
7.307
7.303
7.258
7.254
7.238
7.220
7.212
7.209
7.191
7.174
7.153
7.149
7.133
3.920
3.902
3.897
3.881
3.604
3.476
3.454
3.442
3.419
3.081
3.064
3.047
3.030
CO2Me
Ph
4.05
5.28
5.06
1.00
3.02
1.04
0.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


173.928
140.736
140.393
139.099
137.754
129.049
128.879
128.487
128.462
127.466
127.431
127.145
126.533
53.368
52.176
39.899
CO2Me
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

74


7.255
7.233
7.228
7.212
7.206
7.193
7.185
7.181
7.175
7.169
7.158
7.154
7.150
7.048
7.043
7.028
7.024
4.285
4.271
4.259
4.245
3.742
3.635
3.620
3.600
3.586
3.094
3.067
3.058
3.033
F
F
F
F
F
CO2Me
3.26
1.93
1.00
2.95
0.94
1.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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137.668
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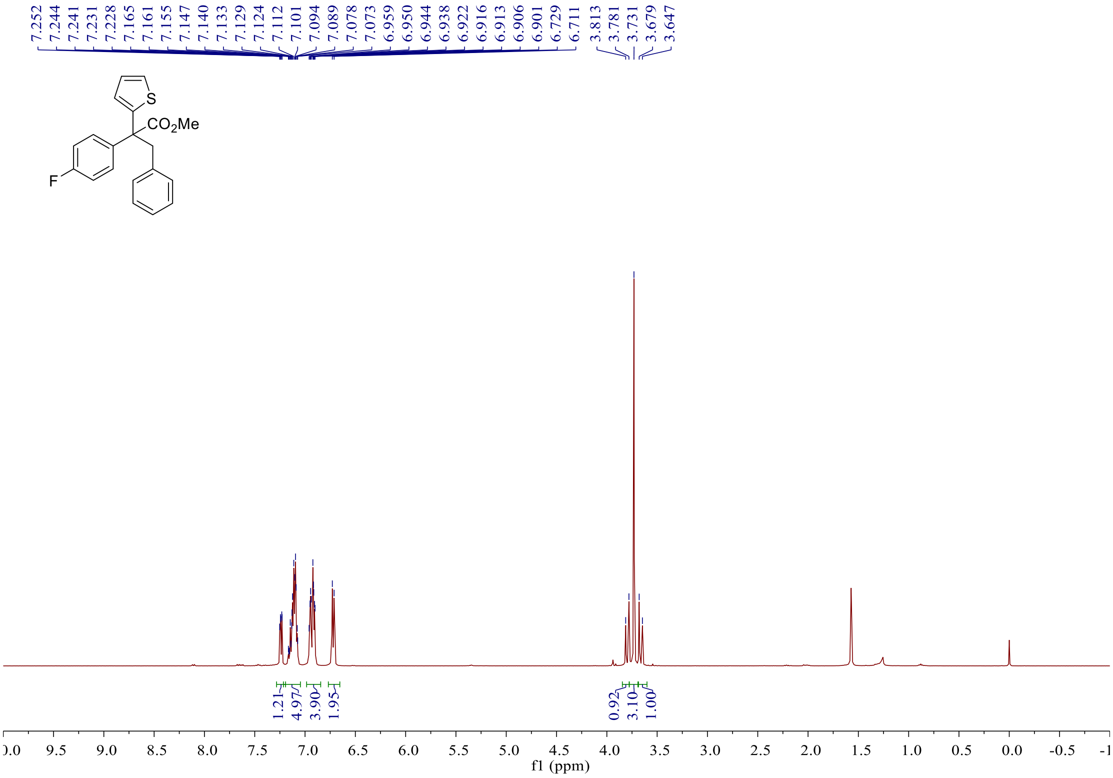
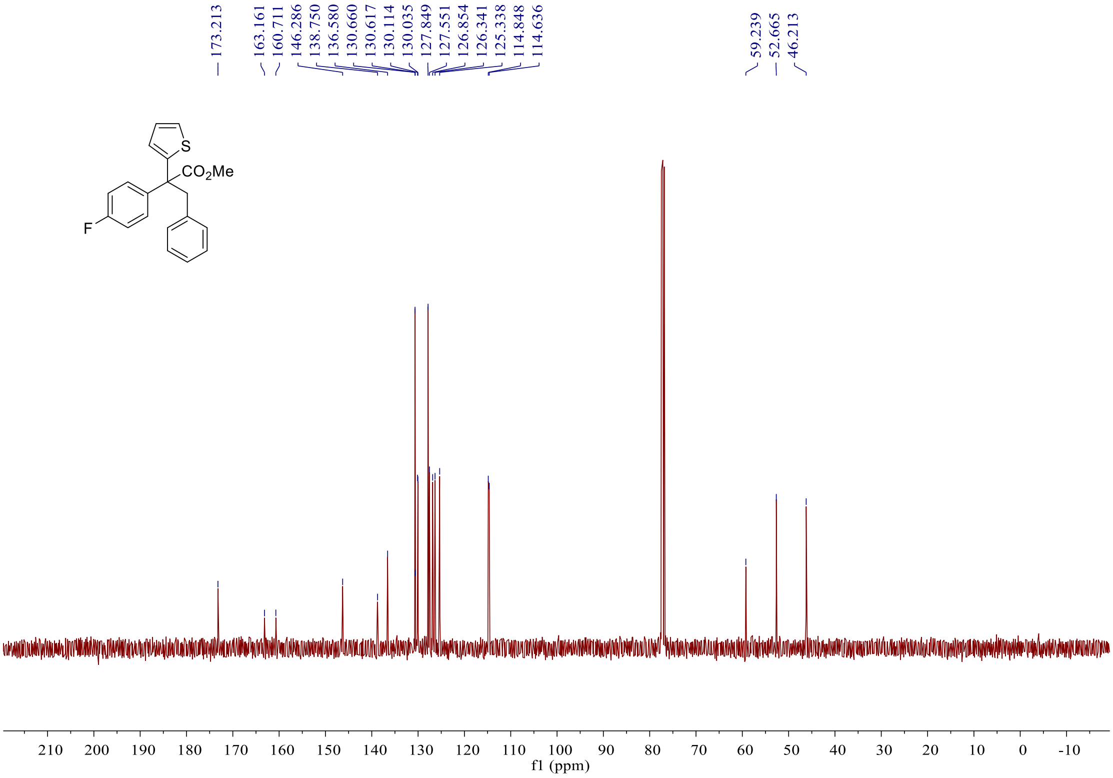
128.691
127.040
52.910
42.406
36.345
F
F
F
F
F
CO2Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

75


7.252
7.244
7.241
7.231
7.228
7.165
7.161
7.155
7.147
7.140
7.133
7.129
7.124
7.112
7.101
7.094
7.089
7.078
7.073
6.959
6.950
6.944
6.938
6.922
6.916
6.913
6.906
6.901
6.729
6.711
3.813
3.781
3.731
3.679
3.647
S
CO$_2$Me
F
1.21
4.97
3.90
1.95
0.92
3.10
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


173.213
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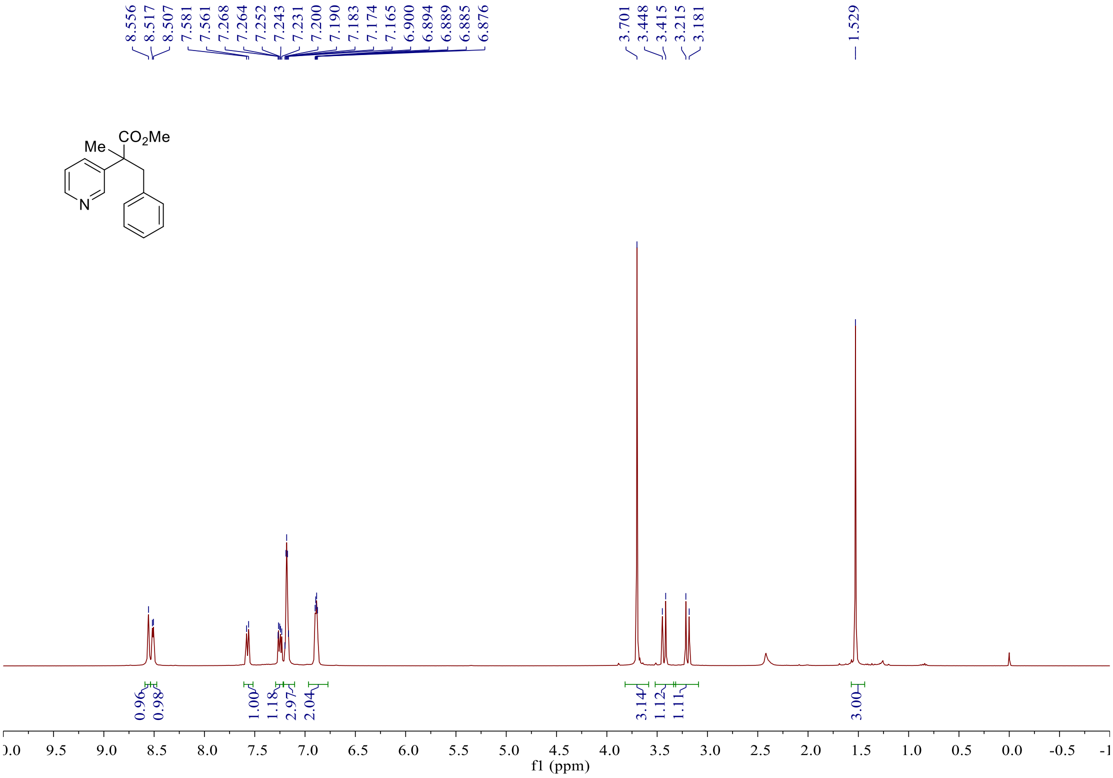
160.711
146.286
138.750
136.580
130.660
130.617
130.114
130.035
127.849
127.551
126.854
126.341
125.338
114.848
114.636
59.239
52.665
46.213
S
CO$_2$Me
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

76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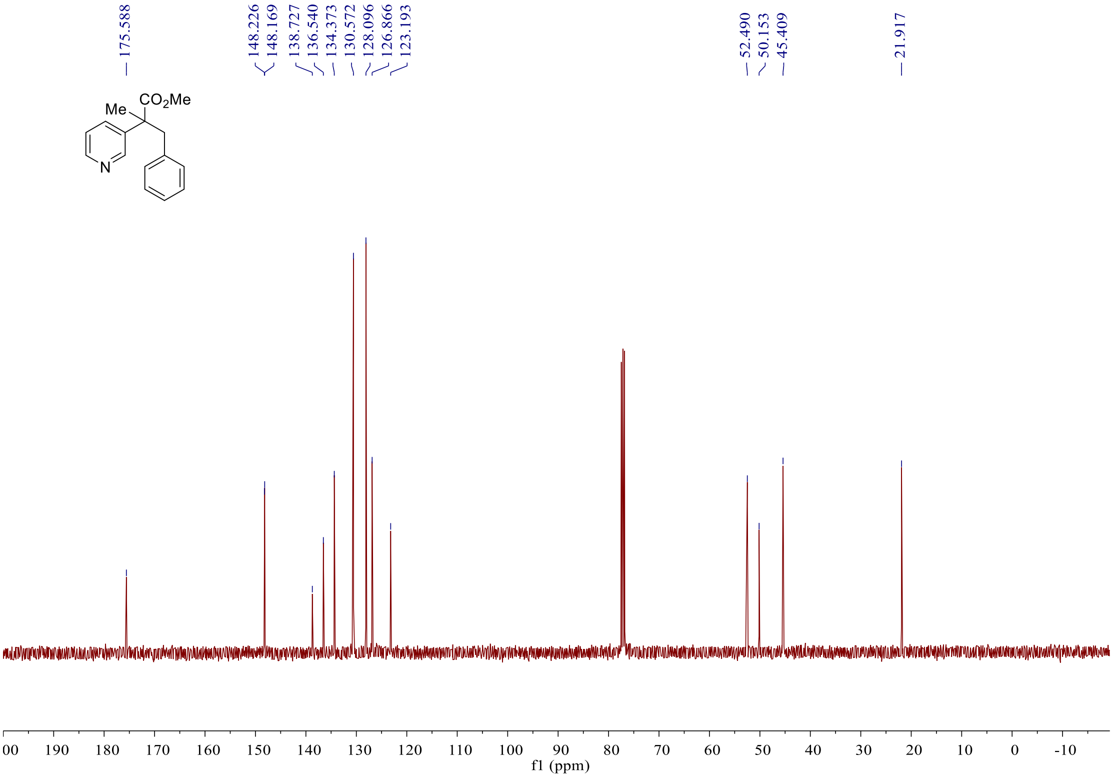
7.264
7.252
7.243
7.231
7.200
7.190
7.183
7.174
7.165
6.900
6.894
6.889
6.885
6.876
3.701
3.448
3.415
3.215
3.181
1.529
Me
CO2Me
N
0.96
0.98
1.00
1.18
2.97
2.04
3.14
1.12
1.11
3.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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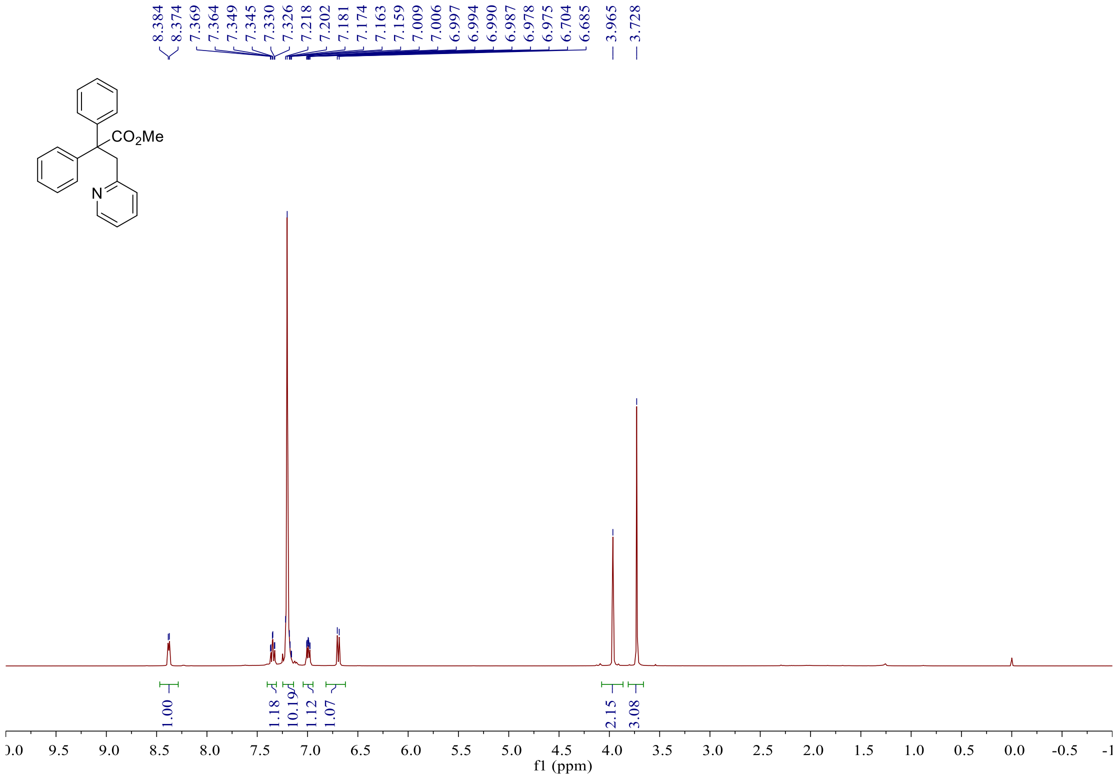
138.727
136.540
134.373
130.572
128.096
126.866
123.193
52.490
50.153
45.409
21.917
Me
CO2Me
N
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

77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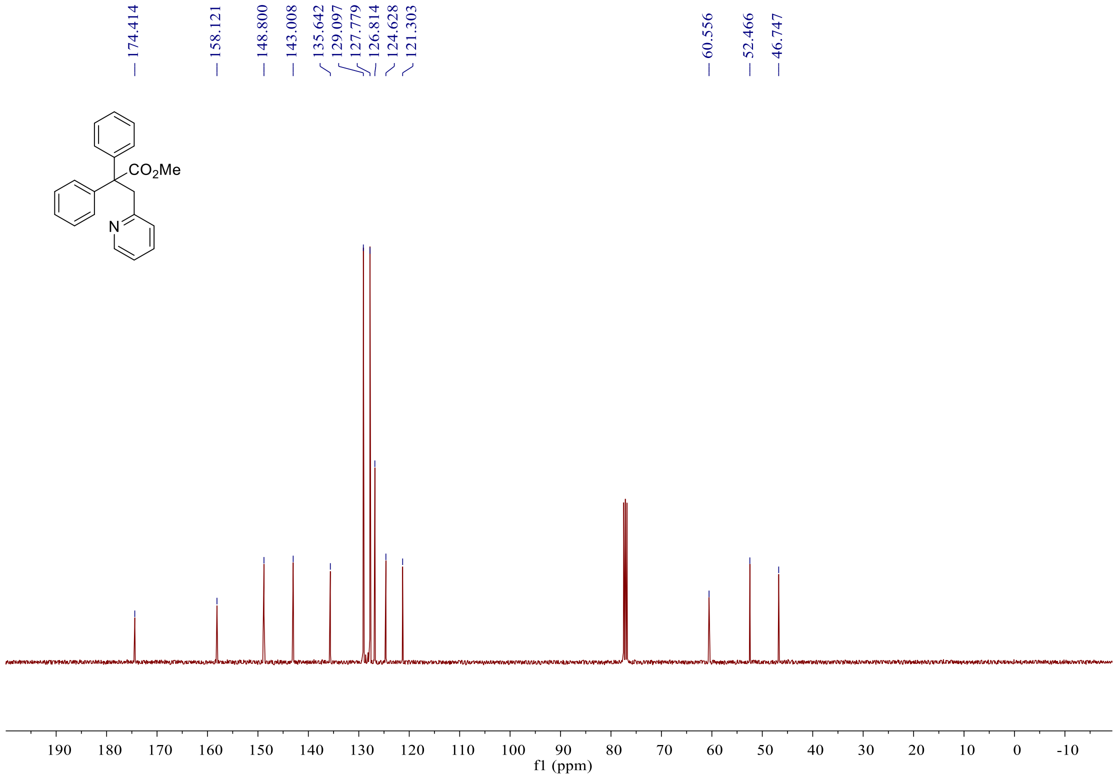
7.345
7.330
7.326
7.218
7.202
7.181
7.174
7.163
7.159
7.009
7.006
6.997
6.994
6.990
6.987
6.978
6.975
6.704
6.685
3.965
3.728
CO2Me
N
1.00
1.18
10.19
1.12
1.07
2.15
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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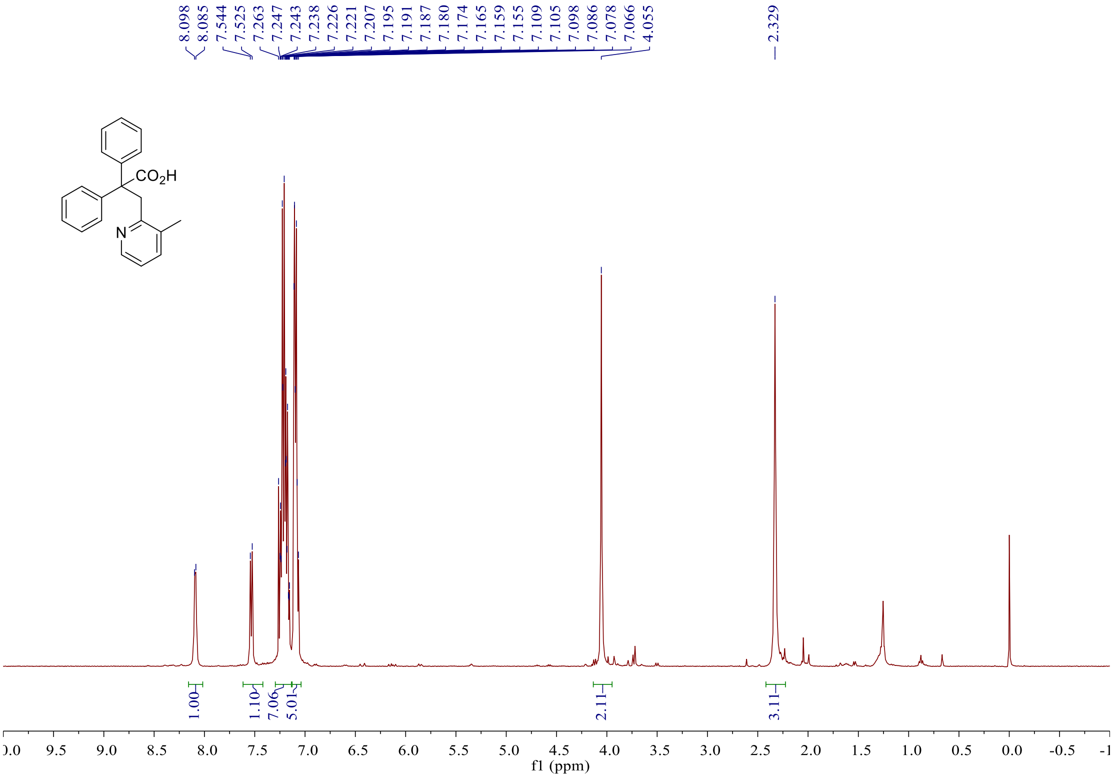
135.642
129.097
127.779
126.814
124.628
121.303
60.556
52.466
46.747
CO2Me
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

78


8.098
8.085
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7.525
7.263
7.247
7.243
7.238
7.226
7.221
7.207
7.195
7.191
7.187
7.180
7.174
7.165
7.159
7.155
7.109
7.105
7.098
7.086
7.078
7.066
4.055
2.329
CO2H
N
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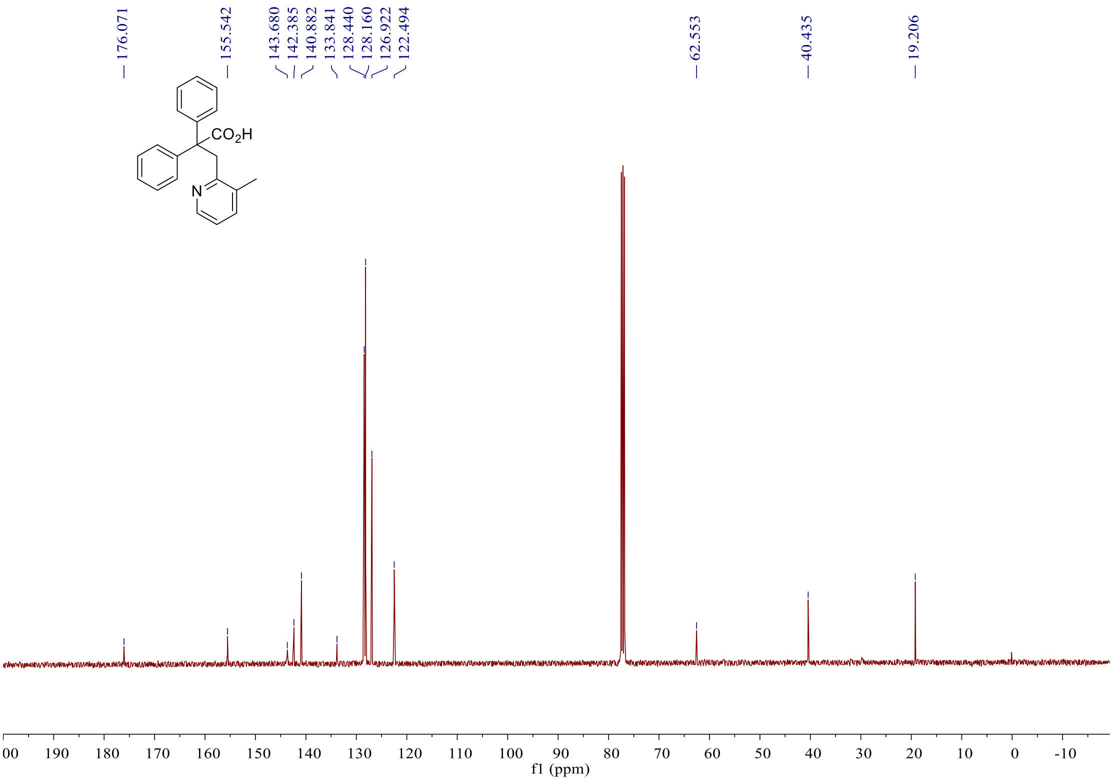
1.10
7.06
5.01
2.11
3.11
f1 (ppm)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140.882
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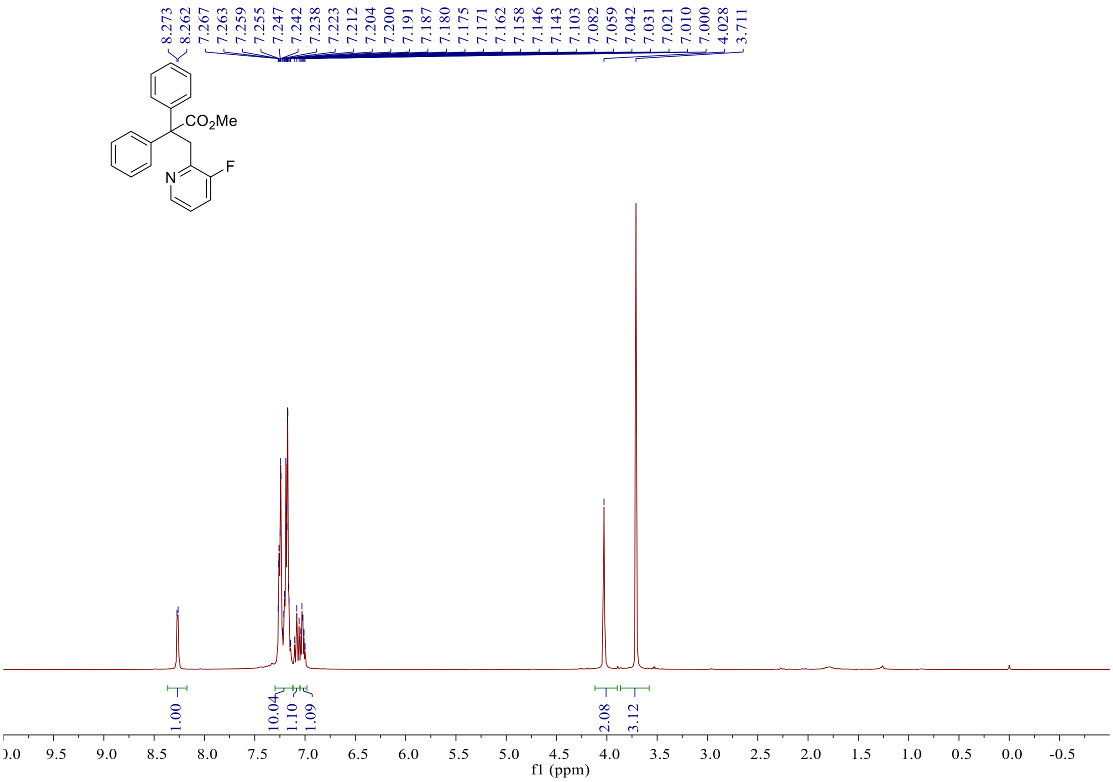
128.440
128.160
126.922
122.494
62.553
40.435
19.206
CO2H
N
f1 (ppm)

79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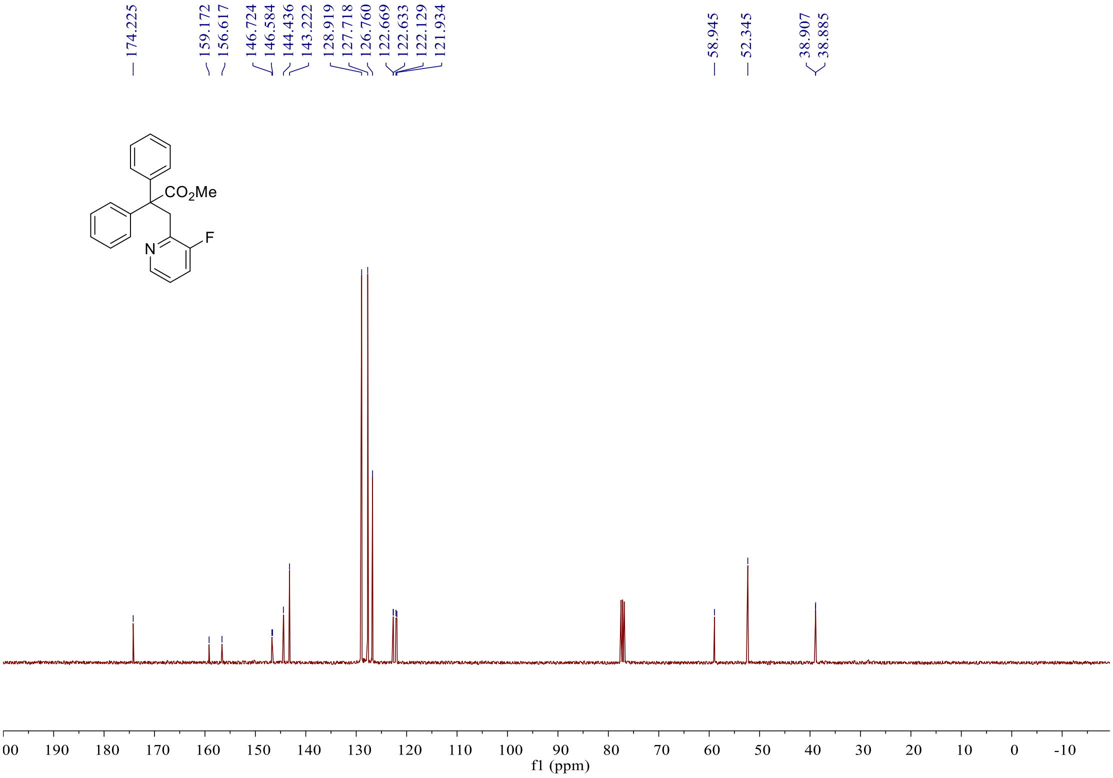
7.267
7.263
7.259
7.255
7.247
7.242
7.238
7.223
7.212
7.204
7.200
7.191
7.187
7.180
7.175
7.171
7.162
7.158
7.146
7.143
7.103
7.082
7.059
7.042
7.031
7.021
7.010
7.000
4.028
3.711
CO2Me
N
F
1.00
10.04
1.10
1.09
2.08
3.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


174.225
159.172
156.617
146.724
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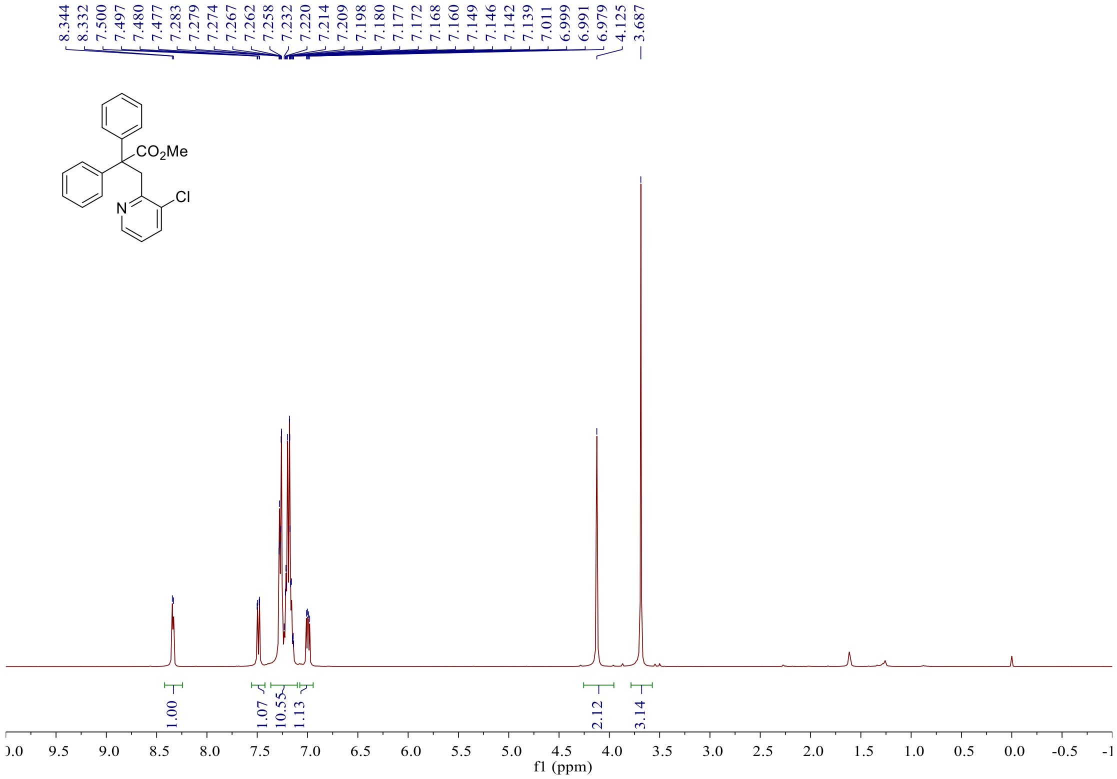
144.436
143.222
128.919
127.718
126.760
122.669
122.633
122.129
121.934
58.945
52.345
38.907
38.885
CO2Me
N
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

80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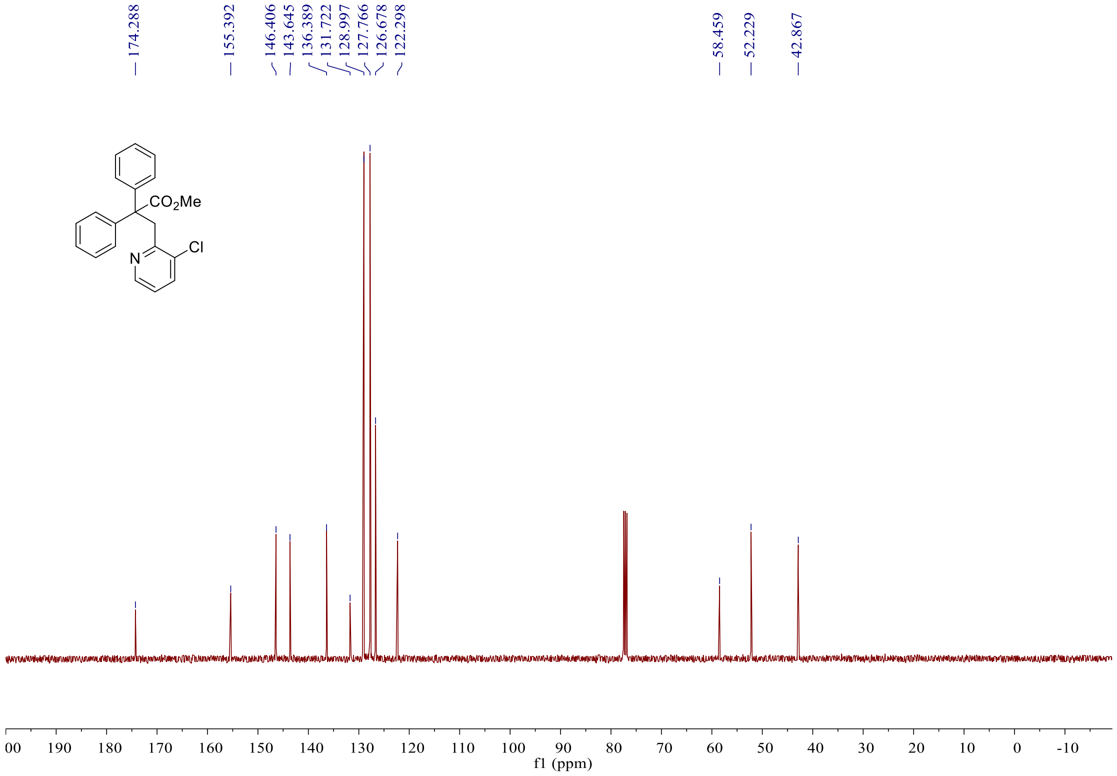
7.232
7.220
7.214
7.209
7.198
7.180
7.177
7.172
7.168
7.160
7.149
7.146
7.142
7.139
7.011
6.999
6.991
6.979
4.125
3.687
CO2Me
N
Cl
1.00
1.07
10.55
1.13
2.12
3.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


174.288
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131.722
128.997
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122.298
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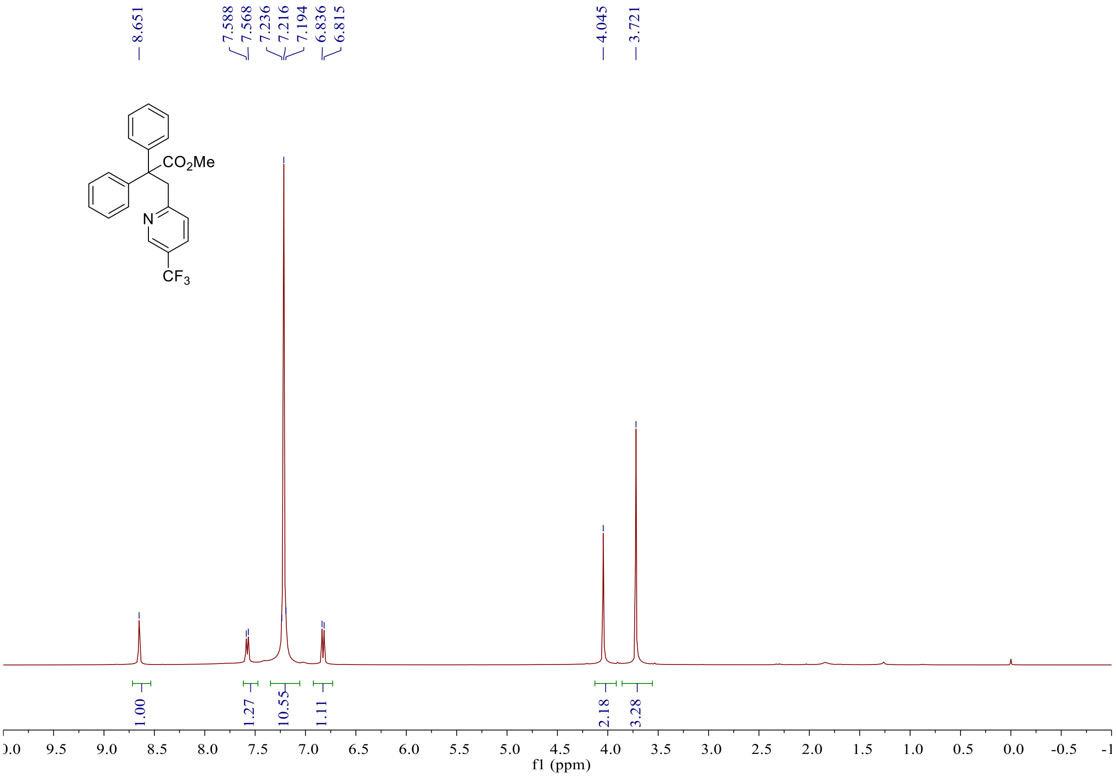
52.229
42.867
CO2Me
N
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

81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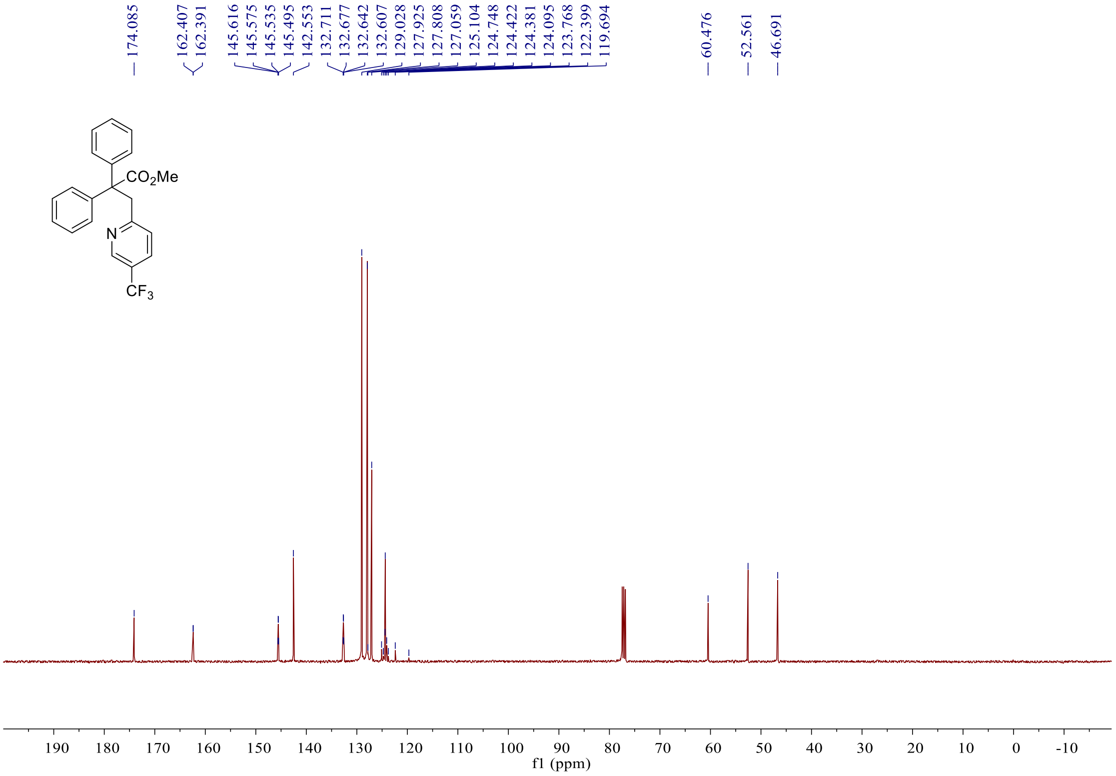
7.236
7.216
7.194
6.836
6.815
4.045
3.721
CO2Me
N
CF3
1.00
1.27
10.55
1.11
2.18
3.28
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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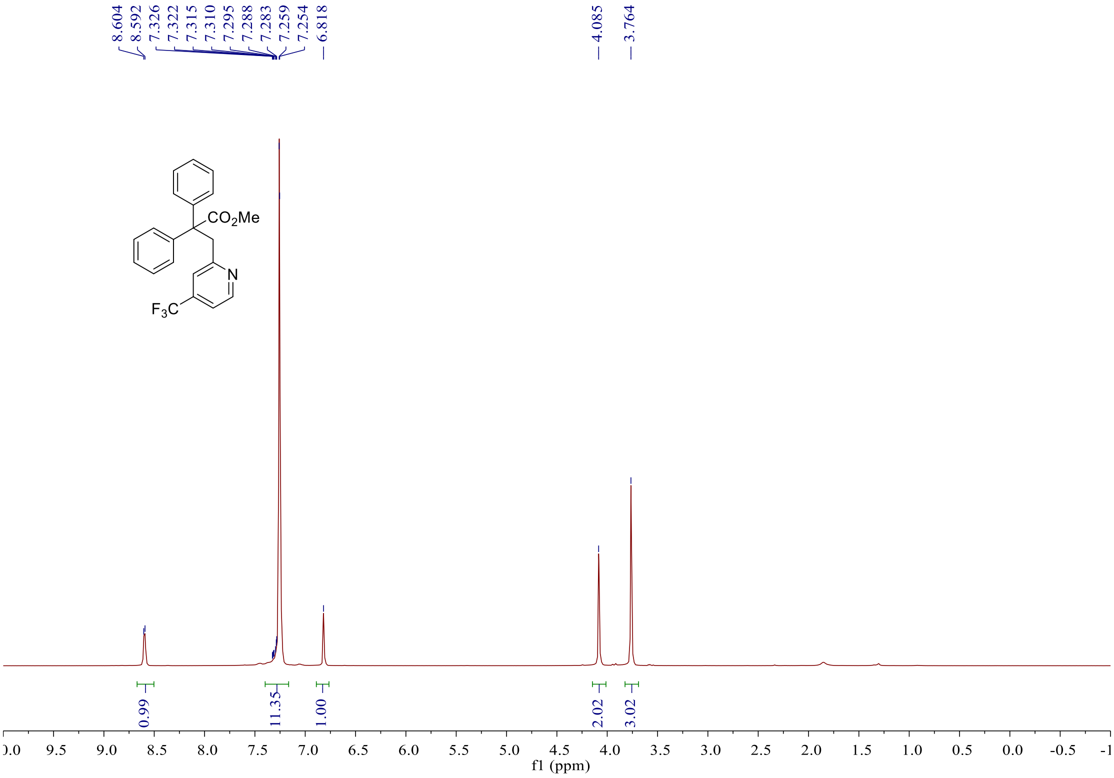
162.407
162.391
145.616
145.575
145.535
145.495
142.553
132.711
132.677
132.642
132.607
129.028
127.925
127.808
127.059
125.104
124.748
124.422
124.381
124.095
123.768
122.399
119.694
60.476
52.561
46.691
CO2Me
N
CF3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

82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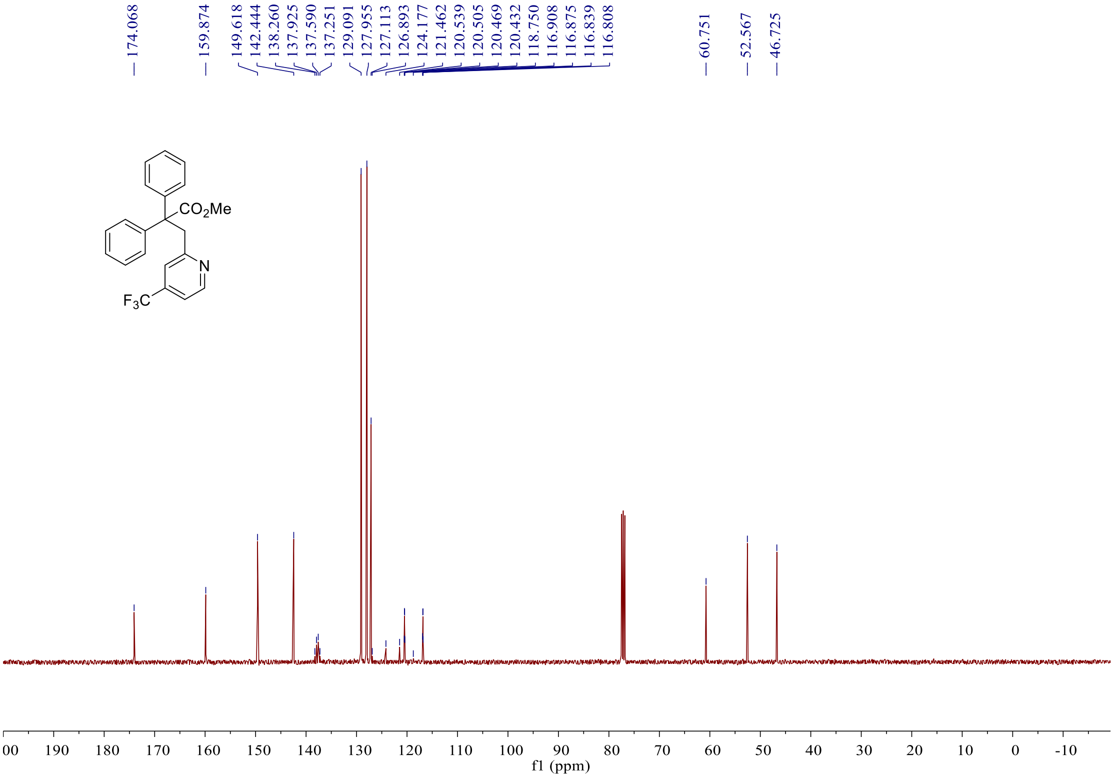
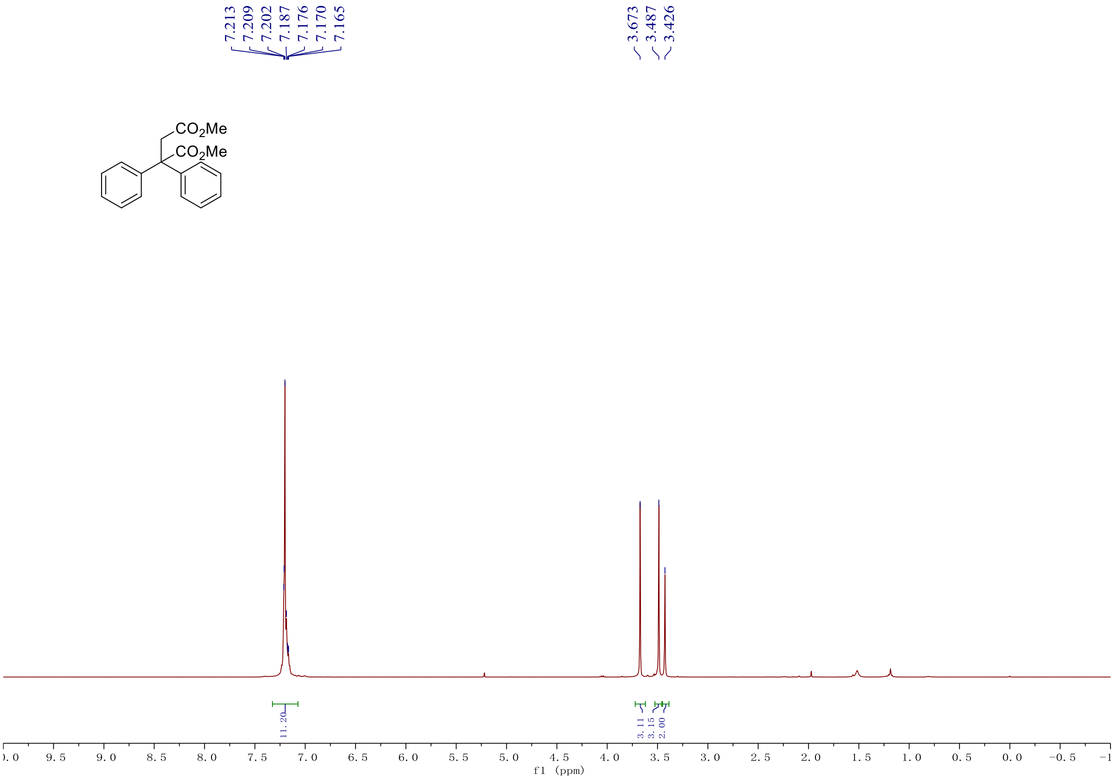
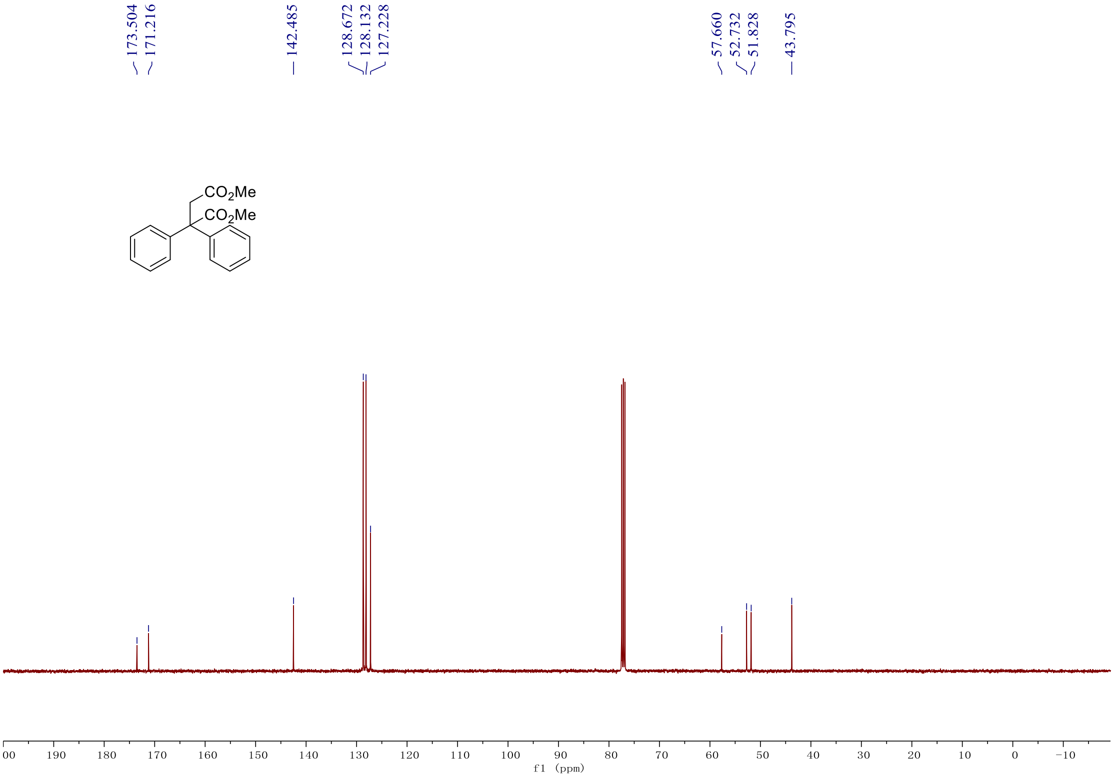
8.592
7.326
7.322
7.315
7.310
7.295
7.288
7.283
7.259
7.254
6.818
4.085
3.764
CO$_2$Me
N
F$_3$C
0.99
11.35
1.00
2.02
3.02
).0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

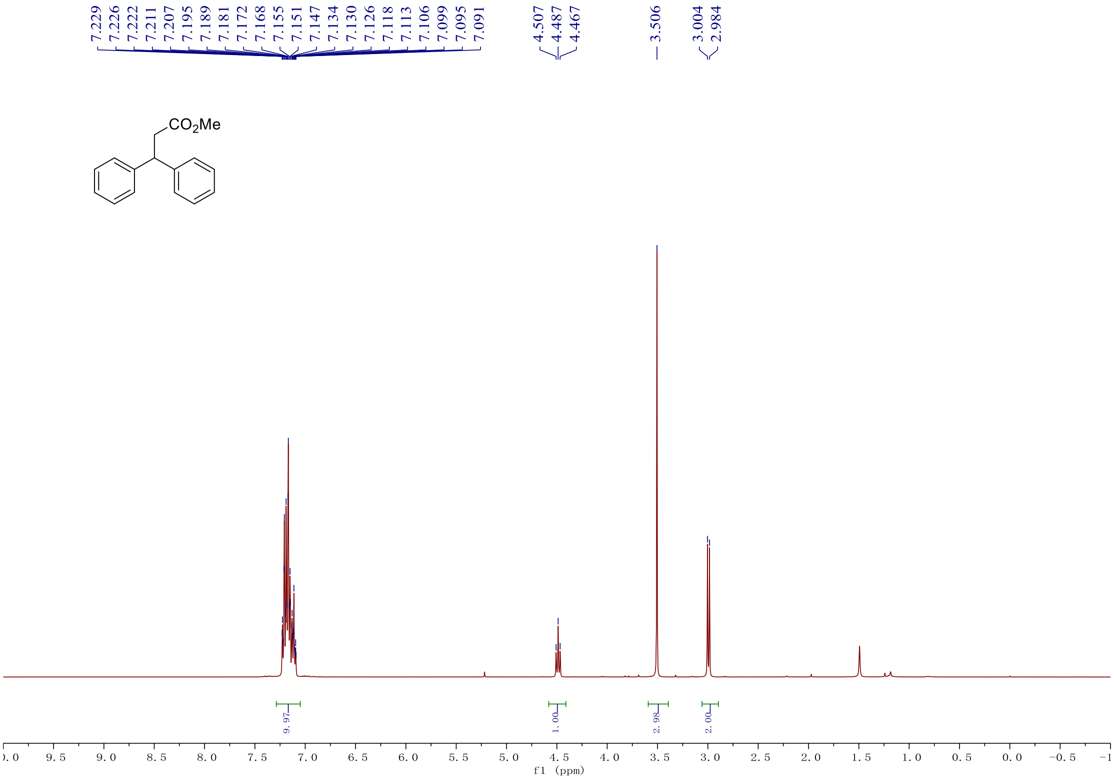

174.068
159.874
149.618
142.444
138.260
137.925
137.590
137.251
129.091
127.955
127.113
126.893
124.177
121.462
120.539
120.505
120.469
120.432
118.750
116.908
116.875
116.839
116.808
60.751
52.567
46.725
CO$_2$Me
N
F$_3$C
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

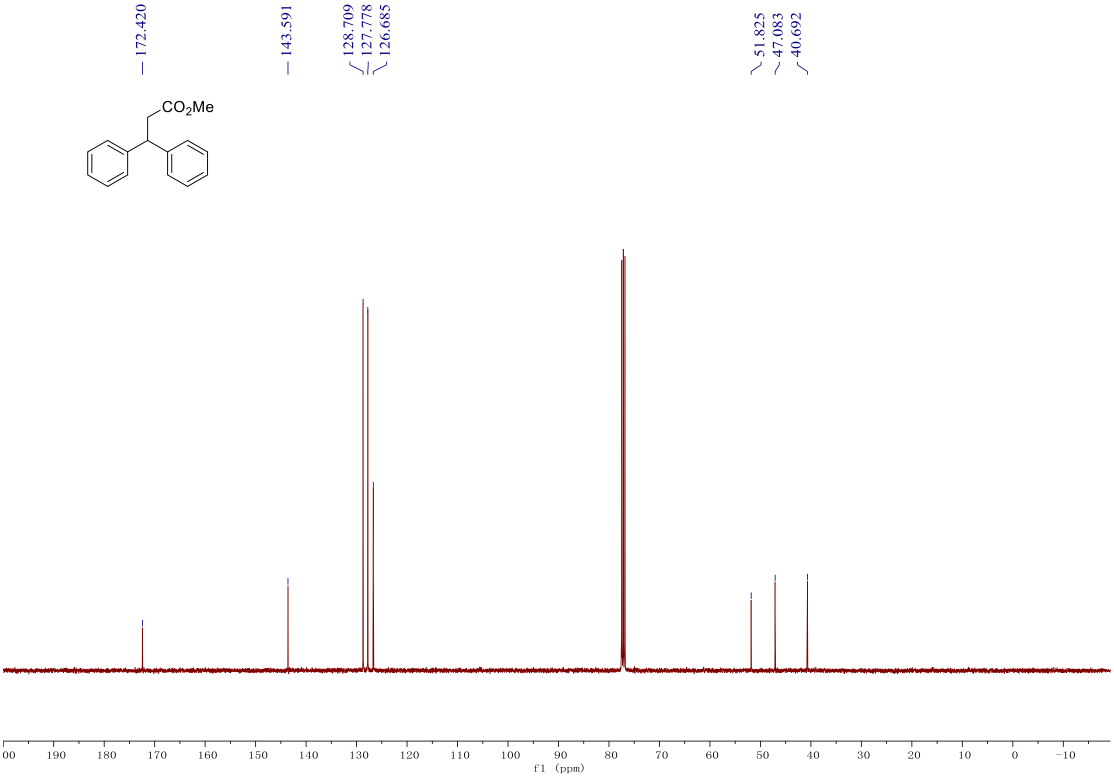
83


7.213
7.209
7.202
7.187
7.176
7.170
7.165
3.673
3.487
3.426
CO2Me
CO2Me
11.20
3.11
3.15
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

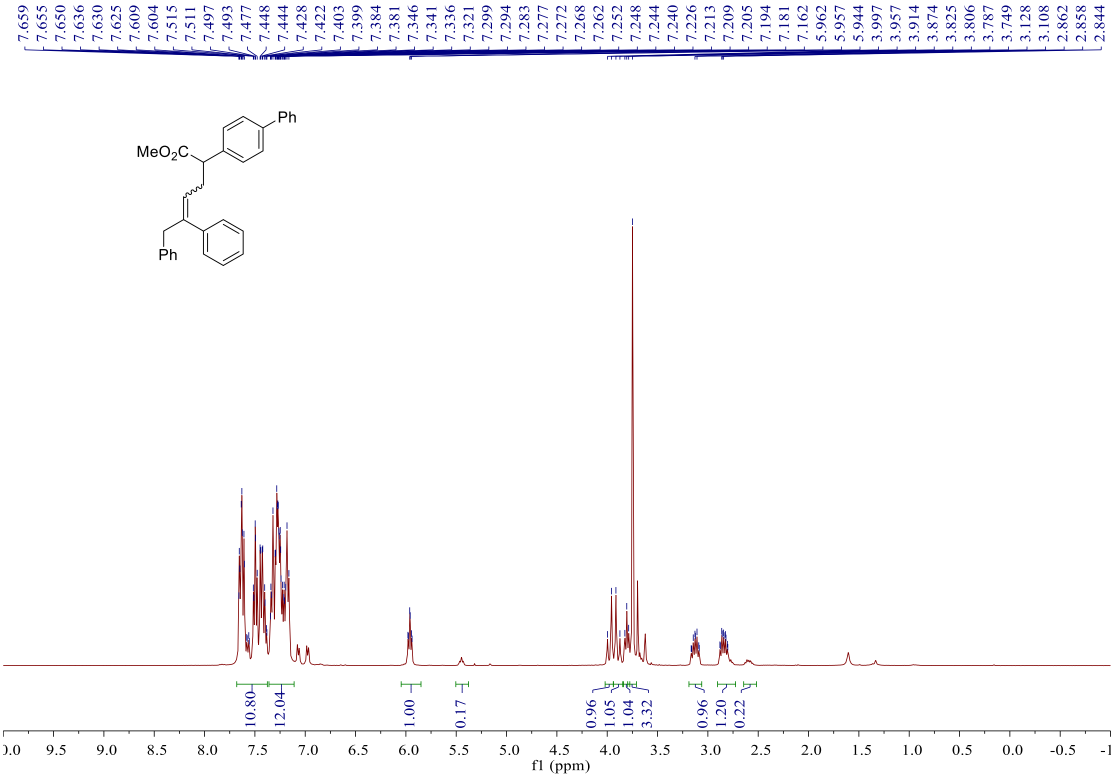

173.504
171.216
142.485
128.672
128.132
127.228
57.660
52.732
51.828
43.795
CO2Me
CO2Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

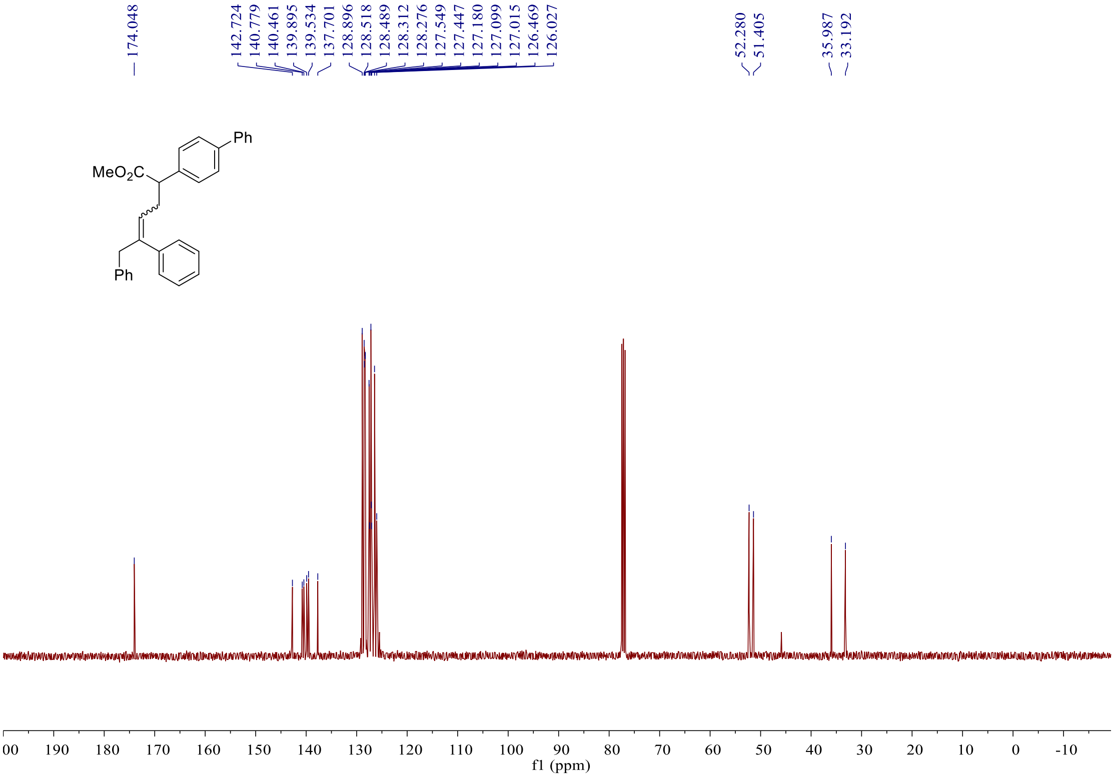
84


7.229
7.226
7.222
7.211
7.207
7.195
7.189
7.181
7.172
7.168
7.155
7.151
7.147
7.134
7.130
7.126
7.118
7.113
7.106
7.099
7.095
7.091
4.507
4.487
4.467
3.506
3.004
2.984
CO2Me
9.97
1.00
2.98
2.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)

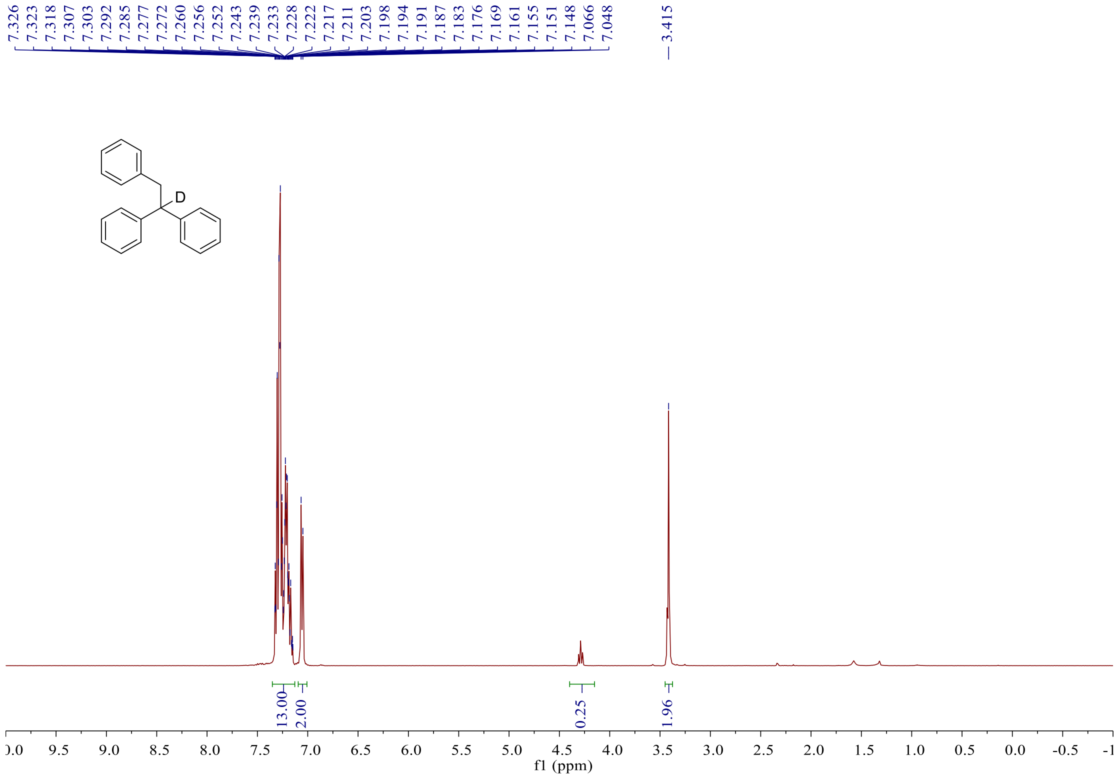

172.420
143.591
128.709
127.778
126.685
51.825
47.083
40.692
CO2Me
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

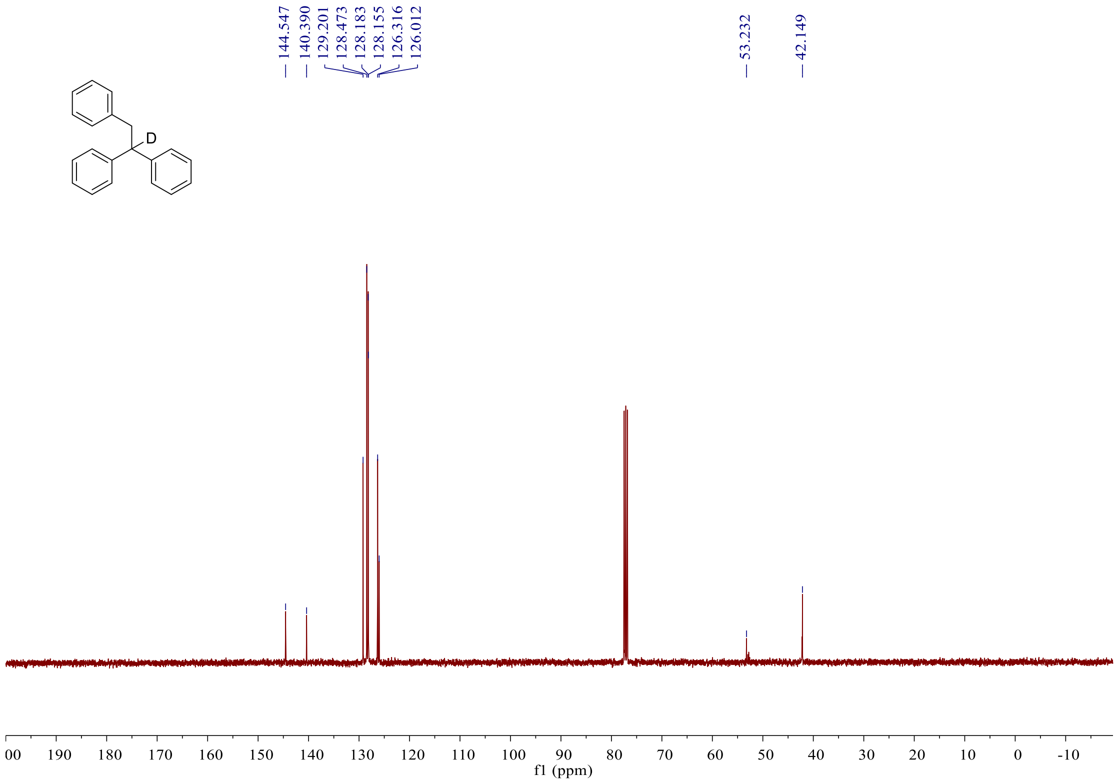
85


7.659
7.655
7.650
7.636
7.630
7.625
7.609
7.604
7.515
7.511
7.497
7.493
7.477
7.448
7.444
7.428
7.422
7.403
7.399
7.384
7.381
7.346
7.341
7.336
7.321
7.299
7.294
7.283
7.277
7.272
7.268
7.262
7.252
7.248
7.244
7.240
7.226
7.213
7.209
7.205
7.194
7.181
7.162
5.962
5.957
5.944
3.997
3.957
3.914
3.874
3.825
3.806
3.787
3.749
3.128
3.108
2.862
2.858
2.844
Ph
MeO2C
Ph
10.80
12.04
1.00
0.17
0.96
1.05
1.04
3.32
0.96
1.20
0.22
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

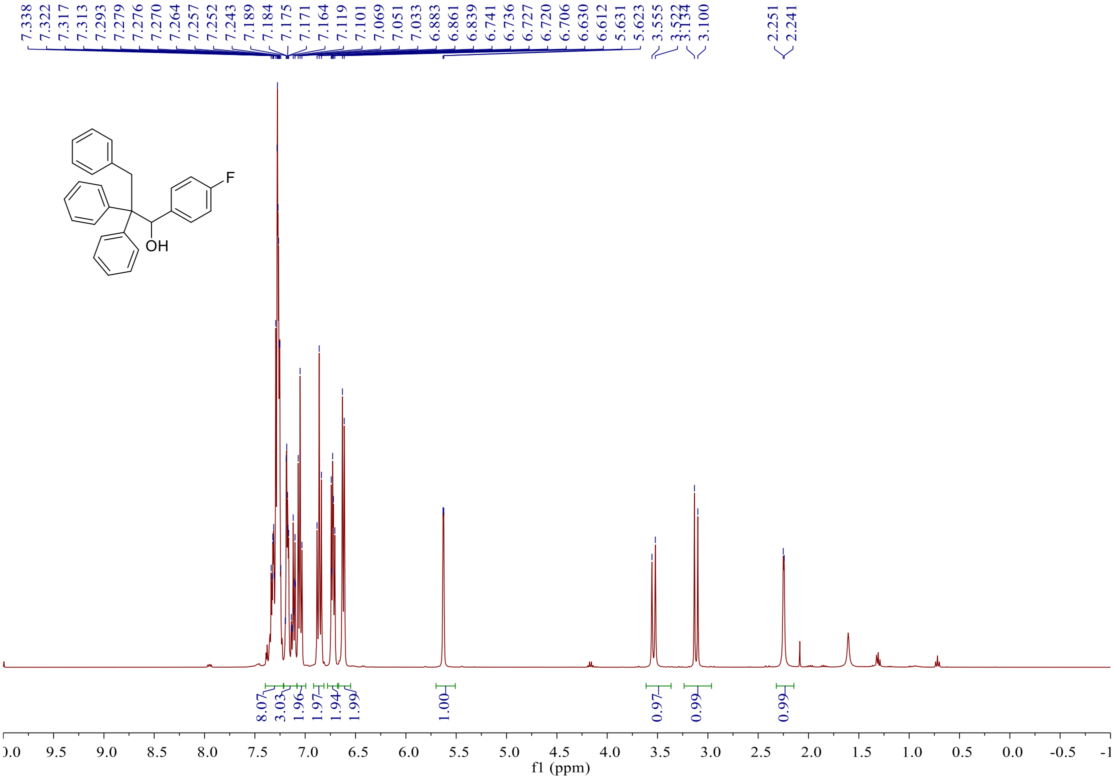

174.048
142.724
140.779
140.461
139.895
139.534
137.701
128.896
128.518
128.489
128.312
128.276
127.549
127.447
127.180
127.099
127.015
126.469
126.027
52.280
51.405
35.987
33.192
Ph
MeO2C
Ph
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

86


7.326
7.323
7.318
7.307
7.303
7.292
7.285
7.277
7.272
7.260
7.256
7.252
7.243
7.239
7.233
7.228
7.222
7.217
7.211
7.203
7.198
7.194
7.191
7.187
7.183
7.176
7.169
7.161
7.155
7.151
7.148
7.066
7.048
3.415
D
13.00
2.00
0.25
1.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


144.547
140.390
129.201
128.473
128.183
128.155
126.316
126.012
53.232
42.149
D
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

87


7.338
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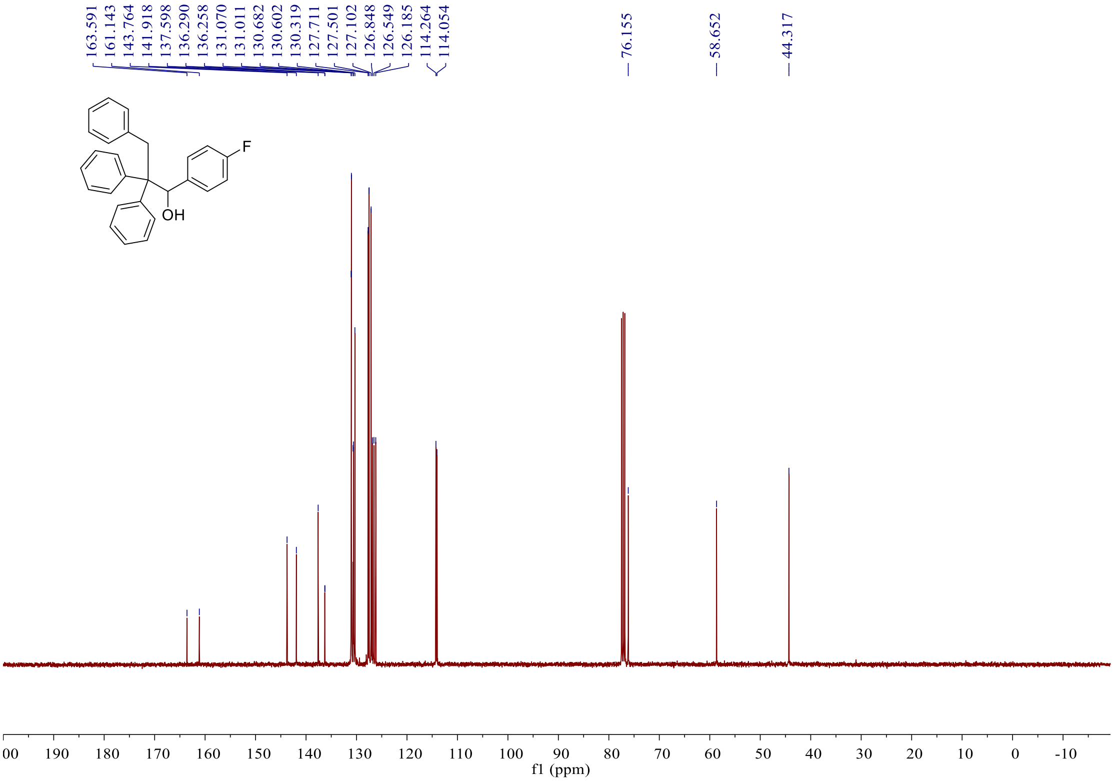
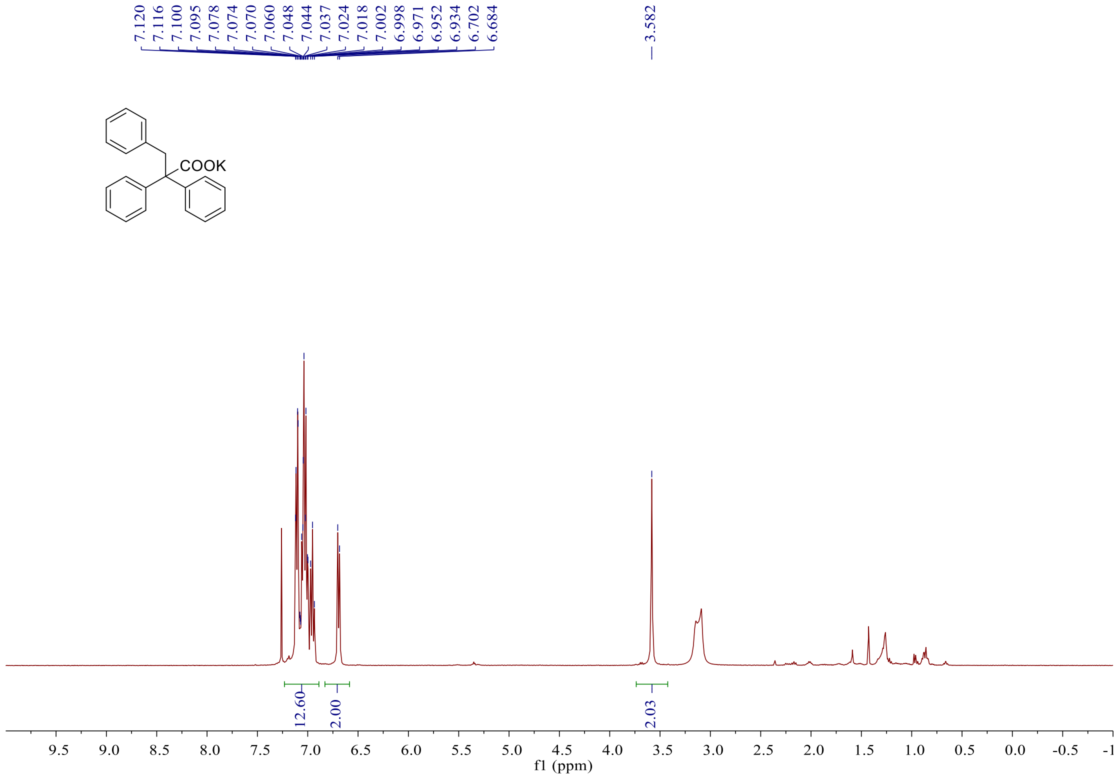
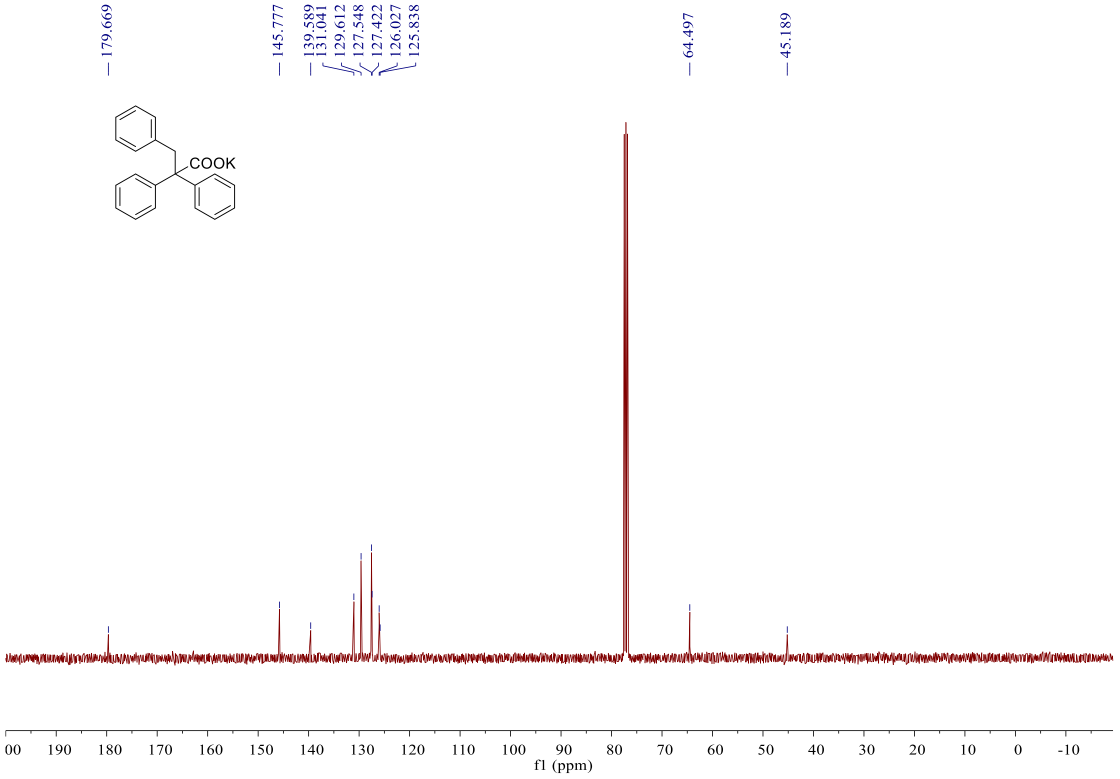
7.317
7.313
7.293
7.279
7.276
7.270
7.264
7.257
7.252
7.243
7.189
7.184
7.175
7.171
7.164
7.119
7.101
7.069
7.051
7.033
6.883
6.861
6.839
6.741
6.736
6.727
6.720
6.706
6.630
6.612
5.631
5.623
3.555
3.522
3.134
3.100
2.251
2.241
F
OH
8.07
3.03
1.96
1.97
1.94
1.99
1.00
0.97
0.99
0.99
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


163.591
161.143
143.764
141.918
137.598
136.290
136.258
131.070
131.011
130.682
130.602
130.319
127.711
127.501
127.102
126.848
126.549
126.185
114.264
114.054
76.155
58.652
44.317
F
OH
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

1-K


7.120
7.116
7.100
7.095
7.078
7.074
7.070
7.060
7.048
7.044
7.037
7.024
7.018
7.002
6.998
6.971
6.952
6.934
6.702
6.684
3.582
COOK
12.60
2.00
2.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


179.669
145.777
139.589
131.041
129.612
127.548
127.422
126.027
125.838
64.497
45.189
COOK
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

5. References

[S1] Combee, L. A.; Johnson, S. L.; Laudenschlager, J. E.; Hilinski, M. K., Rh(II)-Catalyzed Nitrene-Transfer [5 + 1] Cycloadditions of Aryl-Substituted Vinylcyclopropanes. *Org. Lett.* **2019,** *21*, 2307-2311.