Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Visible Light-Induced Aryltrifluoromethylation of Hydroxy Alkenes *via* Radical Trifluoromethylation-Triggered Aryl and Heteroaryl Migration

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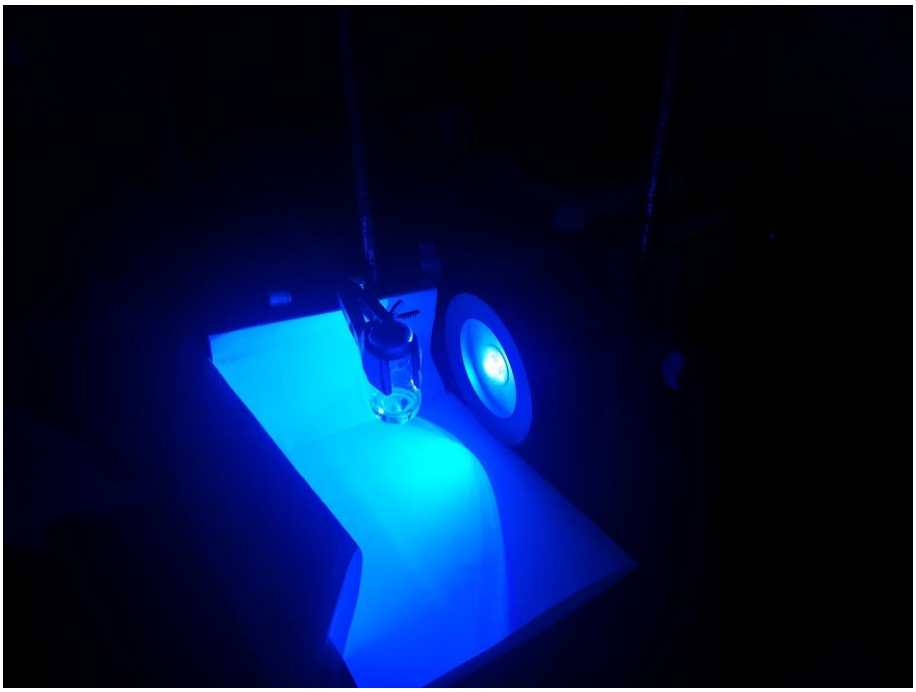
Contents

1. General methods.

DMSO was dried according to Purification of Common Laboratory Chemicals. Other reagents were used without further purification. Thin layer chromatography (TLC) was performed on EMD precoated plates (silica gel 60 F254, Art 5715) and visualized by fluorescence quenching under UV light and by staining with phosphomolybdic acid or potassium permanganate, respectively. Column chromatography was performed on EMD Silica Gel 60 (300–400 Mesh) using a forced flow of 0.5–1.0 bar. ^{1}H NMR (400 MHz), ^{13}C NMR (100MHz) and ^{19}F (376MHz) were measured on a Bruker AVANCE III–400 spectrometer. Chemical shifts are expressed in parts per million (ppm) with respect to the residual solvent peak. Coupling constants are reported as Hertz (Hz), signal shapes and splitting patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet.

Reaction Apparatus

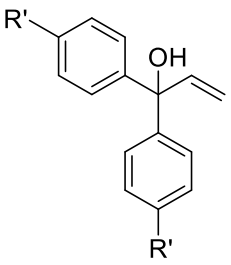
Photochemical reaction was carried out under visible light irradiation by a 48W blue lamp at room temperature (about 25 ºC).



2. General procedure for the difunctionalization of olefins

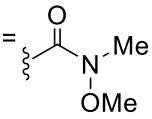
General Procedure. A 10 mL round bottom flask was equipped with a rubber septum and magnetic stir bar and was charged with **1a** (0.2 mmol, 1.0 equiv), **IV** (0.4 mmol, 2.0 equiv) and K_2HPO_4 (0.3mmol, 1.5 equiv). The flask was evacuated and backfilled with nitrogen for 3 times, DMSO (2.0 mL, 0.1 M) were added with a syringe under nitrogen. The mixture was then irradiated by a 48W blue lamp. After the reaction was complete (as judged by TLC analysis), the mixture was poured into a separatory funnel containing 20 mL of H_2O and 20 mL of Et_2O. The layers were separated and the aqueous layer was extracted with Et_2O (2 × 20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure after filtration. The crude product was purified by flash chromatography on silica gel to afford the desired product **2a**.

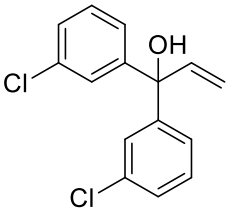
The structures of substrates **1**



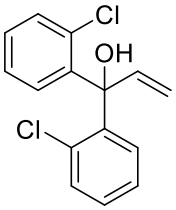
1a: R' = H
1b: R' = Me
1c: R' = OMe
1d: R' = F
1e: R' = Cl
1f: R' = CO_2Et
1g: R' = $CONEt_2$

1h: R' =

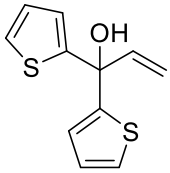




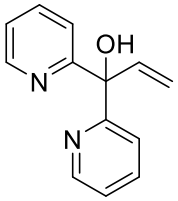
1i



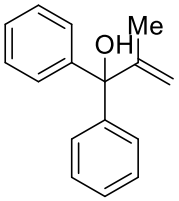
1j



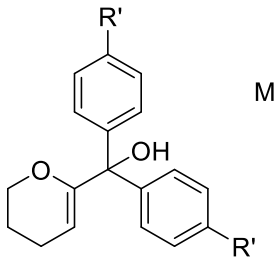
1k



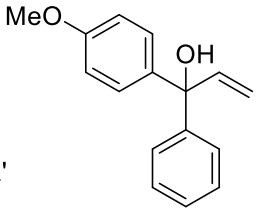
1l



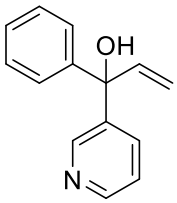
1m



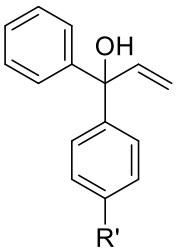
1n: R' = H
1o: R' = F
1p: R' = Cl



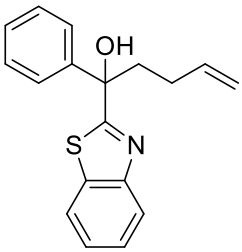
1q



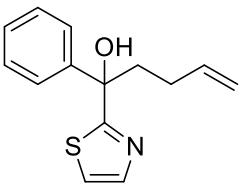
1r



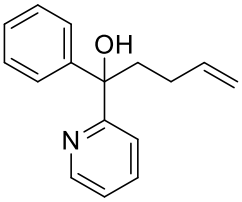
1s: R' = CF_3
1t: R' = CN



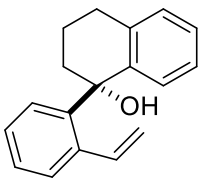
1u



1v



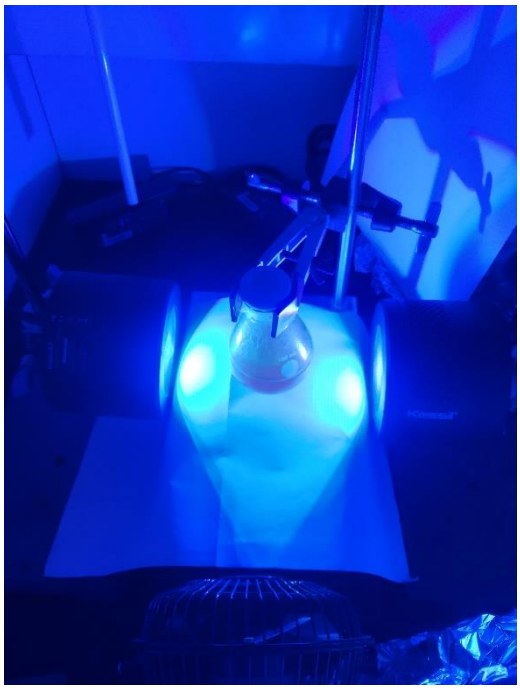
1w



1x

3. Scale-up Experiment

A 100 mL round bottom flask was equipped with a rubber septum and magnetic stir bar and was charged with **1s** (1.11g, 4 mmol, 1.0 equiv), **IV** (5.51g, 8.0 mmol, 2.0 equiv) and K_2HPO_4 (1.05g, 6.0 mmol, 1.5 equiv). The flask was evacuated and backfilled with nitrogen for 3 times, DMSO (40.0 mL, 0.1 M) were added with a syringe under nitrogen. The mixture was then irradiated by a 96 W blue lamps(two 48 W blue lamps). After the reaction was complete (as judged by TLC analysis), the mixture was poured into a separatory funnel containing 100 mL of H_2O and 100 mL of Et_2O. The layers were separated and the aqueous layer was extracted with Et_2O (2 × 100 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure after filtration. The crude product was purified by flash chromatography on silica gel to afford the desired product **2s** in 90% yield (1.25g).

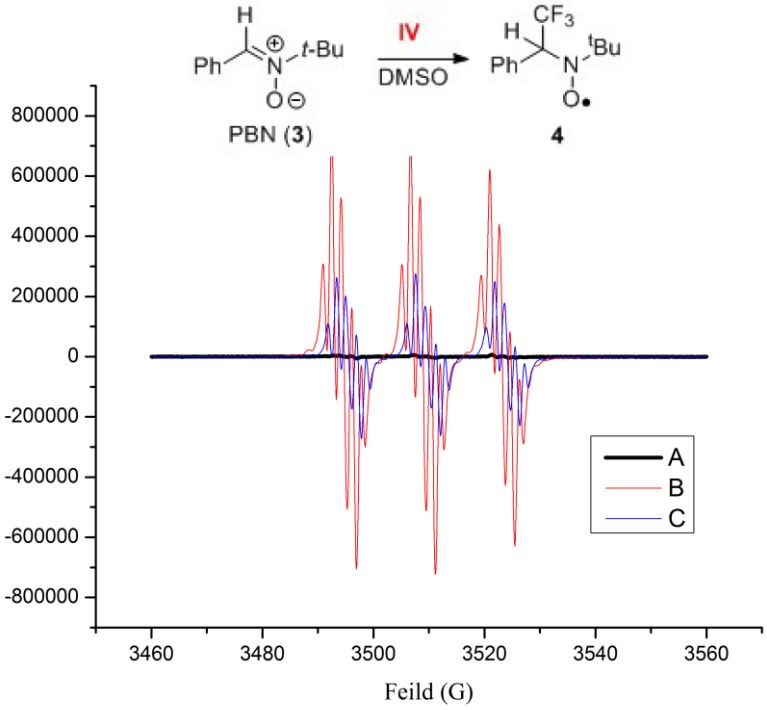


4. EPR Experiment.

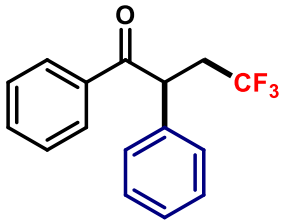
Line A: A 10 mL round bottom flask equipped magnetic stir bar was charged with PBN (0.2 mmol) and DMSO (1 mL). EPR spectrum was recorded by Bruker EMX-10/12 EPR spectrometer immediately.

Line B: A 10 mL round bottom flask equipped magnetic stir bar was charged with PBN (0.2mmol), **IV** (0.2mmol), DMSO (1 mL) and was irradiated with 48W blue lamp for 1 hour. EPR spectrum was recorded by Bruker EMX-10/12 EPR spectrometer immediately.

Line C: A 10 mL round bottom flask equipped magnetic stir bar was charged with PBN (0.2mmol), **IV** (0.2mmol), DMSO (1 mL) and was in the dark condition for 1 hour. EPR spectrum was recorded by Bruker EMX-10/12 EPR spectrometer immediately.

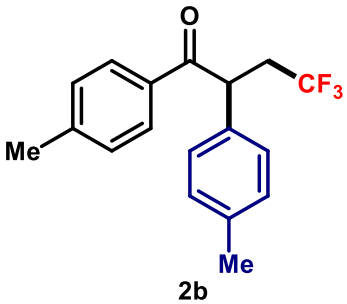


5. Characterization of products



2a

4,4,4-trifluoro-1,2-diphenylbutan-1-one (2a):[1] According to the general procedure: **1a** (0.2 mmol, 42.0 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2a** (44.4 mg, 80%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97-7.94 (m, 2H), 7.52-7.48 (m, 1H), 7.40 (dd, *J* = 8.3, 6.9 Hz, 2H), 7.30 (d, *J* = 4.3 Hz, 4H), 7.26-7.21 (m, 1H), 4.91 (dd, *J* = 7.7, 5.4 Hz, 1H), 3.31 (dqd, *J* = 15.0, 10.8, 7.7 Hz, 1H), 2.54 (dqd, *J* = 15.1, 10.7, 5.5 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.61. ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.73, 137.42, 135.70, 133.36, 129.34, 128.82, 128.67, 128.05, 126.40 (q, *J* = 277.3 Hz), 47.20 (q, *J* = 2.5 Hz), 37.38 (q, *J* = 28.2 Hz).

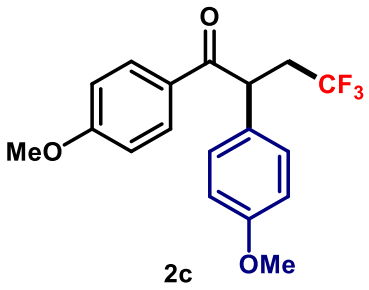


2b

4,4,4-trifluoro-1,2-di-p-tolylbutan-1-one (2b):[1] According to the general procedure: **1b** (0.2 mmol, 47.6 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2b** (49.3 mg, 81%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.19 (d, *J* = 3.2 Hz,2H), 7.17 (d, *J* = 3.1 Hz,

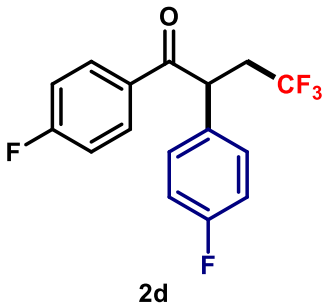
[1] Liu, X.; Xiong, F.; Huang, X.; Xu, L.; Li, P.; Wu, X. *Angew. Chem., Int. Ed.* **2013**, *52*, 6962.

2H), 7.10 (d, *J* = 7.9 Hz, 2H), 4.84 (dd, *J* = 7.6, 5.5 Hz, 1H), 3.34-3.20 (m, 1H), 2.51 (dqd, *J* = 15.0, 10.8, 5.5 Hz, 1H), 2.34 (s, 3H), 2.27 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.55. ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.42, 144.21, 137.50, 134.65, 133.17, 129.97, 129.34, 128.96, 128.87, 126.40 (q, *J* = 277.3 Hz), 46.63 (q, *J* = 2.6 Hz), 37.34 (q, *J* = 28.0 Hz), 6.93, 21.61, 21.02.



2c

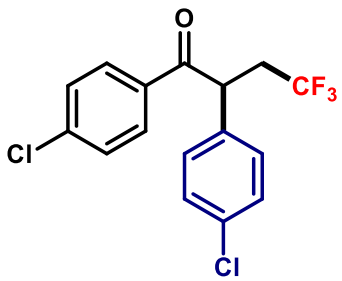
4,4,4-trifluoro-1,2-bis(4-methoxyphenyl)butan-1-one (2c): [2] According to the general procedure: **1c** (0.2 mmol, 54.0 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2c** (42.1 mg, 62%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 9.0 Hz, 2H), 7.21 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 4.82-4.79 (m, 1H), 3.81 (s, 3H), 3.74 (s, 3H), 3.24 (dqd, *J* = 15.0, 10.9, 7.5 Hz, 1H), 2.57-2.44 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.50. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.37, 163.61, 159.04, 131.15, 129.82, 129.05, 128.59, 126.53 (q, *J* = 277.4 Hz), 114.65, 113.85, 55.44, 55.21, 45.95 (q, *J* = 2.5 Hz), 37.39 (q, *J* = 27.9 Hz).



2d

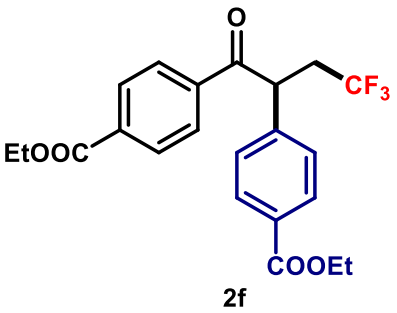
[2] Egami, H.; Shimizu, R.; Usui, Y.; Sodeoka, M. *Chem. Commun.* **2013**, *49*, 7346.

4,4,4-trifluoro-1,2-bis(4-fluorophenyl)butan-1-one (2d):[2] According to the general procedure: **1d** (0.2 mmol, 49.2 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2d** (44.2 mg, 70%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99-7.95 (m, 2H), 7.28-7.25 (m, 2H), 7.10-7.06 (m, 2H), 7.03-6.99 (m, 2H), 4.85 (dd, *J* = 7.4, 5.9 Hz, 1H), 3.24 (dqd, *J* = 15.1, 10.7, 7.4 Hz, 1H), 2.53 (dqd, *J* = 15.0, 10.6, 5.8 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.50, -104.01, -113.80. ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.07, 165.86 (d, *J* = 256.2 Hz), 162.31 (d, *J* = 247.6 Hz), 132.93 (d, *J* = 3.0 Hz), 131.81 (d, *J* = 2.9 Hz), 131.48 (d, *J* = 9.5 Hz), 129.63 (d, *J* = 8.2 Hz), 126.25 (d, *J* = 277.2 Hz), 116.42 (d, *J* = 21.6 Hz), 115.95 (d, *J* = 21.9 Hz), 46.35 (d, *J* = 2.8 Hz), 37.39 (q, *J* = 28.3 Hz).



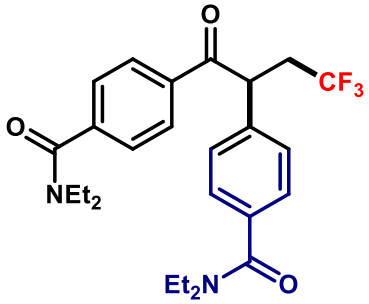
2e

1,2-bis(4-chlorophenyl)-4,4,4-trifluorobutan-1-one (2e):[1] According to the general procedure: **1e** (0.2 mmol, 55.6 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2e** (55.3 mg, 80%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87-7.85 (m, 2H), 7.39-7.37 (m, 1H), 7.30-7.27 (m, 2H), 7.23-7.21 (m, 2H), 4.82 (dd, *J* = 7.3, 6.0 Hz, 1H), 3.24 (dqd, *J* = 15.1, 10.7, 7.3 Hz, 1H), 2.53 (dqd, *J* = 15.0, 10.6, 5.9 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.45. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.22, 140.17, 135.48, 134.13, 133.65, 130.16, 129.67, 129.33, 129.13, 126.19 (d, *J* = 277.3 Hz), 46.58 (q, *J* = 2.7 Hz), 37.20 (q, *J* = 28.3 Hz).



2f

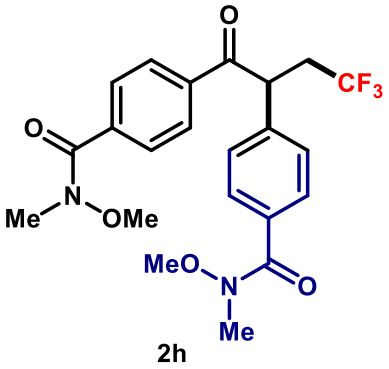
diethyl 4,4'-(4,4,4-trifluoro-1-oxobutane-1,2-diyl)dibenzoate (2f): According to the general procedure: **1f** (0.2 mmol, 70.8 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2f** (50.6 mg, 60%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 8.5 Hz, 2H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.96 (d, *J* = 8.5 Hz, 2H), 7.37 (d, *J* = 8.3 Hz, 2H), 4.96 (t, *J* = 6.6 Hz, 1H), 4.40-4.32 (m, 3H), 3.37-3.23 (m, 1H), 2.66-2.52 (m, 1H), 1.40-1.34(m, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.41. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.81, 165.84, 165.39, 141.60, 138.51, 134.65, 130.65, 130.35, 129.87, 128.64, 128.12, 126.16 (d, *J* = 277.3 Hz), 61.51, 61.13, 47.65, 37.05 (q, *J* = 28.6 Hz), 14.27, 14.23. HRMS (DART Positive) ($[M+H]^+$) Calcd for $C_{22}H_{22}F_3O_5$: 423.1414; found: 423.1413.



2g

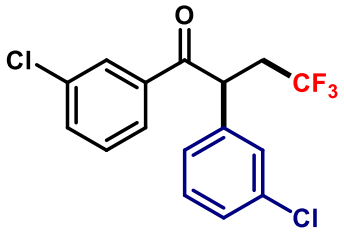
4,4'-(4,4,4-trifluoro-1-oxobutane-1,2-diyl)bis(N,N-diethylbenzamide) (2g): According to the general procedure: **1g** (0.2 mmol, 81.6 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2g** (92.8 mg, 97%) as a white solid after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. m.p. 135-136 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.36-7.33 (m, 4H), 4.94 (dd, *J* = 7.8, 5.4 Hz,

1H), 3.56-3.51 (m, 4H), 3.38-3.26 (1H), 3.24-3.16 (4H), 2.62-2.49 (1H), 1.27-1.21 (m, 6H), 1.13-1.07 (m, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.55. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.68, 170.44, 169.82, 142.17, 137.92, 136.97, 135.66, 129.07, 128.15, 127.43, 126.61, 126.20 (d, *J* = 277.2 Hz), 46.92 (d, *J* = 2.9 Hz), 43.28, 43.19, 39.25, 37.19 (q, *J* = 28.3 Hz), 14.17, 12.81. HRMS (DART Positive) ([M+H]$^+$) Calcd for $C_{26}H_{32}F_3N_2O_3$: 477.2360; found: 477.2356.



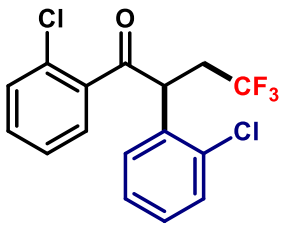
2h

4,4'-(4,4,4-trifluoro-1-oxobutane-1,2-diyl)bis(N-methoxy-N-methylbenzamide) (2h): According to the general procedure: **1a** (0.2 mmol, 76.8 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2h** (88.7 mg, 98%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 8.5 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 4.95 (dd, *J* = 7.6, 5.6 Hz, 1H), 3.50 (s, 6H), 3.34 (s, 3H), 3.33-3.24 (m, 4H), 2.64-2.51 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.50. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.80, 168.99, 168.53, 139.34, 138.85, 136.71, 133.80, 129.32, 128.47, 128.42, 127.78, 126.19 (d, *J* = 277.2 Hz), 61.30, 61.08, 47.18 (q, *J* = 2.3 Hz), 37.16 (q, *J* = 28.5 Hz), 33.57, 33.30. HRMS (DART Positive) ([M+Na]$^+$) Calcd for $C_{26}H_{31}F_3N_2O_3Na$: 475.1451; found: 475.1452.



2i

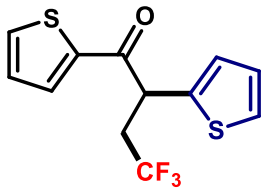
1,2-bis(3-chlorophenyl)-4,4,4-trifluorobutan-1-one (2i):[1] According to the general procedure: **1i** (0.2 mmol, 55.6 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2i** (54.6 mg, 79%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (t, *J* = 1.9 Hz, 1H), 7.80 (dt, *J* = 7.8, 1.3 Hz, 1H), 7.51 (ddd, *J* = 8.0, 2.1, 1.1 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.29-7.23 (m, 3H), 7.19 (dt, *J* = 6.9, 1.9 Hz, 1H), 4.81 (dd, *J* = 7.7, 5.5 Hz, 1H), 3.26 (dqd, *J* = 15.0, 10.6, 7.6 Hz, 1H), 2.60-2.47 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.59. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.01, 138.67, 136.91, 135.30, 135.25, 133.61, 130.73, 130.10, 128.87, 128.44, 128.04, 127.44, 126.80, 126.26, 126.07 (d, *J* = 277.1 Hz), 46.90 (q, *J* = 2.5 Hz), 37.28 (q, *J* = 28.6 Hz).



2j

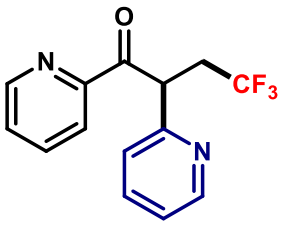
1,2-bis(2-chlorophenyl)-4,4,4-trifluorobutan-1-one (2j):[1] According to the general procedure: **1j** (0.2 mmol, 55.6 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2j** (49.2 mg, 71%) as a colorless oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35-7.15 (m, 8H), 5.39 (t, *J* = 6.5 Hz, 1H), 3.31 (dqd, *J* = 15.1, 10.7, 6.7 Hz, 1H), 2.56 (dqd, *J* = 15.1, 10.6, 6.4 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.57. ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.43, 137.63, 134.22,

133.75, 131.96, 131.28, 130.55, 130.23, 129.39, 129.30, 129.00, 127.61, 126.61, 126.23 (d, *J* = 277.2 Hz), 35.33 (q, *J* = 29.0 Hz).



2k

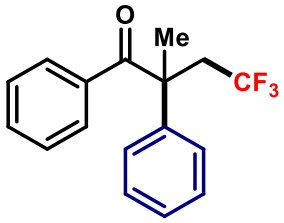
4,4,4-trifluoro-1,2-di(thiophen-2-yl)butan-1-one (2k): According to the general procedure: **1k** (0.2 mmol, 44.4 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2k** (30.1 mg, 52%) a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (dd, *J* = 3.9, 1.1 Hz, 1H), 7.67 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.22 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.12 (dd, *J* = 4.9, 3.9 Hz, 1H), 6.99 (ddd, *J* = 3.5, 1.3, 0.6 Hz, 1H), 6.93 (dd, *J* = 5.1, 3.5 Hz, 1H), 5.01 (dd, *J* = 8.3, 5.0 Hz, 1H), 3.37-3.23 (m, 1H), 2.70-2.57 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.86. ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.34, 142.10, 139.18, 135.05, 133.14, 128.37, 127.31, 126.38, 125.89 (d, *J* = 277.4 Hz), 125.82, 43.21, 37.82 (q, *J* = 28.6 Hz). HRMS (DART Positive) ([M+H]$^+$) Calcd for $C_{12}H_{10}F_3OS_2$: 291.0120; found: 291.0118.



2l

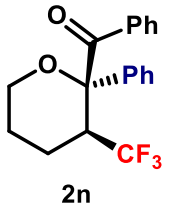
4,4,4-trifluoro-1,2-di(pyridin-2-yl)butan-1-one (2l): According to the general procedure: **1l** (0.2 mmol, 42.4 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2l** (33.9 mg, 61%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.64 (ddd, *J* = 4.8, 1.7, 0.9 Hz, 1H), 8.49 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 8.05 (m, 1H), 7.78 (td, *J* = 7.7, 1.7 Hz, 1H), 7.59 (td, *J* = 7.6, 1.8

Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 2H), 7.41 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 7.09 (ddd, *J* = 7.4, 4.8, 1.4 Hz, 1H), 5.88 (t, *J* = 6.6 Hz, 1H), 3.27 (dqd, *J* = 15.2, 11.0, 6.7 Hz, 1H), 2.90 (dqd, *J* = 15.2, 10.9, 6.5 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.50. ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.80, 156.95, 151.97, 149.66, 148.81, 136.94, 136.67, 127.27, 126.84 (d, *J* = 276.8 Hz), 124.97, 123.11, 122.11, 47.29 (q, *J* = 2.4 Hz), 35.00 (q, *J* = 28.6 Hz). HRMS (DART Positive) ([M+Na]$^+$) Calcd for Chemical Formula: C14H11F3N2ONa: Exact Mass: 303.0716; found: 303.0709.



2m

4,4,4-trifluoro-2-methyl-1,2-diphenylbutan-1-one (2m):[2] According to the general procedure: **1m** (0.2 mmol, 44.8 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2m** (29.5 mg, 50%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42-7.31 (m, 8H), 7.24-7.20 (m, 2H), 3.06 (dq, *J* = 15.5, 11.1 Hz, 1H), 2.83 (dq, *J* = 15.5, 11.2 Hz, 1H), 1.82 (d, *J* = 1.4 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -58.58. ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.42, 140.81, 136.04, 131.85, 129.34, 129.26, 128.10, 127.77, 126.43 (d, *J* = 277.2 Hz), 126.30, 51.88, 43.41 (q, *J* = 26.8 Hz), 22.02.

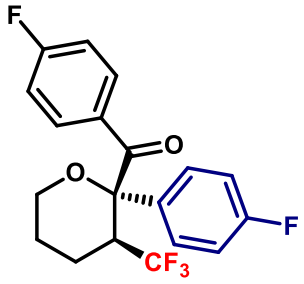


2n

phenyl(2-phenyl-3-(trifluoromethyl)tetrahydro-2H-pyran-2-yl)methanone (2n):[3] According to the general procedure: **1n** (0.2 mmol, 53.2 mg), **IV** (0.4 mmol, 175.3

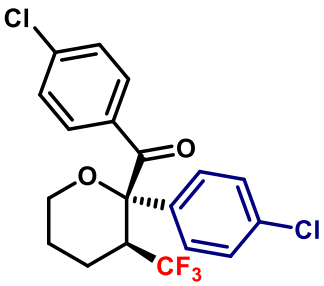
[3] Chen, Z.- M.; Bai, W.; Wang, S.-H.; Yang, B.-M.; Tu, Y.-Q.; Zhang, F.-M. *Angew. Chem., Int. Ed.* **2013**, *52*, 9781.

mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2n** (44.3 mg, 66%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.48-7.44 (m, 1H), 7.41-7.38 (m, 2H), 7.35-7.27 (m, 5H), 3.85-3.80 (m, 1H), 3.55 (ddd, *J* = 12.3, 8.9, 3.6 Hz, 1H), 3.09-2.99 (m, 1H), 2.22-2.12 (m, 1H), 2.07-1.99 (m, 1H), 1.87-1.80 (m, 1H), 1.76-1.65 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.08. ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.31, 139.88, 135.19, 132.71, 130.44, 128.44, 128.28, 127.92, 126.87, 126.30 (d, *J* = 281.6 Hz), 86.27, 64.15, 49.95 (q, *J* = 25.9 Hz), 23.61, 21.00 (q, *J* = 3.2 Hz).



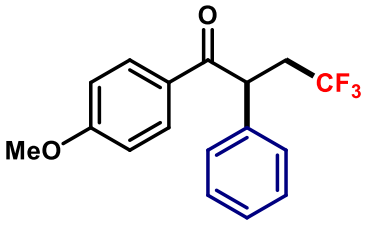
2o

(4-fluorophenyl)(2-(4-fluorophenyl)-3-(trifluoromethyl)tetrahydro-2H-pyran-2-yl)methanone (2o):[3] According to the general procedure: **1o** (0.2 mmol, 60.4 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2o** (33.9 mg, 46%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02-7.98 (m, 2H), 7.35 (dd, *J* = 8.6, 5.2 Hz, 2H), 7.04-6.96 (m, 4H), 3.84 (dtd, *J* = 12.2, 4.6, 1.1 Hz, 1H), 3.52 (ddd, *J* = 12.5, 9.5, 3.5 Hz, 1H), 2.92 (pd, *J* = 10.0, 3.9 Hz, 1H), 2.16 (dtd, *J* = 14.3, 10.0, 4.5 Hz, 1H), 2.06-1.99 (m, 1H), 1.87-1.79 (m, 1H), 1.78-1.69(m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.25, -104.77, -113.27. ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.27, 165.48 (d, *J* = 255.6 Hz), 162.47 (d, *J* = 248.2 Hz), 135.72 (d, *J* = 3.5 Hz), 133.32 (d, *J* = 9.3 Hz), 131.13 (d, *J* = 3.2 Hz), 128.63 (d, *J* = 8.4 Hz), 126.07 (d, *J* = 281.3 Hz), 115.46 (d, *J* = 21.7 Hz), 115.17 (d, *J* = 21.7 Hz), 85.76, 64.37, 23.77, 20.97 (q, *J* = 2.7 Hz)..



2p

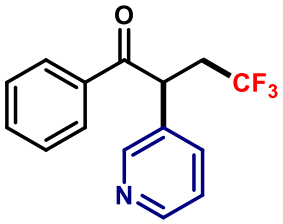
(4-chlorophenyl)(2-(4-chlorophenyl)-3-(trifluoromethyl)tetrahydro-2H-pyran-2-yl)methanone (2p):[3] According to the general procedure: **1p** (0.2 mmol, 66.8 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2p** (33.0 mg, 41%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 8.7 Hz, 1H), 7.34-7.28 (m, 6H), 3.84 (dt, *J* = 12.1, 4.7 Hz, 1H), 3.53 (ddd, *J* = 12.4, 9.2, 3.5 Hz, 1H), 2.93 (pd, *J* = 9.9, 3.9 Hz, 1H), 2.21-2.11 (m, 1H), 2.05-1.98 (m, 1H), 1.89-1.81 (m, 1H), 1.78-1.67 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.17. ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.58, 139.52, 138.28, 134.46, 133.03, 131.94, 128.75, 128.41, 128.21, 126.03 (d, *J* = 281.5 Hz), 85.75, 64.36, 50.19 (q, *J* = 26.0 Hz), 23.60, 20.89 (q, *J* = 2.8 Hz).



2q

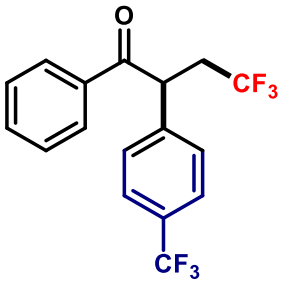
4,4,4-trifluoro-1-(4-methoxyphenyl)-2-phenylbutan-1-one (2q):[1] According to the general procedure: **1q** (0.2 mmol, 48.0 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2q**、**2q'** (48.6 mg, 79%, 5:1) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.9 Hz, 2H), 7.32-7.20 (m, 5H), 6.87 (d, *J* = 8.9 Hz, 2H), 4.86 (dd, *J* = 7.6, 5.5 Hz, 1H), 3.81 (s, 3H), 3.29 (dqd, *J* = 15.0, 10.9, 7.6 Hz, 1H), 2.53 (dqd, *J* = 15.0, 10.8, 5.5 Hz, 1H). ^{19}F NMR (376 MHz,

$CDCl_3$) δ -64.57. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.16, 163.68, 137.91, 131.19, 129.26, 128.56, 127.96, 127.71, 126.47 (d, *J* = 277.2 Hz), 113.87, 55.46, 46.80 (q, *J* = 2.5 Hz), 37.37 (q, *J* = 28.1 Hz).



2r

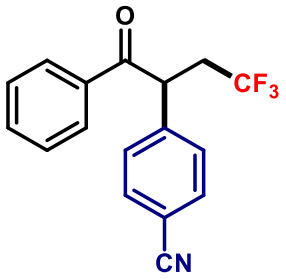
4,4,4-trifluoro-1-phenyl-2-(pyridin-3-yl)butan-1-one (2r):[1] According to the general procedure: **1r** (0.2 mmol, 42.2 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2r**、**2r'** (52.0 mg, 93%, 3.5:1) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.65 (d, *J* = 2.4 Hz, 1H), 8.51 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.97-7.94 (m, 2H), 7.62 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.57-7.52 (m, 1H), 7.45-7.41 (m, 2H), 7.27-7.23 (m, 1H), 4.97 (t, *J* = 6.7 Hz, 1H), 3.27 (dqd, *J* = 15.1, 10.6, 7.2 Hz, 1H), 2.59 (dqd, *J* = 15.1, 10.5, 6.2 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.39. ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.13, 149.78, 149.34, 135.08, 135.08, 133.84, 133.14, 128.90, 128.78, 126.14 (q, *J* = 277.2 Hz), 124.05, 44.40 (q, *J* = 2.7 Hz), 37.18 (q, *J* = 28.5 Hz).



2s

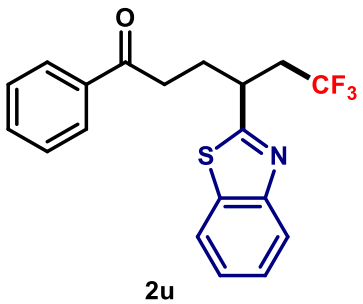
4,4,4-trifluoro-1-phenyl-2-(4-(trifluoromethyl)phenyl)butan-1-one (2s):[1] According to the general procedure: **1s** (0.2 mmol, 55.6 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2s** (58.1 mg, 84%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction

time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96-7.93 (m, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.54-7.52 (m, 1H), 7.46-7.41 (m, 4H), 4.99 (t, *J* = 6.6 Hz, 1H), 3.29 (dqd, *J* = 15.1, 10.7, 7.3 Hz, 1H), 2.58 (dqd, *J* = 15.0, 10.6, 5.9 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.77, -64.50. ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.14, 141.28, 135.29, 133.78, 130.22 (q, *J* = 32.7 Hz), 128.86, 128.79, 128.50, 126.30 (q, *J* = 3.8 Hz), 126.19 (q, *J* = 277.2 Hz), 123.81 (q, *J* = 272.2 Hz), 46.85 (q, *J* = 2.6 Hz), 37.28 (q, *J* = 28.6 Hz).



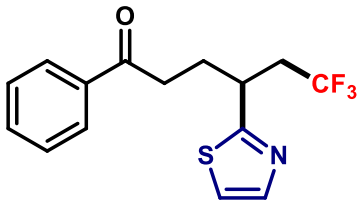
2t

4-(4,4,4-trifluoro-1-oxo-1-phenylbutan-2-yl)benzonitrile (2t):[1] According to the general procedure: **1t** (0.2 mmol, 47.0 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2t** (46.1 mg, 76%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.58-7.53(m, 1H), 7.47-7.41 (m, 4H), 4.99 (t, *J* = 6.7 Hz, 1H), 3.32-3.18 (m, 1H), 2.66-2.53 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.33. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.80, 142.46, 135.10, 133.96, 133.07, 128.96, 128.93, 128.77, 126.10 (d, *J* = 277.2 Hz), 118.20, 112.06, 47.00 (q, *J* = 2.7 Hz), 37.16 (q, *J* = 28.6 Hz).



2u

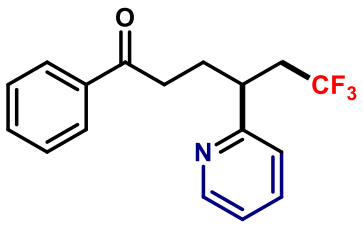
4-(benzo[d]thiazol-2-yl)-6,6,6-trifluoro-1-phenylhexan-1-one (2u)[4]: According to the general procedure: **1u** (0.2 mmol, 59.0 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2u** (64.1 mg, 88%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.87-7.84 (m, 3H), 7.54-7.46 (m, 2H), 7.42-7.36 (m, 3H), 3.75-3.65 (m, 1H),3.03-2.88 (m, 3H), 2.70-2.57(m, 1H), 2.47-2.28 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.05. ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.62, 172.04, 153.07, 136.56, 134.67, 133.21, 128.59, 127.96, 126.23, 126.12 (d, *J* = 277.4 Hz), 125.24, 123.00, 121.74, 39.35 (q, *J* = 28.5 Hz), 37.96 (q, *J* = 2.7 Hz), 35.28, 30.00.



2v

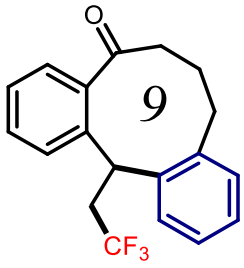
6,6,6-trifluoro-1-phenyl-4-(thiazol-2-yl)hexan-1-one (2v):[4] According to the general procedure: **1v** (0.2 mmol, 49.0 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2v** (58.9 mg, 94%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88-7.85 (m, 2H), 7.74 (d, *J* = 3.3 Hz, 1H), 7.56-7.52(m, 1H), 7.45-7.41 (m, 2H), 7.25 (d, *J* = 3.3 Hz, 1H), 3.67-3.60 (m, 1H), 2.93-2.88 (m, 2H), 2.87-2.77 (m, 1H), 2.64-2.51 (m, 1H), 2.39-2.19 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.10. ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.73, 171.11, 142.74, 136.60, 133.19, 128.60, 127.93, 126.14 (d, *J* = 277.4 Hz), 118.55, 39.61 (q, *J* = 28.3 Hz), 36.90 (q, *J* = 2.7 Hz), 35.24, 30.27.

[4] Wu, Z.; Wang, D.; liu, Y.; Huan, L.; Zhu, C. *J. Am. Chem. Soc.* **2017**, *139*, 1388.



2w

6,6,6-trifluoro-1-phenyl-4-(pyridin-2-yl)hexan-1-one (2w):[4] According to the general procedure: **1w** (0.2 mmol, 47.8 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2w** (42.4 mg, 69%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 7.85-7.82 (m, 2H), 7.61 (td, *J* = 7.6, 1.9 Hz, 1H), 7.55-7.51 (m, 1H), 7.44-7.39 (m, 2H), 7.18-7.12 (m, 2H), 3.26-3.19 (m, 1H), 2.91-2.71 (m, 3H), 2.54-2.40 (m, 1H), 2.22 (q, *J* = 7.4 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.02. ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.31, 161.32, 149.81, 136.69, 136.56, 133.08, 128.56, 127.94, 126.66 (q, *J* = 277.3 Hz), 123.55, 122.05, 40.64, 38.96 (q, *J* = 27.6 Hz), 35.61, 29.85.



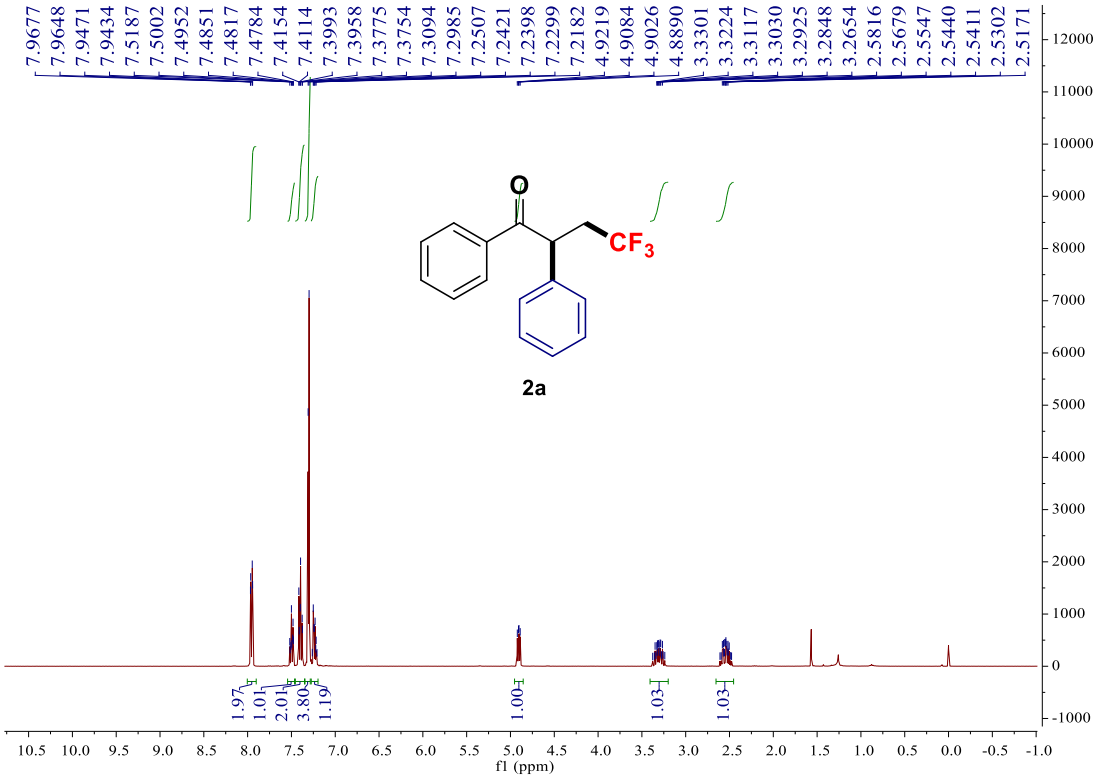
2x

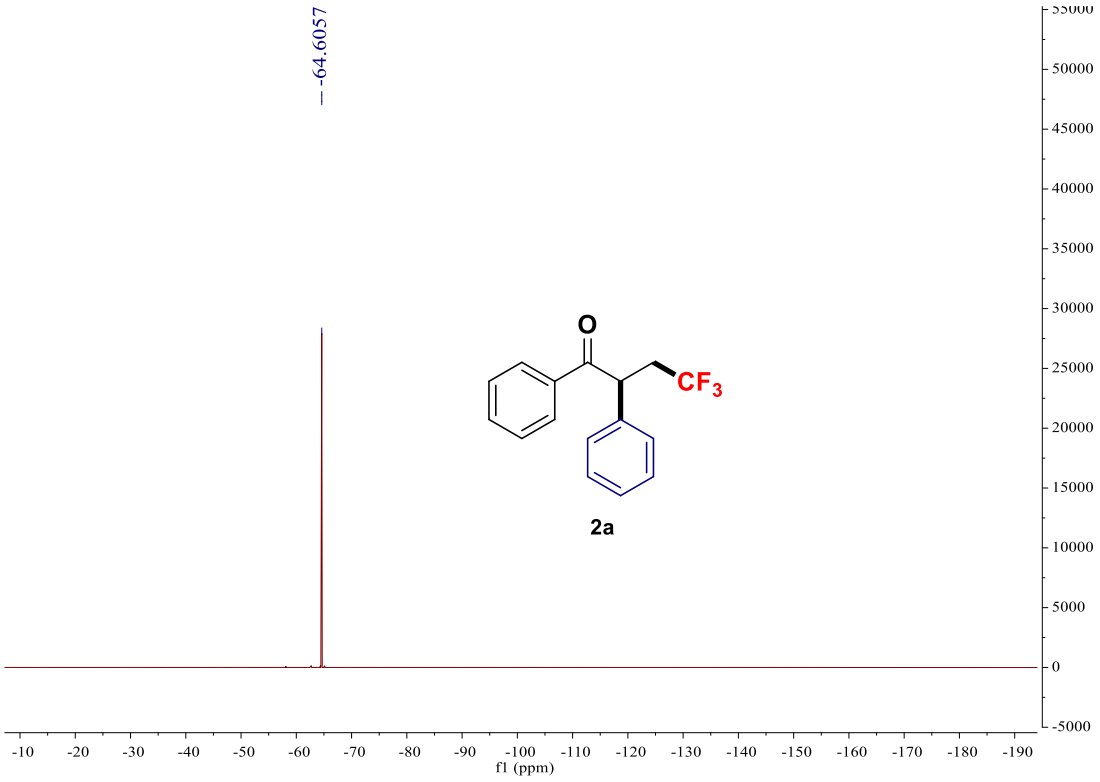
13-(2,2,2-trifluoroethyl)-6,7,8,13-tetrahydro-5H-dibenzo[a,d][9]annulen-5-one (2x):[5] According to the general procedure: **1x** (0.2 mmol, 52.8 mg), **IV** (0.4 mmol, 175.3 mg), K_2HPO_4 (0.3 mmol, 52.3 mg) in DMSO (2.0 mL) afforded **2x** (23.2 mg, 35%) as a yellow oil after purification on silica gel (Petroleum ether: EtOAc = 10:1). Reaction time: 10 h. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.32 (td, *J* = 7.4, 1.7 Hz, 1H), 7.28 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.25-7.19 (m, 1H), 7.18-7.11 (m, 4H), 3.36-3.30 (m, 2H), 3.25-3.11 (m, 2H), 2.93-2.85 (m, 1H),

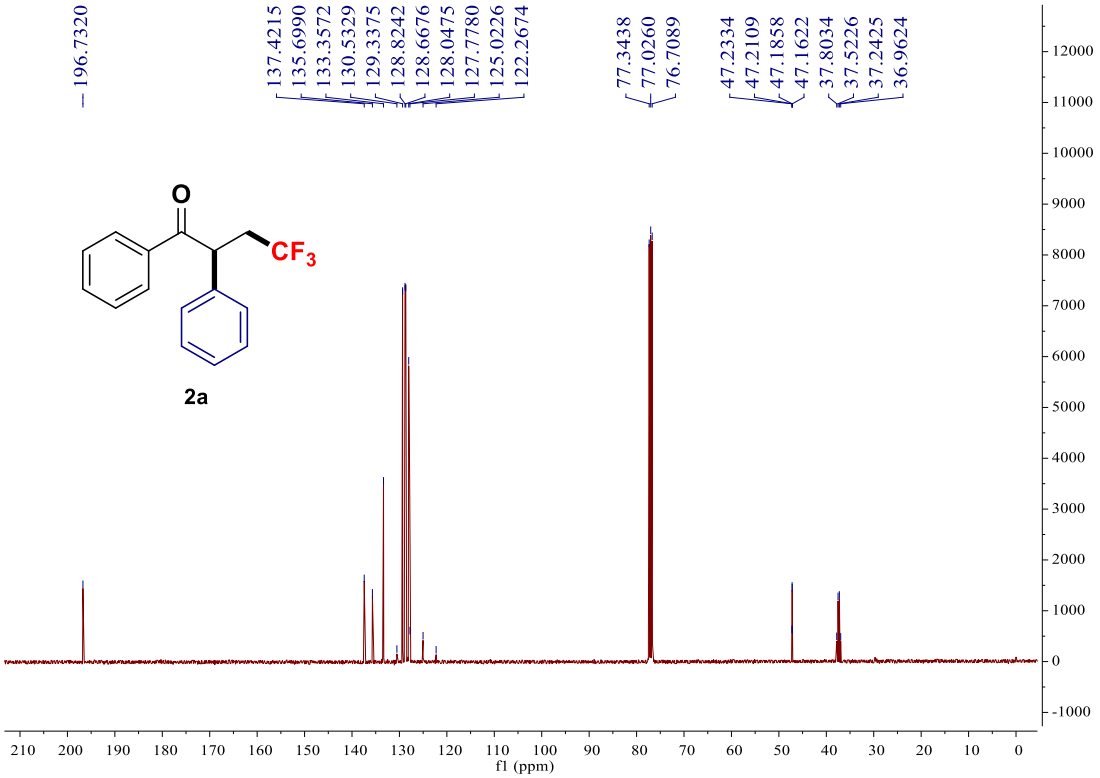
[5] Li, L.; Li, Z.-L.; Wang, F.-L.; Guo, Z.; Cheng, Y.-F.; Wang, N.; Dong, X.-W.; Fang, C.; Liu, J.; Hou, C.; Tan, B.; Liu, X.-Y. *Nat. Commun.* **2016**, *7*, 13852.

2.74-2.64 (m, 2H), 2.54-2.31 (m, 3H), 1.72-1.63 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.15. ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.91, 141.90, 140.37, 139.48, 137.64, 131.20, 130.89, 130.73, 129.23, 127.24, 126.94, 126.03 (q, *J* = 277.6 Hz), 125.45, 44.27, 39.84 (q, *J* = 27.5 Hz), 38.09, 36.24 (q, *J* = 2.4 Hz), 29.17, 26.77.

6. NMR spectra for all compounds



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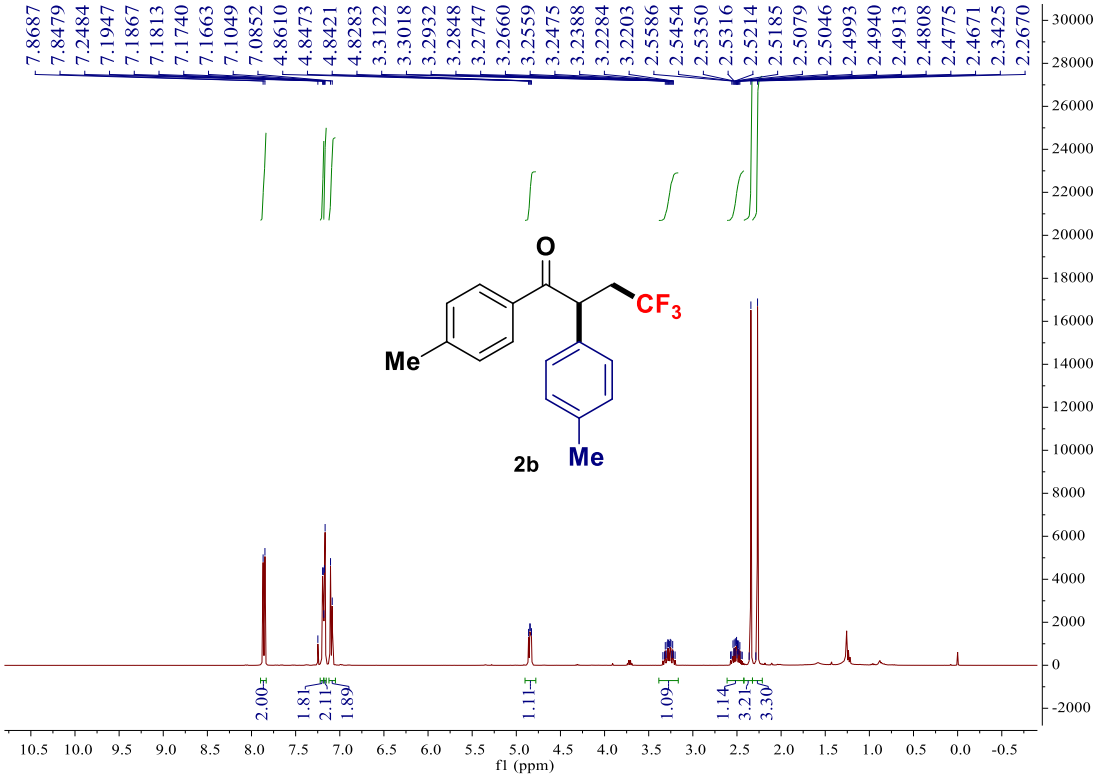
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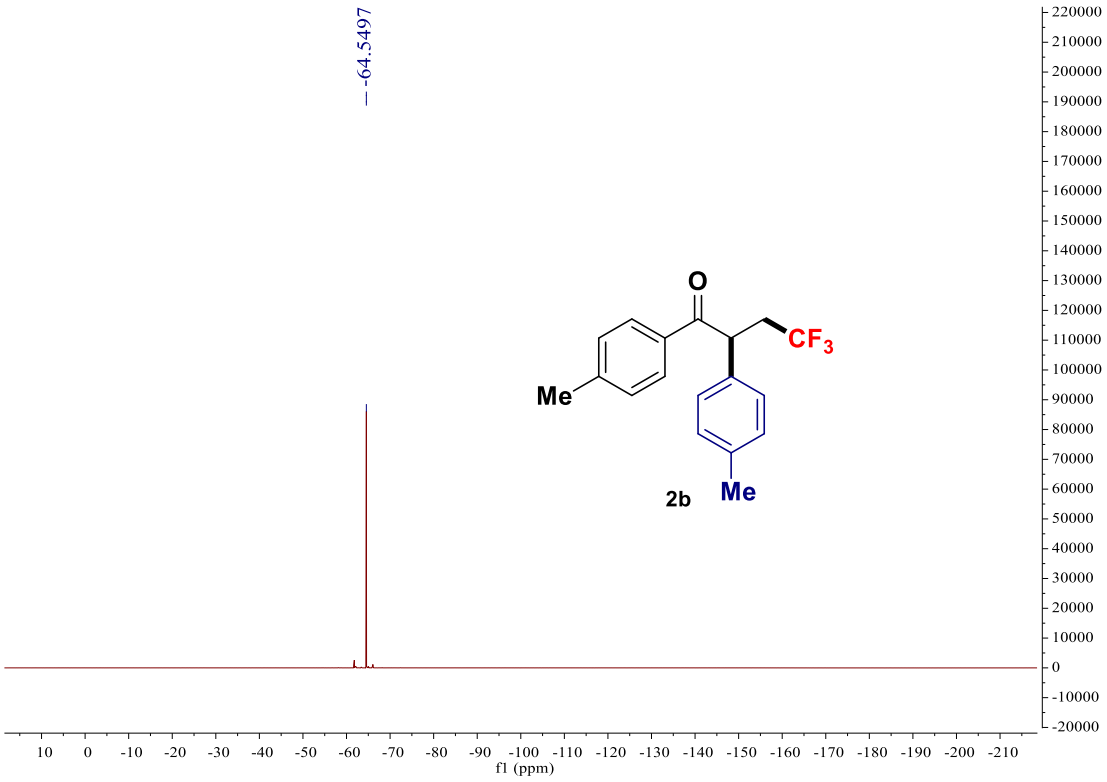
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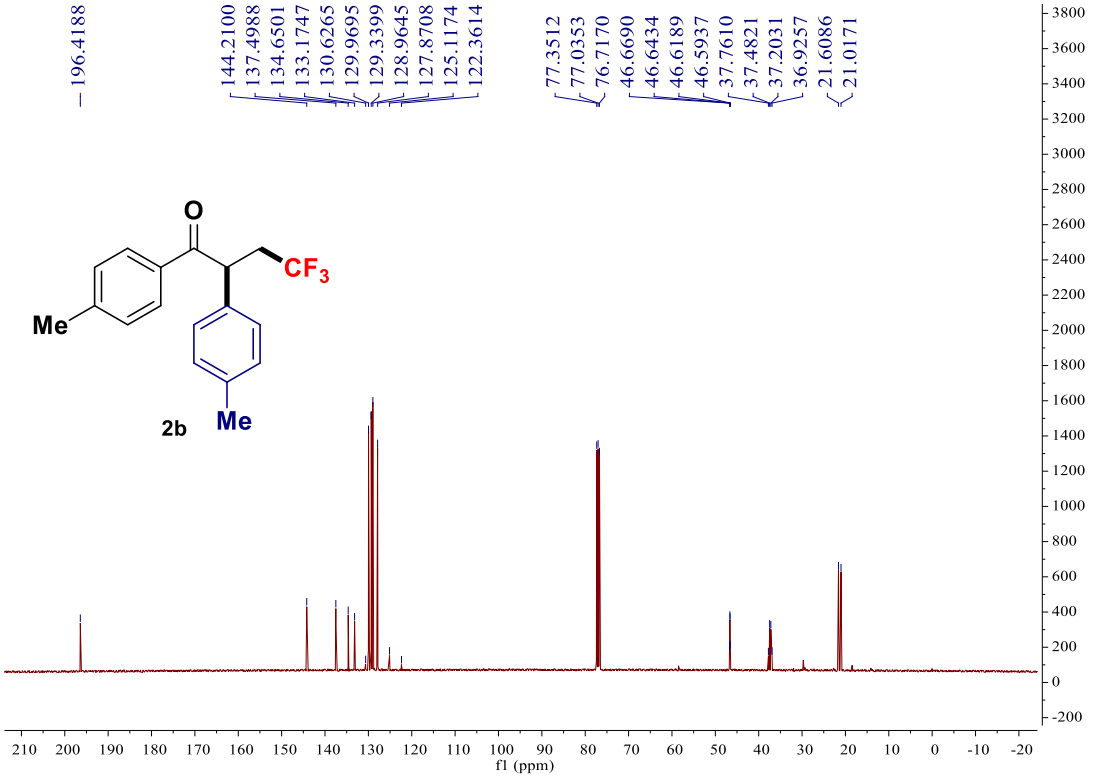
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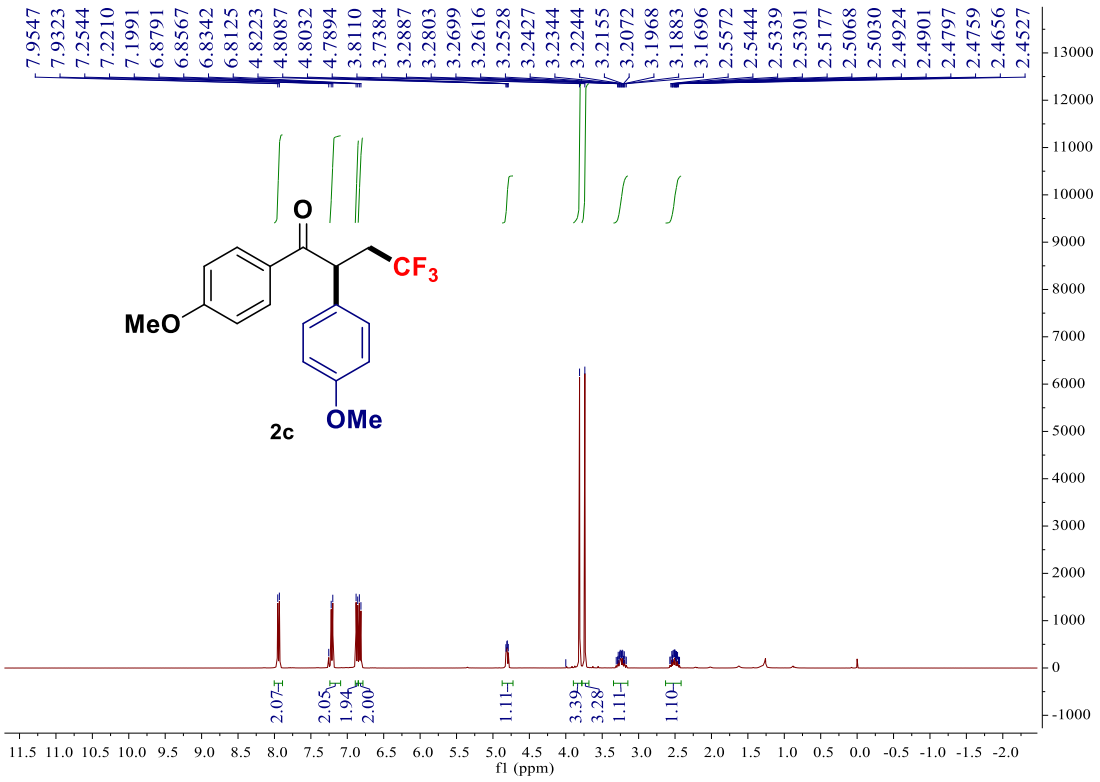
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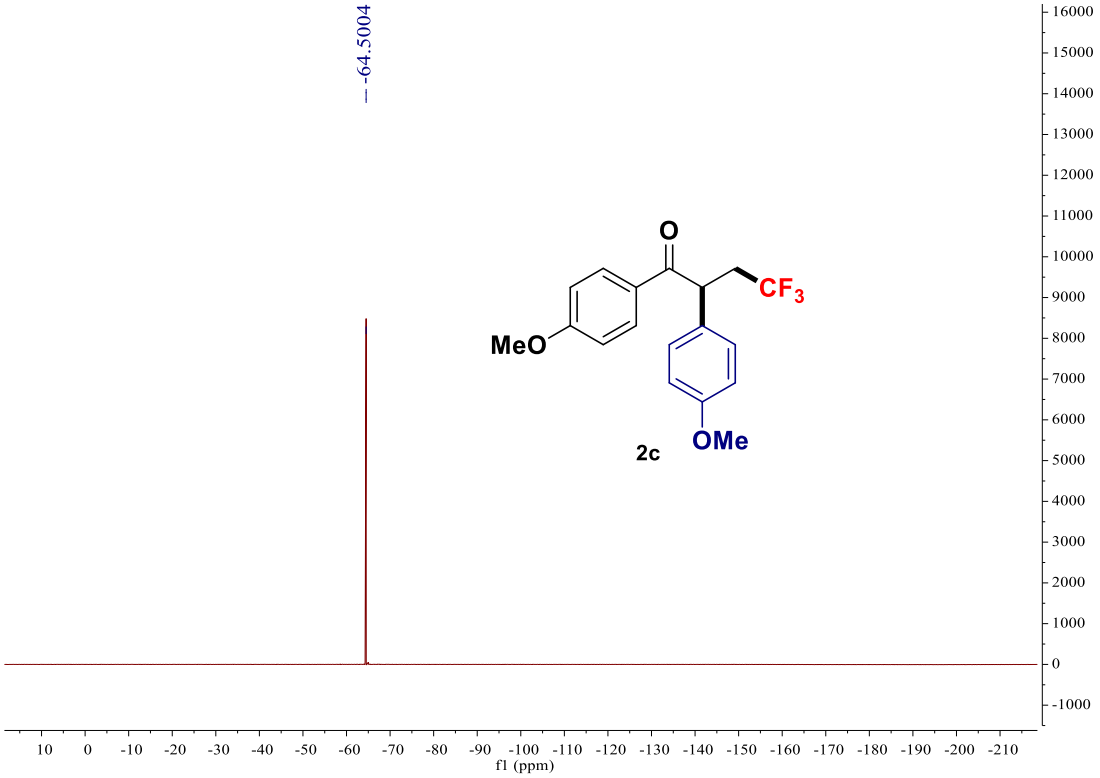
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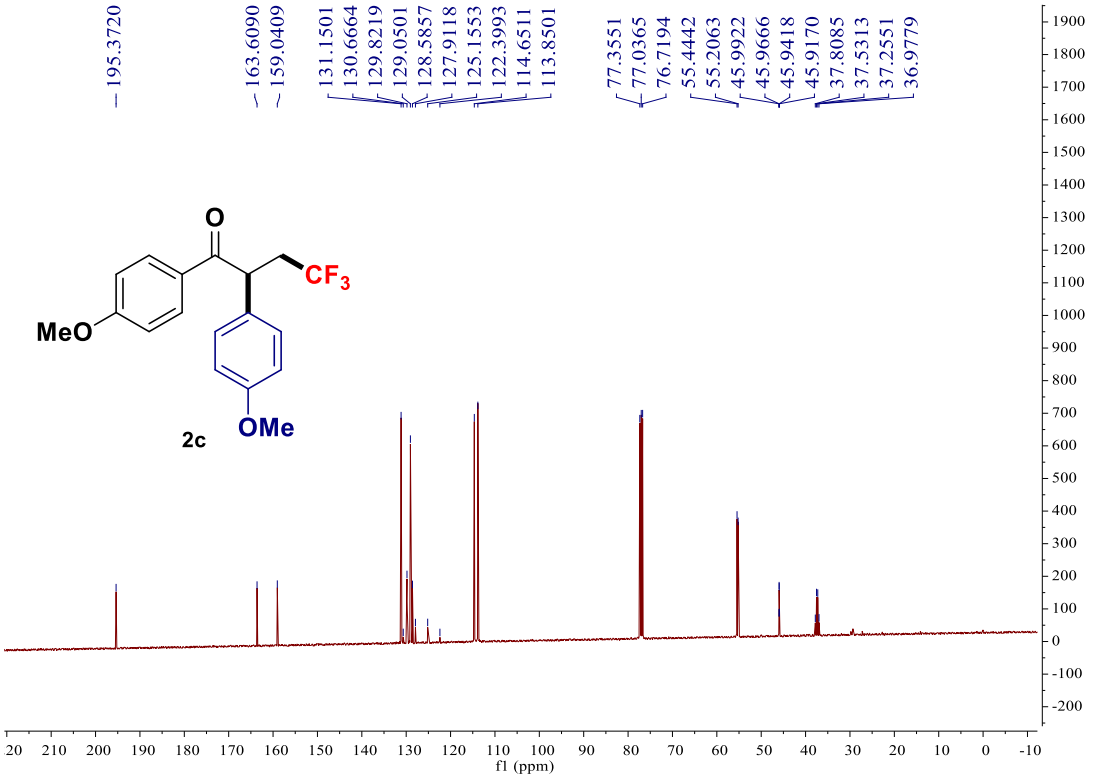
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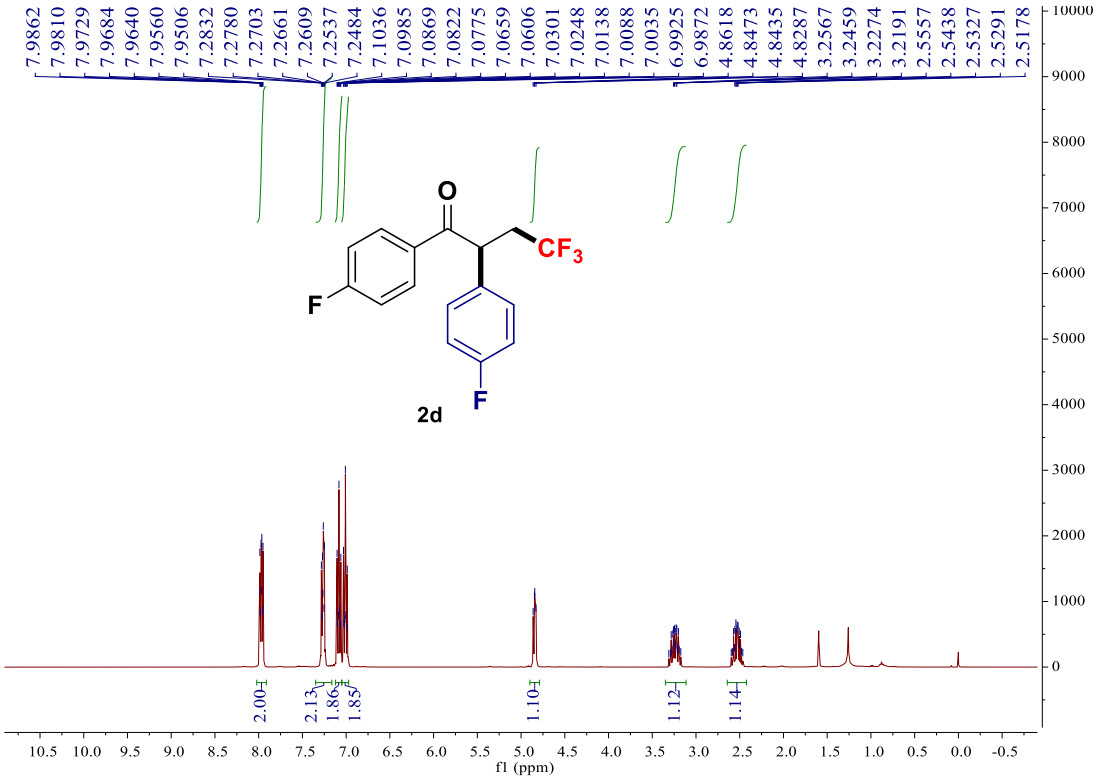
f1 (ppm)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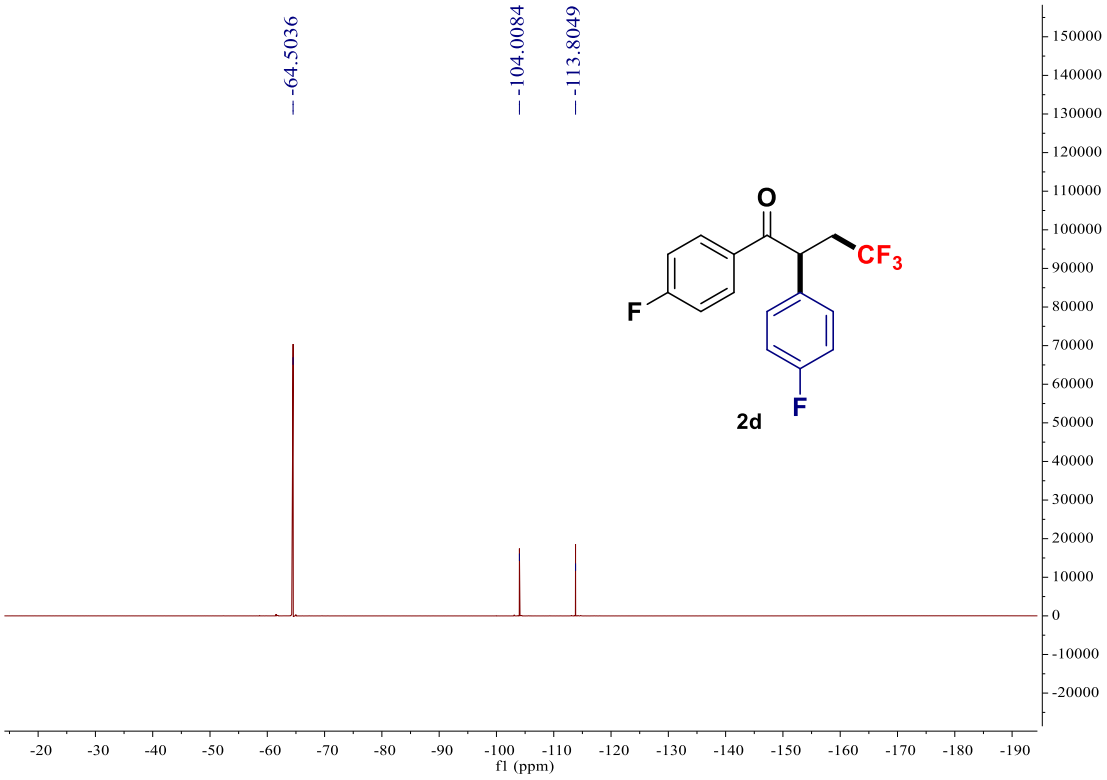
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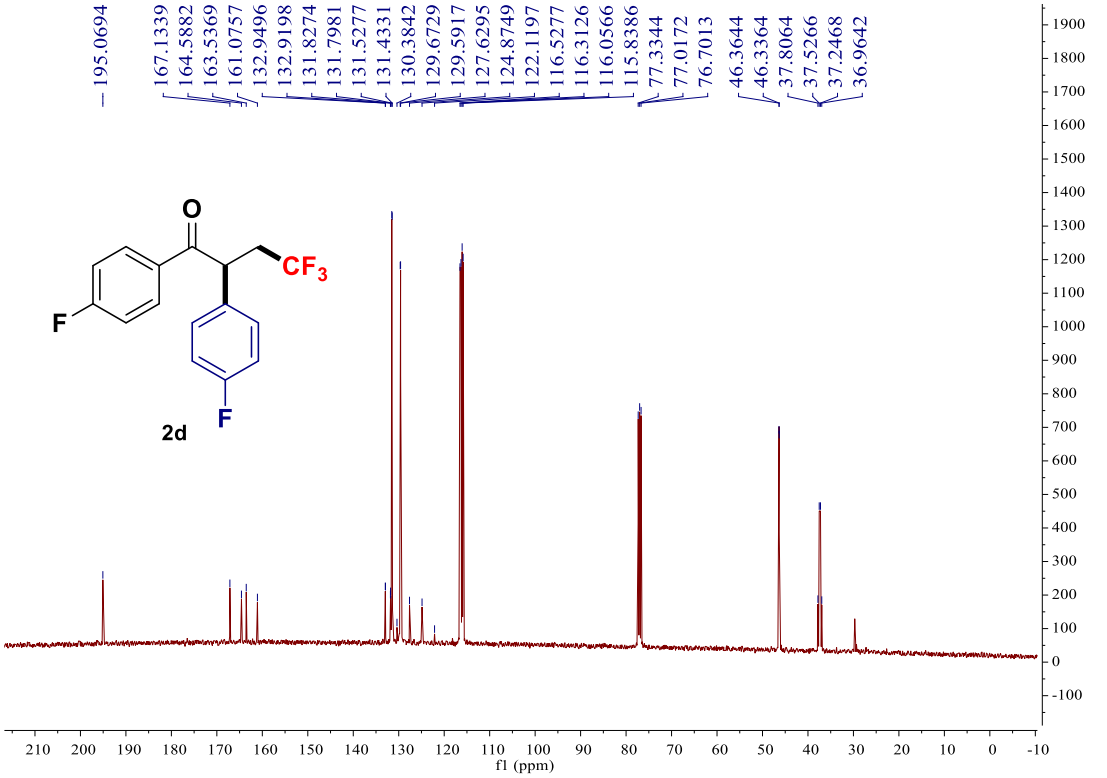
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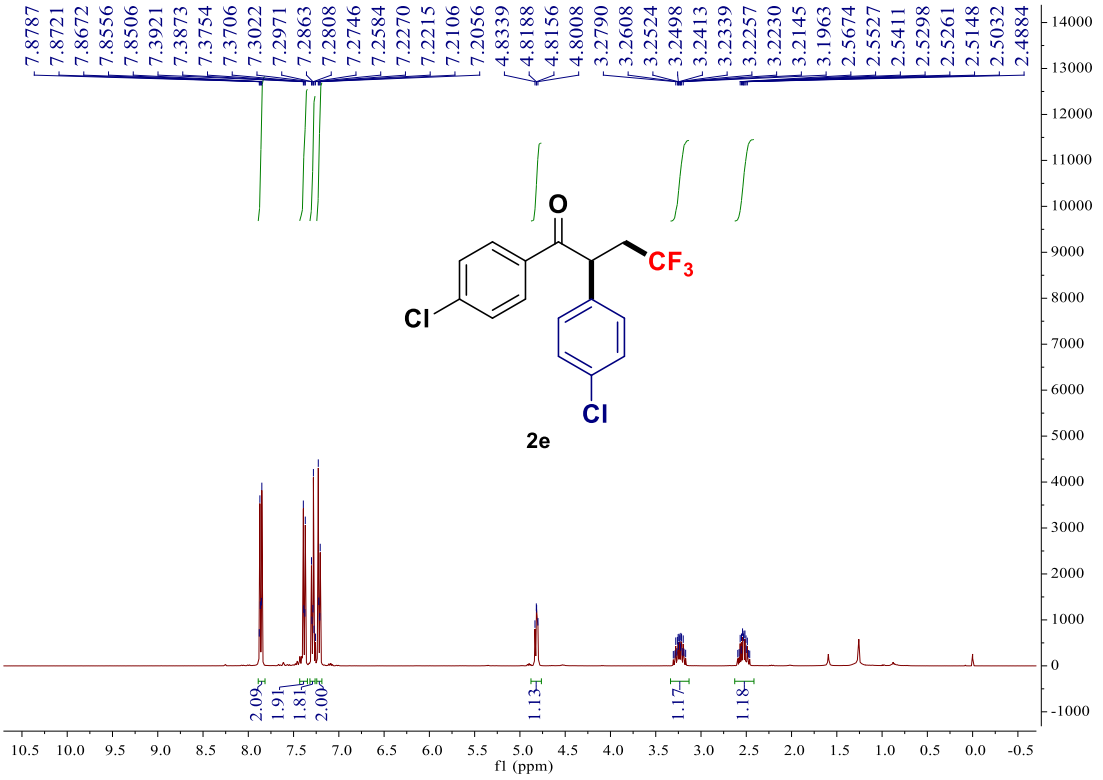
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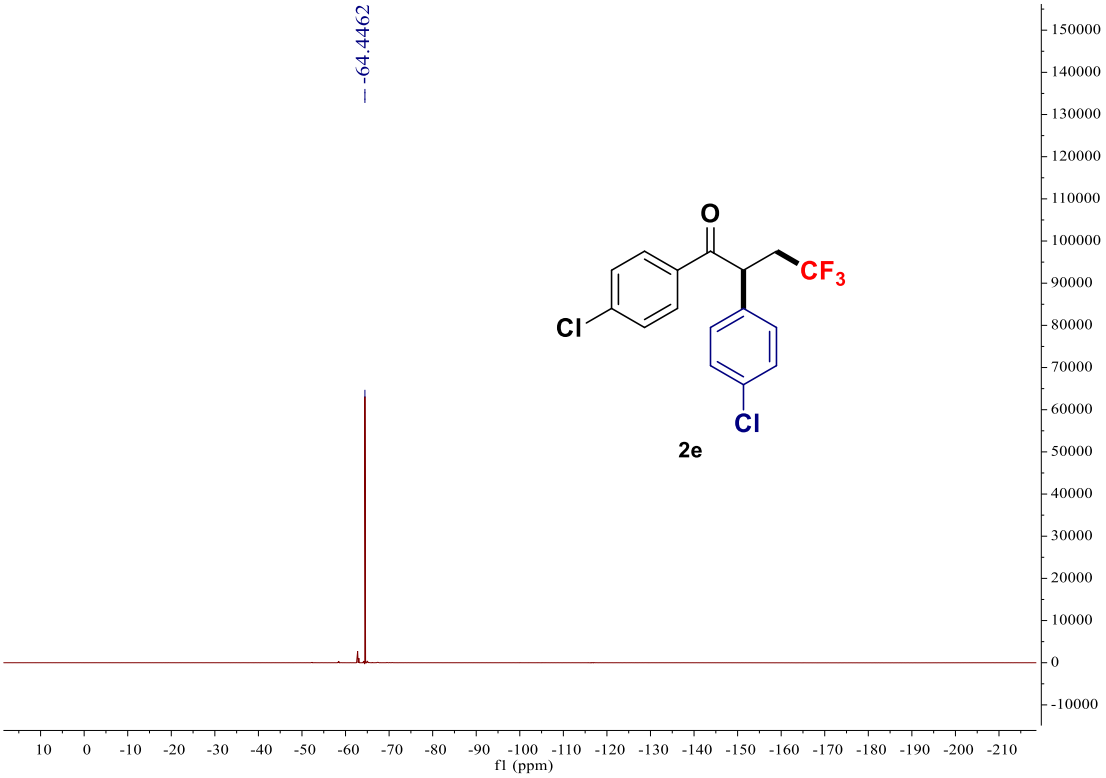
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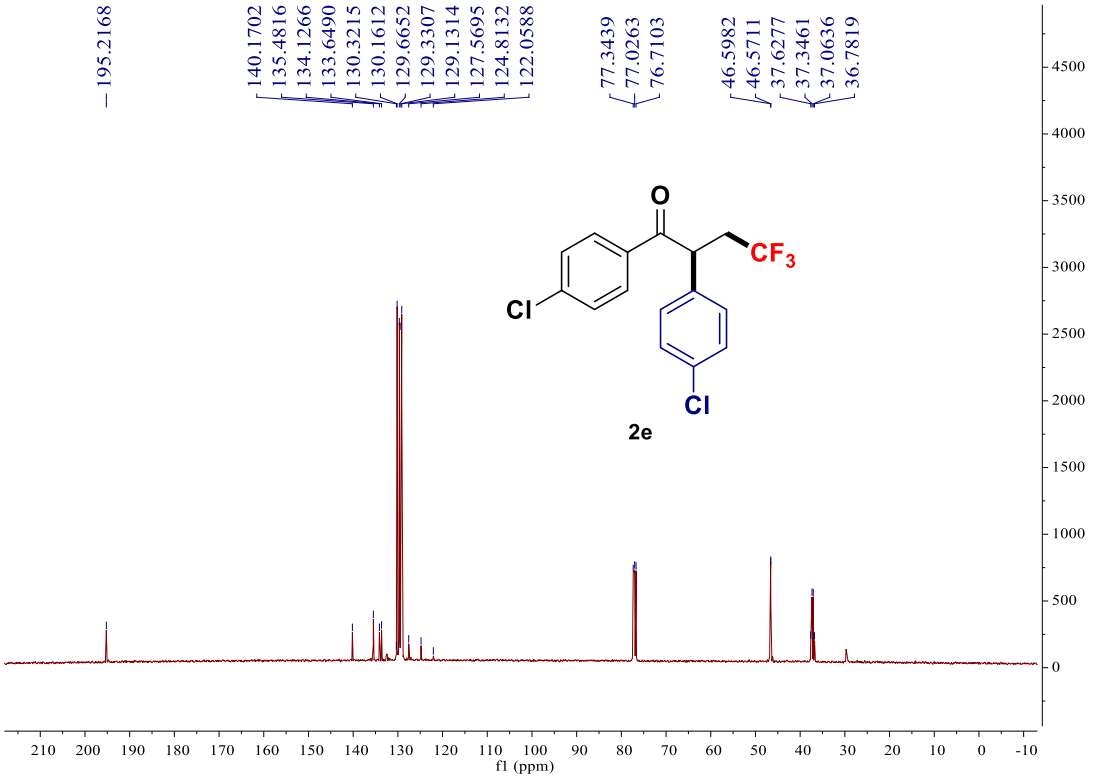
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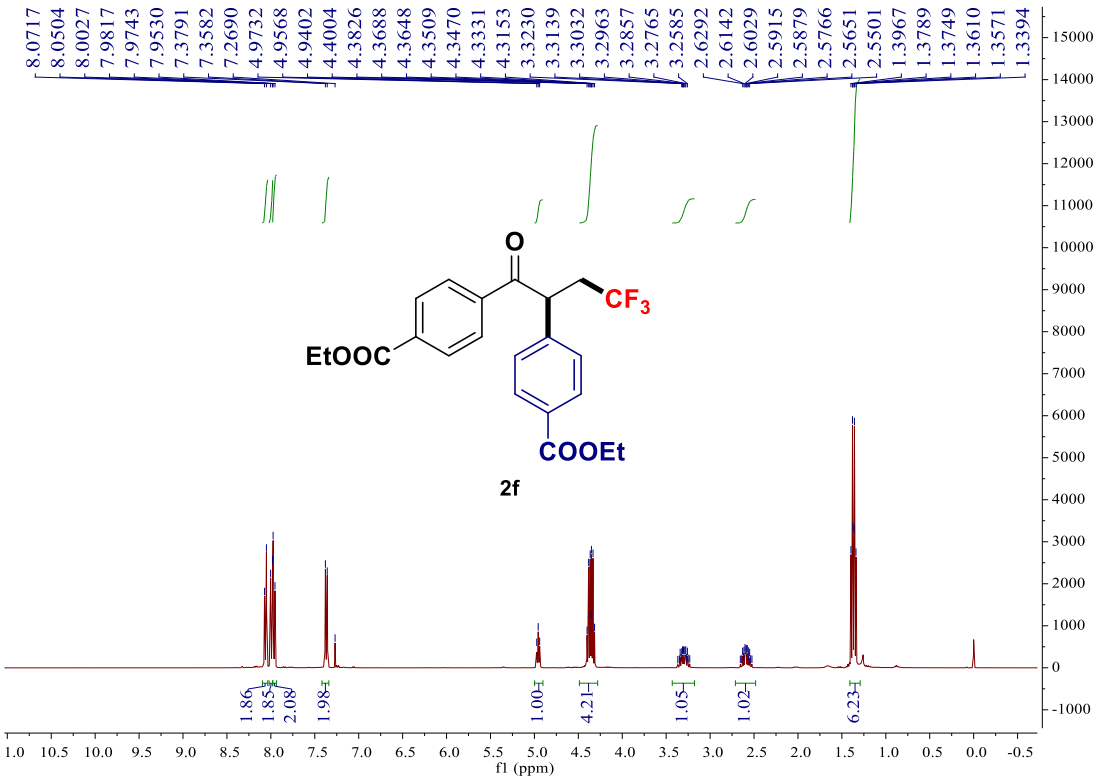
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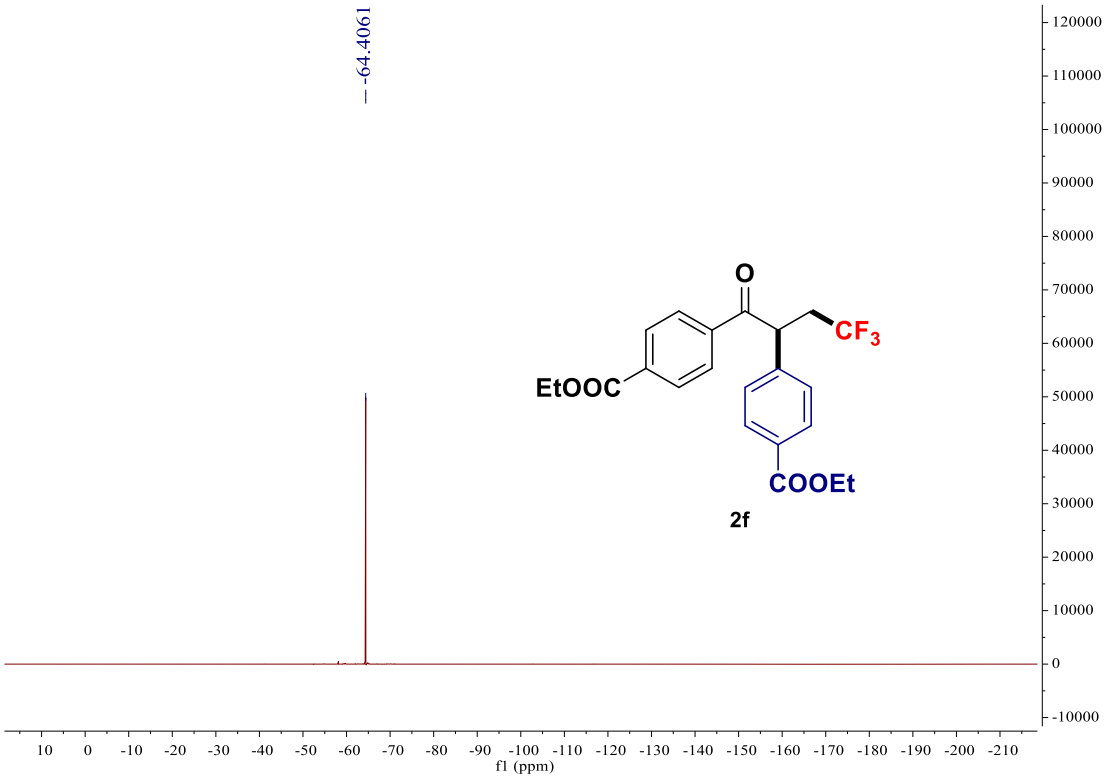
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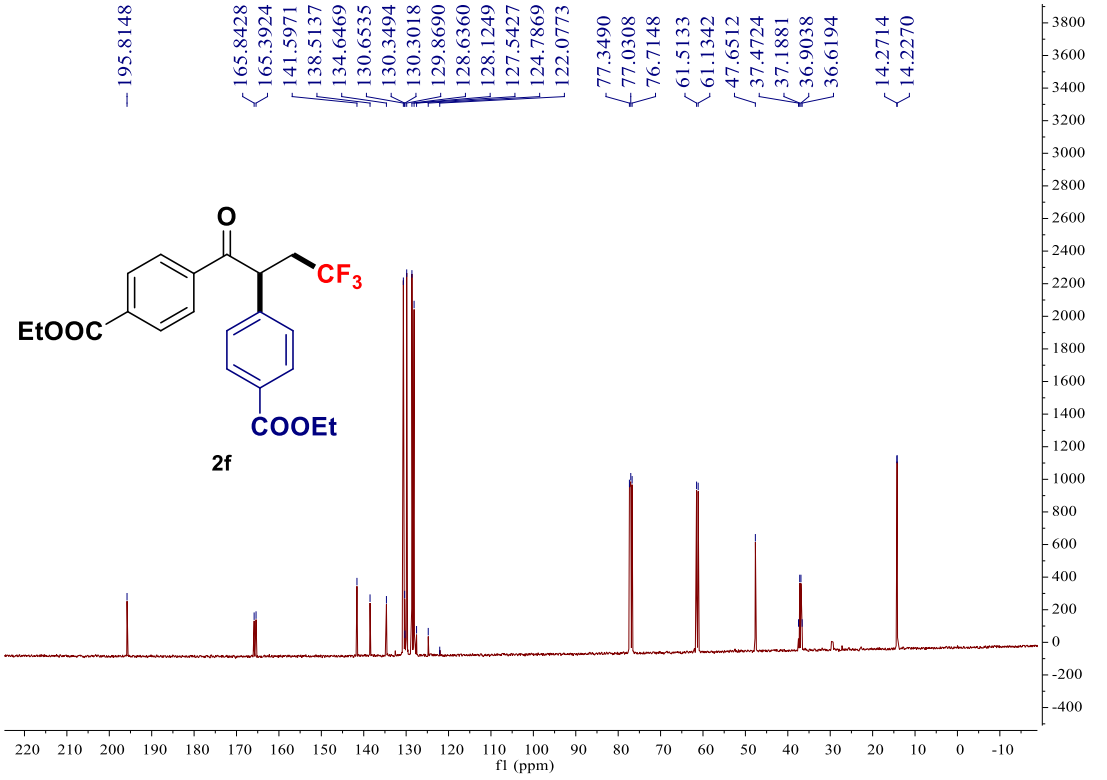
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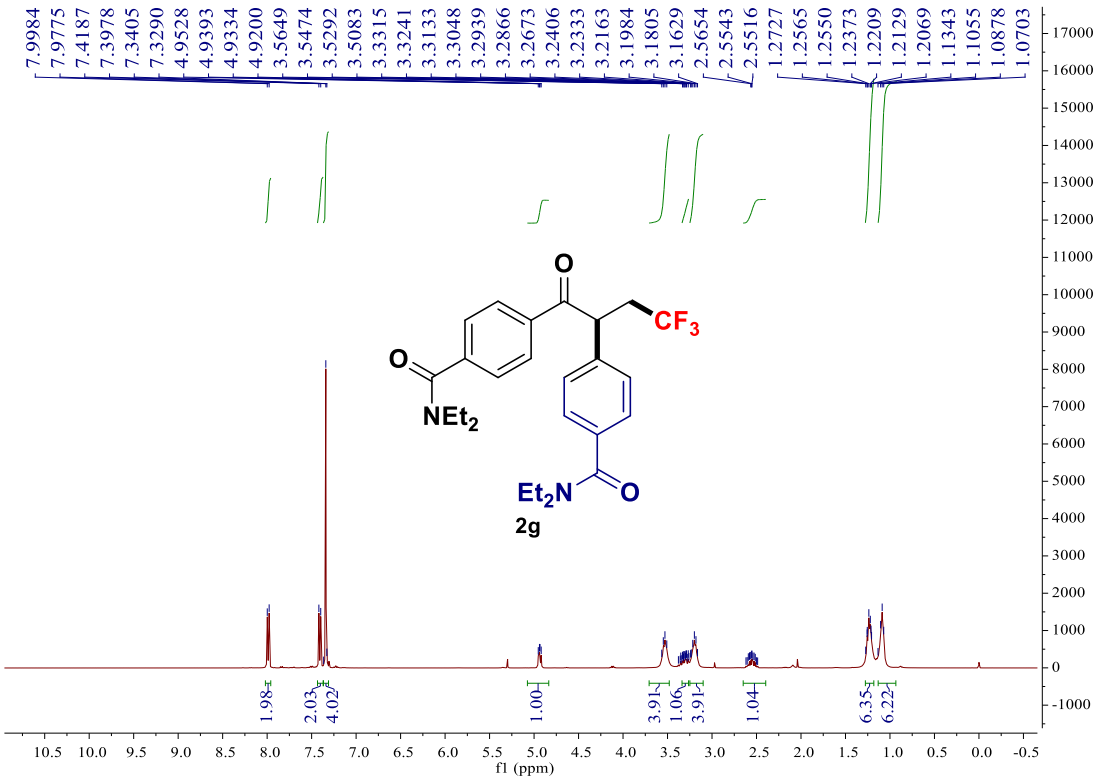
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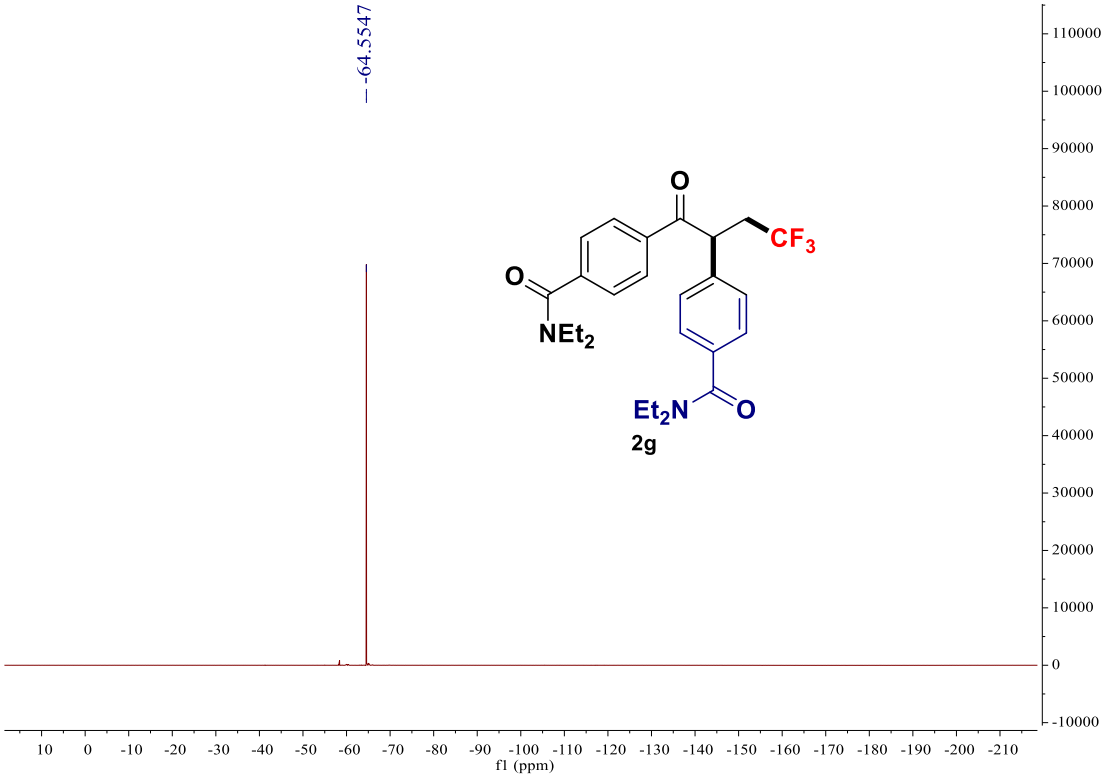
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O
2g
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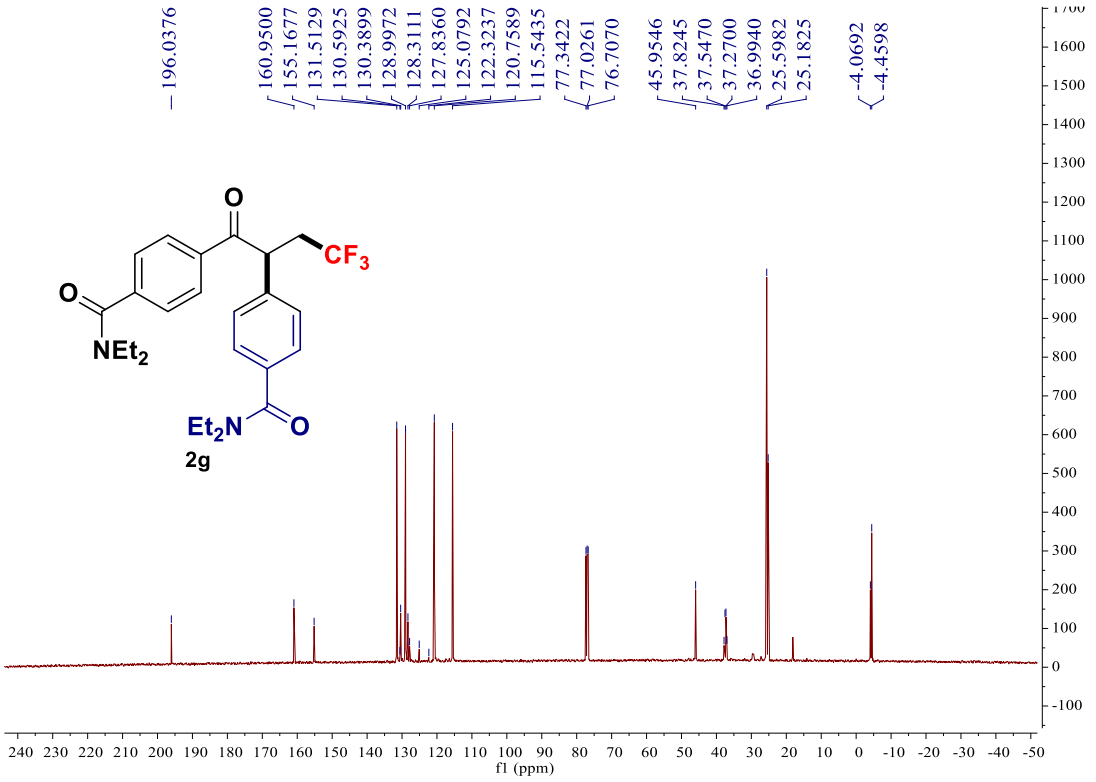
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115.5435
77.3422
77.0261
76.7070
45.9546
37.8245
37.5470
37.2700
36.9940
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CF3
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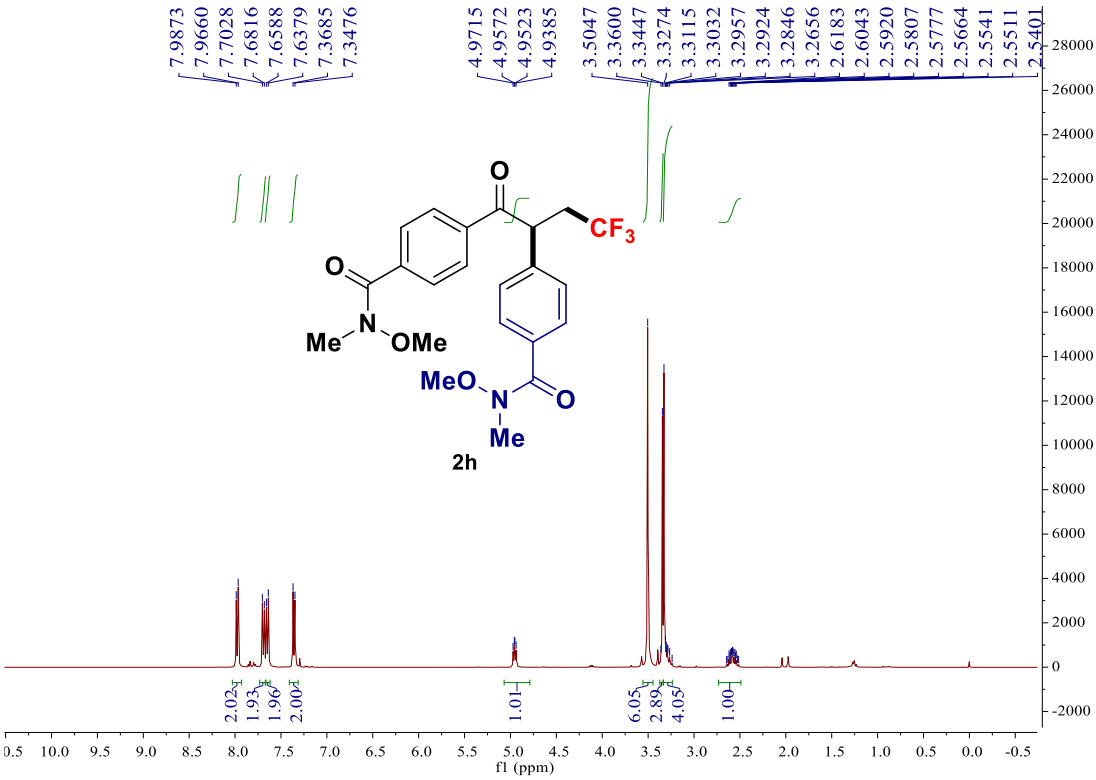
NEt2
Et2N
O
2g
f1 (ppm)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3.5047
3.3600
3.3447
3.3274
3.3115
3.3032
3.2957
3.2924
3.2846
3.2656
2.6183
2.6043
2.5920
2.5807
2.5777
2.5664
2.5541
2.5511
2.5401
O
CF3
O
N
Me
OMe
MeO
N
O
Me
2h
2.02
1.93
1.96
2.00
1.01
6.05
2.89
4.05
1.00
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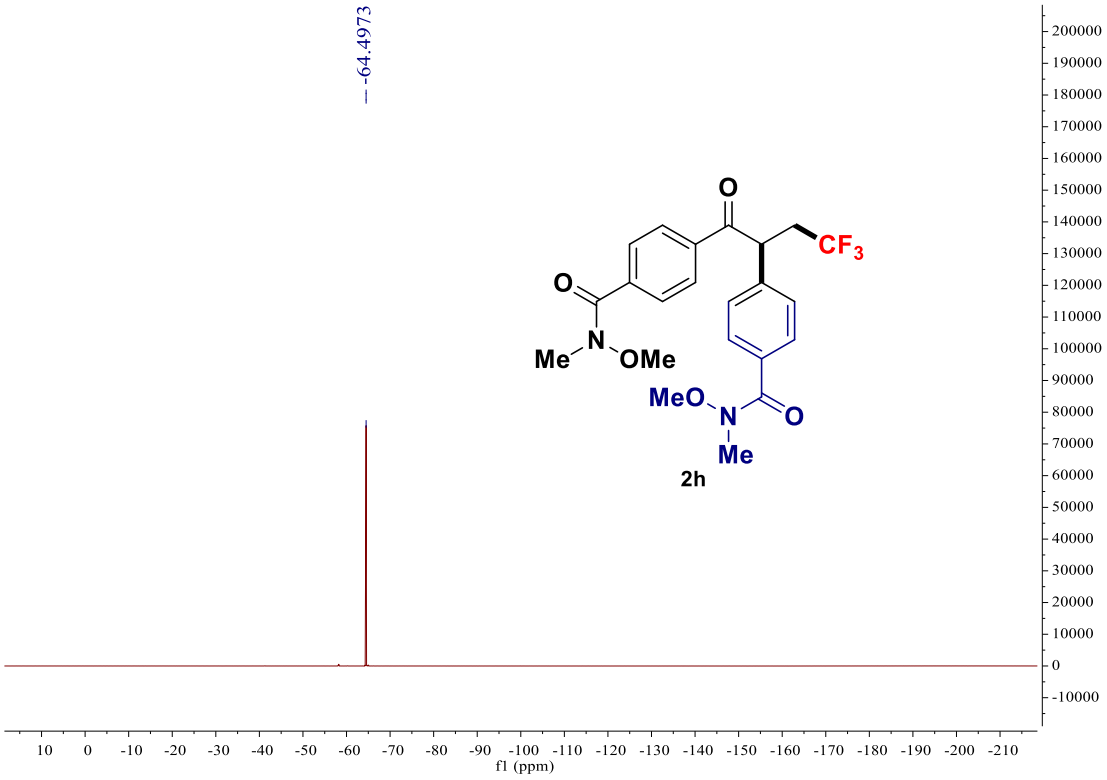
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OMe
MeO
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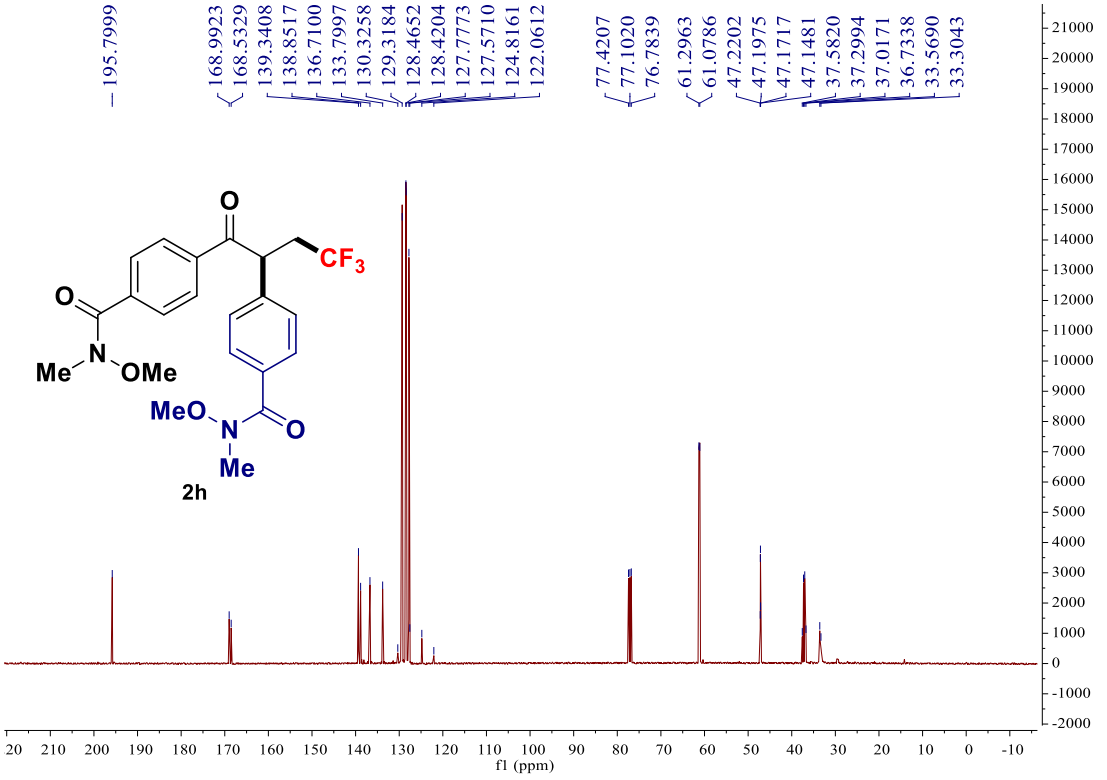
Me
2h
fl (ppm)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77.1020
76.7839
61.2963
61.0786
47.2202
47.1975
47.1717
47.1481
37.5820
37.2994
37.0171
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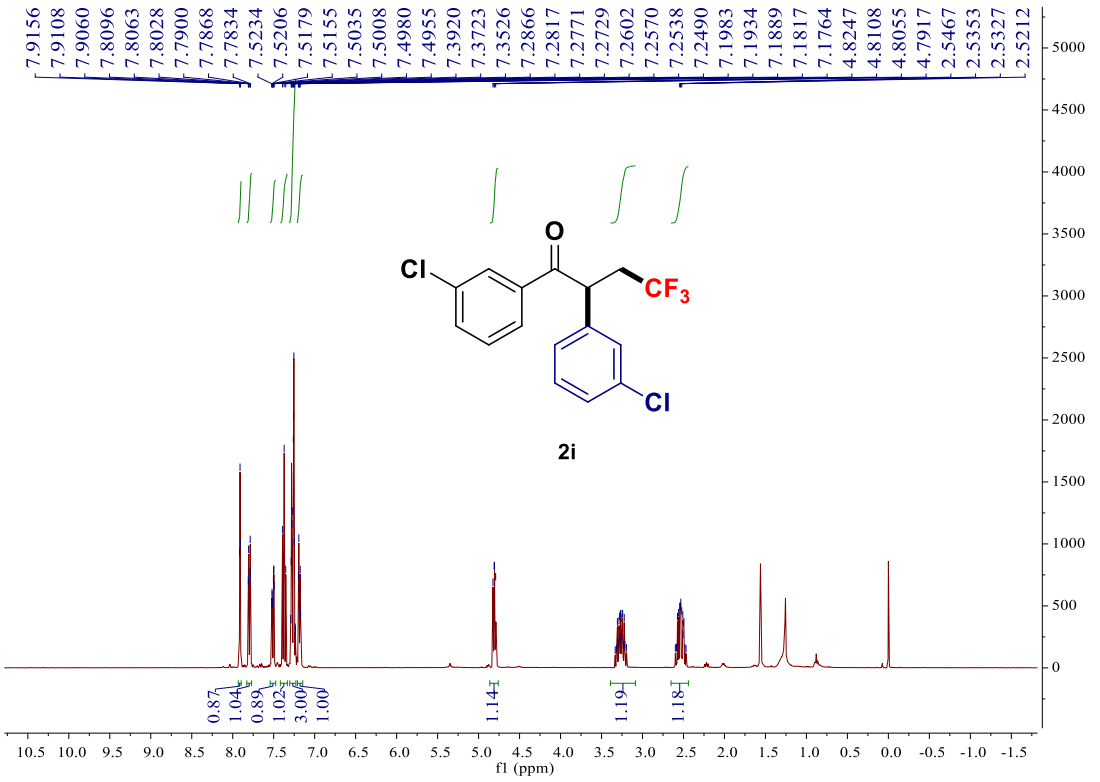
CF3
O
N
Me
OMe
MeO
N
O
Me
2h
fl (ppm)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7.5206
7.5179
7.5155
7.5035
7.5008
7.4980
7.4955
7.3920
7.3723
7.3526
7.2866
7.2817
7.2771
7.2729
7.2602
7.2570
7.2538
7.2490
7.1983
7.1934
7.1889
7.1817
7.1764
4.8247
4.8108
4.8055
4.7917
2.5467
2.5353
2.5327
2.5212
O
Cl
CF3
Cl
2i
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3.00
1.00
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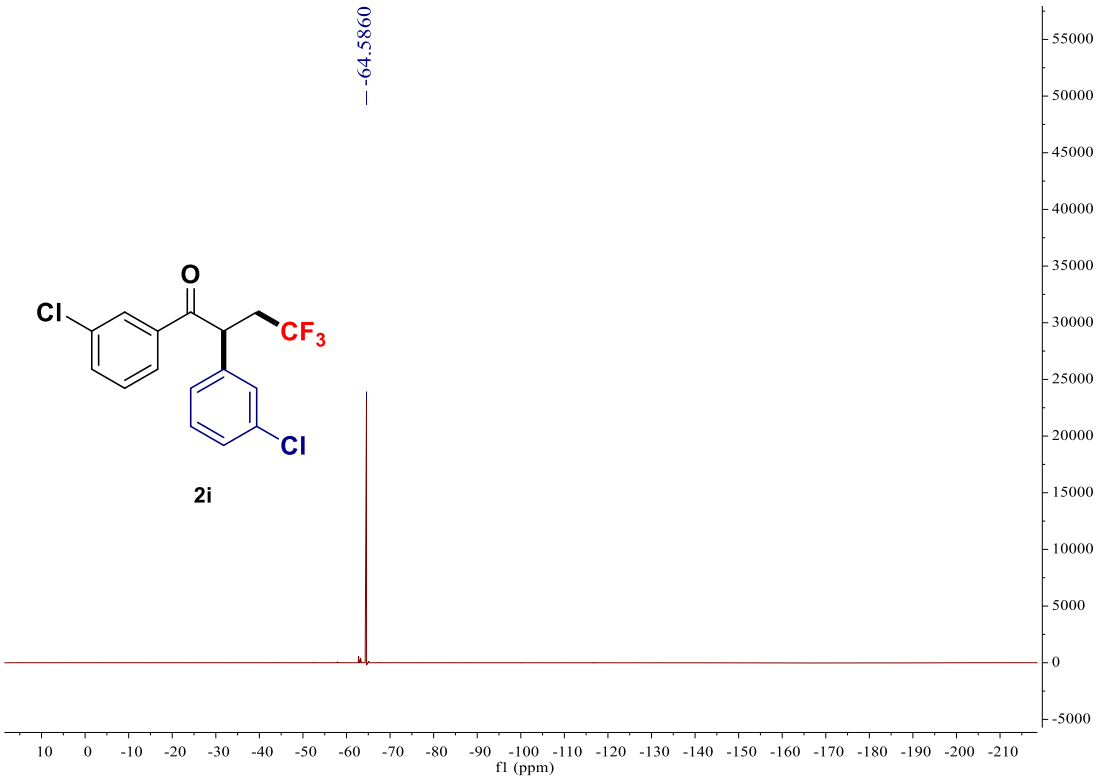
1.19
1.18
fl (ppm)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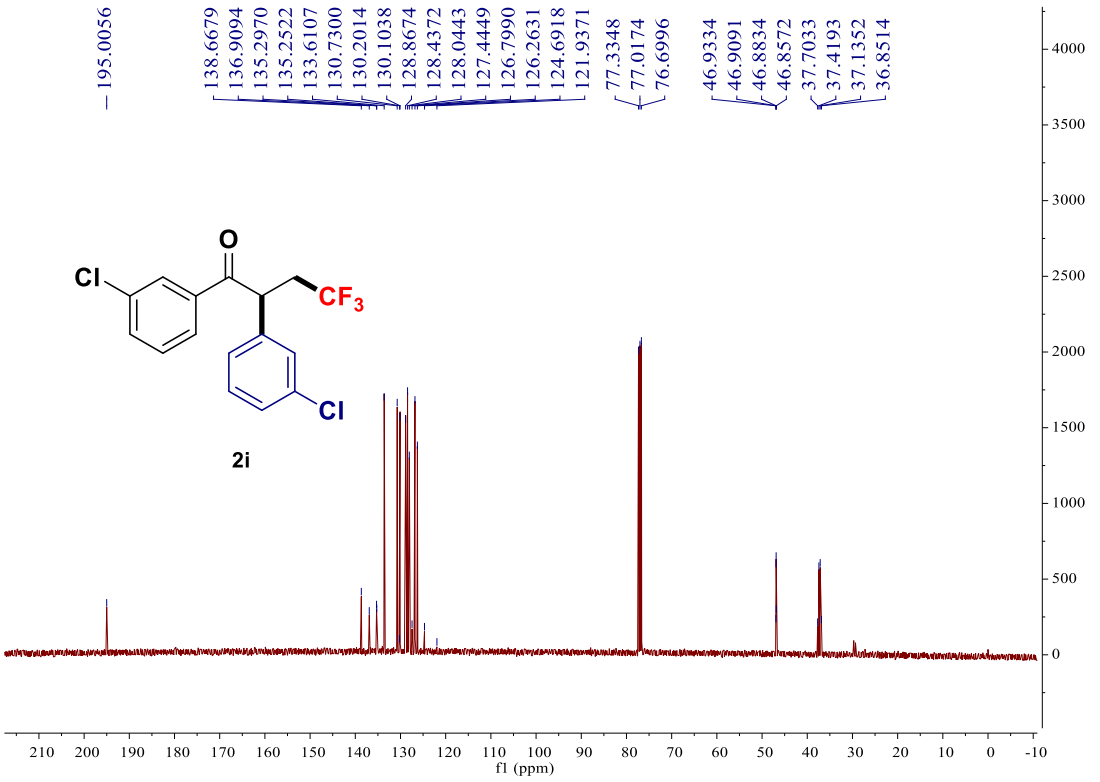
fl (ppm)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128.4372
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127.4449
126.7990
126.2631
124.6918
121.9371
77.3348
77.0174
76.6996
46.9334
46.9091
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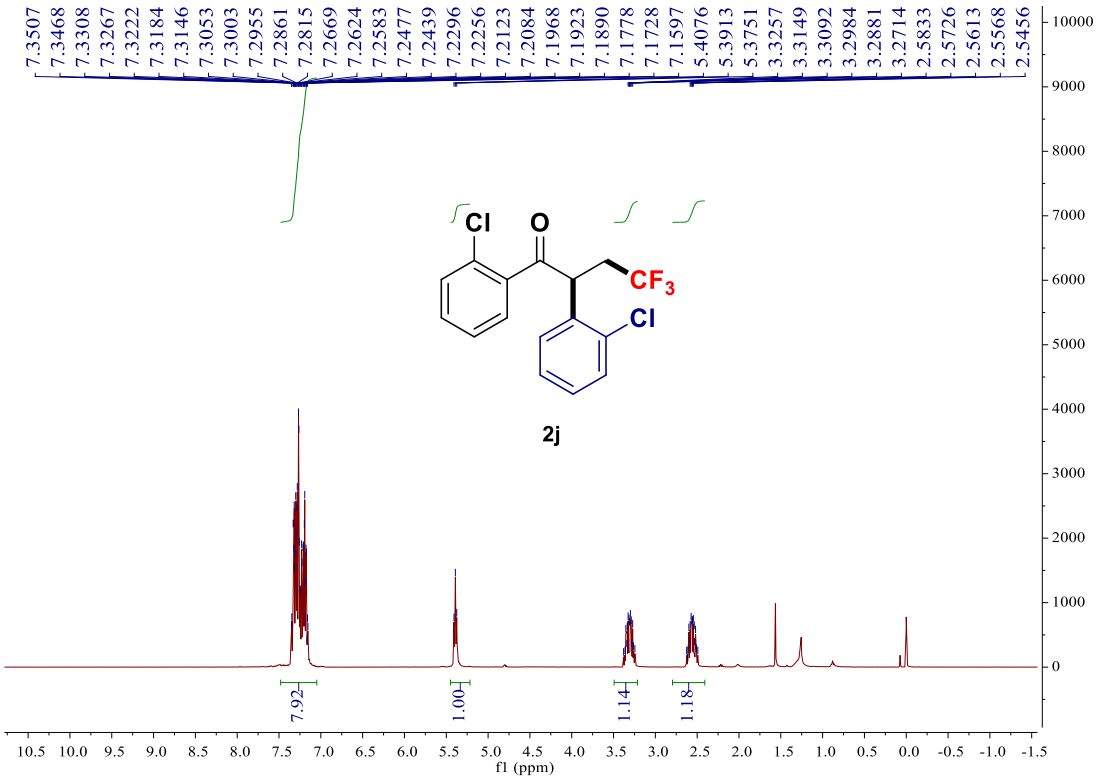
37.4193
37.1352
36.8514
Cl
O
CF3
Cl
2i
fl (ppm)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7.2815
7.2669
7.2624
7.2583
7.2477
7.2439
7.2296
7.2256
7.2123
7.2084
7.1968
7.1923
7.1890
7.1778
7.1728
7.1597
5.4076
5.3913
5.3751
3.3257
3.3149
3.3092
3.2984
3.2881
3.2714
2.5833
2.5726
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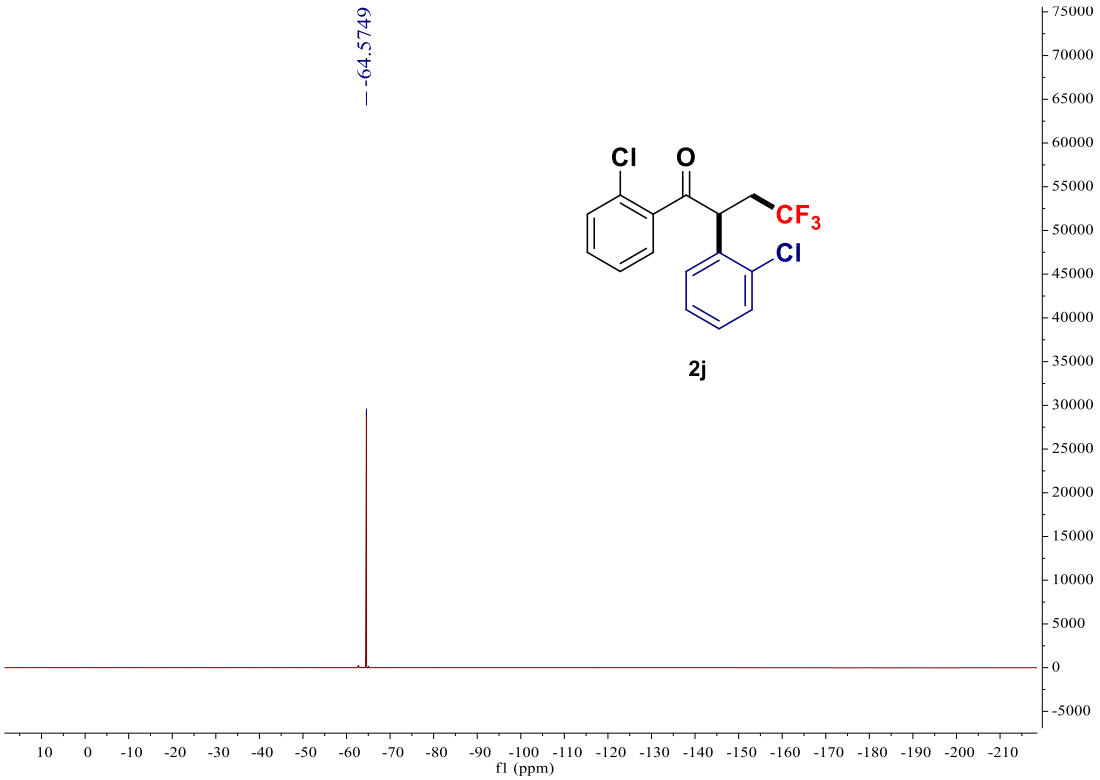
2.5456
Cl
O
CF3
Cl
2j
7.92
1.00
1.14
1.18
fl (ppm)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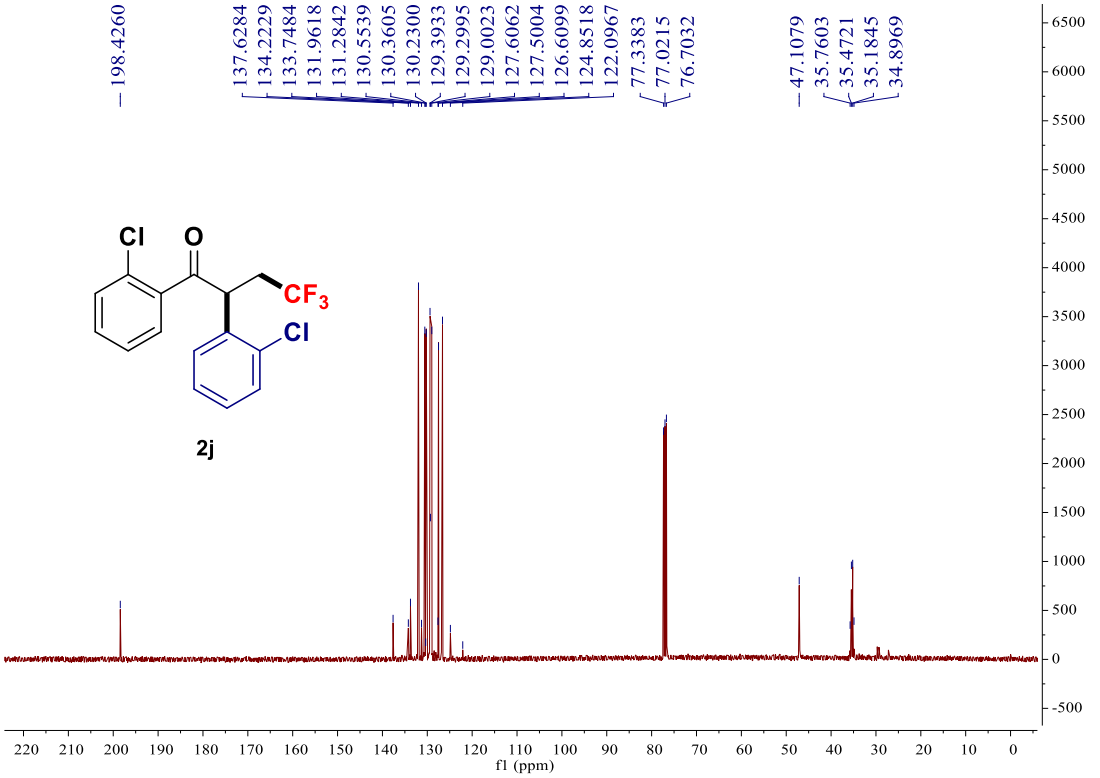
O
CF3
Cl
2j
fl (ppm)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129.0023
127.6062
127.5004
126.6099
124.8518
122.0967
77.3383
77.0215
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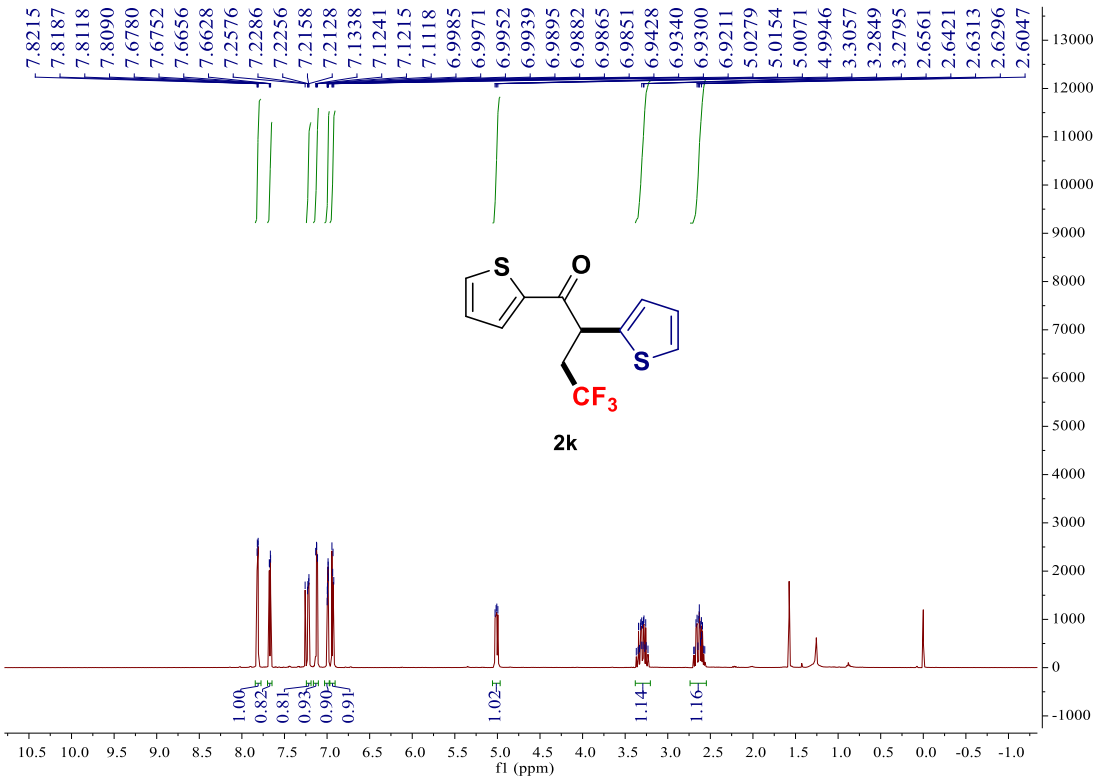
Cl
O
CF3
Cl
2j
fl (ppm)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7.2256
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7.2128
7.1338
7.1241
7.1215
7.1118
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6.9971
6.9952
6.9939
6.9895
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2.6421
2.6313
2.6296
2.6047
S
O
S
CF3
2k
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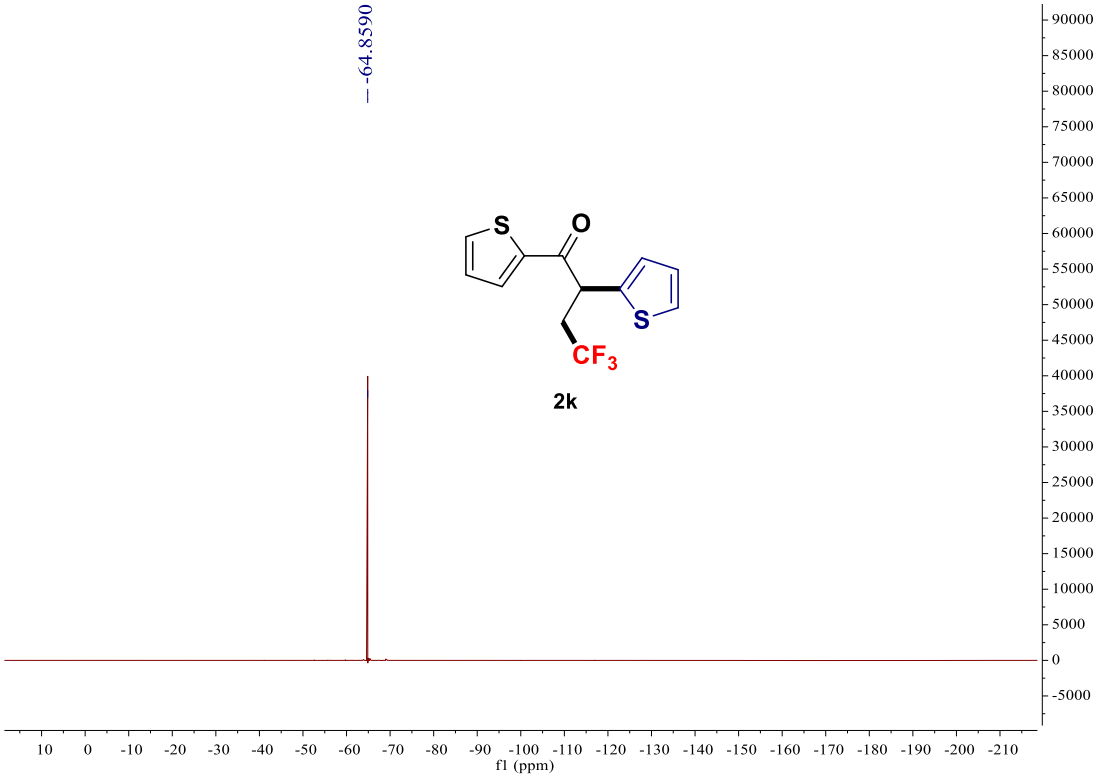
0.81
0.93
0.90
0.91
1.02
1.14
1.16
f1 (ppm)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O
S
CF3
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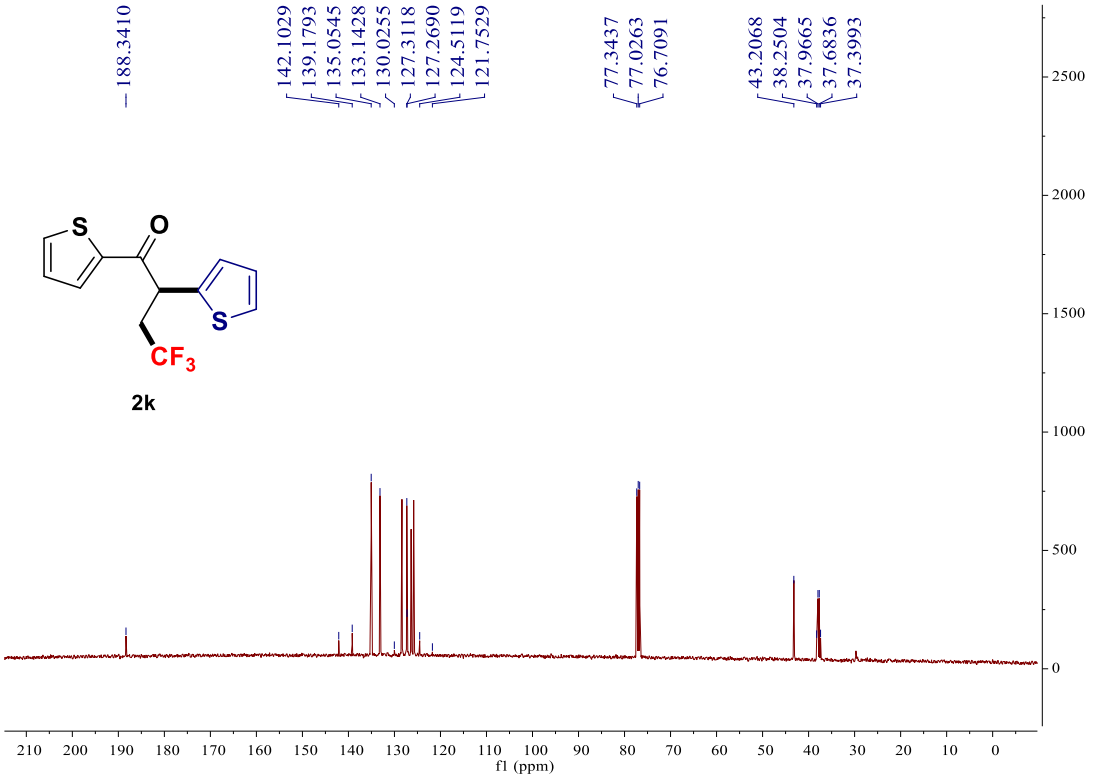
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77.3437
77.0263
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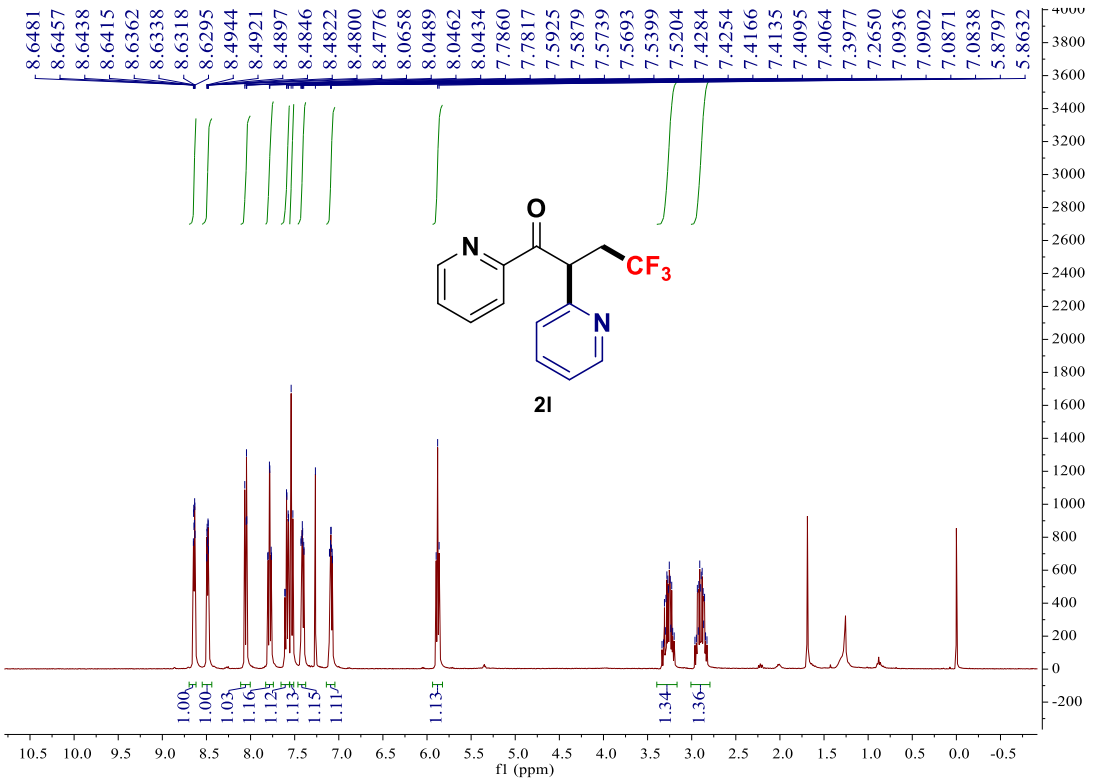
38.2504
37.9665
37.6836
37.3993
S
O
S
CF3
2k
fl (ppm)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8.6318
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8.4846
8.4822
8.4800
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8.0658
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7.4254
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7.4064
7.3977
7.2650
7.0936
7.0902
7.0871
7.0838
5.8797
5.8632
O
N
CF3
N
2l
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1.00
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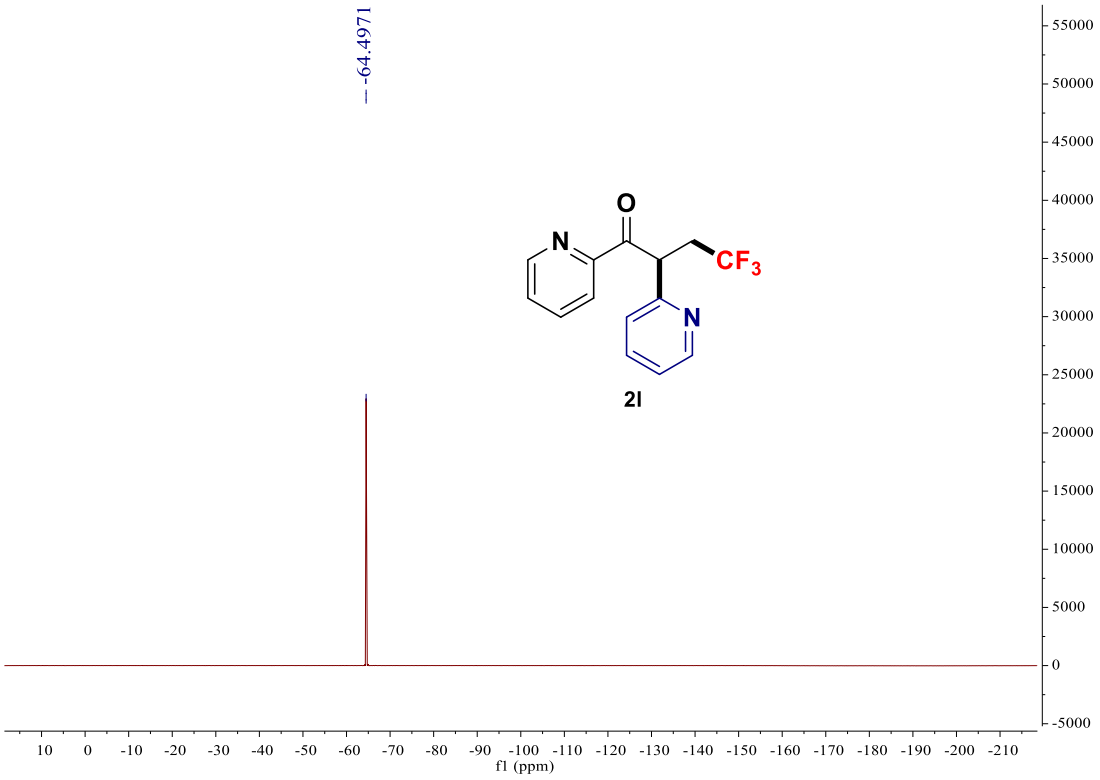
1.16
1.12
1.13
1.15
1.11
1.13
1.34
1.36
fl (ppm)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N
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45000
40000
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25000
20000
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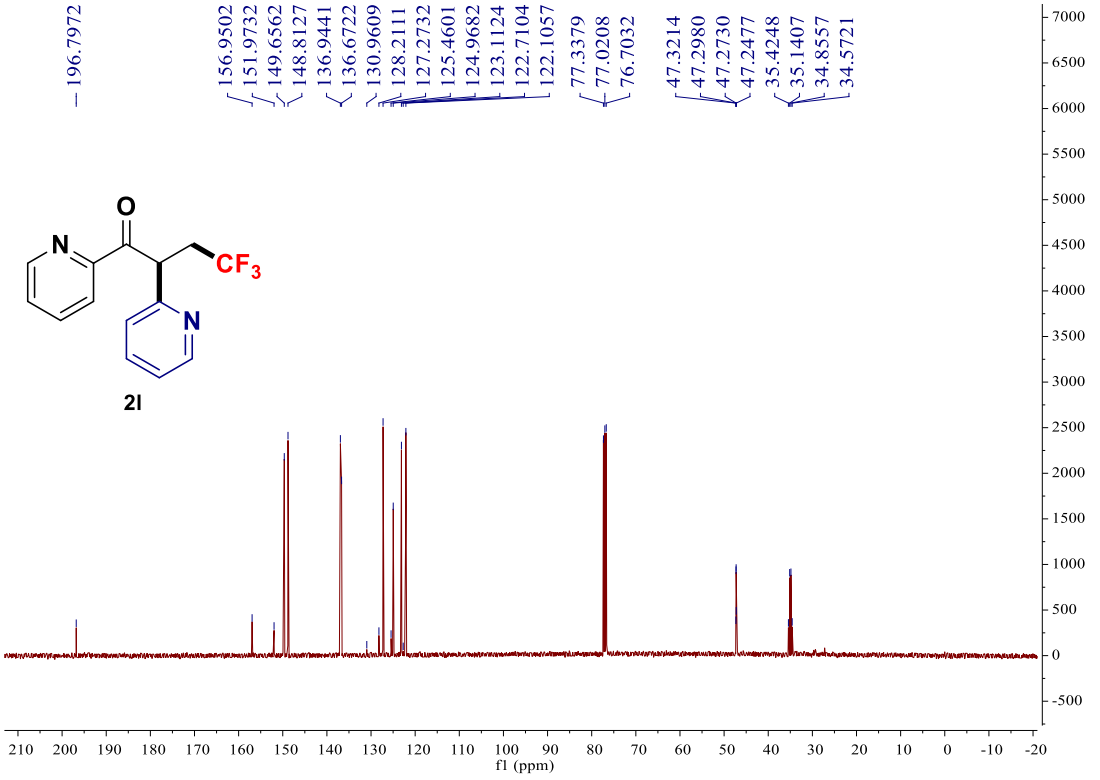
10000
5000
0
-5000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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124.9682
123.1124
122.7104
122.1057
77.3379
77.0208
76.7032
47.3214
47.2980
47.2730
47.2477
35.4248
35.1407
34.8557
34.5721
O
N
CF3
N
2l
7000
6500
6000
5500
5000
4500
4000
3500
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2500
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1500
1000
500
0
-500
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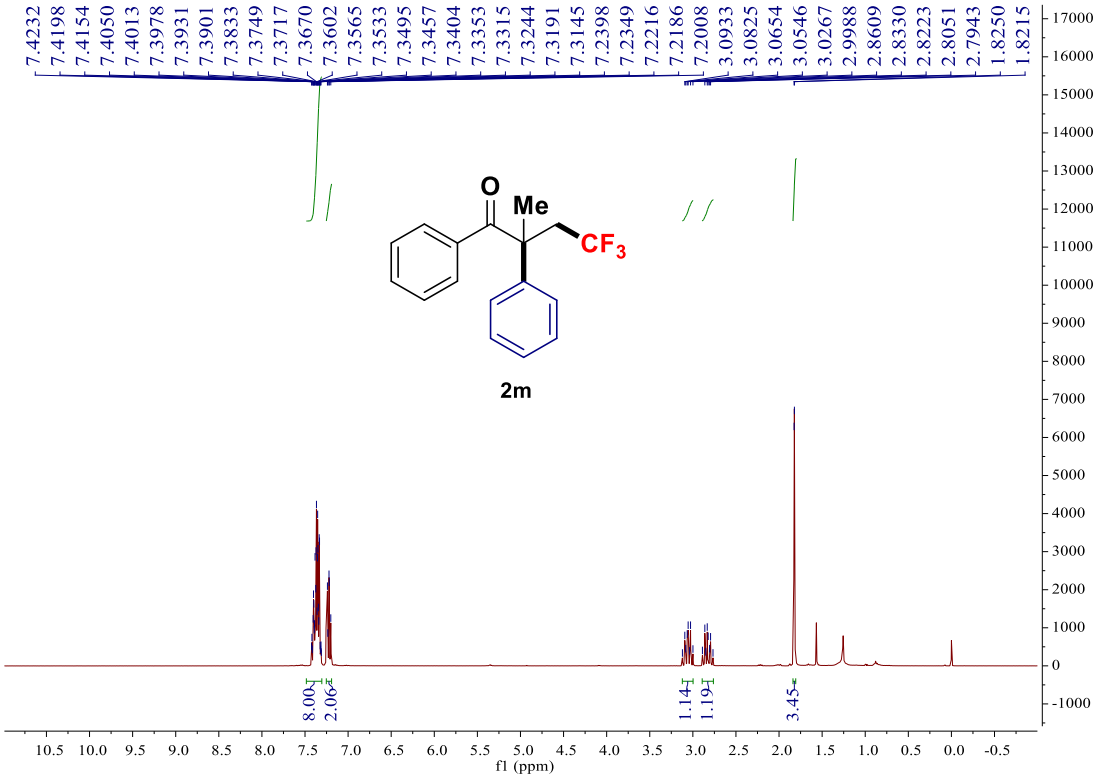
f1 (ppm)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7.2008
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3.0825
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3.0267
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2.8330
2.8223
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2.7943
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Me
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2m
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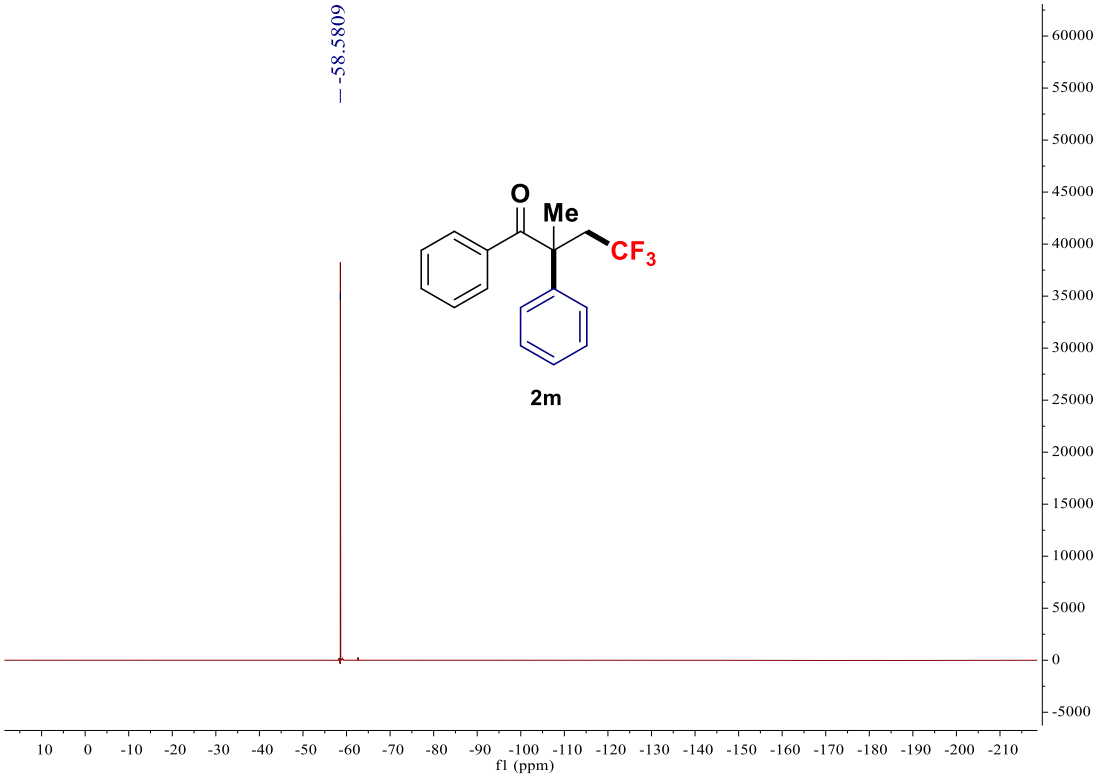
1.14
1.19
3.45
f1 (ppm)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CF3
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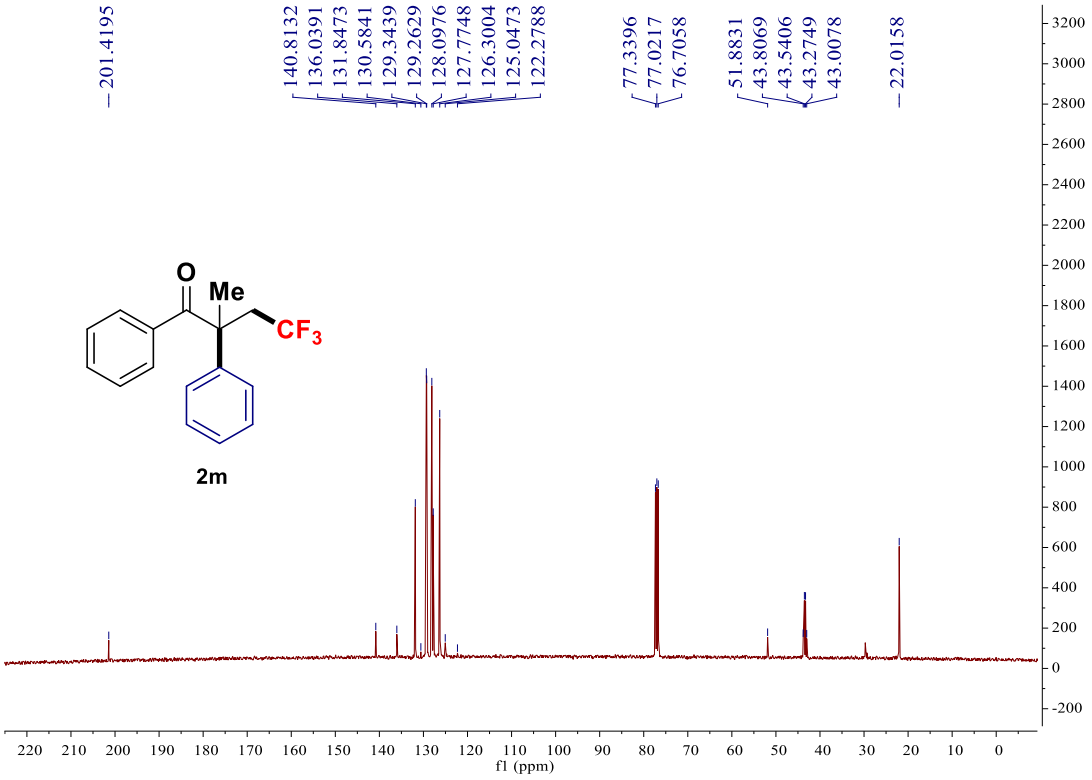
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77.0217
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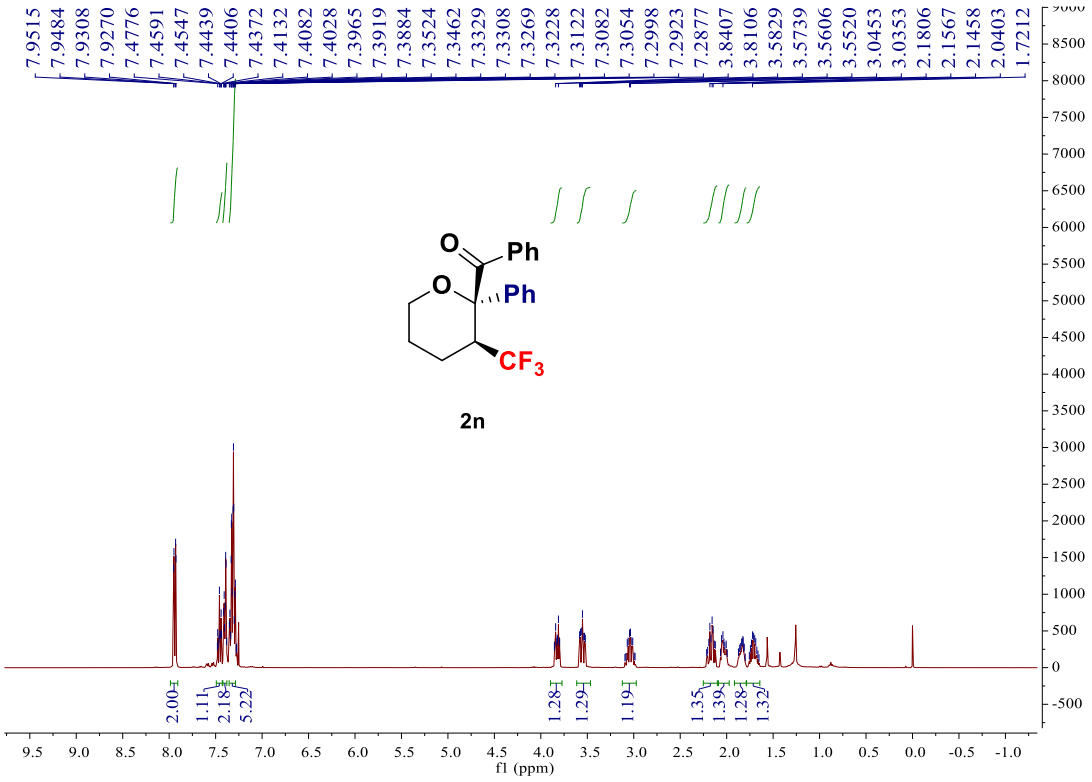
43.0078
22.0158
O
Me
CF3
2m
fl (ppm)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3.5829
3.5739
3.5606
3.5520
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3.0353
2.1806
2.1567
2.1458
2.0403
1.7212
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Ph
O
Ph
CF3
2n
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5.22
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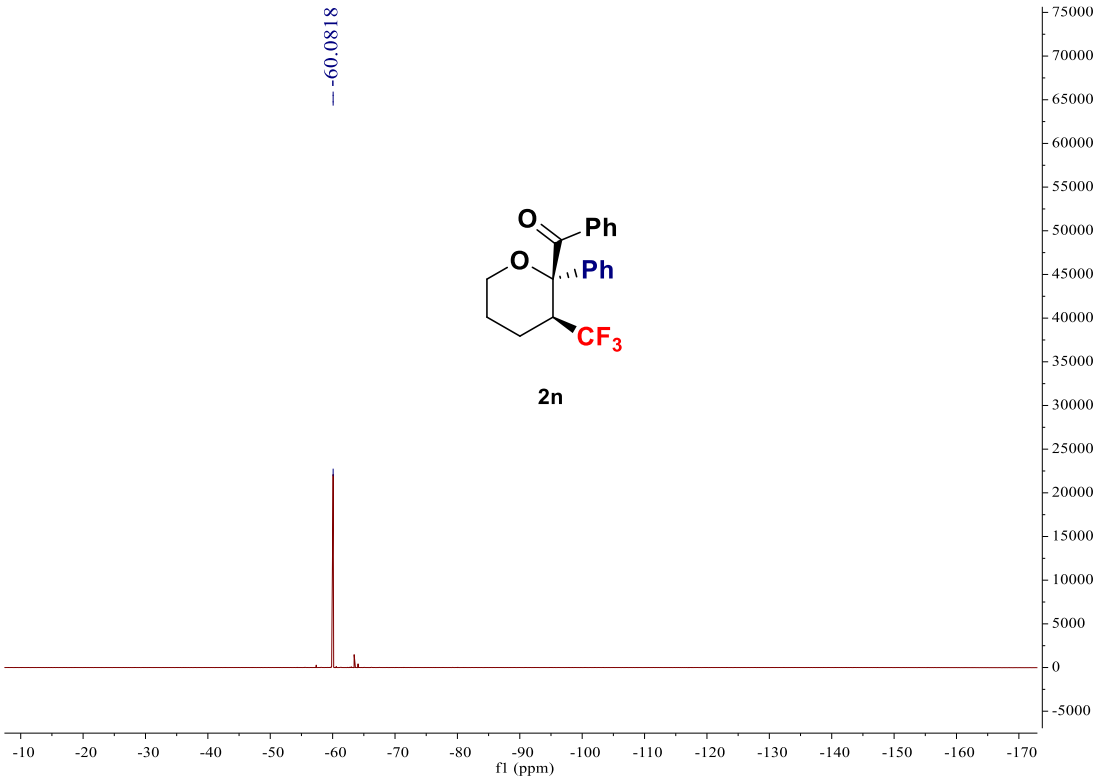
1.29
1.19
1.35
1.39
1.28
1.32
fl (ppm)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O
Ph
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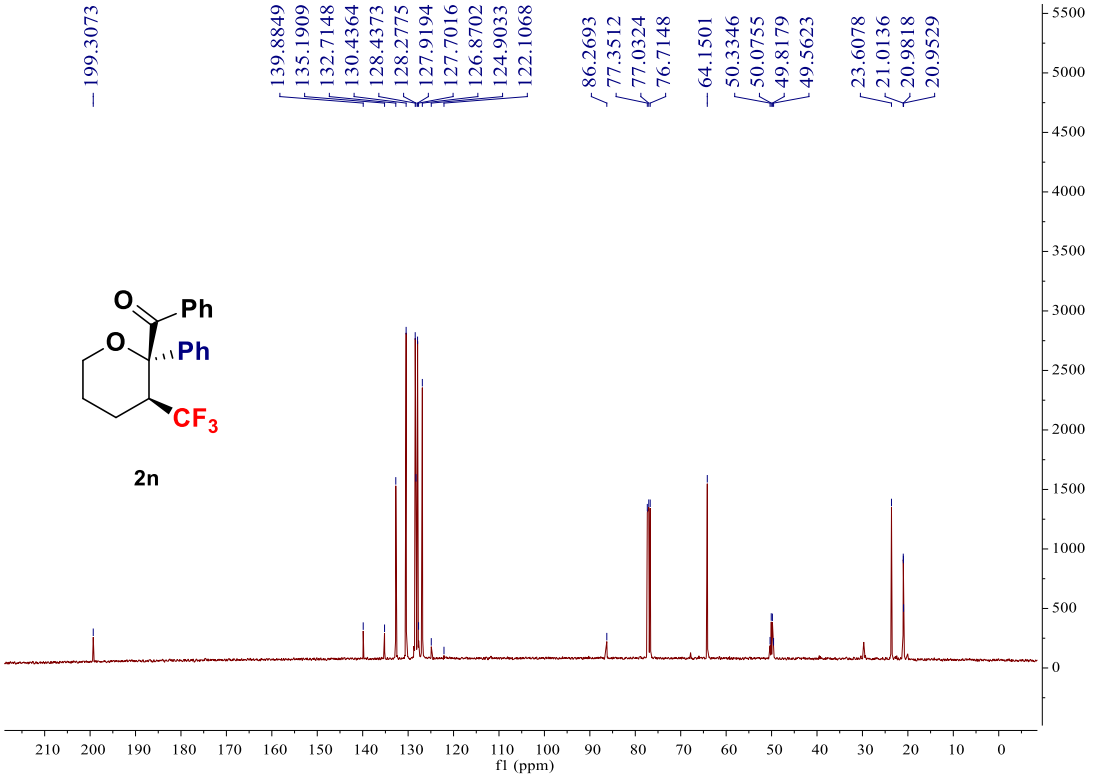
2n
fl (ppm)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124.9033
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86.2693
77.3512
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76.7148
64.1501
50.3346
50.0755
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23.6078
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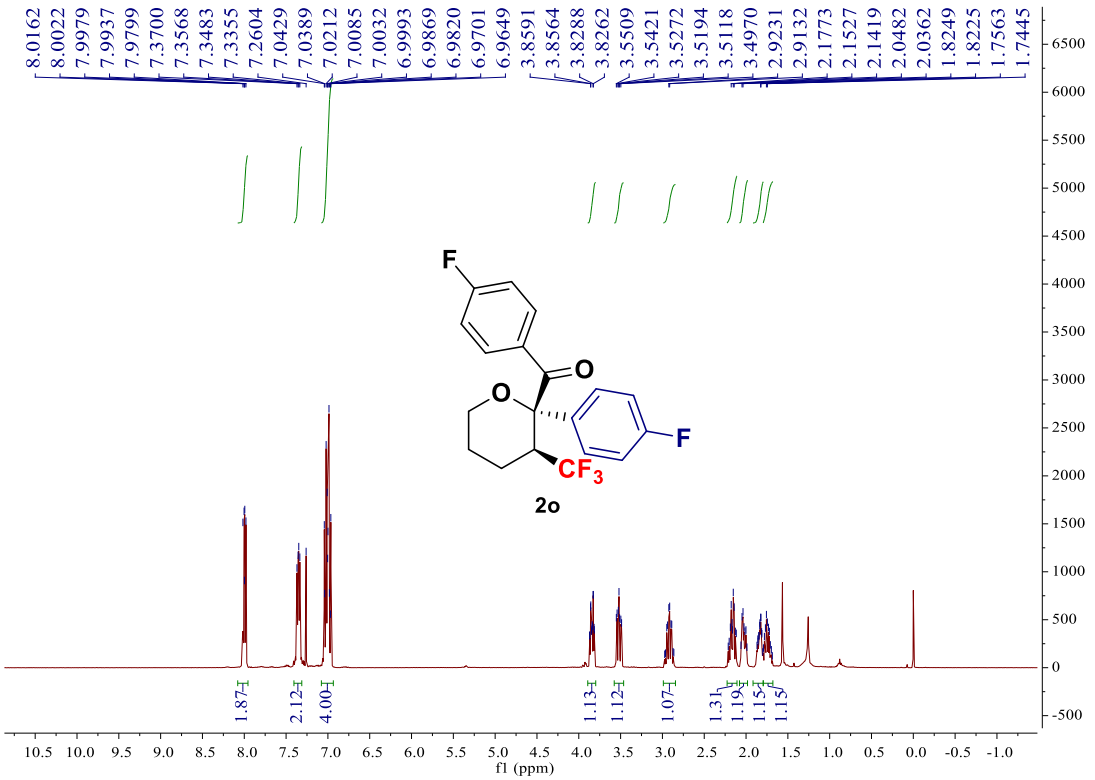
O
Ph
O
Ph
CF3
2n
fl (ppm)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7.2604
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7.0212
7.0085
7.0032
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3.4970
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2.1527
2.1419
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2.0362
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1.8225
1.7563
1.7445
F
O
O
F
CF3
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4.00
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1.19
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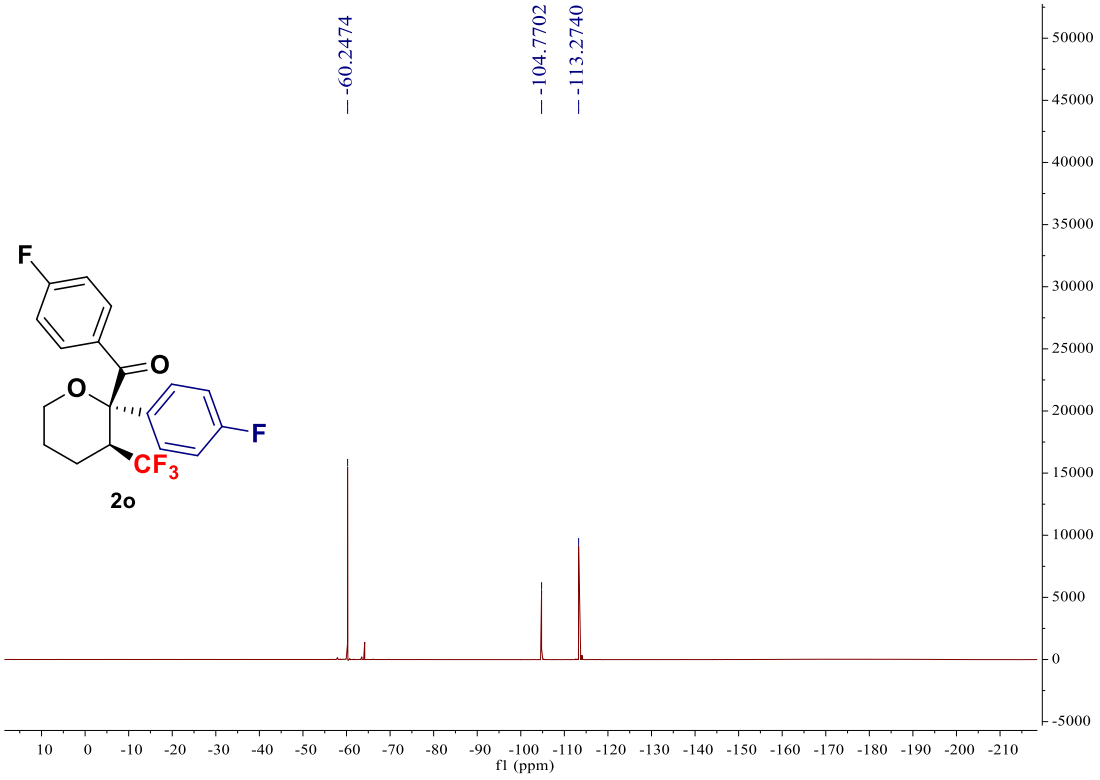
1.15
f1 (ppm)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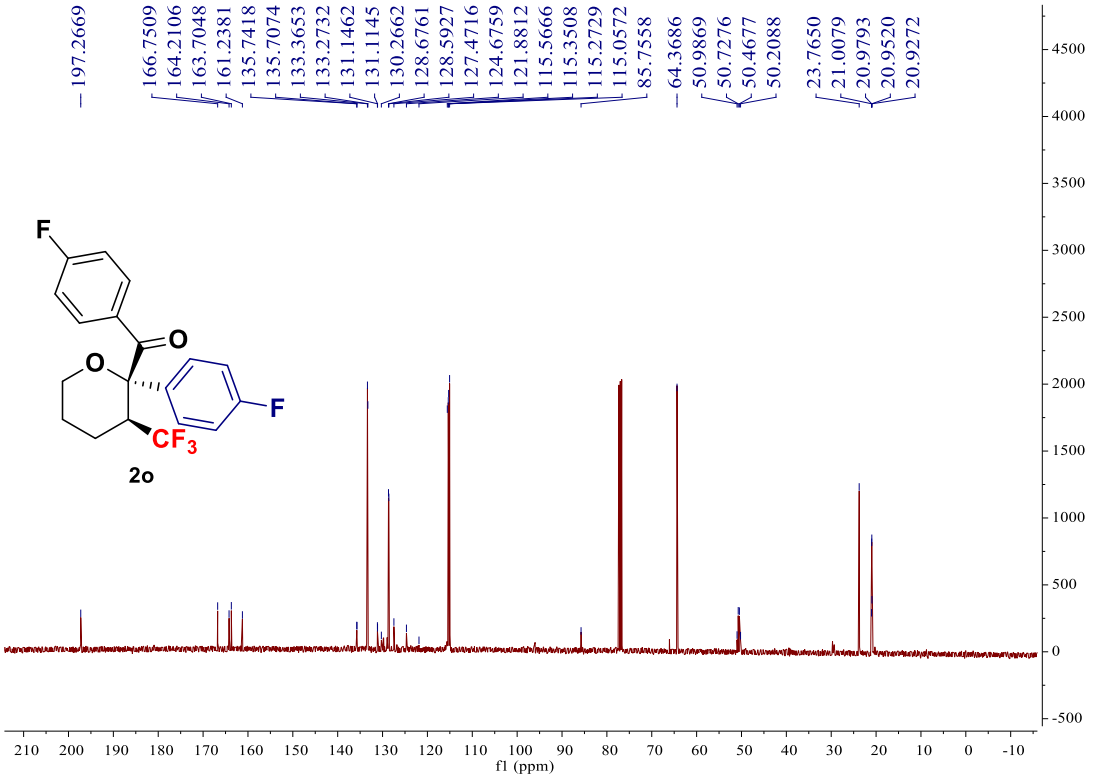
O
O
F
CF3
2o
f1 (ppm)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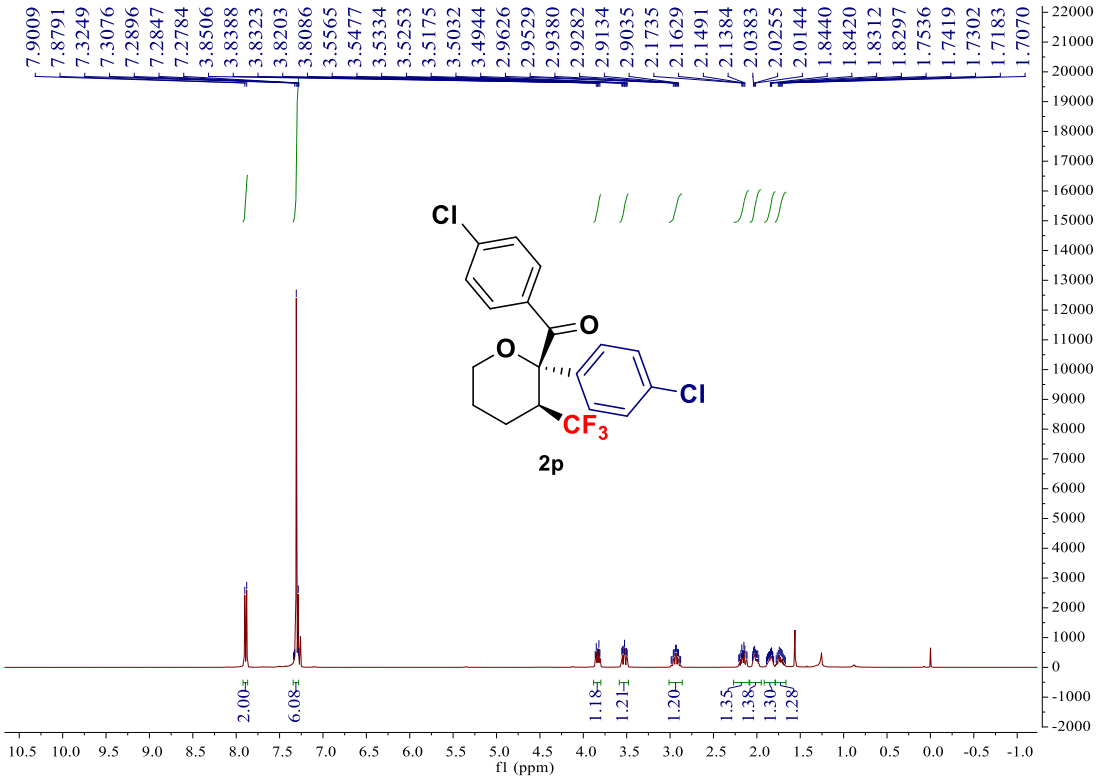
O
O
F
CF3
2o
f1 (ppm)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3.8388
3.8323
3.8203
3.8086
3.5565
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3.5253
3.5175
3.5032
3.4944
2.9626
2.9529
2.9380
2.9282
2.9134
2.9035
2.1735
2.1629
2.1491
2.1384
2.0383
2.0255
2.0144
1.8440
1.8420
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1.8297
1.7536
1.7419
1.7302
1.7183
1.7070
Cl
O
O
Cl
CF3
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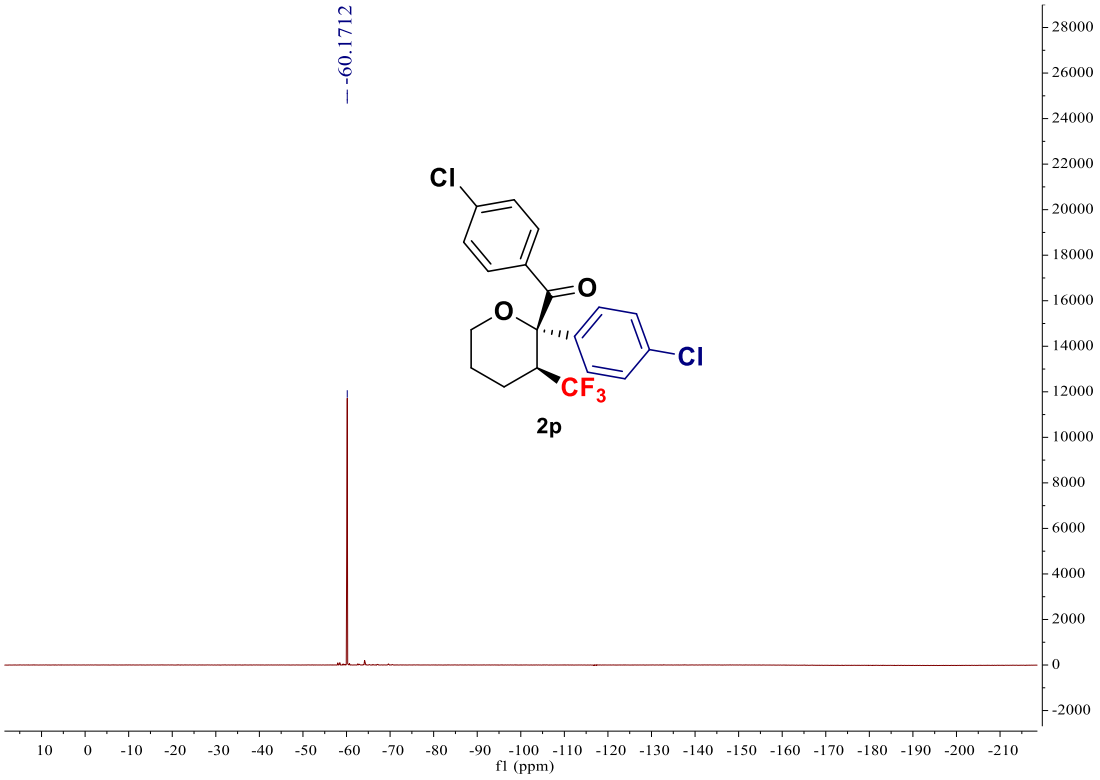
1.38
1.30
1.28
f1 (ppm)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O
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CF3
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26000
24000
22000
20000
18000
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12000
10000
8000
6000
4000
2000
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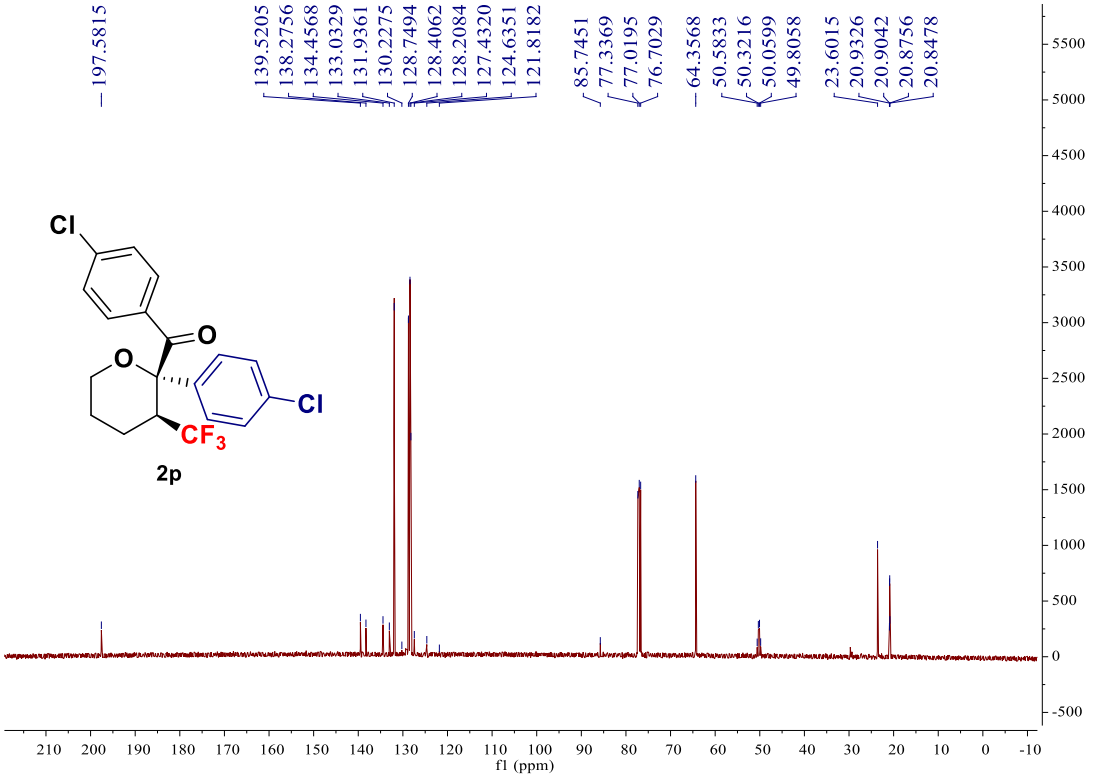
f1 (ppm)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121.8182
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77.0195
76.7029
64.3568
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50.3216
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49.8058
23.6015
20.9326
20.9042
20.8756
20.8478
Cl
O
O
Cl
CF3
2p
5500
5000
4500
4000
3500
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1500
1000
500
0
-500
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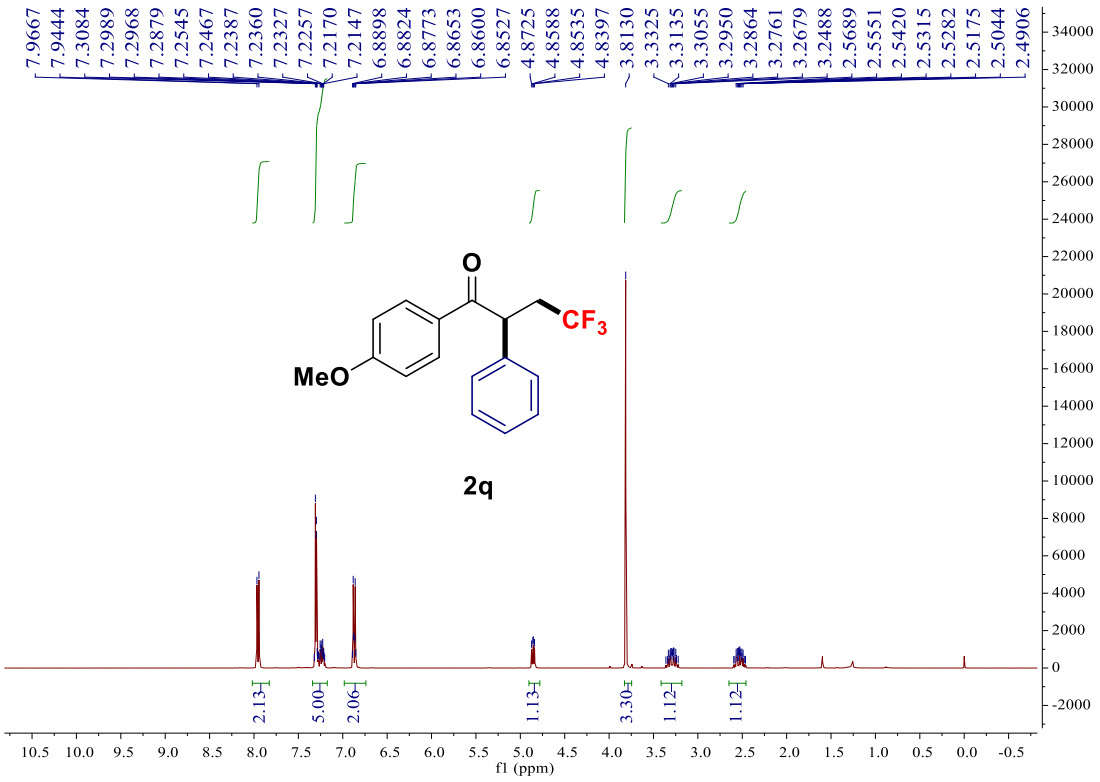
f1 (ppm)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7.2147
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6.8824
6.8773
6.8653
6.8600
6.8527
4.8725
4.8588
4.8535
4.8397
3.8130
3.3325
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3.3055
3.2950
3.2864
3.2761
3.2679
3.2488
2.5689
2.5551
2.5420
2.5315
2.5282
2.5175
2.5044
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MeO
2q
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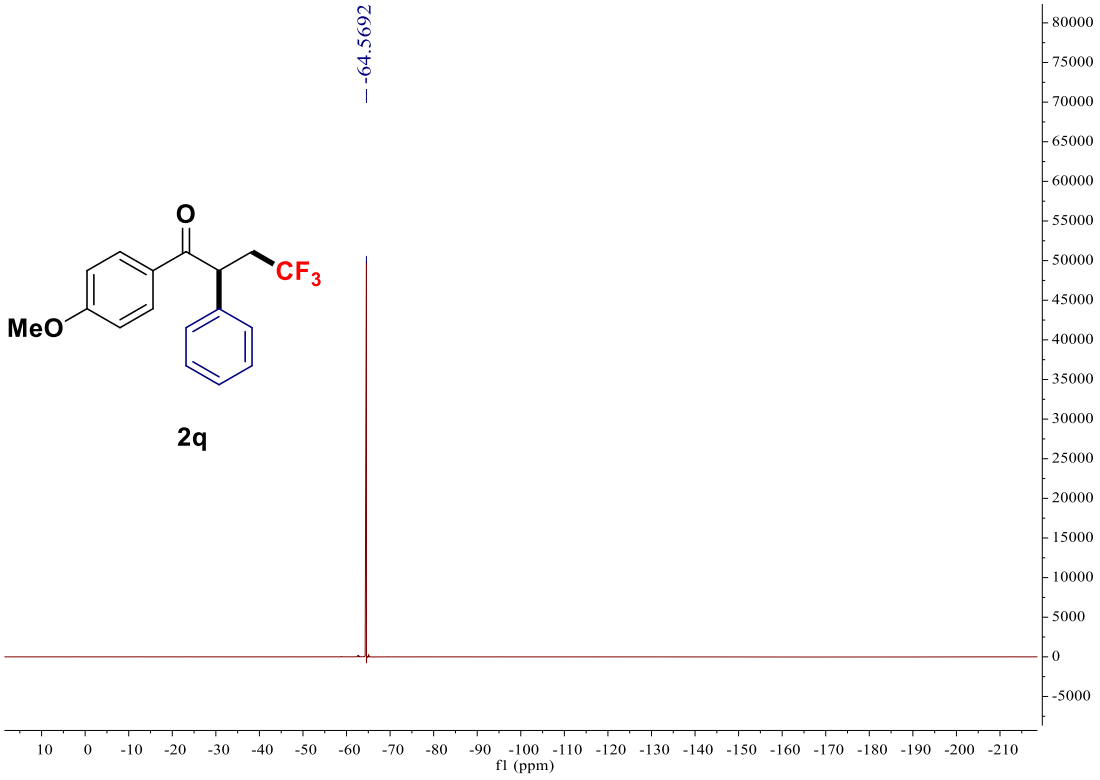
5.00
2.06
1.13
3.30
1.12
1.12
fl (ppm)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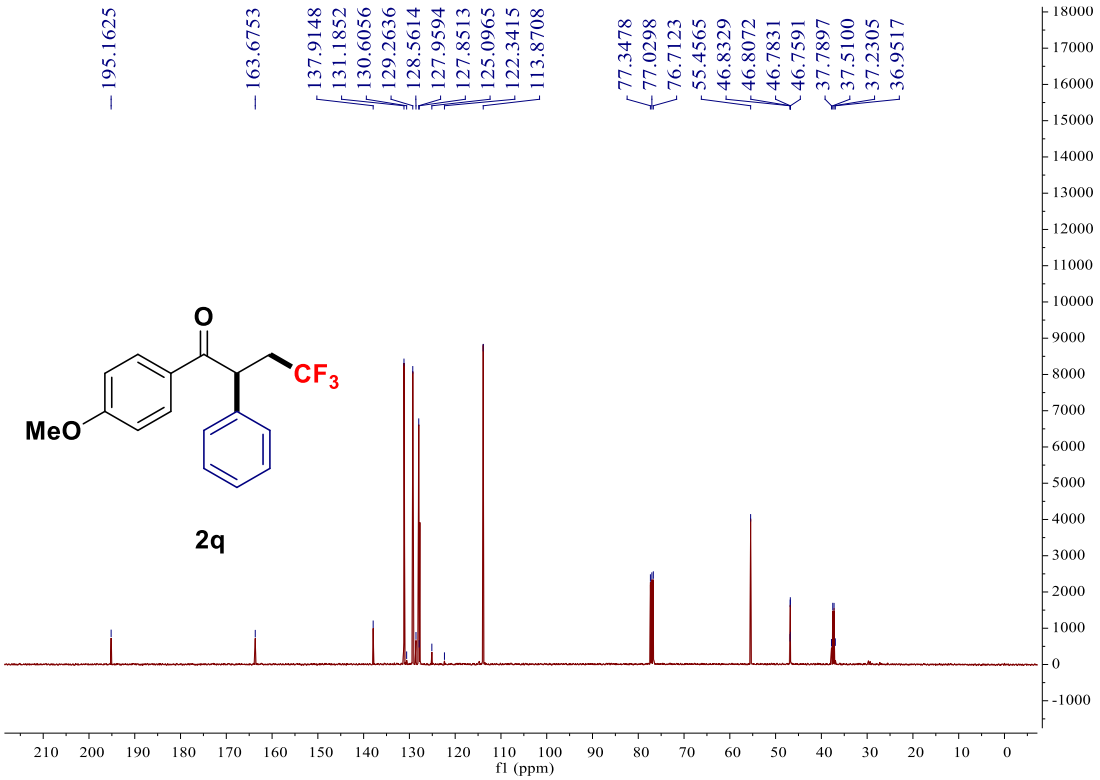
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77.0298
76.7123
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46.8329
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37.7897
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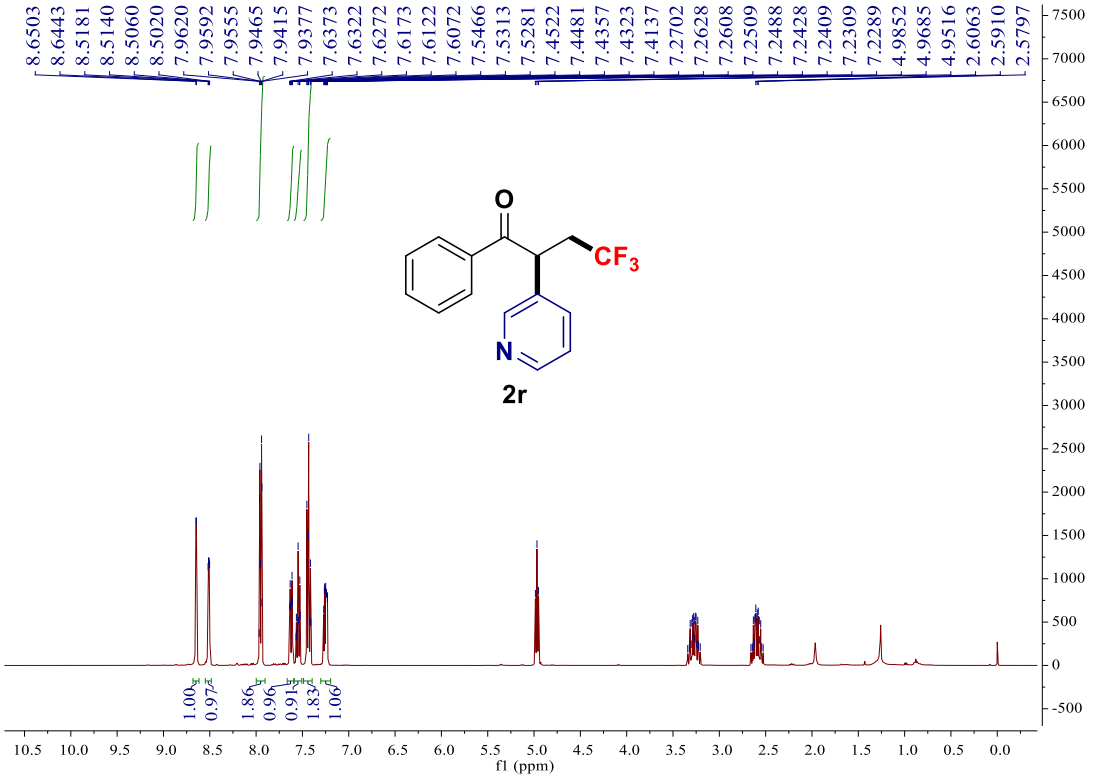
36.9517
O
CF3
MeO
2q
fl (ppm)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7.6373
7.6322
7.6272
7.6173
7.6122
7.6072
7.5466
7.5313
7.5281
7.4522
7.4481
7.4357
7.4323
7.4137
7.2702
7.2628
7.2608
7.2509
7.2488
7.2428
7.2409
7.2309
7.2289
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4.9685
4.9516
2.6063
2.5910
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N
2r
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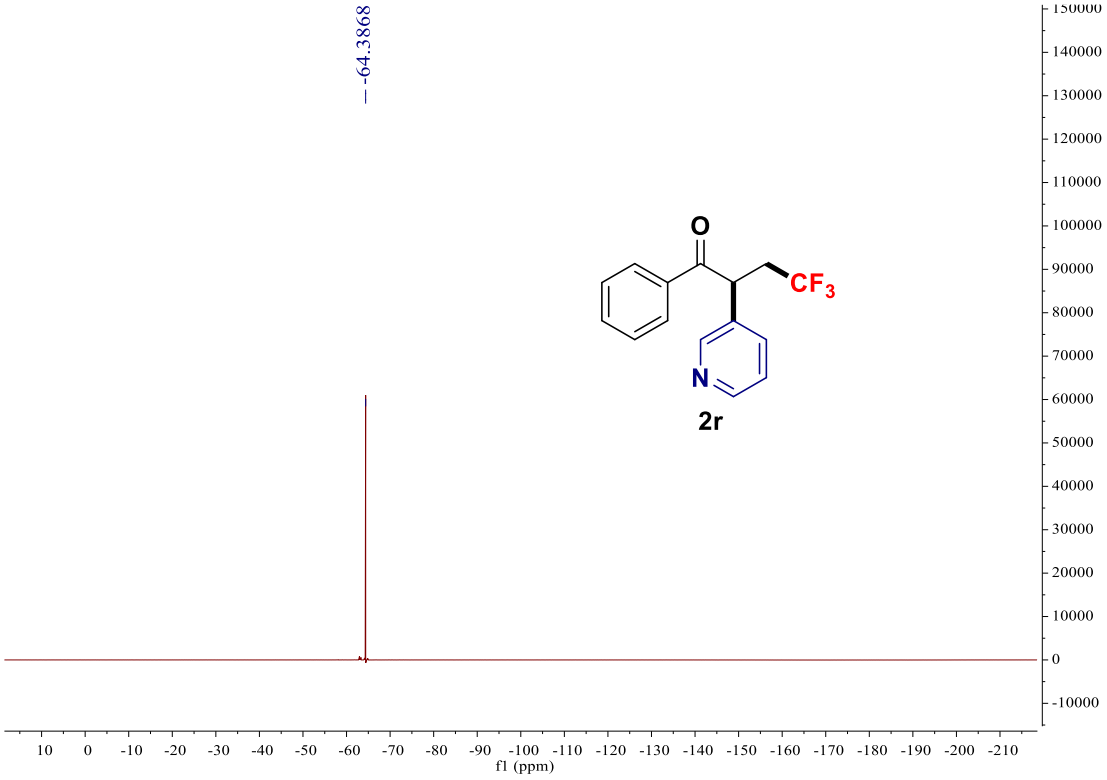
0.96
0.91
1.83
1.06
fl (ppm)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2r
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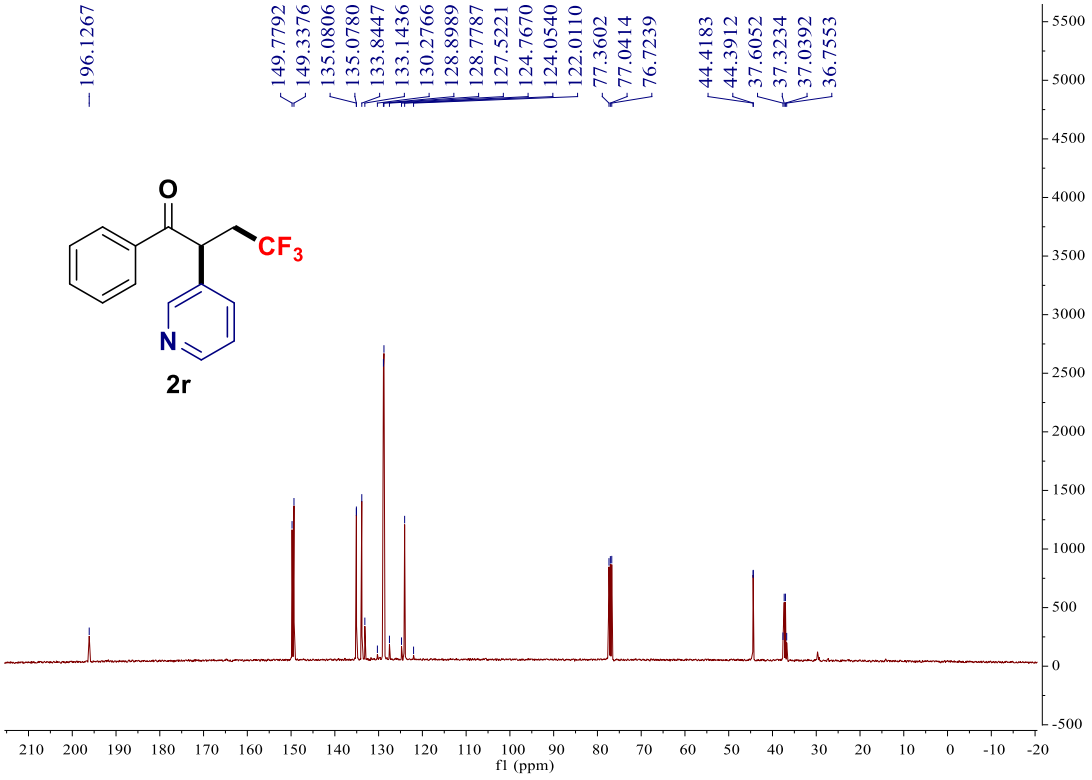
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122.0110
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77.0414
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44.3912
37.6052
37.3234
37.0392
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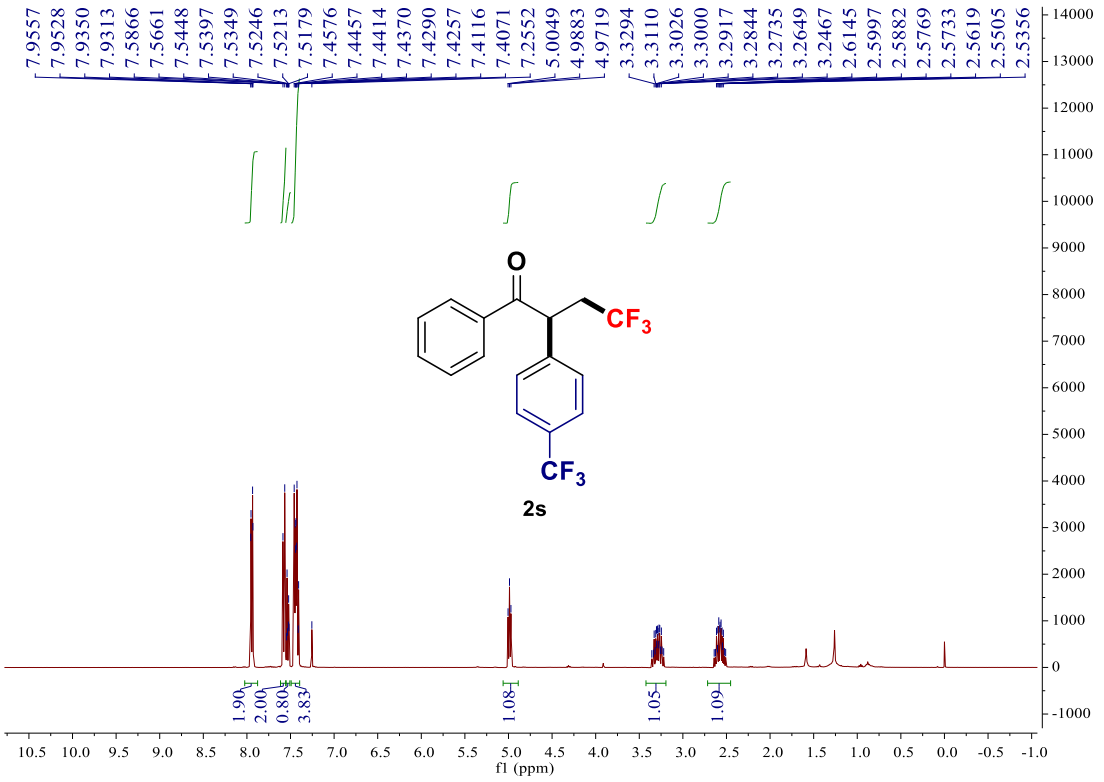
O
CF3
N
2r
f1 (ppm)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7.5349
7.5246
7.5213
7.5179
7.4576
7.4457
7.4414
7.4370
7.4290
7.4257
7.4116
7.4071
7.2552
5.0049
4.9883
4.9719
3.3294
3.3110
3.3026
3.3000
3.2917
3.2844
3.2735
3.2649
3.2467
2.6145
2.5997
2.5882
2.5769
2.5733
2.5619
2.5505
2.5356
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CF3
CF3
2s
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2.00
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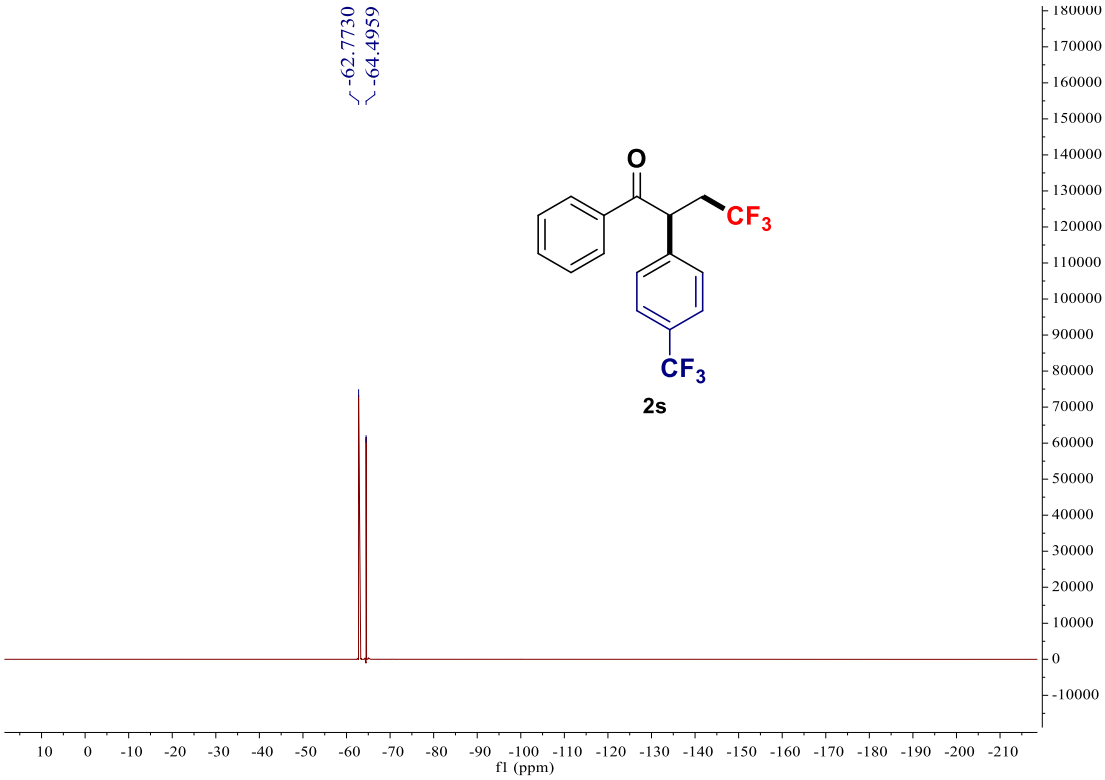
3.83
1.08
1.05
1.09
f1 (ppm)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CF3
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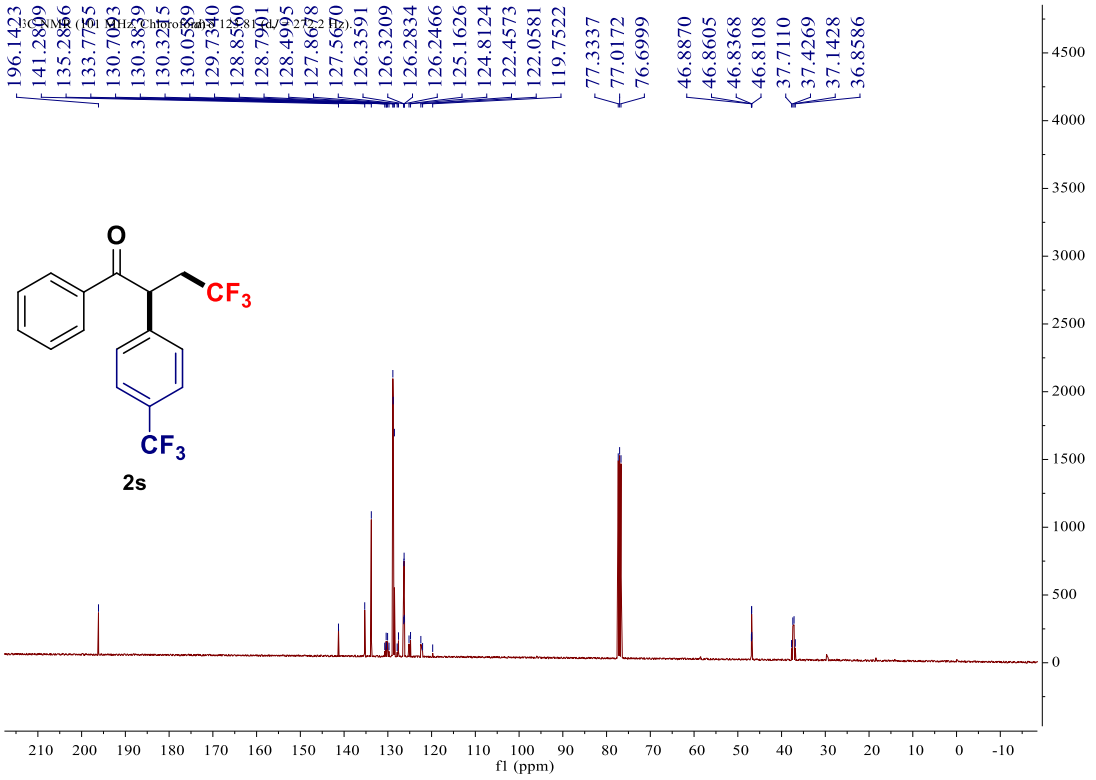
2s
f1 (ppm)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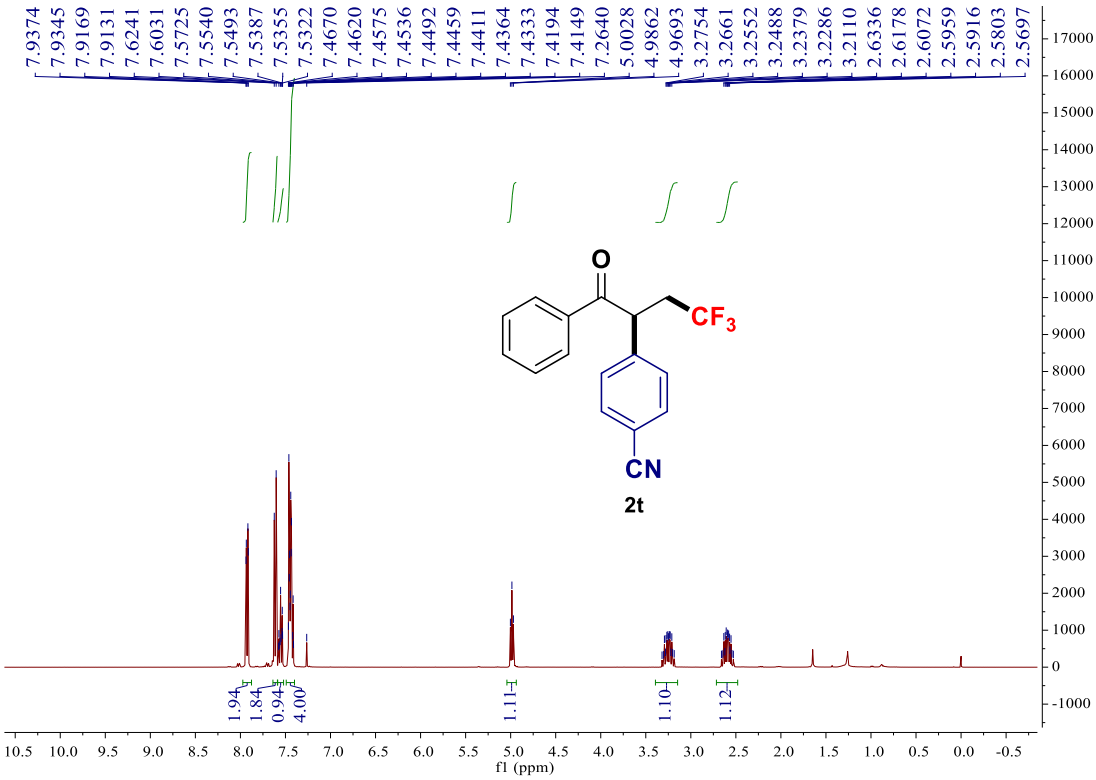
O
CF3
CF3
2s
fl (ppm)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7.5355
7.5322
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7.4620
7.4575
7.4536
7.4492
7.4459
7.4411
7.4364
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5.0028
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3.2661
3.2552
3.2488
3.2379
3.2286
3.2110
2.6336
2.6178
2.6072
2.5959
2.5916
2.5803
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CN
2t
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1.84
0.94
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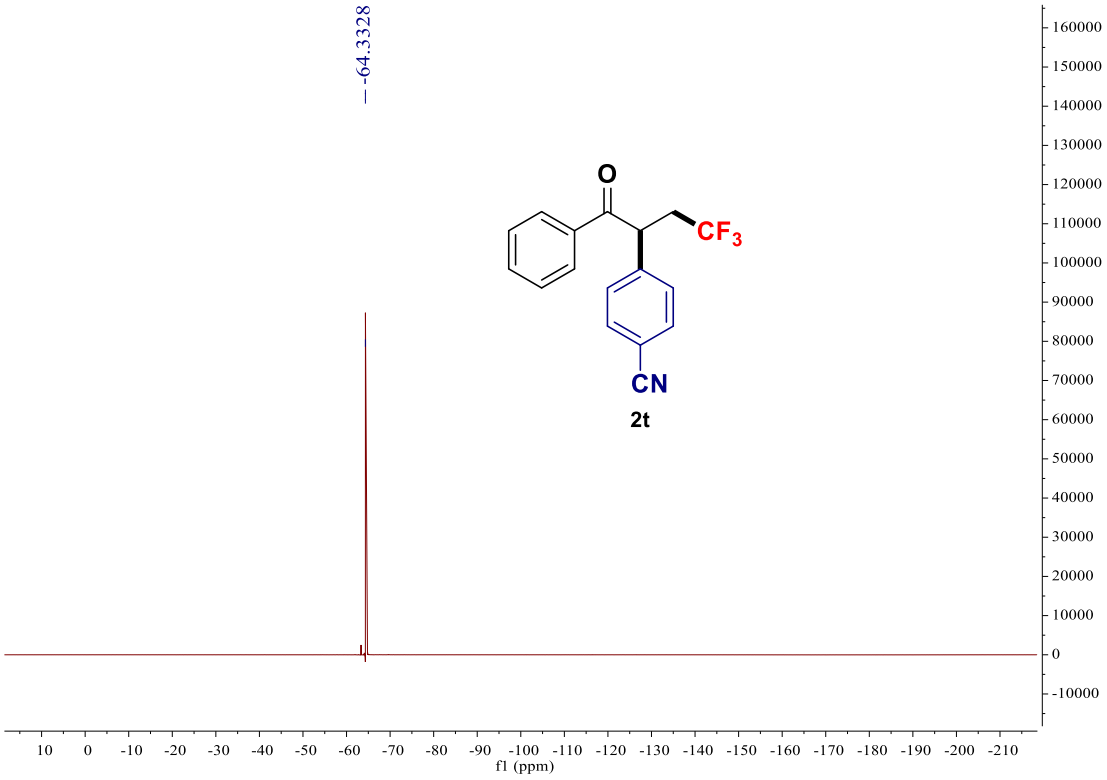
1.11
1.10
1.12
fl (ppm)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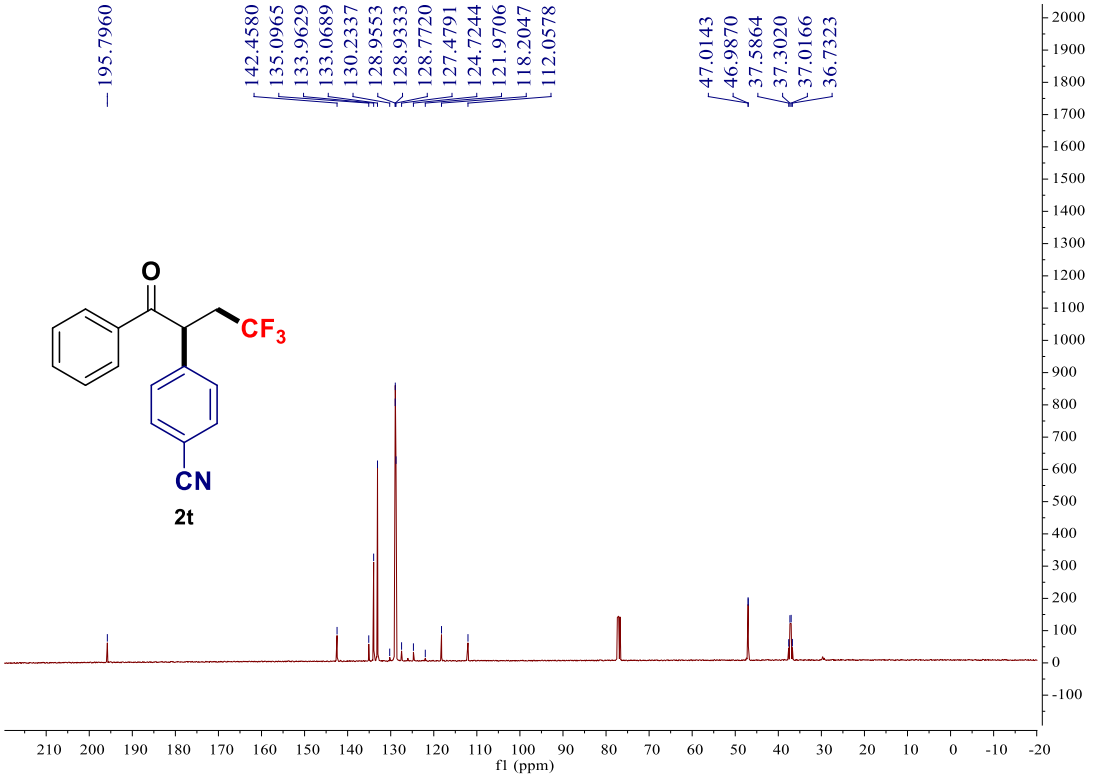
fl (ppm)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118.2047
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47.0143
46.9870
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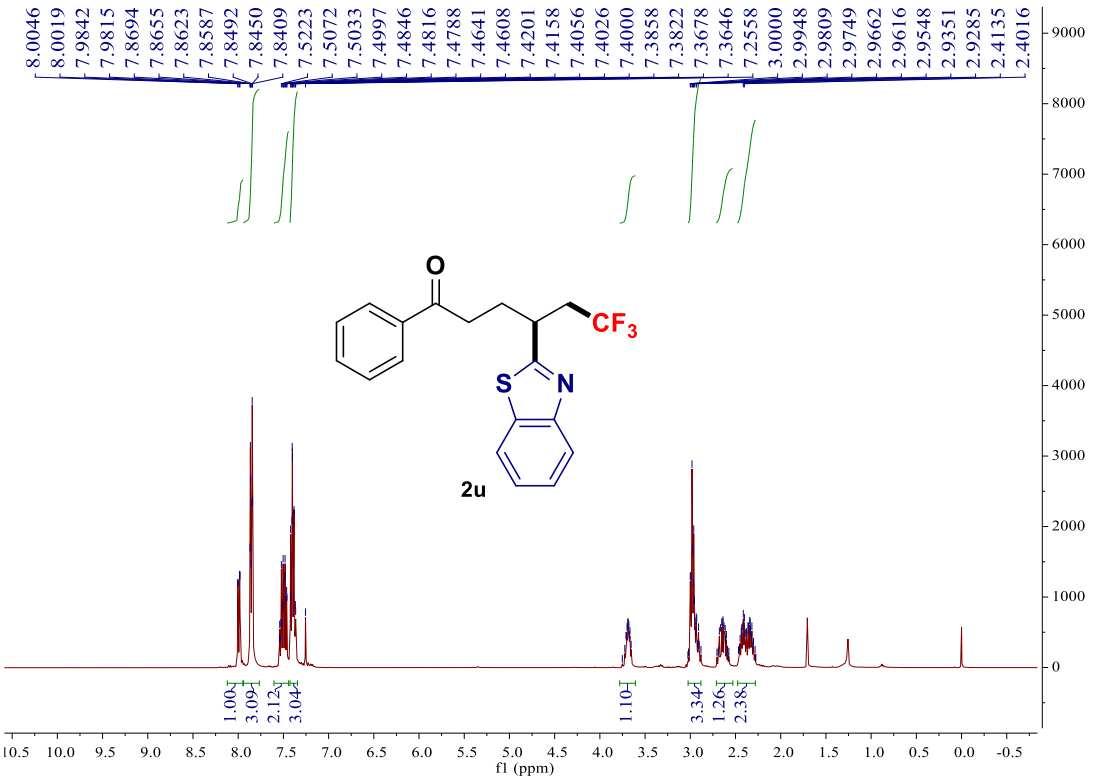
37.3020
37.0166
36.7323
O
CF3
CN
2t
fl (ppm)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7.4846
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7.4026
7.4000
7.3858
7.3822
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7.3646
7.2558
3.0000
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2.9809
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2.9662
2.9616
2.9548
2.9351
2.9285
2.4135
2.4016
O
CF3
S
N
2u
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2.12
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1.10
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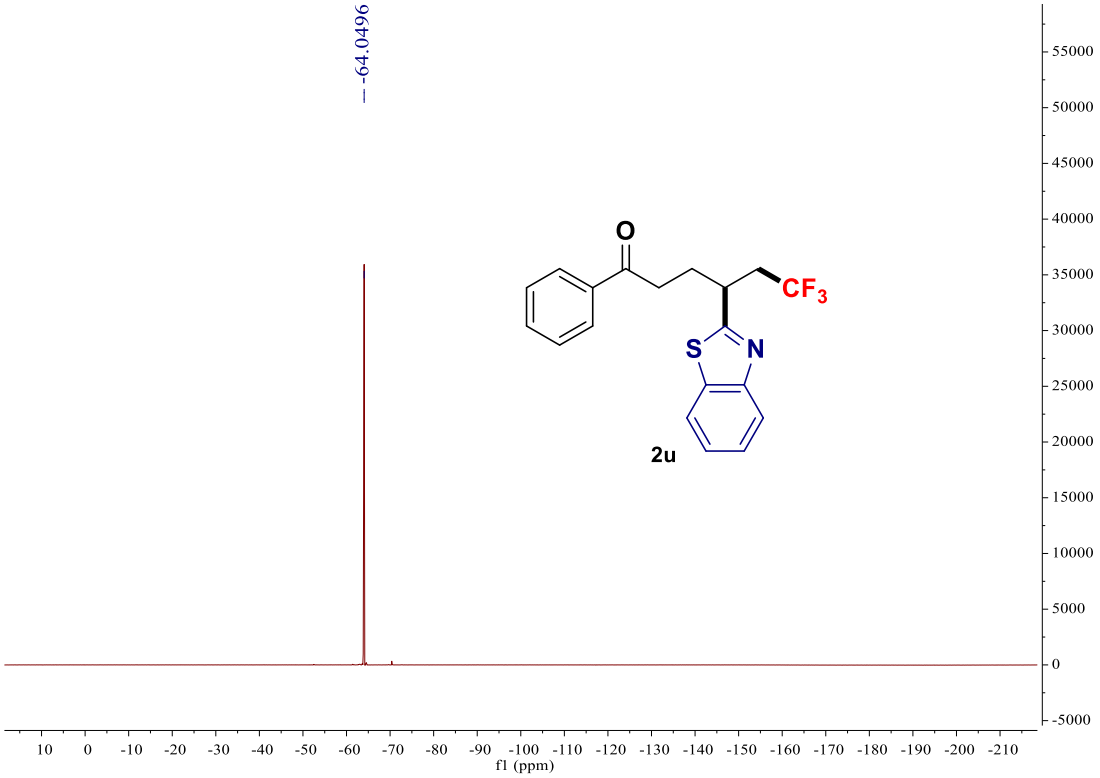
1.26
2.38
f1 (ppm)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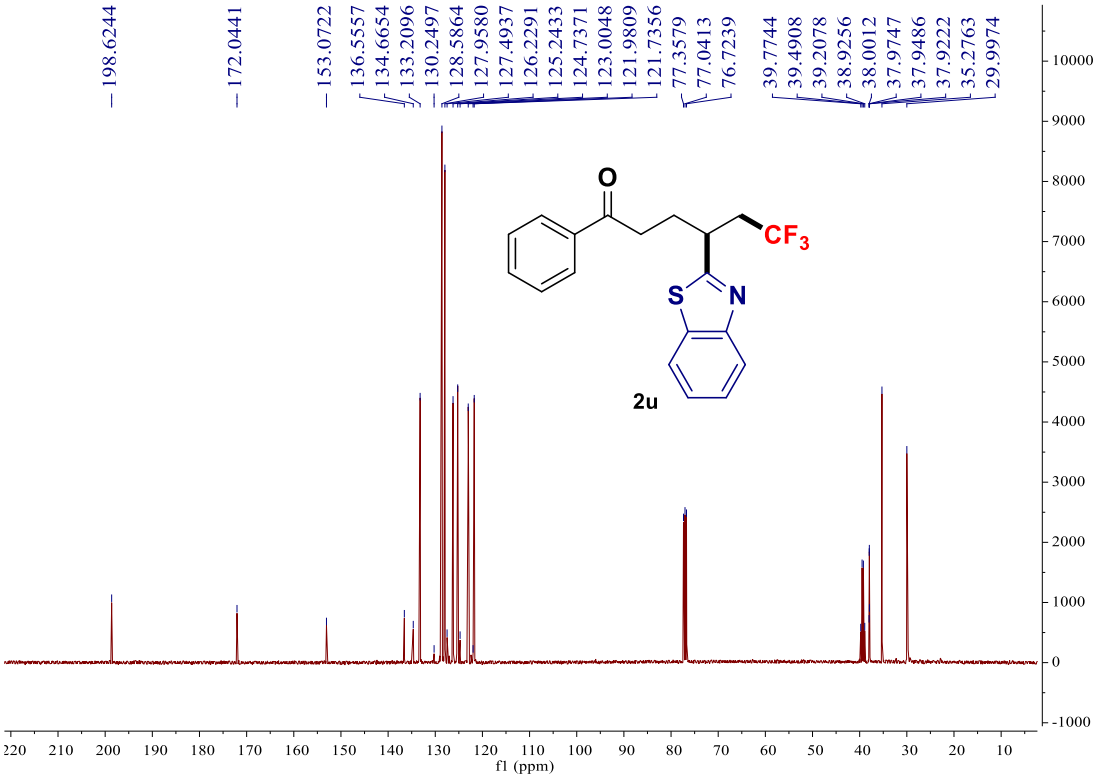
2u
f1 (ppm)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77.0413
76.7239
39.7744
39.4908
39.2078
38.9256
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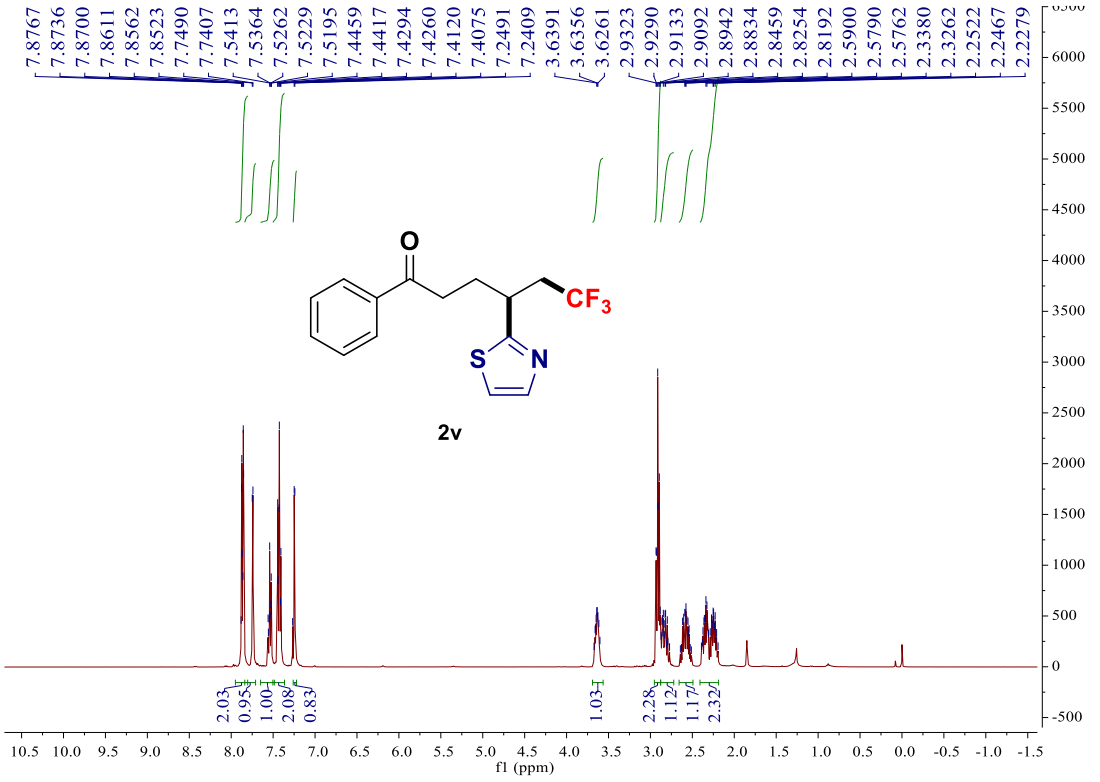
O
CF3
S
N
2u
f1 (ppm)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2.2467
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O
CF3
S
N
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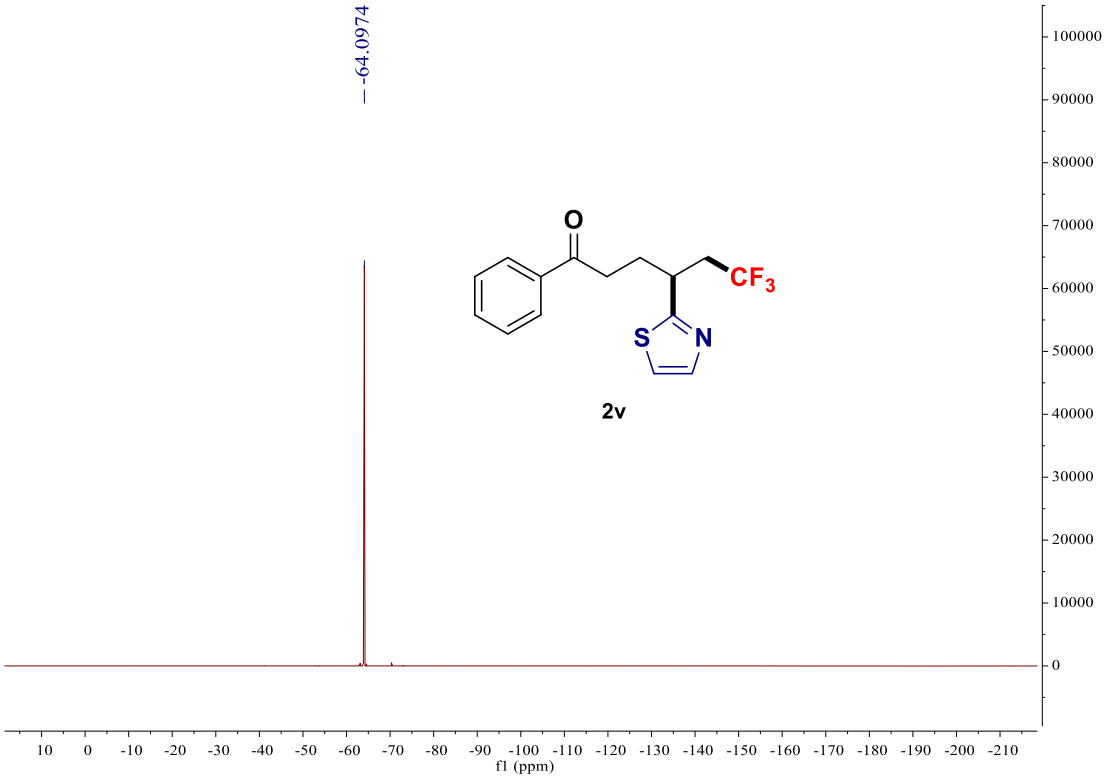
2.32
f1 (ppm)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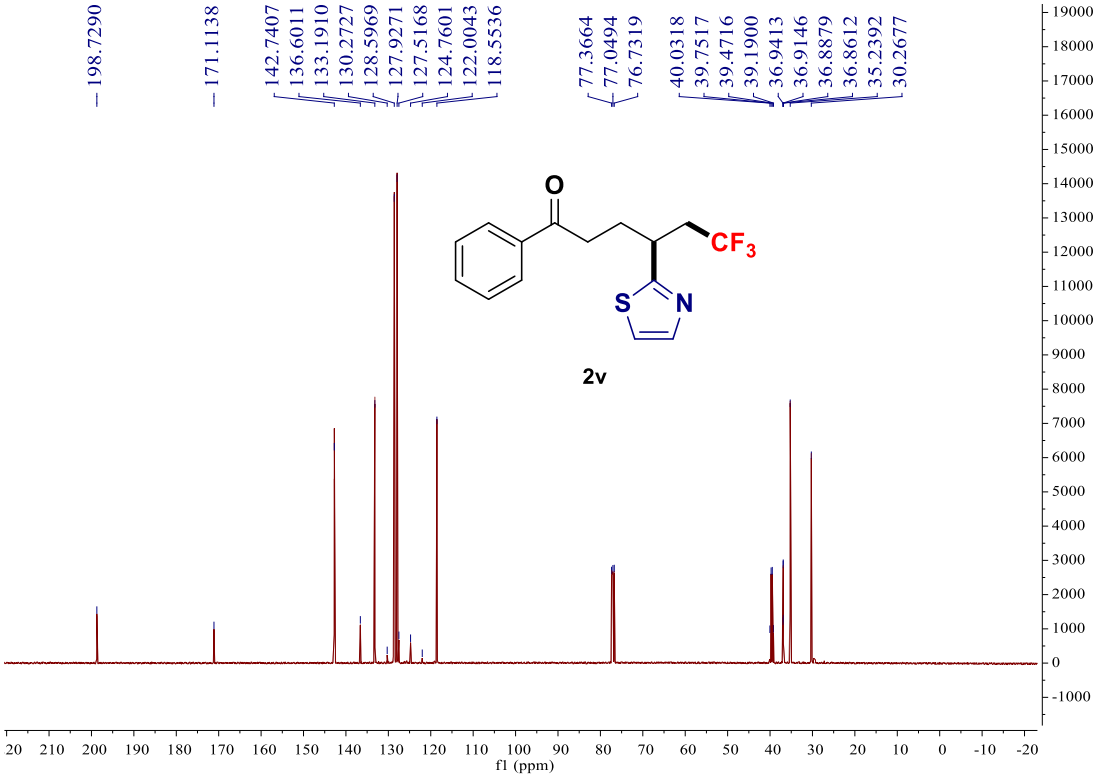
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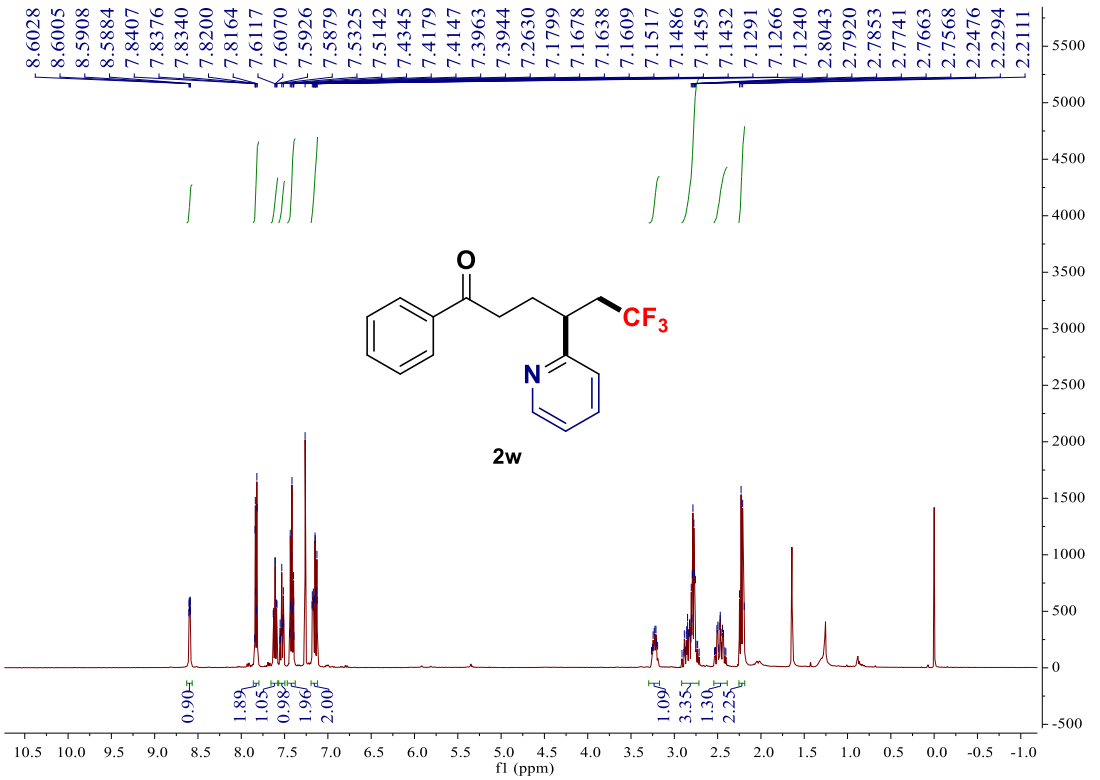
CF3
S
N
2v
f1 (ppm)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7.1609
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CF3
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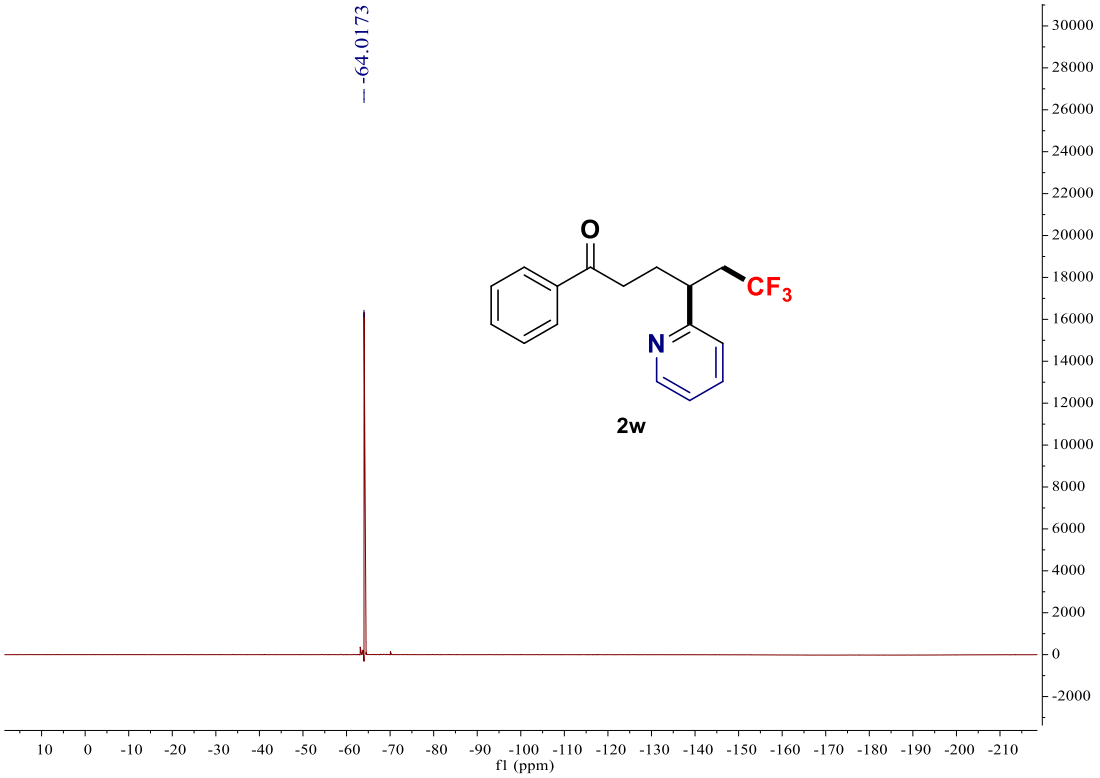
fl (ppm)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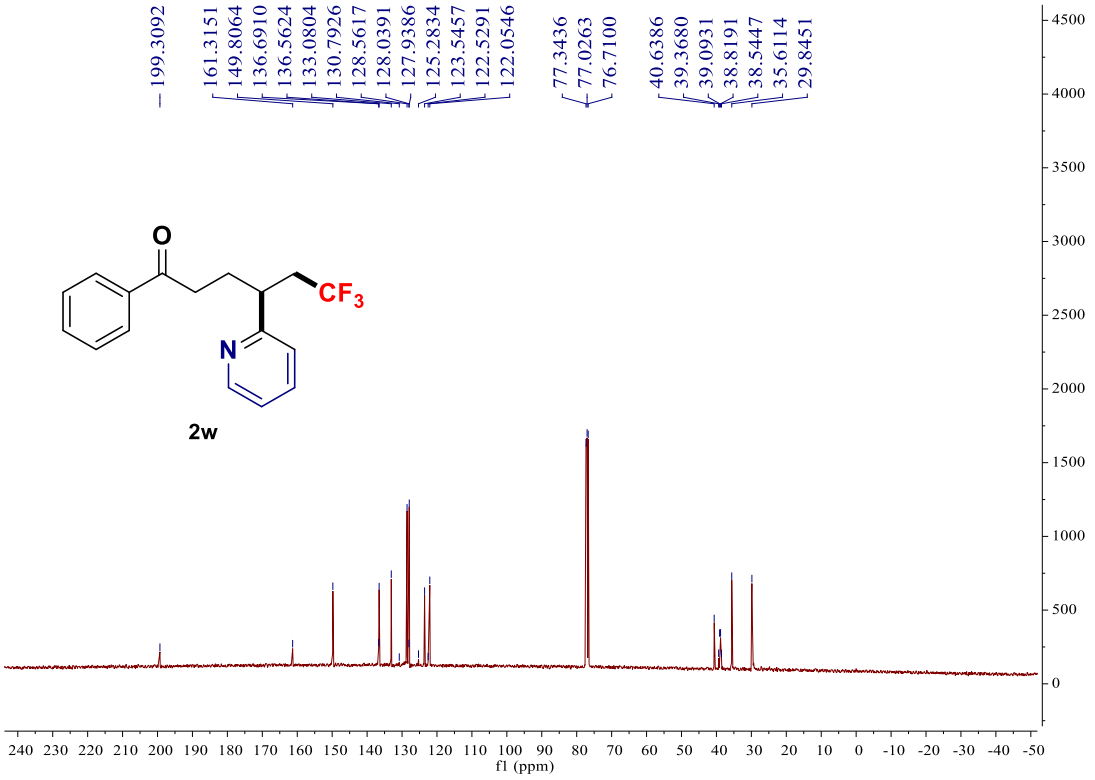
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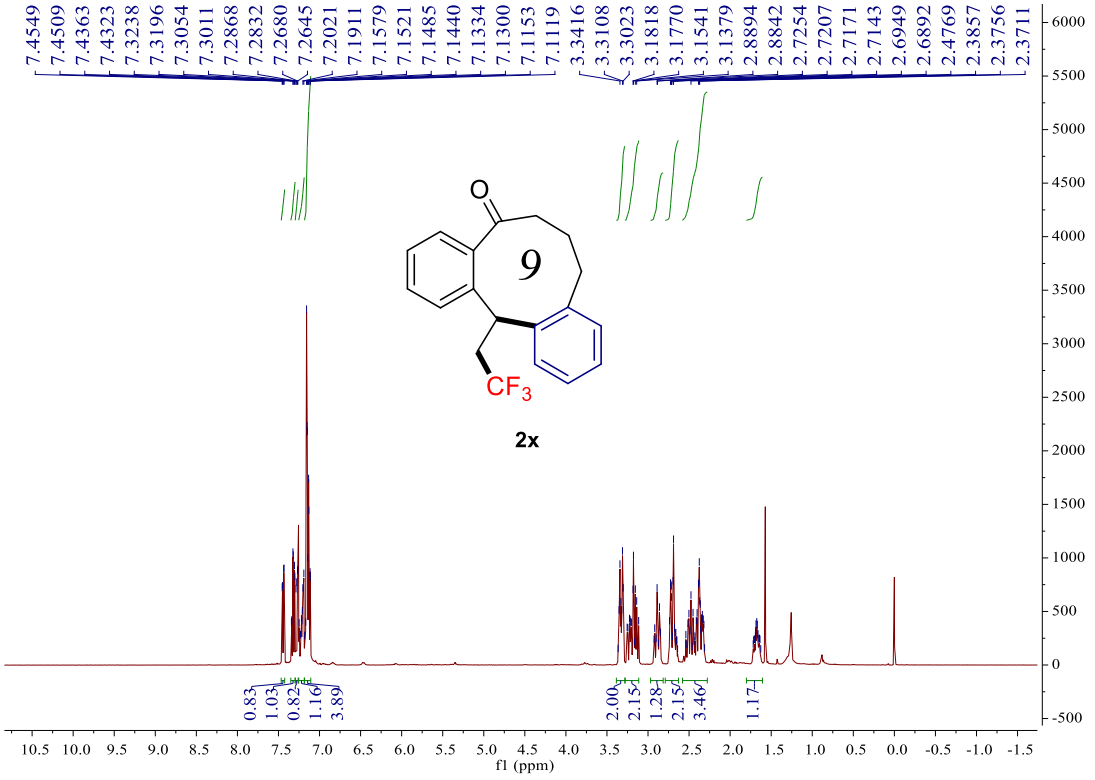
O
CF3
N
2w
f1 (ppm)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7.2645
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7.1911
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7.1521
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7.1300
7.1153
7.1119
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3.3108
3.3023
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2.7171
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2.3857
2.3756
2.3711
O
9
CF3
2x
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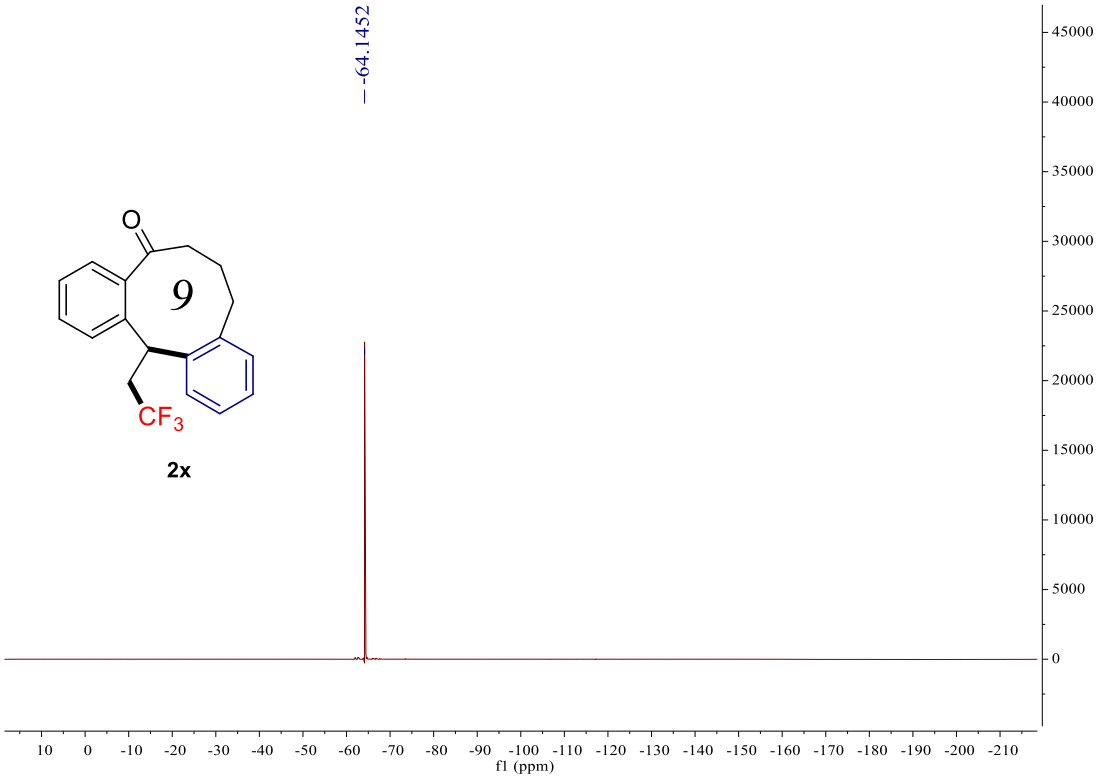
1.28
2.15
3.46
1.17
f1 (ppm)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10000
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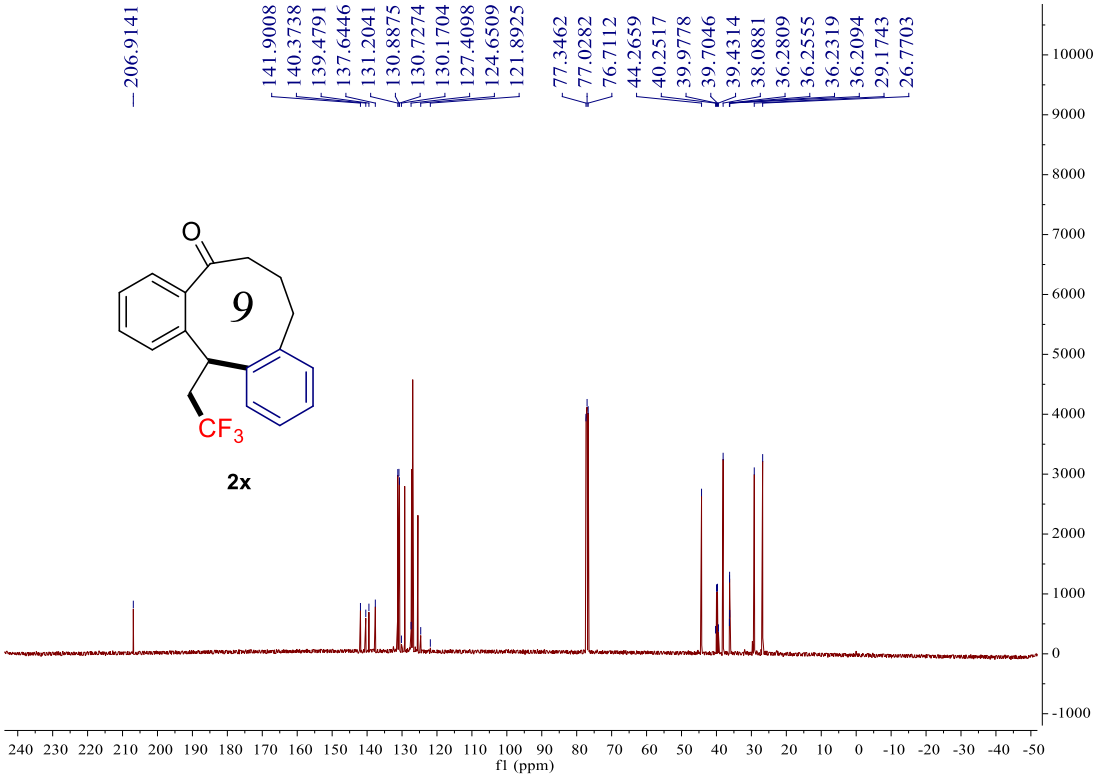
0
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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130.7274
130.1704
127.4098
124.6509
121.8925
77.3462
77.0282
76.7112
44.2659
40.2517
39.9778
39.7046
39.4314
38.0881
36.2809
36.2555
36.2319
36.2094
29.1743
26.7703
O
9
CF3
2x
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50
f1 (ppm)