Electronic Supplementary Material (ESI) for ChemComm.

Pd-Catalyzed Direct C(sp^2)-H Fluorination of Aromatic Ketones: Concise Access to Anacetrapib

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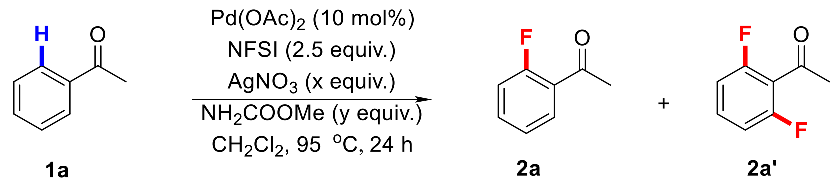
I. General

All experiments were carried out under air atmosphere unless specified noted. The reagents and solvents were purchased from commercial suppliers and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were obtained on Bruker AVANCE III 600/500/400 instrument in $CDCl_3$ using TMS as an internal standard, operating at 600/500/400 MHz and 126/101 MHz, respectively. Chemical shifts (δ) are expressed in ppm and coupling constants J are given in Hz. For $CDCl_3$ solutions the chemical shifts are reported as parts per million (ppm) to residual protium or carbon of the solvents; $CHCl_3$ δH (7.26 ppm) and $CDCl_3$ δC (77.03 ppm); ^{19}F NMR spectra were recorded on a Bruker AVANCE III or Ascend 400. Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet. GC experiments were carried out using Agilent 7890B GC. GC-MS experiments that used dodecane as an internal standard were performed with a Thermo DSQ II, Trace GC Ultra. High resolution mass spectra (HRMS (ESI-TOF)) were obtained on an Agilent 6545 Q-TOF LCMS spectrometer equipped with an ESI source or recorded in the EI mode on Waters GCT Premier TOF MS.

II. Optimization of the fluorination conditions

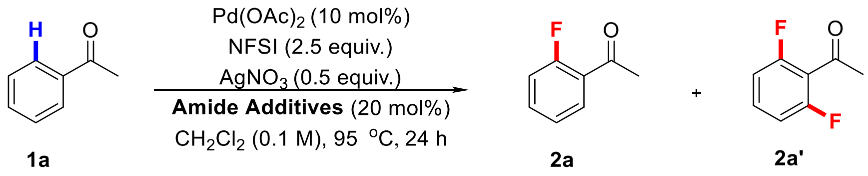
Table S1. Optimizing the additive amount of NH_2COOMe and $AgNO_3$[a]



Entry	AgNO₃ (x)	NH₂COOMe (y)	Yield of 2a [%][b]	Yield of 2a' [%][b]
1	0.3	0.4	34	0
2	0.3	0	15	0
3	0	0.4	14	0
4	0	0	5	0
5	0.3	0.8	38	0
6	0.3	0.2	55	0
7	**0.5**	**0.2**	**85**	**trace**
8	0.5	0.4	44	2
9	0.5	0.8	32	12
10	**0.75**	**0.2**	**83**	**5**
11	0.75	0.4	52	4
12	0.75	0.8	50	2
13	1.0	0.2	69	5
14	1.0	0.4	56	9
15	1.0	0.8	29	31
16[c]	0.75	0.2	82	2
17[d]	0.75	0.2	82	3
18[e]	0.75	0.2	72	0
19[f]	0.75	0.2	77	0
20[g]	0.5	0.2	74	trace

[a]Reaction conditions: **1a** (0.1 mmol), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol), NFSI = N-fluorobenzenesulfonimide (78.8 mg, 0.25 mmol), $AgNO_3$ (x equiv.), NH_2COOMe (y equiv.), CH_2Cl_2 (1.0 mL) at 95 °C for 24 h, under air. [b]GC yield. [c]The reaction time is 12 h. [d]$Pd(OAc)_2$ (3.3 mg, 0.15 mmol). [e]NFSI (63.1 mg, 0.2 mmol). [f]75 °C, 12 h. [g]$AgNO_3$ (0.5 equiv.), 12 h.

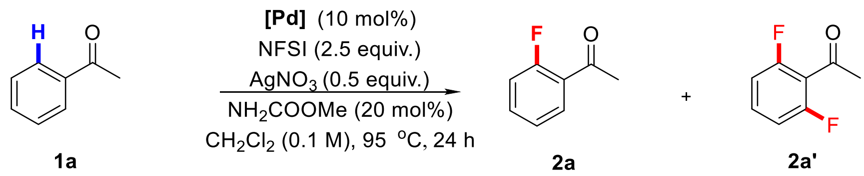
Table S2. Screening of amide additives[a]



Entry	Amide additives (0.2 equiv.)	Yield of 2a [%][b]	Yield of 2a' [%][b]
1	Formamide	0	0
2	Acetamide	25	0
3	Methyl carbamate	85	trace
4	Benzyl carbamate	68	3
5	tert-Butyl carbamate	10	0
6	Trifluoroacetamide	11	0
7	Benzamide	8	0
8	Sulfamic acid	12	0

[a]Reaction conditions: **1a** (0.1 mmol), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol), NFSI = N-fluorobenzenesulfonimide (78.8 mg, 0.25 mmol), $AgNO_3$ (8.5 mg, 0.05 mmol), amide additives (0.02 mmol), CH_2Cl_2 (1.0 mL) at 95 °C for 24 h, under air. [b]GC yield.

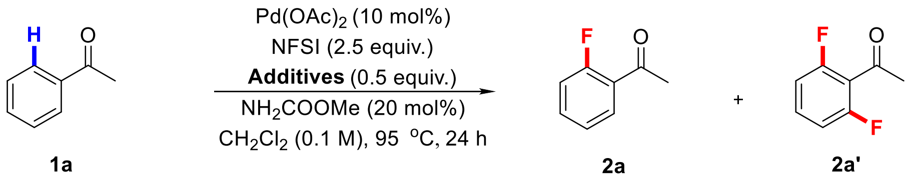
Table S3. Screening of [Pd] catalysts[a]



Entry	[Pd] (10 mol%)	Yield of 2a [%][b]	Yield of 2a' [%][b]
1	-	0	0
2	$Pd(OAc)_2$	85	trace
3	$Pd(dba)_2$	56	6
4	$Pd(TFA)_2$	59	0
5	$[Pd(Cl)(C_3H_5)]_2$	13	0
6	$Pd(PPh_3)_4$	49	0
7	$PdCl_2(cod)$	26	4
8	$PdCl_2$	79	3

[a]Reaction conditions: **1a** (0.1 mmol), [Pd] (2.2 mg, 0.01 mmol), NFSI = N-fluorobenzenesulfonimide (78.8 mg, 0.25 mmol), $AgNO_3$ (8.5 mg, 0.05 mmol), NH_2COOMe (1.5 mg, 0.02 mmol), CH_2Cl_2 (1.0 mL) at 95 °C for 24 h, under air. [b]GC yield.

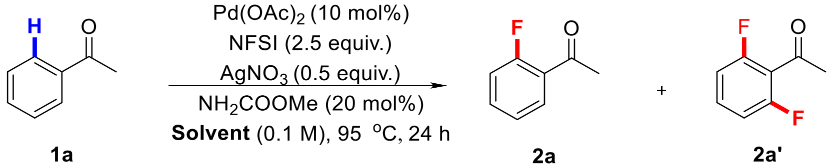
Table S4. Screening of additives[a]



Entry	Additives	Yield of 2a [%][b]	Yield of 2a' [%][b]
1	$AgNO_2$	59	0
2	KNO_3	56	0
3	Ag_2CO_3	12	0
4	$AgNO_3$	85	trace

[a]Reaction conditions: **1a** (0.1 mmol), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol), NFSI = N-fluorobenzenesulfonimide (1 mg, 0.25 mmol), additive (8.5 mg, 0.05 mmol), NH_2COOMe (1.5 mg, 0.02 mmol), CH_2Cl_2 (1.0 mL) at 95 °C for 24 h, under air. [b]GC yield.

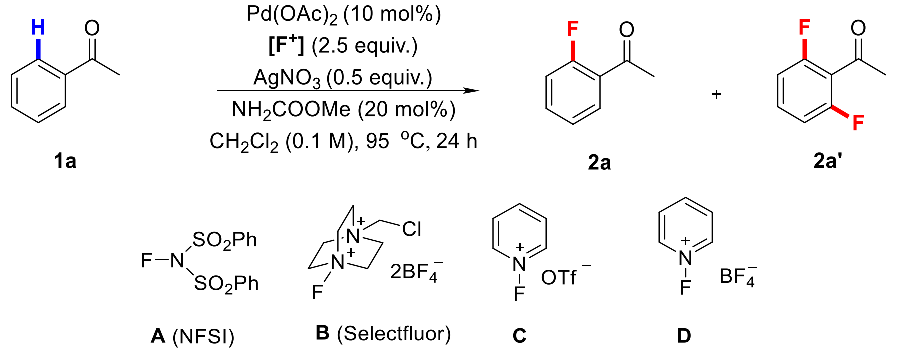
Table S5. Screening of solvents[a]



Entry	Solvents	Yield of 2a [%][b]	Yield of 2a' [%][b]
1	CH_2Cl_2	85	trace
2	DCE	57	2
3	acetone	0	0
4	toluene	3	0
5	DMF	0	0
6	1,4-dioxane	0	0
7	THF	0	0
8	$CHCl_3$	25	0
9	CH_3CN	0	0
10	EtOAc	15	0

[a]Reaction conditions: **1a** (0.1 mmol), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol), NFSI = N-fluorobenzenesulfonimide (78.8 mg, 0.25 mmol), $AgNO_3$ (8.5 mg, 0.05 mmol), NH_2COOMe (1.5 mg, 0.02 mmol), solvent (1.0 mL) at 95 °C for 24 h, under air. [b]GC yield.

Table S6. Screening of fluorination agents [a]



Entry	[F$^+$]	Yield of 2a [%][b]	Yield of 2a' [%][b]
1	A	85	trace
2	B	0	0
3	C	0	0
4	D	0	0

[a]Reaction conditions: **1a** (0.1 mmol), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol), [F$^+$] (0.25 mmol), $AgNO_3$ (8.5 mg, 0.05 mmol), NH_2COOMe (1.5 mg, 0.02 mmol), CH_2Cl_2 (1.0 mL) at 95 °C for 24 h, under air. [b]GC yield.

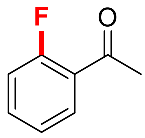
III. General procedure for the substrate scope research

In a 10 mL test tube equipped with a stir bar, substrate (0.2 mmol), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol), NFSI (158.0 mg, 0.5 mmol), $AgNO_3$ (16.9 mg, 0.1 mmol), NH_2COOMe (3.0 mg, 0.04 mmol) and DCM (2.0 mL) were added successively. Then the tube was sealed and stirred at the 95 °C for 24 h. Upon completion, the resulting mixture was cooled to room temperature, diluted with DCM and concentrated under reduced pressure. The residue was purified by silica gel chromatography to afford the desired fluorinated products. (The products of **2a**, **2b**, **2g**, **2j**, **2k**, **2m**, **2n**, **2o**, **2q**, **2r, 2s, 2u** and **2x** require further purification by preparative thin-layer chromatography to afford the desired fluorinated products, and **2aa** should be further purified by recycling preparative HPLC (CH_3CN: H_2O=70: 30, 5.0 mL/min)).

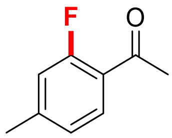
IV. Characterization of fluorination products

1. Characterization of fluorination products

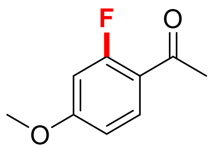
The products **2a**, **2b**, **2c**, **2i**, **2j, 2k**, **2n**, **2o**, **2p**, **2r, 2s, 2v** and **2aa** are known compounds and commercially available. The spectral data of products, **2d**, **2e**, **2h**, **2z** and **2ab** are consistent with those of previous reports.[1-5]



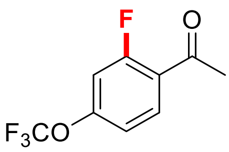
1-(2-fluorophenyl)ethan-1-one (2a): Following the general condition, $AgNO_3$ (0.15 mmol) was added and the reaction time was 12 h; Colorless oil (22.6 mg, 82%); R_f = 0.23 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89 (td, *J* = 7.7, 1.8 Hz, 1H), 7.56-7.51 (m , 1H), 7.26-7.21 (m, 1H), 7.15 (dd, *J* = 11.6, 7.9 Hz, 1H), 2.66 (d, *J* = 4.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.0 (d, *J* = 3.3 Hz), 162.3 (d, *J* = 254.9 Hz), 134.7 (d, *J* = 9.0 Hz), 130.6 (d, *J* = 2.3 Hz), 125.7 (d, *J* = 12.8 Hz), 124.4 (d, *J* = 3.4 Hz), 116.7 (d, *J* = 23.8 Hz), 31.5 (d, *J* = 7.3 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -109.40 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_8H_7FO, 138.0481; found 138.0487.



1-(2-fluoro-4-methylphenyl)ethan-1-one (2b): Following the general condition, $AgNO_3$ (0.15 mmol) was added and the reaction time was 12 h; Colorless oil (27.1 mg, 89%); R_f = 0.33 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 (t, *J* = 8.0 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.95 (d, *J* = 12.2 Hz, 1H), 2.63 (d, *J* = 4.9 Hz, 3H), 2.41 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.6 (d, *J* = 31.25 Hz), 162.32 (d, *J* = 254.7 Hz), 146.4 (d, *J* = 9.1 Hz), 130.4 (d, *J* = 2.8 Hz), 125.2 (d, *J* = 2.8 Hz), 123.0 (d, *J* = 12.8 Hz), 117.0 (d, *J* = 23.7 Hz), 31.4 (d, *J* = 7.5 Hz), 21.4 (d, *J* = 1.2 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -109.98 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_9H_9FO, 152.0637; found 152.0644.

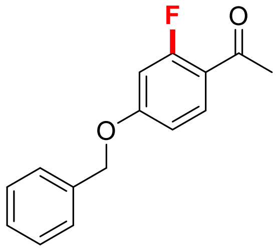


1-(2-fluoro-4-methoxyphenyl)ethan-1-one (2c): Following the general condition, $AgNO_3$ (0.15 mmol) was added; Colorless solid (26.2 mg, 78%); R_f = 0.25 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 (t, *J* = 8.8 Hz, 1H), 6.76 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.63 (dd, *J* = 13.1, 2.4 Hz, 1H), 3.87 (s, 3H), 2.61 (d, *J* = 5.2 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.5 (d, *J* = 4.0 Hz), 164.9 (d, *J* = 1.7 Hz), 163.8 (d, *J* = 245.5 Hz), 132.1 (d, *J* = 4.4 Hz), 118.6 (d, *J* = 12.9 Hz), 110.7 (d, *J* = 2.4 Hz), 101.7 (d, *J* = 27.7 Hz), 55.9, 31.2 (d, *J* = 7.8 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -105.78 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_9H_9FO_2$, 168.0587; found 168.0595.

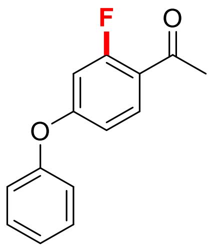


1-(2-fluoro-4-(trifluoromethoxy)phenyl)ethan-1-one (2d): Following the general condition, $AgNO_3$ (0.15 mmol) was added; Colorless solid (26.7 mg, 60%); R_f = 0.42 (petroleum ether-EtOAc = 5:1); **^{1}H**

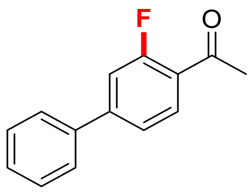
NMR (500 MHz, $CDCl_3$) δ 7.98 (t, *J* = 8.5 Hz, 1H), 7.11 (d, *J* = 7.8 Hz, 1H), 7.04 (d, *J* = 11.2 Hz, 1H), 2.66 (d, *J* = 5.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.2 (d, *J* = 3.9 Hz), 162.5 (d, *J* = 257.1 Hz), 153.1 (dd, *J* = 11.3, 2.0 Hz), 132.5-131.8 (m), 123.9 (d, *J* = 13.1 Hz), 120.2 (q, *J* = 257.1 Hz), 116.3-116.2 (m), 109.0 (d, *J* = 27.4 Hz), 31.4 (d, *J* = 7.4 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -57.81 (s, 3F), -105.08 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_9H_6F_4O_2$, 222.0304; found 222.0315.



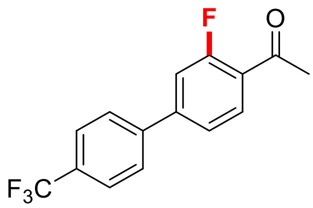
1-(4-(benzyloxy)-2-fluorophenyl)ethan-1-one (2e): Following the general condition, $AgNO_3$ (0.15 mmol) was added; Difluorination product has also been determined by GC-MS (3%); Colorless solid (36.6 mg, 75%); R_f = 0.50 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 (t, *J* = 8.8 Hz, 1H), 7.45-7.40 (m, 4H), 7.39-7.36 (m, 1H), 6.84 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.71 (dd, *J* = 13.0, 2.4 Hz, 1H), 5.13 (s, 2H), 2.61 (d, *J* = 5.1 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.6 (d, *J* = 3.8 Hz), 164.0 (d, *J* = 11.7 Hz), 163.8 (d, *J* = 255.4 Hz), 135.7, 132.2 (d, *J* = 4.3 Hz), 128.8, 128.5, 127.5, 118.9 (d, *J* = 12.9 Hz), 111.4 (d, *J* = 2.7 Hz), 102.7 (d, *J* = 27.7 Hz), 70.6, 31.3 (d, *J* = 7.7 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -105.71 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{15}H_{13}FO_2$, 244.0900; found 244.0907.



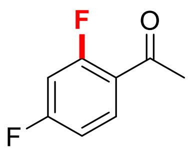
1-(2-fluoro-4-phenoxyphenyl)ethan-1-one (2f): Following the general condition, $AgNO_3$ (0.15 mmol) was added; Difluorination product has also been determined by GC-MS (4%); Colorless solid (23.9 mg, 52%); R_f = 0.29 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (t, *J* = 8.7 Hz, 1H), 7.45-7.39 (m, 2H), 7.26-7.22 (m, 1H), 7.09 (dd, *J* = 8.6, 1.0 Hz, 2H), 6.80 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.65 (dd, *J* = 12.6, 2.3 Hz, 1H), 2.60 (d, *J* = 5.1 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.5 (d, *J* = 3.8 Hz), 163.6 (d, *J* = 256.0 Hz), 163.4 (d, *J* = 11.5 Hz), 154.8, 132.3 (d, *J* = 4.1 Hz), 130.3, 125.3, 120.6, 120.1 (d, *J* = 13.0 Hz), 113.4 (d, *J* = 2.8 Hz), 105.1 (d, *J* = 27.8 Hz), 31.3 (d, *J* = 7.6 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -105.54 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{14}H_{11}FO_2$, 230.0743; found 230.0748.



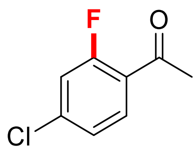
1-(3-fluoro-[1,1'-biphenyl]-4-yl)ethan-1-one (2g): Difluorination product has also been determined by GC-MS (14%); Colorless solid (39.5 mg, 82%); R_f = 0.40 (petroleum ether-EtOAc = 10:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (t, *J* = 8.0 Hz, 1H), 7.65-7.61 (m, 2H), 7.52-7.43 (m, 4H), 7.38 (dd, *J* = 12.4, 1.7 Hz, 1H), 2.70 (d, *J* = 4.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.4 (d, *J* = 3.5 Hz), 162.6 (d, *J* = 254.8 Hz), 148.0 (d, *J* = 8.8 Hz), 138.6, 131.1 (d, *J* = 3.1 Hz), 129.0, 128.8, 127.1, 124.1 (d, *J* = 13.1 Hz), 122.9 (d, *J* = 2.9 Hz), 114.9 (d, *J* = 24.9 Hz), 31.4 (d, *J* = 7.4 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -108.93 (s, 1F); **HRMS** (EI): $[M^+]$ calcd. for $C_{14}H_{11}FO$, 214.0794; found 214.0804. (*It contains minor di-fluorination product, which was difficult to be separated from the mono-fluorination product.*)



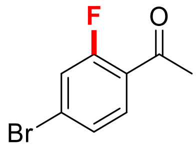
1-(3-fluoro-4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)ethan-1-one (2h): Difluorination product has also been determined by GC-MS (6%); Colorless solid (42.9 mg, 76%); R_f = 0.52 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 (t, *J* = 7.9 Hz, 1H), 7.78-7.70 (m, 4H), 7.48 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.39 (dd, *J* = 12.1, 1.6 Hz, 1H), 2.70 (d, *J* = 4.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.3 (d, *J* = 3.5 Hz), 162.5 (d, *J* = 255.4 Hz), 146.3 (d, *J* = 8.7 Hz), 142.1, 131.4 (d, *J* = 3.0 Hz), 130.8 (q, *J* = 32.6 Hz), 127.6, 126.0 (q, *J* = 3.7 Hz), 124.9 (d, *J* = 13.1 Hz), 123.1 (d, *J* = 3.1 Hz), 115.3 (d, *J* = 25.2 Hz), 111.0 (d, *J* = 26.8 Hz), 31.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.65 (s, 3F), -108.54 (s, 1F); **HRMS** (EI): $[M^+]$ calcd. for $C_{15}H_{10}F_4O$, 282.0668; found 282.0664. (*It contains a minor di-fluorination product, which was difficult to be separated from the mono-fluorination product.*)



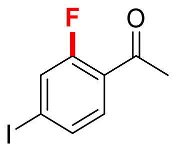
1-(2,4-difluorophenyl)ethan-1-one (2i): Colorless solid (21.2 mg, 68%); R_f = 0.18 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.96 (td, *J* = 8.7, 6.7 Hz, 1H), 7.01-6.93 (m, 1H), 6.92-6.86 (m, 1H), 2.64 (d, *J* = 5.2 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.3 (d, *J* = 3.7 Hz),167.0-164.8 (m), 164.1-161.9 (m), 132.6 (dd, *J* = 10.6, 4.0 Hz), 122.3 (d, *J* = 3.4 Hz), 112.2 (dd, *J* = 21.4, 3.4 Hz), 104.7 (dd, *J* = 27.7, 25.4 Hz), 31.3 (d, *J* = 7.5 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -101.90 (s, 1F), -104.44 (s, 1F); **HRMS** (EI): $[M^+]$ calcd. for $C_8H_6F_2O$, 156.0387; found 156.0391.



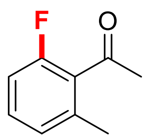
1-(4-chloro-2-fluorophenyl)ethan-1-one (2j): Difluorination product has also been determined by GC-MS (3%); Yellow solid (23.0 mg, 67%); R_f = 0.29 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (t, *J* = 8.2 Hz, 1H), 7.26-7.15 (m, 2H), 2.64 (d, *J* = 5.1 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.5, 162.0 (d, *J* = 258.3 Hz), 140.2 (d, *J* = 10.6 Hz), 131.7 (d, *J* = 3.4 Hz), 125.9 (d, *J* = 3.4 Hz), 124.1 (d, *J* = 13.0 Hz), 117.4 (d, *J* = 27.5 Hz), 31.4 (d, *J* = 7.4 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -107.0 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_8H_6ClFO, 172.0091; found 172.0100.



1-(4-bromo-2-fluorophenyl)ethan-1-one (2k): Colorless oil (29.8 mg, 69%); R_f = 0.49 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (t, *J* = 8.2 Hz, 1H), 7.43-7.31 (m, 2H), 2.64 (d, *J* = 5.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.7 (d, *J* = 3.6 Hz), 161.8 (d, *J* = 259.2 Hz), 131.8 (d, *J* = 3.1 Hz), 128.2 (d, *J* = 9.8 Hz), 128.0 (d, *J* = 3.5 Hz), 124.6 (d, *J* = 12.9 Hz), 120.3 (d, *J* = 27.2 Hz), 31.4 (d, *J* = 7.4 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -107.15 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_8H_6BrFO, 215.9586; found 230.9595.

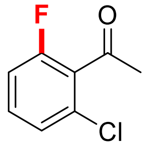


1-(2-fluoro-4-iodophenyl)ethan-1-one (2l): Difluorination product has also been determined by GC-MS (5%); Colorless solid (39.6 mg, 75%); R_f = 0.46 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (t, *J* = 8.2 Hz, 1H), 7.26-7.16 (m, 2H), 2.64 (d, *J* = 5.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.5 (d, *J* = 3.6 Hz), 162.1 (d, *J* = 261.25 Hz), 140.2 (d, *J* = 10.6 Hz), 131.7 (d, *J* = 3.4 Hz), 125.1 (d, *J* = 3.4 Hz), 124.1 (d, *J* = 12.5 Hz), 117.4 (d, *J* = 27.4 Hz), 31.4 (d, *J* = 7.4 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -107.51 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_8H_6FIO, 263.9447; found 263.9436.

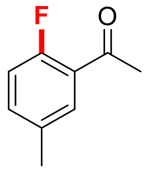


1-(2-fluoro-6-methylphenyl)ethan-1-one (2m): Following the general condition, $AgNO_3$ (0.15 mmol) was added and the reaction time was 12 h; Colorless oil (24.3 mg, 80%); R_f = 0.33 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.27 (td, *J* = 8.1, 6.0 Hz, 1H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.94 (t, 1H), 2.57 (d, *J* = 3.0 Hz, 3H), 2.35 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 201.2, 160.2

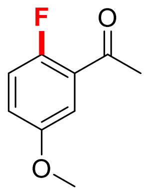
(d, J = 247.2 Hz), 138.1 (d, J = 3.5 Hz), 131.0 (d, J = 9.3 Hz), 128.6 (d, J = 16.2 Hz), 126.7 (d, J = 2.8 Hz), 113.2 (d, J = 22.6 Hz), 32.5 (d, J = 4.4 Hz), 19.6 (d, J = 2.3 Hz); ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -114.78 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_9H_9FO, 152.0637; found 152.0646.



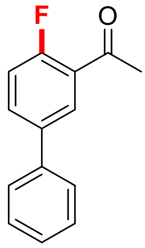
1-(2-chloro-6-fluorophenyl)ethan-1-one (2n): Colorless oil (21.3 mg, 62%); R_f = 0.42 (petroleum ether-EtOAc = 20:1); ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.32 (td, J = 8.2, 6.1 Hz, 1H), 7.22 (d, J = 8.1 Hz, 1H), 7.07 -7.02 (m, 1H), 2.59 (d, J = 1.2 Hz, 3H); ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 197.7, 159.1 (d, J = 250.5 Hz), 131.1 (d, J = 9.2 Hz), 130.8 (d, J = 6.0 Hz), 129.3 (d, J = 21.5 Hz), 125.8 (d, J = 3.4 Hz), 114.5 (d, J = 21.9 Hz), 32.0 (d, J = 1.5 Hz); ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -114.05 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_8H_6ClFO, 172.0091; found 172.0101.



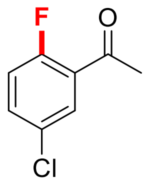
1-(2-fluoro-5-methylphenyl)ethan-1-one (2o): Following the general condition, $AgNO_3$ (0.15 mmol) was added and the reaction time was 12 h; Colorless oil (26.8 mg, 88%); R_f = 0.42 (petroleum ether-EtOAc = 20:1); ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.66 (dd, J = 7.1, 2.0 Hz, 1H), 7.33-7.21 (m, 1H), 7.02 (dd, J = 10.9, 8.4 Hz, 1H), 2.64 (d, J = 4.9 Hz, 3H), 2.35 (s, 3H); ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 196.2 (d, J = 3.4 Hz), 160.6 (d, J = 252.3 Hz), 135.2 (d, J = 8.7 Hz), 133.9 (d, J = 3.4 Hz), 130.5 (d, J = 2.3 Hz), 125.2 (d, J = 12.9 Hz), 116.4 (d, J = 24.0 Hz), 53.4, 31.4 (d, J = 7.5 Hz); ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -114.55 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_9H_9FO, 152.0637; found 152.0642.



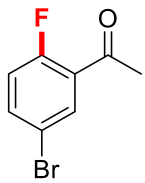
1-(2-fluoro-5-methoxyphenyl)ethan-1-one (2p): Following the general condition, $AgNO_3$ (0.15 mmol) was added; Colorless solid (17.8 mg, 53%); R_f = 0.31 (petroleum ether-EtOAc = 20:1); ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.36-7.34 (m, 2.1 Hz, 1H), 7.07 (d, J = 2.6 Hz, 1H), 7.06 (d, J = 1.8 Hz, 1H), 3.83 (s, 3H), 2.65 (d, J = 5.2 Hz, 3H); ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 195.7 (d, J = 3.8 Hz), 156.9 (d, J = 247.9 Hz), 155.7 (d, J = 1.7 Hz), 125.7 (d, J = 14.5 Hz), 121.7 (d, J = 8.7 Hz), 117.6 (d, J = 26.3 Hz), 112.7 (d, J = 2.6 Hz), 55.9, 31.4 (d, J = 8.1 Hz); ^{19}**F NMR** (471 MHz, $CDCl_3$) δ -119.42 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_9H_9FO_2$, 168.0587; found 168.0593.



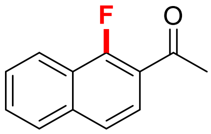
1-(4-fluoro-[1,1'-biphenyl]-3-yl)ethan-1-one (2q): Difluorination product has also been determined by GC-MS (4%); Colorless solid (32.5 mg, 76%); R_f = 0.41 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (dd, *J* = 7.0, 2.5 Hz, 1H), 7.77-7.73 (m, 1H), 7.59 (d, *J* = 7.2 Hz, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.4 Hz, 1H), 7.23 (dd, *J* = 10.7, 8.6 Hz, 1H), 2.71 (d, *J* = 5.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.9 (d, *J* = 3.5 Hz), 161.8 (d, *J* = 255.3 Hz), 139.1, 137.7 (d, *J* = 3.4 Hz), 133.1 (d, *J* = 9.0 Hz), 129.0 (d, *J* = 2.6 Hz), 128.9, 127.8, 127.0, 125.7 (d, *J* = 13.3 Hz), 117.1 (d, *J* = 24.3 Hz), 31.2 (d, *J* = 7.5 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -112.19 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{14}H_{11}FO$, 214.0794; found 214.0802.



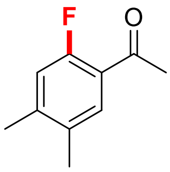
1-(5-chloro-2-fluorophenyl)ethan-1-one (2r): Colorless oil (24.1 mg, 70%); R_f = 0.33 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 6.2, 2.8 Hz, 1H), 7.50-7.47 (m,1H), 7.12 (dd, *J* = 10.2, 8.8 Hz, 1H), 2.65 (d, *J* = 5.0 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.5, 160.6 (d, *J* = 254.7 Hz), 134.4 (d, *J* = 9.2 Hz), 130.2 (d, *J* = 2.8 Hz), 130.0 (d, *J* = 3.2 Hz), 126.7 (d, *J* = 14.7 Hz), 118.3 (d, *J* = 26.0 Hz), 31.3 (d, *J* = 7.5 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -112.30 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_8H_6ClFO, 172.0091; found 172.0092.



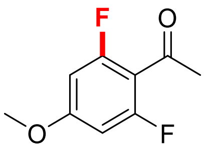
1-(5-bromo-2-fluorophenyl)ethan-1-one (2s): Colorless solid (26.4 mg, 61%); R_f = 0.42 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 6.4, 2.6 Hz, 1H), 7.63-7.60 (m, 1H), 7.06 (dd, *J* = 10.4, 8.7 Hz, 1H), 2.64 (d, *J* = 4.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.4 (d, *J* = 3.7 Hz), 161.2 (d, *J* = 255.2 Hz), 137.3 (d, *J* = 9.1 Hz), 133.3 (d, *J* = 2.4 Hz), 127.1 (d, *J* = 14.4 Hz), 118.7 (d, *J* = 25.5 Hz), 117.3 (d, *J* = 3.0 Hz), 31.3 (d, *J* = 7.5 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -111.78 (s, 1F); **HRMS** (EI): [M^+] calcd. for C_8H_6BrFO, 215.9586; found 215.9592.



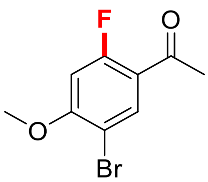
1-(1-fluoronaphthalen-2-yl)ethan-1-one (2t): Difluorination product has also been determined by GC-MS (6%); Colorless solid (30.5 mg, 81%); R_f = 0.31 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 7.4 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.64-7.58 (m, 1H), 7.56-7.49 (m, 2H), 2.75 (d, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.2 (d, *J* = 3.6 Hz), 158.8 (d, *J* = 251.7 Hz), 136.2 (d, *J* = 9.6 Hz), 132.6 (d, *J* = 3.7 Hz), 129.7, 129.7, 129.2, 126.9 (d, *J* = 5.1 Hz), 126.3, 126.1 (d, *J* = 2.5 Hz), 112.5 (d, *J* = 23.1 Hz), 31.4 (d, *J* = 7.3 Hz); **^{19}F NMR** (471 MHz, $CDCl_3$) δ -114.96 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{12}H_9FO$, 188.0637; found 188.0644.



1-(2-fluoro-4,5-dimethylphenyl)ethan-1-one (2u): Colorless oil (30.2 mg, 91%); R_f = 0.33 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.7 Hz, 1H), 6.91 (d, *J* = 11.8 Hz, 1H), 2.61 (d, *J* = 4.9 Hz, 3H), 2.29 (s, 3H), 2.25 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.8 (d, *J* = 3.6 Hz), 160.6 (d, *J* = 252.6 Hz), 144.8 (d, *J* = 8.7 Hz), 132.7 (d, *J* = 3.0 Hz), 130.9 (d, *J* = 2.5 Hz), 122.8 (d, *J* = 12.4 Hz), 117.3 (d, *J* = 23.8 Hz), 31.4 (d, *J* = 7.5 Hz), 20.0, 18.8; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -114.20 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{10}H_{11}FO$, 166.0794; found 166.0803.

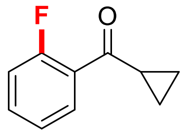


1-(2,6-difluoro-4-methoxyphenyl)ethan-1-one (2v): Colorless solid (34.6 mg, 93%); R_f = 0.41 (petroleum ether-EtOAc = 10:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.51-6.43 (m, 2H), 3.84 (s, 3H), 2.57 (t, *J* = 2.3 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.7, 163.4-163.1 (m), 162.2 (d, *J* = 254.6 Hz), 162.1 (d, *J* = 254.6 Hz), 111.0-110.7 (m), 98.6 (d, *J* = 18.3), 98.6 (dd, *J* = 28.7, 1.5 Hz), 56.0, 32.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -109.05 (s, 2F); **HRMS** (EI): [M^+] calcd. for $C_9H_8F_2O_2$, 186.0492; found 186.0498.

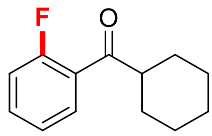


1-(5-bromo-2-fluoro-4-methoxyphenyl)ethan-1-one (2w): Colorless solid (38.4 mg, 78%); R_f = 0.50 (petroleum ether-EtOAc = 10:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 7.9 Hz, 1H), 6.65 (d, *J* = 12.5 Hz, 1H), 3.96 (s, 3H), 2.60 (d, *J* = 5.2 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.2 (d, *J* = 4.1

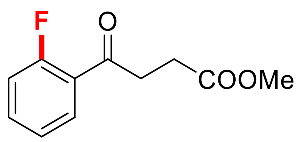
Hz), 162.8 (d, J = 256.1 Hz), 160.6 (d, J = 10.9 Hz), 134.7 (d, J = 4.1 Hz), 119.1 (d, J = 14.0 Hz), 107.1 (d, J = 2.9 Hz), 100.3 (d, J = 29.8 Hz), 56.9, 31.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -105.92 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_9H_8BrFO_2$, 245.9692; found 245.9695.



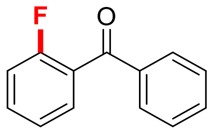
cyclopropyl(2-fluorophenyl)methanone (2x): Colorless oil (28.9 mg, 88%); R_f = 0.40 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (td, J = 7.6, 1.8 Hz, 1H), 7.53-7.49 (m, 1.8 Hz, 1H), 7.23 (td, J = 7.7, 0.9 Hz, 1H), 7.19-7.14 (m, 1H), 2.70-2.65 (m, 1H), 1.30 (q, J = 3.8 Hz, 2H), 1.10-1.06 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.7 (d, J = 3.2 Hz), 161.7 (d, J = 253.8 Hz), 133.9 (d, J = 8.8 Hz), 130.3 (d, J = 2.7 Hz), 127.2 (d, J = 12.8 Hz), 124.3 (d, J = 3.5 Hz), 116.6 (d, J = 23.4 Hz), 21.4 (d, J = 8.8 Hz), 12.5; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -111.50 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{10}H_9FO$, 164.0637; found 164.0647.



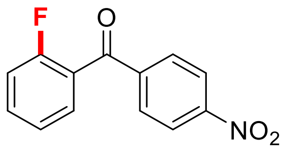
cyclohexyl(2-fluorophenyl)methanone (2y): Difluorination product has also been determined by GC-MS (5%); Colorless solid (31.7 mg, 77%); R_f = 0.47 (petroleum ether-EtOAc = 20:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 (td, J = 7.6, 1.8 Hz, 1H), 7.51-7.47 (m, 1H), 7.22 (td, J = 7.7, 1.0 Hz, 1H), 7.14-7.10 (m, 1H), 3.22-3.07 (m, 1H), 1.95 (d, J = 12.0 Hz, 2H), 1.84-1.80 (m, 2H), 1.76-1.68 (m, 1H), 1.42-1.37 (m, 2H), 1.37-1.32 (m, 1H), 1.31-1.21 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 202.9 (d, J = 4.1 Hz), 161.1 (d, J = 253.0 Hz), 133.8 (d, J = 8.9 Hz), 130.8 (d, J = 3.0 Hz), 126.1 (d, J = 13.7 Hz), 124.5 (d, J = 3.4 Hz), 116.5 (d, J = 23.9 Hz), 50.1 (d, J = 6.1 Hz), 28.8, 26.0, 25.8; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -111.70 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{13}H_{15}FO$, 206.1107; found 206.1102. (*It contains a minor di-fluorination product, which was difficult to be separated from the mono-fluorination product.*)



methyl 4-(2-fluorophenyl)-4-oxobutanoate (2z): Following the general condition, $AgNO_3$ (0.15 mmol) was added; Colorless oil (27.7 mg, 66%); R_f = 0.28 (petroleum ether-EtOAc = 10:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 (td, J = 7.6, 1.8 Hz, 1H), 7.58-7.50 (m, 1H), 7.24 (t, J = 7.6 Hz, 1H), 7.15 (dd, J = 10.9, 8.7 Hz, 3H), 3.71 (s, 3H), 3.35-3.30 (m, 2H), 2.76 (t, J = 6.5 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.3 (d, J = 4.1 Hz), 173.2, 162.2 (d, J = 254.9 Hz), 134.7 (d, J = 9.0 Hz), 130.7 (d, J = 2.6 Hz), 125.1 (d, J = 13.0 Hz), 124.5 (d, J = 3.4 Hz), 116.7 (d, J = 23.9 Hz), 51.8, 38.3, 28.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -108.90 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{11}H_{11}FO_3$, 210.0692; found 210.0701.

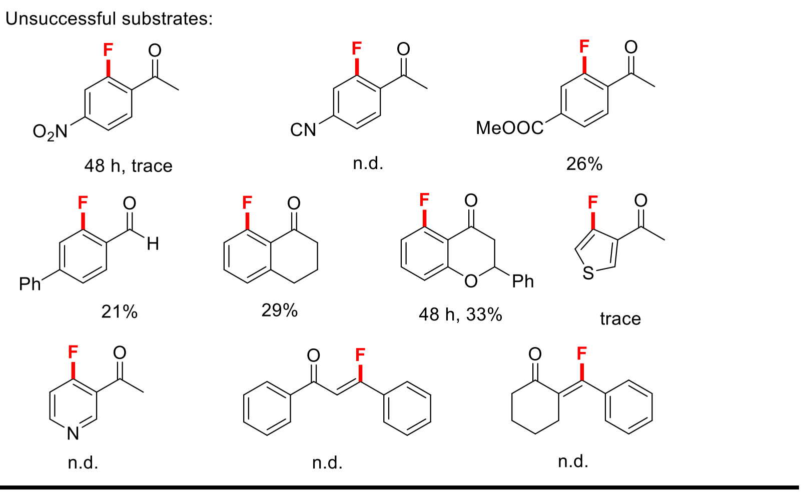


(2-fluorophenyl)(phenyl)methanone (2aa): Following the general condition, $AgNO_3$ (0.15 mmol) was added and the reaction time was 12 h; Difluorination product has also been determined by GC-MS (8%); Colorless solid (30.0 mg, 75%); R_f = 0.58 (petroleum ether-EtOAc = 10:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.647.60 (m, 1H), 7.59-7.56 (m, 1H), 7.63-7.56 (m 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 1H), 7.18 (t, *J* = 9.1 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.6, 160.1 (d, *J* = 252.4 Hz), 137.3, 133.5, 133.2 (d, *J* = 8.3 Hz), 130.8 (d, *J* = 2.9 Hz), 129.9 (d, *J* = 0.7 Hz)), 128.5, 127.0 (d, *J* = 14.3 Hz), 124.3 (d, *J* = 3.6 Hz), 116.3 (d, *J* = 21.7 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -110.99 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{13}H_9FO$, 200.0637; found 200.0634. (*It contains a minor di-fluorination product, which was difficult to be separated from the mono-fluorination product.*)



(2-fluorophenyl)(4-nitrophenyl)methanone (2ab): Following the general condition, $AgNO_3$ (0.15 mmol) was added; Yellow solid (33.3 mg, 68%); R_f = 0.64 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.8 Hz, 2H), 7.98 (d, *J* = 9.9 Hz, 2H), 7.69-7.59 (m, 2H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.24-7.15 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 191.8, 160.4 (d, *J* = 253.7 Hz), 150.4, 142.5, 134.4 (d, *J* = 8.5 Hz), 131.1 (d, *J* = 2.2 Hz), 130.4 (d, *J* = 1.2 Hz), 125.7 (d, *J* = 14.1 Hz), 124.8 (d, *J* = 3.6 Hz), 123.7, 116.6 (d, *J* = 21.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -109.16 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{13}H_8FNO_3$, 245.0488; found 245.0496.

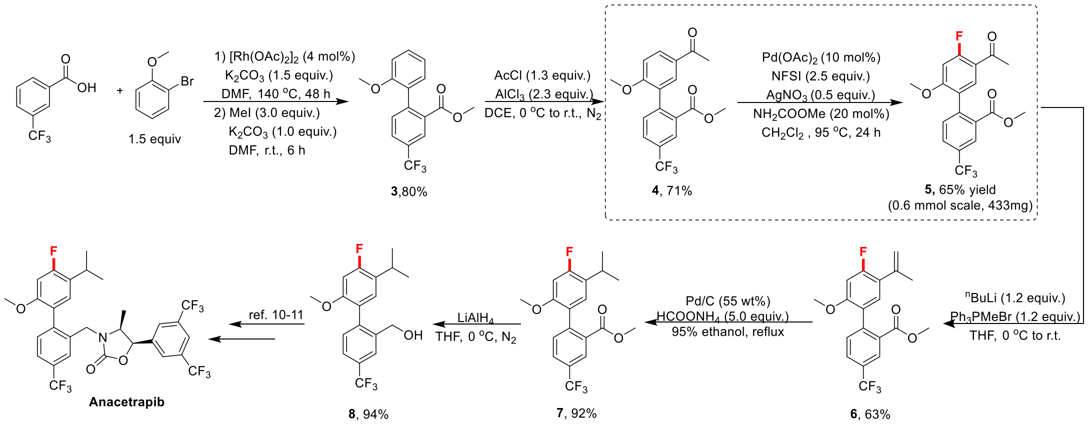
2. The unsuccessful substrates in direct *ortho*-C-H bond fluorination of ketones



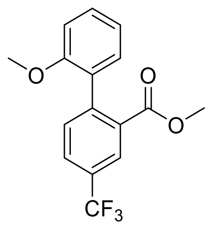
[a]Reaction conditions: ketone (0.1 mmol), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol), NFSI (0.25 mmol), $AgNO_3$ (8.5 mg, 0.075 mmol), NH_2COOMe (1.5 mg, 0.02 mmol), CH_2Cl_2 (1.0 mL) at 95 °C for 24-48 h, under air. [b]GC-MS yield.

V. The application of direct *ortho*-C(sp^2)-H bond fluorination in the synthesis of Anacetrapib

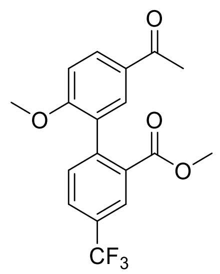
1. Synthetic routine



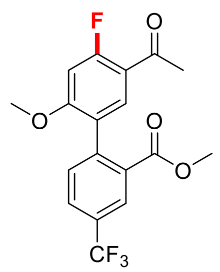
2. Characterization of the products



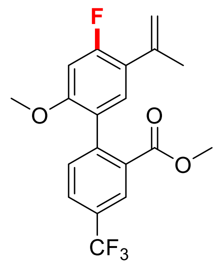
methyl 2'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate (3): The biarly **3** was prepared according to the literature.[6] An oven-dried 25 mL thick wall tubes equipped with a stir bar was charged with $[Rh(OAc)_2]_2$ (22.1 mg, 0.05 mmol), 3-trifluoromethylbenzoic (237.5 mg, 1.25 mmol), K_2CO_3 (262.4 mg, 1.9 mmol), and closed with a sealing cap. After the vessel was flushed with three alternating vacuum and nitrogen purge cycles, dry DMF (2 mL) and an *O*-bromoanisole (350.6 mg, 1.9 mmol) were added via syringe. The resulting mixture was stirred at 140 ℃ for 48 h. After cooling down to room temperature, K_2CO_3 (172.8 mg, 1.25 mmol) and MeI (234 μL, 3.75 mmol) were added and stirred at room temperature for 6 h. Another five tubes were gave the same operation and after the reaction was completed, the combined mixture of six tubes were filtered, diluted with EtOAc (30 mL) and washed with water and brine (30 mL each), then the aqueous phases were extracted with EtOAc (3×20 mL). The combined organic phases were dried over anhydrous $MgSO_4$, filtered, and the volatiles were removed under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/ethyl acetate = 10/1) to give the product **3** as a colorless oil (1.86 g, 80% yield), R_f = 0.66 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.85-7.75 (m, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.43-7.38 (m, 1H), 7.32-7.25 (m, 1H), 7.13-7.07 (m, 1H), 6.95 (dd, *J* = 8.3, 1.0 Hz, 1H), 3.75 (s, 3H), 3.73 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.3, 155.9, 142.5, 132.3, 132.0, 129.8, 129.6, 129.4 (d, *J* = 33.1 Hz), 129.1, 128.0 (q, *J* = 3.6 Hz), 126.4 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 273.6 Hz), 120.6, 110.3, 55.2, 52.0; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd. for $C_{16}H_{13}F_3O_3Na$ 333.0714; found: 333.0715.



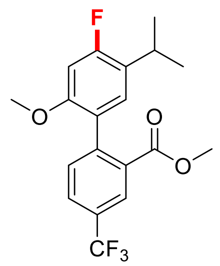
methyl 5'-acetyl-2'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate (4): The product of **4** was prepared according to the literature.[7] A dried 50 mL round bottle flask with a magnetic stir bar was charged with **3** (1.71 g, 5.5 mmol), and dried DCE (25 mL) under an N_2 atmosphere. Acetyl chloride (0.55 g, 7.0 mmol) was added dropwise to the mixture at 0 ^{o}C under stirring. The resulting mixture was stirred at 0 ^{o}C for 5 min and then $AlCl_3$ (1.67 g, 12.5 mmol) was slowly added into the reaction mixture. The reaction mixture was stirred at room temperature for 24 h. Purification was conducted by column chromatography on silica gel to provide the desired product **4** as a colorless solid (1.37 g, 71% yield), R_f = 0.27 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.20 (s, 1H), 8.05 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.90 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 8.7 Hz, 1H), 3.82 (s, 3H), 3.73 (s, 3H), 2.61 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.5, 166.8, 159.9, 141.6, 132.0, 131.9, 130.9, 130.4, 130.1, 129.4 (d, *J* = 33.3 Hz), 129.5, 128.4 (q, *J* = 3.3 Hz), 126.7 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 272.3 Hz), 109.7, 55.6, 52.1, 26.3; **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd. for $C_{18}H_{15}F_3O_4Na$ 375.0820; found: 375.0820.



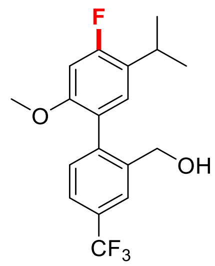
methyl 5'-acetyl-4'-fluoro-2'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate (5): In a 25 mL test tube equipped with a stir bar, substrate **4** (211.2 mg, 0.6 mmol), $Pd(OAc)_2$ (13.4 mg, 0.06 mmol), NFSI (473 mg, 1.5 mmol), NH_2COOMe (4.5 mg, 0.12 mmol), $AgNO_3$ (50.7 mg, 0.3 mmol) and DCM (2.5 mL) were added successively. Then the tube was sealed and stirred at the 95 ^{o}C for 24 h. Another two tubes were gave the same operation and after the reaction was complete, the combined mixture of three tubes were combined, the resulting mixture was cooled to room temperature, diluted with DCM and concentrated under reduced pressure. Then the residue was purified by silica gel chromatography to afford the desired fluorination product **5** as a colorless solid (433 mg, 65% yield), R_f = 0.45 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 6.68 (d, *J* = 12.8 Hz, 1H), 3.80 (s, 3H), 3.76 (s, 3H), 2.66 (d, *J* = 5.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.3 (d, *J* = 4.0 Hz), 166.7, 164.0 (d, *J* = 257.2 Hz), 161.3 (d, *J* = 10.8 Hz), 140.8, 132.2, 131.7, 131.5 (d, *J* = 4.3 Hz), 130.1 (q, *J* = 33.2 Hz), 128.5 (q, *J* = 3.6 Hz), 126.8 (q, *J* = 3.7 Hz), 126.1 (d, *J* = 2.9 Hz), 123.6 (q, *J* = 272.4 Hz), 118.1 (d, *J* = 13.0 Hz), 98.9 (d, *J* = 28.9 Hz), 56.1, 52.2, 31.4 (d, *J* = 7.8 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.75 (s, 3F), -104.48 (s, 1F); **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd. for $C_{18}H_{14}F_4O_4Na$ 393.0726; found: 393.0725.



methyl 4'-fluoro-2'-methoxy-5'-(prop-1-en-2-yl)-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate (6): The product of **6** was prepared according to the literature.[8] In a dry round bottom flask, a dissolved methyltriphenylphosphonium bromide (750 mg, 2.1 mmol) in dry THF solution (10 mL) was added dropwise n-Butyl lithium (1.3 mL, 2.0 mmol, 1.6 mol/L in hexane) in THF solution under N_2 protection at -30 ºC. After addition, the mixture was continued to stir for 30 minutes at the same temperature then the **5** (370 mg, 1.0 mmol) in 1 mL THF was added dropwise by syringe. The mixture was allowed to warm to room temperature and stirred for 24 h. The resulting solution was quenched with saturated NH_4Cl (2 mL) at 0 ºC and extracted with EtOAc. The combined organic layer was washed with brine, dried over anhydrous $MgSO_4$ and filtered. The filtrate was concentrated in vacuo, purified by silica gel chromatography to afford the desired product **6** as a colorless solid (232 mg, 63% yield), R_f = 0.64 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.80 (d, *J* = 9.4 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 8.7 Hz, 1H), 6.65 (d, *J* = 12.7 Hz, 1H), 5.25 (d, *J* = 32.9 Hz, 2H), 3.75 (s, 3H), 3.73 (s, 3H), 2.17 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.2, 160.6 (d, *J* = 250.4 Hz), 156.1 (d, *J* = 10.3 Hz), 141.5, 139.2, 132.2, 132.1, 130.1 (d, *J* = 6.3 Hz), 129.6 (q, *J* = 32.8 Hz), 128.1 (q, *J* = 3.7 Hz), 126.6 (q, *J* = 3.7 Hz), 124.8 (d, *J* = 3.7 Hz), 123.7 (q, *J* = 273.3 Hz), 122.2 (d, *J* = 13.7 Hz), 115.9 (d, *J* = 4.7 Hz), 99.2 (d, *J* = 28.2 Hz), 55.6, 52.1, 23.2 (d, *J* = 3.4 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.75 (s, 3F), -104.48 (s, 1F) ; **HRMS** (EI): [M^+] calcd. for $C_{19}H_{16}F_4O_3$, 368.1036; found 368.1034.



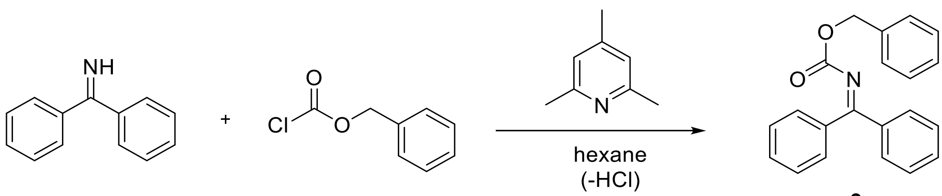
methyl 4'-fluoro-5'-isopropyl-2'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate (7): The product of **7** was prepared according to the literature.[9] In a dry round bottom flask, substrate **6** (184 mg, 0.5 mmol) was added to 95% ethanol (10 mL), followed by addition of ammonium formate (94.5 mg, 1.5 mmol). Pd/C (55 wt%, 10 mg) was then added, and the reaction was heated under reflux for 8 h. Afterwards the reaction was cooled, followed by filtration. The solution was diluted with 0.1 M KOH (aq) (10 mL), followed by extraction with dichloromethane (4 × 10 mL). The combined organic fractions were dried over anhydrous $MgSO_4$, then evaporated in vacuo to give the desired product **7** as a colorless solid (170 mg, 92% yield), R_f = 0.67 (petroleum ether-EtOAc = 5:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.5 Hz, 1H), 6.64 (d, *J* = 12.0 Hz, 1H), 3.75 (s, 3H), 3.72 (s, 3H), 3.30-3.18 (m, 1H), 1.29 (d, *J* = 6.9 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.5, 161.0 (d, *J* = 246.3 Hz), 154.8 (d, *J* = 10.1 Hz), 141.9, 132.3, 132.1, 129.4 (q, *J* = 33.1 Hz), 123.8 (q, *J* = 274.4 Hz), 128.2 (d, *J* = 7.4 Hz), 128.0 (q, *J* = 3.5 Hz), 127.1 (d, *J* = 15.4 Hz), 126.1 (q, J = 3.7 Hz), 124.6 (d, J = 3.5 Hz), 98.8 (d, J = 27.7 Hz), 55.6, 52.2, 26.7, 22.8; ^{19}**F NMR** (376 MHz, $CDCl_3$) δ -62.61 (s, 3F), -116.14 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{19}H_{18}F_4O_3$, 370.1192; found 370.1181.



(4'-fluoro-5'-isopropyl-2'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)methanol (8): The product of **8** was prepared according to the literature.[9] In a dry round bottom flask, to a stirred suspension of $LiAlH_4$ (0.4 mL, 0.4 mmol, 1.0 mol/L in THF) in THF (20 mL) at 0 ℃ was added a solution of **7** (130 mg, 0.35 mmol) in THF (2 mL). The reaction was stirred at room temperature and was monitored by TLC to determine the consumption of the **7**. The reaction mixture was quenched at 0 ℃ with 1N HCl and was then extracted with EtOAc (3 × 5 mL). The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to afford the desired product **8** as a colorless solid (113 mg, 94% yield), R_f = 0.48 (petroleum ether-EtOAc = 5:1); ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.33 (d, J = 7.9 Hz, 1H), 7.02 (d, J = 8.6 Hz, 1H), 6.71 (d, J = 12.0 Hz, 1H), 4.61-4.39 (m, 2H), 3.76 (s, 3H), 3.17-3.30 (m, 1H), 2.17 (s, 1H), 1.27 (d, J = 5.6 Hz, 6H); ^{13}**C NMR** (101 MHz, $CDCl_3$) δ 160.9 (d, J = 246.3 Hz), 155.0 (d, J = 10.1 Hz), 140.5, 140.3, 131.0, 130.0 (q, J = 32.5 Hz), 129.1 (d, J = 7.3 Hz), 127.4 (d, J = 15.3 Hz), 124.7 (q, J = 3.7 Hz), 124.2 (q, J = 272.2 Hz), 124.2 (q, J = 3.7 Hz), 123.8 (d, J = 3.6 Hz), 99.4 (d, J = 27.7 Hz), 62.9, 56.0, 26.7 (d, J = 1.1 Hz), 22.8; ^{19}**F NMR** (376 MHz, $CDCl_3$) δ -62.43 (s, 3F), -116.17 (s, 1F); **HRMS** (EI): [M^+] calcd. for $C_{18}H_{18}F_4O_2$, 342.1243; found 342.1240.

VI. Experimental studies on the role of carbamate

1. The synthesis of complex 9

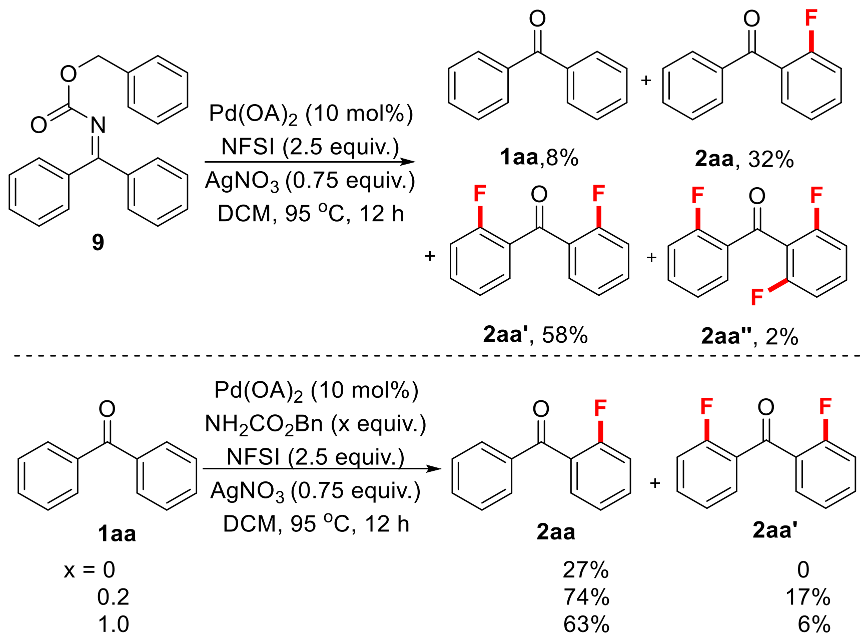


9

benzyl (diphenylmethylene)carbamate (9): The product of **9** was prepared according to the literature.[12] Benzyl carbonochloridate (1.28 g, 7.5 mmol) was added dropwise to a stirred solution of diphenylmethanimine (0.91 g, 5.0 mmol) and 2,4,6-trimethylpyridine (0.81 g, 6.7 mmol) in dry hexane (25 mL) at room temperature under the nitrogen atmosphere. The mixture was refluxed for 24 h. The white precipitate was then filtered off and washed with hot hexane (30 mL). The filtrate and washings were combined and the volatile components removed in vacuo. The residue was crystallized from pentane to afford the desired product **9** as a colorless solid (1.10 g, 70% yield), R_f = 0.40 (petroleum ether-EtOAc = 10:1); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85-7.80 (m, 2H), 7.63-7.59 (m, 1H), 7.53-7.46 (m, 4H), 7.41-7.33 (m, 5H), 7.32-7.28 (m, 2H), 5.11 (d, *J* = 17.2 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.78, 156.7, 137.6, 136.2, 132.4, 130.1, 128.6, 128.3, 128.2, 128.1, 67.0; **HRMS** (EI): [M^+] calcd. for $C_{21}H_{17}NO_2$ 315.1259; found: 315.1260.

2. Experimental studies on the role of carbamate

Table S7. Experimental studies on the role of carbamate



VII. X-Ray data for 2e and 2ab

1. X-Ray data for 2e

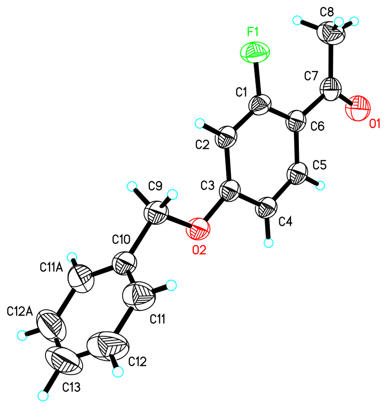


Table S8. Crystal data and structure refinement for d8v18818.

Identification code	d8v18818	
Empirical formula	$C_{15} H_{13} F O_2$	
Formula weight	244.25	
Temperature	190(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n m a	
Unit cell dimensions	a = 8.2060(8) Å	α = 90 °.
	b = 6.9192(6) Å	β = 90 °.
	c = 22.420(2) Å	γ = 90 °.
Volume	1273.0(2) $Å^3$	
Z	4	
Density (calculated)	1.274 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	512	
Crystal size	0.200 x 0.170 x 0.130 mm^3	
Theta range for data collection	2.643 to 25.987 °.	
Index ranges	-10<=h<=9, -8<=k<=8, -23<=l<=27	
Reflections collected	6041	
Independent reflections	1348 [R(int) = 0.0502]	
Completeness to theta = 25.242 °	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6035	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1348 / 0 / 111
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0429, wR2 = 0.1140
R indices (all data)	R1 = 0.0616, wR2 = 0.1351
Extinction coefficient	0.088(16)
Largest diff. peak and hole	0.145 and -0.114 e.Å^{-3}

2. X-Ray data for 2ab

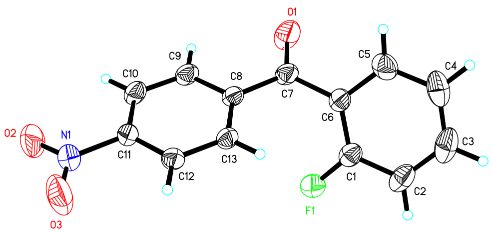


Table S9. Crystal data and structure refinement for dd19334.

Identification code	dd19334	
Empirical formula	$C_{13} H_8 F N O_3$	
Formula weight	245.20	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 4.1258(2) Å	α = 90 °.
	b = 22.7811(8) Å	β = 93.5990(10) °.
	c = 11.8050(7) Å	γ = 90 °.
Volume	1107.37(9) Å^3	
Z	4	
Density (calculated)	1.471 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	504	
Crystal size	0.180 x 0.150 x 0.130 mm^3	
Theta range for data collection	2.487 to 25.998 °.	
Index ranges	-5<=h<=5, -28<=k<=28, -14<=l<=14	
Reflections collected	16486	
Independent reflections	2144 [R(int) = 0.0320]	
Completeness to theta = 25.242 °	98.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6695
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2144 / 2 / 177
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0451, wR2 = 0.1156
R indices (all data)	R1 = 0.0538, wR2 = 0.1251
Extinction coefficient	0.044(17)
Largest diff. peak and hole	0.180 and -0.181 e.$Å^{-3}$

VIII. References

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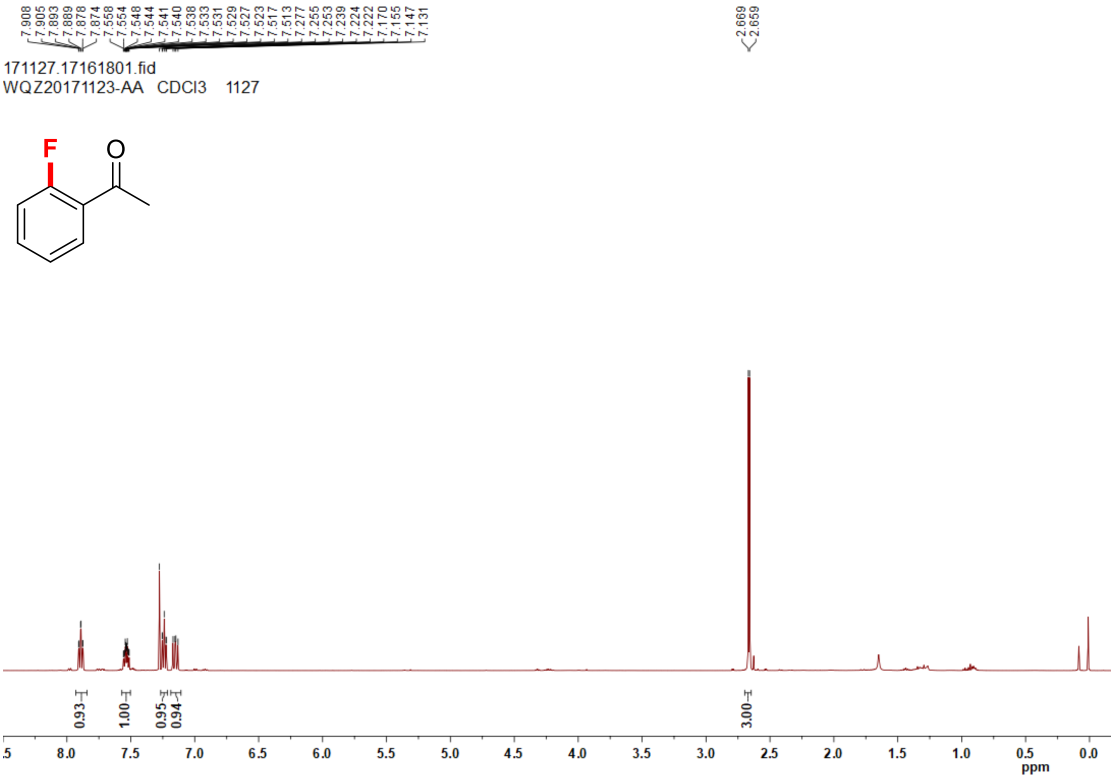
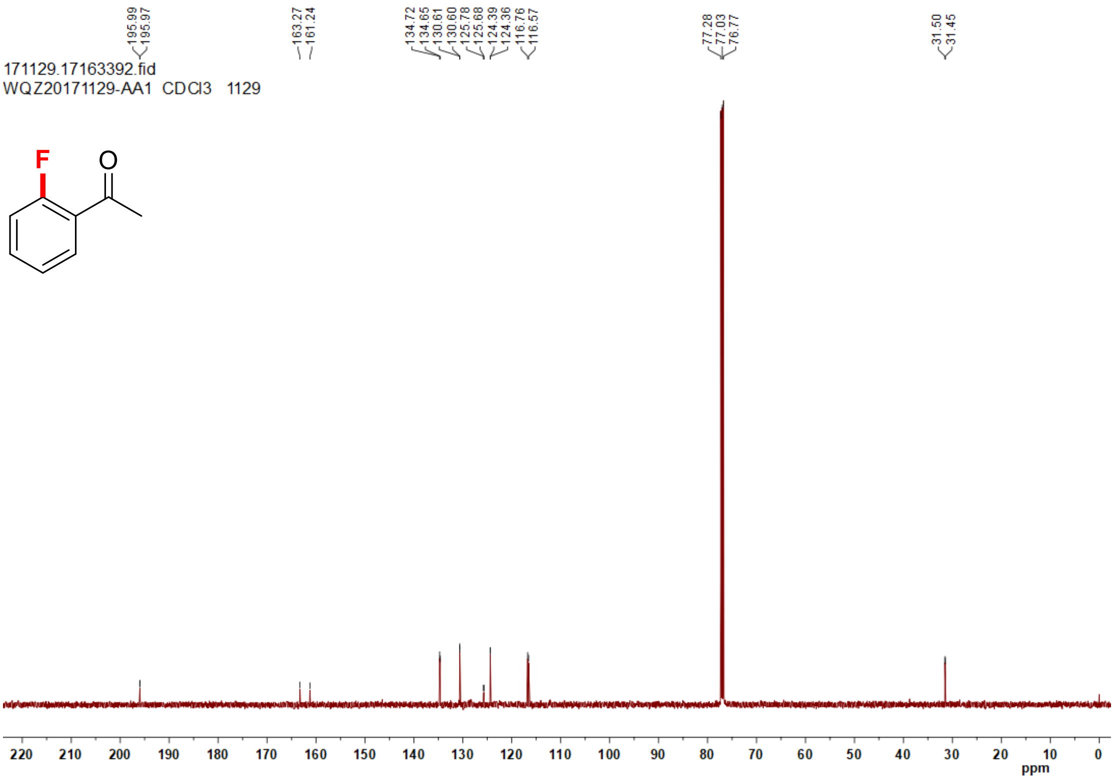
IX. NMR Spectra





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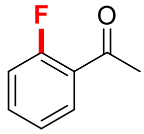

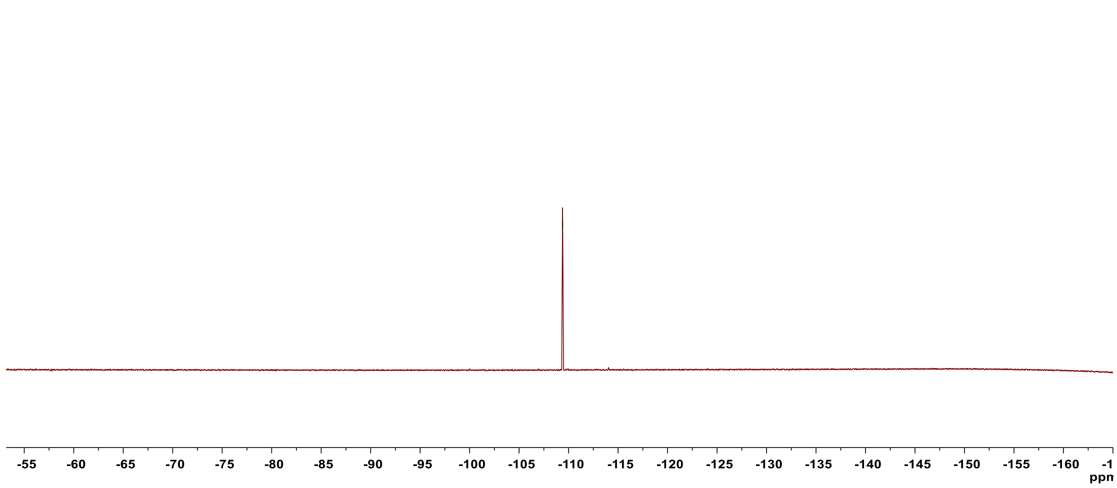

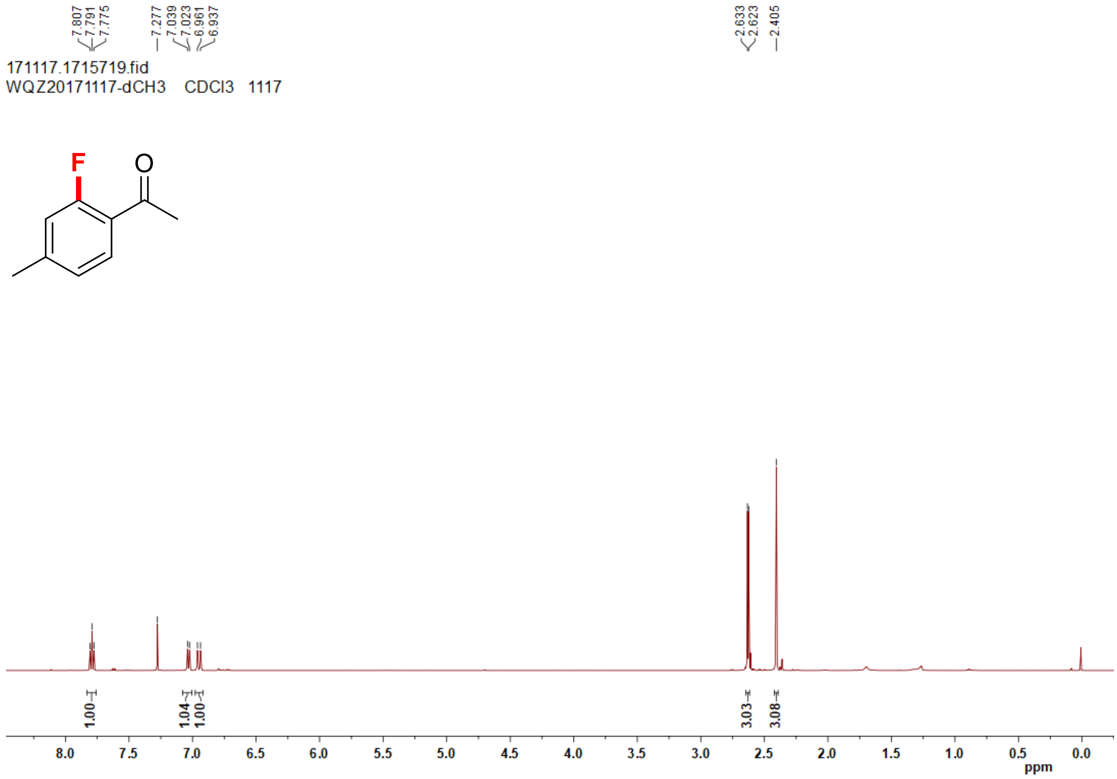
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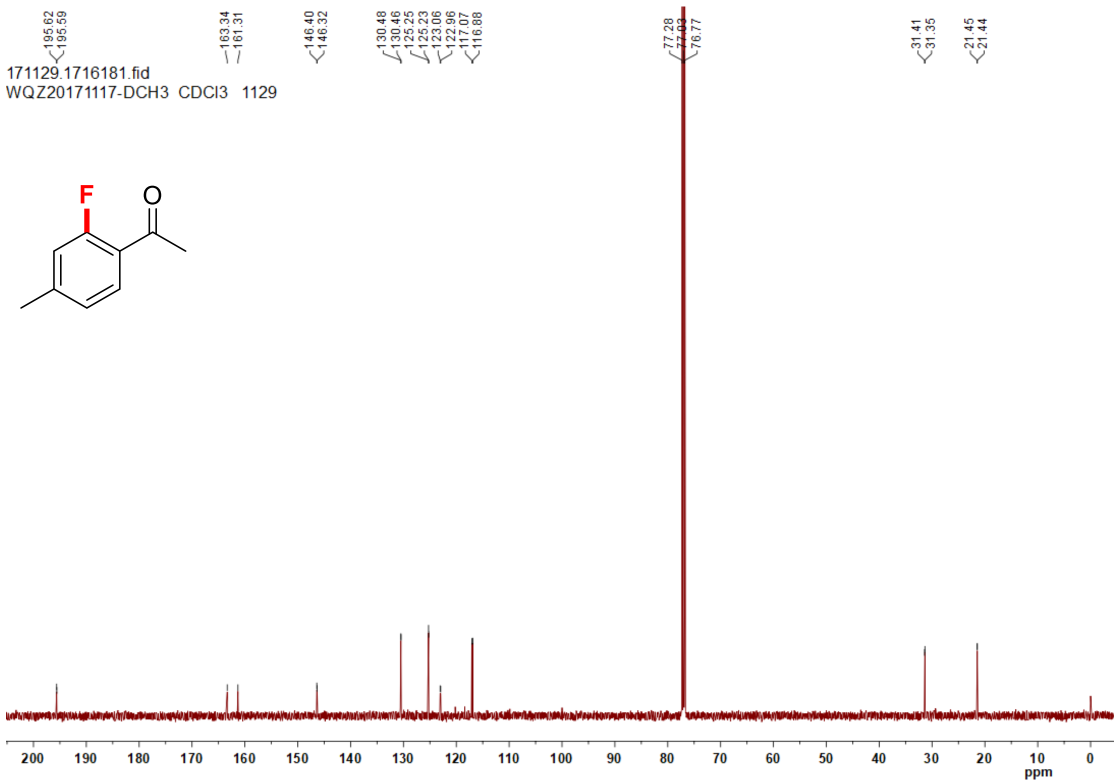
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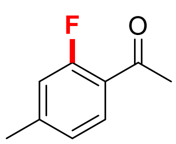
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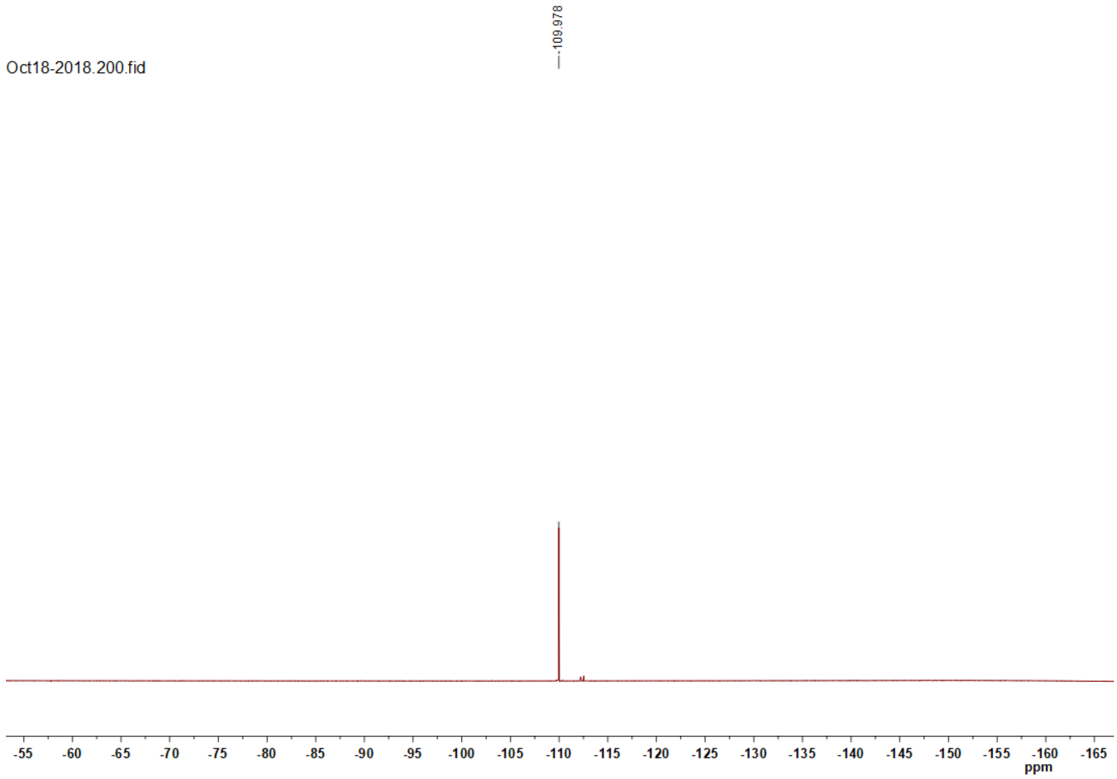
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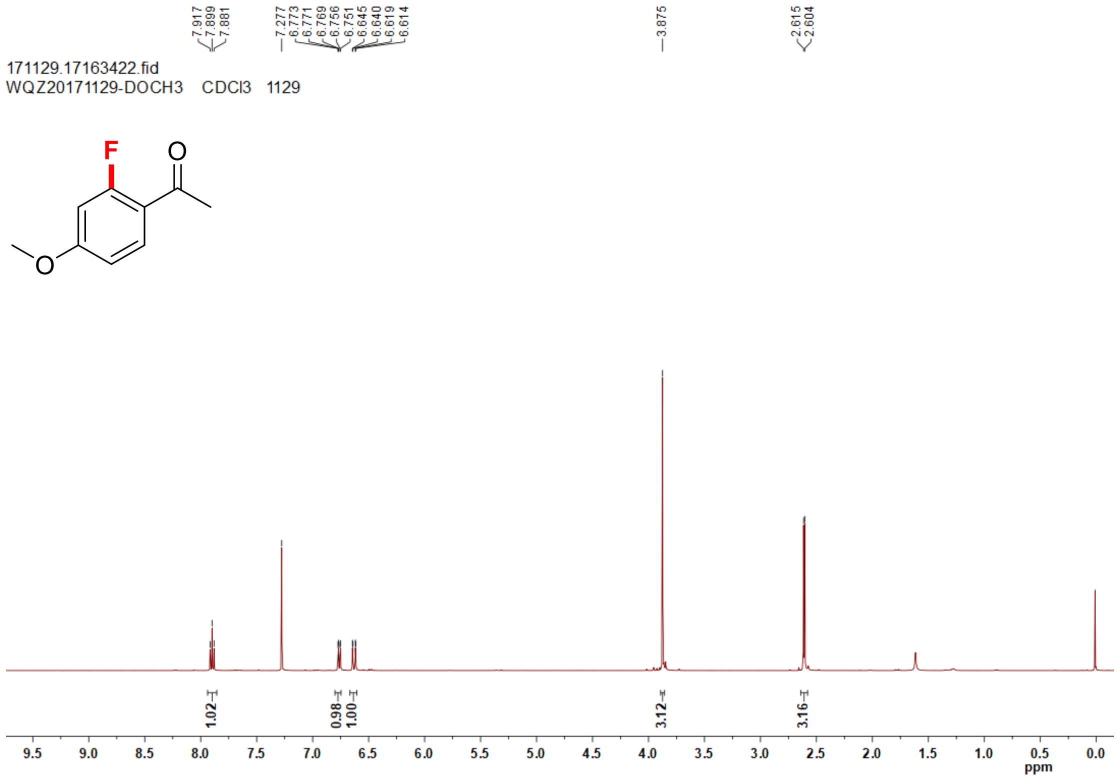
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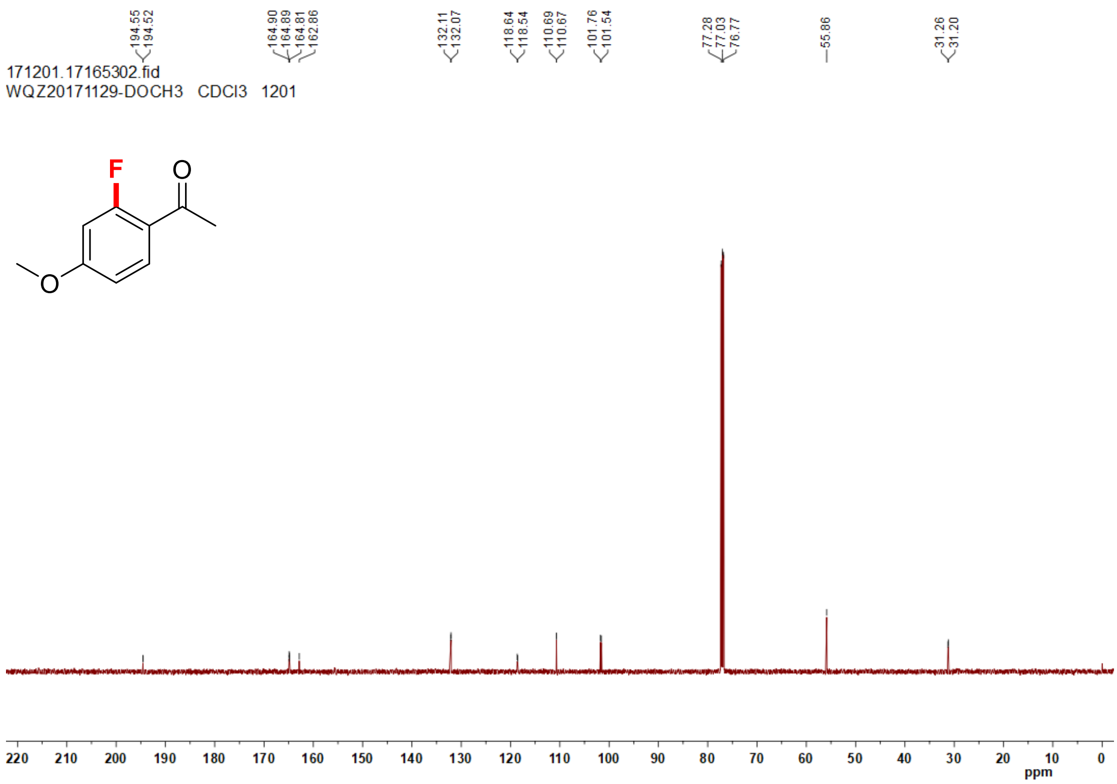
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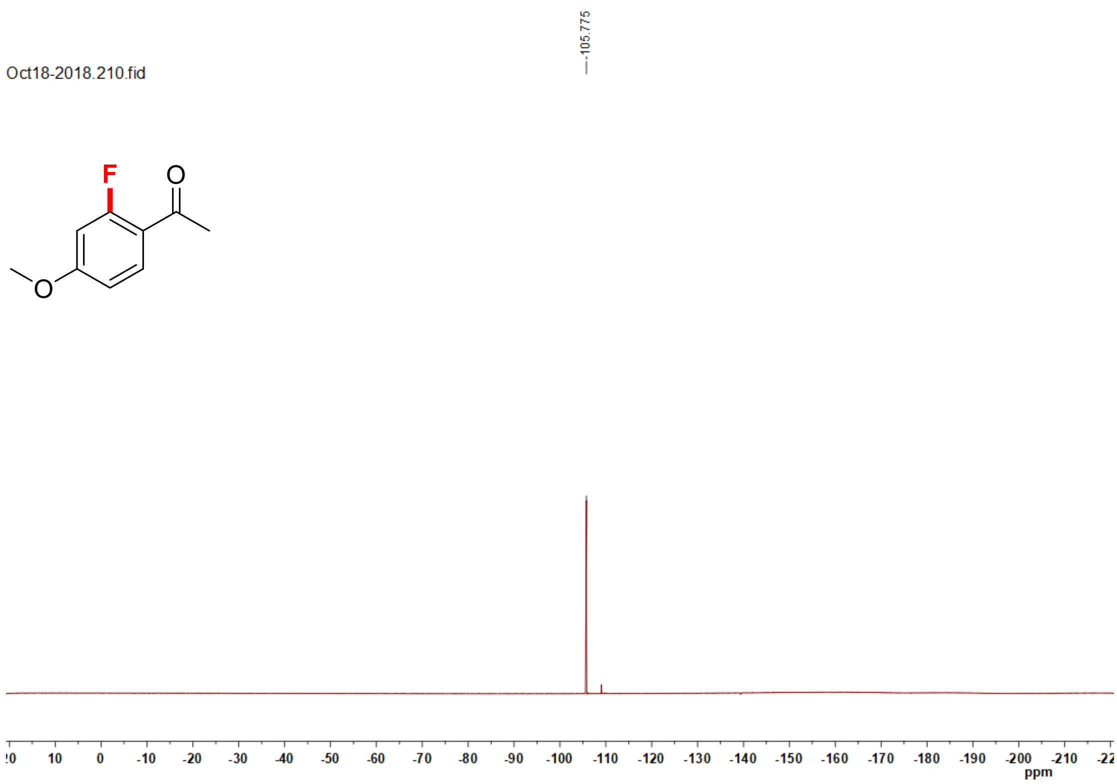
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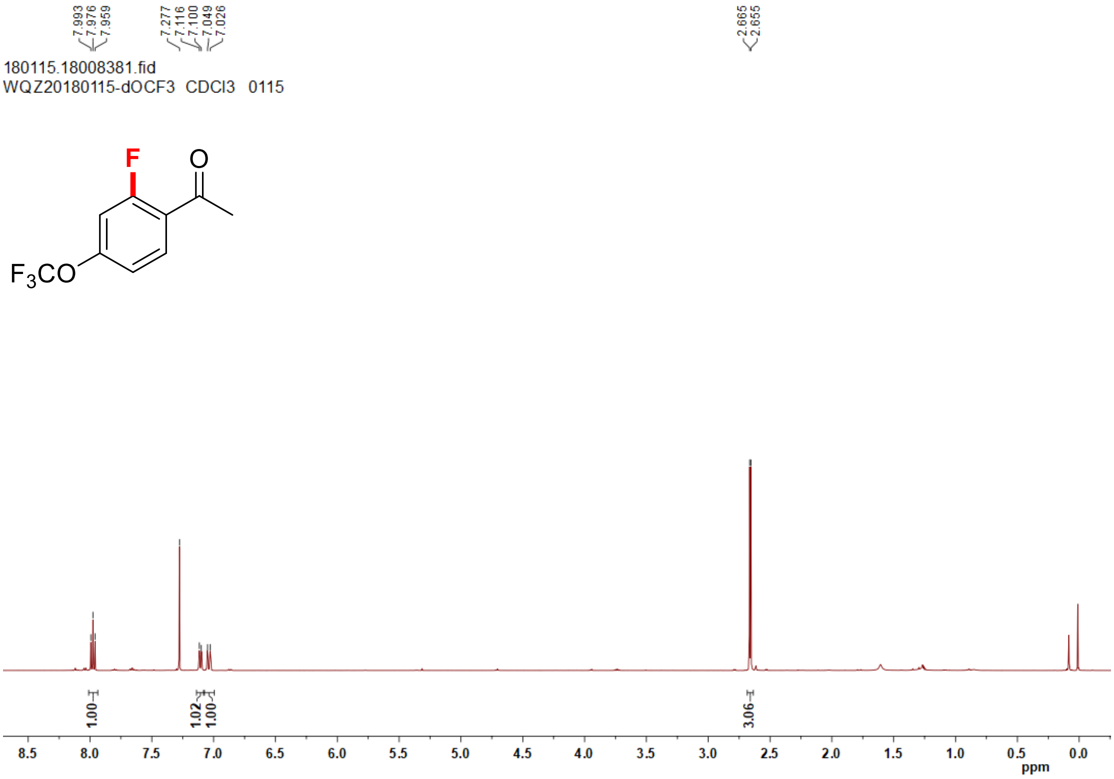

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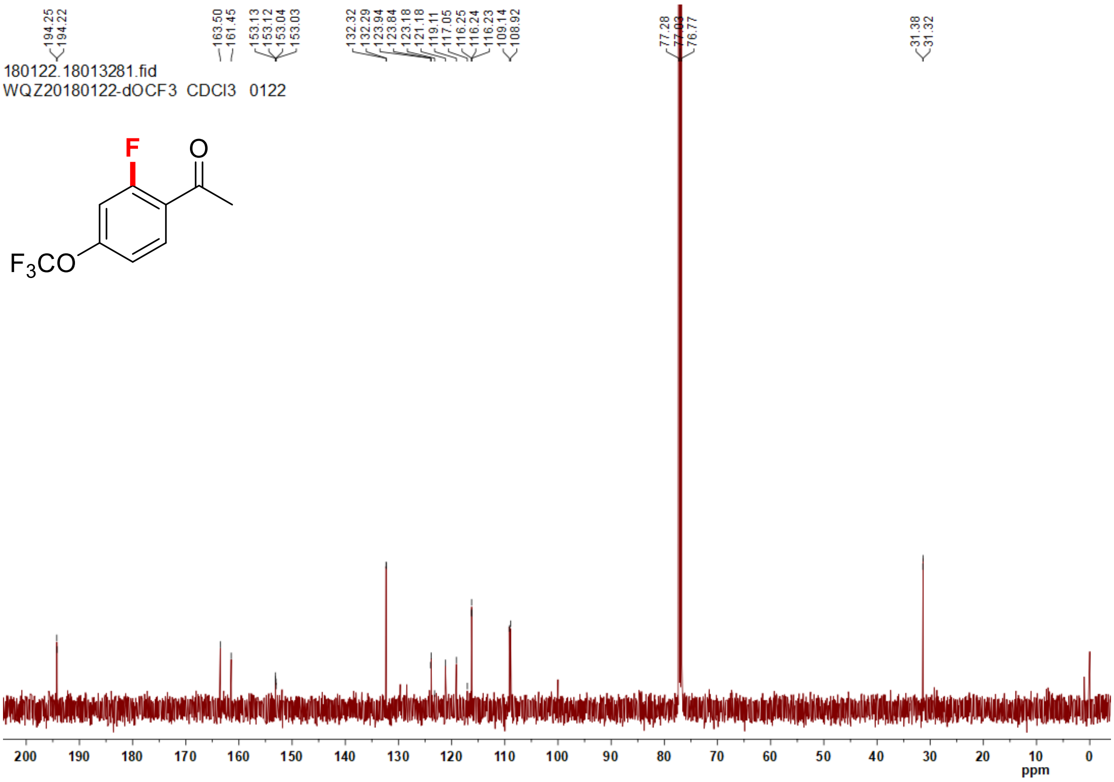

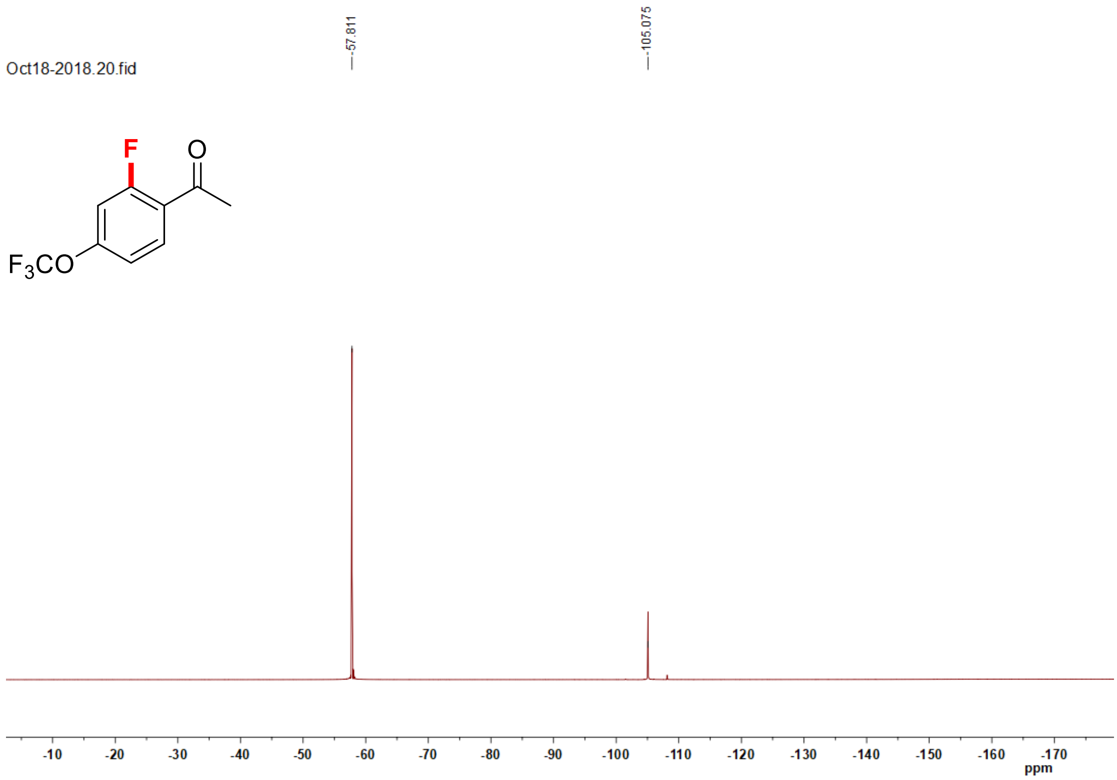

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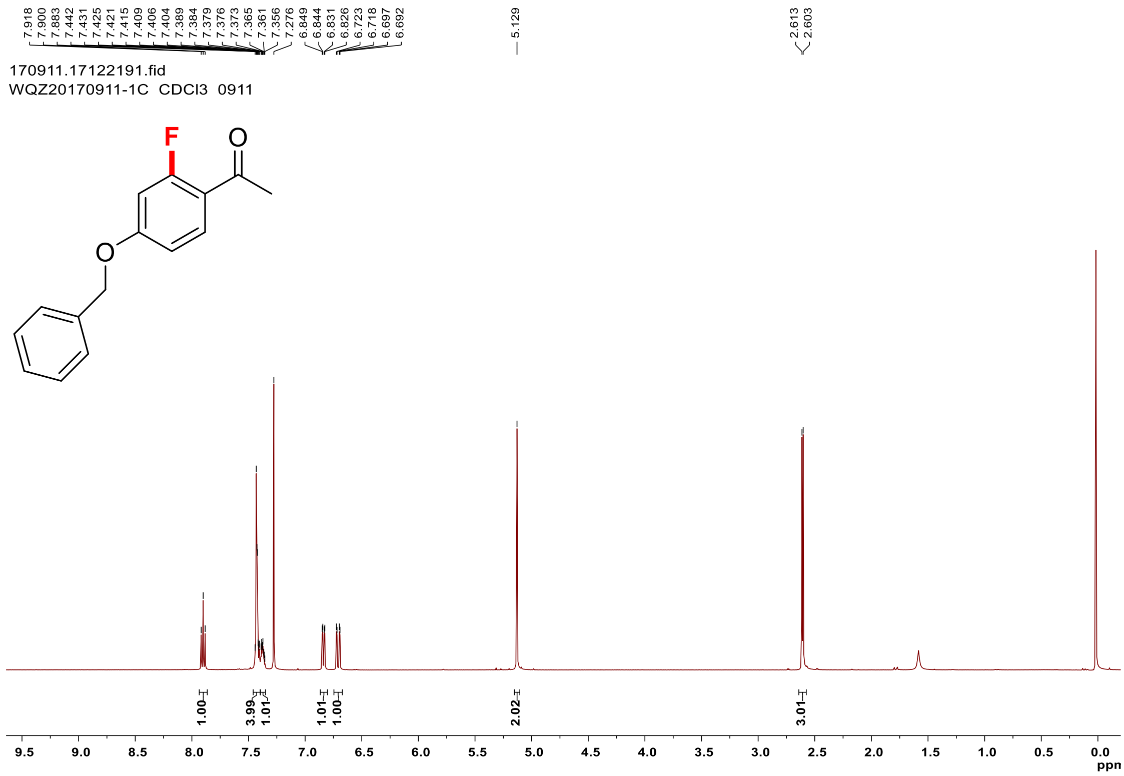

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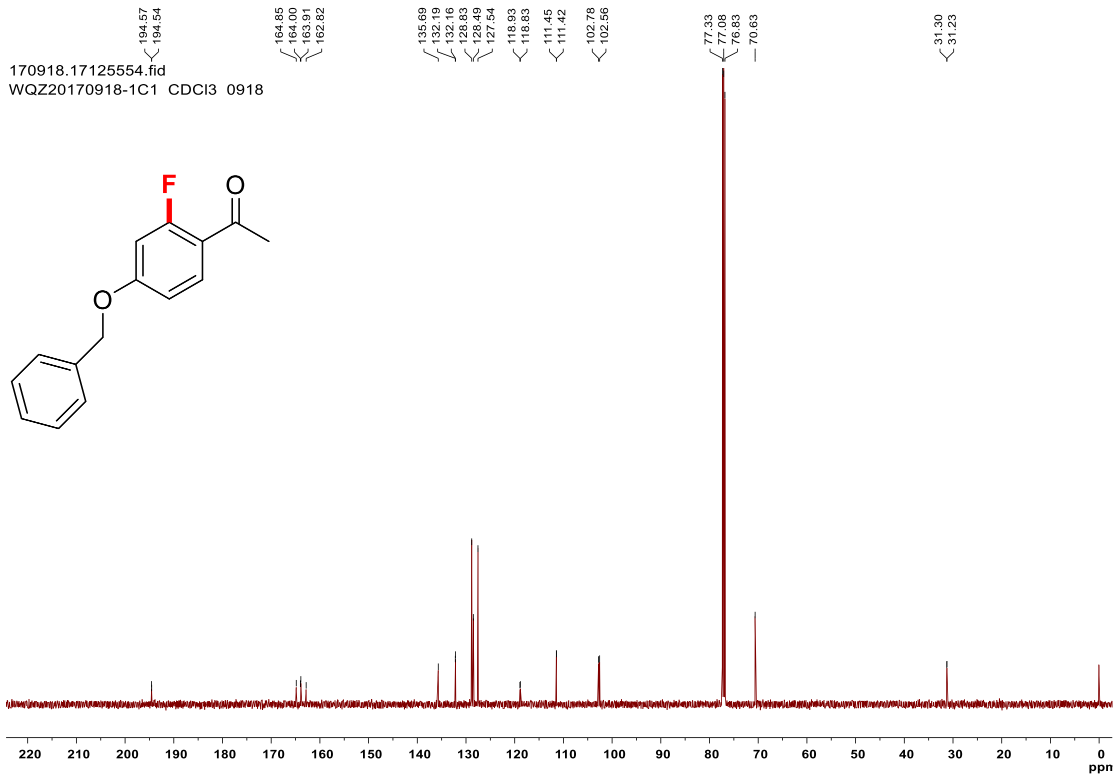
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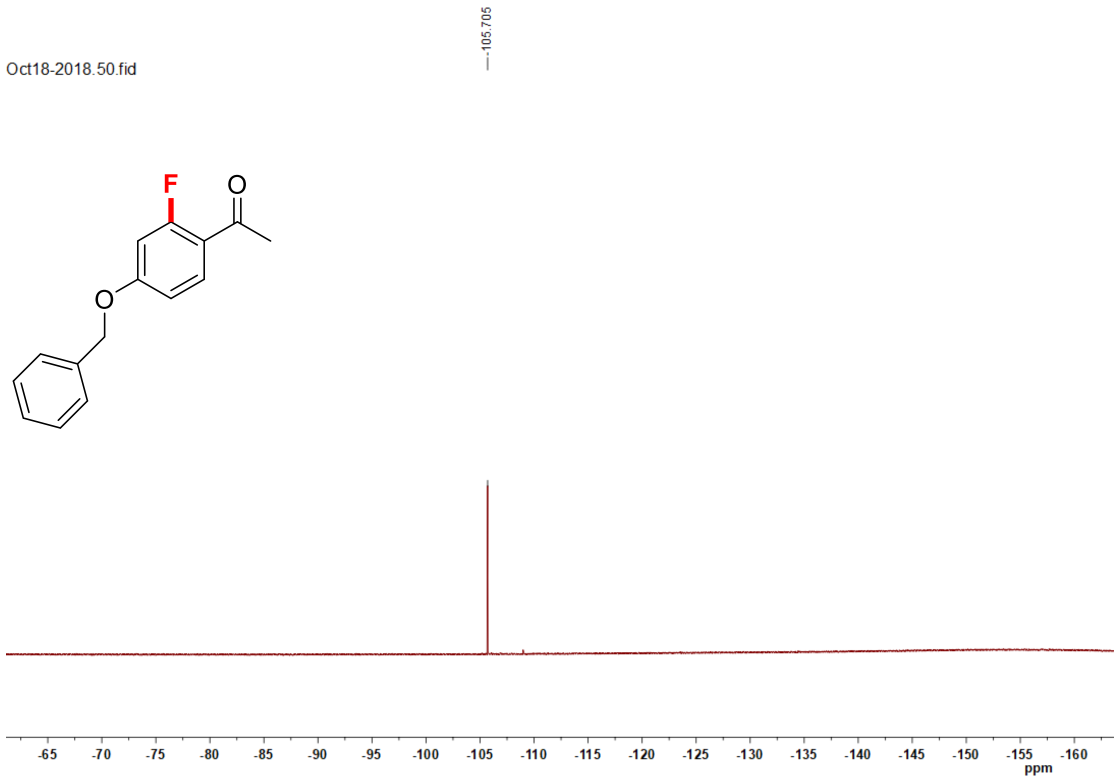
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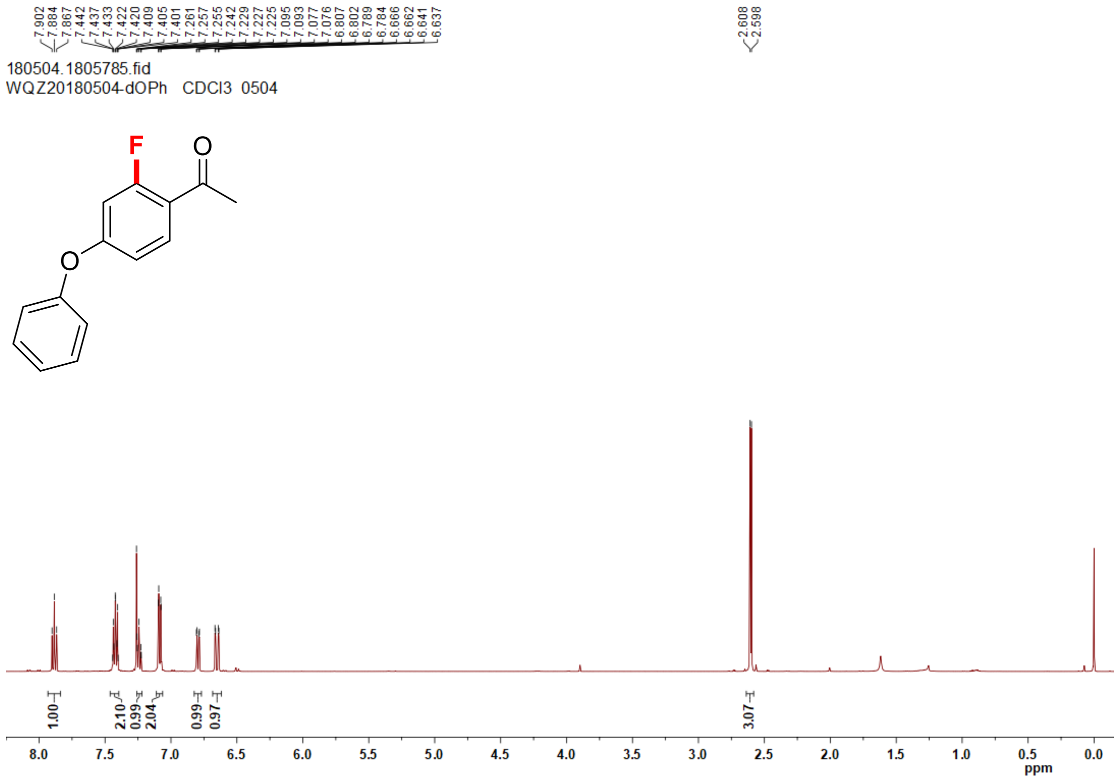
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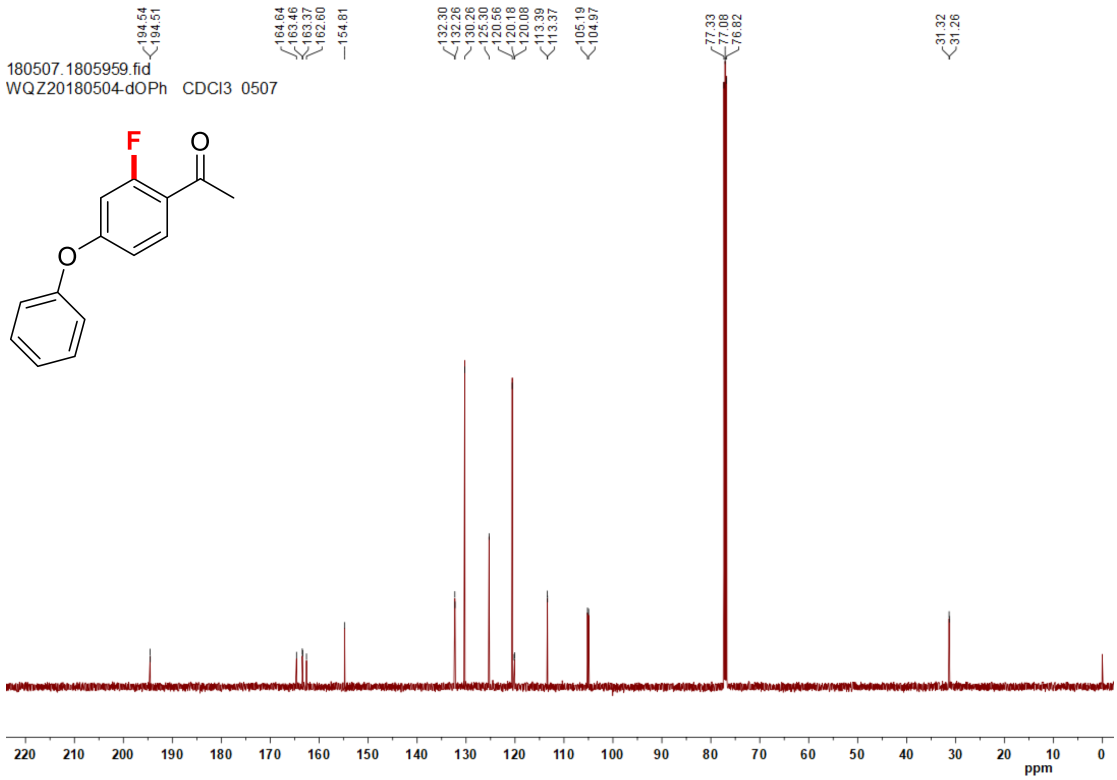
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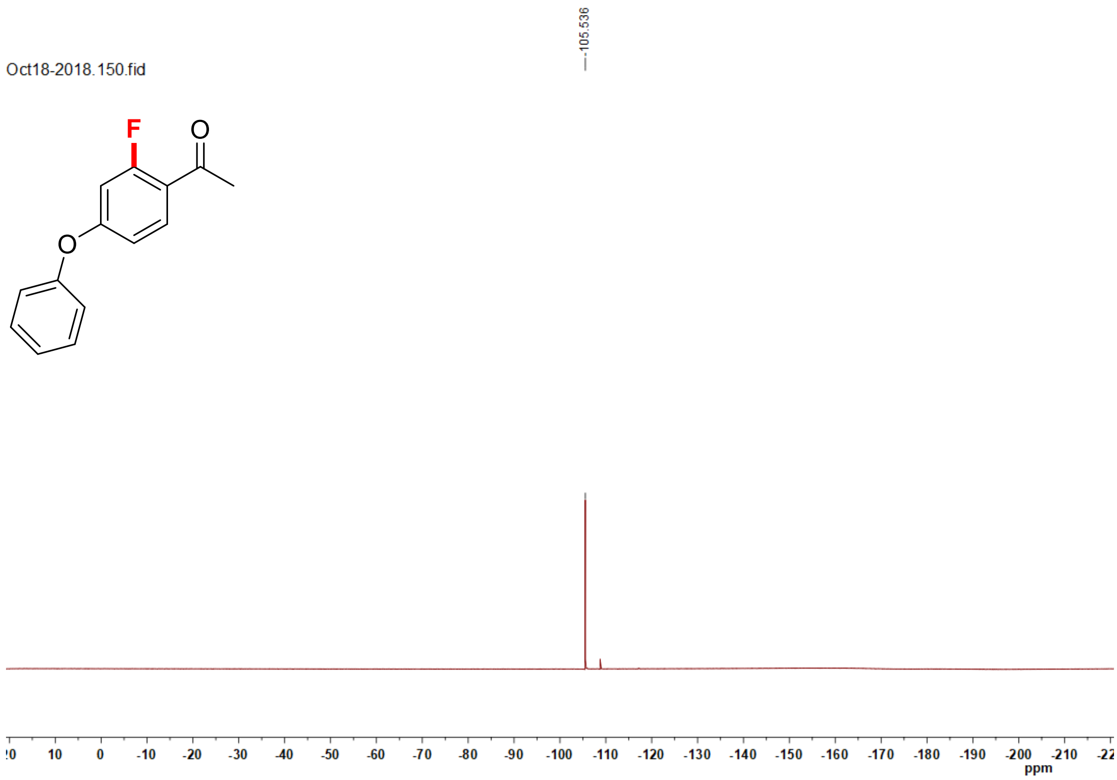
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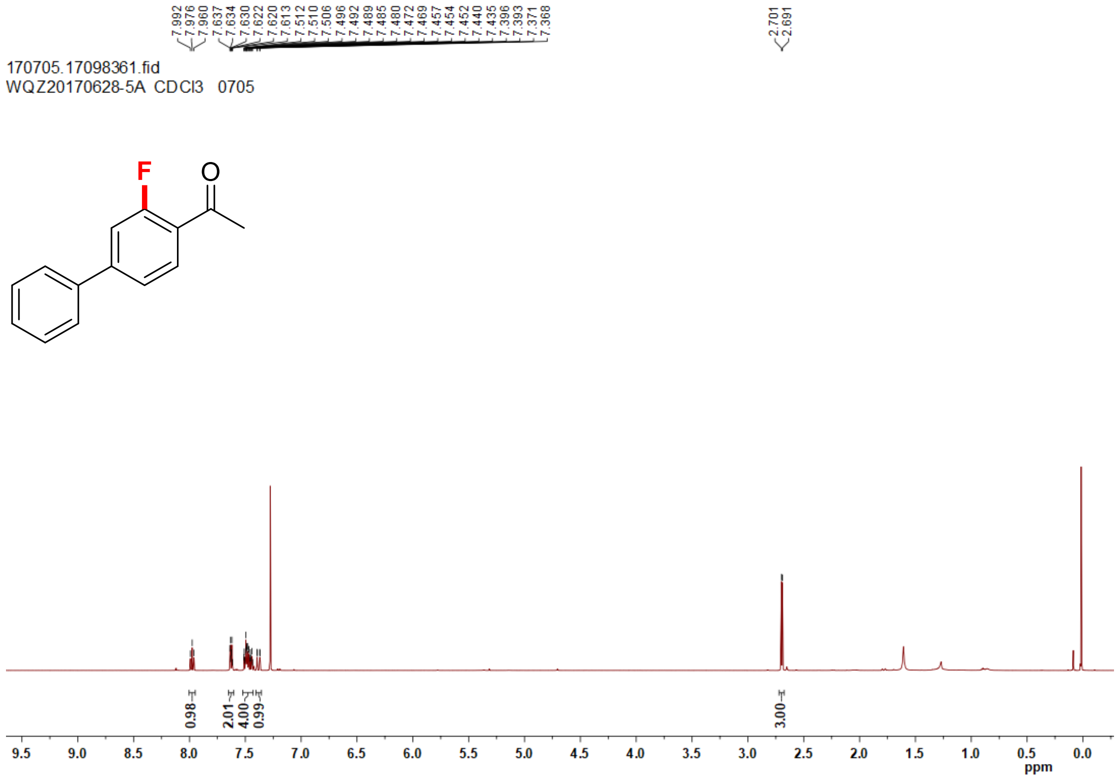
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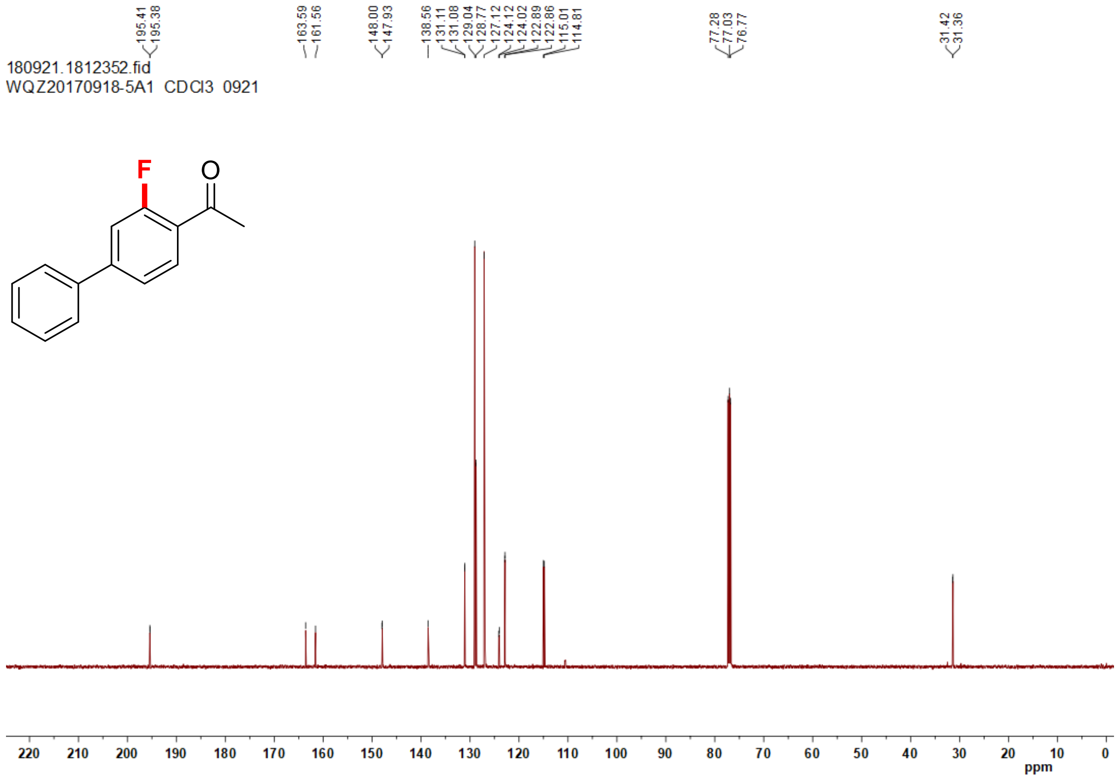
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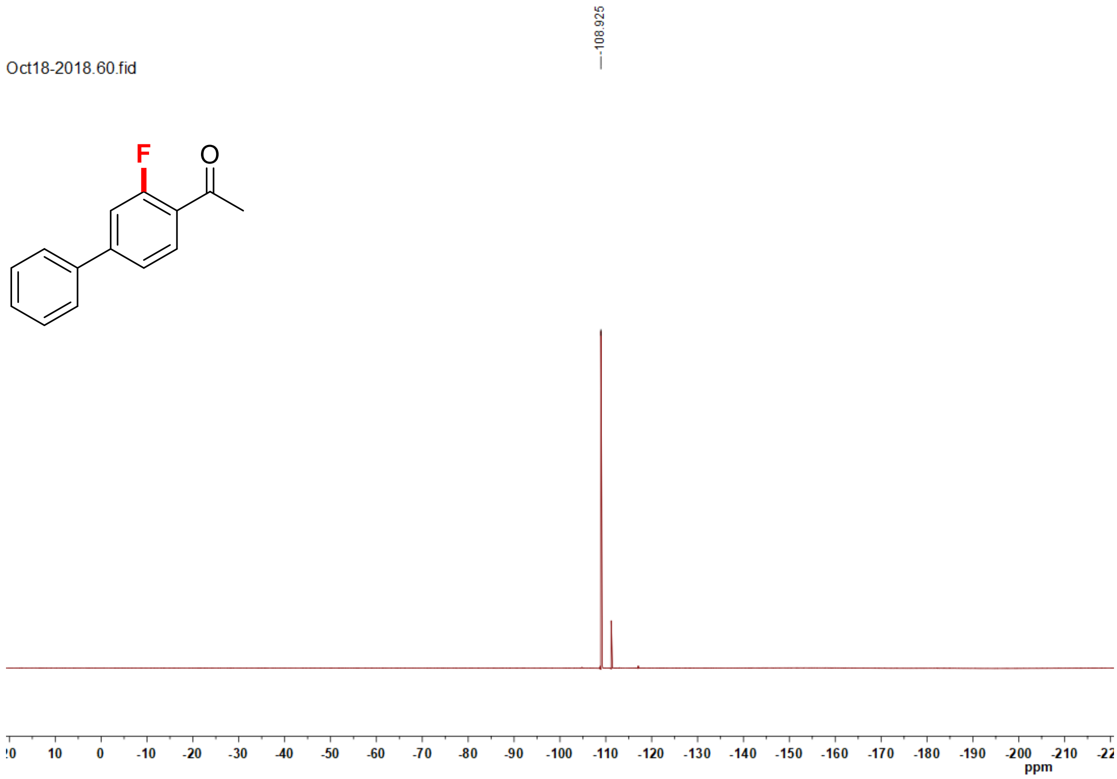
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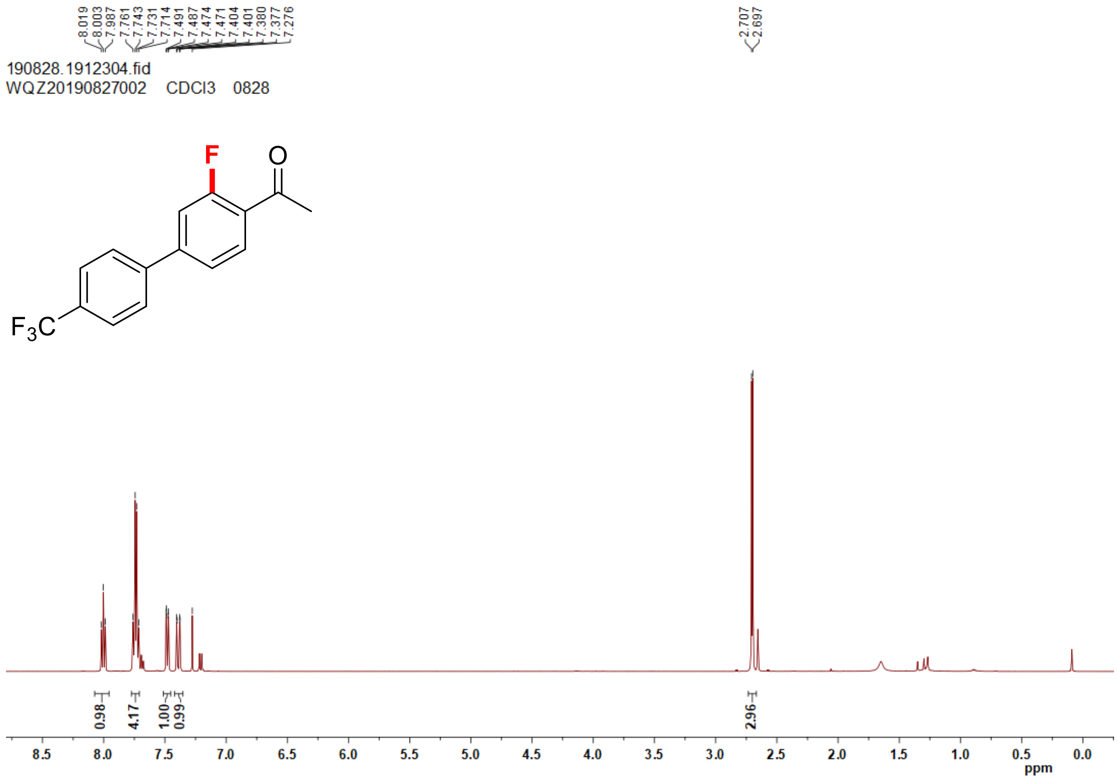
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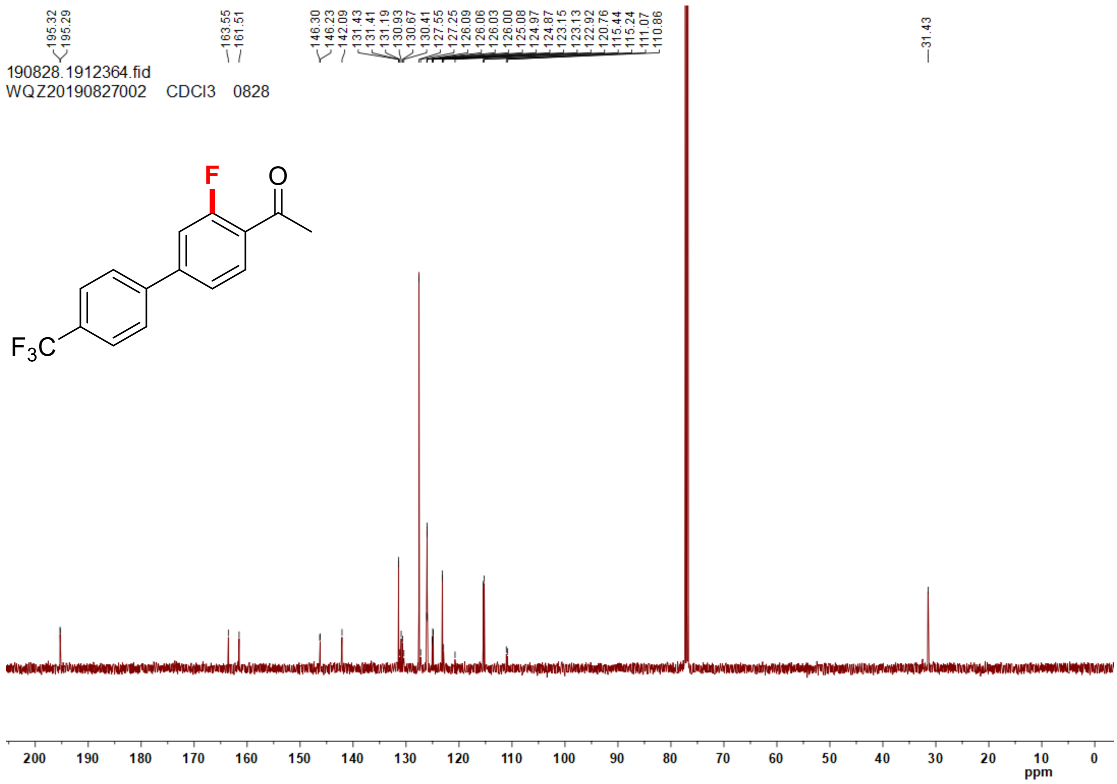
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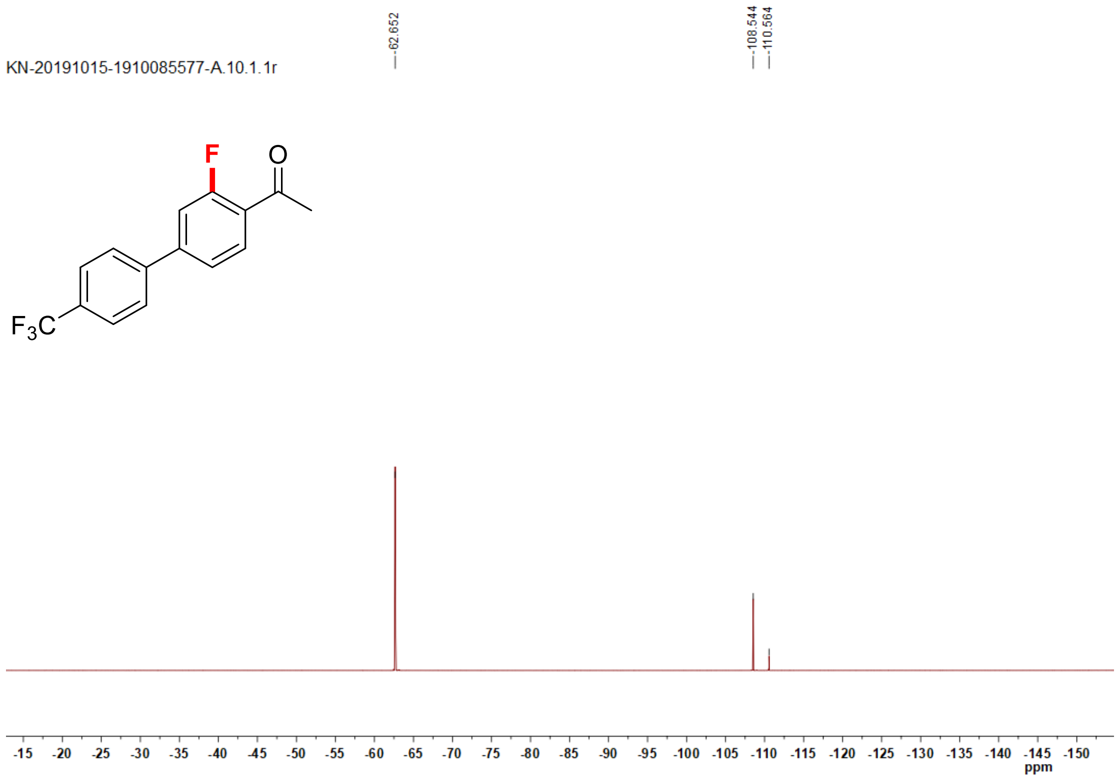
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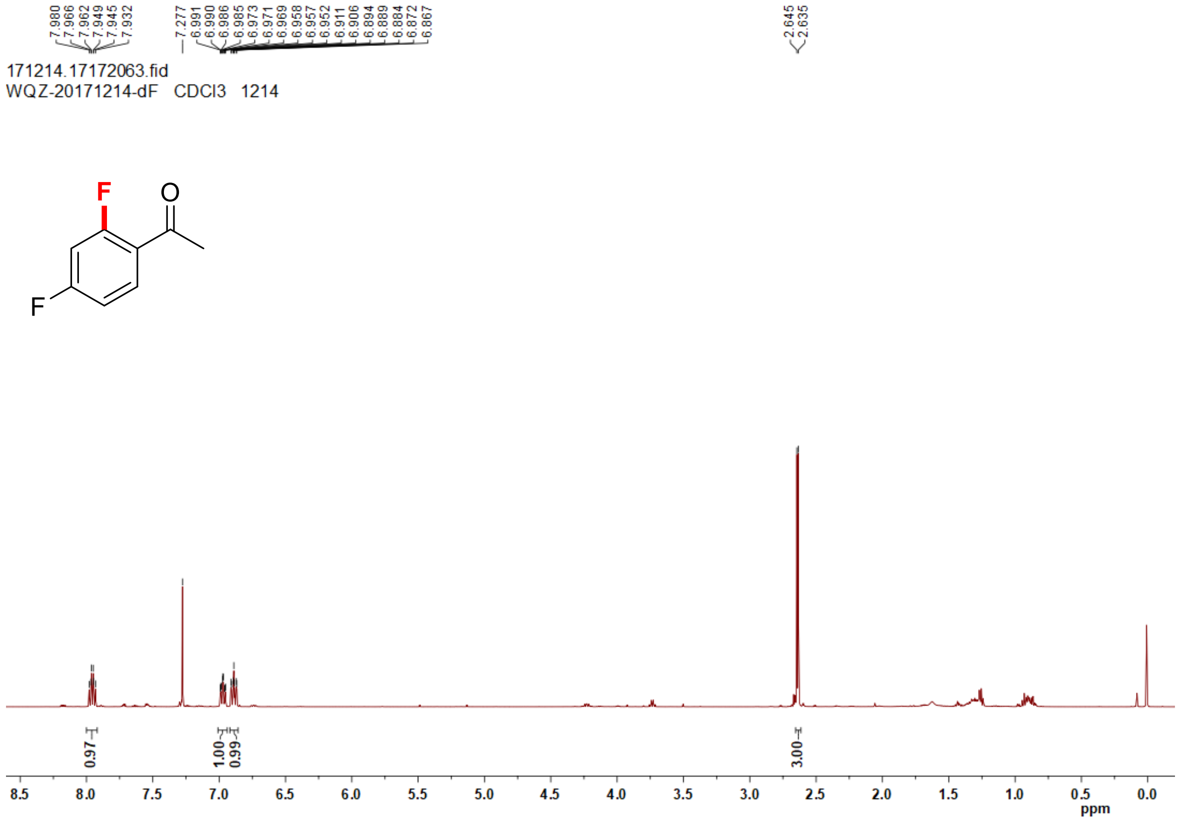
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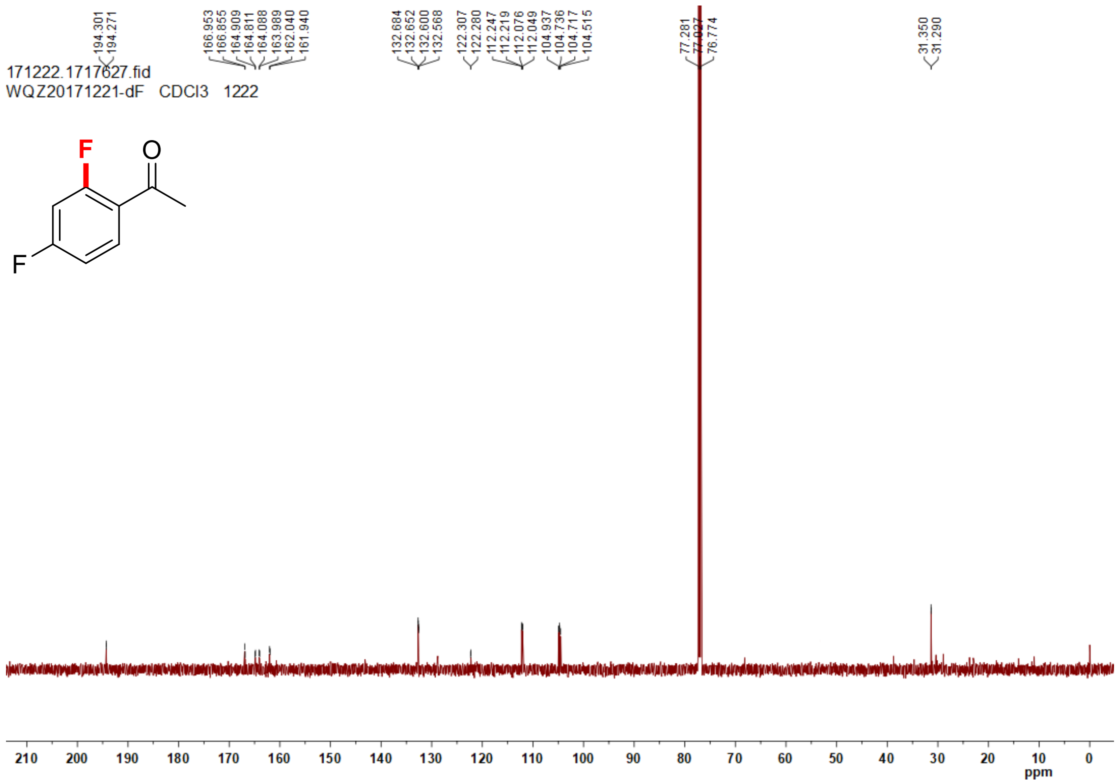
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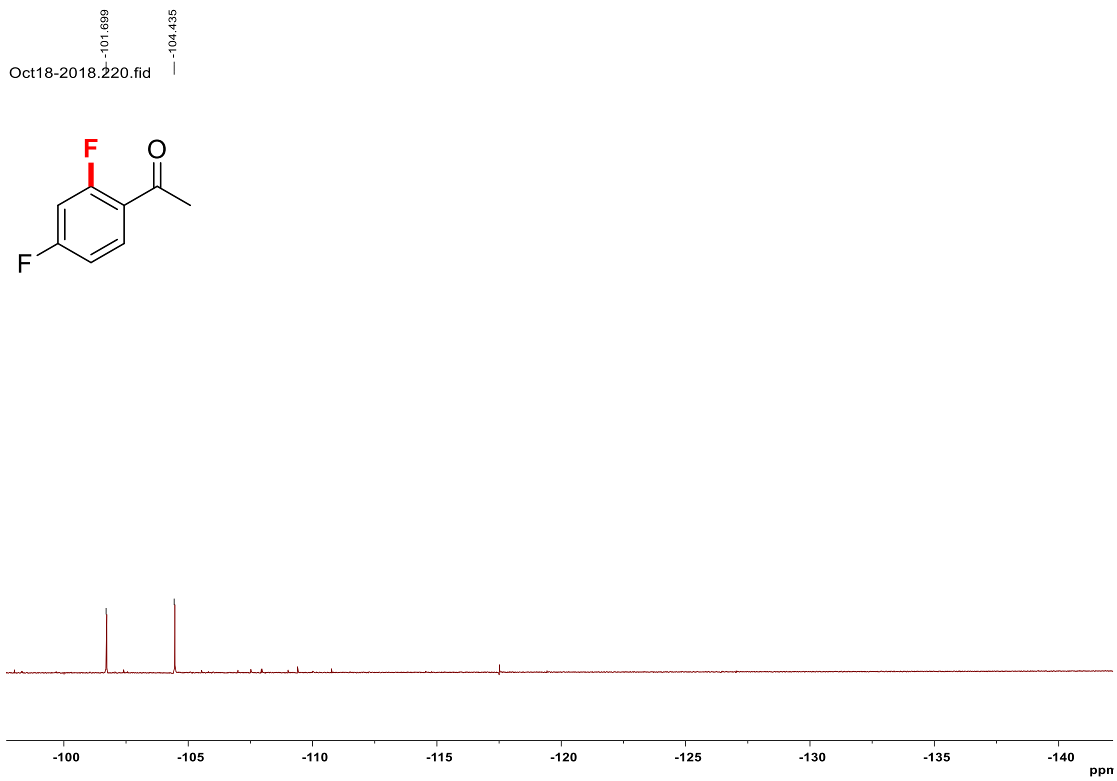
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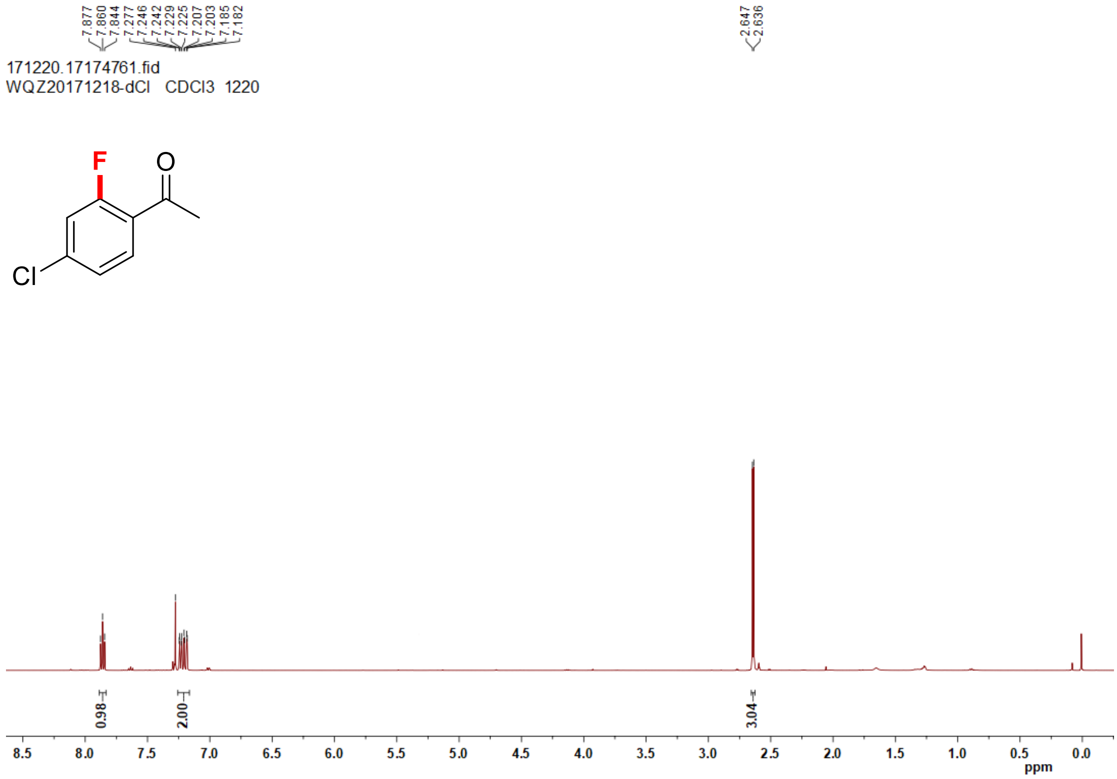
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7.182
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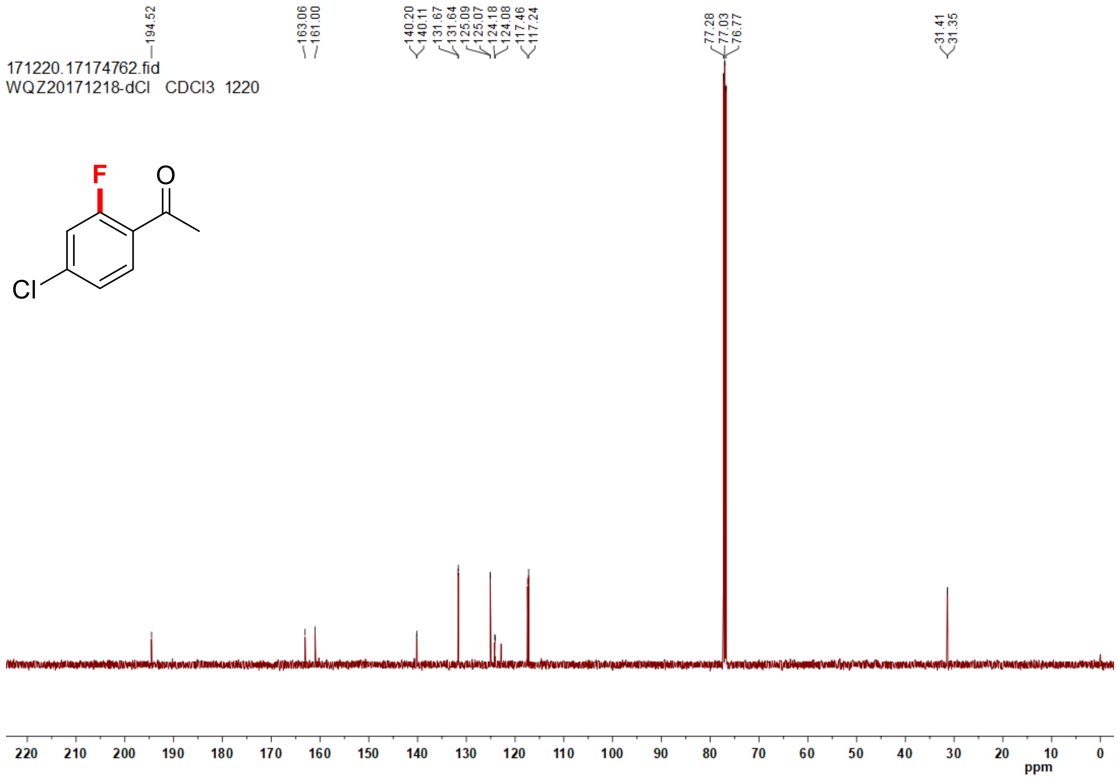
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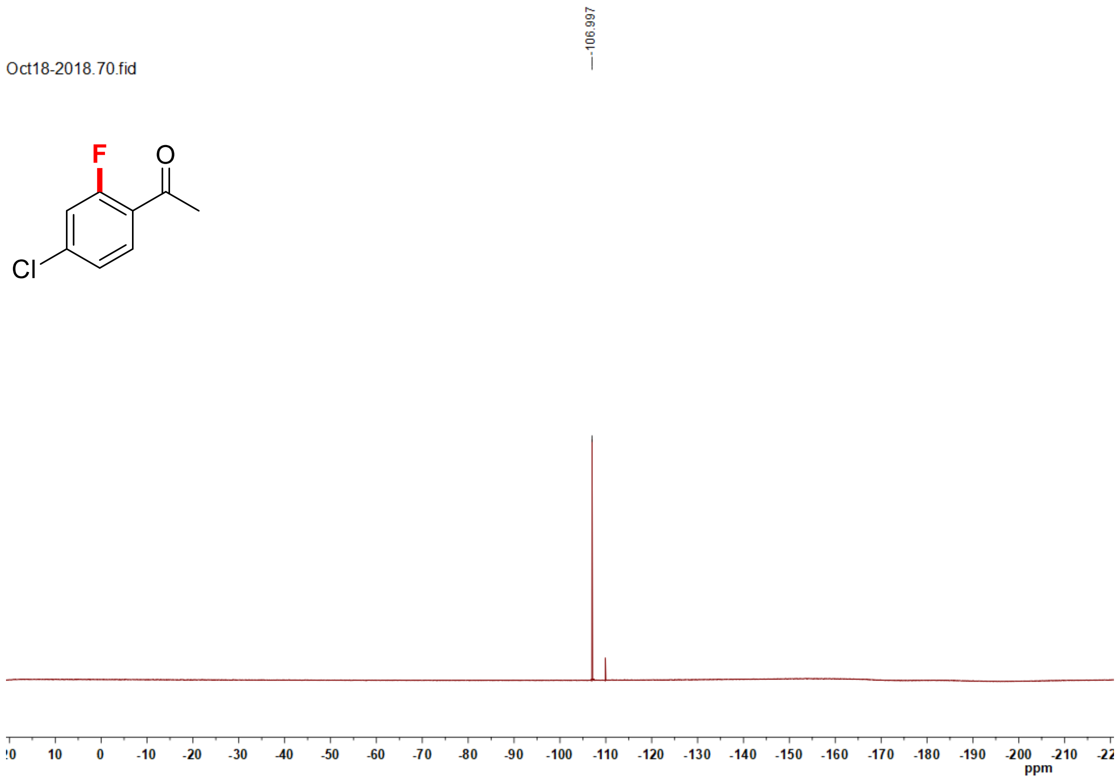
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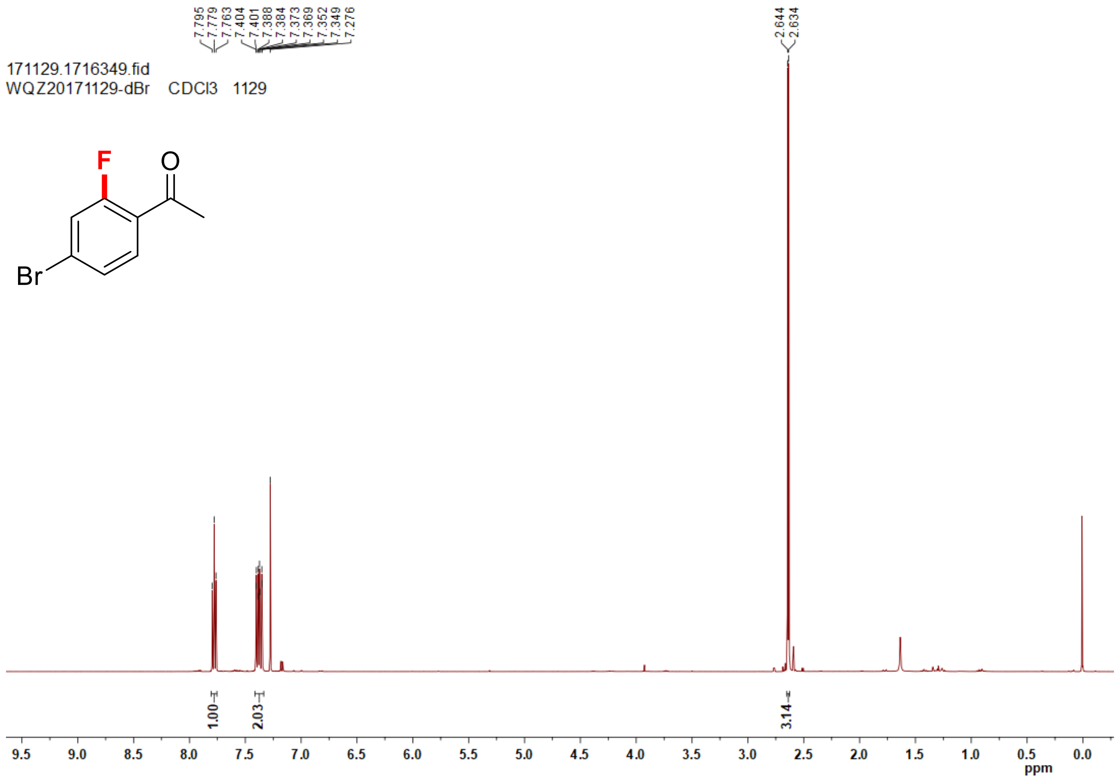
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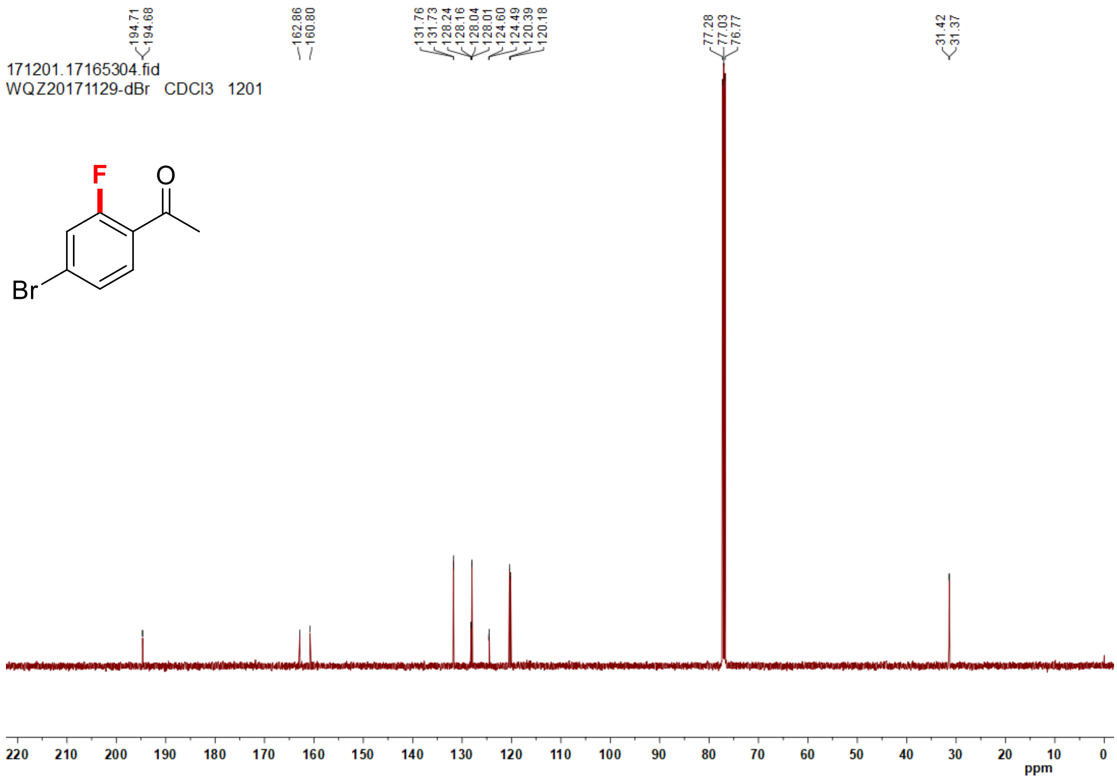
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77.03
76.77
31.42
31.37
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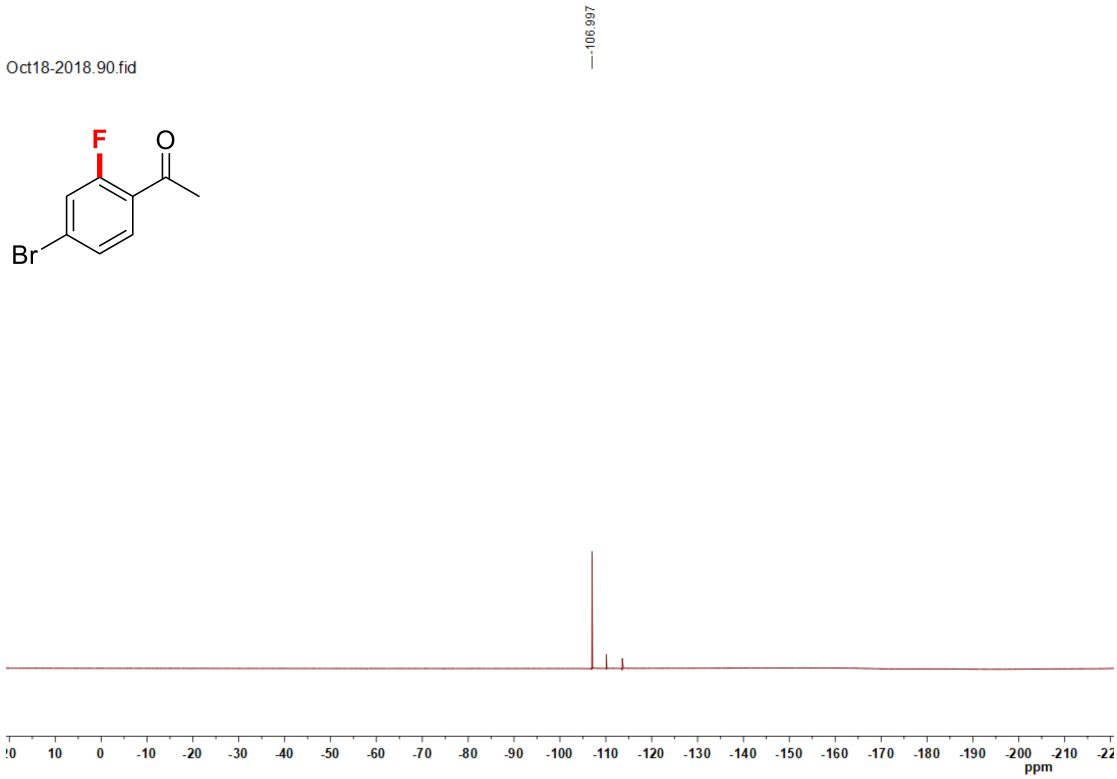
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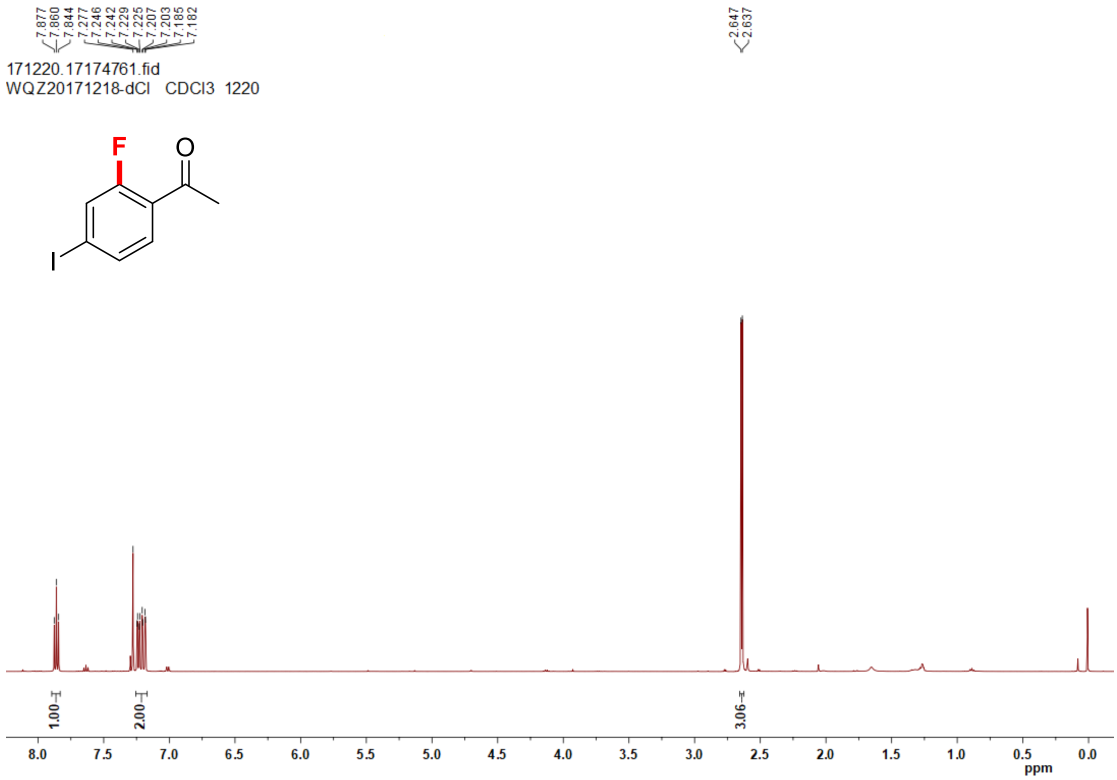
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O
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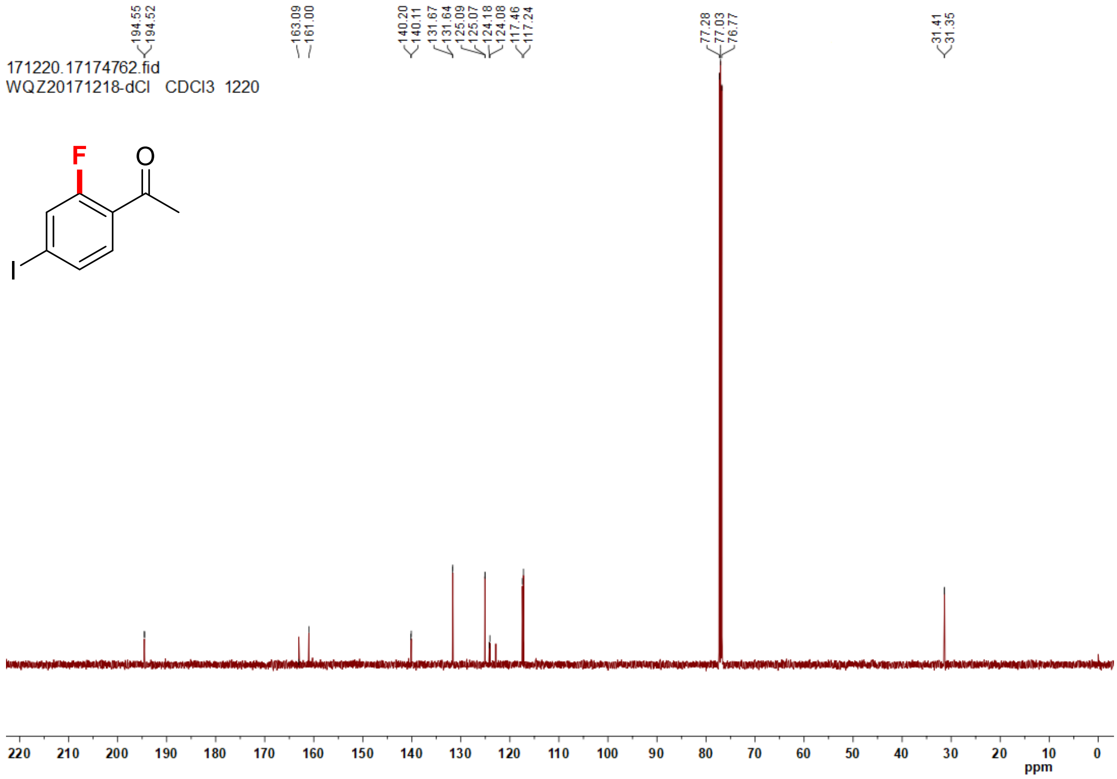
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117.24
77.28
77.03
76.77
31.41
31.35
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F
O
I
220
210
200
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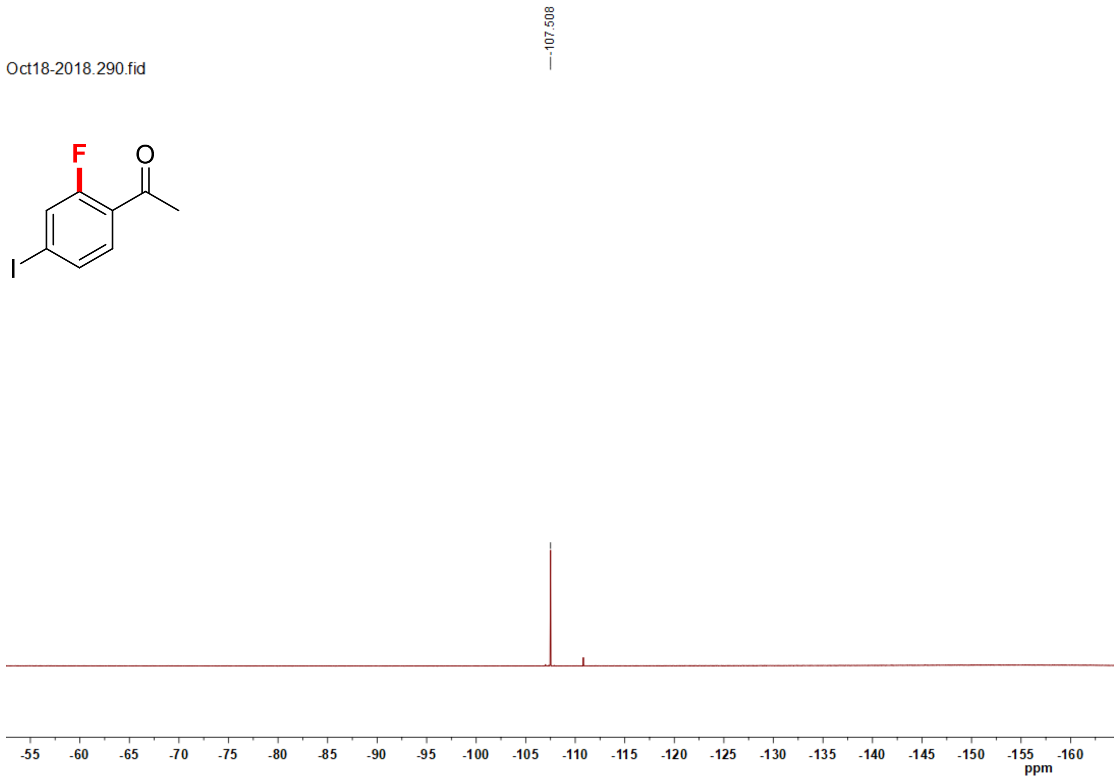
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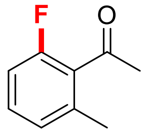

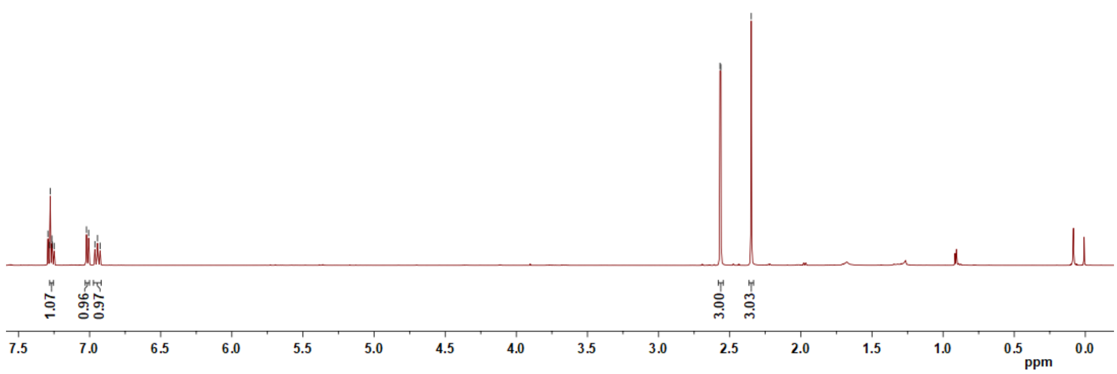

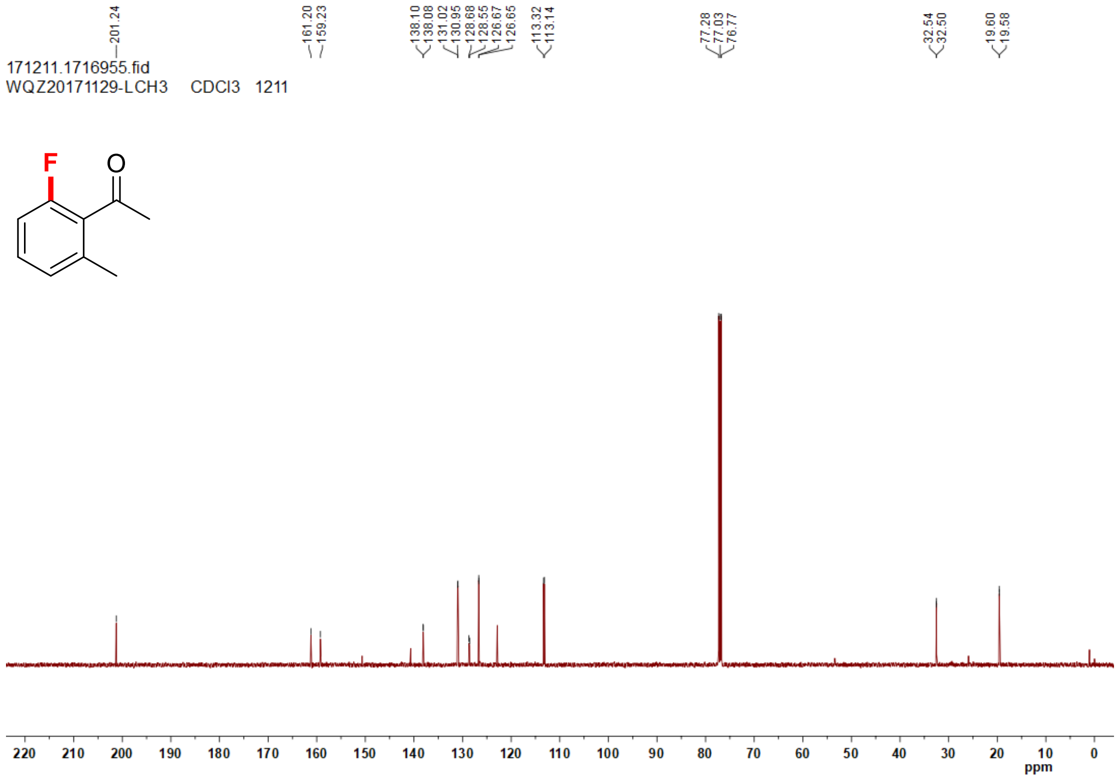

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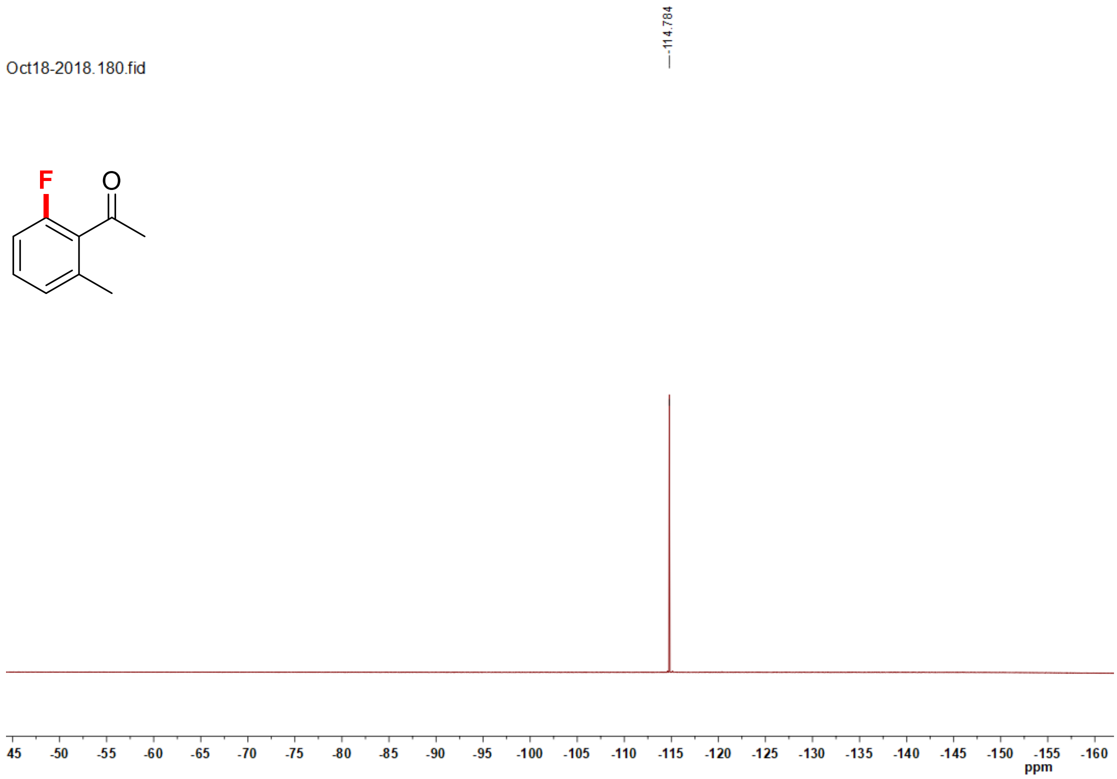
O
ppm



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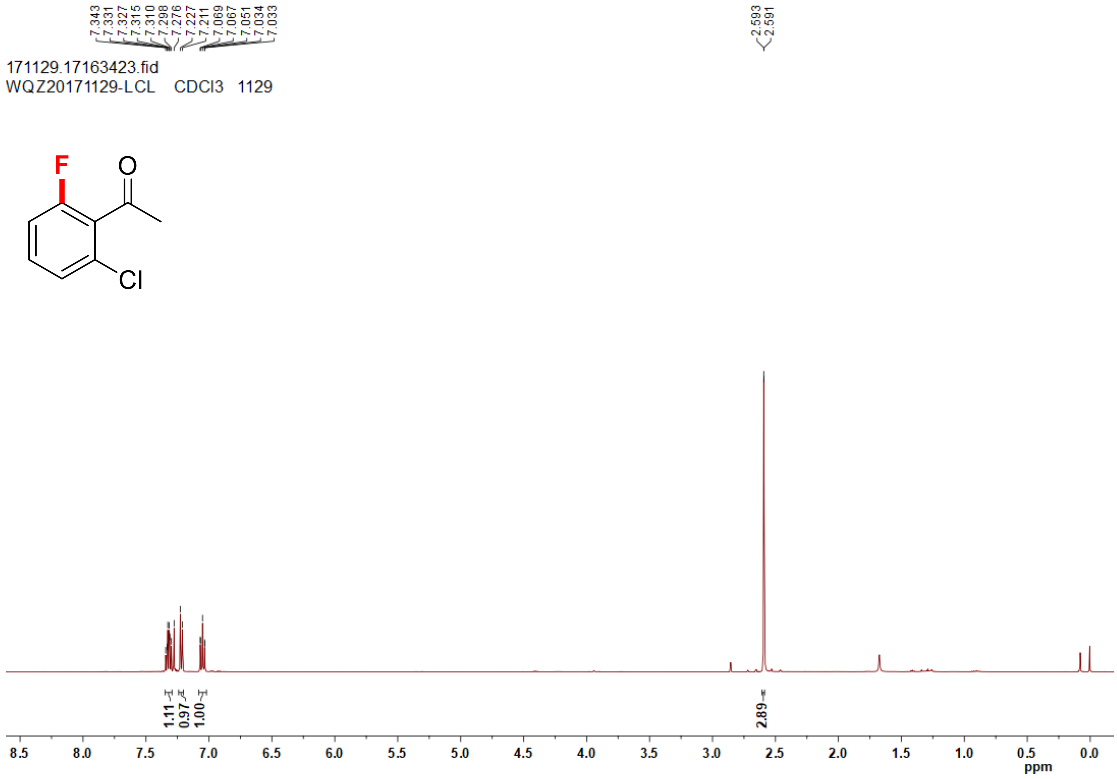
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2.593
2.591
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F
O
Cl
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0.97
1.00
2.89
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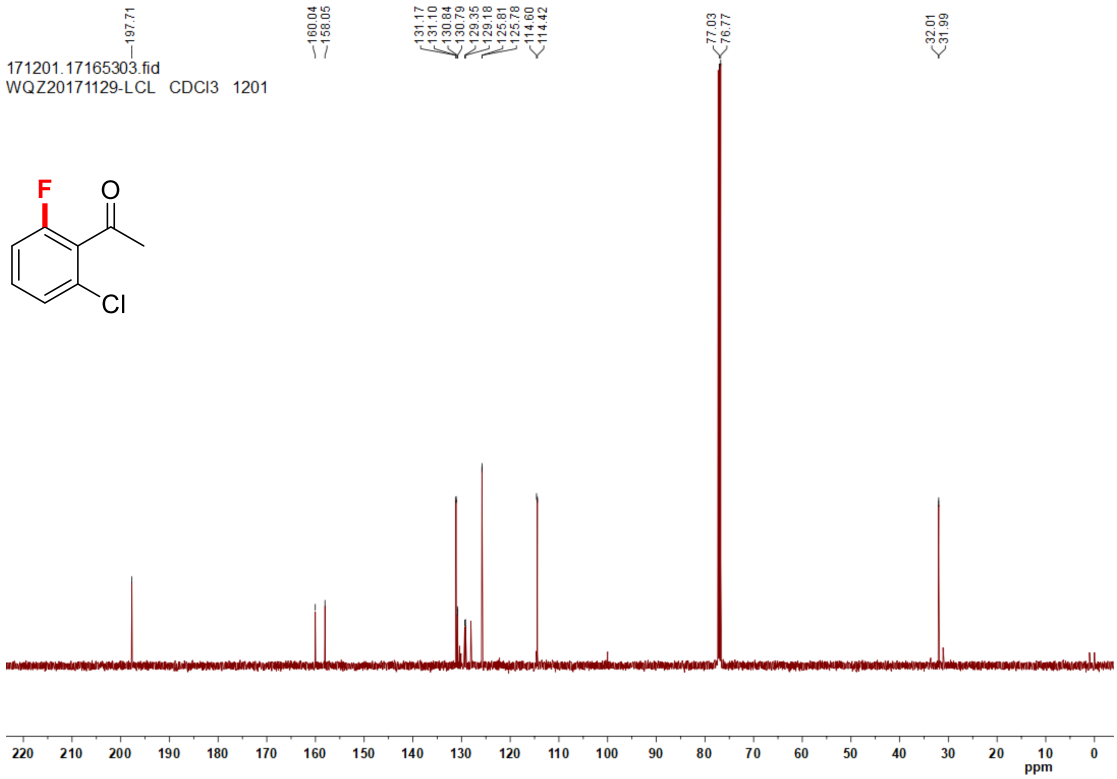
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O
Cl
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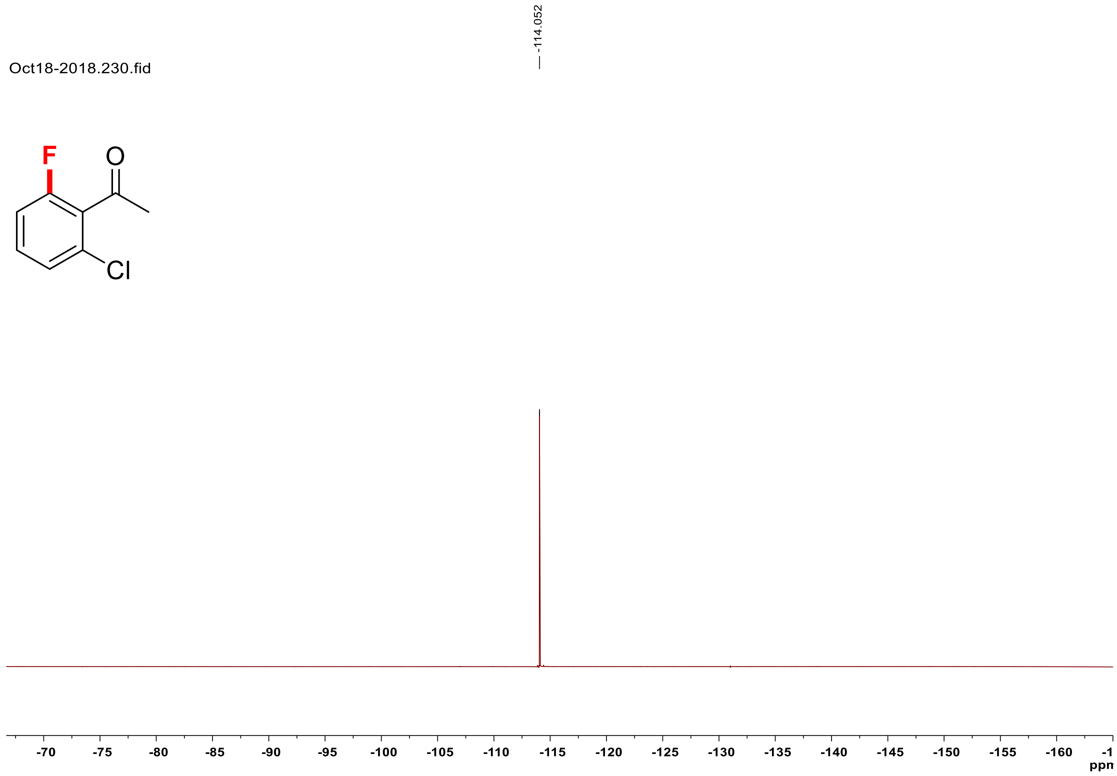

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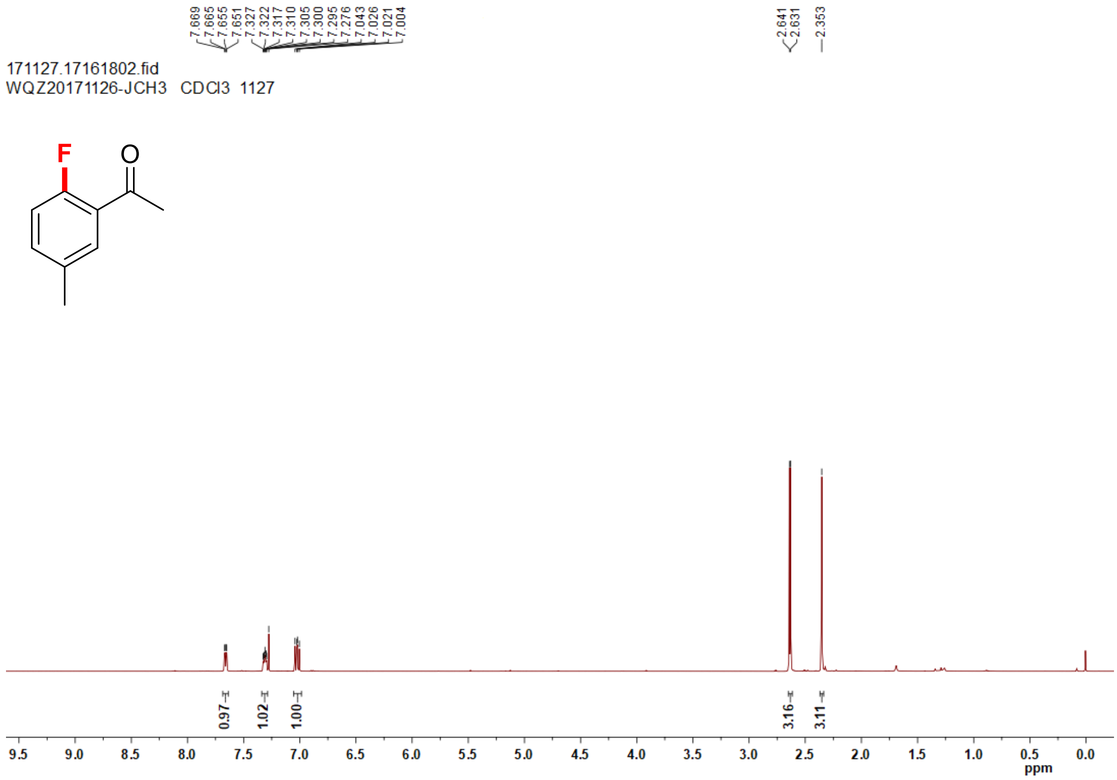

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2.631
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F
O
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1.00
3.16
3.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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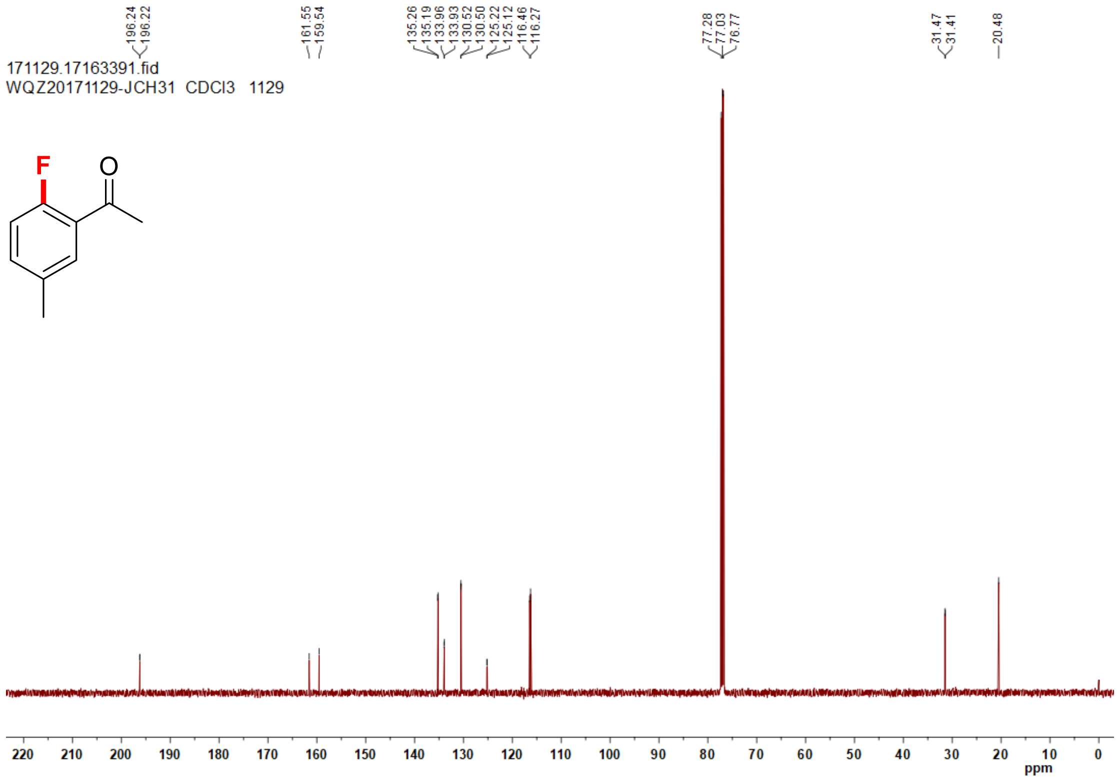
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O
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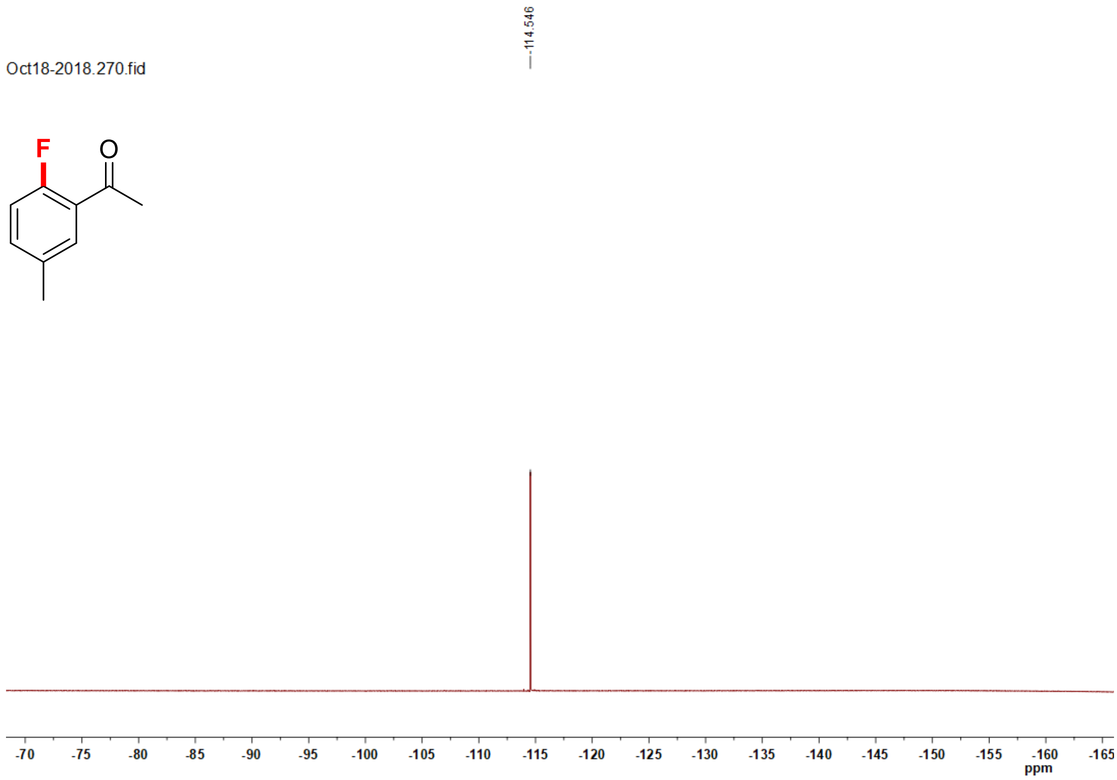
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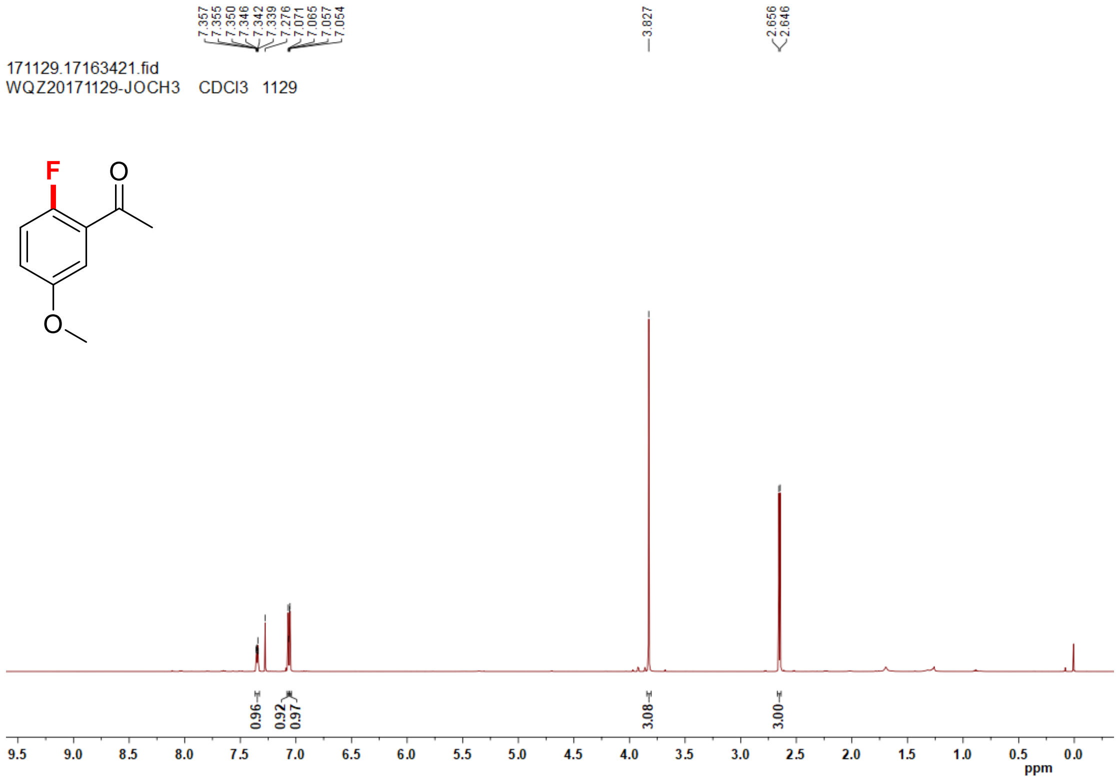
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2.646
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WQZ20171129-JOCH3 CDCl3 1129
F
O
O
0.96
0.92
0.97
3.08
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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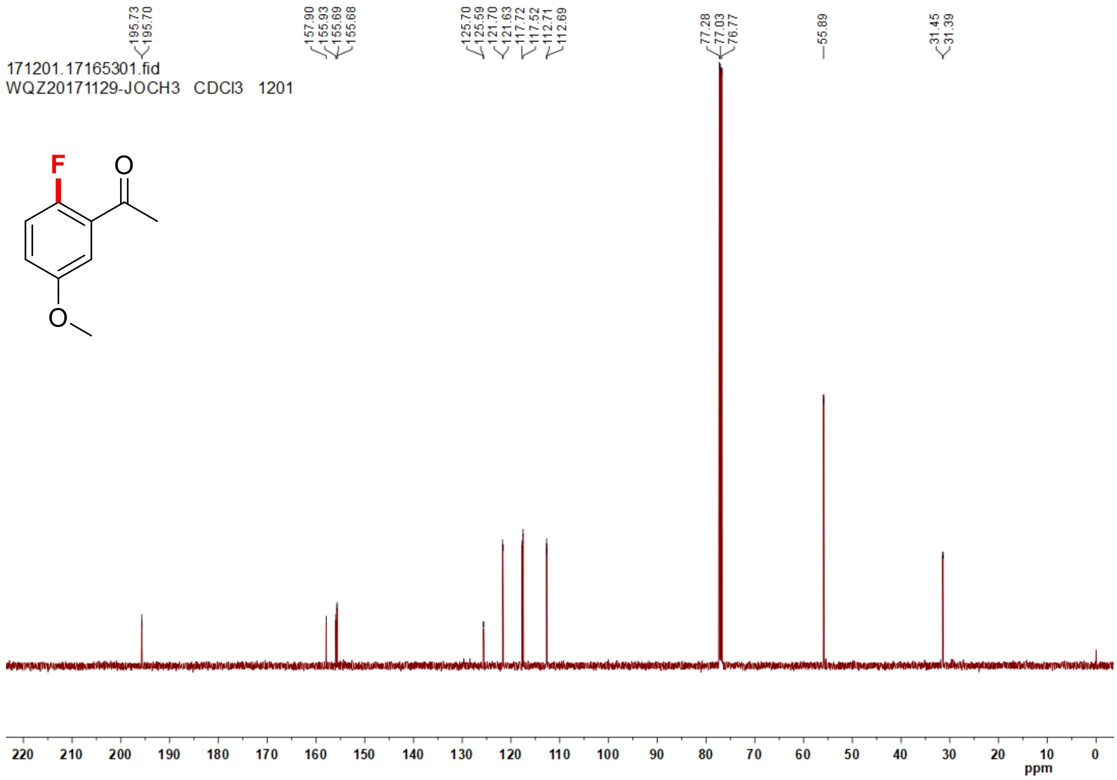
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77.03
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31.39
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O
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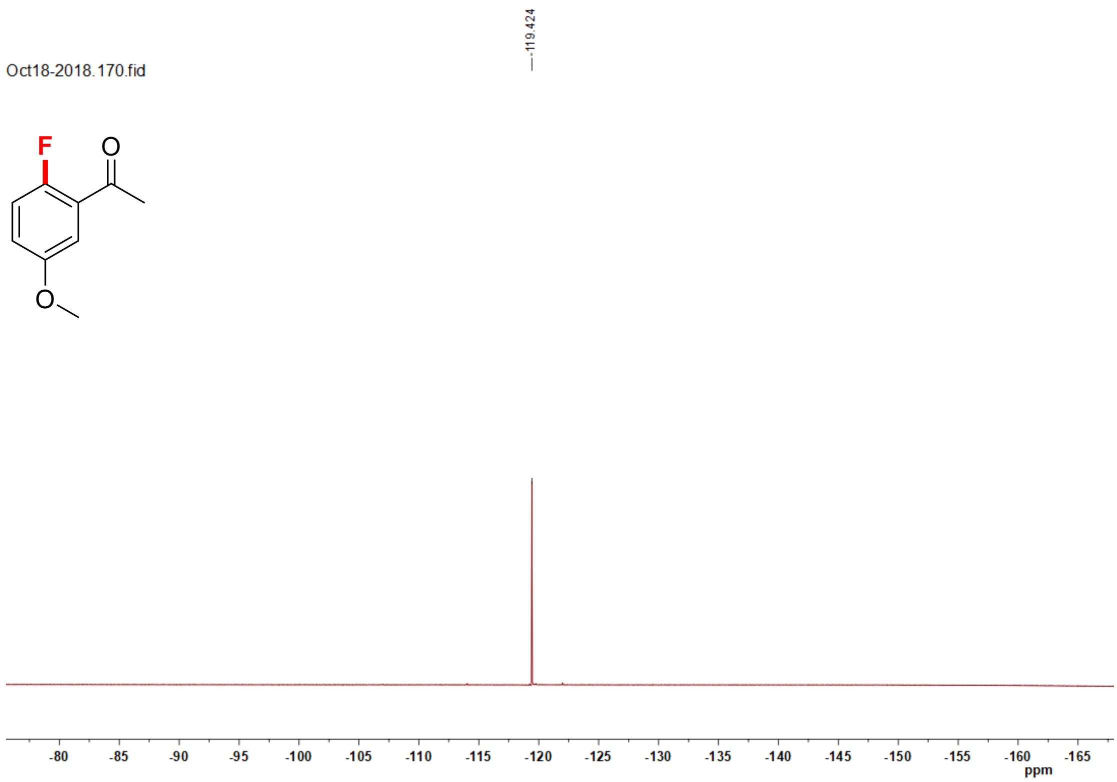
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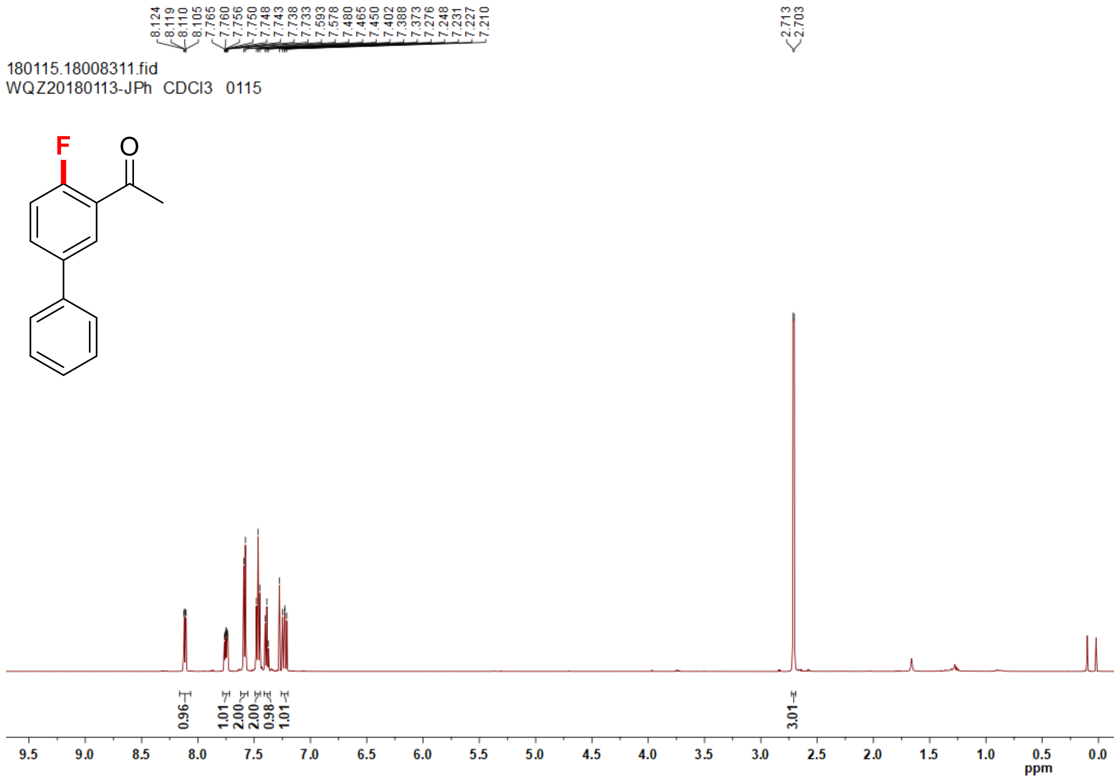
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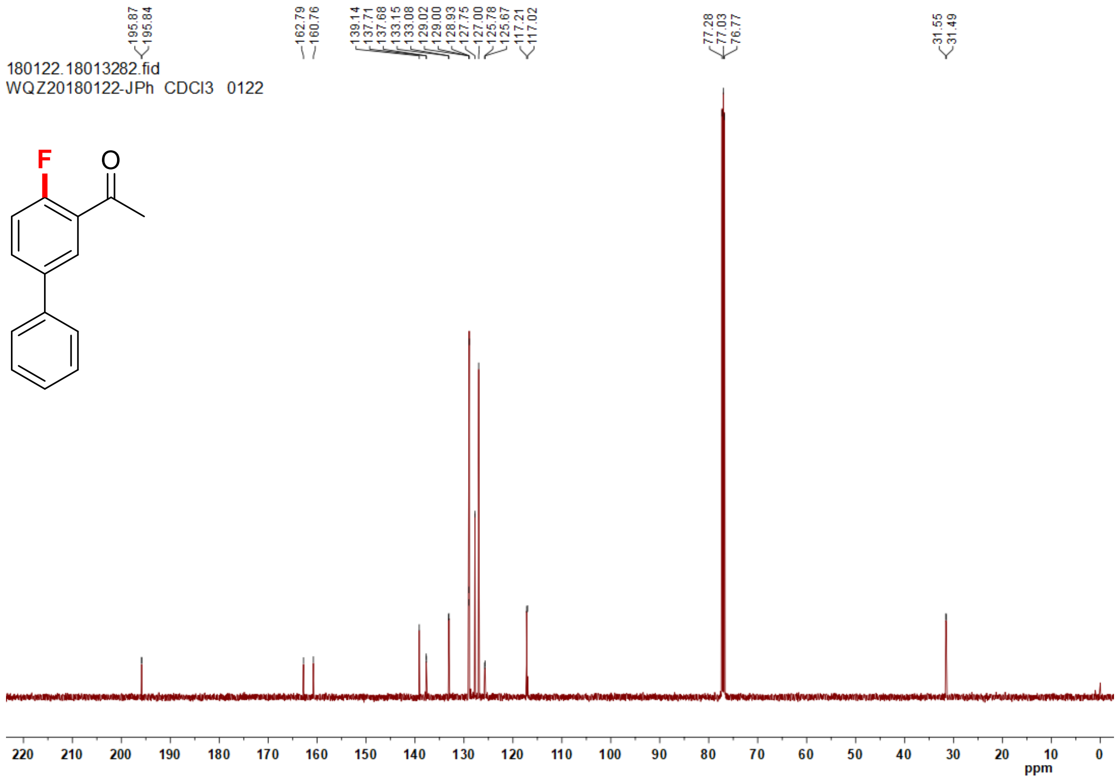
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77.03
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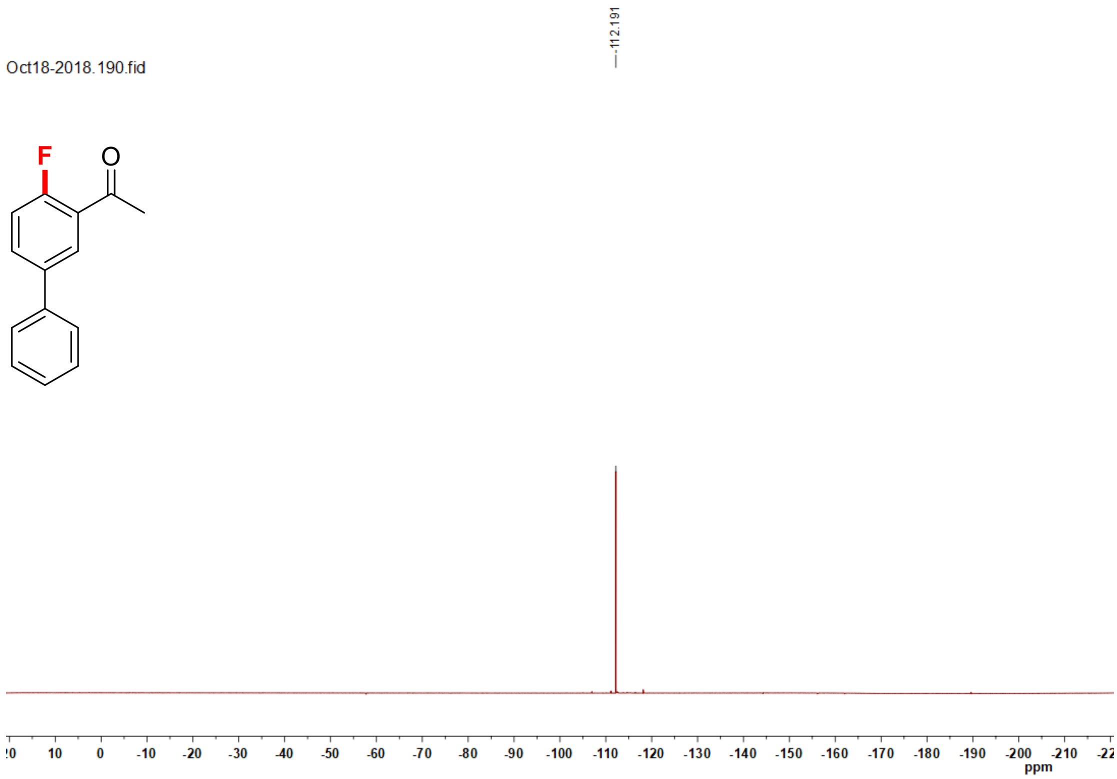
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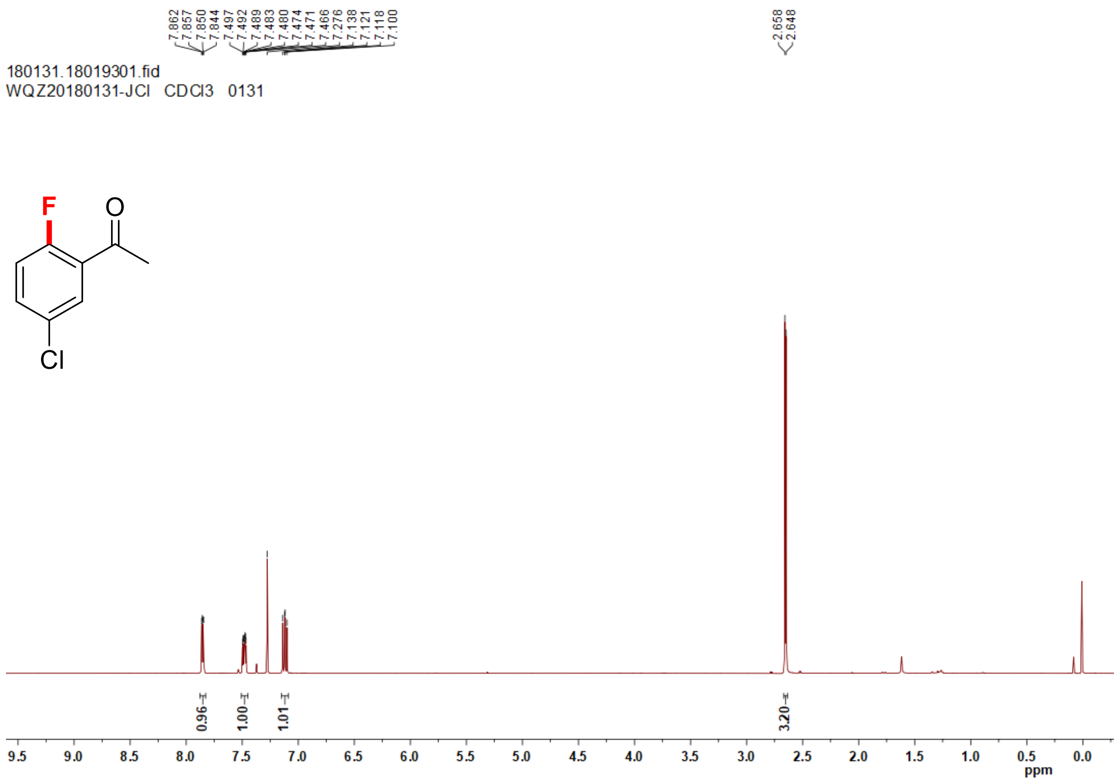
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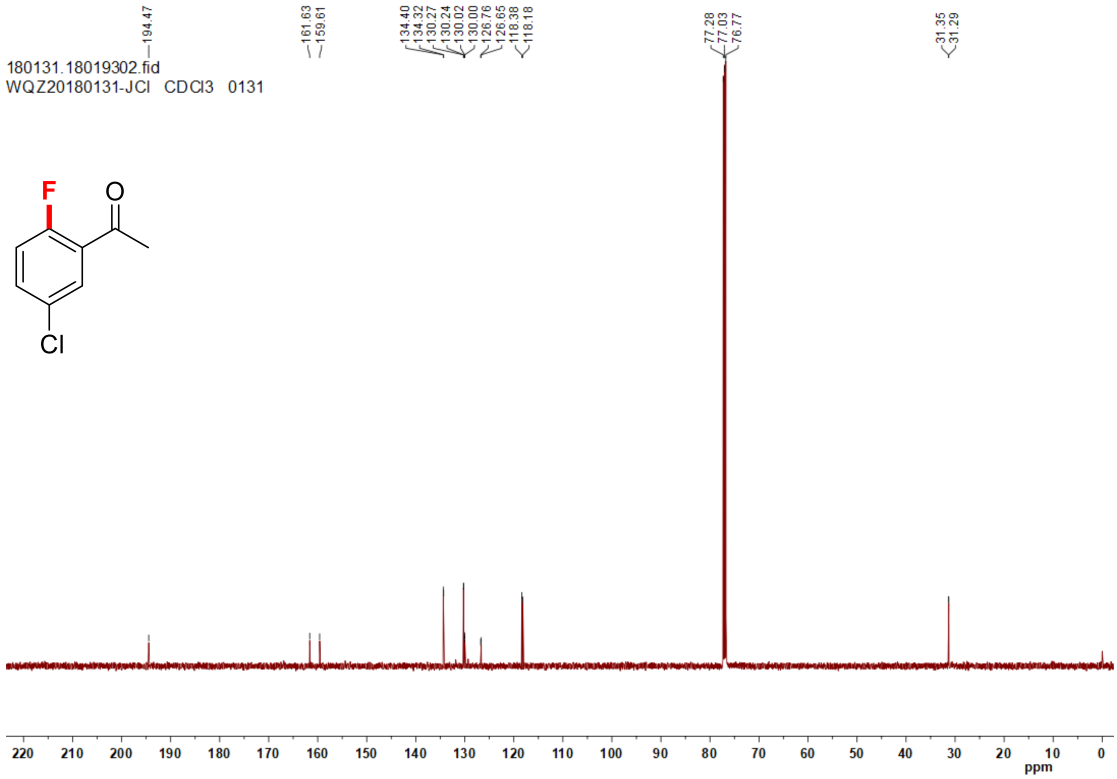
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77.03
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31.35
31.29
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Cl
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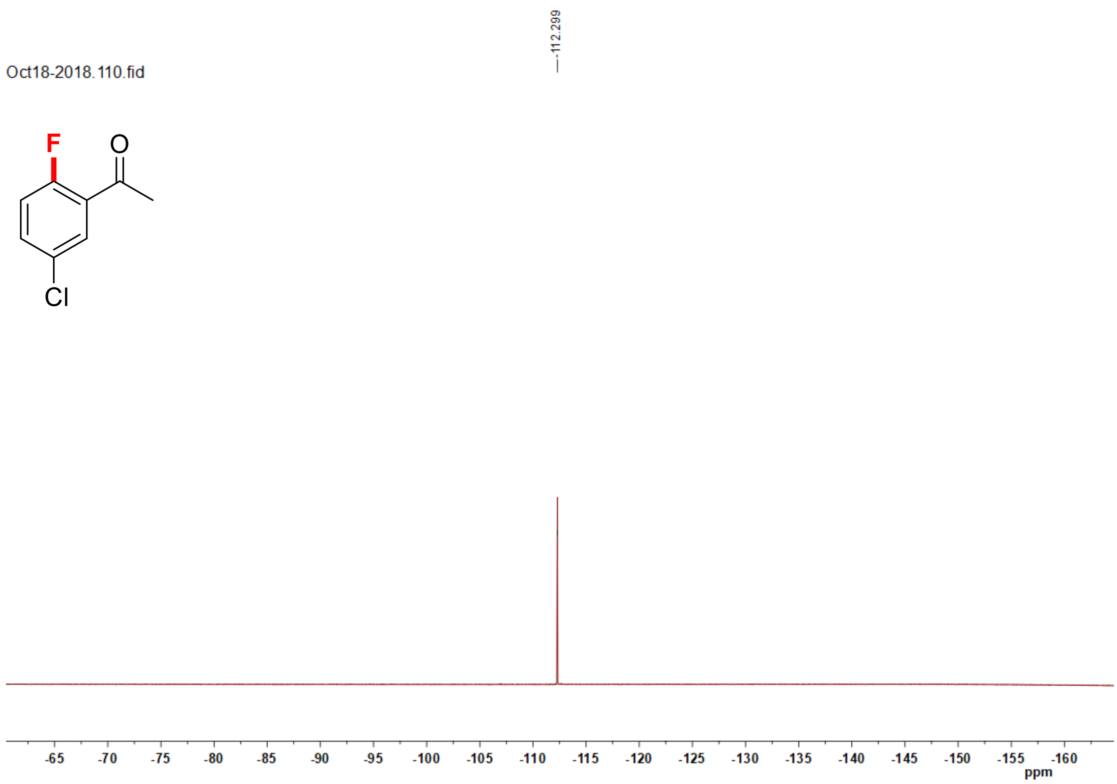

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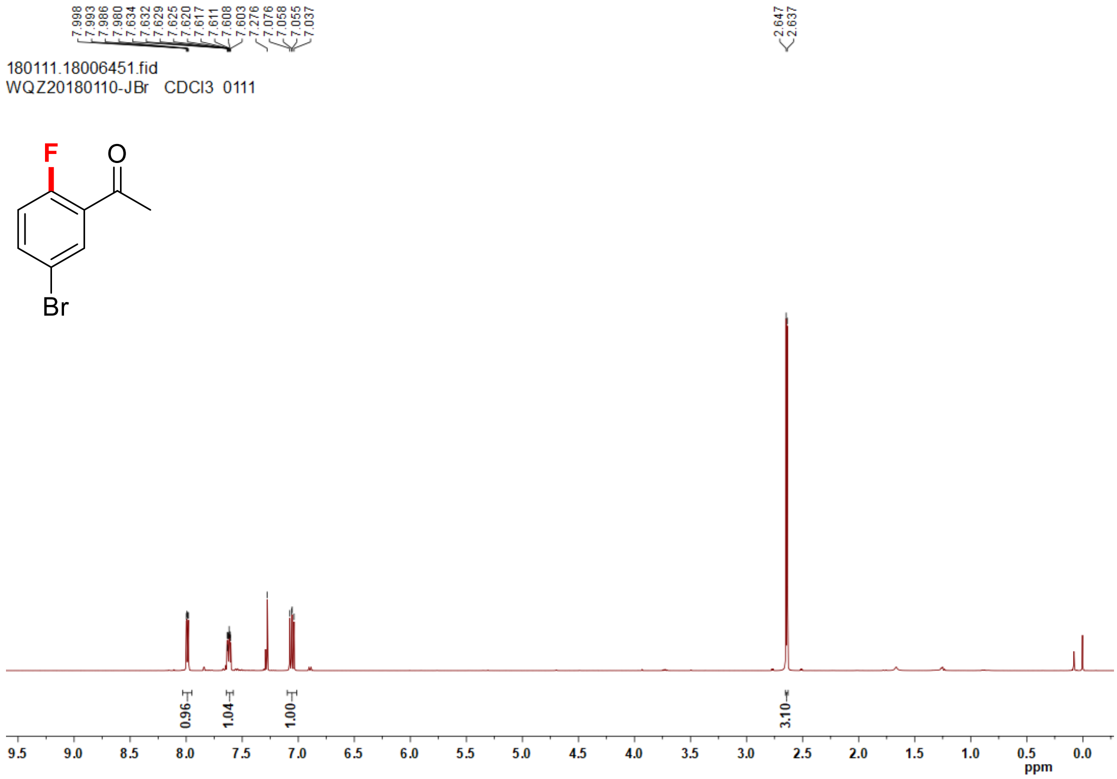

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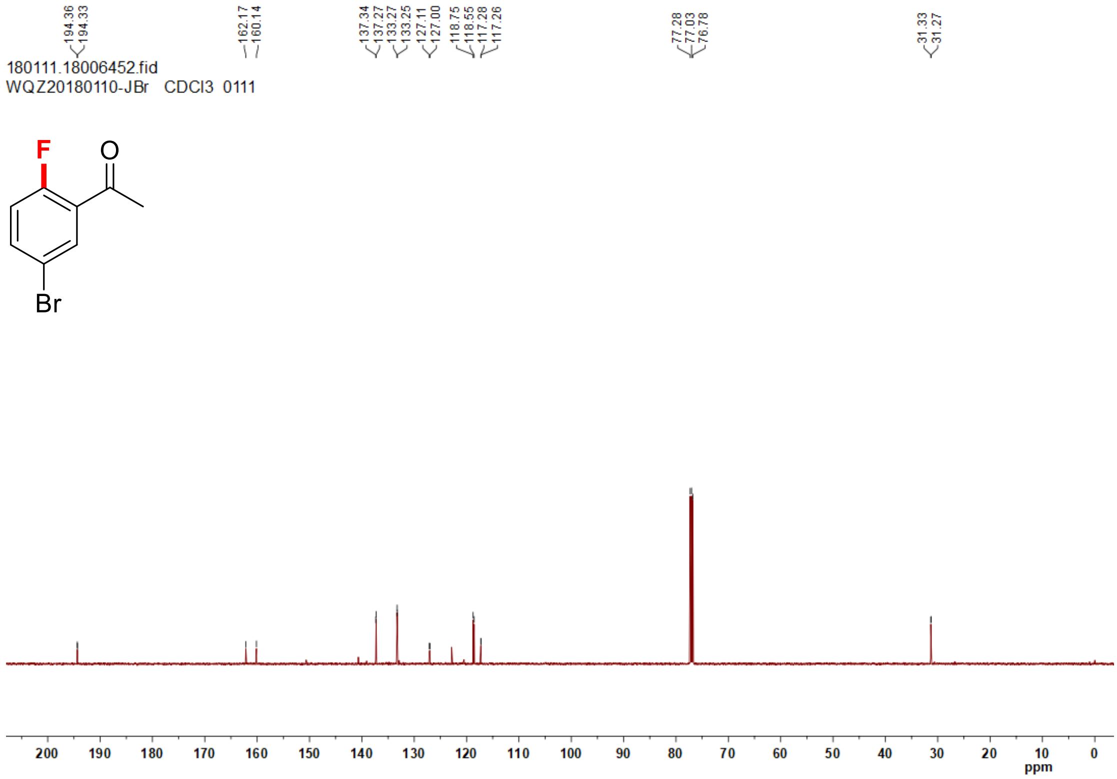

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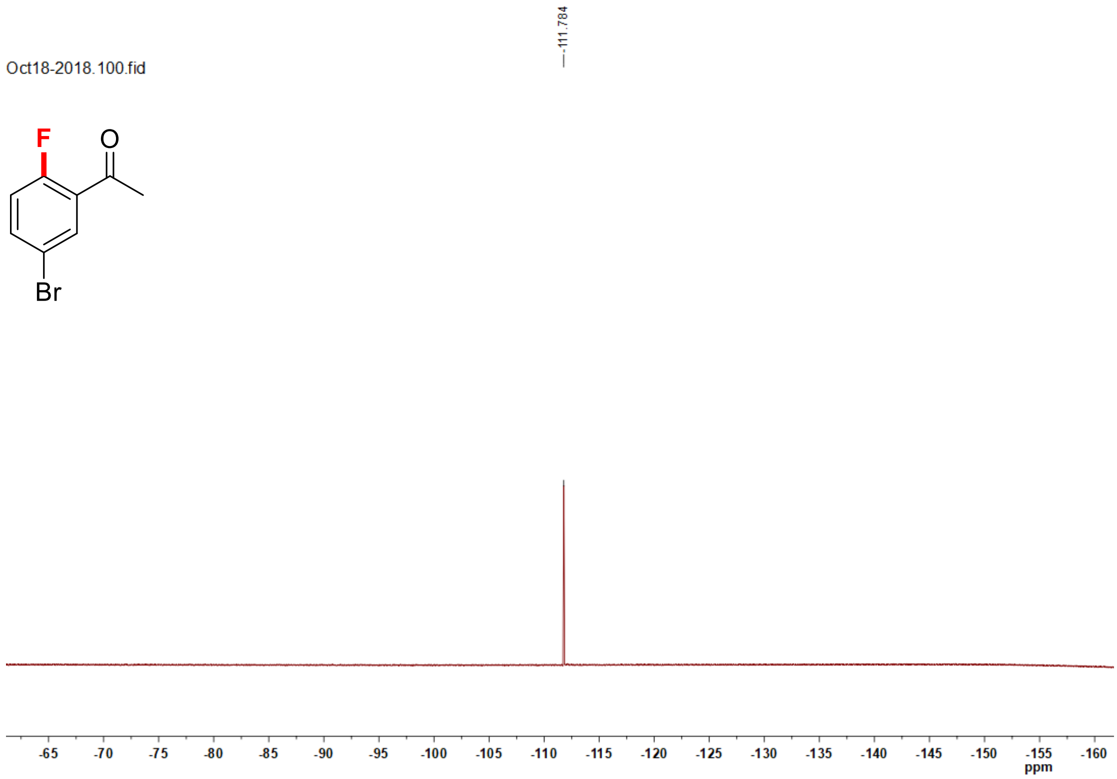

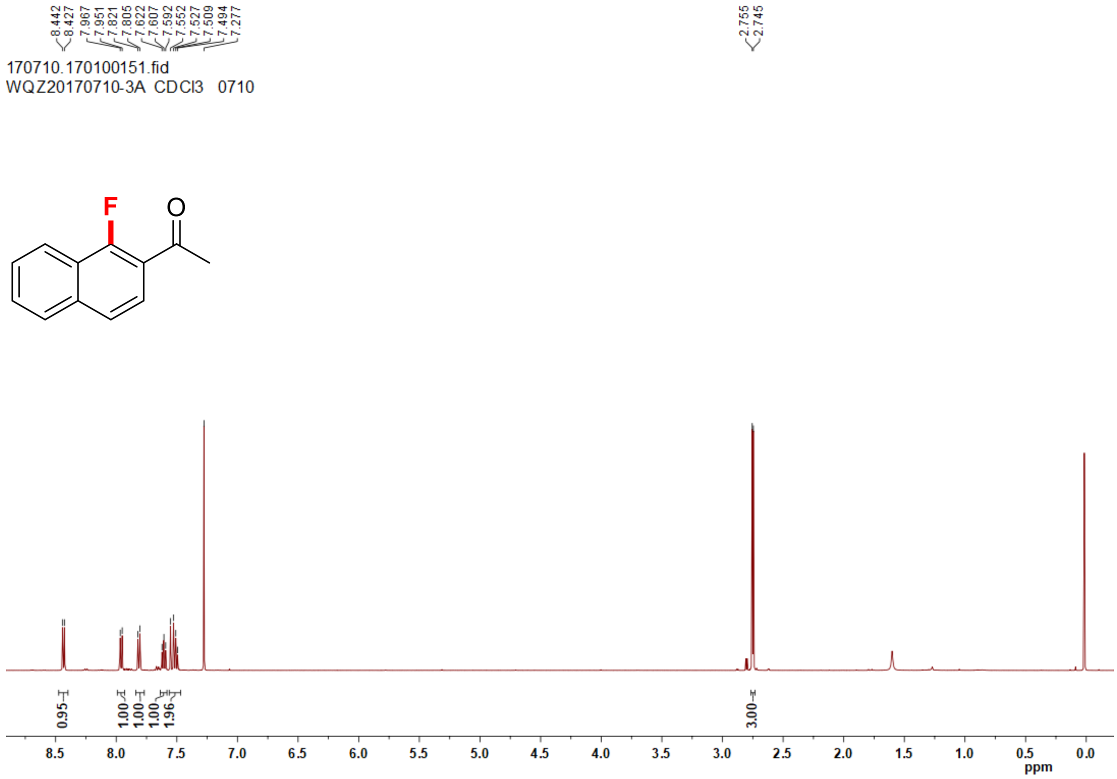
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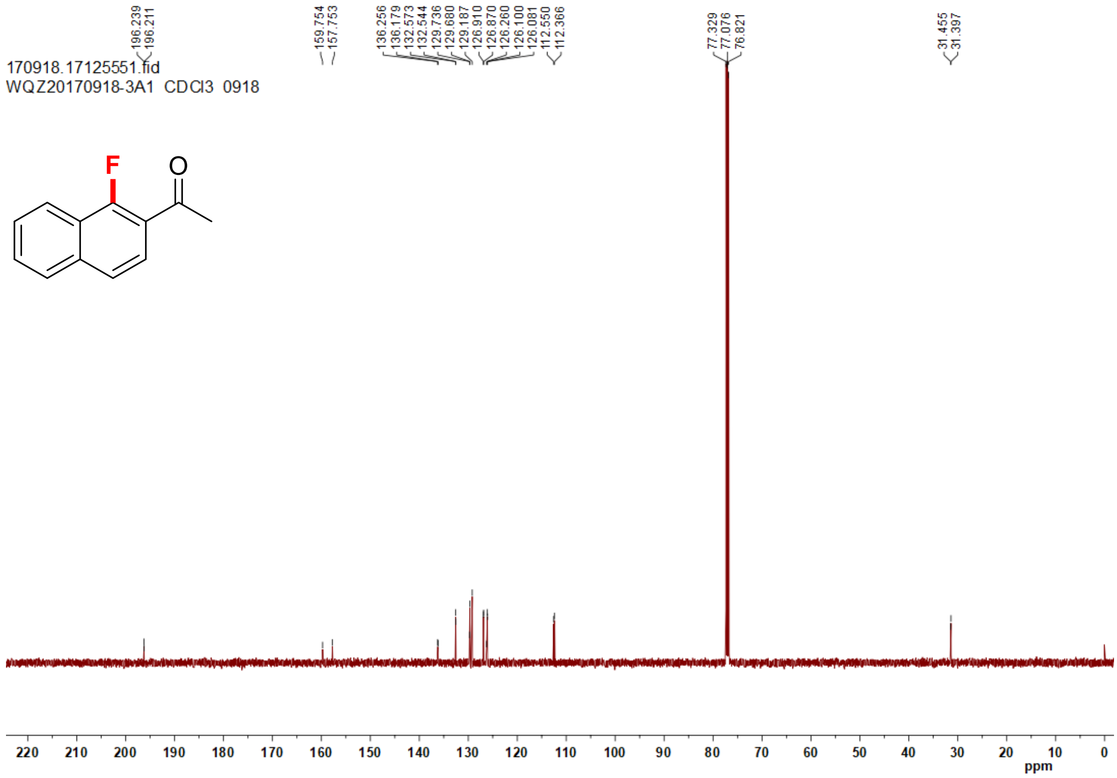
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O
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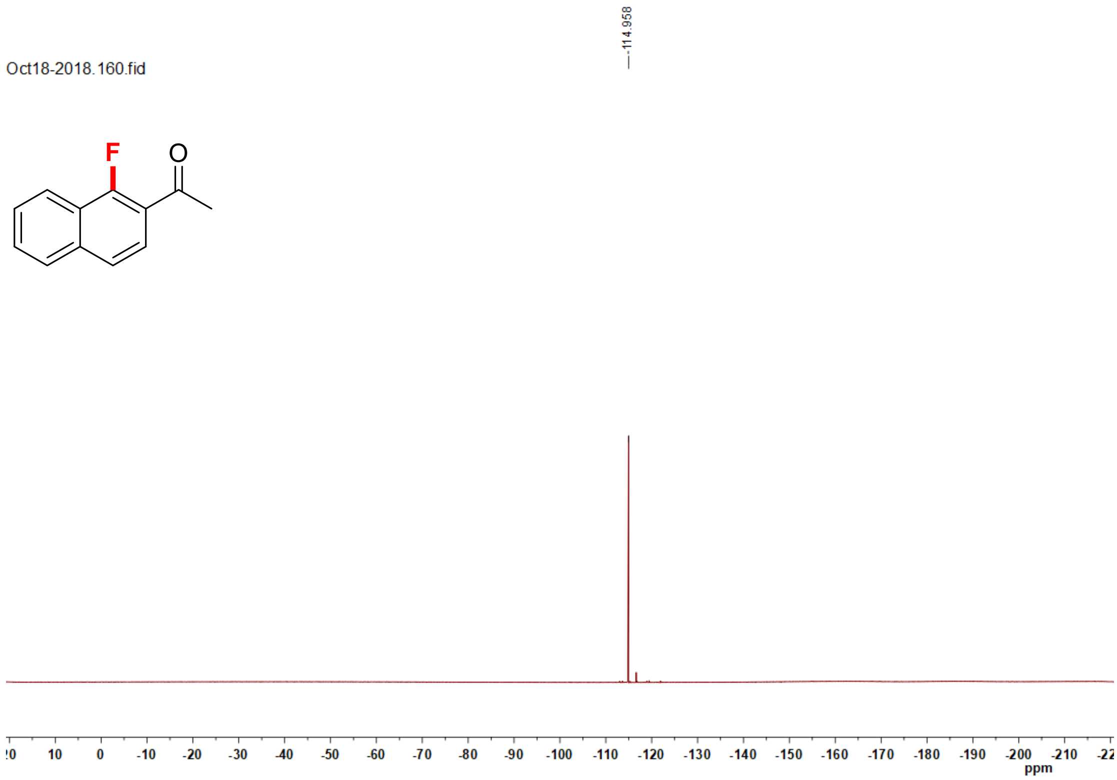

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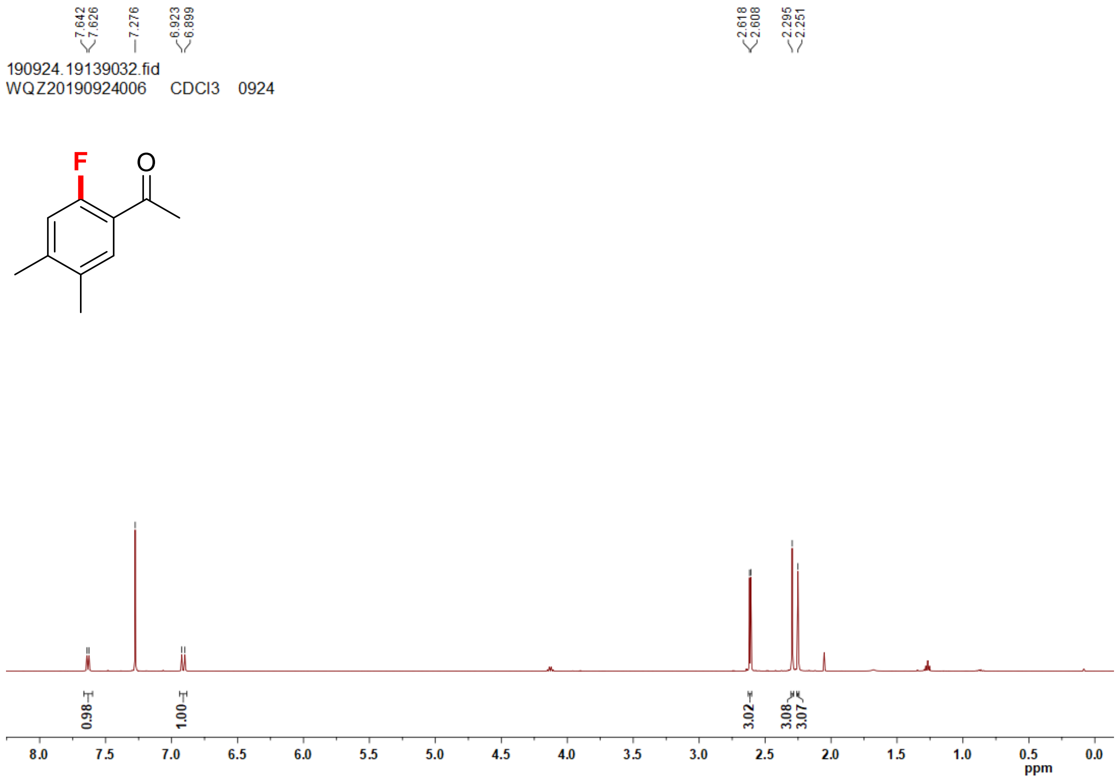

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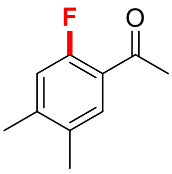

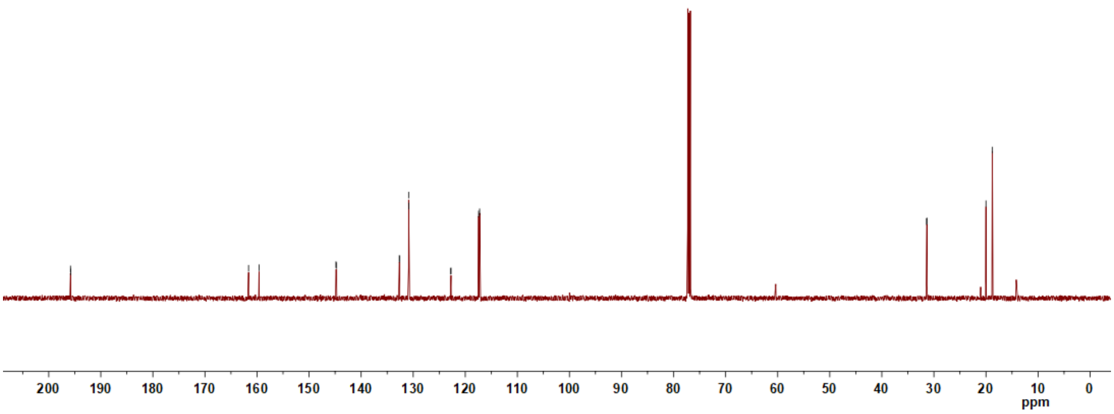

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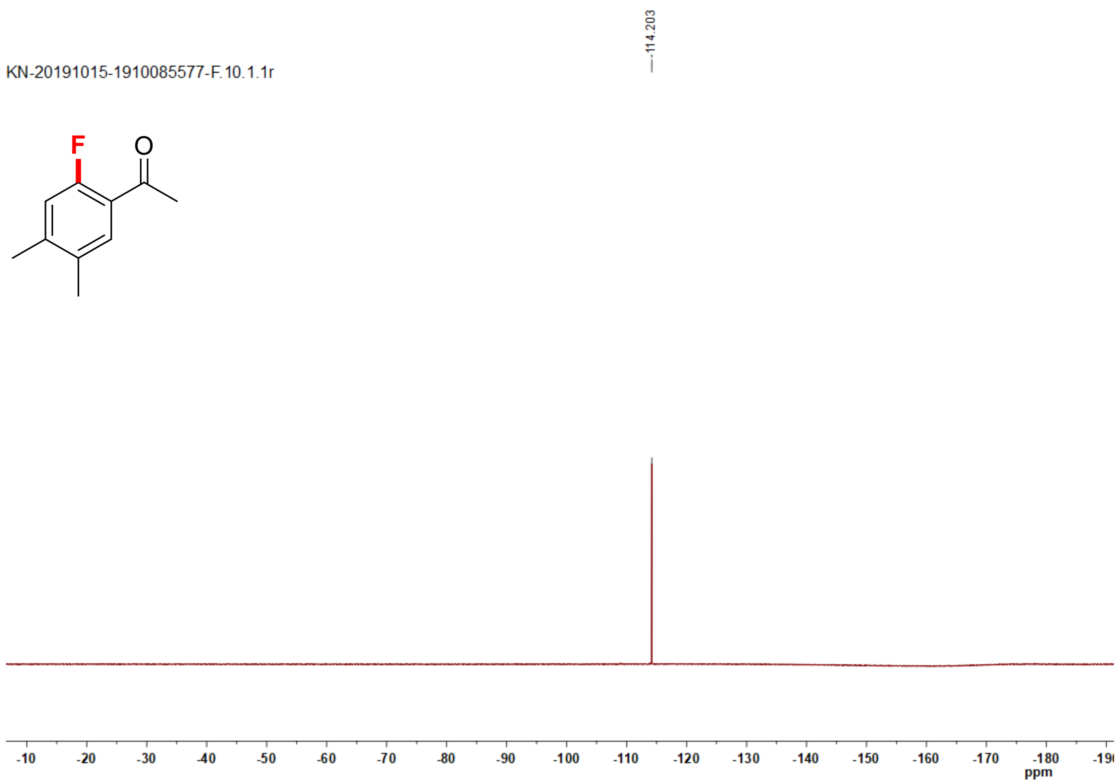

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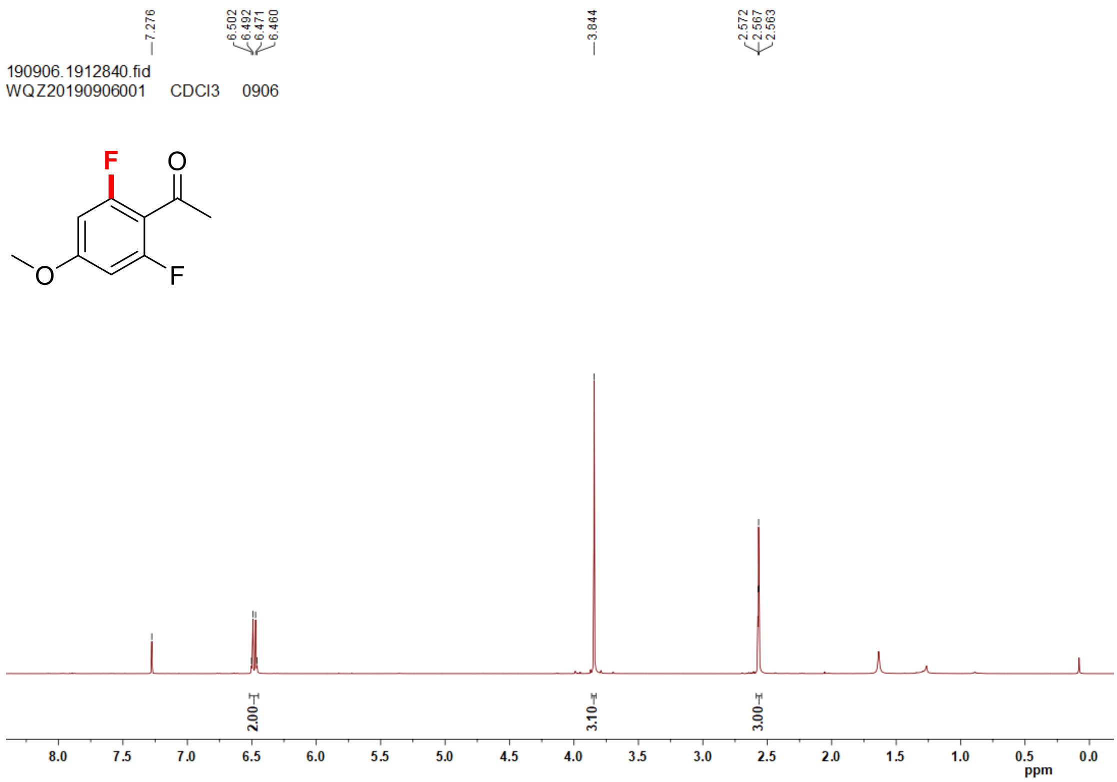

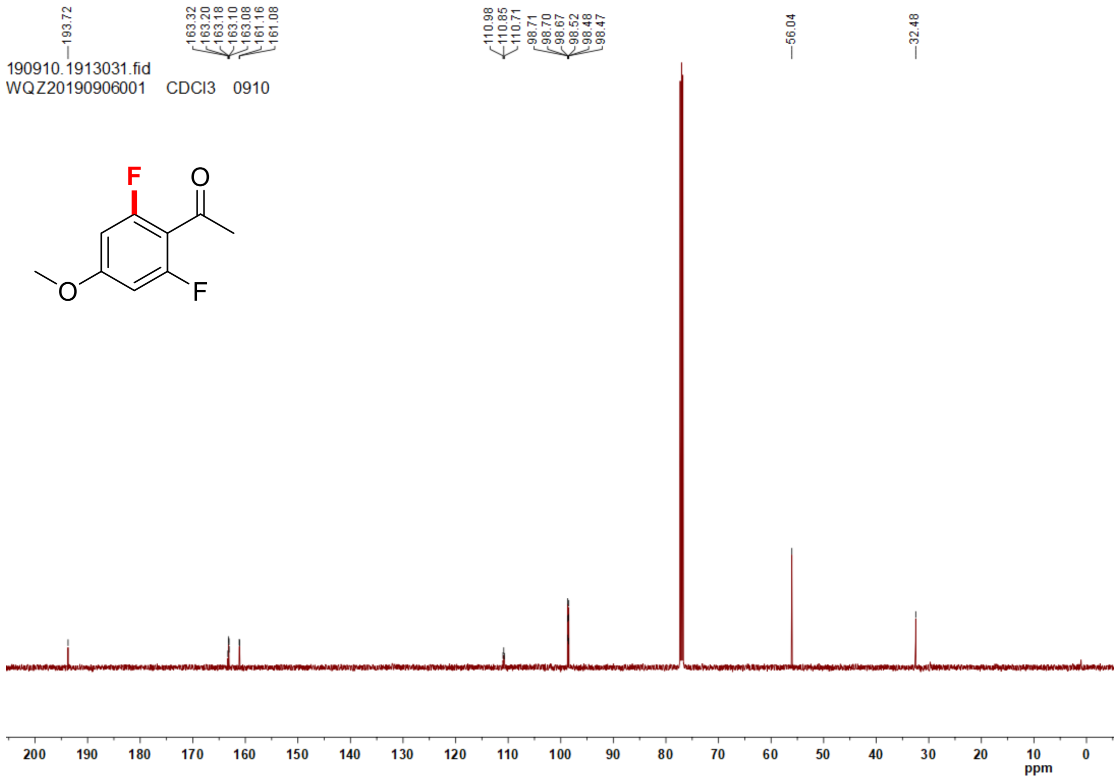

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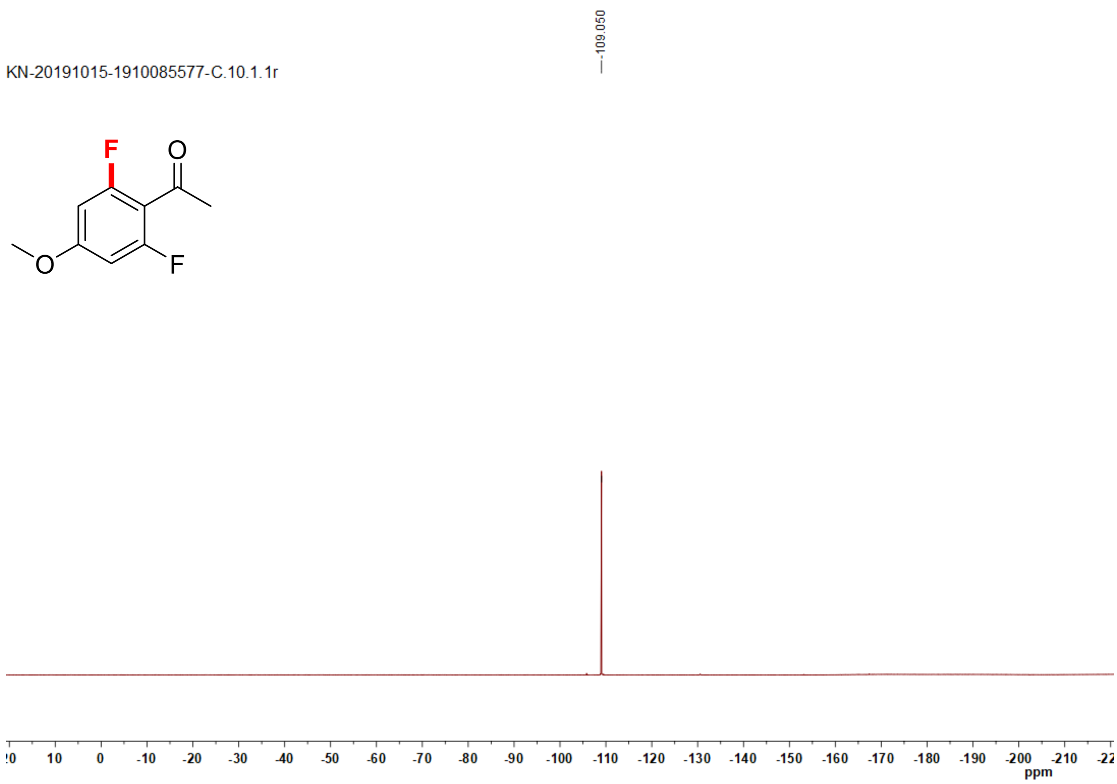

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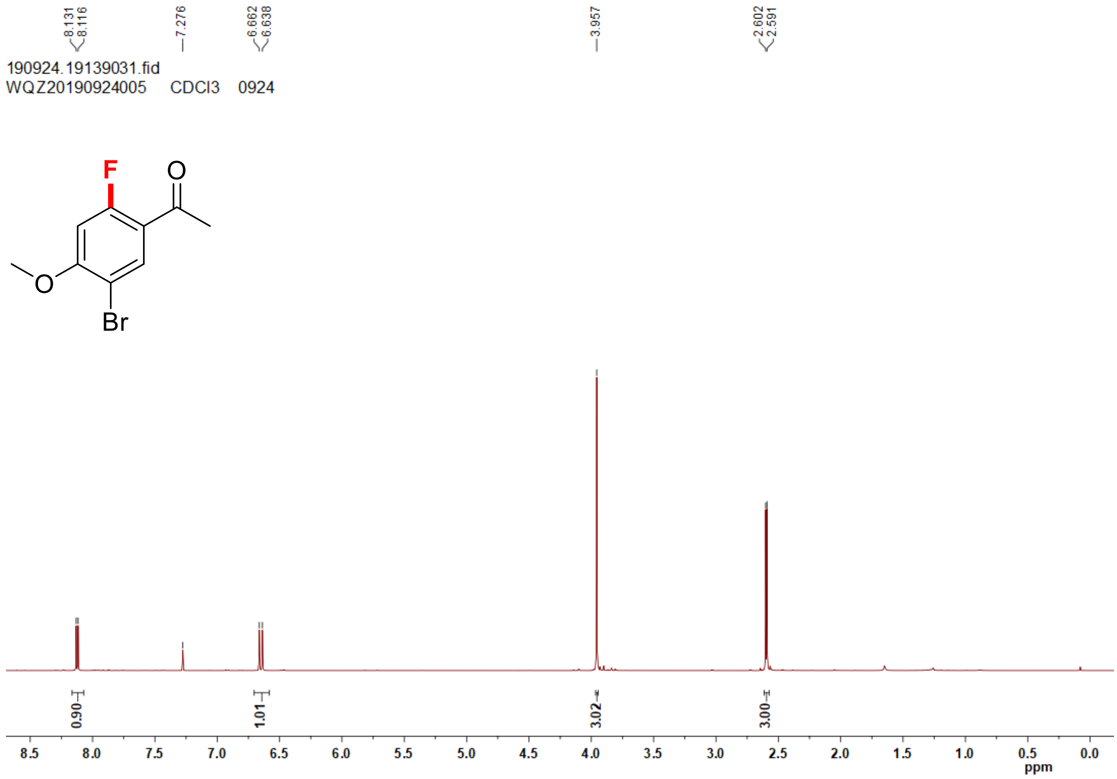

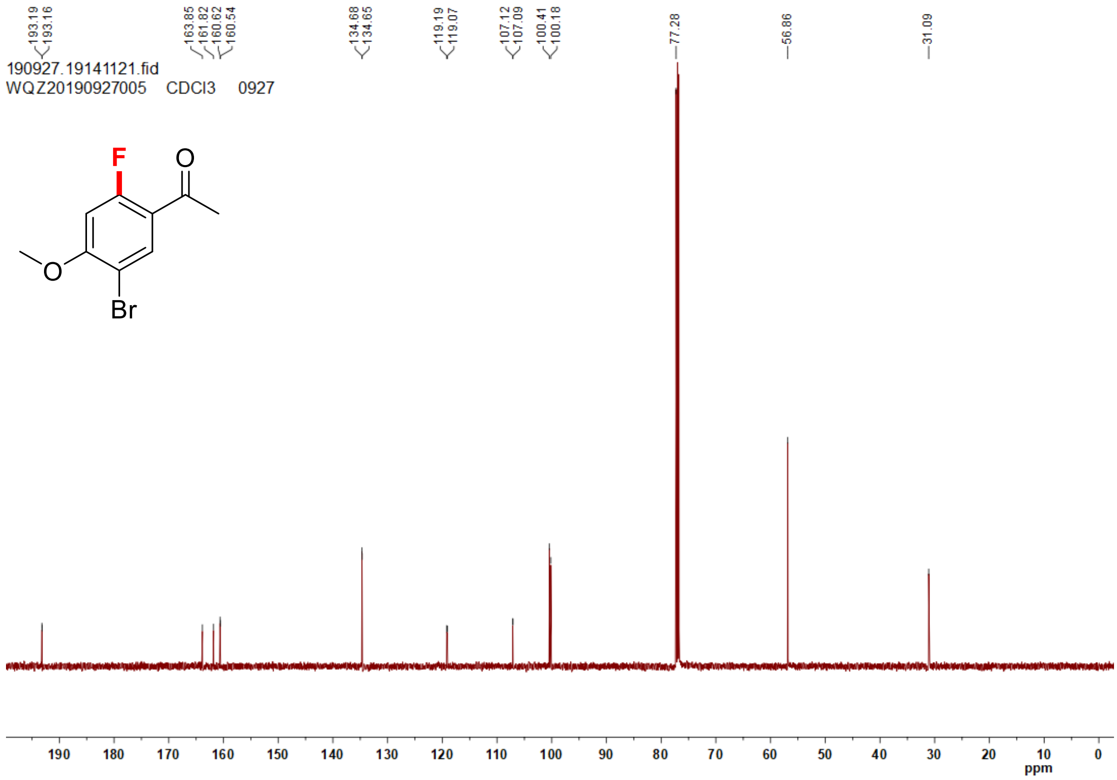
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Br
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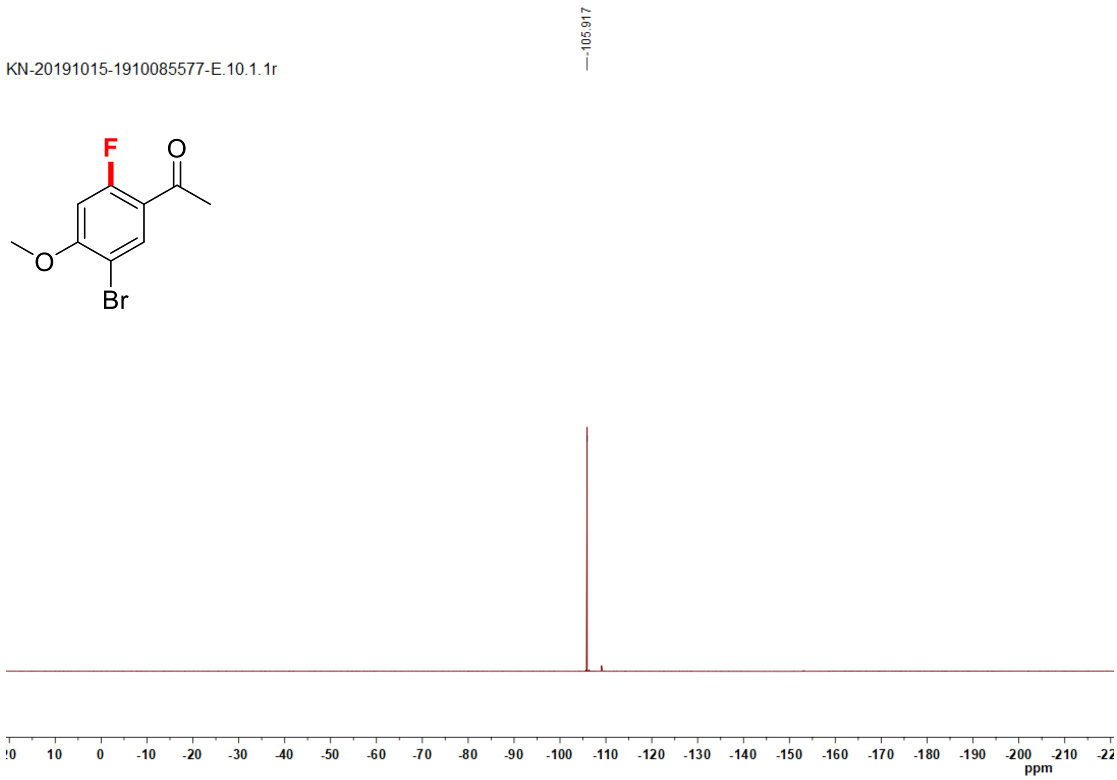
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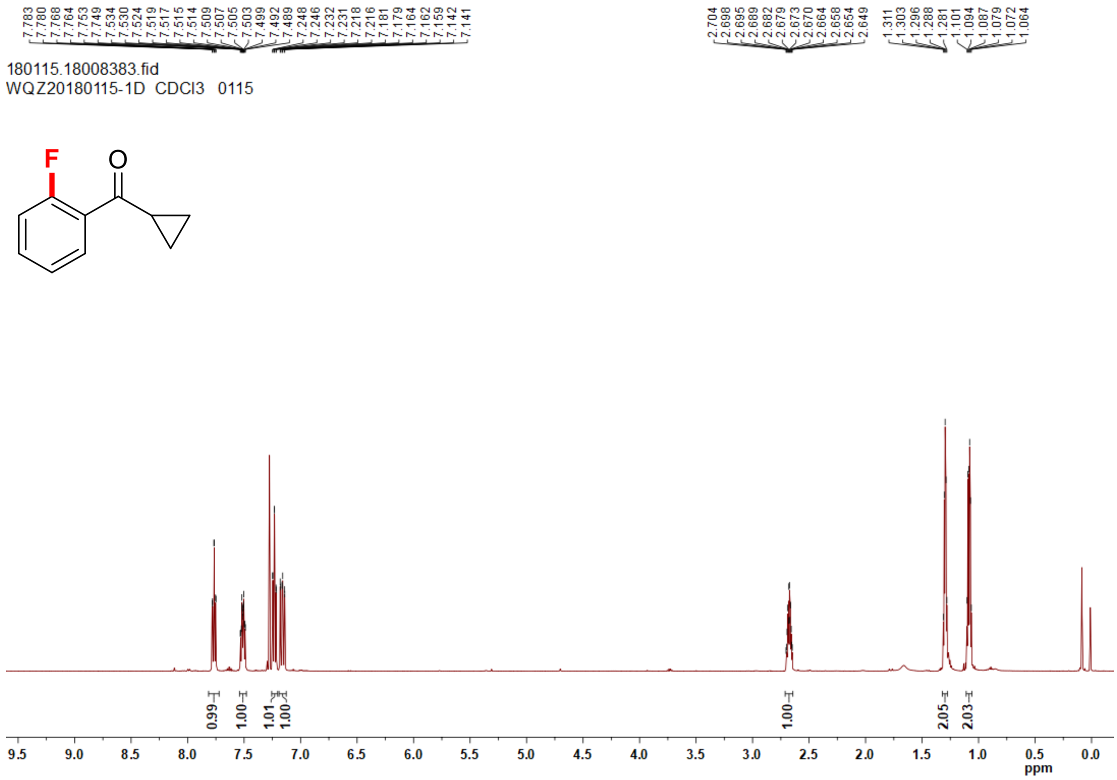
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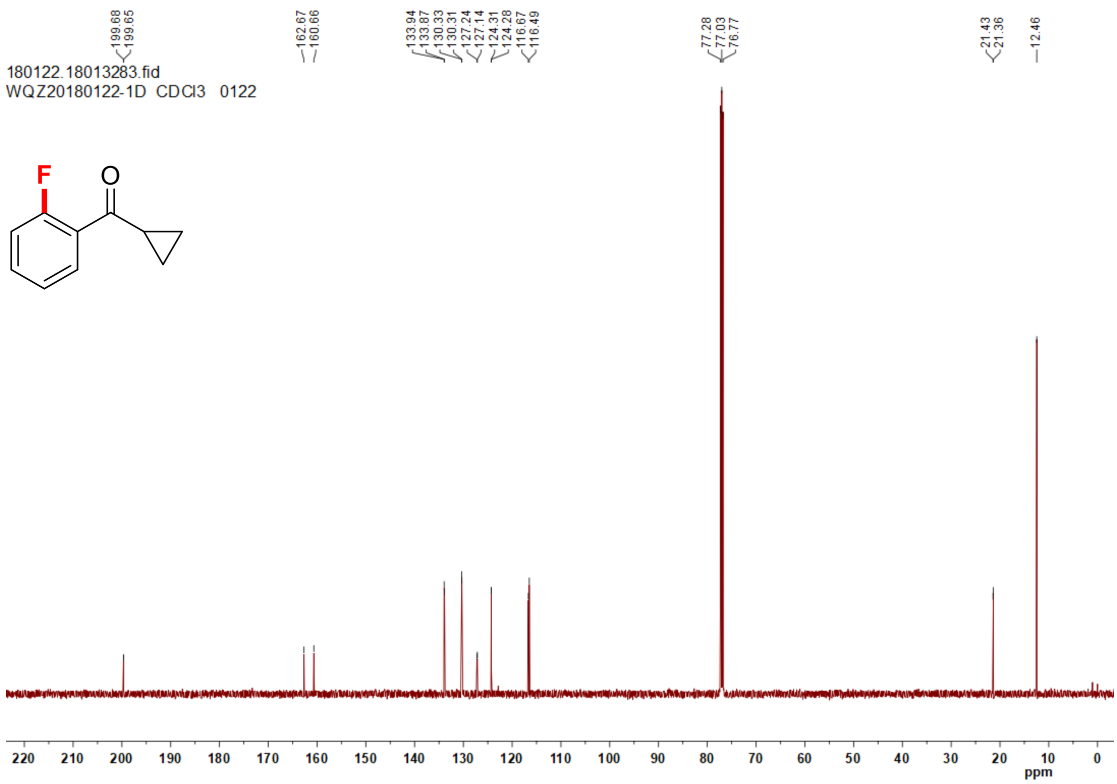
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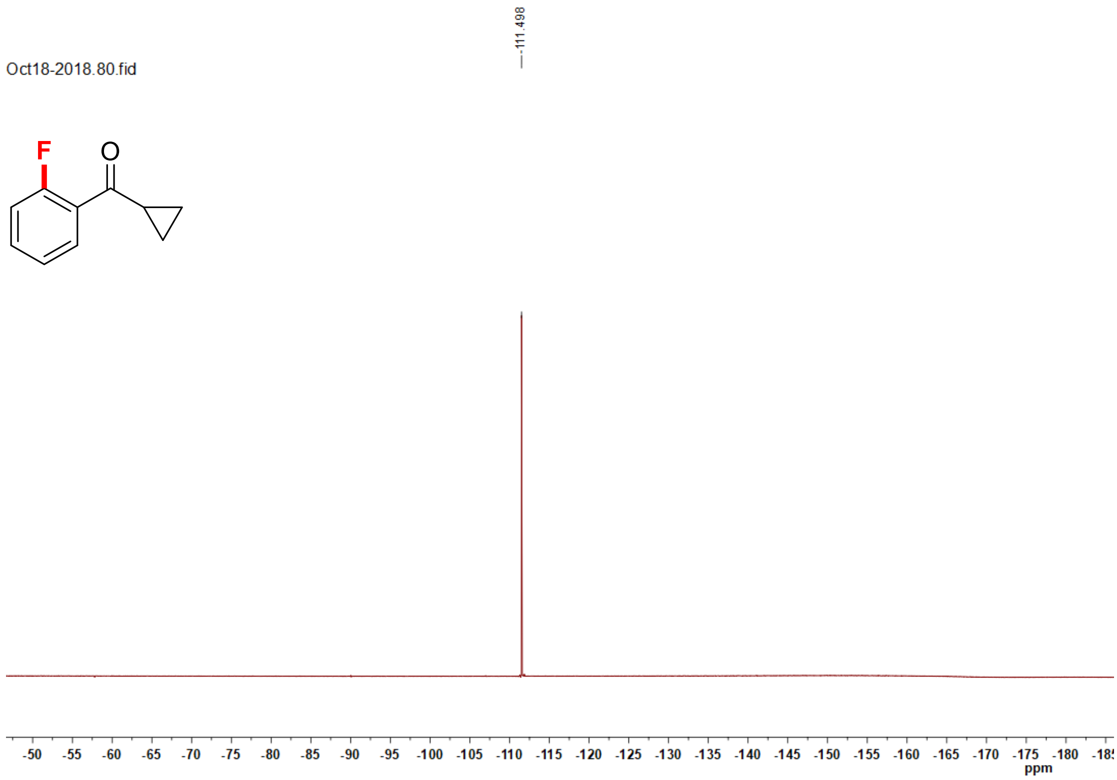
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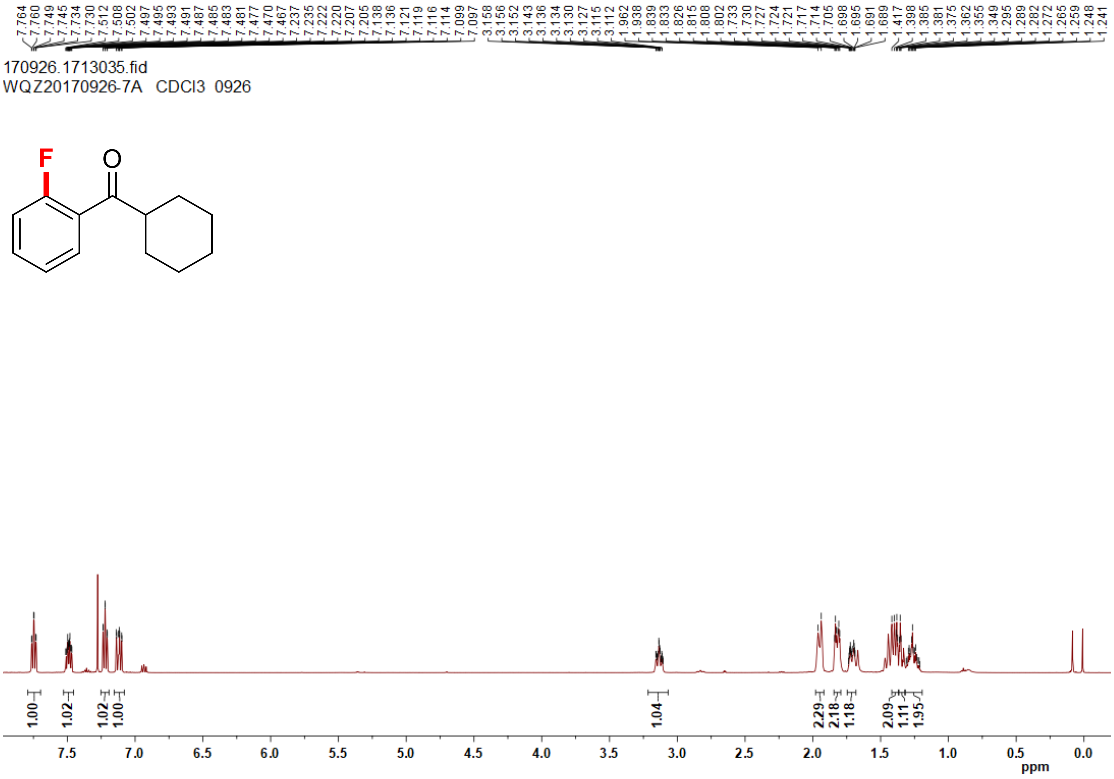
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170926.1713035.fid
WQZ20170926-7A CDCl3 0926
F
O
1.00 1.02 1.02 1.00 1.04 2.29 2.18 1.18 2.09 1.11 1.95
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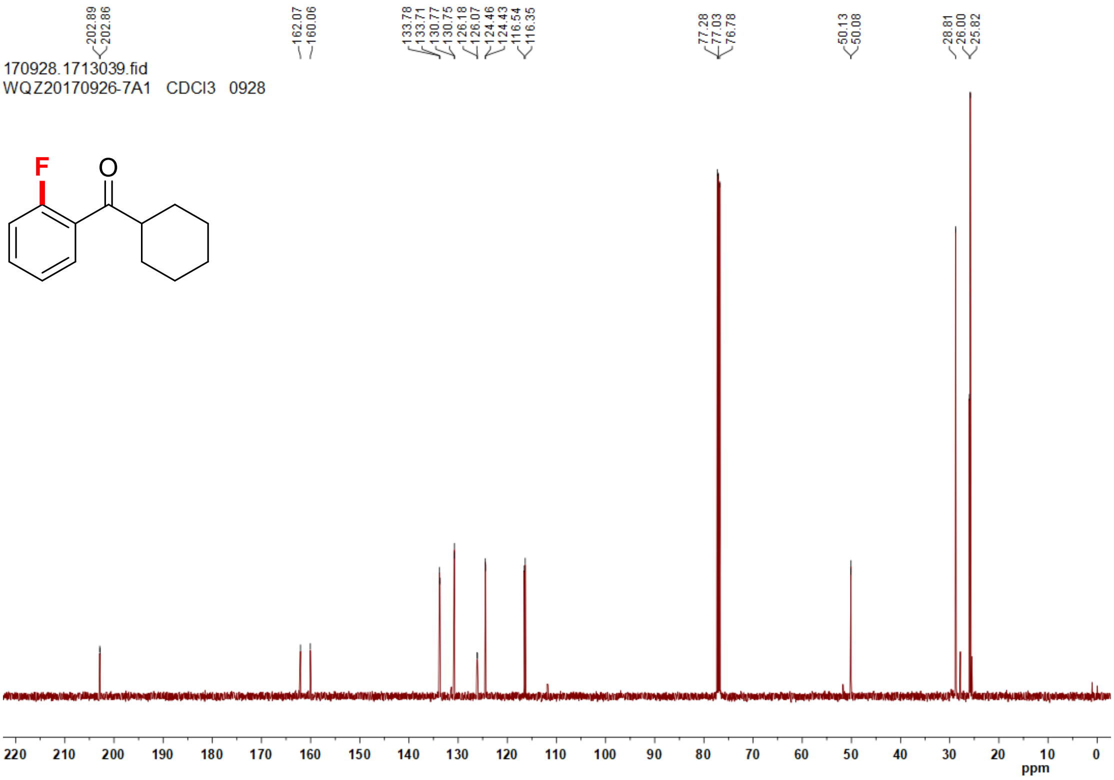
202.89 202.86 162.07 160.06 133.78 133.71 130.77 130.75 126.18 126.07 124.46 124.43 116.54 116.35 77.28 77.03 76.78 50.13 50.08 28.81 26.00 25.82
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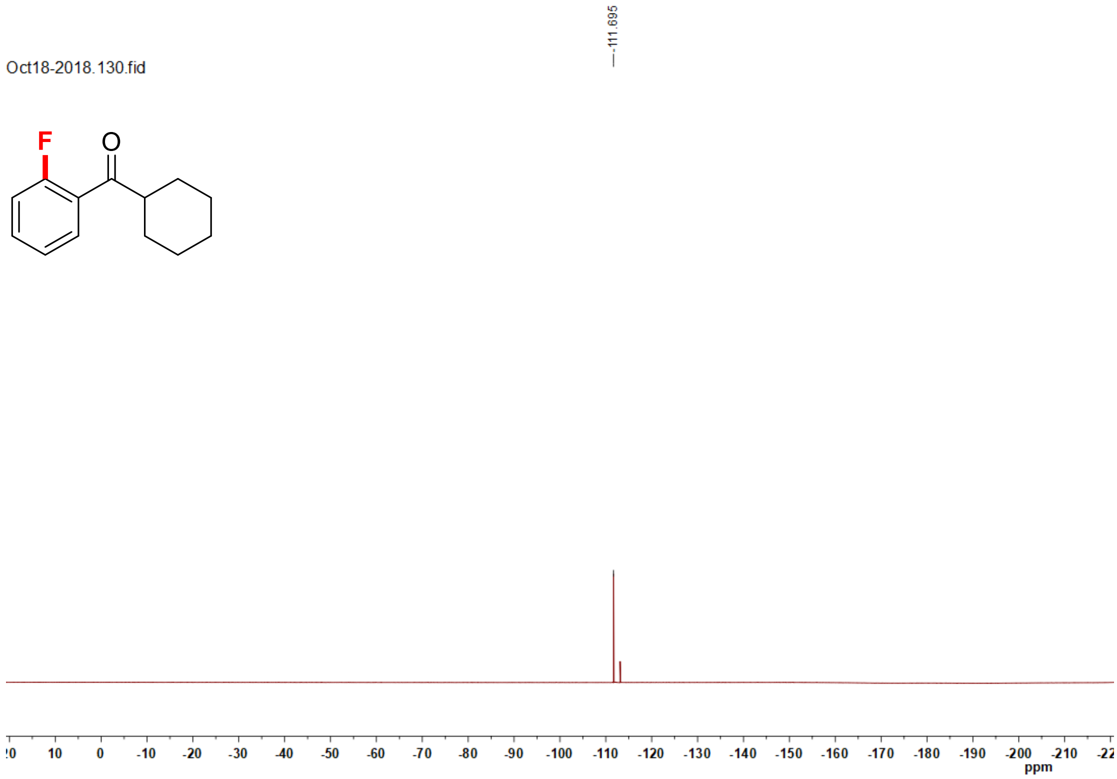
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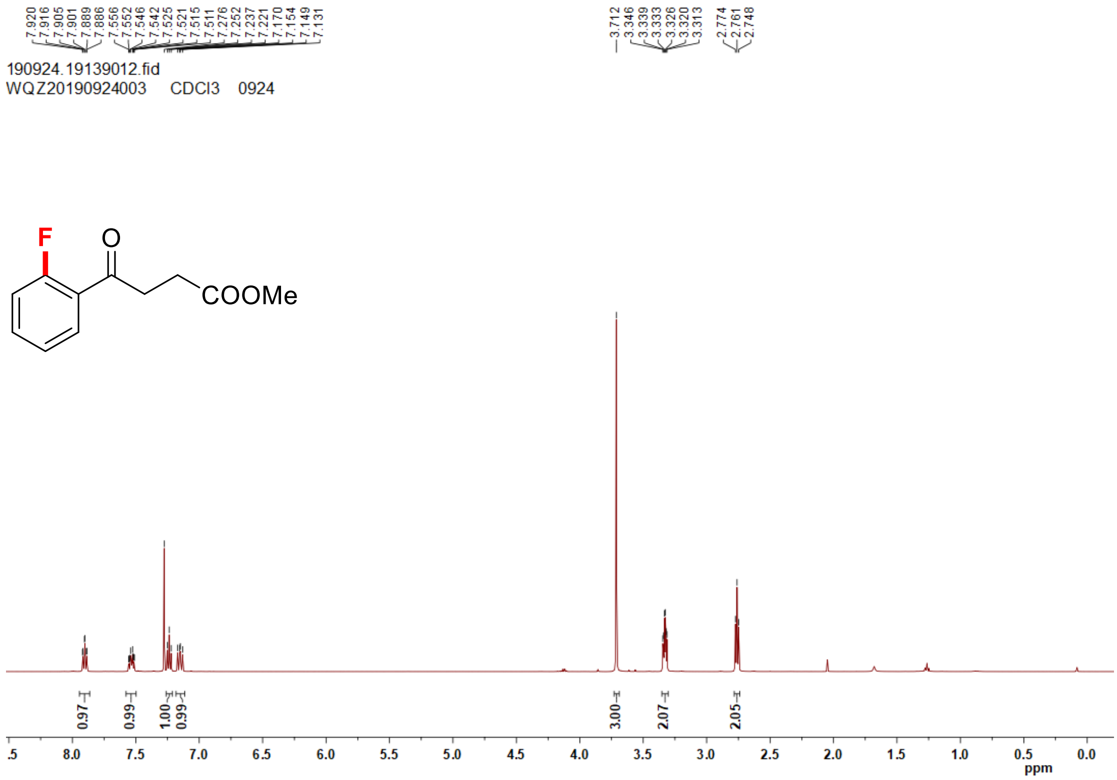
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7.521
7.515
7.511
7.276
7.252
7.237
7.221
7.170
7.154
7.149
7.131
3.712
3.346
3.339
3.333
3.326
3.320
3.313
2.774
2.761
2.748
190924.19139012.fid
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O
COOMe
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0.99
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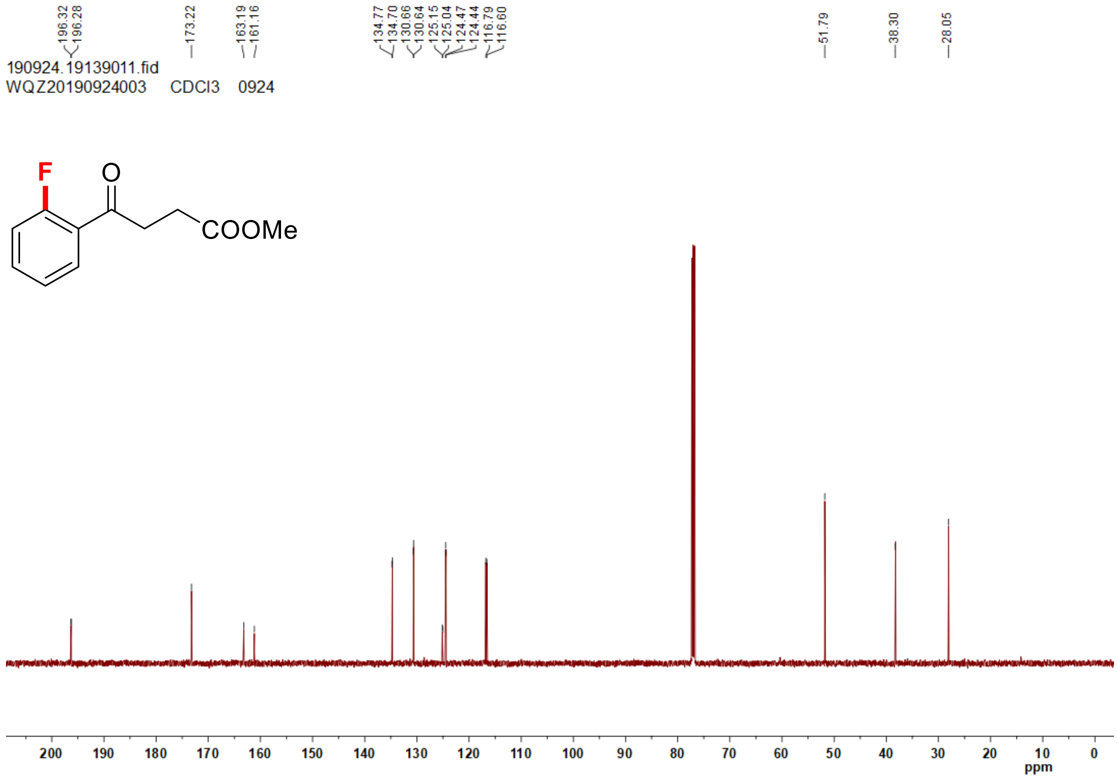
0.99
3.00
2.07
2.05
ppm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196.28
173.22
163.19
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134.77
134.70
130.66
130.64
125.15
125.04
124.47
124.44
116.79
116.60
51.79
38.30
28.05
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F
O
COOMe
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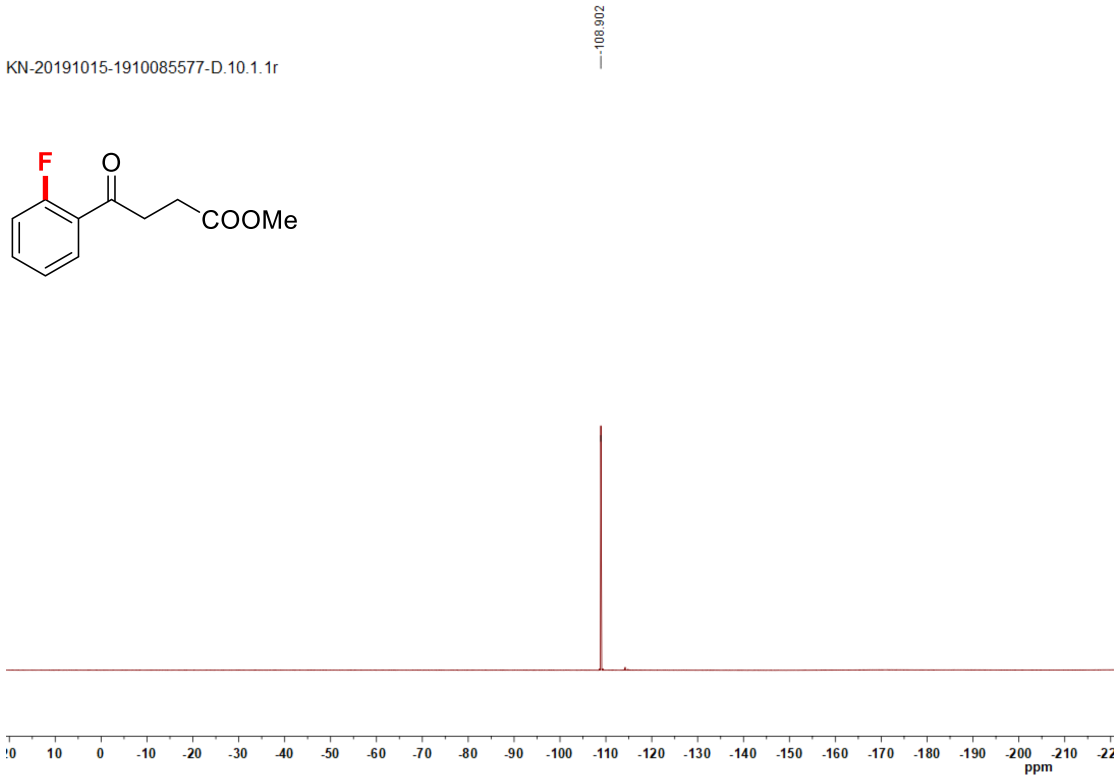
ppm


KN-20191015-1910085577-D.10.1.1r
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F
O
COOMe
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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-140
-150
-160
-170
-180
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-210
-22
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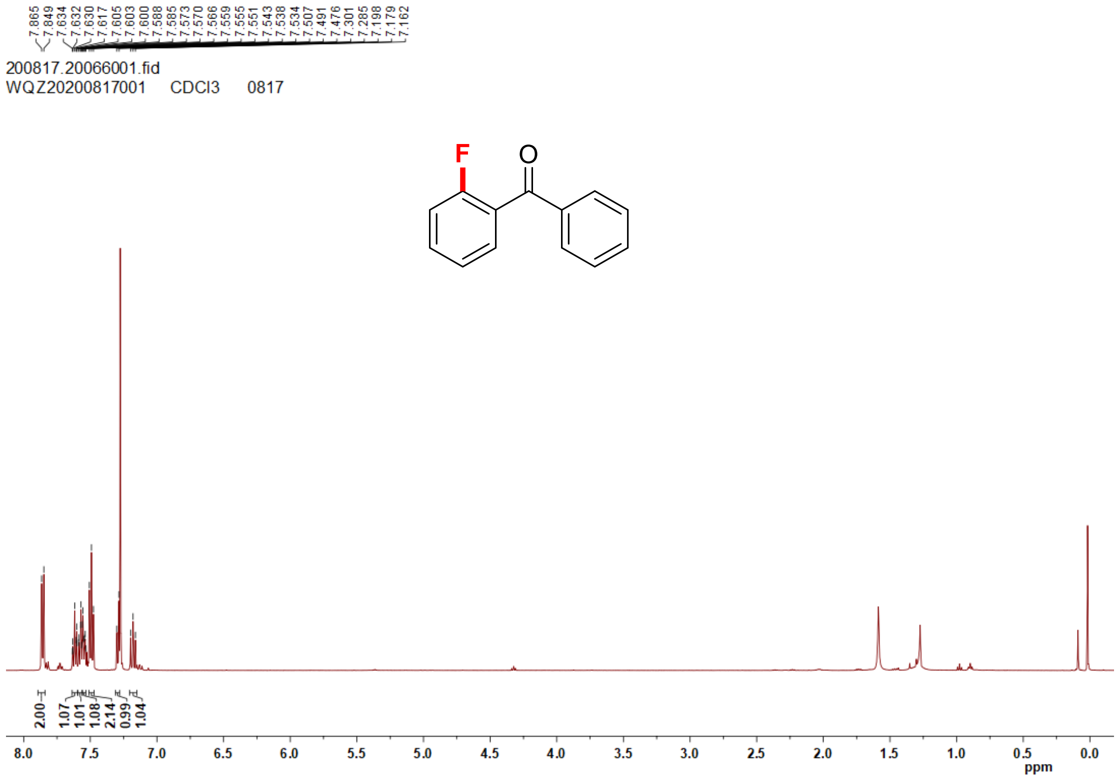
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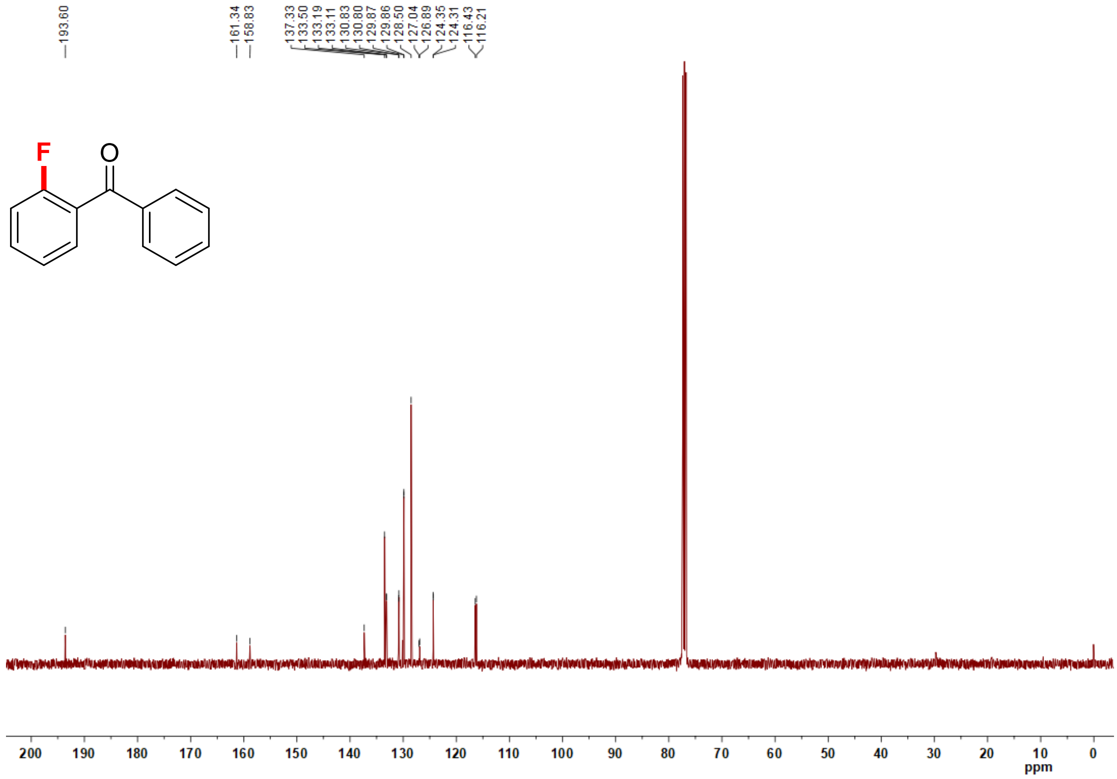
7.849
7.634
7.632
7.630
7.617
7.605
7.603
7.600
7.588
7.585
7.573
7.570
7.566
7.559
7.555
7.551
7.543
7.538
7.534
7.507
7.491
7.476
7.301
7.285
7.198
7.179
7.162
200817.20066001.fid
WQZ20200817001 CDCl3 0817
F
O
2.00
1.07
1.01
1.08
2.14
0.99
1.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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137.33
133.50
133.19
133.11
130.83
130.80
129.87
129.86
128.50
127.04
126.89
124.35
124.31
116.43
116.21
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O
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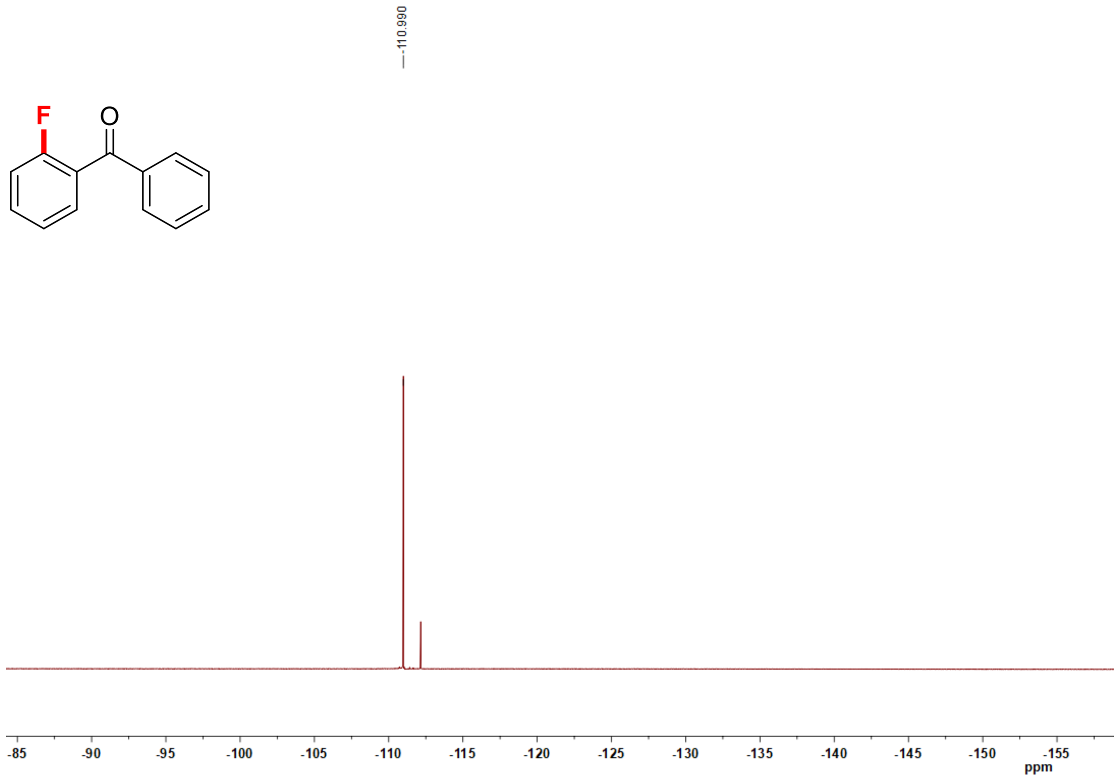
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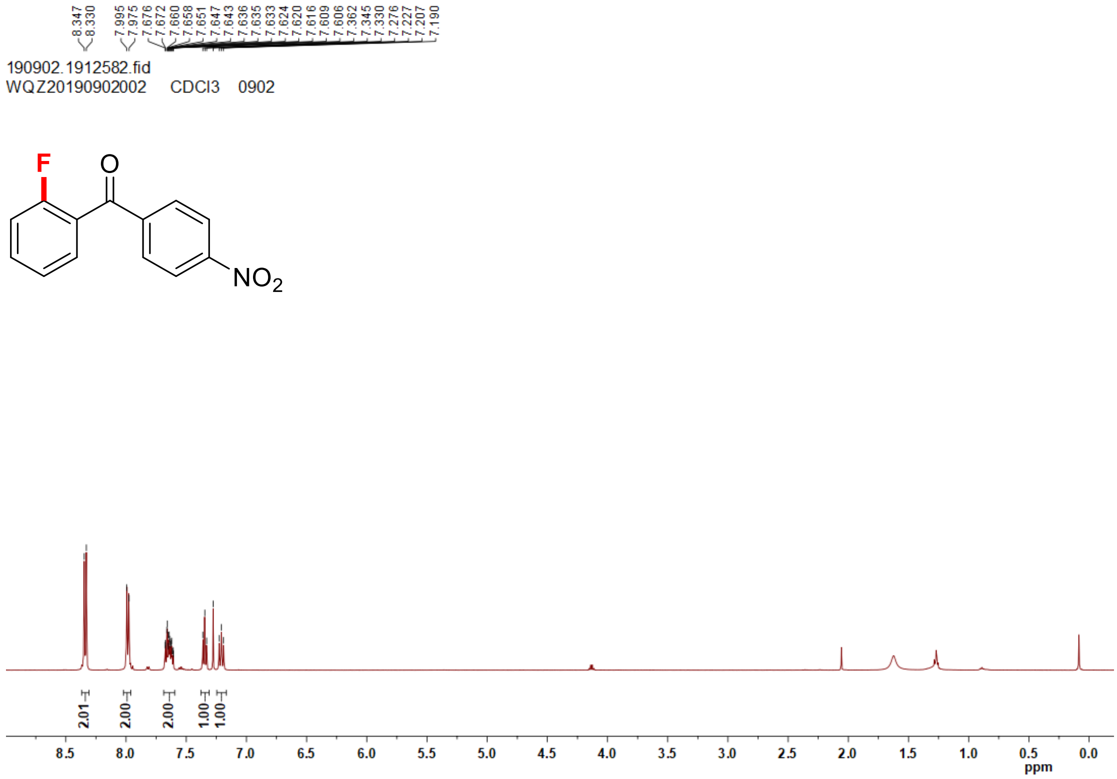
O
-85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155
ppm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O
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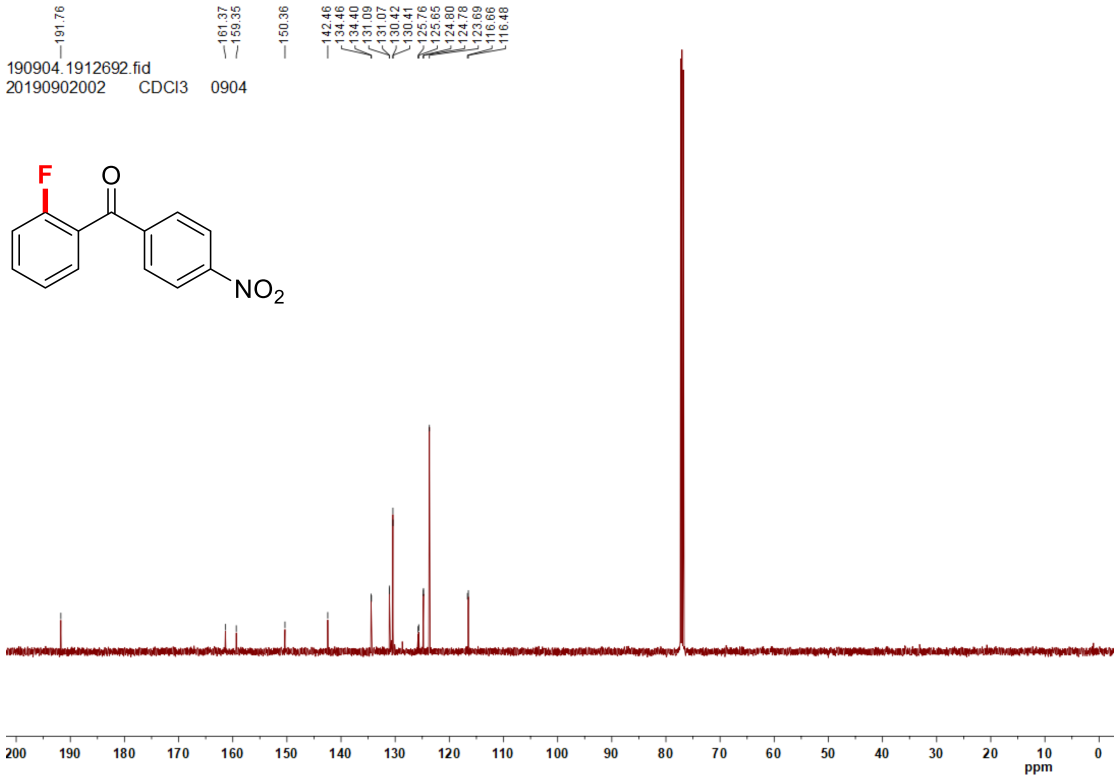
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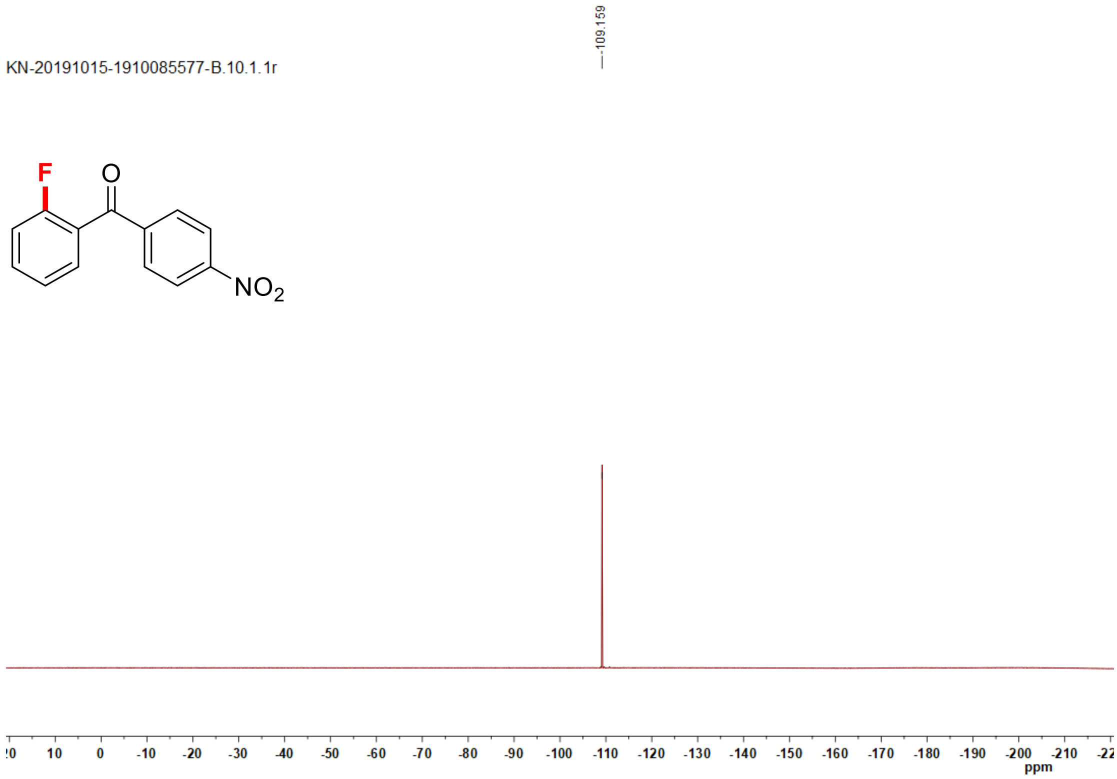
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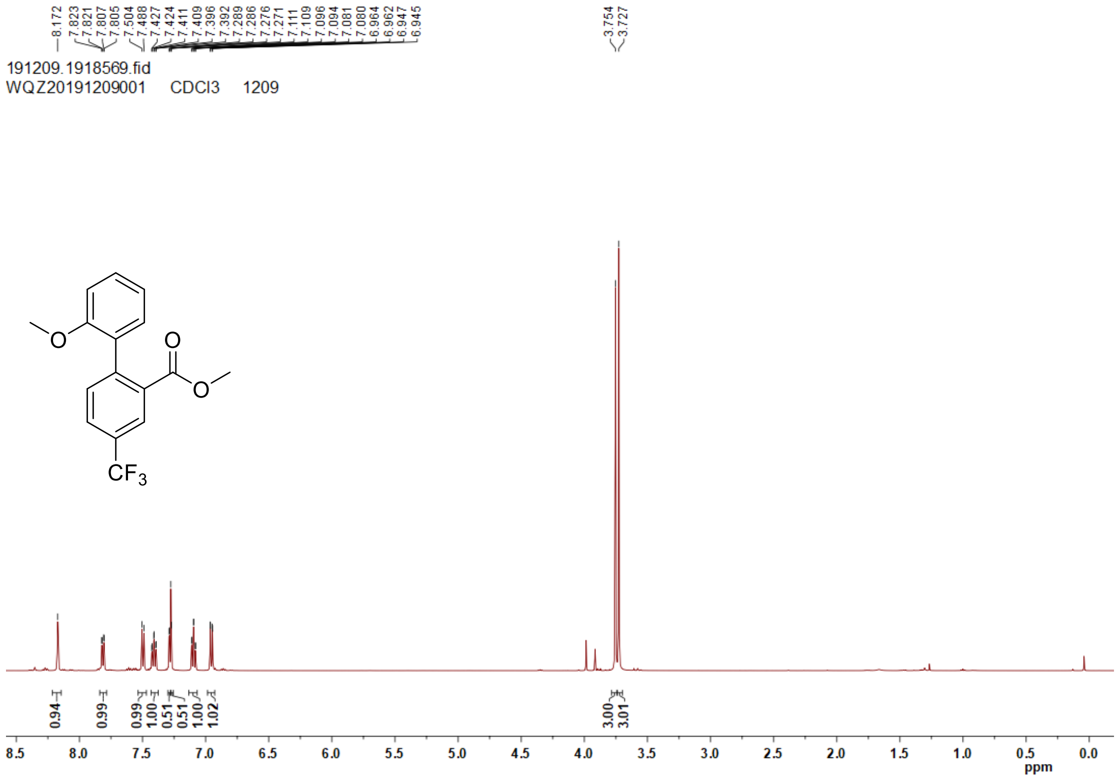
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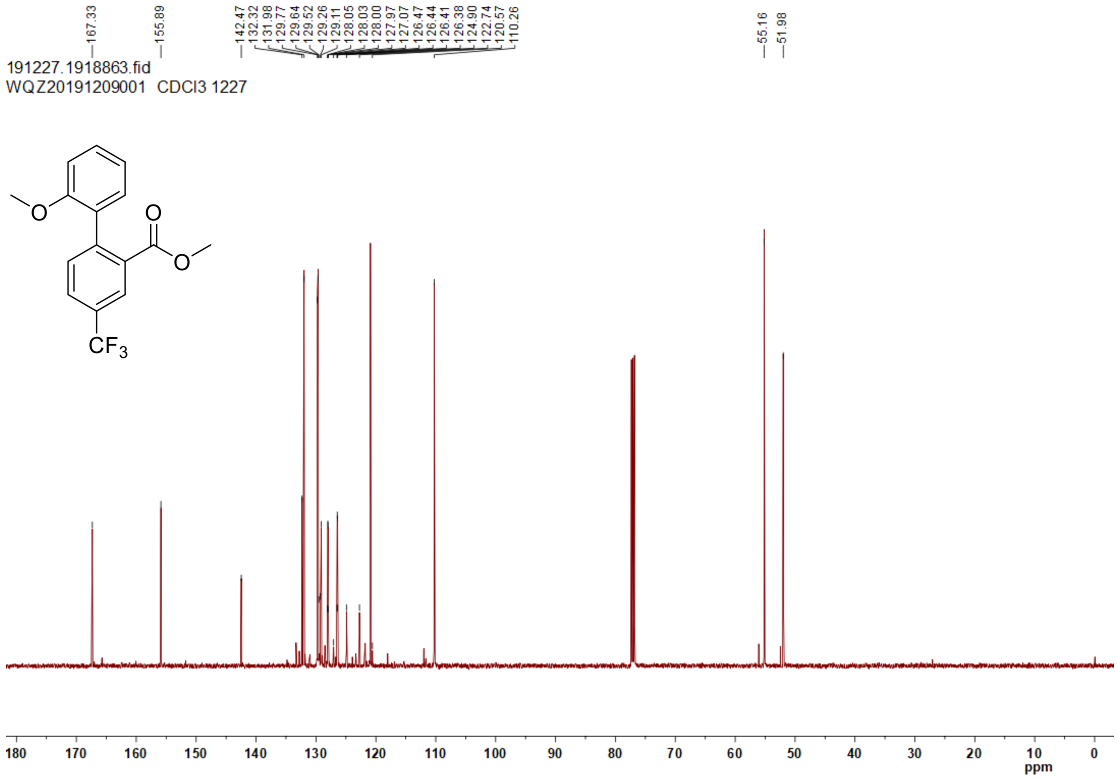
O
O
CF3
ppm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129.64
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129.11
128.05
128.03
128.00
127.97
127.07
126.47
126.44
126.41
126.38
124.90
122.74
120.57
110.26
55.16
51.98
O
O
O
CF3
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140
130
120
110
100
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80
70
60
50
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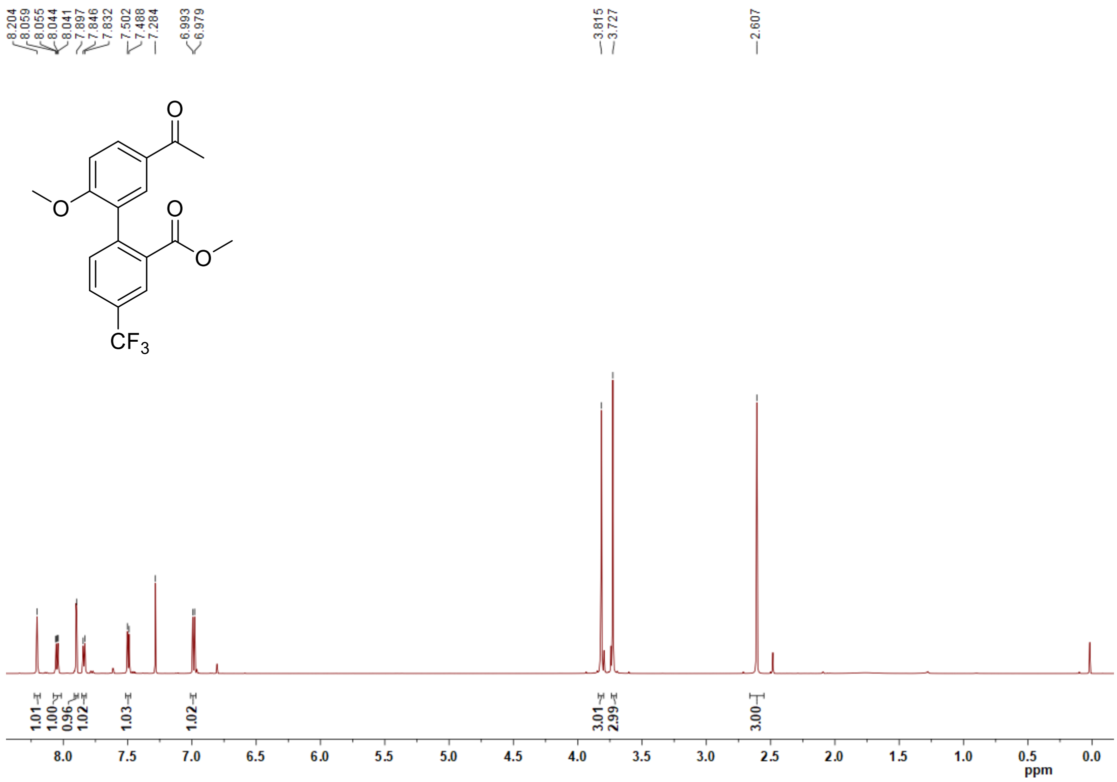
30
20
10
0
ppm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7.832
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7.488
7.284
6.993
6.979
3.815
3.727
2.607
O
O
O
O
CF3
1.01
1.00
0.96
1.02
1.03
1.02
3.01
2.99
3.00
8.0
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
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1.5
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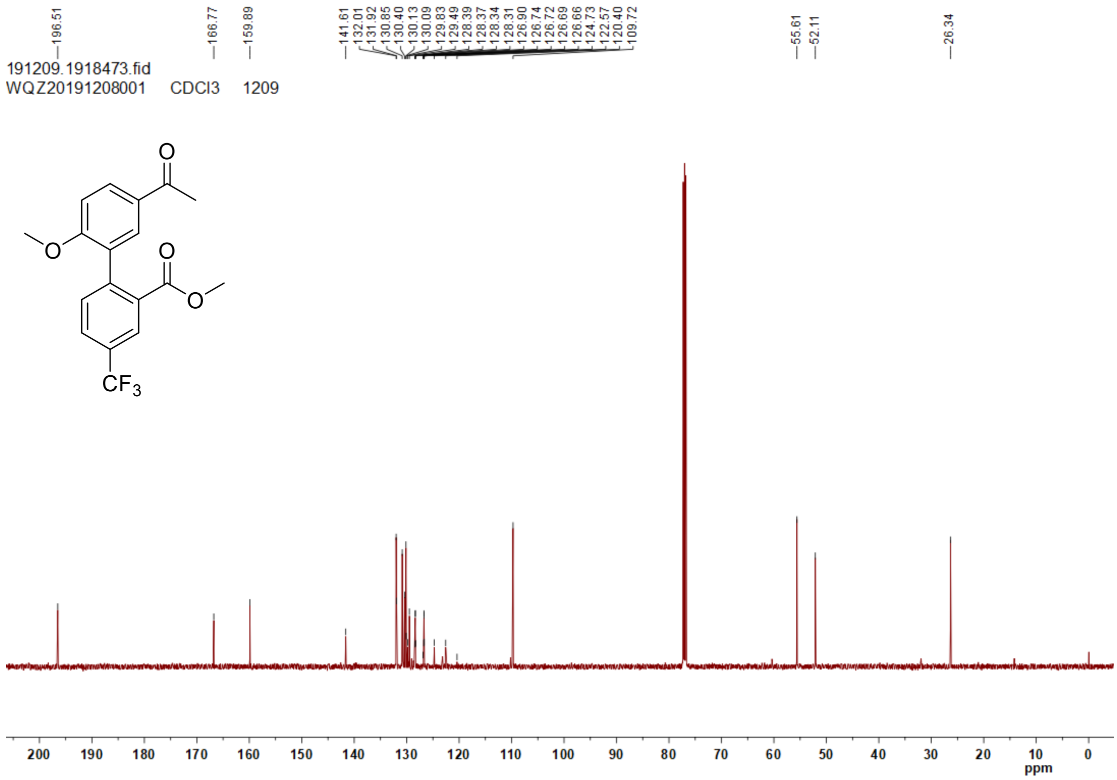
0.5
0.0
ppm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130.09
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129.49
128.39
128.37
128.34
128.31
126.90
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126.72
126.69
126.66
124.73
122.57
120.40
109.72
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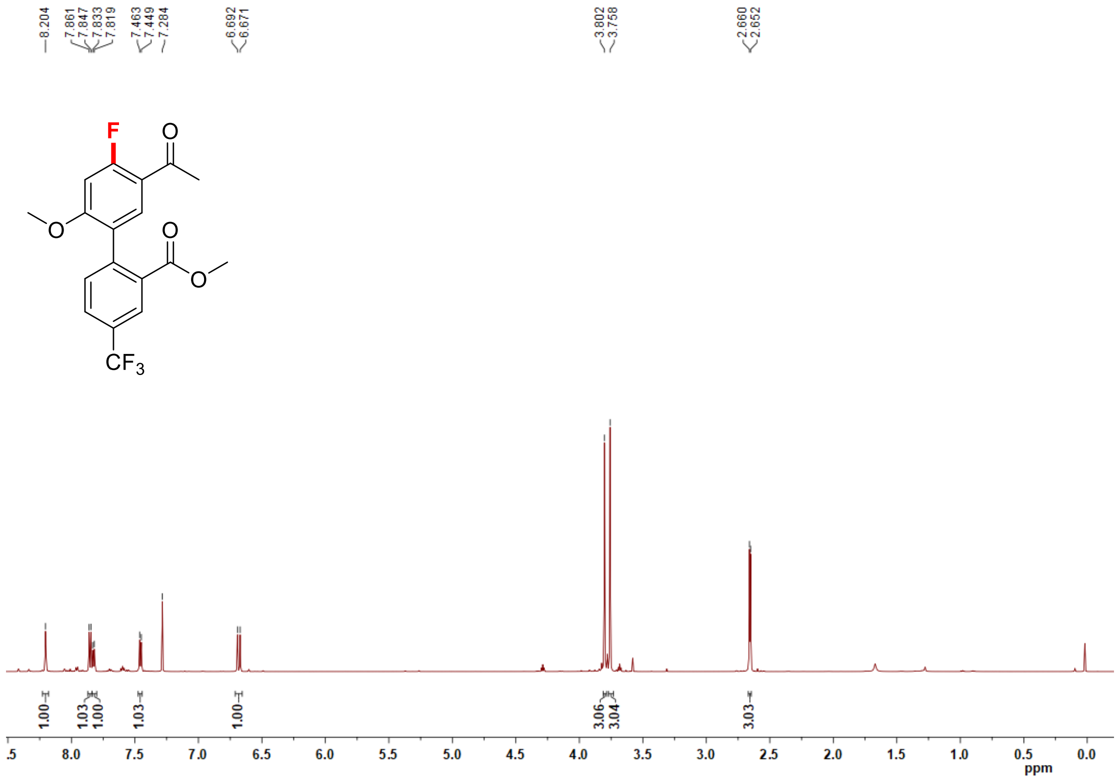
O
O
O
CF_3
ppm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2.660
2.652
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1.00
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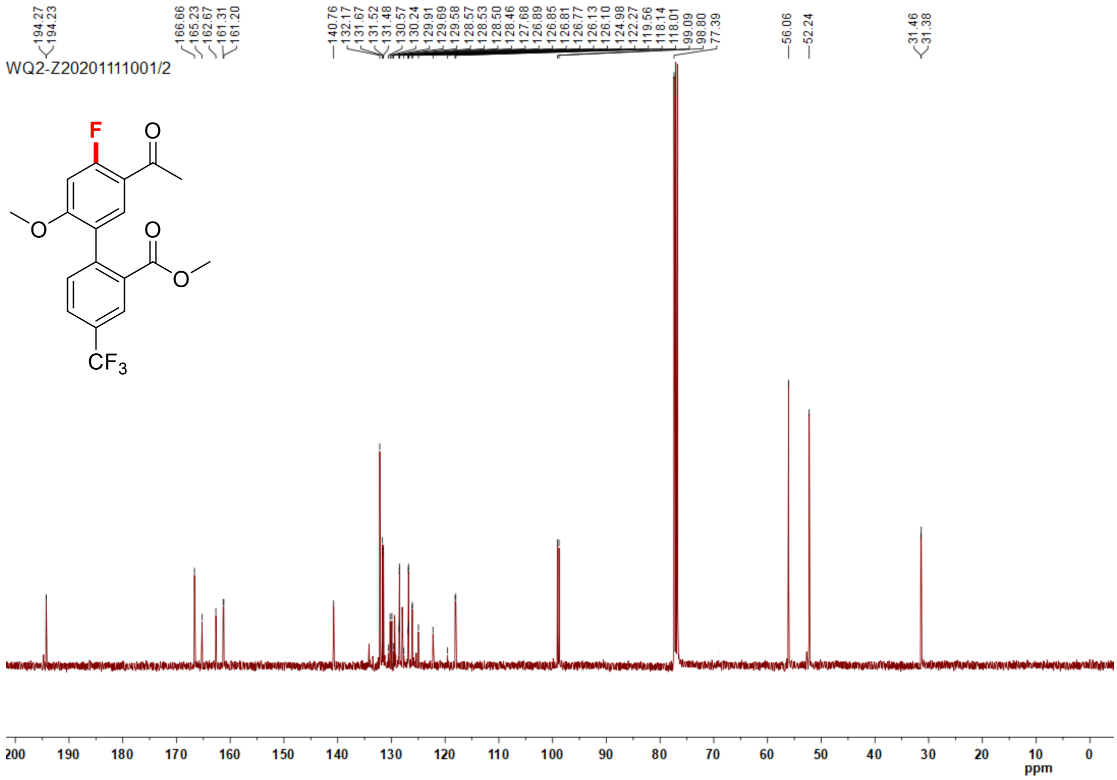
3.04
3.03
ppm



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128.57
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126.85
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126.81
126.77
126.13
126.10
124.98
122.27
119.56
118.14
118.01
99.09
98.80
77.39
56.06
52.24
31.46
31.38
WQ2-Z20201111001/2
F
O
O
O
O
CF3
200
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20
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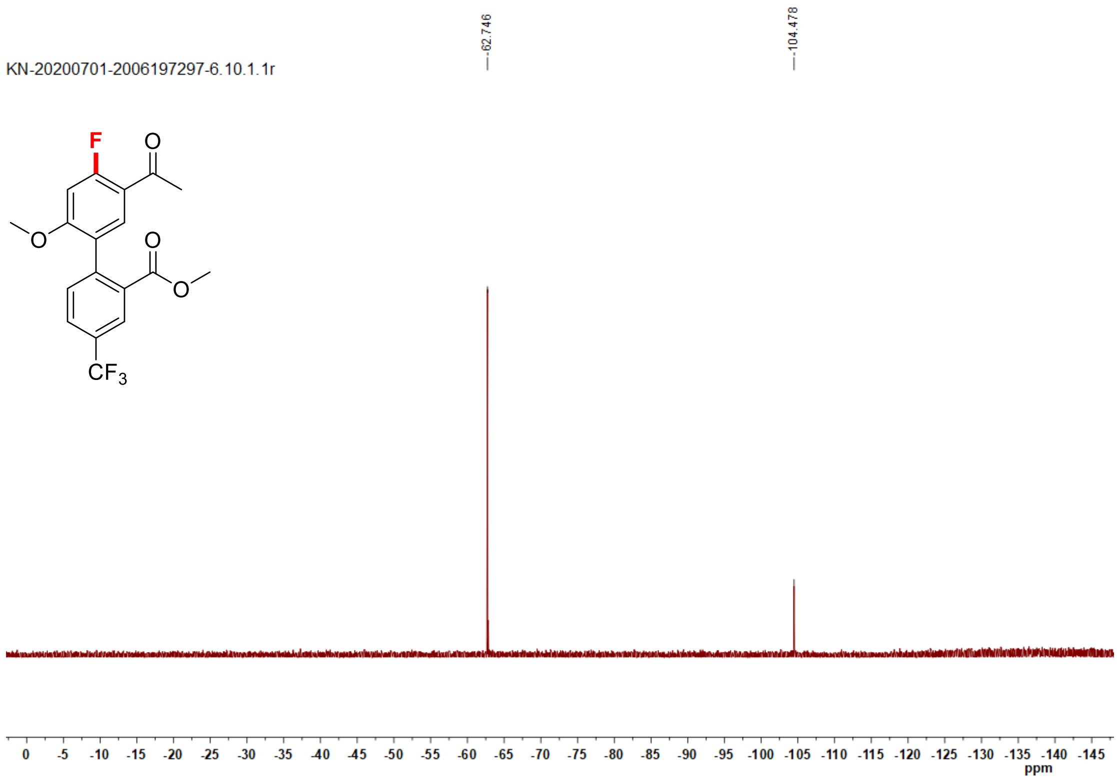

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O
O
O
O
CF3
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-35
-40
-45
-50
-55
-60
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-70
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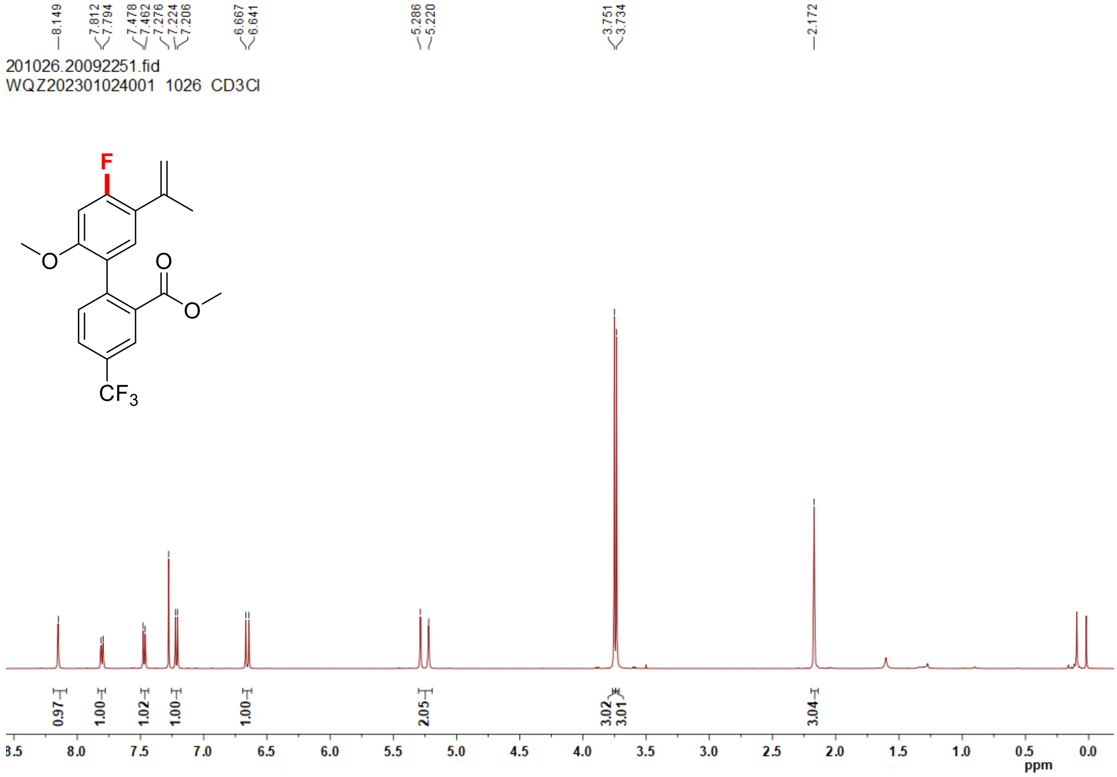
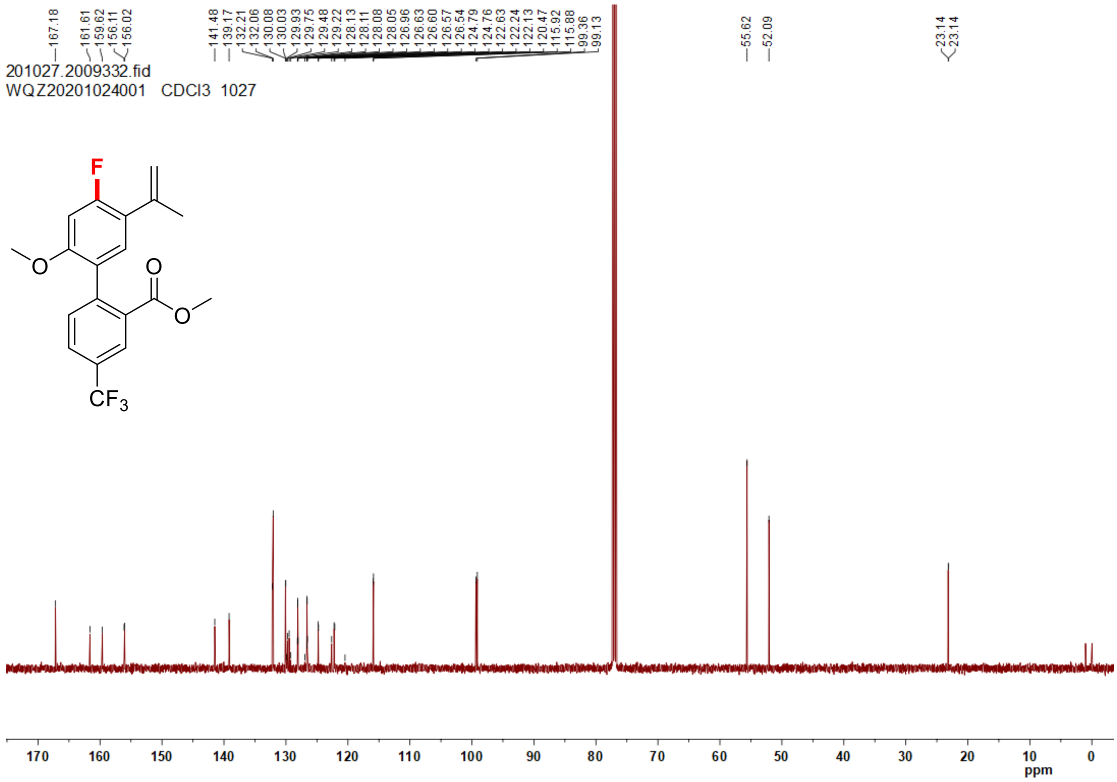
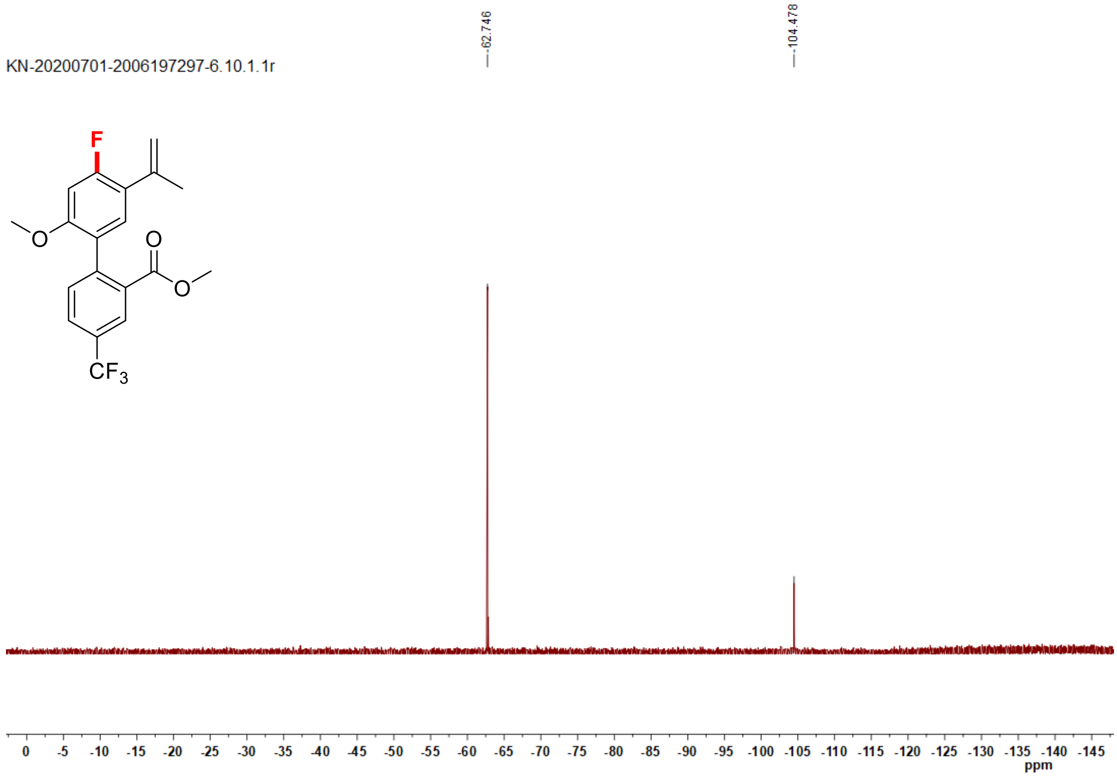
-140
-145
ppm



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O
O
CF3
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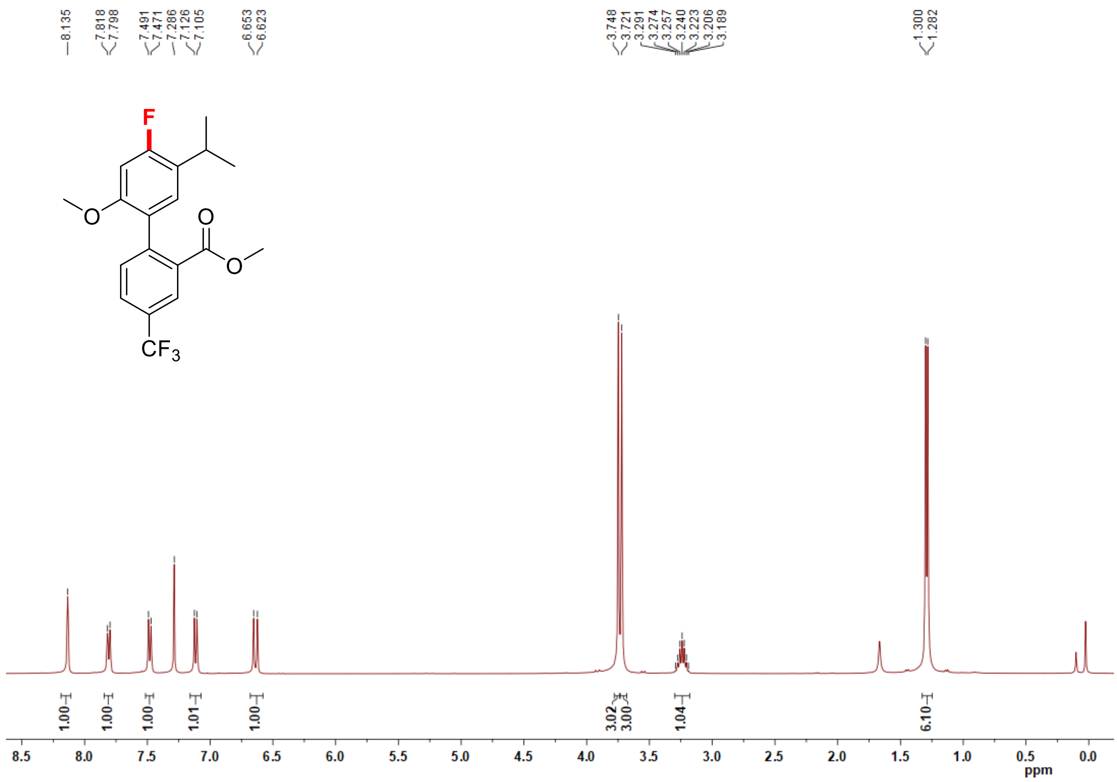
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6.623
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3.721
3.291
3.274
3.257
3.240
3.223
3.206
3.189
1.300
1.282
F
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O
O
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1.00
1.00
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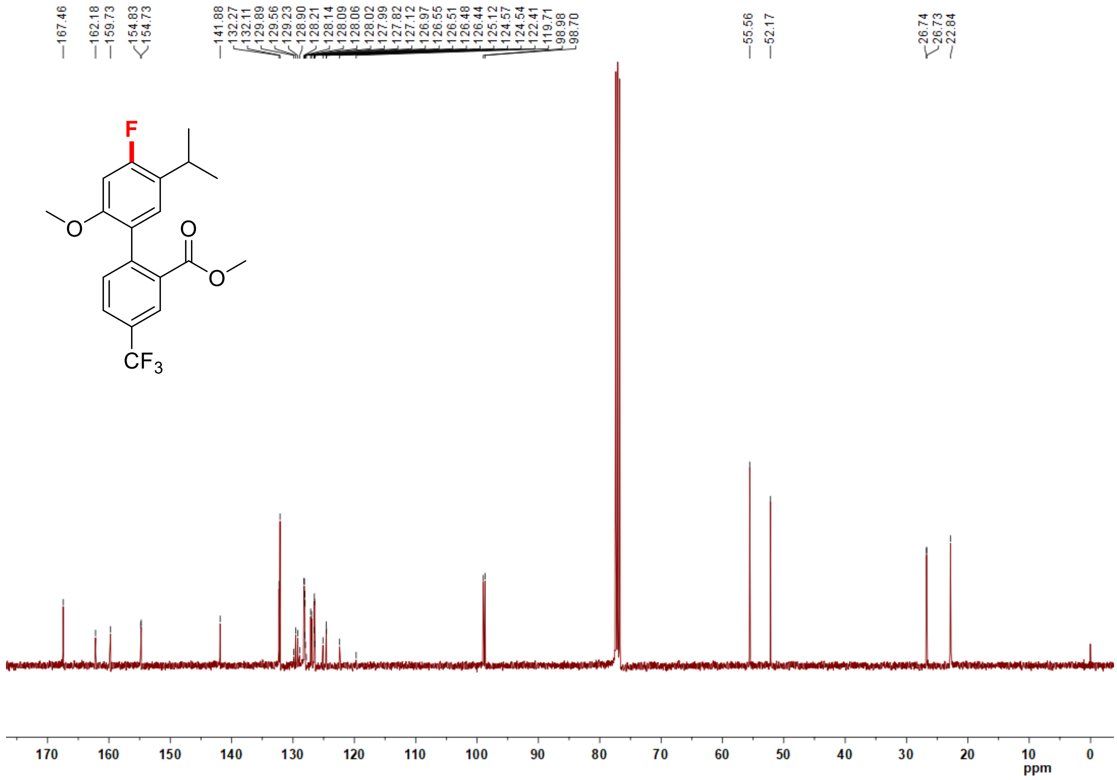
3.02
3.00
1.04
6.10
ppm



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128.21
128.14
128.09
128.06
128.02
127.99
127.82
127.12
126.97
126.55
126.51
126.48
126.44
125.12
124.57
124.54
122.41
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22.84
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O
O
CF_3
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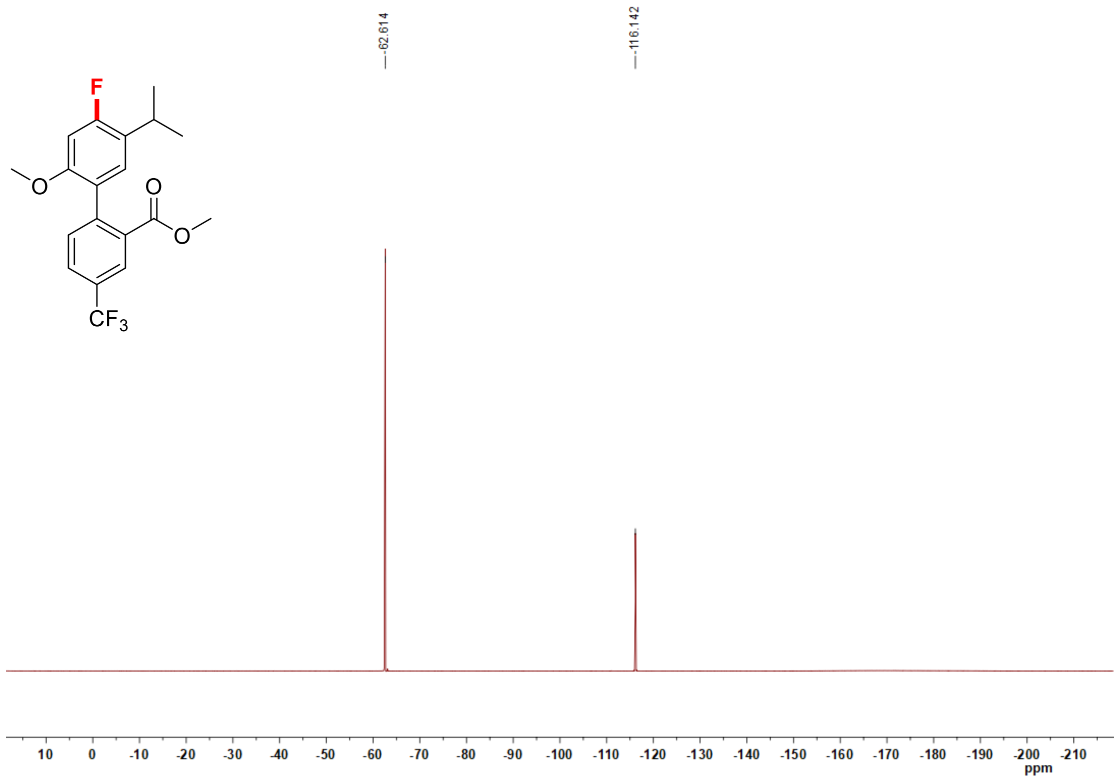

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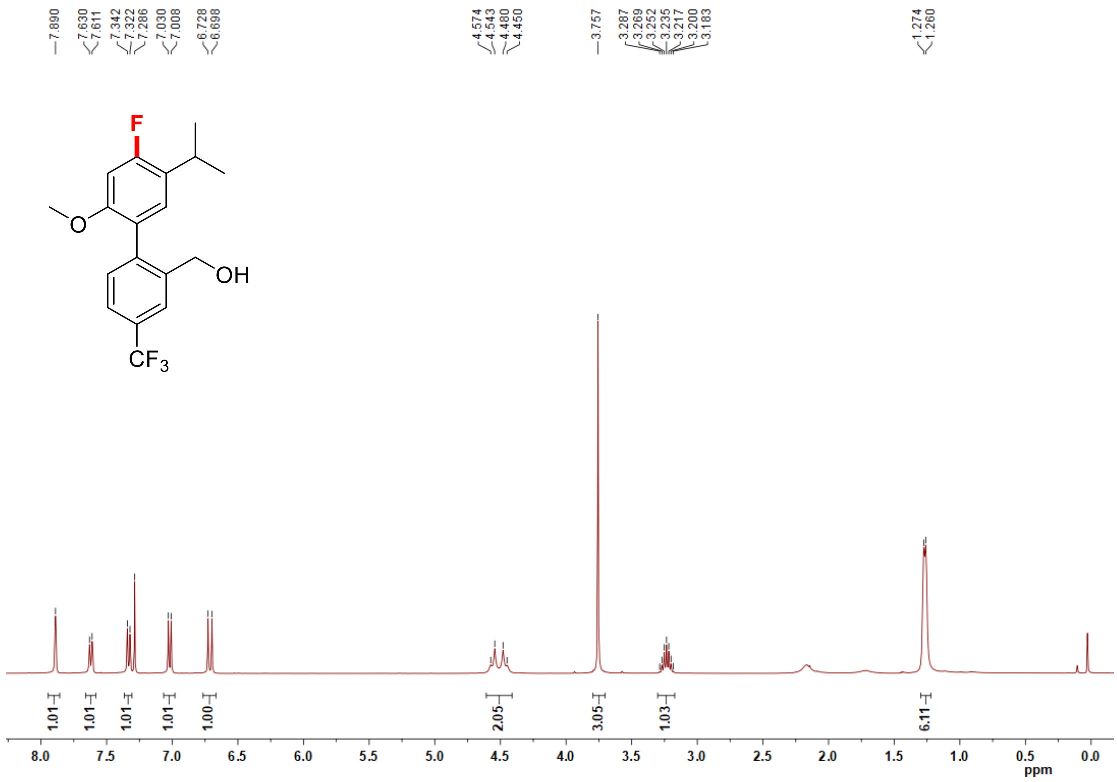
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6.698
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4.450
3.757
3.287
3.269
3.252
3.235
3.217
3.200
3.183
1.274
1.260
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O
OH
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1.01
1.01
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2.05
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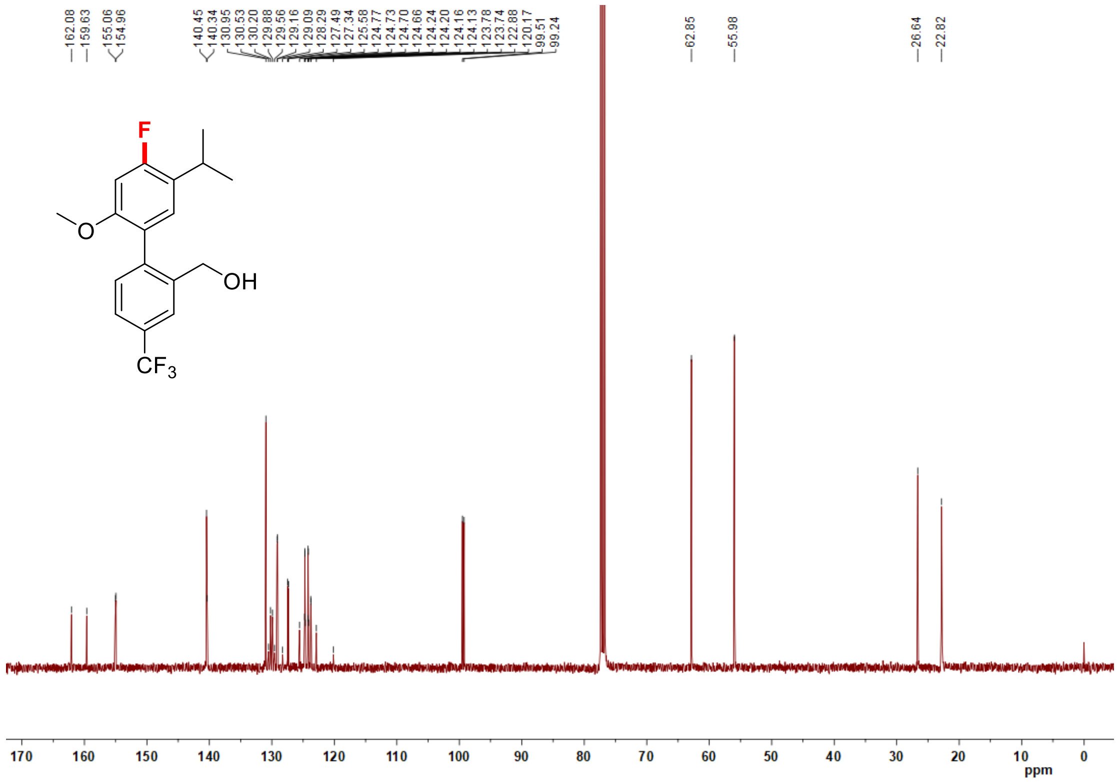
6.11
ppm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129.09
128.29
127.49
127.34
125.58
124.77
124.73
124.70
124.66
124.24
124.20
124.16
124.13
123.78
123.74
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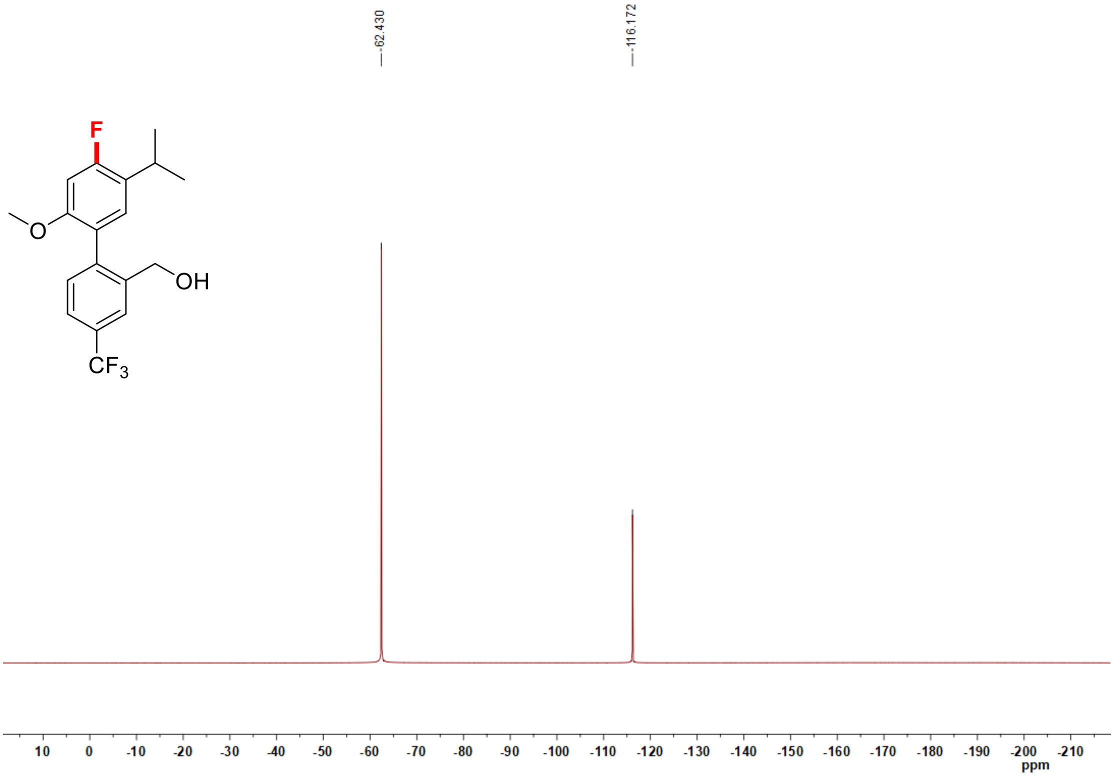
62.85
55.98
26.64
22.82
F
O
OH
CF3
ppm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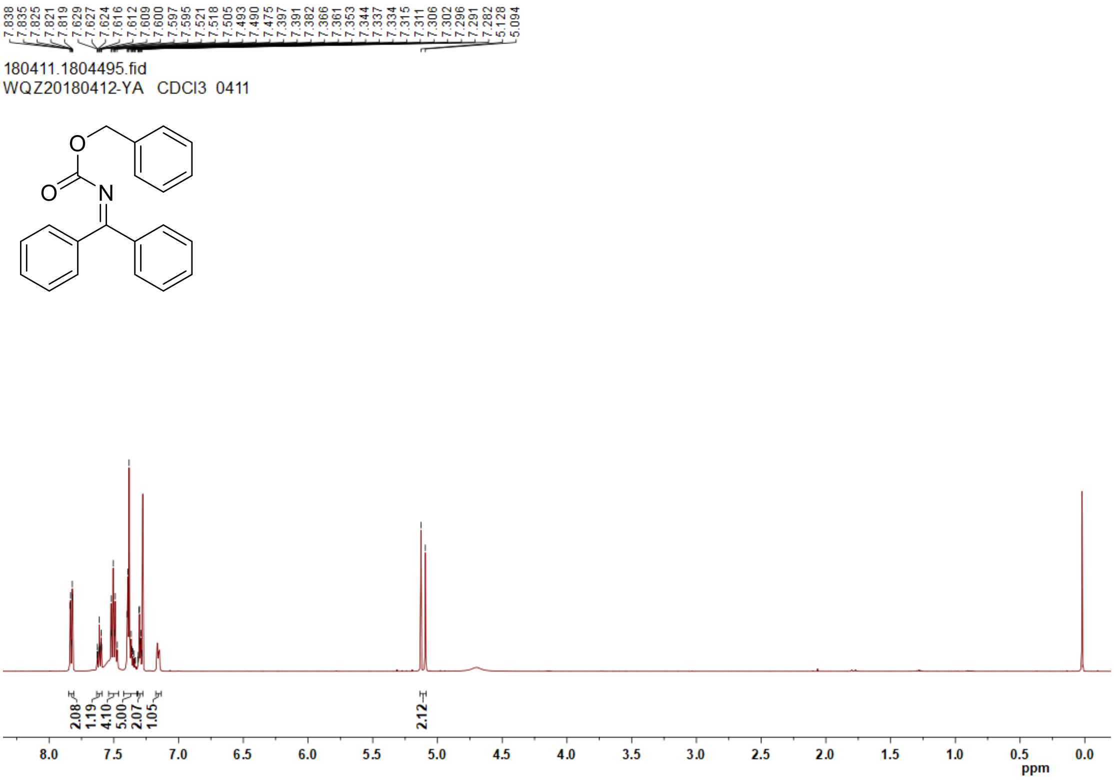
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O
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1.19
4.10
5.00
2.07
1.05
2.12
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