Supporting Information

Current-controlled Nickel-catalyzed Multi-electrophile Electroreductive Cross-Coupling

Shentong Xie[a], Yuqing Yin[a], Ya Wang[a], Jiannan Wang[a], Xiaoqian He[b], Ruopeng Bai*[b] and Renyi Shi*[a]

[a] School of Chemical Engineering and Technology

Xi'an Jiaotong University

Xi'an 710049 (P. R. China)

E-mail: renyi.shi@xjtu.edu.cn

[b] School of Chemistry and Chemical Engineering, Chongqing Key Laboratory of Theoretical and Computational Chemistry

Chongqing University

Chongqing 400030 (P. R. China)

E-mail: ruopeng@cqu.edu.cn

General Analytical Information

Nuclear Magnetic Resonance spectra were recorded on a Bruker Avance 400 MHz instruments at ambient temperature. All ^{1}H NMR spectra were measured in part per million (ppm) relative to the signals of tetramethylsilane (TMS, 0.00 ppm) added into the deuterated chloroform ($CDCl_3$, 7.30 ppm) unless otherwise stated. Data for ^{1}H NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets), coupling constants, and integration. All ^{13}C NMR spectra were reported in ppm relative to tetramethylsilane (0.00 ppm) unless otherwise stated, and were obtained with complete ^{1}H decoupling. All GC analyses were performed on a Perkin-Elmer Clarus 400 GC system with an FID detector. High-resolution mass spectra were obtained with an AB Triple 5600 mass spectrometer by ESI on a TOF mass analyzer.

General Reagent Information

Unless otherwise noted, all chemicals used in the preparations of starting materials and in the nickel catalyzed electroreductive carbonylative cross-coupling reactions were commercially available and were used as received without further purifications or prepared according to previous work. Solvents transferred to the glove box without exposure to air. Anhydrous dimethylacetamide (DMA) (99.8% purity) were purchased from China National Pharmaceutical Group Corporation.

General Procedure for Electroreductive Carbonylative Cross-electrophile

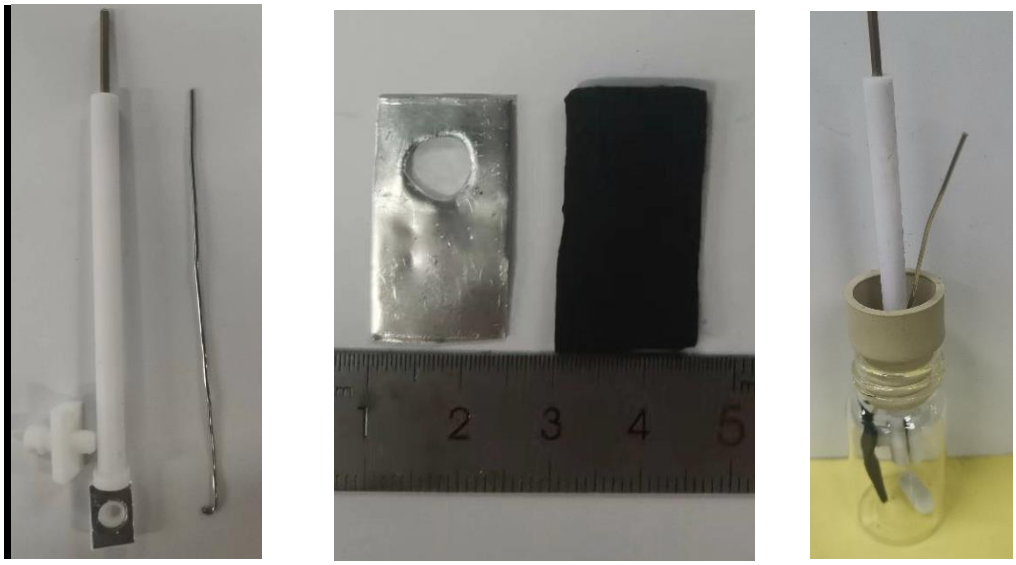


Figure S1 Hand-made electrochemical cell

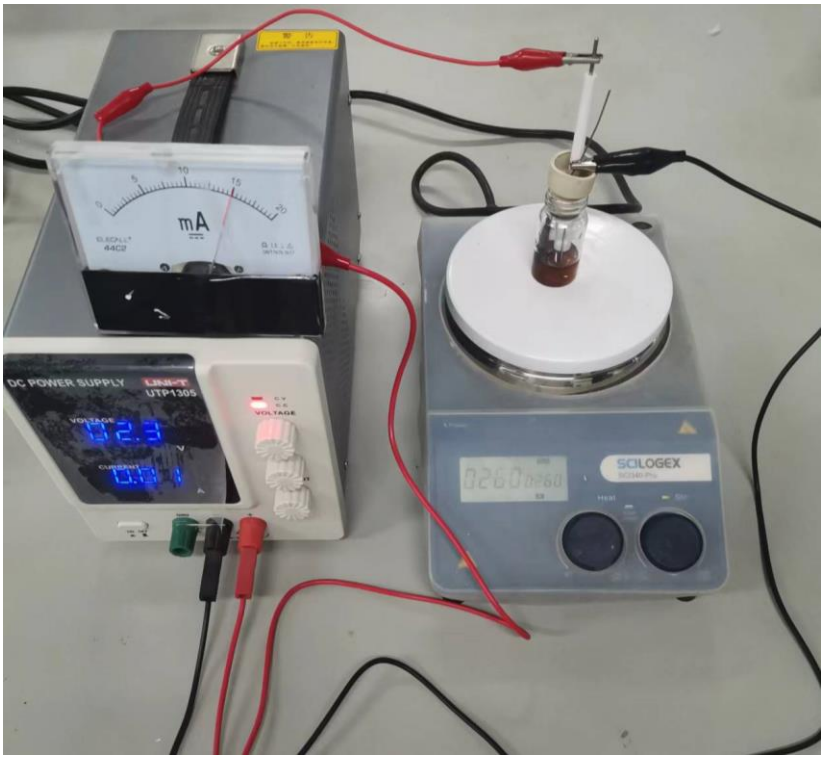
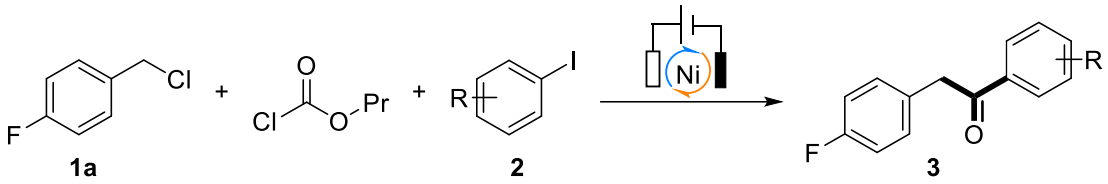


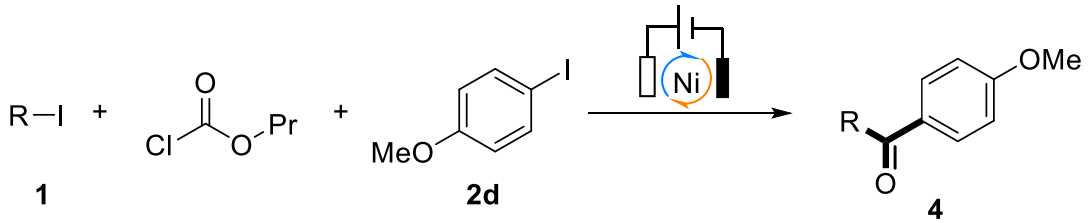
Figure S2 Electrochemical reactor

General procedure A (Electroreductive Carbonylative of benzyl chlorides and iodobenzenes)



An oven-dried 20 mL re-sealable screw-cap test tube equipped with a Teflon-coated magnetic stir bar was sequentially charged with dtbpy (15 mol%), $NiCl_2$·dme (10 mol%), LiOTf (0.2 M) in the glove. Then DMA (6 mL), benzyl chloride (0.75 mmol), ClCOOPr (1.5 mmol.), iodobenzene (0.5 mmol) were added into the tube in turn. All these procedures were conducted in the glovebox. Screw the vial cap with electrode (Zn anode (12 mm X 15 mm), graphite felt cathode (12 mm X 15 mm)) onto the vial to finger tight and adapt the electrochemical cell. Then removed from the glove box. The reaction mixture was stirred and electrolyzed at a constant current (15 mA) at room temperature for 4h. After electrolysis, the product was extracted from the crude reaction mixture with ethyl acetate (4 X 30 mL). The organic layers were combined, and washed with brine (60 mL). Dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

General procedure B (Electroreductive Carbonylative of alkyl iodides and iodobenzenes)



An oven-dried 20 mL re-sealable screw-cap test tube equipped with a Teflon-coated magnetic stir bar was sequentially charged with dtbpy (15 mol%), $NiCl_2$·dme (10 mol%), LiOTf (0.2 M), KF (2 mmol) in the glove. Then 4 mL DMA and 2 mL dioxane, alkyl iodides (0.6 mmol), ClCOOPr (2 mmol.), iodobenzenes (0.5 mmol) were added into the tube in turn. All these procedures were conducted in the glovebox. Screw the vial cap with electrode (Zn anode (12 mm X 15 mm), graphite felt cathode (12 mm X 15 mm)) onto the vial to finger tight and adapt the electrochemical cell. Then removed from the glove box. The reaction mixture was stirred and electrolyzed at a constant current (15 mA) at room temperature for 4h. After electrolysis, the product was extracted from the crude reaction mixture with ethyl acetate (4 X 30 mL). The organic layers were combined, and washed with brine (60 mL). Dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v)

as an eluent.

Large Scale Reaction procedure

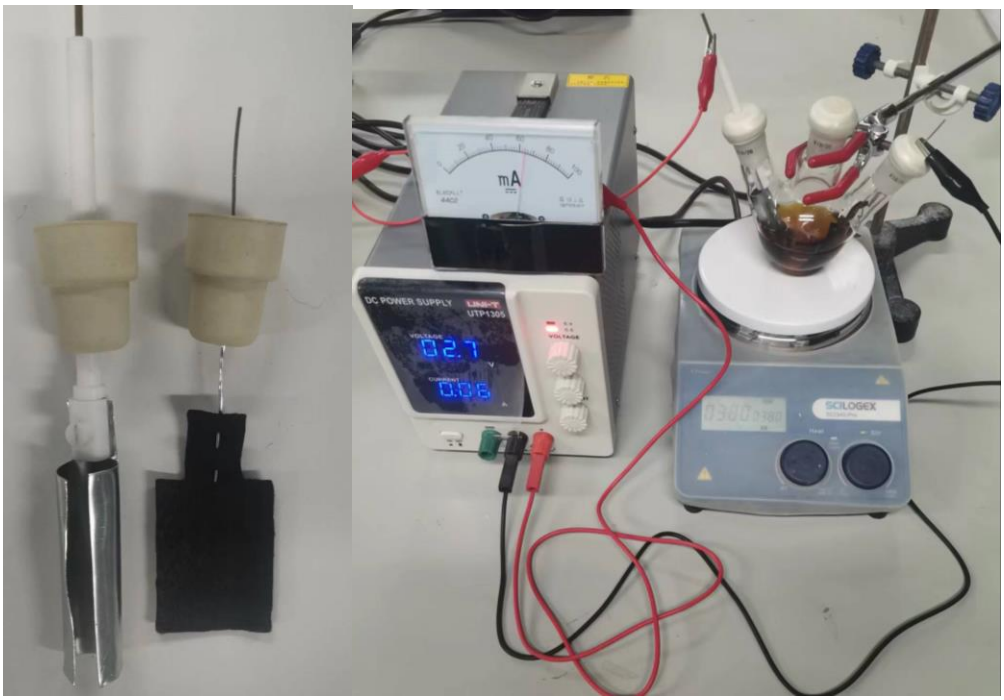
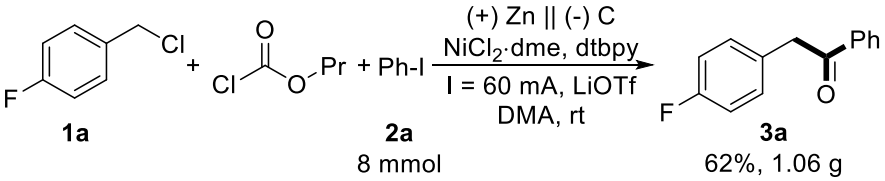


Figure S3 Scale reaction set-up

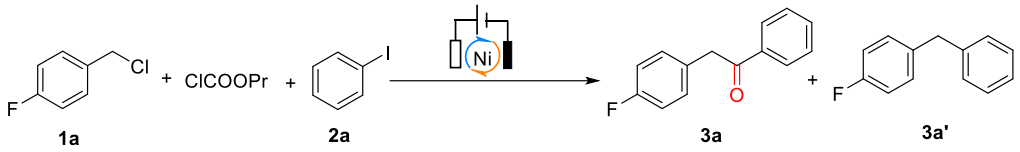


An oven-dried 100 mL three-necked flask equipped with a Teflon-coated magnetic stir bar was sequentially charged with dtbpy (15 mol%), $NiCl_2$·dme (10 mol%), LiOTf (0.2 M) in the glove. Then 60 mL DMA, 1-(chloromethyl)-4-fluorobenzene **1a** (12 mmol), ClCOOPr (24 mmol.), iodobenzene **2a** (8 mmol) were added into the three-necked flask in turn. All these procedures were conducted in the glovebox. Screw the vial cap with electrode onto the vial to finger tight and adapt the electrochemical cell. Then removed from the glove box. The reaction mixture was stirred and electrolyzed at a constant current (60 mA) at room temperature for 12h. After electrolysis, the product was extracted from the crude reaction mixture with ethyl acetate (4 X 80 mL). The organic layers were combined, and washed with brine (160 mL). Dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

Optimizations of Ni-Catalyzed Electroreductive Carbonylation

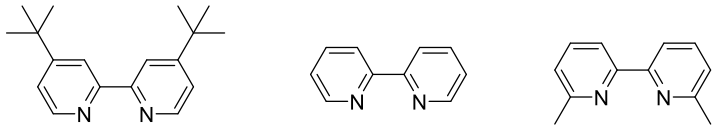
Optimizations of electroreductive carbonylation of 1a and 2a

Table 1. Screening of the Reaction Conditions



1a 2a 3a 3a'

entry	deviation from standard conditions	yield **3a** [%]	yield **3a'** [%]
1	**none**	**85 (78)**[c]	**14**
2[b]	Zn powder, 12h	48	42
3	I = 0 mA, 12h	4	66
4	I = 3 mA, 12h	44	53
5	I = 5 mA, 12h	53	40
6	I = 10 mA, 8h	66	32
7	I = 20 mA, 3h	78	15
8	Mg instead of Zn	37	59
9	Fe instead of Zn	11	46
10	Ni foam instead of graphite felt	35	21
11	using 12 mmol% dtbpy	72 (62)[c]	23
12	bpy instead of dtbpy	62	24
13	dmbpy instead of dtbpy	0	0
14	$^{n}Bu_4NBr$ instead of LiOTf	31	67
15	$^{n}BuNPF_6$ instead of LiOTf	75	20
16	CO instead of ClCOO^{n}Pr	8	trace
17	No $NiCl_2$·dme / No dtbbpy ligand	0	0

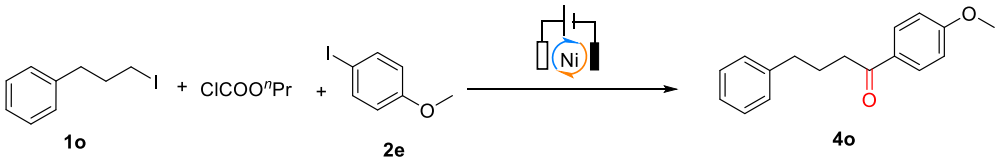


dtbpy bpy dmbpy

[a] Reaction condition 1: 0.75 mmol **1a**, 1.5 mmol ClCOOPr, 0.5 mmol **2a**, 0.2 M LiOTf, 10 mol% $NiCl_2$·dme, 15 mol% dtbpy, 6 mL DMAc, Zn anode, graphite felt cathode, undivided cell, constant current of 15 mA, rt, 4h. Conversion was measured by GC using naphthalene as an internal standard. [b] No electrode and electrolyte, 3 equiv. Zn powder. [c] Isolated yield.

Optimizations of electroreductive carbonylation of 1o and 2d

Table 2. Screening of the Reaction Conditions



1o 2e 4o

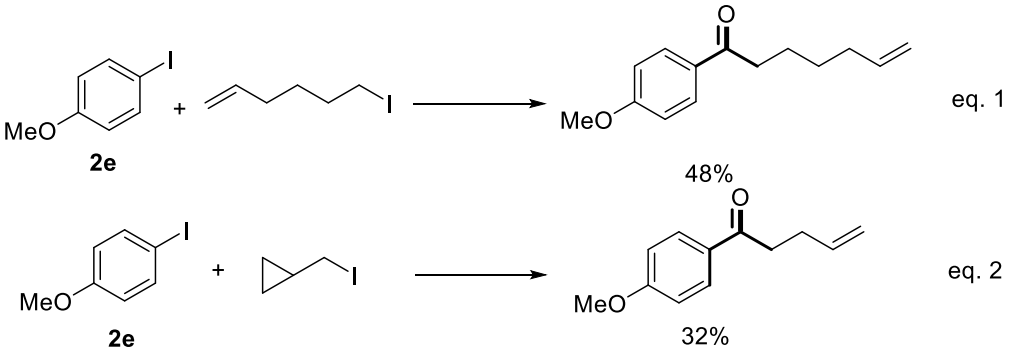
entry	**1o** (mmol)	ClCOOPr (mmol)	Solvent	yield **4o** [%]
1	0.75	1.5	DMAc	54

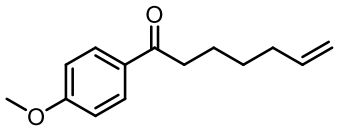
2	0.6	1.5	DMAc	53
3[b]	0.6	1.5	DMAc	52
4[c]	0.6	1.5	DMAc	0
5	0.6	2	DMAc	60
6[d]	0.6	2	DMAc	42
7[e]	0.6	2	DMAc	55
8	0.6	2	DMAc/dioxane 4/2	72
9	0.6	2	DMAc/dioxane 2/4	57
10[f]	**0.6**	**2**	**DMAc/dioxane 4/2**	**79(71)**

[a] Reaction condition: (3-iodopropyl)benzene **1o**, ClCOOPr, 0.5 mmol **2e**, 0.2 M LiOTf, 10 mol% $NiCl_2$·dme, 15 mol% dtbpy, 6 mL solvent, Zn anode, graphite felt cathode, undivided cell, constant current of 15 mA, rt, 4h. Conversion was measured by GC using naphthalene as an internal standard. [b] $NiBr_2$·dme. [c] Ligand: 3,2':6',3"-terpyridine. [d] 5 mol% $NiCl_2$·dme, 7.5 mol% dtbpy. [e] I= 10 mA. [f] 1.5 mmol KF as an additive.

Control Experiments

Eq.1 followed the General Procedure B using 6-iodohex-1-en-1-ylium as the substrate; Eq.2 followed the General Procedure B using (iodomethyl)cyclopropane as the substrate.

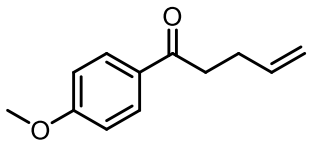




1-(4-methoxyphenyl)hept-6-en-1-one[1] The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.94 (m, 2H), 6.97 – 6.93 (m, 2H), 5.89 – 5.79 (m, 1H), 5.07 – 4.96 (m, 2H), 3.89 (s, 3H), 2.96 – 2.90 (m, 2H), 2.16 – 2.10 (m, 2H), 1.79 – 1.75 (m, 2H), 1.54 – 1.47 (m, 2H).

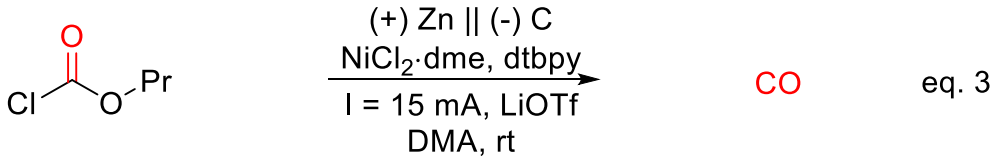
^{13}C NMR (101 MHz, $CDCl_3$) δ 199.0, 163.3, 138.6, 130.3, 130.2, 114.6, 113.7, 55.5, 38.1, 33.6, 28.7, 24.1.

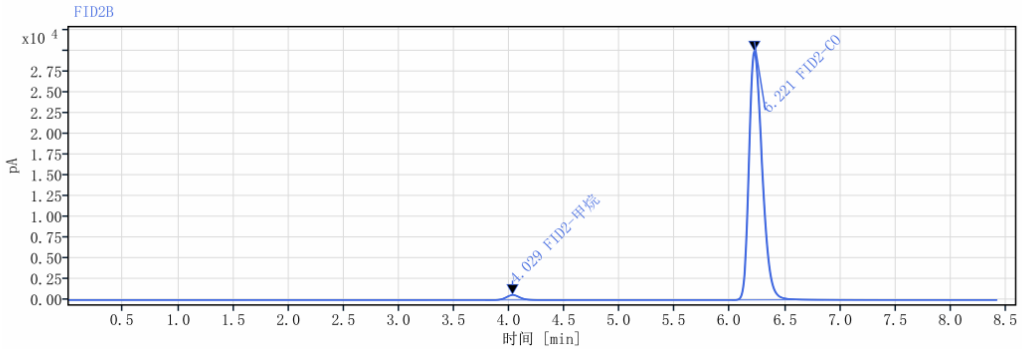


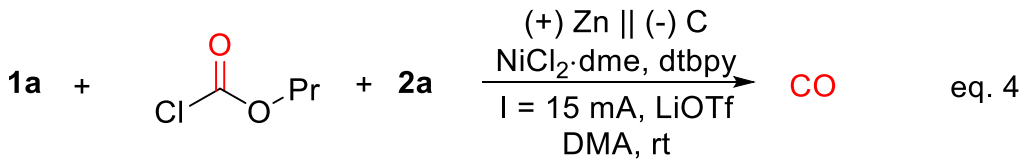
1-(4-methoxyphenyl)pent-4-en-1-one[2] The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

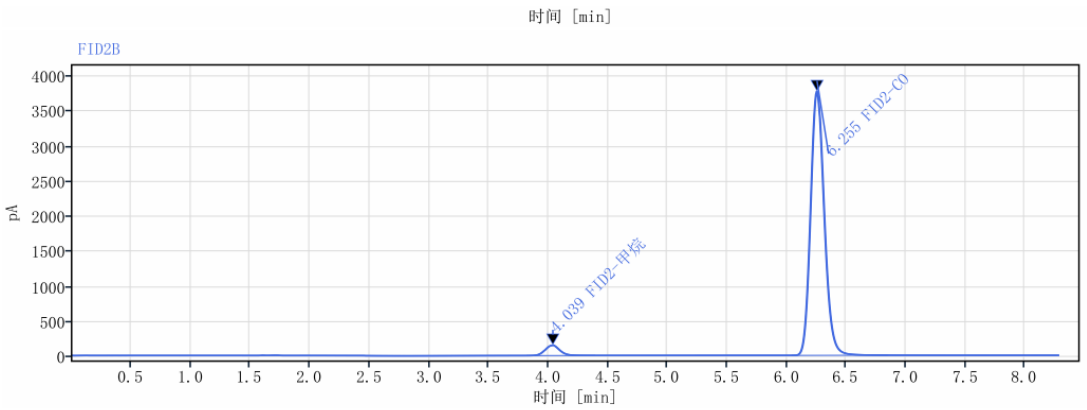
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.96 (m, 2H), 6.98 – 6.94 (m, 2H), 14 – 5.02 (m, 2H),.98 – 5.88 (m, 1H), 3.90 (s, 3H), 3.05 (t, *J* = 7.5 Hz, 2H), 2.54 – 2.48 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.1, 163.4, 137.5, 130.3, 130.1, 115.2, 113.7, 55.5, 37.4, 28.4.

Eq.3 Without 1-(chloromethyl)-4-fluorobenzene iodobenzene **1a** and iodobenzene **2a**, the electrolysis of $ClCO_2Pr$ followed the General Procedure A CO could be detected after the reaction using GC; Eq.4 followed the General Procedure A, using **1a** and **2a** as the substrate, CO could be still detected after the reaction using GC.

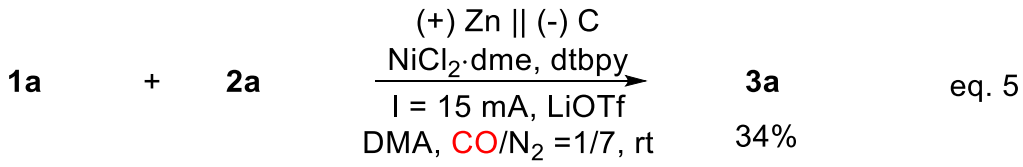








Eq.5 Without $ClCO_2Pr$, run the reaction followed the General Procedure A under the atmosphere CO/N_2 (1:7). The desired product 2-(4-fluorophenyl)-1-phenylethan-1-one **3a** was obtained with a yield of 36%.



Kinetic experiments

An oven-dried 20 mL re-sealable screw-cap test tube equipped with a Teflon-coated magnetic stir bar was sequentially charged with dtbpy (15 mol%), $NiCl_2$·dme (10 mol%), naphthalene (30 mg) as an internal standard, LiOTf (0.2 M) in the glove. Then 6mL DMA, **1a** (0.75 mmol), ClCOOPr (1.5 mmol.), **2a** (0.5 mmol) were added into the tube in turn. All these procedures were conducted in the glovebox. Screw the vial cap with electrode (Zn anode (12 mm X 15 mm), graphite felt cathode (12 mm X 15 mm)) onto the vial to finger tight and adapt the electrochemical cell. Then removed from the glove box. The reaction mixture was stirred and electrolyzed at a constant current (3mA and 15 mA) at room temperature. The yields of **3a** and **3a'** were detected using GC at different times.

Table 3. Monitor the reaction of nickel-catalyzed electroreductive carbonylation of 1a and 2a

I=3mA			I=15mA		
T/h	yield **3a** [%]	yield **3a'** [%]	T/h	yield **3a** [%]	yield **3a'** [%]
1	5	1	0.5	5	2
2	11	7	1	10	9

4	28	18	1.5	12	24
6	39	30	2	13	35
8	44	37	2.5	14	48
10	49	41	3	15	60
12	53	44	3.5	15	73

Conversion was measured by GC using naphthalene as an internal standard.

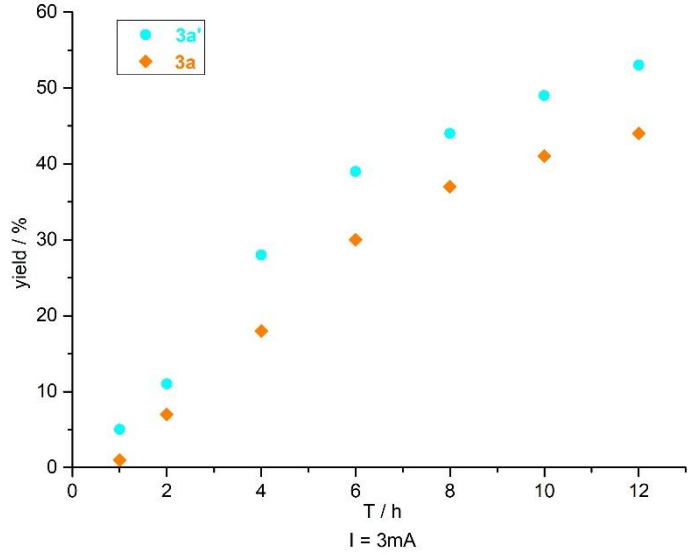


Figure S4 Kinetic plots at I = 3 mA

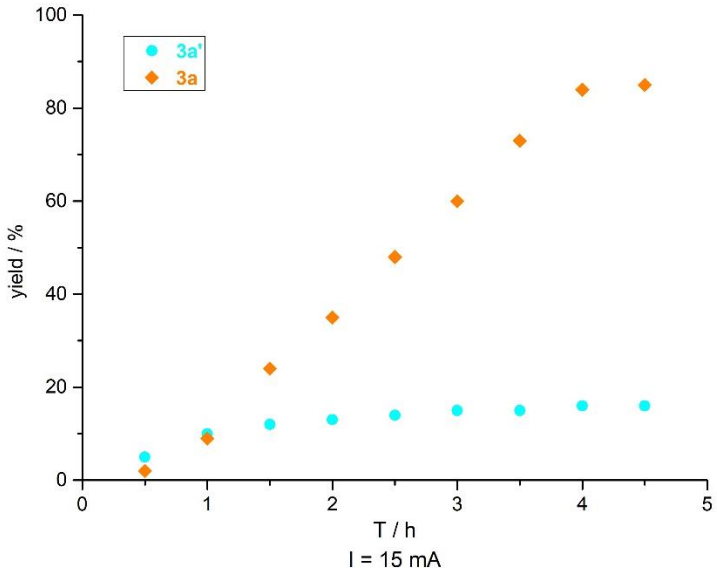


Figure S5 Kinetic plots at I = 15 mA

Cyclic Voltammetry

Cyclic voltammograms in solvent (10 mL) by using glassy carbon as the working electrode, Pt wire as the counter electrode and Ag/AgCl as the reference electrode under N_2 at room temperature. DMA (10mL) containing 0.1 M $^{n}Bu_4PF_6$ was poured into the electro chemical cell in all experiments. The scan rate was 100 mV s^{-1}.

1) Cathodic reduction

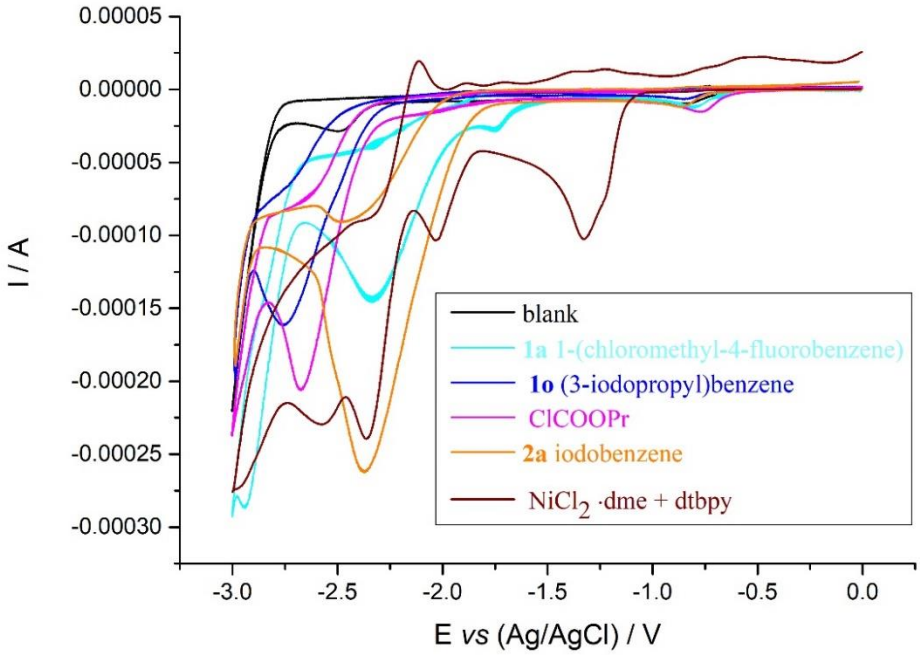


Figure S6: Cyclic voltammograms recorded on a glassy carbon electrode at 100 mVs^{-1} in: (a) DMAc (10 mL), $^{n}Bu_4PF_6$ (1 mol); (b) **1a** (0.1 mmol), DMA (10 mL), $^{n}Bu_4PF_6$ (1 mol); (c) **1o** (0.1 mmol), DMA (10 mL), $^{n}Bu_4PF_6$ (1 mol); (d) ClCOOPr (0.1 mmol), DMA (10 mL), $^{n}Bu_4PF_6$ (1 mol); (d) **2a** (0.1 mmol), DMA (10 mL), $^{n}Bu_4PF_6$ (1 mol); (f) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), DMA (10 mL), $^{n}Bu_4PF_6$ (1 mol).

2) Interaction between [Ni] cat. and 2a iodobenzene

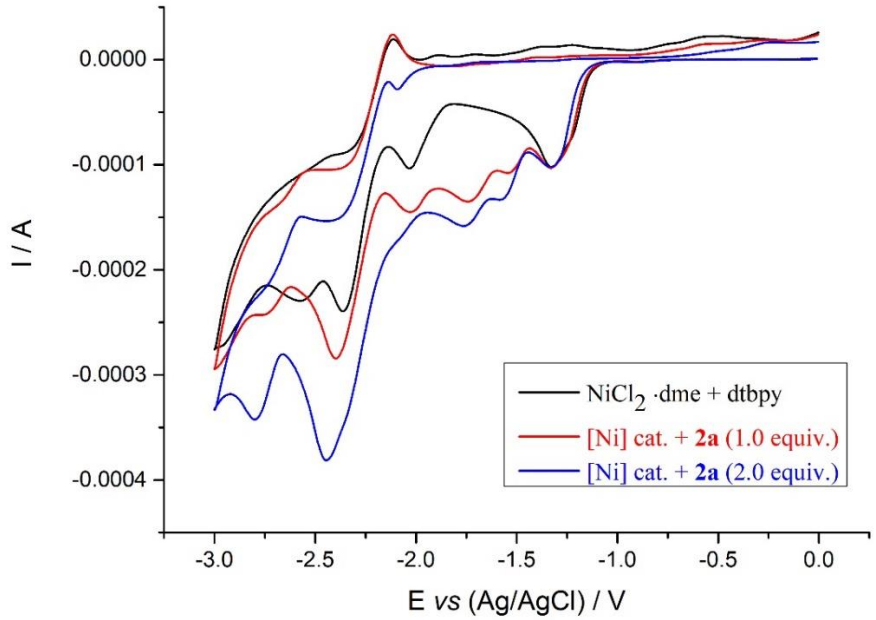


Figure S7: Cyclic voltammograms recorded on a glassy carbon electrode at 100 mVs^{-1} in: (a) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (b) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), **2a** (0.1 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (c) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), **2a** (0.2 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol).

3) Interaction between [Ni] cat. and ClCOOEt

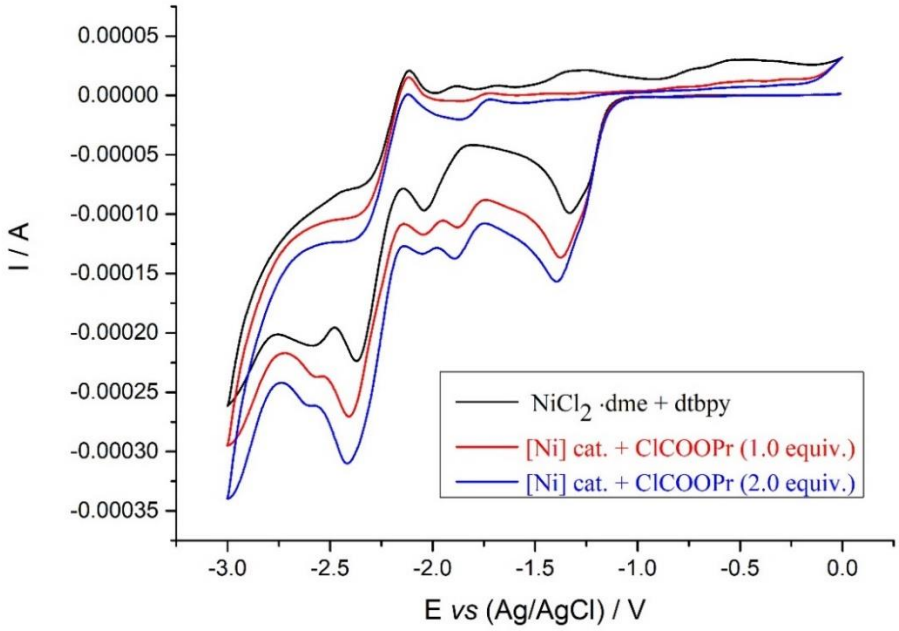


Figure S8: Cyclic voltammograms recorded on a glassy carbon electrode at 100 mVs^{-1} in: (a) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (b) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), ClCOOPr (0.1 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (c) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), ClCOOPr (0.2 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol).

4) Interaction between [Ni] cat, 2a and ClCOOPr

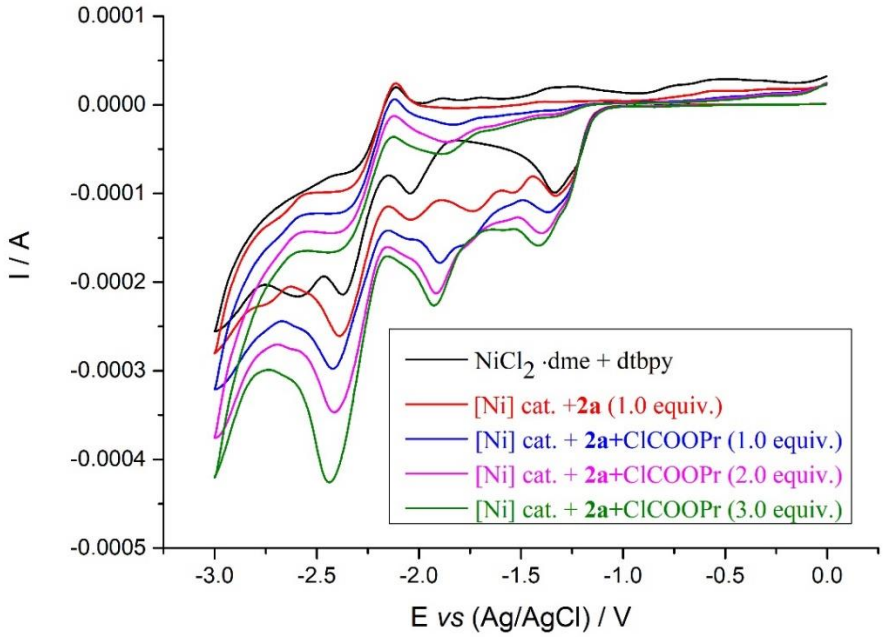


Figure S9: Cyclic voltammograms recorded on a glassy carbon electrode at 100 mVs^{-1} in: (a) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (b) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), **2a** (0.1 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (c) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), **2a** (0.1 mmol), ClCOOPr (0.1 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (d) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), **2a** (0.1 mmol), ClCOOPr (0.2 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (e) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), **2a** (0.1 mmol), ClCOOPr (0.3 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol).

5) Interaction between [Ni] cat, ClCOOPr and 2a

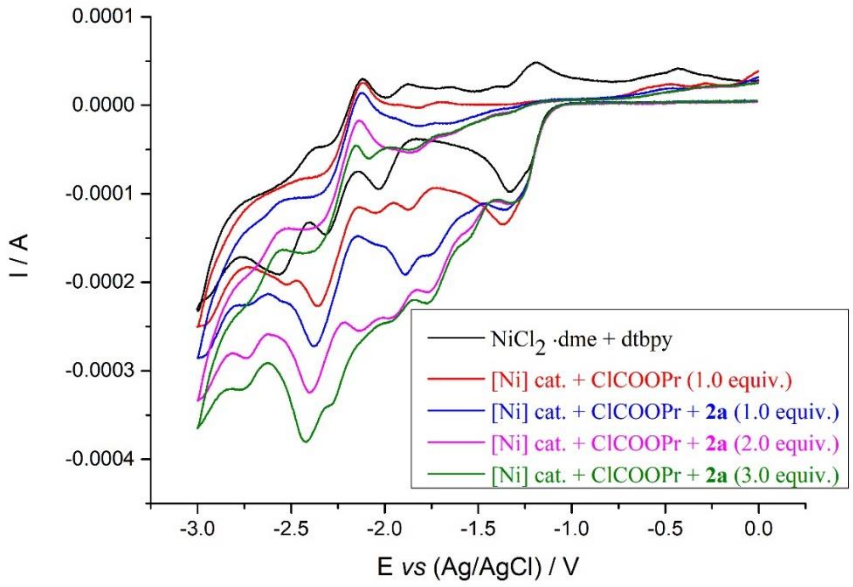


Figure S10: Cyclic voltammograms recorded on a glassy carbon electrode at 100 mVs^{-1} in: (a) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (b) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), ClCOOPr (0.1 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (c) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), ClCOOPr (0.1 mmol), **2a** (0.1 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol); (d) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), ,ClCOOPr (0.1 mmol), **2a** (0.2 mmol) DMA (10 mL), $^nBu_4PF_6$ (1 mol); (e) $NiCl_2$·dme (0.05 mmol), dtbpy (0.15 mmol), ClCOOPr (0.1 mmol), **2a** (0.3 mmol), DMA (10 mL), $^nBu_4PF_6$ (1 mol).

DFT Calculations

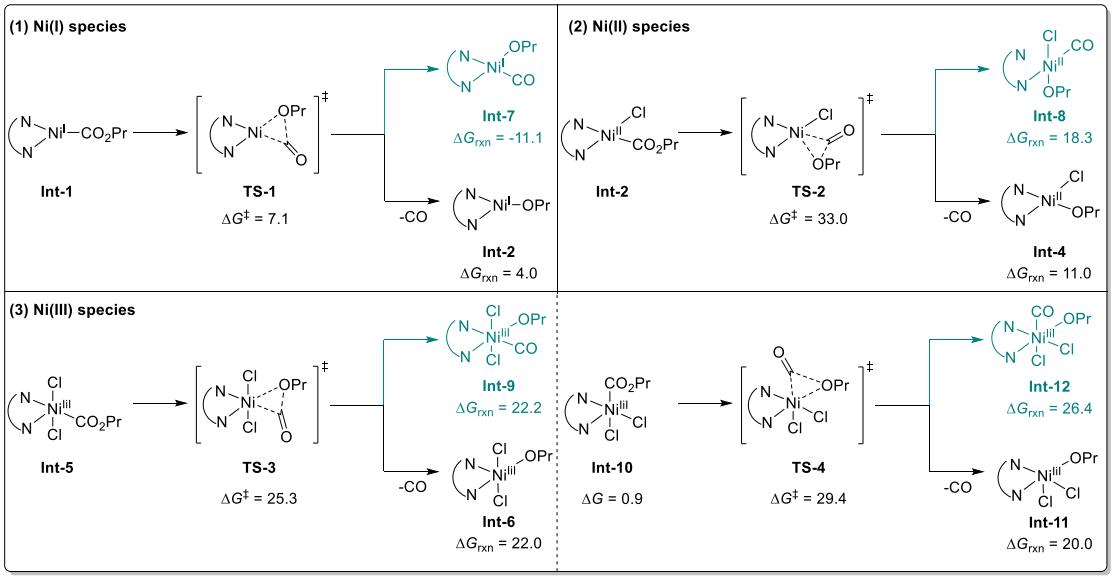


Figure S11. DFT-computed energy profiles of the decarbonylation. Calculations were performed using Gaussian 16 at the M06-L/SDD-6-311+G(d, p)/SMD(DMA)//B3LYP-D3(BJ)/LANL2DZ-6-31G(d) level of theory and the values are shown in kcal/mol.

Computational Details

a) Computational methods

All DFT calculations were carried out using the Gaussian 16 series of programs[3]. Geometries of intermediates and transition states were optimized using dispersion-corrected B3LYP-D3(BJ) functional[4] with a mixed basis set of LANL2DZ for Ni and 6-31G(d) for other atoms in the gas phase. Vibrational frequency calculations were performed for all stationary points to confirm if each optimized structure is a local minimum or a transition state structure. All optimized transition state structures have only one imaginary (negative) frequency, and all minima (reactants, products, and intermediates) have no imaginary frequencies. The M06-L functional[5] with a mixed basis set of SDD for Ni and 6-311+G(d,p) for other atoms was used for single-point energy calculations in solution. Solvation energy corrections were calculated in N, N-dimethylacetamide as solvent with the SMD continuum solvation model[6] based on the gas-phase optimized geometries.

b) Cartesian coordinates (Å) and energies of optimized structures

Int-1

B3LYP-D3(BJ) SCF energy: -1286.44123339 a.u.
B3LYP-D3(BJ) enthalpy: -1285.915223 a.u.
B3LYP-D3(BJ) free energy: -1286.010599 a.u.
M06-L SCF energy in solution: -1288.18479433 a.u.
M06-L enthalpy in solution: -1287.658784 a.u.
M06-L free energy in solution: -1287.754160 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.457280	0.604630	-0.000132
C	-1.802105	1.113823	-0.000156
C	-1.533949	2.482672	-0.000165
C	-0.211367	2.937193	-0.000152
C	0.791783	1.956375	-0.000132
C	1.444803	-0.500507	-0.000129
C	1.740007	-2.795184	-0.000336
C	3.125797	-2.667589	-0.000158
C	3.706990	-1.395151	0.000053
C	2.823517	-0.307253	0.000061
H	-2.809919	0.708883	-0.000120

H	-2.366600	3.174679	-0.000169
H	1.833476	2.253991	-0.000148
H	1.269844	-3.773583	-0.000499
H	3.730466	-3.565413	-0.000210
H	3.216700	0.701916	0.000230
N	0.904616	-1.747182	-0.000313
N	-0.830387	0.197330	-0.000144
Ni	-1.088266	-1.838382	-0.000245
C	5.218998	-1.157885	0.000295
C	5.603236	-0.354041	-1.261702
C	5.602831	-0.354170	1.262495
C	6.010356	-2.475761	0.000335
H	5.335738	-0.902348	-2.171384
H	5.100529	0.617971	-1.294404
H	6.683798	-0.172461	-1.276381
H	5.334995	-0.902534	2.172046
H	6.683392	-0.172628	1.277569
H	5.100133	0.617854	1.295113
H	7.083484	-2.258766	0.000448
H	5.794250	-3.079066	0.888837
H	5.794433	-3.079003	-0.888259
C	0.169692	4.420423	-0.000119
C	1.005752	4.726738	1.262088
C	1.006264	4.726728	-1.261974
C	-1.065987	5.334976	-0.000370
H	0.434198	4.511180	2.171256
H	1.926109	4.134670	1.294944
H	1.288329	5.785452	1.277908
H	0.435131	4.511074	-2.171381
H	1.288754	5.785466	-1.277723
H	1.926705	4.134766	-1.294387
H	-0.746664	6.382373	-0.000333
H	-1.687189	5.177502	-0.888742
H	-1.687553	5.177527	0.887743
C	-2.957618	-2.328720	-0.000204
O	-3.430686	-3.455810	-0.001059
O	-3.858708	-1.240267	0.000938
C	-5.252273	-1.571269	0.000689
C	-6.047714	-0.273771	0.000487
H	-5.491035	-2.180739	0.881488
H	-5.490685	-2.180868	-0.880101
H	-5.763449	0.317400	0.881299
H	-5.763136	0.317281	-0.880297
C	-7.559030	-0.520402	0.000246

H	-8.118546	0.421866	0.000094
H	-7.865988	-1.091695	-0.884256
H	-7.866290	-1.091580	0.884719

TS-1

B3LYP-D3(BJ) SCF energy: -1286.43252526 a.u.
B3LYP-D3(BJ) enthalpy: -1285.908793 a.u.
B3LYP-D3(BJ) free energy: -1286.002969 a.u.
M06-L SCF energy in solution: -1288.17243171 a.u.
M06-L enthalpy in solution: -1287.648699 a.u.
M06-L free energy in solution: -1287.742875 a.u.
Imaginary frequency: -50.0659 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.431855	0.758862	-0.175778
C	1.652664	1.734546	-0.435163
C	1.117747	3.015520	-0.329496
C	-0.258611	3.182021	-0.136711
C	-1.027823	2.011877	-0.062269
C	-1.167098	-0.526857	-0.109918
C	-0.959964	-2.827297	-0.208334
C	-2.328931	-3.005832	-0.017767
C	-3.160855	-1.891437	0.135728
C	-2.541688	-0.634062	0.084909
H	2.714749	1.565626	-0.584187
H	1.784231	3.865695	-0.399120
H	-2.098843	2.082145	0.084500
H	-0.286030	-3.670210	-0.327937
H	-2.724757	-4.013074	0.008902
H	-3.138011	0.263247	0.199136
N	-0.386225	-1.622565	-0.254287
N	0.903721	0.628462	-0.359948
Ni	1.612232	-1.228786	-0.495819
C	-4.673402	-1.992874	0.350675
C	-5.036771	-1.332027	1.698813
C	-5.396595	-1.256115	-0.798396
C	-5.157286	-3.451760	0.376115
H	-4.529901	-1.834371	2.529755
H	-4.755565	-0.274218	1.723103
H	-6.117577	-1.394799	1.868553
H	-5.149466	-1.704063	-1.766907
H	-6.481879	-1.317442	-0.659537
H	-5.124119	-0.196486	-0.838288

H	-6.240886	-3.475639	0.531259
H	-4.946132	-3.966023	-0.567786
H	-4.693226	-4.019188	1.190154
C	-0.931563	4.551229	-0.009158
C	-1.974332	4.707835	-1.138076
C	-1.636535	4.641192	1.362431
C	0.079517	5.704355	-0.114870
H	-1.498030	4.642383	-2.122237
H	-2.748981	3.935865	-1.087055
H	-2.468211	5.683010	-1.060587
H	-0.916942	4.527046	2.180291
H	-2.125731	5.615865	1.470033
H	-2.403032	3.868063	1.478186
H	-0.444236	6.660959	-0.017937
H	0.833296	5.657231	0.678634
H	0.594808	5.705130	-1.081568
C	2.994532	-2.569991	-0.559490
O	3.658746	-3.531643	-0.335432
O	3.788842	-1.188950	-0.781966
C	5.077618	-1.092675	-0.201503
C	5.033333	-0.381801	1.152019
H	5.735598	-0.548502	-0.894917
H	5.485746	-2.106112	-0.080474
H	4.583367	0.612105	1.017576
H	4.357576	-0.942595	1.810651
C	6.415794	-0.250685	1.795945
H	7.099034	0.320848	1.154961
H	6.362997	0.259261	2.764668
H	6.867096	-1.236426	1.961697

CO

B3LYP-D3(BJ) SCF energy: -113.30764 a.u.
B3LYP-D3(BJ) enthalpy: -113.2993 a.u.
B3LYP-D3(BJ) free energy: -113.32174 a.u.
M06-L SCF energy in solution: -113.32564 a.u.
M06-L enthalpy in solution: -113.317298 a.u.
M06-L free energy in solution: -113.339741 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	-0.650132
O	0.000000	0.000000	0.487599

Int-2

B3LYP-D3(BJ) SCF energy: -1173.11029355 a.u.
B3LYP-D3(BJ) enthalpy: -1172.596546 a.u.
B3LYP-D3(BJ) free energy: -1172.686510 a.u.
M06-L SCF energy in solution: -1174.83175090 a.u.
M06-L enthalpy in solution: -1174.318003 a.u.
M06-L free energy in solution: -1174.407967 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.973977	-0.438279	-0.174256
C	-1.347158	-2.718215	-0.347286
C	-2.709701	-2.559541	-0.132491
C	-3.240996	-1.279211	0.086182
C	-2.330696	-0.217533	0.058523
C	0.041727	0.625214	-0.237116
C	2.287096	1.072183	-0.586509
C	2.089215	2.438055	-0.422116
C	0.805851	2.929949	-0.140791
C	-0.219878	1.982660	-0.050982
H	-0.914576	-3.701293	-0.504090
H	-3.340784	-3.439189	-0.132647
H	-2.681834	0.795506	0.215249
H	3.271704	0.662525	-0.787624
H	2.940072	3.101447	-0.510917
H	-1.231651	2.304452	0.165517
N	1.295648	0.175119	-0.496020
N	-0.479437	-1.692184	-0.366670
Ni	1.487327	-1.831177	-0.578892
C	0.500131	4.416494	0.063540
C	-0.527990	4.871177	-0.995849
C	-0.088734	4.622831	1.476538
C	1.758261	5.289481	-0.072094
H	-0.134235	4.729981	-2.008202
H	-1.465683	4.311335	-0.918797
H	-0.760665	5.934027	-0.863649
H	0.621743	4.302802	2.246337
H	-0.316002	5.682664	1.638995
H	-1.015082	4.056687	1.617906
H	1.493689	6.340840	0.081912
H	2.517142	5.025786	0.672653
H	2.206934	5.202874	-1.067734
C	-4.727184	-1.014716	0.341337
C	-4.892023	-0.340248	1.721161
C	-5.270809	-0.077254	-0.759491

C	-5.554471	-2.310437	0.330290
H	-4.509554	-0.985386	2.519479
H	-4.356420	0.613169	1.774028
H	-5.951371	-0.140674	1.919406
H	-5.161117	-0.532656	-1.749653
H	-6.334772	0.125098	-0.591124
H	-4.745554	0.883310	-0.771307
H	-6.607627	-2.075318	0.516411
H	-5.494805	-2.821681	-0.636793
H	-5.227318	-3.007107	1.109891
O	2.949954	-2.873926	-0.664558
C	4.011715	-3.059117	0.206453
C	4.636466	-1.745990	0.700579
H	4.807779	-3.646226	-0.292473
H	3.714243	-3.650867	1.096454
H	4.939192	-1.160955	-0.179998
H	3.855232	-1.165222	1.212122
C	5.834242	-1.956508	1.630357
H	6.631439	-2.517000	1.126270
H	6.259912	-1.004367	1.968573
H	5.545190	-2.526725	2.522194

Int-3

B3LYP-D3(BJ) SCF energy: -1746.70699464 a.u.
B3LYP-D3(BJ) enthalpy: -1746.175844 a.u.
B3LYP-D3(BJ) free energy: -1746.271667 a.u.
M06-L SCF energy in solution: -1748.47402929 a.u.
M06-L enthalpy in solution: -1747.942879 a.u.
M06-L free energy in solution: -1748.038702 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.770314	0.819678	-0.151390
C	-1.171733	2.017189	-0.559544
C	-0.503821	3.228363	-0.403427
C	0.859188	3.248492	-0.097824
C	1.486001	2.000491	0.014732
C	1.381981	-0.522951	-0.097542
C	0.986037	-2.782212	-0.405261
C	2.312713	-3.094164	-0.113767
C	3.217078	-2.078979	0.212002
C	2.715622	-0.769312	0.214316
H	-2.220399	1.977698	-0.825587
H	-1.068244	4.143222	-0.529554

H	2.547559	1.948124	0.221475
H	0.244942	-3.536808	-0.649722
H	2.617462	-4.132397	-0.141752
H	3.369315	0.056986	0.464783
N	0.528553	-1.527679	-0.398062
N	-0.563889	0.829581	-0.418584
C	4.685781	-2.337122	0.557637
C	5.580721	-1.576888	-0.446103
C	4.962410	-1.826313	1.989036
C	5.040171	-3.831586	0.494339
H	5.396369	-1.917224	-1.470720
H	5.404966	-0.496703	-0.412977
H	6.637005	-1.750750	-0.212388
H	4.333237	-2.347132	2.718744
H	6.011094	-2.002354	2.253459
H	4.769772	-0.752680	2.083573
H	6.096678	-3.968012	0.747101
H	4.450447	-4.419200	1.206181
H	4.883096	-4.244009	-0.508206
C	1.664649	4.534809	0.094252
C	2.280115	4.535355	1.511159
C	2.792130	4.584806	-0.960706
C	0.791489	5.790328	-0.061362
H	1.498831	4.494235	2.277686
H	2.949131	3.682583	1.665726
H	2.863340	5.449979	1.665443
H	2.379631	4.577460	-1.975260
H	3.380124	5.500999	-0.836579
H	3.475356	3.734307	-0.868391
H	1.405344	6.684064	0.090257
H	0.350848	5.857222	-1.061962
H	-0.018528	5.815080	0.675693
C	-3.148516	-0.280011	-0.650385
O	-3.623307	0.448241	-1.506753
O	-3.851241	-0.648414	0.446688
C	-5.229826	-0.222253	0.489310
C	-5.848494	-0.797169	1.751646
H	-5.740036	-0.581384	-0.410842
H	-5.273412	0.873728	0.479112
H	-5.739139	-1.887827	1.729726
H	-5.281339	-0.440842	2.620843
Ni	-1.393174	-0.932864	-0.615770
Cl	-2.197006	-2.949708	-0.996602
C	-7.324301	-0.411898	1.888157

H	-7.910963	-0.781459	1.038549
H	-7.758674	-0.832658	2.801277
H	-7.450351	0.677110	1.929495

TS-2

B3LYP-D3(BJ) SCF energy: -1746.64639030 a.u.
B3LYP-D3(BJ) enthalpy: -1746.118979 a.u.
B3LYP-D3(BJ) free energy: -1746.214322 a.u.
M06-L SCF energy in solution: -1748.41822158 a.u.
M06-L enthalpy in solution: -1747.890810 a.u.
M06-L free energy in solution: -1747.986153 a.u.
Imaginary frequency: -373.5490 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	0.714486	0.834883	-0.167411
C	-1.141249	2.233617	-0.277282
C	-0.341370	3.358343	-0.100192
C	1.046157	3.229686	0.028979
C	1.559621	1.925889	0.004603
C	1.127544	-0.573004	-0.132190
C	0.355883	-2.759756	-0.172359
C	1.646927	-3.252305	-0.008439
C	2.734561	-2.377875	0.087454
C	2.438303	-1.010191	0.021107
H	-2.223763	2.268475	-0.336579
H	-0.822493	4.326971	-0.063483
H	2.621552	1.757519	0.134563
H	-0.506945	-3.408748	-0.263276
H	1.781418	-4.325222	0.037928
H	3.233820	-0.278304	0.090480
N	0.091068	-1.447367	-0.236004
N	-0.619465	1.002817	-0.336452
C	4.181720	-2.844786	0.255665
C	5.015882	-2.334261	-0.940260
C	4.749255	-2.263117	1.569540
C	4.290716	-4.377116	0.310948
H	4.627763	-2.728905	-1.885343
H	5.011146	-1.241226	-1.003993
H	6.057247	-2.658467	-0.835641
H	4.168121	-2.605114	2.432633
H	5.786836	-2.587991	1.704937
H	4.739852	-1.168252	1.569020
H	5.340069	-4.664881	0.431563

H	3.733566	-4.793674	1.157113
H	3.922810	-4.843892	-0.609158
C	1.989039	4.421577	0.208169
C	2.733237	4.277456	1.554386
C	3.010527	4.431288	-0.950743
C	1.234103	5.760655	0.207037
H	2.027615	4.257326	2.391766
H	3.331080	3.361121	1.594905
H	3.411905	5.125410	1.698645
H	2.505078	4.526886	-1.917701
H	3.696269	5.278293	-0.837755
H	3.610934	3.515970	-0.973175
H	1.947181	6.582116	0.330408
H	0.699248	5.924341	-0.734761
H	0.513366	5.821727	1.029598
C	-3.086047	0.198626	-1.769069
O	-4.050274	0.390485	-2.374908
O	-3.296974	0.578806	0.187852
C	-4.473503	0.070577	0.745312
C	-4.212216	-0.630886	2.081786
H	-4.966953	-0.641353	0.059541
H	-5.192368	0.895300	0.908918
H	-3.495766	-1.440693	1.899176
H	-3.726951	0.082958	2.761920
Ni	-1.638373	-0.604460	-0.587186
Cl	-2.737029	-2.519708	-0.771130
C	-5.488162	-1.188894	2.717077
H	-5.964499	-1.923165	2.056052
H	-5.279594	-1.686441	3.671478
H	-6.219325	-0.393078	2.909567

Int-4

B3LYP-D3(BJ) SCF energy: -1633.36627581 a.u.
B3LYP-D3(BJ) enthalpy: -1632.847216 a.u.
B3LYP-D3(BJ) free energy: -1632.937445 a.u.
M06-L SCF energy in solution: -1635.11024918 a.u.
M06-L enthalpy in solution: -1634.591189 a.u.
M06-L free energy in solution: -1634.681418 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.375698	0.834618	0.000161
C	-1.770649	1.721775	0.000595
C	-1.270950	3.021258	0.000433

C	0.110589	3.245524	0.000115
C	0.932613	2.109684	-0.000016
C	1.136409	-0.426033	0.000134
C	0.964224	-2.736106	0.000716
C	2.349834	-2.874478	0.000487
C	3.173637	-1.745165	-0.000015
C	2.524719	-0.503079	-0.000180
H	-2.826801	1.466900	0.000815
H	-1.973815	3.844324	0.000561
H	2.009990	2.220533	-0.000244
H	0.292523	-3.587089	0.001000
H	2.764053	-3.874428	0.000679
H	3.105160	0.411375	-0.000549
N	0.359814	-1.540939	0.000513
N	-0.964850	0.657454	0.000461
C	4.702195	-1.813991	-0.000358
C	5.237200	-1.102644	-1.263000
C	5.237765	-1.102145	1.261768
C	5.214767	-3.263208	-0.000191
H	4.864268	-1.586022	-2.172330
H	4.939835	-0.049402	-1.294911
H	6.332100	-1.141471	-1.278902
H	4.865234	-1.585163	2.171454
H	6.332673	-1.140968	1.277202
H	4.940411	-0.048892	1.293389
H	6.309591	-3.264019	-0.000472
H	4.883029	-3.811051	0.888439
H	4.882567	-3.811411	-0.888426
C	0.736334	4.642542	-0.000074
C	1.612662	4.801623	1.262164
C	1.612297	4.801459	-1.262583
C	-0.327196	5.752480	0.000006
H	1.013792	4.684780	2.171748
H	2.420808	4.063648	1.293726
H	2.068860	5.797736	1.278162
H	1.013161	4.684527	-2.171981
H	2.068513	5.797561	-1.278826
H	2.420420	4.063465	-1.294300
H	0.164949	6.730456	-0.000114
H	-0.966084	5.702780	-0.888356
H	-0.965846	5.702882	0.888545
Ni	-1.597424	-1.200662	0.000391
Cl	-2.141832	-3.340205	-0.000030
O	-3.272007	-0.542451	0.000270

C	-4.459033	-1.286280	-0.000236
C	-5.638169	-0.307242	-0.000733
H	-4.531494	-1.941403	0.882157
H	-4.530755	-1.941395	-0.882667
H	-5.552639	0.342708	0.880811
H	-5.552181	0.342380	-0.882471
C	-6.991538	-1.022664	-0.000949
H	-7.824127	-0.309562	-0.001390
H	-7.098891	-1.662895	-0.885077
H	-7.099422	-1.662432	0.883448

Int-5

B3LYP-D3(BJ) SCF energy: -2206.92509840 a.u.
B3LYP-D3(BJ) enthalpy: -2206.391023 a.u.
B3LYP-D3(BJ) free energy: -2206.494080 a.u.
M06-L SCF energy in solution: -2208.72052145 a.u.
M06-L enthalpy in solution: -2208.186446 a.u.
M06-L free energy in solution: -2208.289503 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.156148	0.759107	-0.000003
C	-0.386452	2.488588	-0.000028
C	0.624686	3.447760	-0.000013
C	1.963898	3.050467	0.000063
C	2.208481	1.670076	0.000025
C	1.344696	-0.709979	-0.000049
C	0.271819	-2.759910	-0.000179
C	1.481682	-3.448961	-0.000148
C	2.684534	-2.735416	-0.000058
C	2.588530	-1.337306	-0.000006
H	-1.437243	2.755185	-0.000062
H	0.344956	4.493218	-0.000044
H	3.228077	1.306184	0.000048
H	-0.678483	-3.283696	-0.000243
H	1.466078	-4.530994	-0.000215
H	3.490576	-0.738660	0.000057
N	0.206472	-1.430156	-0.000125
N	-0.128034	1.180860	-0.000023
C	4.059971	-3.407524	-0.000014
C	4.834021	-2.968333	-1.262676
C	4.833904	-2.968361	1.262735
C	3.953803	-4.941098	-0.000022
H	4.298880	-3.261884	-2.172058

H	4.981497	-1.883991	-1.294277
H	5.822514	-3.440820	-1.278693
H	4.298675	-3.261915	2.172066
H	5.822389	-3.440860	1.278851
H	4.981381	-1.884018	1.294368
H	4.958081	-5.377049	0.000016
H	3.431713	-5.312073	0.888696
H	3.431745	-5.312096	-0.888745
C	3.135562	4.035282	0.000058
C	3.992776	3.796464	1.262781
C	3.992830	3.796347	-1.262608
C	2.660687	5.497286	-0.000034
H	3.402394	3.952006	2.172051
H	4.398229	2.780003	1.294626
H	4.837592	4.494082	1.278908
H	3.402532	3.951961	-2.171915
H	4.837737	4.493866	-1.278667
H	4.398203	2.779851	-1.294400
H	3.529188	6.163905	-0.000077
H	2.063923	5.730175	-0.888587
H	2.063942	5.730292	0.888505
C	-3.218930	0.606952	0.000029
O	-3.337842	1.804773	0.000039
O	-4.180303	-0.298953	0.000048
C	-5.543080	0.219272	0.000014
C	-6.477524	-0.974451	0.000052
H	-5.670186	0.844441	-0.889387
H	-5.670213	0.844529	0.889355
H	-6.263375	-1.590290	-0.881252
H	-6.263370	-1.590211	0.881420
Cl	-1.864999	-0.601643	-2.230575
Ni	-1.529745	-0.338140	0.000013
Cl	-1.864873	-0.602077	2.230561
C	-7.944997	-0.534789	0.000040
H	-8.181200	0.066759	-0.885803
H	-8.610538	-1.403914	0.000089
H	-8.181190	0.066852	0.885822

TS-3

B3LYP-D3(BJ) SCF energy: -2206.87357239 a.u.

B3LYP-D3(BJ) enthalpy: -2206.343053 a.u.

B3LYP-D3(BJ) free energy: -2206.444887 a.u.

M06-L SCF energy in solution: -2208.67782147 a.u.

M06-L enthalpy in solution: -2208.147302 a.u.

M06-L free energy in solution: -2208.249136 a.u.
Imaginary frequency: -177.2754 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-1.292784	-0.275327	0.032325
C	-1.301515	-2.583825	0.185187
C	-2.675310	-2.637971	-0.035966
C	-3.394184	-1.456298	-0.241172
C	-2.664158	-0.260224	-0.199967
C	-0.448456	0.933554	0.119605
C	1.715574	1.695920	0.492148
C	1.301726	3.024285	0.443196
C	-0.044536	3.325488	0.211558
C	-0.920302	2.240298	0.058681
H	-0.718642	-3.485290	0.336852
H	-3.161536	-3.604582	-0.049573
H	-3.168580	0.685715	-0.353672
H	2.743532	1.408221	0.682733
H	2.037827	3.803377	0.590870
H	-1.977100	2.417450	-0.096713
N	0.864640	0.689760	0.313464
N	-0.630680	-1.435985	0.217450
C	-0.582442	4.756418	0.136935
C	-1.236664	4.974278	-1.245521
C	-1.636590	4.955532	1.248681
C	0.528892	5.802102	0.322923
H	-0.508698	4.829831	-2.050948
H	-2.069257	4.284383	-1.416697
H	-1.628350	5.995035	-1.316323
H	-1.197211	4.794151	2.238776
H	-2.030616	5.977147	1.210471
H	-2.481143	4.267688	1.138866
H	0.099613	6.806881	0.255458
H	1.010741	5.713555	1.302668
H	1.299145	5.718256	-0.451514
C	-4.901852	-1.424237	-0.502214
C	-5.586164	-0.593807	0.606196
C	-5.158544	-0.768256	-1.877137
C	-5.516948	-2.832957	-0.509206
H	-5.409423	-1.035581	1.592673
H	-5.219523	0.437581	0.628560
H	-6.667726	-0.560213	0.434203
H	-4.672977	-1.335266	-2.678413

H	-6.234611	-0.737611	-2.081325
H	-4.781715	0.258909	-1.916092
H	-6.592690	-2.760880	-0.699137
H	-5.083371	-3.461349	-1.294753
H	-5.383826	-3.339171	0.453134
C	2.237274	-2.830005	0.716230
O	2.691429	-3.861908	0.886066
O	3.384035	-1.012562	0.604321
C	4.250318	-1.092522	-0.500675
C	4.417510	0.246545	-1.220818
H	3.856087	-1.813289	-1.233408
H	5.219330	-1.476854	-0.143207
H	3.430250	0.567440	-1.569701
H	4.787559	0.996772	-0.508270
Cl	1.413912	-1.588992	-2.005182
Ni	1.397986	-1.193031	0.396596
Cl	1.142681	-1.350724	2.793702
C	5.375238	0.127457	-2.408746
H	4.987068	-0.583130	-3.147245
H	5.506447	1.093042	-2.909115
H	6.365778	-0.221520	-2.091650

Int-6

B3LYP-D3(BJ) SCF energy: -2093.55692492 a.u.
B3LYP-D3(BJ) enthalpy: -2093.036044 a.u.
B3LYP-D3(BJ) free energy: -2093.133701 a.u.
M06-L SCF energy in solution: -2095.33793851 a.u.
M06-L enthalpy in solution: -2094.817058 a.u.
M06-L free energy in solution: -2094.914715 a.u.

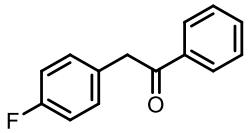
Cartesian coordinates

ATOM	X	Y	Z
C	-1.174759	-0.265551	0.022518
C	-1.368325	-2.571894	0.180945
C	-2.743412	-2.513698	-0.023426
C	-3.368100	-1.277127	-0.217802
C	-2.544477	-0.143600	-0.191134
C	-0.233841	0.872867	0.085398
C	1.988024	1.462788	0.412476
C	1.685888	2.818623	0.307364
C	0.366929	3.223317	0.075727
C	-0.598169	2.210556	-0.029756
H	-0.851053	-3.512544	0.329625
H	-3.305921	-3.437929	-0.028690

H	-2.973925	0.839630	-0.337209
H	2.988996	1.093764	0.603649
H	2.486558	3.539066	0.411710
H	-1.636520	2.469613	-0.194857
N	1.052251	0.524243	0.291718
N	-0.610774	-1.477326	0.203373
C	-0.049939	4.690454	-0.054160
C	-0.690578	4.908938	-1.442873
C	-1.078453	5.020114	1.050520
C	1.145565	5.646067	0.089151
H	0.018891	4.673402	-2.243372
H	-1.578937	4.285223	-1.585738
H	-0.995930	5.955389	-1.552782
H	-0.649011	4.862034	2.045478
H	-1.386701	6.068600	0.972546
H	-1.977652	4.400882	0.969670
H	0.800797	6.680011	-0.013399
H	1.625083	5.552894	1.069589
H	1.901004	5.470566	-0.684518
C	-4.873007	-1.124270	-0.451016
C	-5.467460	-0.244174	0.670918
C	-5.102686	-0.446883	-1.820304
C	-5.598818	-2.479315	-0.447073
H	-5.306432	-0.700185	1.653509
H	-5.020266	0.755025	0.686133
H	-6.546185	-0.125323	0.520287
H	-4.680292	-1.049482	-2.631451
H	-6.176528	-0.329702	-2.003520
H	-4.645918	0.547084	-1.866033
H	-6.668563	-2.320950	-0.617428
H	-5.231398	-3.139342	-1.240401
H	-5.489368	-2.995979	0.512611
O	3.212864	-1.343702	0.833626
C	4.244022	-1.747919	-0.012863
C	4.624335	-0.727053	-1.084469
H	4.022732	-2.723011	-0.470736
H	5.102060	-1.922710	0.665148
H	3.730777	-0.508580	-1.678802
H	4.932175	0.206653	-0.592493
Cl	1.587637	-2.336372	-1.613560
Ni	1.377066	-1.474206	0.494867
Cl	0.918855	-1.678859	2.744483
C	5.745434	-1.238418	-1.992128
H	5.430967	-2.144863	-2.522426

H 6.022552 -0.491430 -2.743884
H 6.647522 -1.482836 -1.416898

Analytical Data of Substrates and Products

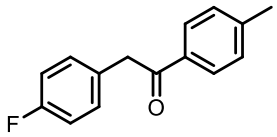


2-(4-fluorophenyl)-1-phenylethan-1-one[7] Light yellow solid (83.5 mg, 78% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 8.02 (m, 2H), 7.63 – 7.59 (m, 1H), 7.53 – 7.49 (m, 2H), 7.29 – 7.23 (m, 2H), 7.03 – 6.09 (m, 2H), 4.30 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.5, 161.9 (d, *J* = 245.2 Hz), 136.4, 133.4, 131.1 (d, *J* = 8.0 Hz), 130.2 (d, *J* = 3.3 Hz), 128.7, 128.5, 115.5 (d, *J* = 21.5 Hz), 44.5.

^{19}F NMR (377 MHz, $CDCl_3$) δ -115.93.

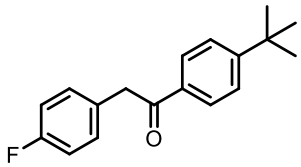


2-(4-fluorophenyl)-1-(p-tolyl)ethan-1-one[8] White solid (94.7 mg, 83% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 2H), 7.31 – 7.24 (m, 4H), 7.08 – 7.02 (m, 2H), 4.27 (s, 2H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.1, 161.9 (d, *J* = 245.0 Hz), 144.2, 134.0, 131.0 (d, *J* = 8.0 Hz), 130.4 (d, *J* = 3.3 Hz), 129.4, 128.7, 115.5 (d, *J* = 21.5 Hz), 44.4, 21.7.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.07.



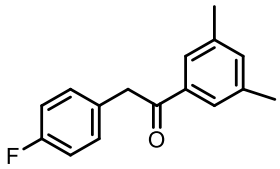
1-(4-(tert-butyl)phenyl)-2-(4-fluorophenyl)ethan-1-one White solid (110.7 mg, 82% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.98 (m, 2H), 7.54 – 7.51 (m, 2H), 7.30 – 7.25 (m, 2H), 7.07 – 7.03 (m, 2H), 4.28 (s, 2H), 1.38 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.1, 161.9 (d, *J* = 245.0 Hz), 157.1, 133.9, 131.0 (d, *J* = 8.0 Hz), 130.4 (d, *J* = 3.3 Hz), 128.6, 125.7, 115.5 (d, *J* = 21.3 Hz), 44.5, 35.2, 31.1.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.05.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{19}FNaO^+$ 293.1312; Found 293.1310.



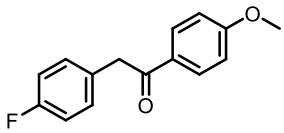
1-(3,5-dimethylphenyl)-2-(4-fluorophenyl)ethan-1-one Light yellow oil (92.1 mg, 76% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 1.7 Hz, 2H), 7.28 – 7.24 (m, 3H), 7.08 – 7.04 (m, 2H), 4.28 (s, 2H), 2.42 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 161.9 (d, *J* = 245.0 Hz), 138.4, 136.7, 135.0, 131.1 (d, *J* = 7.9 Hz), 130.4 (d, *J* = 3.3 Hz), 126.3, 115.5 (d, *J* = 21.4 Hz), 44.5, 21.3.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.07.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{15}FNaO^+$ 265.0999; Found 265.0997.

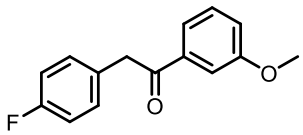


2-(4-fluorophenyl)-1-(4-methoxyphenyl)ethan-1-one[9] Light yellow oil (107.4 mg, 88% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.27 – 7.23 (m, 2H), 7.06 – 7.02 (m, 2H), 6.98 – 6.96 (m, 2H), 4.24 (s, 2H), 3.90 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.0, 163.7, 161.9 (d, *J* = 245.0 Hz), 131.0 (d, *J* = 8.0 Hz), 130.9, 130.6 (d, *J* = 3.3 Hz), 129.5, 115.5 (d, *J* = 21.4 Hz), 113.9, 55.5, 44.3.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.15.



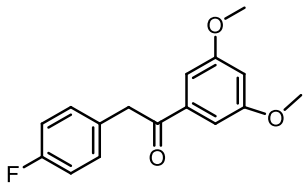
2-(4-fluorophenyl)-1-(3-methoxyphenyl)ethan-1-one Yellow oil (74.6 mg, 61% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (ddd, *J* = 7.7, 1.6, 1.0 Hz, 1H), 7.55 (dd, *J* = 2.7, 1.6 Hz, 1H), 7.41 (t, *J* = 7.9 Hz, 1H), 7.29 – 7.22 (m, 2H), 7.15 (ddd, *J* = 8.2, 2.7, 1.0 Hz, 1H), 7.08 – 7.02 (m, 2H), 4.28 (s, 2H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.3, 161.9 (d, *J* = 245.1 Hz), 159.9, 137.8, 131.1 (d, *J* = 8.0 Hz), 130.2 (d, *J* = 3.4 Hz), 129.7, 121.2, 119.7, 115.5 (d, *J* = 21.3 Hz), 112.9, 55.4, 44.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -115.97.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{13}FNaO_2^+$ 267.0792; Found 267.0789.



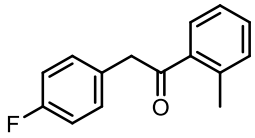
1-(3,5-dimethoxyphenyl)-2-(4-fluorophenyl)ethan-1-one Yellow oil (97.3 mg, 71% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.23 (m, 2H), 7.16 (d, *J* = 2.3 Hz, 2H), 7.07 – 7.01 (m, 2H), 6.68 (t, *J* = 2.3 Hz, 1H), 4.24 (s, 2H), 3.85 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.14, 161.9 (d, *J* = 245.1 Hz), 160.9, 138.4, 131.0 (d, *J* = 8.0 Hz), 130.2 (d, *J* = 3.3 Hz), 115.5 (d, *J* = 21.5 Hz), 106.4, 105.4, 55.6, 44.6.

^{19}F NMR (377 MHz, $CDCl_3$) δ -115.93.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{15}FNaO_3^+$ 297.0897; Found 297.0902.



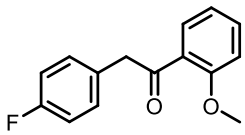
2-(4-fluorophenyl)-1-(o-tolyl)ethan-1-one Light yellow oil (44.5 mg, 39% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.41 (td, *J* = 7.5, 1.4 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.24 – 7.21 (m, 2H), 7.07 – 7.02 (m, 2H), 4.22 (s, 2H), 2.48 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 201.2, 161.9 (d, *J* = 245.3 Hz), 138.6, 137.4, 132.1, 131.5, 131.1 (d, *J* = 8.0 Hz), 130.1 (d, *J* = 3.5 Hz), 128.6, 125.7, 115.5 (d, *J* = 21.4 Hz), 47.4, 21.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -116.61.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{13}FNaO^+$ 251.0842; Found 251.0852.



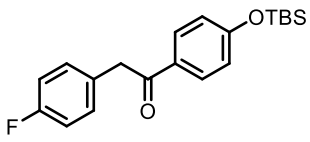
2-(4-fluorophenyl)-1-(2-methoxyphenyl)ethan-1-one Light yellow oil (51.2 mg, 42% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.50 (ddd, *J* = 8.4, 7.3, 1.9 Hz, 1H), 7.25 – 7.19 (m, 2H), 7.05 – 6.99 (m, 4H), 4.31 (s, 2H), 3.96 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 199.9, 161.8 (d, *J* = 244.4 Hz), 158.4, 133.7, 131.2 (d, *J* = 7.8 Hz), 130.9 (d, *J* = 3.3 Hz), 130.7, 128.0, 120.8, 115.2 (d, *J* = 21.3 Hz), 111.5, 55.5, 49.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -116.01.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{13}FNaO_2^+$ 267.0792; Found 267.0790.



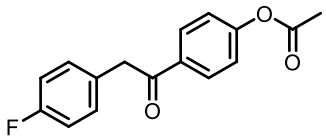
1-(4-((tert-butyldimethylsilyl)oxy)phenyl)-2-(4-fluorophenyl)ethan-1-one White solid (134.2 mg, 78% yield). mp 140.6−141.3 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.95 (m, 2H), 7.28 – 7.23 (m, 2H), 7.07 – 7.01 (m, 2H), 6.93 – 6.89 (m, 2H), 4.24 (s, 2H), 1.02 (s, 9H), 0.27 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.1, 161.9 (d, *J* = 244.9 Hz), 160.5, 131.0 (d, *J* = 8.0 Hz), 130.8, 130.5 (d, *J* = 3.3 Hz), 130.0, 120.0, 115.5 (d, *J* = 21.3 Hz), 44.2, 25.6, 18.3, -4.3.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.17.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{25}FNaO_2Si^+$ 367.1500; Found 367.1503.



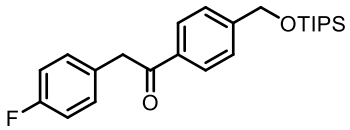
4-(2-(4-fluorophenyl)acetyl)phenyl acetate Yellow solid (103.4 mg, 76% yield). mp 114.7−115.3 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 8/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 8.05 (m, 2H), 7.26 – 7.22 (m, 4H), 7.08 – 7.02 (m, 2H), 4.27 (s, 2H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.2, 168.9, 162.0 (d, *J* = 245.3 Hz), 154.5, 134.0, 131.1 (d, *J* = 8.0 Hz), 130.2, 130.0 (d, *J* = 3.3 Hz), 121.94, 115.6 (d, *J* = 21.4 Hz), 44.5, 21.2.

^{19}F NMR (377 MHz, $CDCl_3$) δ -115.82.

HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{16}H_{14}FO_3^+$ 273.0921; Found 273.0915.



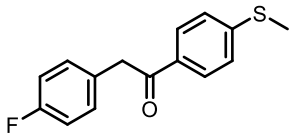
2-(4-fluorophenyl)-1-(4(((triisopropylsilyl)oxy)methyl)phenyl)ethan-1-one White solid (118.1 mg, 59% yield). mp 90.1−90.9 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.01 (m, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.28 – 7.24 (m, 2H), 7.07 – 7.03 (m, 2H), 4.93 (s, 2H), 4.29 (s, 2H), 1.27 – 1.18 (m, 3H), 1.14 (d, *J* = 6.7 Hz, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.1, 161.9 (d, *J* = 245.2 Hz), 147.6, 135.1, 131.1 (d, *J* = 8.0 Hz), 130.3 (d, *J* = 3.3 Hz), 128.6, 125.7, 115.5 (d, *J* = 21.3 Hz), 64.6, 44.5, 18.0, 12.0.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.01.

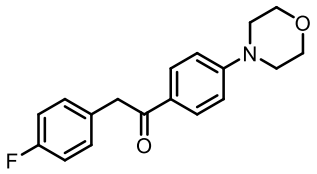
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{24}H_{33}FNaO_2Si^+$ 423.2126; Found 423.2122.



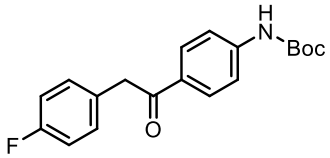
2-(4-fluorophenyl)-1-(4-(methylthio)phenyl)ethan-1-one[10] Light yellow solid (70.2 mg, 54% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 10/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 2H), 7.31 – 7.22 (m, 4H), 7.07 – 7.01 (m, 2H), 4.25 (s, 2H), 2.55 (s, 3H).

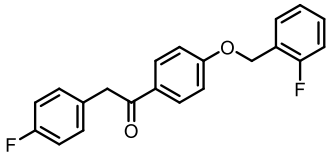
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.4, 161.9 (d, *J* = 245.2 Hz), 146.3, 132.7, 131.0 (d, *J* = 7.9 Hz), 130.3 (d, *J* = 3.4 Hz), 129.0, 125.0, 115.5 (d, *J* = 21.3 Hz) 44.4, 14.7.
^{19}F NMR (377 MHz, $CDCl_3$) δ -115.95.



2-(4-fluorophenyl)-1-(4-morpholinophenyl)ethan-1-one Gray solid (101.7 mg, 68% yield). mp 127.7−128.6 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 5/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.95 (m, 2H), 7.28 – 7.22 (m, 2H), 7.06 – 7.00 (m, 2H), 6.91 – 6.88 (m, 2H), 4.21 (s, 2H), 3.90 – 3.87 (m, 4H), 3.35 – 3.33 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 195.7, 161.8 (d, *J* = 244.7 Hz), 154.3, 130.9 (d, *J* = 3.4 Hz), 130.9, 130.7, 127.1, 115.4 (d, *J* = 21.3 Hz), 113.3, 66.6, 47.4, 44.1.
^{19}F NMR (377 MHz, $CDCl_3$) δ -116.32.
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{18}FNNaO_2^+$ 322.1214; Found 322.1213.



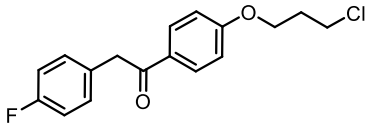
tert-butyl (4-(2-(4-fluorophenyl)acetyl)phenyl)carbamate White solid (88.9 mg, 54% yield). mp 169.8−170.4 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 3/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.82 (s, 1H), 8.00 – 7.96 (m, 2H), 7.64 – 7.61 (m, 2H), 7.32 – 7.29 (m, 2H), 7.16 – 7.11 (m, 2H), 4.33 (s, 2H), 1.51 (s, 9H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 196.5, 161.5 (d, *J* = 242.1 Hz), 153.0, 144.8, 132.0, 132.0 (d, *J* = 8.3 Hz), 130.3 (d, *J* = 28.5 Hz), 117.7, 115.4 (d, *J* = 21.1 Hz), 80.2, 43.8, 28.5.
^{19}F NMR (377 MHz, $CDCl_3$) δ -116.11.
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{20}FNNaO_3^+$ 352.1319; Found 322.1322.



1-(4-((2-fluorobenzyl)oxy)phenyl)-2-(4-fluorophenyl)ethan-1-one White solid (126.7 mg, 75% yield). mp 132.7−132.3 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 8.01 (m, 2H), 7.54 – 7.50 (m, 1H), 7.40 – 7.35 (m, 1H), 7.27 – 7.12 (m, 4H), 7.08 – 7.02 (m, 4H), 5.23 (s, 2H), 4.24 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.0, 162.5, 161.9 (d, *J* = 245.0 Hz), 160.5 (d, *J* = 247.3 Hz) 131.0 (d, *J* = 8.0 Hz), 130.9, 130.5 (d, *J* = 3.3 Hz), 130.1 (d, *J* = 8.1 Hz), 129.9, 129.7 (d, *J* = 3.8 Hz), 124.4 (d, *J* = 3.6 Hz), 123.3 (d, *J* = 14.2 Hz), 115.5 (d, *J* = 21.0 Hz), 115.5 (d, *J* = 21.4 Hz), 114.6, 63.9(d, *J* = 4.6 Hz), 44.3.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.11, -118.45.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{16}F_2NaO_2^+$ 361.1011; Found 361.1008.



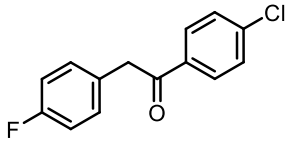
1-(4-(3-chloropropoxy)phenyl)-2-(4-fluorophenyl)ethan-1-one White solid (93.3 mg, 61% yield). mp 73.3−75.7 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.27 – 7.24 (m, 2H), 7.07 – 6.96 (m, 4H), 4.24 – 4.19 (m, 4H), 3.78 (t, *J* = 6.2 Hz, 2H), 2.29 (p, *J* = 6.1 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.0, 161.8 (d, *J* = 244.9 Hz), 160.6, 131.0 (d, *J* = 7.9 Hz), 130.91, 130.6 (d, *J* = 3.3 Hz), 129.7, 115.5 (d, *J* = 21.3 Hz), 114.3, 64.5, 44.2, 41.3, 32.0.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.09.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{16}ClFNaO_2^+$ 329.0715; Found 329.0706.

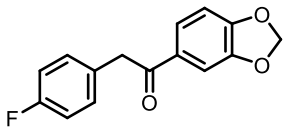


1-(4-chlorophenyl)-2-(4-fluorophenyl)ethan-1-one[11] White solid (44.7 mg, 36% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.95 (m, 2H), 7.48 – 7.46 (m, 2H), 7.26 – 7.22 (m, 2H), 7.08 –7.03 (m, 2H), 4.27 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.22, 162.0 (d, *J* = 245.5 Hz), 139.8, 134.7, 131.0 (d, *J* = 8.0 Hz), 130.0, 129.8 (d, *J* = 3.5 Hz), 129.2, 115.6 (d, *J* = 21.5 Hz), 44.5.

^{19}F NMR (377 MHz, $CDCl_3$) δ -115.65.



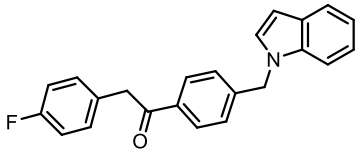
1-(benzo[d][1,3]dioxol-5-yl)-2-(4-fluorophenyl)ethan-1-one White solid (91.6 mg, 71% yield). mp 92.6−94.9 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 15/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.49 (d, *J* = 1.7 Hz, 1H), 7.27 – 7.22 (m, 2H), 7.07 – 7.01 (m, 2H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.08 (s, 2H), 4.21 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.5, 161.9 (d, *J* = 245.1 Hz), 152.0, 148.3, 131.3, 130.9 (d, *J* = 8.0 Hz), 130.4 (d, *J* = 3.3 Hz), 124.9, 115.5 (d, *J* = 21.5 Hz), 108.3, 108.0, 101.9, 44.3.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.04.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{11}FNaO_3^+$ 281.0584; Found 281.0594.



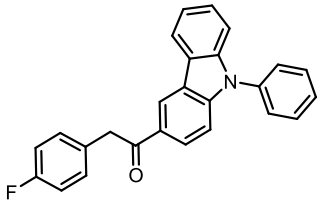
1-(4-((1H-indol-1-yl)methyl)phenyl)-2-(4-fluorophenyl)ethan-1-one Yellow solid (101.2 mg, 59% yield). mp 80.5−81.2 °C. (The product was purified by silica gel column chromatography, using petroleum ether /EA = 8/1 (v/v) as an eluent.)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.95 (m, 2H), 7.75 (dd, *J* = 7.0, 1.5 Hz, 1H), 7.30 – 7.18 (m, 8H), 7.09 – 7.03 (m, 2H), 6.66 (d, *J* = 3.1 Hz, 1H), 5.40 (s, 2H), 4.23 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 161.9 (d, *J* = 245.1 Hz), 143.3, 136.2, 135.8, 131.1 (d, *J* = 8.0 Hz), 130.1 (d, *J* = 3.3 Hz), 129.1, 128.9, 128.3, 126.9, 122.0, 121.2, 119.9, 115.6 (d, *J* = 21.4 Hz), 109.6, 102.3, 49.8, 44.6.

^{19}F NMR (377 MHz, $CDCl_3$) δ -115.79.

HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{23}H_{19}FNO^+$ 344.1445; Found 344.1446.



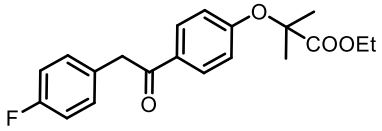
2-(4-fluorophenyl)-1-(9-phenyl-9H-carbazol-3-yl)ethan-1-one White solid (136.5 mg, 72% yield). mp 102.4−103.6 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 6/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 1.7 Hz, 1H), 8.24 (dt, *J* = 7.8, 1.0 Hz, 1H), 8.14 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.59 – 7.49 (m, 4H), 7.46 – 7.32 (m, 5H), 7.09 – 7.05 (m, 2H), 4.44 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 161.9 (d, *J* = 245.0 Hz), 143.7, 141.8, 136.9, 131.1 (d, *J* = 8.0 Hz), 131.0 (d, *J* = 3.3 Hz), 130.1, 128.9, 128.2, 127.1, 127.0, 126.9, 123.4, 123.3, 122.0, 121.0, 120.6, 115.5 (d, *J* = 21.3 Hz), 110.4, 109.6, 44.6.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.15.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{26}H_{18}FNNaO^+$ 402.1265; Found 402.1264.



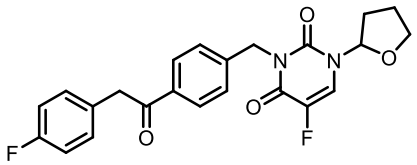
ethyl 2-(4-(2-(4-fluorophenyl)acetyl)phenoxy)-2-methylpropanoate White solid (130.7 mg, 76% yield). mp 101.7−102.5 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 8/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.94 (m, 2H), 7.26 – 7.21 (m, 2H), 7.06 – 7.01 (m, 2H), 6.88 – 6.84 (m, 2H), 4.28 – 4.22 (m, 4H), 1.68 (s, 6H), 1.24 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.0, 173.7, 161.9 (d, *J* = 245.0 Hz), 160.0, 131.0 (d, *J* = 8.0 Hz), 130.5, 130.4, 130.0, 117.4, 115.5 (d, *J* = 21.3 Hz), 79.4, 6.73, 44.2, 25.4, 14.0.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.13.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{21}FNaO_4^+$ 367.1316; Found 367.1316.



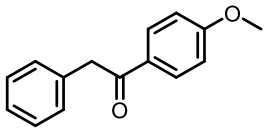
5-fluoro-3-(4-(2-(4-fluorophenyl)acetyl)benzyl)-1-(tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione 1-(3,5-dimethylphenyl)-2-(4-fluorophenyl)ethan-1-one Yellow oil (140.6 mg, 66% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 5/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.95 (m, 2H), 7.58 – 7.56 (m, 2H), 7.44 (d, *J* = 5.8 Hz, 1H), 7.25 – 7.20 (m, 2H), 7.06 – 7.00 (m, 2H), 6.00 (ddd, *J* = 6.3, 3.0, 1.4 Hz, 1H), 5.23 – 5.12 (m, 2H), 4.27 – 4.22 (m, 3H), 4.01 (td, *J* = 8.4, 6.4 Hz, 1H), 2.48 – 2.38 (m, 1H), 2.12 – 2.03 (m, 2H), 1.98 – 1.89 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 161.9 (d, *J* = 245.3 Hz), 157.1 (d, *J* = 25.6 Hz), 149.0, 141.5, 139.9 (d, *J* = 234.7 Hz), 135.9, 131.0 (d, *J* = 7.9 Hz), 130.1 (d, *J* = 3.3 Hz), 129.3, 128.8, 122.1 (d, *J* = 34.0 Hz), 115.5 (d, *J* = 21.3 Hz), 88.2, 70.4, 44.6, 44.4, 33.0, 23.8.

^{19}F NMR (377 MHz, $CDCl_3$) δ -116.0, -164.1.

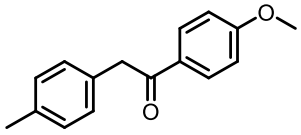
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{20}F_2N_2NaO_4^+$ 449.1283; Found 449.1284.



1-(4-methoxyphenyl)-2-phenylethan-1-one[12] White solid (96.0 mg, 85% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 8.01 (m, 2H), 7.38 – 7.26 (m, 5H), 6.98 – 6.95 (m, 2H), 4.27 (s, 2H), 3.89 (s, 3H).

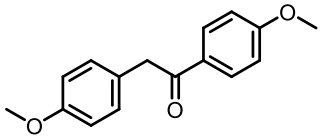
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 163.5, 135.0, 131.0, 129.7, 129.4, 128.7, 126.8, 113.8, 55.5, 45.3.



1-(4-methoxyphenyl)-2-(p-tolyl)ethan-1-one1-one[13] Light yellow oil (97.2 mg, 81% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

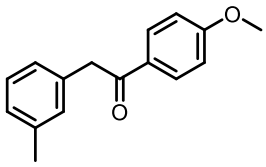
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.01 (m, 2H), 7.20 – 7.14 (m, 4H), 6.97 – 6.93 (m, 2H), 4.22 (s, 2H), 3.89 (s, 3H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.5, 163.5, 136.4, 131.9, 131.0, 129.7, 129.4, 129.2, 113.8, 55.5, 44.9, 21.1.

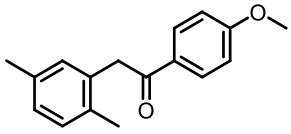


1,2-bis(4-methoxyphenyl)ethan-1-one[9] White solid (92.2 mg, 72% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 15/1 (v/v) as an eluent.

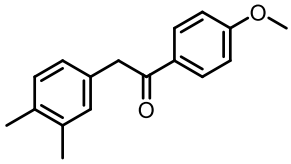
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 8.00 (m, 2H), 7.24 – 7.20 (m, 2H), 6.98 – 6.94 (m, 2H), 6.91 – 6.87 (m, 2H), 4.21 (s, 2H), 3.89 (s, 3H), 3.81 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.6, 163.5, 158.5, 131.0, 130.4, 129.6, 127.0, 114.1, 113.8, 55.5, 55.3, 44.4.



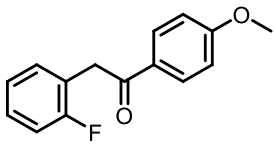
1-(4-methoxyphenyl)-2-(m-tolyl)ethan-1-one[14] White solid (94.8 mg, 79% yield). (The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 8.03 (m, 2H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.11 (dd, *J* = 12.1, 5.5 Hz, 3H), 6.98 – 6.95 (m, 2H), 4.23 (s, 2H), 3.89 (s, 3H), 2.36 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.4, 163.5, 138.3, 134.9, 131.0, 130.1, 129.7, 128.6, 127.6, 126.4, 113.8, 55.5, 45.3, 21.4.



2-(2,5-dimethylphenyl)-1-(4-methoxyphenyl)ethan-1-one Yellow oil (83.8 mg, 66% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 8.04 (m, 2H), 7.14 (d, *J* = 7.7 Hz, 1H), 7.05 – 6.98 (m, 4H), 4.26 (s, 2H), 3.91 (s, 3H), 2.33 (s, 3H), 2.27 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 163.5, 135.5, 133.7, 133.6, 131.0, 130.7, 130.2, 130.0, 127.9, 113.8, 55.5, 43.1, 21.0, 19.4.
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{18}NaO_2^+$ 277.1199; Found 277.1199.



2-(3,4-dimethylphenyl)-1-(4-methoxyphenyl)ethan-1-one White solid (106.7 mg, 84% yield). mp 49.0−50.4 ºC. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 8.02 (m, 2H), 7.13 – 7.09 (m, 2H), 7.04 (dd, *J* = 7.7, 2.0 Hz, 1H), 6.98 – 6.94 (m, 2H), 4.21 (s, 2H), 3.89 (s, 3H), 2.27 (d, *J* = 4.0 Hz, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.63, 163.5, 136.9, 135.1, 132.3, 131.0, 130.6, 129.9, 129.7, 126.7, 113.8, 55.5, 44.9, 19.8, 19.4.
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{18}NaO_2^+$ 277.1199; Found 277.1198.



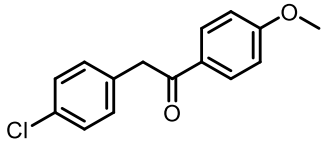
2-(2-fluorophenyl)-1-(4-methoxyphenyl)ethan-1-one White solid (69.5 mg, 57% yield). mp 75.3−76.9 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.04 (m, 2H), 7.32 – 7.26 (m, 2H), 7.16 – 7.08 (m, 2H), 7.00 – 6.97 (m, 2H), 4.31 (s, 2H), 3.90 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 160.9 (d, *J* = 245.4 Hz), 159.7, 131.6 (d, *J* = 4.2 Hz), 129.5, 128.8 (d, *J* = 8.1 Hz), 124.2 (d, *J* = 3.5 Hz), 122.3, 122.1, 115.4 (d, *J* = 22.0 Hz), 113.9, 55.5, 38.3 (d, *J* = 2.2 Hz).

^{19}F NMR (377 MHz, $CDCl_3$) δ -117.20.

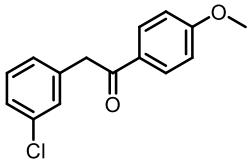
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{13}FNaO_2^+$ 267.0792; Found 267.0796.



2-(4-chlorophenyl)-1-(4-methoxyphenyl)ethan-1-one[15] Light yellow solid (84.5 mg, 65% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 8.00 (m, 2H), 7.33 – 7.30 (m, 2H), 7.24 – 7.22 (m, 2H), 6.98 – 6.96 (m, 2H), 4.24 (s, 2H), 3.90 (s, 3H.

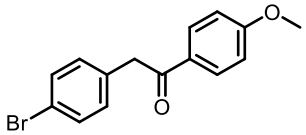
^{13}C NMR (101 MHz, $CDCl_3$) δ 195.7, 163.7, 133.4, 132.8, 130.9, 130.8, 129.4, 128.8, 113.9, 55.5, 44.4.



2-(3-chlorophenyl)-1-(4-methoxyphenyl)ethan-1-one[16] White solid (87.1 mg, 67% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.99 (m, 2H), 7.30 – 7.21 (m, 3H), 7.18 (dt, *J* = 6.8, 1.9 Hz, 1H), 6.99 – 6.95 (m, 2H), 4.23 (s, 2H), 3.89 (s, 3H).

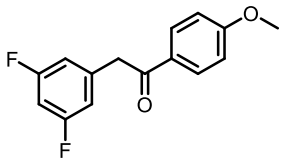
^{13}C NMR (101 MHz, $CDCl_3$) δ 195.5, 163.7, 136.9, 134.4, 130.9, 129.8, 129.6, 129.4, 127.7, 127.1, 113.9, 55.5, 44.7.



2-(4-bromophenyl)-1-(4-methoxyphenyl)ethan-1-one[17] White solid (77.5 mg, 51% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.99 (m, 2H), 7.49 – 7.46 (m, 2H), 7.19 – 7.15 (m, 2H), 6.99 – 6.95 (m, 2H), 4.22 (s, 2H), 3.90 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.6, 163.7, 133.9, 131.7, 131.2, 130.9, 129.4, 120.9, 113.9, 55.5, 44.5.



2-(3,5-difluorophenyl)-1-(4-methoxyphenyl)ethan-1-one Light yellow solid (81.2 mg, 62% yield). mp 77.2−79.6 ºC. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

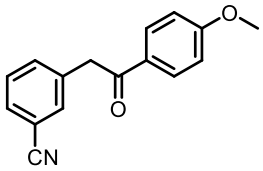
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.98 (m, 2H), 7.00 – 6.96 (m, 2H), 6.85 – 6.80 (m, 2H), 6.73 (tt, *J* = 9.0, 2.4 Hz, 1H), 4.24 (s, 2H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.8, 163.9, 163.0 (dd, *J* = 248.3, 13.0 Hz), 138.5 (t, *J* = 9.6 Hz), 130.9, 129.2, 114.0, 112.7 – 112.4 (m), 102.4 (t, *J* = 25.2 Hz), 55.5, 44.6 (t, *J* = 2.1 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 163.5, 135.0, 131.0, 129.7, 129.4, 128.7, 126.8, 113.8, 55.5, 45.3.

^{19}F NMR (377 MHz, $CDCl_3$) δ -110.00.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{12}F_2NaO_2^+$ 285.0698; Found 285.0697.

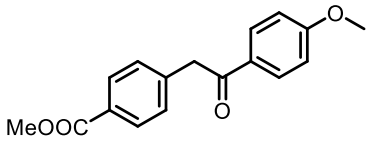


3-(2-(4-methoxyphenyl)-2-oxoethyl)benzonitrile Light yellow solid (77.8 mg, 62% yield). mp 81.4−82.7 ºC. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.60 – 7.45 (m, 4H), 7.01 – 7.68 (m, 2H), 4.31 (s, 2H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.8, 163.9, 136.3, 134.3, 133.2, 130.8, 130.6, 129.3, 129.2, 118.8, 114.0, 112.6, 55.6, 44.3.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{13}NNaO_2^+$ 274.0838; Found 274.0836.

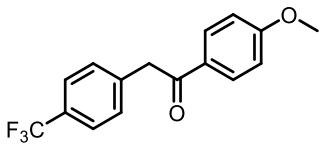


methyl 4-(2-(4-methoxyphenyl)-2-oxoethyl)benzoate White solid (63.9 mg, 45% yield). mp 155.5−156.1 ºC. (The product was purified by silica gel column chromatography, using petroleum ether /EA = 10/1 (v/v) as an eluent.)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.99 (m, 4H), 7.38 – 7.36 (m, 2H), 6.99 – 6.95 (m, 2H), 4.32 (s, 2H), 3.93 (s, 3H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.4, 167.0, 163.7, 140.3, 130.9, 129.9, 129.6, 129.4, 128.8, 113.9, 55.5, 52.1, 45.2.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{13}NNaO_2^+$ 307.0941; Found 307.0955.

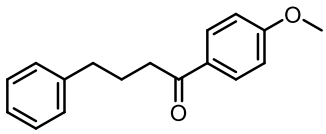


1-(4-methoxyphenyl)-2-(4-(trifluoromethyl)phenyl)ethan-1-one[18] Light yellow solid (122.1 mg, 83% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.02 (m, 2H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.00 – 6.98 (m, 2H), 4.33 (s, 2H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 163.8, 139.0 (d, *J* = 1.5 Hz), 130.9, 129.9, 129.2 (d, *J* = 32.6 Hz), 128.98, 125.5 (q, *J* = 3.8 Hz), 122.9, 114.0, 55.5, 44.8.

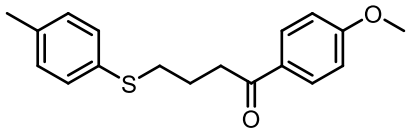
^{19}F NMR (377 MHz, $CDCl_3$) δ -62.41.



1-(4-methoxyphenyl)-4-phenylbutan-1-one[19] White solid (90.2 mg, 71% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.93 (m, 2H), 7.33 (dd, *J* = 8.1, 6.7 Hz, 2H), 7.26 – 7.22 (m, 3H), 6.98 – 6.94 (m, 2H), 3.90 (s, 3H), 2.97 (t, *J* = 7.3 Hz, 2H), 2.76 (t, *J* = 7.6 Hz, 2H), 2.12 (p, *J* = 7.5 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 198.8, 163.4, 141.8, 130.3, 130.1, 128.6, 128.4, 126.0, 113.7, 55.5, 37.4, 35.3, 26.0.

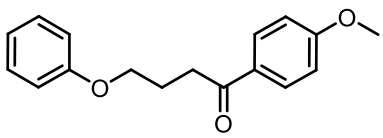


1-(4-methoxyphenyl)-4-(p-tolylthio)butan-1-one Yellow oil (84.0 mg, 56% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 15/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.93 (m, 2H), 7.32 – 7.29 (m, 2H), 7.14 – 7.11 (m, 2H), 6.97 – 6.93 (m, 2H), 3.89 (s, 3H), 3.10 (t, *J* = 7.1 Hz, 2H), 3.02 (t, *J* = 7.0 Hz, 2H), 2.34 (s, 3H), 2.08 (p, *J* = 7.0 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 198.1, 163.5, 136.2, 132.3, 130.3, 130.1, 130.0, 129.7, 113.7, 55.5, 36.6, 33.9, 23.7, 21.0.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{20}NaO_2S^+$ 323.1076; Found 323.1080.

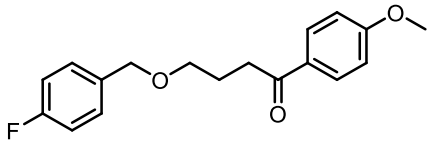


1-(4-methoxyphenyl)-4-phenoxybutan-1-one White solid (72.9 mg, 54% yield). mp 60.1−61.2 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.99 (m, 2H), 7.34 – 7.29 (m, 2H), 7.00 – 6.90 (m, 5H), 4.10 (t, *J* = 6.0 Hz, 2H), 3.90 (s, 3H), 3.19 (t, *J* = 7.1 Hz, 2H), 2.30 – 2.24 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 198.3, 163.5, 158.9, 130.3, 130.1, 129.5, 120.7, 114.5, 113.7, 66.9, 55.5, 34.6, 24.0.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{18}NaO_3^+$ 293.1148; Found 293.1152.



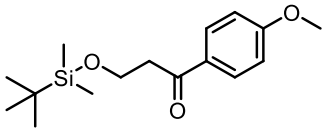
4-((4-fluorobenzyl)oxy)-1-(4-methoxyphenyl)butan-1-one White solid (77.1 mg, 51% yield). mp 54.5−55.1 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.88 (m, 2H), 7.36 – 7.24 (m, 2H), 7.08 – 7.00 (m, 2H), 6.98 – 6.91 (m, 2H), 4.48 (s, 2H), 3.89 (s, 3H), 3.59 (t, *J* = 6.1 Hz, 2H), 3.07 (t, *J* = 7.2 Hz, 2H), 2.14 – 2.02 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 198.5, 162.3 (d, *J* = 245.4 Hz), 161.1, 134.2 (d, *J* = 3.3 Hz), 130.3, 130.1, 129.4 (d, *J* = 8.1 Hz), 115.2 (d, *J* = 21.3 Hz), 113.7, 72.2, 69.5, 55.5, 34.7, 24.5.

^{19}F NMR (377 MHz, $CDCl_3$) δ -114.97.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{19}FNaO_3^+$ 325.1210; Found 325.1207.

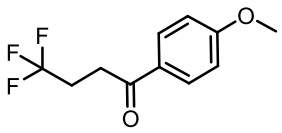


3-((tert-butyldimethylsilyl)oxy)-1-(4-methoxyphenyl)propan-1-one White solid (91.2 mg, 62% yield). mp 41.3−42.3 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.9 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 4.07 (t, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 3.18 – 3.15 (m, 2H), 0.89 (s, 9H), 0.07 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 163.5, 130.5, 130.5, 113.7, 59.5, 55.5, 41.4, 25.9, 18.3, -5.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{26}NaO_3Si^+$ 317.1543; Found 317.1553.

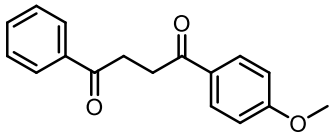


4,4,4-trifluoro-1-(4-methoxyphenyl)butan-1-one[20] Light yellow solid (40.6 mg, 35% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 25/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.97 (m, 2H), 7.00 – 6.95 (m, 2H), 3.91 (s, 3H), 3.26 – 3.22 (m, 2H), 2.67 – 2.54 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 163.9, 130.3, 129.2, 127.2 (q, J = 275.9 Hz), 113.9, 55.5, 30.8 (q, J = 2.6 Hz), 28.5 (q, J = 29.6 Hz).

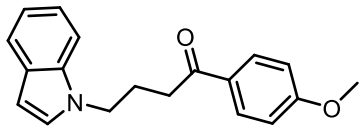
^{19}F NMR (377 MHz, $CDCl_3$) δ -66.37.



1-(4-methoxyphenyl)-4-phenylbutane-1,4-dione[21] Whoite solid (88.5 mg, 66% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 15/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.03 (m, 4H), 7.62 – 7.58 (m, 1H), 7.52 – 7.48 (m, 2H), 7.00 – 6.96 (m, 2H), 3.90 (s, 3H), 3.50 – 3.42 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 198.9, 197.2, 163.6, 136.8, 133.1, 130.4, 129.9, 128.6, 128.1, 113.8, 55.5, 32.7, 32.2.

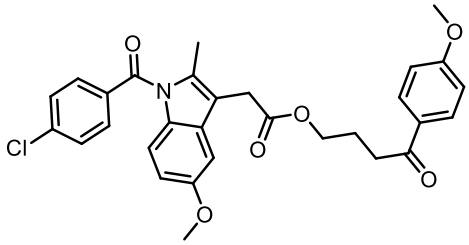


4-(1H-indol-1-yl)-1-(4-methoxyphenyl)butan-1-one Yellow solid (64.5 mg, 44% yield). mp 68.8−70.6 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 15/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.7 Hz, 2H), 7.68 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.43 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.17 – 7.13 (m, 2H), 6.96 – 6.92 (m, 2H), 6.54 (d, *J* = 3.1 Hz, 1H), 4.30 (t, *J* = 6.8 Hz, 2H), 3.89 (s, 3H), 2.91 (t, *J* = 6.8 Hz, 2H), 2.33 (p, *J* = 6.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 163.6, 136.0, 130.3, 129.8, 128.7, 127.9, 121.6, 121.0, 119.4, 113.8, 109.5, 101.2, 55.5, 45.5, 34.6, 24.6.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{19}NNaO_2^+$ 316.1308; Found 316.1308.

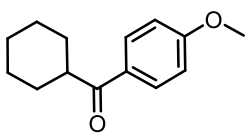


4-(4-methoxyphenyl)-4-oxobutyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetate White solid (138.6 mg, 52% yield). mp 133.3−134.0 °C. The product was purified by silica gel column chromatography, using petroleum ether /EA = 3/1 (v/v) as an eluent.

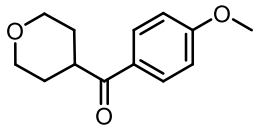
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.79 (m, 2H), 7.65 – 7.62 (m, 2H), 7.47 – 7.44 (m, 2H), 7.01 (d, *J* = 2.5 Hz, 1H), 6.92 – 6.88 (m, 3H), 6.69 (dd, *J* = 9.0, 2.6 Hz, 1H), 4.23 (t, *J* = 6.3 Hz, 2H), 3.88 (s, 3H), 3.82 (s, 3H), 3.68 (s, 2H), 2.89 (t, *J* = 7.2 Hz, 2H), 2.40 (s, 3H), 2.12 – 2.05 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.5, 170.8, 168.3, 163.5, 156.1, 139.2, 135.9, 133.9, 131.2, 130.8, 130.6, 130.2, 129.8, 129.1, 115.0, 113.7, 112.7, 111.7, 101.3, 64.4, 55.7, 55.5, 34.2, 30.5, 23.3, 13.4.

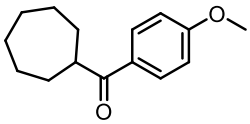
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{30}H_{28}ClNNaO_6^+$ 566.1497; Found 566.1509.



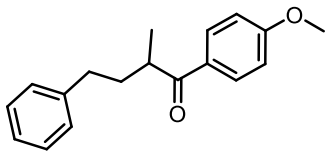
cyclohexyl(4-methoxyphenyl)methanone[22] White solid (62.2 mg, 57% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.95 (m, 2H), 6.98 – 6.94 (m, 2H), 3.89 (s, 3H), 3.25 (tt, *J* = 11.5, 3.2 Hz, 1H), 1.92 – 1.73 (m, 5H), 1.57 – 1.22 (m, 5H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 202.5, 163.2, 130.5, 129.3, 113.7, 55.5, 45.3, 29.6, 26.0, 25.9.



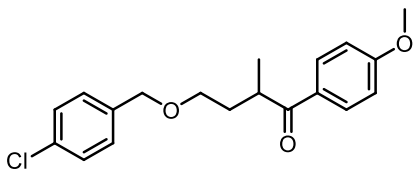
(4-methoxyphenyl)(tetrahydro-2H-pyran-4-yl)methanone[23] Light yellow solid (46.3 mg, 42% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 5/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.94 (m, 2H), 6.99 – 6.94 (m, 2H), 4.08 (ddd, *J* = 11.5, 4.3, 2.4 Hz, 2H), 3.90 (s, 3H), 3.58 (td, *J* = 11.6, 2.4 Hz, 2H), 3.49 (tt, *J* = 11.2, 3.9 Hz, 1H), 1.96 – 1.86 (m, 2H), 1.81 – 1.76 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 200.4, 163.5, 130.6, 128.7, 113.9, 67.4, 55.5, 42.3, 29.2.



cycloheptyl(4-methoxyphenyl)methanone[24] Colorless oil (60.3 mg, 52% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.94 (m, 2H), 6.98 – 6.95 (m, 2H), 3.90 (s, 3H), 3.42 (tt, *J* = 9.6, 4.0 Hz, 1H), 1.97 – 1.91 (m, 2H), 1.86 – 1.55 (m, 10H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 203.0, 163.2, 130.6, 129.3, 113.7, 55.5, 46.3, 31.0, 28.4, 26.9.



1-(4-methoxyphenyl)-2-methyl-4-phenylbutan-1-one[25] Colorless oil (72.4 mg, 54% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.88 (m, 2H), 7.33– 7.29 (m, 2H), 7.25 – 7.18 (m, 3H), 6.98 – 6.93 (m, 2H), 3.90 (s, 3H), 3.51 – 3.42 (m, 1H), 2.70 – 2.65 (m, 2H), 2.25– 2.16 (m, 1H), 1.83 – 1.75 (m, 1H), 1.26 (d, *J* = 6.9 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 202.7, 163.4, 141.9, 130.6, 129.5, 128.5, 128.4, 125.9, 113.8, 55.5, 39.3, 35.4, 33.5, 17.5.



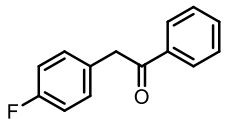
4-((4-chlorobenzyl)oxy)-1-(4-methoxyphenyl)-2-methylbutan-1-one Colorless oil (59.7 mg, 36% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 20/1 (v/v) as an eluent.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.97 (m, 2H), 7.29 – 7.19 (m, 4H), 6.97 – 6.93 (m, 2H), 4.41 (d, *J* = 3.7 Hz, 2H), 3.90 (s, 3H), 3.74 – 3.69 (td, *J* = 7.4, 6.1 Hz, 1H), 3.55 (ddd, *J* = 9.5, 6.7, 5.3 Hz, 1H), 3.45 (ddd, *J* = 9.5, 7.1, 5.2 Hz, 1H), 2.23 – 2.15 (m, 1H), 1.81 – 1.72 (m, 1H), 1.22 (d, *J* = 6.9 Hz, 3H).

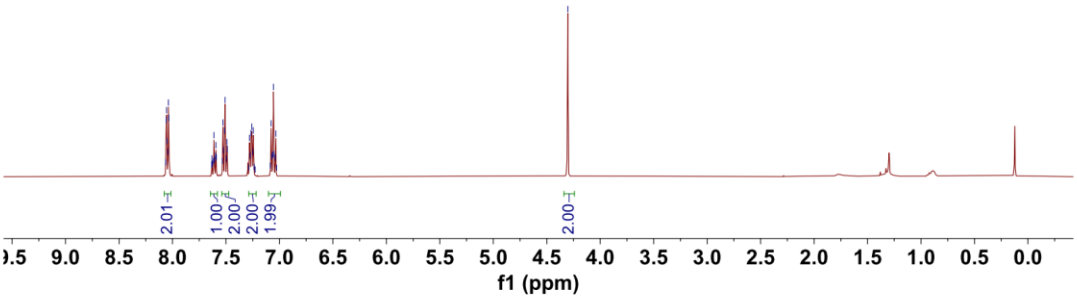
^{13}C NMR (101 MHz, $CDCl_3$) δ 202.7, 163.4, 136.9, 133.2, 130.7, 129.6, 128.9, 128.5, 113.8, 72.1, 68.2, 55.5, 36.8, 33.7, 17.9.

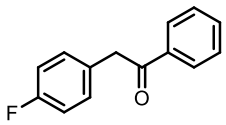
HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{21}ClNaO_3^+$ 355.1071; Found 355.1081.

NMR Spectra of Substrates and Products



^{1}H NMR





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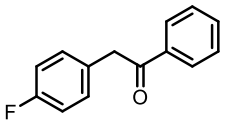
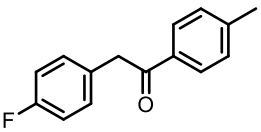
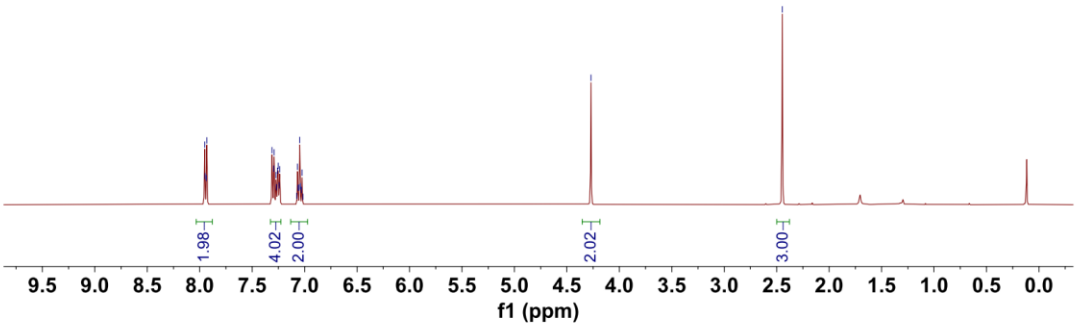
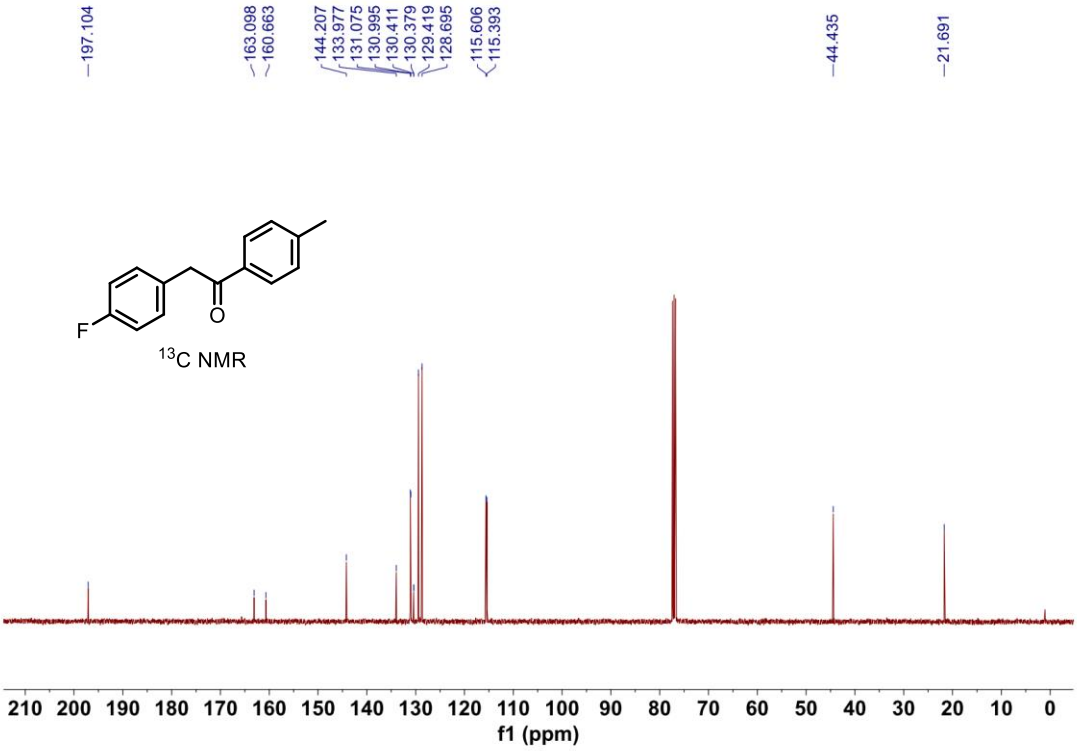


^{19}F NMR



^{1}H NMR

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131.075
130.995
130.411
130.379
129.419
128.695
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115.393
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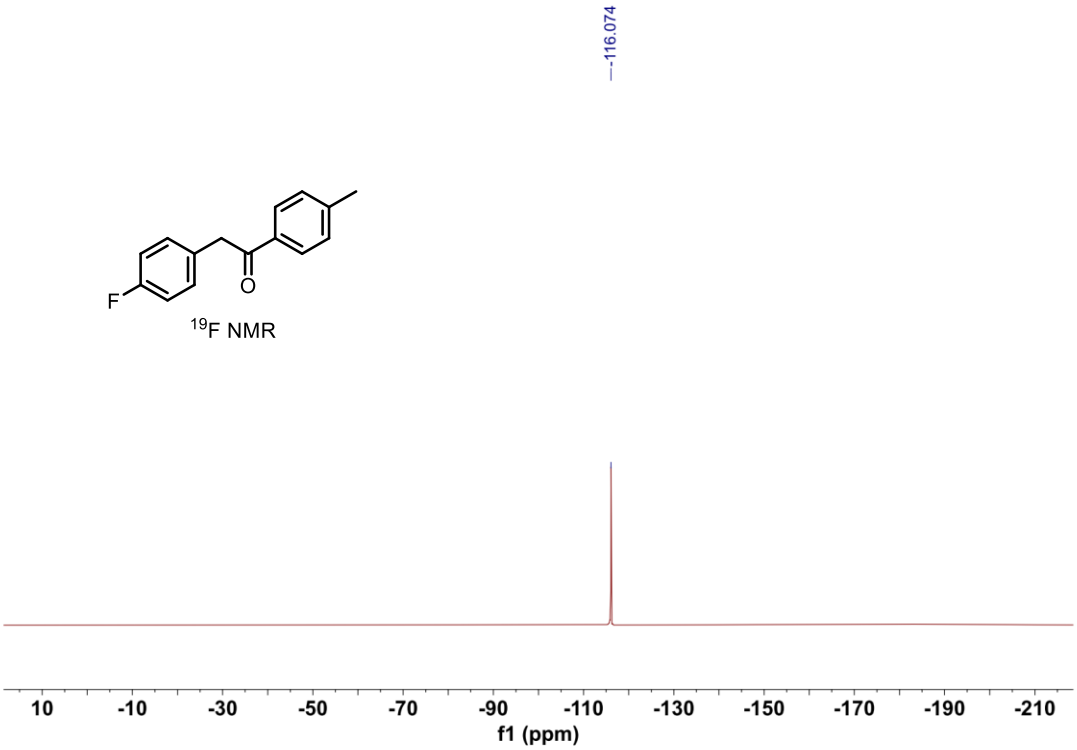
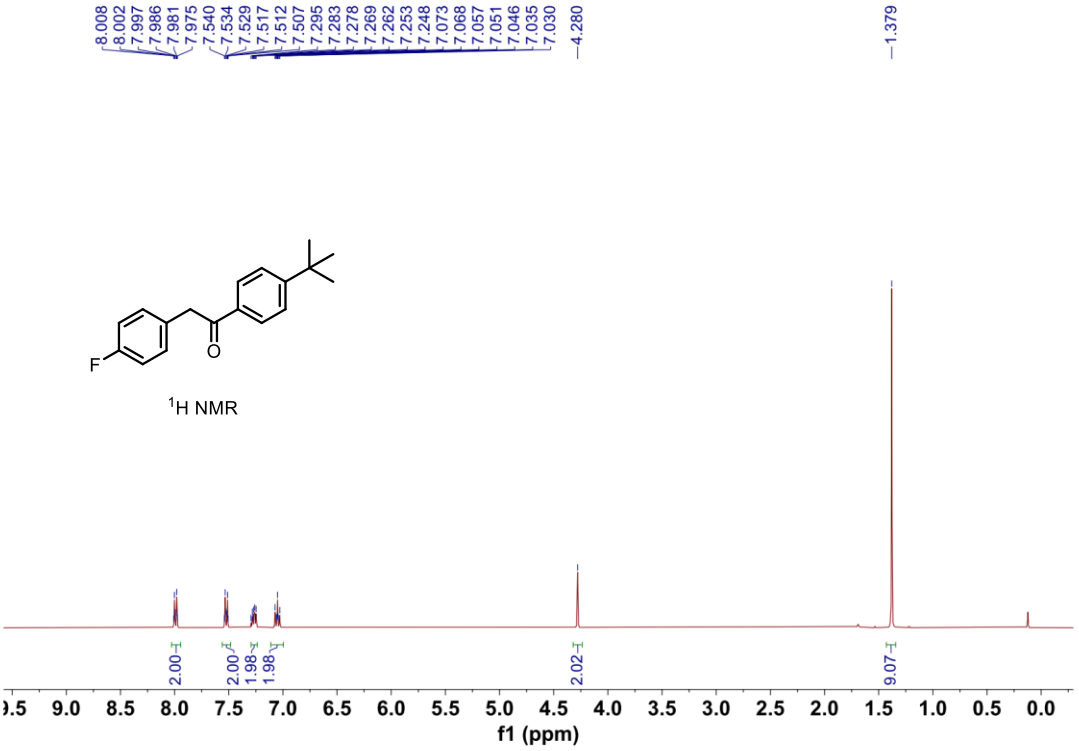
21.691
F
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


116.074
F
O
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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8.002
7.997
7.986
7.981
7.975
7.540
7.534
7.529
7.517
7.512
7.507
7.295
7.283
7.278
7.269
7.262
7.253
7.248
7.073
7.068
7.057
7.051
7.046
7.035
7.030
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F
O
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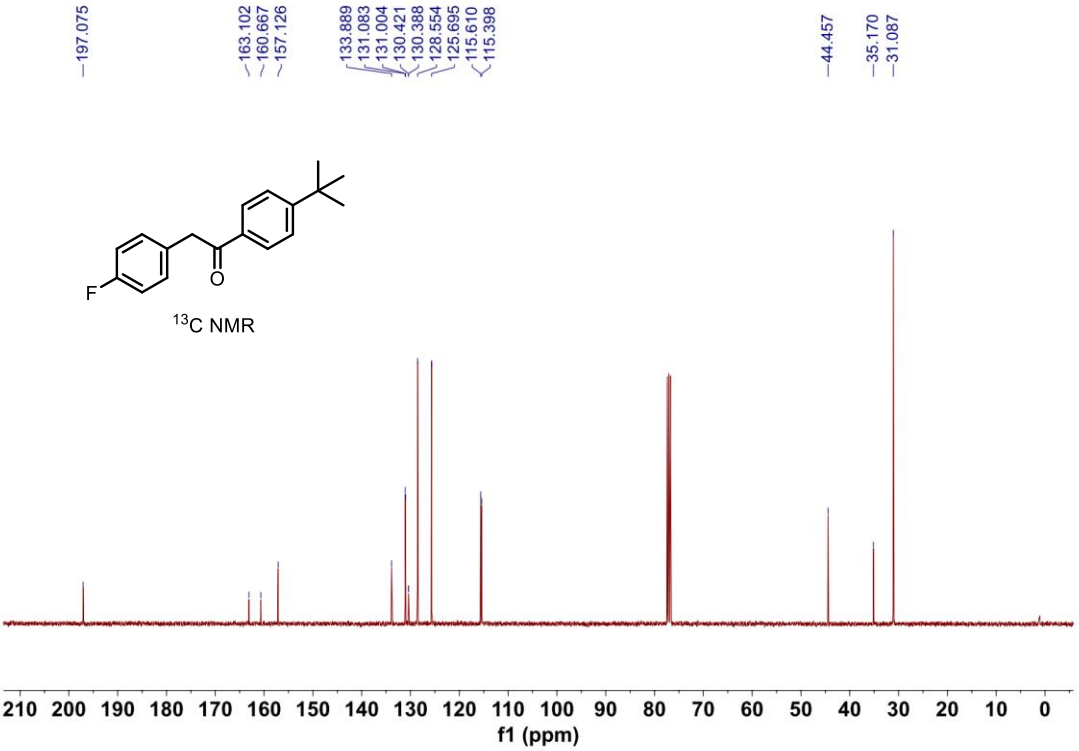
2.00
2.00
1.98
1.98
2.02
9.07
f1 (ppm)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157.126
133.889
131.083
131.004
130.421
130.388
128.554
125.695
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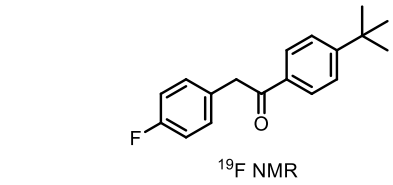
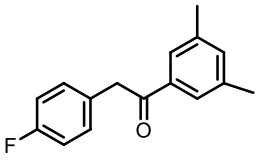
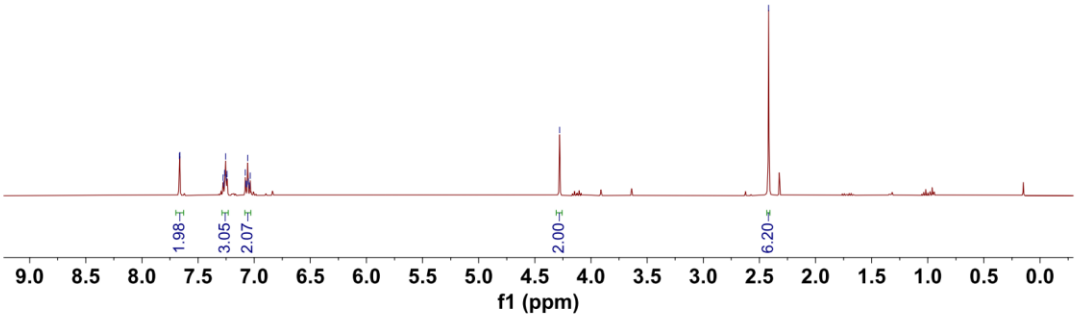
115.398
44.457
35.170
31.087
F
O
13C NMR
f1 (ppm)

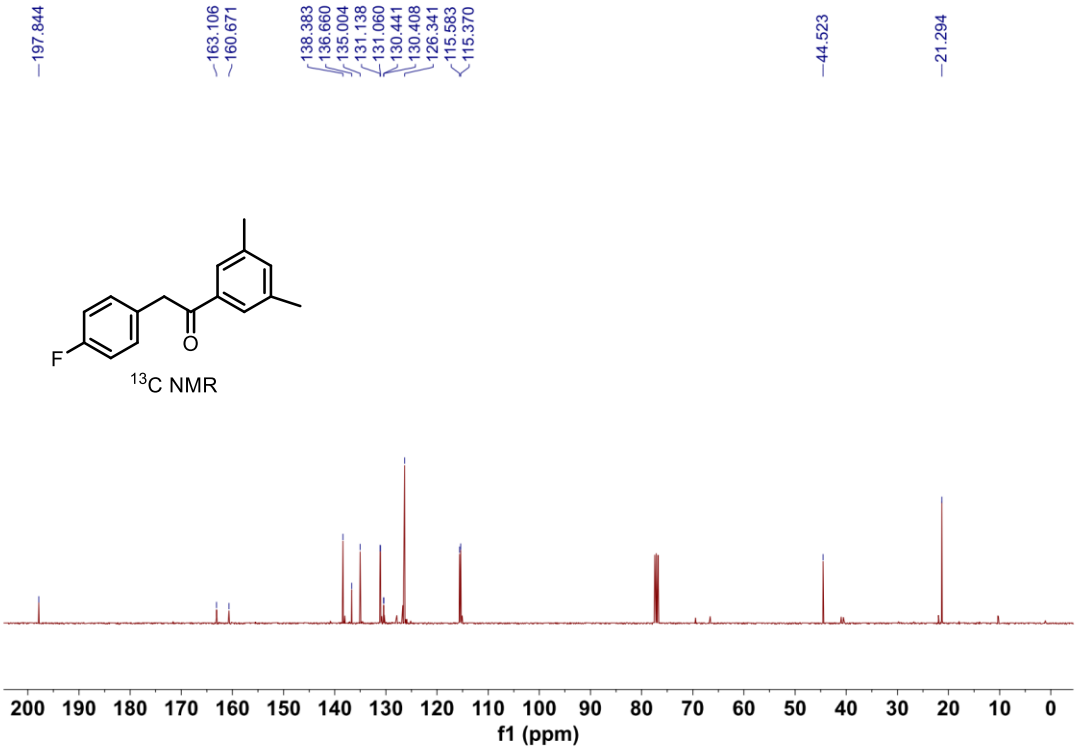


^{19}F NMR



^{1}H NMR

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136.660
135.004
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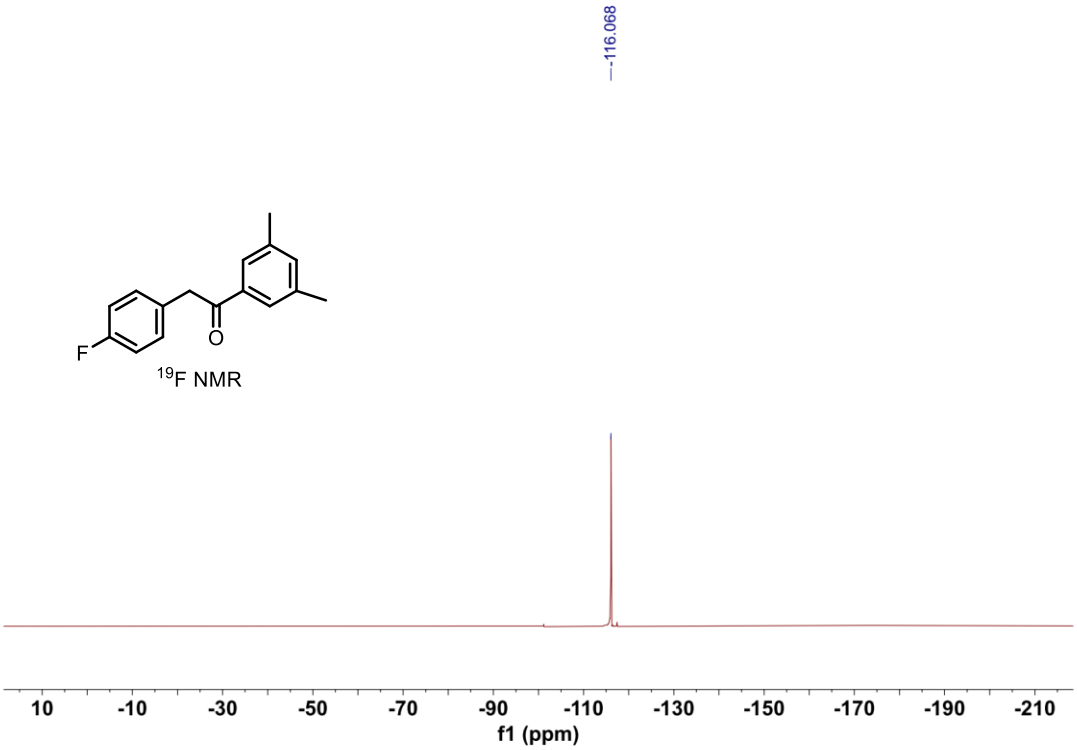
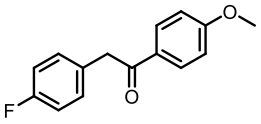
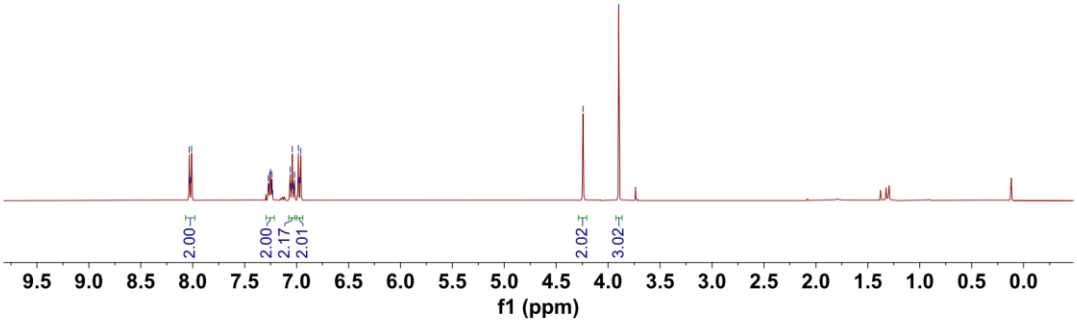
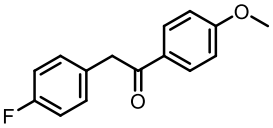
130.408
126.341
115.583
115.370
44.523
21.294
O
F
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


116.068
O
F
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

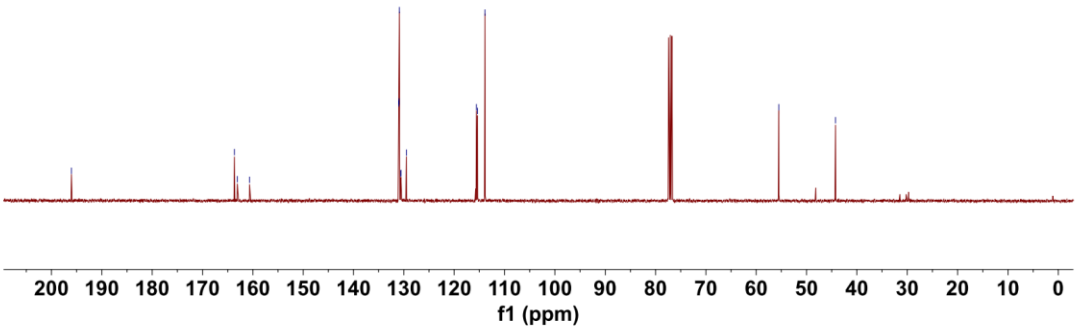


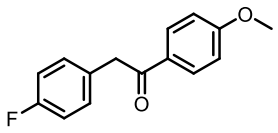
^{1}H NMR



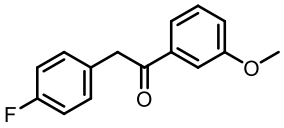


^{13}C NMR

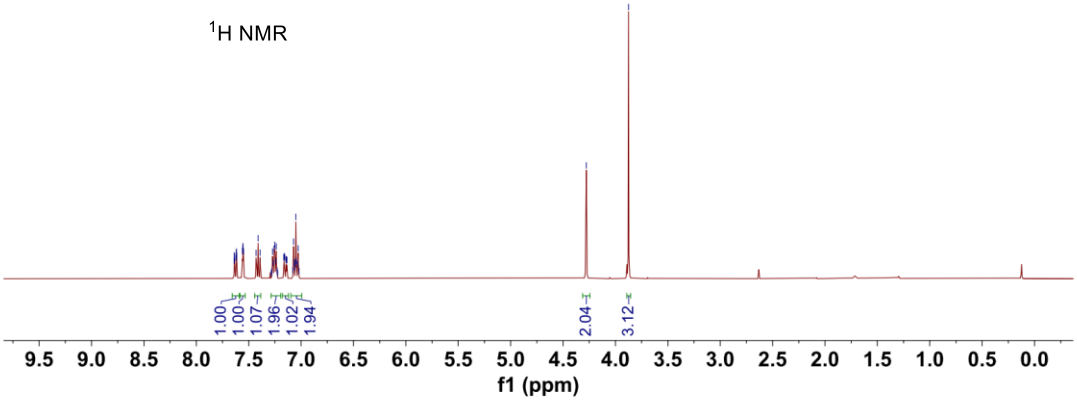


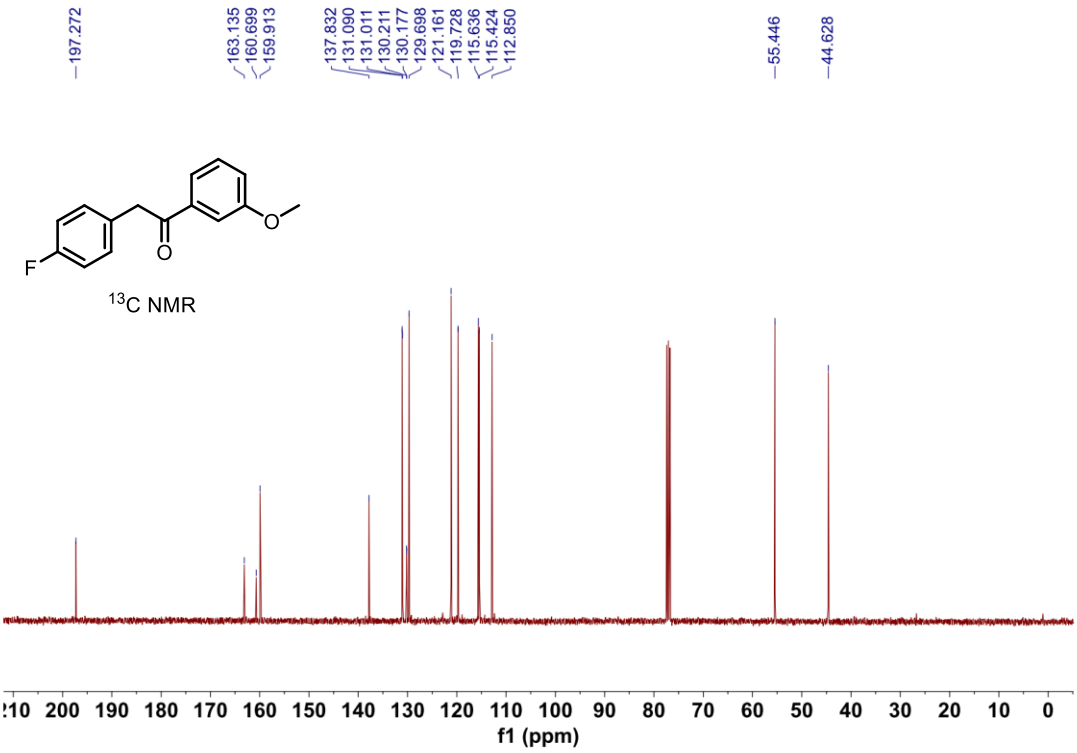


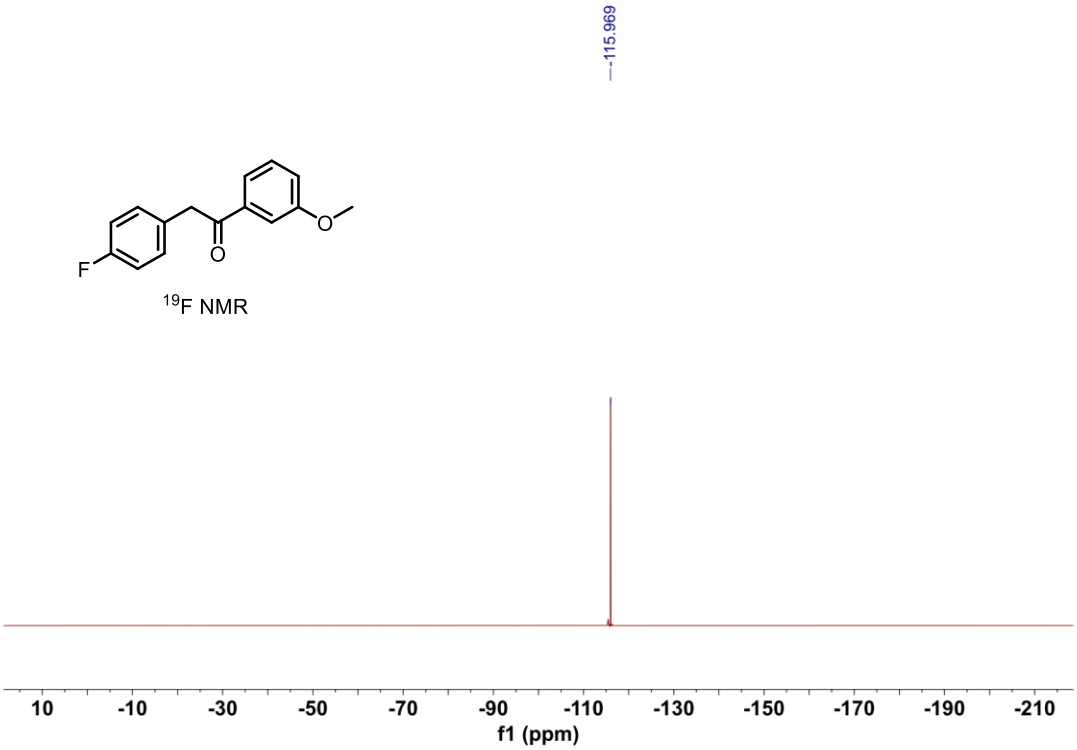
^{19}F NMR

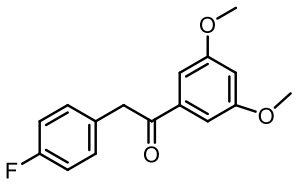


^{1}H NMR

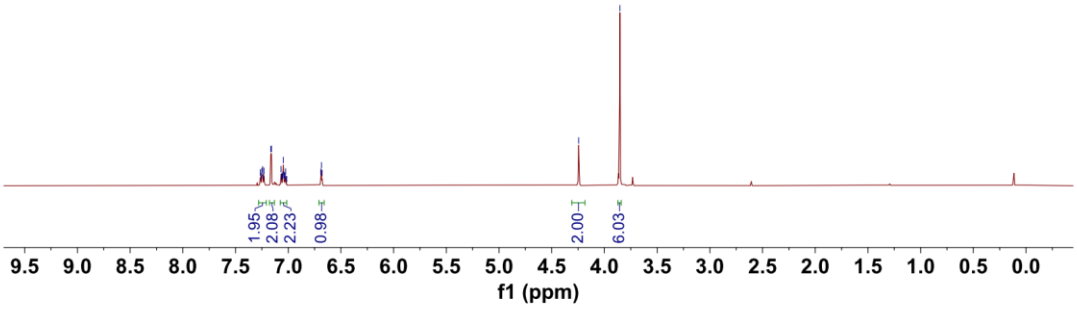


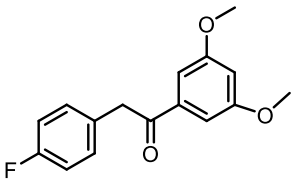

197.272
163.135
160.699
159.913
137.832
131.090
131.011
130.211
130.177
129.698
121.161
119.728
115.636
115.424
112.850
55.446
44.628
O
O
F
13C NMR
f1 (ppm)


115.969
O
O
F
19F NMR
f1 (ppm)

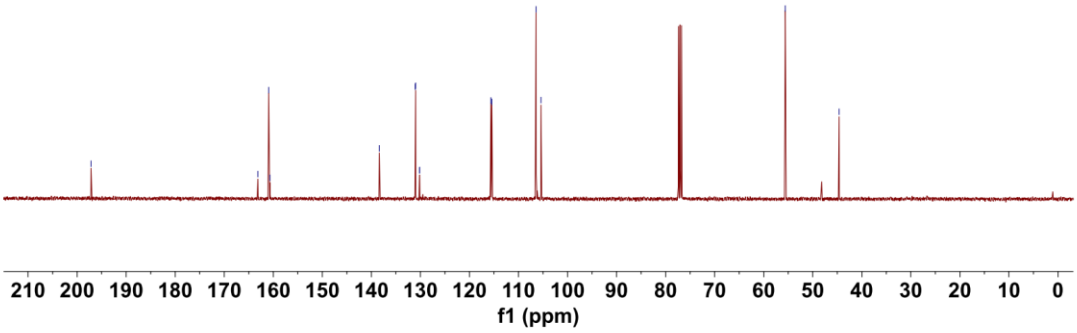


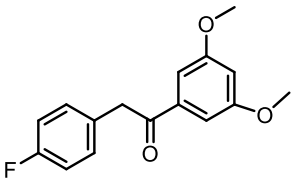
^{1}H NMR



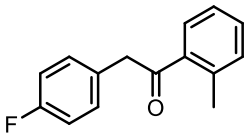


^{13}C NMR

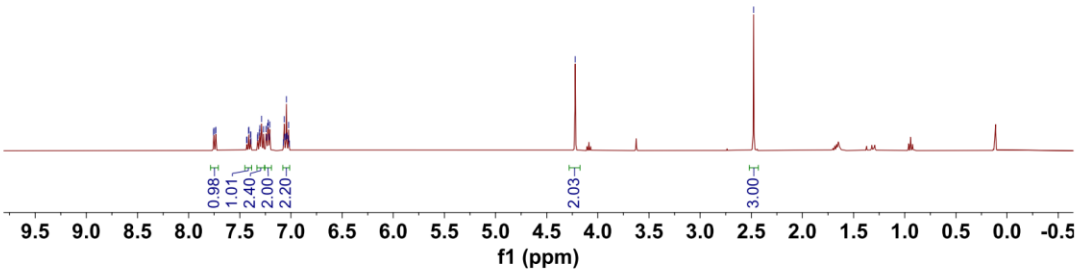


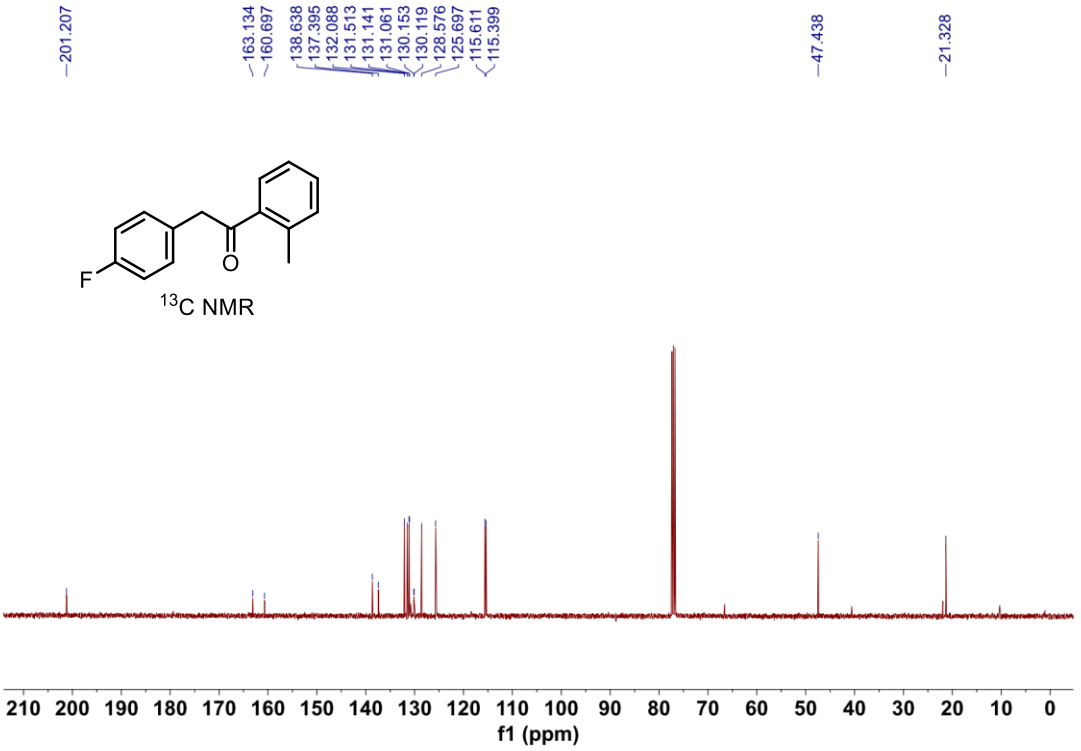


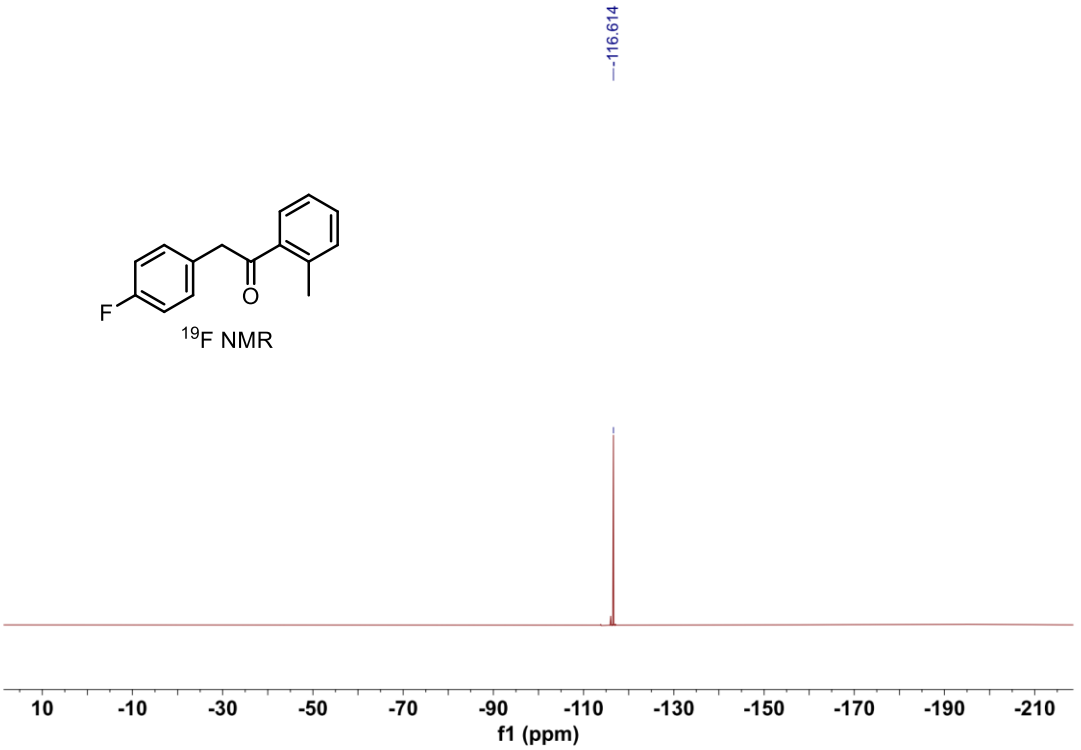
^{19}F NMR

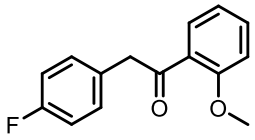


^{1}H NMR

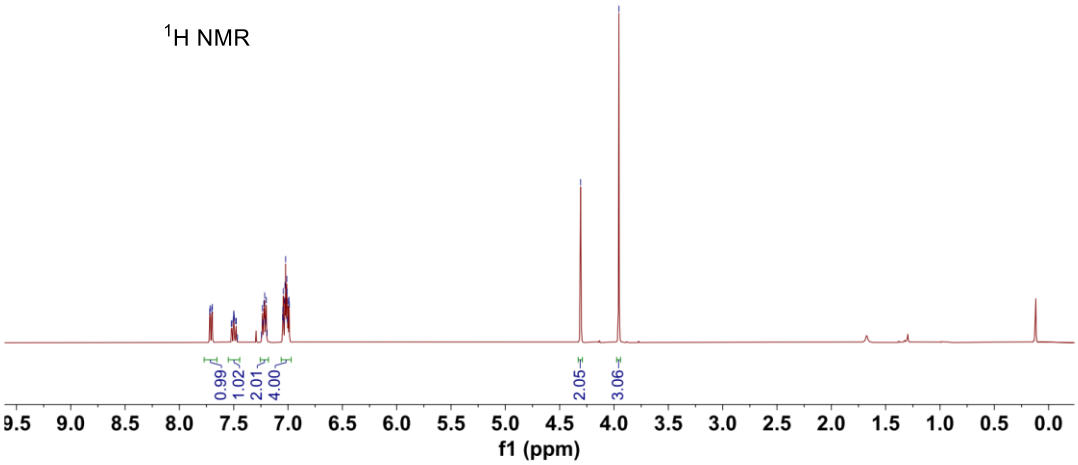


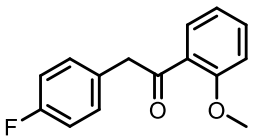

201.207
163.134
160.697
138.638
137.395
132.088
131.513
131.141
131.061
130.153
130.119
128.576
125.697
115.611
115.399
47.438
21.328
F
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


116.614
F
O
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

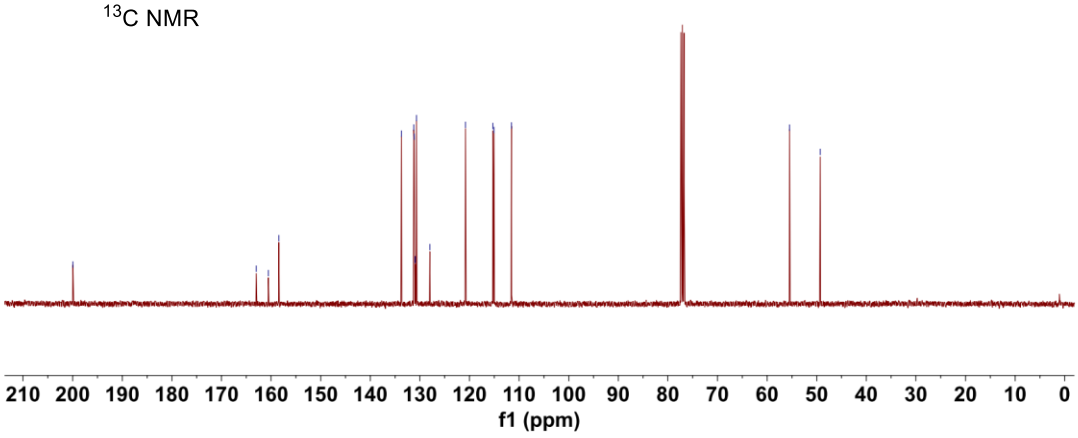


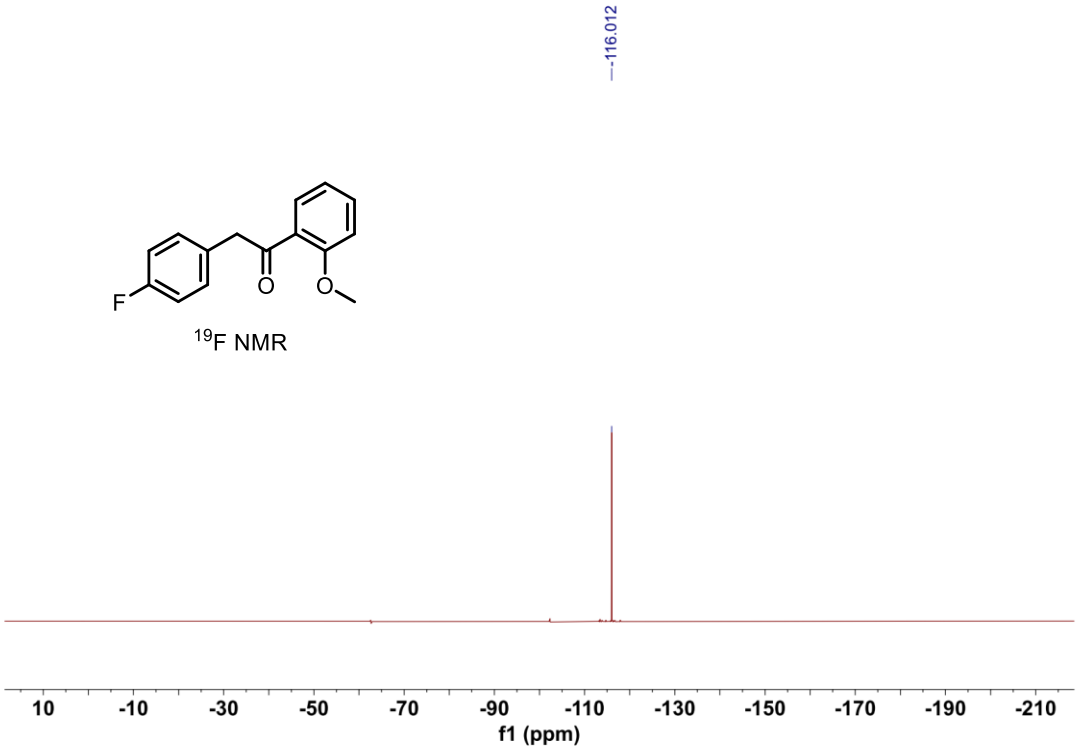
^{1}H NMR

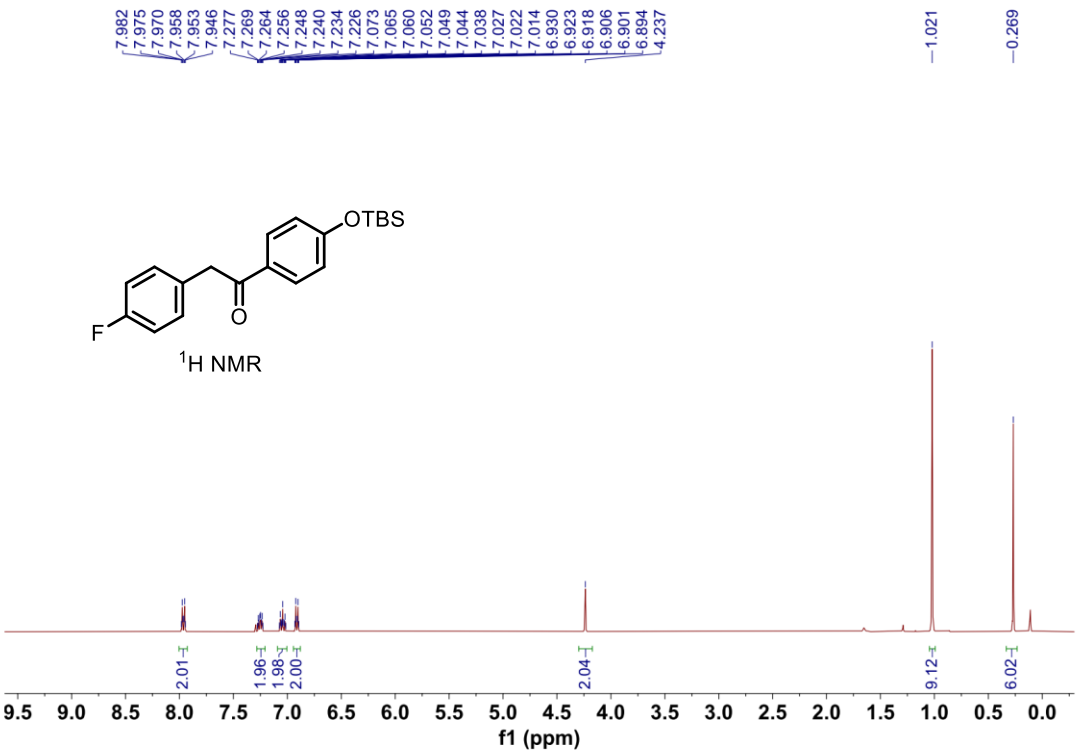


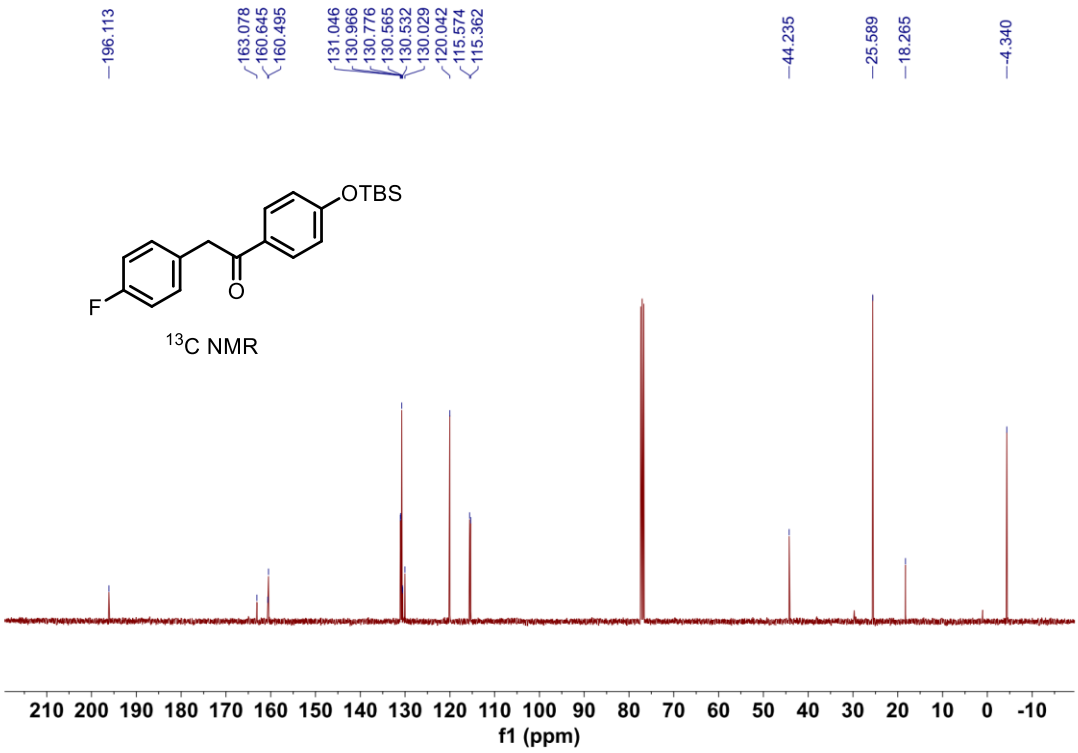


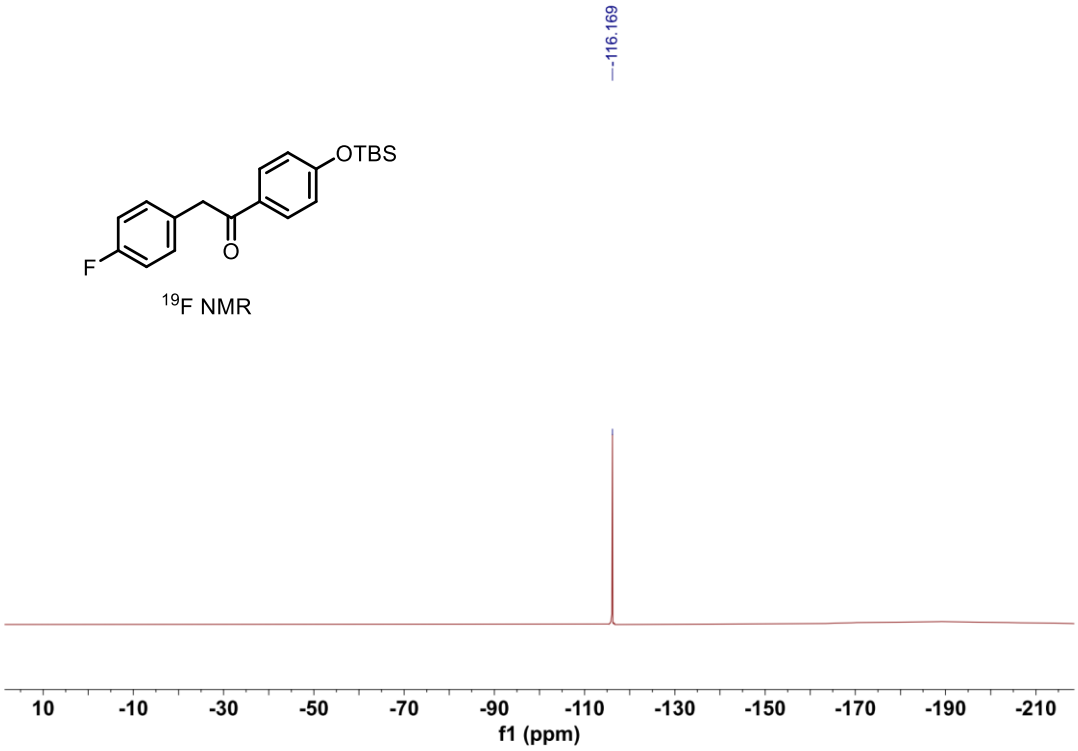
^{13}C NMR

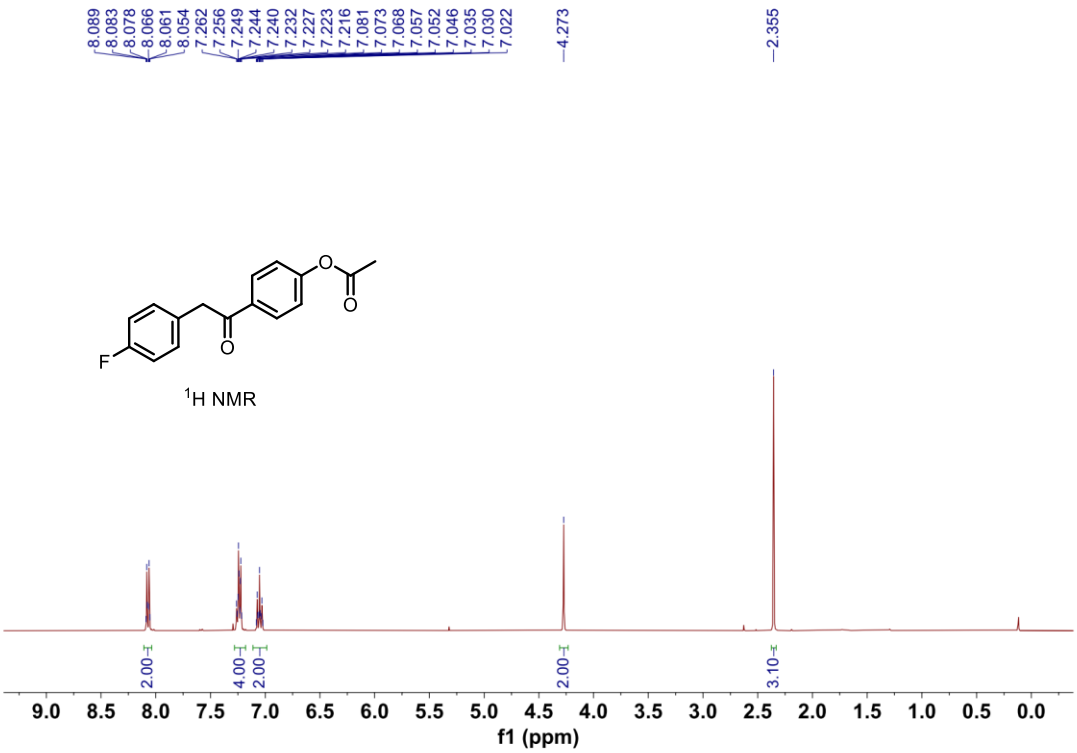


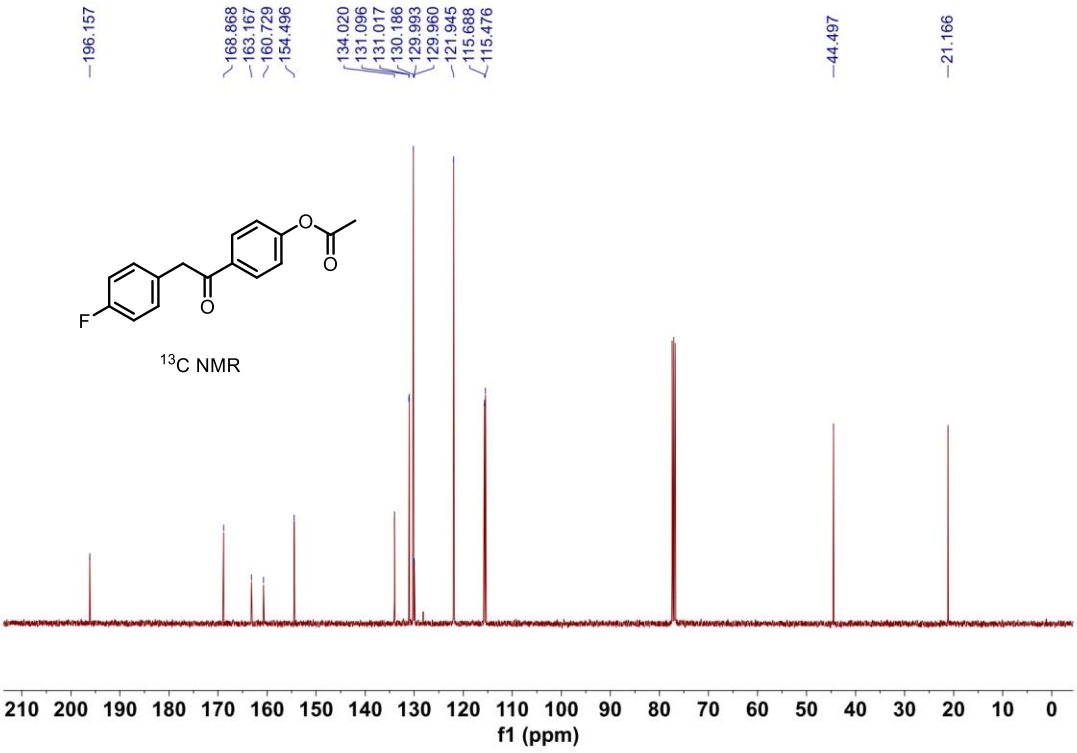

-116.012
F
O
O
19F NMR
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

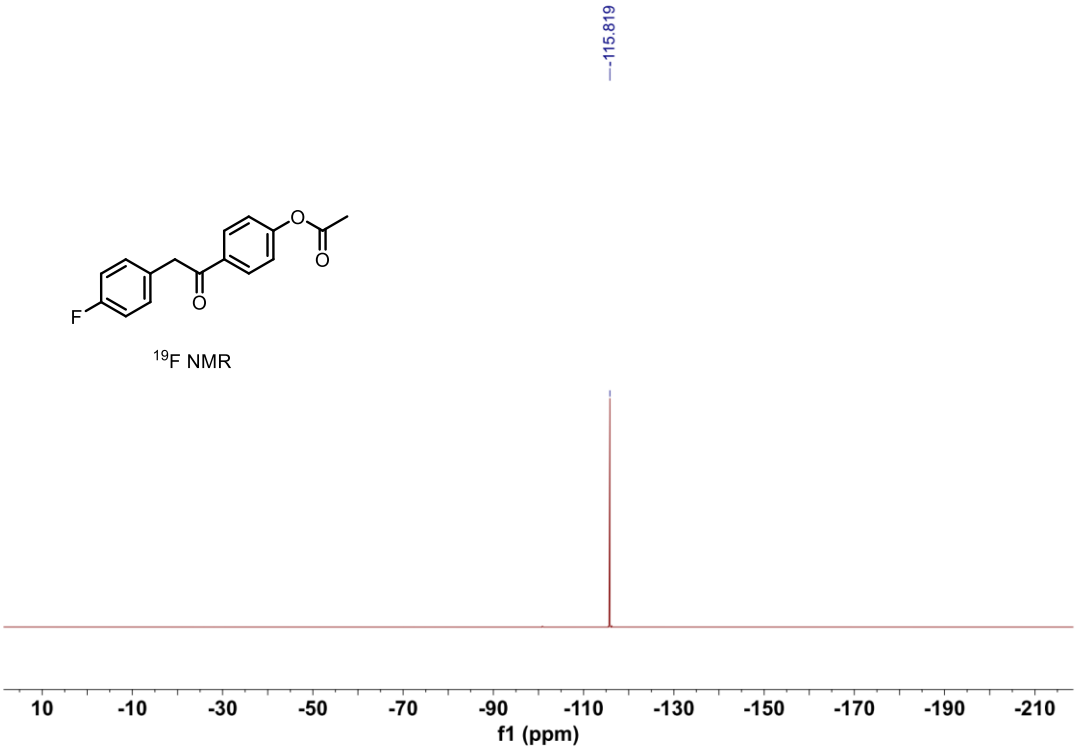

7.982
7.975
7.970
7.958
7.953
7.946
7.277
7.269
7.264
7.256
7.248
7.240
7.234
7.226
7.073
7.065
7.060
7.052
7.049
7.044
7.038
7.027
7.022
7.014
6.930
6.923
6.918
6.906
6.901
6.894
4.237
1.021
0.269
OTBS
F
O
1H NMR
2.01
1.96
1.98
2.00
2.04
9.12
6.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

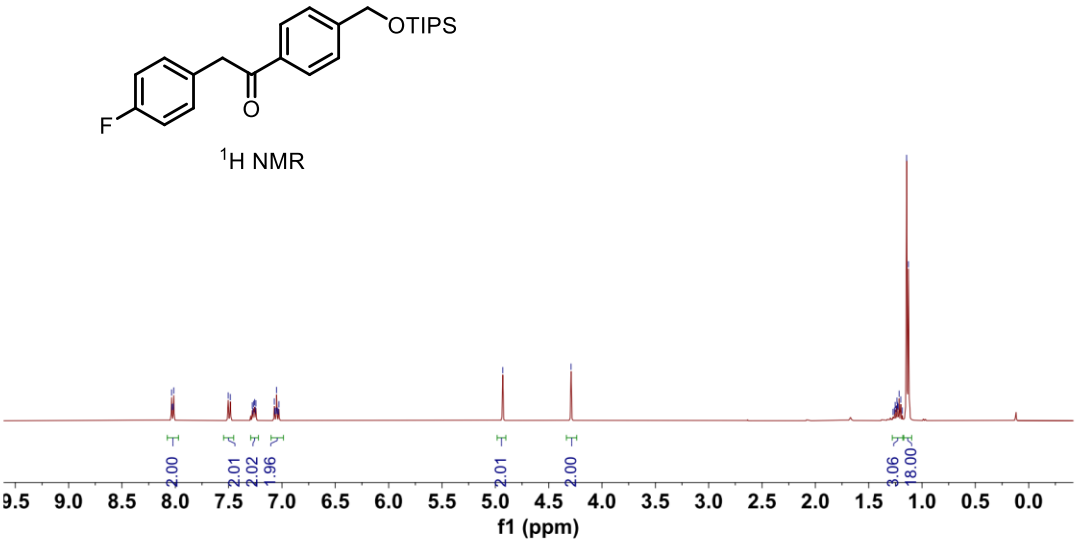

196.113
163.078
160.645
160.495
131.046
130.966
130.776
130.565
130.532
130.029
120.042
115.574
115.362
44.235
25.589
18.265
-4.340
OTBS
O
F
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

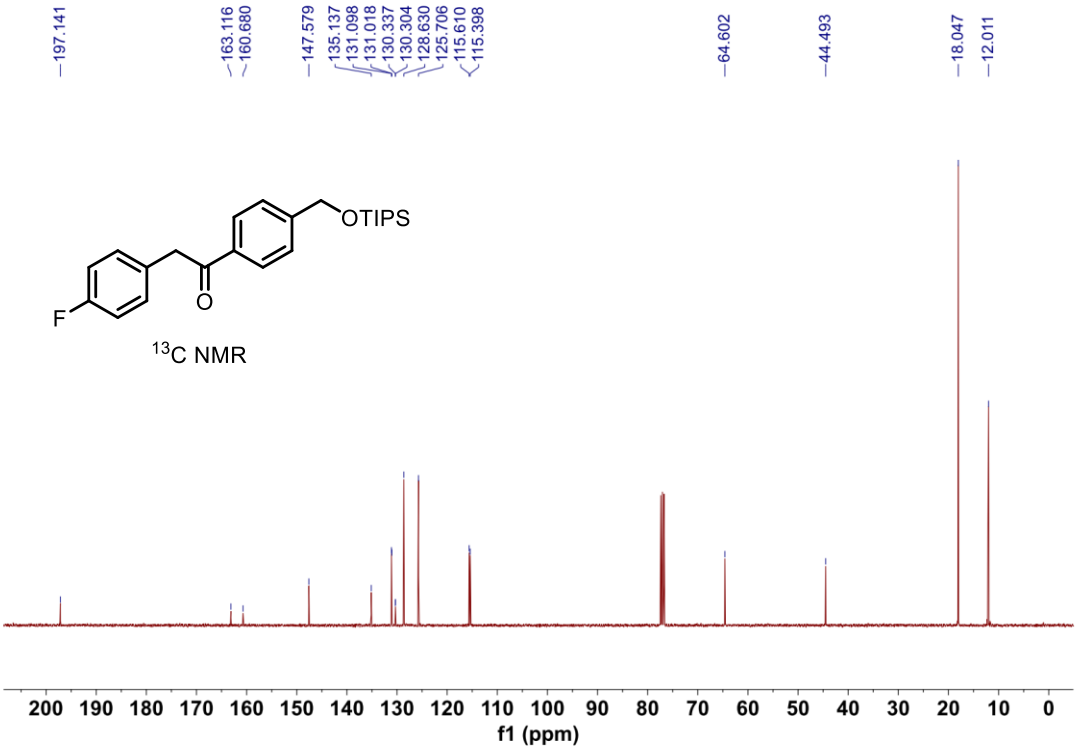

-116.169
OTBS
O
F
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


8.089
8.083
8.078
8.066
8.061
8.054
7.262
7.256
7.249
7.244
7.240
7.232
7.227
7.223
7.216
7.081
7.073
7.068
7.057
7.052
7.046
7.035
7.030
7.022
4.273
2.355
O
O
F
O
1H NMR
2.00
4.00
2.00
2.00
3.10
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
f1 (ppm)

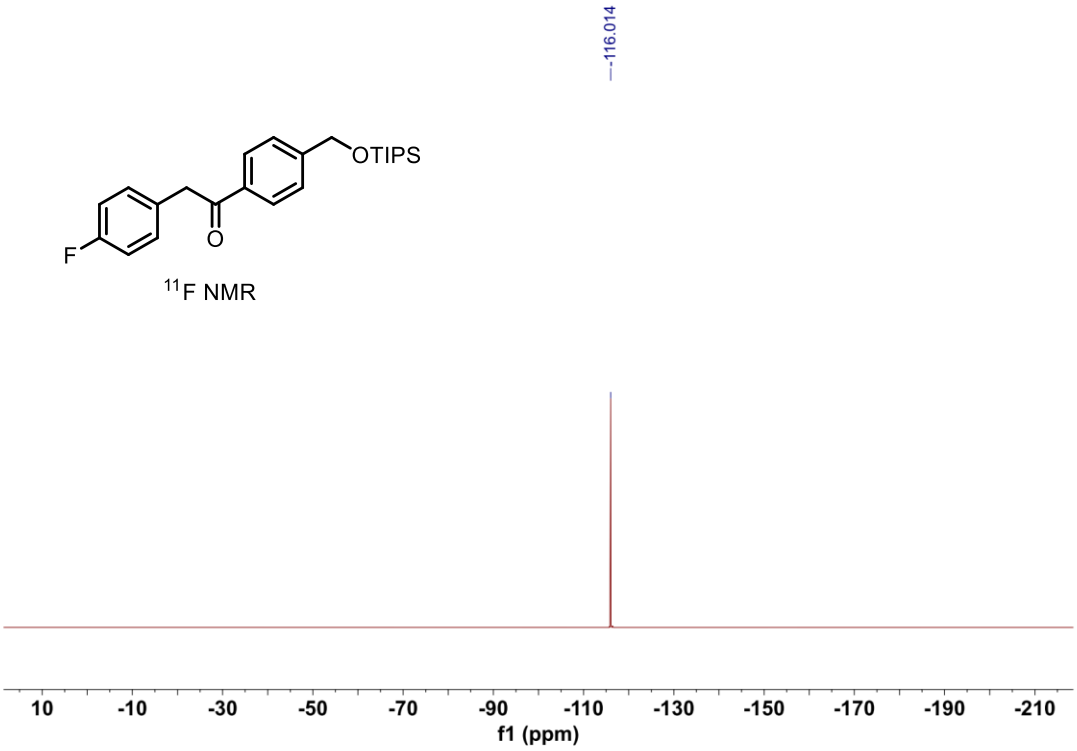

196.157
168.868
163.167
160.729
154.496
134.020
131.096
131.017
130.186
129.993
129.960
121.945
115.688
115.476
44.497
21.166
O
O
F
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-115.819
O
O
F
19F NMR
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)
8.035
8.031
8.019
8.015
7.504
7.484
7.279
7.273
7.265
7.258
7.249
7.244
7.072
7.066
7.056
7.050
7.044
7.034
7.028
4.931
4.290
1.272
1.258
1.252
1.242
1.235
1.232
1.224
1.215
1.199
1.184
1.144
1.128

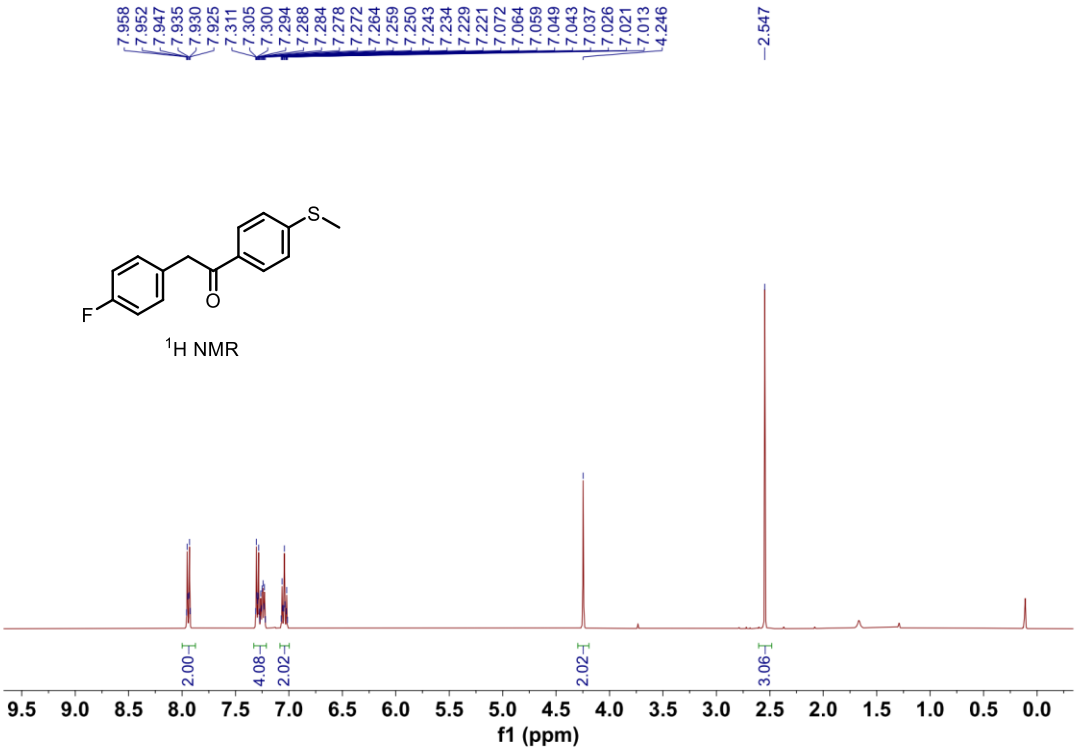

OTIPS
O
F
1H NMR
2.00
2.01
2.02
1.96
2.01
2.00
3.06
18.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



^{13}C NMR



^{11}F NMR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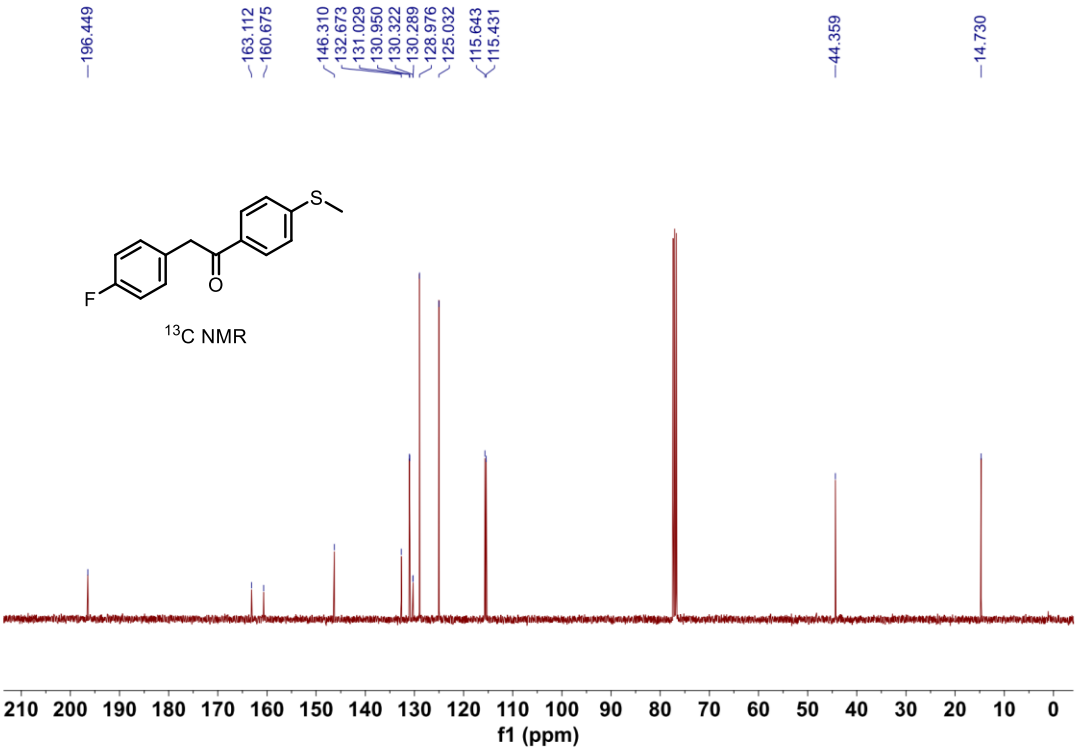
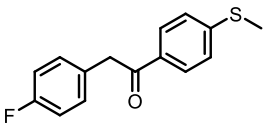
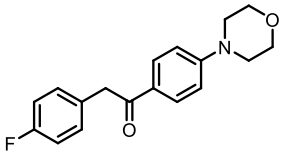
7.952
7.947
7.935
7.930
7.925
7.311
7.305
7.300
7.294
7.288
7.284
7.278
7.272
7.264
7.259
7.250
7.243
7.234
7.229
7.221
7.072
7.064
7.059
7.049
7.043
7.037
7.026
7.021
7.013
4.246
2.547
S
O
F
1H NMR
2.00
4.08
2.02
2.02
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

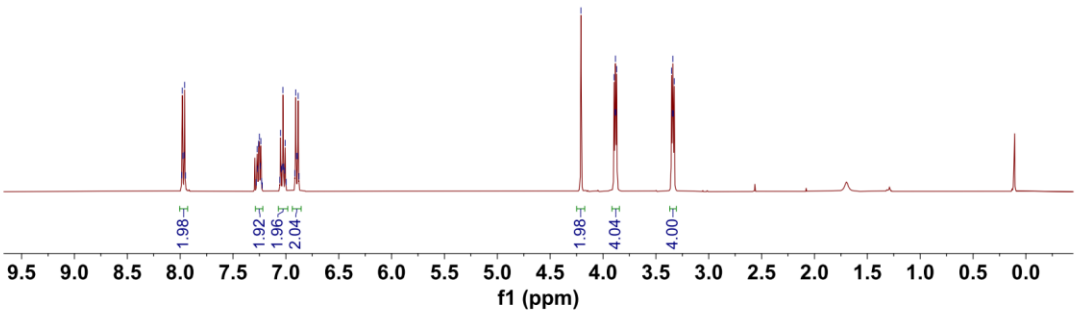

196.449
163.112
160.675
146.310
132.673
131.029
130.950
130.322
130.289
128.976
125.032
115.643
115.431
44.359
14.730
S
O
F
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

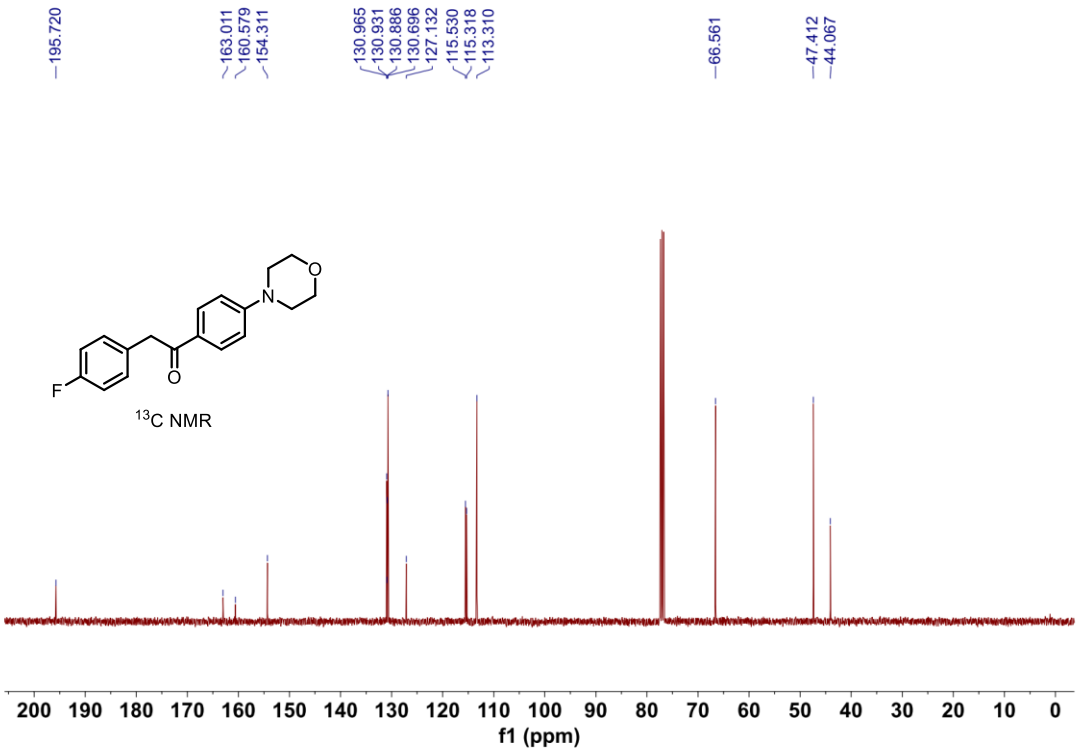


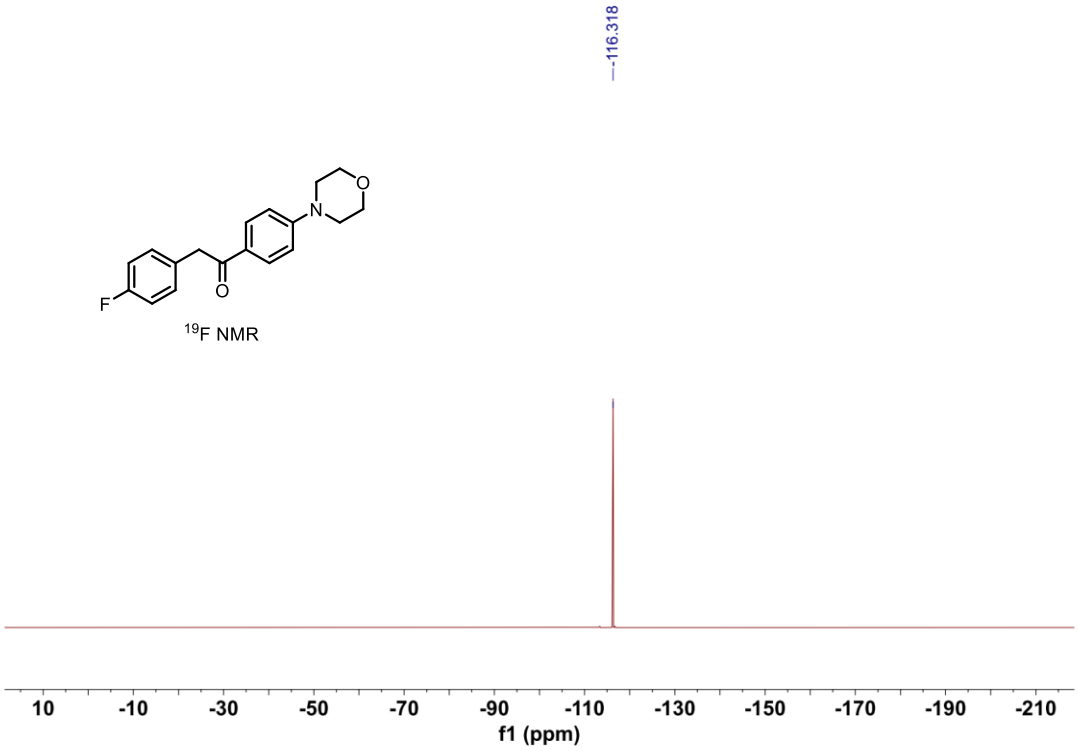
^{19}F NMR

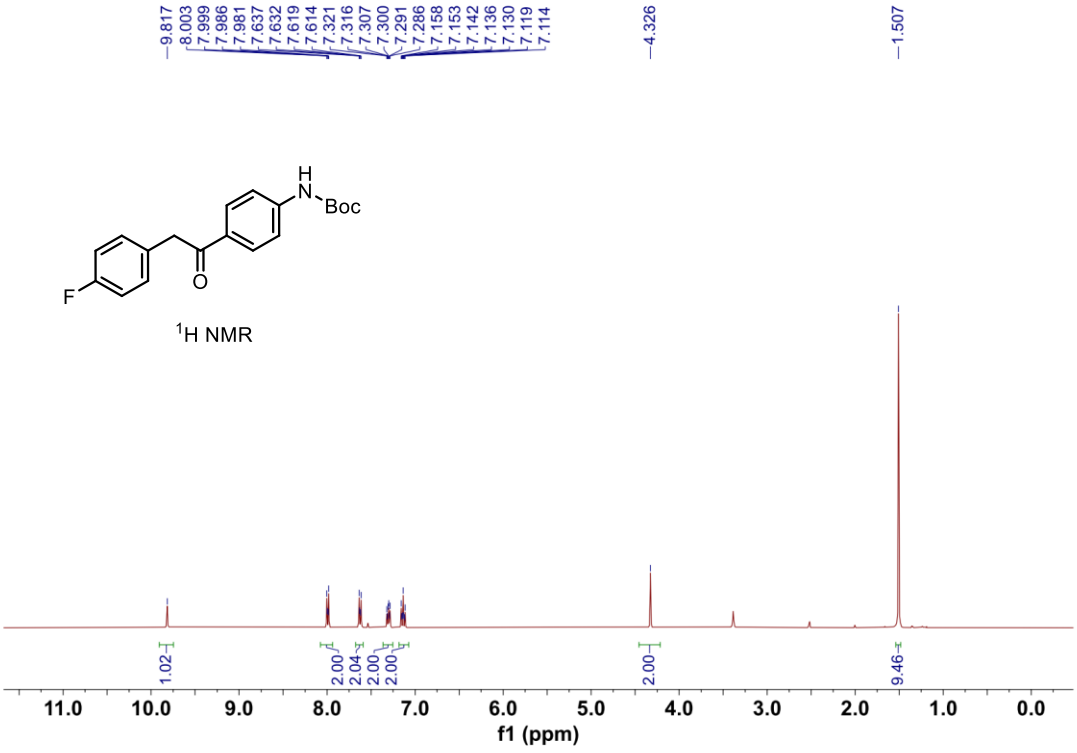


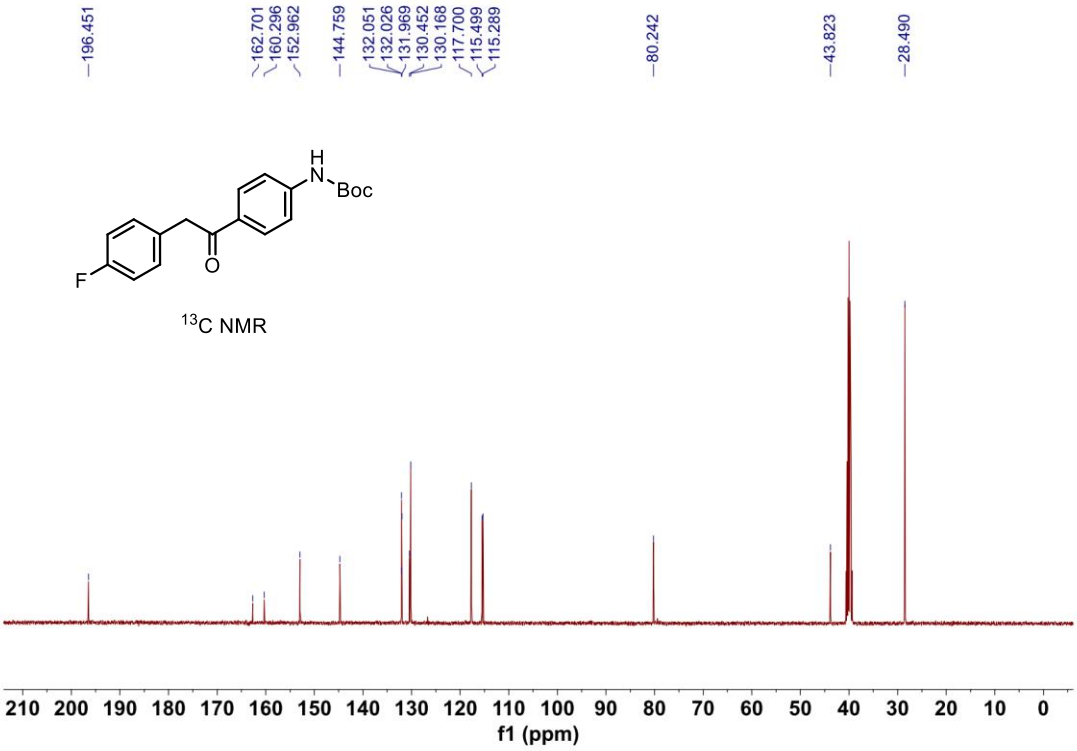
^{1}H NMR

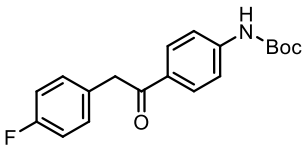



195.720
163.011
160.579
154.311
130.965
130.931
130.886
130.696
127.132
115.530
115.318
113.310
66.561
47.412
44.067
O
N
O
F
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

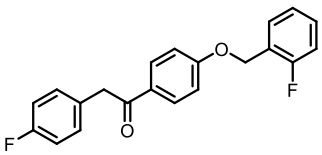

116.318
O
N
O
F
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


9.817
8.003
7.999
7.986
7.981
7.637
7.632
7.619
7.614
7.321
7.316
7.307
7.300
7.291
7.286
7.158
7.153
7.142
7.136
7.130
7.119
7.114
4.326
1.507
H
N
Boc
O
F
1H NMR
1.02
2.00
2.04
2.00
2.00
2.00
9.46
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

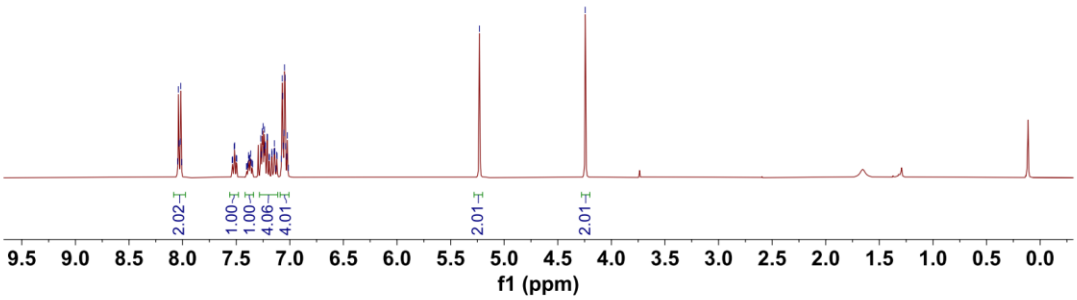

196.451
162.701
160.296
152.962
144.759
132.051
132.026
131.969
130.452
130.168
117.700
115.499
115.289
80.242
43.823
28.490
H
N
Boc
O
F
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

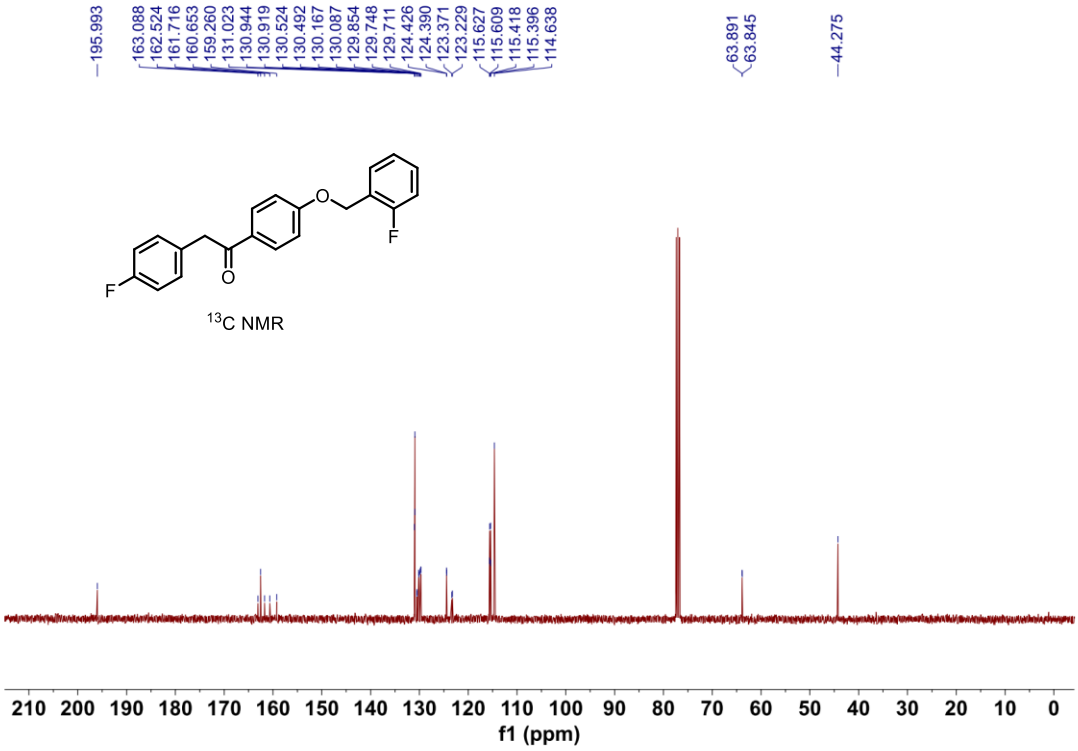


^{19}F NMR

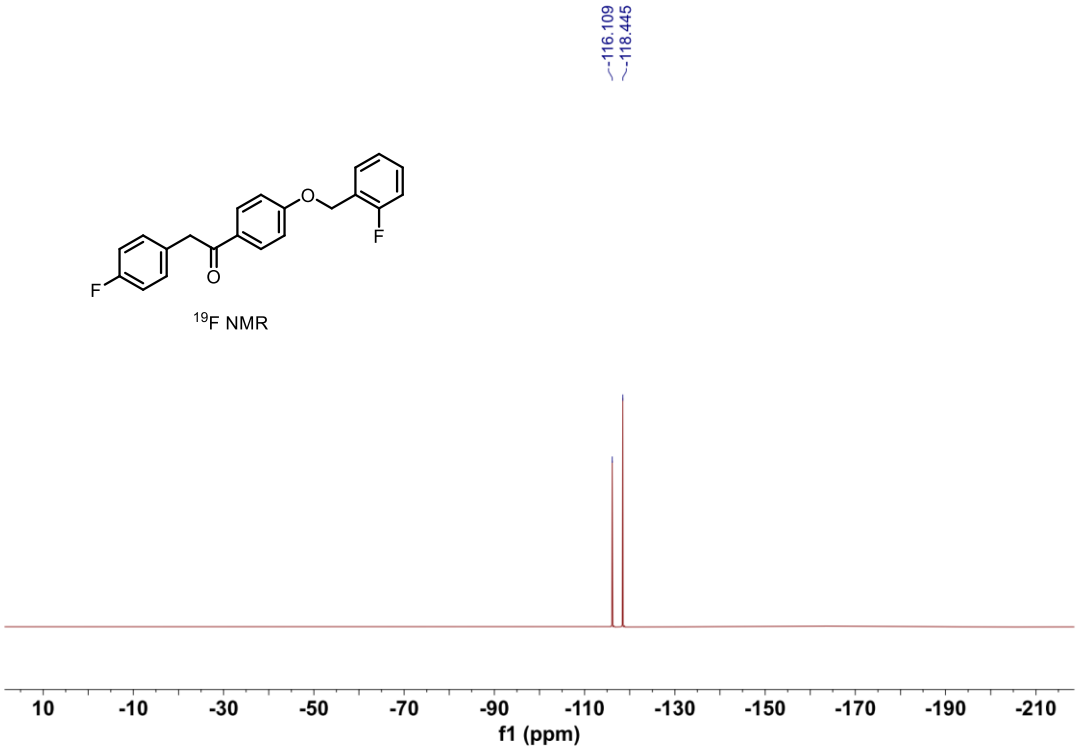


^{1}H NMR

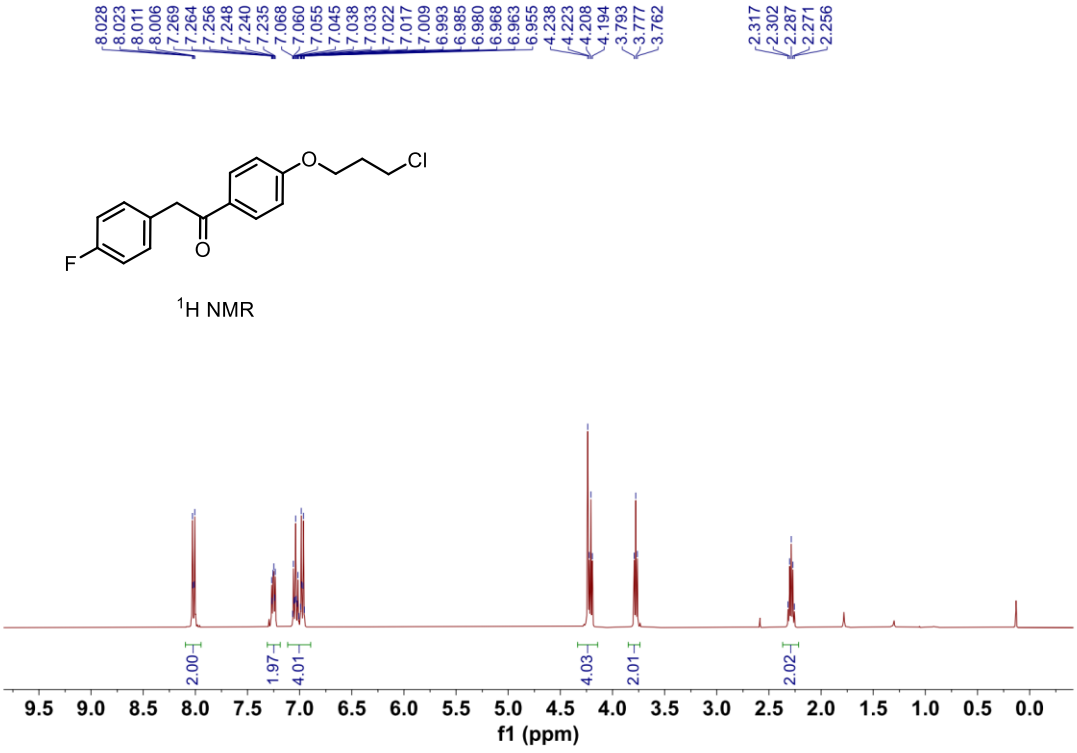




^{13}C NMR



^{19}F NMR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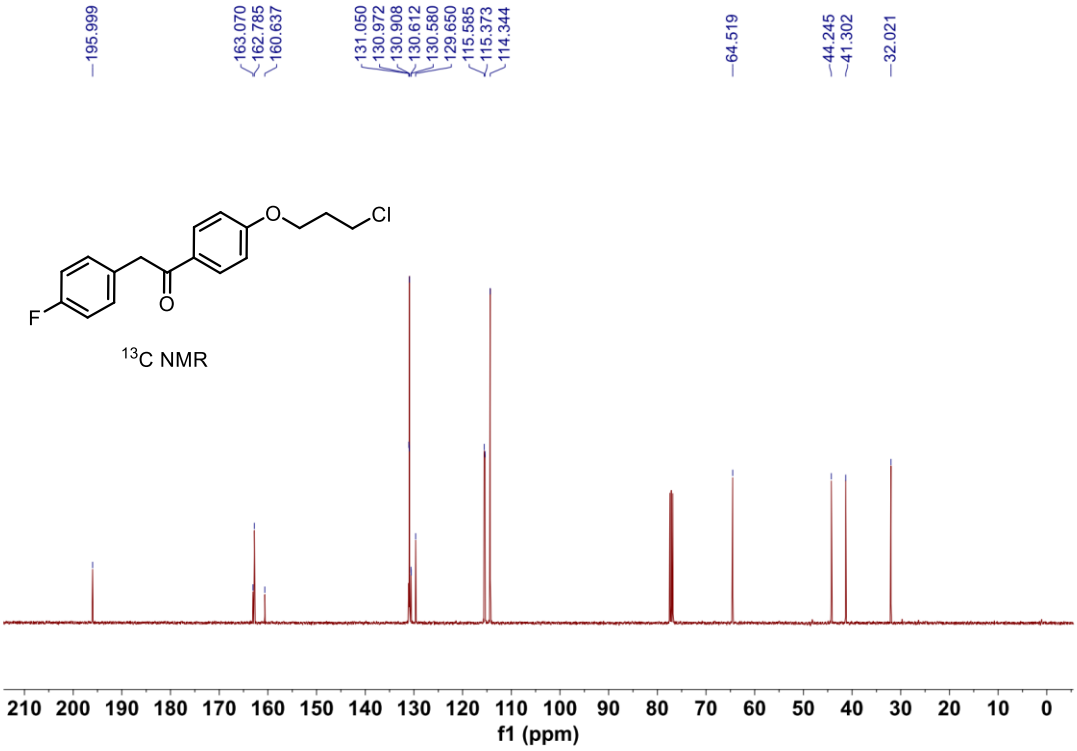
8.023
8.011
8.006
7.269
7.264
7.256
7.248
7.240
7.235
7.068
7.060
7.055
7.045
7.038
7.033
7.022
7.017
7.009
6.993
6.985
6.980
6.968
6.963
6.955
4.238
4.223
4.208
4.194
3.793
3.777
3.762
2.317
2.302
2.287
2.271
2.256
O
Cl
F
O
1H NMR
2.00
1.97
4.01
4.03
2.01
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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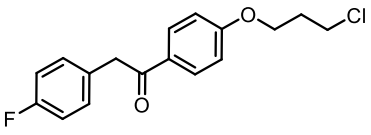
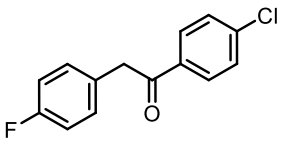
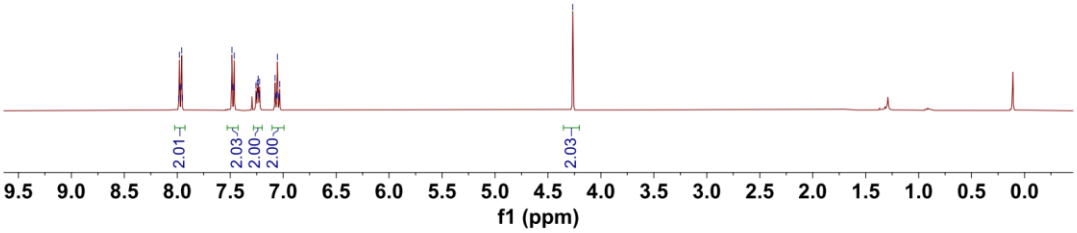
163.070
162.785
160.637
131.050
130.972
130.908
130.612
130.580
129.650
115.585
115.373
114.344
64.519
44.245
41.302
32.021
O
Cl
F
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

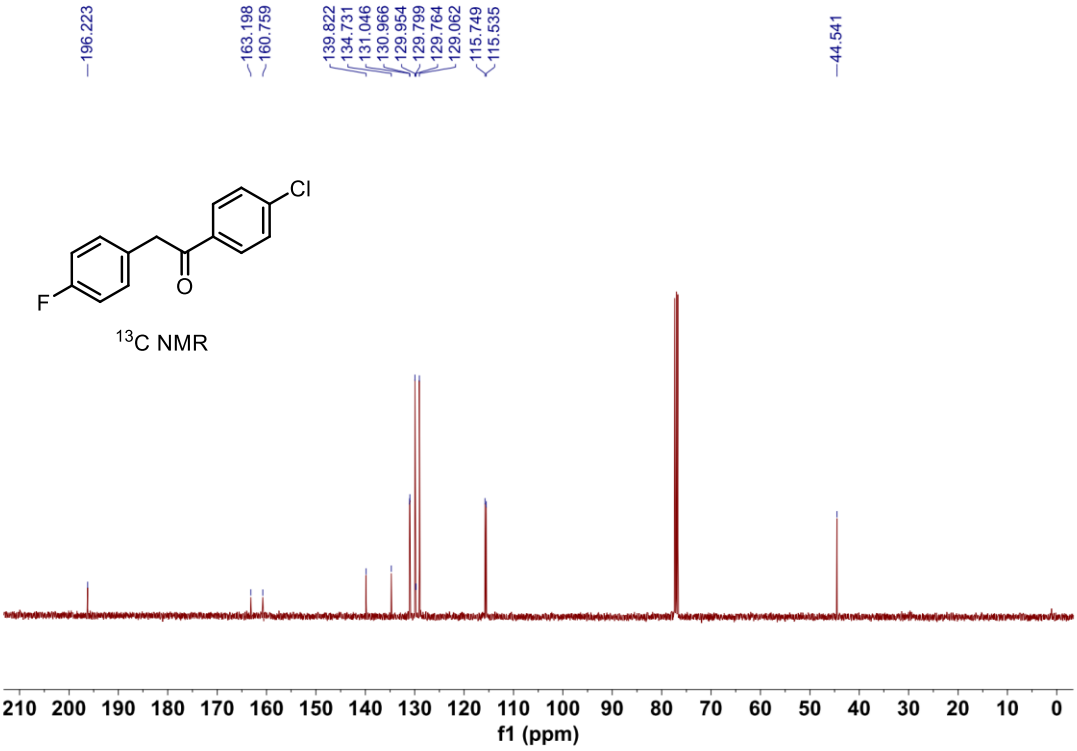


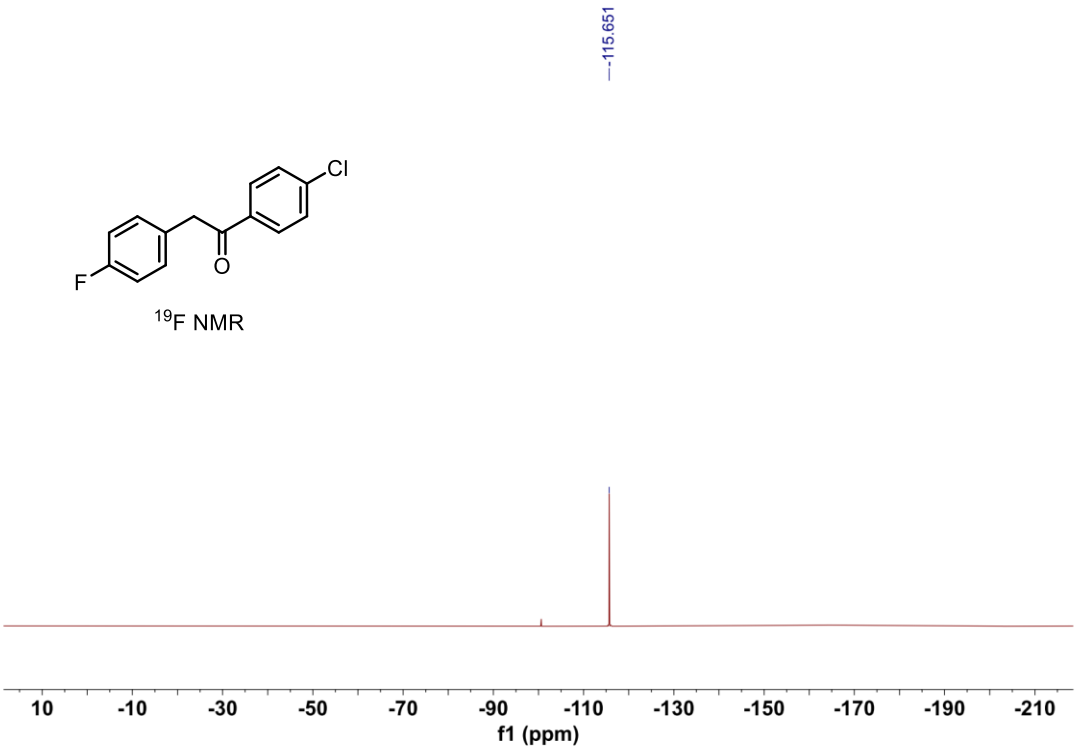
^{19}F NMR

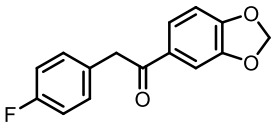


^{1}H NMR

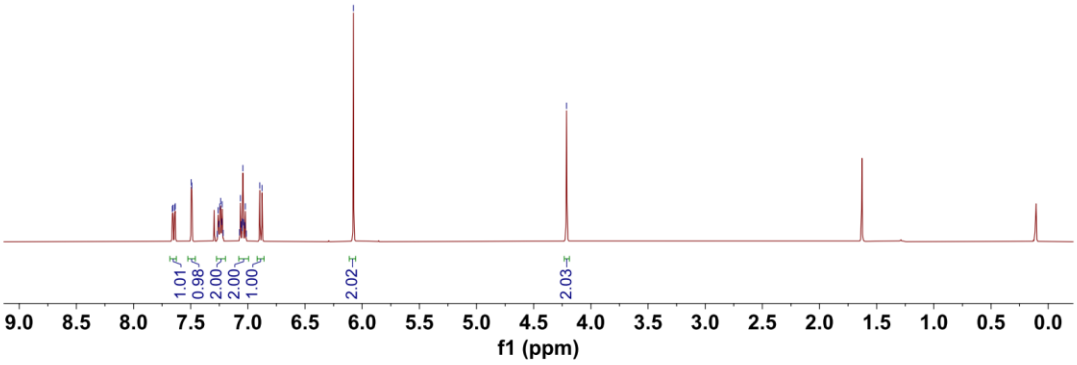


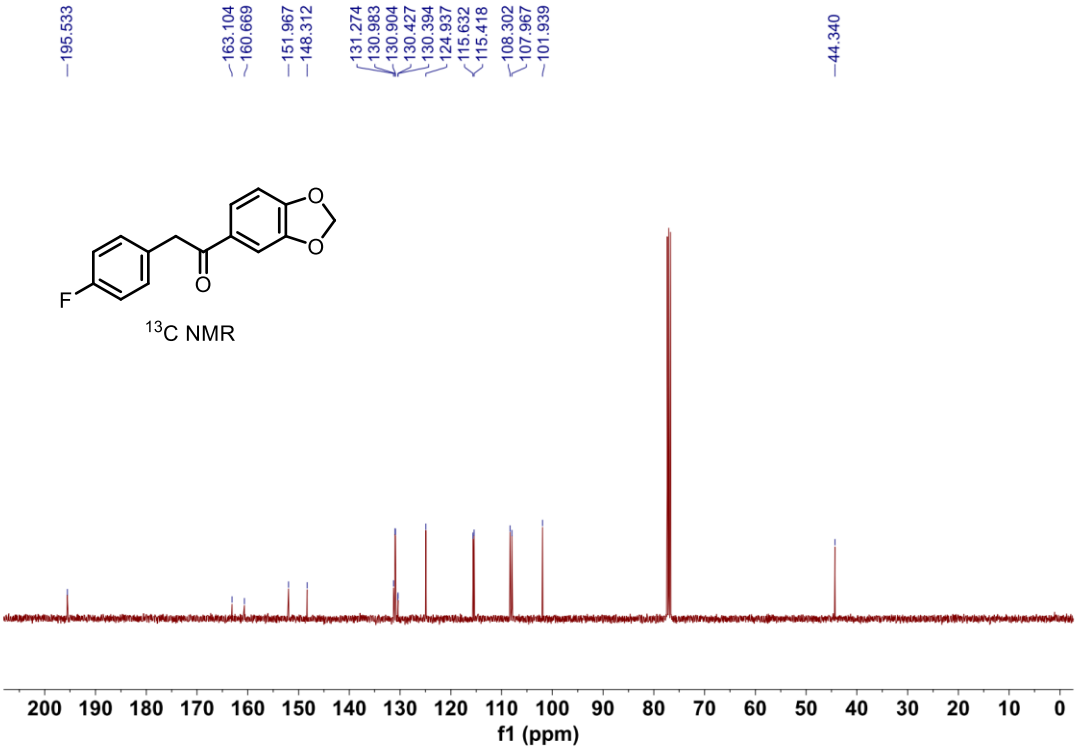

196.223
163.198
160.759
139.822
134.731
131.046
130.966
129.954
129.799
129.764
129.062
115.749
115.535
44.541
Cl
O
F
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


115.651
Cl
O
F
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

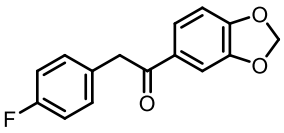


^{1}H NMR

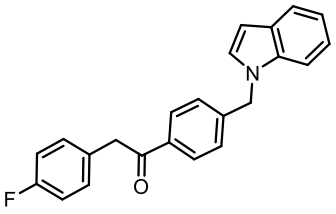




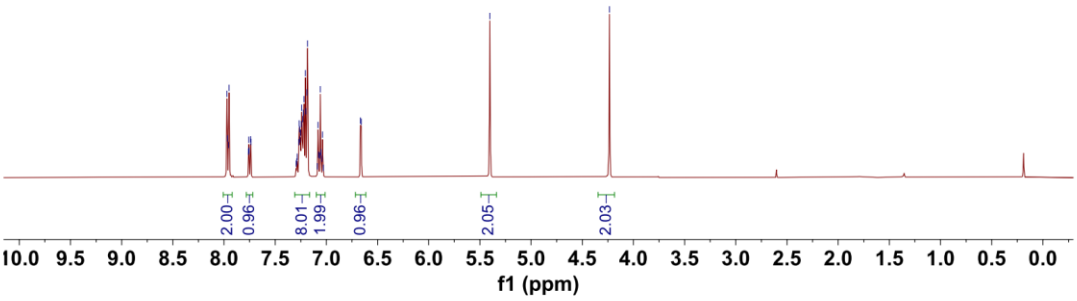
^{13}C NMR

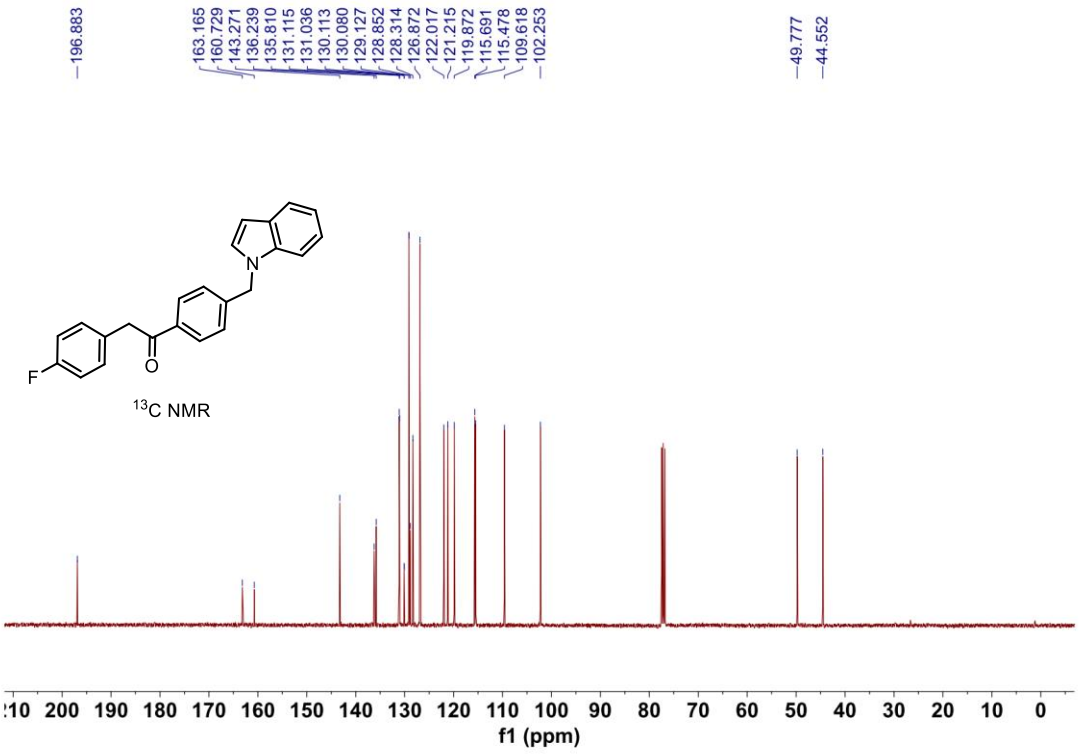


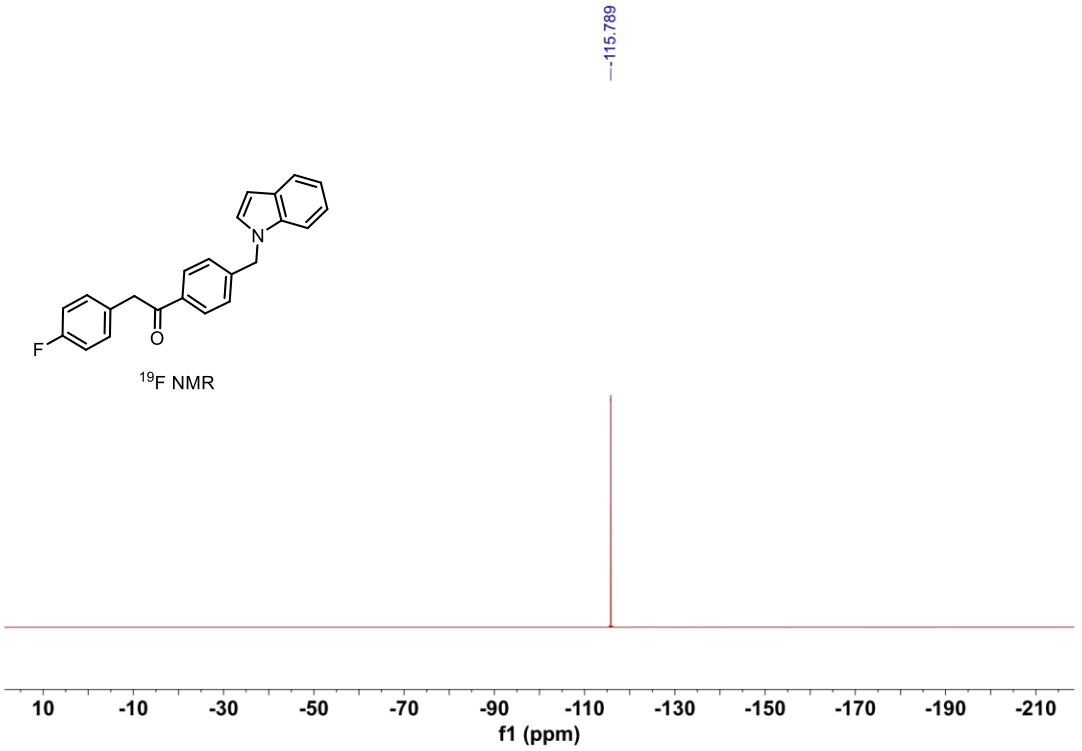
^{19}F NMR



^{1}H NMR




196.883
163.165
160.729
143.271
136.239
135.810
131.115
131.036
130.113
130.080
129.127
128.852
128.314
126.872
122.017
121.215
119.872
115.691
115.478
109.618
102.253
49.777
44.552
F
O
N
13C NMR
f1 (ppm)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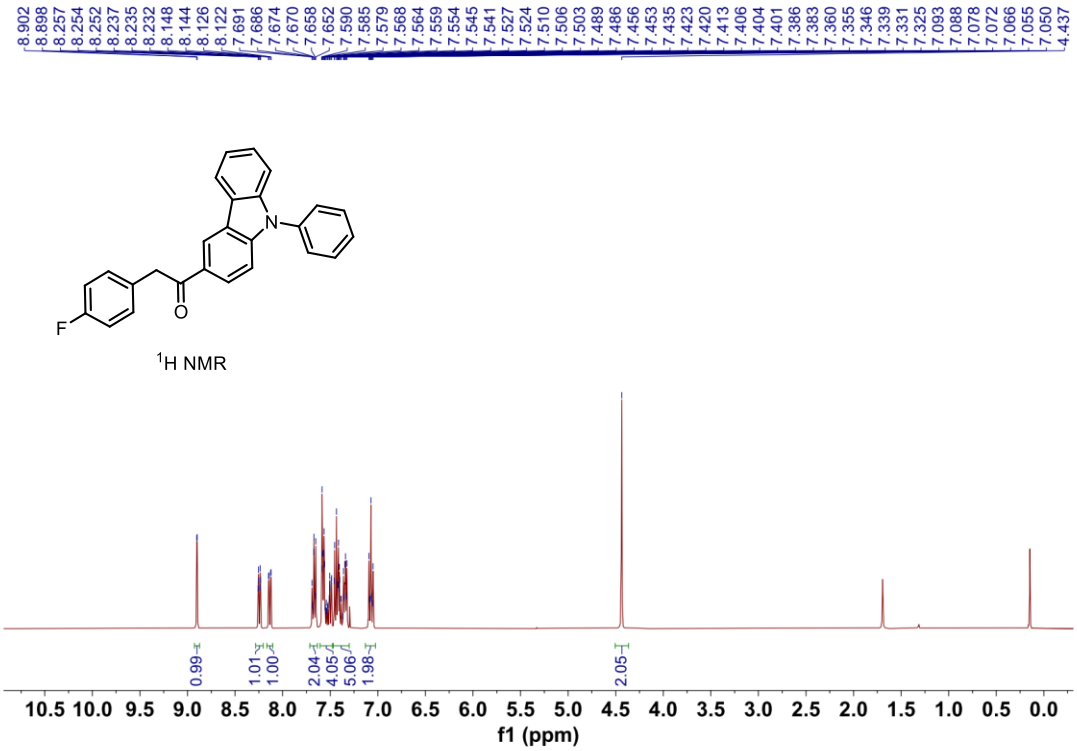
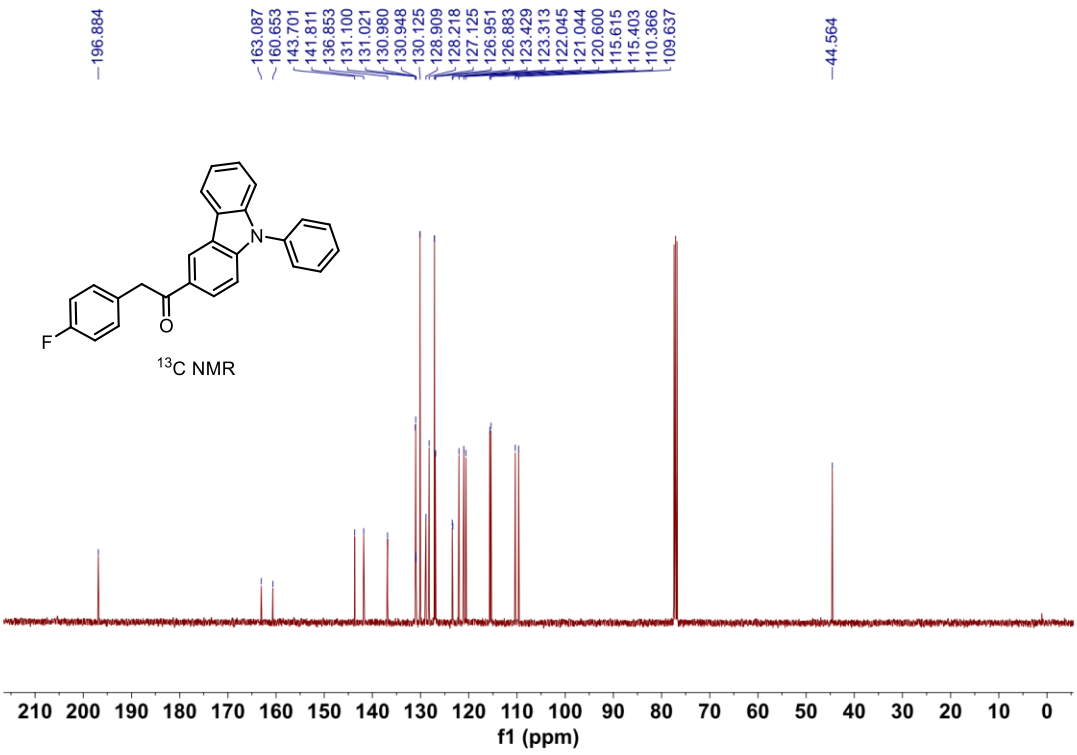
F
O
N
19F NMR
f1 (ppm)


8.902
8.898
8.257
8.254
8.252
8.237
8.235
8.232
8.148
8.144
8.126
8.122
7.691
7.686
7.674
7.670
7.658
7.652
7.590
7.585
7.579
7.568
7.564
7.559
7.554
7.545
7.541
7.527
7.524
7.510
7.506
7.503
7.489
7.486
7.456
7.453
7.435
7.423
7.420
7.413
7.406
7.404
7.401
7.386
7.383
7.360
7.355
7.346
7.339
7.331
7.325
7.093
7.088
7.078
7.072
7.066
7.055
7.050
4.437
F
O
N
1H NMR
0.99
1.01
1.00
2.04
4.05
5.06
1.98
2.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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163.087
160.653
143.701
141.811
136.853
131.100
131.021
130.980
130.948
130.125
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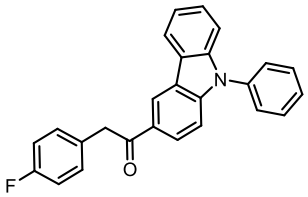
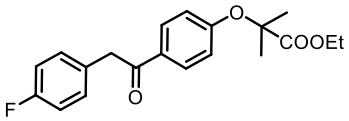
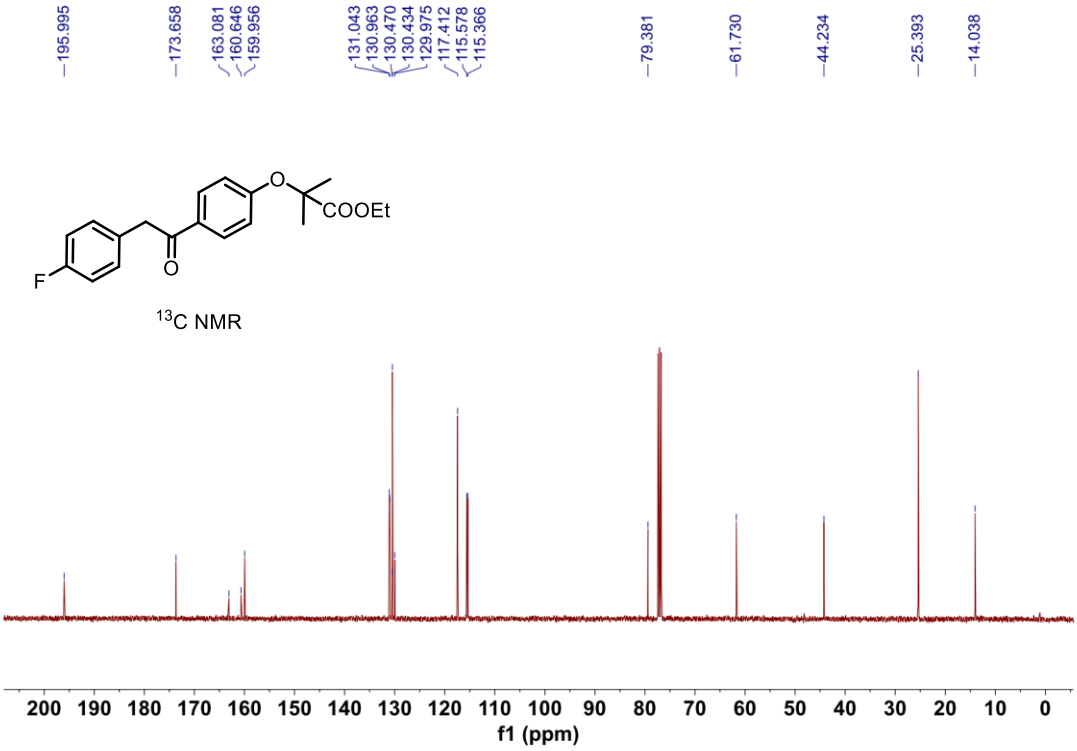
128.218
127.125
126.951
126.883
123.429
123.313
122.045
121.044
120.600
115.615
115.403
110.366
109.637
44.564
F
O
N
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



^{19}F NMR



^{1}H NMR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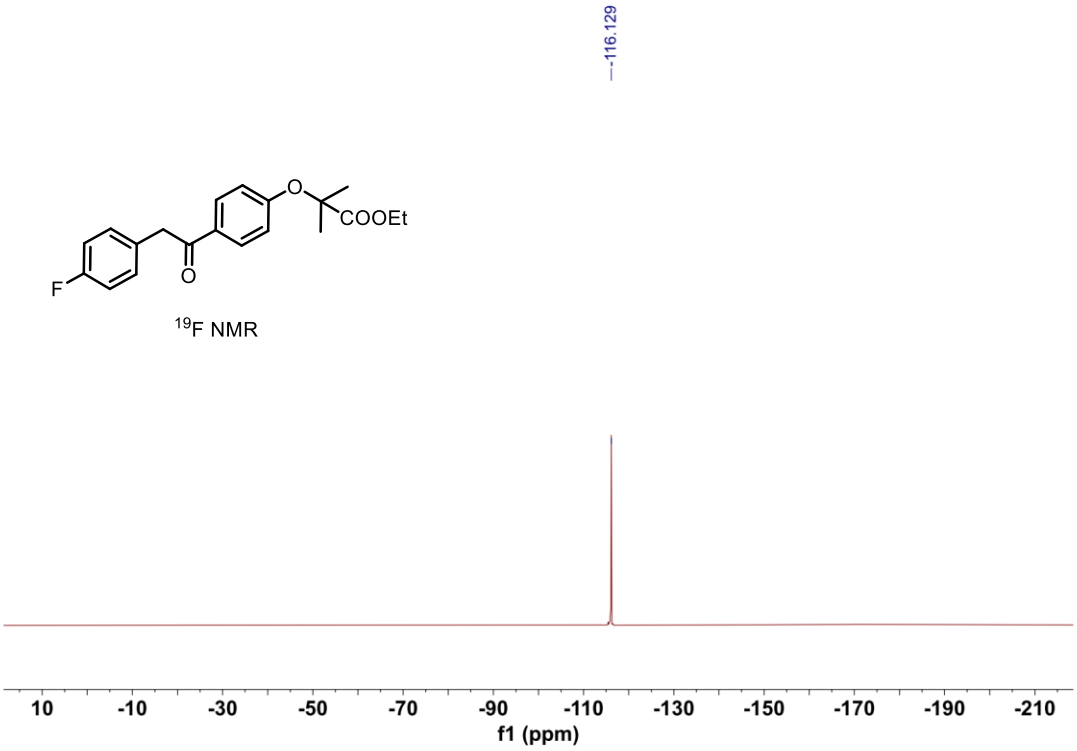
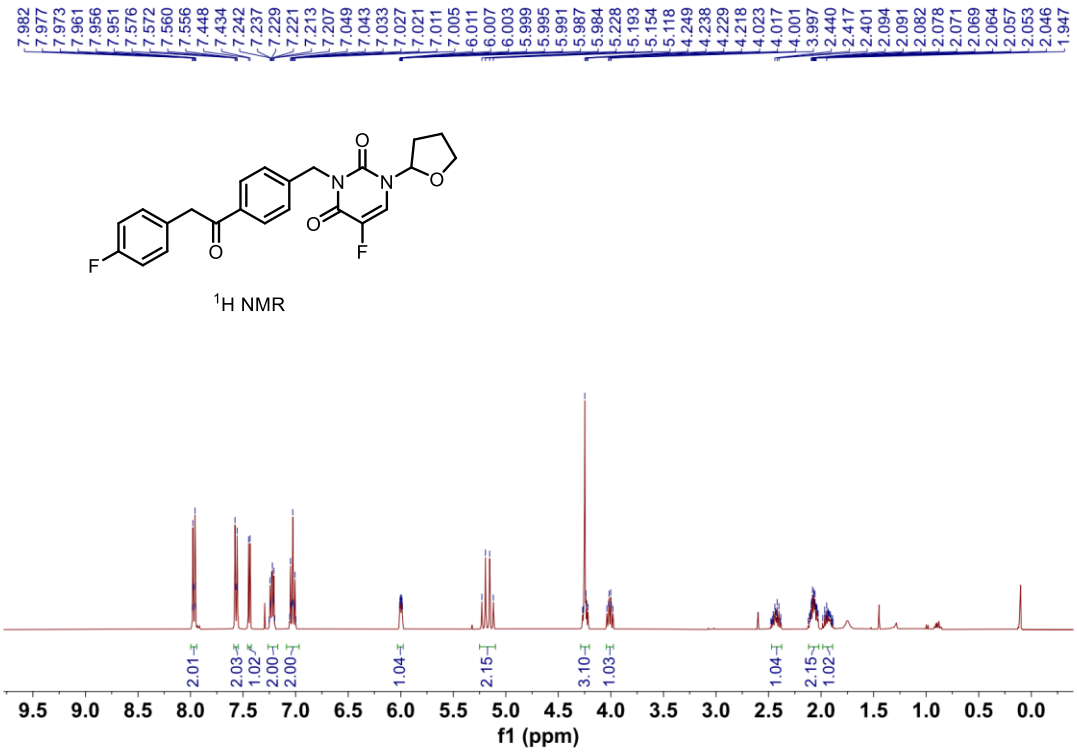
173.658
163.081
160.646
159.956
131.043
130.963
130.470
130.434
129.975
117.412
115.578
115.366
79.381
61.730
44.234
25.393
14.038
O
COOEt
F
O
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


116.129
O
COOEt
F
O
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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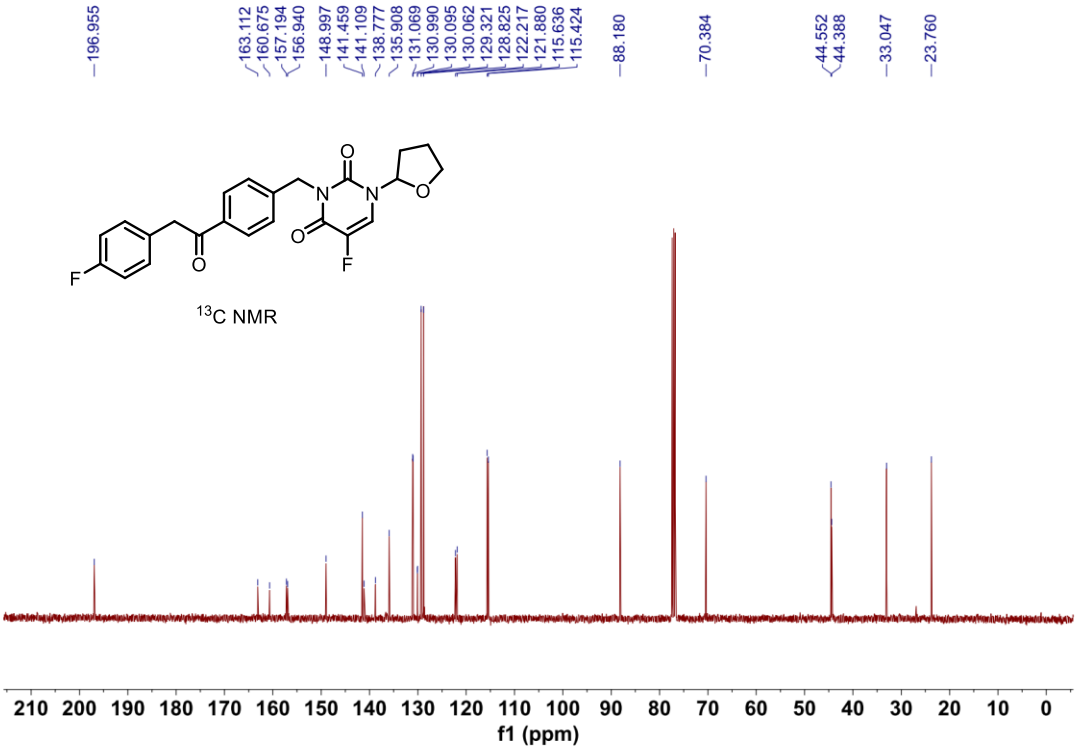
7.973
7.961
7.956
7.951
7.576
7.572
7.560
7.556
7.448
7.434
7.242
7.237
7.229
7.221
7.213
7.207
7.049
7.043
7.033
7.027
7.021
7.011
7.005
6.011
6.007
6.003
5.999
5.995
5.991
5.987
5.984
5.228
5.193
5.154
5.118
4.249
4.238
4.229
4.218
4.023
4.017
4.001
3.997
2.440
2.417
2.401
2.094
2.091
2.082
2.078
2.071
2.069
2.064
2.057
2.053
2.046
1.947
O
N
N
O
O
F
O
F
1H NMR
2.01
2.03
1.02
2.00
2.00
1.04
2.15
3.10
1.03
1.04
2.15
1.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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163.112
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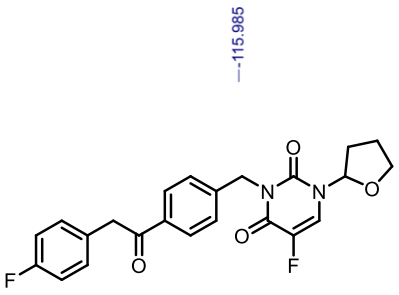
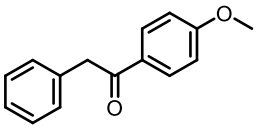
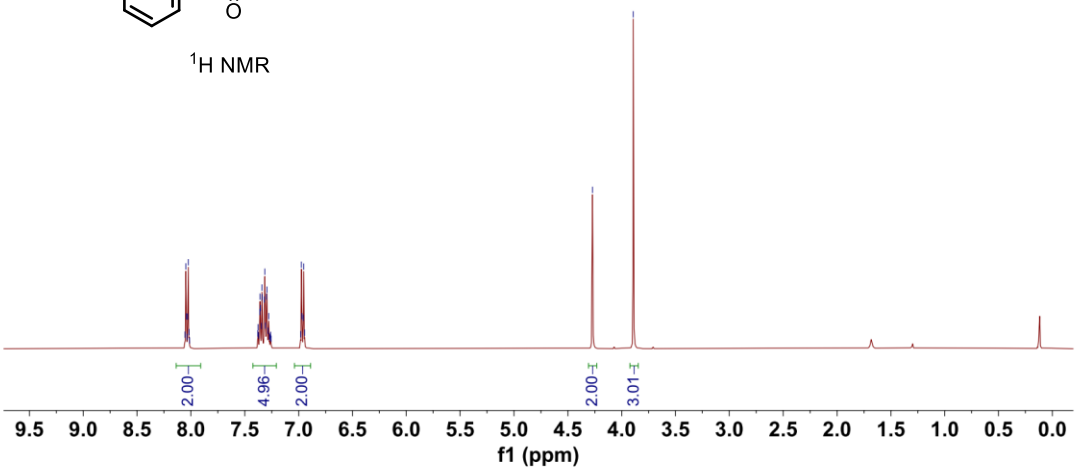
157.194
156.940
148.997
141.459
141.109
138.777
135.908
131.069
130.990
130.095
130.062
129.321
128.825
122.217
121.880
115.636
115.424
88.180
70.384
44.552
44.388
33.047
23.760
O
N
N
O
O
F
O
F
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

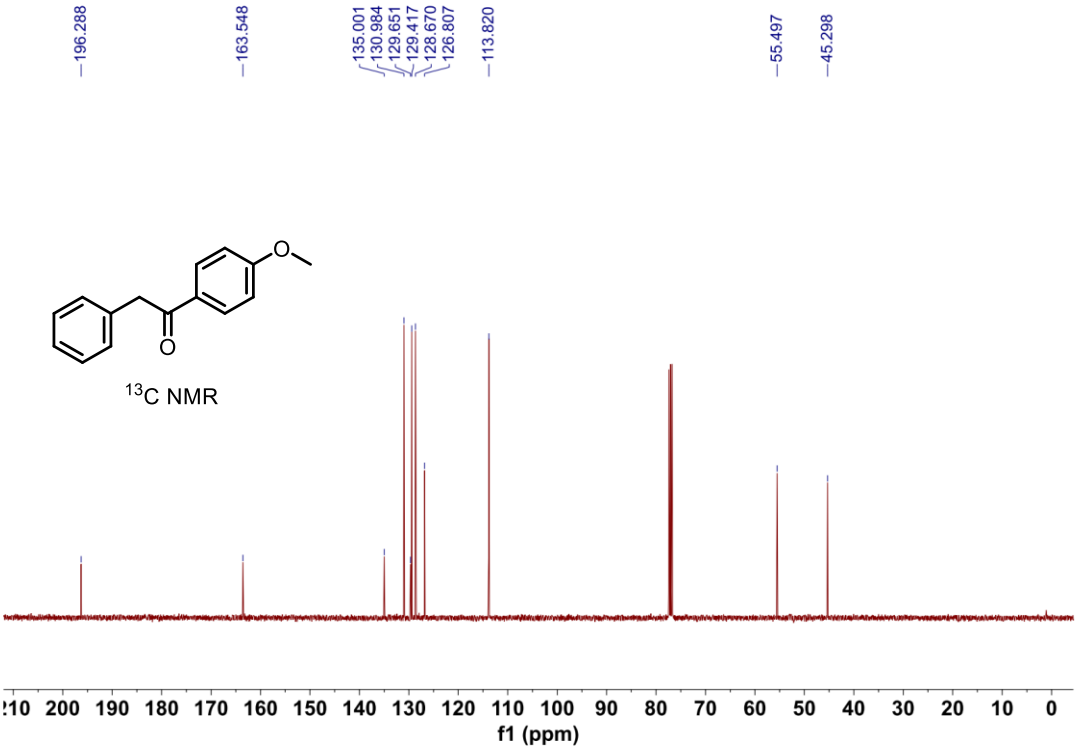


^{19}F NMR



^{1}H NMR

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163.548
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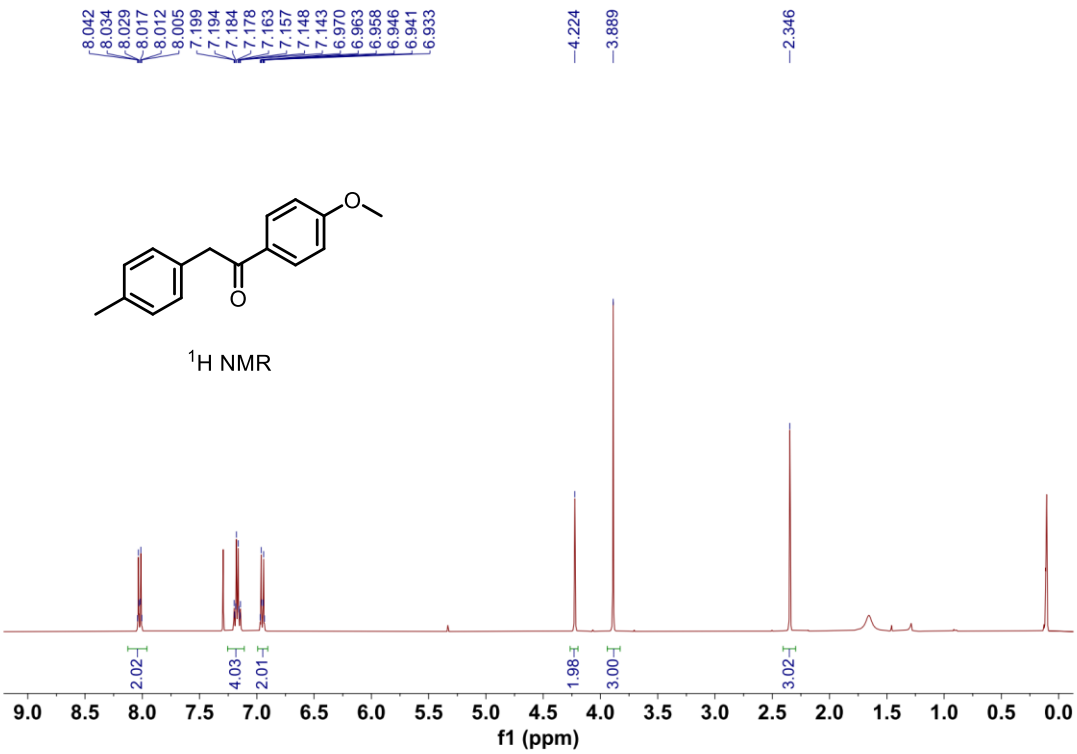
129.651
129.417
128.670
126.807
113.820
55.497
45.298
O
O
13C NMR
f1 (ppm)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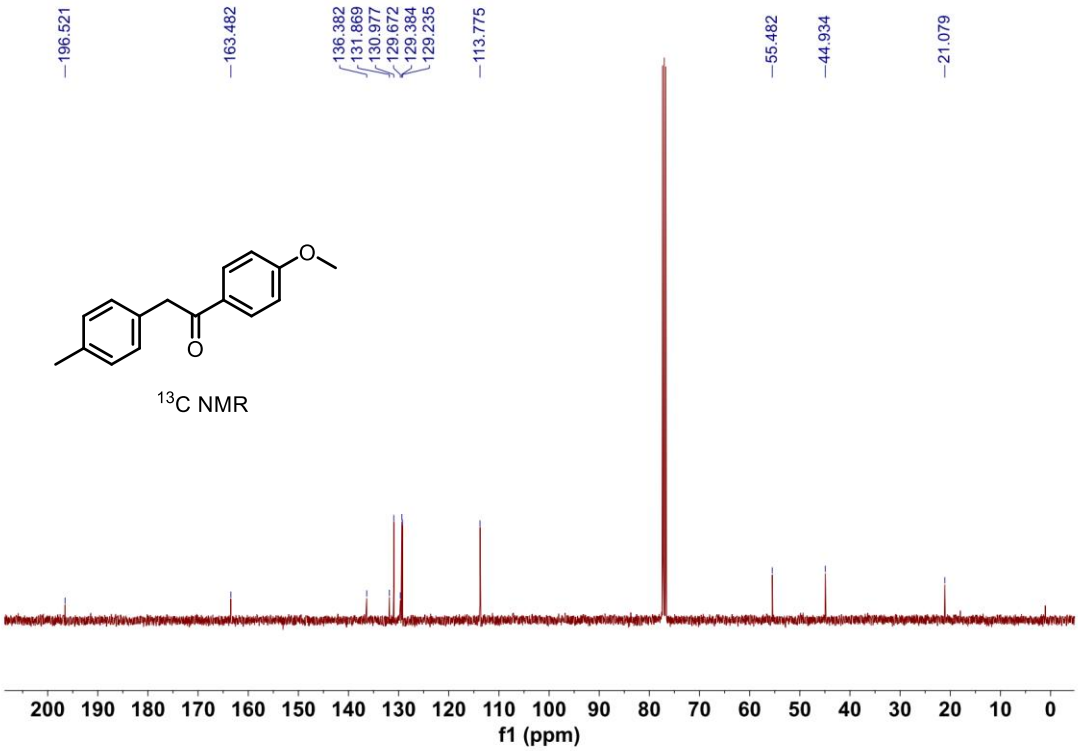
8.017
8.012
8.005
7.199
7.194
7.184
7.178
7.163
7.157
7.148
7.143
6.970
6.963
6.958
6.946
6.941
6.933
4.224
3.889
2.346
O
O
1H NMR
2.02
4.03
2.01
1.98
3.00
3.02
f1 (ppm)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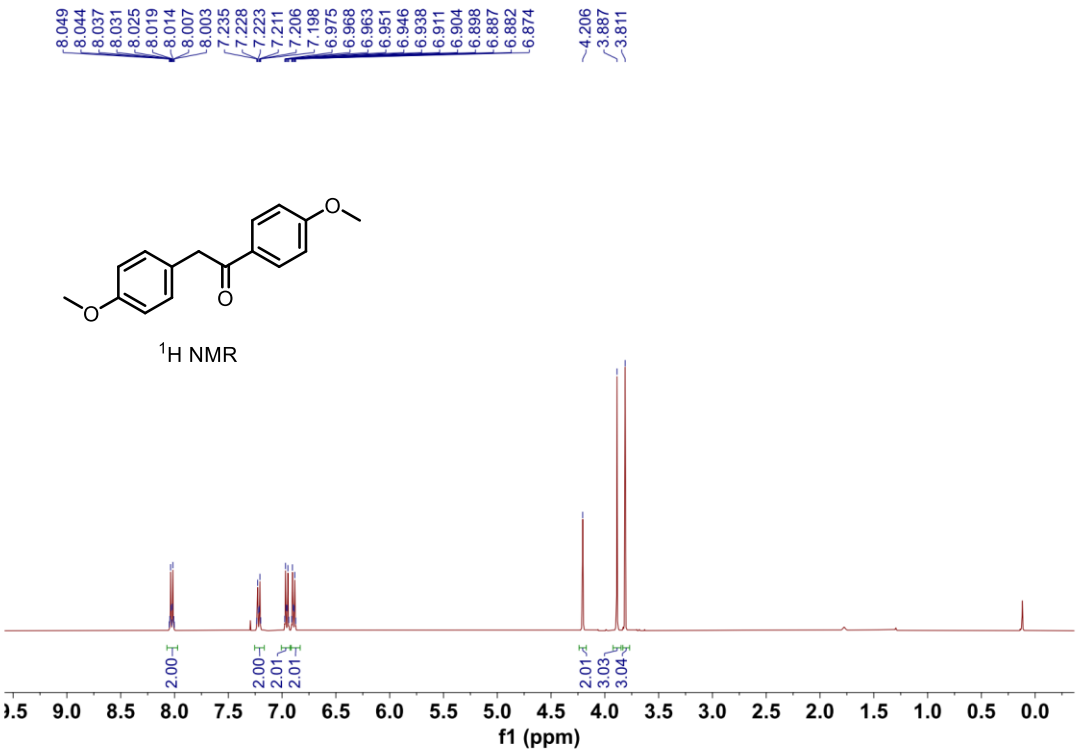
136.382
131.869
130.977
129.672
129.384
129.235
113.775
55.482
44.934
21.079
O
O
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.044
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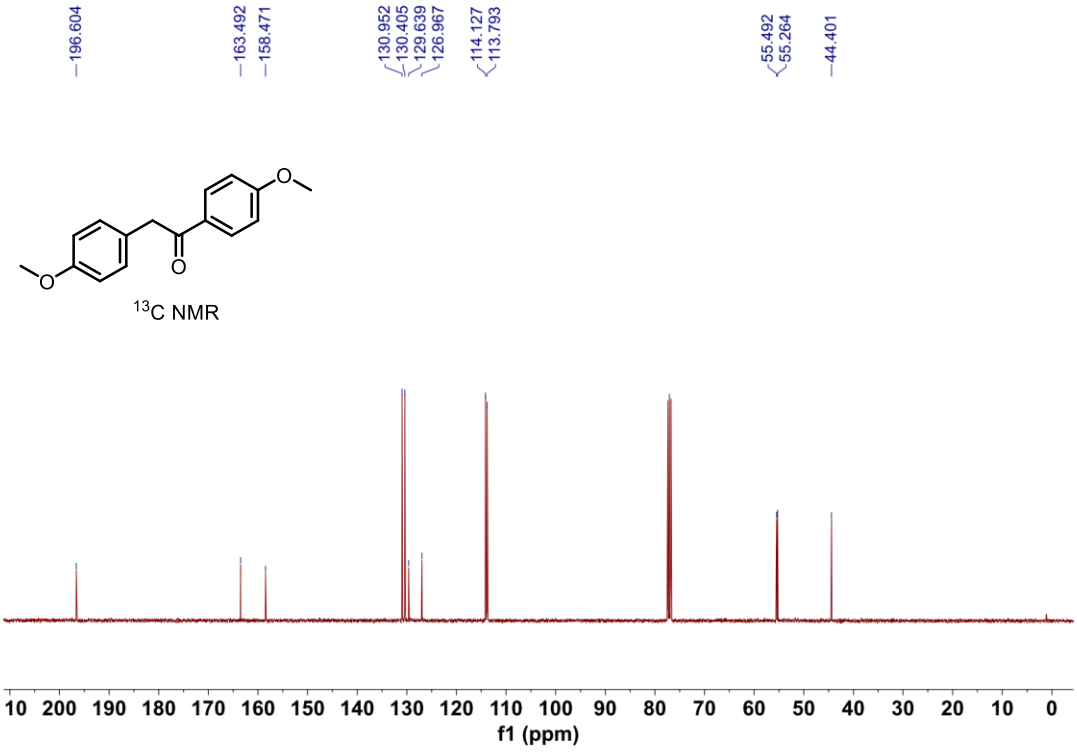
8.031
8.025
8.019
8.014
8.007
8.003
7.235
7.228
7.223
7.211
7.206
7.198
6.975
6.968
6.963
6.951
6.946
6.938
6.911
6.904
6.898
6.887
6.882
6.874
4.206
3.887
3.811
O
O
O
1H NMR
2.00
2.00
2.01
2.01
2.01
3.03
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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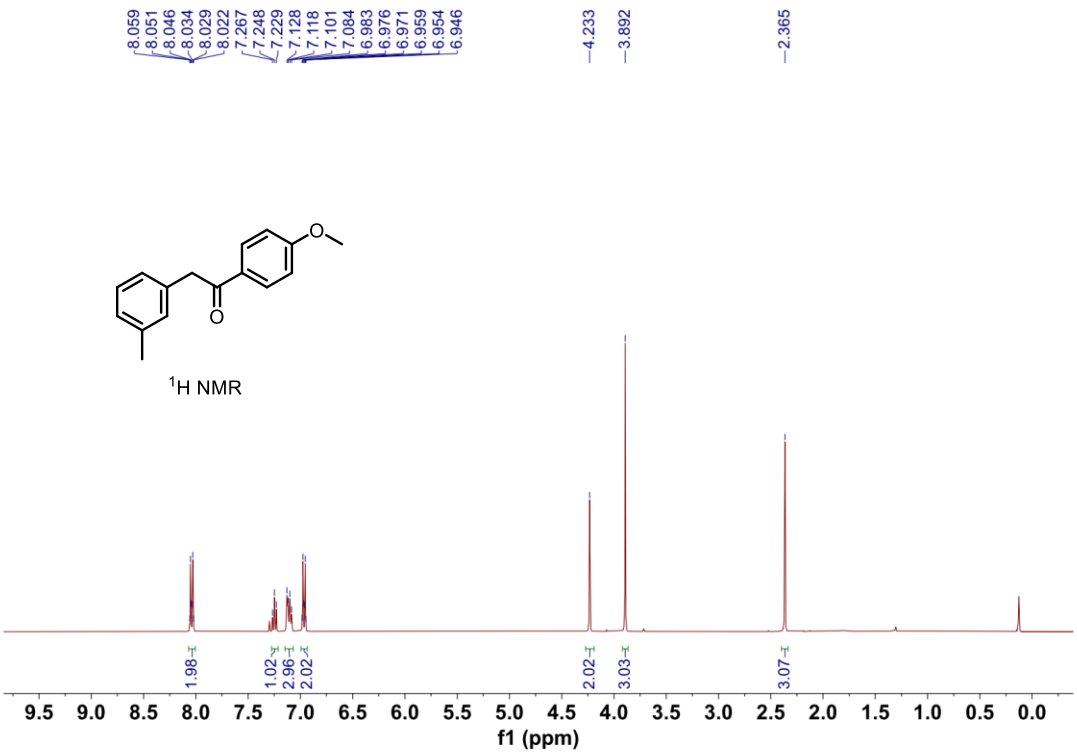
130.405
129.639
126.967
114.127
113.793
55.492
55.264
44.401
O
O
O
13C NMR
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.051
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8.029
8.022
7.267
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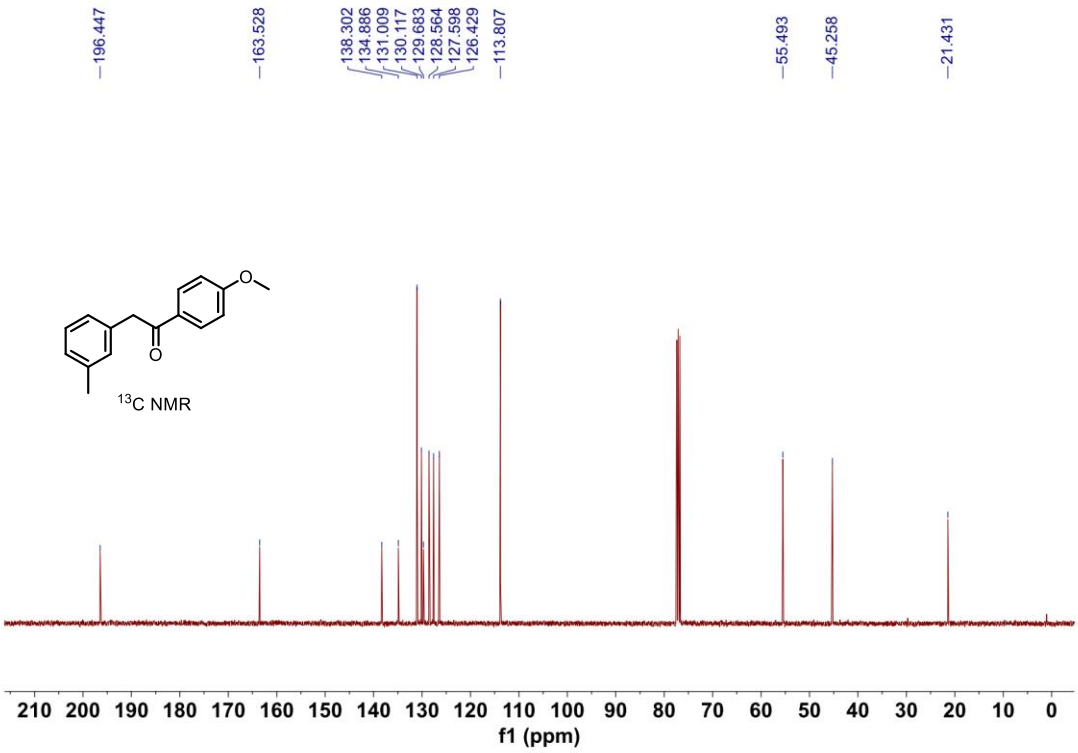
7.128
7.118
7.101
7.084
6.983
6.976
6.971
6.959
6.954
6.946
4.233
3.892
2.365
O
O
1H NMR
1.98
1.02
2.96
2.02
2.02
3.03
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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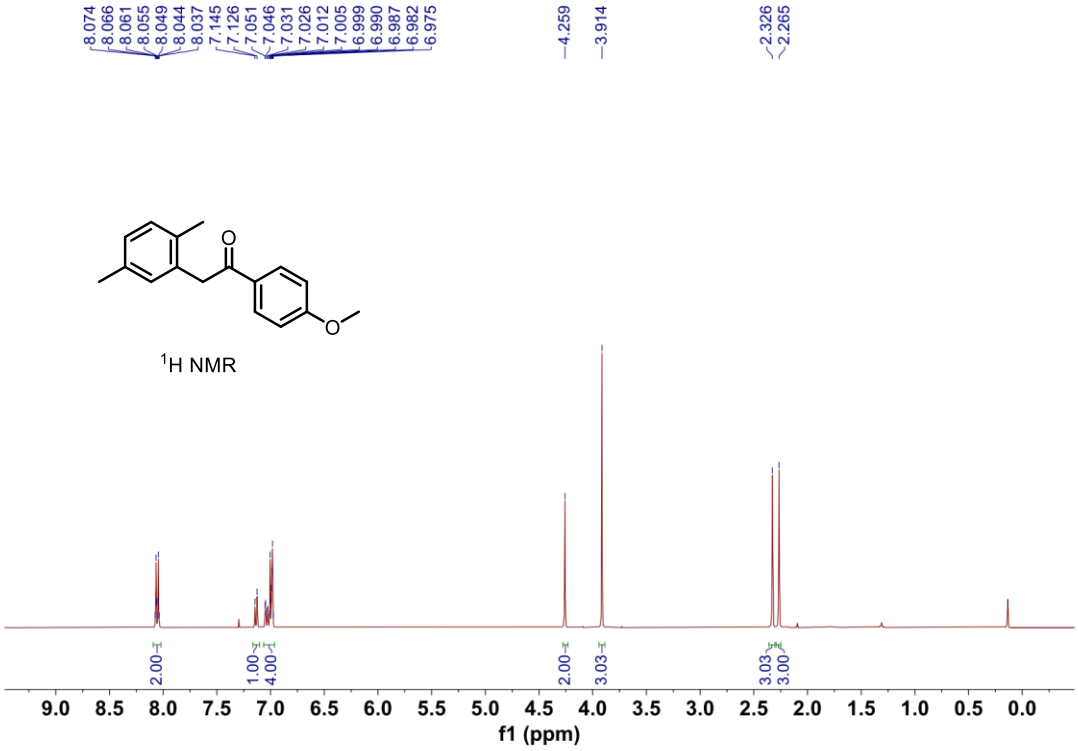
134.886
131.009
130.117
129.683
128.564
127.598
126.429
113.807
55.493
45.258
21.431
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.066
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8.055
8.049
8.044
8.037
7.145
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7.051
7.046
7.031
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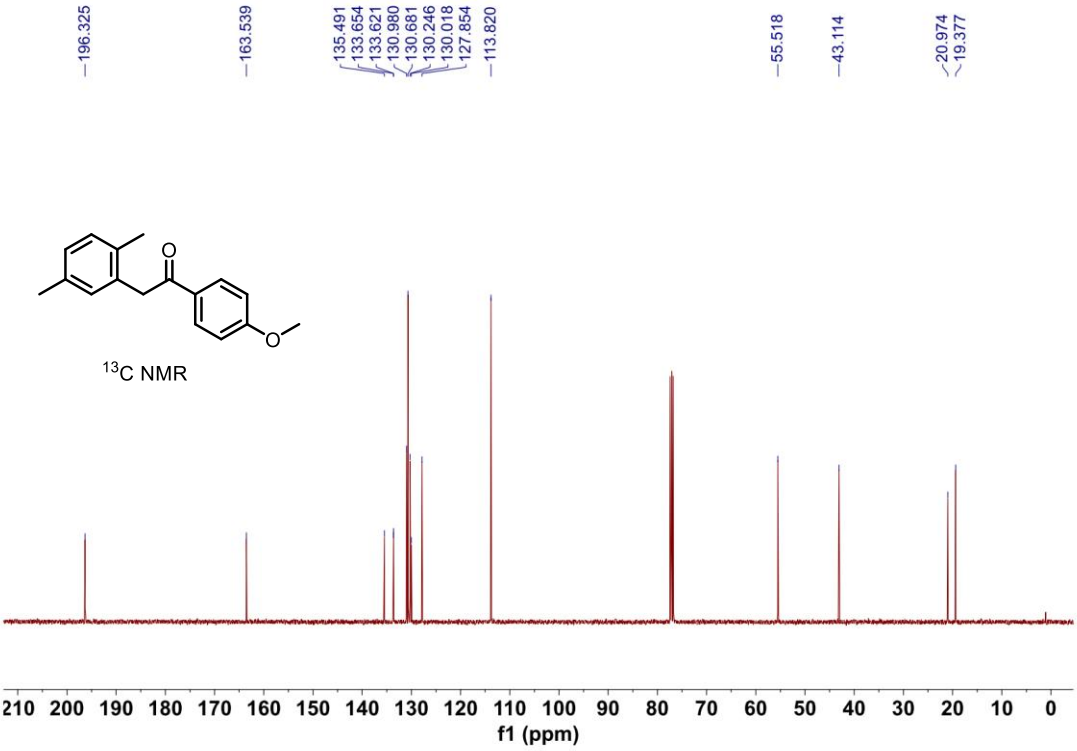
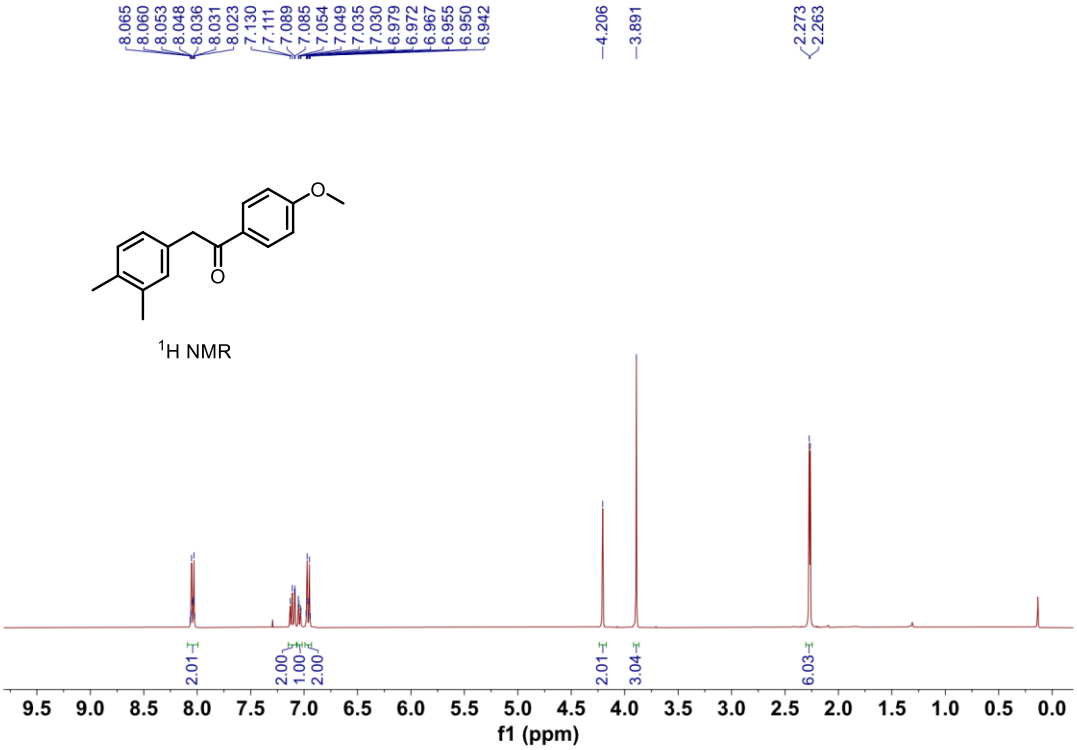
7.012
7.005
6.999
6.990
6.987
6.982
6.975
4.259
3.914
2.326
2.265
O
O
1H NMR
2.00
1.00
4.00
2.00
3.03
3.03
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


196.325
163.539
135.491
133.654
133.621
130.980
130.681
130.246
130.018
127.854
113.820
55.518
43.114
20.974
19.377
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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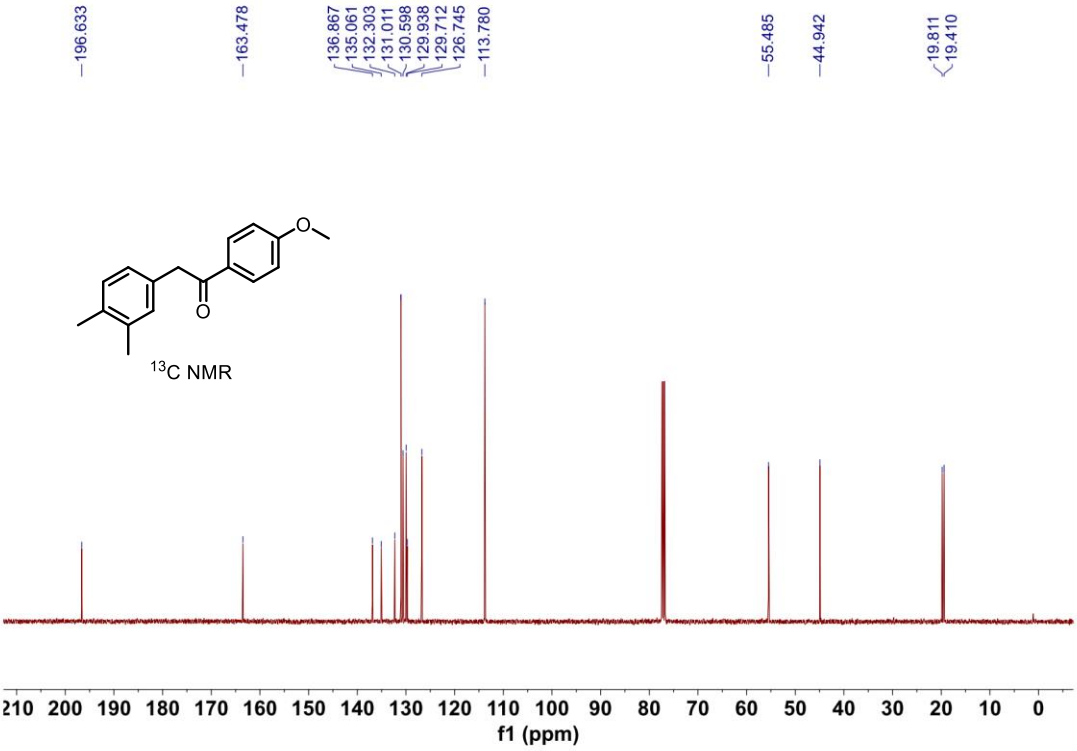
8.060
8.053
8.048
8.036
8.031
8.023
7.130
7.111
7.089
7.085
7.054
7.049
7.035
7.030
6.979
6.972
6.967
6.955
6.950
6.942
4.206
3.891
2.273
2.263
O
O
1H NMR
2.01
2.00
1.00
2.00
2.01
3.04
6.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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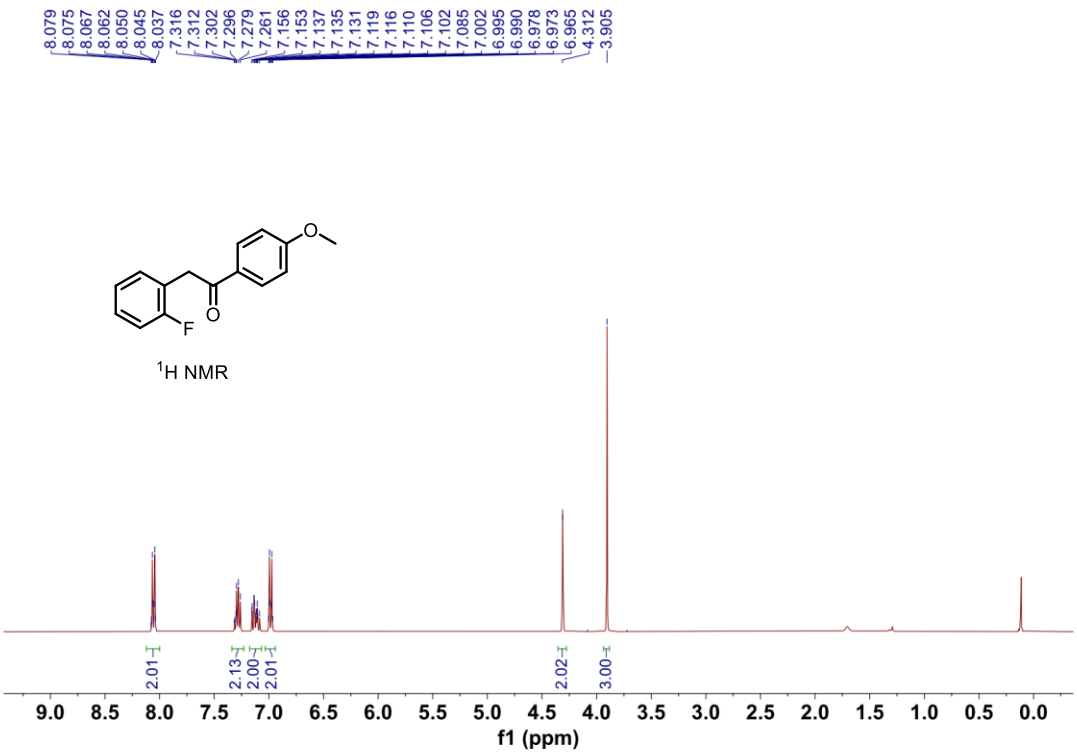
163.478
136.867
135.061
132.303
131.011
130.598
129.938
129.712
126.745
113.780
55.485
44.942
19.811
19.410
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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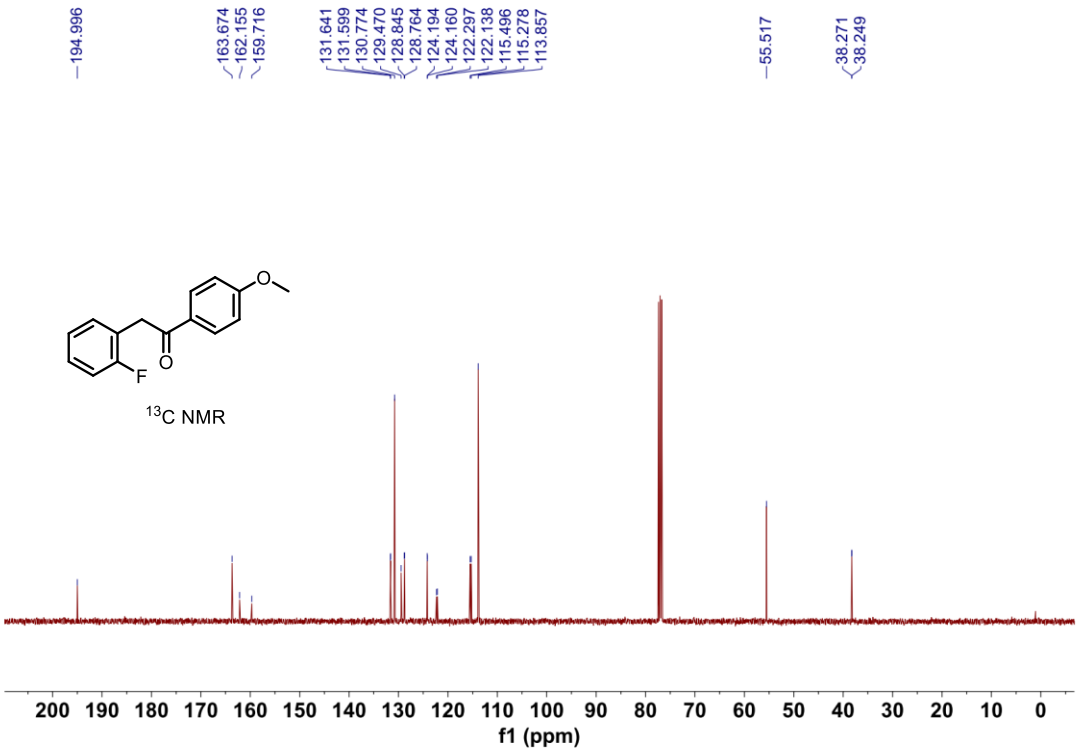
8.075
8.067
8.062
8.050
8.045
8.037
7.316
7.312
7.302
7.296
7.279
7.261
7.156
7.153
7.137
7.135
7.131
7.119
7.116
7.110
7.106
7.102
7.085
7.002
6.995
6.990
6.978
6.973
6.965
4.312
3.905
O
O
F
1H NMR
2.01
2.13
2.00
2.01
2.02
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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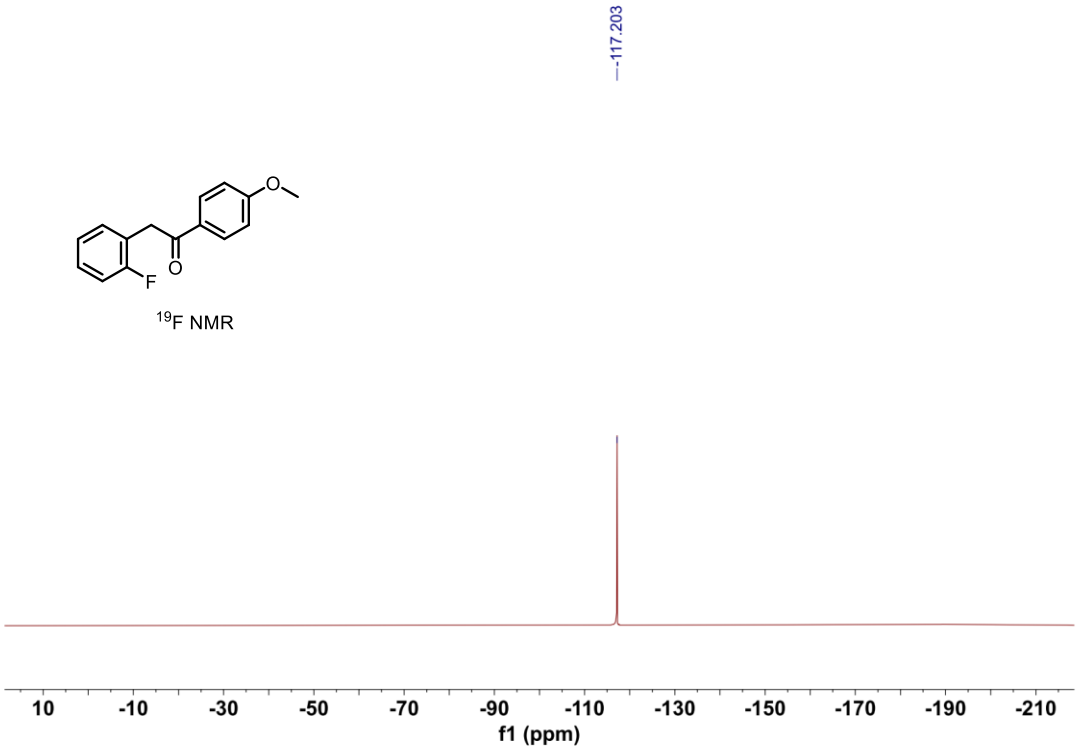
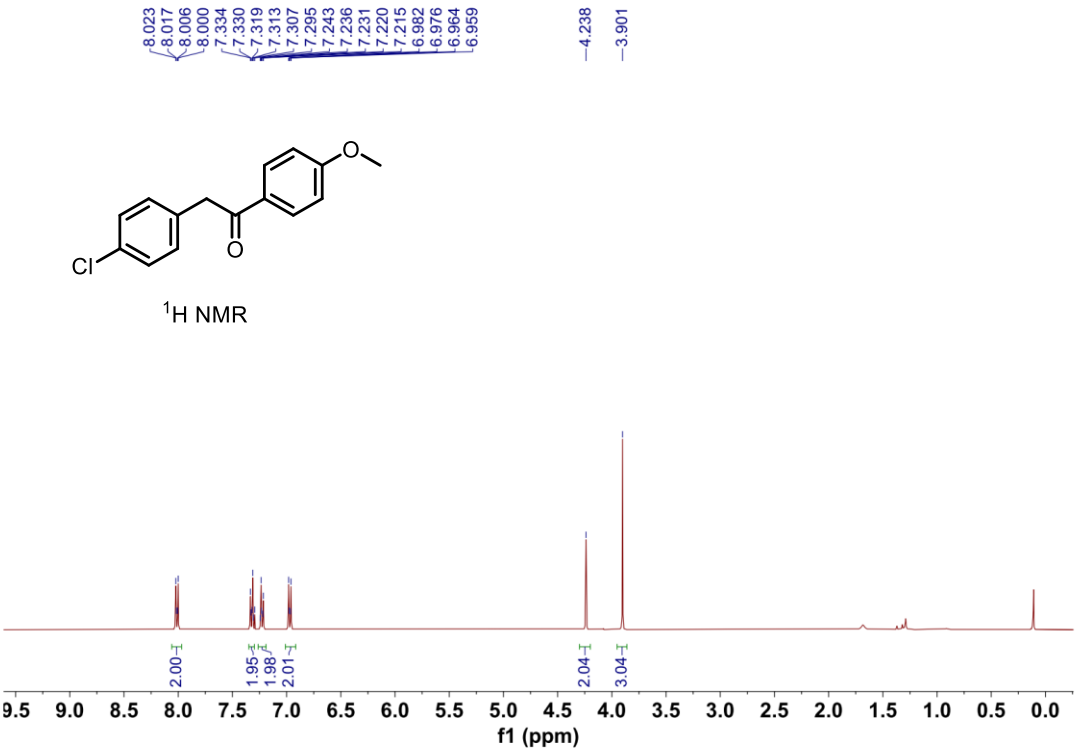
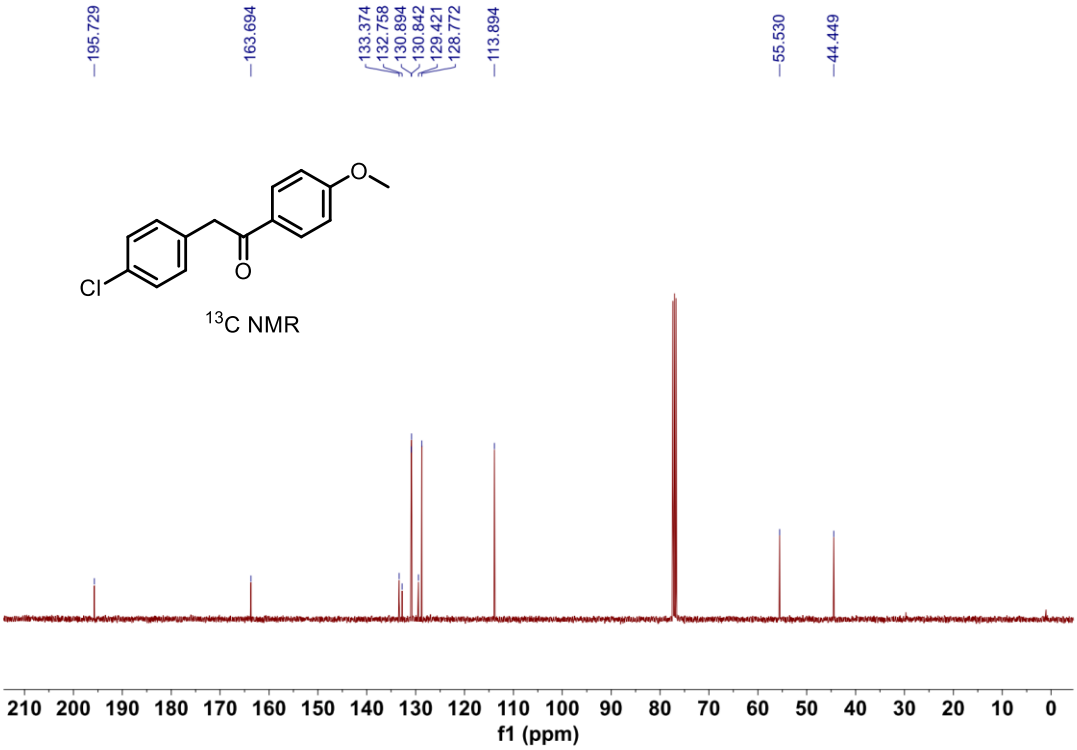
163.674
162.155
159.716
131.641
131.599
130.774
129.470
128.845
128.764
124.194
124.160
122.297
122.138
115.496
115.278
113.857
55.517
38.271
38.249
O
O
F
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

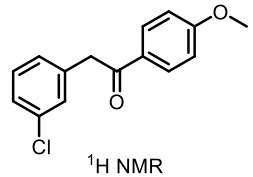

117.203
O
O
F
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)



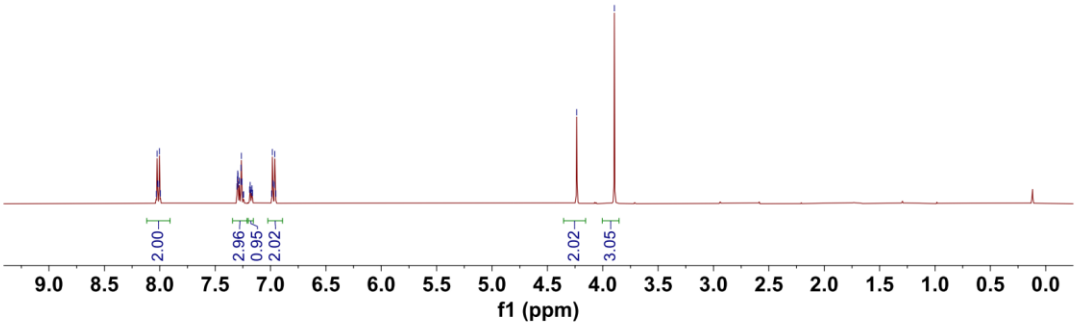
^{1}H NMR

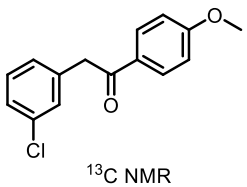


^{13}C NMR

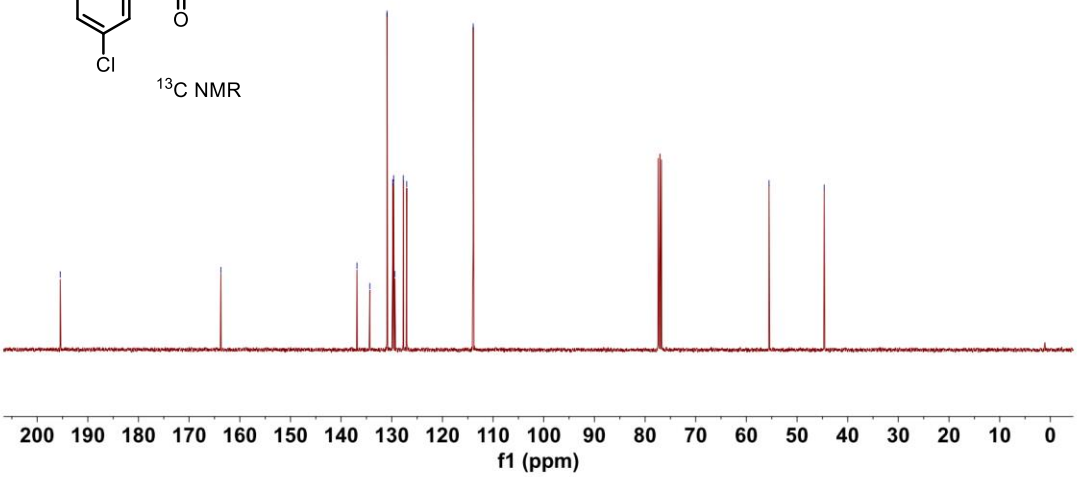


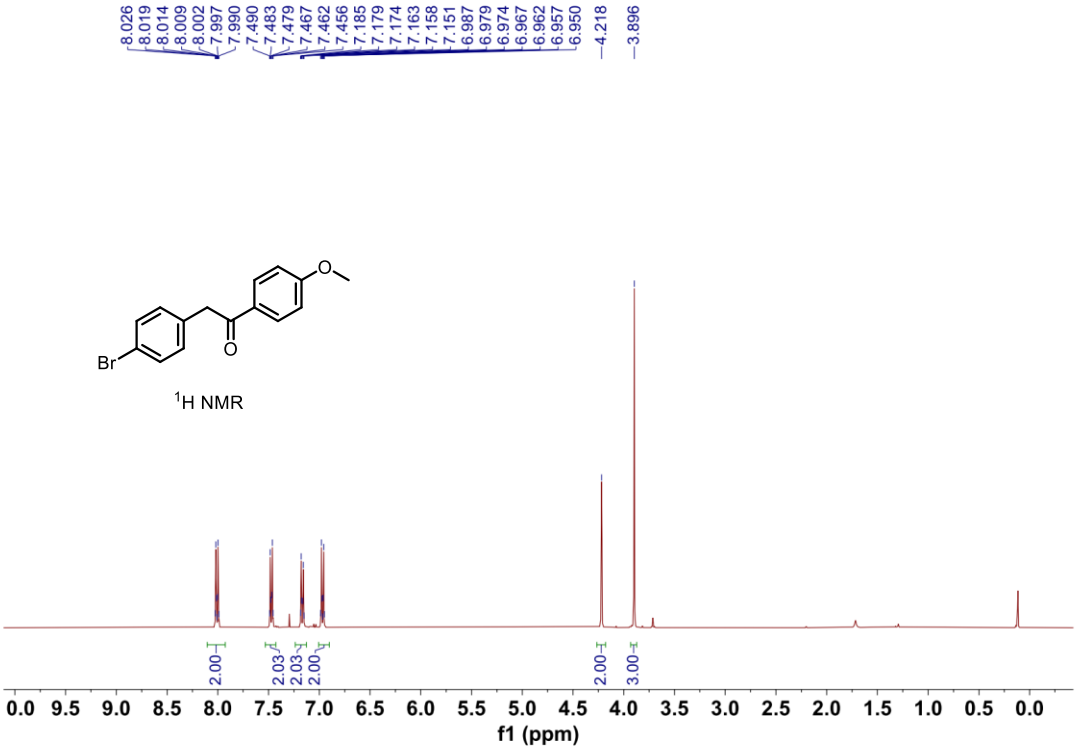
^{1}H NMR





^{13}C NMR

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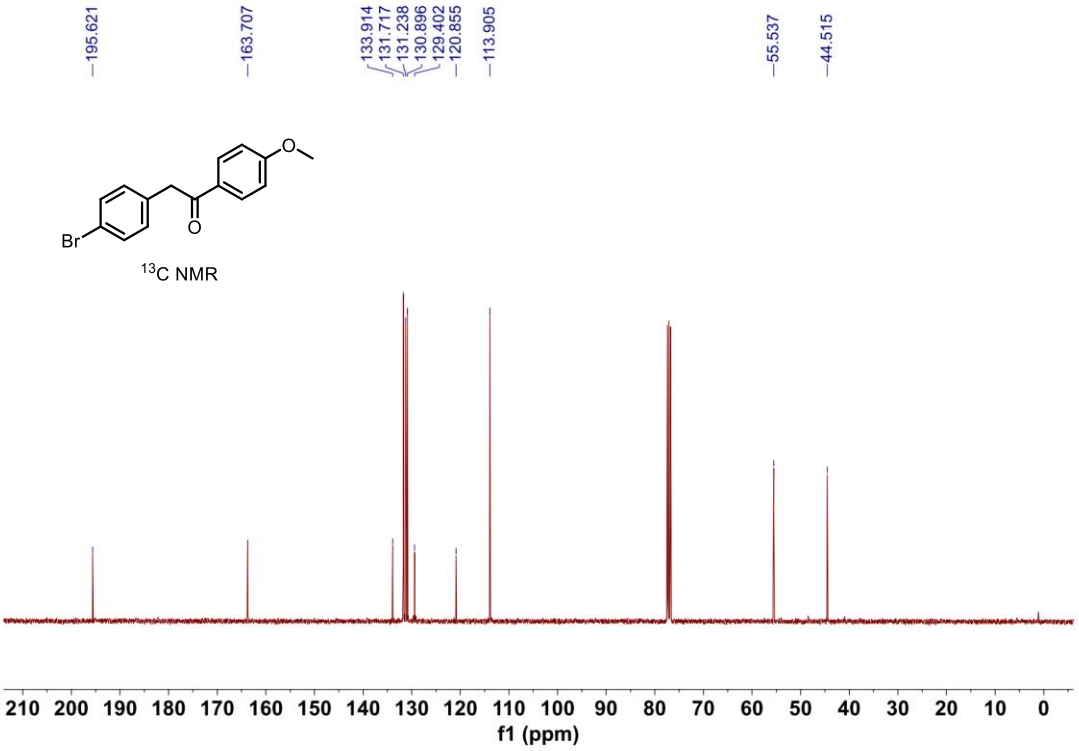
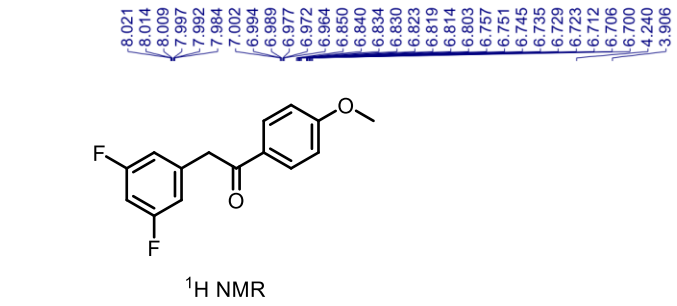
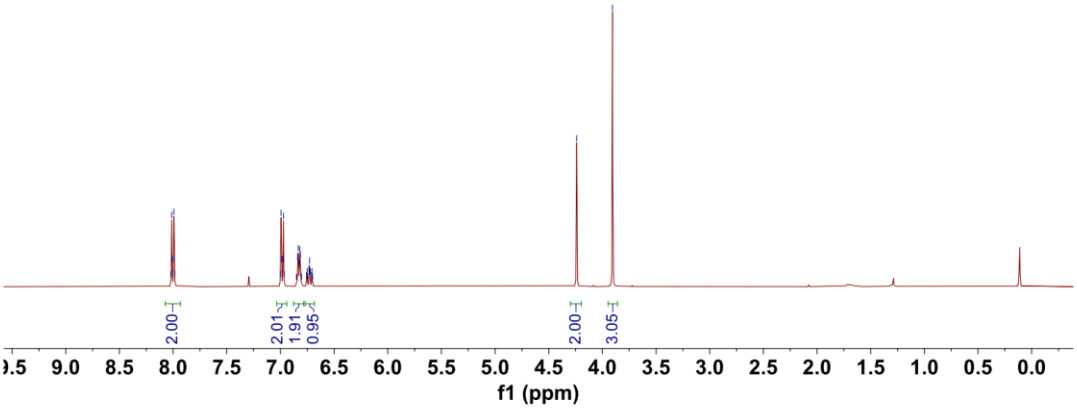
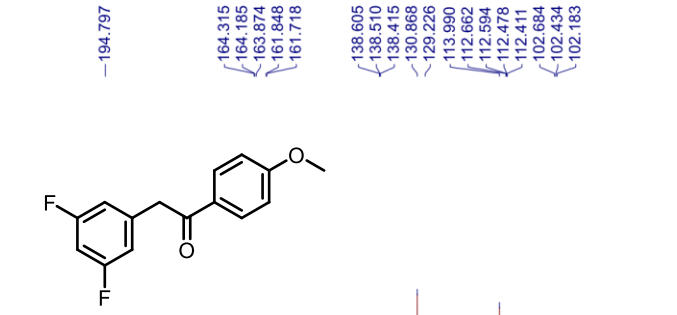
8.019
8.014
8.009
8.002
7.997
7.990
7.490
7.483
7.479
7.467
7.462
7.456
7.185
7.179
7.174
7.163
7.158
7.151
6.987
6.979
6.974
6.967
6.962
6.957
6.950
4.218
3.896
O
Br
1H NMR
2.00
2.03
2.03
2.00
2.00
3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


195.621
163.707
133.914
131.717
131.238
130.896
129.402
120.855
113.905
55.537
44.515
O
Br
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

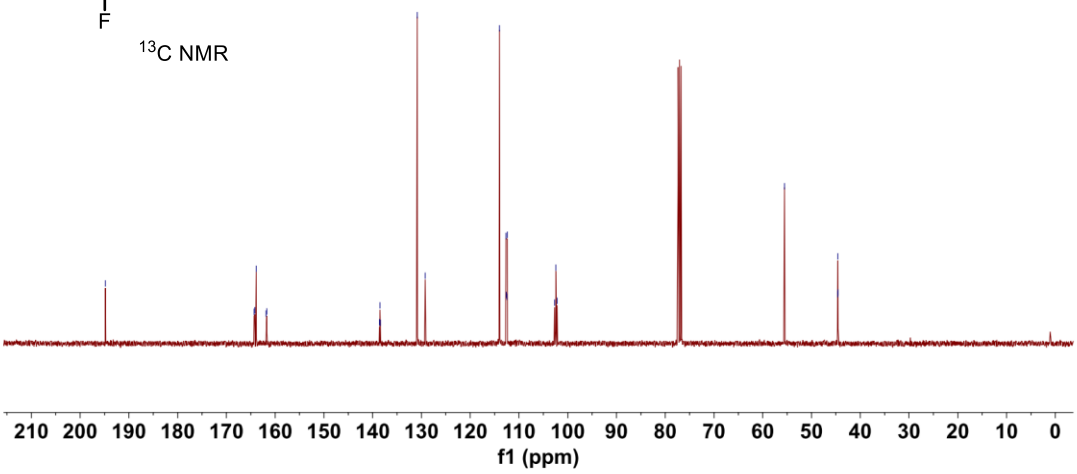


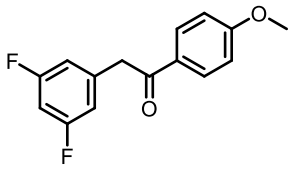
^{1}H NMR



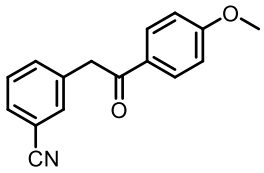


^{13}C NMR

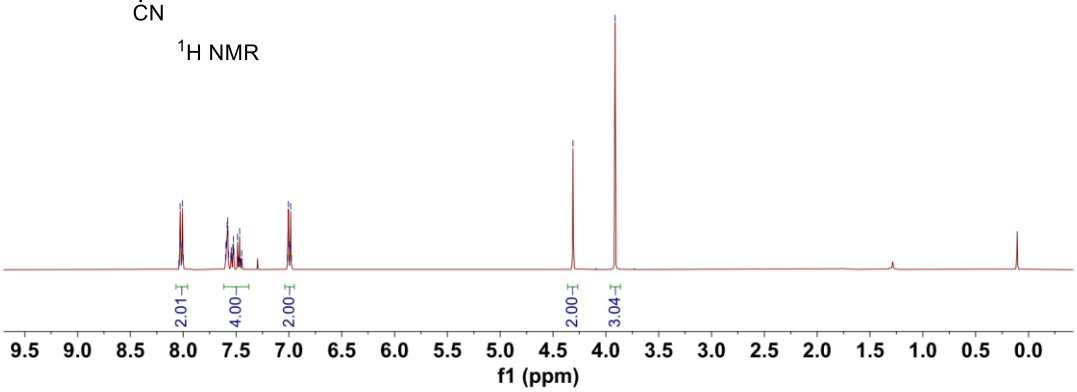


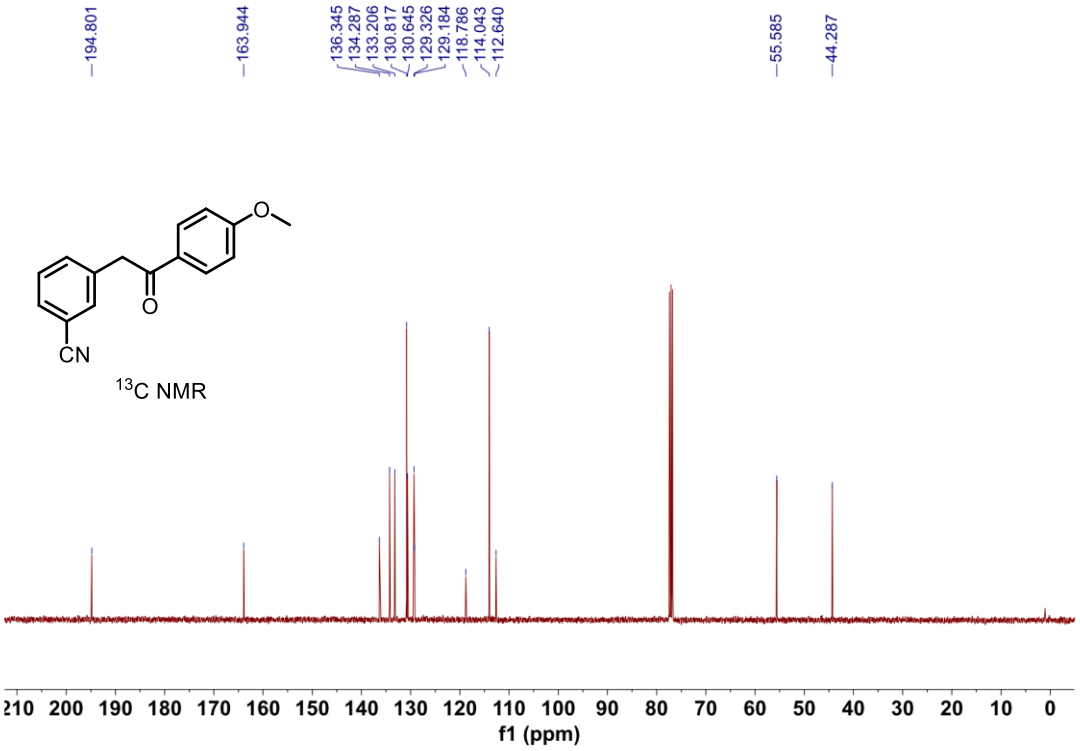


^{19}F NMR



^{1}H NMR

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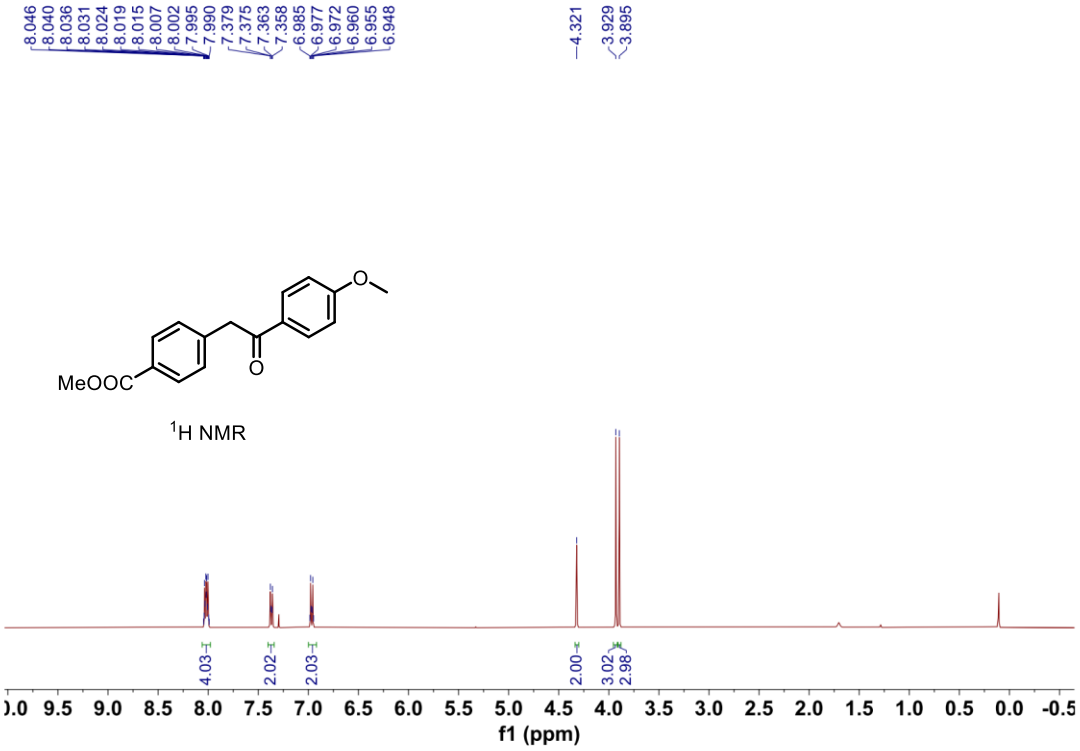
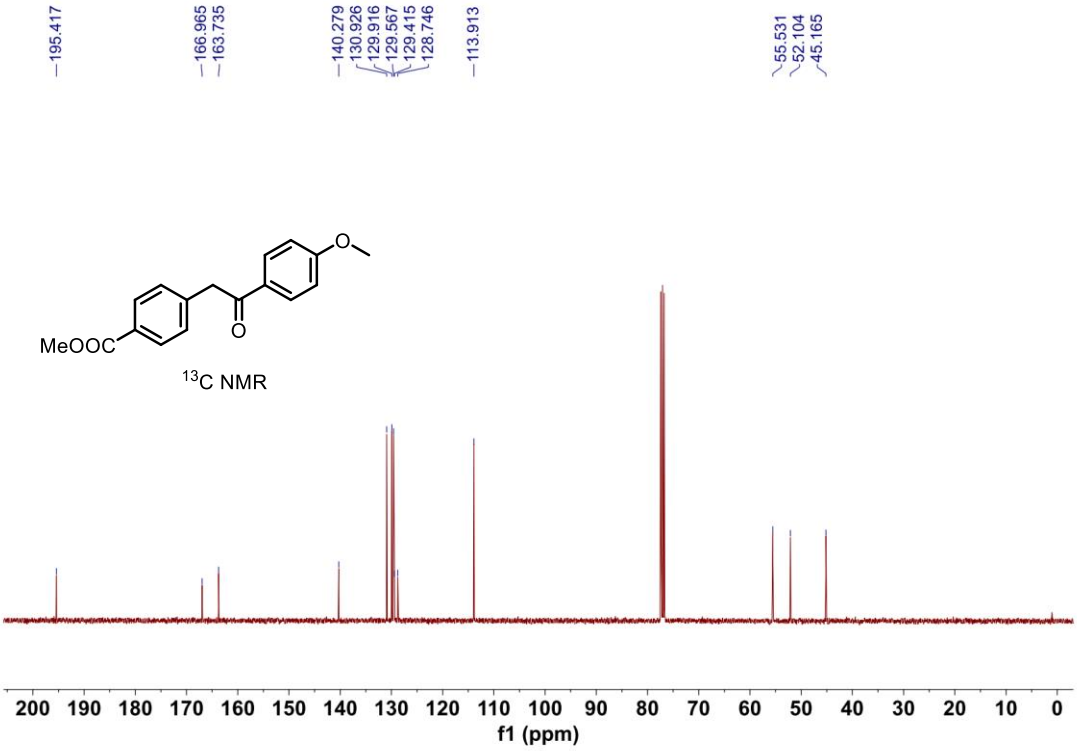
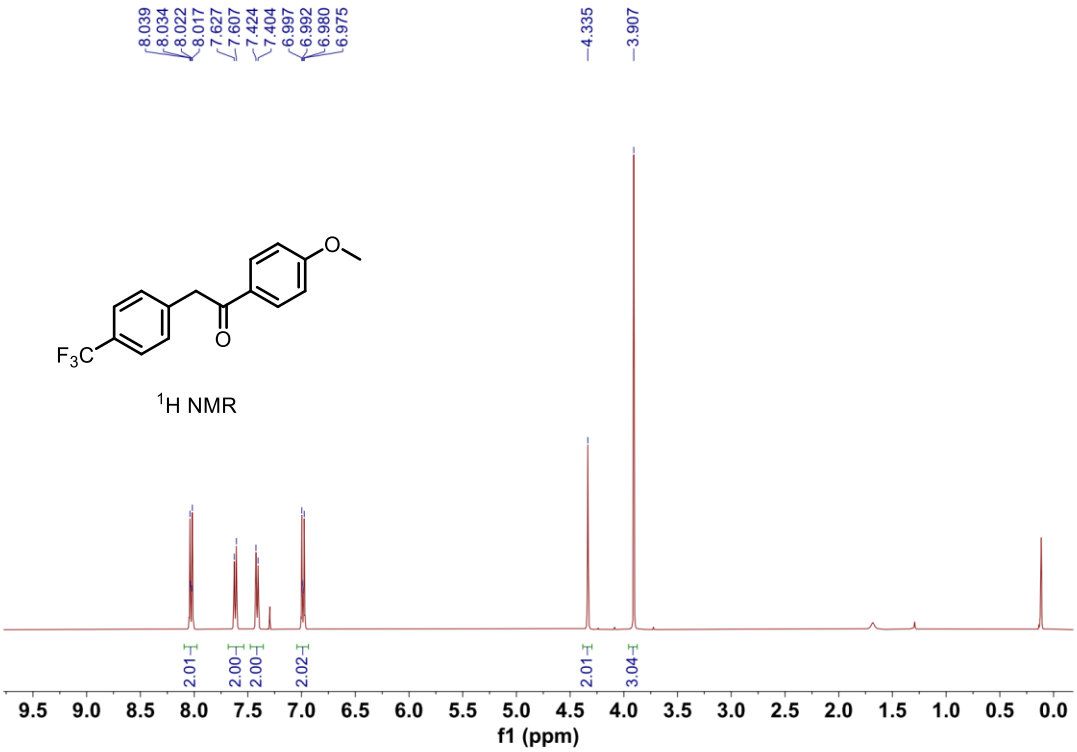
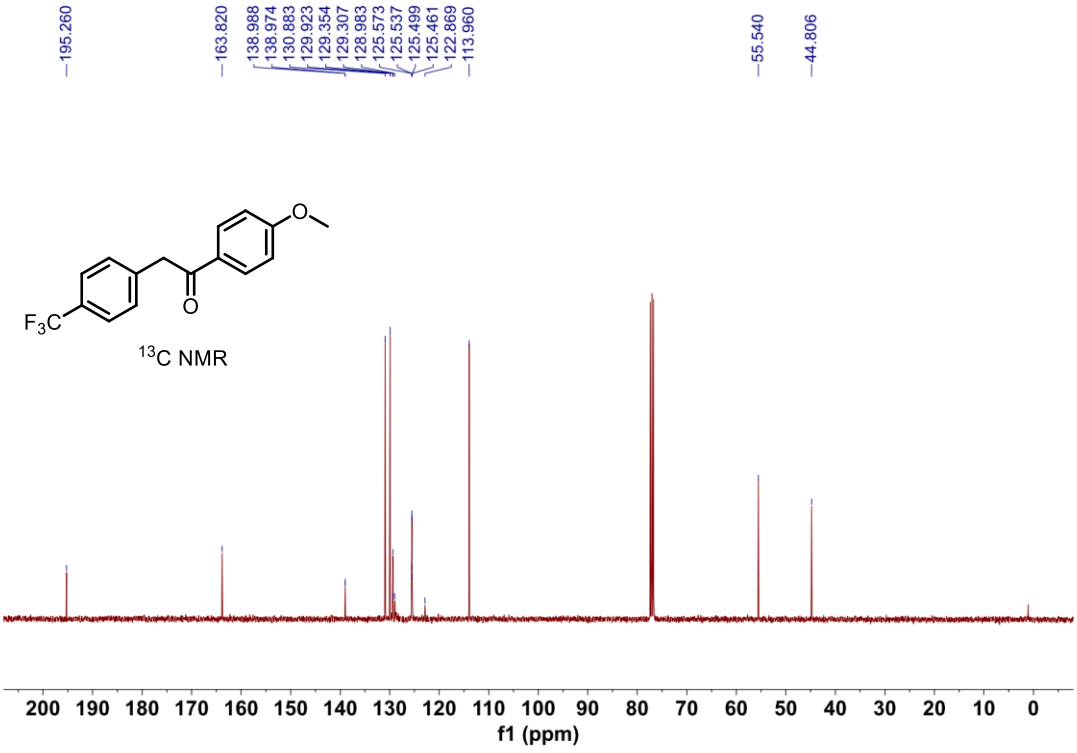
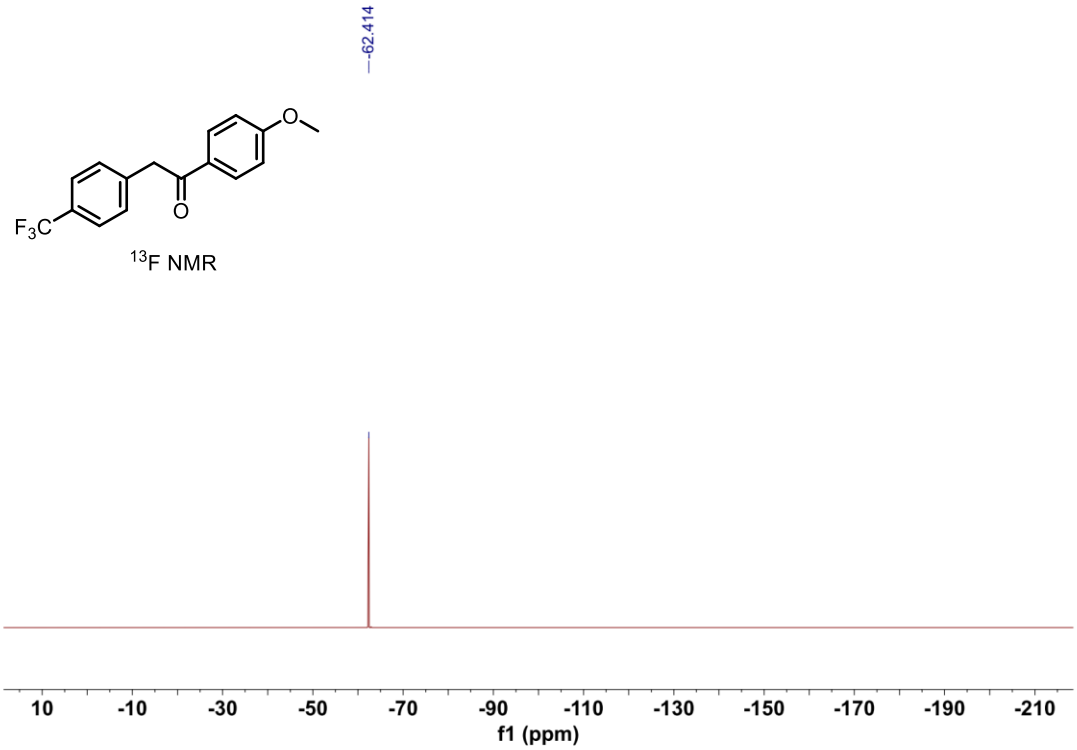
163.944
136.345
134.287
133.206
130.817
130.645
129.326
129.184
118.786
114.043
112.640
55.585
44.287
O
O
CN
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

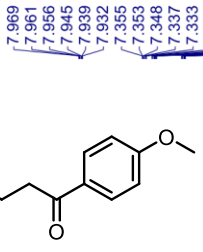

8.046
8.040
8.036
8.031
8.024
8.019
8.015
8.007
8.002
7.995
7.990
7.379
7.375
7.363
7.358
6.985
6.977
6.972
6.960
6.955
6.948
4.321
3.929
3.895
O
O
MeOOC
1H NMR
4.03
2.02
2.03
2.00
3.02
2.98
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


195.417
166.965
163.735
140.279
130.926
129.916
129.567
129.415
128.746
113.913
55.531
52.104
45.165
MeOOC
O
O
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

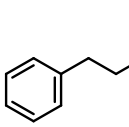

8.039
8.034
8.022
8.017
7.627
7.607
7.424
7.404
6.997
6.992
6.980
6.975
4.335
3.907
F3C
O
O
1H NMR
2.01
2.00
2.00
2.02
2.01
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


195.260
163.820
138.988
138.974
130.883
129.923
129.354
129.307
128.983
125.573
125.537
125.499
125.461
122.869
113.960
55.540
44.806
O
O
F3C
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

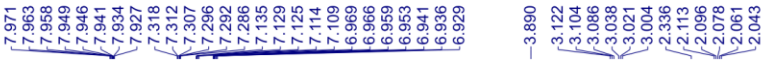

62.414
O
O
F3C
13F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

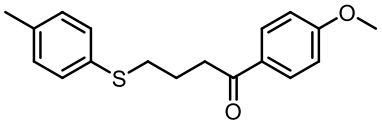


^{1}H NMR

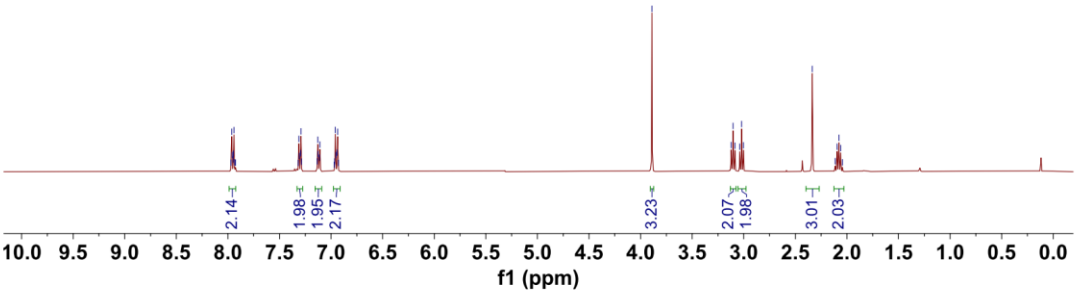


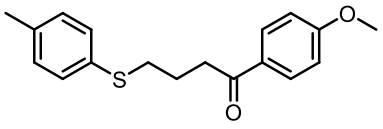
^{13}C NMR



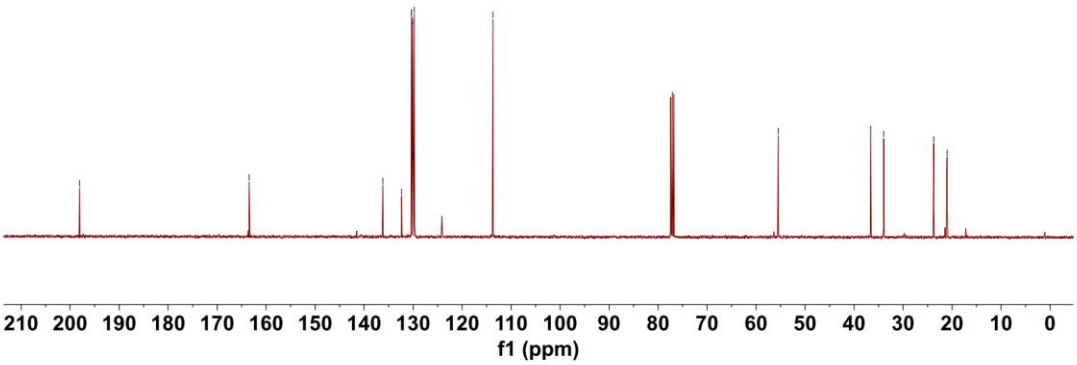


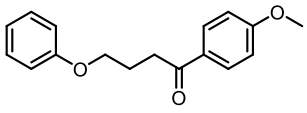
^{1}H NMR



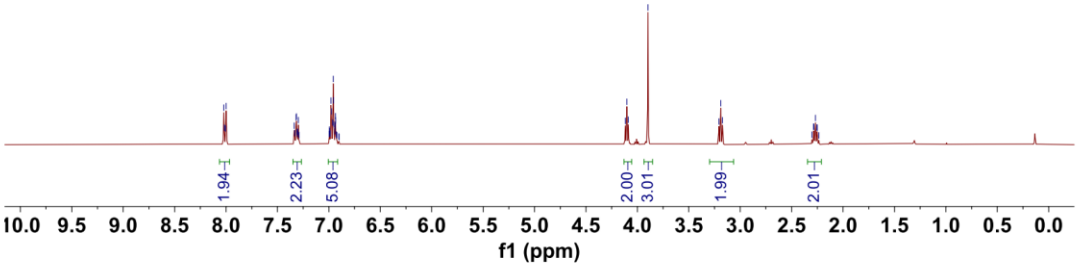


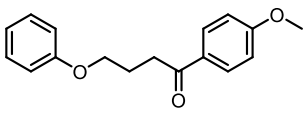
^{13}C NMR



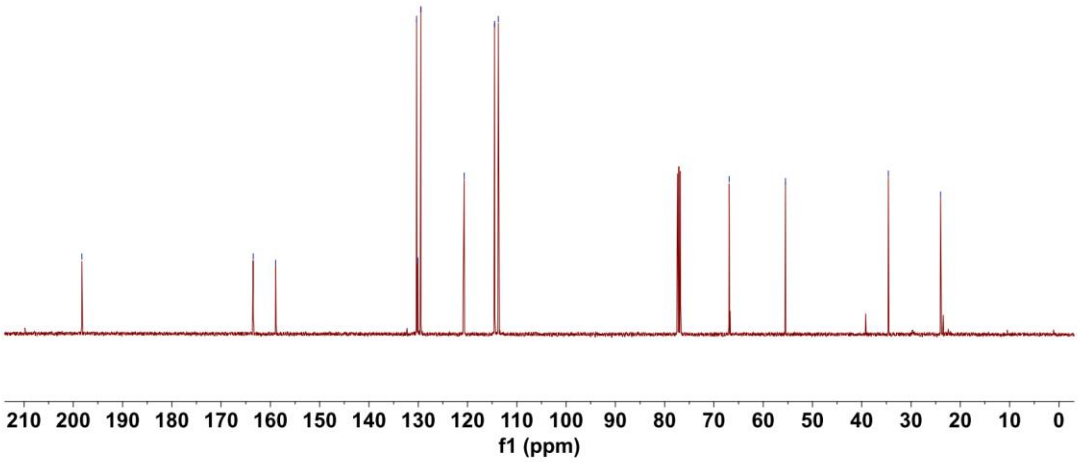


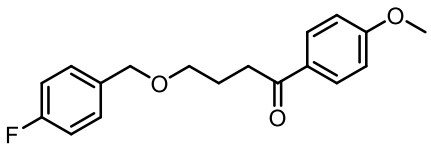
^{1}H NMR



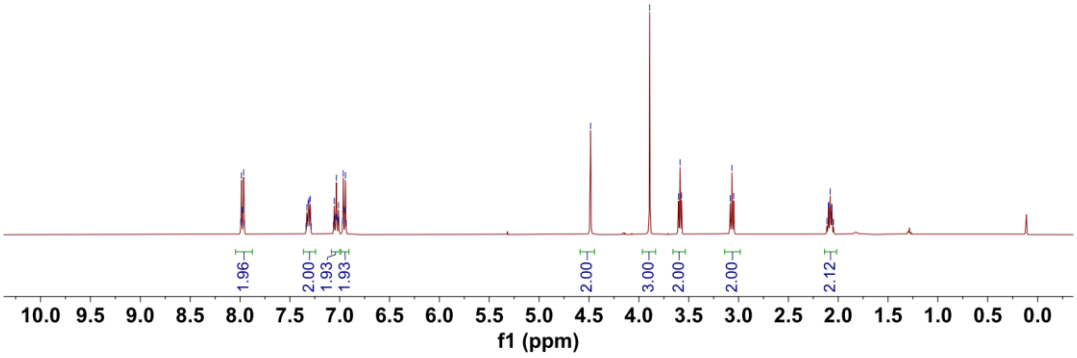


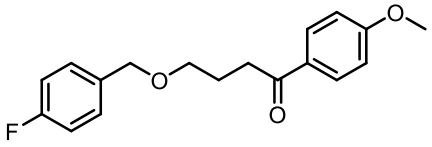
^{13}C NMR



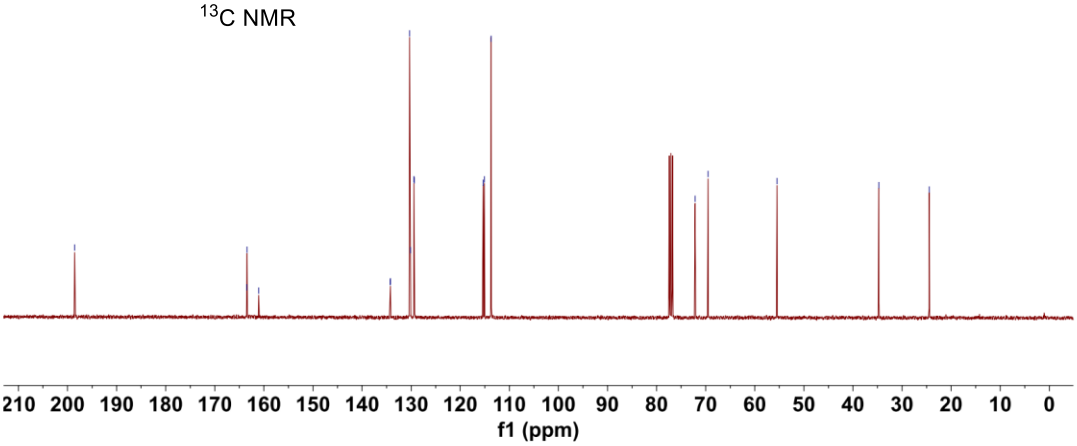


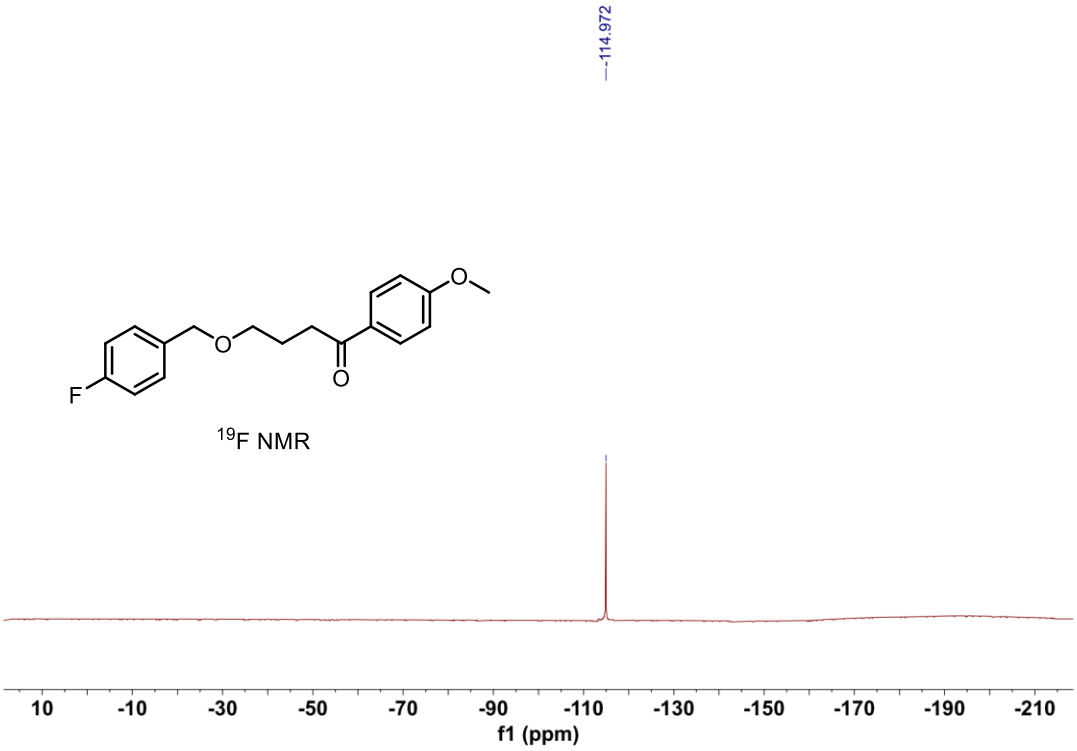
^{1}H NMR

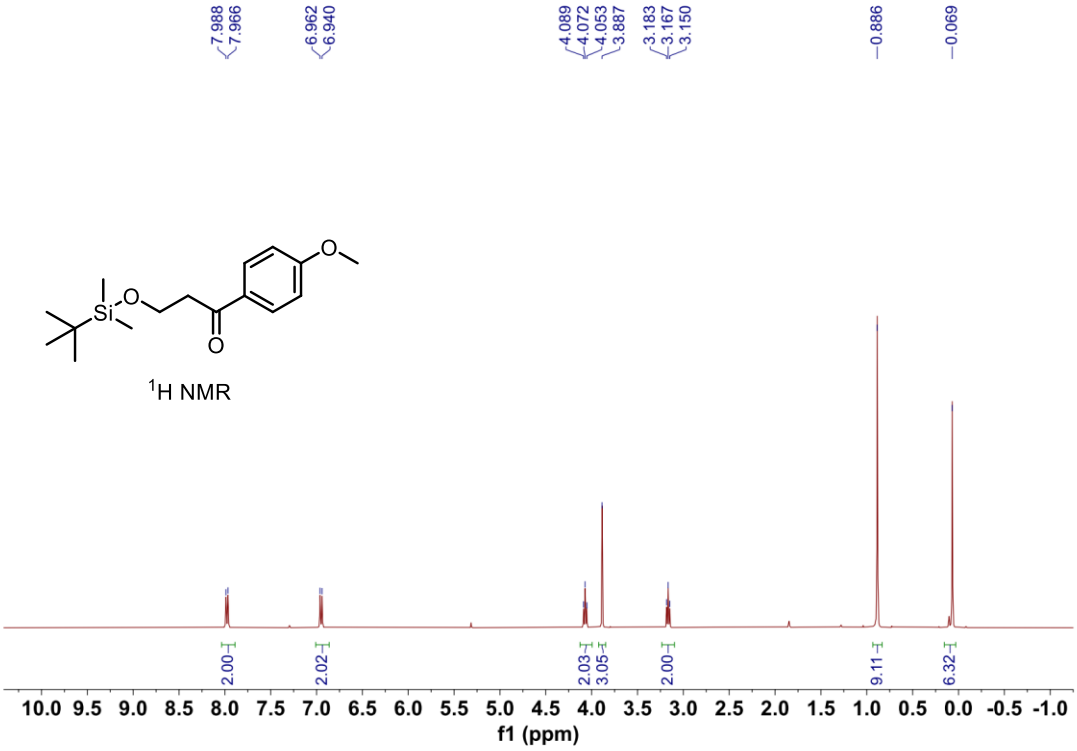


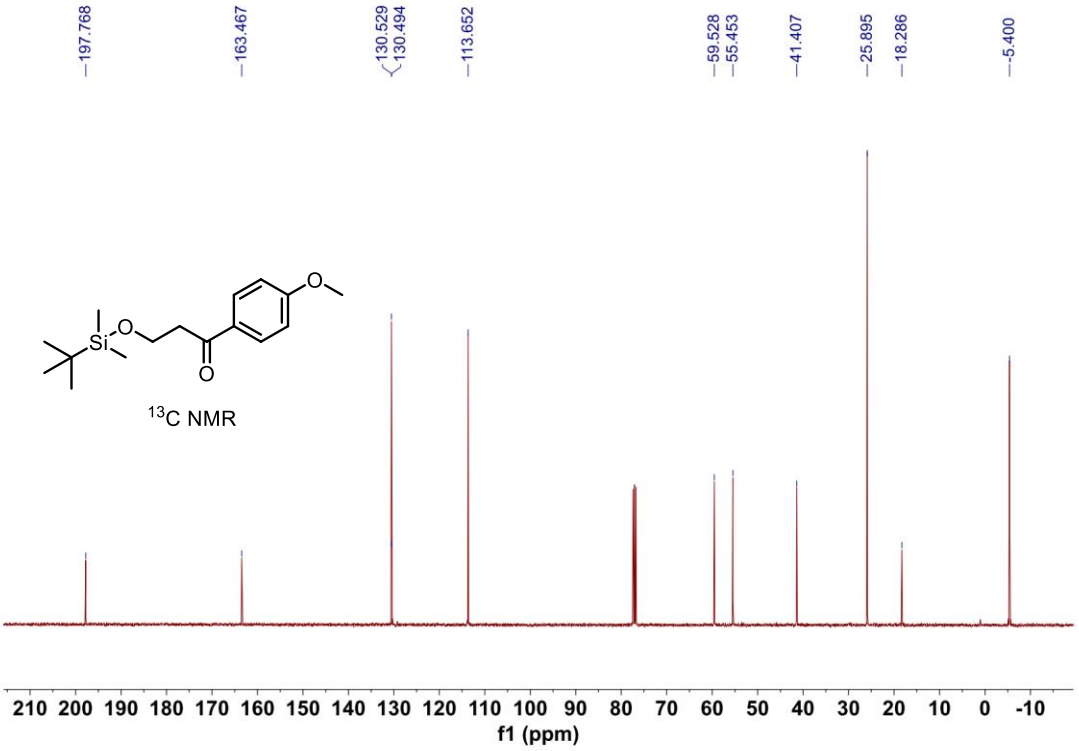


^{13}C NMR




-114.972
O
O
O
F
19F NMR
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


7.988
7.966
6.962
6.940
4.089
4.072
4.053
3.887
3.183
3.167
3.150
0.886
0.069
O
Si
O
O
1H NMR
2.00
2.02
2.03
3.05
2.00
9.11
6.32
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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163.467
130.529
130.494
113.652
59.528
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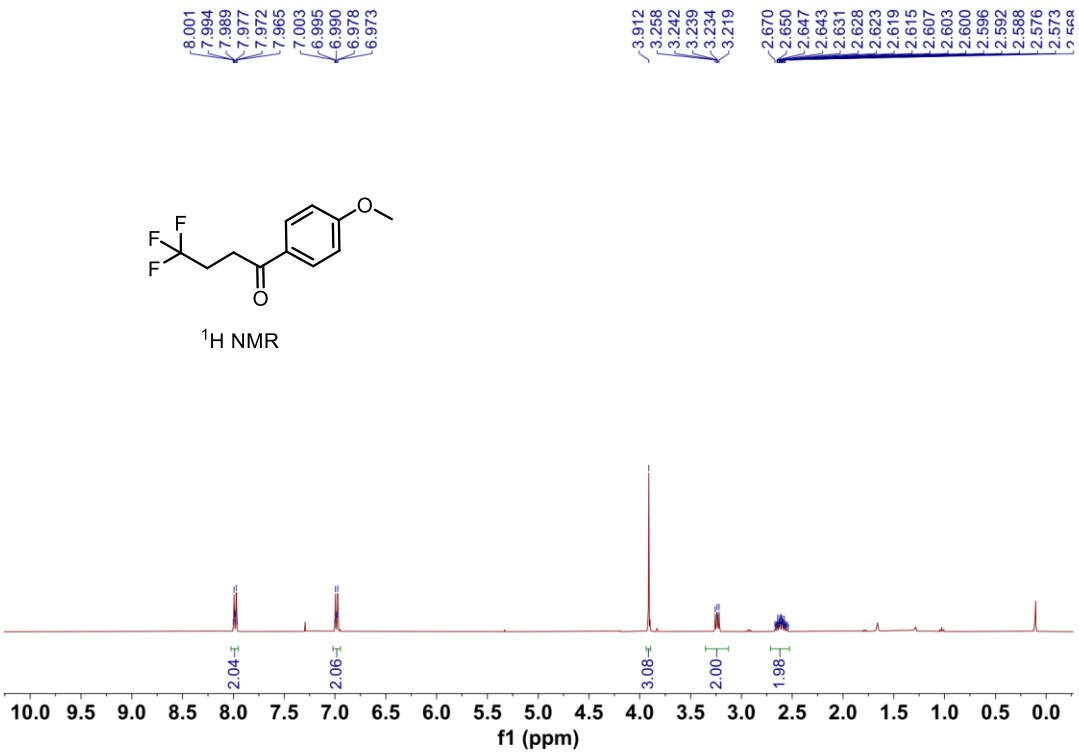
41.407
25.895
18.286
-5.400
Si
O
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.972
7.965
7.003
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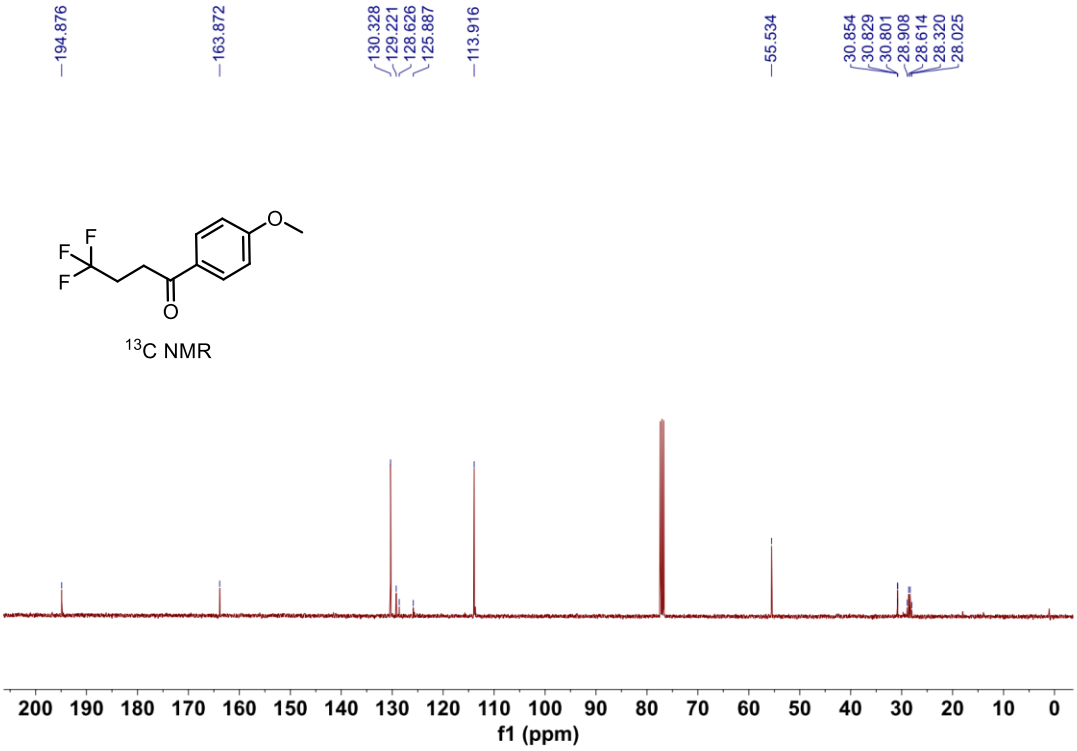
6.978
6.973
3.912
3.258
3.242
3.239
3.234
3.219
2.670
2.650
2.647
2.643
2.631
2.628
2.623
2.619
2.615
2.607
2.603
2.600
2.596
2.592
2.588
2.576
2.573
F
F
F
O
O
1H NMR
2.04
2.06
3.08
2.00
1.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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163.872
130.328
129.221
128.626
125.887
113.916
55.534
30.854
30.829
30.801
28.908
28.614
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F
F
O
O
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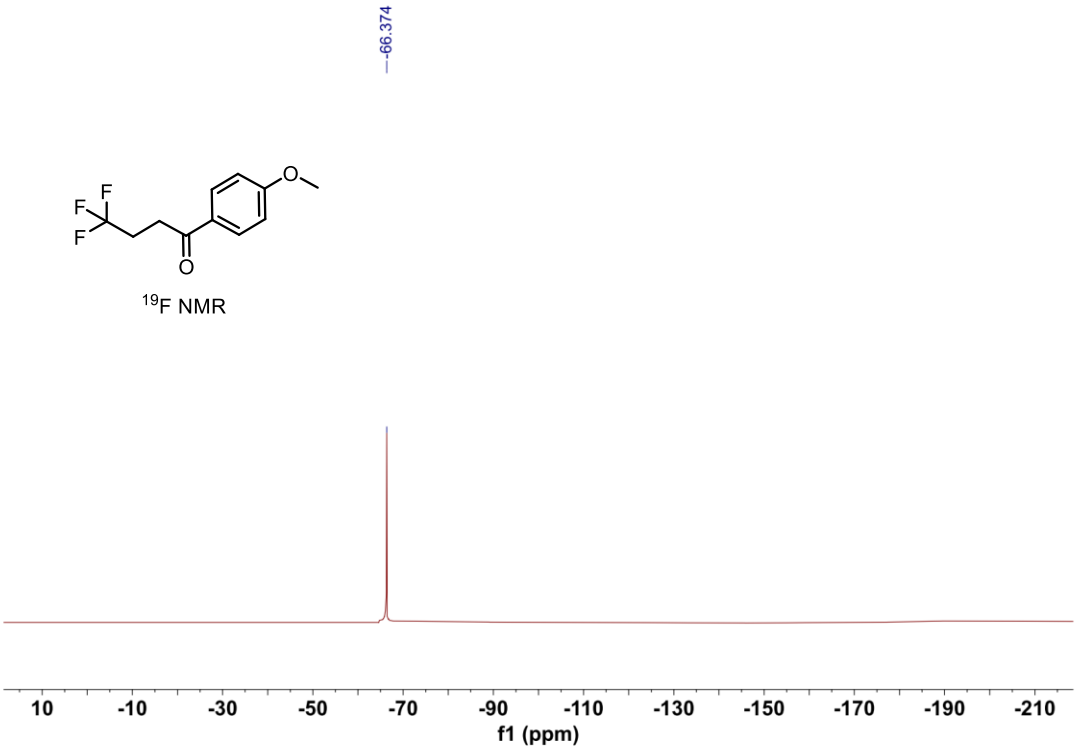
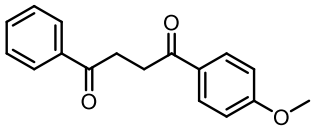
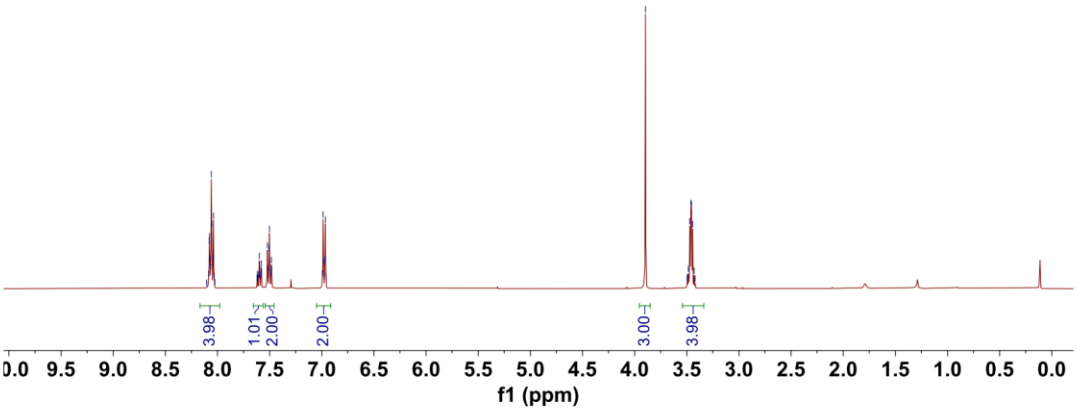
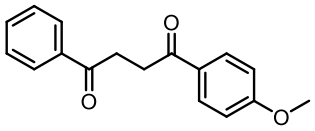
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


66.374
F
F
F
O
O
19F NMR
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

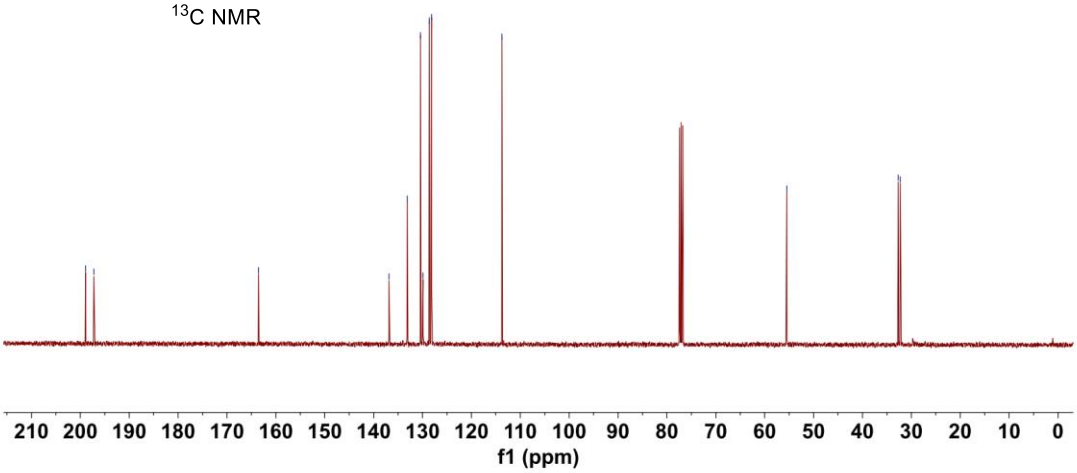


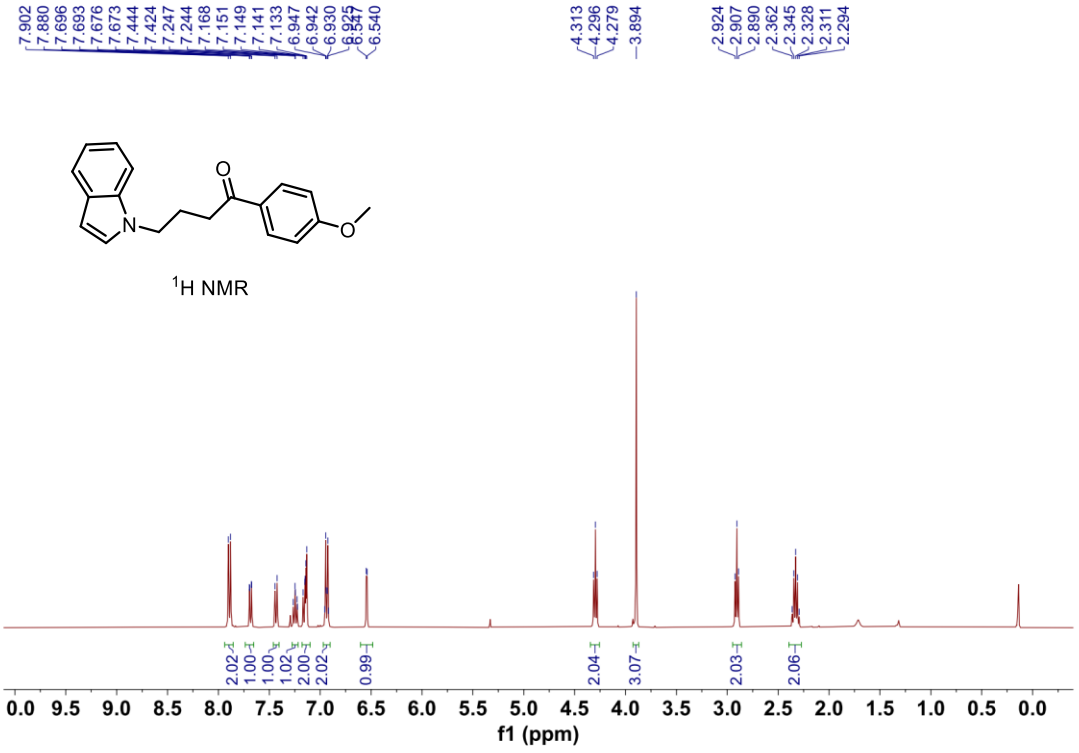
^{1}H NMR





^{13}C NMR

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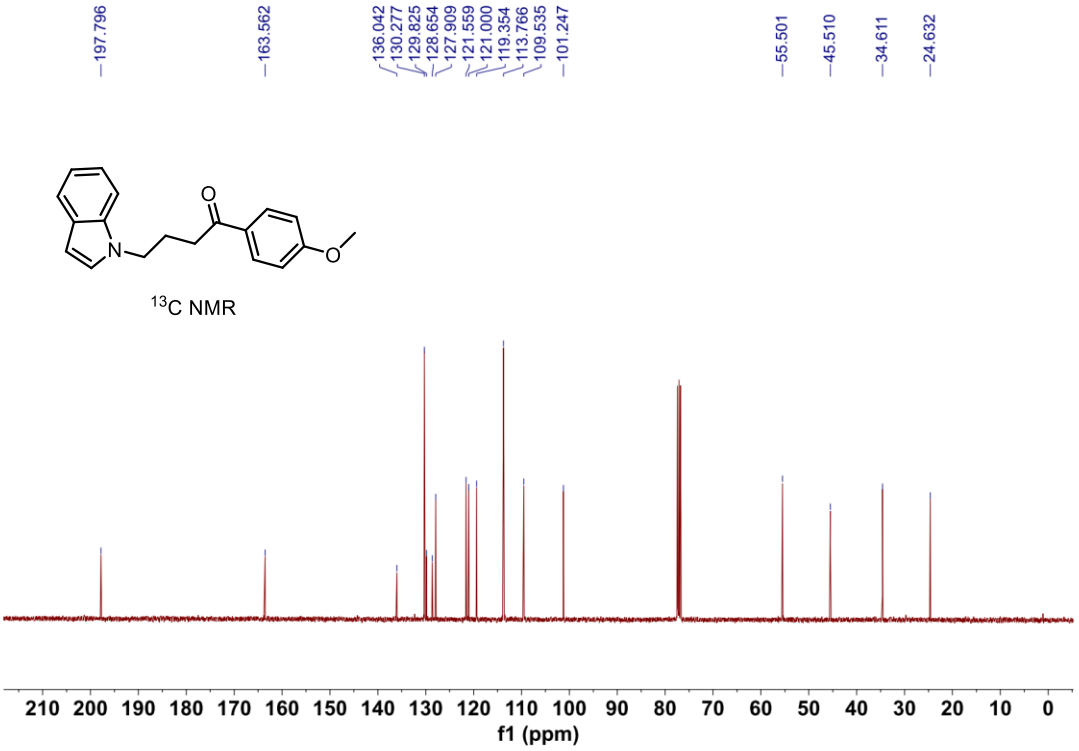
7.696
7.693
7.676
7.673
7.444
7.424
7.247
7.244
7.168
7.151
7.149
7.141
7.133
6.947
6.942
6.930
6.540
4.313
4.296
4.279
3.894
2.924
2.907
2.890
2.362
2.345
2.328
2.311
2.294
O
N
O
1H NMR
2.02
1.00
1.00
1.02
2.00
2.02
0.99
2.04
3.07
2.03
2.06
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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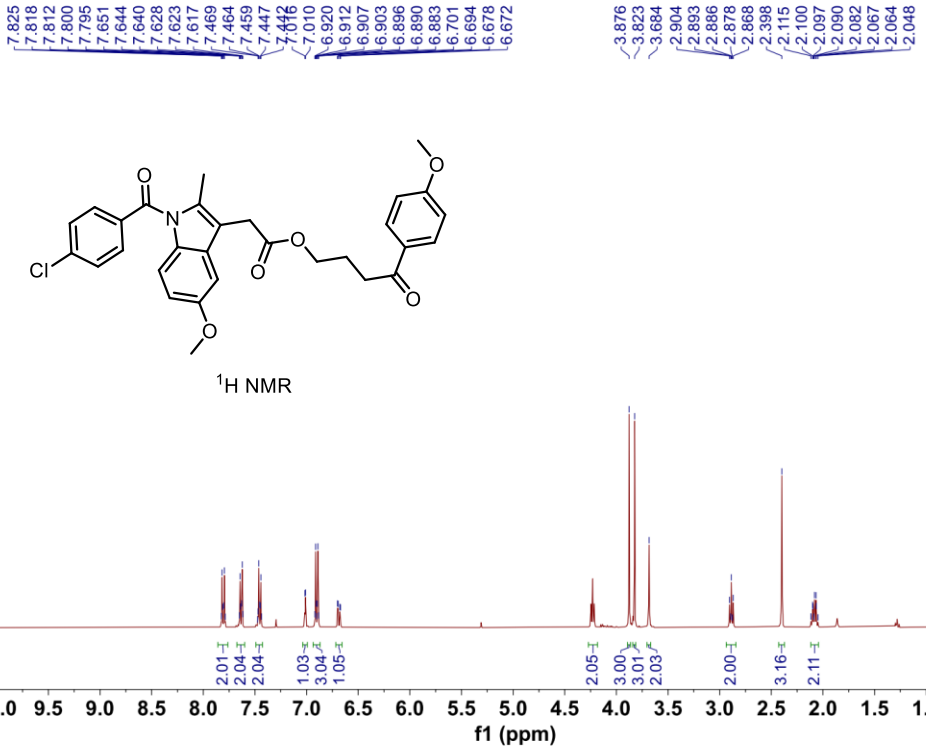
163.562
136.042
130.277
129.825
128.654
127.909
121.559
121.000
119.354
113.766
109.535
101.247
55.501
45.510
34.611
24.632
O
N
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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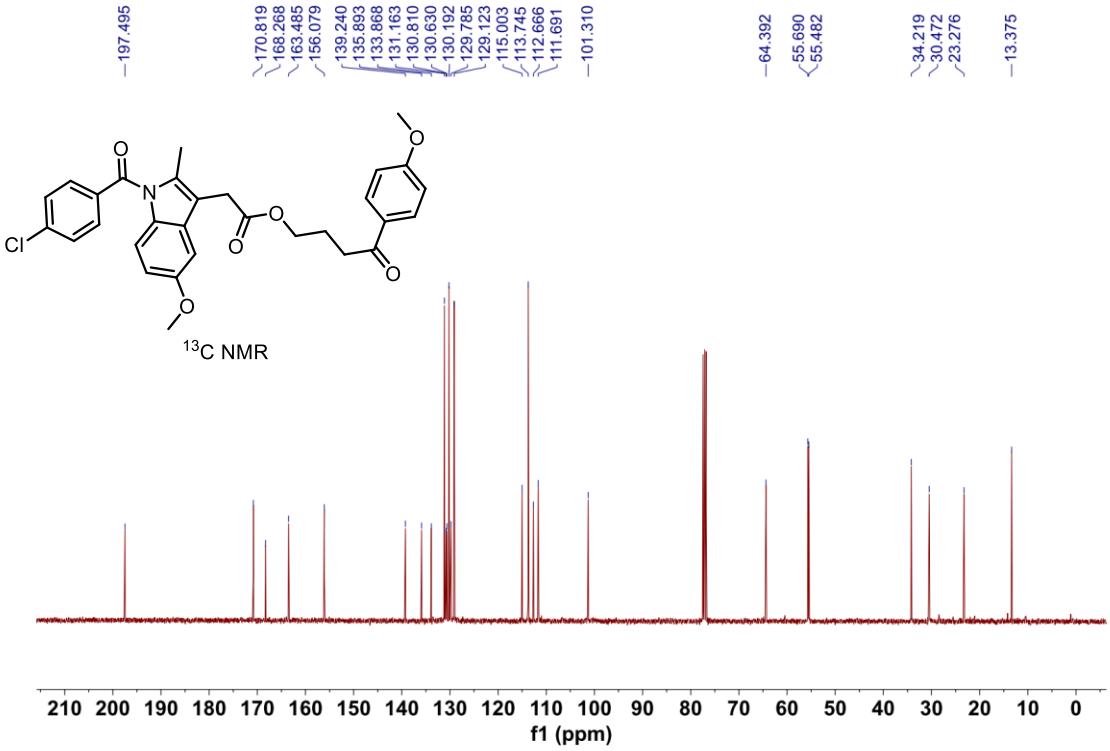
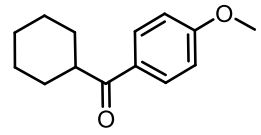
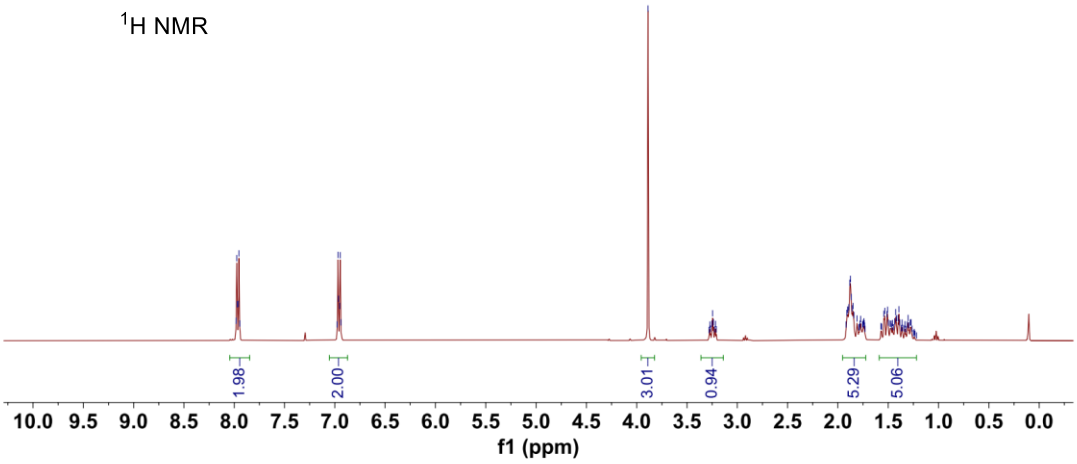
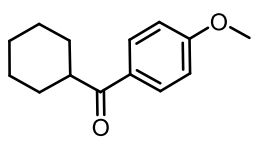
7.818
7.812
7.800
7.795
7.651
7.644
7.640
7.628
7.623
7.617
7.469
7.464
7.459
7.447
7.442
7.010
6.920
6.912
6.907
6.903
6.896
6.890
6.883
6.701
6.694
6.678
6.672
3.876
3.823
3.684
2.904
2.893
2.886
2.878
2.868
2.398
2.115
2.100
2.097
2.090
2.082
2.067
2.064
2.048
Cl
O
N
O
O
O
O
O
O
1H NMR
2.01
2.04
2.04
1.03
3.04
1.05
2.05
3.00
3.01
2.03
2.00
3.16
2.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


197.495
170.819
168.268
163.485
156.079
139.240
135.893
133.868
131.163
130.810
130.630
130.192
129.785
129.123
115.003
113.745
112.666
111.691
101.310
64.392
55.690
55.482
34.219
30.472
23.276
13.375
Cl
O
N
O
O
O
O
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

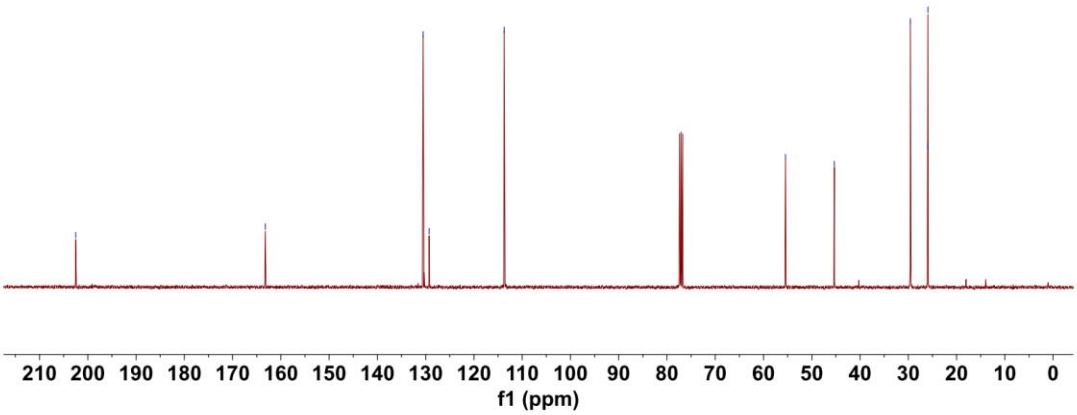


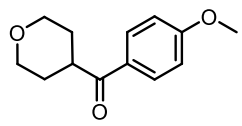
^{1}H NMR



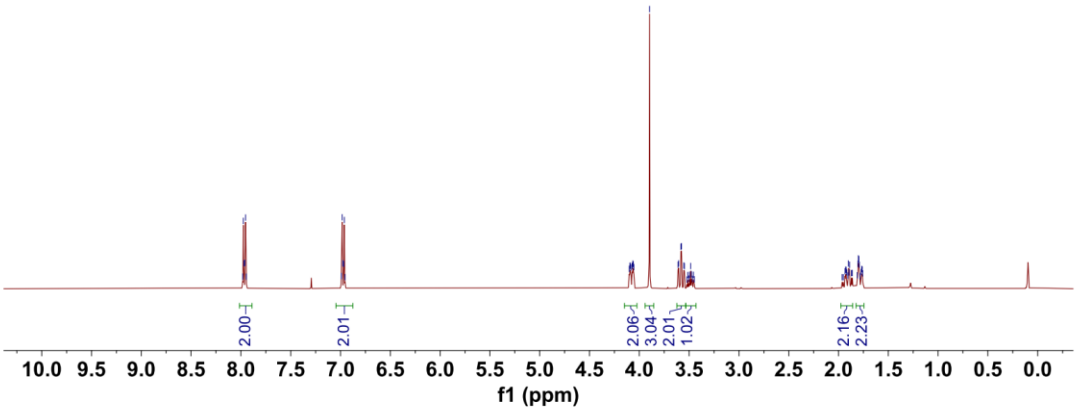


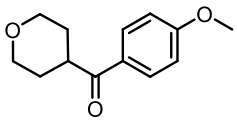
^{13}C NMR



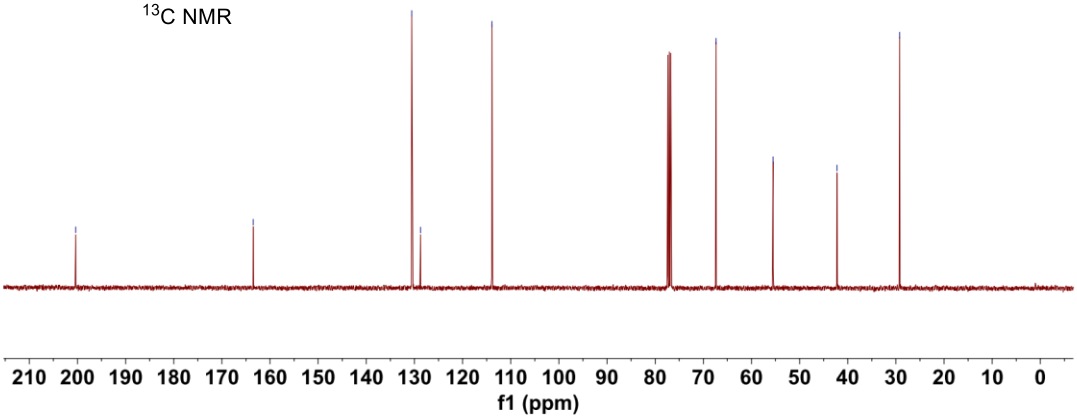


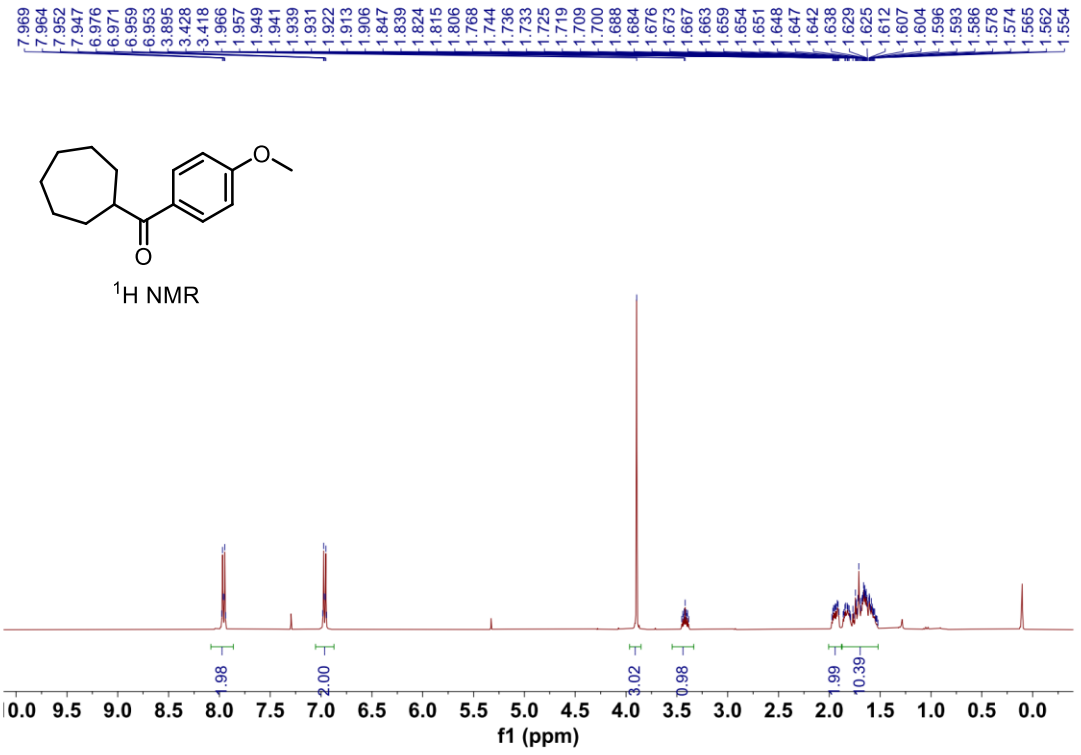
^{1}H NMR





^{13}C NMR

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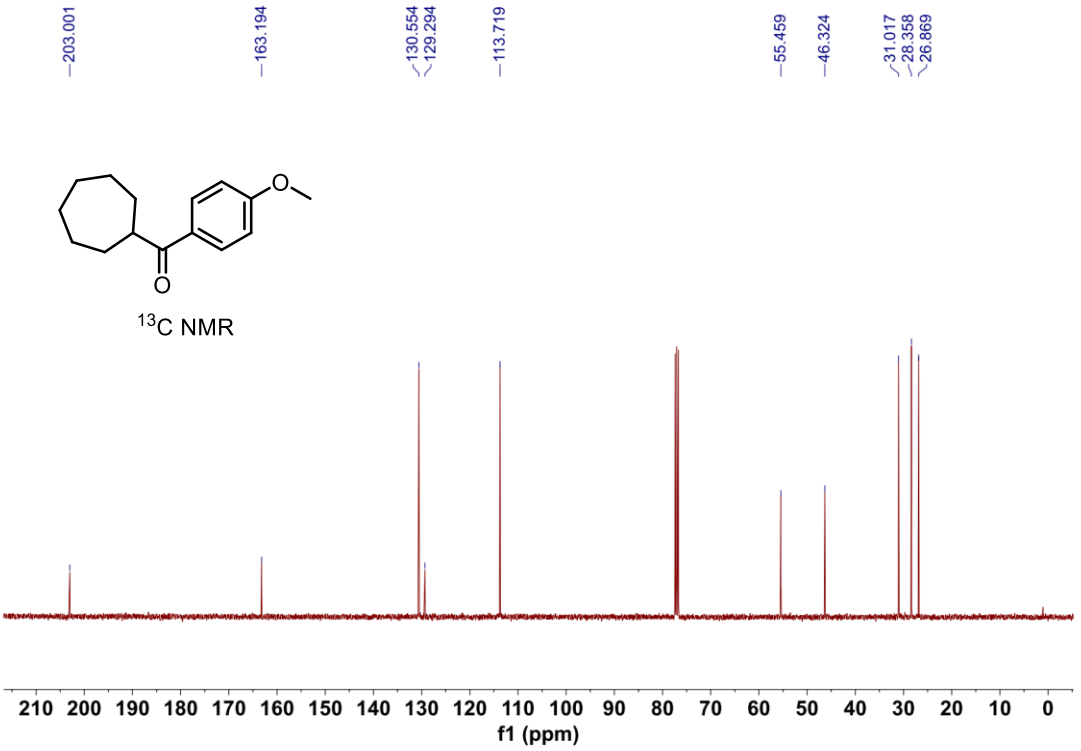
3.418
1.966
1.957
1.949
1.941
1.939
1.931
1.922
1.913
1.906
1.847
1.839
1.824
1.815
1.806
1.768
1.744
1.736
1.733
1.725
1.719
1.709
1.700
1.688
1.684
1.676
1.673
1.667
1.663
1.659
1.654
1.651
1.648
1.647
1.642
1.638
1.629
1.625
1.612
1.607
1.604
1.596
1.593
1.586
1.578
1.574
1.565
1.562
1.554
O
O
1H NMR
1.98
2.00
3.02
0.98
1.99
10.39
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


203.001
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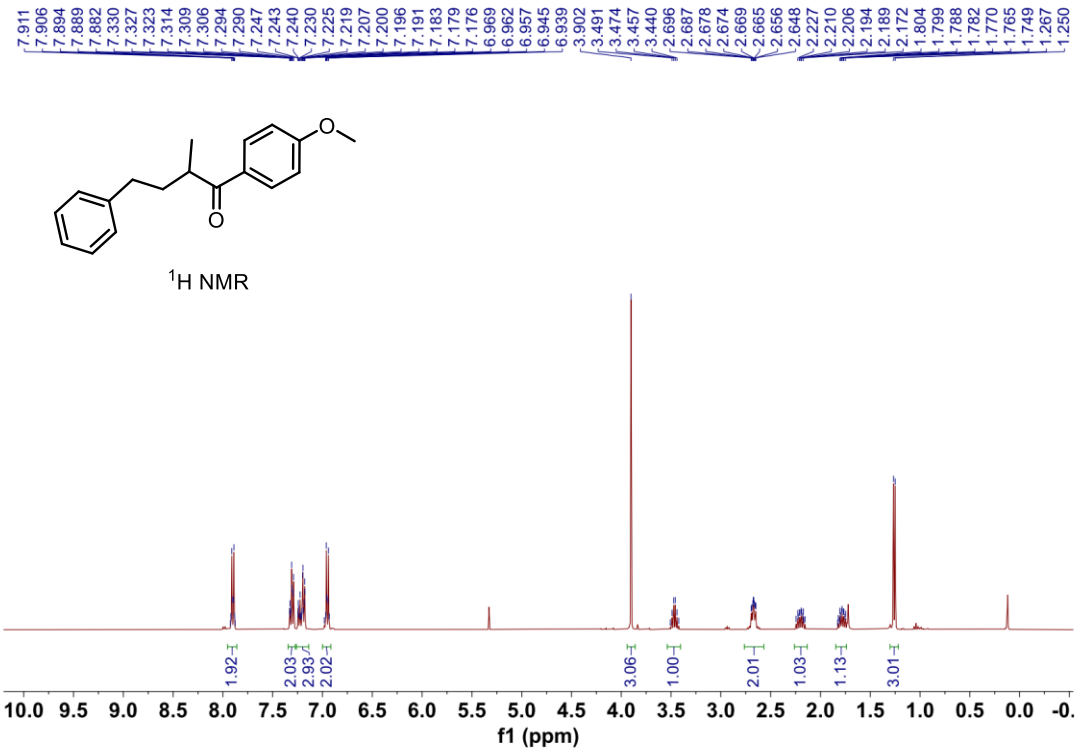
130.554
129.294
113.719
55.459
46.324
31.017
28.358
26.869
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.243
7.240
7.230
7.225
7.219
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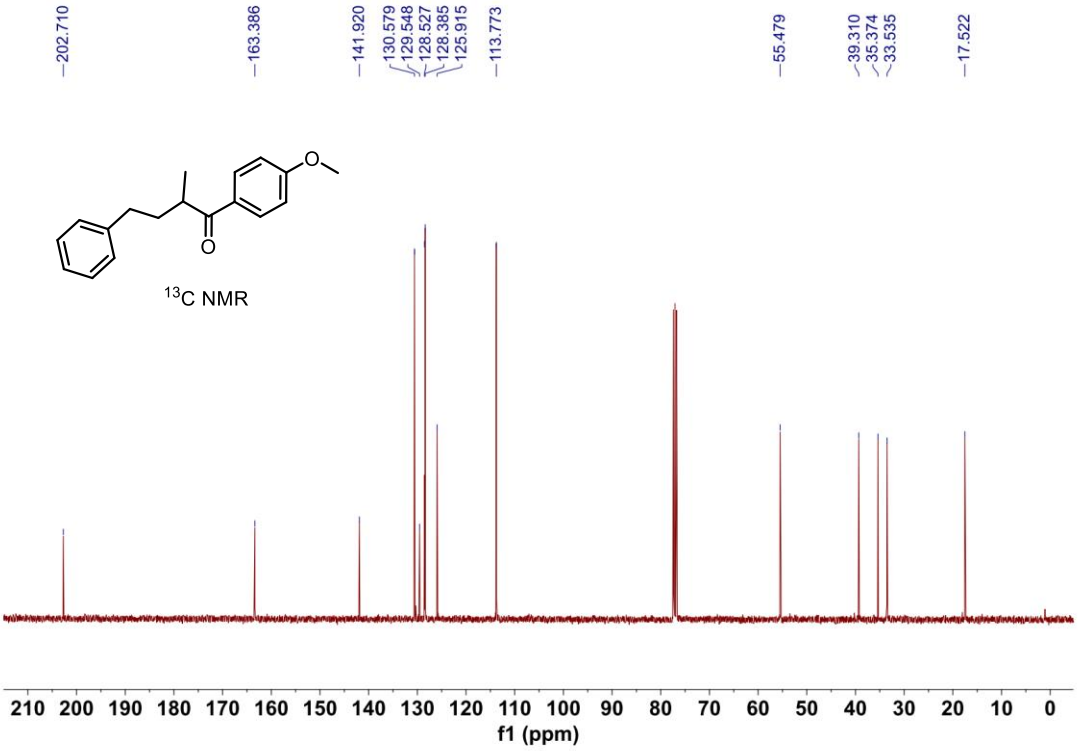
7.200
7.196
7.191
7.183
7.179
7.176
6.969
6.962
6.957
6.945
6.939
3.902
3.491
3.474
3.457
3.440
2.696
2.687
2.678
2.674
2.669
2.665
2.656
2.648
2.227
2.210
2.206
2.194
2.189
2.172
1.804
1.799
1.788
1.782
1.770
1.765
1.749
1.267
1.250
O
O
1H NMR
1.92
2.03
2.93
2.02
3.06
1.00
2.01
1.03
1.13
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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128.385
125.915
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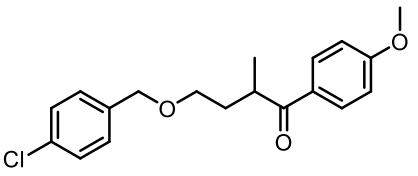
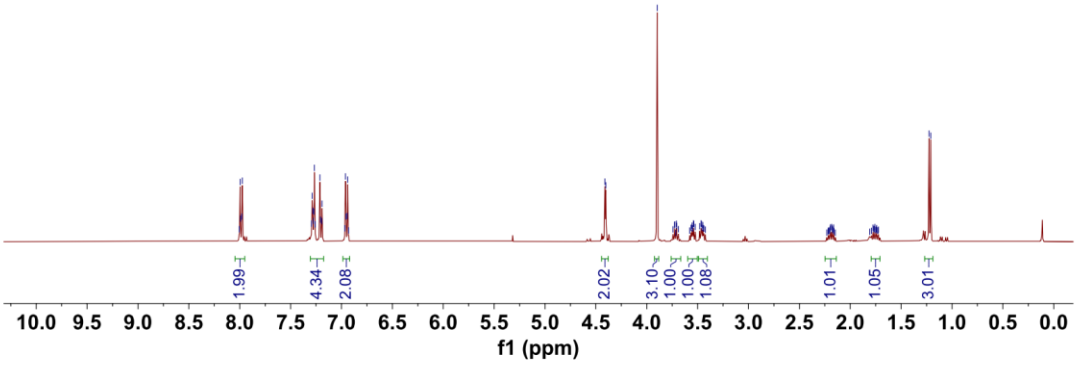
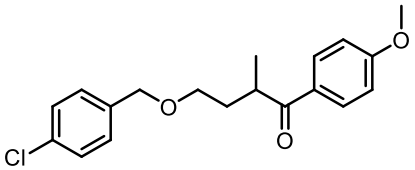
39.310
35.374
33.535
17.522
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

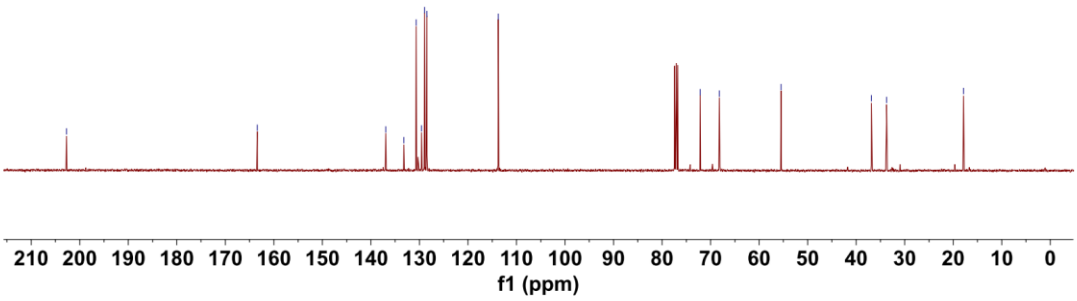


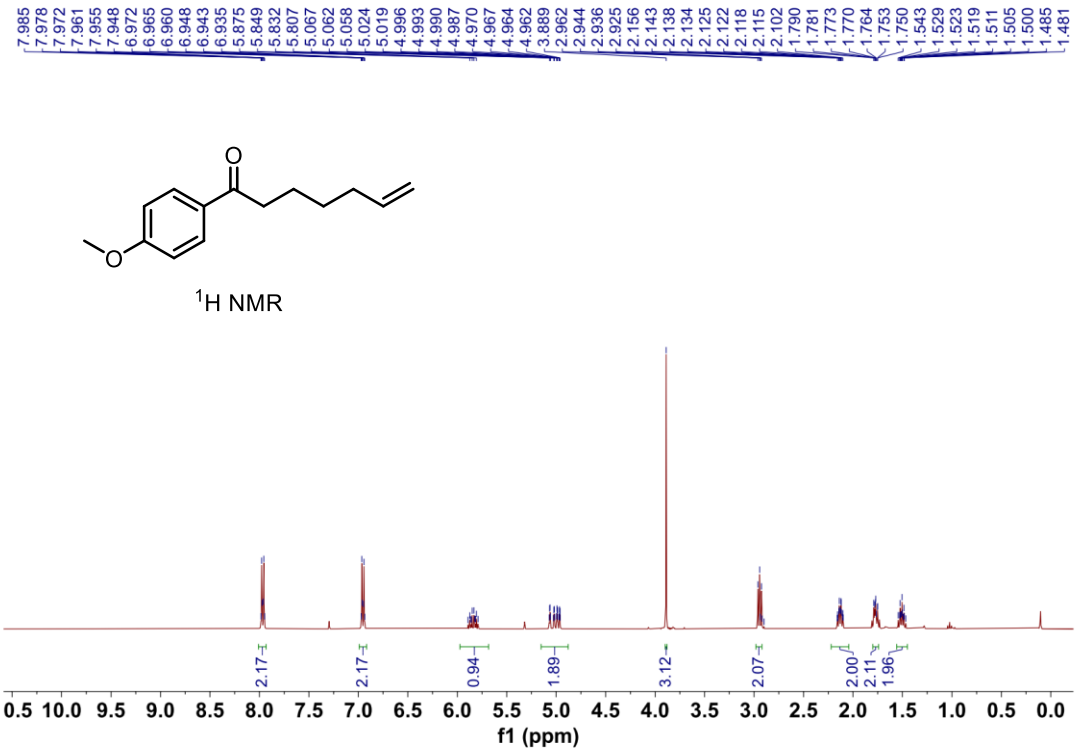
^{1}H NMR





^{13}C NMR

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6.960
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6.943
6.935
5.875
5.849
5.832
5.807
5.067
5.062
5.058
5.024
5.019
4.996
4.993
4.990
4.987
4.970
4.967
4.964
4.962
3.889
2.962
2.944
2.936
2.925
2.156
2.143
2.138
2.134
2.125
2.122
2.118
2.115
2.102
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1.781
1.773
1.770
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1.750
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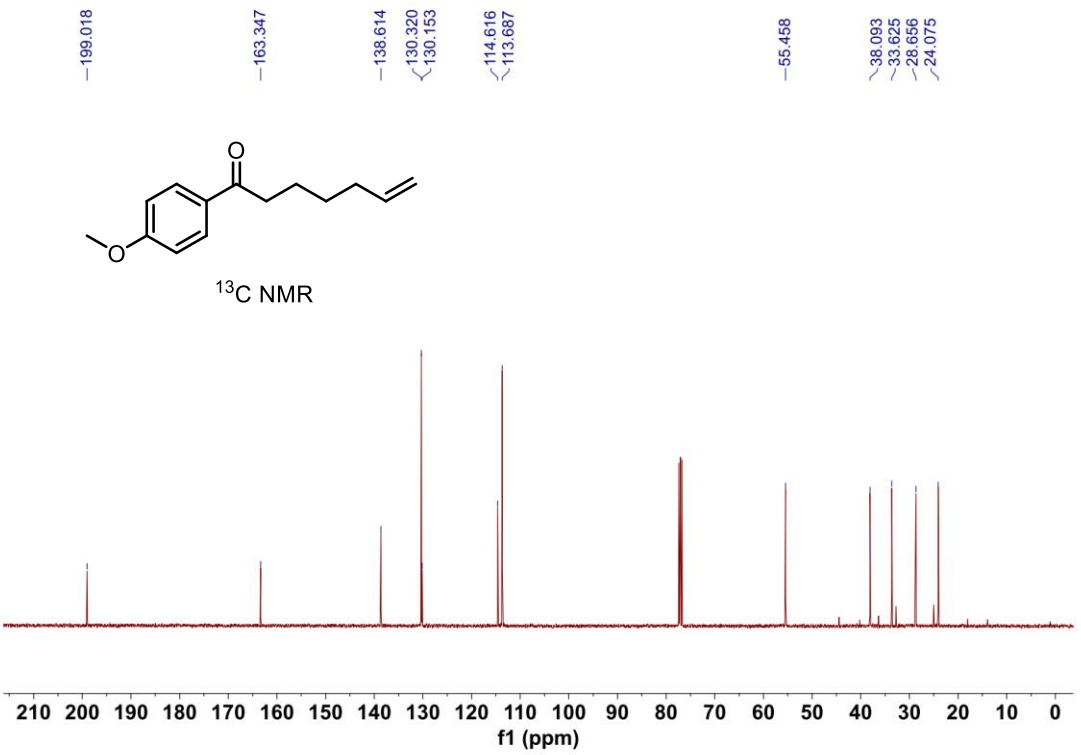
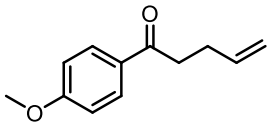
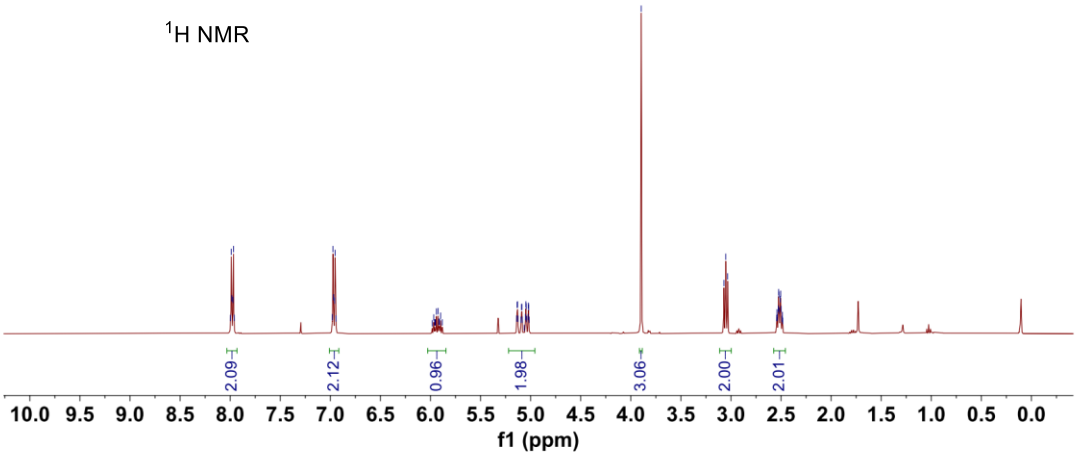
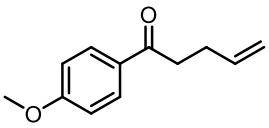
1.529
1.523
1.519
1.511
1.505
1.500
1.485
1.481
O
O
1H NMR
2.17
2.17
0.94
1.89
3.12
2.07
2.00
2.11
1.96
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


199.018
163.347
138.614
130.320
130.153
114.616
113.687
55.458
38.093
33.625
28.656
24.075
O
O
13C NMR
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

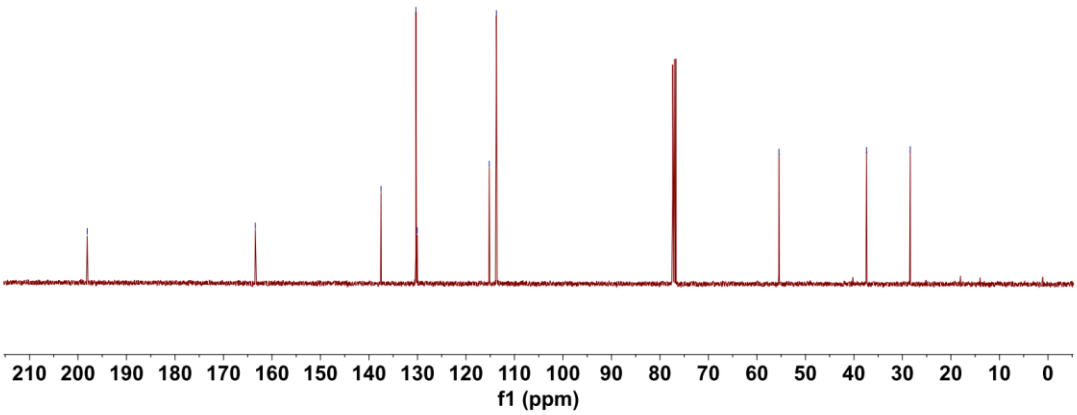


^{1}H NMR





^{13}C NMR



References

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