Supporting Information

Benzoyl Cyanide, A General Radical Acylating Reagent for Photoredox-catalyzed Benzylic Site-selective Acylation Reactions

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I. Experimental Section

Part 1. General Information

1. Chemicals and Reagents

All manipulations were carried out under an atmosphere of nitrogen using standard Schlenk techniques. Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (98% purity, Bidepharm) Ir(ppy)$_2$(dtbbbp)PF_6 (97% purity, Bidepharm) were purchased and used directly. Potassium benzoate (>99% purity, Adamas), sodium bromide (>99% purity, Adamas), zinc bromide (99% purity, Bidepharm), anhydrous sodium carbonate (>99% purity, Adamas), potassium carbonate (99% purity, Bidepharm) and sodium trifluoromethanesulfinate (99% purity, Bidepharm) were used as received. MeCN (acetonitrile, 99.9% purity, extra dry, Adamas), DMF (*N*,*N*-dimethylformamide, 99.8% purity, extra dry, Adamas) and Acetone (>99.5% purity, Greagent) were purchased and used directly. Deuterated solvents were used as received ($CDCl_3$ from Energy-chemical). Water was deionized and brine referred to a saturated aqueous solution of NaCl. Unless otherwise noted, starting materials, and other reagents were purchased from commercial sources and used without further purification.

2. Physical Method

Column chromatography was performed using silica gel 300-400 mesh (purchased from Qingdao-Haiyang Co., China) as the solid support. Thin layer chromatography (TLC) was used to monitor reaction progress and analyze fractions from column chromatography. Compounds were visualised under UV light or by staining with aqueous basic potassium permanganate or an ethanolic solution of phosphomolybdic acid (PMA). All NMR spectra were recorded on a Bruker 400 MHz spectrometer and Bruker 500 MHz spectrometer at STP, unless otherwise indicated. ^{1}H NMR and ^{13}C NMR chemical shifts are reported in δ units, parts per million (ppm) relative to the chemical shift of residual solvent. Reference peaks for $CDCl_3$ in ^{1}H NMR and ^{13}C NMR spectra were set at 7.26 ppm and 77.16 ppm, respectively. Coupling constants (*J*) are given in Hertz (Hz) and refer to apparent multiplicities (s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, h = heptet, m = multiplet, dd = doublet of doublets, etc.). The ^{1}H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constants, number of protons). High-resolution mass spectra were recorded on a Bruker impact II UPLC-QTOF

instruments at Central Analytical Lab, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University. Gas chromatography (GC) was performed on an Agilent Technologies 8860 GC System using an Agilent HP-5 column (15 m × 0.25 mm × 0.25 μm).

3. Photochemical Equipment

The blue LEDs was used RLH-18 8-position Photo Reaction System (Beijing Rogertech Co. ltd, Beijing, PRC), which equipped with 8 blue light 10 W LEDs (peak wavelength = 455 nm). Reaction mixtures were prepared under a nitrogen atmosphere in 10 mL Schlenk tube before sealing with parafilm placing in the photoreactor (Figure S1). The LED intensity was set to 10 W and the stirring speed set to 550 rpm. The temperature was controlled by stirrer.

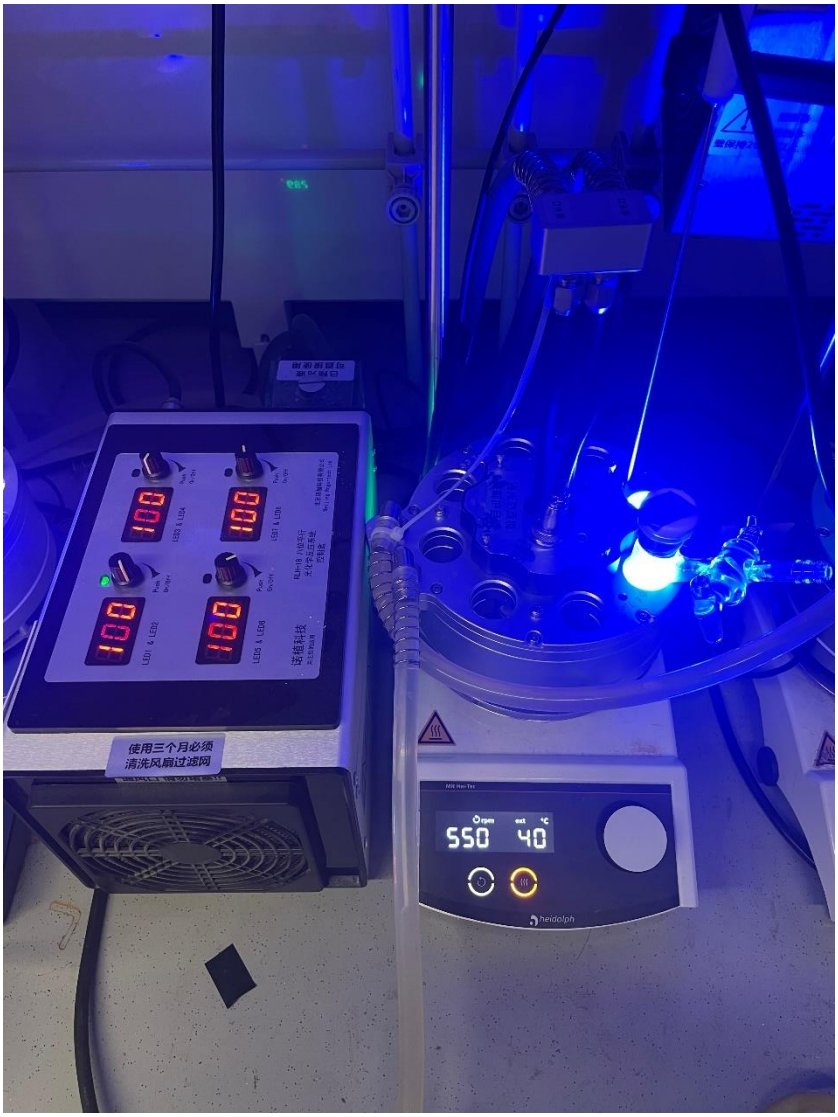
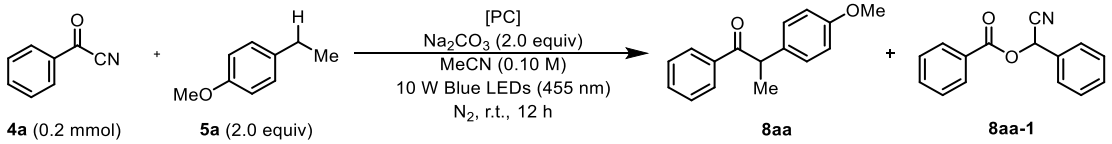


Figure S1. Photochemical Equipment

Part 2. Details of Optimization and Control Experiments

1. Typical procedure for optimization of acyl cyanide coupling with electron-rich ethylbenzene: To an oven-dried Schlenk tube equipped with a stirring bar was added Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (2.2 mg, 0.002 mmol, 1 mol%) and potassium benzoate (64.0 mg, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation at r.t. for 12 hours under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The yield was determined by ^{1}H NMR spectroscopy using 2,5-dimethyl furan as the internal standard, unless otherwise noted. (Note: The solid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

Table S1. Photocatalyst screening for the reaction of benzoyl cyanide and 1-ethyl-4-methoxy -benzene

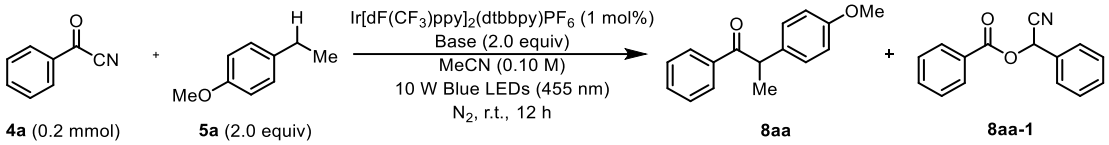


4a (0.2 mmol) **5a** (2.0 equiv) **8aa** **8aa-1**

entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	[Mes-Acr-Me]$^+$(ClO_4^-) (5 mol%)	0%	0%
2	4CzIPN (5 mol%)	32%	44%
3	Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (1 mol%)	42%	38%
4	Eosin Y (5 mol%)	0%	0%
5	TBADT (5 mol%) 390 nm	0%	0%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

Table S2. Base screening for the reaction of benzoyl cyanide and 1-ethyl-4-methoxybenzene

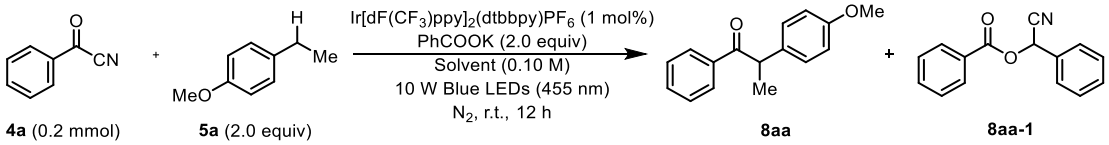


4a (0.2 mmol) **5a** (2.0 equiv) **8aa** **8aa-1**

entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	Na_2CO_3	42%	38%
2	$NaHCO_3$	45%	48%
3	Li_2CO_3	41%	38%
4	K_2CO_3	0%	0%
5	Cs_2CO_3	0%	0%
6	Na_2HPO_4	45%	40%
7	K_2HPO_4	52%	22%
8	Na_3PO_4	46%	20%
9	K_3PO_4	31%	10%
10	PhCOOK	68%	36%
11	PhCOONa	13%	< 1%
12	HCOONa	42%	46%
13	CH_3COOK	25%	32%
14	Pyridine	12%	< 1%
15	2,6-Lutidine	12%	< 1%
16	DBU	0%	0%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

Table S3. Solvent screening for the reaction of benzoyl cyanide and 1-ethyl-4-methoxy-benzene



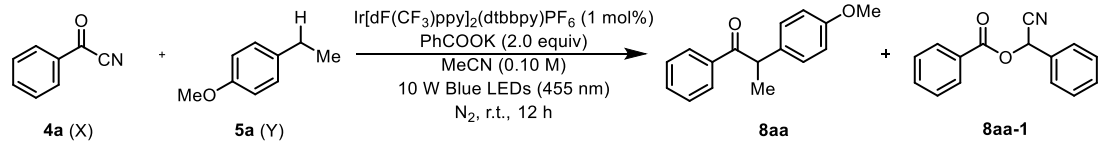
4a (0.2 mmol) **5a** (2.0 equiv) **8aa** **8aa-1**

entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	MeCN	68%	36%
2	THF	0%	0%
3	Acetone	38%	< 1%

4	Toluene	25%	< 1%
5	EtOAc	24%	< 1%
6	DCE	24%	< 1%
7	DMF	< 1%	0%
8	DMSO	0%	0%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

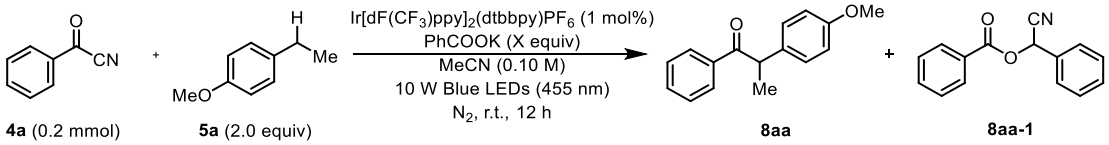
Table S4. Optimization of the ratio of benzoyl cyanide and 1-ethyl-4-methoxybenzene



entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	0.2 mmol : 0.2 mmol	49%	48%
2	0.2 mmol : 0.3 mmol	62%.	42%
3	0.2 mmol : 0.4 mmol	68%	36%
4	0.3 mmol : 0.2 mmol	56%	58%[b]
5	0.4 mmol : 0.2 mmol	50%	50%[b]
6	0.2 mmol : 0.5 mmol	56%	9%
7	0.2 mmol : 0.6 mmol	54%	4%
8	0.4 mmol : 0.8 mmol	55%	4%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography. [b] Yield was determined based on the scale of **4a**.

Table S5. Optimization of the amount of potassium benzoate for the reaction of benzoyl cyanide and 1-ethyl-4-methoxybenzene

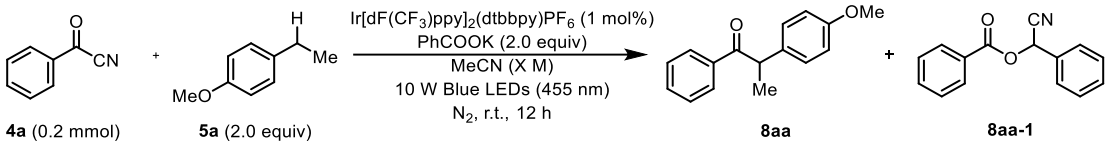


entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	0.5 equiv	41%	10%
2	1.0 equiv	45%	14%
3	1.5 equiv	47%	16%

4	2.0 equiv	68%	36%
5	2.5 equiv	47%	14%
6	3.0 equiv	46%.	16%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

Table S6. Optimization of the concentration of MeCN for the reaction of benzoyl cyanide and 1-ethyl-4-methoxybenzene

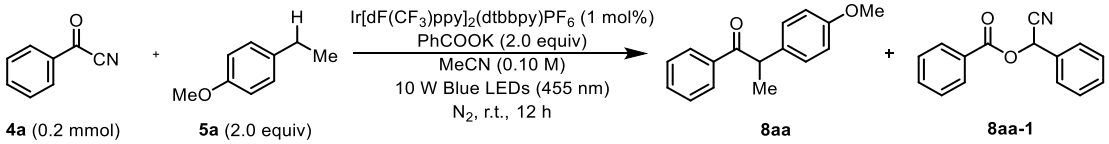


4a (0.2 mmol) **5a** (2.0 equiv) **8aa** **8aa-1**

entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	0.2 M	47%	28%
2	0.15 M	63%	40%
3	0.1 M	68%	36%
4	0.075 M	64%	28%
5	0.05 M	46%.	32%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

Table S7. Control experiments of benzoyl cyanide and 1-ethyl-4-methoxybenzene



4a (0.2 mmol) **5a** (2.0 equiv) **8aa** **8aa-1**

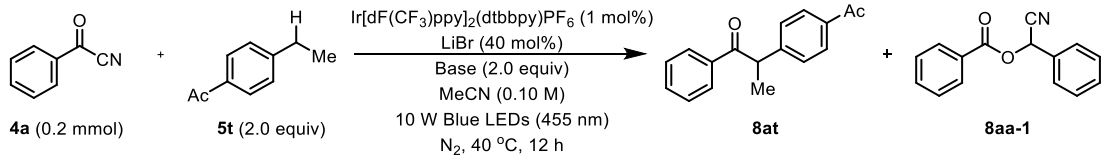
entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	none	68% (65%)[b]	36% (26%)[b]
2	w/o Ir[dF(CF$_3$)ppy]$_2$(dtbbpy)PF$_6$	< 1%	< 1%
3	w/o PhCOOK	49%	28%
4	w/o Blue LEDs	0%	0%
5	40 ℃	41%	36%
6	60 ℃	28%	44%
7	5 W Blue LEDs	62%	28%
8	35 W Blue LEDs	44%	26%

9	6 h	54%	28%
10	Ir[dF(CF$_3$)ppy]$_2$(dtbbpy)PF$_6$ (2 mol%)	48%	30%
11	4CzIPN (5 mol%) instead Ir	40%	30%
12	Benzoic anhydride instead of **4a**	0%	0%
13	Benzoyl fluoride instead of **4a**	0%	0%
14	Benzoyl chloride instead of **4a**	< 1%	0%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography. [b] Isolated yield.

2. Typical procedure for optimization of acyl cyanide coupling with electron-deficient and -neutral ethylbenzene: To an oven-dried Schlenk tube equipped with a stirring bar was added Ir[dF(CF$_3$)ppy]$_2$(dtbbpy)PF$_6$ (2.2 mg, 0.002 mmol, 1 mol%), sodium bromide (8.2 mg, 0.080 mmol, 40 mol%) and anhydrous sodium carbonate (42.4 mg, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethylacetophenone (59.3 mg, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation in an aluminum module at 40 ℃ for 12 hours under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The yield was determined by ^{1}H NMR spectroscopy using 2,5-dimethyl furan as the internal standard, unless otherwise noted. (Note: The solid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

Table S8. Base screening for the reaction of benzoyl cyanide and 4-ethylacetophenone

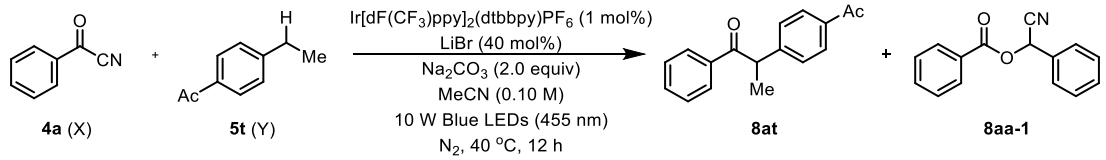


entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	Na_2CO_3	65%	28%
2	$NaHCO_3$	39%	16%

3	Li_2CO_3	20%	4%
4	K_2CO_3	49%	12%
5	Cs_2CO_3	0%	0%
6	Na_2HPO_4	20%	12%
7	K_2HPO_4	55%	24%
8	Na_3PO_4	58%	24%
9	K_3PO_4	26%	22%
10	PhCOOK	48%	20%
11	PhCOONa	39%	26%
12	CH_3COOK	27%	26%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

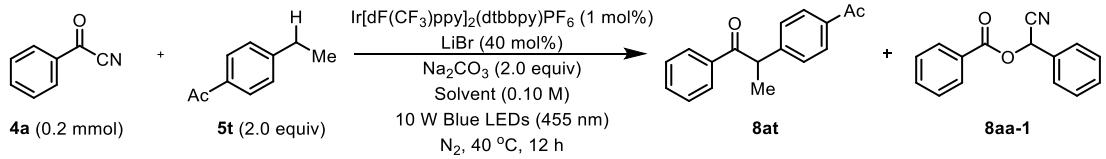
Table S9. Optimization of the ratio of benzoyl cyanide and 4-ethylacetophenone



entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	0.2 mmol : 0.2 mmol	37%	38%
2	0.2 mmol : 0.3 mmol	47%.	34%
3	0.2 mmol : 0.4 mmol	65%	28%
4	0.3 mmol : 0.2 mmol	48%	37%[b]
5	0.4 mmol : 0.2 mmol	39%	40%[b]

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography. [b] Yield was determined based on the scale of **4a**.

Table S10. Solvent screening for the reaction of benzoyl cyanide and 4-ethylacetophenone

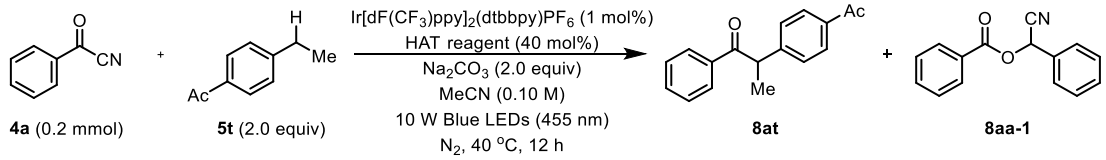


entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	MeCN	65%	28%
2	EtOAc	49%	40%

3	DCE	51%	< 1%
4	Acetone	25%	< 1%
5	Chlorobenzene	58%	< 1%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

Table S11. HAT reagent screening for the reaction of benzoyl cyanide and 4-ethylacetophenone

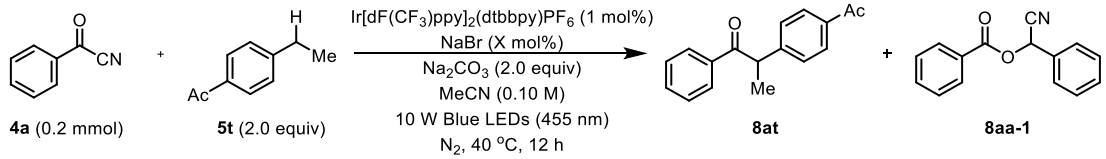


4a (0.2 mmol) **5t** (2.0 equiv) **8at** **8aa-1**

entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	LiBr	65%	28%
2	LiCl	25%	52%
3	TBAB	12%	26%
4	CH_2Br_2	56%	32%
5	NaBr	79%	24%
6	Quinuclidine	8%	24%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

Table S12. Optimization of the amount of NaBr for the reaction of benzoyl cyanide and 4-ethylacetophenone

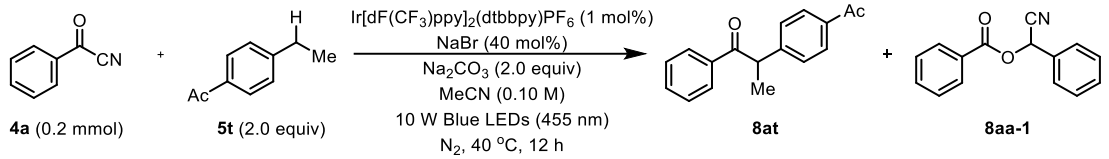


4a (0.2 mmol) **5t** (2.0 equiv) **8at** **8aa-1**

entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	10 mol%	61%	20%
2	20 mol%	62%	22%
3	30 mol%	58%	24%
4	40 mol%	79%	24%
5	60 mol%	77%	22%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography.

Table S13. Control experiments of benzoyl cyanide and 4-ethylacetophenone



4a (0.2 mmol) + **5t** (2.0 equiv) → **8at** + **8aa-1**

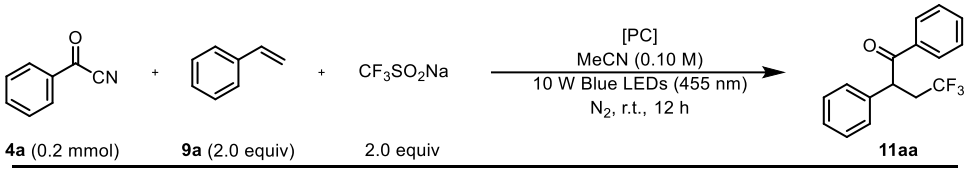
entry	variation from the standard condition	yield (%)[a]	yield (%)[a]
1	none	79% (74%)[b]	24% (26%)[b]
2	w/o $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$	0%	0%
3	w/o NaBr	< 1%	< 1%
4	w/o Na_2CO_3	51%	34%
5	w/o Blue LEDs	0%	0%
6	r.t.	68%	24%
7	LiBr instead of NaBr	65%	28%
8	$Ir[dF(CF_3)ppy]_2(5,5'\text{-}dCF_3bpy)PF_6$ instead of Ir	68%	6%
9	4CzIPN (5 mol%) instead Ir	58%	34%
10	Benzoic anhydride instead of **4a**	22%	0%
11	Benzoyl fluoride instead of **4a**	24%	0%
12	Benzoyl chloride instead of **4a**	26%	0%

[a] ^{1}H-NMR yield using 2,5-dimethyl furan as the internal standard from a mixture containing other impurities after quick flash column chromatography. [b] Isolated yield.

3. Typical procedure for optimization of acylfluoroalkylation of styrene with benzoyl cyanide: To an oven-dried Schlenk tube equipped with a stirring bar was added $Ir(ppy)_2(dtbbpy)PF_6$ (1.8 mg, 0.002 mmol, 1 mol%) and sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), styrene (41.7 mg, 0.400 mmol, 200 mol%), Acetone (3 mL) and DMF (0.3 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation at r.t. for 12 hours under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The yield was determined by GC-FID using 1,3,5-trimethoxybenzene as the internal standard, unless otherwise noted. (Note: The solid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL)

carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

Table S14. Photocatalyst screening for the reaction of acylfluoroalkylation of styrene with benzoyl cyanide

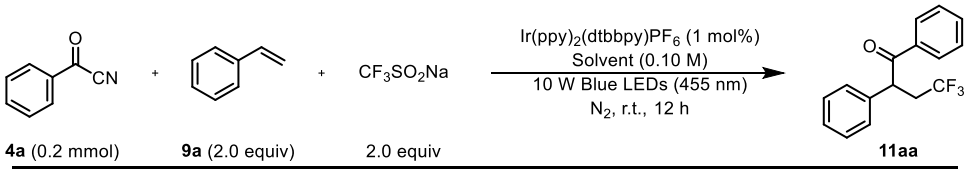


4a (0.2 mmol) **9a** (2.0 equiv) 2.0 equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	4CzIPN (5 mol%)	18%[b]
2	Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (1 mol%)	9.2%
3	Ir[dF(CF_3)ppy]$_2$(5,5'-dCF_3bpy)PF_6 (1 mol%)	14.6%
4	Ir(ppy)$_2$(dtbbpy)PF_6 (1 mol%)	23.5%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard. [b] Isolated yield.

Table S15. Solvent screening for the reaction of acylfluoroalkylation of styrene with benzoyl cyanide



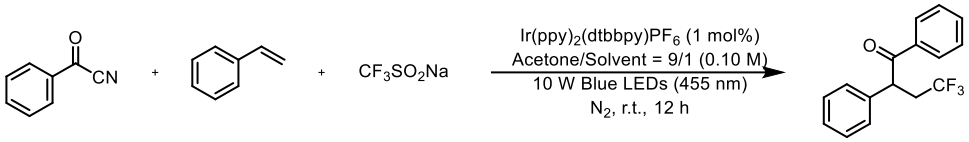
4a (0.2 mmol) **9a** (2.0 equiv) 2.0 equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	MeCN	23.5%
2	DCM	13.6%
3	PhCl	1.3%
4	THF	23.8%
5	Acetone	40.5%
6	DCE	18.9%
7	EtOAc	20.6%
8	DMF	23.6%
9	DMSO	16.4%
10	DMA	21.7%
11	2-Butanone	30.8%

12	DME	14.3%
13	$PhCF_3$	1.1%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard.

Table S16. Co-solvent screening for the reaction of acylfluoroalkylation of styrene with a benzoyl cyanide

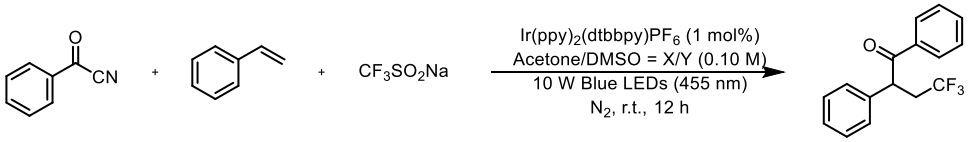


4a (0.2 mmol) **9a** (2.0 equiv) 2.0 equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	Acetone	40.5%
2	DMF	47.4%
3	DMSO	47.4%
4	DMA	45.8%
5	MeCN	41.2%
6	DCE	44.9%
7	PhCl	43.6%
8	THF	40.3%
9	DME	41.7%
10	EtOAc	45.3%
11	DCM	39.7%
12	2-Butanone	43.8%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard.

Table S17. Acetone/DMSO co-solvent screening for the reaction of acylfluoroalkylation of styrene with benzoyl cyanide



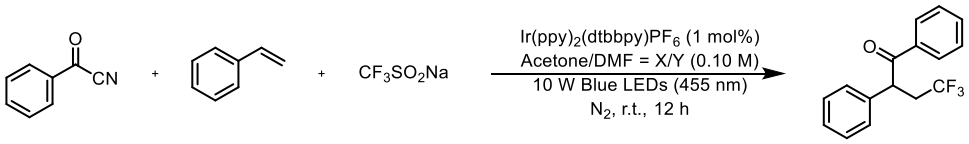
4a (0.2 mmol) **9a** (2.0 equiv) 2.0 equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	5/5	25.1%
2	6/4	26.3%
3	7/3	31.2%

4	8/2	38.8%
5	9/1	47.4%
6	10/1 (2.2 mL)	48.1%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard.

Table S18. Acetone/DMF co-solvent screening for the reaction of acylfluoroalkylation of styrene with benzoyl cyanide

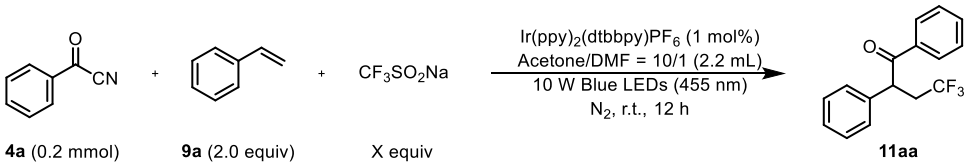


4a (0.2 mmol) **9a** (2.0 equiv) 2.0 equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	5/5	37.5%
2	6/4	42.8%
3	7/3	45.8%
4	8/2	46.2%
5	9/1	47.4%
6	10/1 (2.2 mL)	50.1%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard.

Table S19. Optimization of the ratio of CF_3SO_2Na for the reaction of acylfluoroalkylation of styrene with benzoyl cyanide

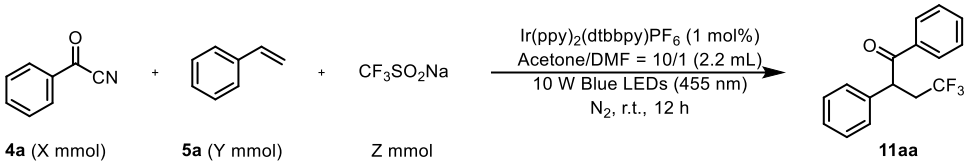


4a (0.2 mmol) **9a** (2.0 equiv) X equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	1.5 equiv	46.2%
2	2.0 equiv	50.1%
3	2.5 equiv	47.4%
4	3.0 equiv	37.6%
5	4.0 equiv	28.8%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard.

Table S20. Optimization of the ratio of benzoyl cyanide, styrene and CF_3SO_2Na for the reaction of acylfluoroalkylation of styrene with benzoyl cyanide

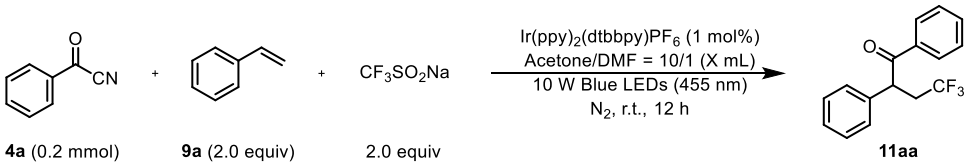


4a (X mmol) **5a** (Y mmol) Z mmol **11aa**

entry	variation from the standard condition	yield (%)[a]
1	0.2 : 0.4 : 0.4	50.1%
2	0.2 : 0.3 : 0.4	49.6%
3	0.2 : 0.2 : 0.4	29.7%
4	0.3 : 0.2 : 0.4	35.8%
5	0.4 : 0.2 : 0.4	38.6%
6	0.2 : 0.5 : 0.4	41.3%
7	0.2 : 0.6 : 0.4	39.6%
8	0.2 : 0.3 : 0.3	45.5%
9	0.2 : 0.2 : 0.2	34.5%
10	0.3 : 0.2 : 0.2	35.9%
11	0.4 : 0.2 : 0.2	36.3%
12	0.2 : 0.5 : 0.5	46.8%
13	0.2 : 0.6 : 0.6	45.8%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard.

Table S21. Optimization of the concentration of co-solvent for the reaction of acylfluoroalkylation of styrene with benzoyl cyanide



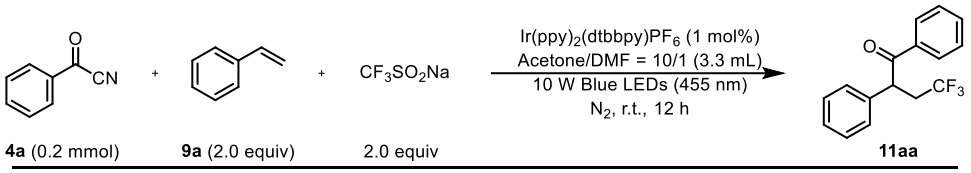
4a (0.2 mmol) **9a** (2.0 equiv) 2.0 equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	1.1 mL	42.5%
2	1.65 mL	41.5%
3	2.2 mL	50.1%
4	2.75 mL	51.2%
5	3.3 mL	52.6%
6	3.85 mL	51.6%

7	4.4 mL	46.0%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard.

Table S22. Control experiments of the reaction of acylfluoroalkylation of styrene with benzoyl cyanide



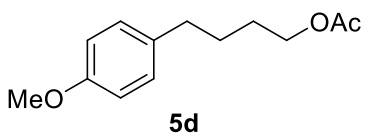
4a (0.2 mmol) **9a** (2.0 equiv) 2.0 equiv **11aa**

entry	variation from the standard condition	yield (%)[a]
1	none	52.6% (55%)[b]
2	w/o Ir	17.3%
3	w/o Blue LEDs	0%
4	40 °C	43.1%
5	5 W Blue LEDs	45.6%
6	4CzIPN (5 mol%) instead of Ir	47.1%
7	$Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ instead of Ir	47.4%
8	$Ir(ppy)_2(bpy)PF_6$ instead of Ir	42.8%
9	Acetone instead of co-solvent	50.2%
10	DMF instead of co-solvent	17.5%
11	Benzoic anhydride instead of **4a**	0%
12	Benzoyl fluoride instead of **4a**	0.1%
13	Benzoyl chloride instead of **4a**	0%

[a] GC-FID yield using1,3,5-trimethoxybenzene as the internal standard. [b] Isolated yield.

Part 3. Preparation of Starting Materials

4-(4-Methoxyphenyl)butyl acetate (5d).



5d

Following a reported procedure,[1] in an oven-dried 100 mL round-bottom flask at room temperature under nitrogen, 4-(4-methoxyphenyl)butan-1-ol (1.80 g, 10 mmol), pyridine (12 mL), 4-dimethylaminopyridine (61 mg, 0.5 mmol) and acetic anhydride (2.04 g, 20 mmol) were added. The reaction was stirred overnight at room temperature then slowly quenched with $NaHCO_3$ (sat.)

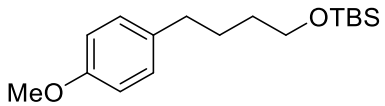
until bubbling ceased. The mixture was extracted with EtOAc (3 x 50 mL). The organic extracts were combined and washed with $CuSO_4$ (sat) (3 x 30 mL), H_2O (2 x 50 mL) then brine (1 x 50 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 85% yield (1.88 g, 8.5 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.05 (m, 2H), 6.88-6.78 (m, 2H), 4.07 (t, *J* = 6.2 Hz, 2H), 3.79 (s, 3H), 2.59 (t, *J* = 7.0 Hz, 2H), 2.04 (s, 3H), 1.72-1.59 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 157.8, 134.1, 129.3, 113.8, 64.4, 55.2, 34.5, 28.2, 28.0, 21.0.

HRMS (ESI^+, m/z) calcd for $C_{13}H_{18}NaO_3$ ($[M+Na]^+$): 245.1148. Found: 245.1148.

tert-Butyl(4-(4-methoxyphenyl)butoxy)dimethylsilane (5e).



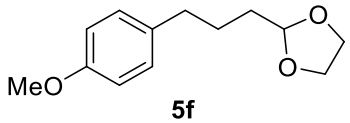
5e

Following a reported procedure,[2] to a solution of 4-(4-methoxyphenyl)butan-1-ol (1.80 g, 10 mmol) in DCM (20 mL), triethylamine (2.02 g, 20 mmol) and 4-dimethylaminopyridine (122 mg, 1 mmol) were added. Then TBSCl (1.66 g, 11 mmol) was added dropwise. The reaction was stirred overnight at room temperature. Then, water was added and extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), compound **5e** was isolated in 90% yield (2.65 g, 9.0 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14-7.03 (m, 2H), 6.89-6.77 (m, 2H), 3.79 (s, 3H), 3.62 (t, *J* = 6.3 Hz, 2H), 2.57 (t, *J* = 7.5 Hz, 2H), 1.70-1.49 (m, 4H), 0.89 (s, 9H), 0.04 (s, 6H).

Spectroscopic data are in accordance with those described in literature.[2]

2-(3-(4-Methoxyphenyl)propyl)-1,3-dioxolane (5f).



5f

Step 1: Following a reported procedure,[3] to a solution of 1-(4-methoxyphenyl)-4-butanol (1.80 g, 10 mmol) in DCM (20 mL) was added Dess-Martin periodinate (4.24 g, 10 mmol). The reaction was allowed to stir for 1 h at room temperature. It was then quenched with sodium metabisulfate and extracted with DCM, dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the product 4-(4-methoxyphenyl)butanal was isolated in 88% yield (1.57 g, 8.8 mmol) as a colorless oil.

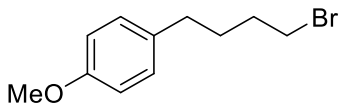
Step 2: Following a reported procedure,[4] a mixture of 4-(4-methoxyphenyl)butanal (1.57 g, 8.8 mmol), ethylene glycol (0.66 g, 10.6 mmol), and p-toluenesulfonic acid (151.5 mg, 0.88 mmol) in toluene (50 mL) was heated at reflux for 24 h using a Dean-Stark trap. The mixture was cooled to r.t. and quenched with saturated aqueous sodium bicarbonate solution. The resulting mixture was extracted with EtOAc. The combined organic layers were washed with saturated aqueous sodium bicarbonate solution, brine, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), compound **5f** was isolated in 50% yield (976 mg, 4.4 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14-7.05 (m, 2H), 6.87-6.76 (m, 2H), 4.37 (t, *J* = 5.1 Hz, 1H), 3.78 (s, 3H), 3.29 (s, 4H), 2.57 (t, *J* = 6.9 Hz, 2H), 1.69-1.58 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 134.4, 129.4, 113.9, 104.6, 55.4, 52.8, 34.9, 32.2, 26.8.

HRMS (ESI^+, m/z) calcd for $C_{13}H_{18}NaO_3$ ($[M+Na]^+$): 245.1148. Found: 245.1148.

1-(4-Bromobutyl)-4-methoxybenzene (5g).



5g

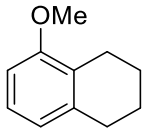
Following a reported procedure,[5] bromine (2.08 g, 13 mmol) was added to a suspension of PPh_3 (3.41 g, 13 mmol) and imidazole (0.88 g, 13 mmol) in anhydrous DCM (50 mL) at 0 ºC.

4-(4-Methoxyphenyl)butan-1-ol (1.80 g, 10 mmol) was then added slowly by syringe. The resulting mixture was allowed to warm to room temperature and stirred overnight. Completion of the reaction was monitored by TLC. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ and extracted with DCM. The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), compound **5g** was isolated in 86% yield (2.10 g, 8.6 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16-7.03 (m, 2H), 6.92-6.76 (m, 2H), 3.79 (s, 3H), 3.42 (t, *J* = 6.7 Hz, 2H), 2.59 (t, *J* = 7.5 Hz, 2H), 1.95-1.82 (m, 2H), 1.82-1.66 (m, 2H).

Spectroscopic data are in accordance with those described in literature.[5]

5-Methoxy-1,2,3,4-tetrahydronaphthalene (5k).



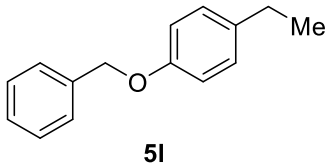
5k

Following a reported procedure,[6] 5,6,7,8-Tetrahydronaphthalenol (0.45 g, 3 mmol), iodomethane (0.2 mL, 3.3 mmol,) and K_2CO_3 (1.04 g, 7.5 mmol) were dissolved in acetone and refluxed overnight. The reaction was quenched with MeOH (0.4 mL), cooled to room temperature, filtered and concentrated under reduced pressure. Then, water was added and extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), compound **5k** was isolated in 45% yield (219 mg, 1.35 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (t, *J* = 7.9 Hz, 1H), 6.75-6.62 (m, 2H), 3.82 (s, 3H), 2.77 (t, *J* = 5.9 Hz, 2H), 2.66 (t, *J* = 6.0 Hz, 2H), 1.90-1.68 (m, 4H).

Spectroscopic data are in accordance with those described in literature.[6]

1-(Benzyloxy)-4-ethylbenzene (5l).



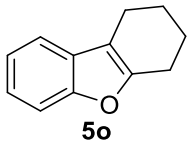
5l

Following a reported procedure,[7] a mixture of 4-ethylphenol (1.22 g, 10 mmol), benzyl bromide (1.88 g, 11 mmol), and Cs_2CO_3 (3.58 g, 11 mmol) was dissolved in MeCN (25 mL). The mixture was stirred at room temperature for 3 h under a nitrogen atmosphere. After 3 h, the reaction mixture was diluted with DCM. The organic solution was washed with water and brine, dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: petroleum ether), compound **5l** was isolated in 56% yield (1.19 g, 5.6 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.43 (m, 2H), 7.43-7.36 (m, 2H), 7.36-7.30 (m, 1H), 7.18-7.08 (m, 2H), 6.98-6.86 (m, 2H), 5.06 (s, 2H), 2.61 (q, *J* = 7.6 Hz, 2H), 1.23 (t, *J* = 7.6 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[7]

1,2,3,4-tetrahydrodibenzo[*b,d*]furan (5o).



5o

Step 1: Following a reported procedure,[8] to a solution of phenol (508.2 mg, 5.4 mmol) in acetone (54 mL), potassium carbonate (1.5 g, 10.8 mmol) and 2-bromocyclohexan-1-one (1.16 g, 6.5 mmol) were added. The reaction was stirred overnight at 60 ℃. After completing of the reaction, the reaction mixture was filtered and the filtrate was concentrated under reduced pressure to give a residue. The residue was diluted with water and extracted with EtOAc. The combined organic layers were washed with brine, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the product 2-phenoxycyclohexan-1-one was isolated in 48% yield (489.7 mg, 2.57 mmol) as a colorless oil.

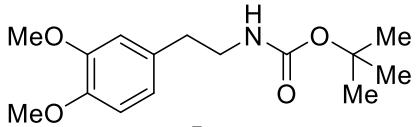
Step 2: Following a reported procedure,[8] to a 25 mL two necked flask equipped with a reflux condenser, fresh distilled dichloromethane (30 mL), 2-phenoxycyclohexan-1-one (489.7 mg, 2.57

mmol), and titanium tetrachloride (487.5 mg, 2.57 mmol) were added under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 6 h. After completion of the reaction (monitored by TLC), it was quenched with a saturated aqueous solution of NH_4Cl. The reaction mixture was partitioned between water and dichloromethane. After extraction with dichloromethane, the organic layer was dried over anhydrous sodium sulfate and evaporated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 60% yield (265.2 mg, 1.54 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 -7.31 (m, 2H), 7.25-7.12 (m, 2H), 2.82-2.70 (m, 2H), 2.70-2.53 (m, 2H), 2.00-1.89 (m, 2H), 1.92-1.80 (m, 2H).

Spectroscopic data are in accordance with those described in literature.[8]

tert-Butyl (3,4-dimethoxyphenethyl)carbamate (5p).



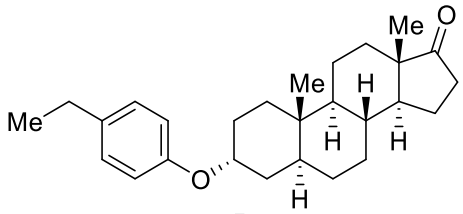
5p

Following a reported procedure,[9] to a solution of 2-(3,4-dimethoxyphenyl)ethan-1-amine (905 mg, 5 mmol) in DCM (10 mL), triethylamine (1.01 g, 10 mmol) was added and the mixture was stirred for 15 min at room temperature. After that, Boc_2O (1.20 g, 5.5 mmol) was added. The mixture was stirred at room temperature for 20 h. Then the reaction mixture was directly concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2: 20% ethyl acetate in petroleum ether), compound **5p** was isolated in 80% yield (1.13 g, 4.0 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84-6.77 (m, 1H), 6.77-6.65 (m, 2H), 4.54 (s, 1H), 3.87 (s, 6H), 3.86 (s, 6H), 3.35 (q, J = 6.8 Hz, 2H), 2.74 (t, J = 7.1 Hz, 2H), 1.43 (s, 9H).

Spectroscopic data are in accordance with those described in literature.[9]

(3R,5S,8R,9S,10S,13S,14S)-3-(4-ethylphenoxy)-10,13-dimethylhexadecahydro-17 H-cyclopenta[*a*]phenanthren-17-one (5q).



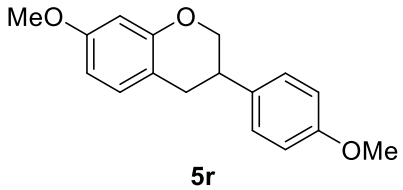
5q

Following a reported procedure,[10] to a solution of epiandrosterone (1.0 g, 3.44 mmol), PPh_3 (1.80 g, 6.89 mmol) and 4-ethylphenol (756 mg, 6.20 mmol) in THF (30 mL), DIAD (1.39 g, 6.89 mmol) was added dropwise with cooling in an ice bath and the mixture was allowed to warm to room temperature. After stirring overnight, water was added, and the organic layer was separated. The aqueous layer was extracted with EtOAc twice, and the combined organic layers were washed with brine, and dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure, and the residue was purified by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), compound **5q** was isolated in 33% yield (447.9 mg, 1.14 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.05 (m, 2H), 6.86-6.79 (m, 2H), 4.49 (p, *J* = 2.7 Hz, 1H), 2.58 (q, *J* = 7.6 Hz, 2H), 2.44 (dd, *J* = 19.2, 8.7 Hz, 1H), 2.13-2.01 (m, 1H), 1.99-1.85 (m, 2H), 1.83-1.73 (m, 2H), 1.72-1.60 (m, 4H), 1.60-1.36 (m, 5H), 1.34-1.18 (m, 8H), 1.08-0.95 (m, 1H), 0.91-0.79 (m, 1H), 0.86 (s, 3H), 0.84 (s, 3H).

Spectroscopic data are in accordance with those described in literature.[10]

7-Methoxy-3-(4-methoxyphenyl)chromane (5r).



5r

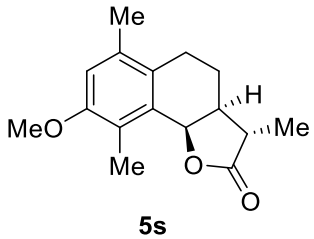
Following a reported procedure,[11] to a solution of 3-(4-hydroxyphenyl)chroman-7-ol (484.5 mg, 2 mmol) in acetone (10 mL), potassium carbonate (691.0 mg, 5 mmol) and iodomethane (709.7 mg, 5 mmol) were added. The reaction was stirred overnight at 60 °C. The mixture was passed through a short silica gel pad with EtOAc as an eluent, and the solvent was removed on a rotary evaporator. The resulting residue was purified by column chromatography (SiO_2: 10% ethyl acetate in

petroleum ether), compound **5r** was isolated in 80% yield (432.3 mg, 1.6 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.13 (m, 2H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.94-6.86 (m, 2H), 6.48 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.43 (d, *J* = 2.6 Hz, 1H), 4.35-4.27 (m, 1H), 3.98 (t, *J* = 10.5 Hz, 1H), 3.81 (s, 3H), 3.78 (s, 3H), 3.25-3.12 (m, 1H), 2.99-2.88 (m, 2H).

Spectroscopic data are in accordance with those described in literature.[11]

(3*S*,3*aS*,9*bR*)-8-methoxy-3,6,9-trimethyl-3a,4,5,9b-tetrahydronaphtho[1,2-*b*]furan-2(3*H*)-one (5s).



5s

Step 1: Following a reported procedure,[12] the mixture of α-santonin (2.5 g, 10 mmol), acetic anhydride (13 mL) was stirred at 0 ℃ and H_2SO_4 (1.25 mL, 23 mmol) was added dropwise and allowed to react for 3 h. After the reaction completed, saturated aqueous sodium bicarbonate solution was added to quench the reaction at 0 ℃. The resulting mixture was extracted with EtOAc. The combined organic layers were washed with brine, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 20% ethyl acetate in petroleum ether), the product α-desmotroposantonin acetate was isolated in 85% yield (2.44 g, 8.5 mmol) as a white solid.

Step 2: Following a reported procedure,[12] α-desmotroposantonin acetate (2.44 g, 8.5 mmol) was added to the solution of ammonium hydroxide and MeOH (1:1). The reaction was stirred at r.t. for about 2 h. The resulting mixture was extracted with EtOAc. The combined organic layers were washed with brine, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 50% ethyl acetate in petroleum ether), the product α-desmotroposantonin was isolated in 80% yield (1.67 g, 6.8 mmol) as a white solid.

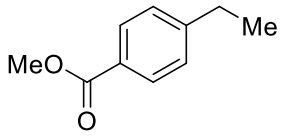
Step 3: Following a reported procedure,[12] to a solution of α-desmotroposantonin (1.67 g, 6.8 mmol) in acetone (20 mL), potassium carbonate (1.88 g, 13.6 mmol) and iodomethane (1.93 g, 13.6 mmol) were added. The reaction was stirred overnight at 60 ℃. The mixture was passed through a

short silica gel pad with EtOAc as an eluent, and the solvent was removed on a rotary evaporator. The resulting residue was purified by column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), compound **5s** was isolated in 94% yield (1.66 g, 6.4 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.74 (s, 1H), 5.63 (d, *J* = 6.3 Hz, 1H), 3.81 (s, 3H), 2.77-2.67 (m, 1H), 2.60-2.46 (m, 2H), 2.46-2.37 (m, 1H), 2.27 (s, 3H), 2.24 (s, 3H), 1.97-1.87 (m, 1H), 1.79-1.67 (m, 1H), 1.39 (d, *J* = 7.4 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[12]

Methyl 4-ethylbenzoate (5w).



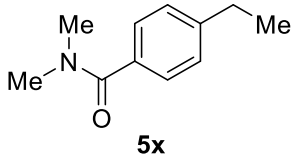
5w

Following a reported procedure,[13] 4-ethylbenzoic acid (1.50 g, 10 mmol) was dissolved in 20 mL of methanol. Concentrated sulphuric acid (5 drops) was slowly added and the reaction mixture was stirred at 80 °C for 5 h. Then saturated aqueous sodium bicarbonate solution was added to quench the reaction and the mixture was extracted with EtOAc. The combined organic layers were washed with brine, dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), compound **5w** was isolated in 80% yield (1.31 g, 8.0 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.92 (m, 2H), 7.31-7.22 (m, 3H), 3.90 (s, 3H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[13]

4-Ethyl-*N*,*N*-dimethylbenzamide (5x).



5x

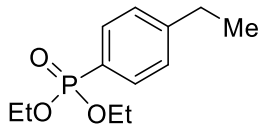
Following a reported procedure,[14] to a solution of dimethylamine (2.0 M in THF) (3.3 mL, 6.5 mmol) and triethylamine (1.04 mL, 7.5 mmol) in dry DCM (20 mL), 4-ethylbenzoyl chloride

(0.74 mL, 5.0 mmol) was added dropwise at 0 °C and the reaction mixture was stirred at room temperature for 12 h. Then water (40 mL) was added, the organic layer was separated and the aqueous layer was extracted with DCM (3 x 30 mL). The combined organic layer was washed with saturated aqueous $NaHCO_3$ (30 mL) solution followed by water (30 mL). The combined organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), compound **5x** was isolated in 90% yield (796.5 mg, 4.5 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 2H), 7.23-7.16 (m, 2H), 3.02 (s, 6H), 2.64 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[15]

Diethyl (4-ethylphenyl)phosphonate (5d').



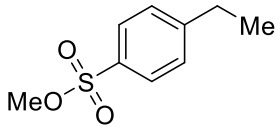
5d'

Following a reported procedure,[16] diethyl phosphite (0.57 mL, 4.4 mmol), triethylamine (0.61 mL, 4.4 mmol), and tetrakis(triphenylphosphine)palladium (231.0 mg, 0.20 mmol) were dissolved under nitrogen in 3 mL of toluene, and the solution was cooled to 0 °C. The 1-bromo-4-ethylbenzene (0.55 mL, 4.0 mmol) was then added, and the reaction mixture was brought to reflux overnight. After the mixture was cooled to room temperature, 25 mL of diethyl ether was added and the unsoluble solids were filtered off. The filtrate was evaporated to dryness and the residue was purified by column chromatography (SiO_2: 50% ethyl acetate in petroleum ether), compound **5d'** was isolated in 72% yield (697.0 mg, 2.88 mmol) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.65 (m, 2H), 7.36-7.22 (m, 2H), 4.20-3.97 (m, 4H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.1 Hz, 6H), 1.23 (t, *J* = 7.6 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[17]

Methyl 4-ethylbenzenesulfonate (5e').



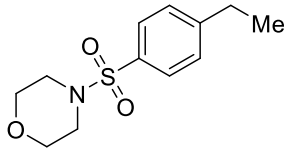
5e'

Following a reported procedure,[18] to a solution of MeOH (160.0 mg, 5.0 mmol.) in DCM (15 ml) were added 4-ethylbenzenesulfonyl chloride (1.53 g, 7.5 mmol), triethylamine (757.5 mg, 7.5 mmol) and DMAP (61 mg, 0.5 mmol). After stirring for 24 h at r.t. under an atmosphere of argon, the mixture was washed with 1N HCl, aq. sat. $NaHCO_3$ and brine. The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), compound **5e'** was isolated in 70% yield (700 mg, 3.5 mmol) as a light-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 3.74 (s, 3H), 2.74 (q, *J* = 7.6 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[19]

4-((4-Ethylphenyl)sulfonyl)morpholine (5f').



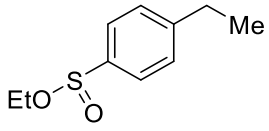
5f'

Following a reported procedure,[20] to a solution of the morpholine (174.2 mg, 2.0 mmol) in pyridine (5 mL) were added 4-ethylbenzenesulfonyl chloride (225.1 mg, 1.1 mmol) at 0 °C. The reaction was stirred at ambient temperature for 2-3 h. After the reaction completed, pyridine was removed by rotary evaporator. The residue was poured into water and extracted with DCM. The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 20% ethyl acetate in petroleum ether), compound **5f'** was isolated in 90% yield (252.8 mg, 0.99 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.62 (m, 2H), 7.40-7.31 (m, 2H), 3.74 (t, *J* = 4.7 Hz, 4H), 2.98 (t, *J* = 4.6 Hz, 4H), 2.73 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[21]

Ethyl 4-ethylbenzenesulfinate (5g').



5g'

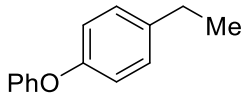
Following a reported procedure,[22] to a solution of 4-ethylbenzenesulfonyl chloride (1.02 g, 5 mmol) in DCM (15 mL) was added ethanol (0.44 mL, 7.5 mmol), triethylamine (1.04 mL, 7.5 mmol) at 0 °C. Triphenylphosphine (1.3 g, 5 mmol) was dissolved in DCM (10 mL) and it was slowly added dropwise using a dropping funnel. The reaction was stirred at 0 °C for 3 h. Then the solvent was removed by rotary evaporator. The resulting residue was purified by column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), compound **5g'** was isolated in 64% yield (633.6 mg, 3.2 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.58 (m, 2H), 7.39-7.31 (m, 2H), 4.10 (dq, *J* = 9.9, 7.1 Hz, 1H), 3.72 (dq, *J* = 9.9, 7.0 Hz, 1H), 2.71 (q, *J* = 7.7 Hz, 2H), 1.33-1.20 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 142.0, 128.6, 125.3, 60.8, 28.9, 15.6, 15.4.

HRMS (ESI^+, m/z) calcd for $C_{10}H_{14}NaO_2S$ ($[M+Na]^+$): 221.0607. Found: 221.0606.

1-Ethyl-4-phenoxybenzene (5h').



5h'

Following a reported procedure,[23] to an oven-dried 100 mL Schlenk flask CuI (190.5 mg, 1 mmol), 2-picolinic acid (307.5 mg, 2.5 mmol), iodobenzene (2.04 g, 10 mmol), 4-ethylphenol (1.59 g, 13 mmol), K_3PO_4 (4.24 g, 20 mmol), and anhydrous DMSO (12 mL) were added. The reaction was heated at 100 ºC for 24 h under N_2. The reaction mixture was cooled to room temperature and diluted with DCM (70 mL) and transferred to a separatory funnel (250 mL). The organic mixture was washed with saturated NH_4Cl (aq) (3 x 50 mL). The organic layer was collected, and dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: petroleum ether), compound **5h'** was isolated in 56% yield (0.99 g, 5.0 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.28 (m, 2H), 7.21-7.14 (m, 2H), 7.12-7.04 (m, 1H), 7.03-6.98

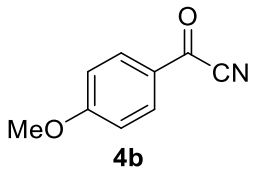
(m, 2H), 6.98-6.91 (m, 2H), 2.65 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H).

Spectroscopic data are in accordance with those described in literature.[23]

Part 4. Preparation of Acyl Cyanides

A general procedure for the preparation of acyl cyanides (GP): Following a reported procedure,[24] under an argon atmosphere, to a stirred suspension of copper(I) cyanide (3.59 g, 40 mmol) in dry acetonitrile (40 mL) was added aroyl chloride (10 mmol). After refluxing overnight, the resulting clear solution was cooled down to room temperature and concentrated in vacuo. The residue was washed with ethyl acetate, filtrated and concentrated in vacuo again. The residue was purified by flash column chromatography to separate copper salt. After additional distillation under reduced pressure, the desired product was obtained. (Note: The conversion of acyl chlorides to acyl cyanides was a highly efficient reaction. However, hydrolysis was inevitable during the work-up process. It usually achieved > 90% purity mixed with its corresponding acid after FCC. For pure spectrum, additional distillation was necessary. The yield shown below was the yield after distillation. The solid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (50 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

4-Methoxybenzoyl cyanide (4b).



4b

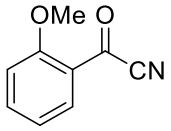
This compound was prepared according to the ***GP*** using 4-methoxybenzoyl chloride (1.71 g, 10.0 mmol). Distillation afforded the title product in 25% yield (402.5 mg, 2.5 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.07 (m, 2H), 7.09-7.01 (m, 2H), 3.94 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 166.2, 133.3, 126.9, 115.1, 113.2, 56.1.

Spectroscopic data are in accordance with those described in literature.[25]

2-Methoxybenzoyl cyanide (4c).



4c

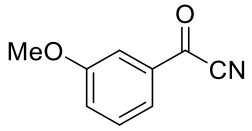
This compound was prepared according to the ***GP*** using 2-methoxybenzoyl chloride (1.71 g, 10.0 mmol). Distillation afforded the title product in 28% yield (450.8 mg, 2.8 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.73-7.65 (m, 1H), 7.15-7.02 (m, 2H), 4.01 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 161.4, 138.4, 132.7, 122.7, 121.2, 114.4, 112.6, 56.2.

Spectroscopic data are in accordance with those described in literature.[26]

3-Methoxybenzoyl cyanide (4d).



4d

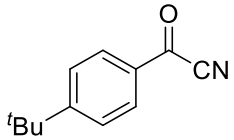
This compound was prepared according to the ***GP*** using 3-methoxybenzoyl chloride (1.71 g, 10.0 mmol). Distillation afforded the title product in 66% yield (1.06 g, 6.6 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.57 (t, *J* = 2.6 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.32 (dd, *J* = 8.3, 2.7 Hz, 1H), 3.89 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 160.5, 134.8, 130.7, 124.3, 124.2, 112.9, 112.9, 55.8.

Spectroscopic data are in accordance with those described in literature.[25]

4-(*tert*-Butyl)benzoyl cyanide (4e).



4e

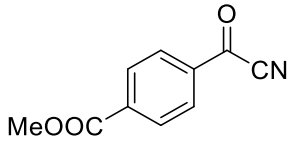
This compound was prepared according to the ***GP*** using 4-(*tert*-butyl)benzoyl chloride (1.96 g, 10.0 mmol). Distillation afforded product **4e** in 52% yield (972.4 mg, 5.2 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-8.05 (m, 2H), 7.65-7.58 (m, 2H), 1.37 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 161.7, 131.1, 130.7, 126.7, 113.1, 35.9, 31.0.

Spectroscopic data are in accordance with those described in literature.[25]

Methyl 4-(cyanocarbonyl)benzoate (4f).



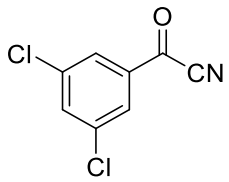
4f

This compound was prepared according to the ***GP*** using methyl 4-(chlorocarbonyl)benzoate (1.99 g, 10.0 mmol). Distillation afforded product **4f** in 22% yield (415.8 mg, 2.2 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29-8.18 (m, 4H), 3.99 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 165.5, 137.3, 136.2, 130.6, 130.5, 112.6, 53.0.

3,5-Dichlorobenzoyl cyanide (4g).



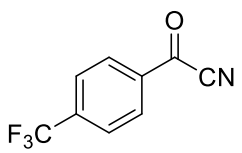
4g

This compound was prepared according to the ***GP*** using 3,5-dichlorobenzoyl chloride (2.09 g, 10.0 mmol). Distillation afforded product **4g** in 47% yield (940 mg, 4.7 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 1.9 Hz, 2H), 7.75 (t, *J* = 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 137.0, 136.6, 135.6, 128.5, 112.1.

4-(Trifluoromethyl)benzoyl cyanide (4h).



4h

This compound was prepared according to the ***GP*** using 4-(trifluoromethyl)benzoyl chloride (2.0 g, 10.0 mmol). Distillation afforded product **4h** in 52% yield (1.04 g, 5.2 mmol) as a colorless oil.

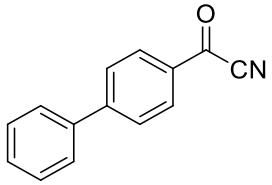
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.1 Hz, 2H), 7.89 (d, *J* = 8.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 137.8 (q, $^{2}J_{C\text{-}F}$ = 33.4 Hz), 135.9, 130.9, 126.8 (q, $^{3}J_{C\text{-}F}$ = 3.7 Hz), 123.1 (q, $^{1}J_{C\text{-}F}$ = 274.4 Hz), 112.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.59.

Spectroscopic data are in accordance with those described in literature.[24]

[1,1'-Biphenyl]-4-carbonyl cyanide (4i).



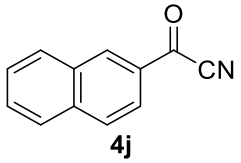
4i

This compound was prepared according to the ***GP*** using [1,1'-biphenyl]-4-carbonyl chloride (2.16 g, 10.0 mmol). Distillation afforded product **4i** in 47% yield (972.9 mg, 4.7 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24-8.19 (m, 2H), 7.85-7.79 (m, 2H), 7.69-7.64 (m, 2H), 7.56-7.43 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 149.8, 138.9, 132.3, 131.2, 129.4, 129.4, 128.2, 127.6, 113.0.

2-Naphthoyl cyanide (4j).



4j

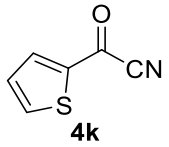
This compound was prepared according to the ***GP*** using 2-naphthoyl chloride (1.91 g, 10.0 mmol). Distillation afforded the title product in 55% yield (995.5 mg, 5.5 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.08-8.01 (m, 2H), 7.97-7.90 (m, 2H), 7.77-7.70 (m, 1H), 7.70-7.63 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 137.3, 135.7, 132.3, 131.1, 131.0, 130.4, 129.8, 128.3, 128.1, 122.9, 113.1.

Spectroscopic data are in accordance with those described in literature.[25]

Thiophene-2-carbonyl cyanide (4k).



4k

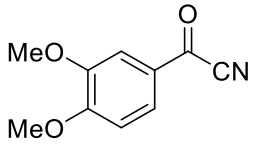
This compound was prepared according to the ***GP*** using thiophene-2-carbonyl chloride (1.5 g, 10.0 mmol). Distillation afforded product **4k** in 44% yield (602.8 mg, 4.4 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 4.0, 1.2 Hz, 1H), 7.99 (dd, *J* = 4.9, 1.2 Hz, 1H), 7.34-7.29 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 141.1, 140.0, 139.6, 129.6, 112.6.

Spectroscopic data are in accordance with those described in literature.[24]

3,4-Dimethoxybenzoyl cyanide (4l).



4l

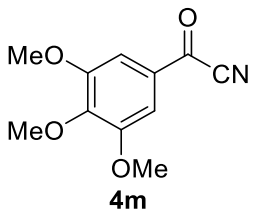
This compound was prepared according to the ***GP*** using 3,4-dimethoxybenzoyl chloride (2.0 g, 10.0 mmol). Distillation afforded the title product in 19% yield (362.0 mg, 1.9 mmol) as a bright yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.52 (d, *J* = 2.1 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 4.02 (s, 3H), 3.95 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 156.9, 150.0, 128.2, 127.1, 113.2, 110.8, 110.0, 56.7, 56.3.

Spectroscopic data are in accordance with those described in literature.[27]

3,4,5-Trimethoxybenzoyl cyanide (4m).



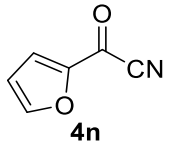
4m

This compound was prepared according to the ***GP*** using 3,4,5-trimethoxybenzoyl chloride (2.3 g, 10.0 mmol). Distillation afforded the title product in 44% yield (972.0 mg, 4.4 mmol) as a bright yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (s, 2H), 3.99 (s, 3H), 3.93 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 153.6, 146.2, 128.3, 112.9, 107.7, 61.4, 56.5.

Furan-2-carbonyl cyanide (4n).



4n

This compound was prepared according to the ***GP*** using furan-2-carbonyl chloride (1.31 g, 10.0 mmol). Distillation afforded the title product in 55% yield (660.0 mg, 5.5 mmol) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.65 (dd, *J* = 3.8, 0.8 Hz, 1H), 6.75 (dd, *J* = 3.8, 1.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 153.2, 151.7, 150.6, 126.3, 114.3, 112.6.

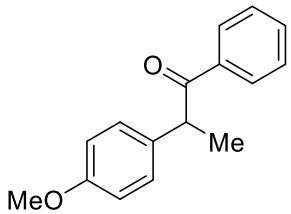
Spectroscopic data are in accordance with those described in literature.[24]

Part 5. Coupling of Acyl Cyanides with Alkylbenzenes

General Procedure A (GPA) for acyl cyanides with electron-rich ethylbenzenes: To an oven-dried Schlenk tube equipped with a stirring bar was added $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (2.2 mg, 0.002 mmol, 1 mol%), potassium benzoate (64.0 mg, 0.400 mmol, 200 mol%), ethylbenzene (if solid, 0.400 mmol, 200 mol%) and acyl cyanide (if solid, 0.200 mmol, 100 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Acyl cyanide (if liquid, 0.200 mmol, 100 mol%), ethylbenzene (if liquid, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under blue

LEDs irradiation at r.t. for 12 hours under N_2 atmosphere. After the reaction completed, the mixture was added 30 mL of EtOAc and washed with brine. The organic phase was dried over Na_2SO_4, filtered, and evaporated under vacuum. The residue was purified by silica gel column chromatography to give the target product. (Note: The liquid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

2-(4-Methoxyphenyl)-1-phenylpropan-1-one (8aa).



8aa

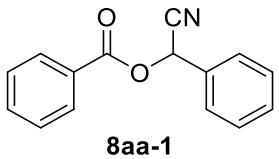
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetone in petroleum ether), the title compound **8aa** was isolated in 65% yield (31.2 mg, 0.130 mmol) as a colorless oil. At the same time, the byproduct **8aa-1** was isolated in 26% yield (6.2 mg, 0.026 mmol) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.91 (m, 2H), 7.51-7.44 (m, 1H), 7.42-7.34 (m, 2H), 7.23-7.17 (m, 2H), 6.88-6.79 (m, 2H), 4.65 (q, *J* = 6.8 Hz, 1H), 3.75 (s, 3H), 1.51 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.7, 158.6, 136.7, 133.6, 132.8, 128.9, 128.9, 128.6, 114.5, 55.3, 47.1, 19.6.

Spectroscopic data are in accordance with those described in literature.[28]

Cyano(phenyl)methyl benzoate (8aa-1).



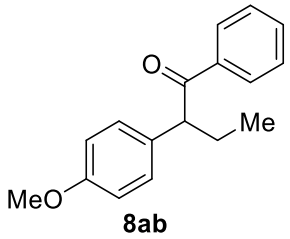
8aa-1

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.05 (m, 2H), 7.67-7.58 (m, 3H), 7.53-7.43 (m, 5H), 6.68 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 134.3, 132.0, 130.6, 130.2, 129.4, 128.8, 128.2, 128.0, 116.3, 63.5.

Spectroscopic data are in accordance with those described in literature.[29]

2-(4-Methoxyphenyl)-1-phenylbutan-1-one (8ab).



8ab

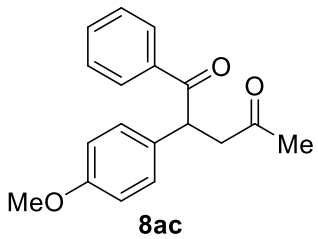
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-methoxy-4-propylbenzene (60.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 51% yield (25.9 mg, 0.102 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-7.90 (m, 2H), 7.52-7.44 (m, 1H), 7.43-7.35 (m, 2H), 7.25-7.19 (m, 2H), 6.89-6.79 (m, 2H), 4.40 (t, J = 7.2 Hz, 1H), 3.75 (s, 3H), 2.26-2.10 (m, 1H), 1.92-1.76 (m, 1H), 0.90 (t, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.5, 158.7, 137.2, 132.8, 131.8, 129.4, 128.7, 128.6, 114.4, 55.3, 54.6, 27.2, 12.4.

Spectroscopic data are in accordance with those described in literature.[30]

2-(4-Methoxyphenyl)-1-phenylpentane-1,4-dione (8ac).



8ac

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-(4-methoxyphenyl)butan-2-one (71.3 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 56% yield (31.6 mg, 0.112 mmol) as a light yellow oil.

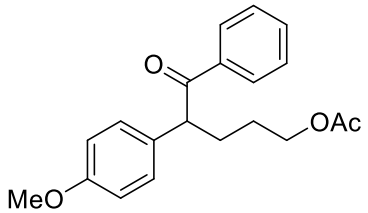
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.91 (m, 2H), 7.51-7.41 (m, 1H), 7.40-7.31 (m, 2H),

7.21-7.13 (m, 2H), 6.85-6.74 (m, 2H), 5.05 (dd, *J* = 10.0, 4.2 Hz, 1H), 3.73 (s, 3H), 3.57 (dd, *J* = 17.9, 9.9 Hz, 1H), 2.73 (dd, *J* = 18.0, 4.1 Hz, 1H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 207.1, 199.2, 158.9, 136.4, 133.0, 130.6, 129.3, 129.0, 128.6, 114.7, 55.3, 48.2, 48.0, 30.2.

Spectroscopic data are in accordance with those described in literature.[10]

4-(4-Methoxyphenyl)-5-oxo-5-phenylpentyl acetate (8ad).



8ad

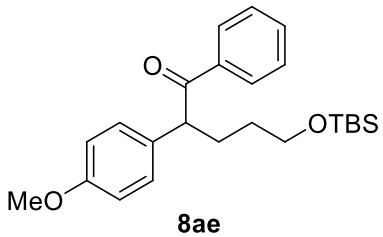
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-(4-methoxyphenyl)butyl acetate (88.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 66% yield (43.1 mg, 0.132 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.90 (m, 2H), 7.51-7.44 (m, 1H), 7.42-7.34 (m, 2H), 7.24-7.15 (m, 2H), 6.86-6.77 (m, 2H), 4.51 (t, *J* = 7.3 Hz, 1H), 4.06 (t, *J* = 6.5 Hz, 2H), 3.74 (s, 3H), 2.26-2.13 (m, 1H), 2.00 (s, 3H), 1.93-1.81 (m, 1H), 1.72-1.48 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 171.3, 158.8, 136.8, 133.0, 131.3, 129.3, 128.8, 128.6, 114.5, 64.4, 55.3, 52.3, 30.4, 26.7, 21.1.

HRMS (ESI^+, m/z) calcd for $C_{20}H_{22}NaO_4$ ($[M+Na]^+$): 349.1410. Found: 349.1407.

5-((*tert*-Butyldimethylsilyl)oxy)-2-(4-methoxyphenyl)-1-phenylpentan-1-one (8ae).



8ae

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), *tert*-butyl(4-(4-methoxy phenyl)butoxy)dimethylsilane (117.8 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% acetone in petroleum ether), the

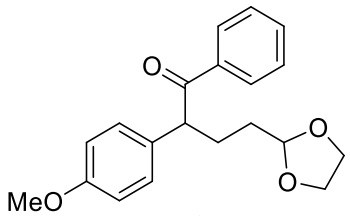
title compound was isolated in 51% yield (40.7 mg, 0.102 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.88 (m, 2H), 7.52-7.43 (m, 1H), 7.42-7.34 (m, 2H), 7.25-7.16 (m, 2H), 6.88-6.76 (m, 2H), 4.53 (t, *J* = 7.3 Hz, 1H), 3.75 (s, 3H), 3.61 (t, *J* = 6.4 Hz, 2H), 2.27-2.11 (m, 1H), 1.95-1.80 (m, 1H), 1.59-1.39 (m, 2H), 0.87 (s, 9H), 0.02 (d, *J* = 3.3 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.3, 158.7, 137.1, 132.9, 131.8, 129.4, 128.8, 128.6, 114.4, 63.2, 55.3, 52.5, 30.8, 30.5, 26.1, 18.5, -5.2.

HRMS (ESI^+, m/z) calcd for $C_{24}H_{34}NaO_3Si$ ($[M+Na]^+$): 421.2169. Found: 421.2162.

4-(1,3-Dioxolan-2-yl)-2-(4-methoxyphenyl)-1-phenylbutan-1-one (8af).



8af

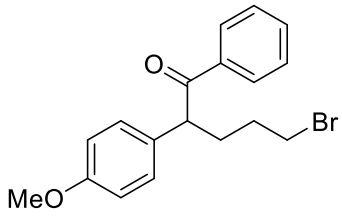
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 2-(3-(4-methoxyphenyl)propyl)-1,3-dioxolane (88.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 48% yield (31.3 mg, 0.096 mmol) as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.89 (m, 2H), 7.52-7.44 (m, 1H), 7.42-7.34 (m, 2H), 7.25-7.16 (m, 2H), 6.87-6.77 (m, 2H), 4.51 (t, *J* = 7.3 Hz, 1H), 4.36 (t, *J* = 5.7 Hz, 1H), 3.74 (s, 3H), 3.27 (s, 2H), 3.25 (s, 2H), 2.27-2.10 (m, 1H), 1.94-1.79 (m, 1H), 1.66-1.49 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0, 158.7, 136.9, 132.9, 131.5, 129.4, 128.8, 128.6, 114.5, 104.6, 55.3, 52.9, 52.8, 52.5, 30.6, 29.1.

HRMS (ESI^+, m/z) calcd for $C_{20}H_{22}NaO_4$ ($[M+Na]^+$): 349.1410. Found: 349.1411.

5-Bromo-2-(4-methoxyphenyl)-1-phenylpentan-1-one (8ag).



8ag

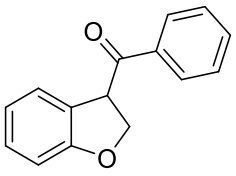
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-(4-bromobutyl)-4-methoxybenzene (97.3 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 61% yield (42.4 mg, 0.112 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.89 (m, 2H), 7.52-7.44 (m, 1H), 7.43-7.34 (m, 2H), 7.24-7.17 (m, 2H), 6.88-6.78 (m, 2H), 4.50 (t, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 3.39 (t, *J* = 6.9, 2H), 2.33-2.19 (m, 1H), 2.03-1.72 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 158.9, 136.7, 133.0, 131.1, 129.3, 128.8, 128.7, 114.6, 55.3, 52.1, 33.6, 32.6, 30.9.

HRMS (ESI^+, m/z) calcd for $C_{18}H_{19}BrNaO_2$ ($[M+Na]^+$): 369.0461. Found: 369.0458.

(2,3-Dihydrobenzofuran-3-yl)(phenyl)methanone (8ah).



8ah

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 2,3-dihydrobenzofuran (48.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 56% yield (25.1 mg, 0.112 mmol) as a white solid.

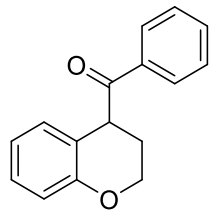
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-8.01 (m, 2H), 7.72-7.62 (m, 1H), 7.61-7.52 (m, 2H), 7.21-7.10 (m, 1H), 7.04-6.94 (m, 1H), 6.86 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.76 (td, *J* = 7.5, 1.0 Hz, 1H), 5.30 (dd, *J* = 9.5, 6.5 Hz, 1H), 5.12 (dd, *J* = 8.9, 6.5 Hz, 1H), 4.78 (t, *J* = 9.2 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 196.4, 160.2, 136.2, 133.9, 129.4, 129.2, 129.1, 125.3, 125.1,

120.5, 110.3, 72.6, 49.5.

Spectroscopic data are in accordance with those described in literature.[10]

Chroman-4-yl(phenyl)methanone (8ai).



8ai

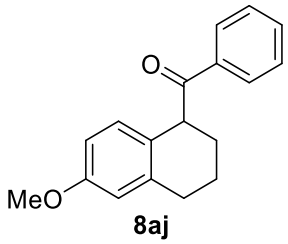
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), chromane (53.7 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 48% yield (22.9 mg, 0.096 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-7.96 (m, 2H), 7.67-7.57 (m, 1H), 7.52 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.16 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 1H), 6.96-6.87 (m, 2H), 6.82 (td, *J* = 7.4, 1.3 Hz, 1H), 4.84 (t, *J* = 6.0 Hz, 1H), 4.38-4.15 (m, 2H), 2.41-2.19 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 201.1, 155.3, 136.3, 133.5, 130.0, 129.0, 128.9, 128.6, 120.7, 120.0, 117.5, 63.5, 42.4, 26.2.

Spectroscopic data are in accordance with those described in literature.[10]

(6-Methoxy-1,2,3,4-tetrahydronaphthalen-1-yl)(phenyl)methanone (8aj).



8aj

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 6-methoxy-1,2,3,4-tetrahydronaphthalene (64.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 59% yield (31.4 mg, 0.118 mmol) as a white solid.

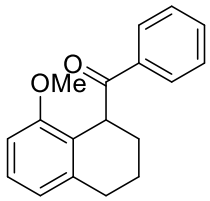
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-7.96 (m, 2H), 7.63-7.55 (m, 1H), 7.53-7.44 (m, 2H), 6.84 (d,

J = 8.3 Hz, 1H), 6.74-6.63 (m, 2H), 4.77 (t, *J* = 6.6 Hz, 1H), 3.78 (s, 3H), 2.95-2.72 (m, 2H), 2.21-2.01 (m, 2H), 1.99-1.84 (m, 1H), 1.82-1.71 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 202.9, 158.2, 139.1, 136.7, 133.1, 130.5, 128.9, 128.8, 127.0, 114.0, 112.4, 55.3, 46.8, 29.8, 27.9, 20.7.

Spectroscopic data are in accordance with those described in literature.[10]

(8-Methoxy-1,2,3,4-tetrahydronaphthalen-1-yl)(phenyl)methanone (8ak).



8ak

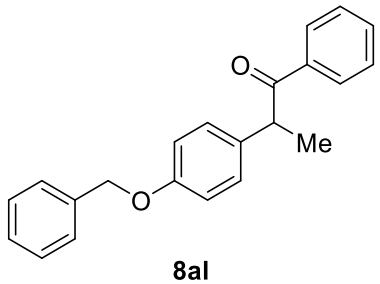
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 5-methoxy-1,2,3,4-tetrahydronaphthalene (64.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 3% ethyl acetate in petroleum ether), the title compound was isolated in 31% yield (16.5 mg, 0.062 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-7.97 (m, 2H), 7.61-7.53 (m, 1H), 7.53-7.45 (m, 2H), 7.16 (t, *J* = 7.9 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 6.65 (d, *J* = 8.1 Hz, 1H), 4.87 (t, *J* = 6.3 Hz, 1H), 3.58 (s, 3H), 2.95-2.70 (m, 2H), 2.16-2.03 (m, 1H), 2.01-1.79 (m, 2H), 1.78-1.65 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 203.0, 156.8, 139.5, 137.1, 132.5, 128.6, 128.5, 127.3, 124.6, 121.8, 107.6, 55.3, 42.0, 29.5, 27.1, 20.1.

Spectroscopic data are in accordance with those described in literature.[10]

2-(4-(Benzyloxy)phenyl)-1-phenylpropan-1-one (8al).



8al

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol,

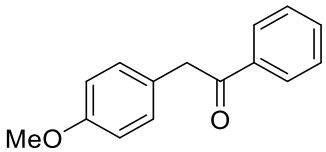
100 mol%), 1-(benzyloxy)-4-ethylbenzene (84.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 40% yield (25.3 mg, 0.080 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.92 (m, 2H), 7.53-7.43 (m, 2H), 7.43-7.28 (m, 7H), 7.24-7.16 (m, 2H), 6.96-6.86 (m, 2H), 5.00 (s, 2H), 4.65 (q, *J* = 6.8 Hz, 1H), 1.51 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.7, 157.9, 137.1, 136.6, 133.9, 132.9, 129.0, 128.9, 128.7, 128.6, 128.1, 127.6, 115.4, 70.1, 47.1, 19.7.

Spectroscopic data are in accordance with those described in literature.[10]

2-(4-Methoxyphenyl)-1-phenylethan-1-one (8am).



8am

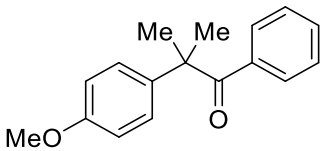
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-methoxy-4-methylbenzene (48.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 51% yield (23.1 mg, 0.102 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-7.97 (m, 2H), 7.62-7.51 (m, 1H), 7.50-7.41 (m, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 4.23 (s, 2H), 3.79 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 158.7, 136.7, 133.2, 130.6, 128.8, 128.7, 126.6, 114.3, 55.4, 44.8.

Spectroscopic data are in accordance with those described in literature.[31]

2-(4-Methoxyphenyl)-2-methyl-1-phenylpropan-1-one (8an).



8an

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol,

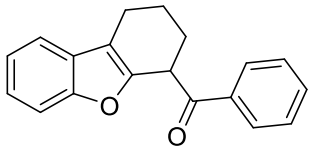
100 mol%), 1-isopropyl-4-methoxybenzene (60.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 13% yield (6.6 mg, 0.026 mmol) as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.44 (m, 2H), 7.40-7.31 (m, 1H), 7.26-7.19 (m, 4H), 6.93-6.86 (m, 2H), 3.81 (s, 3H), 1.57 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.2, 158.5, 137.4, 136.6, 131.7, 129.8, 128.1, 127.0, 114.5, 55.4, 50.8, 28.0.

Spectroscopic data are in accordance with those described in literature.[32]

Phenyl(1,2,3,4-tetrahydrodibenzo[b,d]furan-4-yl)methanone (8ao).



8ao

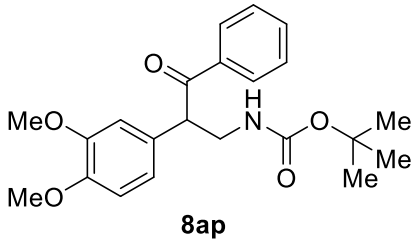
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1,2,3,4-tetrahydrodibenzo[*b,d*]furan (68.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 39% yield (21.6 mg, 0.078 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.01 (m, 2H), 7.66-7.58 (m, 1H), 7.56-7.50 (m, 2H), 7.49-7.44 (m, 1H), 7.40-7.33 (m, 1H), 7.25-7.18 (m, 2H), 4.86 (t, *J* = 6.1 Hz, 1H), 2.84-2.66 (m, 2H), 2.32-2.18 (m, 2H), 2.12-1.98 (m, 1H), 1.95-1.82 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 154.8, 150.6, 136.3, 133.5, 128.9, 128.9, 128.3, 123.8, 122.4, 119.0, 116.1, 111.3, 42.8, 27.8, 20.8, 20.5.

HRMS (ESI$^+$, m/z) calcd for $C_{19}H_{16}NaO_2$ ([M+Na]$^+$): 299.1043. Found: 299.1041.

tert-Butyl (2-(3,4-dimethoxyphenyl)-3-oxo-3- phenylpropyl)carbamate (8ap).



8ap

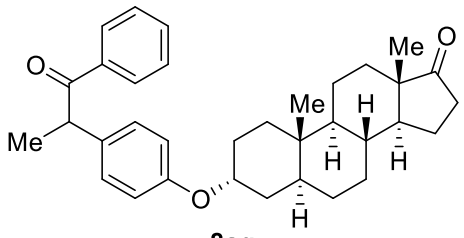
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), *tert*-butyl (3,4-dimethoxyphenethyl)carbamate (112.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 20% ethyl acetate in petroleum ether), the title compound was isolated in 55% yield (42.4 mg, 0.110 mmol) as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.88 (m, 2H), 7.51-7.43 (m, 1H), 7.36 (t, *J* = 7.7 Hz, 2H), 6.83-6.69 (m, 3H), 4.96 (d, *J* = 6.6 Hz, 1H), 4.82 (dd, *J* = 8.6, 5.6 Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.69-3.52 (m, 2H), 1.40 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 156.1, 149.5, 148.5, 136.4, 133.3, 129.4, 128.9, 128.6, 120.8, 111.7, 111.1, 79.4, 56.0, 55.9, 53.6, 43.9, 28.5.

Spectroscopic data are in accordance with those described in literature.[10]

(*3R,5S,8R,9S,10S,13S,14S*)-10,13-Dimethyl-3-(4-(1-oxo-1-phenylpropan-2-yl)phenoxy)hexadecahydro-17H-cyclopenta[a]phenanthren-17-one (8aq).



8aq

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%),

(*3R,5S,8R,9S,10S,13S,14S*)-3-(4-ethylphenoxy)-10,13-dimethylhexadecahydro-17H-cyclopenta[a]phenanthren-17-one (157.8 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 54% yield (53.8 mg, 0.108 mmol) as a white solid.

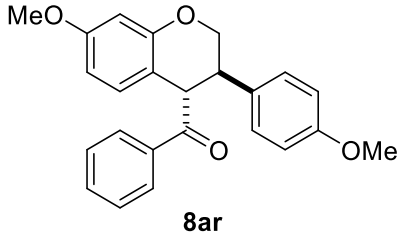
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.91 (m, 2H), 7.52-7.43 (m, 1H), 7.37 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 6.85-6.76 (m, 2H), 4.63 (q, *J* = 6.8 Hz, 1H), 4.45 (t, *J* = 2.8 Hz, 1H), 2.42 (dd, *J* = 19.2, 8.7 Hz, 1H), 2.10-2.01 (m, 1H), 1.92-1.76 (m, 4H), 1.72-1.55 (m, 6H), 1.50 (d, *J* = 6.9 Hz, 3H), 1.44-1.14 (m, 8H), 1.00 (dq, *J* = 12.1, 6.8 Hz, 1H), 0.90-0.78 (m, 1H), 0.85 (s, 3H), 0.83 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 221.6, 200.7, 156.8, 136.7, 133.1, 133.1, 132.8, 128.9, 128.5,

116.4, 72.0, 71.9, 54.4, 51.6, 47.9, 47.0, 39.7, 36.0, 36.0, 35.1, 32.8, 32.7, 31.7, 30.9, 28.2, 25.7, 21.9, 20.2, 19.6, 13.9, 11.5.

Spectroscopic data are in accordance with those described in literature.[10]

(7-Methoxy-3-(4-methoxyphenyl)chroman-4-yl)(phenyl)methanone (8ar).



8ar

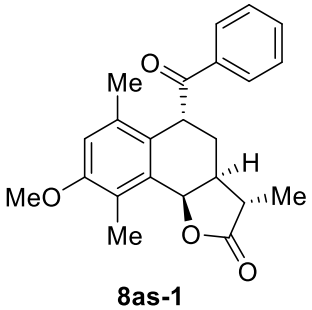
This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 7-methoxy-3-(4-methoxyphenyl)chromane (108.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 45% yield (33.7 mg, 0.090 mmol, d.r. > 20:1) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.83 (m, 2H), 7.58-7.50 (m, 1H), 7.48-7.40 (m, 2H), 7.15-7.07 (m, 2H), 6.84-6.76 (m, 3H), 6.51 (d, *J* = 2.6 Hz, 1H), 6.47-6.38 (m, 1H), 4.92 (d, *J* = 7.8 Hz, 1H), 4.38 (dd, *J* = 10.9, 3.6 Hz, 1H), 4.17 (dd, *J* = 10.9, 8.5 Hz, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 3.60 (td, *J* = 8.2, 3.5 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 201.2, 159.9, 158.9, 155.6, 137.2, 133.3, 132.0, 129.7, 128.9, 128.9, 128.8, 114.4, 113.0, 108.3, 102.0, 69.2, 55.4, 55.3, 49.5, 41.3.

HRMS (ESI$^+$, m/z) calcd for $C_{24}H_{22}NaO_4$ ([M+Na]$^+$): 397.1410. Found: 397.1413.

(*3S,3aS,5R,9bR*)-5-Benzoyl-8-methoxy-3,6,9-trimethyl-3a,4,5,9b-tetrahydronapth o[1,2-*b*]furan-2(3*H*)-one (8as-1).



8as-1

This compound was prepared according to the ***GPA*** using benzoyl cyanide (26.2 mg, 0.200 mmol,

100 mol%),

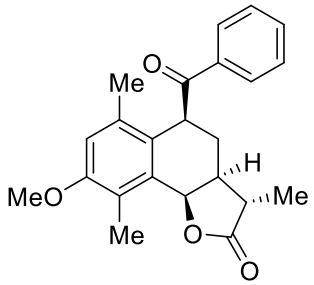
(*3S,3aS,9bR*)-8-methoxy-3,6,9-trimethyl-3a,4,5,9b-tetrahydronaphtho[1,2-*b*]furan-2(3*H*)-one (104.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), the title compound **8as-1** was isolated in 54% yield (39.4 mg, 0.108 mmol) as a light yellow solid. At the same time, the isomer **8as-2** was isolated in 17% yield (12.3 mg, 0.034 mmol) as a light yellow solid. The total yield was 71%, d.r. = 3.2:1. The d.r. value was confirmed by isolated yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.07 (m, 2H), 7.69-7.62 (m, 1H), 7.61-7.52 (m, 2H), 6.76 (s, 1H), 5.68 (d, *J* = 5.0 Hz, 1H), 5.03 (dd, *J* = 6.2, 2.1 Hz, 1H), 3.82 (s, 3H), 2.45-2.35 (m, 1H), 2.33 (s, 3H), 2.31-2.24 (m, 1H), 2.17-2.10 (m, 1H), 2.10 (s, 3H), 2.06-1.92 (m, 1H), 1.38 (d, *J* = 7.7 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 179.5, 156.7, 135.5, 133.8, 133.8, 131.5, 129.2, 128.5, 126.1, 125.9, 113.8, 75.3, 55.7, 43.4, 43.4, 37.9, 28.0, 20.3, 15.1, 11.6.

HRMS (ESI$^+$, m/z) calcd for $C_{23}H_{24}NaO_4$ ([M+Na]$^+$): 387.1567. Found: 387.1562.

(*3S,3aS,5S,9bR*)-5-Benzoyl-8-methoxy-3,6,9-trimethyl-3a,4,5,9b-tetrahydronapht ho[1,2-*b*]furan-2(3*H*)-one (8as-2).



8as-2

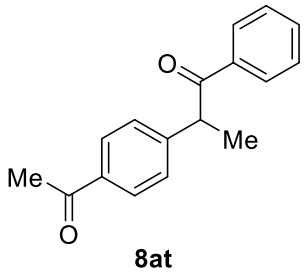
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.91 (m, 2H), 7.64-7.55 (m, 1H), 7.52-7.43 (m, 2H), 6.74 (s, 1H), 5.65 (d, *J* = 6.3 Hz, 1H), 4.71 (t, *J* = 7.3 Hz, 1H), 3.83 (s, 3H), 2.61 (qd, *J* = 7.3, 5.4 Hz, 1H), 2.53-2.43 (m, 1H), 2.34 (s, 3H), 2.32-2.24 (m, 1H), 2.15-2.07 (m, 1H), 2.03 (s, 3H), 1.25 (d, *J* = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 202.2, 179.1, 156.8, 135.7, 135.1, 133.5, 131.5, 129.0, 128.6, 126.2, 126.2, 114.1, 75.6, 55.8, 45.7, 41.0, 40.6, 28.0, 21.4, 14.2, 11.9.

HRMS (ESI$^+$, m/z) calcd for $C_{23}H_{24}NaO_4$ ([M+Na]$^+$): 387.1567. Found: 387.1564.

General Procedure B (GPB) for acyl cyanide coupling with electron-deficient and -neutral ethylbenzene: To an oven-dried Schlenk tube equipped with a stirring bar was added $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (2.2 mg, 0.002 mmol, 1 mol%), sodium bromide (8.2 mg, 0.080 mmol, 40 mol%), anhydrous sodium carbonate (42.4 mg, 0.400 mmol, 200 mol%), acyl cyanide (if solid, 0.200 mmol, 100 mol%) and ethyl benzene (if solid, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Acyl cyanide (if liquid, 0.200 mmol, 100 mol%), ethyl benzene (if liquid, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation in an aluminum module at 40 ℃ for 12 hours under N_2 atmosphere. After the reaction completed, the mixture was added 30 mL of EtOAc and washed with brine. The organic phase was dried over Na_2SO_4, filtered, and evaporated under vacuum. The residue was purified by silica gel column chromatography to give the target product. (Note: The liquid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

2-(4-Acetylphenyl)-1-phenylpropan-1-one (8at).



8at

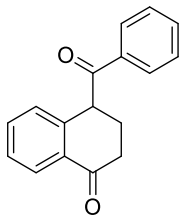
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethylacetophenone (59.3 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 74% yield (37.3 mg, 0.148 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.82 (m, 4H), 7.55-7.44 (m, 1H), 7.43-7.33 (m, 4H), 4.76 (q, J = 6.9 Hz, 1H), 2.54 (s, 3H), 1.55 (d, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 197.7, 146.9, 136.3, 136.0, 133.2, 129.2, 128.8, 128.7, 128.1, 47.9, 26.7, 19.4.

HRMS (ESI$^+$, m/z) calcd for $C_{17}H_{16}NaO_2$ ([M+Na]$^+$): 275.1043. Found: 275.1041.

4-Benzoyl-3,4-dihydronaphthalen-1(2*H*)-one (8au).



8au

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 3,4-dihydronaphthalen-1(2*H*)-one (58.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 47% yield (23.5 mg, 0.094 mmol) as a light yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 7.8, 1.6 Hz, 1H), 8.10-8.02 (m, 2H), 7.69-7.60 (m, 1H), 7.58-7.51 (m, 2H), 7.47 (td, *J* = 7.5, 1.6 Hz, 1H), 7.40 (td, *J* = 7.5, 1.3 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 5.05 (t, *J* = 5.3 Hz, 1H), 2.84-2.71 (m, 1H), 2.67-2.58 (m, 1H), 2.57-2.41 (m, 2H).

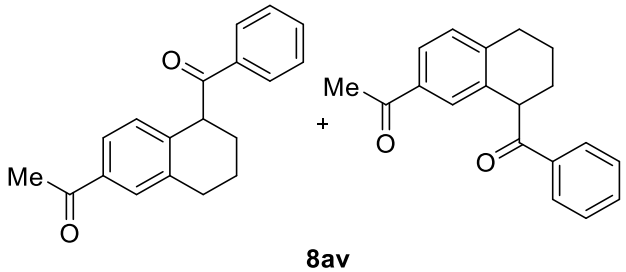
^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 197.2, 141.8, 136.1, 133.8, 133.7, 133.4, 129.1, 128.8, 127.9, 127.7, 46.5, 35.4, 26.8.

HRMS (ESI$^+$, m/z) calcd for $C_{17}H_{14}NaO_2$ ([M+Na]$^+$): 273.0886. Found: 273.0885.

The mixture of isomers

1-(5-benzoyl-5,6,7,8-tetrahydronaphthalen-2-yl)ethan-1-one and

1-(8-benzoyl-5,6,7,8-tetrahydronaphthalen-2-yl)ethan-1-one (8av).



8av

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-(5,6,7,8-tetrahydronaphthalen-2-yl)ethan-1-one (69.7 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 54% yield (28.9 mg, 0.108 mmol, r.r. = 1:1) as a colorless oil. The r.r.

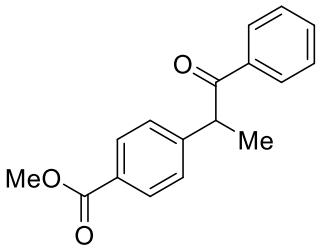
value was determined by ^{1}H NMR analysis.

^{1}H NMR (400 MHz, $CDCl_3$, for all isomers) δ 8.08-7.97 (m, 4H), 7.79-7.73 (m, 2H), 7.67 (dd, J = 8.0, 1.9 Hz, 1H), 7.64-7.57 (m, 2H), 7.56-7.46 (m, 5H), 7.27-7.23 (m, 1H), 7.01 (d, *J* = 8.1 Hz, 1H), 4.92 (t, *J* = 6.2 Hz, 1H), 4.88 (t, *J* = 6.5 Hz, 1H), 3.04-2.90 (m, 2H), 2.90-2.78 (m, 2H), 2.57 (s, 3H), 2.49 (s, 3H), 2.26-2.15 (m, 2H), 2.15-2.03 (m, 2H), 2.00-1.86 (m, 2H), 1.86-1.77 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, for all isomers) δ 202.0, 201.9, 198.3, 198.0, 144.0, 140.5, 138.4, 136.3, 136.2, 135.6, 135.1, 135.1, 133.4, 133.4, 129.9, 129.7, 129.5, 128.9, 128.8, 128.8, 126.7, 125.9, 47.5, 47.0, 29.5, 29.4, 27.5, 27.4, 26.7, 26.6, 20.5, 20.0.

HRMS (ESI^+, m/z) calcd for $C_{19}H_{18}NaO_2$ ($[M+Na]^+$): 301.1199. Found: 301.1196.

Methyl 4-(1-oxo-1-phenylpropan-2-yl)benzoate (8aw).



8aw

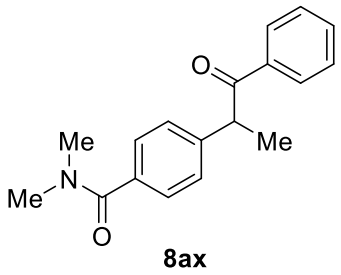
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), methyl 4-ethylbenzoate (65.7 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 58% yield (31.1 mg, 0.116 mmol) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.87 (m, 4H), 7.53-7.44 (m, 1H), 7.44-7.32 (m, 4H), 4.75 (q, *J* = 6.9 Hz, 1H), 3.87 (s, 3H), 1.55 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 166.9, 146.7, 136.3, 133.2, 130.4, 129.0, 128.8, 128.7, 128.0, 52.2, 48.0, 19.4.

Spectroscopic data are in accordance with those described in literature.[33]

N,N-dimethyl-4-(1-oxo-1-phenylpropan-2-yl)benzamide (8ax).



8ax

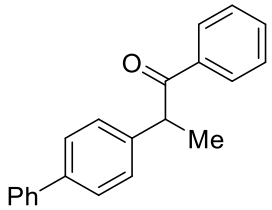
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethyl-*N,N*-dimethylbenzamide (70.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 33% ethyl acetate in petroleum ether), the title compound was isolated in 56% yield (31.5 mg, 0.112 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.88 (m, 2H), 7.53-7.45 (m, 1H), 7.42-7.28 (m, 6H), 4.71 (q, *J* = 6.8 Hz, 1H), 3.05 (s, 3H), 2.95 (s, 3H), 1.52 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 171.4, 143.1, 136.3, 135.0, 133.1, 128.9, 128.7, 127.9, 127.9, 47.7, 39.7, 35.5, 19.6.

HRMS (ESI^+, m/z) calcd for $C_{18}H_{19}NNaO_2$ ($[M+Na]^+$): 304.1308. Found: 304.1303.

2-([1,1'-Biphenyl]-4-yl)-1-phenylpropan-1-one (8ay).



8ay

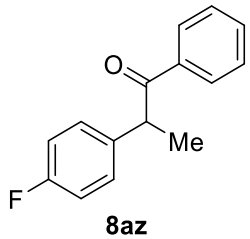
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethyl-1,1'-biphenyl (72.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 51% yield (29.2 mg, 0.102 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.7 Hz, 2H), 7.59-7.51 (m, 4H), 7.50-7.46 (m, 1H), 7.45 -7.29 (m, 7H), 4.75 (q, *J* = 6.9 Hz, 1H), 1.59 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.4, 140.7, 140.6, 139.9, 136.6, 133.0, 128.9, 128.9, 128.7, 128.3, 127.8, 127.4, 127.1, 47.6, 19.6.

Spectroscopic data are in accordance with those described in literature.[28]

2-(4-Fluorophenyl)-1-phenylpropan-1-one (8az).



8az

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-fluorobenzene (49.7 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 52% yield (23.7 mg, 0.104 mmol) as a colorless oil.

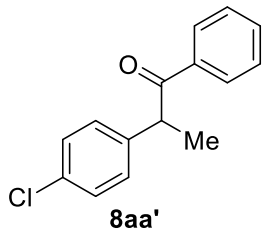
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.89 (m, 2H), 7.54-7.45 (m, 1H), 7.44-7.34 (m, 2H), 7.31-7.20 (m, 2H), 7.03-6.93 (m, 2H), 4.69 (q, J = 6.9 Hz, 1H), 1.52 (d, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.4, 161.9 (C-F, d, $^1J_{C\text{-}F}$ = 246.4 Hz), 137.2 (C-F, d, $^4J_{C\text{-}F}$ = 3.2 Hz), 136.4, 133.1, 129.4 (C-F, d, $^3J_{C\text{-}F}$ = 8.0 Hz), 128.9, 128.7, 116.0 (C-F, d, $^2J_{C\text{-}F}$ = 21.4 Hz), 47.1, 19.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -115.84.

Spectroscopic data are in accordance with those described in literature.[33]

2-(4-Chlorophenyl)-1-phenylpropan-1-one (8aa').



8aa'

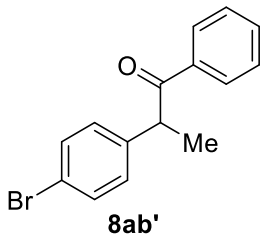
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%),1-chloro-4-ethylbenzene (56.2 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 61% yield (29.9 mg, 0.122 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.88 (m, 2H), 7.53-7.47 (m, 1H), 7.44-7.35 (m, 2H), 7.30-7.20 (m, 4H), 4.68 (q, J = 6.9 Hz, 1H), 1.52 (d, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 140.0, 136.3, 133.1 132.9, 129.3, 129.3, 128.8, 128.7, 47.2, 19.6.

Spectroscopic data are in accordance with those described in literature.[28]

2-(4-Bromophenyl)-1-phenylpropan-1-one (8ab').



8ab'

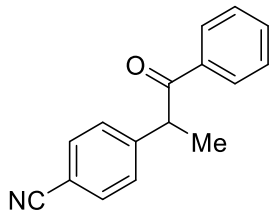
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%),1-bromo-4-ethylbenzene (74.0 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 60% yield (34.7 mg, 0.120 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.89 (m, 2H), 7.53-7.47 (m, 1H), 7.45-7.34 (m, 4H), 7.22-7.12 (m, 2H), 4.66 (q, *J* = 6.9 Hz, 1H), 1.52 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0, 140.5, 136.3, 133.2, 132.2, 129.6, 128.8, 128.7, 121.0, 47.3, 19.5.

Spectroscopic data are in accordance with those described in literature.[34]

4-(1-Oxo-1-phenylpropan-2-yl)benzonitrile (8ac').



8ac'

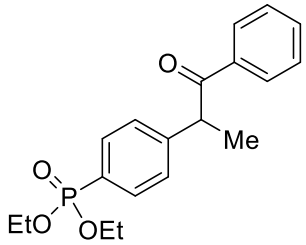
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.3 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 3% ethyl acetate in petroleum ether), the title compound was isolated in 89% yield (41.9 mg, 0.178 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.88 (m, 2H), 7.64-7.56 (m, 2H), 7.56-7.49 (m, 1H), 7.47-7.34 (m, 4H), 4.77 (q, *J* = 6.9 Hz, 1H), 1.55 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 146.8, 136.0, 133.5, 132.9, 128.9, 128.8, 118.8, 111.1, 47.7, 19.4.

Spectroscopic data are in accordance with those described in literature.[35]

Diethyl (4-(1-oxo-1-phenylpropan-2-yl)phenyl)phosphonate (8ad').



8ad'

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), diethyl (4-ethylphenyl)phosphonate (96.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 33% ethyl acetate in petroleum ether), the title compound was isolated in 51% yield (35.3 mg, 0.102 mmol) as a colorless oil.

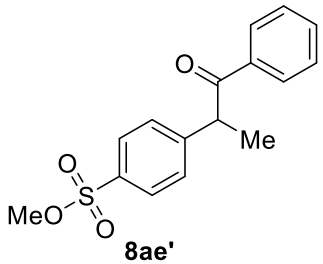
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.88 (m, 2H), 7.78-7.67 (m, 2H), 7.53-7.46 (m, 1H), 7.43-7.34 (m, 4H), 4.74 (q, J = 6.9 Hz, 1H), 4.19-3.94 (m, 4H), 1.53 (d, J = 6.9 Hz, 3H), 1.29 (td, J = 7.1, 3.4 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 146.1 (d, J_{C-P} = 3.2 Hz), 136.2, 133.2, 132.5 (d, J_{C-P} = 10.3 Hz), 128.9, 128.7, 128.1 (d, J_{C-P} = 15.4 Hz), 126.9 (d, J_{C-P} = 190.7 Hz), 62.3 (d, J_{C-P} = 5.5 Hz), 47.8, 19.5, 16.4 (d, J_{C-P} = 6.3 Hz).

^{31}P NMR (162 MHz, $CDCl_3$) δ 18.67.

HRMS (ESI$^+$, m/z) calcd for $C_{19}H_{23}NaO_4P$ ([M+Na]$^+$): 369.1226. Found: 369.1226.

Methyl 4-(1-oxo-1-phenylpropan-2-yl)benzenesulfonate (8ae').



8ae'

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), methyl 4-ethylbenzenesulfonate (80.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was

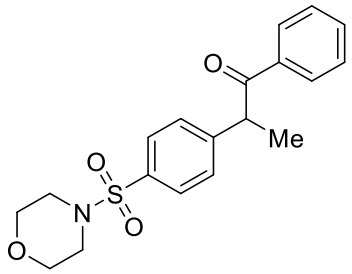
isolated in 36% yield (21.9 mg, 0.072 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.90 (m, 2H), 7.88-7.81 (m, 2H), 7.57-7.47 (m, 3H), 7.46-7.39 (m, 2H), 4.82 (q, *J* = 6.9 Hz, 1H), 3.74 (s, 3H), 1.57 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 147.9, 136.0, 133.9, 133.5, 128.9, 128.8, 128.8, 56.5, 47.5, 19.5.

HRMS (ESI^+, m/z) calcd for $C_{16}H_{16}NaO_4S$ ($[M+Na]^+$): 327.0662. Found: 327.0661.

2-(4-(Morpholinosulfonyl)phenyl)-1-phenylpropan-1-one (8af').



8af'

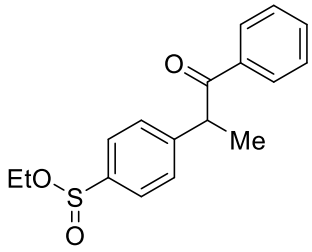
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-((4-ethylphenyl)sulfonyl)morpholine (95.7 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), the title compound was isolated in 57% yield (40.9 mg, 0.114 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.89 (m, 2H), 7.72-7.64 (m, 2H), 7.57 7.51 (m, 1H), 7.51-7.46 (m, 2H), 7.46-7.39 (m, 2H), 4.80 (q, *J* = 6.9 Hz, 1H), 3.72 (t, *J* = 4.8 Hz, 4H), 2.97 (t, *J* = 4.7 Hz, 4H), 1.57 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 147.0, 136.1, 133.8, 133.5, 128.9, 128.8, 128.7, 128.6, 66.2, 47.5, 46.0, 19.6.

HRMS (ESI^+, m/z) calcd for $C_{19}H_{21}NNaO_4S$ ($[M+Na]^+$): 382.1083. Found: 382.1081.

Ethyl 4-(1-oxo-1-phenylpropan-2-yl)benzenesulfinate (8ag').



8ag'

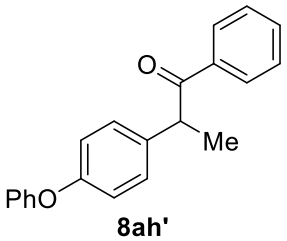
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), ethyl 4-ethylbenzenesulfinate (79.3 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), compound **8ag'** was isolated in 35% yield (21.2 mg, 0.070 mmol) as a white solid. ^{13}C NMR showed the d.r. value is 1:1 (d.r. caused by the chiral center located in sulfur center and benzylic carbon center).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.89 (m, 2H), 7.68-7.60 (m, 2H), 7.54-7.48 (m, 1H), 7.48-7.44 (m, 2H), 7.44-7.37 (m, 2H), 4.78 (q, *J* = 6.9 Hz, 1H), 4.16 -4.03 (m, 1H), 3.80-3.68 (m, 1H), 1.55 (d, *J* = 6.9 Hz, 3H), 1.26 (td, *J* = 7.1, 3.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, for all isomers) δ 199.8, 199.7, 145.9, 145.9, 143.6, 143.6, 136.2, 133.3, 128.8, 128.8, 128.7, 126.0, 126.0, 61.6, 61.6, 47.7, 47.7, 19.6, 15.7.

HRMS (ESI^+, m/z) calcd for $C_{17}H_{18}NaO_3S$ ($[M+Na]^+$): 325.0869. Found: 325.0865.

2-(4-Phenoxyphenyl)-1-phenylpropan-1-one (8ah').



8ah'

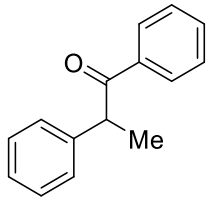
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-phenoxybenzene (79.3 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 47% yield (28.4 mg, 0.094 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.93 (m, 2H), 7.55-7.47 (m, 1H), 7.45-7.37 (m, 2H), 7.35-7.28 (m, 2H), 7.28-7.22 (m, 2H), 7.13-7.06 (m, 1H), 7.02-6.89 (m, 4H), 4.69 (q, *J* = 6.9 Hz, 1H), 1.54 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.5, 157.1, 156.3, 136.5, 136.2, 133.0, 129.9, 129.2, 128.9, 128.7, 123.5, 119.2, 119.1, 47.1, 19.7.

Spectroscopic data are in accordance with those described in literature.[10]

1,2-Diphenylpropan-1-one (8ai').



8ai'

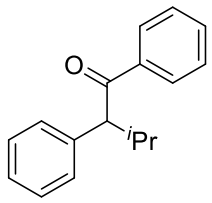
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), ethylbenzene (42.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 43% yield (18.1 mg, 0.086 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.91 (m, 2H), 7.52-7.44 (m, 1H), 7.42-7.34 (m, 2H), 7.33-7.27 (m, 4H), 7.24-7.16 (m, 1H), 4.69 (q, J = 6.8 Hz, 1H), 1.54 (d, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.5, 141.6, 136.6, 132.9, 129.1, 128.9, 128.6, 127.9, 127.0, 48.0, 19.6.

Spectroscopic data are in accordance with those described in literature.[33]

3-Methyl-1,2-diphenylbutan-1-one (8aj').



8aj'

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), isobutylbenzene (53.7 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 27% yield (12.9 mg, 0.054 mmol) as a white solid.

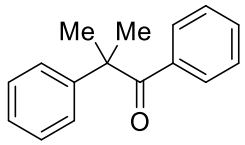
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.94 (m, 2H), 7.52-7.45 (m, 1H), 7.44-7.37 (m, 2H), 7.37-7.31 (m, 2H), 7.31-7.26 (m, 2H), 7.22-7.16 (m, 1H), 4.21 (d, J = 10.1 Hz, 1H), 2.67-2.51 (m, 1H), 1.01 (d,

J = 6.5 Hz, 3H), 0.76 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 138.7, 137.8, 132.9, 128.9, 128.8, 128.6, 127.2, 61.5, 32.0, 22.1, 20.7.

Spectroscopic data are in accordance with those described in literature.[36]

2-Methyl-1,2-diphenylpropan-1-one (8al').



8al'

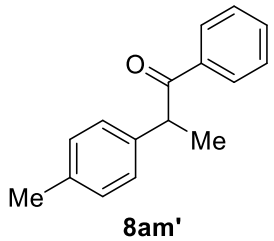
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), cumene (48.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 31% yield (13.9 mg, 0.062 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.46 (m, 2H), 7.41-7.30 (m, 5H), 7.29-7.18 (m, 3H), 1.61 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 203.9, 145.4, 136.4, 131.8, 129.9, 129.1, 128.1, 126.9, 125.8, 51.5, 28.0.

Spectroscopic data are in accordance with those described in literature.[37]

1-Phenyl-2-(p-tolyl)propan-1-one (8am').



8am'

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%),1-ethyl-4-methylbenzene (48.1 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 68% yield (30.5 mg, 0.136 mmol) as a colorless oil.

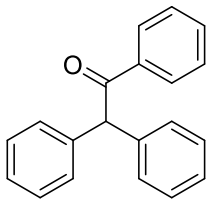
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.90 (m, 2H), 7.51-7.43 (m, 1H), 7.42-7.32 (m, 2H),

7.21-7.14 (m, 2H), 7.13-7.06 (m, 2H), 4.65 (q, *J* = 6.8 Hz, 1H), 2.28 (s, 3H), 1.51 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 138.6, 136.7, 136.7, 132.8, 129.8, 128.9, 128.6, 127.8, 47.6, 21.1, 19.6.

Spectroscopic data are in accordance with those described in literature.[33]

1,2,2-Triphenylethan-1-one (8an').



8an'

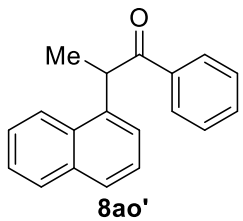
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), diphenylmethane (67.3 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 48% yield (26.1 mg, 0.096 mmol) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.89 (m, 2H), 7.47-7.40 (m, 1H), 7.37-7.29 (m, 2H), 7.27-7.17 (m, 10H), 5.97 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 139.2, 136.9, 133.2, 129.3, 129.1, 128.9, 128.7, 127.3, 59.6.

Spectroscopic data are in accordance with those described in literature.[38]

2-(Naphthalen-1-yl)-1-phenylpropan-1-one (8ao').



8ao'

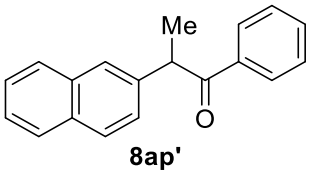
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethylnaphthalene (62.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 52% yield (27.1 mg, 0.104 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31-8.22 (m, 1H), 7.95-7.83 (m, 3H), 7.77-7.71 (m, 1H), 7.67-7.60 (m, 1H), 7.58-7.52 (m, 1H), 7.45-7.38 (m, 1H), 7.37-7.31 (m, 1H), 7.31-7.25 (m, 2H), 7.24 -7.19 (m, 1H), 5.39 (q, *J* = 6.8 Hz, 1H), 1.64 (d, *J* = 6.9 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 138.1, 136.4, 134.5, 132.9, 130.7, 129.5, 128.7, 128.6, 127.7, 126.9, 126.0, 125.9, 125.2, 122.7, 43.8, 18.7.

Spectroscopic data are in accordance with those described in literature.[36]

2-(Naphthalen-2-yl)-1-phenylpropan-1-one (8ap').



8ap'

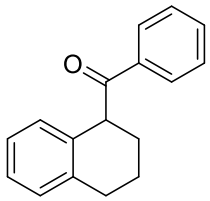
This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 2-ethylnaphthalene (62.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 47% yield (24.5 mg, 0.094 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-7.96 (m, 2H), 7.85-7.75 (m, 3H), 7.73 (s, 1H), 7.51-7.40 (m, 4H), 7.40-7.32 (m, 2H), 4.86 (q, *J* = 6.8 Hz, 1H), 1.62 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.4, 139.1, 136.6, 133.8, 132.9, 132.5, 128.9, 128.6, 127.9, 127.8, 126.6, 126.3, 126.1, 125.9, 48.2, 19.7.

Spectroscopic data are in accordance with those described in literature.[35]

Phenyl(1,2,3,4-tetrahydronaphthalen-1-yl)methanone (8aq').



8aq'

This compound was prepared according to the ***GPB*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1,2,3,4-tetrahydronaphthalene (52.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was

isolated in 40% yield (18.9 mg, 0.080 mmol) as a white solid.

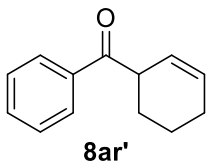
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-7.97 (m, 2H), 7.64-7.55 (m, 1H), 7.53-7.45 (m, 2H), 7.21-7.14 (m, 2H), 7.13-7.05 (m, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 4.84 (t, *J* = 6.7 Hz, 1H), 3.00-2.75 (m, 2H), 2.25-2.02 (m, 2H), 2.02-1.88 (m, 1H), 1.86-1.73 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 202.7, 137.8, 136.7, 134.9, 133.1, 129.6, 129.5, 128.9, 128.8, 126.8, 126.0, 47.5, 29.4, 27.7, 20.8.

Spectroscopic data are in accordance with those described in literature.[39]

Procedure for cyclohexene allylic acylation reaction with benzoyl cyanide: To an oven-dried Schlenk tube equipped with a stirring bar was added $Ir[dF(CF_3)ppy)_2(dtbbpy)PF_6$ (2.2 mg, 0.002 mmol, 1 mol%), $ZnBr_2$ (18.0 mg, 0.080 mmol, 40 mol%), and K_2CO_3 (55.3, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), cyclohexene (164.3 mg, 2.000 mmol, 1000 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation at r.t. for 12 hours under N_2 atmosphere. After the reaction completed, the mixture was added 30 mL of EtOAc and washed with brine. The organic phase was dried over Na_2SO_4, filtered, and evaporated under vacuum. The residue was purified by silica gel column chromatography to give the target product. (Note: The liquid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

Cyclohex-2-en-1-yl(phenyl)methanone (8ar').



8ar'

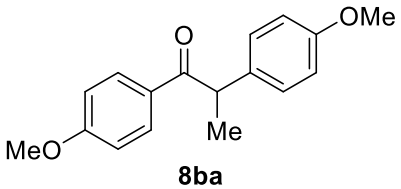
This compound was prepared according to the procedure mentioned above using benzoyl cyanide After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 53% yield (19.7 mg, 0.106 mmol) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00-7.91 (m, 2H), 7.59-7.51 (m, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 5.96-5.87 (m, 1H), 5.78-5.70 (m, 1H), 4.13-4.04 (m, 1H), 2.15-2.01 (m, 2H), 2.00-1.93 (m, 1H), 1.91-1.79 (m, 2H), 1.74-1.62 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 201.9, 136.3, 133.0, 130.2, 128.8, 128.6, 124.8, 44.0, 26.0, 24.9, 21.0.

Spectroscopic data are in accordance with those described in literature.[40]

1,2-Bis(4-methoxyphenyl)propan-1-one (8ba).



8ba

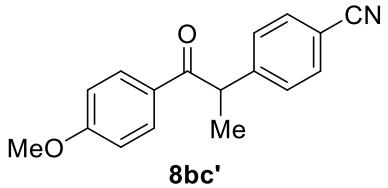
This compound was prepared according to the ***GPA*** using 4-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 84% yield (45.4 mg, 0.168 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.89 (m, 2H), 7.23-7.15 (m, 2H), 6.90-6.77 (m, 4H), 4.60 (q, *J* = 6.8 Hz, 1H), 3.81 (s, 3H), 3.75 (s, 3H), 1.49 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 163.3, 158.5, 134.1, 131.2, 129.5, 128.8, 114.4, 113.7, 55.5, 55.3, 46.7, 19.7.

Spectroscopic data are in accordance with those described in literature.[33]

4-(1-(4-Methoxyphenyl)-1-oxopropan-2-yl)benzonitrile (8bc').



8bc'

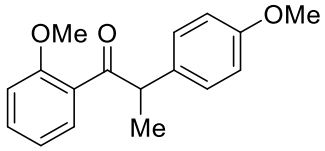
This compound was prepared according to the ***GPB*** using 4-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 71% yield (37.7 mg, 0.142 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.87 (m, 2H), 7.62-7.55 (m, 2H), 7.45-7.37 (m, 2H), 6.92-6.84 (m, 2H), 4.72 (q, *J* = 6.9 Hz, 1H), 3.83 (s, 3H), 1.53 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 163.8, 147.2, 132.8, 131.1, 129.0, 128.7, 118.8, 114.0, 110.9, 55.6, 47.4, 19.5.

HRMS (ESI^+, m/z) calcd for $C_{17}H_{15}NNaO_2$ ($[M+Na]^+$): 288.0995. Found: 288.0991.

1-(2-Methoxyphenyl)-2-(4-methoxyphenyl)propan-1-one (8ca).



8ca

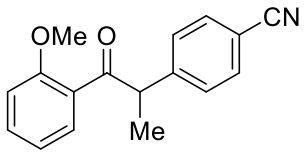
This compound was prepared according to the ***GPA*** using 2-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 81% yield (43.8 mg, 0.162 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.39-7.32 (m, 1H), 7.17-7.09 (m, 2H), 6.93-6.84 (m, 2H), 6.82-6.75 (m, 2H), 4.67 (q, *J* = 7.0 Hz, 1H), 3.85 (s, 3H), 3.74 (s, 3H), 1.48 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 158.4, 157.6, 133.5, 132.8, 130.5, 129.3, 129.1, 120.7, 113.9, 111.4, 55.5, 55.3, 51.0, 18.8.

HRMS (ESI^+, m/z) calcd for $C_{17}H_{18}NaO_3$ ($[M+Na]^+$): 293.1148. Found: 293.1147.

4-(1-(2-Methoxyphenyl)-1-oxopropan-2-yl)benzonitrile (8cc').



8cc'

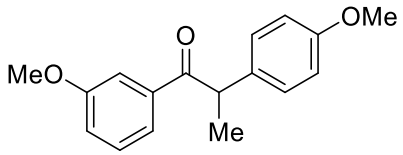
This compound was prepared according to the ***GPB*** using 2-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 26% yield (13.8 mg, 0.052 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.53 (m, 2H), 7.52 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.44-7.38 (m, 1H), 7.37 -7.32 (m, 2H), 6.95 (t, *J* = 7.5, 1.0 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 4.80 (q, *J* = 7.0 Hz, 1H), 3.84 (s, 3H), 1.50 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 202.7, 157.8, 147.2, 133.7, 132.3, 130.8, 129.1, 128.2, 121.0, 119.0, 111.5, 110.6, 55.5, 51.9, 19.0.

HRMS (ESI^+, m/z) calcd for $C_{17}H_{15}NNaO_2$ ($[M+Na]^+$): 288.0995. Found: 288.0994.

1-(3-Methoxyphenyl)-2-(4-methoxyphenyl)propan-1-one (8da).



8da

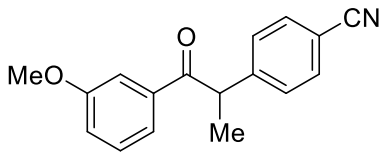
This compound was prepared according to the ***GPA*** using 3-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 47% yield (25.4 mg, 0.094 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.50 (m, 1H), 7.50-7.46 (m, 1H), 7.30-7.26 (m, 1H), 7.23-7.16 (m, 2H), 7.02 (dd, *J* = 8.2, 2.7 Hz, 1H), 6.87-6.79 (m, 2H), 4.62 (q, *J* = 6.8 Hz, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 1.50 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.5, 159.8, 158.6, 138.0, 133.6, 129.5, 128.9, 121.5, 119.3, 114.5, 113.2, 55.5, 55.3, 47.2, 19.7.

HRMS (ESI^+, m/z) calcd for $C_{17}H_{18}NaO_3$ ($[M+Na]^+$): 293.1148. Found: 293.1146.

4-(1-(3-Methoxyphenyl)-1-oxopropan-2-yl)benzonitrile (8dc').



8dc'

This compound was prepared according to the ***GPB*** using 3-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was

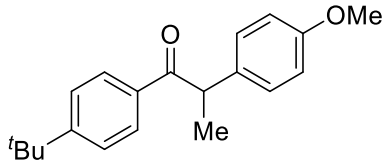
isolated in 33% yield (17.5 mg, 0.066 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.56 (m, 2H), 7.51-7.43 (m, 2H), 7.43-7.37 (m, 2H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.06 (dd, *J* = 8.0, 2.6 Hz, 1H), 4.74 (q, *J* = 6.9 Hz, 1H), 3.82 (s, 3H), 1.55 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 160.0, 146.8, 137.4, 132.9, 129.8, 128.8, 121.3, 119.8, 118.8, 113.3, 111.1, 55.6, 47.9, 19.4.

HRMS (ESI^+, m/z) calcd for $C_{17}H_{15}NNaO_2$ ($[M+Na]^+$): 288.0995. Found: 288.0995.

1-(4-(*tert*-Butyl)phenyl)-2-(4-methoxyphenyl)propan-1-one (8ea).



8ea

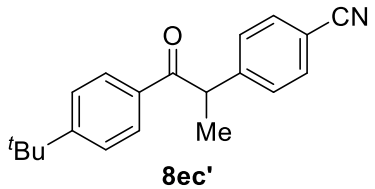
This compound was prepared according to the ***GPA*** using 4-(*tert*-butyl)benzoyl cyanide (37.5 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetone in petroleum ether), the title compound was isolated in 68% yield (40.3 mg, 0.136 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.86 (m, 2H), 7.44-7.37 (m, 2H), 7.25-7.17 (m, 2H), 6.88-6.79 (m, 2H), 4.64 (q, *J* = 6.8 Hz, 1H), 3.75 (s, 3H), 1.50 (d, *J* = 6.8 Hz, 3H), 1.30 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 158.5, 156.5, 134.0, 133.9, 128.9, 128.9, 125.6, 114.5, 55.3, 46.9, 35.2, 31.2, 19.7.

HRMS (ESI^+, m/z) calcd for $C_{20}H_{24}NaO_2$ ($[M+Na]^+$): 319.1669. Found: 319.1667.

4-(1-(4-(*tert*-Butyl)phenyl)-1-oxopropan-2-yl)benzonitrile (8ec').



8ec'

This compound was prepared according to the ***GPB*** using 4-(*tert*-butyl)benzoyl cyanide (37.5 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 3% ethyl acetate in petroleum ether), the title compound was

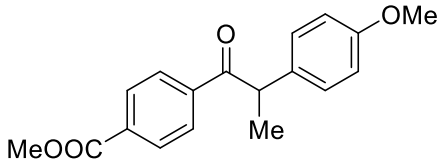
isolated in 72% yield (42.0 mg, 0.144 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.83 (m, 2H), 7.63-7.55 (m, 2H), 7.46-7.39 (m, 4H), 4.76 (q, *J* = 6.9 Hz, 1H), 1.54 (d, *J* = 7.0 Hz, 3H), 1.30 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 157.3, 147.0, 133.4, 132.8, 128.8, 125.8, 118.8, 111.0, 47.6, 35.3, 31.1, 19.5.

HRMS (ESI^+, m/z) calcd for $C_{20}H_{21}NNaO$ ($[M+Na]^+$): 314.1515. Found: 314.1514.

Methyl 4-(2-(4-methoxyphenyl)propanoyl)benzoate (8fa).



8fa

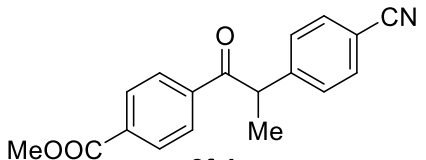
This compound was prepared according to the ***GPA*** using methyl 4-(cyanocarbonyl)benzoate (37.8 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 48% yield (28.6 mg, 0.096 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.00 (m, 2H), 8.00-7.93 (m, 2H), 7.21-7.12 (m, 2H), 6.86-6.78 (m, 2H), 4.62 (q, *J* = 6.8 Hz, 1H), 3.90 (s, 3H), 3.74 (s, 3H), 1.51 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 166.3, 158.7, 140.0, 133.5, 133.0, 129.8, 128.9, 128.7, 114.6, 55.3, 52.5, 47.6, 19.5.

HRMS (ESI^+, m/z) calcd for $C_{18}H_{18}NaO_4$ ($[M+Na]^+$): 321.1097. Found: 321.1095.

Methyl 4-(2-(4-cyanophenyl)propanoyl)benzoate (8fc').



8fc'

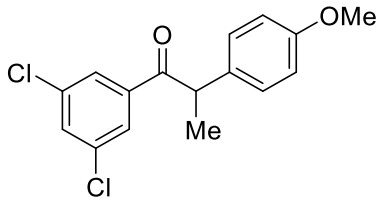
This compound was prepared according to the ***GPB*** using methyl 4-(cyanocarbonyl)benzoate (37.8 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 51% yield (29.9 mg, 0.102 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09-8.02 (m, 2H), 7.99-7.91 (m, 2H), 7.64-7.53 (m, 2H), 7.44-7.36 (m, 2H), 4.75 (q, *J* = 6.9 Hz, 1H), 3.92 (s, 3H), 1.56 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 166.1, 146.2, 139.3, 134.1, 133.0, 130.0, 128.8, 128.7, 118.6, 111.3, 52.6, 48.2, 19.3.

HRMS (ESI^+, m/z) calcd for $C_{18}H_{15}NNaO_3$ ($[M+Na]^+$): 316.0944. Found: 316.0945.

1-(3,5-Dichlorophenyl)-2-(4-methoxyphenyl)propan-1-one (8ga).



8ga

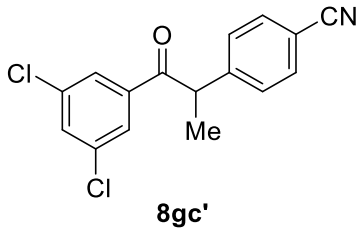
This compound was prepared according to the ***GPA*** using 3,5-dichlorobenzoyl cyanide (40.0 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 61% yield (37.7 mg, 0.122 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 1.9 Hz, 2H), 7.44 (t, *J* = 1.9 Hz, 1H), 7.18-7.12 (m, 2H), 6.88-6.82 (m, 2H), 4.50 (q, *J* = 6.8 Hz, 1H), 3.77 (s, 3H), 1.49 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 158.9, 139.2, 135.6, 132.5, 132.4, 128.9, 127.3, 114.8, 55.4, 47.6, 19.5.

HRMS (ESI^+, m/z) calcd for $C_{16}H_{14}Cl_2NaO_2$ ($[M+Na]^+$): 331.0263. Found: 331.0262.

4-(1-(3,5-Dichlorophenyl)-1-oxopropan-2-yl)benzonitrile (8gc').



8gc'

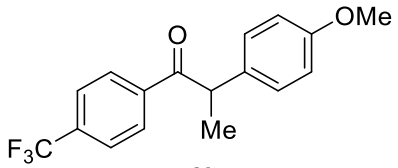
This compound was prepared according to the ***GPB*** using 3,5-dichlorobenzoyl cyanide (40.0 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 3% ethyl acetate in petroleum ether), the title compound was isolated in 40% yield (24.3 mg, 0.080 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 1.8 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.50 (t, *J* = 1.8 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 4.64 (q, *J* = 6.8 Hz, 1H), 1.55 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 145.6, 138.5, 136.0, 133.2, 133.1, 128.7, 127.2, 118.6, 111.6, 48.1, 19.3.

HRMS (ESI^+, m/z) calcd for $C_{16}H_{11}Cl_2NNaO$ ($[M+Na]^+$): 326.0110. Found: 326.0107.

2-(4-Methoxyphenyl)-1-(4-(trifluoromethyl)phenyl)propan-1-one (8ha).



8ha

This compound was prepared according to the ***GPA*** using 4-(trifluoromethyl)benzoyl cyanide (39.8 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the title compound was isolated in 55% yield (33.9 mg, 0.110 mmol) as a colorless oil.

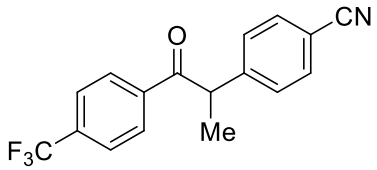
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.1 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.23-7.12 (m, 2H), 6.90-6.78 (m, 2H), 4.60 (q, *J* = 6.8 Hz, 1H), 3.75 (s, 3H), 1.52 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 158.8, 139.4, 134.0 (q, $^{2}J_{C\text{-}F}$ = 32.7 Hz), 132.9, 129.2, 128.9, 125.7 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 123.7 (q, $^{1}J_{C\text{-}F}$ = 273.8 Hz), 114.7, 55.3, 47.7, 19.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.15.

HRMS (ESI^+, m/z) calcd for $C_{17}H_{15}F_3NaO_2$ ($[M+Na]^+$): 331.0916. Found: 331.0916.

4-(1-Oxo-1-(4-(trifluoromethyl)phenyl)propan-2-yl)benzonitrile (8hc').



8hc'

This compound was prepared according to the ***GPB*** using 4-(trifluoromethyl)benzoyl cyanide (39.8 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% acetone in petroleum ether), the title compound was isolated in 56% yield (33.4 mg, 0.112 mmol) as a light yellow oil.

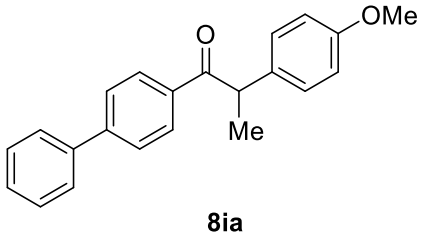
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.63-7.57 (m, 2H), 7.43-7.36 (m, 2H), 4.74 (q, *J* = 6.9 Hz, 1H), 1.57 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 146.0, 138.7, 134.7 (q, $^{2}J_{C-F}$ = 32.8 Hz), 133.1, 129.1, 128.8, 126.0 (q, $^{3}J_{C-F}$ = 3.7 Hz), 123.5 (q, $^{1}J_{C-F}$ = 273.8 Hz), 118.6, 111.5, 48.3, 19.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.24.

Spectroscopic data are in accordance with those described in literature.[41]

1-([1,1'-Biphenyl]-4-yl)-2-(4-methoxyphenyl)propan-1-one (8ia).



8ia

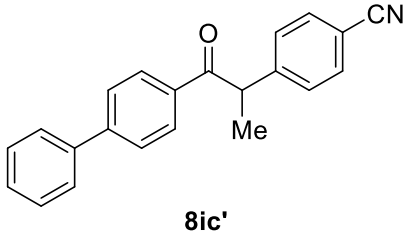
This compound was prepared according to the ***GPA*** using [1,1'-biphenyl]-4-carbonyl cyanide (41.4 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 66% yield (41.7 mg, 0.132 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.01 (m, 2H), 7.67-7.55 (m, 4H), 7.50-7.42 (m, 2H), 7.41-7.35 (m, 1H), 7.30-7.21 (m, 2H), 6.92-6.82 (m, 2H), 4.69 (q, *J* = 6.8 Hz, 1H), 3.76 (s, 3H), 1.55 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 158.6, 145.4, 140.0, 135.2, 133.7, 129.5, 129.0, 128.9, 128.3, 127.3, 127.2, 114.5, 55.3, 47.1, 19.7.

HRMS (ESI^+, m/z) calcd for $C_{22}H_{20}NaO_2$ ($[M+Na]^+$): 339.1356. Found: 339.1351.

4-(1-([1,1'-Biphenyl]-4-yl)-1-oxopropan-2-yl)benzonitrile (8ic').



8ic'

This compound was prepared according to the ***GPB*** using [1,1'-biphenyl]-4-carbonyl cyanide (41.4 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.5 mg, 0.400 mmol, 200 mol%). After

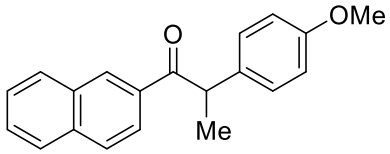
purification by column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated in 54% yield (33.6 mg, 0.108 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ8.07-7.97 (m, 2H), 7.68-7.55 (m, 6H), 7.49-7.42 (m, 4H), 7.42-7.36 (m, 1H), 4.80 (q, *J* = 6.9 Hz, 1H), 1.58 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 146.8, 146.1, 139.6, 134.6, 132.9, 129.4, 129.1, 128.8, 128.5, 127.5, 127.3, 118.8, 111.0, 47.7, 19.4.

HRMS (ESI$^+$, m/z) calcd for $C_{22}H_{17}NNaO$ ([M+Na]$^+$): 334.1202. Found: 334.1198.

2-(4-Methoxyphenyl)-1-(naphthalen-2-yl)propan-1-one (8ja).



8ja

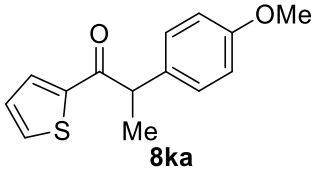
This compound was prepared according to the ***GPA*** using 2-naphthoyl cyanide (36.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 40% yield (23.2 mg, 0.080 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.02 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.86-7.79 (m, 2H), 7.60-7.49 (m, 2H), 7.32-7.23 (m, 2H), 6.88-6.80 (m, 2H), 4.82 (q, *J* = 6.8 Hz, 1H), 3.74 (s, 3H), 1.58 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.7, 158.6, 135.5, 133.9, 133.7, 132.6, 130.5, 129.7, 128.9, 128.5, 128.4, 127.8, 126.7, 124.7, 114.5, 55.3, 47.1, 19.7.

HRMS (ESI$^+$, m/z) calcd for $C_{20}H_{18}NaO_2$ ([M+Na]$^+$): 313.1199. Found: 313.1199.

2-(4-Methoxyphenyl)-1-(thiophen-2-yl)propan-1-one (8ka).



8ka

This compound was prepared according to the ***GPA*** using thiophene-2-carbonyl cyanide (27.4 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%). After

purification by column chromatography (SiO_2: 2% acetone in petroleum ether), the title compound was isolated in 46% yield (22.7 mg, 0.056 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.55 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.29-7.21 (m, 2H), 7.05 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.89-6.81 (m, 2H), 4.46 (q, *J* = 6.9 Hz, 1H), 3.77 (s, 3H), 1.52 (d, *J* = 6.9 Hz, 3H).

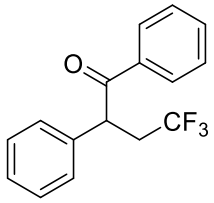
^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7, 158.8, 143.9, 133.6, 133.5, 132.5, 128.9, 128.1, 114.5, 55.4, 48.6, 19.3.

HRMS (ESI^+, m/z) calcd for $C_{14}H_{14}NaO_2S$ ($[M+Na]^+$): 269.0607. Found: 269.0607.

Part 6. Acylfluoroalkylation of Styrenes with Acyl Cyanides

General Procedure C (GPC) for acylfluoroalkylation of styrenes with acyl cyanides: To an oven-dried Schlenk tube equipped with a stirring bar was added $Ir(ppy)_2(dtbbpy)PF_6$ (1.8 mg, 0.002 mmol, 1 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%), styrenes (if solid, 0.400 mmol, 200 mol%) and acyl cyanide (if solid, 0.200 mmol, 100 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Acyl cyanide (if liquid, 0.200 mmol, 100 mol%), styrenes (if liquid, 0.400 mmol, 200 mol%), Acetone (3 mL) and DMF (0.3 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation at r.t. for 12 hours under N_2 atmosphere. After the reaction completed, the mixture was added 30 mL of EtOAc and washed with brine. The organic phase was dried over Na_2SO_4, filtered, and evaporated under vacuum. The residue was purified by silica gel column chromatography to give the target product. (Note: The liquid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

4,4,4-Trifluoro-1,2-diphenylbutan-1-one (11aa).



11aa

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), styrene (41.7 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 55% yield (30.6 mg, 0.110 mmol) as a colorless oil.

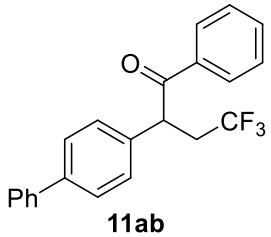
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98-7.92 (m, 2H), 7.53-7.47 (m, 1H), 7.43-7.37 (m, 2H), 7.33-7.28 (m, 4H), 7.27-7.21 (m, 1H), 4.91 (dd, J = 7.7, 5.4 Hz, 1H), 3.38-3.24 (m, 1H), 2.62-2.48 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.9, 137.5, 135.8, 133.5, 129.5, 129.0, 128.8, 128.2, 128.0, 126.5 (q, $^1J_{C\text{-}F}$ = 275.5 Hz), 47.3 (q, $^3J_{C\text{-}F}$ = 2.3 Hz), 37.5 (q, $^2J_{C\text{-}F}$ = 28.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.59.

Spectroscopic data are in accordance with those described in literature.[42]

2-([1,1'-Biphenyl]-4-yl)-4,4,4-trifluoro-1-phenylbutan-1-one (11ab).



11ab

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-vinylbiphenyl (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 74% yield (52.3 mg, 0.148 mmol) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05-7.97 (m, 2H), 7.59-7.50 (m, 5H), 7.46-7.37 (m, 6H),

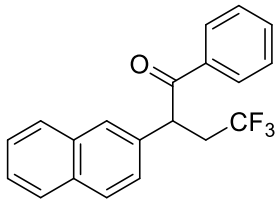
7.36-7.31 (m, 1H), 4.97 (dd, J = 7.8, 5.4 Hz, 1H), 3.43-3.29(m, 1H), 2.66-2.53 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.8, 140.9, 140.3, 136.5, 135.8, 133.6, 129.0, 128.9, 128.9, 128.6, 128.1, 127.7, 127.1, 126.5 (q, $^{1}J_{C\text{-}F}$ = 275.6 Hz), 46.9 (q, $^{3}J_{C\text{-}F}$ = 2.3 Hz), 37.5 (q, $^{2}J_{C\text{-}F}$ = 28.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.53.

Spectroscopic data are in accordance with those described in literature.[42]

4,4,4-Trifluoro-2-(naphthalen-2-yl)-1-phenylbutan-1-one (11ac).



11ac

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 2-vinylnaphthalene (61.7 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 47% yield (30.8 mg, 0.094 mmol) as a light yellow solid.

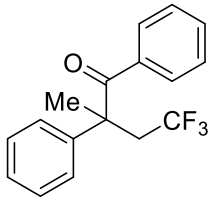
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04-7.97 (m, 2H), 7.85-7.73 (m, 4H), 7.52-7.42 (m, 4H), 7.42-7.35 (m, 2H), 5.08 (dd, J = 7.6, 5.4 Hz, 1H), 3.47-3.34 (m, 1H), 2.71-2.58 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.8, 135.8, 134.9, 133.7, 133.5, 132.8, 129.5, 129.0, 128.8, 128.0, 127.8, 127.4, 126.7, 126.6 (q, $^{1}J_{C\text{-}F}$ = 275.6 Hz), 126.5, 125.7, 47.5 (q, $^{3}J_{C\text{-}F}$ = 2.3 Hz), 37.5 (q, $^{2}J_{C\text{-}F}$ = 28.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.52.

Spectroscopic data are in accordance with those described in literature.[42]

4,4,4-trifluoro-2-methyl-1,2-diphenylbutan-1-one (11ad).



11ad

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), α-methylstyrene (47.3 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 64% yield (37.4 mg, 0.128 mmol) as a colorless oil.

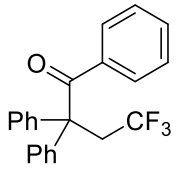
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43-7.31 (m, 8H), 7.25-7.19 (m, 2H), 3.13-3.00 (m, 1H), 2.90-2.77 (m, 1H), 1.83 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 201.6, 141.0, 136.2, 132.0, 129.5, 129.4, 128.2, 127.9, 126.6 (q, $^{1}J_{C\text{-}F}$ = 276.7 Hz), 126.4, 52.0, 43.5 (q, $^{2}J_{C\text{-}F}$ = 26.6 Hz), 22.1 (q, $^{3}J_{C\text{-}F}$ = 1.4 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -58.57.

Spectroscopic data are in accordance with those described in literature.[43]

4,4,4-Trifluoro-1,2,2-triphenylbutan-1-one (11ae).



11ae

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 72% yield (51.0 mg, 0.144 mmol) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61-7.55 (m, 2H), 7.53-7.45 (m, 4H), 7.40-7.27 (m, 7H), 7.22-7.15 (m, 2H), 3.42 (q, J = 10.5 Hz, 2H).

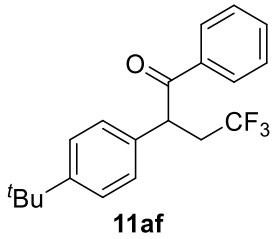
^{13}C NMR (125 MHz, $CDCl_3$) δ 198.5, 138.7, 136.5, 132.0, 130.2, 129.8, 128.5, 127.9, 127.8,

125.8 (q, $^{1}J_{C\text{-}F}$ = 277.1 Hz), 62.1, 45.0 (q, $^{2}J_{C\text{-}F}$ = 27.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.15.

Spectroscopic data are in accordance with those described in literature.[44]

2-(4-(*tert*-Butyl)phenyl)-4,4,4-trifluoro-1-phenylbutan-1-one (11af).



11af

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-*tert*-butylstyrene (64.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 46% yield (30.7 mg, 0.092 mmol) as a colorless oil.

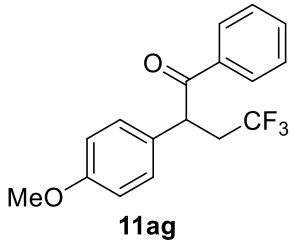
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01-7.96 (m, 2H), 7.54-7.48 (m, 1H), 7.45-7.38 (m, 2H), 7.35-7.30 (m, 2H), 7.25-7.21 (m, 2H), 4.91 (dd, *J* = 8.3, 4.8 Hz, 1H), 3.41-3.28 (m, 1H), 2.58-2.45 (m, 1H), 1.27 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.0, 150.9, 136.0, 134.4, 133.4, 129.0, 128.8, 127.7, 126.5 (q, $^{1}J_{C\text{-}F}$ = 275.6 Hz), 126.4, 46.7 (q, $^{3}J_{C\text{-}F}$ = 2.4 Hz), 37.5 (q, $^{2}J_{C\text{-}F}$ = 28.0 Hz), 34.6, 31.4.

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.76.

Spectroscopic data are in accordance with those described in literature.[45]

4,4,4-Trifluoro-2-(4-methoxyphenyl)-1-phenylbutan-1-one (11ag).



11ag

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-methoxystyrene (53.7 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column

chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 70% yield (43.1 mg, 0.140 mmol) as a colorless oil.

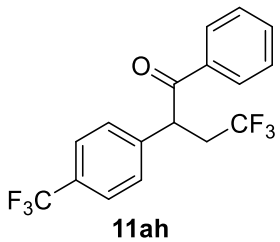
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00-7.91 (m, 2H), 7.54-7.47 (m, 1H), 7.44-7.36 (m, 2H), 7.24-7.17 (m, 2H), 6.87-6.79 (m, 2H), 4.85 (dd, J = 7.6, 5.6 Hz, 1H), 3.75 (s, 3H), 3.32-3.18 (m, 1H), 2.58-2.45 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.1, 159.3, 135.8, 133.4, 129.4, 129.3, 128.9, 128.8, 126.6 (q, $^1J_{C\text{-}F}$ = 275.5 Hz), 114.9, 55.4, 46.5 (q, $^3J_{C\text{-}F}$ = 2.4 Hz), 37.5 (q, $^2J_{C\text{-}F}$ = 27.7 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.52.

Spectroscopic data are in accordance with those described in literature.[42]

4,4,4-Trifluoro-1-phenyl-2-(4-(trifluoromethyl)phenyl)butan-1-one (11ah).



11ah

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-trifluoromethylstyrene (53.7 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (68.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 41% yield (28.4 mg, 0.082 mmol) as a colorless oil.

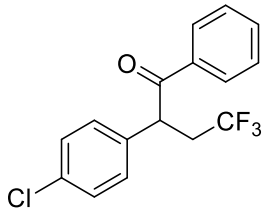
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98-7.90 (m, 2H), 7.62-7.51 (m, 3H), 7.48-7.39 (m, 4H), 4.99 (t, J = 6.6 Hz, 1H), 3.36-3.21 (m, 1H), 2.65-2.50 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.3, 141.4, 135.4, 133.9, 130.4 (q, $^2J_{C\text{-}F}$ = 32.5 Hz), 129.0, 128.9, 128.6, 126.5 (q, $^3J_{C\text{-}F}$ = 3.7 Hz), 126.4 (q, $^1J_{C\text{-}F}$ = 275.4 Hz), 123.9 (q, $^1J_{C\text{-}F}$ = 270.4 Hz), 47.0 (q, $^3J_{C\text{-}F}$ = 2.3 Hz), 37.4 (q, $^2J_{C\text{-}F}$ = 28.3 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -62.75, -64.48.

Spectroscopic data are in accordance with those described in literature.[42]

2-(4-Chlorophenyl)-4,4,4-trifluoro-1-phenylbutan-1-one (11ai).



11ai

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-chlorostyrene (55.4 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (68.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 42% yield (26.2 mg, 0.084 mmol) as a colorless oil.

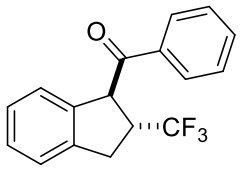
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95-7.89 (m, 2H), 7.56-7.50 (m, 1H), 7.45-7.39 (m, 2H), 7.31-7.27 (m, 2H), 7.26-7.21 (m, 2H), 4.89 (dd, J = 7.3, 5.9 Hz, 1H), 3.31-3.18 (m, 1H), 2.60-2.47 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.6, 136.0, 135.5, 134.1, 133.8, 129.7, 129.6, 128.9, 126.4 (q, $^1J_{C\text{-}F}$ = 275.6 Hz), 46.6 (q, $^3J_{C\text{-}F}$ = 2.3 Hz), 37.4 (q, $^2J_{C\text{-}F}$ = 28.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.46.

Spectroscopic data are in accordance with those described in literature.[42]

***trans*-Phenyl(2-(trifluoromethyl)-2,3-dihydro-1H-inden-1-yl)methanone (11aj).**



11aj

This compound was prepared according to the ***GPC*** using benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), indene (46.5 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (68.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 30% yield (17.4 mg, 0.060 mmol, d.r. > 20:1) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15-8.08 (m, 2H), 7.72-7.66 (m, 1H), 7.63-7.55 (m, 2H), 7.31-7.27 (m, 1H), 7.25-7.20 (m, 1H), 7.08 (t, J = 7.5 Hz, 1H), 6.90 (d, J = 7.7 Hz, 1H), 5.31 (d, J

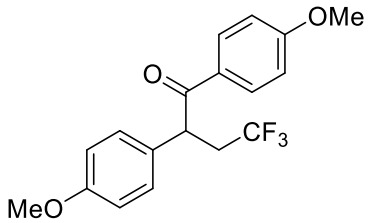
= 6.9 Hz, 1H), 4.08-3.96 (m, 1H), 3.44 (dd, *J* = 16.4, 9.4 Hz, 1H), 3.26 (dd, *J* = 16.4, 7.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.5, 141.2, 139.4, 136.8, 134.0, 129.4, 129.2, 128.3, 127.9 (q, $^{1}J_{C\text{-}F}$ = 275.9 Hz), 127.3, 125.1, 124.3, 52.5 (q, $^{3}J_{C\text{-}F}$ = 2.3 Hz), 44.9 (q, $^{2}J_{C\text{-}F}$ = 27.6 Hz), 32.3 (q, $^{3}J_{C\text{-}F}$ = 2.4 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -70.74.

Spectroscopic data are in accordance with those described in literature.[42]

4,4,4-Trifluoro-1,2-bis(4-methoxyphenyl)butan-1-one (11bg).



11bg

This compound was prepared according to the ***GPC*** using 4-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 4-methoxystyrene (53.7 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (68.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 58% yield (39.2 mg, 0.116 mmol) as a colorless oil.

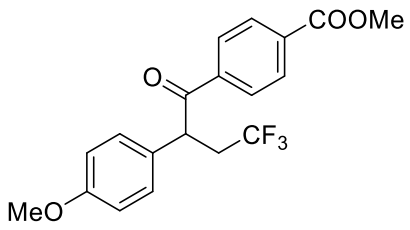
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99-7.91 (m, 2H), 7.25-7.18 (m, 2H), 6.90-6.85 (m, 2H), 6.85-6.80 (m, 2H), 4.81 (dd, *J* = 7.5, 5.7 Hz, 1H), 3.82 (s, 3H), 3.74 (s, 3H), 3.31-3.17 (m, 1H), 2.58-2.44 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 195.5, 163.7, 159.2, 131.3, 129.9, 129.2, 128.7, 126.7 (q, $^{1}J_{C\text{-}F}$ = 275.5 Hz), 114.8, 114.0, 55.6, 55.3, 46.1 (q, $^{3}J_{C\text{-}F}$ = 2.3 Hz), 37.5 (q, $^{2}J_{C\text{-}F}$ = 27.6 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.48.

Spectroscopic data are in accordance with those described in literature.[46]

Methyl 4-(4,4,4-trifluoro-2-(4-methoxyphenyl)butanoyl)benzoate (11fg).



11fg

This compound was prepared according to the ***GPC*** using methyl 4-(cyanocarbonyl)benzoate (37.8 mg, 0.200 mmol, 100 mol%), 4-methoxystyrene (53.7 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (68.9 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% acetate in petroleum ether), the title compound was isolated in 35% yield (25.6 mg, 0.070 mmol) as a colorless oil.

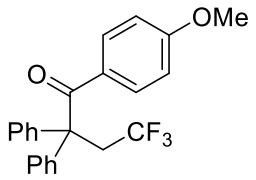
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.02 (m, 2H), 8.00-7.94 (m, 2H), 7.21-7.15 (m, 2H), 6.86-6.80 (m, 2H), 4.83 (dd, J = 7.5, 5.7 Hz, 1H), 3.91 (s, 3H), 3.74 (s, 3H), 3.32- 3.19 (m, 1H), 2.60-2.46 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.6, 166.2, 159.4, 139.2, 134.1, 130.0, 129.3, 128.8, 128.7, 126.5 (q, $^1J_{C\text{-}F}$ = 275.5 Hz), 115.0, 55.4, 52.6, 47.0 (q, $^3J_{C\text{-}F}$ = 2.3 Hz), 37.4 (q, $^2J_{C\text{-}F}$ = 27.9 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -64.49.

HRMS (ESI$^+$, m/z) calcd for $C_{19}H_{18}F_3O_4$ ([M+H]$^+$): 367.1152. Found: 367.1148.

4,4,4-Trifluoro-1-(4-methoxyphenyl)-2,2-diphenylbutan-1-one (11be).



11be

This compound was prepared according to the ***GPC*** using 4-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 92% yield (70.6 mg, 0.184 mmol) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68-7.62 (m, 2H), 7.53-7.45 (m, 4H), 7.38-7.32 (m, 4H),

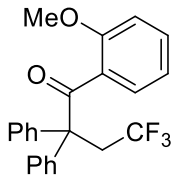
7.31-7.26 (m, 2H), 3.73 (s, 3H), 3.39 (q, J = 10.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.3, 162.5, 139.0, 133.0, 129.8, 128.5, 128.5, 127.7, 125.8 (q, $^1J_{C\text{-}F}$ = 277.2 Hz), 113.0, 61.9, 55.4, 45.6 (q, $^2J_{C\text{-}F}$ = 26.8 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.14.

HRMS (ESI$^+$, m/z) calcd for $C_{23}H_{19}F_3NaO_2$ ([M+Na]$^+$): 407.1229. Found: 407.1226.

4,4,4-Trifluoro-1-(2-methoxyphenyl)-2,2-diphenylbutan-1-one (11ce).



11ce

This compound was prepared according to the ***GPC*** using 2-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 85% yield (65.3 mg, 0.170 mmol) as a white solid.

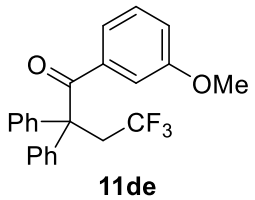
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35-7.20 (m, 10H), 7.19-7.12 (m, 1H), 6.69 (d, J = 8.4 Hz, 1H), 6.60 (t, J = 7.5, 1H), 6.18 (dd, J = 7.5, 1.7 Hz, 1H), 3.55 (s, 3H), 3.27 (q, J = 10.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 203.4, 155.8, 138.3, 130.8, 130.4, 129.7, 128.0, 127.7, 127.0, 126.1 (q, $^1J_{C\text{-}F}$ = 277.0 Hz), 120.1, 111.0, 64.1, 55.7, 39.9 (q, $^2J_{C\text{-}F}$ = 27.3 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -56.62.

HRMS (ESI$^+$, m/z) calcd for $C_{23}H_{19}F_3NaO_2$ ([M+Na]$^+$): 407.1229. Found: 407.1230.

4,4,4-Trifluoro-1-(3-methoxyphenyl)-2,2-diphenylbutan-1-one (11de).



11de

This compound was prepared according to the ***GPC*** using 3-methoxybenzoyl cyanide (32.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium

trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 69% yield (52.9 mg, 0.138 mmol) as a colorless oil.

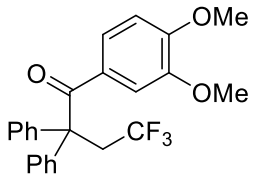
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.42 (m, 4H), 7.38-7.33 (m, 4H), 7.32-7.27 (m, 2H), 7.13-7.10 (m, 1H), 7.10-7.04 (m, 2H), 6.88 (dt, J = 6.9, 2.4 Hz, 1H), 3.65 (s, 3H), 3.39 (q, J = 10.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 198.4, 159.0, 138.8, 137.9, 129.8, 128.9, 128.5, 127.8, 125.8 (q, $^1J_{C\text{-}F}$ = 277.2 Hz), 122.8, 118.5, 114.6, 62.1, 55.3, 45.0 (q, $^2J_{C\text{-}F}$ = 27.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.17.

HRMS (ESI$^+$, m/z) calcd for $C_{23}H_{19}F_3NaO_2$ ([M+Na]$^+$): 407.1229. Found: 407.1212.

1-(3,4-Dimethoxyphenyl)-4,4,4-trifluoro-2,2-diphenylbutan-1-one (11le).



11le

This compound was prepared according to the ***GPC*** using 3,4-dimethoxybenzoyl cyanide (38.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 3% acetate in petroleum ether), the title compound was isolated in 91% yield (75.3 mg, 0.182 mmol) as a white solid.

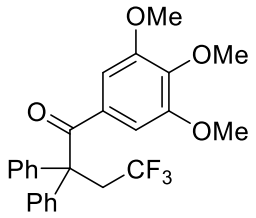
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53-7.45 (m, 4H), 7.38-7.31 (m, 4H), 7.31-7.21 (m, 4H), 6.59 (d, J = 8.5 Hz, 1H), 3.80 (s, 3H), 3.67 (s, 3H), 3.39 (q, J = 10.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.4, 152.3, 148.0, 139.0, 129.7, 128.5, 128.4, 127.7, 125.7 (q, $^1J_{C\text{-}F}$ = 277.3 Hz), 125.5, 113.4, 109.5, 62.0, 55.9, 55.8, 45.6 (q, $^2J_{C\text{-}F}$ = 26.8 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.08.

HRMS (ESI$^+$, m/z) calcd for $C_{24}H_{21}F_3NaO_3$ ([M+Na]$^+$): 437.1335. Found: 437.1326.

4,4,4-Trifluoro-2,2-diphenyl-1-(3,4,5-trimethoxyphenyl)butan-1-one (11me).



11me

This compound was prepared according to the ***GPC*** using 3,4,5-trimethoxybenzoyl cyanide (44.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 3% acetate in petroleum ether), the title compound was isolated in 89% yield (79.0 mg, 0.178 mmol) as a white solid.

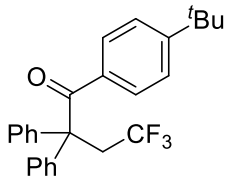
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51-7.44 (m, 4H), 7.39-7.32 (m, 4H), 7.32-7.27 (m, 2H), 6.88 (d, J = 1.2 Hz, 2H), 3.81 (s, 3H), 3.58 (s, 6H), 3.39 (q, J = 10.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.9, 152.1, 141.4, 138.9, 130.9, 129.7, 128.5, 127.8, 125.7 (q, $^1J_{C\text{-}F}$ = 277.3 Hz), 108.3, 62.0, 60.9, 56.0, 45.4 (q, $^2J_{C\text{-}F}$ = 27.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.04.

HRMS (ESI^+, m/z) calcd for $C_{25}H_{23}F_3NaO_4$ ($[M+Na]^+$): 467.1441. Found: 467.1433.

1-(4-(*tert*-Butyl)phenyl)-4,4,4-trifluoro-2,2-diphenylbutan-1-one (11ee).



11ee

This compound was prepared according to the ***GPC*** using 4-(*tert*-butyl)benzoyl cyanide (37.4 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 88% yield (72.1 mg, 0.176 mmol) as a white solid.

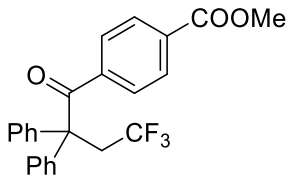
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58-7.52 (m, 2H), 7.52-7.45 (m, 4H), 7.39-7.32 (m, 4H), 7.32-7.27 (m, 2H), 7.24-7.18 (m, 2H), 3.42 (q, J = 10.5 Hz, 2H), 1.24 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.9, 155.6, 139.0, 133.6, 130.3, 129.8, 128.5, 127.7, 125.8 (q, $^{1}J_{C\text{-}F}$ = 277.2 Hz), 124.9, 62.0, 45.2 (q, $^{2}J_{C\text{-}F}$ = 26.8 Hz), 35.0, 31.1.

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.17.

Spectroscopic data are in accordance with those described in literature.[44]

Methyl 4-(4,4,4-trifluoro-2,2-diphenylbutanoyl)benzoate (11fe).



11fe

This compound was prepared according to the ***GPC*** using methyl 4-(cyanocarbonyl)benzoate (37.8 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 2% acetate in petroleum ether), the title compound was isolated in 82% yield (67.5 mg, 0.164 mmol) as a white solid.

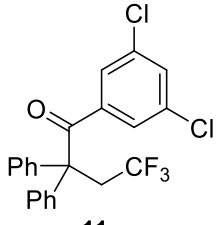
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86-7.80 (m, 2H), 7.57-7.51 (m, 2H), 7.48-7.41 (m, 4H), 7.39-7.27 (m, 6H), 3.86 (s, 3H), 3.38 (q, *J* = 10.4 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 198.3, 166.2, 140.4, 138.2, 132.7, 129.9, 129.7, 129.1, 128.7, 128.0, 125.7 (q, $^{1}J_{C\text{-}F}$ = 277.1 Hz), 62.2, 52.4, 44.7 (q, $^{2}J_{C\text{-}F}$ = 27.1 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.27.

HRMS (ESI^+, m/z) calcd for $C_{24}H_{20}F_3O_3$ ($[M+H]^+$): 413.1359. Found: 413.1355.

1-(3,5-Dichlorophenyl)-4,4,4-trifluoro-2,2-diphenylbutan-1-one (11ge).



11ge

This compound was prepared according to the ***GPC*** using 3,5-dichlorobenzoyl cyanide (40.0 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium

trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 56% yield (47.4 mg, 0.112 mmol) as a white solid.

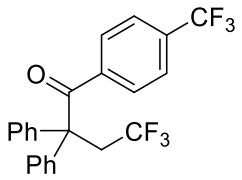
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44-7.32 (m, 12H), 7.30 (t, J = 1.9 Hz, 1H), 3.35 (q, J = 10.3 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.1, 139.1, 137.8, 134.7, 131.7, 129.6, 128.9, 128.4, 128.3, 125.6 (q, $^1J_{C\text{-}F}$ = 277.2 Hz), 62.3, 44.8 (q, $^2J_{C\text{-}F}$ = 27.0 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.35.

HRMS (MALDI$^+$, m/z) calcd for $C_{22}H_{16}Cl_2F_3O$ ([M+H]$^+$): 423.0525. Found: 423.0559.

4,4,4-Trifluoro-2,2-diphenyl-1-(4-(trifluoromethyl)phenyl)butan-1-one (11he).



11he

This compound was prepared according to the ***GPC*** using 4-(trifluoromethyl)benzoyl cyanide (39.8 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 81% yield (68.3 mg, 0.162 mmol) as a colorless oil.

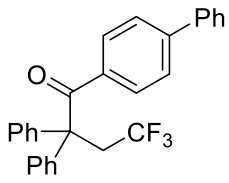
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, J = 8.2 Hz, 2H), 7.50-7.42 (m, 6H), 7.42-7.30 (m, 6H), 3.39 (q, J = 10.3 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.7, 139.7, 138.1, 133.2 (q, $^2J_{C\text{-}F}$ = 32.5 Hz), 130.4, 129.7, 128.8, 128.2, 125.7 (q, $^1J_{C\text{-}F}$ = 277.1 Hz), 125.0 (q, $^3J_{C\text{-}F}$ = 3.7 Hz), 123.6 (q, $^1J_{C\text{-}F}$ = 271.0 Hz), 62.2, 44.8 (q, $^2J_{C\text{-}F}$ = 27.1 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.33, -63.26.

Spectroscopic data are in accordance with those described in literature.[44]

1-([1,1'-Biphenyl]-4-yl)-4,4,4-trifluoro-2,2-diphenylbutan-1-one (11ie).



11ie

This compound was prepared according to the ***GPC*** using [1,1'-biphenyl]-4-carbonyl cyanide (41.4 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 93% yield (79.9 mg, 0.186 mmol) as a white solid.

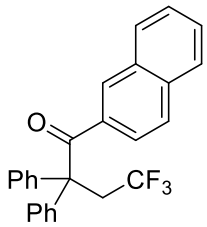
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74-7.67 (m, 2H), 7.57-7.50 (m, 6H), 7.46-7.30 (m, 11H), 3.45 (q, J = 10.4 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.7, 144.6, 139.7, 138.7, 134.9, 131.0, 129.8, 129.0, 128.6, 128.2, 127.8, 127.2, 126.5, 125.8 (q, $^1J_{C\text{-}F}$ = 277.2 Hz), 62.1, 45.3 (q, $^2J_{C\text{-}F}$ = 26.9 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.11.

HRMS (ESI^+, m/z) calcd for $C_{28}H_{21}F_3NaO$ ($[M+Na]^+$): 453.1437. Found: 453.1428.

4,4,4-Trifluoro-1-(naphthalen-2-yl)-2,2-diphenylbutan-1-one (11je).



11je

This compound was prepared according to the ***GPC*** using 2-naphthoyl cyanide (36.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 58% yield (46.9 mg, 0.116 mmol) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.72 (dd, J = 17.8, 8.2 Hz, 2H), 7.68-7.60 (m, 2H), 7.59-7.53 (m, 4H), 7.54-7.48 (m, 1H), 7.47-7.42 (m, 1H), 7.40-7.34 (m, 4H), 7.34-7.28 (m, 2H),

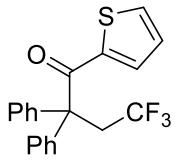
3.48 (q, J = 10.3 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 198.2, 138.8, 134.7, 133.7, 132.1, 132.0, 129.8, 129.7, 128.6, 128.4, 127.8, 127.6, 127.5, 126.6, 126.2, 125.8 (q, $^{1}J_{C\text{-}F}$ = 277.2 Hz), 62.3, 45.3 (q, $^{2}J_{C\text{-}F}$ = 26.9 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.04.

HRMS (ESI$^+$, m/z) calcd for $C_{26}H_{19}F_3NaO$ ([M+Na]$^+$): 427.1280. Found: 427.1274.

4,4,4-Trifluoro-2,2-diphenyl-1-(thiophen-2-yl)butan-1-one (11ke).



11ke

This compound was prepared according to the ***GPC*** using thiophene-2-carbonyl cyanide (27.4 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 76% yield (54.7 mg, 0.152 mmol) as a colorless oil.

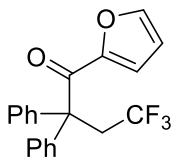
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55-7.47 (m, 4H), 7.45-7.40 (m, 1H), 7.39-7.28 (m, 6H), 7.17-7.12 (m, 1H), 6.82 (t, J = 4.5 Hz, 1H), 3.43 (q, J = 10.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 191.1, 142.0, 138.6, 134.6, 133.5, 130.0, 128.4, 128.0, 127.6, 125.8 (q, $^{1}J_{C\text{-}F}$ = 277.1 Hz), 62.2, 44.4 (q, $^{2}J_{C\text{-}F}$ = 27.1 Hz).

^{19}F NMR (471 MHz, $CDCl_3$) δ -57.28.

Spectroscopic data are in accordance with those described in literature.[44]

4,4,4-Trifluoro-1-(furan-2-yl)-2,2-diphenylbutan-1-one (11ne).



11ne

This compound was prepared according to the ***GPC*** using furan-2-carbonyl cyanide (24.2 mg, 0.200 mmol, 100 mol%), 1,1-diphenylethylene (72.1 mg, 0.400 mmol, 200 mol%), sodium

trifluoromethanesulfinate (62.4 mg, 0.400 mmol, 200 mol%). After purification by column chromatography (SiO_2: 1% acetate in petroleum ether), the title compound was isolated in 82% yield (56.4 mg, 0.164 mmol) as a light yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48-7.40 (m, 4H), 7.38-7.27 (m, 7H), 7.00 (d, J = 3.6 Hz, 1H), 6.33 (dd, J = 3.6, 1.7 Hz, 1H), 3.49 (q, J = 10.5 Hz, 2H).

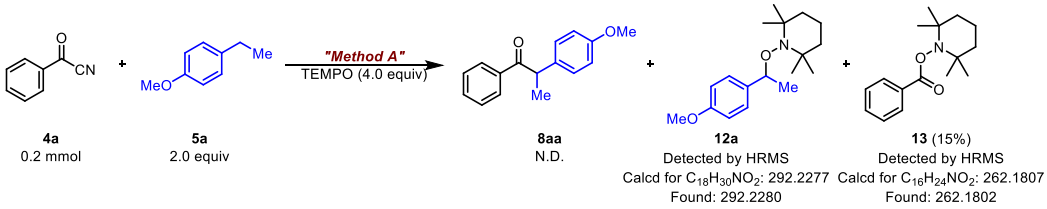
^{13}C NMR (125 MHz, $CDCl_3$) δ 186.1, 151.4, 145.7, 138.8, 129.8, 128.2, 127.7, 125.9 (q, $^1J_{C\text{-}F}$ = 276.9 Hz), 120.4, 112.0, 61.1, 43.1 (q, $^2J_{C\text{-}F}$ = 27.1 Hz).

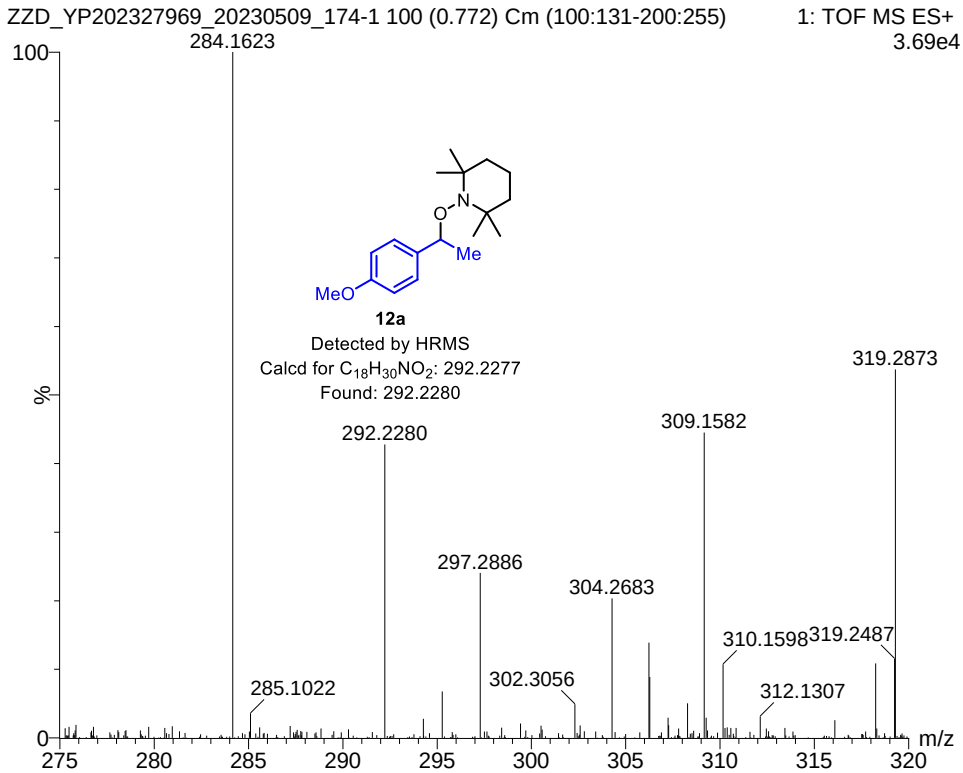
^{19}F NMR (471 MHz, $CDCl_3$) δ -57.63.

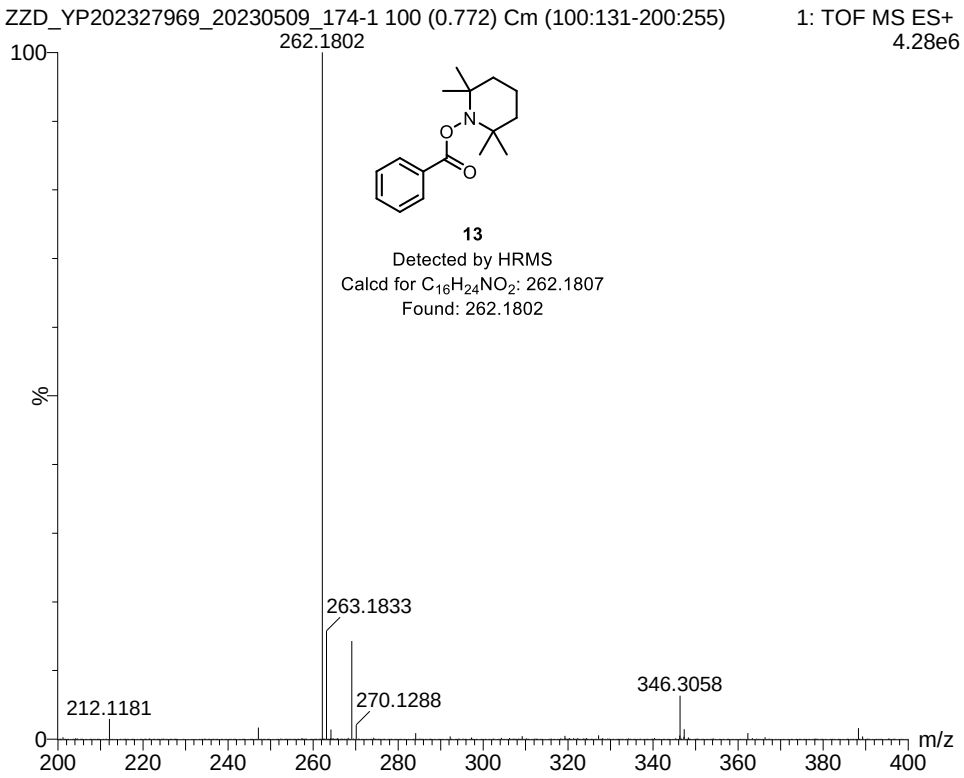
Spectroscopic data are in accordance with those described in literature.[44]

Part 7. Mechanistic Consideration

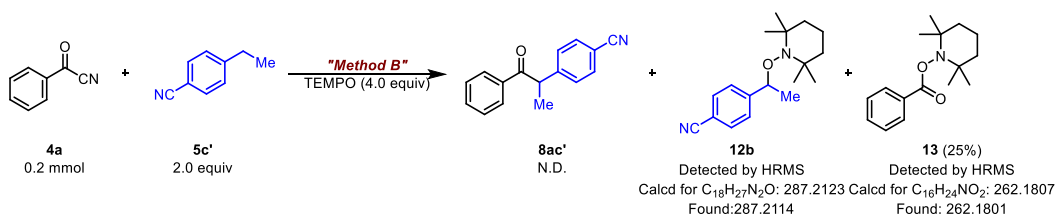
a. Radical Inhibition Experiment

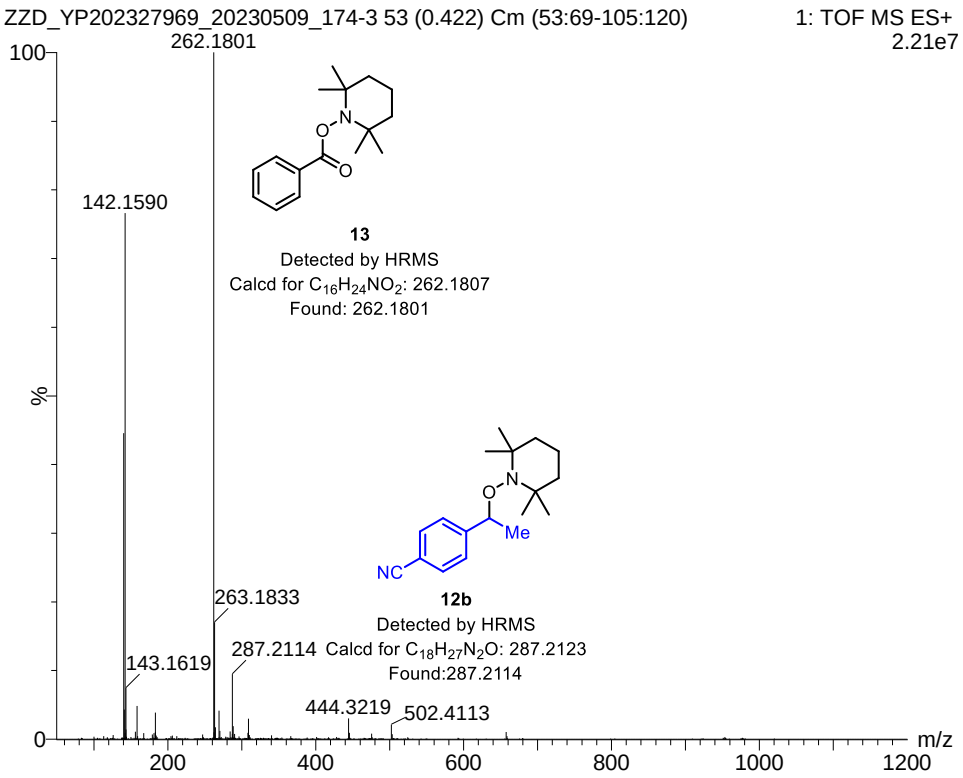






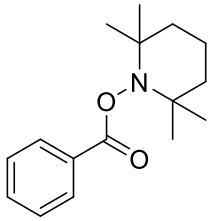
To an oven-dried Schlenk tube equipped with a stirring bar was added Ir[dF(CF$_3$)ppy]$_2$(dtbbpy)PF$_6$ (2.2 mg, 0.002 mmol, 1 mol%), potassium benzoate (64.0 mg, 0.400 mmol, 200 mol%) and TEMPO (125.0 mg, 0.800 mmol, 400 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation at r.t. for 12 hours under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The desired coupling product **8aa** was not detected by ^{1}H NMR. Both the TEMPO trapping benzyl radical product **12a** and the TEMPO trapping benzoyl radical product **13** were found molecular ion peaks on high resolution mass spectrometry, which meant that the reaction might undergo a radical-radical cross-coupling process.





To an oven-dried Schlenk tube equipped with a stirring bar was added Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (2.2 mg, 0.002 mmol, 1 mol%), sodium bromide (8.2 mg, 0.080 mmol, 40 mol%), anhydrous sodium carbonate (42.4 mg, 0.400 mmol, 200 mol%) and TEMPO (125.0 mg, 0.800 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.4 mg, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation in an aluminum module at 40 ℃ for 12 hours under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The desired coupling product **8ac'** was not detected by ^{1}H NMR. The TEMPO trapping benzyl radical product **12b** and the TEMPO trapping benzoyl radical product **13** was found molecular ion peaks on high resolution mass spectrometry, which meant that the reaction might undergo a radical-radical cross-coupling process.

2,2,6,6-tetramethylpiperidin-1-yl benzoate (13).



13

This compound was prepared according to the ***GPA*** using benzoyl cyanide (78.6 mg, 0.600 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (153.5 mg, 1.200 mmol, 200 mol%) and TEMPO (375.0 mg, 2.400 mmol, 400 mol%). The reaction was quenched with sat. aq. Na_2SO_3. After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound **13** was isolated in 15% yield (23.5 mg, 0.090 mmol) as a white solid.

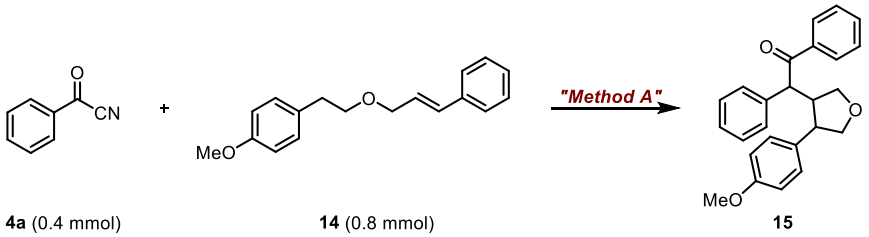
This compound was prepared according to the ***GPB*** using benzoyl cyanide (78.6 mg, 0.600 mmol, 100 mol%), 4-ethylbenzonitrile (156.9 mg, 1.200 mmol, 200 mol%) and TEMPO (375.0 mg, 2.400 mmol, 400 mol%). The reaction was quenched with sat. aq. Na_2SO_3. After purification by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound **13** was isolated in 25% yield (39.2 mg, 0.150 mmol) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.04 (m, 2H), 7.61-7.54 (m, 1H), 7.50-7.42 (m, 2H), 1.85-1.63 (m, 3H), 1.63-1.53 (m, 2H), 1.51-1.41 (m, 1H), 1.28 (s, 6H), 1.12 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 133.0, 129.9, 129.7, 128.6, 60.6, 39.2, 32.1, 21.0, 17.1.

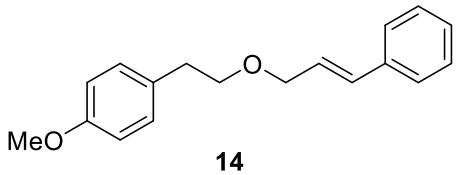
Spectroscopic data are in accordance with those described in literature.[47]

b. Radical Probing Experiment



4a (0.4 mmol) **14** (0.8 mmol) **15**

1-(2-(Cinnamyloxy)ethyl)-4-methoxybenzene (14).



14

Step 1: Following a reported procedure[48], to an oven dried round bottom flask equipped with magnetic stir bar was added cinnamyl alcohol (1.34 g, 10 mmol) and hydrogen bromide (48%) (23 mL) at 0 ºC and the reaction mixture was warmed to room temperature and stirred for 3 hours. The reaction was monitored by TLC. After the complete consumption of the starting material the reaction mixture was quenched by saturated sodium bicarbonate and extracted with EtOAc (2 x 50 mL). The organic layer was separated, dried over Na_2SO_4 and the solvent was removed under reduced pressure to obtain a brown solid (1.81 g, 92%) which was used without further purification.

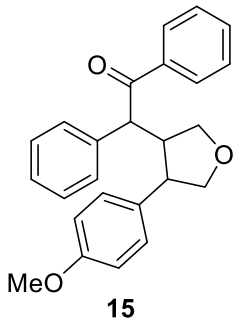
Step 2: Following a reported procedure[49], an oven-dried 50 mL two-neck flask was equipped with a condenser and charged with 2-(4-methoxyphenyl)ethanol (761.0 mg, 5.0 mmol) and THF (dry, 20 mL). The mixture was cooled to 0 °C and sodium hydride (60 wt% on mineral oil, 300 mg, 7.5 mmol) was added in one portion. After 10 min stirring, allyl bromide (1.18 g, 6.0 mmol) was added dropwise at the same temperature. The cooling bath was removed and the suspension was stirred at rt for 30 min. The reaction mixture was then heated at reflux for 16 h. After full conversion, the suspension was cooled to rt and quenched by the addition of a saturated aqueous solution of NH_4Cl (50 mL). The biphasic mixture was then extracted with EtOAc (3 x 50 mL), the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound **14** was isolated in 90% yield (1.21 g, 4.5 mmol) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.3 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 1H), 7.22-7.17 (m, 2H), 6.92-6.85 (m, 2H), 6.61 (d, *J* = 16.0 Hz, 1H), 6.31 (dt, *J* = 15.9, 5.9 Hz, 1H), 4.19 (d, *J* = 5.8 Hz, 2H), 3.82 (s, 3H), 3.70 (t, *J* = 7.2 Hz, 2H), 2.91 (t, *J* = 7.2 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.2, 136.9, 132.3, 131.1, 130.0, 128.6, 127.7, 126.6, 126.3, 113.9, 71.6, 71.6, 55.3, 35.6.

HRMS (ESI^+, m/z) calcd for $C_{18}H_{20}NaO_2$ ($[M+Na]^+$): 291.1356. Found: 291.1357.

2-(4-(4-Methoxyphenyl)tetrahydrofuran-3-yl)-1,2-diphenylethan-1-one (15).



15

This compound was prepared according to the ***GPA*** using benzoyl cyanide (52.5 mg, 0.400 mmol, 100 mol%), 1-(2-(cinnamyloxy)ethyl)-4-methoxybenzene (214.7 mg, 0.800 mmol, 200 mol%). After purification by column chromatography (SiO_2: 3% ethyl acetate in petroleum ether), the title compound **15** was isolated in 9% yield (13.9 mg, 0.037 mmol, d.r. = 3.55:1) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$, for all diastereoisomers) δ 8.01-7.83 (m, 2H), 7.52-7.43 (m, 1H), 7.42-7.27 (m, 3H), 7.25-7.07 (m, 4H), 6.88-6.55 (m, 4H), 4.70-4.54 (m, 1H), 4.34-3.99 (m, 2H), 3.90-3.66 (m, 1H), [3.80 (s) + 3.72 (s), 3H], 3.66-3.57 (m, 1H), 3.30-3.17 (m, 1H), 3.06-2.96 (m, 1H).

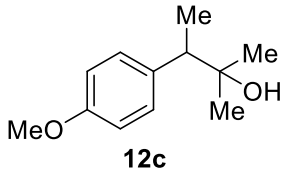
^{13}C NMR (126 MHz, $CDCl_3$, for major diastereoisomer) δ 199.3, 157.9, 137.3, 136.7, 135.3, 133.2, 129.1, 129.0, 128.9, 128.7, 128.2, 127.5, 113.7, 75.7, 74.0, 58.6, 55.3, 51.8, 48.4.

^{13}C NMR (126 MHz, $CDCl_3$, for minor diastereoisomer) δ 199.0, 158.5, 137.0, 137.0, 134.0, 133.1, 130.1, 129.2, 129.1, 128.8, 128.7, 127.7, 114.2, 75.1, 70.9, 56.2, 55.4, 50.7, 49.9.

HRMS (ESI^+, m/z) calcd for $C_{25}H_{24}NaO_3$ ($[M+Na]^+$): 395.1618. Found: 395.1623.

c. Anion Experiment

The synthesis of 3-(4-Methoxyphenyl)-2-methylbutan-2-ol (12c).



12c

Step 1: Following a reported procedure,[50] to a suspension of NaH (60% suspension in mineral oil, 210 mg, 5.25 mmol) in 6 mL of THF at 0 °C was added 1-(4-methoxyphenyl)propan-2-one (821 mg, 5 mmol) in 5 mL of THF. The resulting mixture was warmed to r.t. over a period of 30 min. The reaction mixture was cooled to 0 °C, and iodomethane (0.48 mL, 7.83 mmol) was added. The resulting mixture was stirred at 0 °C for 1 h and r.t. overnight. It was then quenched with H_2O and

extracted with EtOAc, dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2: 1% ethyl acetate in petroleum ether), the product 3-(4-methoxyphenyl)butan-2-one was isolated in 67% yield (592.8 mg, 3.33 mmol) as a light yellow oil.

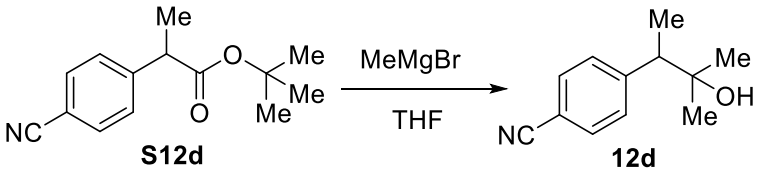
Step 2: Following a reported procedure,[51] an oven-dried round flask was charged with 3-(4-methoxyphenyl)butan-2-one (592.8 mg, 3.33 mmol) and 7 mL THF under N_2 atmosphere. The solution was cooled to 0 °C and MeMgBr (3.0 M in 2-Me-THF, 2.22 mL, 6.66 mmol) was added dropwise. The mixture was warmed to r.t., stirred overnight, quenched with saturated aqueous NH_4Cl, extracted with EtOAc, washed with brine and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 2% ethyl acetate in petroleum ether), the title compound was isolated in 82% yield (529.7 mg, 2.73 mmol) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20-7.14 (m, 2H), 6.88-6.82 (m, 2H), 3.79 (s, 3H), 2.76 (q, *J* = 7.2 Hz, 1H), 1.45 (brs, 1H), 1.31 (d, *J* = 7.2 Hz, 3H), 1.17 (s, 3H), 1.16 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 158.3, 135.4, 130.0, 113.5, 72.8, 55.3, 49.6, 28.1, 26.8, 16.0.

Spectroscopic data are in accordance with those described in literature.[52]

The synthesis of 4-(3-Hydroxy-3-methylbutan-2-yl)benzonitrile (12d).



The starting material *tert*-butyl 2-(4-cyanophenyl)propanoate **S12d** was provided by Prof. Ming Shang from Frontiers Science Center for Transformative Molecules, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, and the spectroscopic data are in accordance with those described in literature.[53]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.5 Hz, 2H), 7.39 (d, *J* = 7.4 Hz, 2H), 3.66 (q, *J* = 7.2 Hz, 1H), 1.45 (d, *J* = 7.2 Hz, 3H), 1.38 (s, 9H).

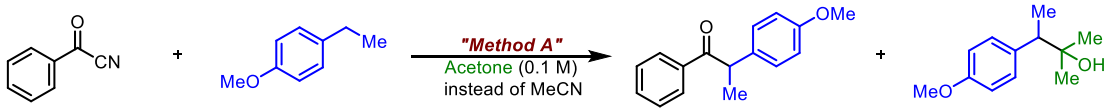
^{13}C NMR (125 MHz, $CDCl_3$) δ 172.7, 146.5, 132.4, 128.5, 118.9, 110.9, 81.4, 46.7, 28.0, 18.3.

An oven-dried round flask was charged with **S12d** (46.3 mg, 0.20 mmol) and 2 mL THF under N_2 atmosphere. The solution was cooled to -30 °C and MeMgBr (3.0 M in 2-Me-THF, 0.20 mL, 0.60 mmol) was added dropwise. The mixture was stirred for 2 h, then warmed to r.t. overnight, quenched with saturated aqueous NH_4Cl, extracted with EtOAc, washed with brine and concentrated under reduced pressure. The resulting residue was purified by column chromatography (SiO_2: 8% ethyl acetate in petroleum ether), compound **12d** was isolated in 15% yield (5.6 mg, 0.03 mmol) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63-7.54 (m, 2H), 7.41-7.34 (m, 2H), 2.84 (q, *J* = 7.2 Hz, 1H), 1.46 (brs, 1H), 1.34 (d, *J* = 7.1 Hz, 3H), 1.21 (s, 3H), 1.15 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 149.6, 131.9, 129.9, 119.2, 110.4, 72.6, 50.6, 28.6, 27.7, 15.8.

HRMS (APCI$^+$, m/z) calcd for $C_{12}H_{15}NNaO$ ([M+Na]$^+$): 212.1051. Found: 212.1053.

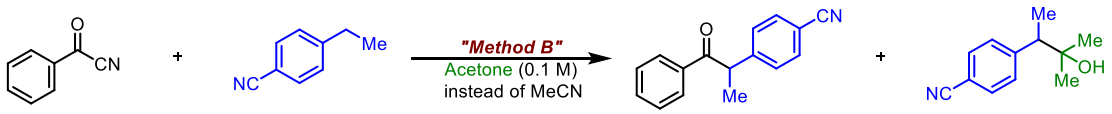


4a 0.2 mmol | **5a** 2.0 equiv | **8aa** 38%[a] | **12c** N.D.[a], 0.84%[b]

[a]NMR yield using 2,5-dimethyl furan as the internal standard. [b]GC yield using 1,3,5-trimethoxybenzene as the internal standard.

To an oven-dried Schlenk tube equipped with a stirring bar was added $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (2.2 mg, 0.002 mmol, 1 mol%), and potassium benzoate (64.0 mg, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%) and acetone (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation at r.t. for 12 hours under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The desired cross-coupling product **8aa** was 38% yield determined by ^{1}H NMR analysis. Acetone trapping benzyl anion product **9c** could not be found by ^{1}H NMR analysis, however, on GC analysis, there was only 0.82% yield was obtained, which meant that further reduction of benzyl radical to benzyl anion and

subsequent nucleophilic substitution with benzoyl cyanide was not the main process of the reaction.



4a
0.2 mmol

5c'
2.0 equiv

8ac'
48%[a]

12d
N.D.[a], 1.73%[b]

[a]NMR yield using 2,5-dimethyl furan as the internal standard. [b]GC yield using 1,3,5-trimethoxybenzene as the internal standard.

To an oven-dried Schlenk tube equipped with a stirring bar was added $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (2.2 mg, 0.002 mmol, 1 mol%), sodium bromide (8.2 mg, 0.080 mmol, 40 mol%), and anhydrous sodium carbonate (42.4 mg, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethylbenzonitrile (52.4 mg, 0.400 mmol, 200 mol%) and acetone (2 mL) were then added via syringes. The reaction mixture was stirred under blue LEDs irradiation in an aluminum module at 40 ℃ for 12 hours under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The desired cross-coupling product **8ac'** was 48% yield determined by ^{1}H NMR analysis. Acetone trapping benzyl anion product **9d** could not be found by ^{1}H NMR analysis, however, on GC analysis, there was only 1.73% yield was obtained, which meant that further reduction of benzyl radical to benzyl anion and subsequent nucleophilic substitution with benzoyl cyanide was not the main process of the reaction.

d. Cyclic Voltammetry Experiments

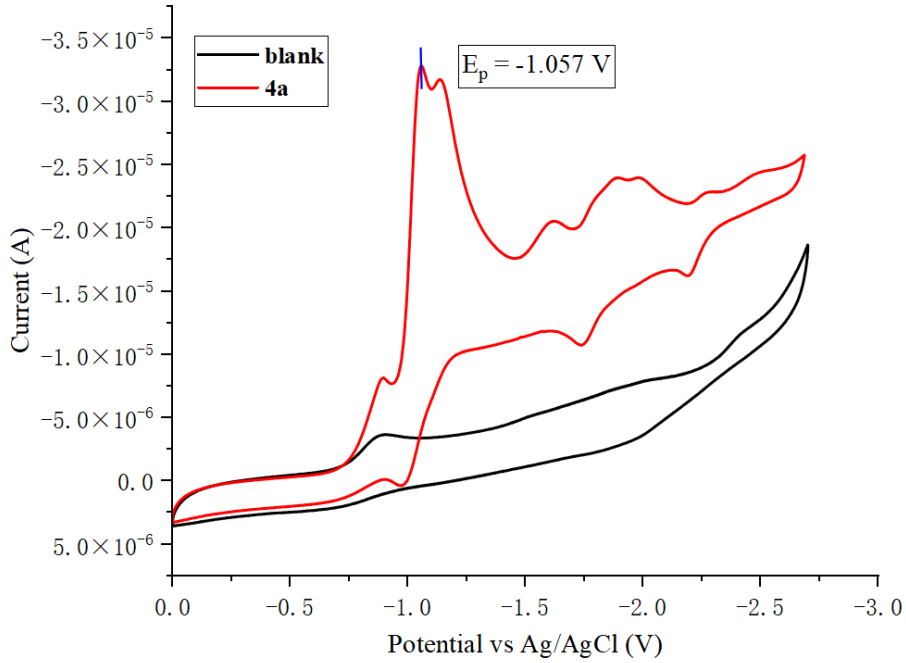


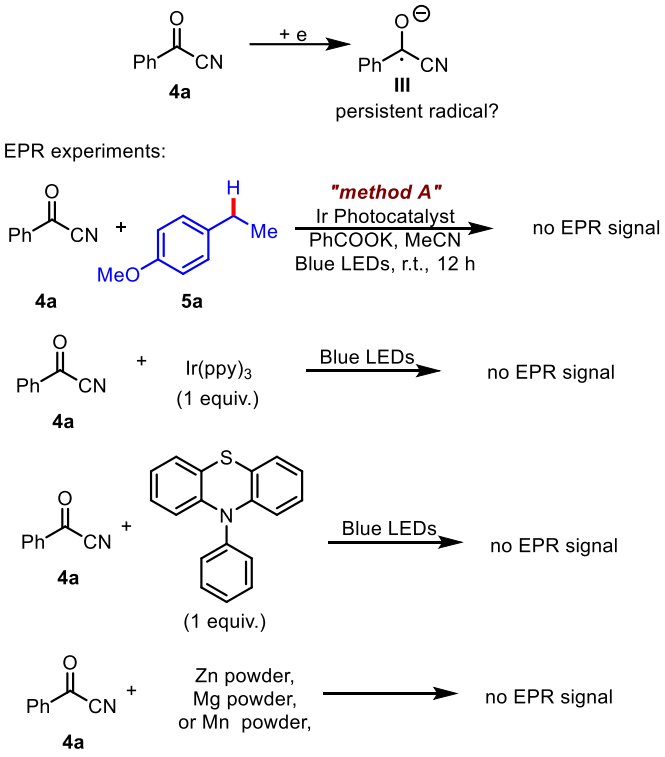
Figure S2. Reduction potential measurement of benzoyl cyanide **4a**

Determination of the reduction potential of **4a** was performed by cyclic voltammetry using a CHI760E potentiostat (CHI Instruments, Shanghai Chenhua Instrument Corp., China). The electrochemical measurements were made using a glassy carbon disk electrode (diameter is 3.0 mm, PTFE shroud) as the working electrode, a Pt electrode as the auxiliary electrode and a Ag/AgCl electrode as the reference electrode. Measurements of **4a** (0.01 M) was performed in 0.1 M of $TBAPF_6$/MeCN with a sweep rate of 100 mV/s.

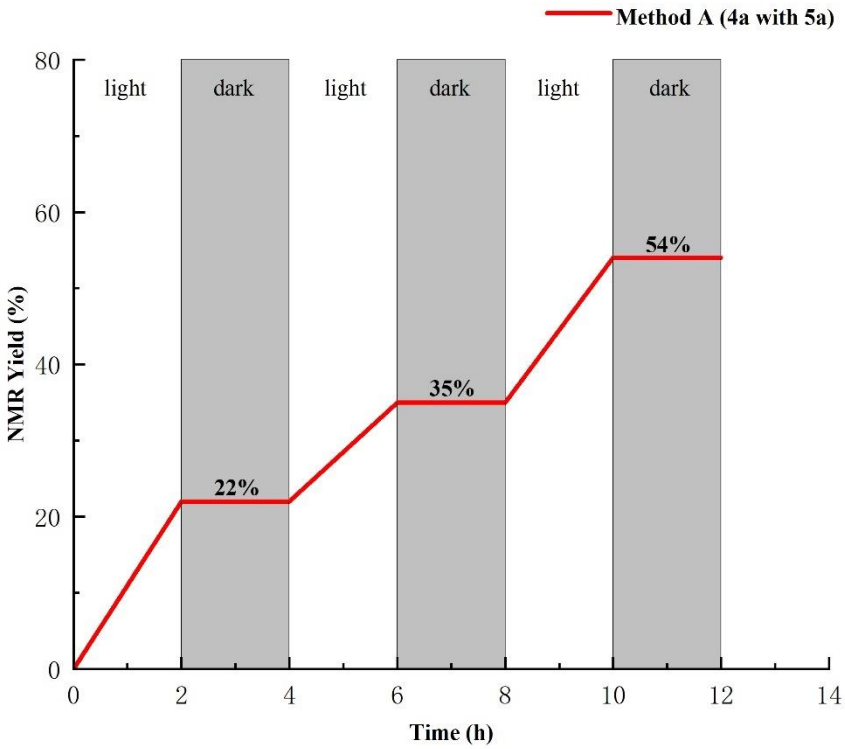
The reduction potential of **4a** is Ep = -1.057 V vs. Ag^+/AgCl (Ep = - 1.100 V vs. SCE), this result suggested that both $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ ($E_{1/2}[Ir^{III/II}]$ = -1.37 V vs. SCE) and $Ir(ppy)_2(dtbbpy)PF_6$ ($E_{1/2}[Ir^{III/II}]$ = -1.51 V vs. SCE) are sufficient to reduce the benzoyl cyanide **4a** to generate the acyl radical intermediate **III**.

e. EPR Experiment

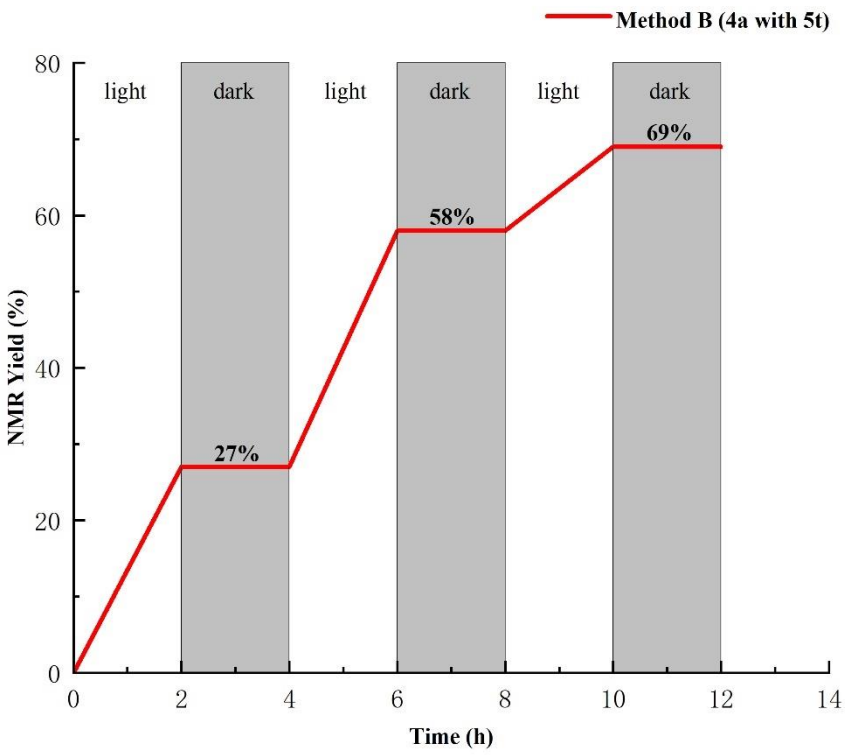
We initially assumed the key anion radical intermediate **III** as a persistent radical, in order to prove this proposal, we performed EPR experiments, including reduction of benzoyl cyanide by stoichiometric photosensitizers and reduction of benzoyl cyanide by metals (Mg, Mn, Zn). However, the signal was not observed by EPR experiments, which indicated that intermediate **III** was unlikely to be a persistent radical.



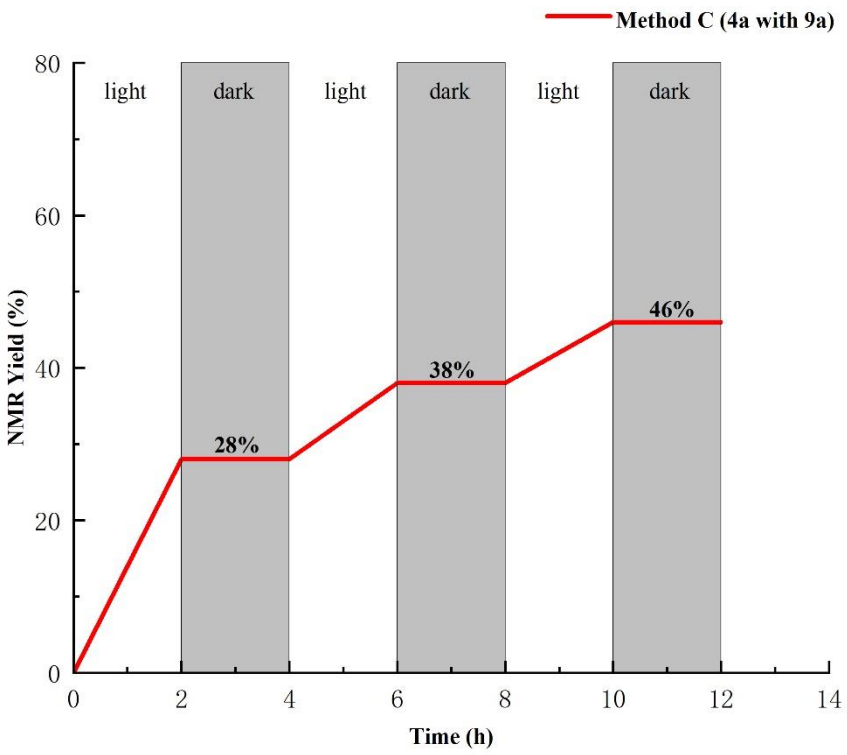
f. Light-on and -off Experiments



According to the ***GPA***, during the light off time, the photochemical equipment was closed and kept in dark environment, and during the light on time, the photochemical equipment was opened in the normal environment. The NMR yield of each period was calculated by using 1,3,5-trimethoxybenzene as the internal standard.



According to the ***GPB***, during the light off time, the photochemical equipment was closed and kept in dark environment, and during the light on time, the photochemical equipment was opened in the normal environment. The NMR yield of each period was calculated by using 1,3,5-trimethoxybenzene as the internal standard.



According to the ***GPC***, during the light off time, the photochemical equipment was closed and kept in dark environment, and during the light on time, the photochemical equipment was opened in the normal environment. The NMR yield of each period was calculated by using 1,3,5-trimethoxybenzene as the internal standard.

f. Measurement of Quantum Yield

According to the procedure of Yoon,[54] the photon flux of the LED was determined by standard ferrioxalate actinometry. A 0.15 M solution of ferrioxalate was prepared by dissolving potassium ferrioxalate hydrate (2.21 g) in 30 mL of a 0.05 M H_2SO_4 solution. A buffered solution of 1,10-phenanthroline was prepared by dissolving 1,10-phenanthroline (50 mg) and sodium acetate (11.25 g) in 50 mL of a 0.5 M solution H_2SO_4. Both solutions were stored in the dark. To determine the photon flux of the LEDs, the ferrioxalate solution (2.0 mL) was placed in a cuvette and irradiated for 90 s at λmax = 465 nm. After irradiation, the phenanthroline solution (0.35 mL) was added to the cuvette and the mixture was allowed to stir in the dark for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. The absorbance of the solution was

measured at 510 nm. A nonirradiated sample was also prepared and the absorbance at 510 nm was measured. Conversion was calculated using eq. 1.

$$\text{mol } Fe^{2+} = \frac{V \bullet \Delta A}{l \bullet \varepsilon} \qquad (1)$$

where V is the total volume (0.00235 L) of the solution after addition of phenanthroline, ΔA is the difference in absorbance at 510 nm between the irradiated and non-irradiated solutions, l is the path length (1.00 cm), and ε is the molar absorptivity of the ferrioxalate actinometer at 510 nm (11,100 L mol^{-1} cm^{-1}).

$$photon\ flux = \frac{mol\ Fe^{2+}}{\Phi \bullet t \bullet f} \qquad (2)$$

where Φ is the quantum yield for the ferrioxalate actinometer (0.93 at λex = 468 nm), t is the irradiation time (90 s), and f is the fraction of light absorbed at λex = 465 nm by the ferrioxalate actinometer. This value is calculated using eq. 3 where A (465 nm) is the absorbance of the ferrioxalate solution at 465 nm.

$$f = 1 - 10^{-A(465\ nm)} \qquad (3)$$

$$\text{mol } Fe^{2+} = \frac{V \bullet \Delta A}{l \bullet \varepsilon} = \frac{0.00235\ L \bullet 1.760}{1\ cm \bullet 11100\ L\ mol^{-1}\ cm^{-1}} = 3.73 \times 10^{-7}\ mol$$

$$f = 1 - 10^{-A(465\ nm)} = 1 - 10^{-0.65} = 0.776$$

$$photon\ flux = \frac{mol\ Fe^{2+}}{\Phi \bullet t \bullet f} = \frac{3.73 \times 10^{-7}}{0.93 \bullet 90 \bullet 0.776} = 5.74 \times 10^{-9}\ einstein \bullet s^{-1}$$

Determination of the Quantum Yield:

Method A (4a with 5a): To an oven-dried 3 mL quartz cuvette equipped with a stirring bar was added $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (2.2 mg, 0.002 mmol, 1 mol%) and potassium benzoate (64.0 mg, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 1-ethyl-4-methoxybenzene (54.5 mg, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under a single blue LED (465 nm) irradiation at r.t. for 7200 s under N_2 atmosphere. After the reaction completed, it was directly

loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The yield was determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard, and the final yield was 9.87% (1.974 x 10^{-5} mol). (Note: The solid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

$$\Phi = \frac{Mol\ product}{photon\ flux \bullet t \bullet f} = \frac{1.974 \text{ x } 10^{-5}}{5.74 \text{ x } 10^{-9} \bullet 7200 \bullet 0.776} = 0.616$$

Method B (4a with 5t): To an oven-dried 3 mL quartz cuvette equipped with a stirring bar was added Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (2.2 mg, 0.002 mmol, 1 mol%), sodium bromide (8.2 mg, 0.080 mmol, 40 mol%) and anhydrous sodium carbonate (42.4 mg, 0.400 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (26.2 mg, 0.200 mmol, 100 mol%), 4-ethylacetophenone (59.3 mg, 0.400 mmol, 200 mol%) and MeCN (2 mL) were then added via syringes. The reaction mixture was stirred under a single blue LED (465 nm) irradiation at r.t. for 7200 s under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The yield was determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard, and the final yield was 6.69% (1.338 x 10^{-5} mol). (Note: The solid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

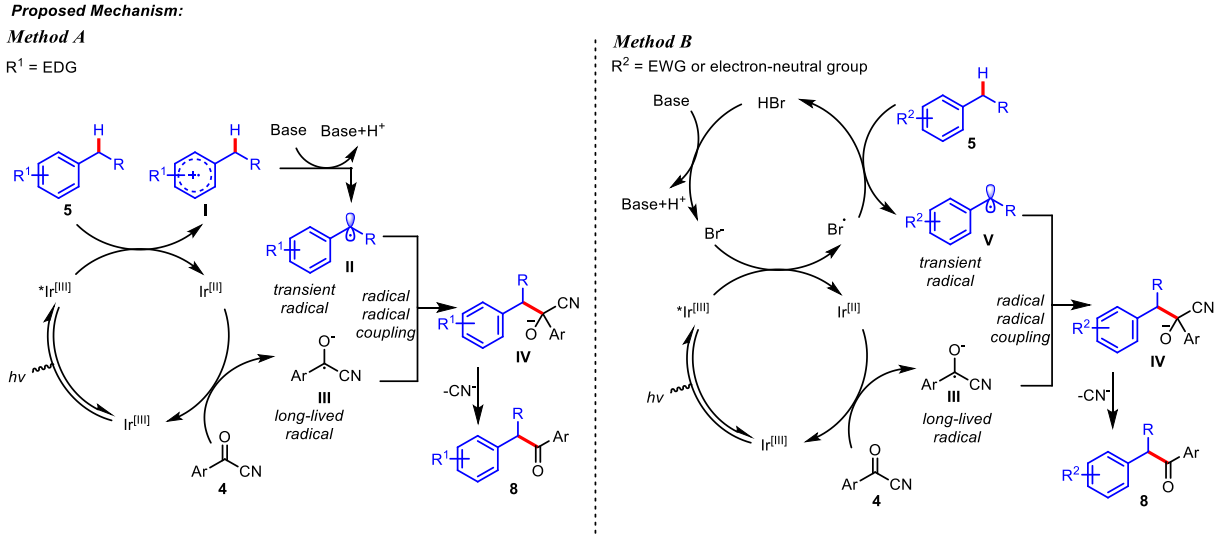
$$\Phi = \frac{Mol\ product}{photon\ flux \bullet t \bullet f} = \frac{1.338 \text{ x } 10^{-5}}{5.74 \text{ x } 10^{-9} \bullet 7200 \bullet 0.776} = 0.417$$

Method C (4a with 9a): To an oven-dried 3 mL quartz cuvette equipped with a stirring bar was added Ir(ppy)$_2$(dtbbpy)PF_6 (0.9 mg, 0.001 mmol, 1 mol%) and sodium trifluoromethanesulfinate (31.2 mg, 0.200 mmol, 200 mol%) under air. The tube was capped with a rubber septum, and it

was evacuated and refilled nitrogen (N_2) three times. Benzoyl cyanide (13.1 mg, 0.100 mmol, 100 mol%), styrene (20.9 mg, 0.200 mmol, 200 mol%), Acetone (1.5 mL) and DMF (0.15 mL) were then added via syringes. The reaction mixture was stirred under a single blue LED (465 nm) irradiation at r.t. for 7200 s under N_2 atmosphere. After the reaction completed, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of EtOAc. Flash column chromatography provided the product as an oil. The yield was determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard, and the final yield was 28.16% (2.816 x 10^{-5} mol). (Note: The solid waste contained highly toxic cyanide ions, it must be oxidized with 30% H_2O_2 (5 mL) carefully and stirred for more than 1 hour, then quenched with saturated aq. Na_2SO_3 before pouring into the waste storage container.)

$$\Phi = \frac{Mol\ product}{photon\ flux \bullet t \bullet f} = \frac{2.816 \text{ x } 10^{-5}}{5.74 \text{ x } 10^{-9} \bullet 7200 \bullet 0.776} = 0.878$$

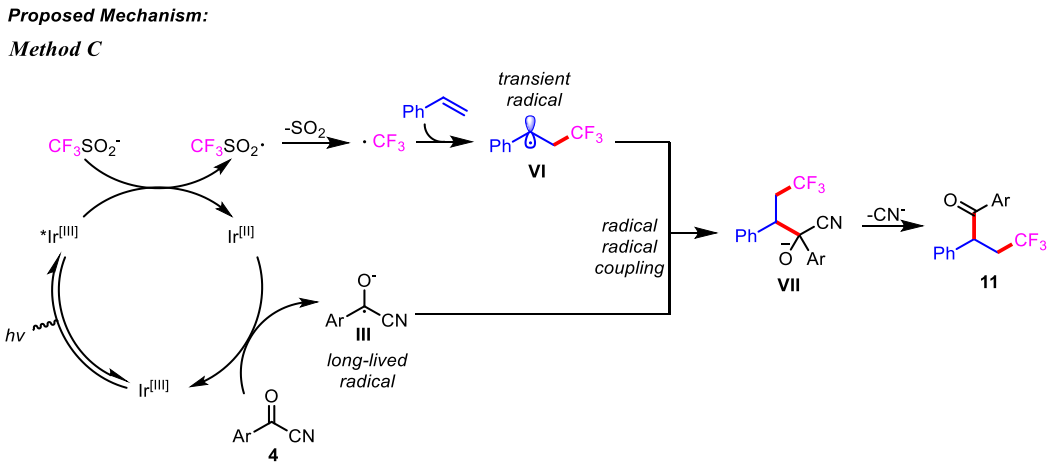
g. Proposed Mechanism



Scheme 1. Plausible reaction mechanism (Method A and B)

According to the above results and previous reports, a possible mechanism is suggested in Scheme 1. In method A, the excited state *Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 is generated by visible-light irradiation. *Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 is a strong oxidant ($E_{1/2}$[$Ir^{*III/II}$] = +1.21 V),[55] and according to the report, 4-ethyl anisole shows a higher oxidation potential ($E_{1/2}$ = +1.52 V),[56] which indicates that the formation of intermediate **I** through photocatalyst oxidation is thermodynamically unfavorable. But due to rapid deprotonation, benzyl radical **II** can be obtained efficiently.[10] We believe that the benzyl radical is similar to a transient radical. In addition, the photocatalyst reduces benzoyl cyanide **4** to form intermediate **III** based on the assumption that intermediate **III** is an anionic radical stabilized by the cyano group and is a long-lived radical[57,58].

Then radical-radical cross-coupling of **II** and **III** forms intermediate **IV**. Finally, the cyanide anion leaves, which generates the desired product **8**. In method B, *Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 can quickly oxidize bromide ($E_{1/2}$ = +0.80 V vs. SCE in MeCN)[59] to generate a bromine radical. Then the electrophilic bromine radicals can rapidly abstract a benzylic hydrogen atoms from an electron-poor/neutral arene to give transient benzyl radical **V**.[60] The obtained hydrogen bromide undergoes deprotonation by the base, which closes the HAT catalytic cycle. Intermediate **III**, formed by photocatalyst reduction of benzoyl cyanide, undergoes coupling with benzyl radical **V**, then expulsing a cyanide anion, which results in the desired product **8**.

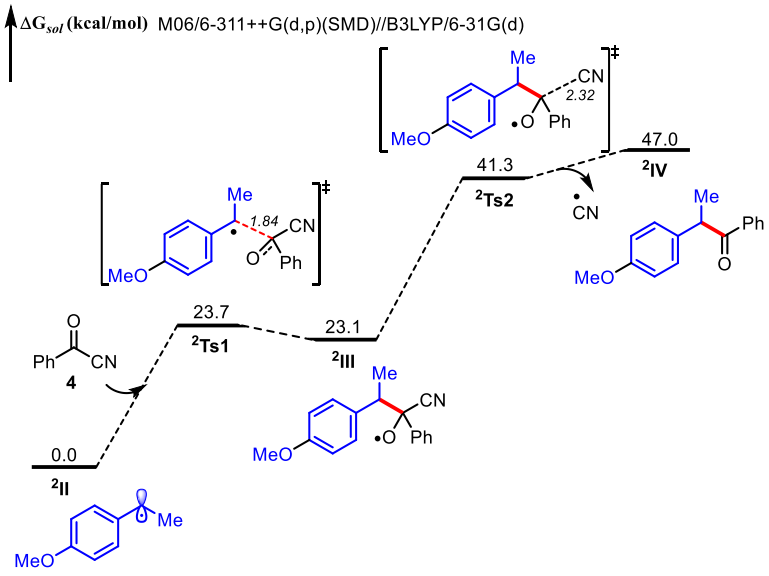


Scheme 2. Plausible reaction mechanism (Method C)

In method C, the excited state *Ir(ppy)$_2$(dtbbpy)PF_6 undergoes known reductive quenching by the trifluoromethanesulfinate anion[61,62] to give the corresponding Ir^{II}-complex ($E_{1/2}[Ir^{III/II}]$ = -1.51 V vs. SCE in MeCN)[55,63] and the trifluoromethylsulfonyl radical, which in turn quickly fragments and expels SO_2 to give the trifluoromethyl radical.[64] Subsequently, the trifluoromethyl radical can add to the double bond of styrene to generate the transient benzyl radical **VI**. Meanwhile, intermediate **III**, which is formed by photocatalyst reduction, couples with benzyl radical **VI** to give intermediate **VII**, then expels a cyanide anion to generate the desired product **11**.

h. DFT Calculations

The B3LYP[65-67] density functional method was employed to carry out all the geometry optimizations. For the geometry optimizations, the 6-31G(d)[68] basis set was used for all atoms. Vibrational frequency analyses at the same level of the theory were performed on all the optimized geometries to characterize them as local minima (no imaginary frequency) or transition states (one imaginary frequency). In addition, intrinsic reaction coordinate (IRC)[69,70] calculations were used to verify that the transition state connect with appropriate reactant and product. Solution phase single-point energies were calculated based on the optimized structures with the M06 method[71-73], SMD[74] solvation model (in acetonitrile) and larger basis sets (6-311++G(d,p) for all atoms). The Gibbs energy was determined by adding the single-point energy and the gas-phase thermal correction to the Gibbs energy obtained from the vibrational frequency analyses. All calculations were carried out with the Gaussian 09 (Revision C.01) suite of programs[75].



Scheme 3. DFT calculation

Cartesian Coordinates and Energies

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.390829	0.608141	0.000135
2	8	0	-1.794957	1.757446	0.000375
3	6	0	-2.387842	-0.491923	-0.000200
4	7	0	-3.196912	-1.325559	-0.000345
5	6	0	0.034071	0.211595	0.000062
6	6	0	1.004974	1.227509	-0.000172
7	6	0	0.426898	-1.135820	0.000210
8	6	0	2.354223	0.895005	-0.000256
9	1	0	0.677459	2.261985	-0.000319
10	6	0	1.781231	-1.462743	0.000205
11	1	0	-0.323969	-1.920836	0.000255
12	6	0	2.742877	-0.449824	-0.000055
13	1	0	3.106264	1.678609	-0.000678
14	1	0	2.086083	-2.504990	0.000640
15	1	0	3.798582	-0.707063	-0.000052

Zero-point correction= 0.108869 (Hartree/Particle)
Thermal correction to Energy= 0.116922
Thermal correction to Enthalpy= 0.117866
Thermal correction to Gibbs Free Energy= 0.075353
Sum of electronic and zero-point Energies= -437.699256
Sum of electronic and thermal Energies= -437.691203
Sum of electronic and thermal Enthalpies= -437.690259
Sum of electronic and thermal Free Energies= -437.732772
M06 /6-311++G(d,p)/SMD//B3LYP /6-31G(d) energy in acetonitrile solvent = -437.625648

^{2}II

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.411767	0.255000	-0.000005
2	6	0	0.688923	-0.946880	-0.000021
3	6	0	-0.701682	-0.922574	-0.000026
4	6	0	-1.433841	0.296854	-0.000010
5	6	0	-0.662471	1.499381	-0.000002
6	6	0	0.716054	1.480629	0.000001
7	1	0	1.201326	-1.902704	-0.000021
8	1	0	-1.239208	-1.866186	-0.000037
9	1	0	-1.184259	2.453598	0.000009

10	1	0	1.293168	2.400445	0.000012
11	6	0	3.529432	-0.851471	0.000029
12	1	0	3.328107	-1.455888	-0.894538
13	1	0	4.577523	-0.546237	0.000027
14	1	0	3.328094	-1.455829	0.894631
15	6	0	-2.846654	0.346091	-0.000012
16	6	0	-3.740560	-0.855455	0.000019
17	1	0	-3.577770	-1.495300	0.881112
18	1	0	-4.794549	-0.562510	-0.000346
19	1	0	-3.577245	-1.495710	-0.880670
20	8	0	2.773959	0.348540	-0.000012
21	1	0	-3.312665	1.328549	0.000079

Zero-point correction= 0.176003 (Hartree/Particle)
Thermal correction to Energy= 0.186033
Thermal correction to Enthalpy= 0.186977
Thermal correction to Gibbs Free Energy= 0.139750
Sum of electronic and zero-point Energies= -424.580239
Sum of electronic and thermal Energies= -424.570210
Sum of electronic and thermal Enthalpies= -424.569265
Sum of electronic and thermal Free Energies= -424.616492

M06 /6-311++G(d,p)/SMD//B3LYP /6-31G(d) energy in acetonitrile solvent = -424.55696

^{2}Ts1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.146942	0.007515	-0.351504
2	6	0	-2.694868	-0.920817	0.599485
3	6	0	-1.400487	-1.424769	0.510008
4	6	0	-0.526321	-1.027639	-0.514752
5	6	0	-0.994117	-0.075554	-1.443297
6	6	0	-2.282537	0.428286	-1.375032
7	1	0	-3.337933	-1.248428	1.408066
8	1	0	-1.056874	-2.122252	1.266907
9	1	0	-0.332635	0.265177	-2.235364
10	1	0	-2.646203	1.151769	-2.097501
11	6	0	-5.313449	0.176911	0.646413
12	1	0	-4.948225	0.443305	1.646345
13	1	0	-6.228782	0.732203	0.435983
14	1	0	-5.524484	-0.899405	0.611363
15	6	0	0.837699	-1.585343	-0.650068
16	6	0	0.988204	-3.090376	-0.493406
17	1	0	0.421185	-3.583202	-1.292980
18	1	0	2.033423	-3.397867	-0.579604
19	1	0	0.603788	-3.443325	0.465547
20	8	0	-4.388729	0.558484	-0.363743
21	1	0	1.319432	-1.226709	-1.563712
22	6	0	1.966991	-0.783321	0.567622
23	8	0	1.562490	-1.292229	1.694461
24	6	0	3.297314	-1.283237	0.108058
25	7	0	4.328311	-1.690559	-0.240049
26	6	0	1.817987	0.718745	0.357466
27	6	0	1.007057	1.444484	1.235711
28	6	0	2.468685	1.380319	-0.690569
29	6	0	0.844991	2.818297	1.062946
30	1	0	0.518448	0.922041	2.050666
31	6	0	2.302663	2.755314	-0.861956
32	1	0	3.120061	0.827513	-1.362890
33	6	0	1.489217	3.477151	0.013124
34	1	0	0.218733	3.377005	1.753409
35	1	0	2.815601	3.261679	-1.675163
36	1	0	1.363670	4.548573	-0.117962

Zero-point correction= 0.287482 (Hartree/Particle)
Thermal correction to Energy= 0.305689
Thermal correction to Enthalpy= 0.306633
Thermal correction to Gibbs Free Energy= 0.239656
Sum of electronic and zero-point Energies= -862.253836
Sum of electronic and thermal Energies= -862.235630
Sum of electronic and thermal Enthalpies= -862.234685

Sum of electronic and thermal Free Energies= -862.301662

M06 /6-311++G(d,p)/SMD//B3LYP /6-31G(d) energy in acetonitrile solvent = -862.169425

^{2}III

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.177194	0.030464	-0.354531
2	6	0	-2.704093	-0.826496	0.650546
3	6	0	-1.405425	-1.325596	0.577250
4	6	0	-0.549751	-0.992648	-0.482311
5	6	0	-1.038109	-0.114873	-1.467771
6	6	0	-2.330633	0.384609	-1.415953
7	1	0	-3.332725	-1.103415	1.488958
8	1	0	-1.046662	-1.969025	1.374540
9	1	0	-0.391805	0.174465	-2.292431
10	1	0	-2.709087	1.053709	-2.182016
11	6	0	-5.330750	0.251109	0.660288
12	1	0	-4.954261	0.586565	1.635164
13	1	0	-6.254444	0.783307	0.427382
14	1	0	-5.532663	-0.826939	0.701037
15	6	0	0.827376	-1.562876	-0.606167
16	6	0	0.912603	-3.084985	-0.486686
17	1	0	0.325345	-3.534696	-1.295306
18	1	0	1.944505	-3.434877	-0.578851
19	1	0	0.512334	-3.442268	0.464573
20	8	0	-4.424666	0.571737	-0.386201
21	1	0	1.274396	-1.236894	-1.551372
22	6	0	1.916770	-0.831387	0.507873
23	8	0	1.527045	-1.302235	1.684909
24	6	0	3.261903	-1.345487	0.100739
25	7	0	4.303903	-1.755658	-0.207229
26	6	0	1.834351	0.689341	0.327835
27	6	0	1.070454	1.441690	1.224172
28	6	0	2.500887	1.329644	-0.722428
29	6	0	0.969403	2.823710	1.065479
30	1	0	0.566790	0.937767	2.041285
31	6	0	2.395240	2.712388	-0.879639
32	1	0	3.117503	0.754786	-1.408764
33	6	0	1.628102	3.462501	0.012969
34	1	0	0.378582	3.403126	1.769900
35	1	0	2.919164	3.201663	-1.696251
36	1	0	1.549869	4.539671	-0.106903

Zero-point correction= 0.288280 (Hartree/Particle)

Thermal correction to Energy= 0.306839

Thermal correction to Enthalpy= 0.307783

Thermal correction to Gibbs Free Energy= 0.240136

Sum of electronic and zero-point Energies= -862.253256

Sum of electronic and thermal Energies= -862.234698

Sum of electronic and thermal Enthalpies= -862.233753

Sum of electronic and thermal Free Energies= -862.301401

M06 /6-311++G(d,p)/SMD//B3LYP /6-31G(d) energy in acetonitrile solvent = -862.1709

^{2}Ts2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.384306	0.177800	0.368191
2	6	0	2.878589	-0.405474	-0.806566
3	6	0	1.599646	-0.950254	-0.805434
4	6	0	0.799878	-0.950962	0.350902
5	6	0	1.313866	-0.330519	1.507466
6	6	0	2.586656	0.212756	1.527365
7	1	0	3.467207	-0.426901	-1.716271
8	1	0	1.203739	-1.371438	-1.724974
9	1	0	0.707942	-0.297791	2.409087
10	1	0	2.994095	0.671197	2.422608
11	6	0	5.475245	0.744397	-0.648192
12	1	0	5.039448	1.311108	-1.479984
13	1	0	6.392620	1.232601	-0.317003

14	1	0	5.702794	-0.276137	-0.979401
15	6	0	-0.556663	-1.605952	0.372329
16	6	0	-0.529452	-3.091617	0.000700
17	1	0	0.139608	-3.626350	0.683030
18	1	0	-1.534818	-3.513795	0.081964
19	1	0	-0.176463	-3.241101	-1.022093
20	8	0	4.610827	0.739981	0.483480
21	1	0	-0.987342	-1.484932	1.366239
22	6	0	-1.467006	-0.778321	-0.687595
23	8	0	-1.434352	-1.165389	-1.847861
24	6	0	-3.339781	-1.768934	0.259053
25	7	0	-4.322573	-2.250081	0.680591
26	6	0	-1.853684	0.628689	-0.335548
27	6	0	-1.865449	1.578870	-1.365814
28	6	0	-2.193897	1.019136	0.967492
29	6	0	-2.208987	2.901448	-1.096161
30	1	0	-1.612272	1.260665	-2.371753
31	6	0	-2.544414	2.341298	1.233341
32	1	0	-2.224008	0.285380	1.766569
33	6	0	-2.546354	3.285994	0.204644
34	1	0	-2.222564	3.631299	-1.900998
35	1	0	-2.820731	2.632871	2.242608
36	1	0	-2.818044	4.317038	0.414251

Zero-point correction= 0.286103 (Hartree/Particle)
Thermal correction to Energy= 0.305253
Thermal correction to Enthalpy= 0.306197
Thermal correction to Gibbs Free Energy= 0.236028
Sum of electronic and zero-point Energies= -862.207621
Sum of electronic and thermal Energies= -862.188471
Sum of electronic and thermal Enthalpies= -862.187527
Sum of electronic and thermal Free Energies= -862.257696
M06 /6-311++G(d,p)/SMD//B3LYP /6-31G(d) energy in acetonitrile solvent = -862.137818

^{2}IV

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.205128	-0.562263	0.122913
2	6	0	-2.565807	0.037281	-0.968227
3	6	0	-1.372957	0.737988	-0.773239
4	6	0	-0.793462	0.858231	0.493777
5	6	0	-1.450074	0.249605	1.575021
6	6	0	-2.637696	-0.449806	1.400138
7	1	0	-2.980141	-0.034679	-1.967431
8	1	0	-0.886042	1.195947	-1.630069
9	1	0	-1.027626	0.331833	2.574631
10	1	0	-3.145599	-0.918070	2.237622
11	6	0	-4.988949	-1.416275	-1.217083
12	1	0	-4.339053	-1.946902	-1.925605
13	1	0	-5.890866	-2.006432	-1.044353
14	1	0	-5.268593	-0.444164	-1.644576
15	6	0	0.486298	1.664797	0.707609
16	6	0	0.221362	3.179743	0.662151
17	1	0	-0.533108	3.449826	1.407997
18	1	0	1.137436	3.743361	0.870508
19	1	0	-0.137775	3.480028	-0.325039
20	8	0	-4.370385	-1.270727	0.051070
21	1	0	0.877515	1.412540	1.700455
22	6	0	1.541290	1.270102	-0.340011
23	8	0	1.695909	1.956453	-1.341215
24	6	0	2.369896	0.035116	-0.137939
25	6	0	3.411402	-0.206914	-1.049037
26	6	0	2.155967	-0.876265	0.907608
27	6	0	4.225669	-1.326669	-0.913431
28	1	0	3.561464	0.503613	-1.855204
29	6	0	2.967719	-2.002804	1.038557
30	1	0	1.343107	-0.725831	1.609585
31	6	0	4.005373	-2.228016	0.132399
32	1	0	5.031806	-1.500178	-1.621231
33	1	0	2.788329	-2.705555	1.847629

34	1	0	4.639540	-3.104256	0.239004

Zero-point correction= 0.281425 (Hartree/Particle)
Thermal correction to Energy= 0.297602
Thermal correction to Enthalpy= 0.298546
Thermal correction to Gibbs Free Energy= 0.236011
Sum of electronic and zero-point Energies= -769.499453
Sum of electronic and thermal Energies= -769.483276
Sum of electronic and thermal Enthalpies= -769.482332
Sum of electronic and thermal Free Energies= -769.544867
M06 /6-311++G(d,p)/SMD//B3LYP /6-31G(d) energy in acetonitrile solvent = -769.438652

-CN radical

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-0.000000	-0.632076
2	7	0	-0.000000	0.000000	0.541779

Zero-point correction= 0.004923 (Hartree/Particle)
Thermal correction to Energy= 0.007284
Thermal correction to Enthalpy= 0.008228
Thermal correction to Gibbs Free Energy= -0.014768
Sum of electronic and zero-point Energies= -92.706824
Sum of electronic and thermal Energies= -92.704463
Sum of electronic and thermal Enthalpies= -92.703519
Sum of electronic and thermal Free Energies= -92.726515
M06 /6-311++G(d,p)/SMD//B3LYP /6-31G(d) energy in acetonitrile solvent = -92.675145

II. Reference

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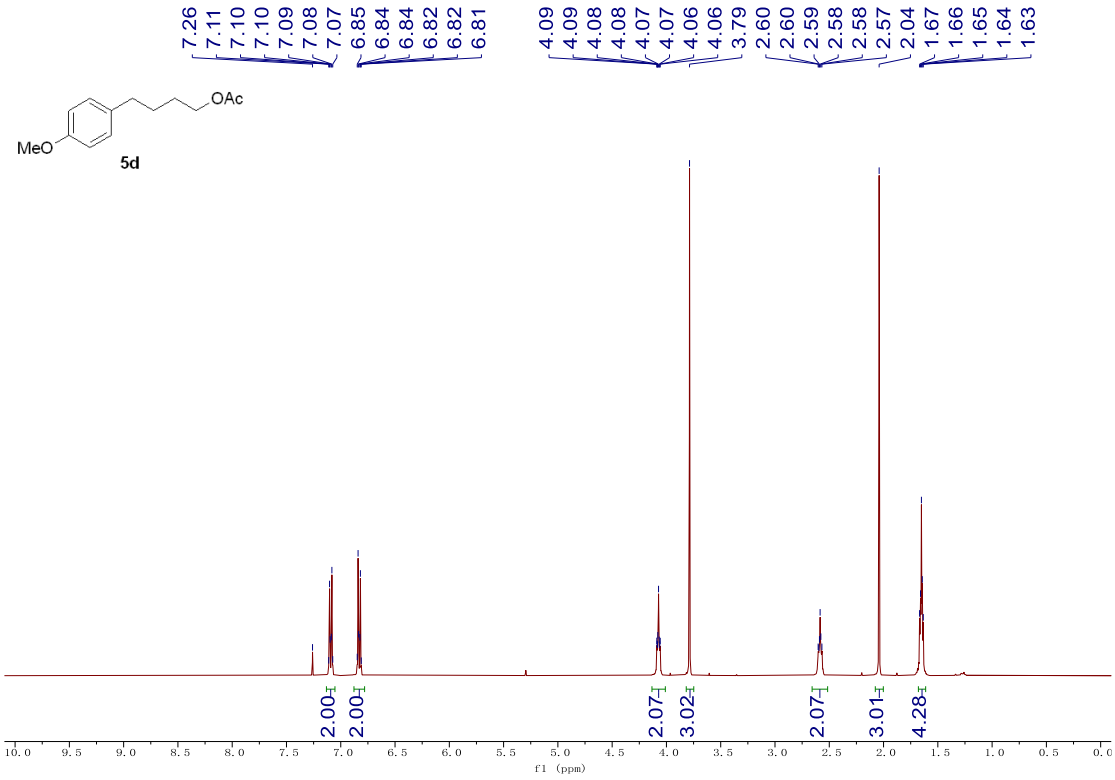
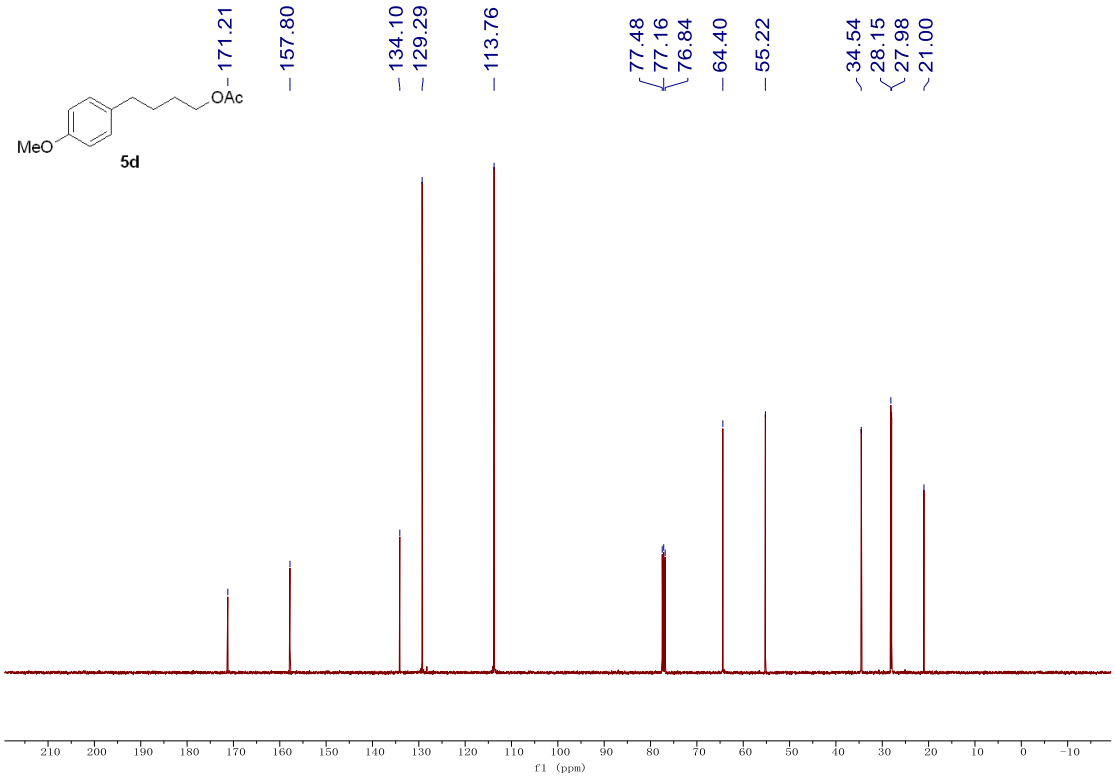
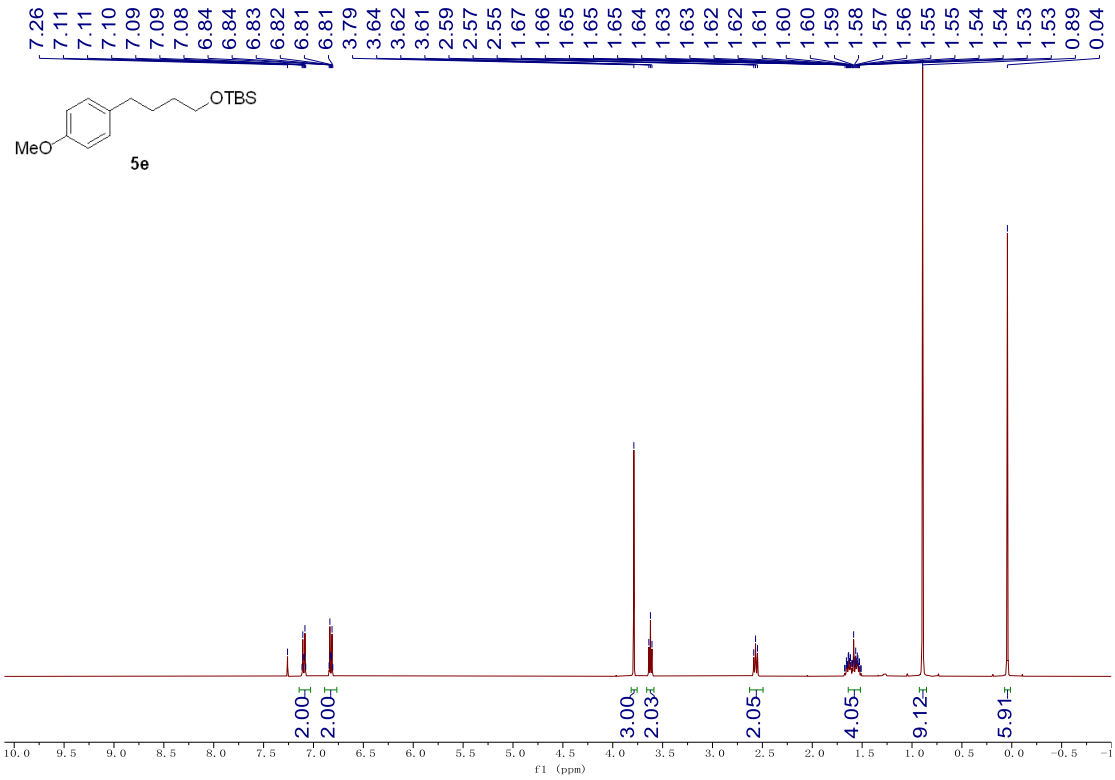
III. Spectral Data for New Compounds



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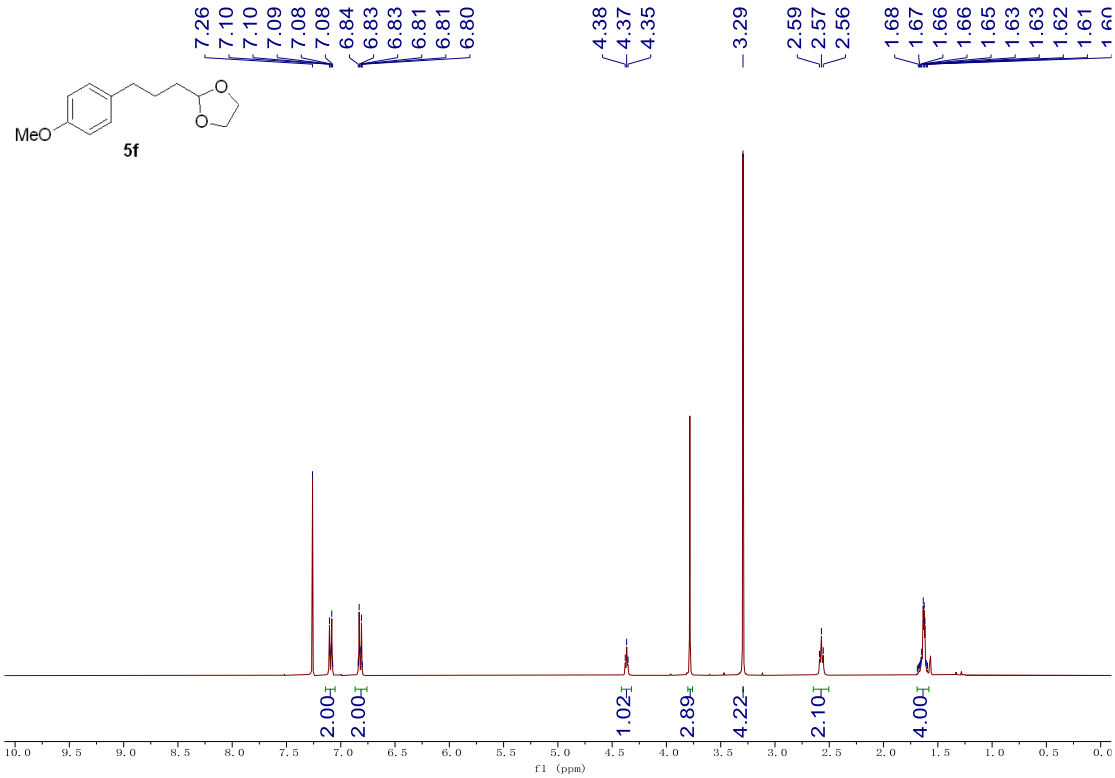
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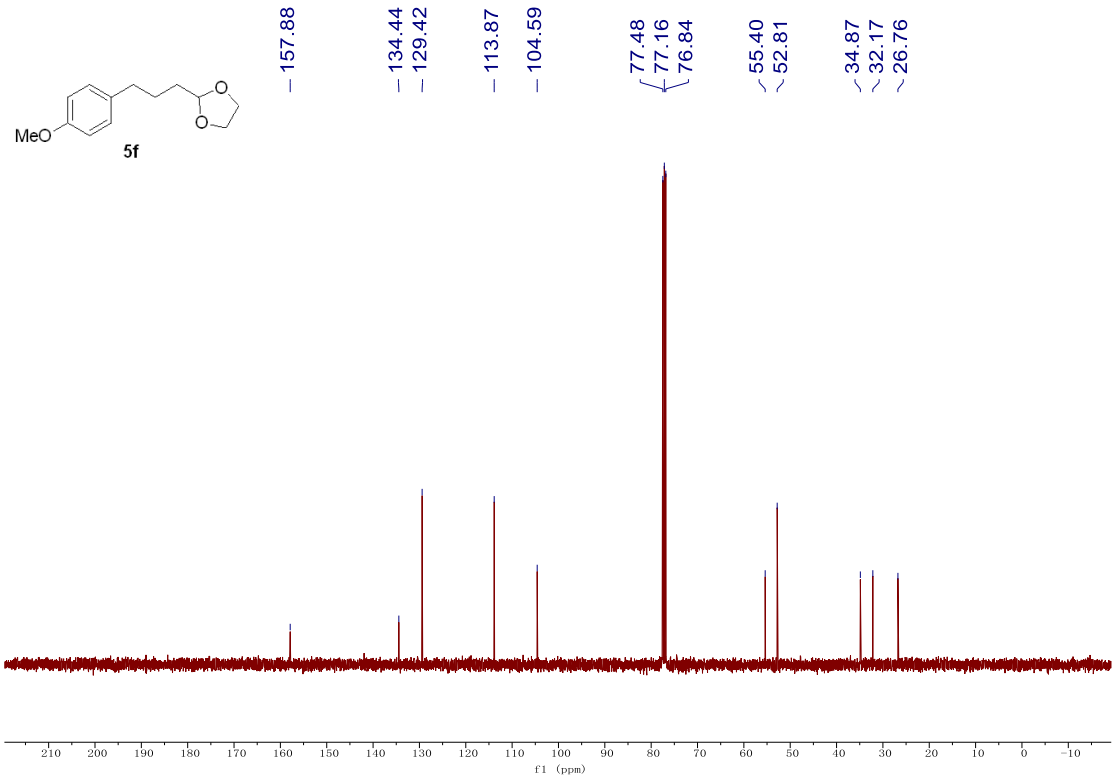
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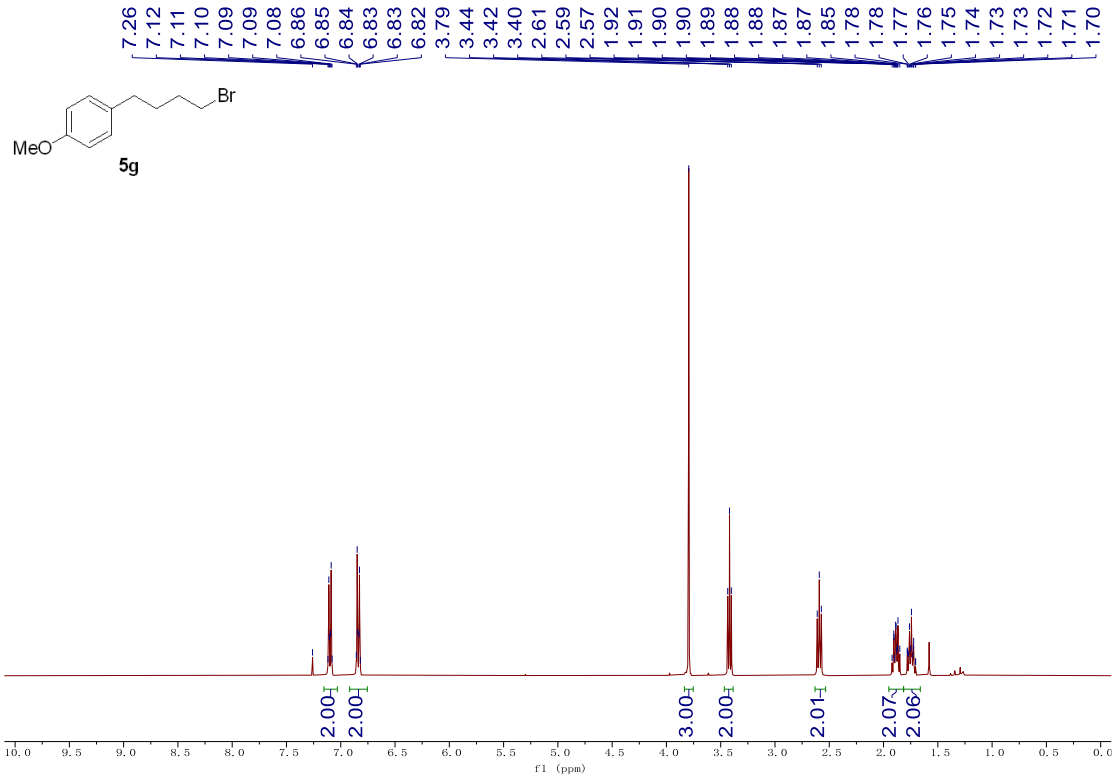
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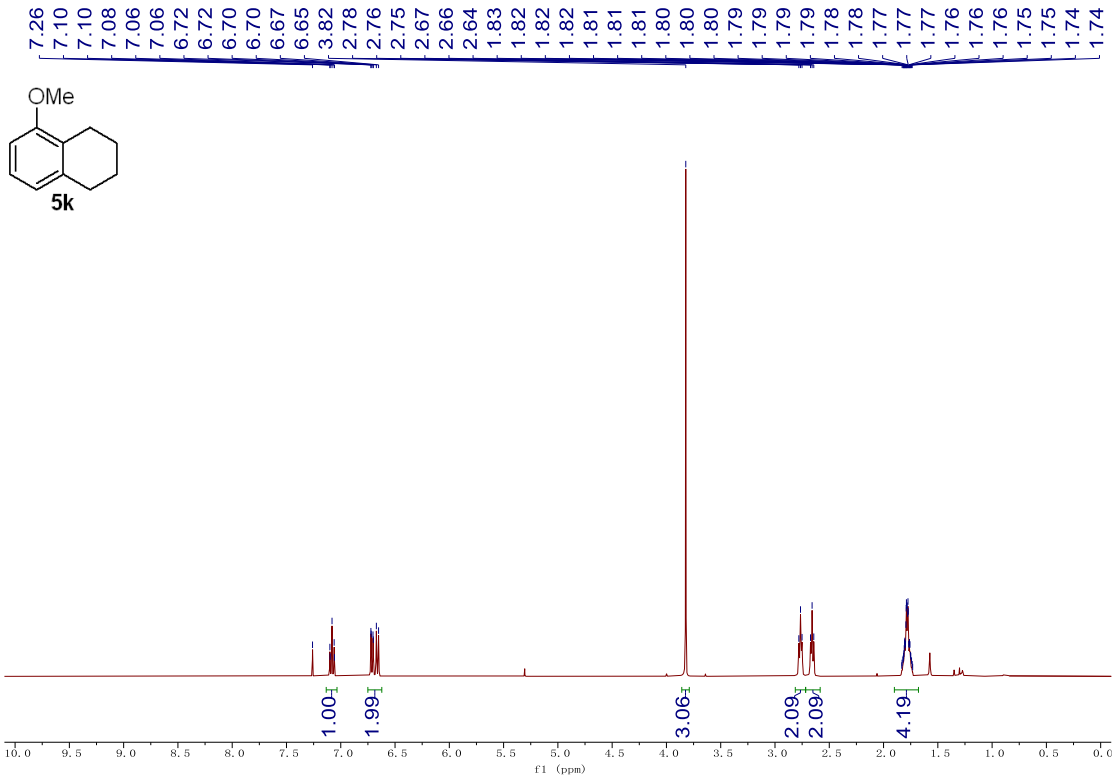
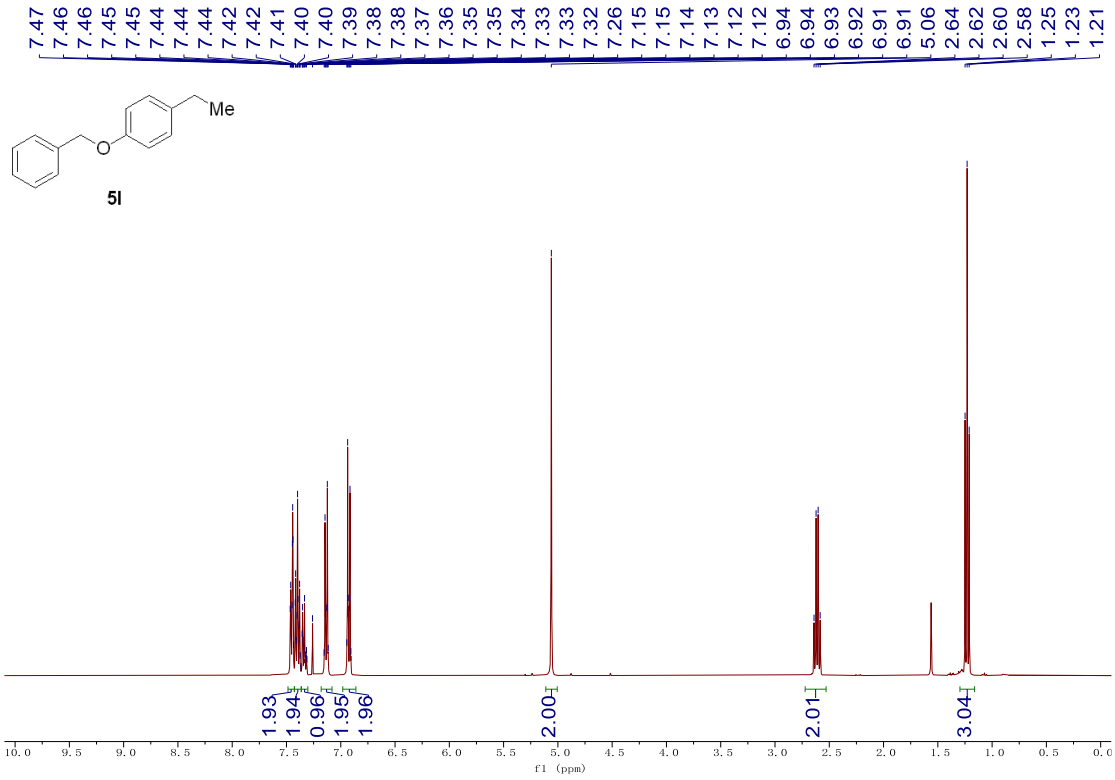

7.26 7.10 7.10 7.08 7.06 7.06 6.72 6.72 6.70 6.70 6.67 6.65 3.82 2.78 2.76 2.75 2.67 2.66 2.64 1.83 1.82 1.82 1.82 1.81 1.81 1.81 1.80 1.80 1.80 1.79 1.79 1.79 1.79 1.78 1.78 1.77 1.77 1.77 1.76 1.76 1.76 1.75 1.75 1.74 1.74
OMe
5k
1.00 1.99 3.06 2.09 2.09 4.19
f1 (ppm)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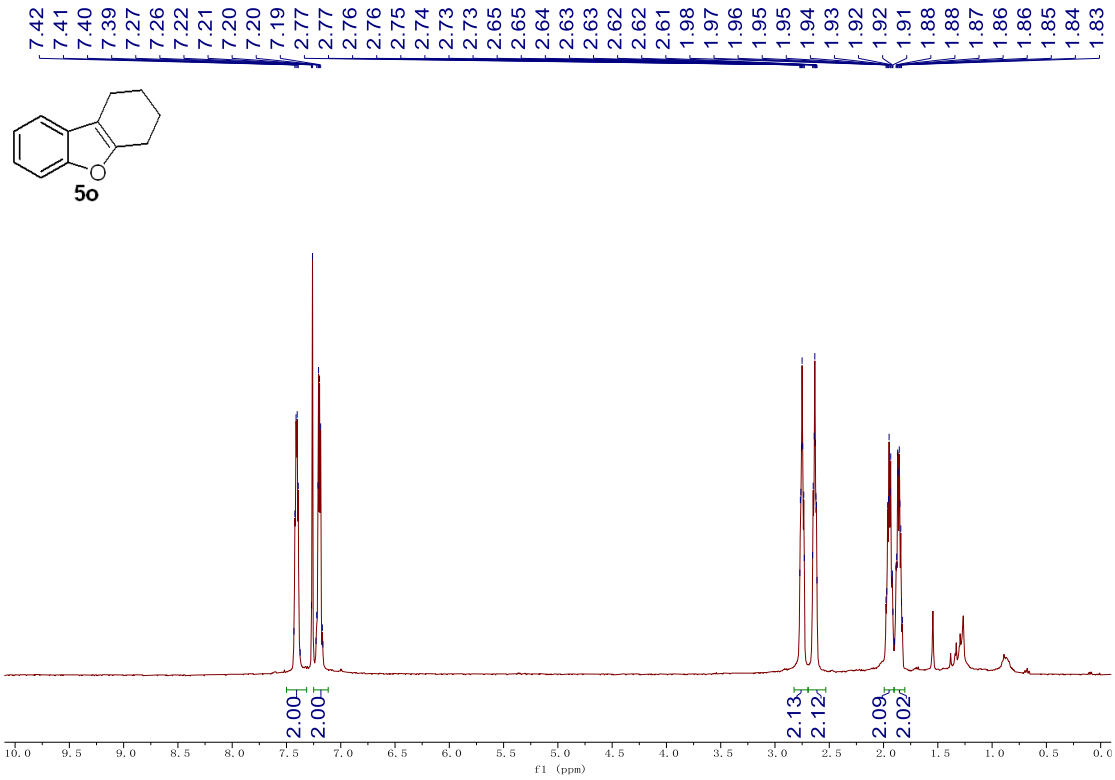
Me
O
5l
1.93 1.94 0.96 1.95 1.96 2.00 2.01 3.04
f1 (ppm)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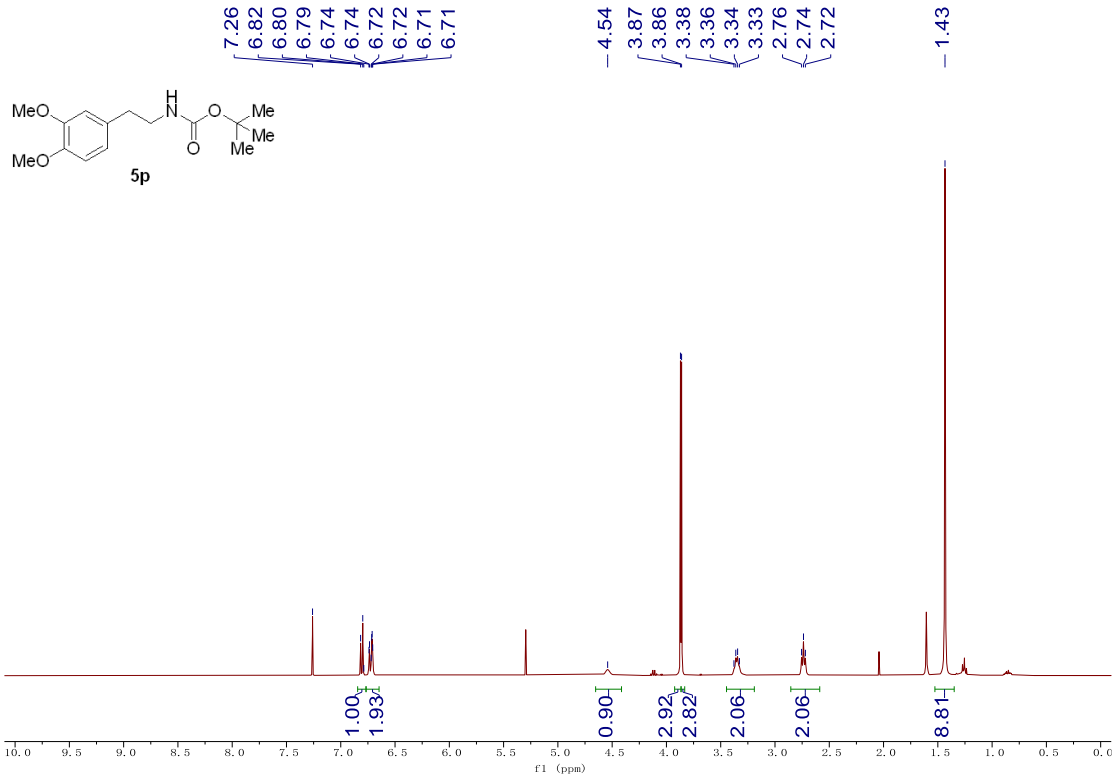
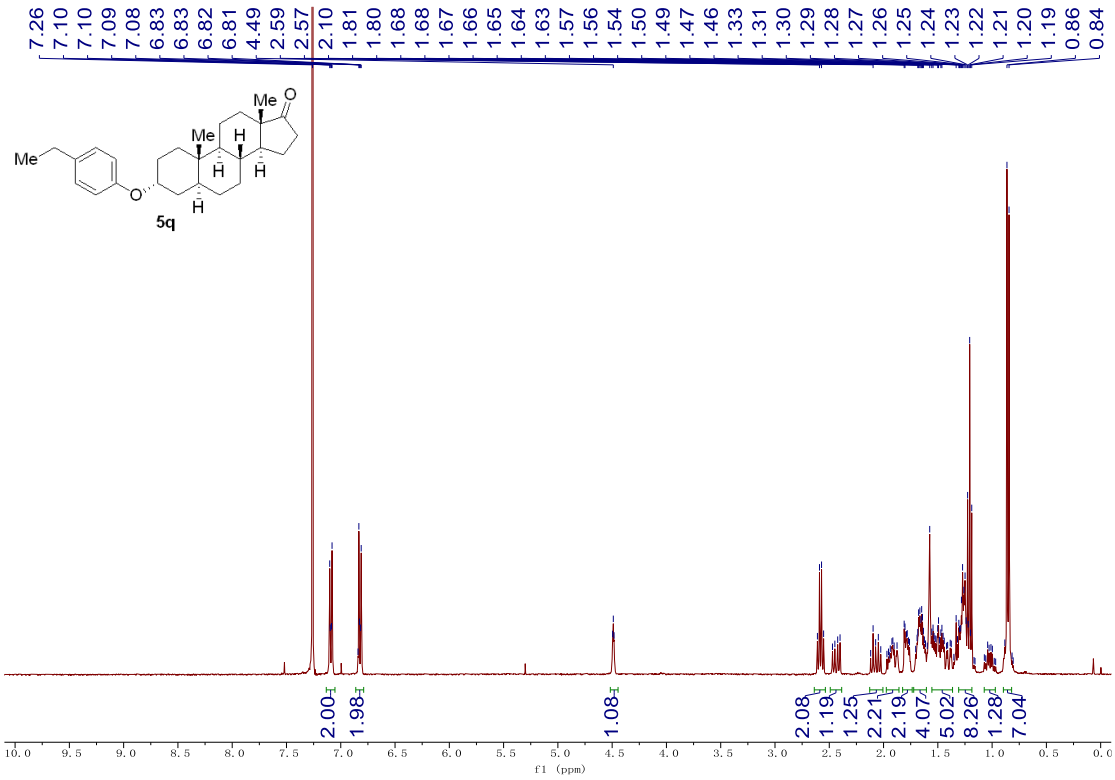
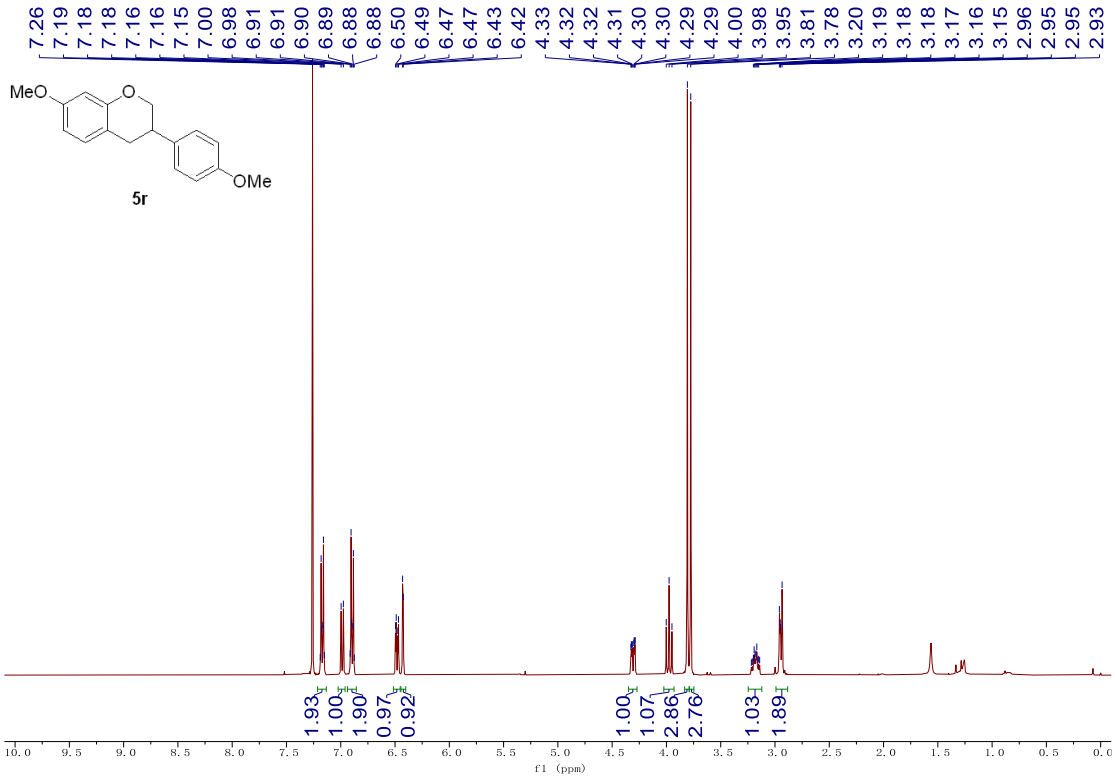
5o
2.00 2.00 2.13 2.12 2.09 2.02
f1 (ppm)


7.26 6.82 6.80 6.79 6.74 6.74 6.72 6.72 6.71 6.71 4.54 3.87 3.86 3.38 3.36 3.34 3.33 2.76 2.74 2.72 1.43
MeO MeO Me Me Me
5p
1.00 1.93 0.90 2.92 2.82 2.06 2.06 8.81
f1 (ppm)


7.26 7.10 7.10 7.09 7.08 6.83 6.83 6.82 6.81 4.49 2.59 2.57 2.10 1.81 1.80 1.68 1.68 1.67 1.66 1.65 1.64 1.63 1.57 1.56 1.54 1.50 1.49 1.47 1.46 1.33 1.31 1.30 1.29 1.28 1.27 1.26 1.25 1.24 1.23 1.22 1.21 1.20 1.19 0.86 0.84
Me
Me
H
H
H
H
O
O
Me
5q
2.00 1.98 1.08 2.08 1.19 1.25 2.21 2.19 4.07 5.02 8.26 1.28 7.04
f1 (ppm)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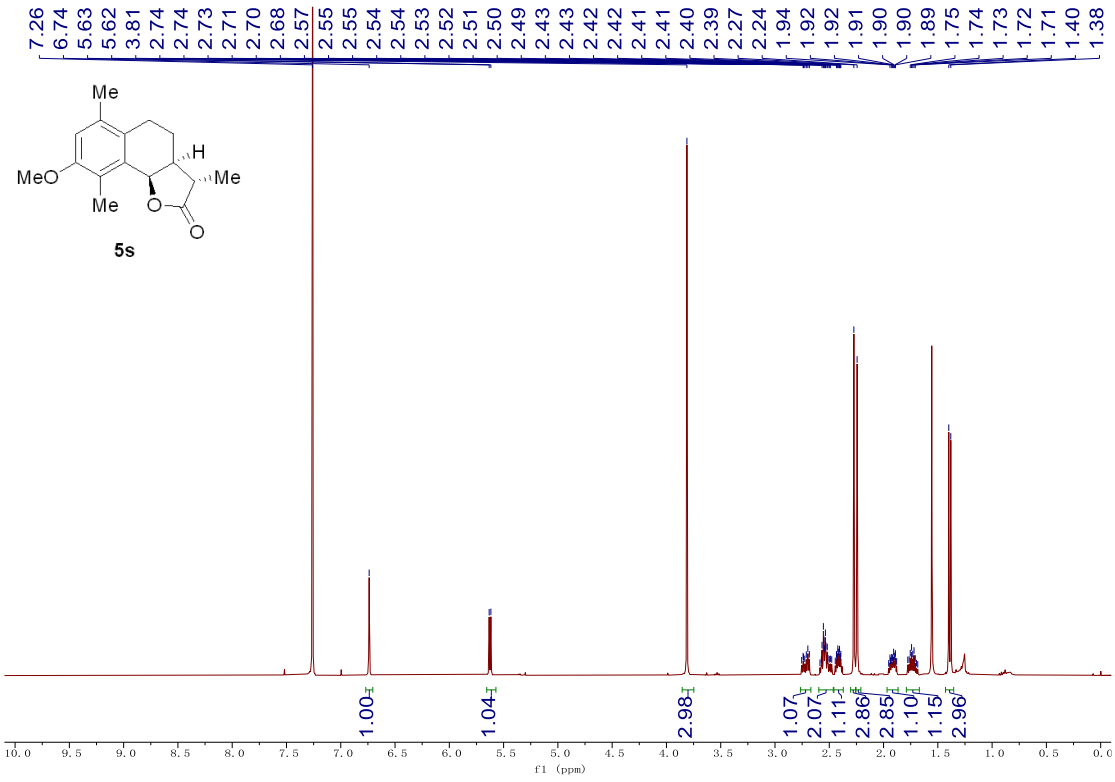
MeO
O
OMe
5r
1.93 1.00 1.90 0.97 0.92 1.00 1.07 2.86 2.76 1.03 1.89
f1 (ppm)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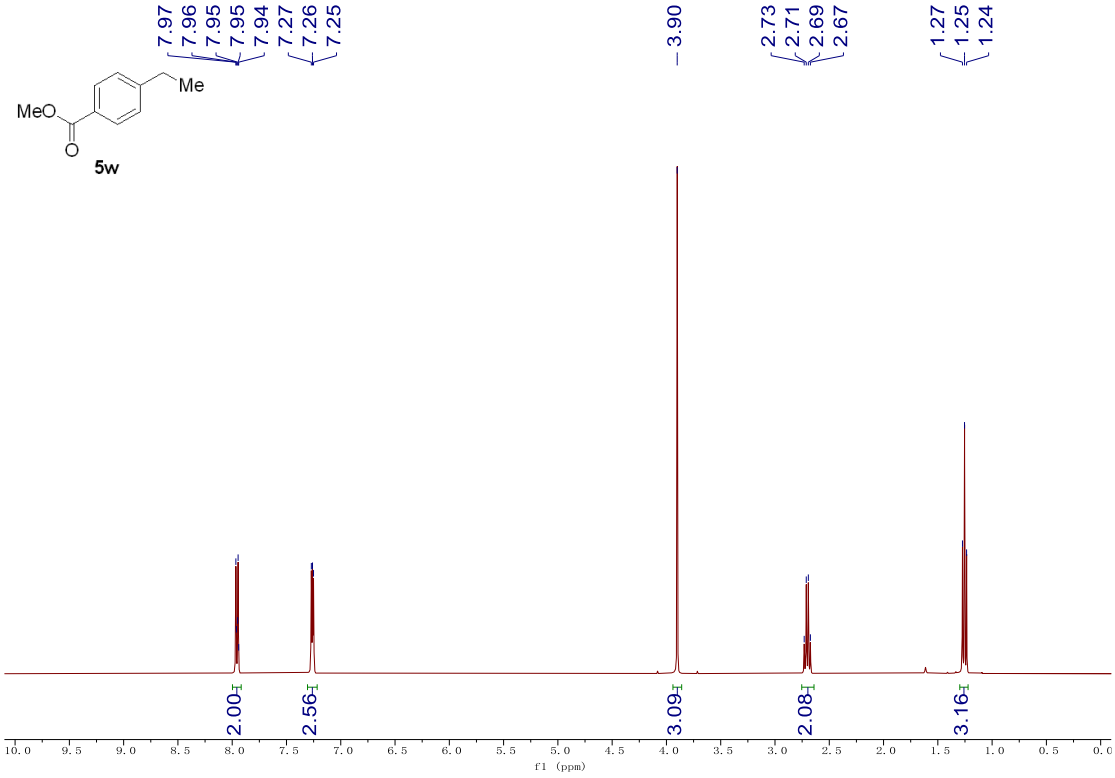
6.74
5.63
5.62
3.81
2.74
2.74
2.73
2.71
2.70
2.68
2.57
2.55
2.55
2.54
2.54
2.53
2.52
2.51
2.50
2.49
2.43
2.43
2.42
2.42
2.41
2.41
2.40
2.39
2.27
2.24
1.94
1.92
1.92
1.91
1.90
1.90
1.89
1.75
1.74
1.73
1.72
1.71
1.40
1.38
Me
MeO
H
Me
Me
O
O
5s
1.00
1.04
2.98
1.07
2.07
1.11
2.86
2.85
1.10
1.15
2.96
f1 (ppm)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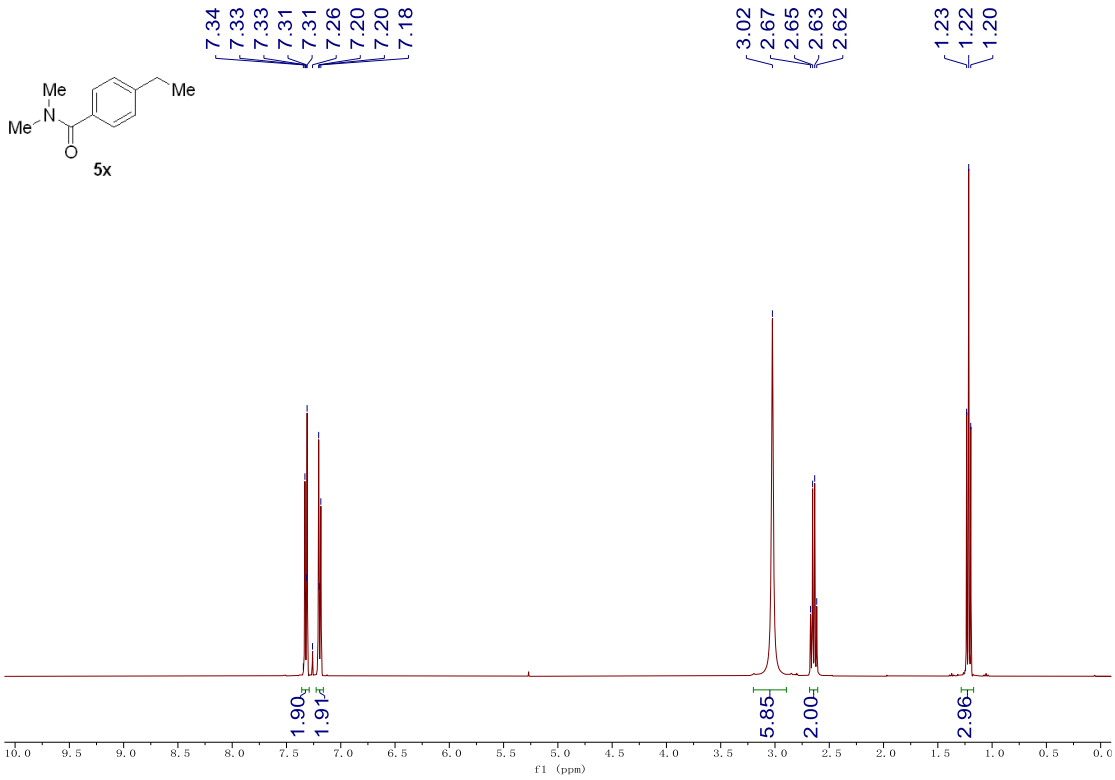
7.96
7.95
7.95
7.94
7.27
7.26
7.25
3.90
2.73
2.71
2.69
2.67
1.27
1.25
1.24
Me
MeO
O
5w
2.00
2.56
3.09
2.08
3.16
f1 (ppm)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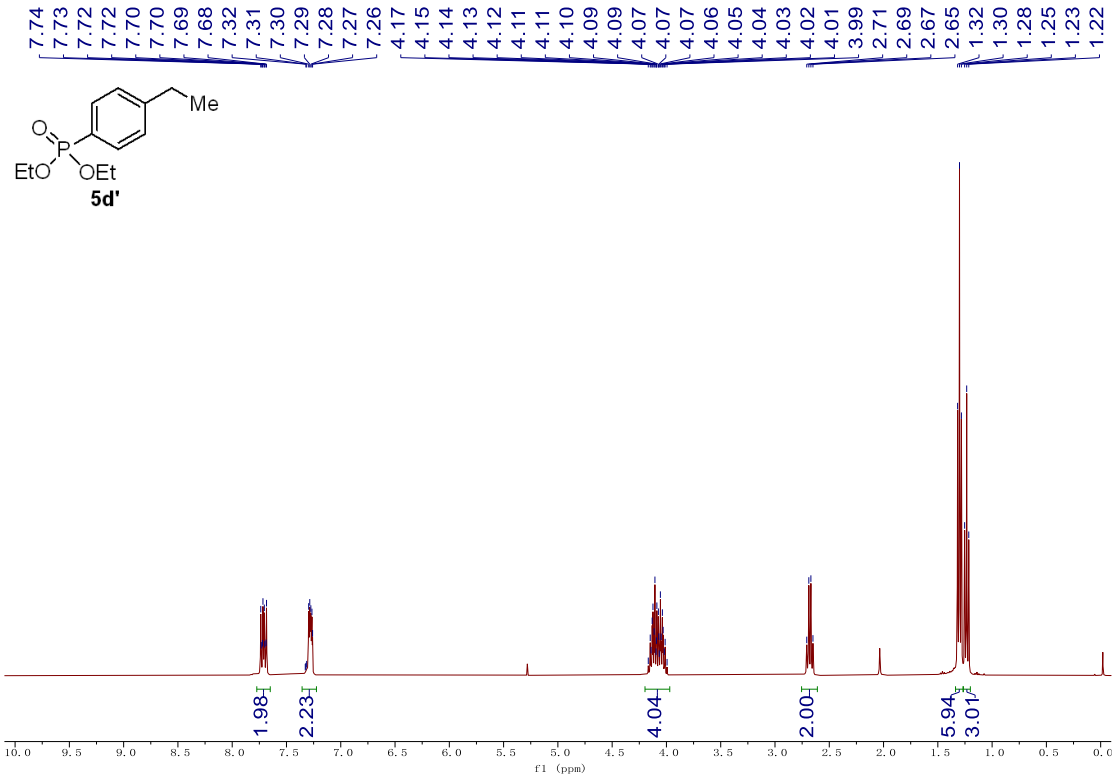
7.33
7.33
7.31
7.31
7.26
7.20
7.20
7.18
3.02
2.67
2.65
2.63
2.62
1.23
1.22
1.20
Me
N
Me
Me
O
5x
1.90
1.91
5.85
2.00
2.96
f1 (ppm)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7.72
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7.70
7.69
7.68
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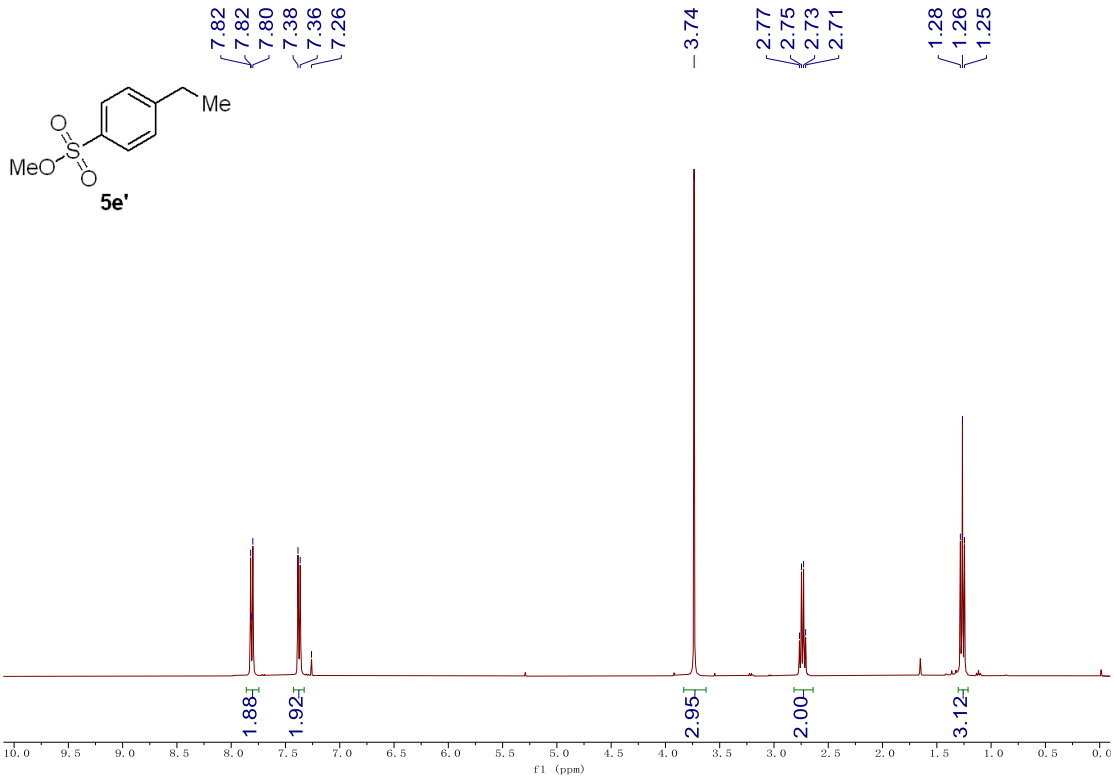
7.31
7.30
7.29
7.28
7.27
7.26
4.17
4.15
4.14
4.13
4.12
4.11
4.11
4.10
4.09
4.09
4.07
4.07
4.07
4.06
4.05
4.04
4.03
4.02
4.01
3.99
2.71
2.69
2.67
2.65
1.32
1.30
1.28
1.25
1.23
1.22
Me
O
P
EtO
OEt
5d'
1.98
2.23
4.04
2.00
5.94
3.01
f1 (ppm)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7.82
7.80
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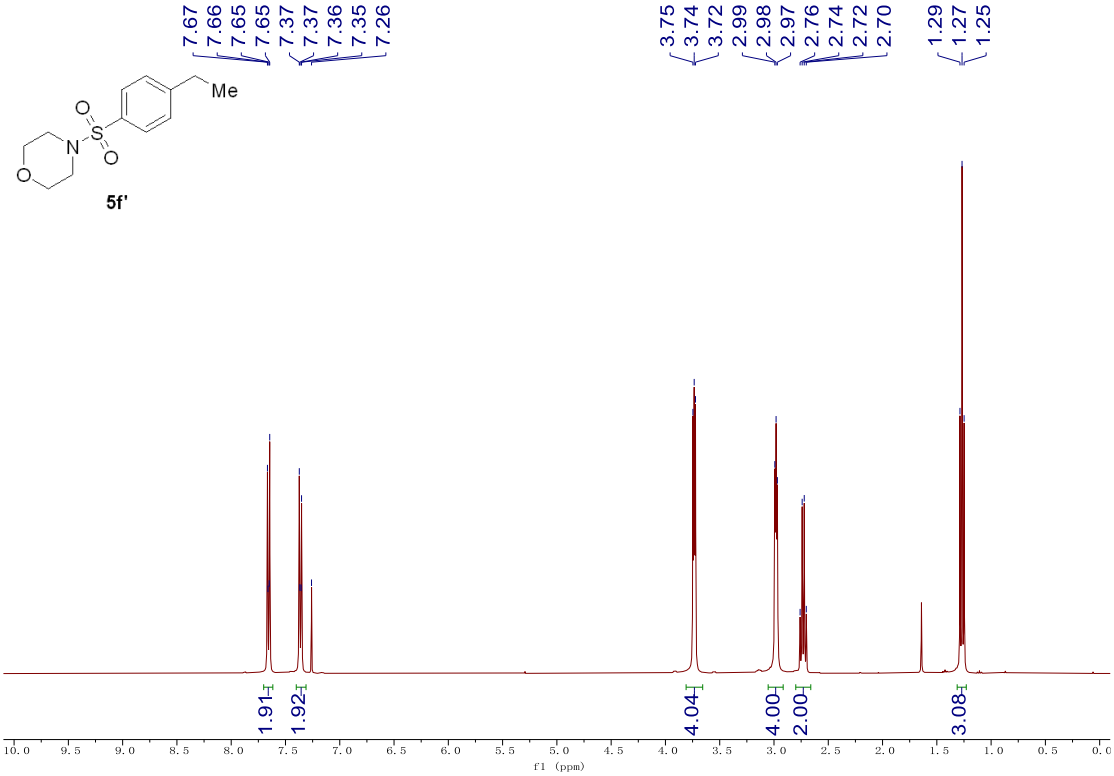
7.36
7.26
3.74
2.77
2.75
2.73
2.71
1.28
1.26
1.25
Me
MeO
5e'
1.88
1.92
2.95
2.00
3.12
f1 (ppm)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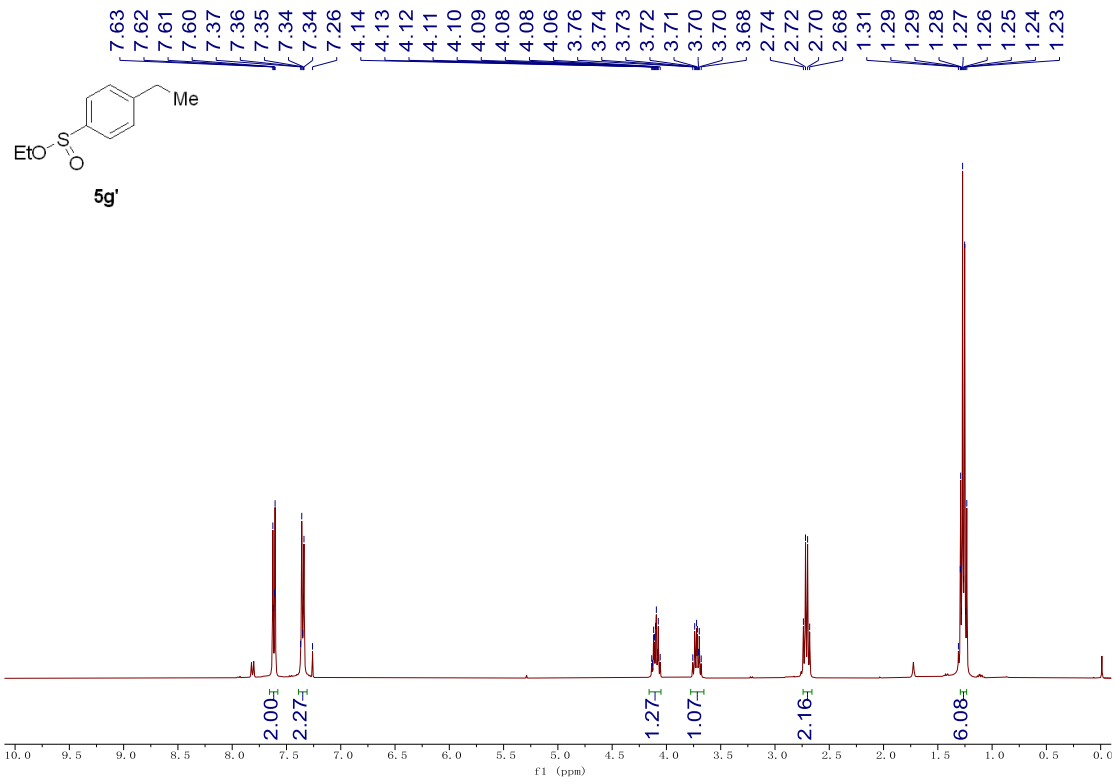
7.65
7.65
7.37
7.37
7.36
7.35
7.26
3.75
3.74
3.72
2.99
2.98
2.97
2.76
2.74
2.72
2.70
1.29
1.27
1.25
Me
N
5f'
1.91
1.92
4.04
4.00
2.00
3.08
f1 (ppm)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7.62
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7.60
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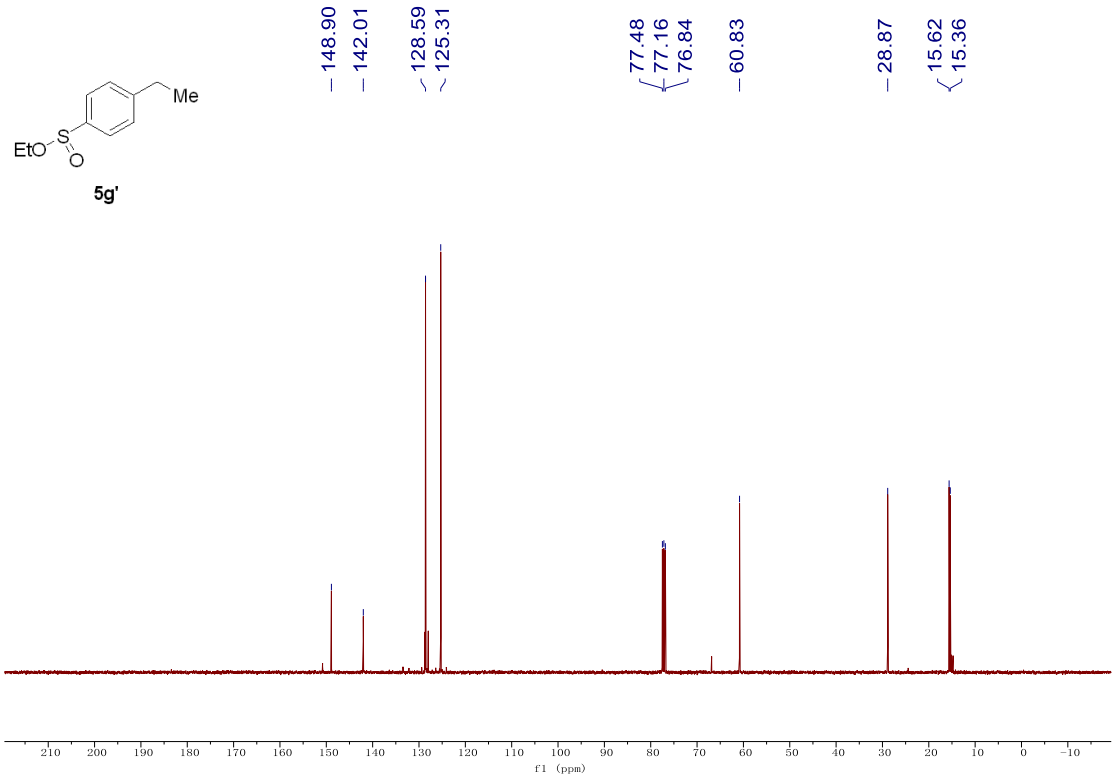
7.36
7.35
7.34
7.34
7.26
4.14
4.13
4.12
4.11
4.10
4.09
4.08
4.08
4.06
3.76
3.74
3.73
3.72
3.71
3.70
3.70
3.68
2.74
2.72
2.70
2.68
1.31
1.29
1.29
1.28
1.27
1.26
1.25
1.24
1.23
Me
EtO
S
O
5g'
2.00
2.27
1.27
1.07
2.16
6.08
f1 (ppm)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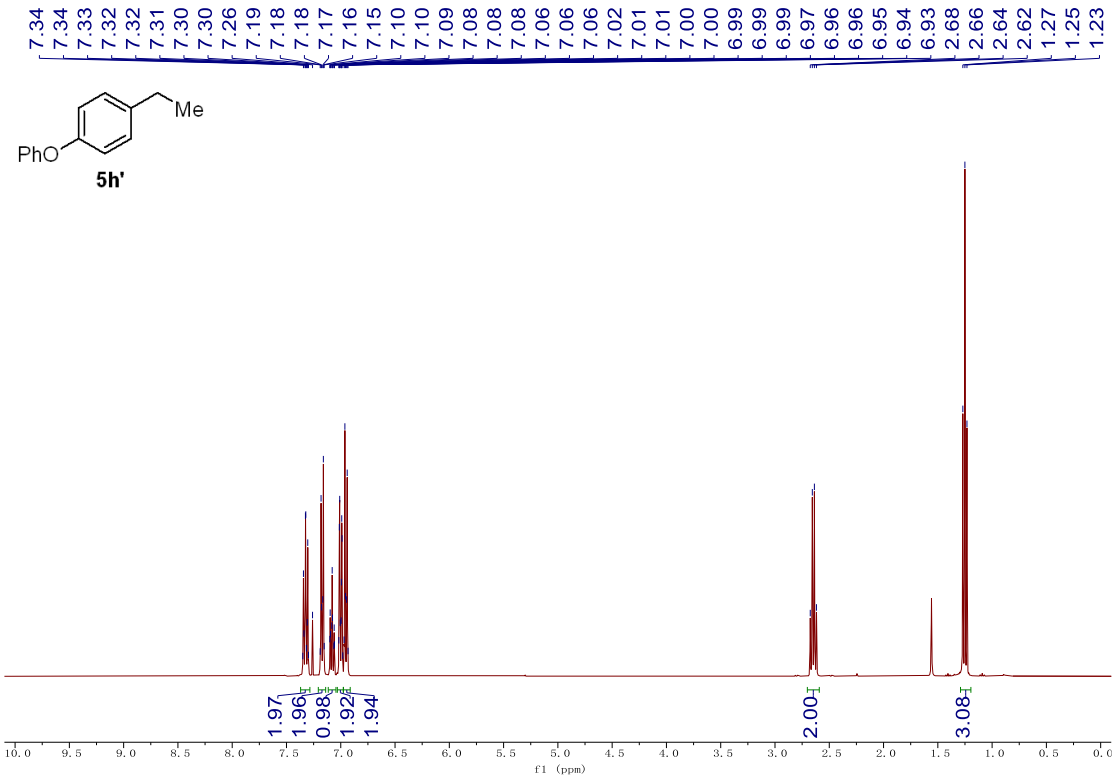
142.01
128.59
125.31
77.48
77.16
76.84
60.83
28.87
15.62
15.36
Me
EtO
S
O
5g'
f1 (ppm)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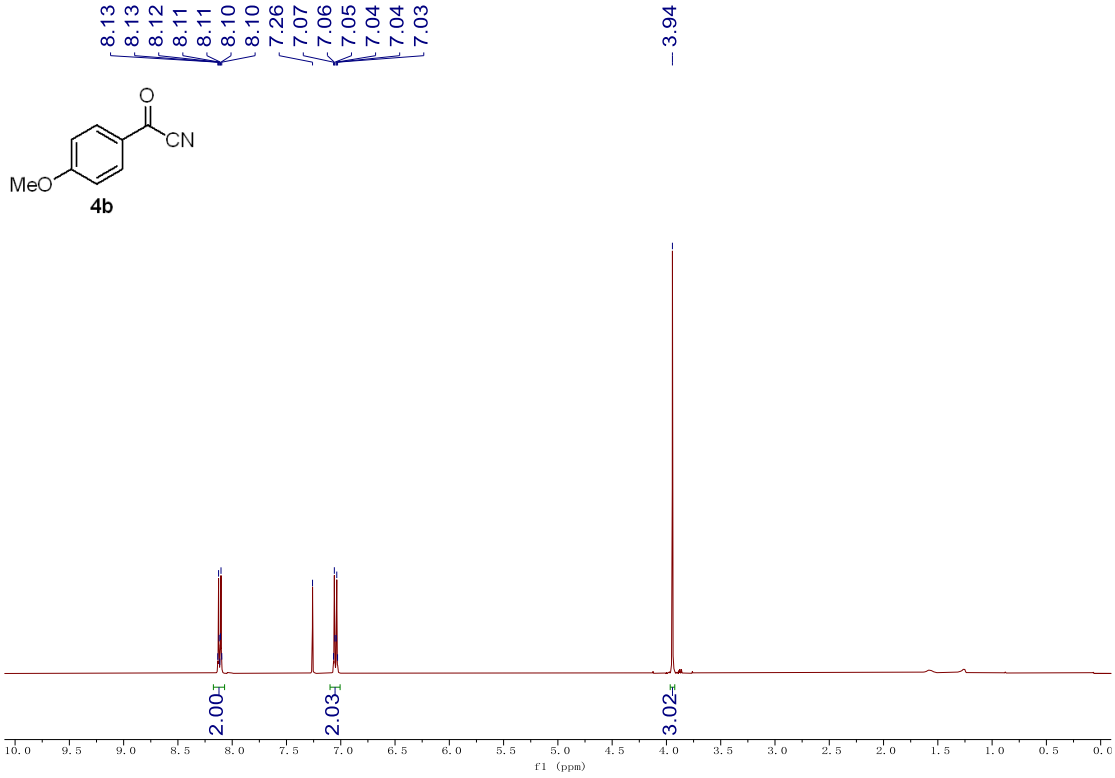
7.32
7.32
7.31
7.30
7.30
7.26
7.19
7.18
7.18
7.17
7.16
7.15
7.10
7.10
7.09
7.08
7.08
7.08
7.06
7.06
7.06
7.02
7.01
7.01
7.00
7.00
6.99
6.99
6.99
6.97
6.96
6.96
6.95
6.94
6.93
2.68
2.66
2.64
2.62
1.27
1.25
1.23
Me
PhO
5h'
1.97
1.96
0.98
1.92
1.94
2.00
3.08
f1 (ppm)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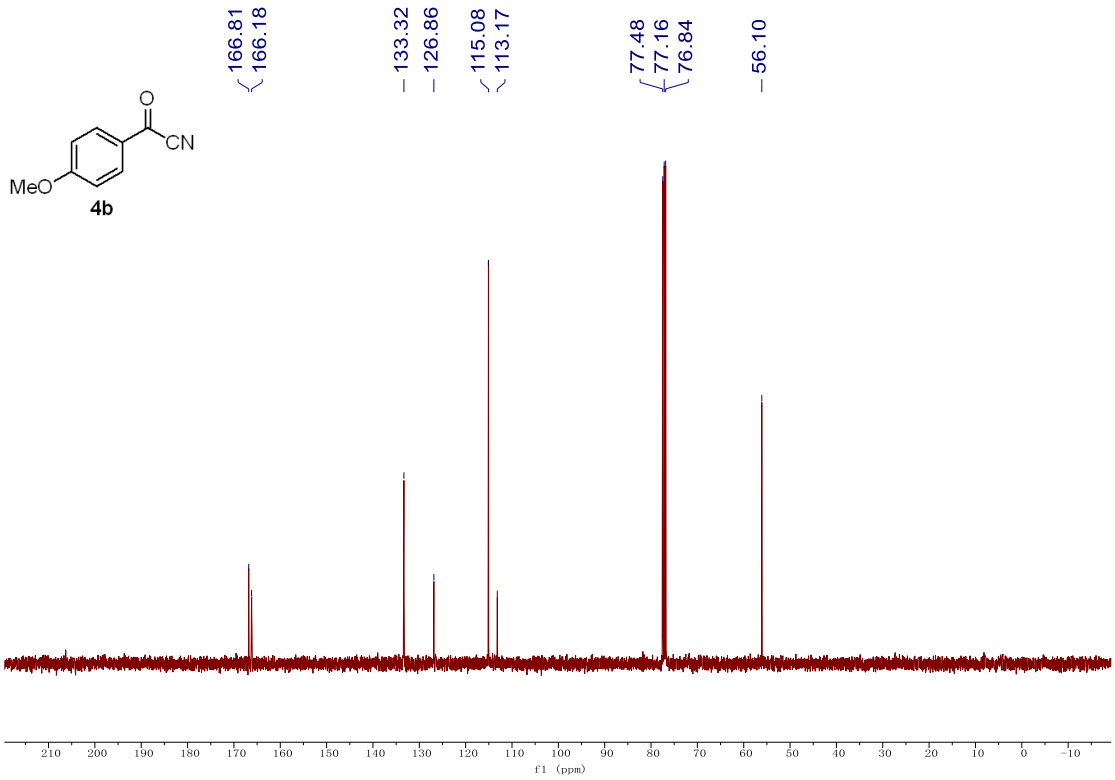
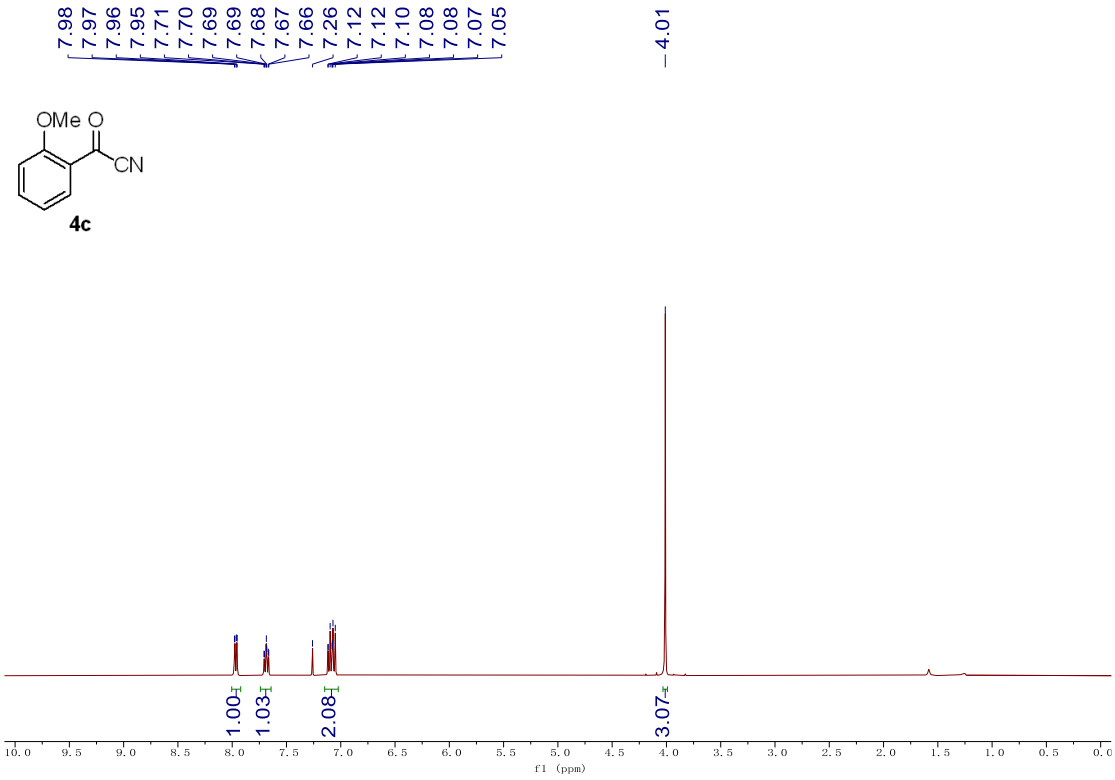
8.13
8.12
8.11
8.11
8.10
8.10
7.26
7.07
7.06
7.05
7.04
7.04
7.03
3.94
O
CN
MeO
4b
2.00
2.03
3.02
f1 (ppm)


166.81
166.18
133.32
126.86
115.08
113.17
77.48
77.16
76.84
56.10
O
CN
MeO
4b
f1 (ppm)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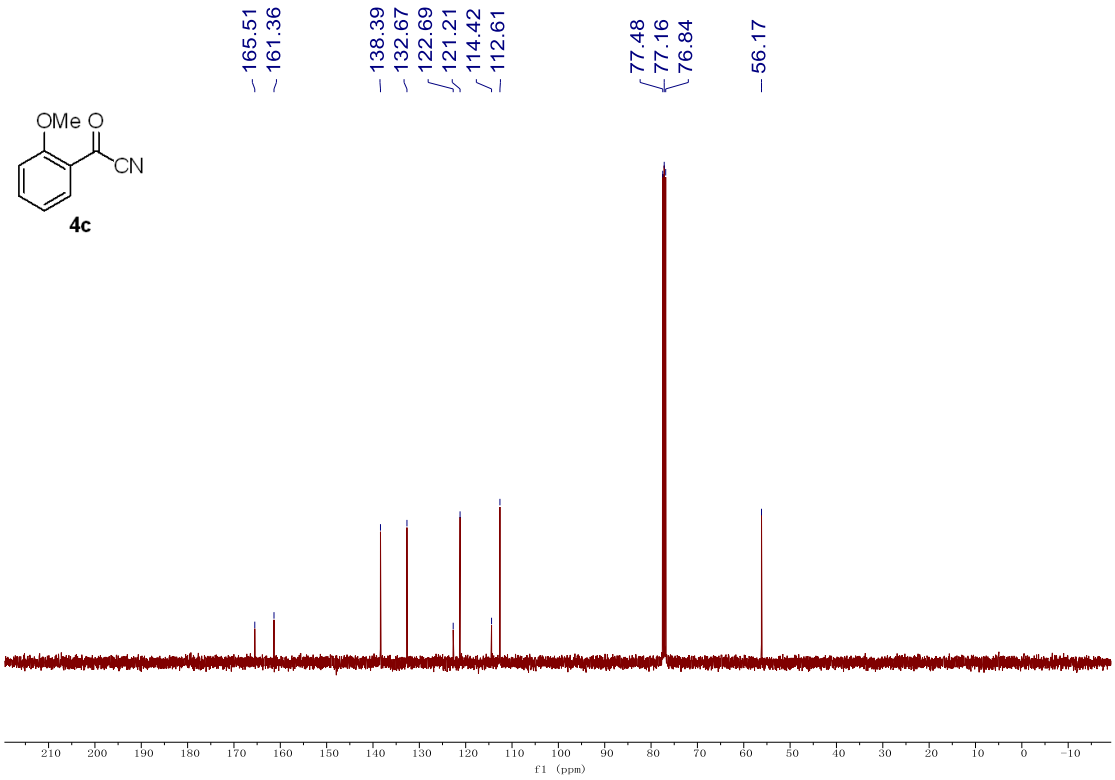
7.71
7.70
7.69
7.69
7.68
7.67
7.66
7.26
7.12
7.12
7.10
7.08
7.08
7.07
7.05
4.01
OMe O
CN
4c
1.00
1.03
2.08
3.07
f1 (ppm)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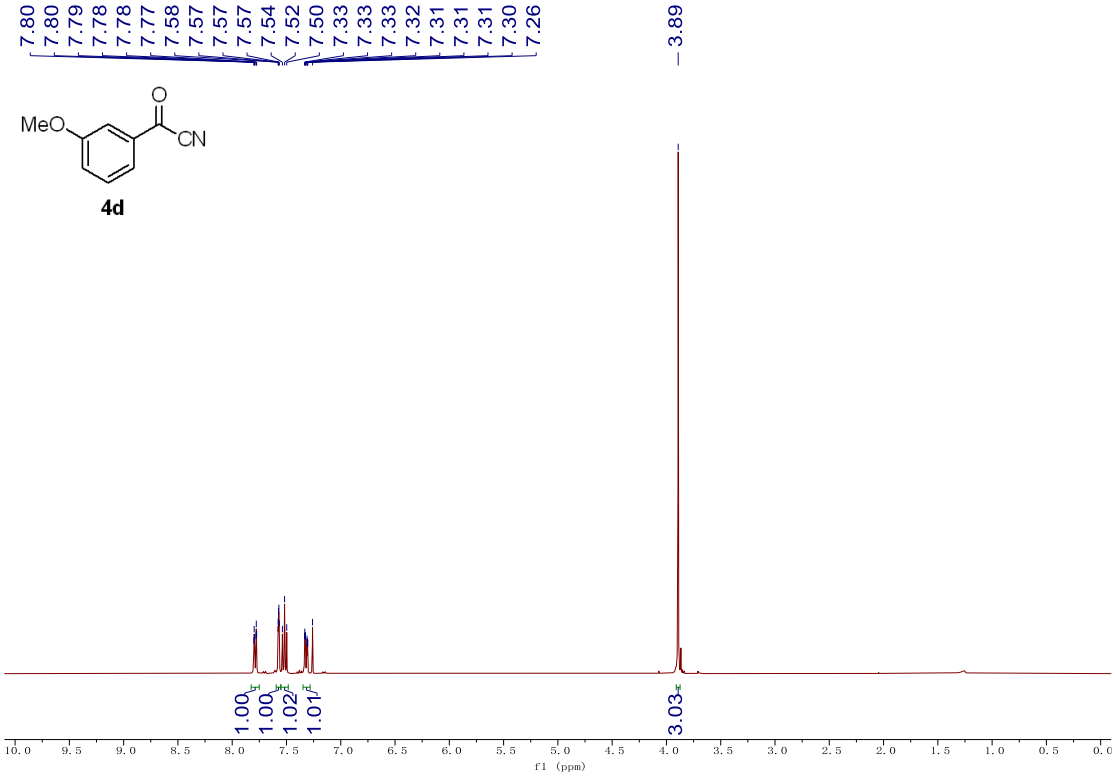
138.39
132.67
122.69
121.21
114.42
112.61
77.48
77.16
76.84
56.17
OMe O
CN
4c
f1 (ppm)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7.57
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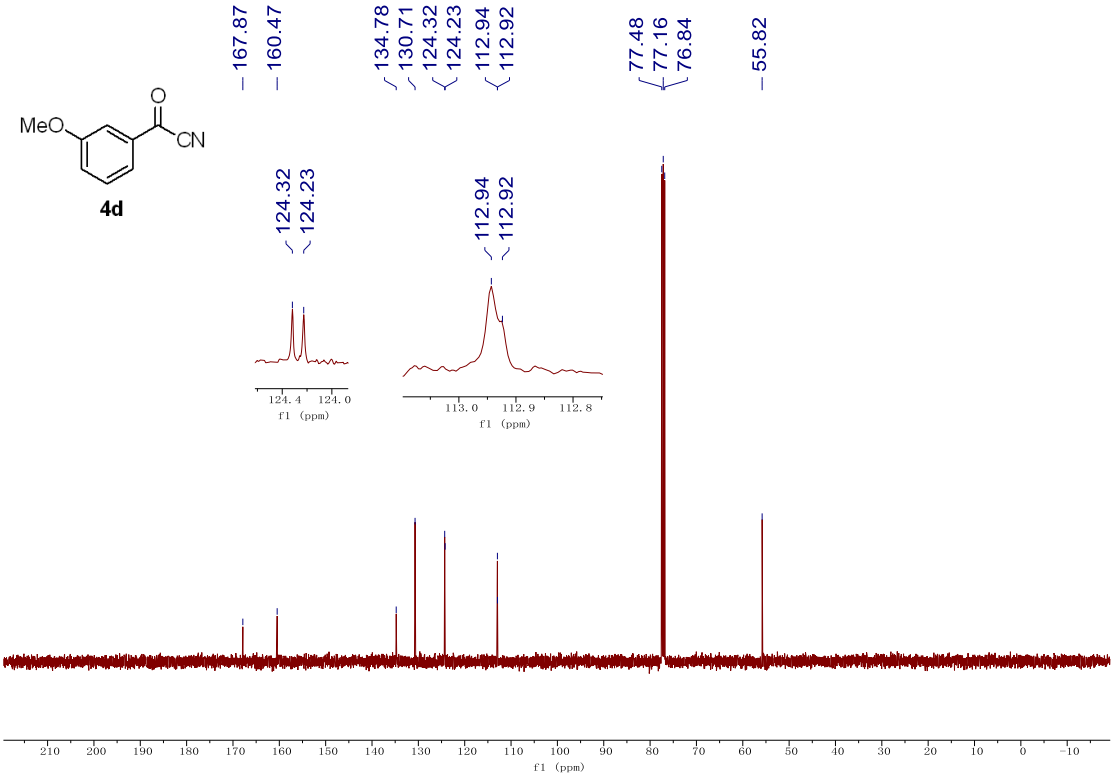
7.52
7.50
7.33
7.33
7.33
7.32
7.31
7.31
7.31
7.30
7.26
3.89
MeO
O
CN
4d
1.00
1.00
1.02
1.01
3.03
f1 (ppm)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130.71
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124.23
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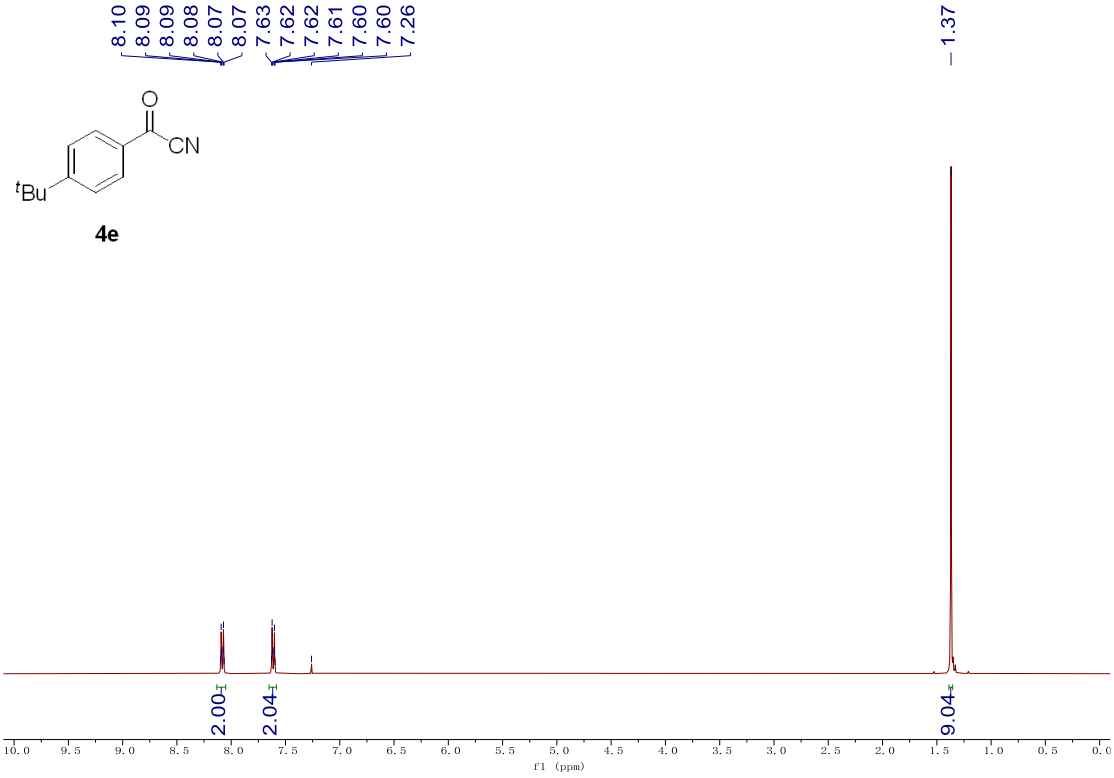
112.92
77.48
77.16
76.84
55.82
MeO
CN
O
4d
f1 (ppm)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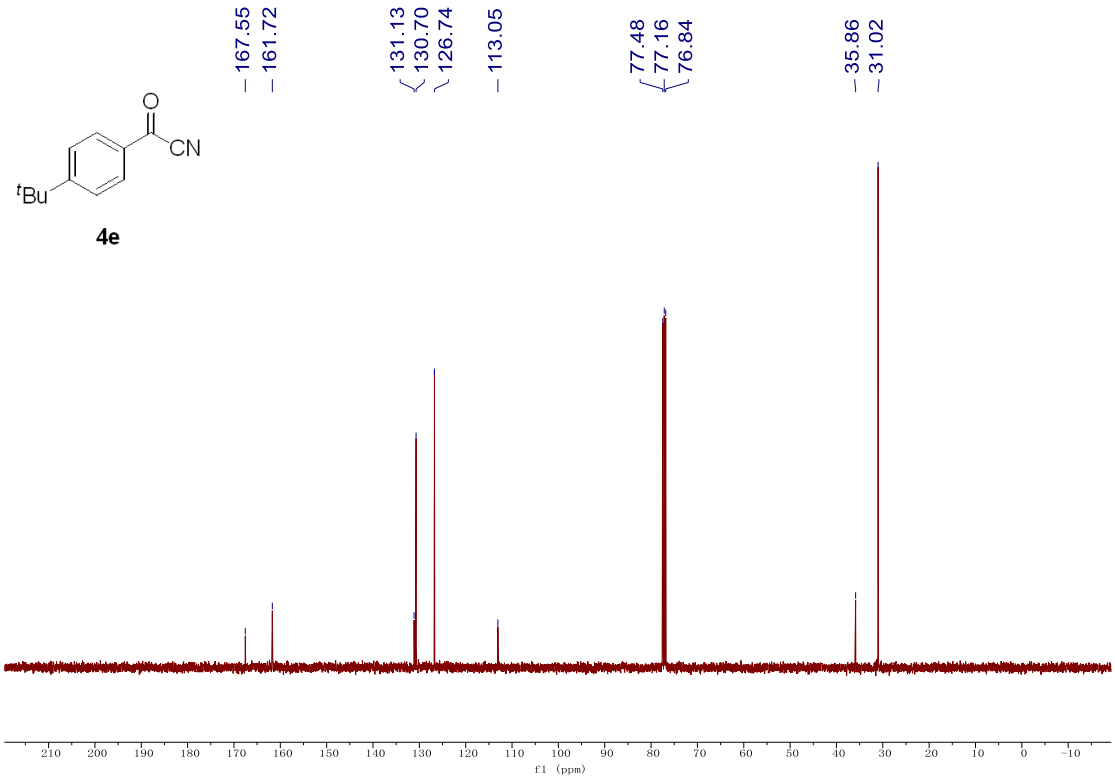
8.09
8.09
8.08
8.07
8.07
7.63
7.62
7.62
7.61
7.60
7.60
7.26
1.37
CN
O
tBu
4e
2.00
2.04
9.04
f1 (ppm)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161.72
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126.74
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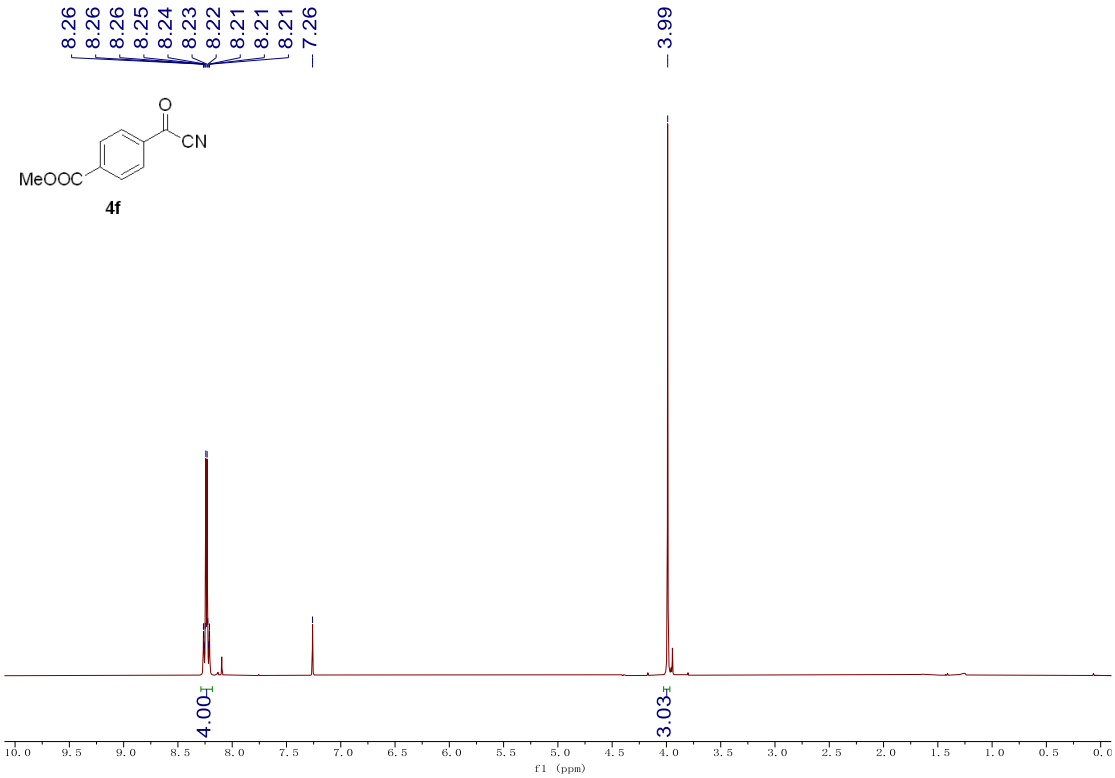
77.48
77.16
76.84
35.86
31.02
O
CN
tBu
4e
f1 (ppm)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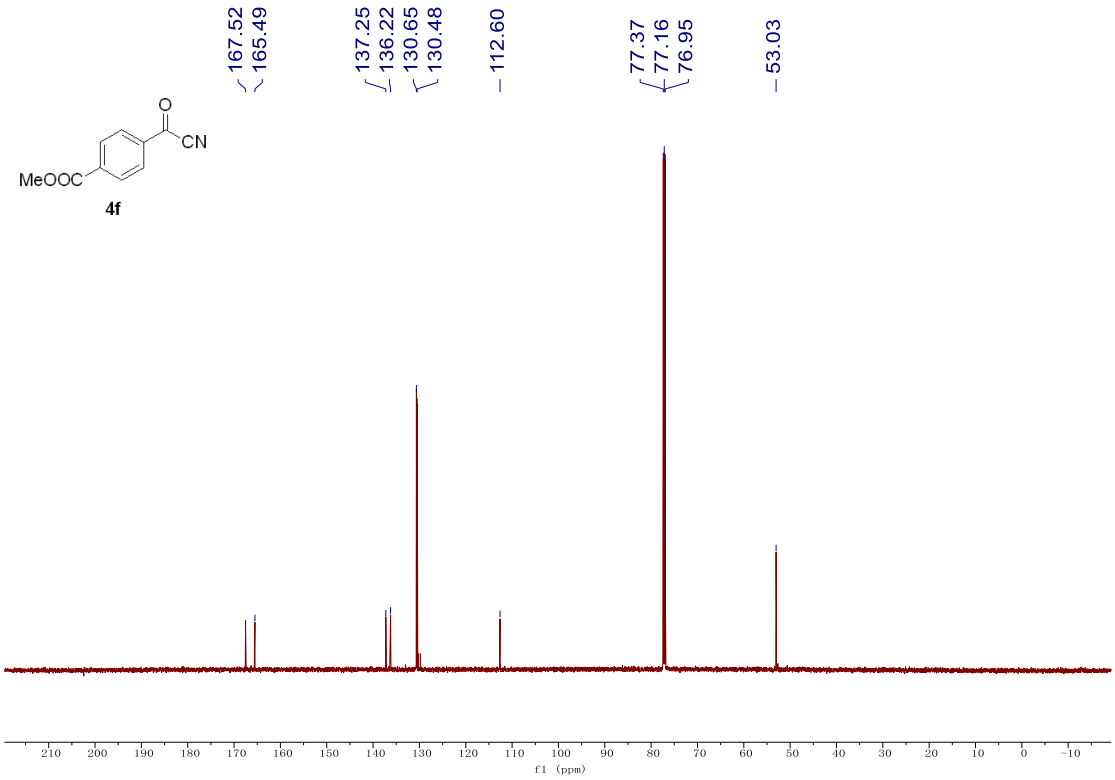
8.26
8.26
8.25
8.24
8.23
8.22
8.21
8.21
8.21
7.26
3.99
O
CN
MeOOC
4f
4.00
3.03
f1 (ppm)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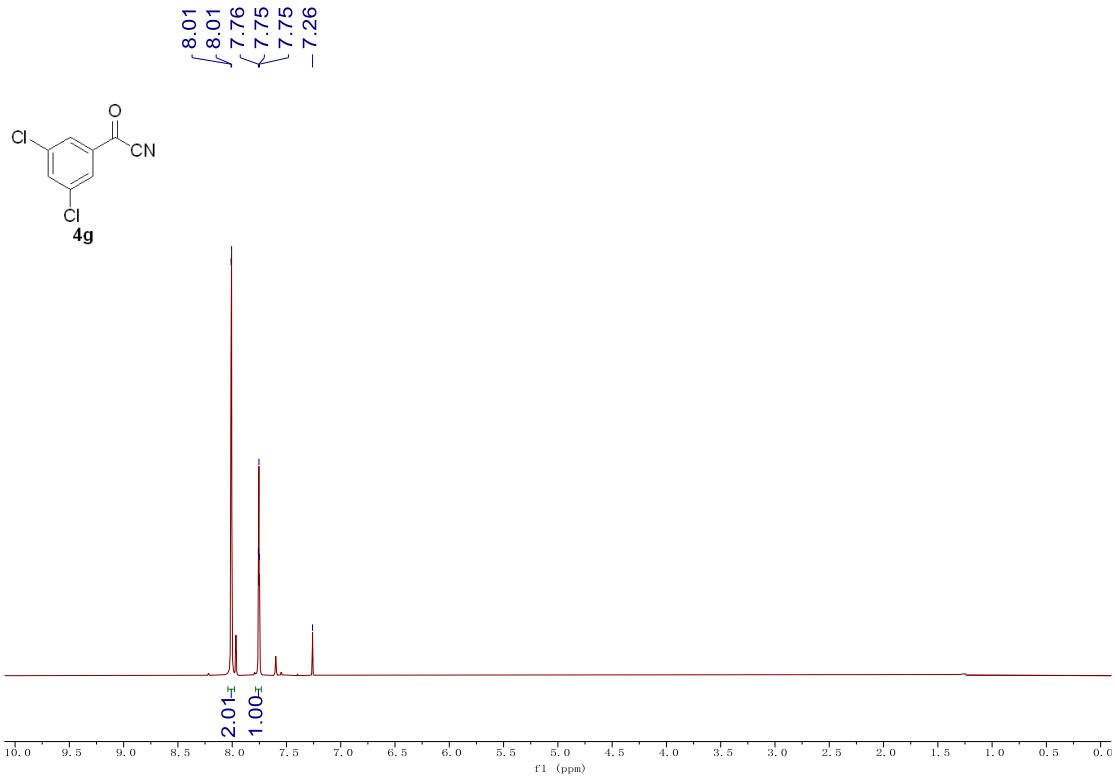
165.49
137.25
136.22
130.65
130.48
112.60
77.37
77.16
76.95
53.03
O
CN
MeOOC
4f
f1 (ppm)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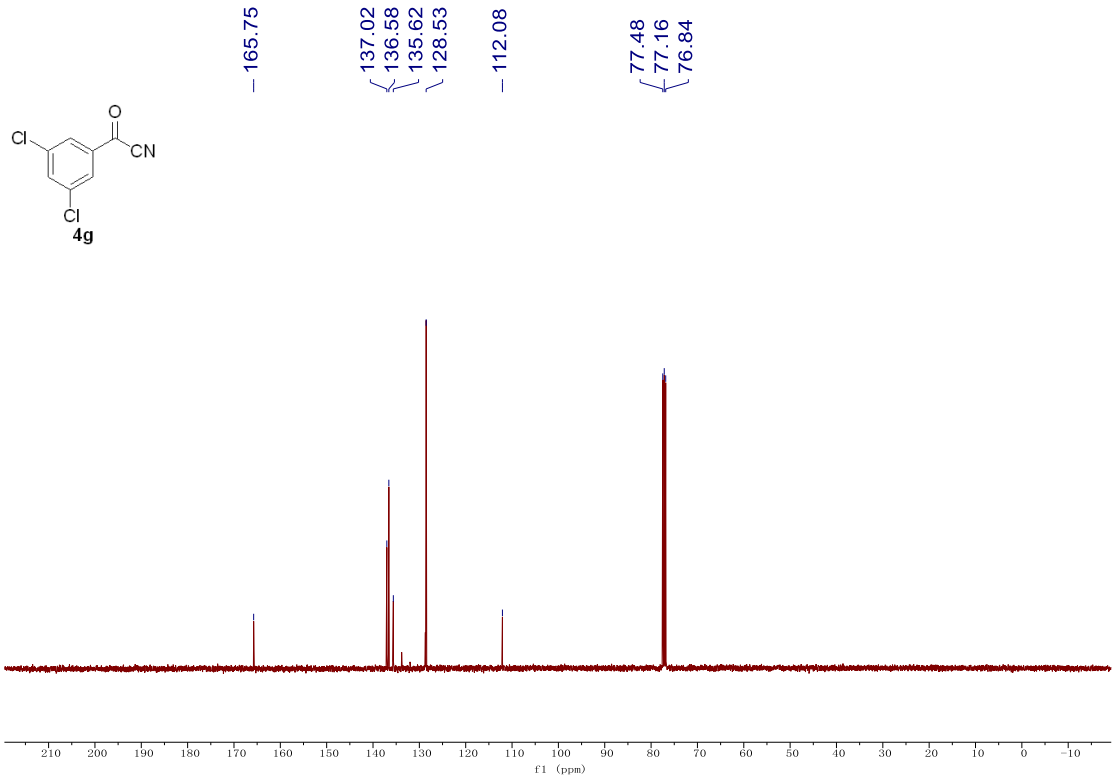
8.01
7.76
7.75
7.75
7.26
O
CN
Cl
Cl
4g
2.01
1.00
f1 (ppm)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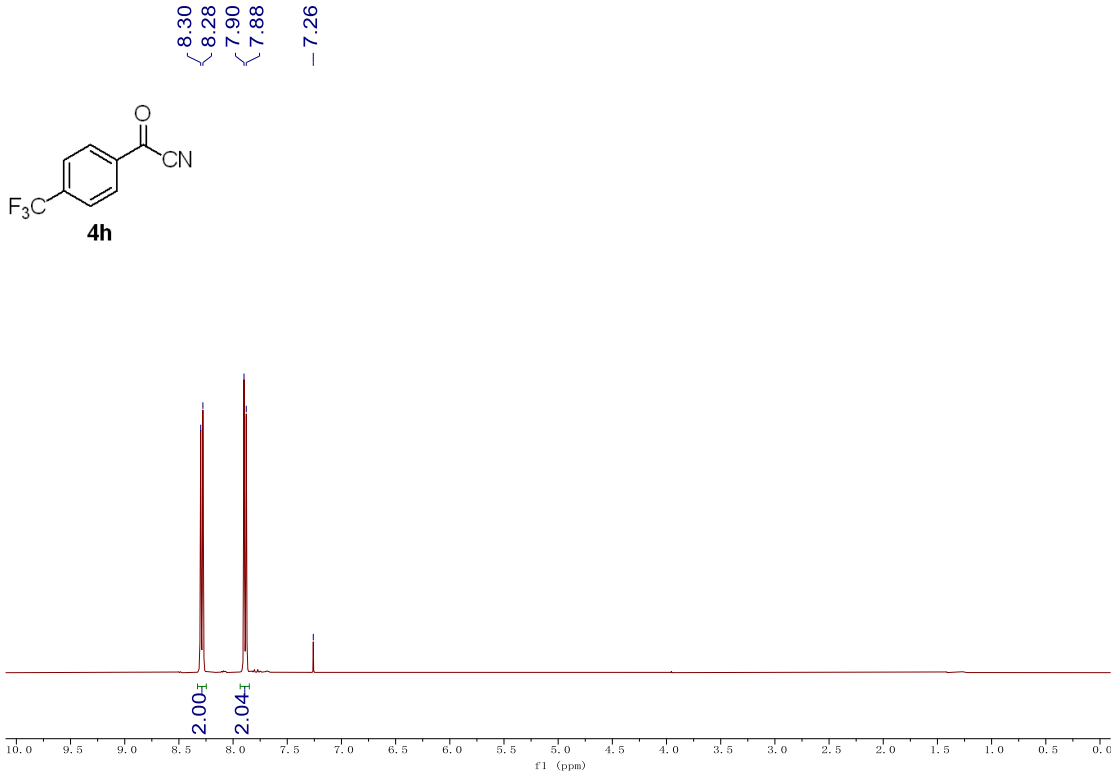
77.16
76.84
Cl
O
CN
Cl
4g
f1 (ppm)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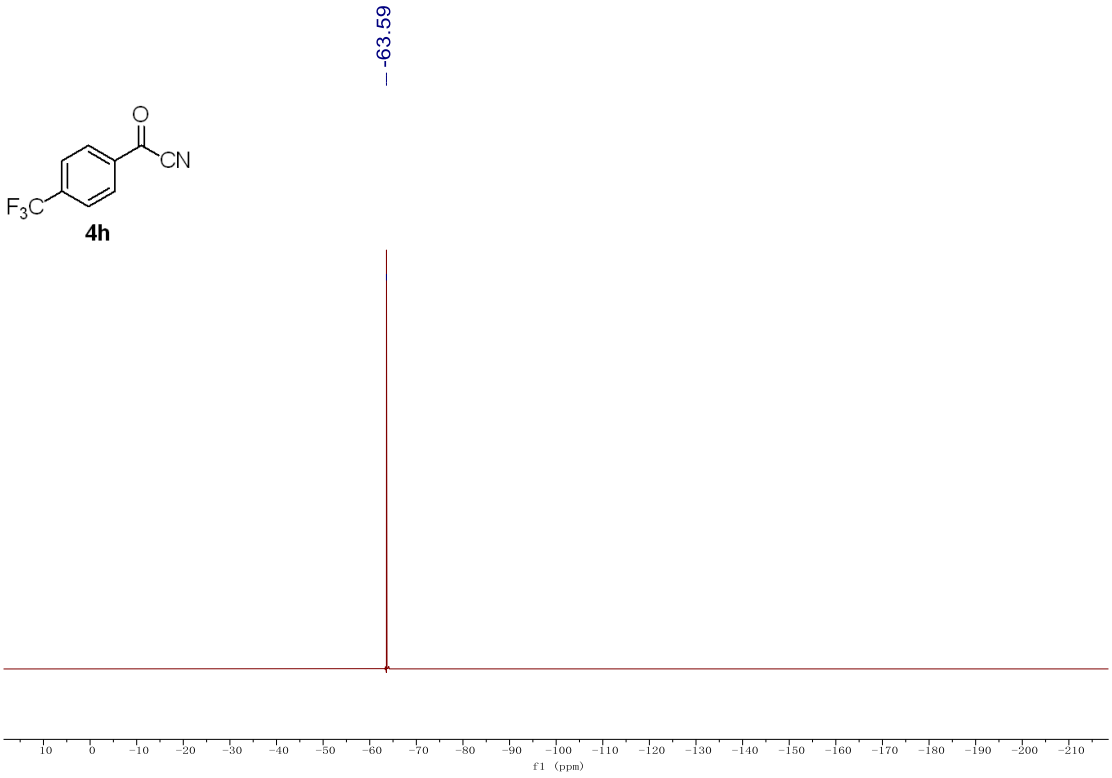
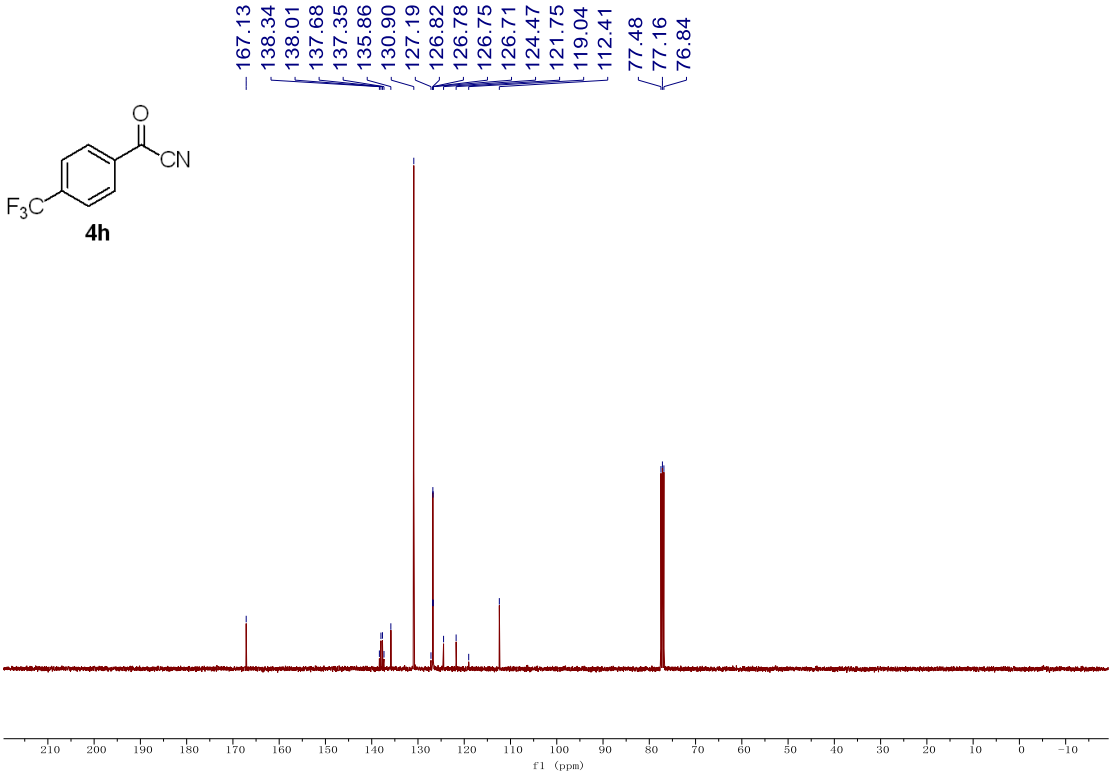
8.28
7.90
7.88
7.26
O
CN
F3C
4h
2.00
2.04
f1 (ppm)


-63.59
O
CN
F3C
4h
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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137.35
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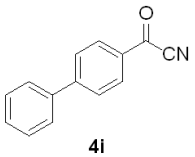
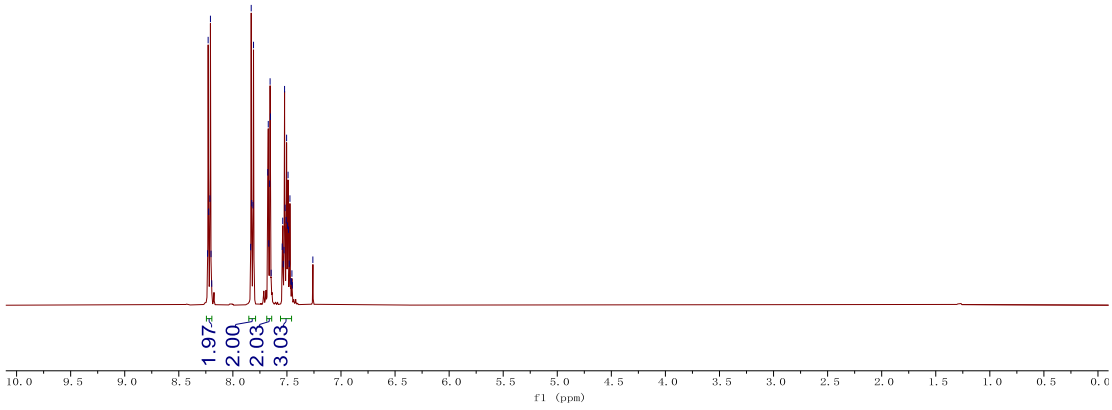
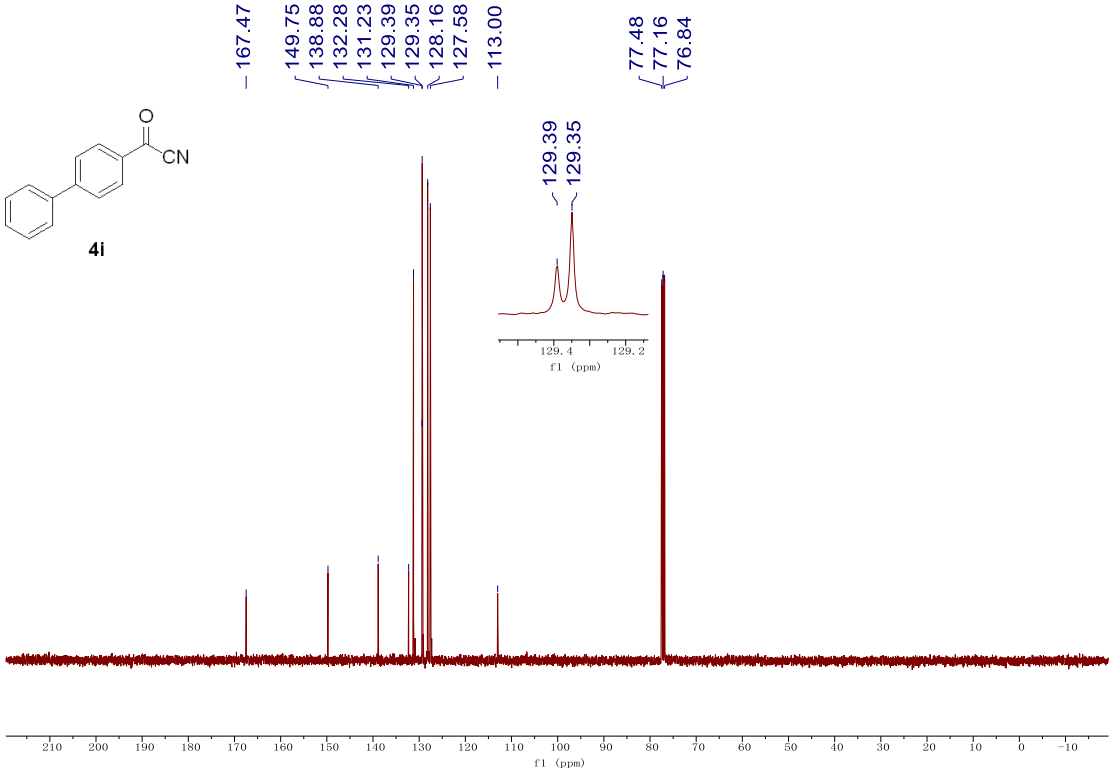
127.19
126.82
126.78
126.75
126.71
124.47
121.75
119.04
112.41
77.48
77.16
76.84
O
CN
F3C
4h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.23
8.23
8.22
8.21
8.21
8.20
8.20
7.84
7.83
7.83
7.81
7.81
7.68
7.67
7.67
7.66
7.66
7.65
7.65
7.54
7.54
7.53
7.53
7.52
7.52
7.51
7.50
7.49
7.49
7.49
7.48
7.47
7.46
7.46
7.45
7.45
7.26

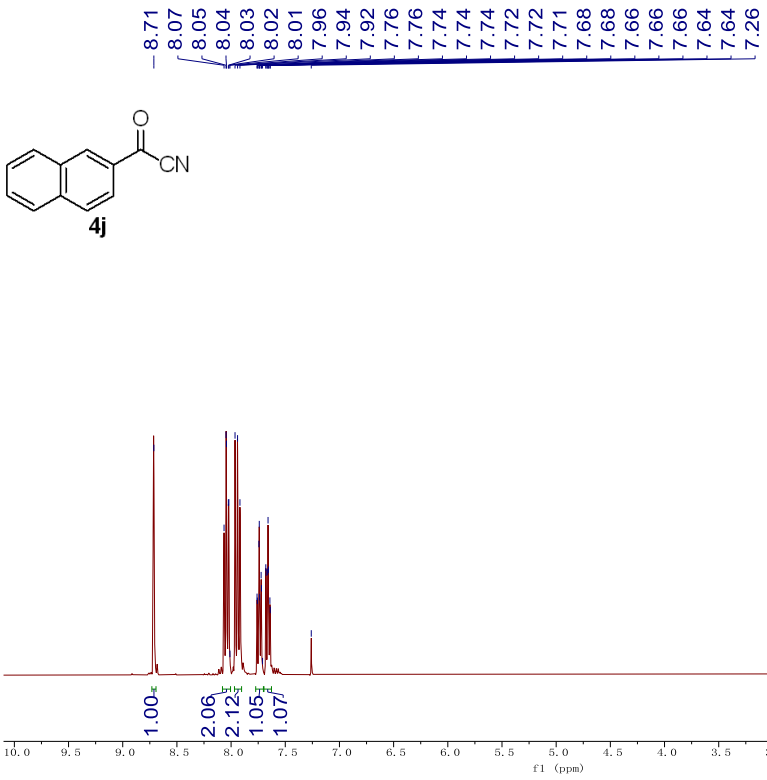

O
CN

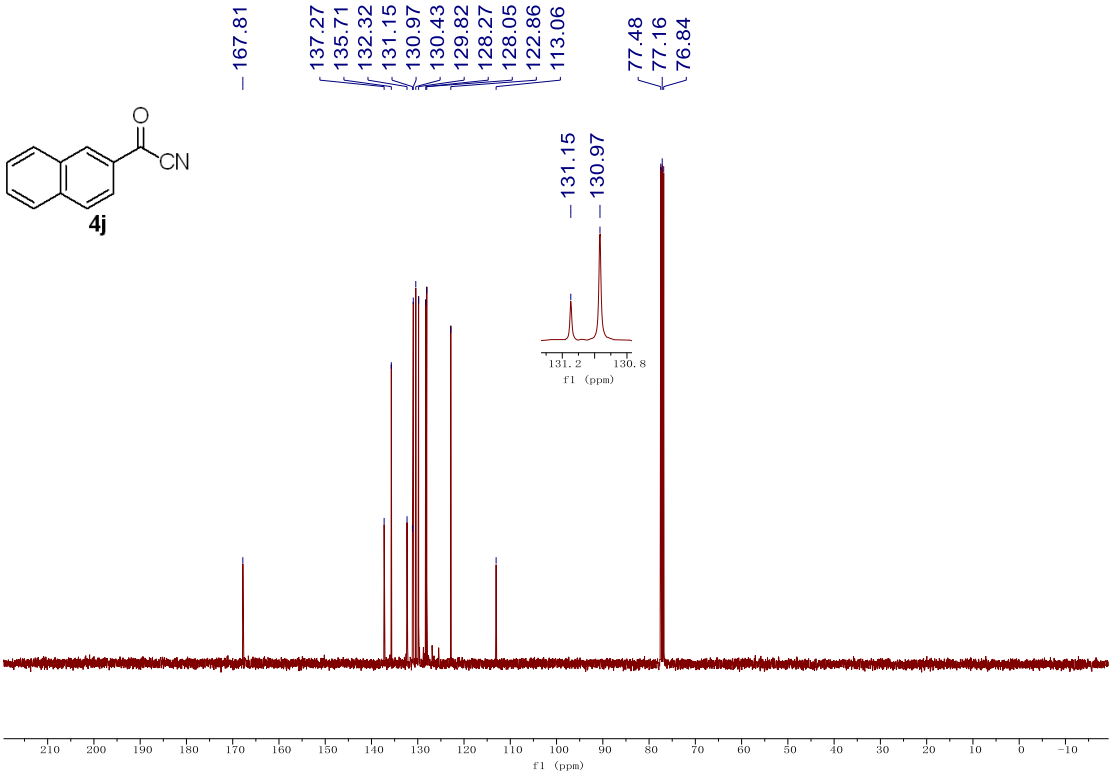
4i


1.97
2.00
2.03
3.03
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)


167.47
149.75
138.88
132.28
131.23
129.39
129.35
128.16
127.58
113.00
77.48
77.16
76.84
O
CN
129.39
129.35
129.4
129.2
f1 (ppm)
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)

4i


8.71
8.07
8.05
8.04
8.03
8.02
8.01
7.96
7.94
7.92
7.76
7.76
7.74
7.74
7.74
7.72
7.72
7.71
7.68
7.68
7.66
7.66
7.66
7.64
7.64
7.26
O
CN
4j
1.00
2.06
2.12
1.05
1.07
f1 (ppm)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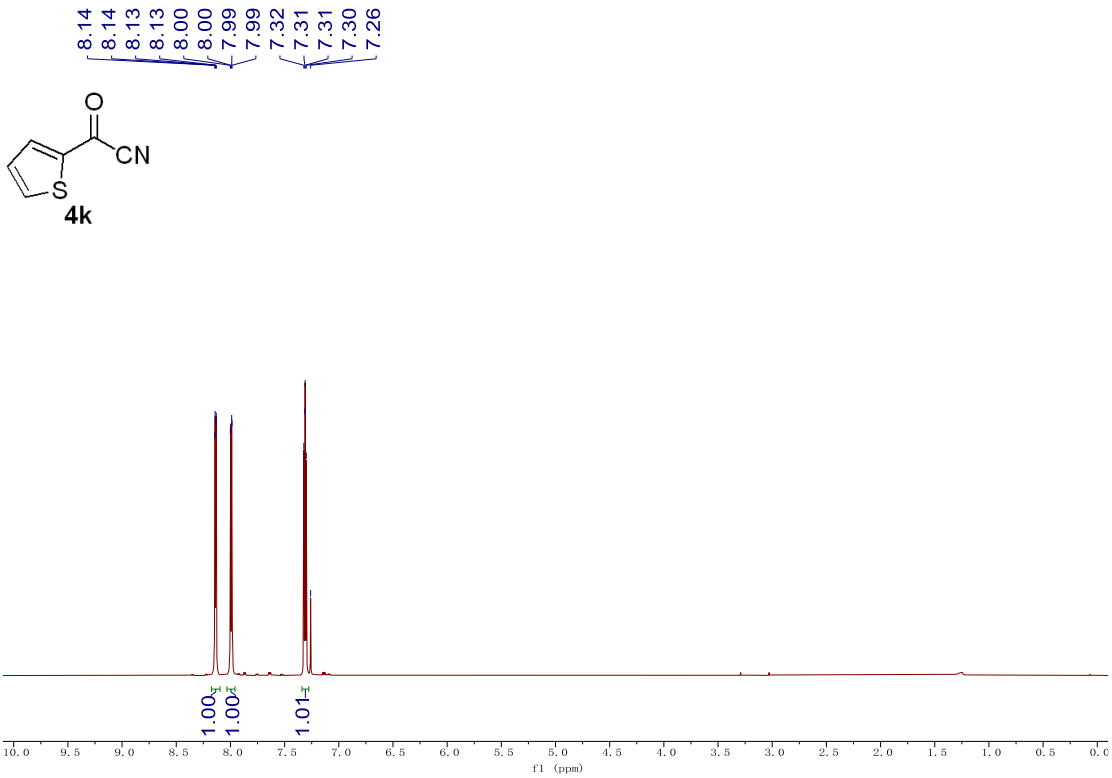
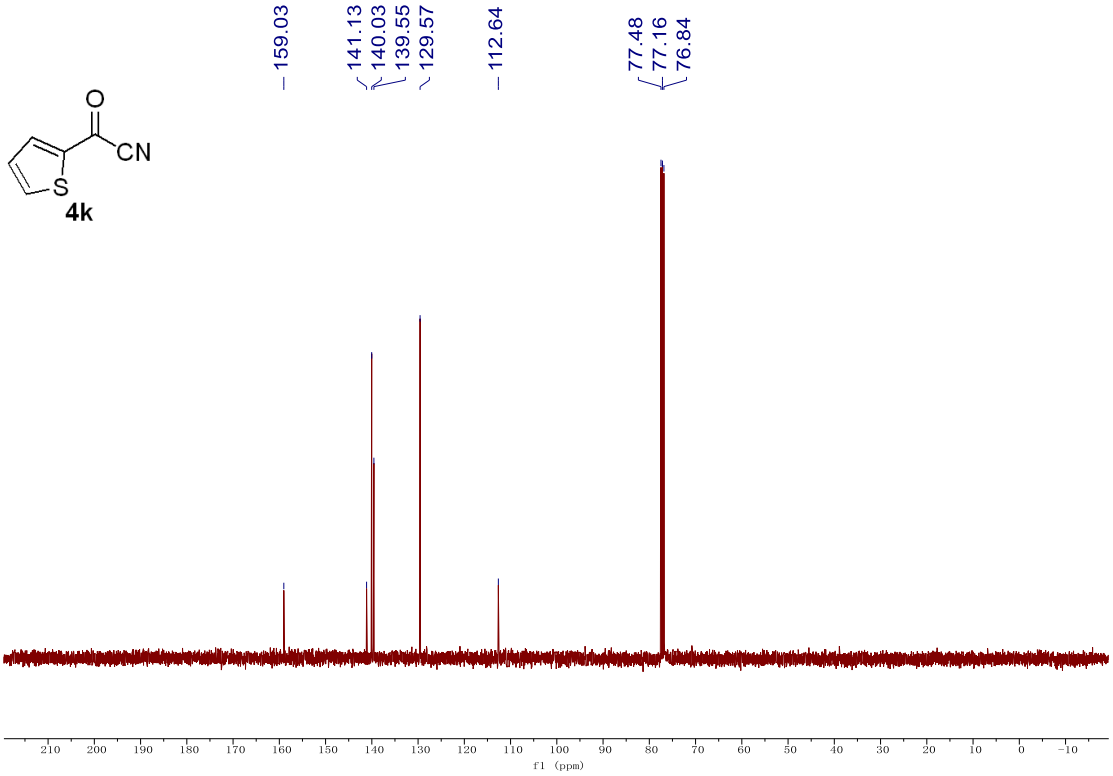
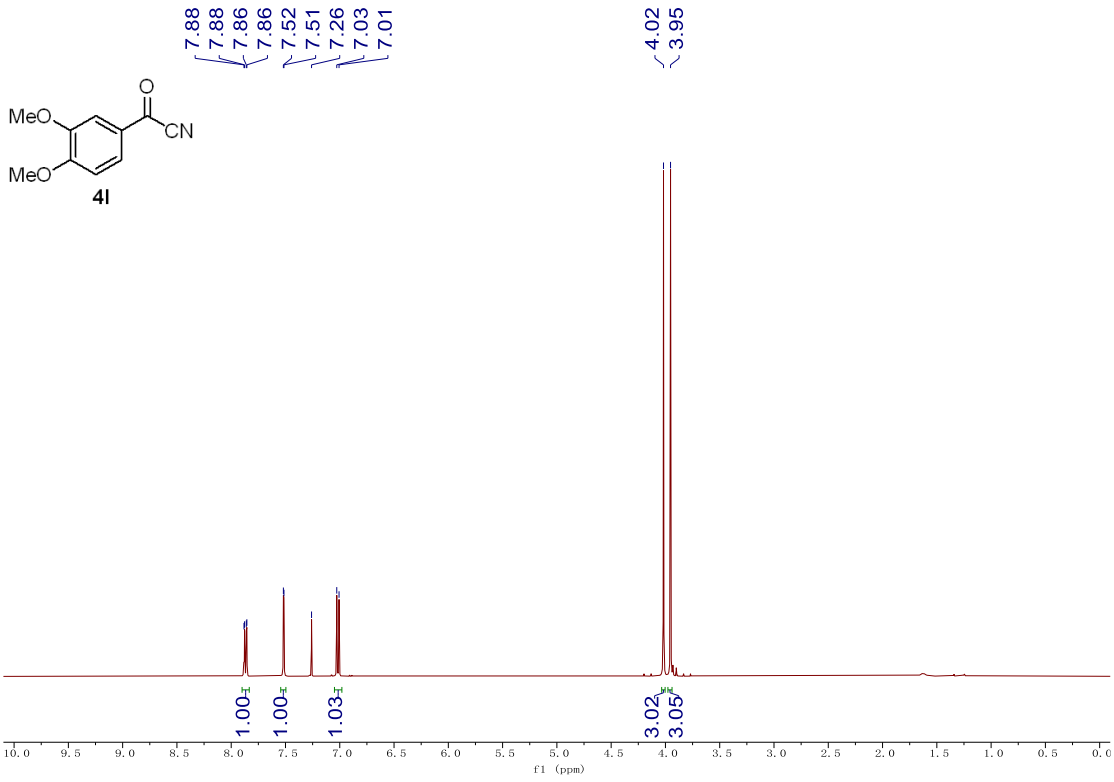
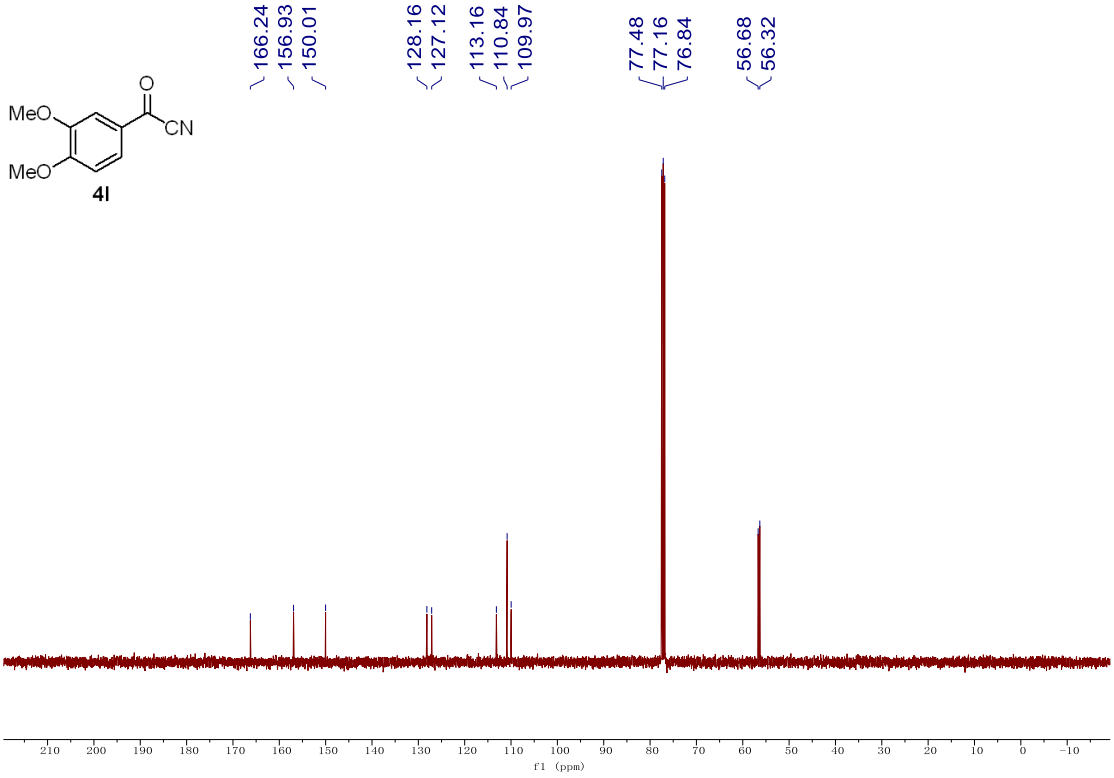
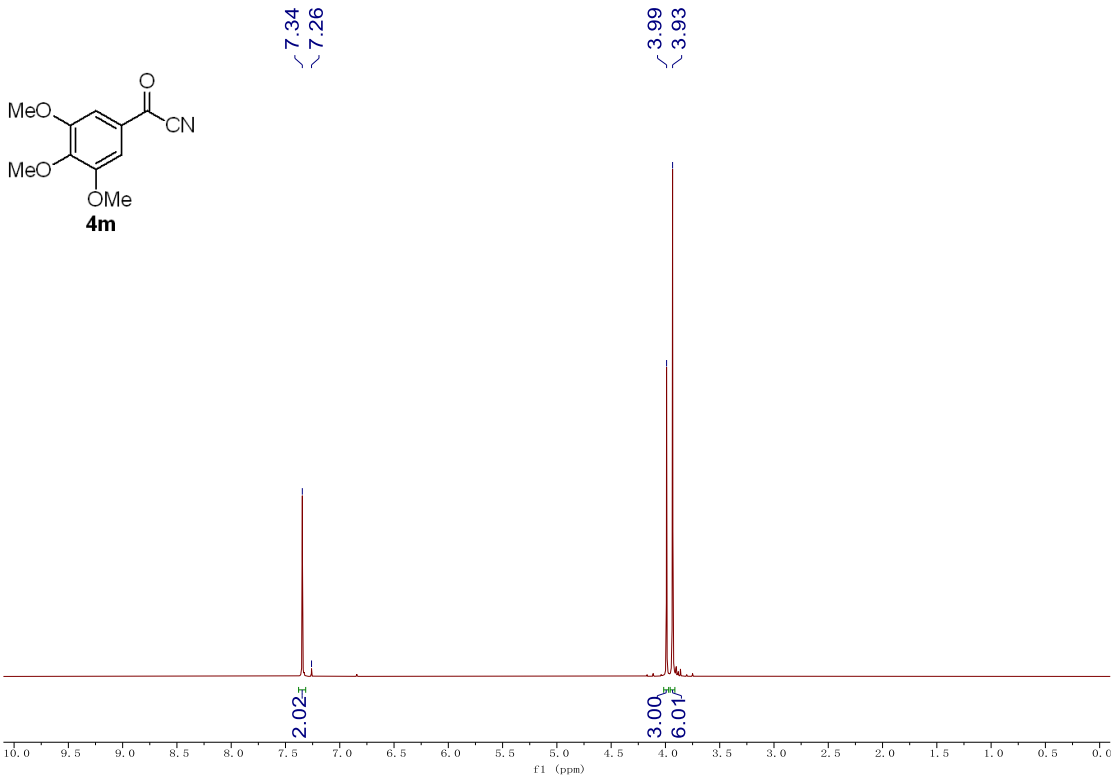
137.27
135.71
132.32
131.15
130.97
130.43
129.82
128.27
128.05
122.86
113.06
77.48
77.16
76.84
131.15
130.97
O
CN
4j
131.2
130.8
f1 (ppm)
f1 (ppm)

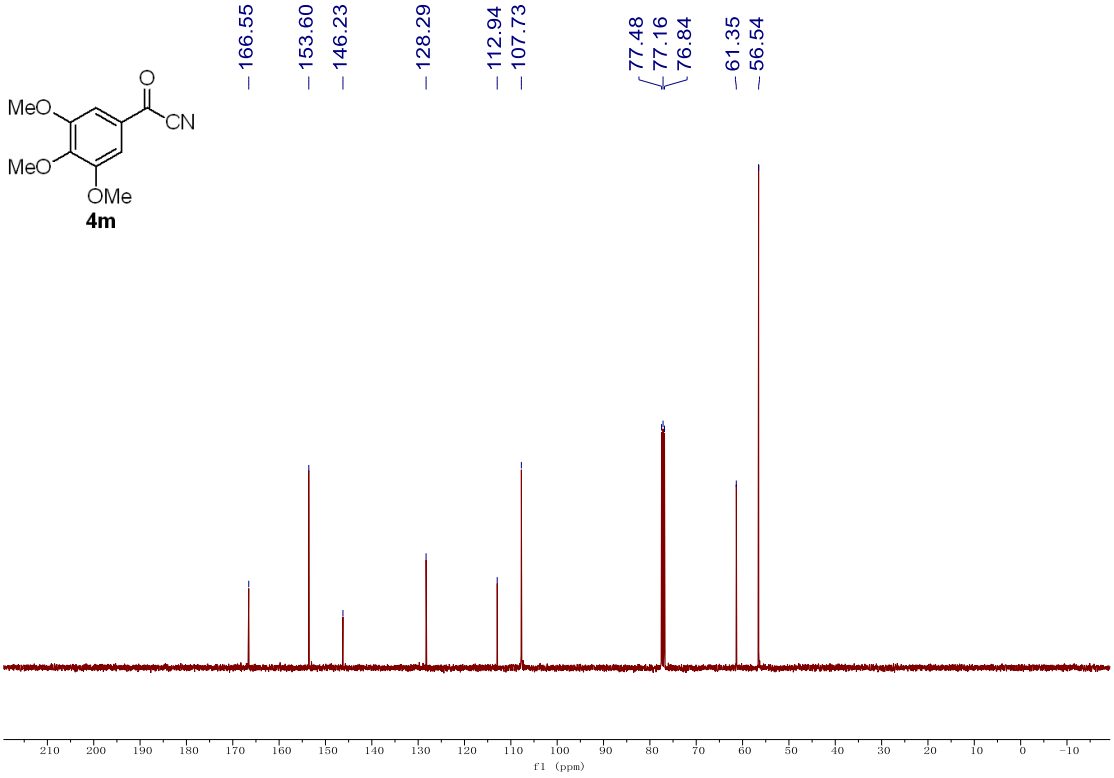

8.14
8.14
8.13
8.13
8.00
8.00
7.99
7.99
7.32
7.31
7.31
7.30
7.26
O
CN
S
4k
1.00
1.00
1.01
f1 (ppm)

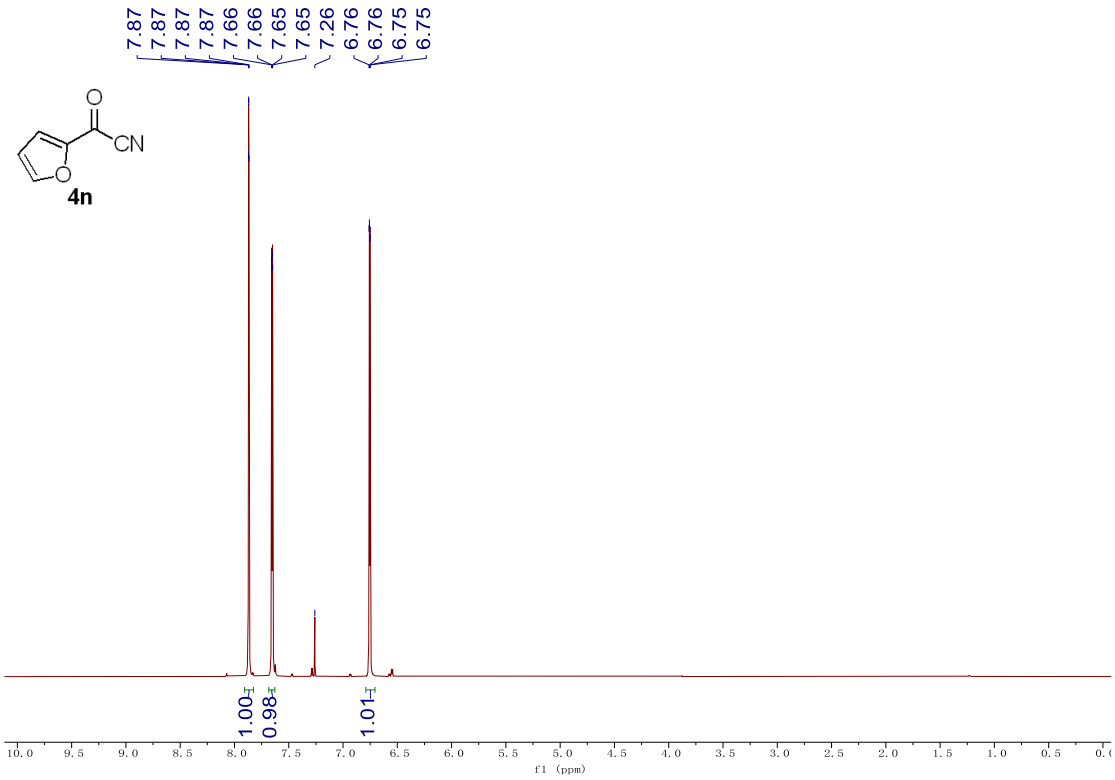

159.03
141.13
140.03
139.55
129.57
112.64
77.48
77.16
76.84
O
CN
S
4k
f1 (ppm)

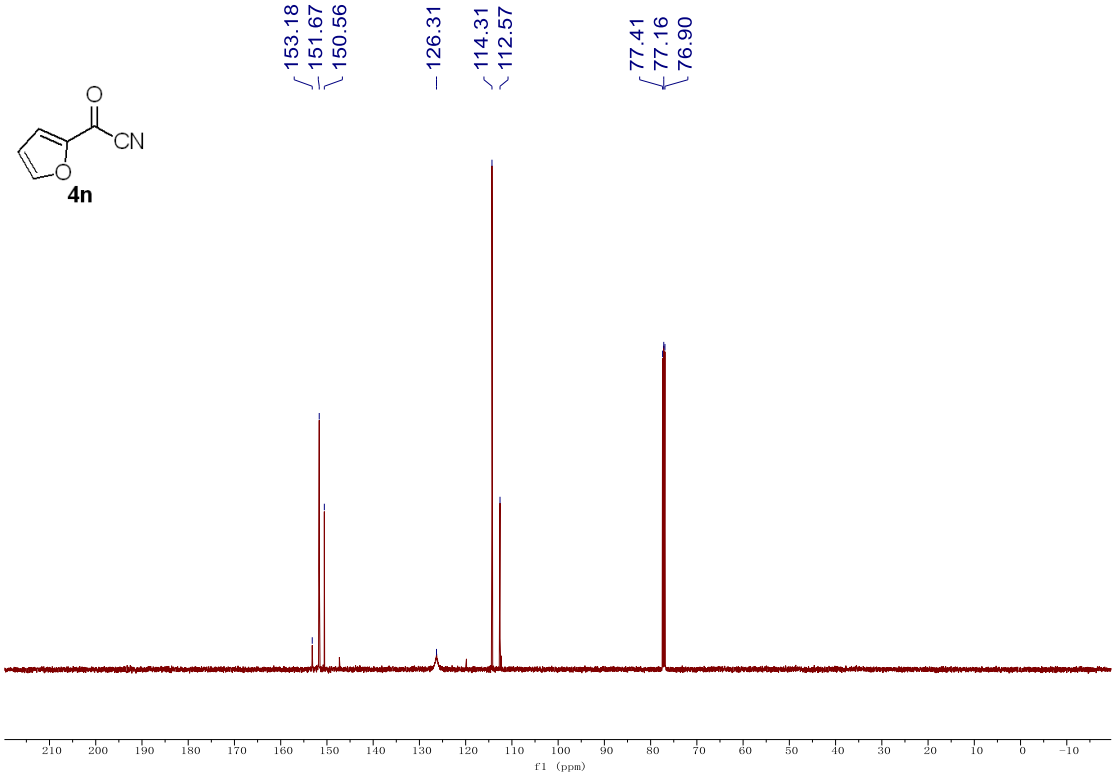

7.88
7.88
7.86
7.86
7.52
7.51
7.26
7.03
7.01
4.02
3.95
MeO
MeO
O
CN
4l
1.00
1.00
1.03
3.02
3.05
f1 (ppm)

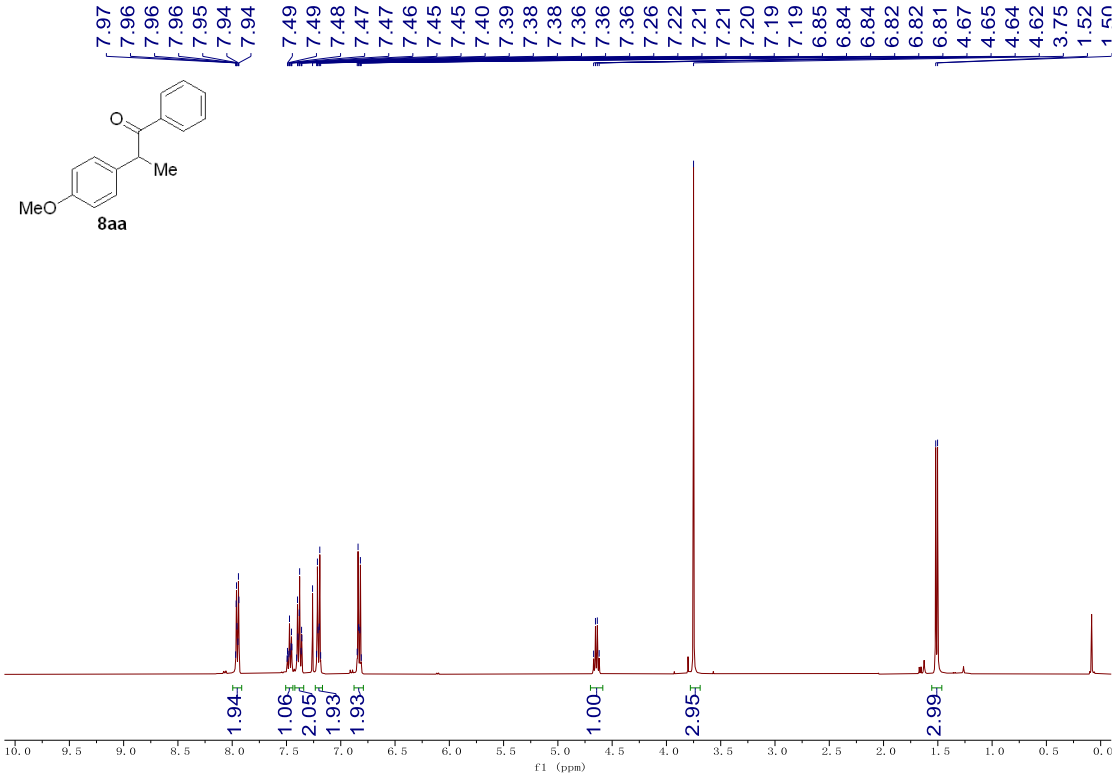

166.24
156.93
150.01
128.16
127.12
113.16
110.84
109.97
77.48
77.16
76.84
56.68
56.32
MeO
MeO
O
CN
4l
f1 (ppm)

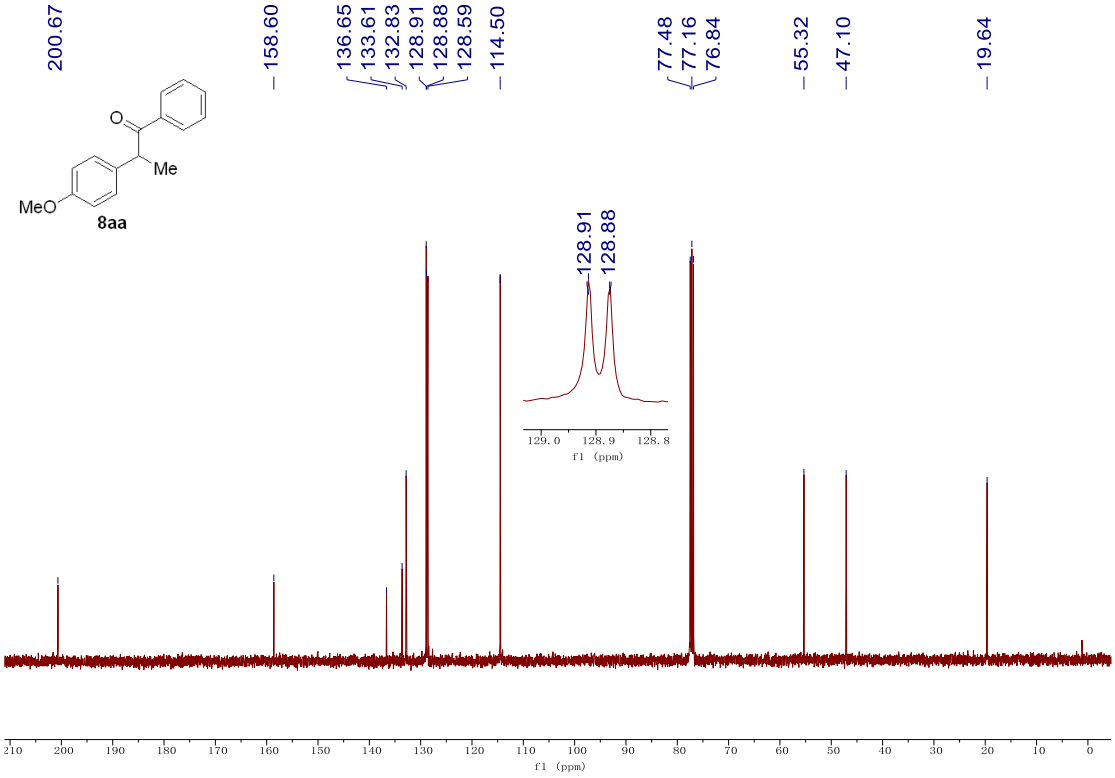

7.34
7.26
3.99
3.93
MeO
MeO
OMe
O
CN
4m
2.02
3.00
6.01
f1 (ppm)


166.55
153.60
146.23
128.29
112.94
107.73
77.48
77.16
76.84
61.35
56.54
MeO
MeO
OMe
O
CN
4m
f1 (ppm)


7.87
7.87
7.87
7.87
7.66
7.66
7.65
7.65
7.26
6.76
6.76
6.75
6.75
O
CN
O
4n
1.00
0.98
1.01
f1 (ppm)


153.18
151.67
150.56
126.31
114.31
112.57
77.41
77.16
76.90
O
CN
O
4n
f1 (ppm)


7.97
7.96
7.96
7.96
7.95
7.94
7.94
7.49
7.49
7.48
7.47
7.47
7.46
7.45
7.45
7.40
7.39
7.38
7.38
7.36
7.36
7.36
7.26
7.22
7.21
7.21
7.20
7.19
7.19
6.85
6.84
6.84
6.82
6.82
6.81
4.67
4.65
4.64
4.62
3.75
1.52
O
Me
MeO
8aa
1.94
1.06
2.05
1.93
1.93
1.00
2.95
2.99
f1 (ppm)


200.67
158.60
136.65
133.61
132.83
128.91
128.88
128.59
114.50
77.48
77.16
76.84
55.32
47.10
19.64
O
Me
MeO
8aa
128.91
128.88
129.0
128.9
128.8
f1 (ppm)
f1 (ppm)


8.09
8.09
8.08
8.07
8.07
8.06
7.65
7.64
7.63
7.62
7.61
7.61
7.60
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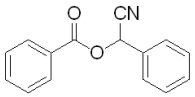
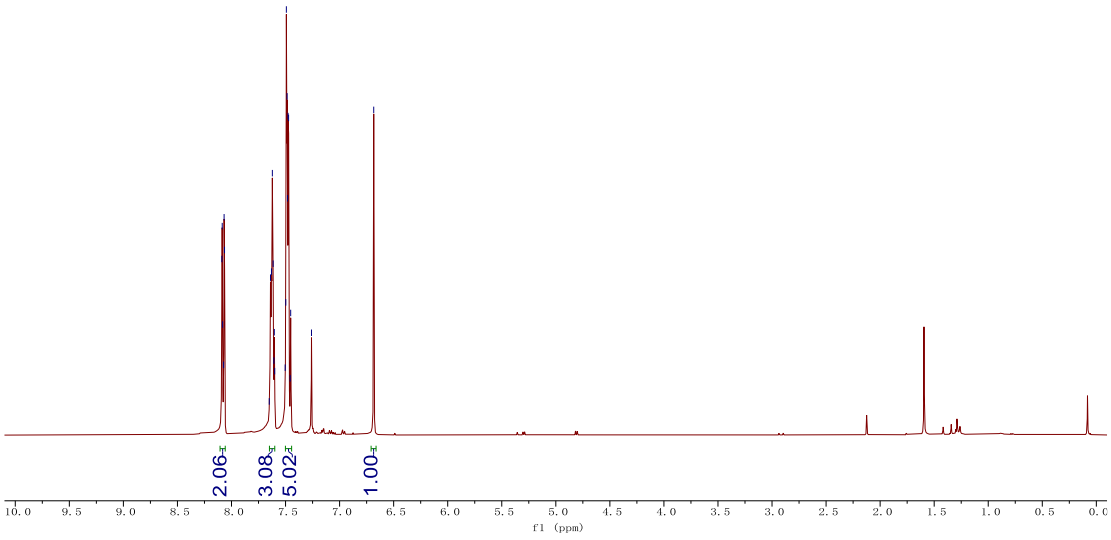
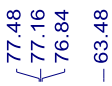
7.48
7.47
7.46
7.45
7.26
6.68

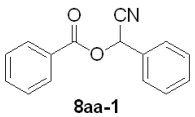

O
CN
O

8aa-1

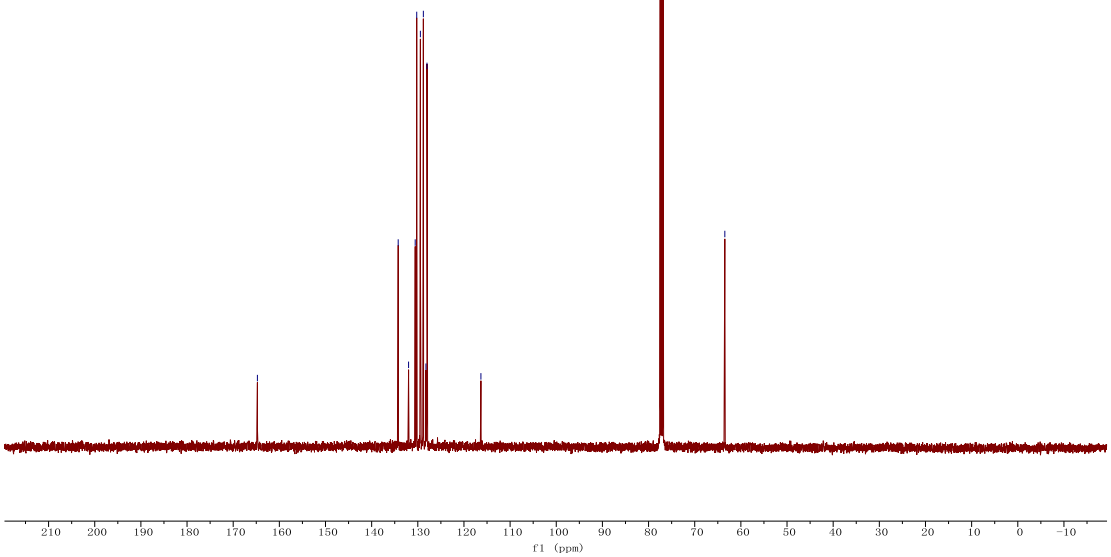

2.06
3.08
5.02
1.00
f1 (ppm)

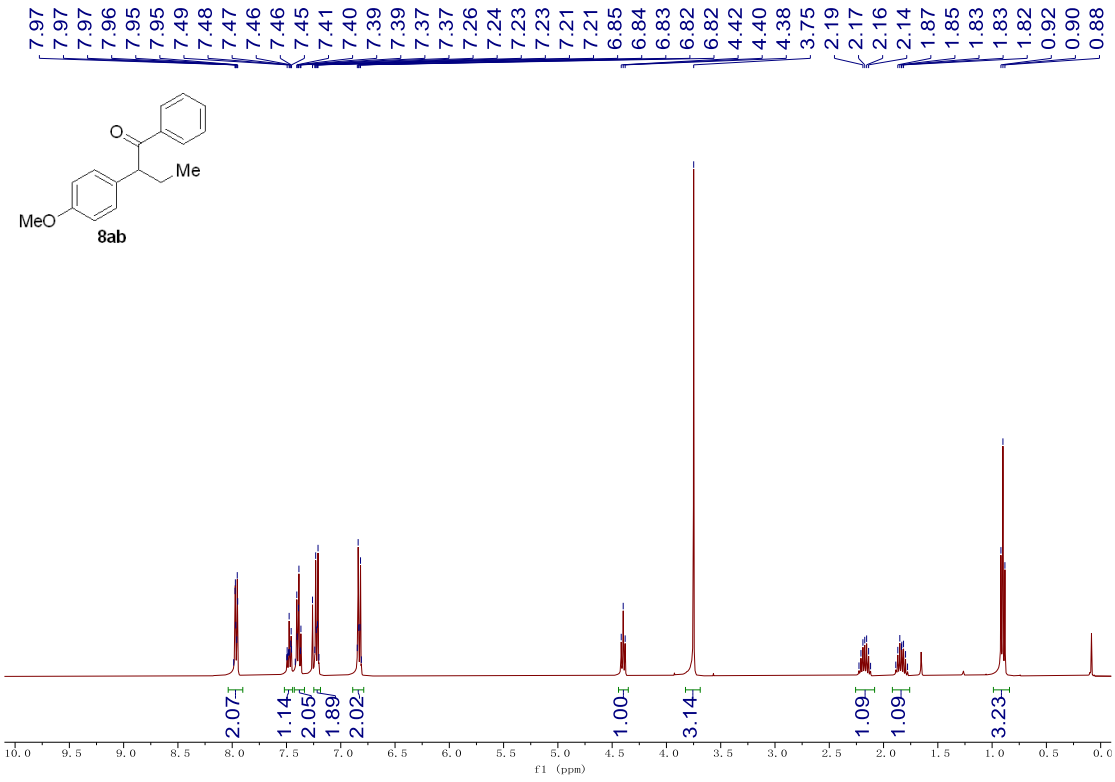

164.75
134.25
132.00
130.56
130.23
129.44
128.80
128.24
128.01
116.33

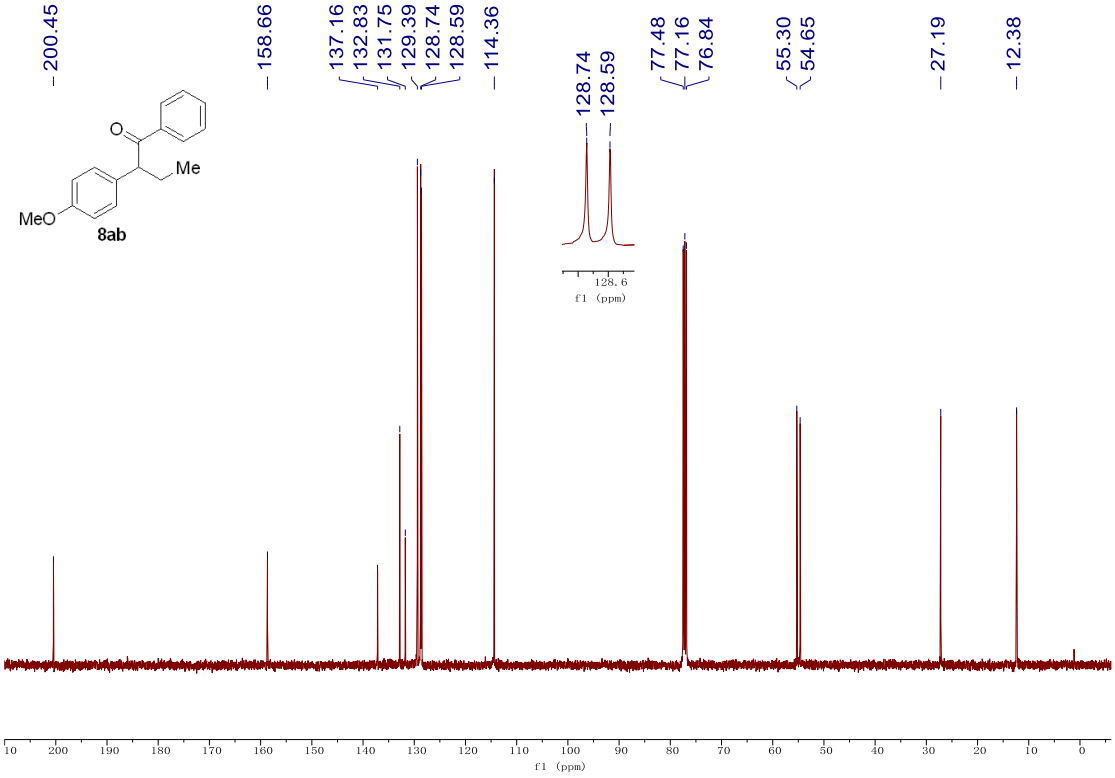

77.48
77.16
76.84
63.48

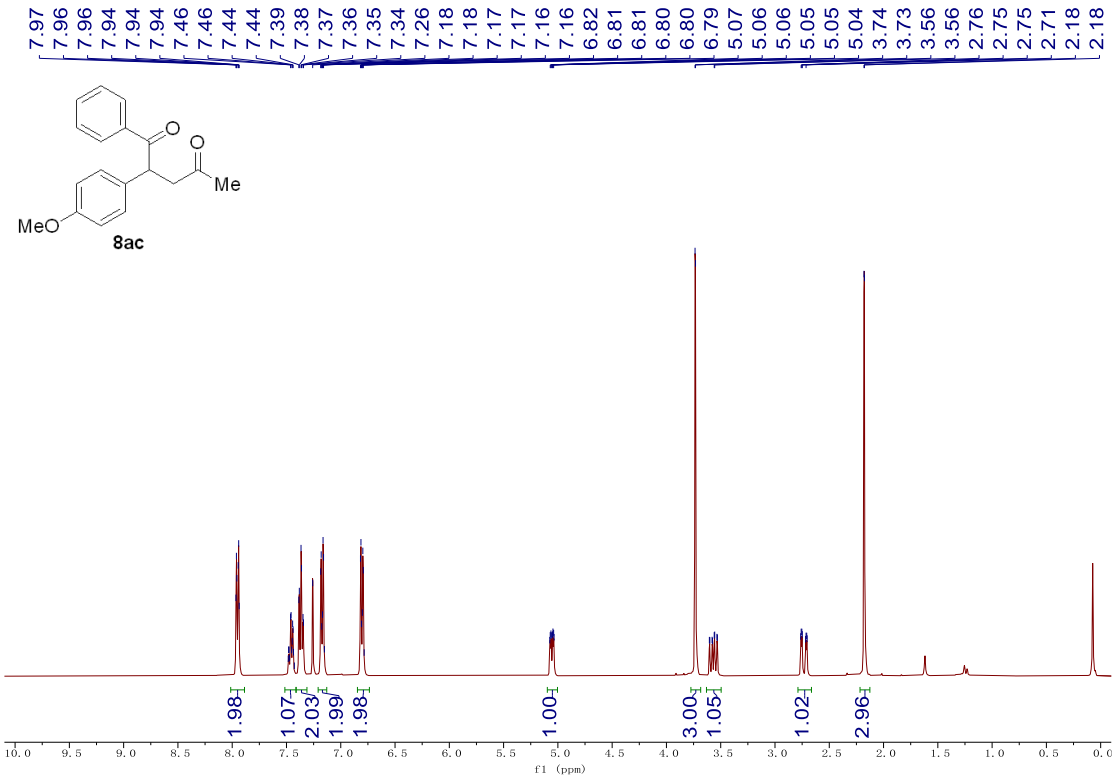

O
CN
O

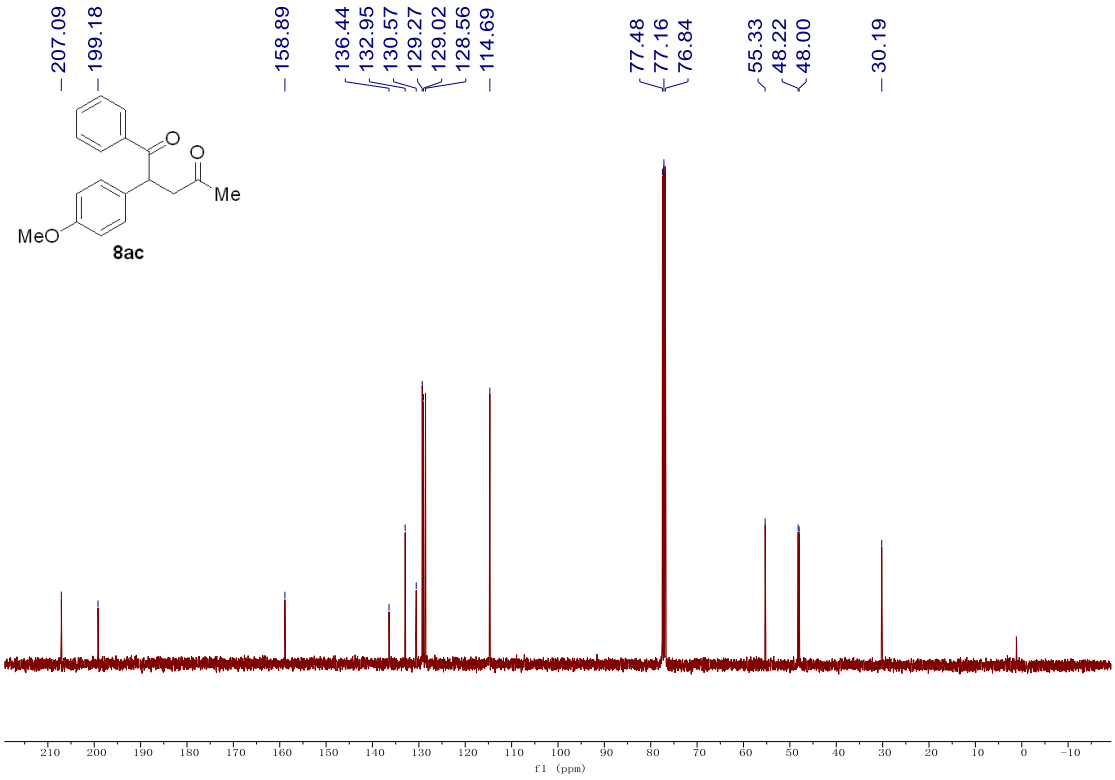
8aa-1

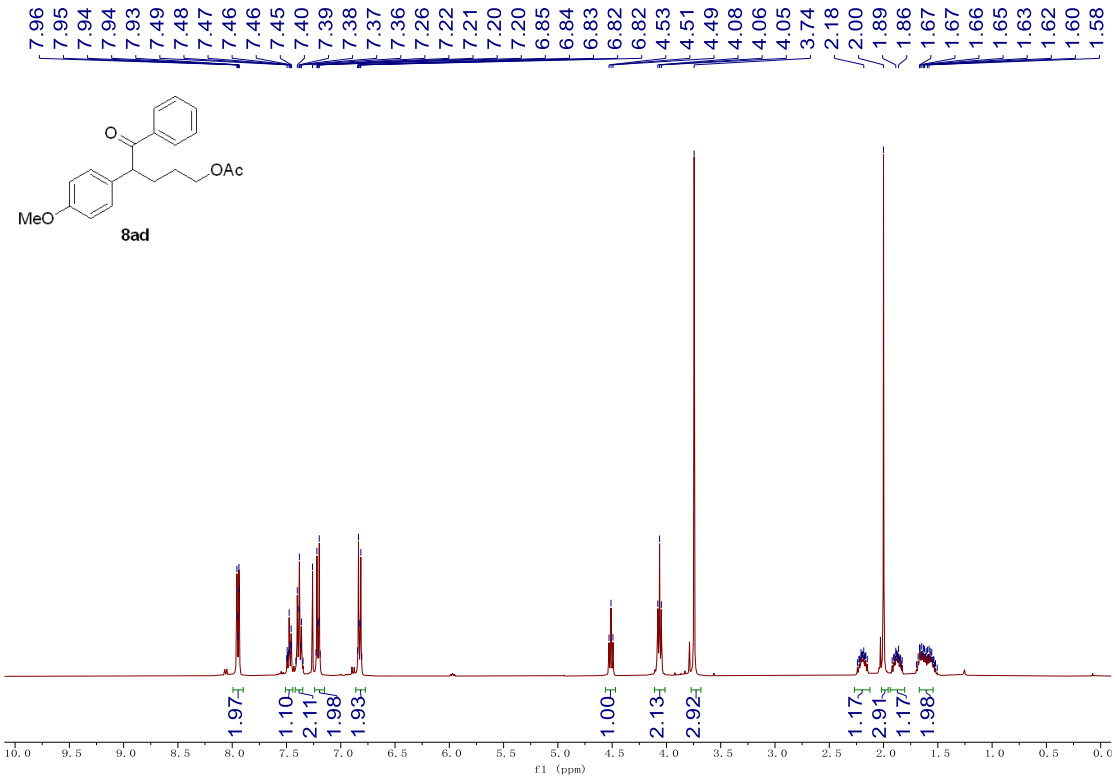

f1 (ppm)

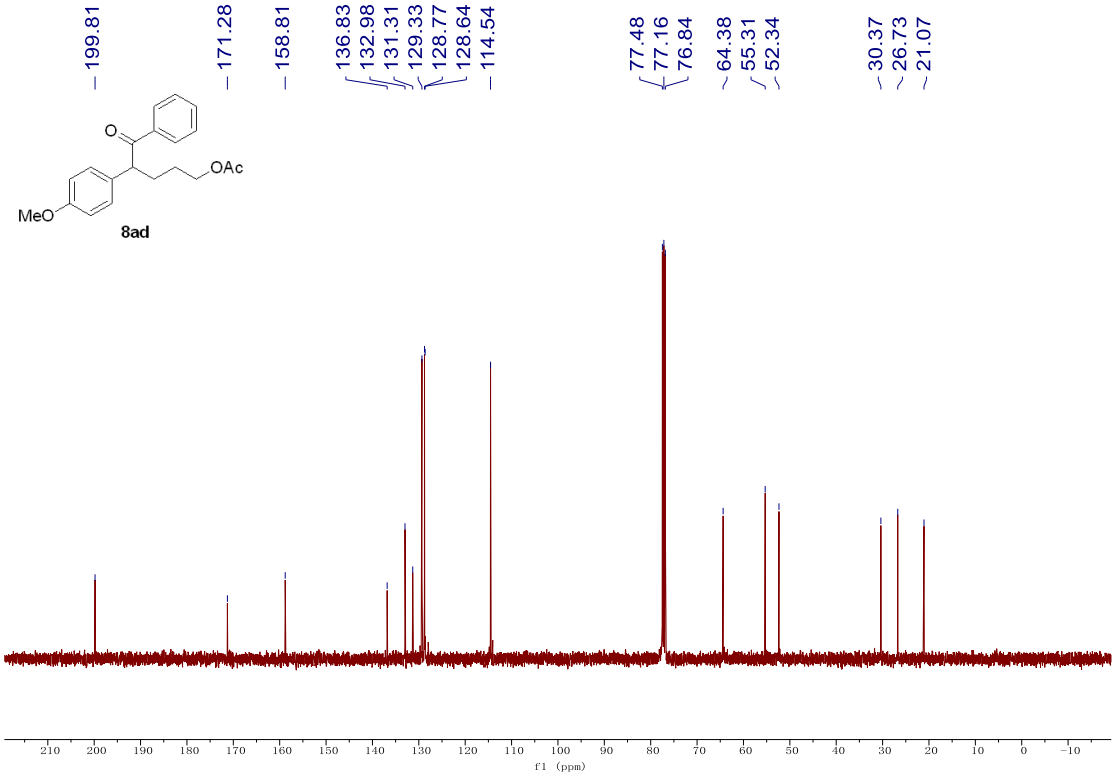

7.97 7.97 7.97 7.96 7.95 7.95 7.49 7.48 7.47 7.46 7.46 7.45 7.41 7.40 7.39 7.39 7.37 7.37 7.26 7.24 7.23 7.23 7.21 7.21 6.85 6.84 6.83 6.82 6.82 4.42 4.40 4.38 3.75 2.19 2.17 2.16 2.14 1.87 1.85 1.83 1.83 1.82 0.92 0.90 0.88
O
Me
MeO
8ab
2.07 1.14 2.05 1.89 2.02 1.00 3.14 1.09 1.09 3.23
f1 (ppm)

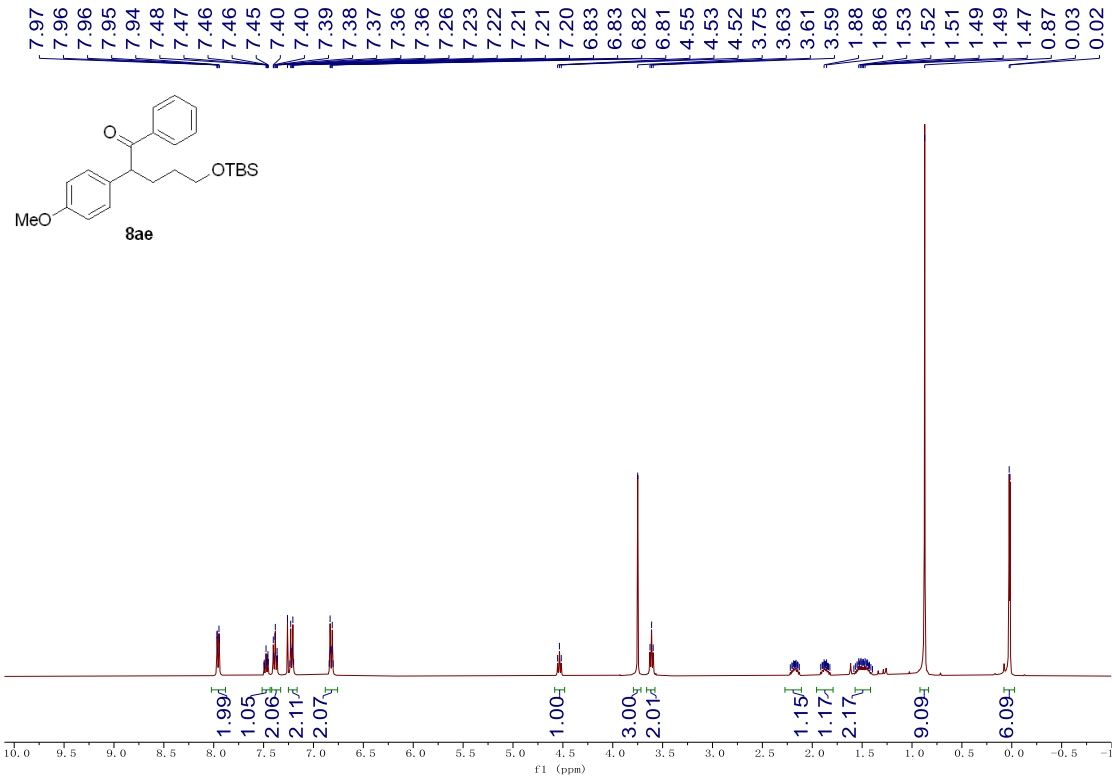

200.45 158.66 137.16 132.83 131.75 129.39 128.74 128.59 114.36 77.48 77.16 76.84 55.30 54.65 27.19 12.38
128.74 128.59
O
Me
MeO
8ab
f1 (ppm)


7.97 7.96 7.96 7.94 7.94 7.94 7.46 7.46 7.44 7.44 7.39 7.38 7.37 7.36 7.35 7.34 7.26 7.18 7.18 7.17 7.17 7.16 7.16 6.82 6.81 6.81 6.80 6.80 6.79 5.07 5.06 5.06 5.05 5.05 5.04 3.74 3.73 3.56 3.56 2.76 2.75 2.75 2.71 2.18 2.18
O
O
Me
MeO
8ac
1.98 1.07 2.03 1.99 1.98 1.00 3.00 1.05 1.02 2.96
f1 (ppm)


207.09 199.18 158.89 136.44 132.95 130.57 129.27 129.02 128.56 114.69 77.48 77.16 76.84 55.33 48.22 48.00 30.19
O
O
Me
MeO
8ac
f1 (ppm)


7.96 7.95 7.94 7.94 7.93 7.49 7.48 7.47 7.46 7.46 7.45 7.40 7.39 7.38 7.37 7.36 7.26 7.22 7.21 7.20 7.20 6.85 6.84 6.83 6.82 6.82 4.53 4.51 4.49 4.08 4.06 4.05 3.74 2.18 2.00 1.89 1.86 1.67 1.67 1.66 1.65 1.63 1.62 1.60 1.58
O
OAc
MeO
8ad
1.97 1.10 2.11 1.98 1.93 1.00 2.13 2.92 1.17 2.91 1.17 1.98
f1 (ppm)


199.81 171.28 158.81 136.83 132.98 131.31 129.33 128.77 128.64 114.54 77.48 77.16 76.84 64.38 55.31 52.34 30.37 26.73 21.07
O
OAc
MeO
8ad
f1 (ppm)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7.96
7.96
7.95
7.94
7.48
7.47
7.46
7.46
7.45
7.40
7.40
7.39
7.38
7.37
7.36
7.36
7.26
7.23
7.22
7.21
7.21
7.20
6.83
6.83
6.82
6.81
4.55
4.53
4.52
3.75
3.63
3.61
3.59
1.88
1.86
1.53
1.52
1.51
1.49
1.49
1.47
0.87
0.03
0.02
O
OTBS
MeO
8ae
1.99
1.05
2.06
2.11
2.07
1.00
3.00
2.01
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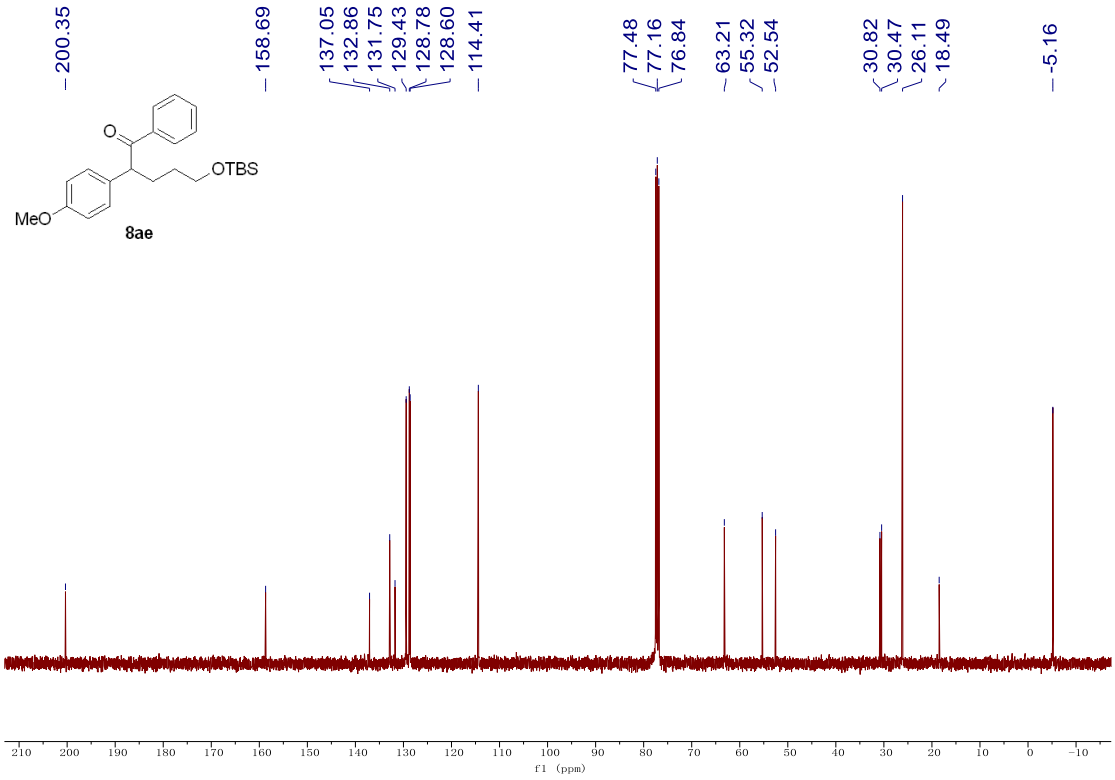
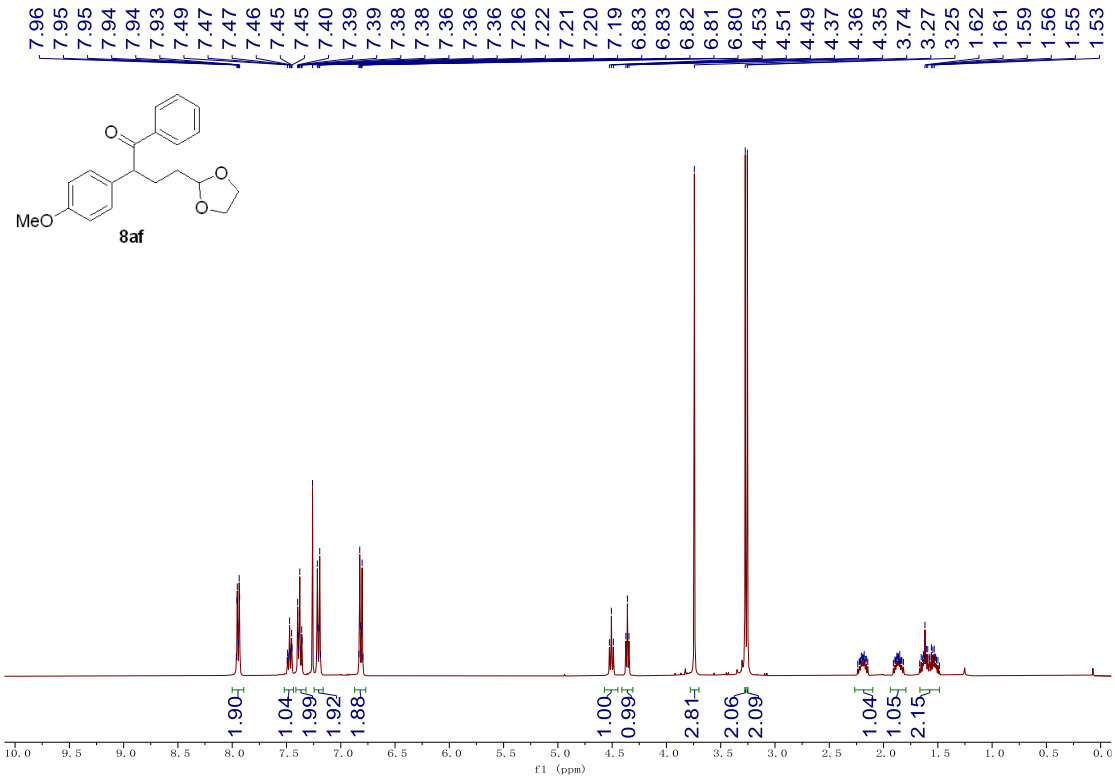
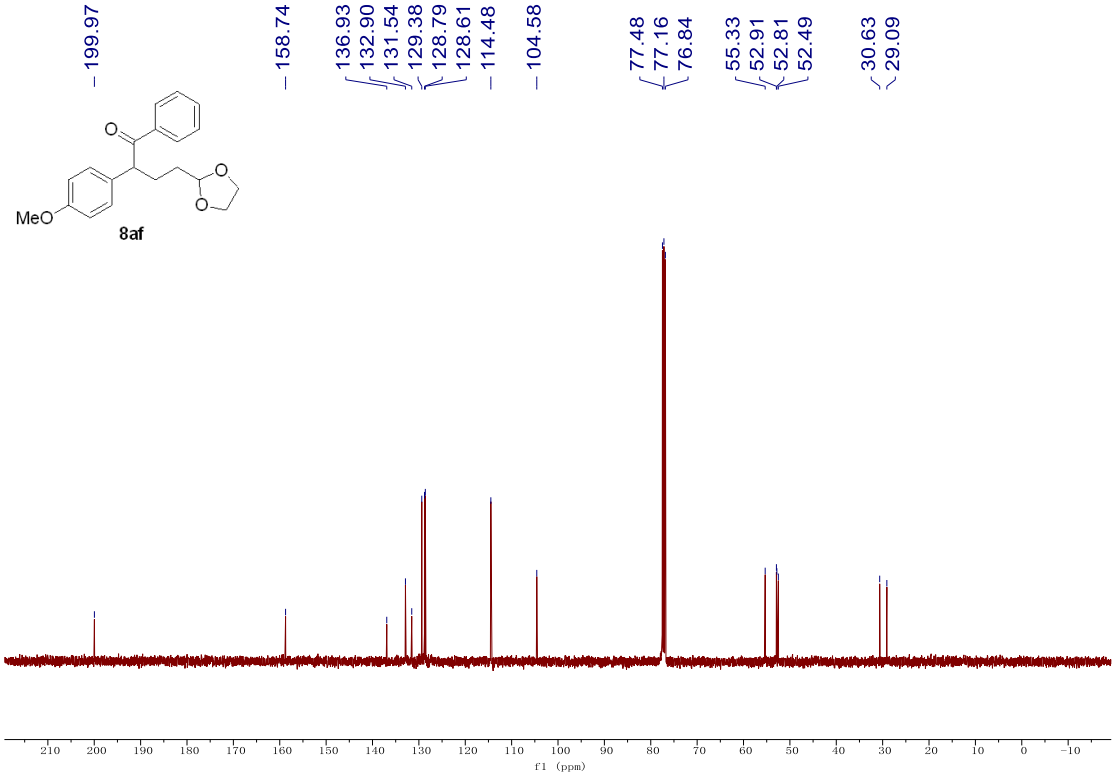
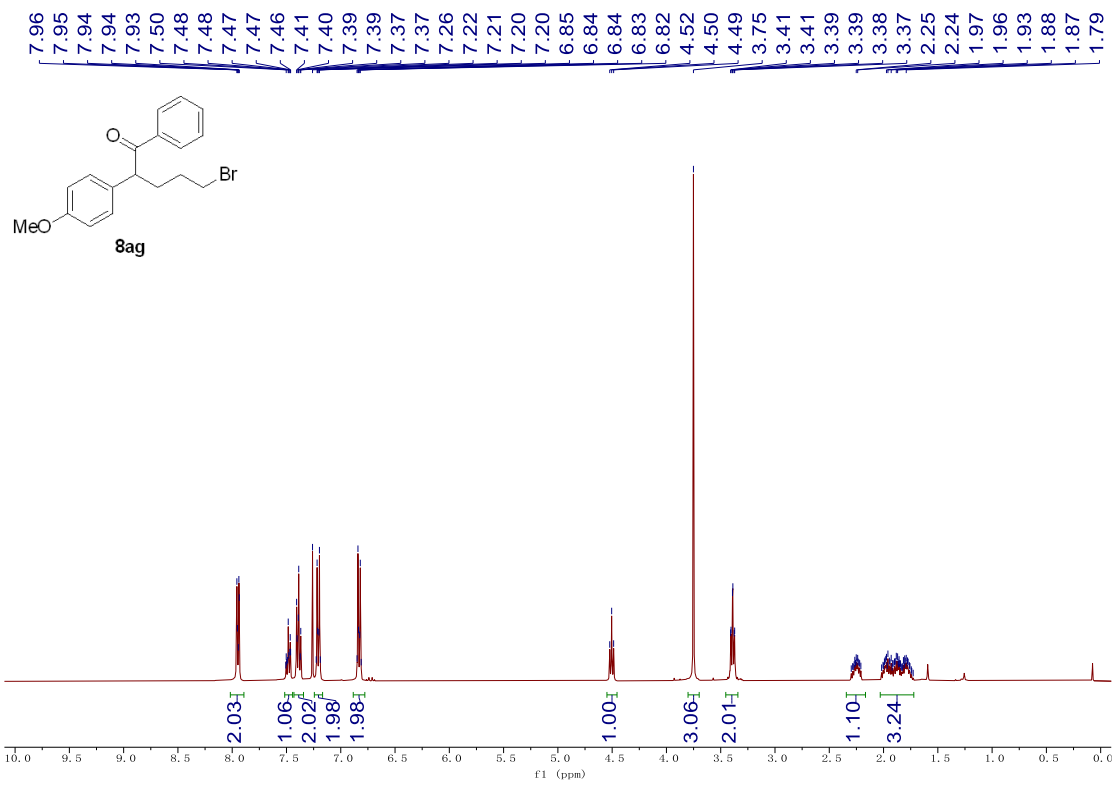
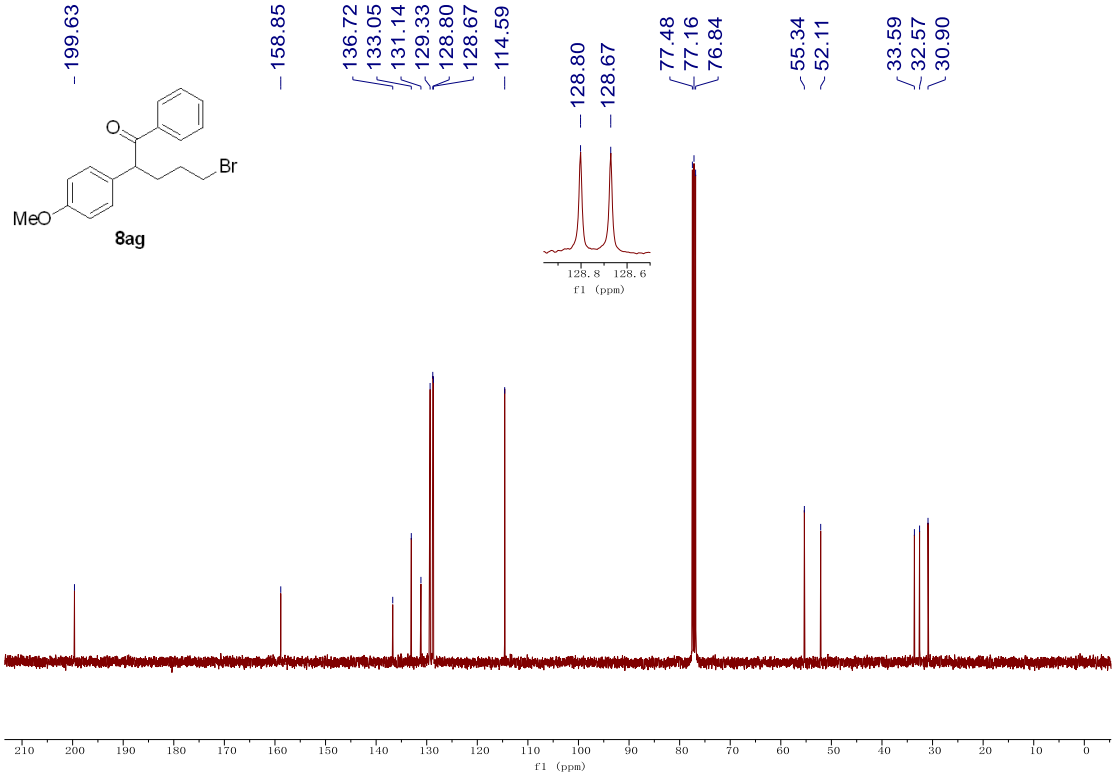
1.17
2.17
9.09
6.09
f1 (ppm)


200.35
158.69
137.05
132.86
131.75
129.43
128.78
128.60
114.41
77.48
77.16
76.84
63.21
55.32
52.54
30.82
30.47
26.11
18.49
-5.16
O
OTBS
MeO
8ae
f1 (ppm)


7.96
7.95
7.95
7.94
7.94
7.93
7.49
7.47
7.47
7.46
7.45
7.45
7.40
7.39
7.39
7.38
7.38
7.36
7.36
7.36
7.26
7.22
7.21
7.20
7.19
6.83
6.83
6.82
6.81
6.80
4.53
4.51
4.49
4.37
4.36
4.35
3.74
3.27
3.25
1.62
1.61
1.59
1.56
1.55
1.53
O
O
O
MeO
8af
1.90
1.04
1.99
1.92
1.88
1.00
0.99
2.81
2.06
2.09
1.04
1.05
2.15
f1 (ppm)


199.97
158.74
136.93
132.90
131.54
129.38
128.79
128.61
114.48
104.58
77.48
77.16
76.84
55.33
52.91
52.81
52.49
30.63
29.09
O
O
O
MeO
8af
f1 (ppm)


7.96 7.95 7.94 7.94 7.93 7.50 7.48 7.48 7.47 7.47 7.46 7.41 7.40 7.39 7.39 7.37 7.37 7.26 7.22 7.21 7.20 7.20 6.85 6.84 6.84 6.83 6.82 4.52 4.50 4.49 3.75 3.41 3.41 3.39 3.39 3.38 3.37 2.25 2.24 1.97 1.96 1.93 1.88 1.87 1.79
O
Br
MeO
8ag
2.03 1.06 2.02 1.98 1.98 1.00 3.06 2.01 1.10 3.24
f1 (ppm)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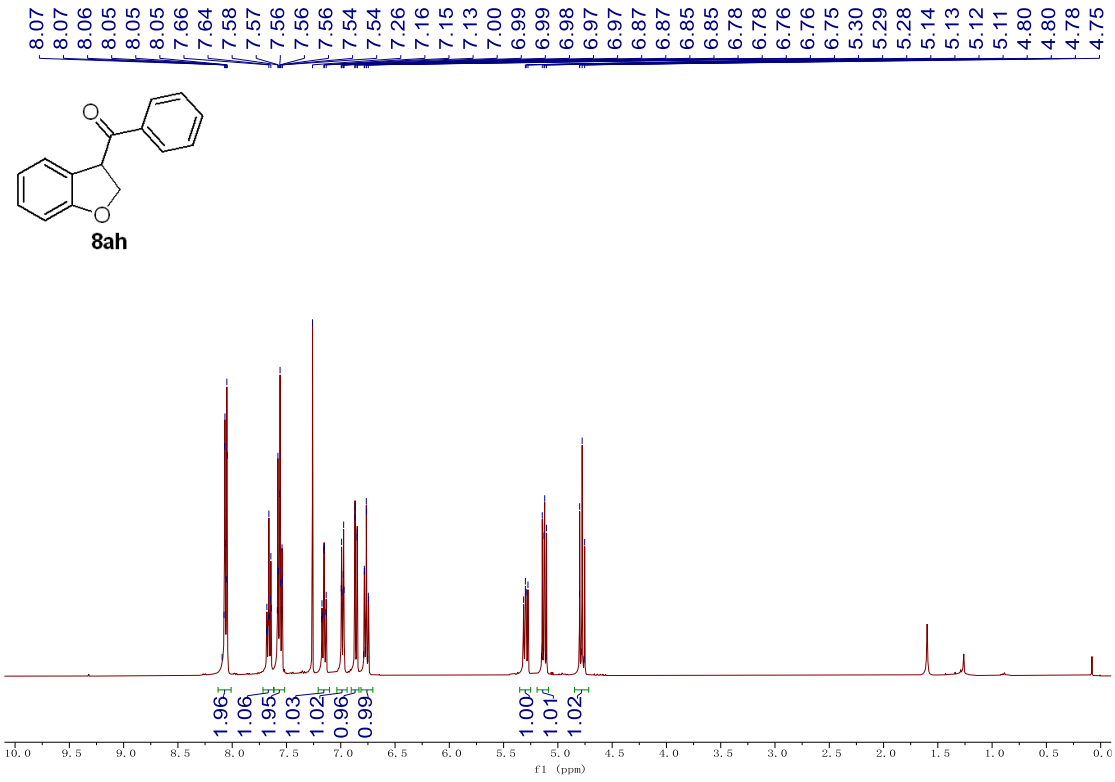
Br
MeO
8ag
128.8 128.6
f1 (ppm)
f1 (ppm)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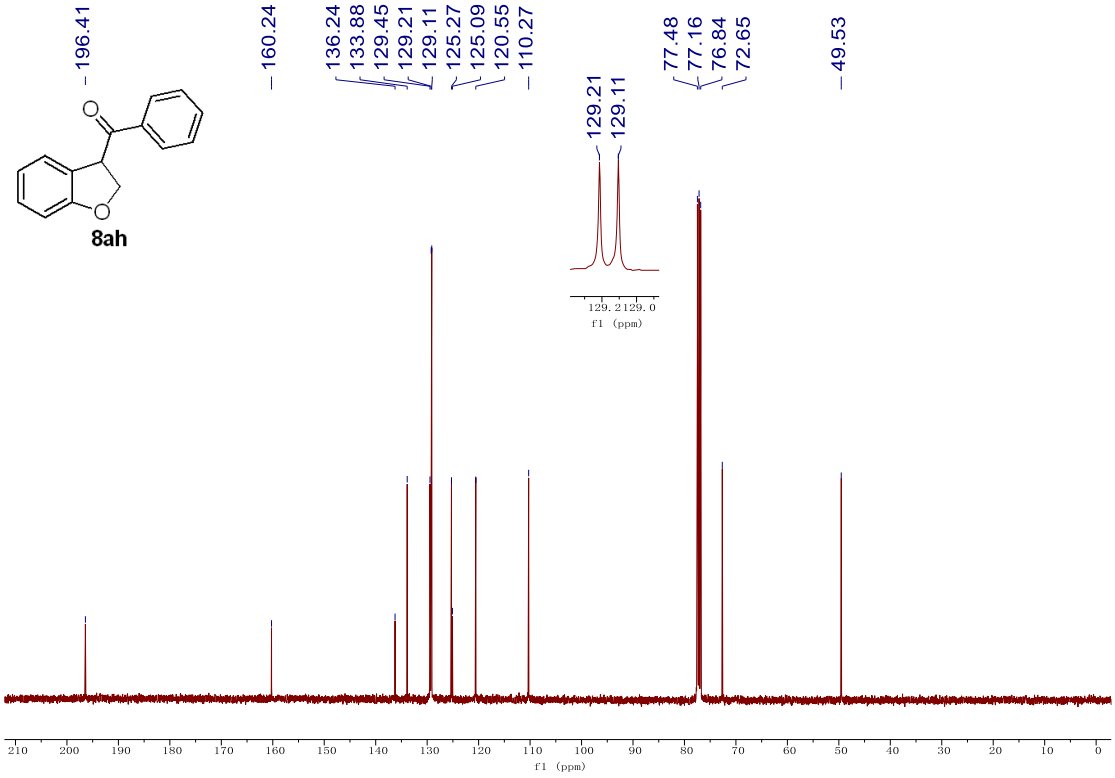
f1 (ppm)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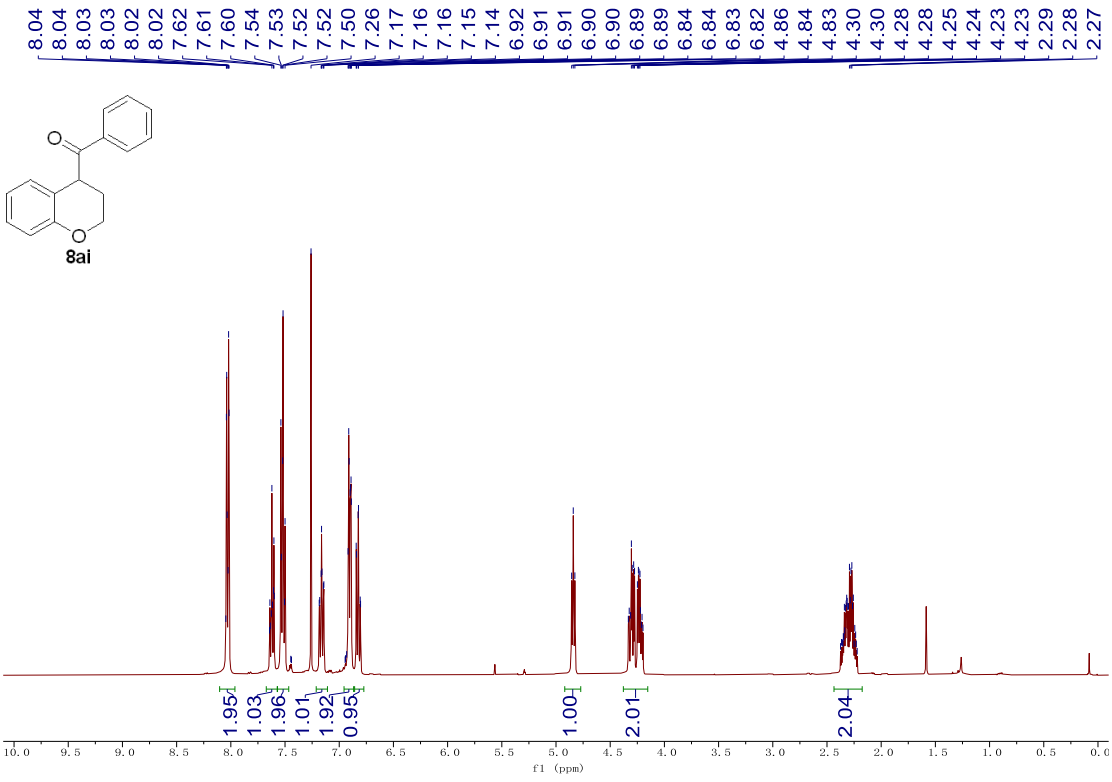
129.2 129.0
f1 (ppm)
f1 (ppm)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8.03
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8.02
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7.50
7.26
7.17
7.16
7.16
7.15
7.14
6.92
6.91
6.91
6.90
6.90
6.89
6.89
6.84
6.84
6.83
6.82
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4.84
4.83
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4.28
4.25
4.24
4.23
4.23
2.29
2.28
2.27
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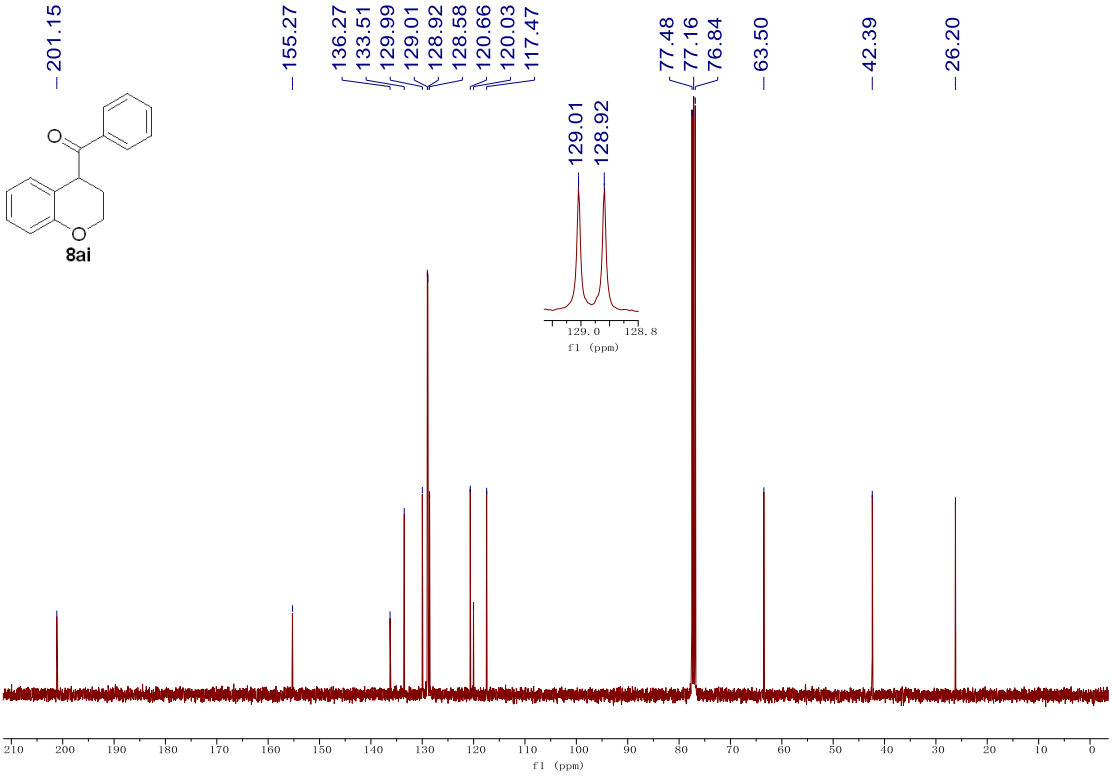
1.03
1.96
1.01
1.92
0.95
1.00
2.01
2.04
f1 (ppm)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128.58
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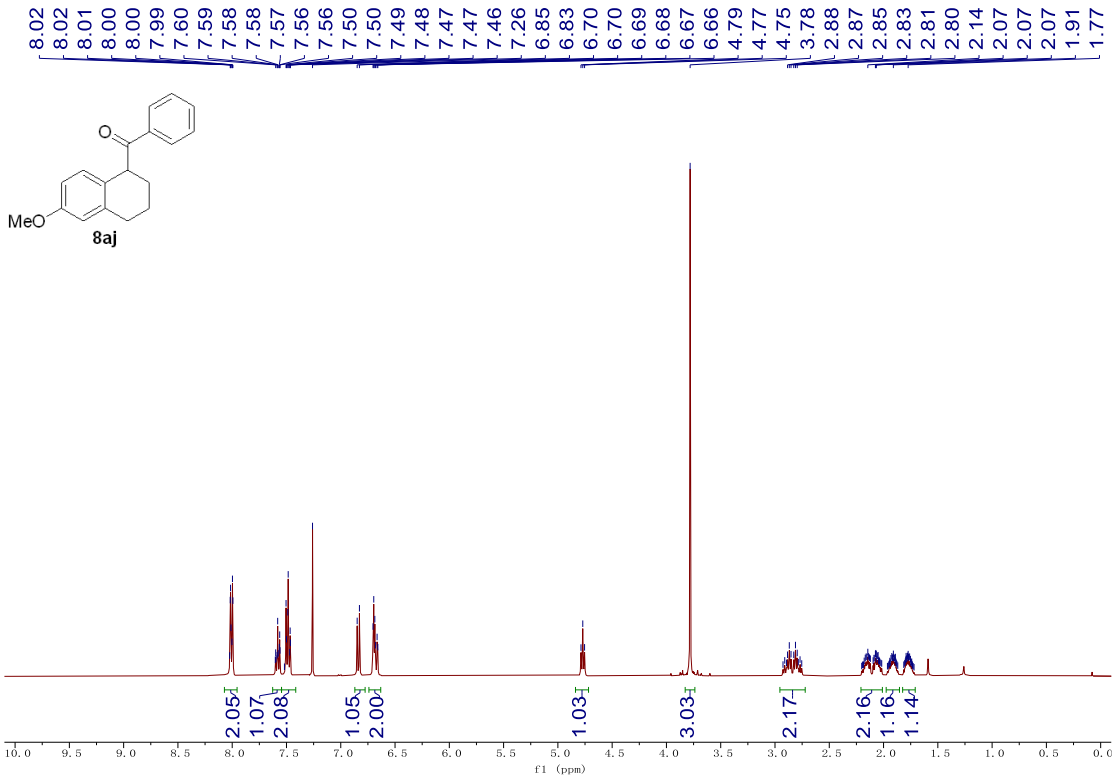
63.50
42.39
26.20
129.01
128.92
8ai
f1 (ppm)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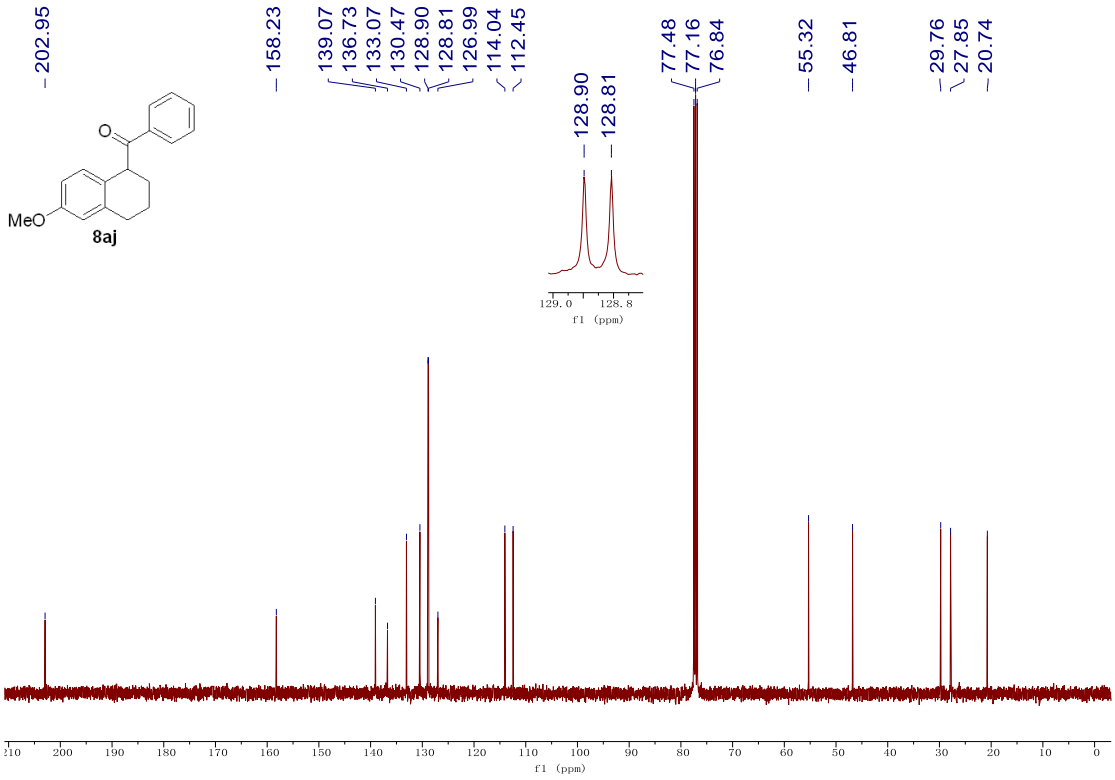
MeO
8aj
2.05 1.07 2.08 1.05 2.00 1.03 3.03 2.17 2.16 1.16 1.14
f1 (ppm)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158.23
139.07 136.73 133.07 130.47 128.90 128.81 126.99 114.04 112.45
128.90 128.81
77.48 77.16 76.84
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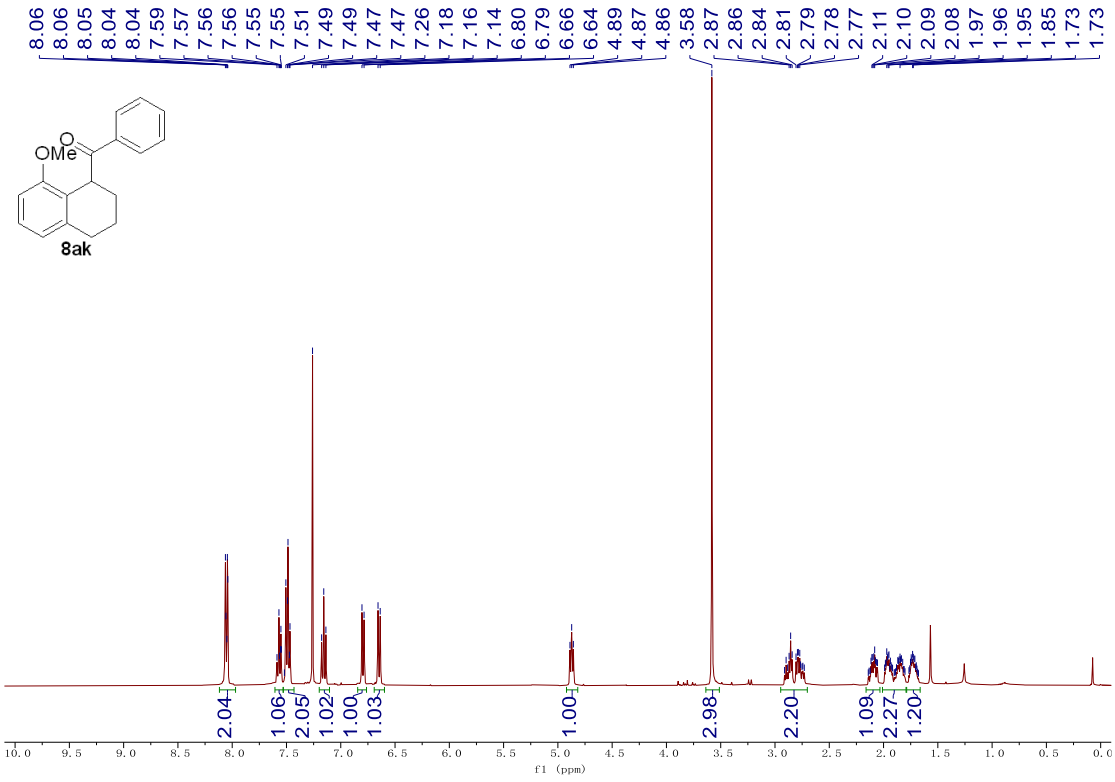
46.81
29.76 27.85 20.74
O
MeO
8aj
129.0 128.8
f1 (ppm)
f1 (ppm)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8.06
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7.51
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7.47
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7.18
7.16
7.14
6.80
6.79
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6.64
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4.86
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2.86
2.84
2.81
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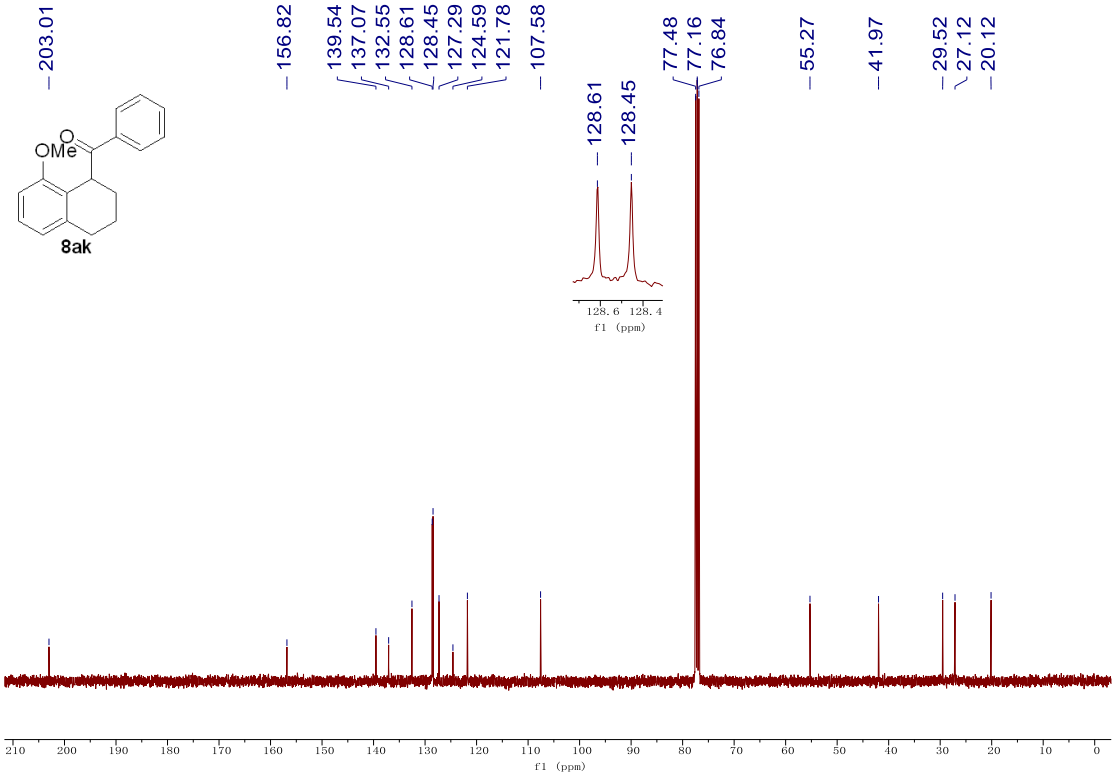
2.78
2.77
2.11
2.10
2.09
2.08
1.97
1.96
1.95
1.85
1.73
1.73
O
OMe
8ak
2.04
1.06
2.05
1.02
1.00
1.03
1.00
2.98
2.20
1.09
2.27
1.20
f1 (ppm)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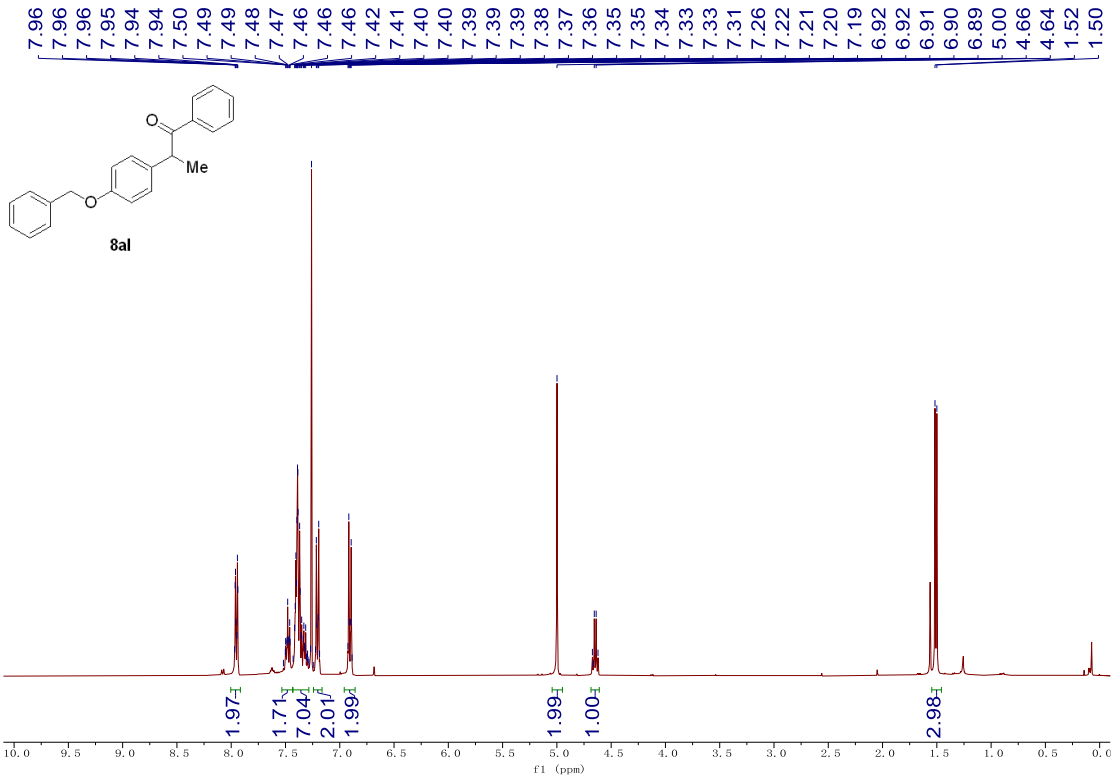
128.45
127.29
124.59
121.78
107.58
77.48
77.16
76.84
55.27
41.97
29.52
27.12
20.12
128.61
128.45
O
OMe
8ak
f1 (ppm)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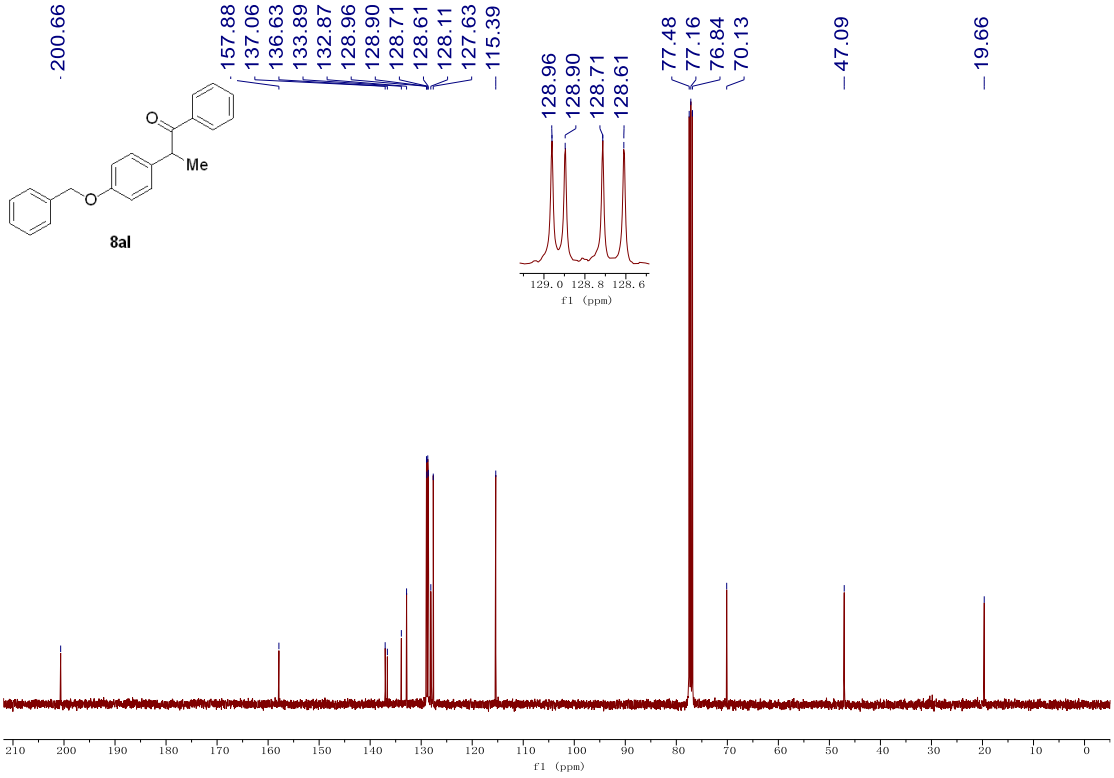
O
Me
O
8al
1.97 1.71 7.04 2.01 1.99 1.99 1.00 2.98
f1 (ppm)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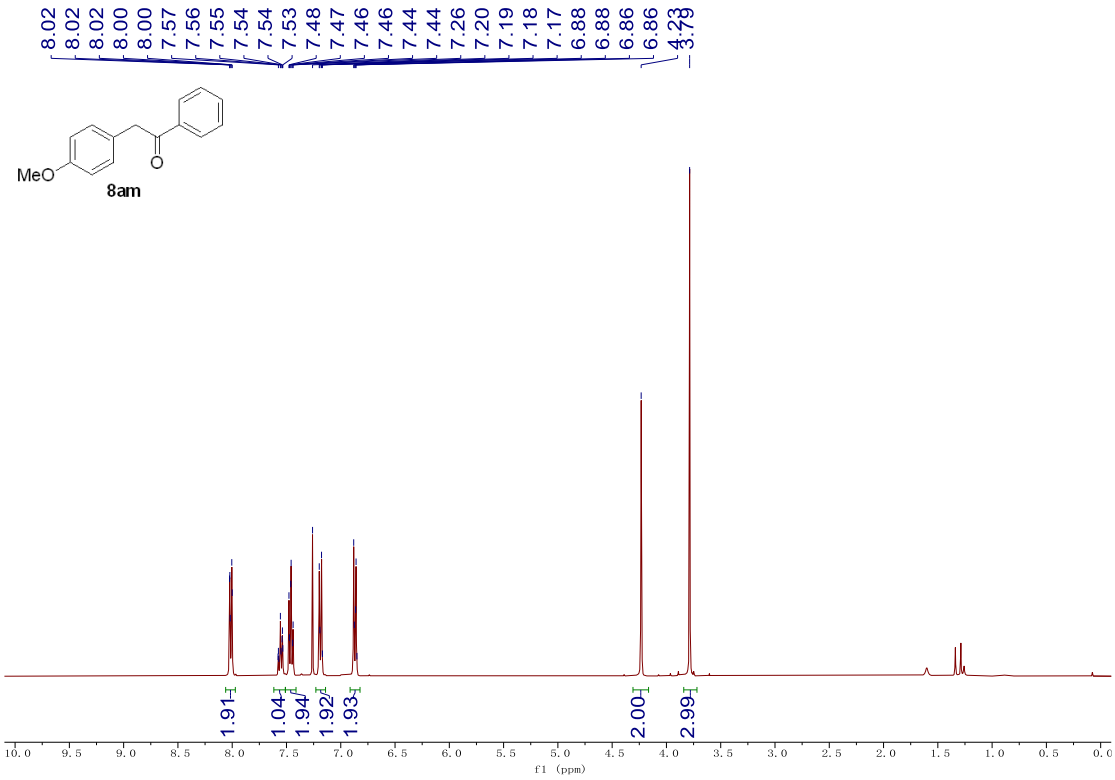
157.88 137.06 136.63 133.89 132.87 128.96 128.90 128.71 128.61 128.11 127.63 115.39
77.48 77.16 76.84 70.13
47.09
19.66
128.96 128.90 128.71 128.61
O
Me
O
8al
f1 (ppm)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8.02
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8.00
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7.46
7.46
7.44
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7.26
7.20
7.19
7.18
7.17
6.88
6.88
6.86
6.86
4.23
3.79
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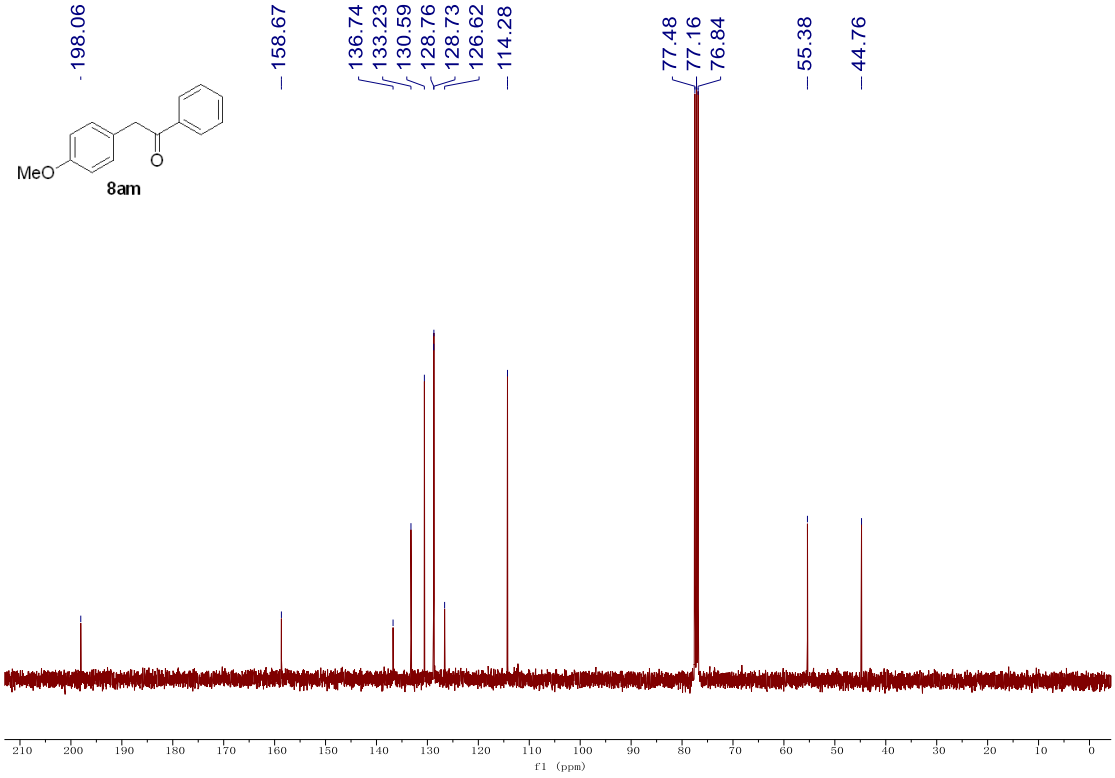
O
8am
1.91
1.04
1.94
1.92
1.93
2.00
2.99
f1 (ppm)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77.16
76.84
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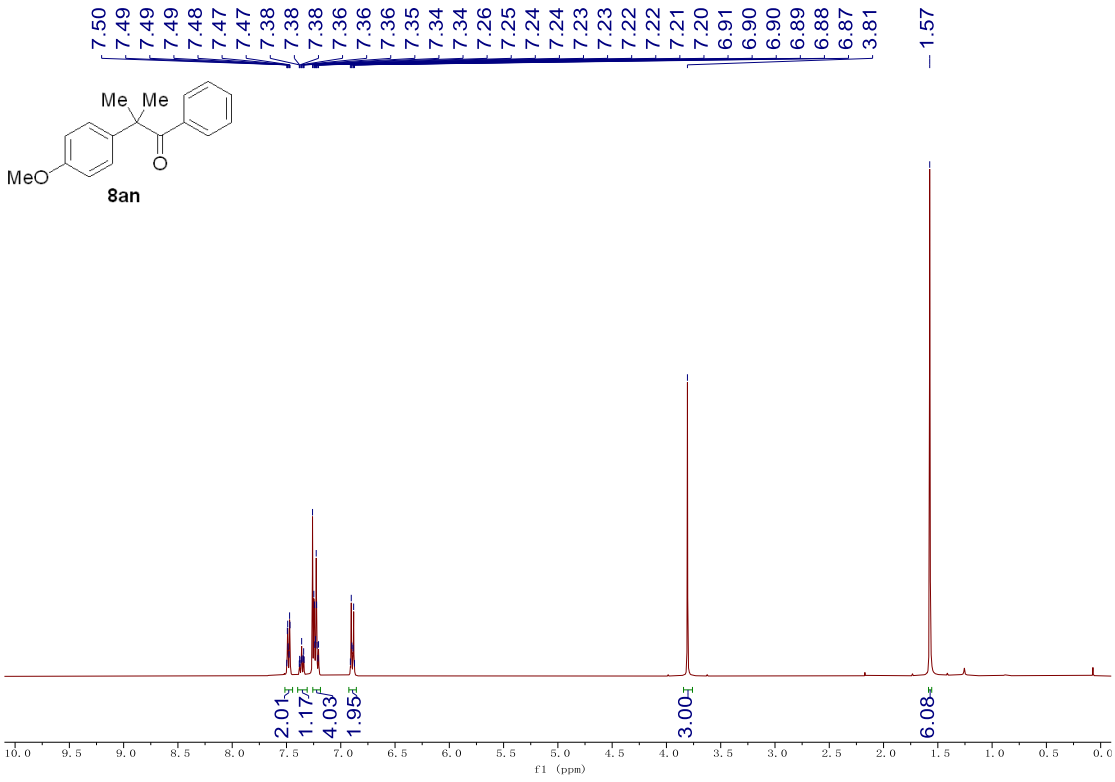
44.76
MeO
O
8am
f1 (ppm)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7.22
7.21
7.20
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6.90
6.90
6.89
6.88
6.87
3.81
1.57
Me
Me
O
MeO
8an
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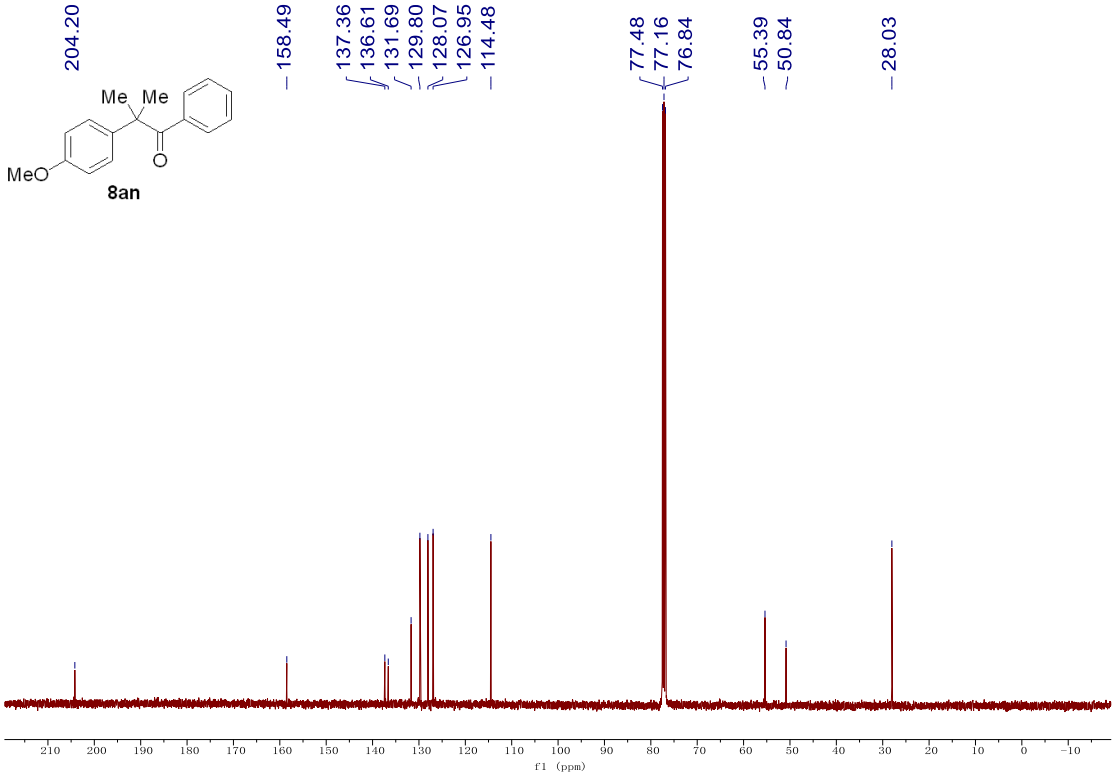
1.17
4.03
1.95
3.00
6.08
f1 (ppm)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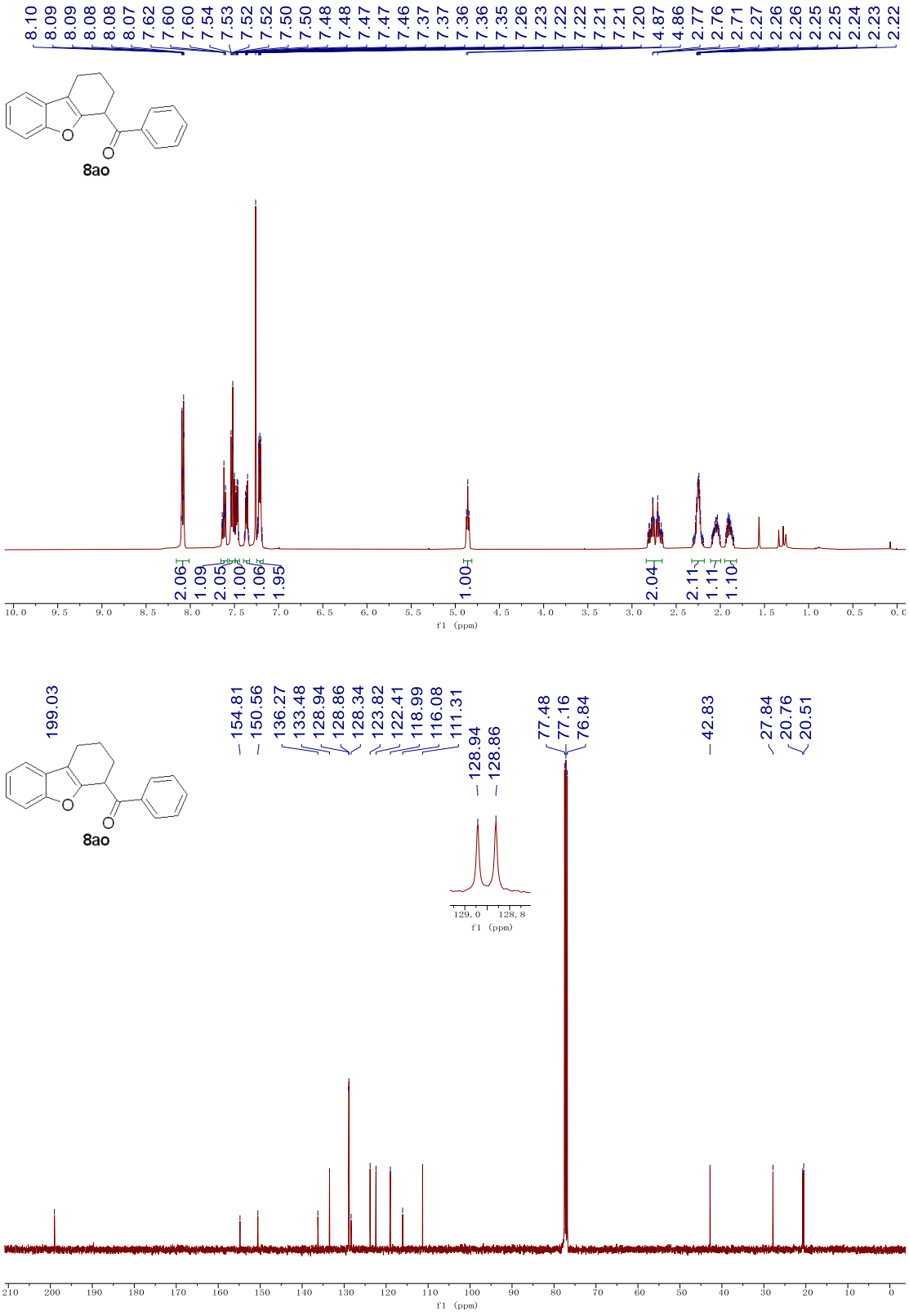
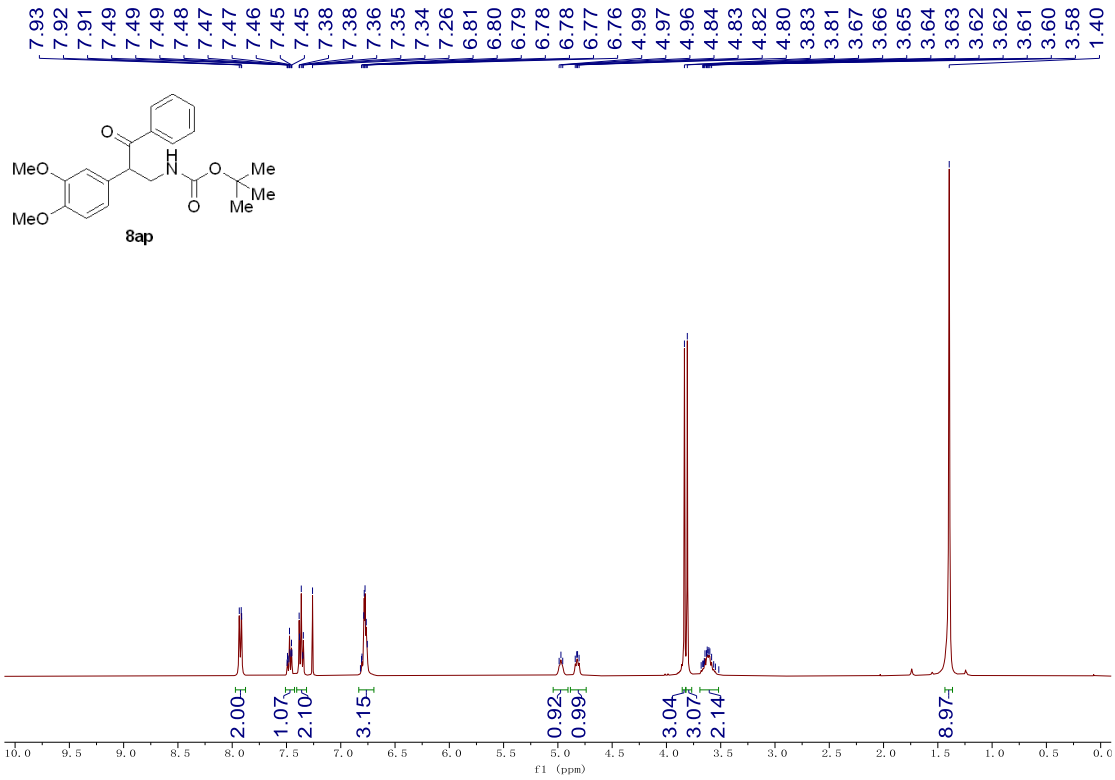
128.07
126.95
114.48
77.48
77.16
76.84
55.39
50.84
28.03
Me
Me
O
MeO
8an
f1 (ppm)


8.10 8.09 8.09 8.08 8.08 8.07 7.62 7.60 7.60 7.54 7.53 7.52 7.52 7.50 7.50 7.48 7.48 7.47 7.47 7.46 7.37 7.37 7.36 7.36 7.35 7.26 7.23 7.22 7.22 7.21 7.21 7.20 4.87 4.86 2.77 2.76 2.71 2.27 2.26 2.26 2.25 2.25 2.24 2.23 2.22
8ao
2.06 1.09 2.05 1.00 1.06 1.95 1.00 2.04 2.11 1.11 1.10
f1 (ppm)
199.03 154.81 150.56 136.27 133.48 128.94 128.86 128.34 123.82 122.41 118.99 116.08 111.31 128.94 128.86 77.48 77.16 76.84 42.83 27.84 20.76 20.51
8ao
f1 (ppm)
f1 (ppm)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7.45
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MeO
MeO
O
H
N
O
O
Me
Me
Me
8ap
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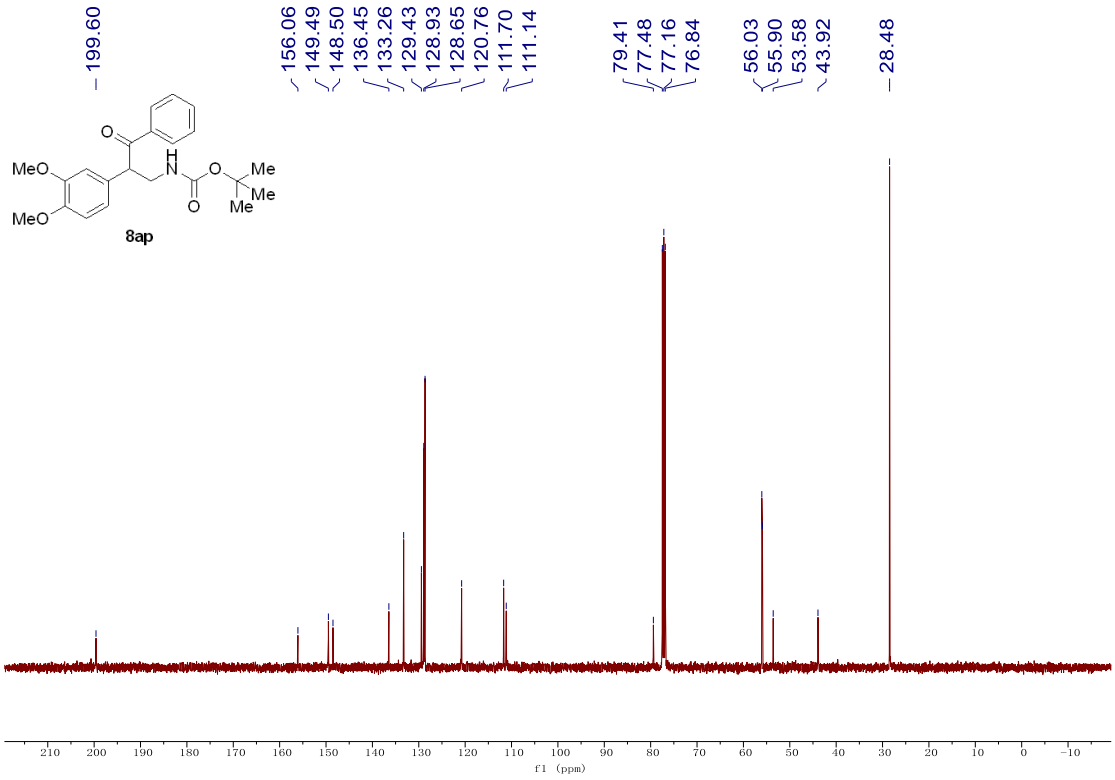
2.10
3.15
0.92
0.99
3.04
3.07
2.14
8.97
f1 (ppm)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120.76
111.70
111.14
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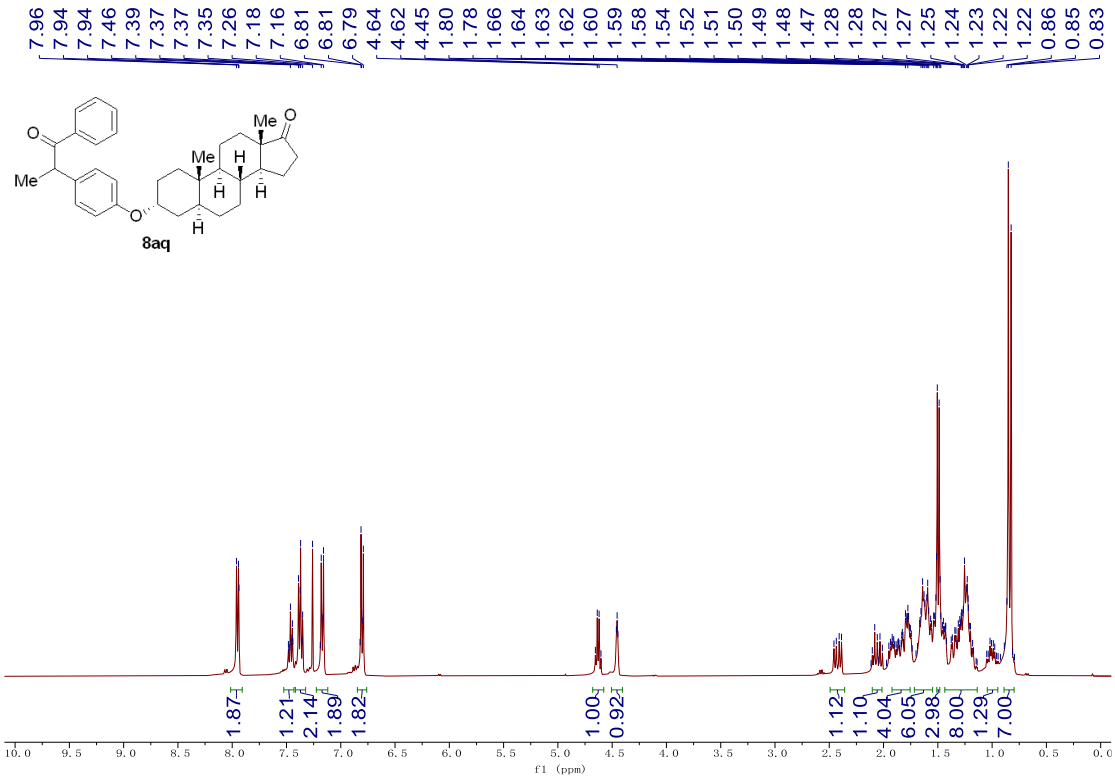
77.48
77.16
76.84
56.03
55.90
53.58
43.92
28.48
MeO
MeO
O
H
N
O
O
Me
Me
Me
8ap
f1 (ppm)


7.96 7.94 7.94 7.46 7.39 7.37 7.37 7.35 7.26 7.18 7.16 6.81 6.79 4.64 4.62 4.45 1.80 1.78 1.66 1.64 1.63 1.62 1.60 1.59 1.58 1.54 1.52 1.51 1.50 1.49 1.48 1.47 1.28 1.28 1.27 1.27 1.25 1.24 1.23 1.22 1.22 0.86 0.85 0.83
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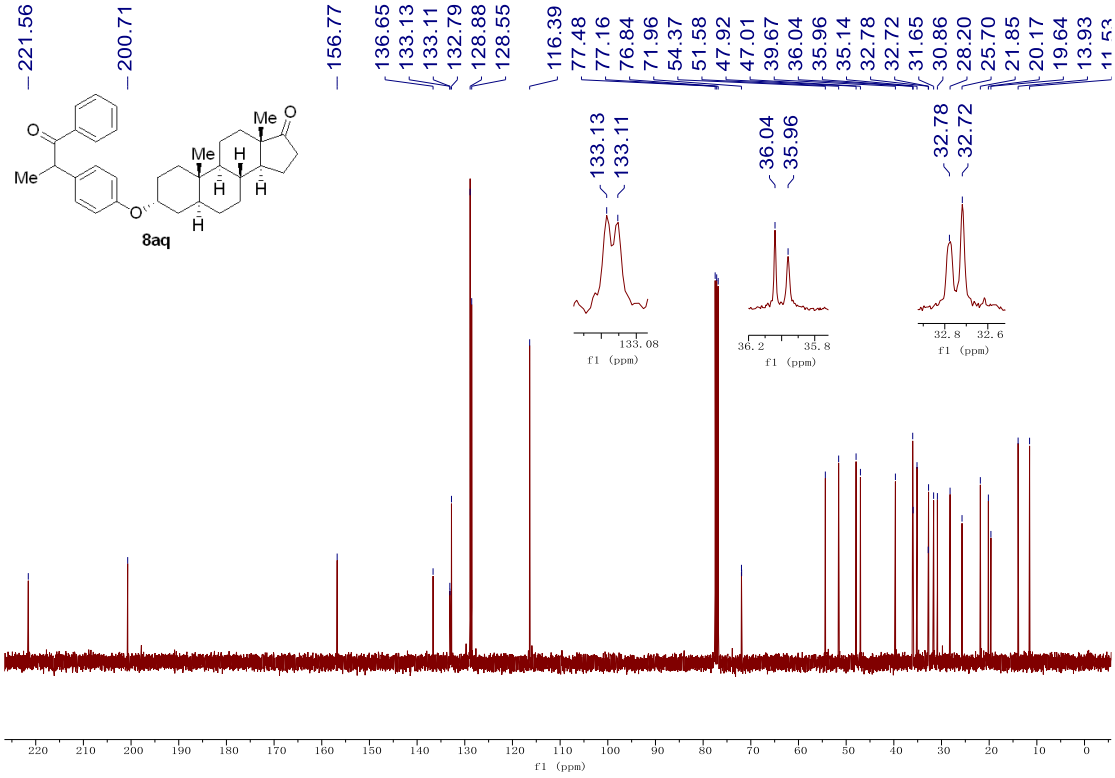
f1 (ppm)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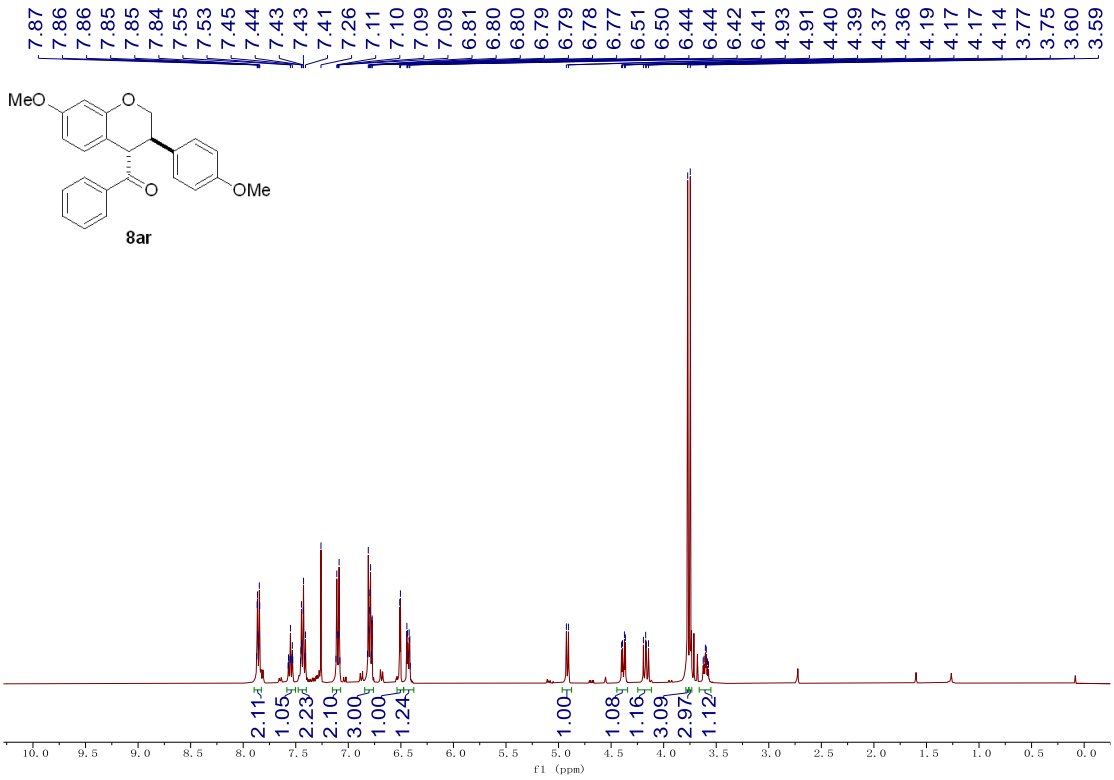
8aq
133.13 133.11
36.04 35.96
32.78 32.72
f1 (ppm)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3.59
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O
O
OMe
8ar
2.11
1.05
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1.00
1.24
1.00
1.08
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3.09
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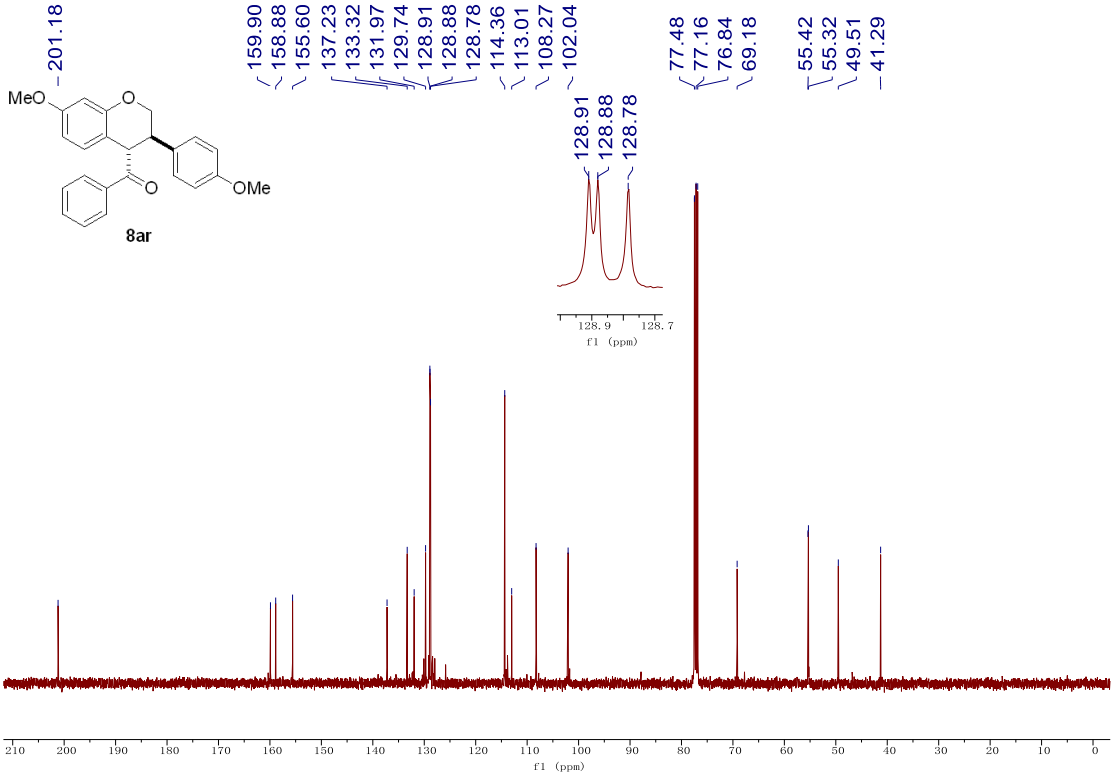
1.12
f1 (ppm)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113.01
108.27
102.04
77.48
77.16
76.84
69.18
55.42
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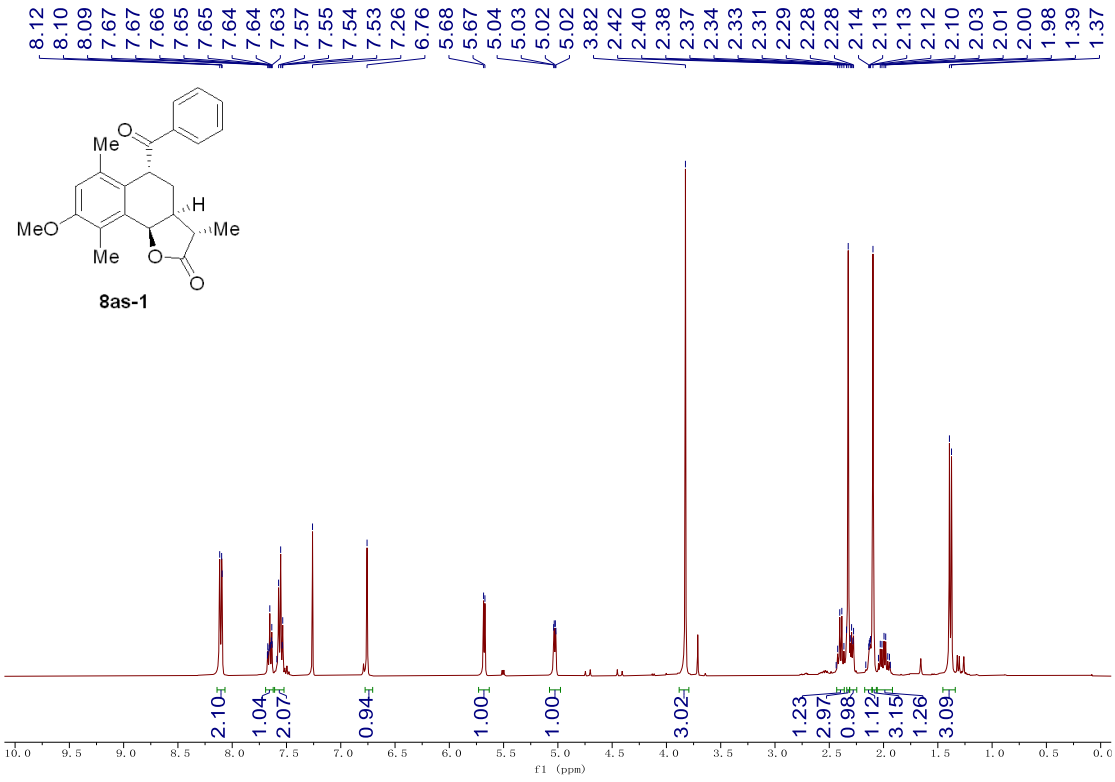
49.51
41.29
MeO
O
O
OMe
8ar
128.91
128.88
128.78
f1 (ppm)
f1 (ppm)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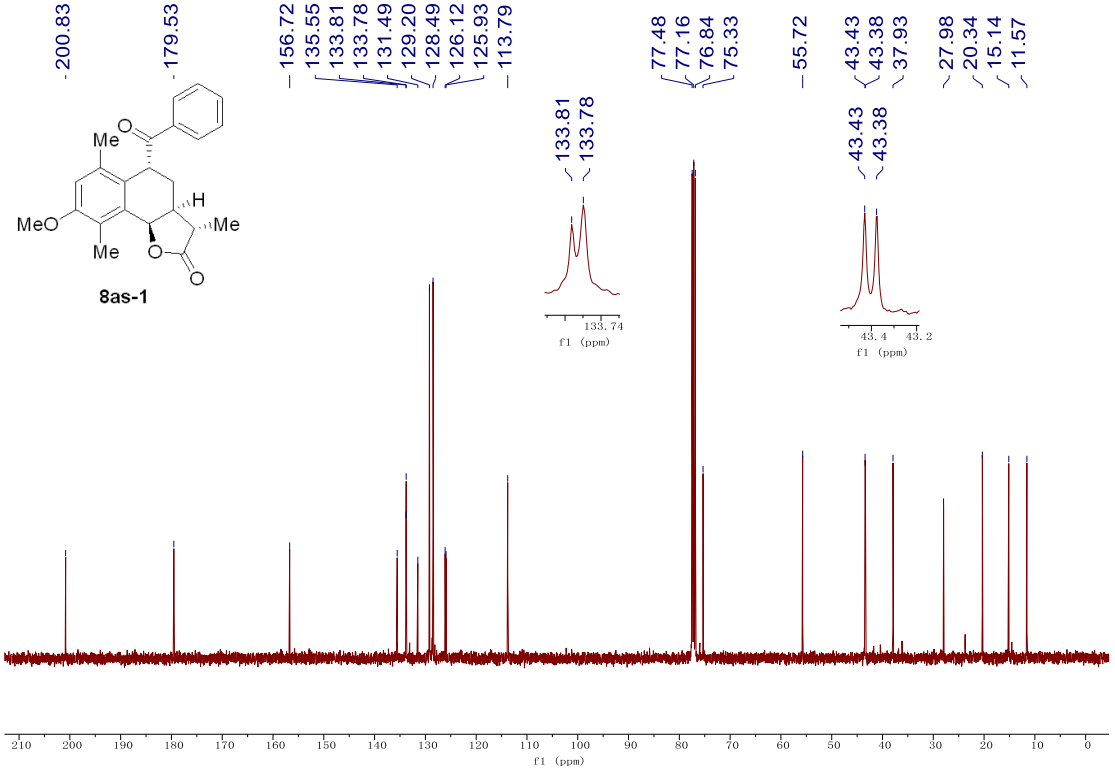
Me
O
H
MeO
Me
Me
O
O
8as-1
2.10 1.04 2.07 0.94 1.00 1.00 3.02 1.23 2.97 0.98 1.12 3.15 1.26 3.09
f1 (ppm)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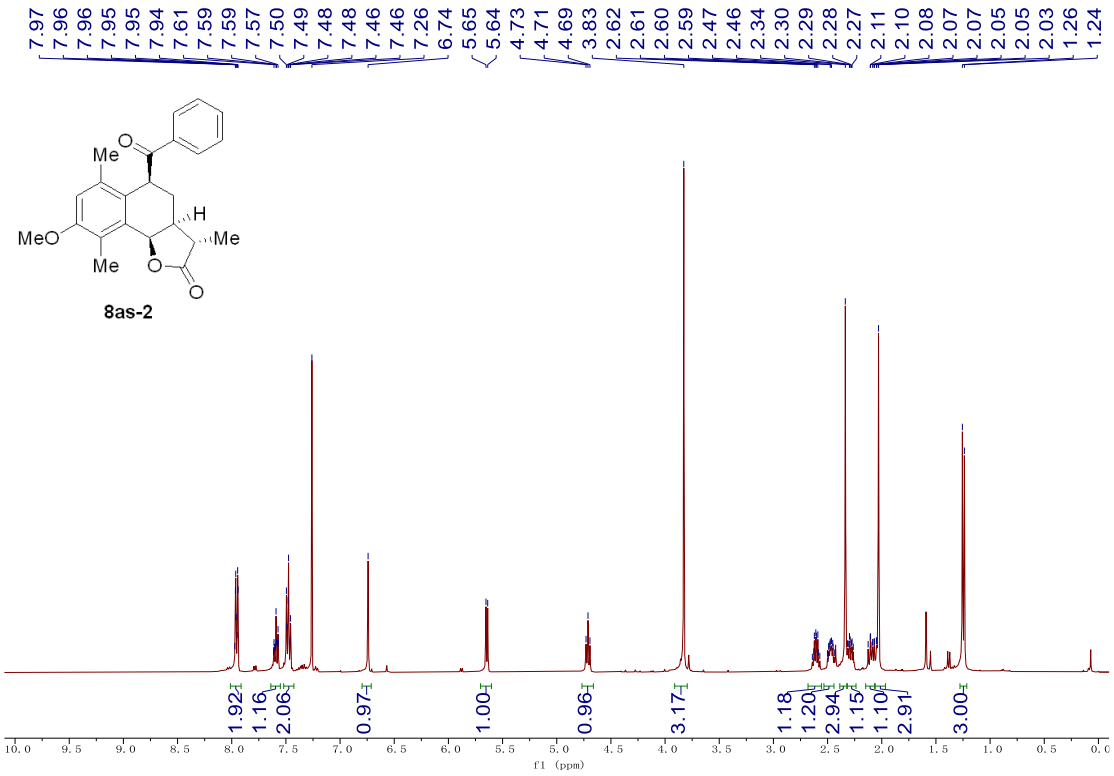
133.81 133.78
43.43 43.38
Me
O
H
MeO
Me
Me
O
O
8as-1
f1 (ppm)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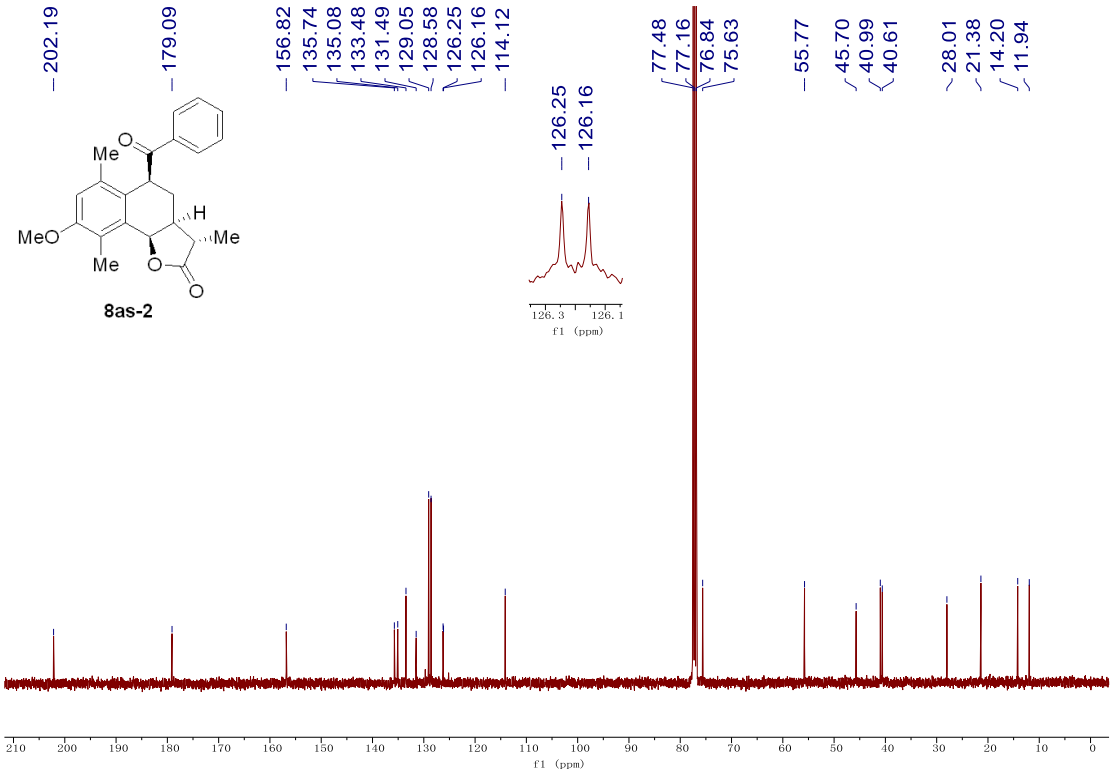
Me
MeO
Me
H
Me
O
O
O
8as-2
1.92 1.16 2.06 0.97 1.00 0.96 3.17 1.18 1.20 2.94 1.15 1.10 2.91 3.00
f1 (ppm)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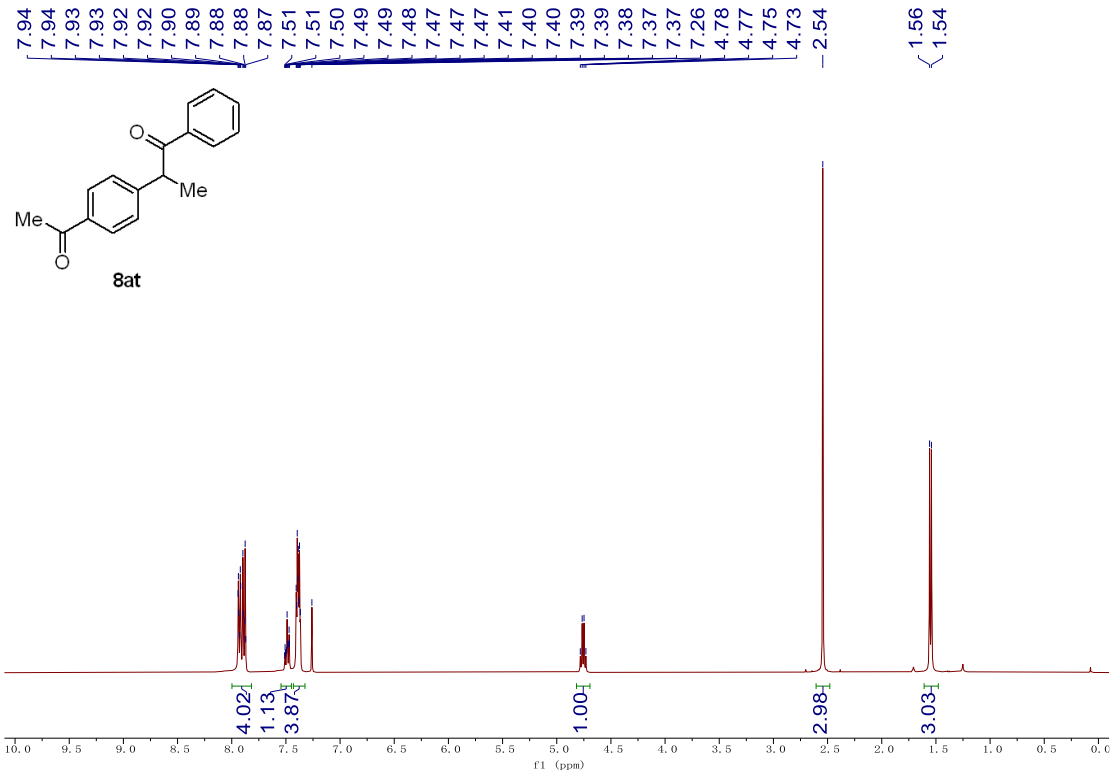
126.25 126.16
126.3 126.1
f1 (ppm)
Me
MeO
Me
H
Me
O
O
O
8as-2
f1 (ppm)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7.88
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7.51
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7.49
7.49
7.48
7.47
7.47
7.47
7.41
7.40
7.40
7.39
7.39
7.38
7.37
7.37
7.26
4.78
4.77
4.75
4.73
2.54
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Me
Me
O
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4.02
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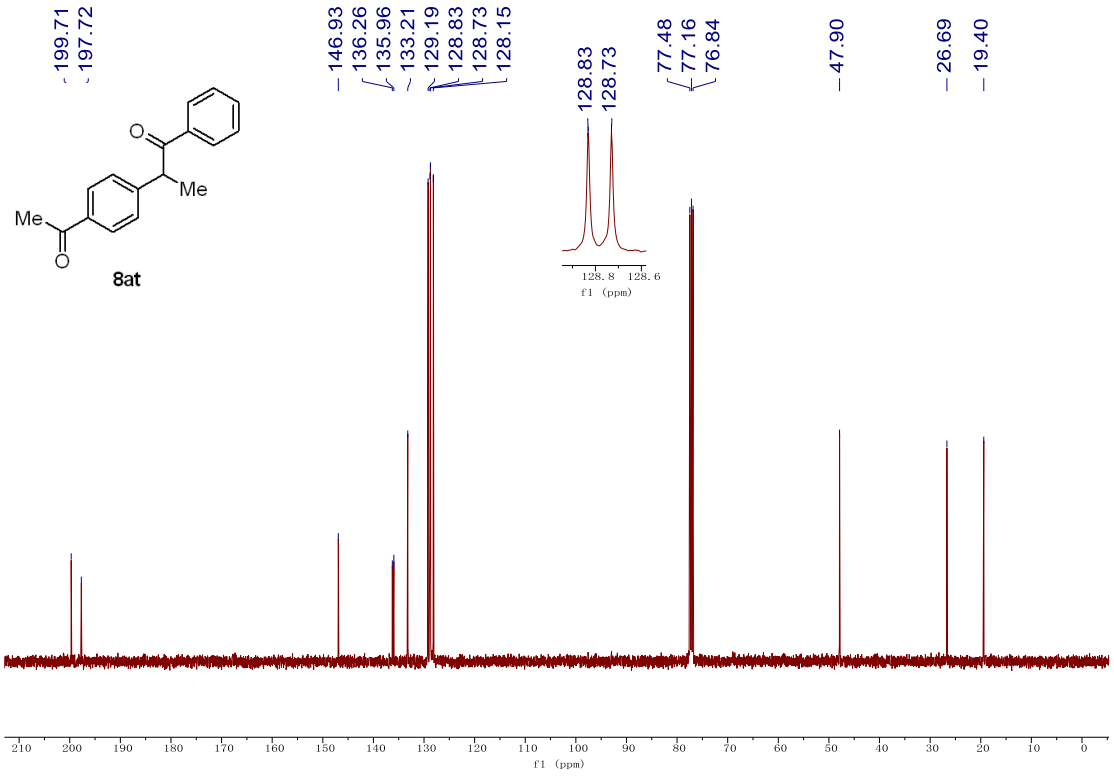
3.87
1.00
2.98
3.03
f1 (ppm)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Me
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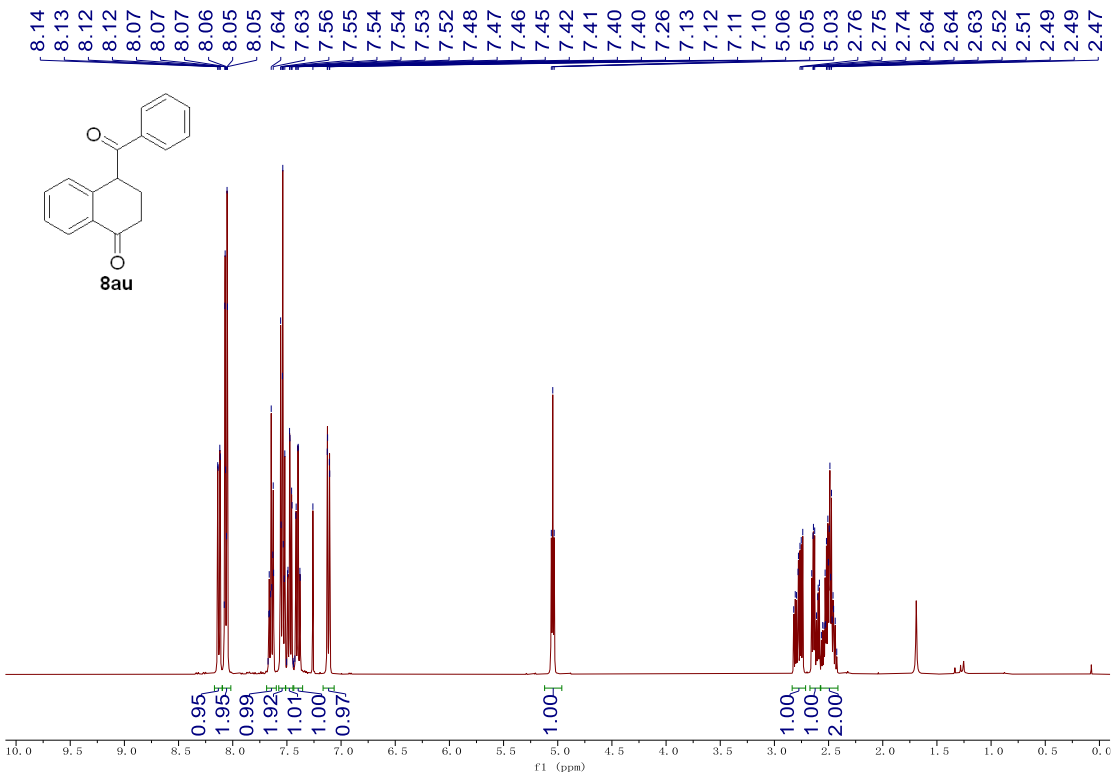
f1 (ppm)
f1 (ppm)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5.05
5.03
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2.75
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2.63
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2.51
2.49
2.49
2.47
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1.00
0.97
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1.00
1.00
2.00
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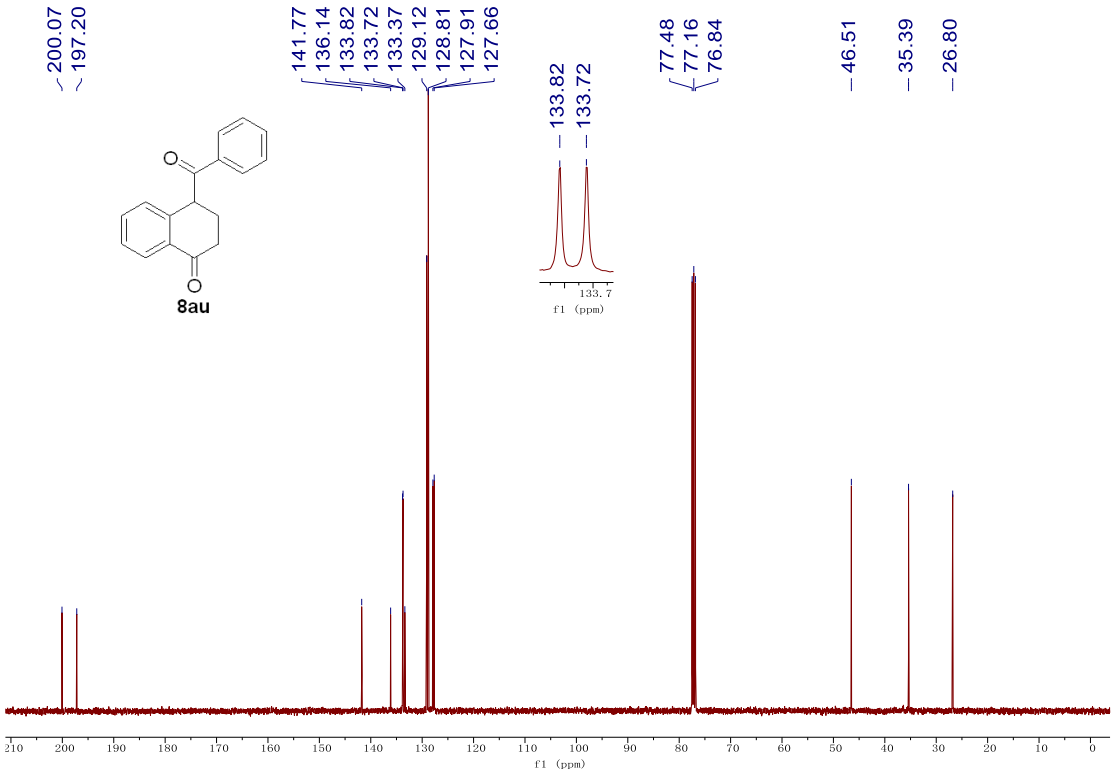
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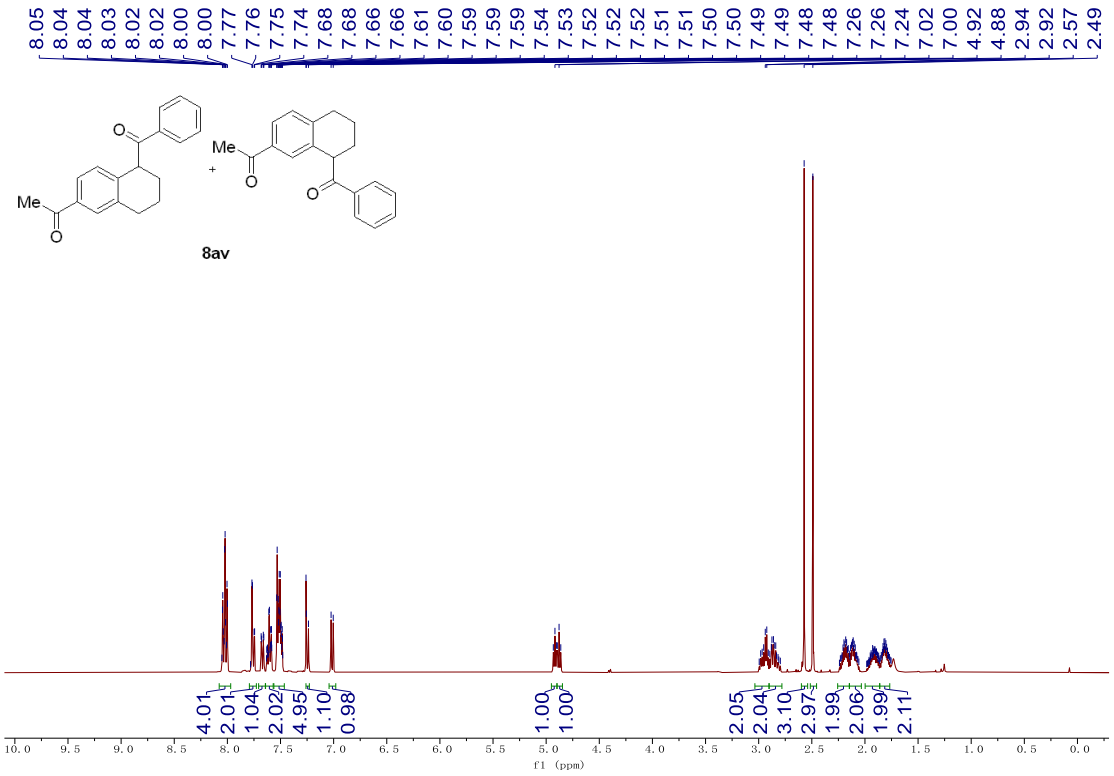
f1 (ppm)
f1 (ppm)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Me
O
Me
O
O
8av
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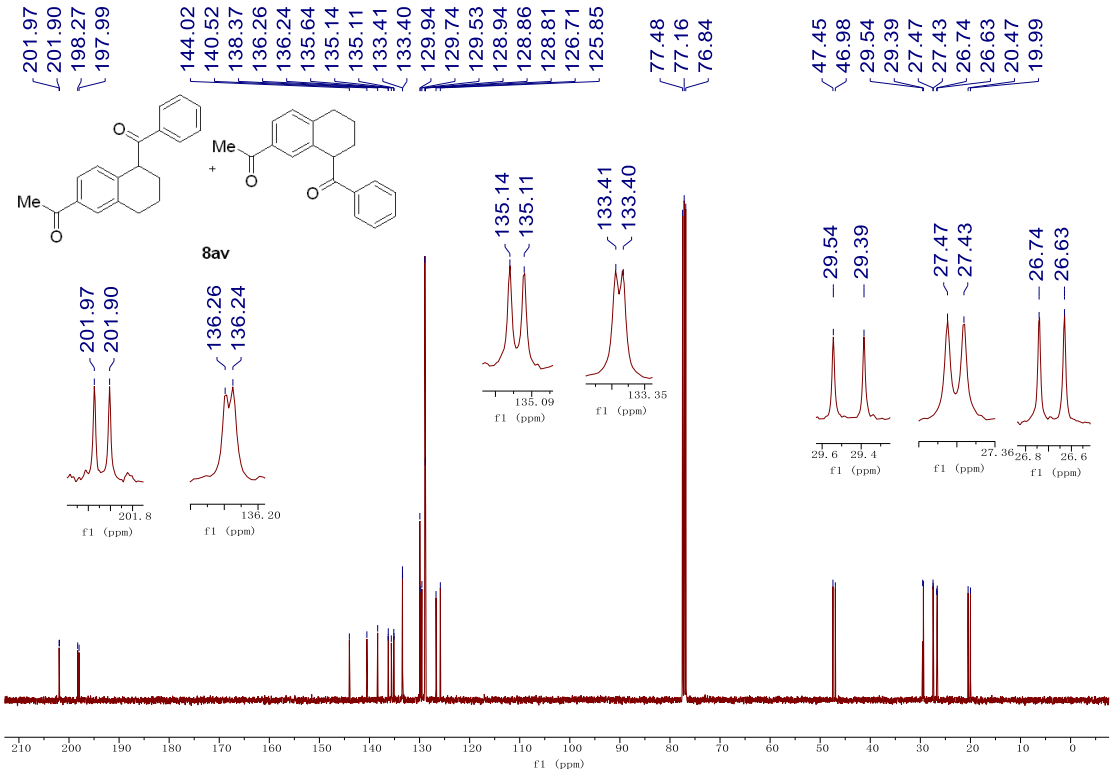
f1 (ppm)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Me
O
Me
O
O
8av
201.97 201.90
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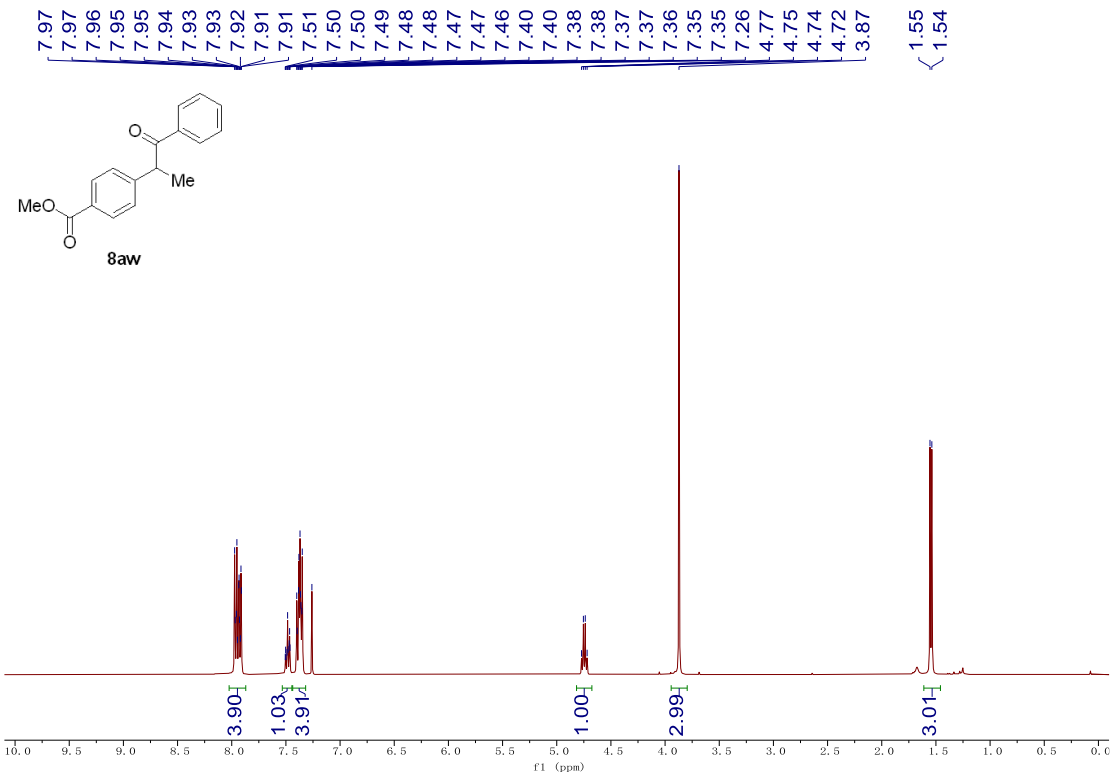
27.47 27.43
26.74 26.63
f1 (ppm)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7.37
7.36
7.35
7.35
7.26
4.77
4.75
4.74
4.72
3.87
1.55
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O
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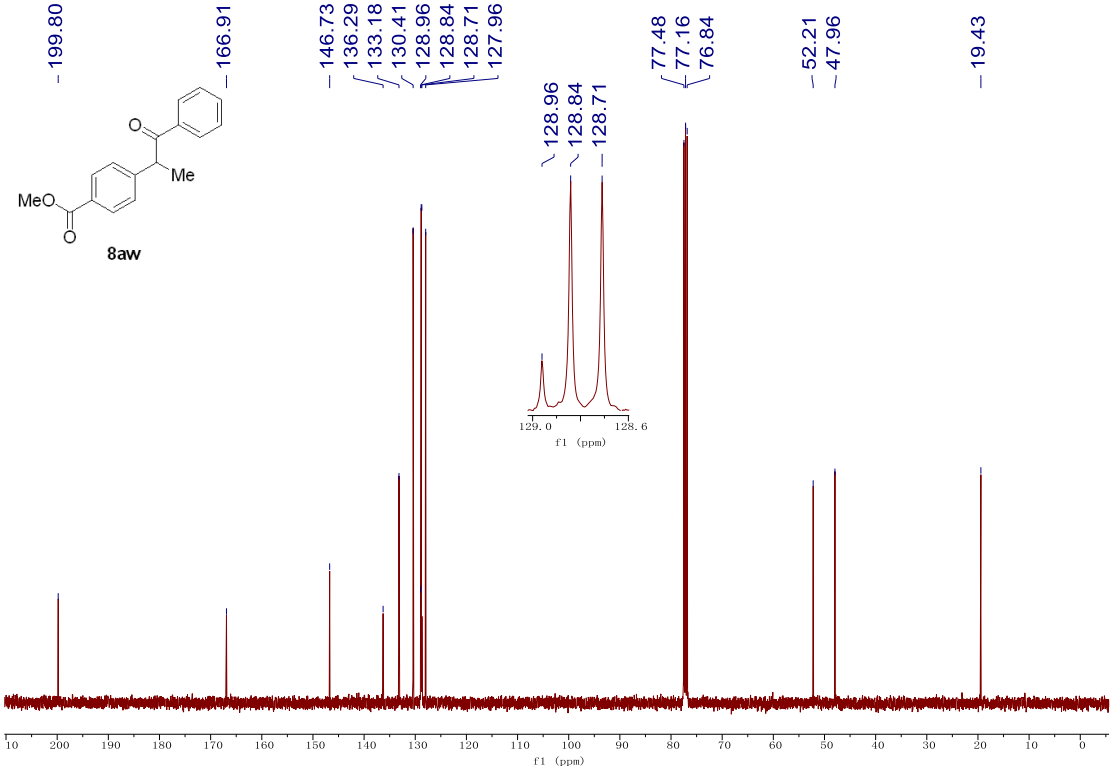
3.91
1.00
2.99
3.01
f1 (ppm)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77.48
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76.84
52.21
47.96
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128.84
128.71
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Me
MeO
O
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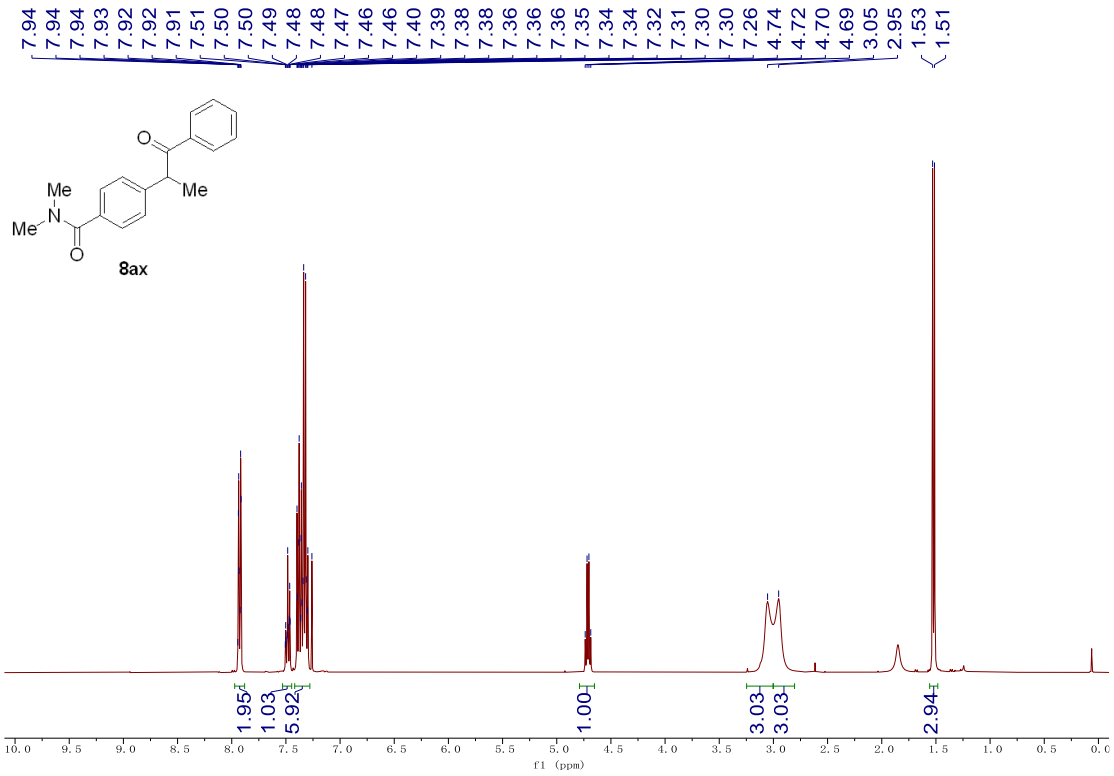
129.0
128.6
f1 (ppm)
f1 (ppm)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7.30
7.30
7.26
4.74
4.72
4.70
4.69
3.05
2.95
1.53
1.51
Me
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8ax
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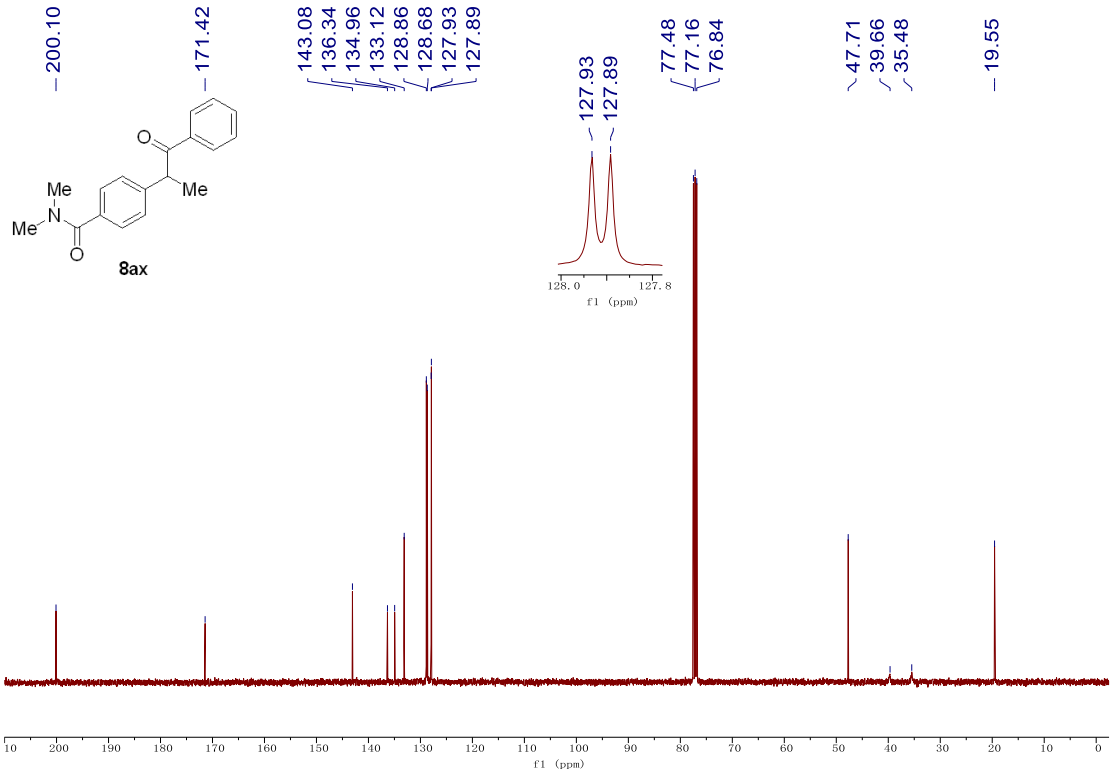
1.03
5.92
1.00
3.03
3.03
2.94
f1 (ppm)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128.68
127.93
127.89
77.48
77.16
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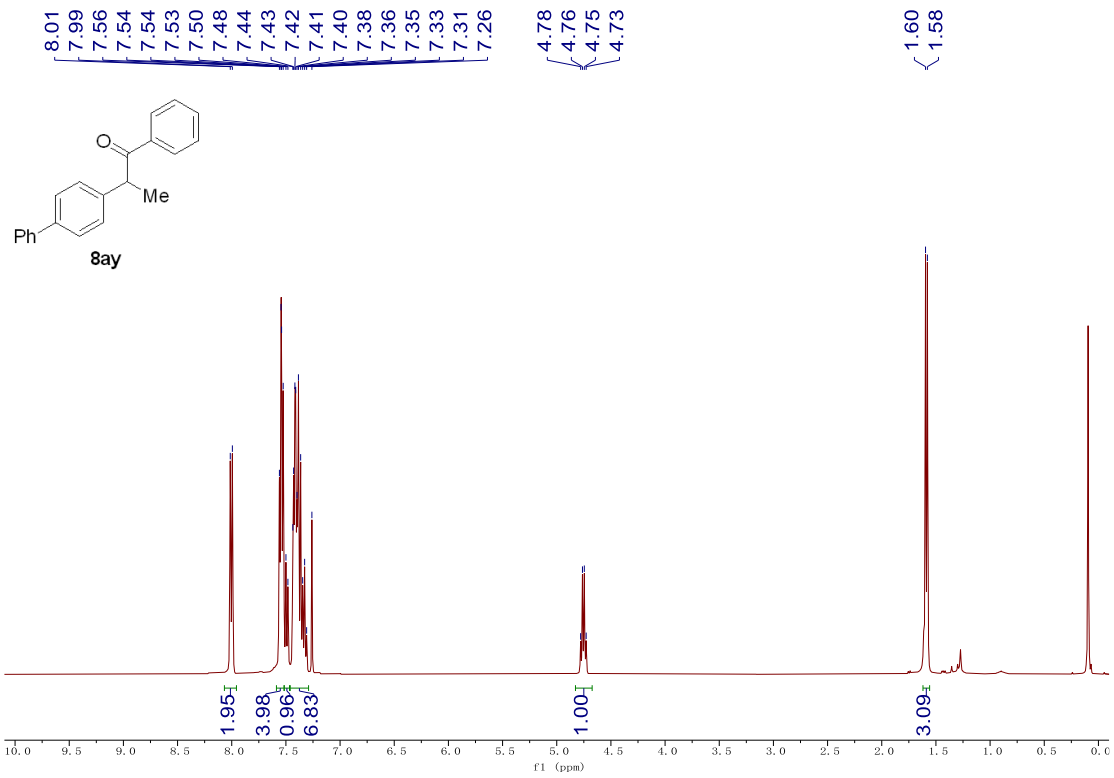
47.71
39.66
35.48
19.55
127.93
127.89
128.0
127.8
f1 (ppm)
Me
N
Me
Me
O
O
8ax
f1 (ppm)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7.38
7.36
7.35
7.33
7.31
7.26
4.78
4.76
4.75
4.73
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O
Me
Ph
8ay
1.95
3.98
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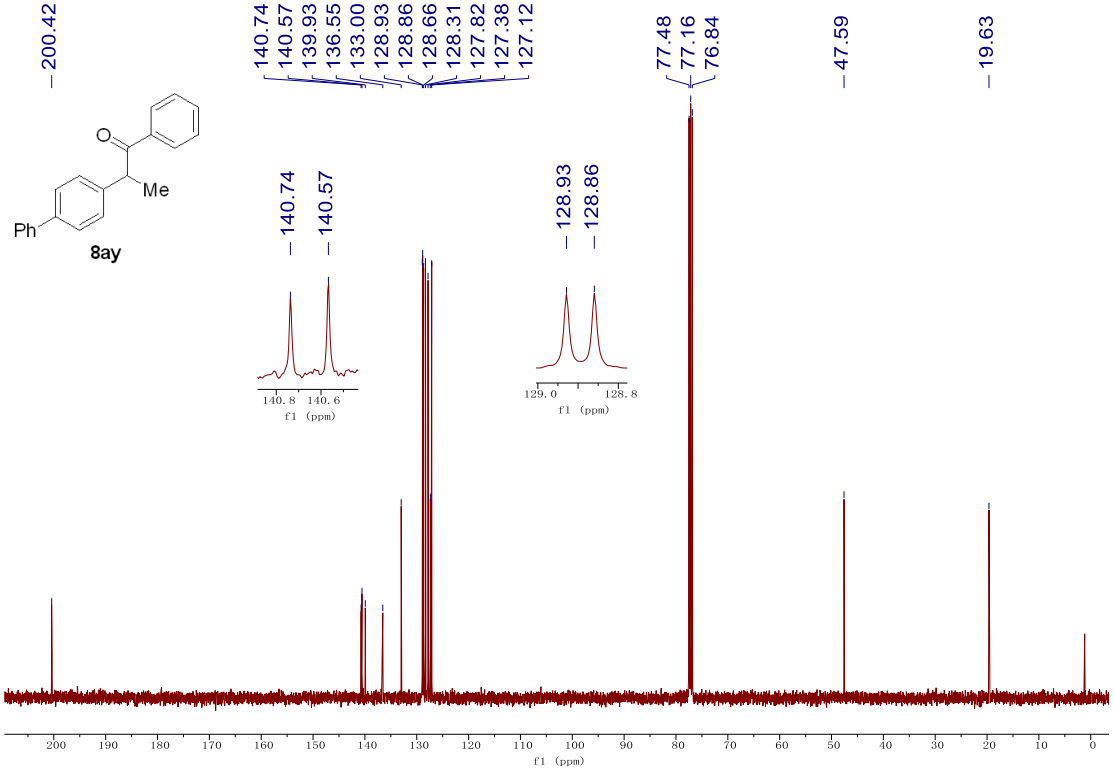
6.83
1.00
3.09
f1 (ppm)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127.12
77.48
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19.63
O
Me
Ph
8ay
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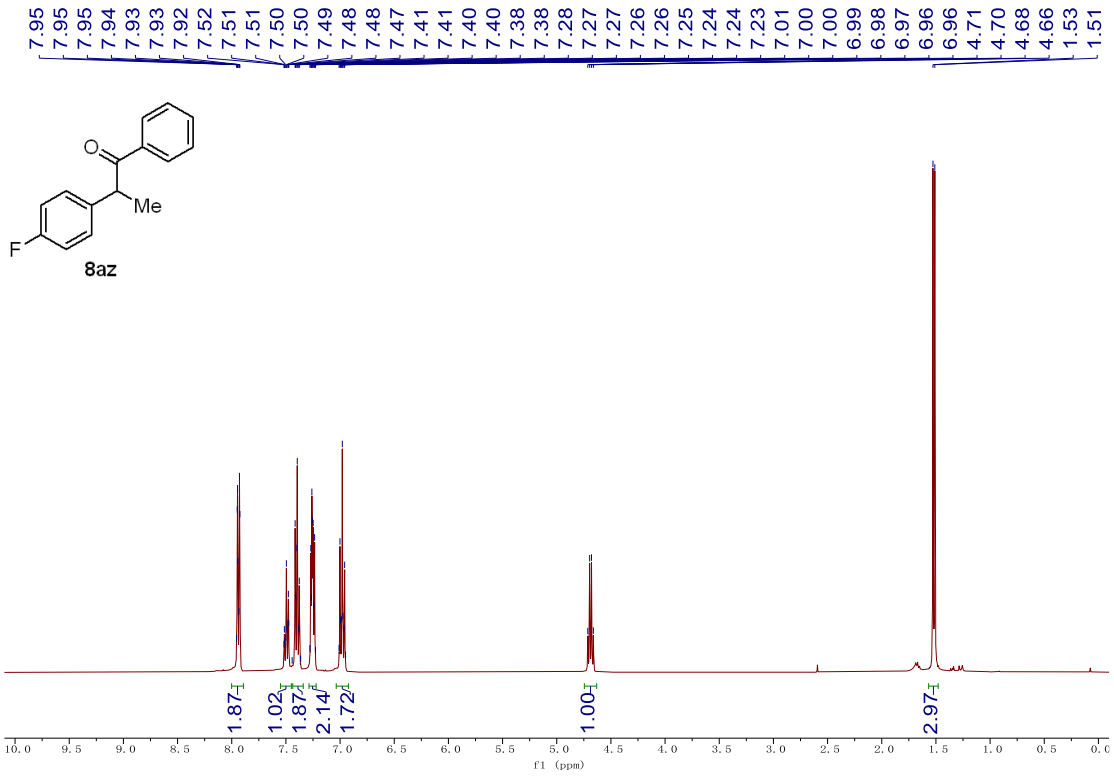
140.57
128.93
128.86
f1 (ppm)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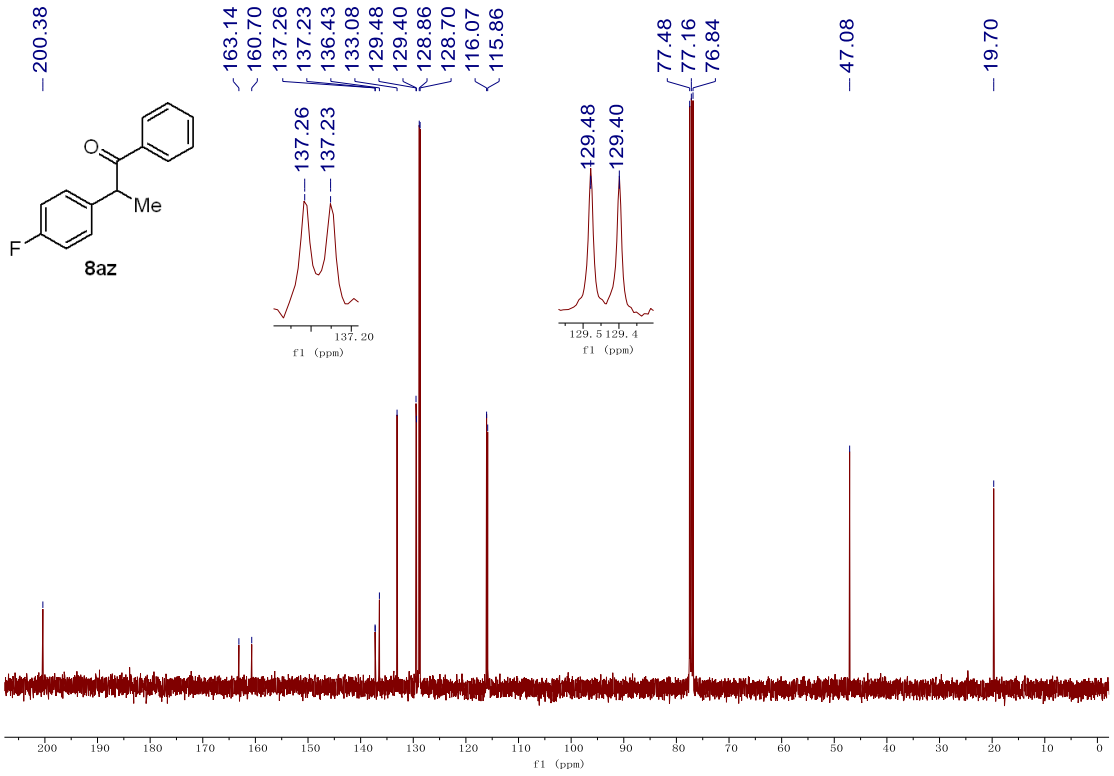
O
Me
F
8az
1.87 1.02 1.87 2.14 1.72 1.00 2.97
f1 (ppm)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47.08
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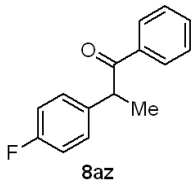
O
Me
F
8az
137.26 137.23
129.48 129.40
f1 (ppm)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Me
F

8az

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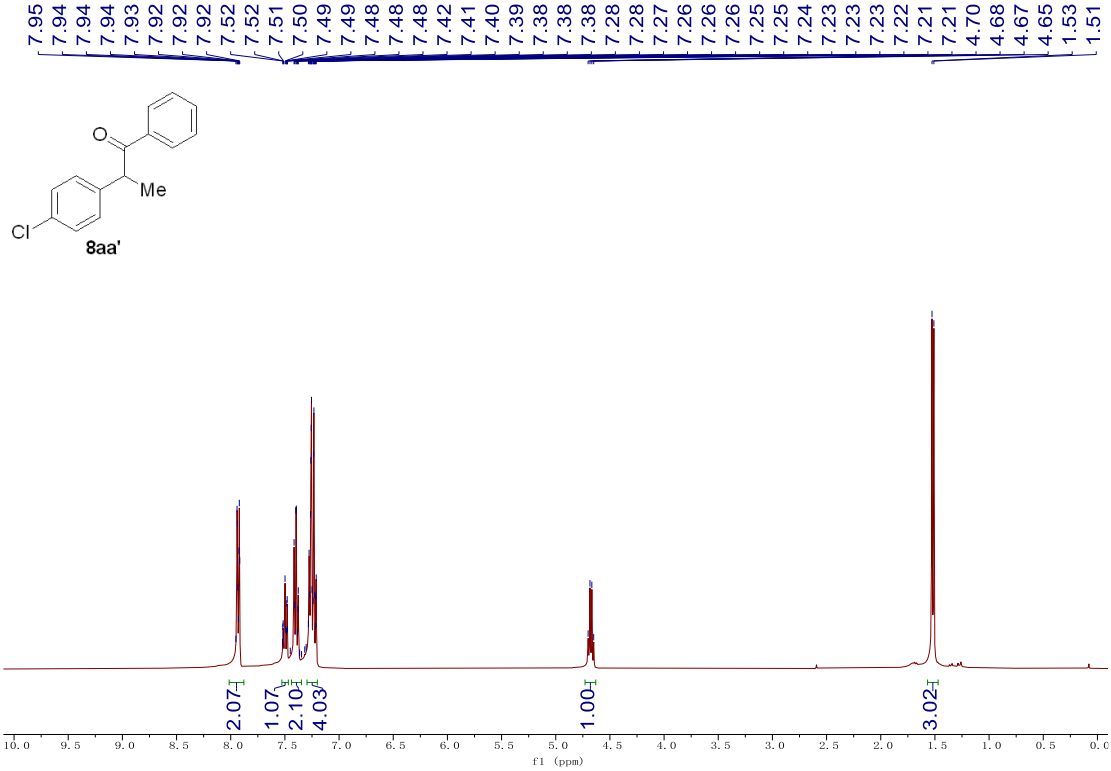
f1 (ppm)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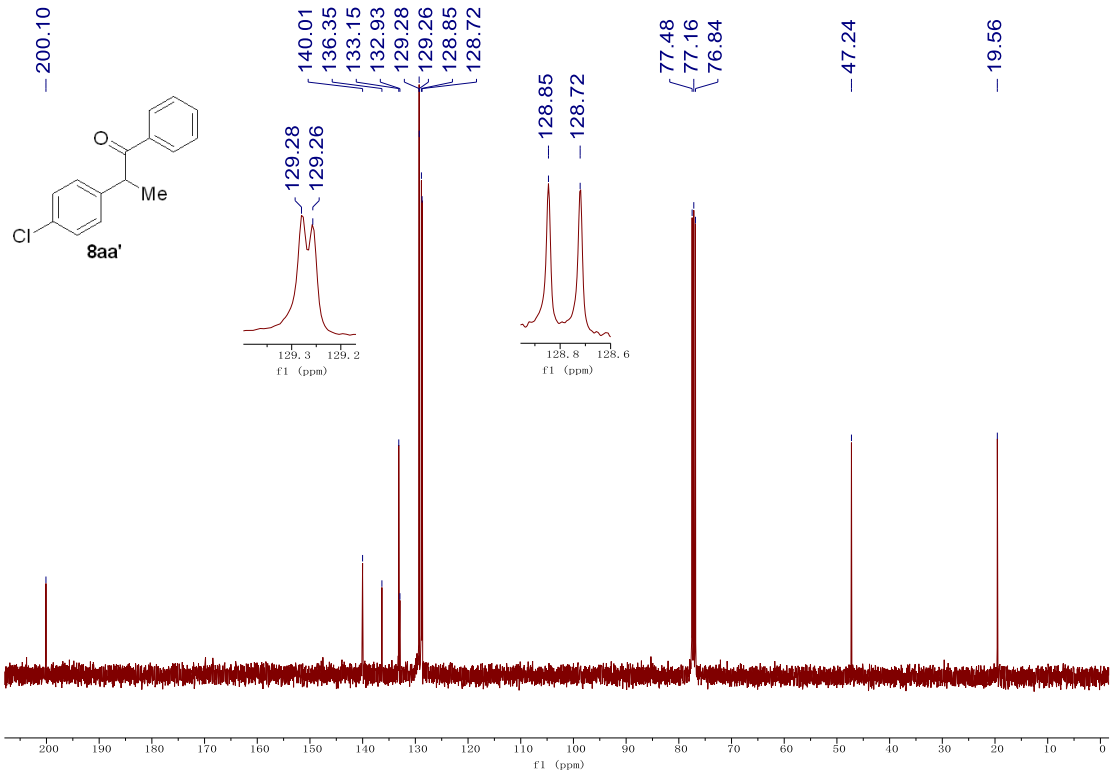
O
Me
Cl
2.07 1.07 2.10 4.03 1.00 3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

8aa'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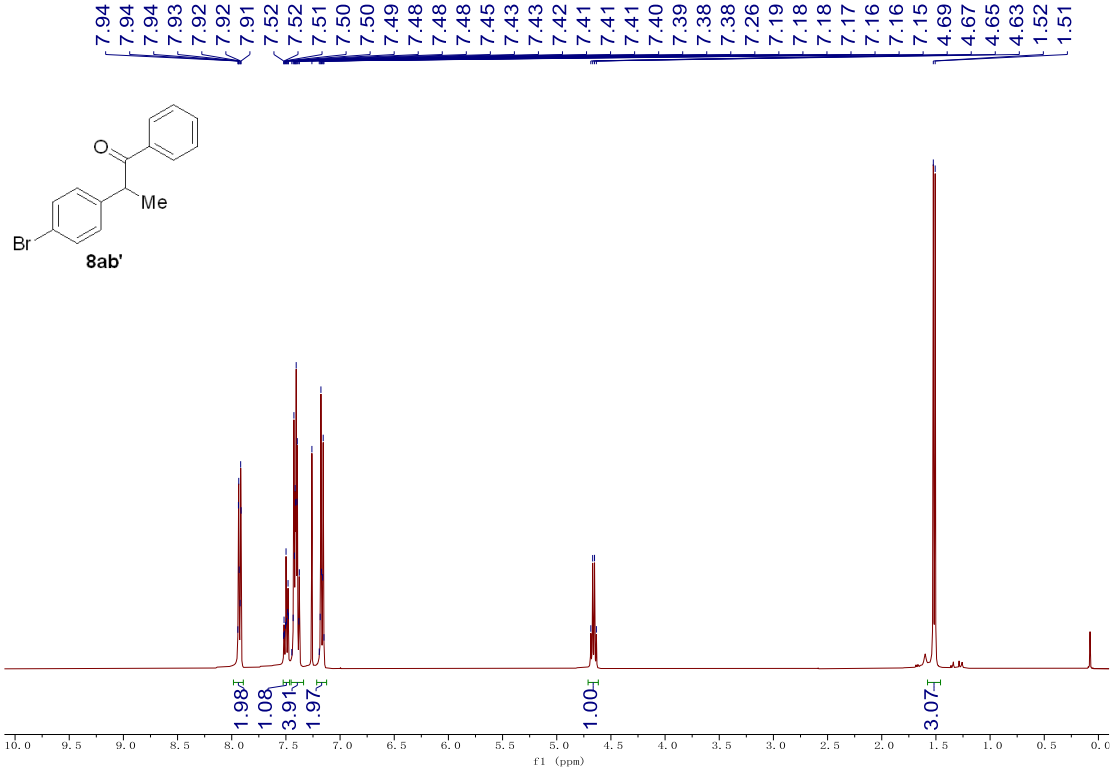
77.16
76.84
47.24
19.56
O
Me
Cl
8aa'
f1 (ppm)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7.16
7.16
7.15
4.69
4.67
4.65
4.63
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Me
Br
8ab'
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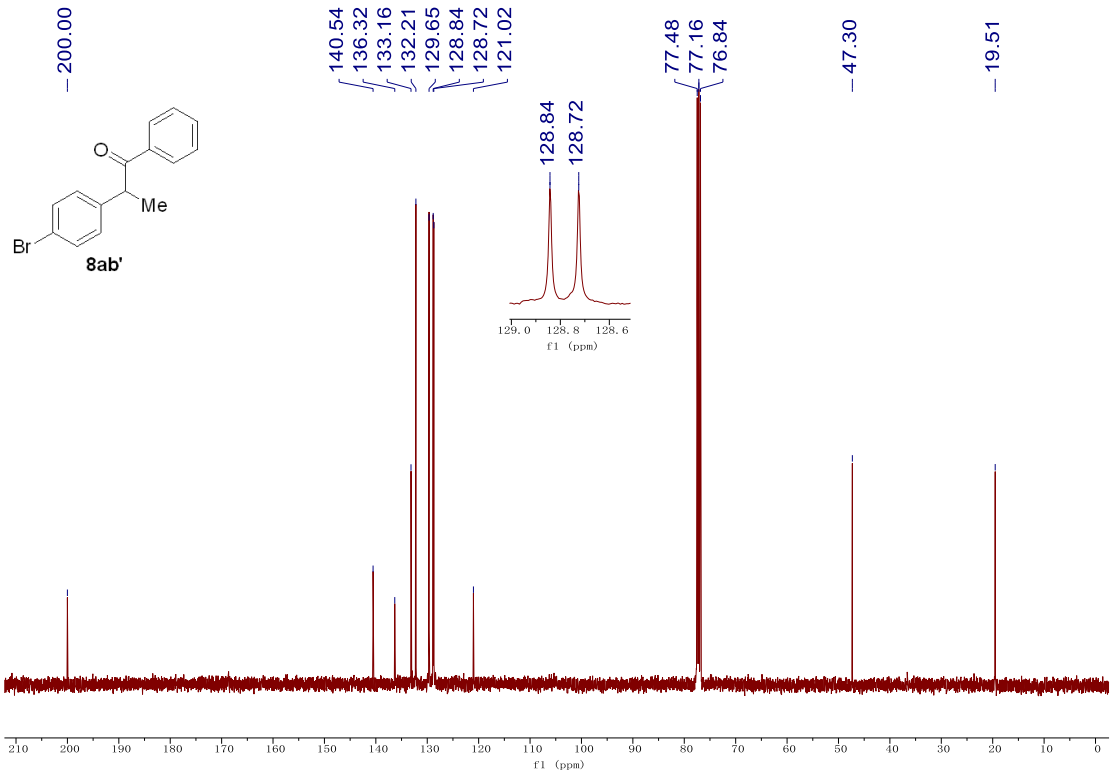
1.08
3.91
1.97
1.00
3.07
f1 (ppm)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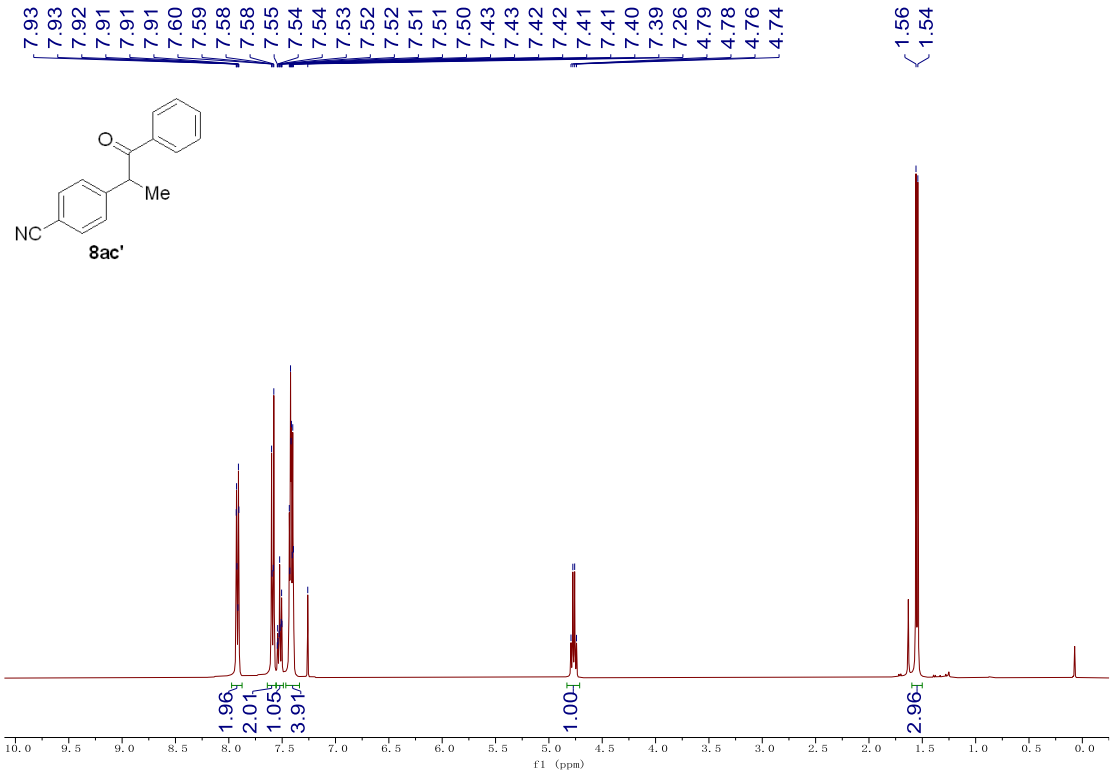
76.84
47.30
19.51
O
Me
Br
8ab'
f1 (ppm)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7.41
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7.39
7.26
4.79
4.78
4.76
4.74
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1.54
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Me
NC
8ac'
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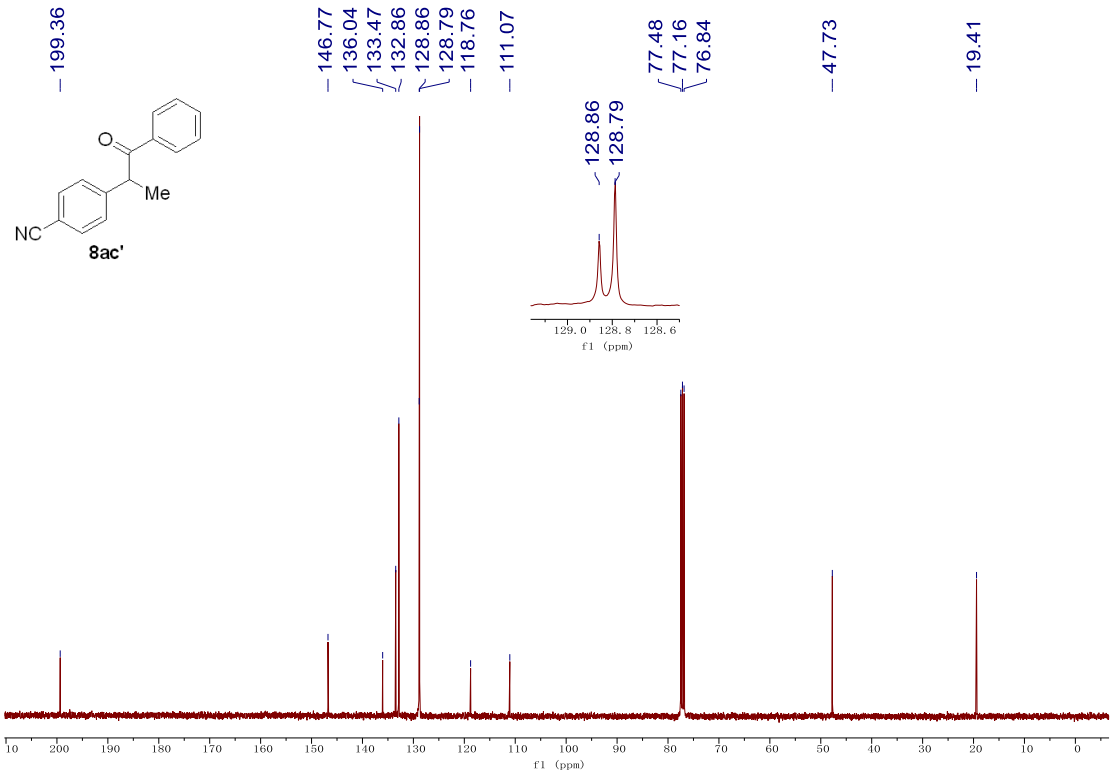
1.05
3.91
1.00
2.96
f1 (ppm)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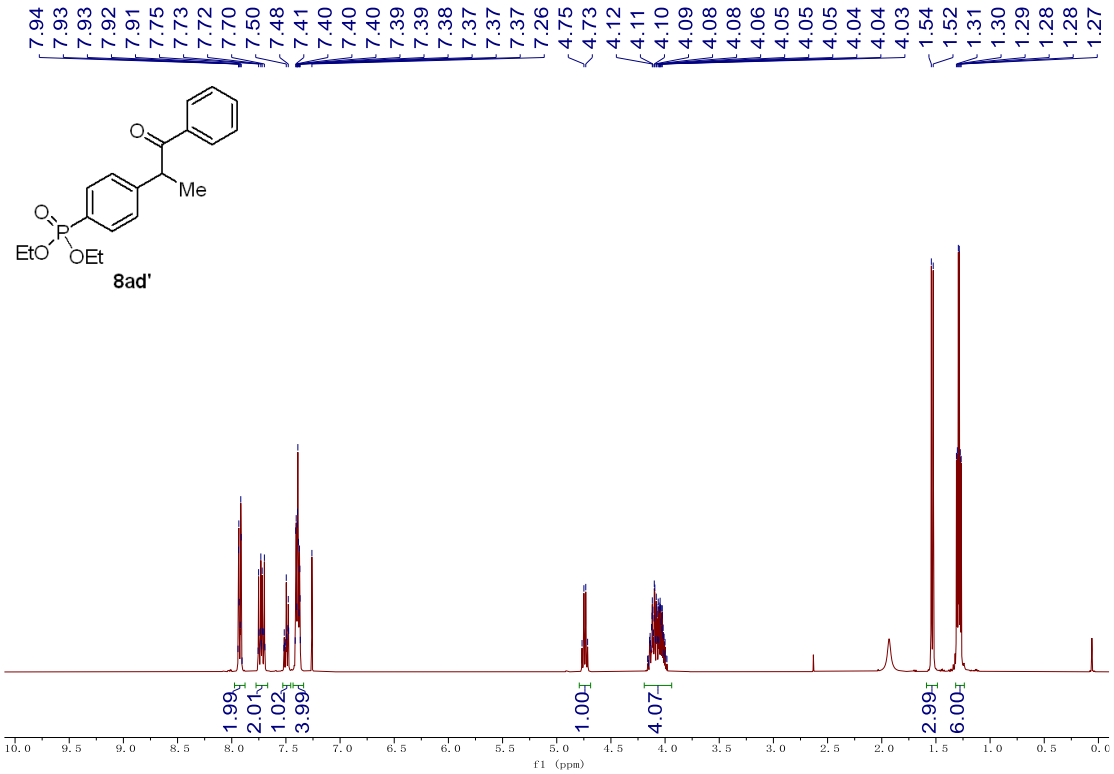
19.41
O
Me
NC
8ac'
f1 (ppm)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4.05
4.04
4.04
4.03
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1.31
1.30
1.29
1.28
1.28
1.27
O
Me
O
P
EtO
OEt
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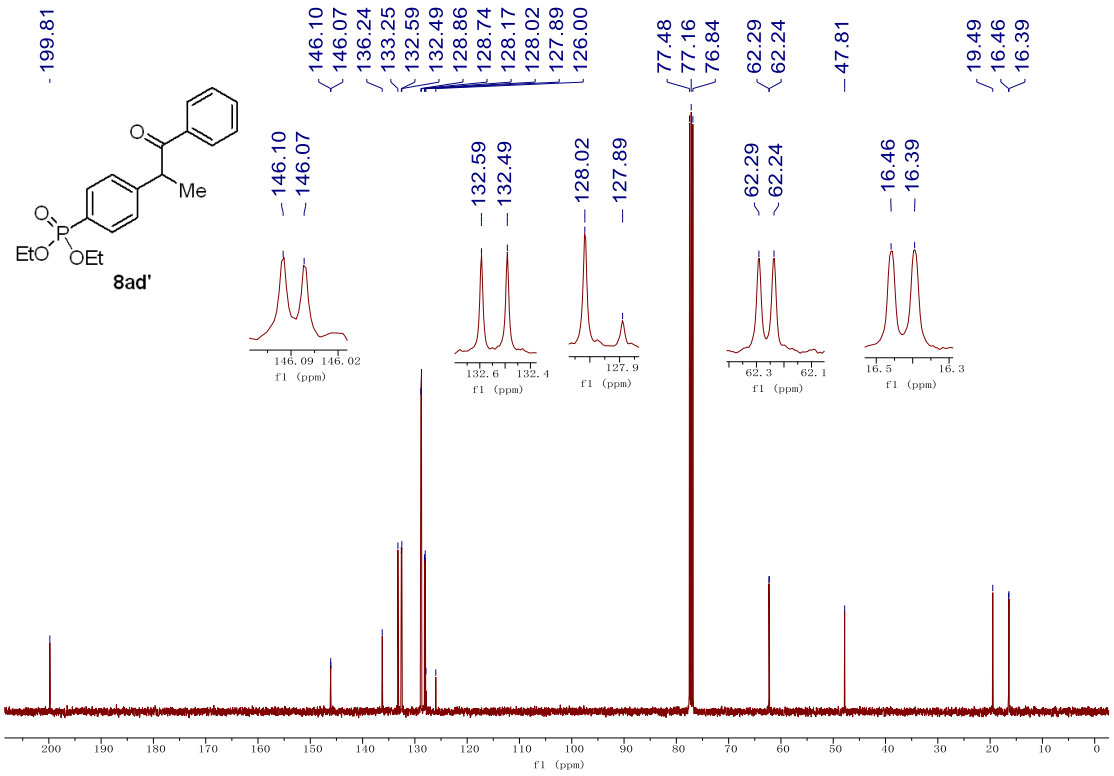
2.01
1.02
3.99
1.00
4.07
2.99
6.00
f1 (ppm)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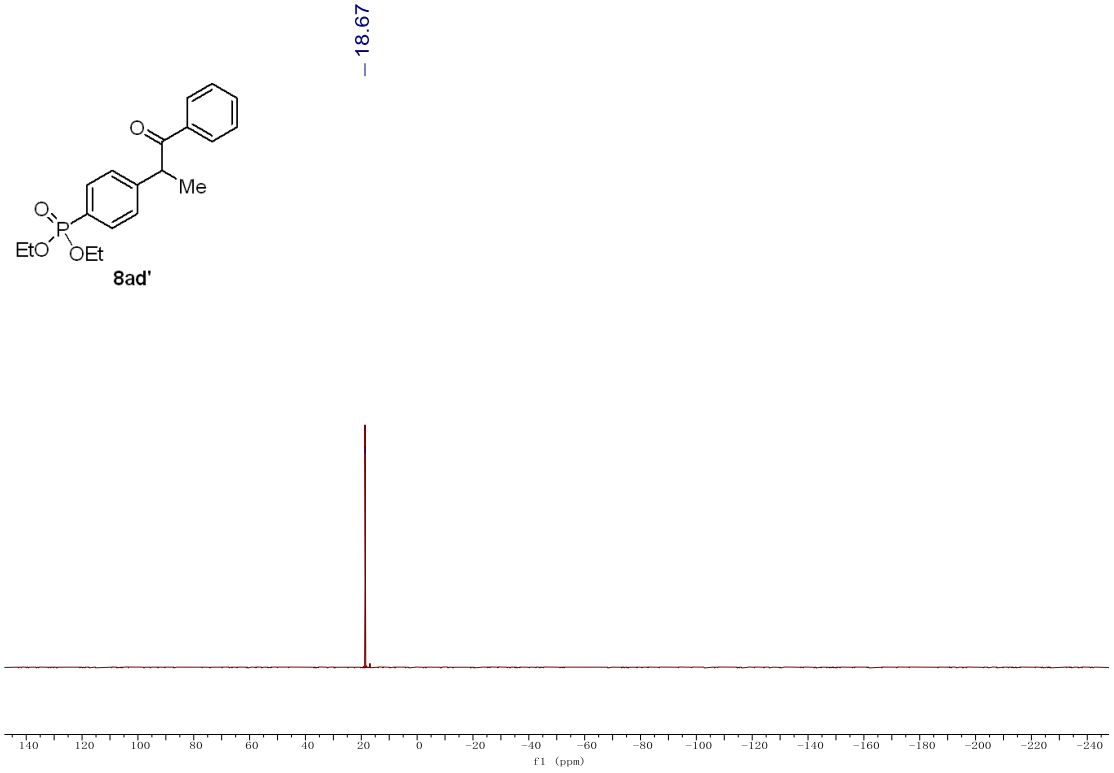
128.86
128.74
128.17
128.02
127.89
126.00
77.48
77.16
76.84
62.29
62.24
47.81
19.49
16.46
16.39
O
Me
O
P
EtO
OEt
8ad'
f1 (ppm)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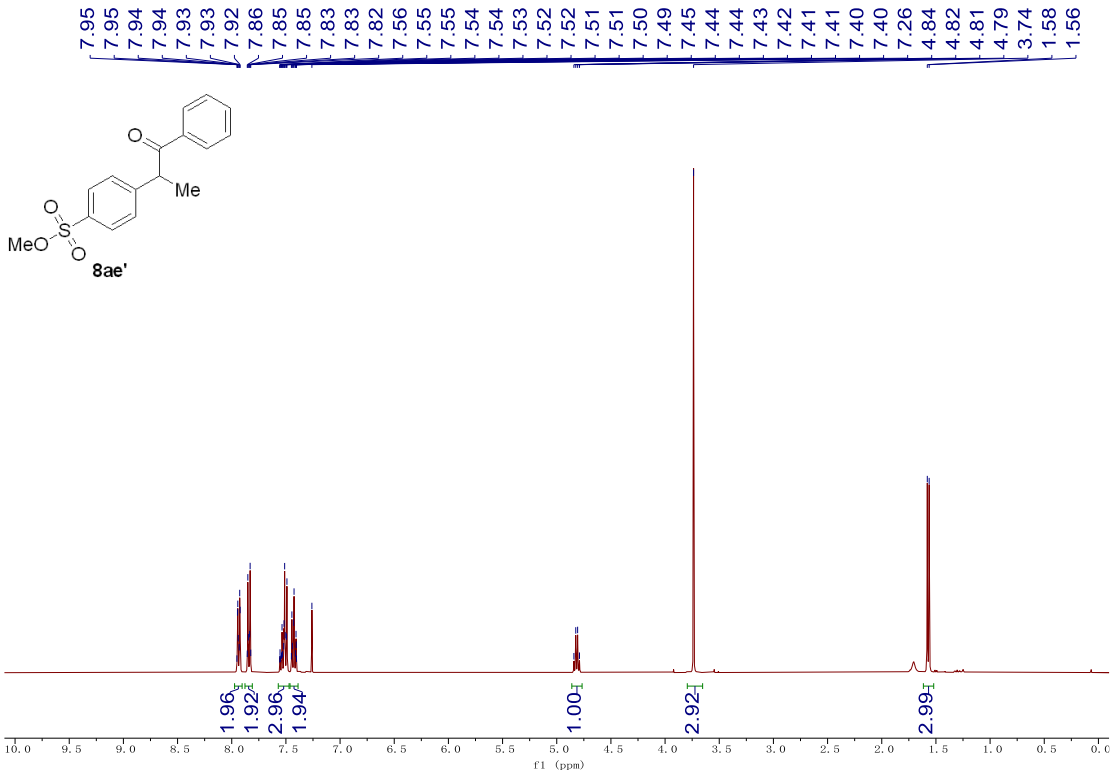
8ad'
f1 (ppm)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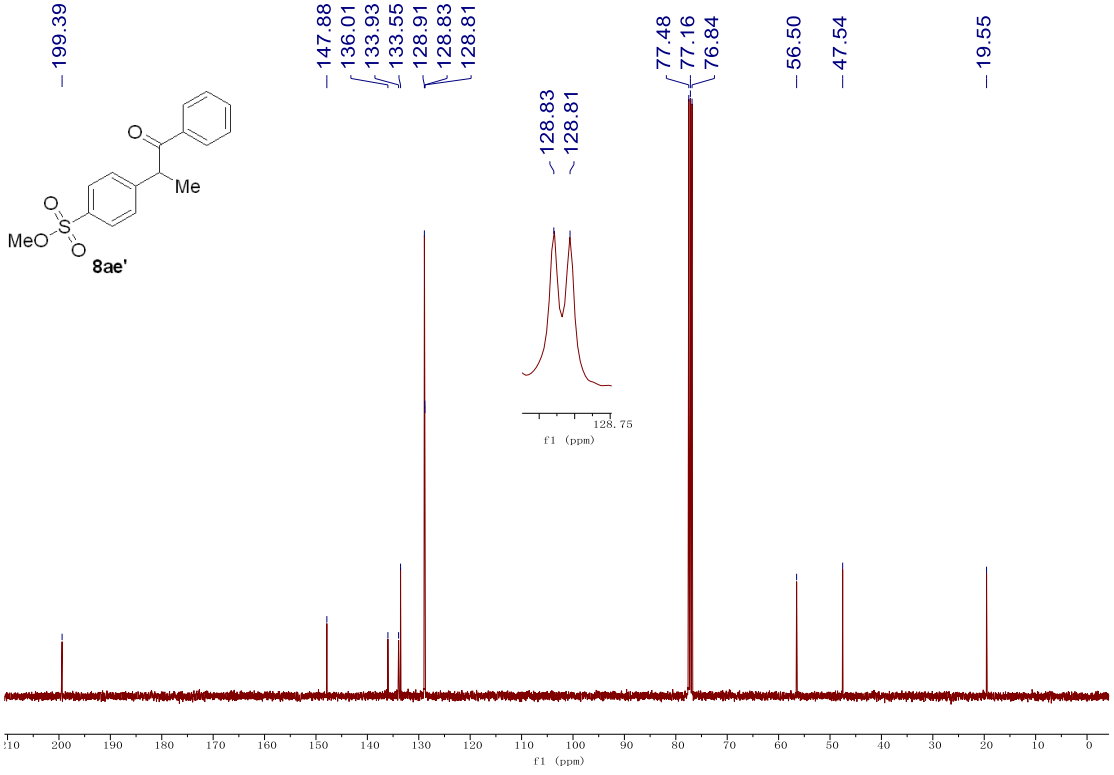
O
Me
O
MeO
S
O
8ae'
1.96 1.92 2.96 1.94 1.00 2.92 2.99
f1 (ppm)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77.48 77.16 76.84
56.50
47.54
19.55
128.83 128.81
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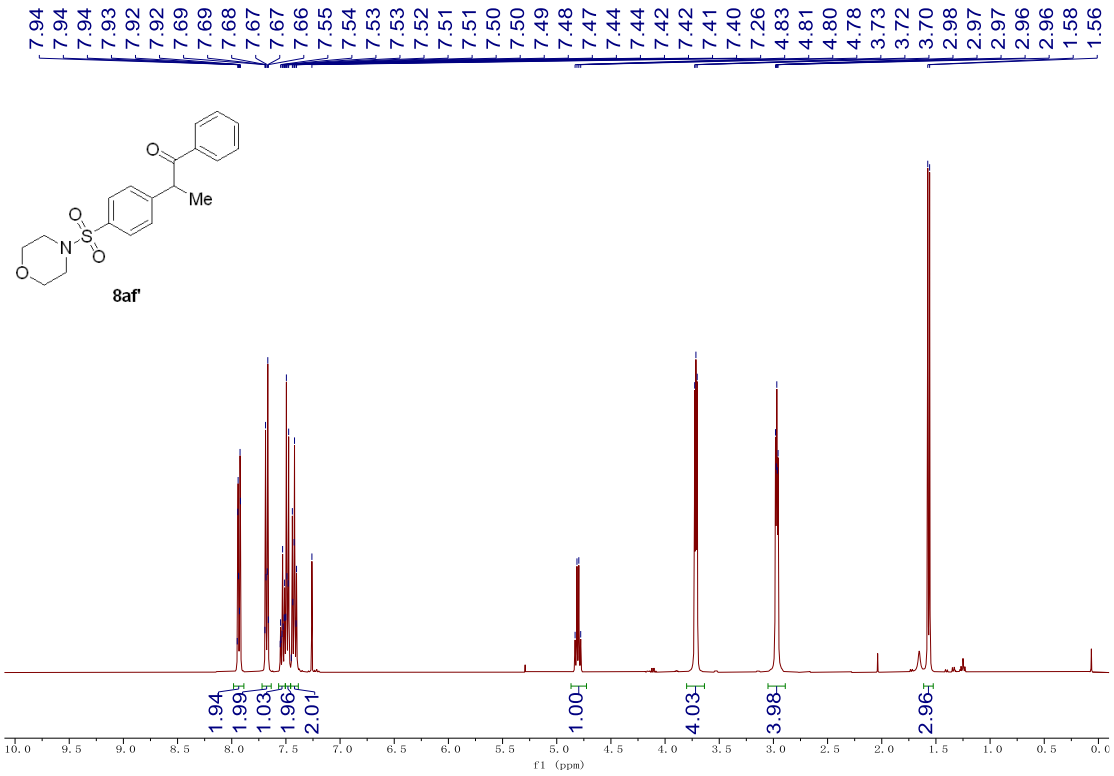
Me
O
MeO
S
O
8ae'
f1 (ppm)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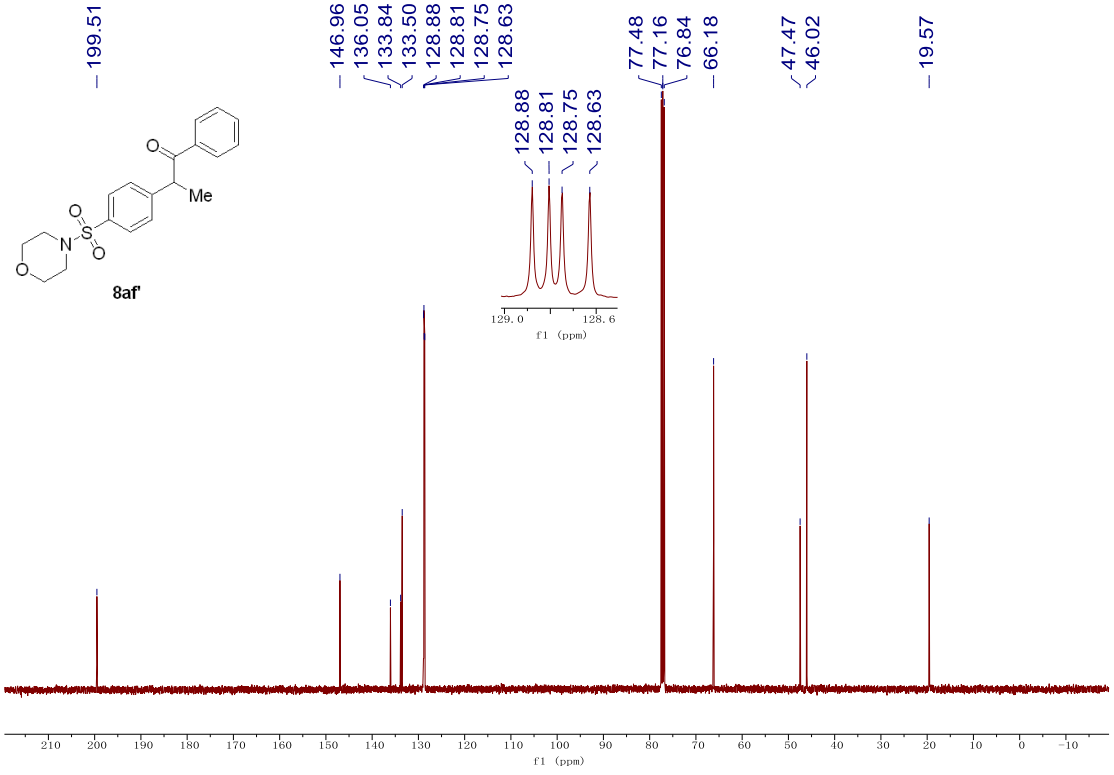
Me
8af'
1.94 1.99 1.03 1.96 2.01 1.00 4.03 3.98 2.96
f1 (ppm)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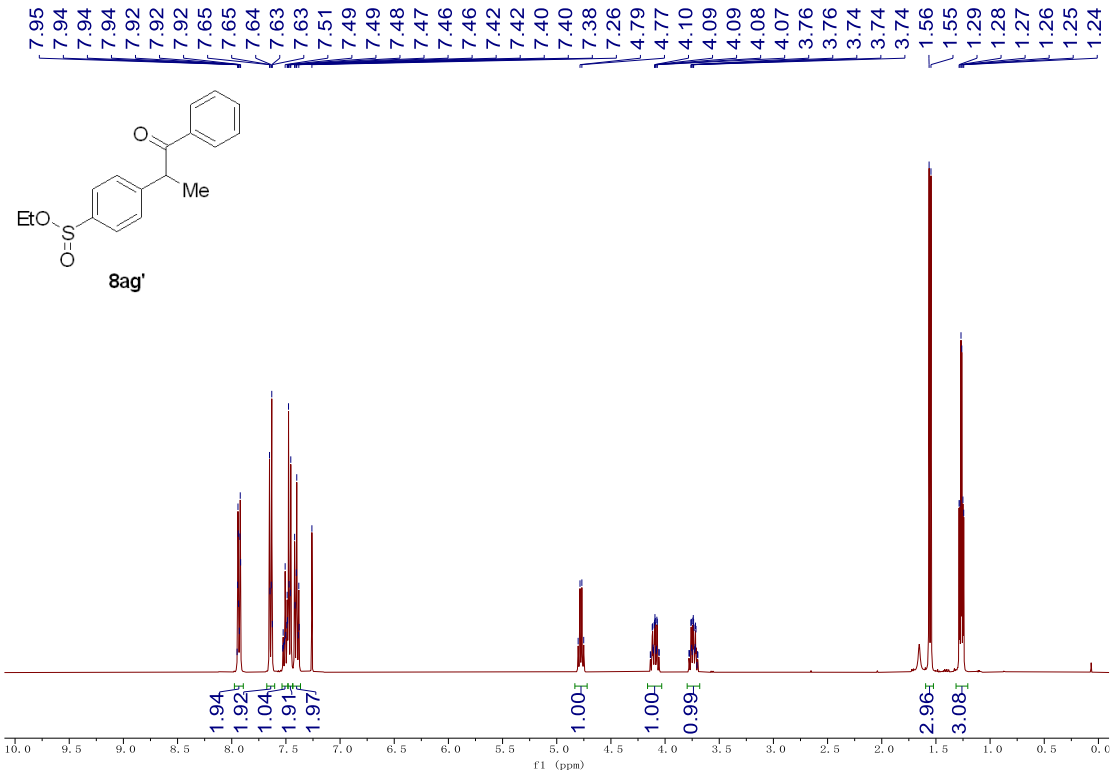
146.96 136.05 133.84 133.50 128.88 128.81 128.75 128.63
77.48 77.16 76.84 66.18 47.47 46.02 19.57
128.88 128.81 128.75 128.63
Me
8af'
f1 (ppm)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O
Me
EtO
S
O=
8ag'
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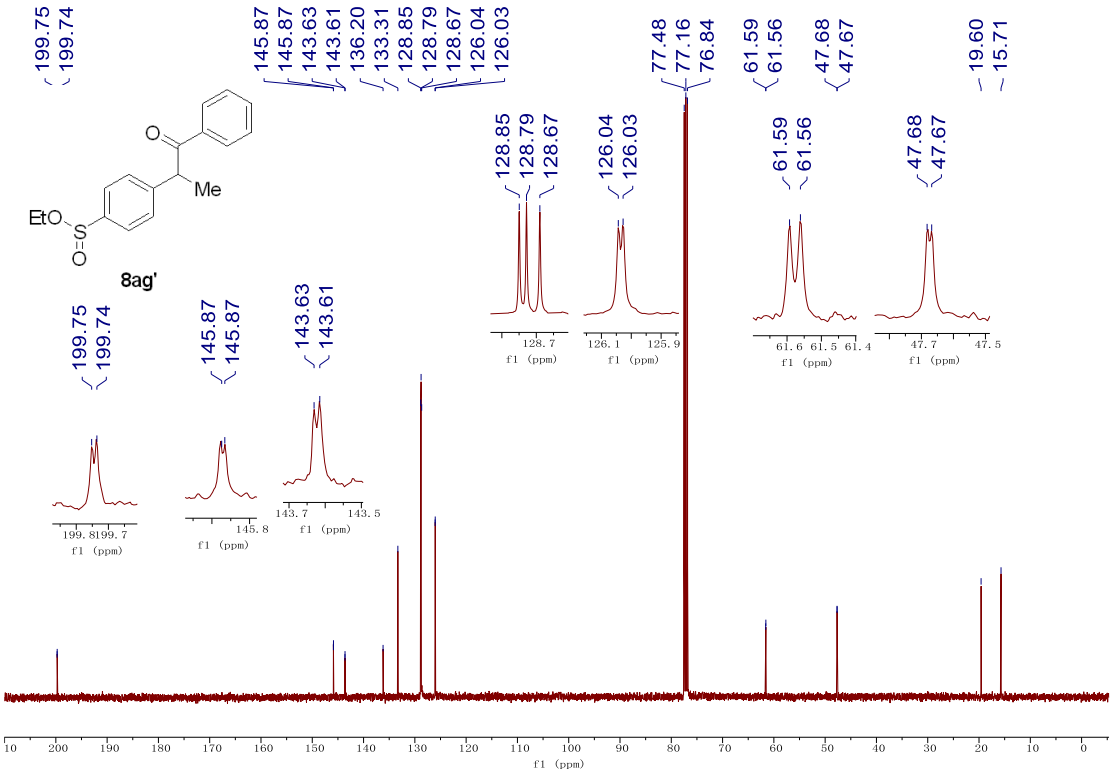
f1 (ppm)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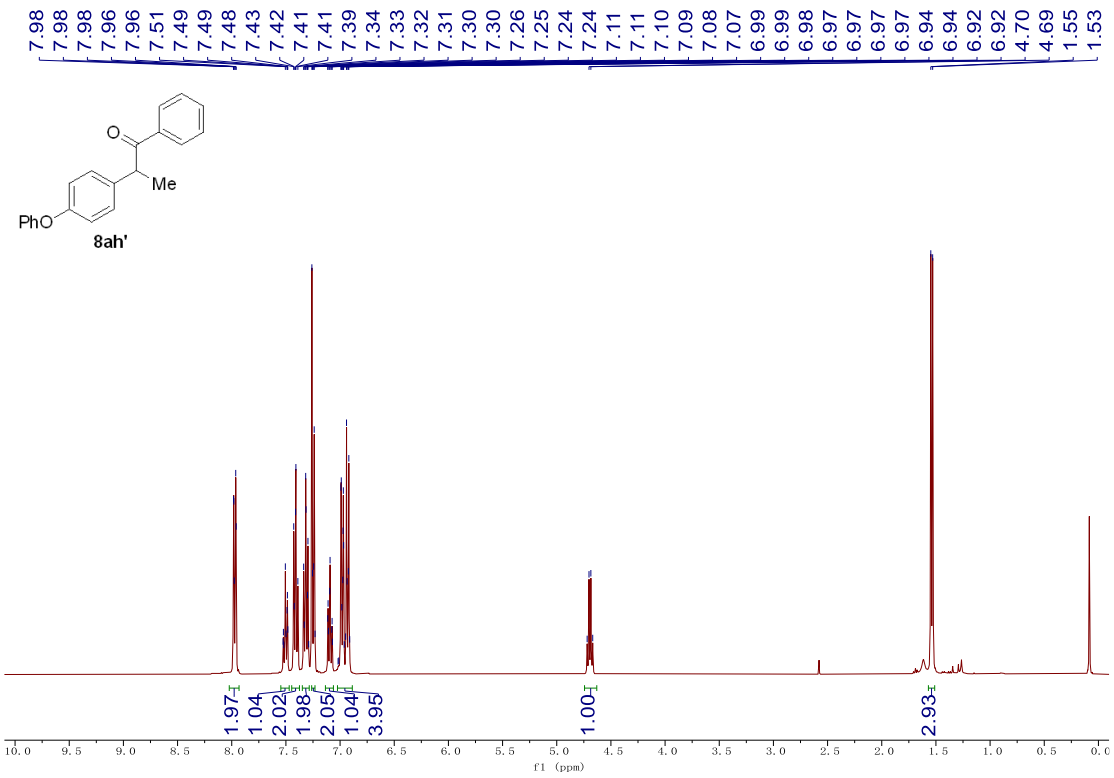
O
Me
EtO
S
O=
8ag'
f1 (ppm)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7.24
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7.11
7.11
7.10
7.09
7.08
7.07
6.99
6.99
6.98
6.97
6.97
6.97
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6.94
6.94
6.92
6.92
4.70
4.69
1.55
1.53
O
Me
PhO
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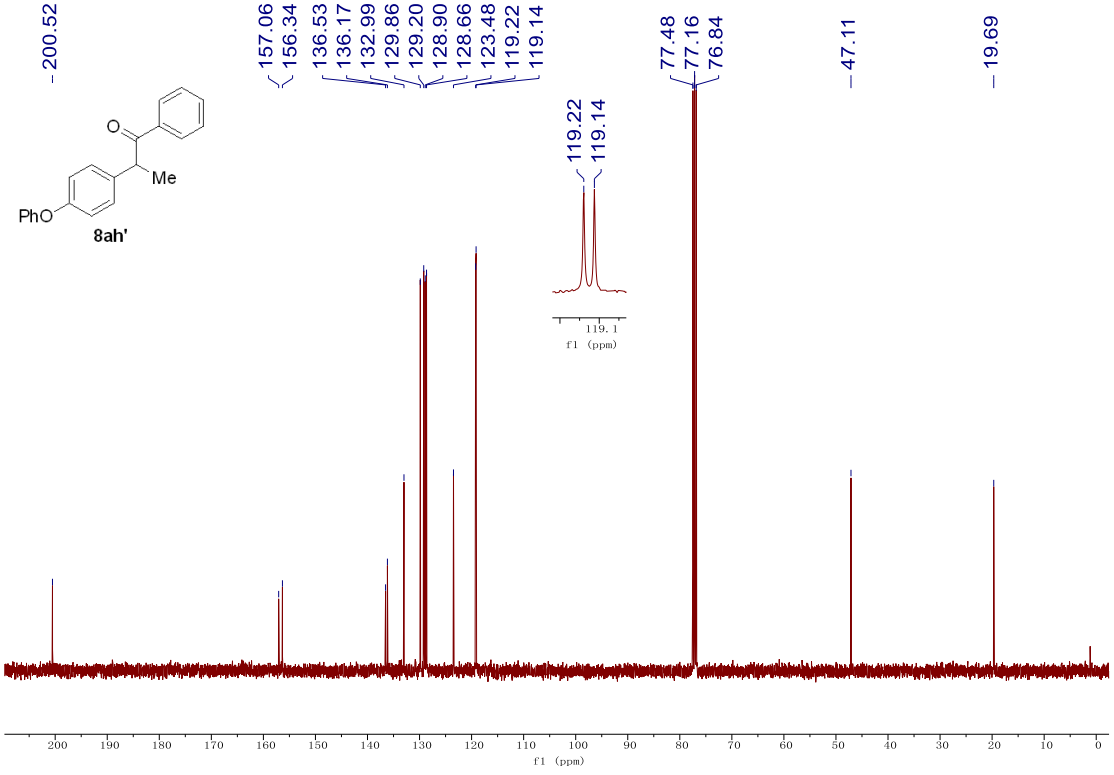
1.04
2.02
1.98
2.05
1.04
3.95
1.00
2.93
f1 (ppm)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77.16
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O
Me
PhO
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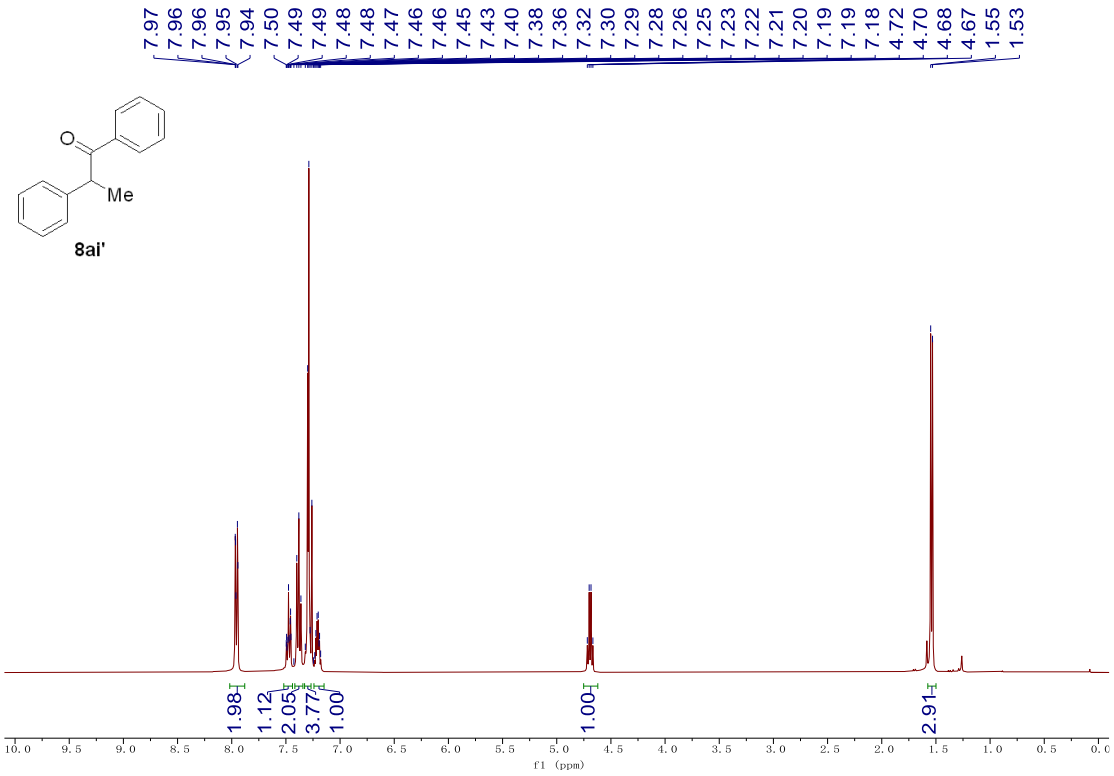
119.22
119.14
119.1
f1 (ppm)
f1 (ppm)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7.21
7.20
7.19
7.19
7.18
4.72
4.70
4.68
4.67
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Me
8ai'
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2.05
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1.00
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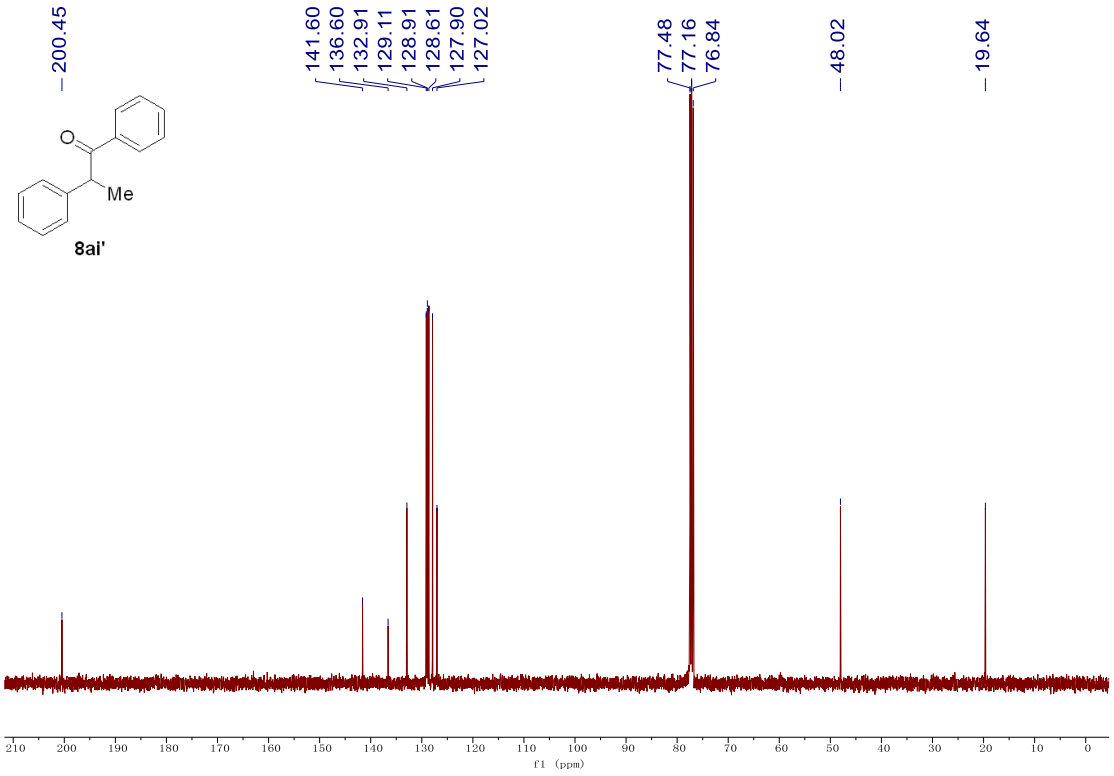
f1 (ppm)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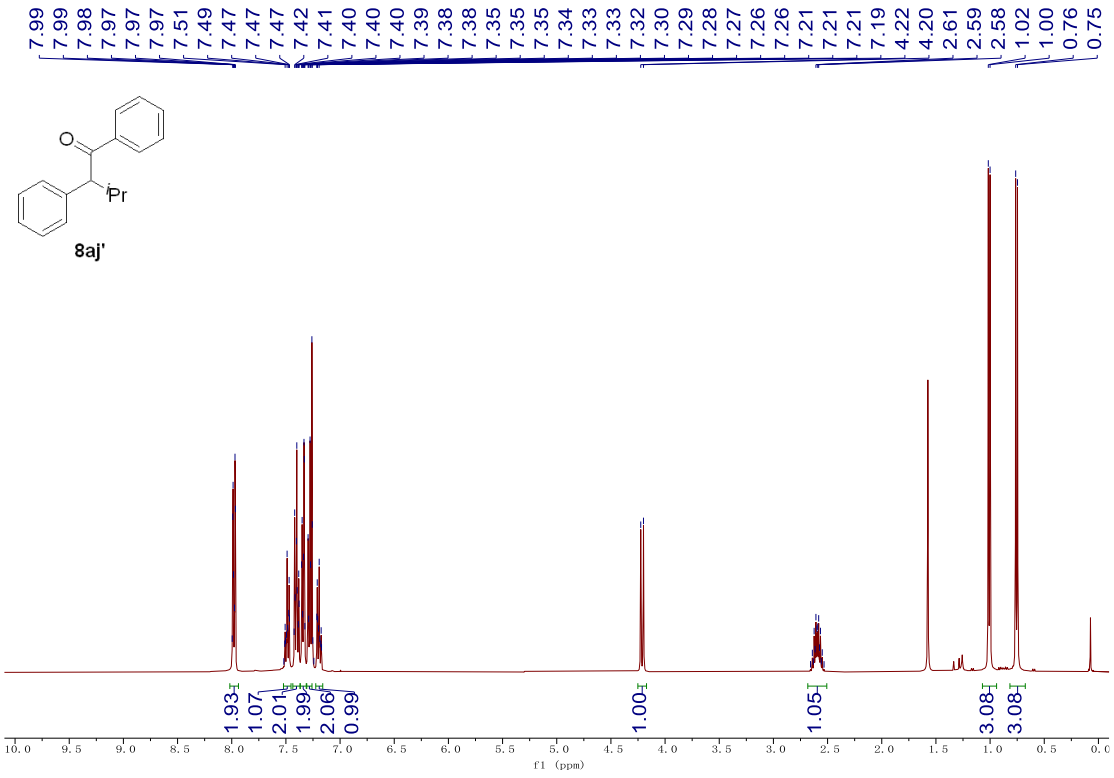
48.02
19.64
O
Me
8ai'
f1 (ppm)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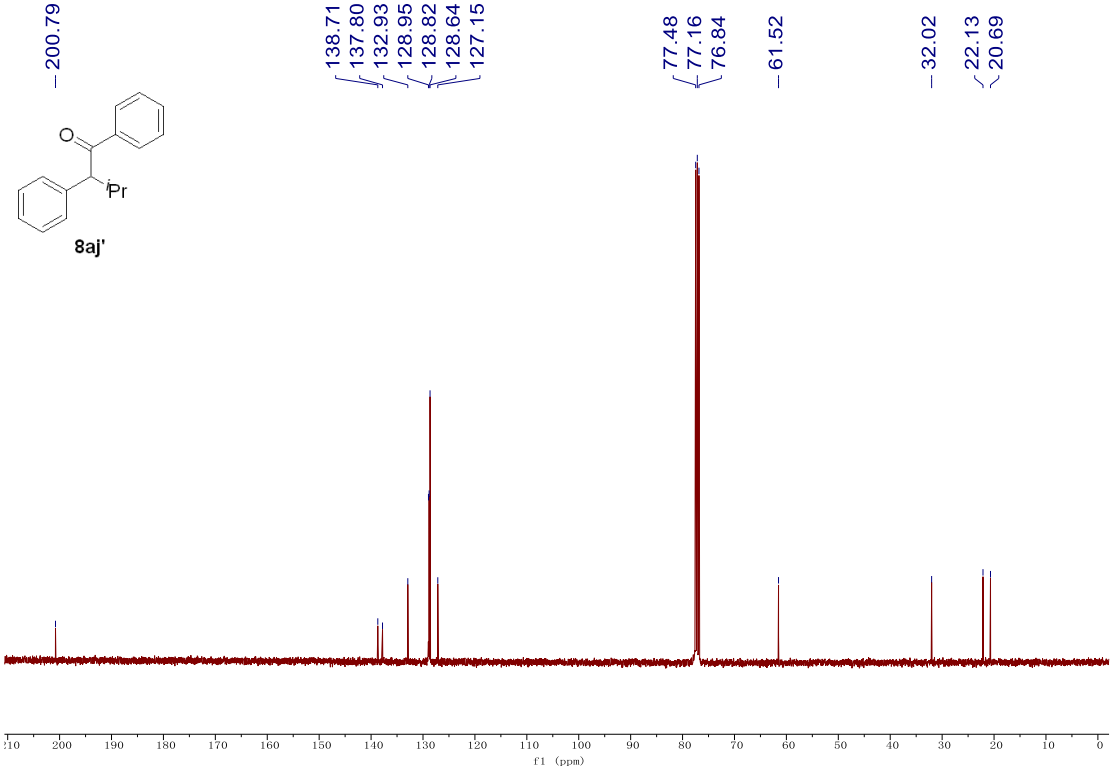
7.21
7.21
7.21
7.19
4.22
4.20
2.61
2.59
2.58
1.02
1.00
0.76
0.75
O
iPr
8aj'
1.93
1.07
2.01
1.99
2.06
0.99
1.00
1.05
3.08
3.08
f1 (ppm)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128.64
127.15
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77.16
76.84
61.52
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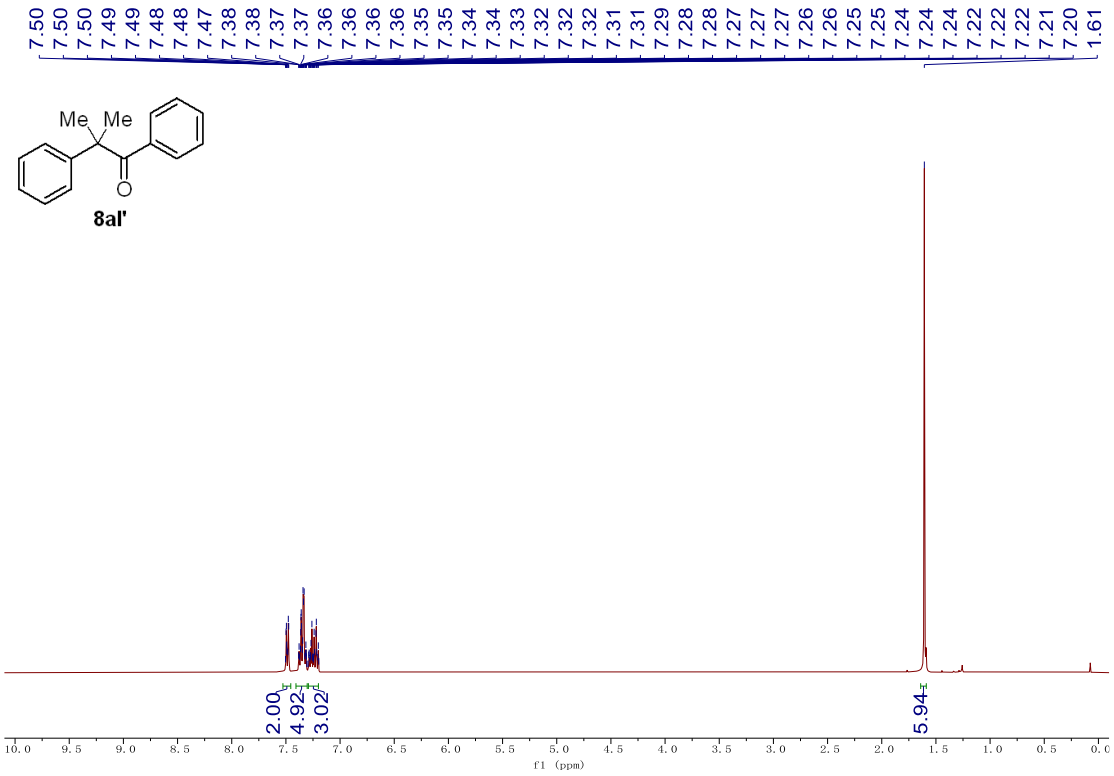
22.13
20.69
O
iPr
8aj'
f1 (ppm)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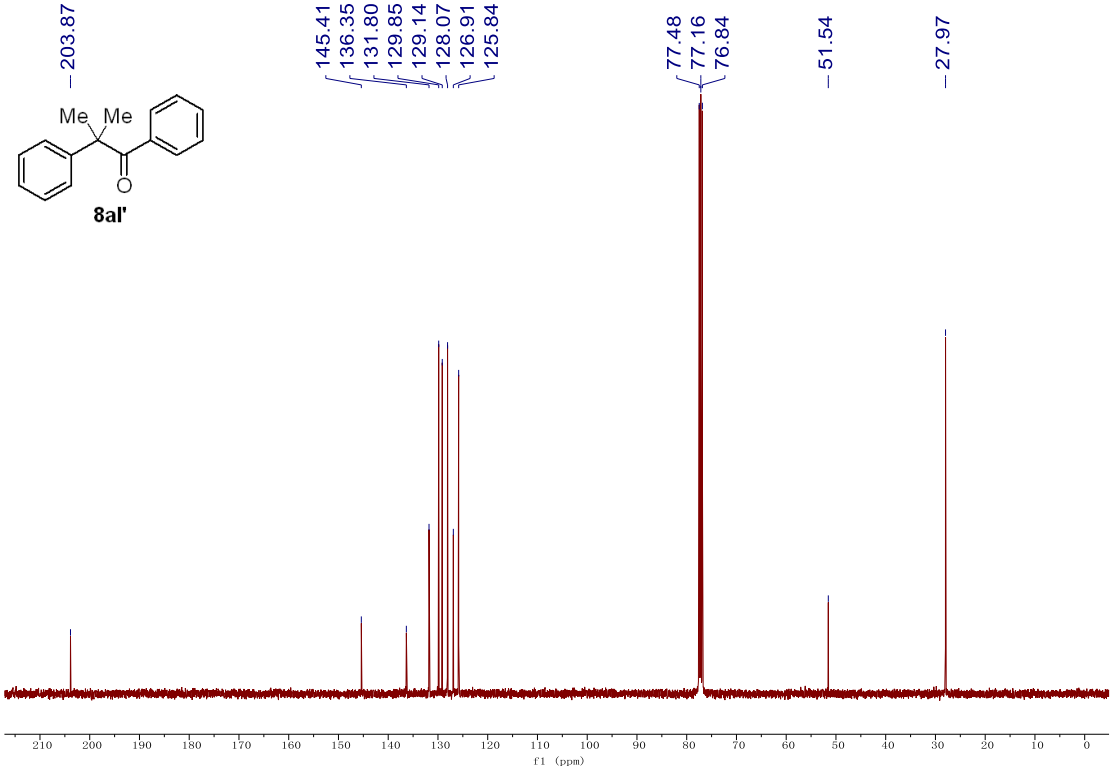
7.26
7.25
7.25
7.24
7.24
7.24
7.22
7.22
7.21
7.20
1.61
Me Me
O
8al'
2.00
4.92
3.02
5.94
f1 (ppm)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129.14
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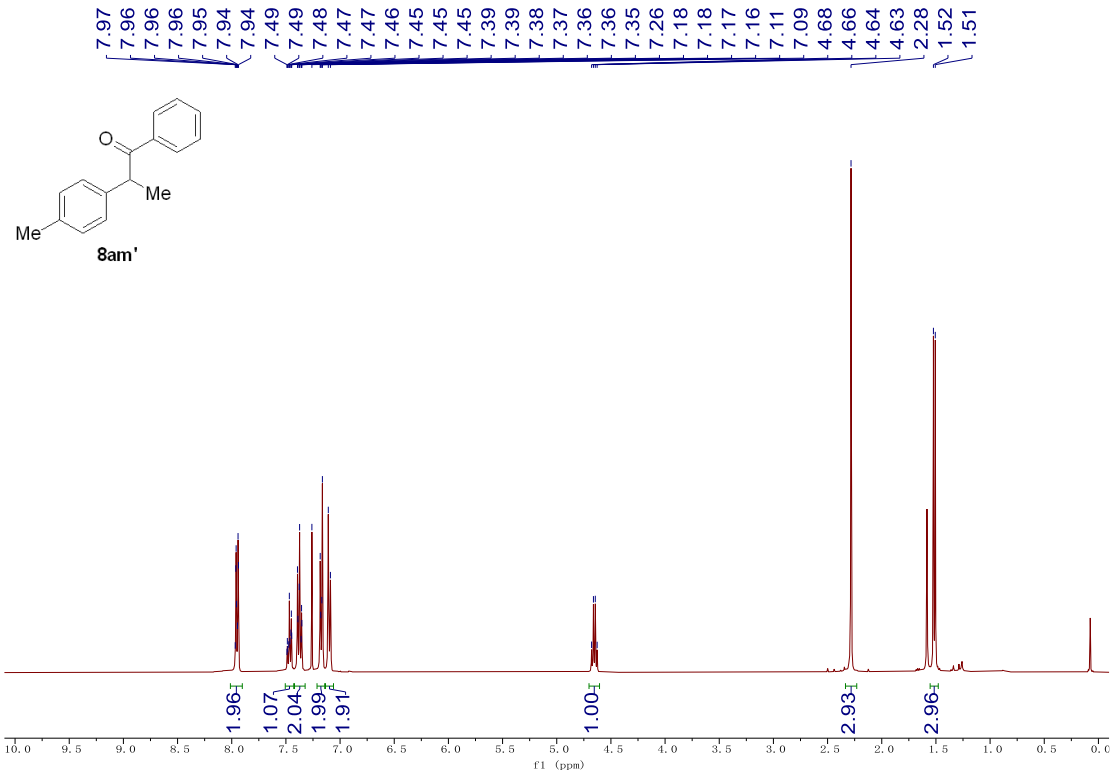
126.91
125.84
77.48
77.16
76.84
51.54
27.97
Me Me
O
8al'
f1 (ppm)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7.18
7.17
7.16
7.11
7.09
4.68
4.66
4.64
4.63
2.28
1.52
1.51
O
Me
Me
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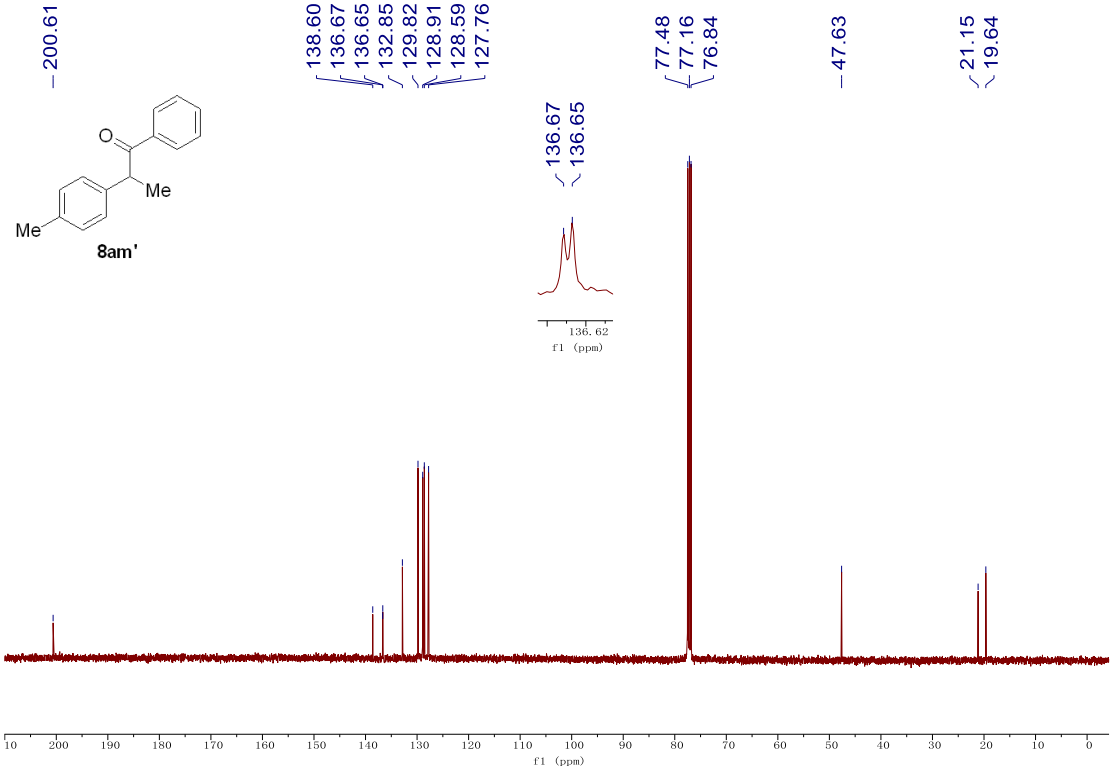
1.96
1.07
2.04
1.99
1.91
1.00
2.93
2.96
f1 (ppm)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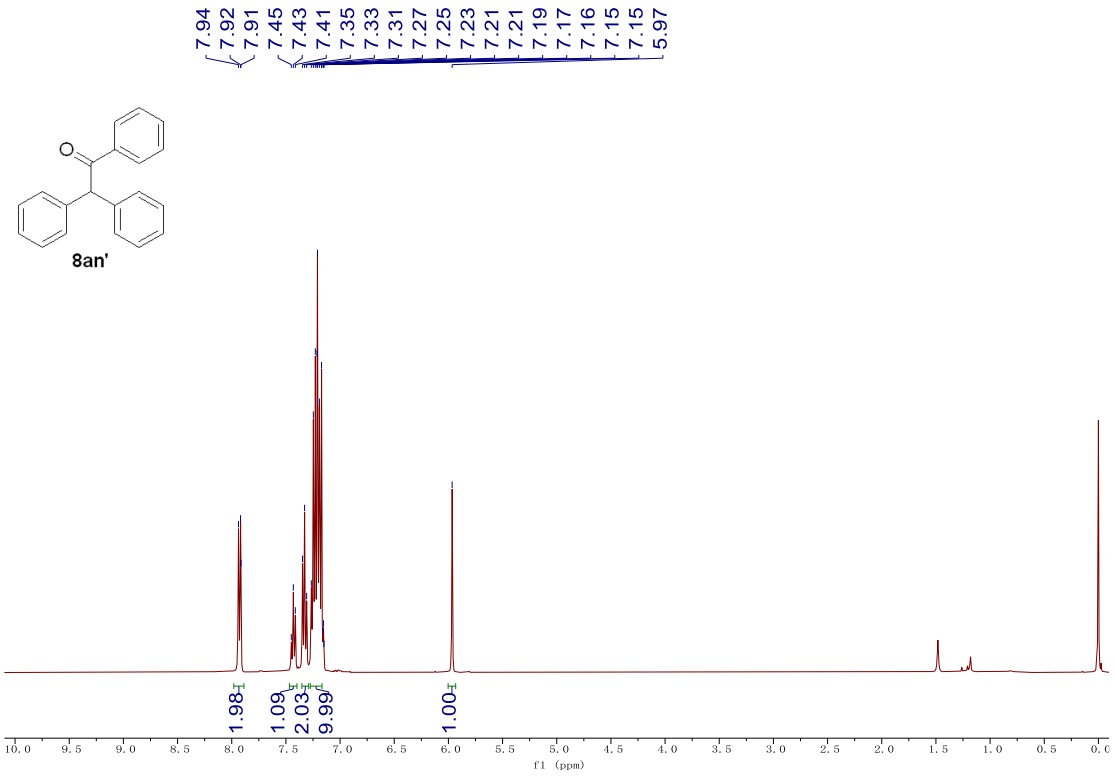
129.82
128.91
128.59
127.76
77.48
77.16
76.84
47.63
21.15
19.64
O
Me
Me
8am'
136.67
136.65
136.62
f1 (ppm)
f1 (ppm)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7.45
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7.31
7.27
7.25
7.23
7.21
7.21
7.19
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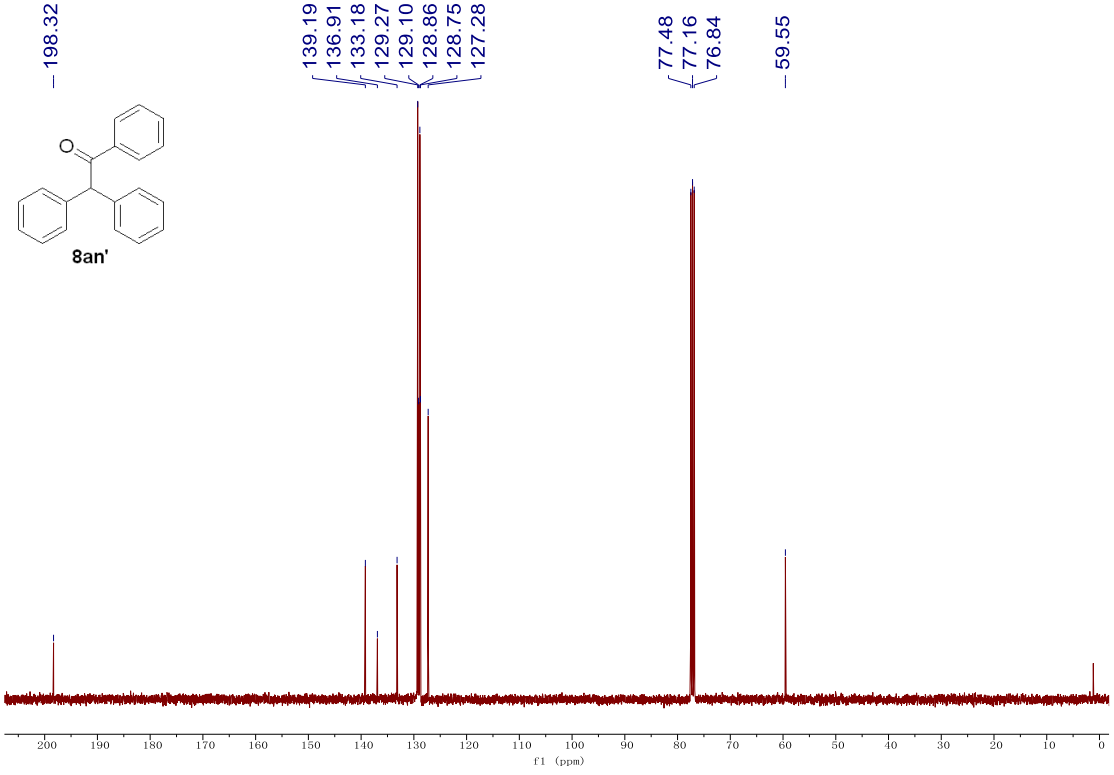
7.15
5.97
8an'
1.98
1.09
2.03
9.99
1.00
f1 (ppm)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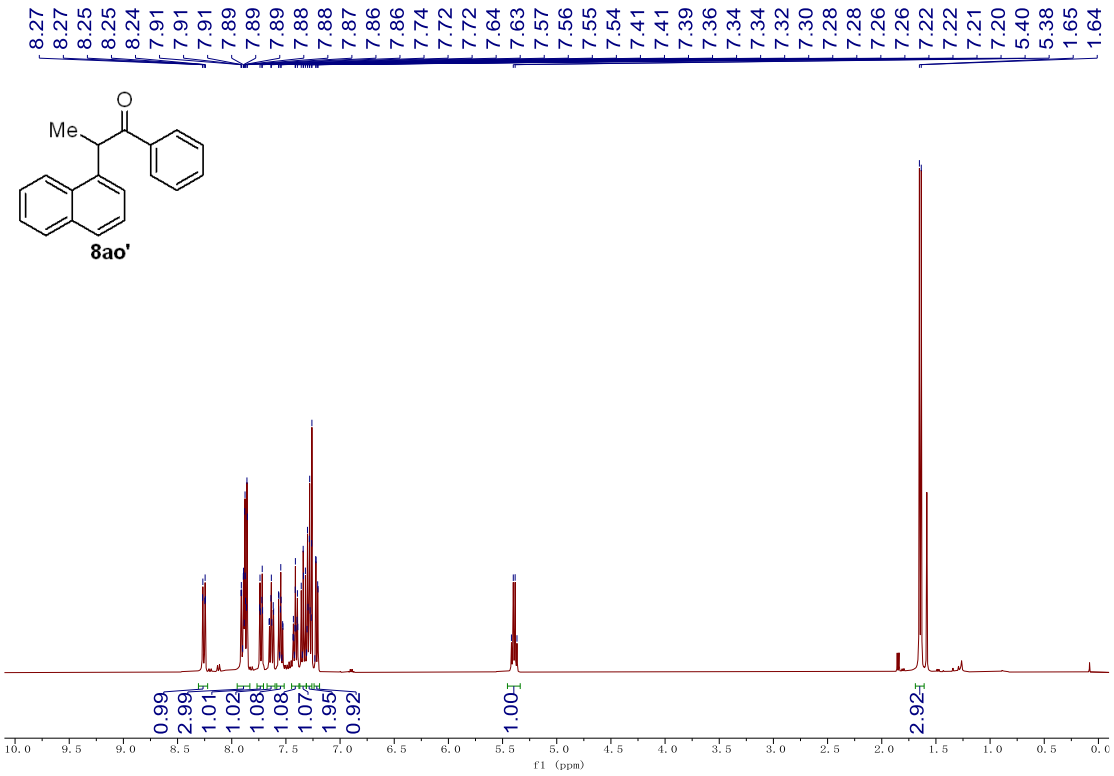
128.75
127.28
77.48
77.16
76.84
59.55
8an'
f1 (ppm)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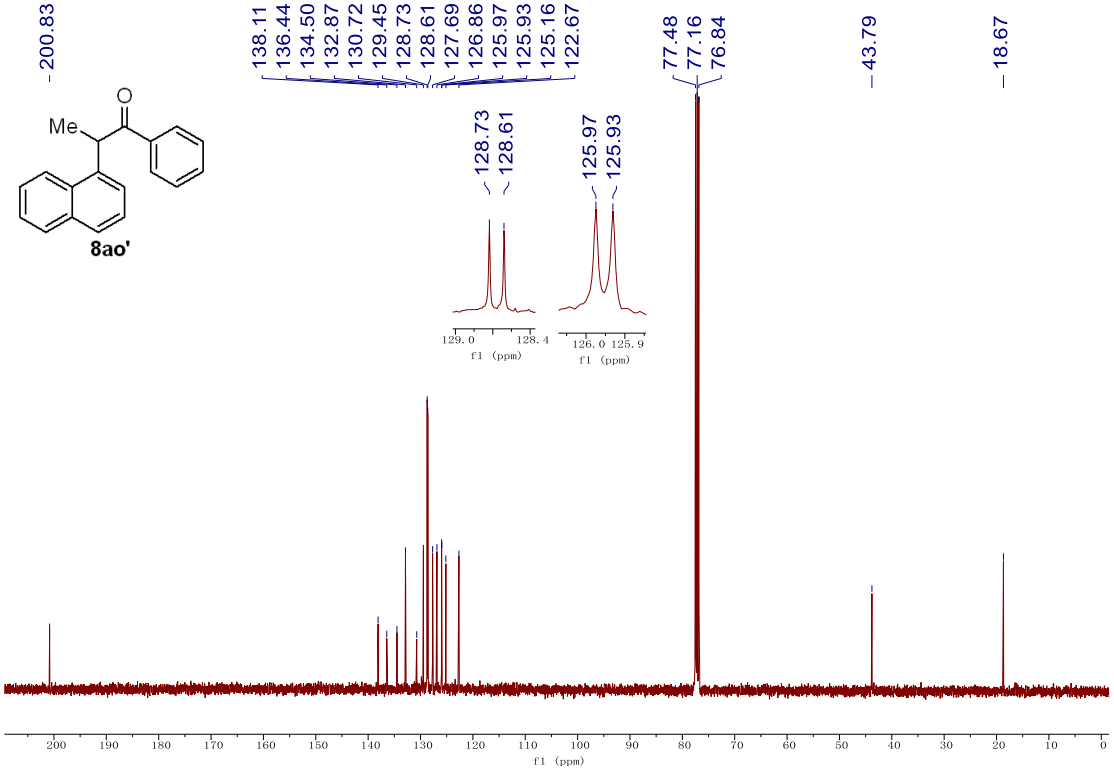
Me
O
8ao'
0.99 2.99 1.01 1.02 1.08 1.08 1.07 1.95 0.92 1.00 2.92
f1 (ppm)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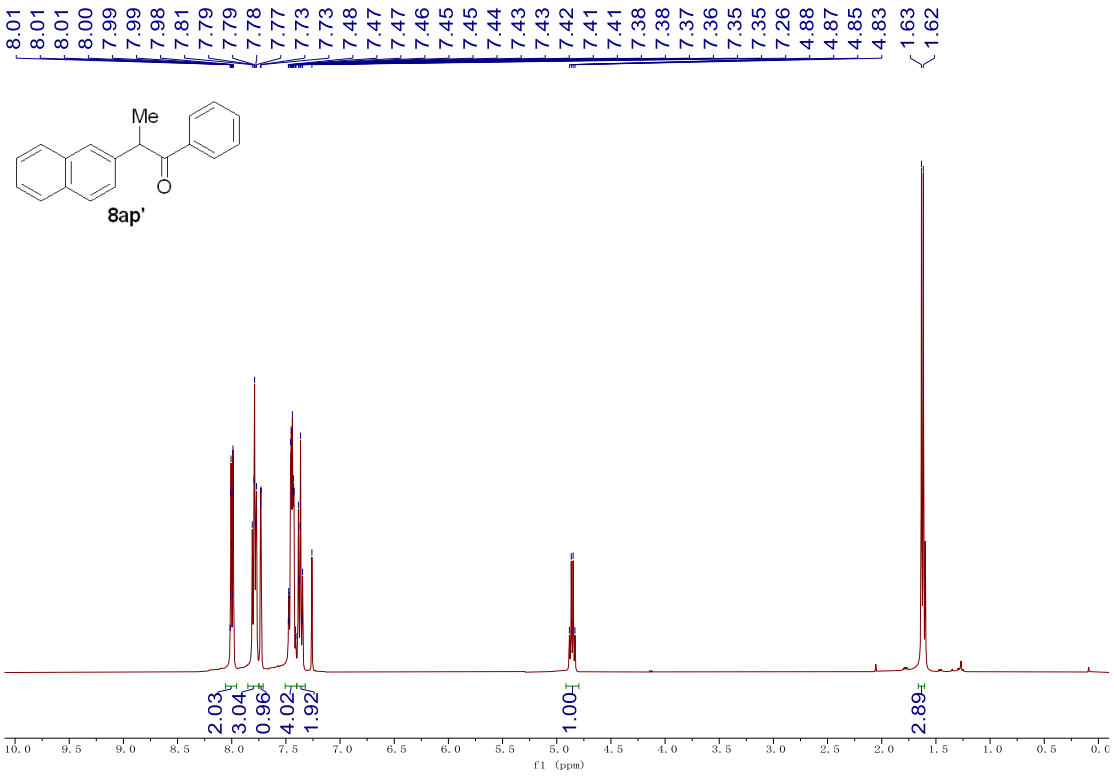
138.11 136.44 134.50 132.87 130.72 129.45 128.73 128.61 127.69 126.86 125.97 125.93 125.16 122.67
77.48 77.16 76.84
43.79
18.67
Me
O
8ao'
128.73 128.61
125.97 125.93
129.0 128.4
126.0 125.9
f1 (ppm)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8.01
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7.37
7.36
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7.35
7.26
4.88
4.87
4.85
4.83
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1.62
Me
O
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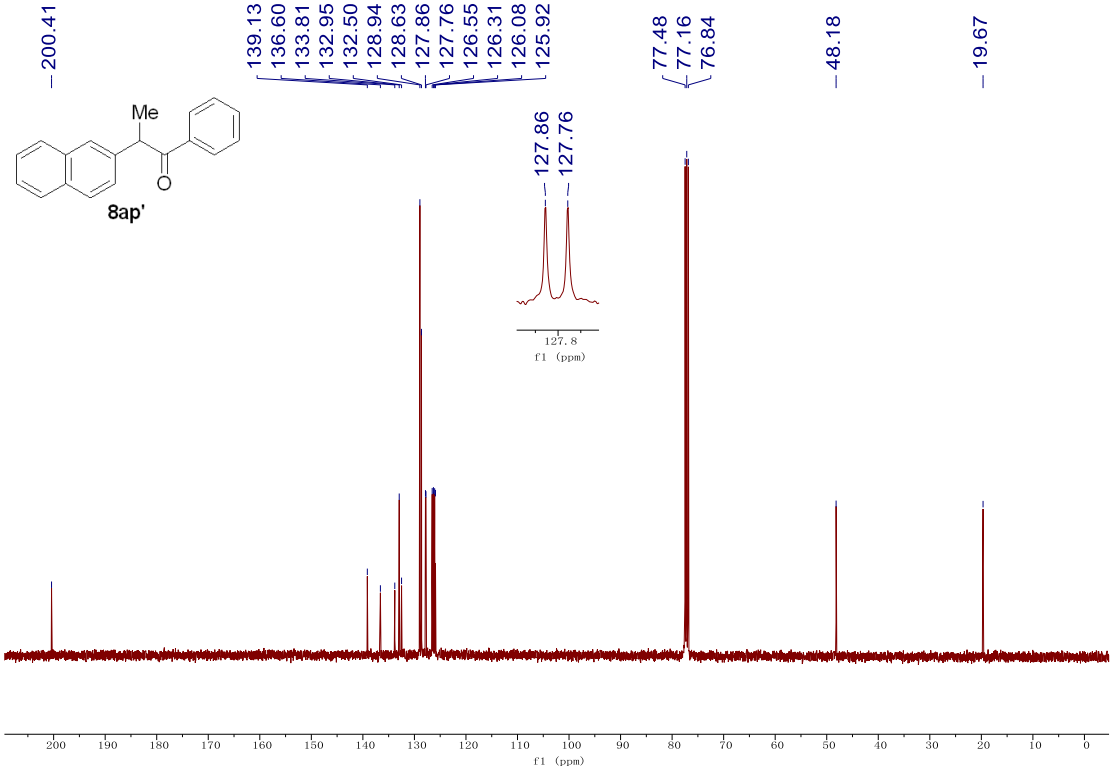
3.04
0.96
4.02
1.92
1.00
2.89
f1 (ppm)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126.08
125.92
77.48
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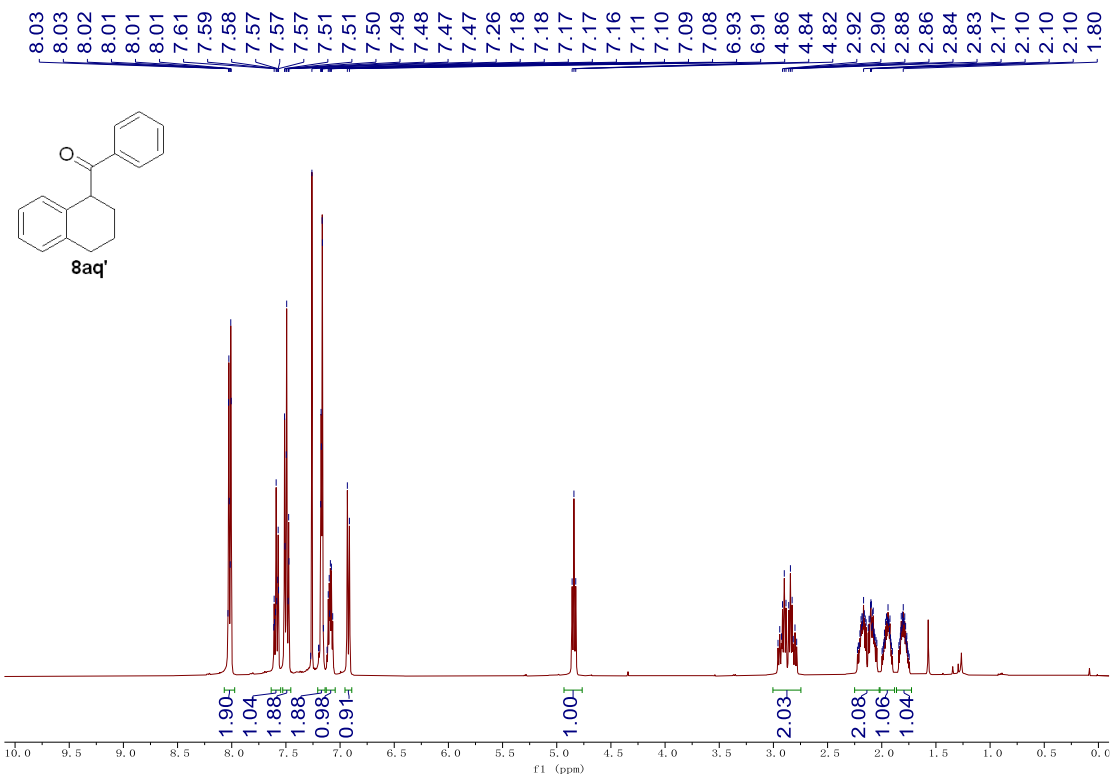
76.84
48.18
19.67
Me
O
8ap'
127.86
127.76
127.8
f1 (ppm)
f1 (ppm)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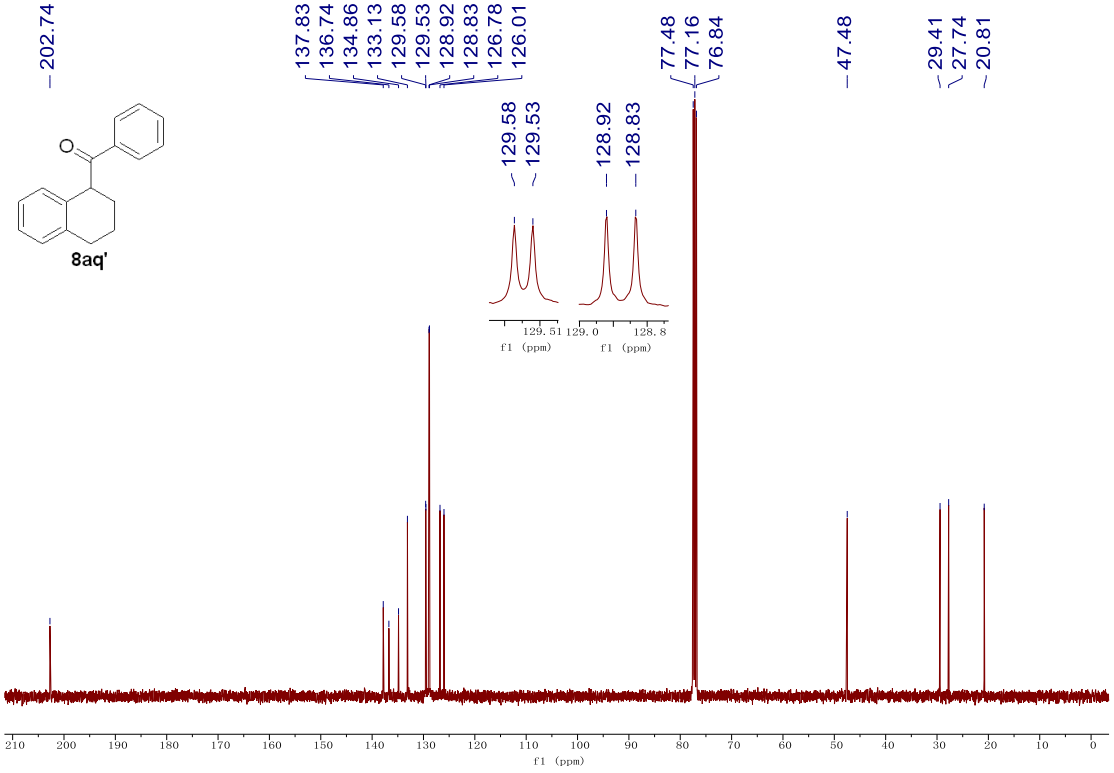
8aq'
1.90 1.04 1.88 1.88 0.99 0.91 1.00 2.03 2.08 1.06 1.04
f1 (ppm)


202.74
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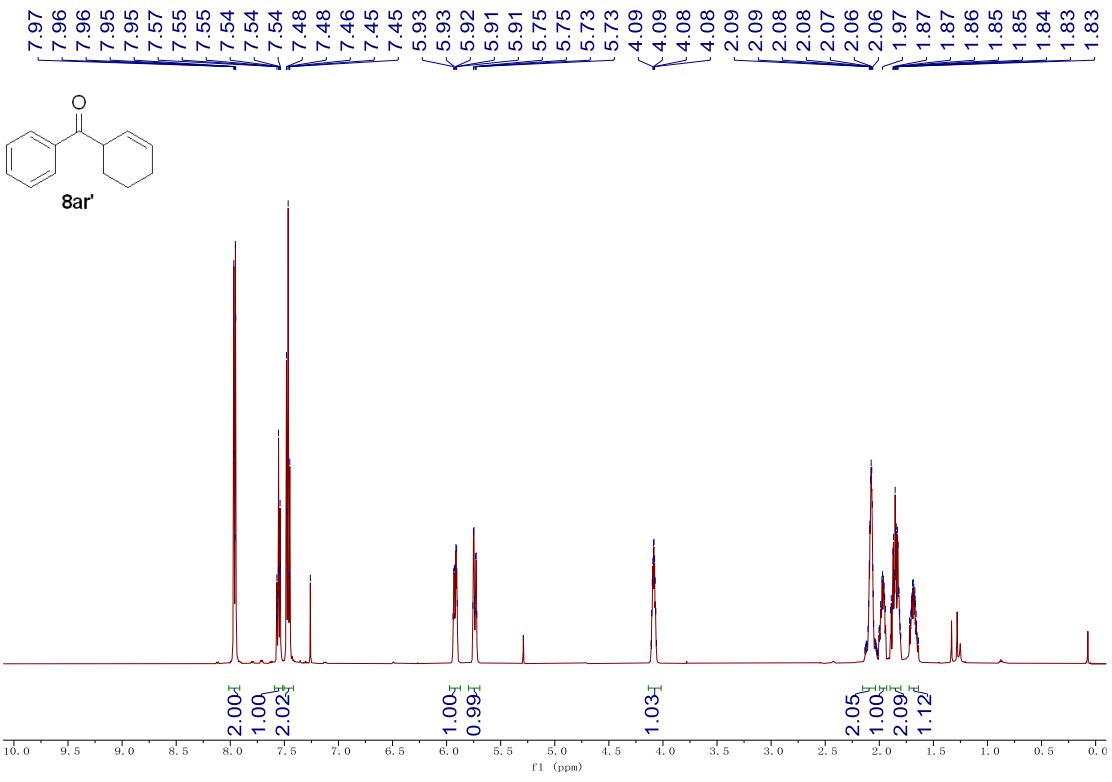
77.48 77.16 76.84
47.48
29.41 27.74 20.81
129.58 129.53 128.92 128.83
8aq'
f1 (ppm)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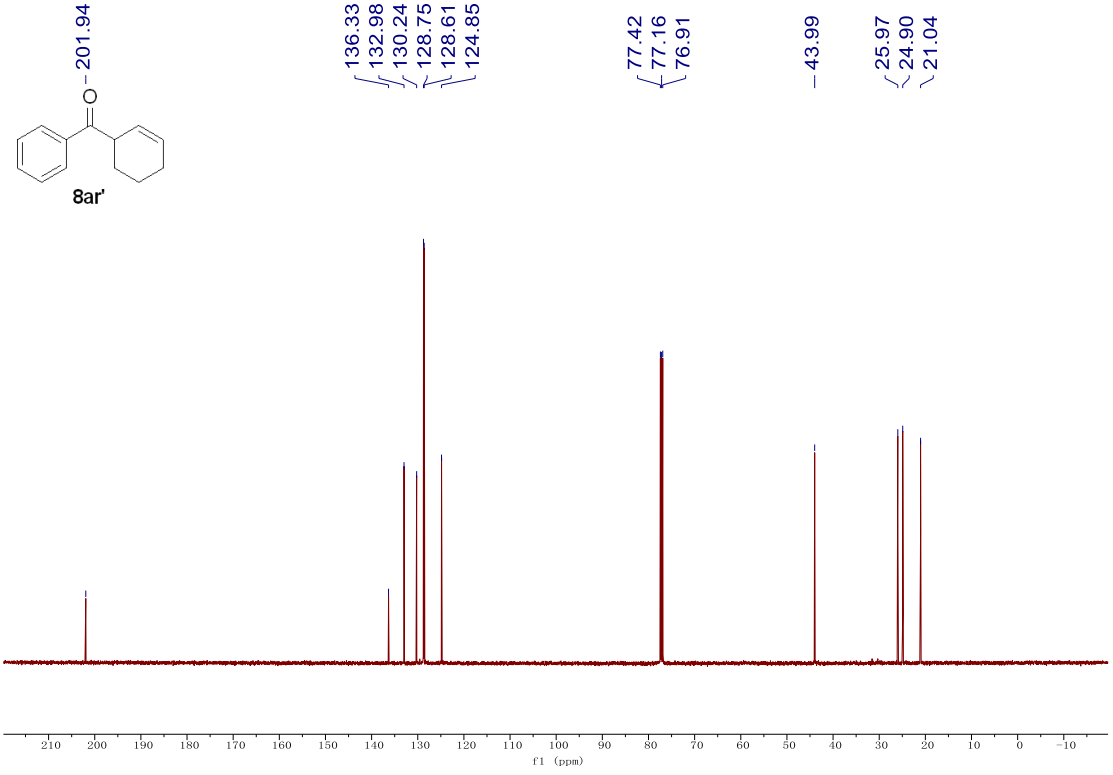
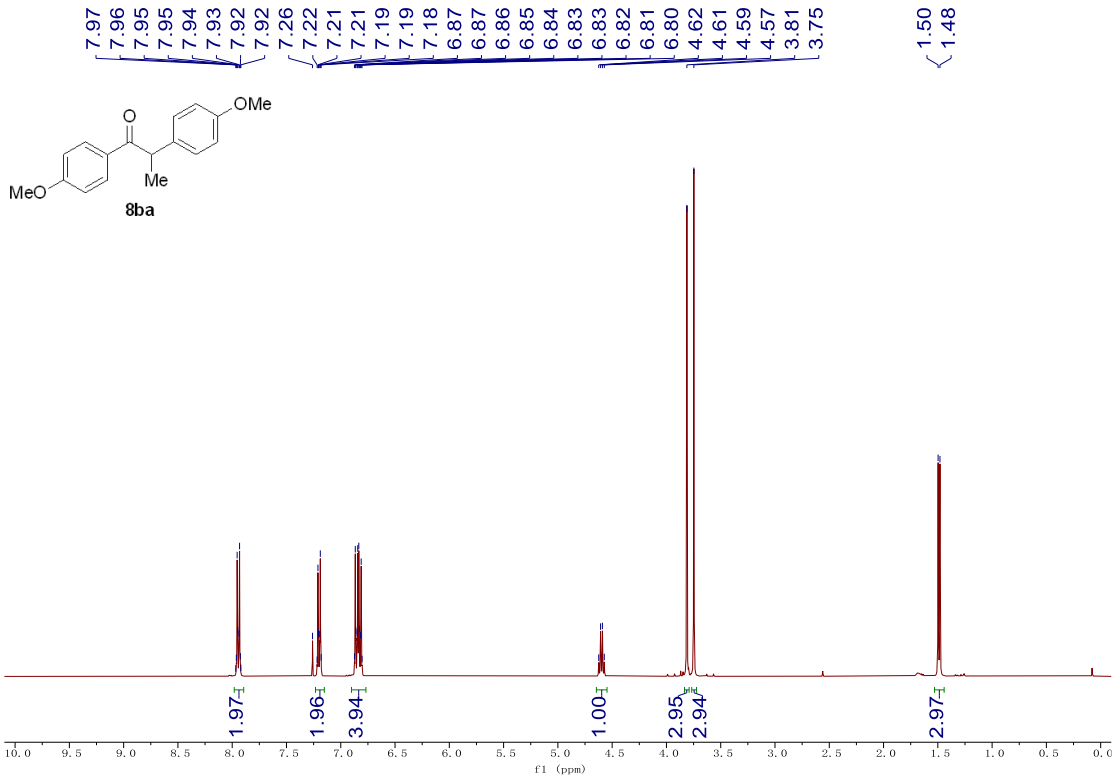
5.93 5.93 5.92 5.91 5.91 5.75 5.75 5.73 5.73
4.09 4.08 4.08
2.09 2.09 2.08 2.08 2.07 2.06 2.06
1.97 1.87 1.87 1.86 1.85 1.85 1.84 1.83 1.83
8ar'
2.00 1.00 2.02 1.00 0.99 1.03 2.05 1.00 2.09 1.12
f1 (ppm)


201.94
136.33 132.98 130.24 128.75 128.61 124.85
77.42 77.16 76.91
43.99
25.97 24.90 21.04
8ar'
f1 (ppm)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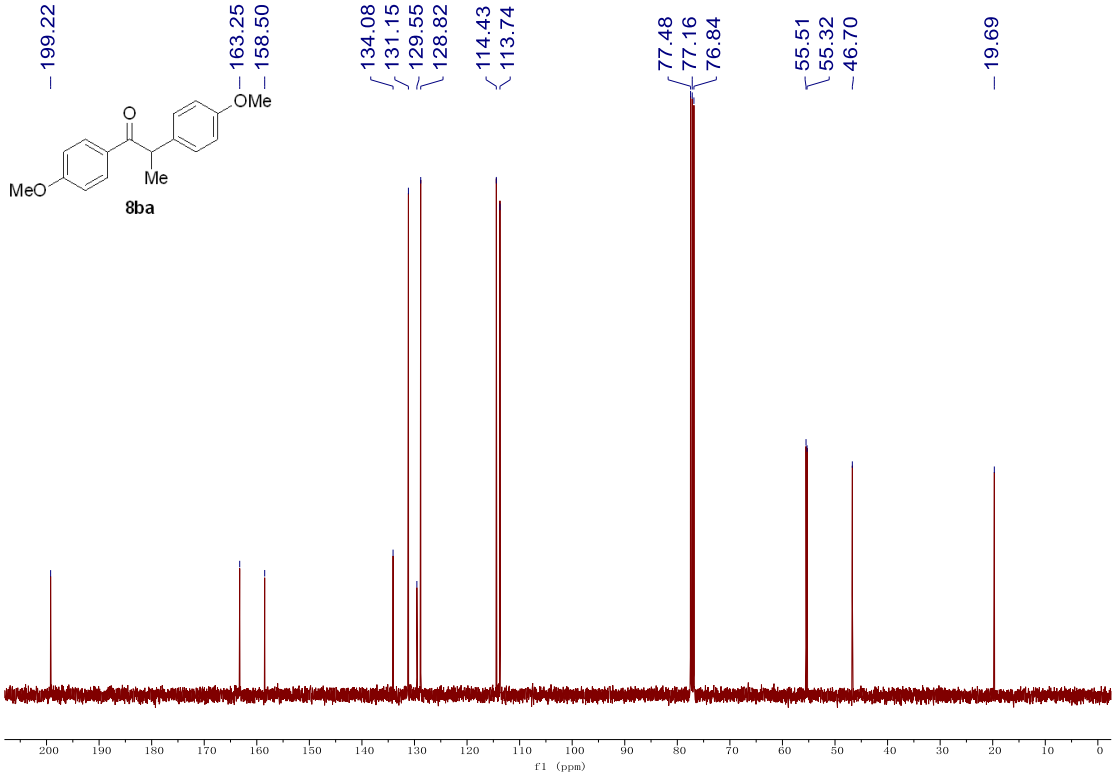
6.82
6.81
6.80
4.62
4.61
4.59
4.57
3.81
3.75
1.50
1.48
O
OMe
Me
MeO
8ba
1.97
1.96
3.94
1.00
2.95
2.94
2.97
f1 (ppm)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55.51
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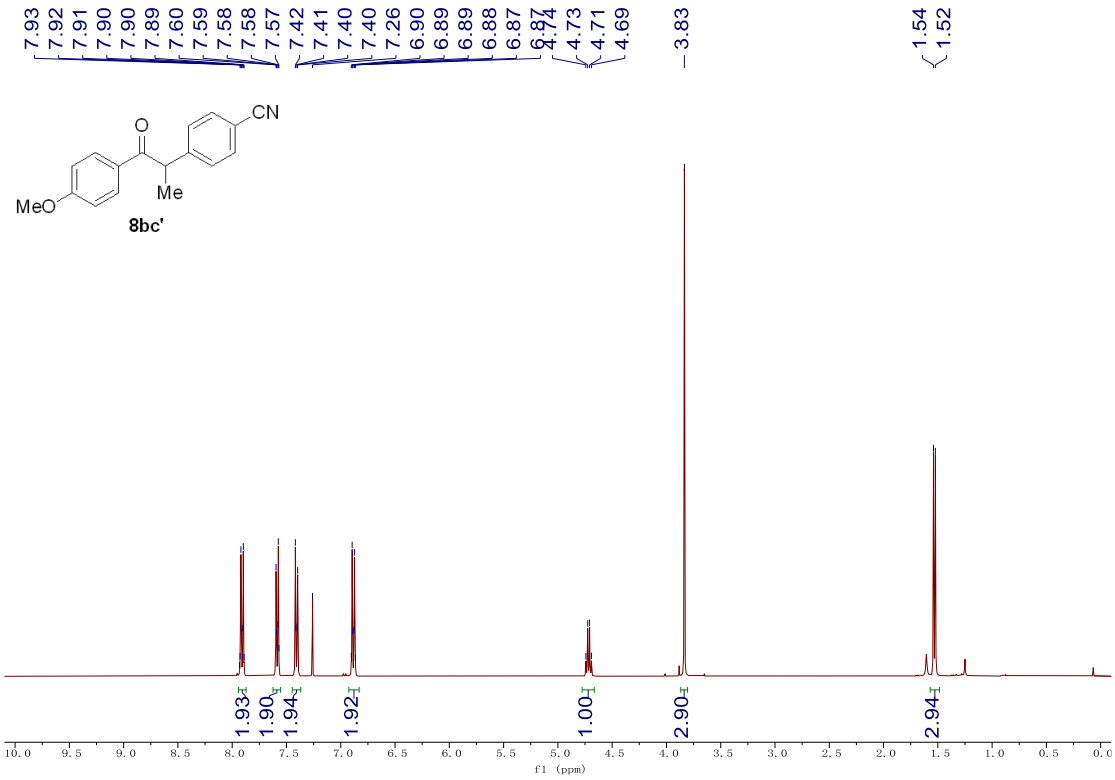
46.70
19.69
O
OMe
Me
MeO
8ba
f1 (ppm)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7.57
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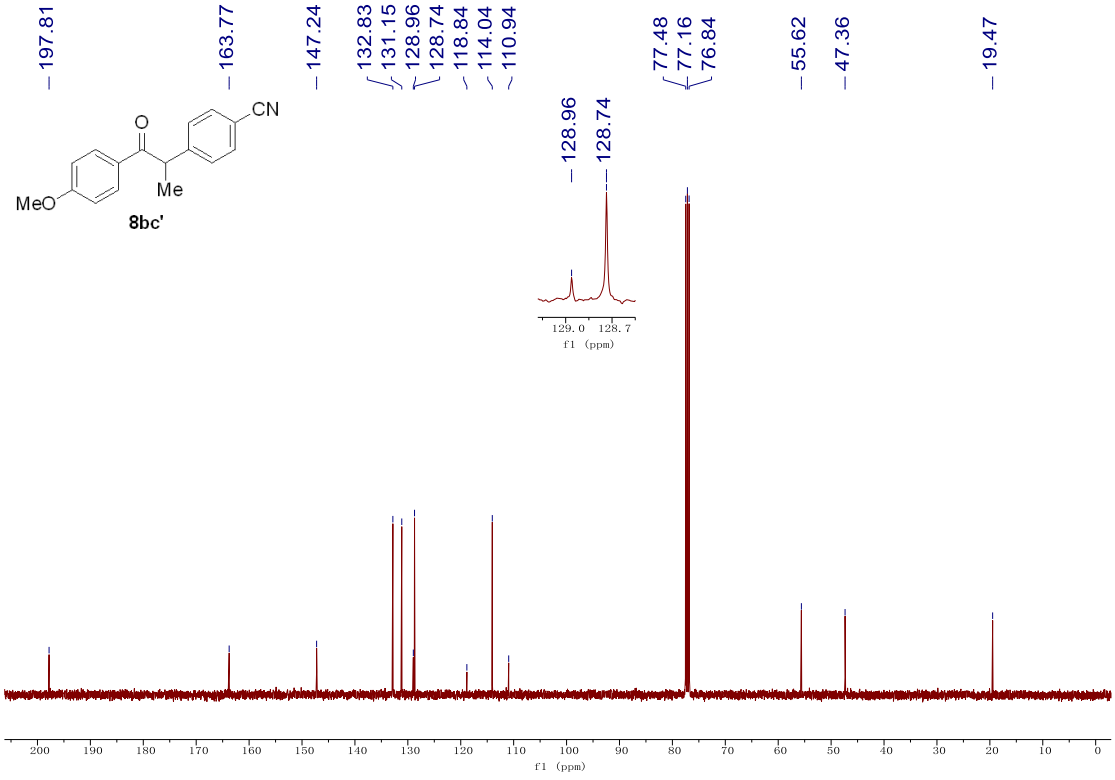
6.89
6.88
6.87
6.87
4.74
4.73
4.71
4.69
3.83
1.54
1.52
O
CN
Me
MeO
8bc'
1.93
1.90
1.94
1.92
1.00
2.90
2.94
f1 (ppm)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118.84
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110.94
77.48
77.16
76.84
55.62
47.36
19.47
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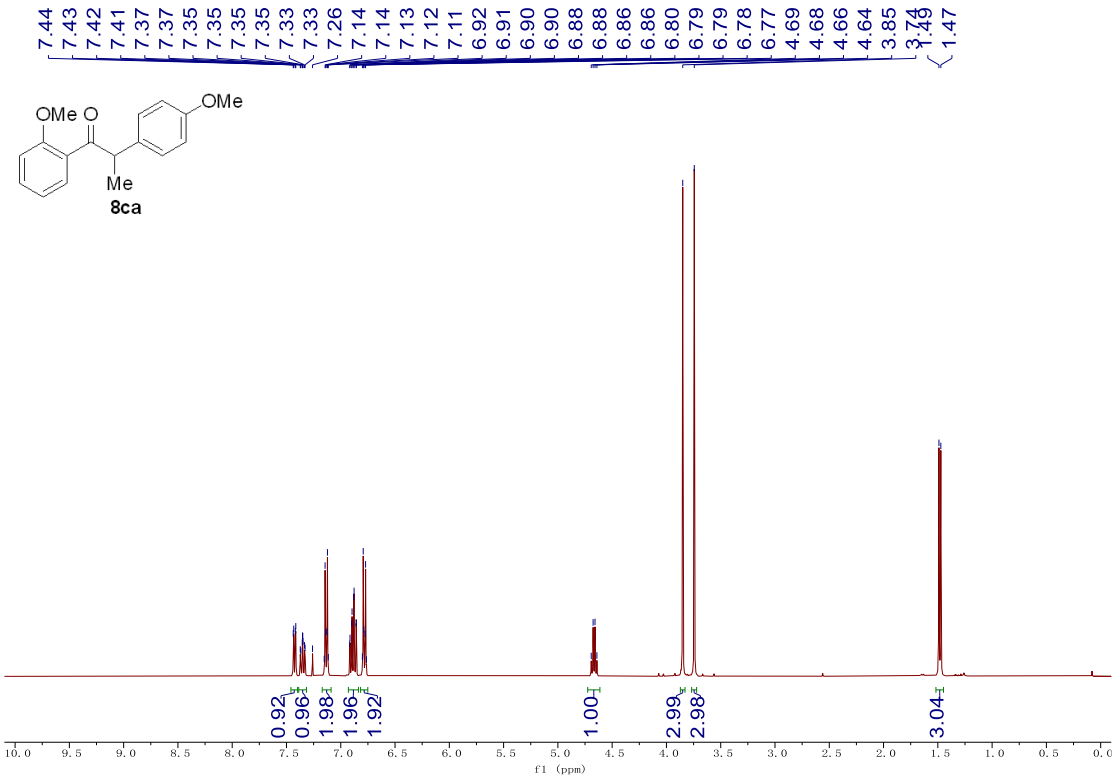
128.74
O
CN
Me
MeO
8bc'
129.0
128.7
f1 (ppm)
f1 (ppm)


7.44 7.43 7.42 7.41 7.37 7.37 7.35 7.35 7.35 7.33 7.33 7.26 7.14 7.14 7.13 7.12 7.11 6.92 6.91 6.90 6.90 6.88 6.88 6.86 6.86 6.80 6.79 6.79 6.78 6.77 4.69 4.68 4.66 4.64 3.85 3.74 1.49 1.47
OMe O
OMe
Me
8ca
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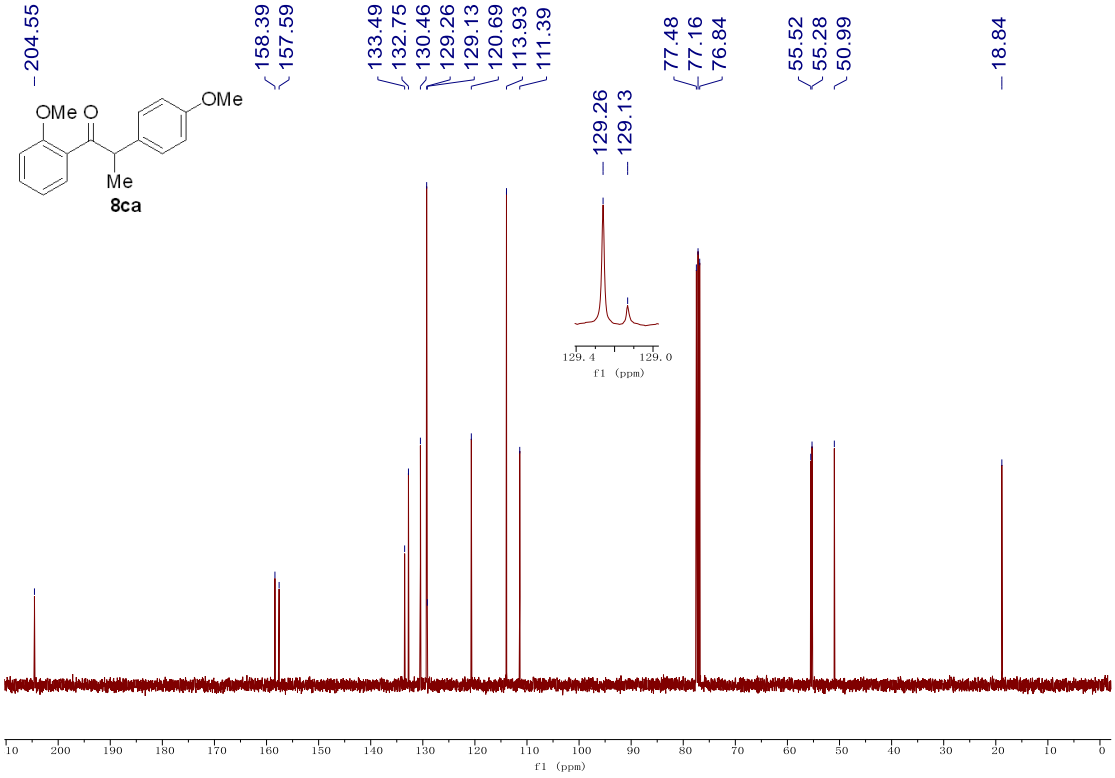
f1 (ppm)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158.39 157.59
133.49 132.75 130.46 129.26 129.13 120.69 113.93 111.39
77.48 77.16 76.84
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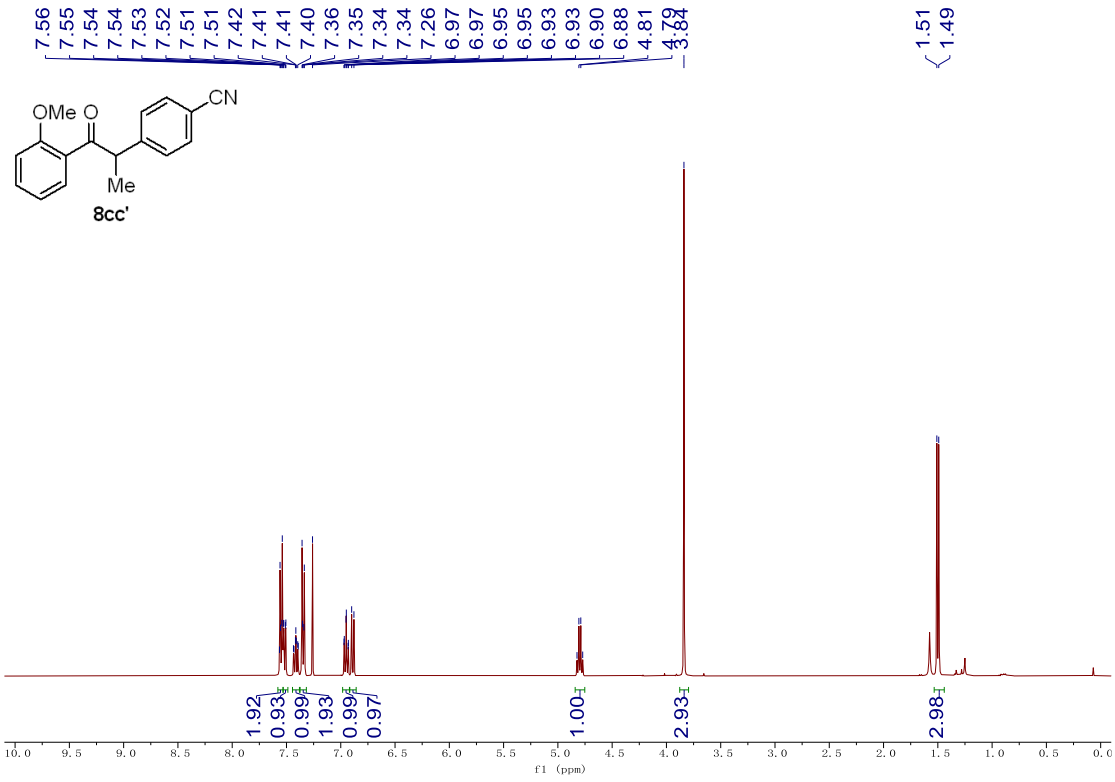
18.84
129.26 129.13
OMe O
OMe
Me
8ca
129.4 129.0
f1 (ppm)
f1 (ppm)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7.36
7.35
7.34
7.34
7.26
6.97
6.97
6.95
6.95
6.93
6.93
6.90
6.88
4.81
4.79
3.84
1.51
1.49
OMe O
CN
Me
8cc'
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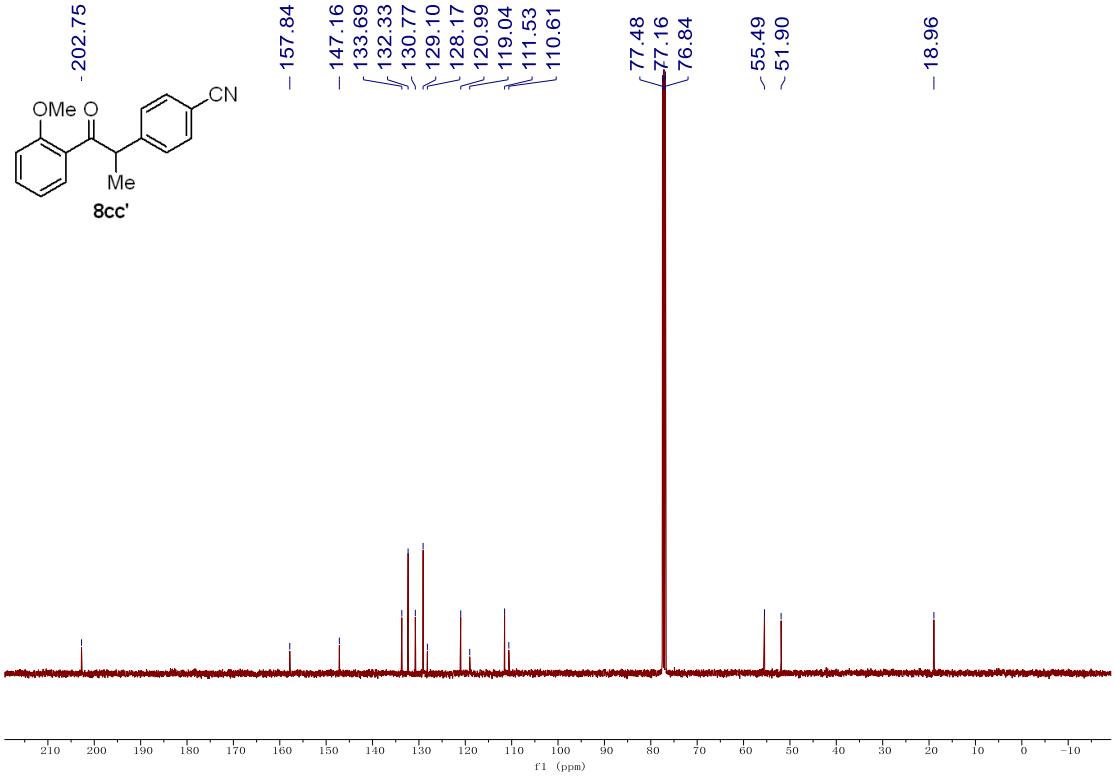
0.93
0.99
1.93
0.99
0.97
1.00
2.93
2.98
f1 (ppm)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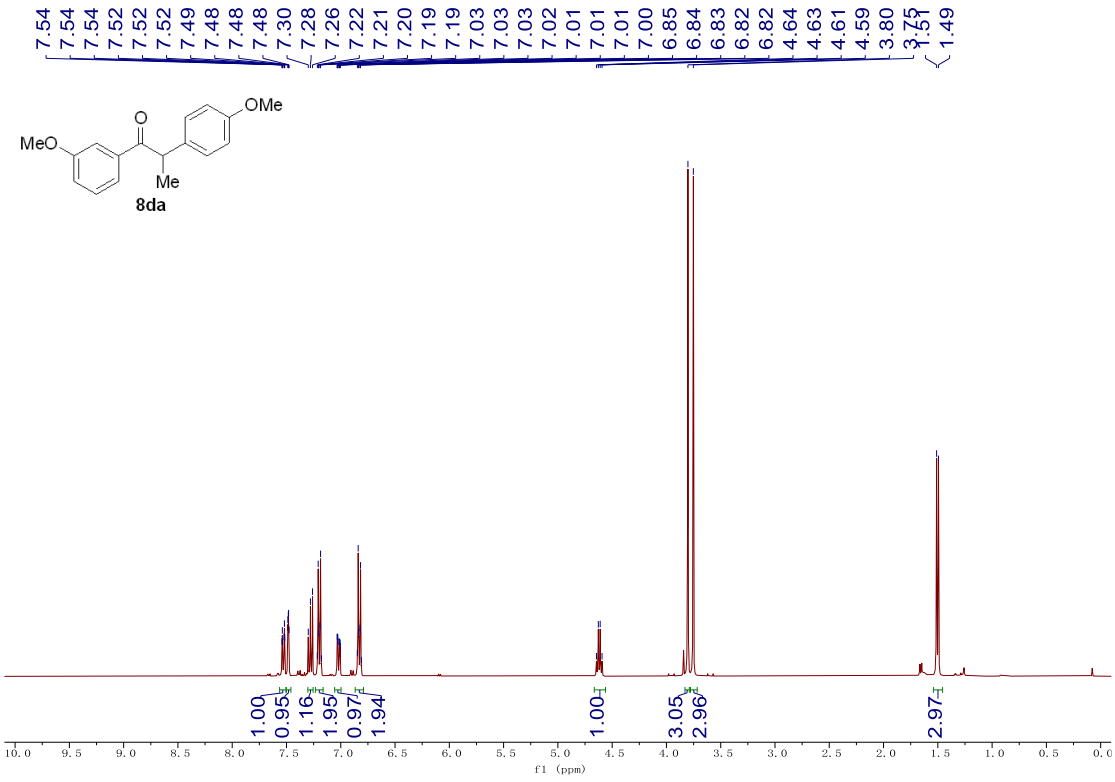
77.16
76.84
55.49
51.90
18.96
OMe O
CN
Me
8cc'
f1 (ppm)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7.21
7.20
7.19
7.19
7.03
7.03
7.03
7.02
7.01
7.01
7.01
7.00
6.85
6.84
6.83
6.82
6.82
4.64
4.63
4.61
4.59
3.80
3.75
1.51
1.49
OMe
O
MeO
Me
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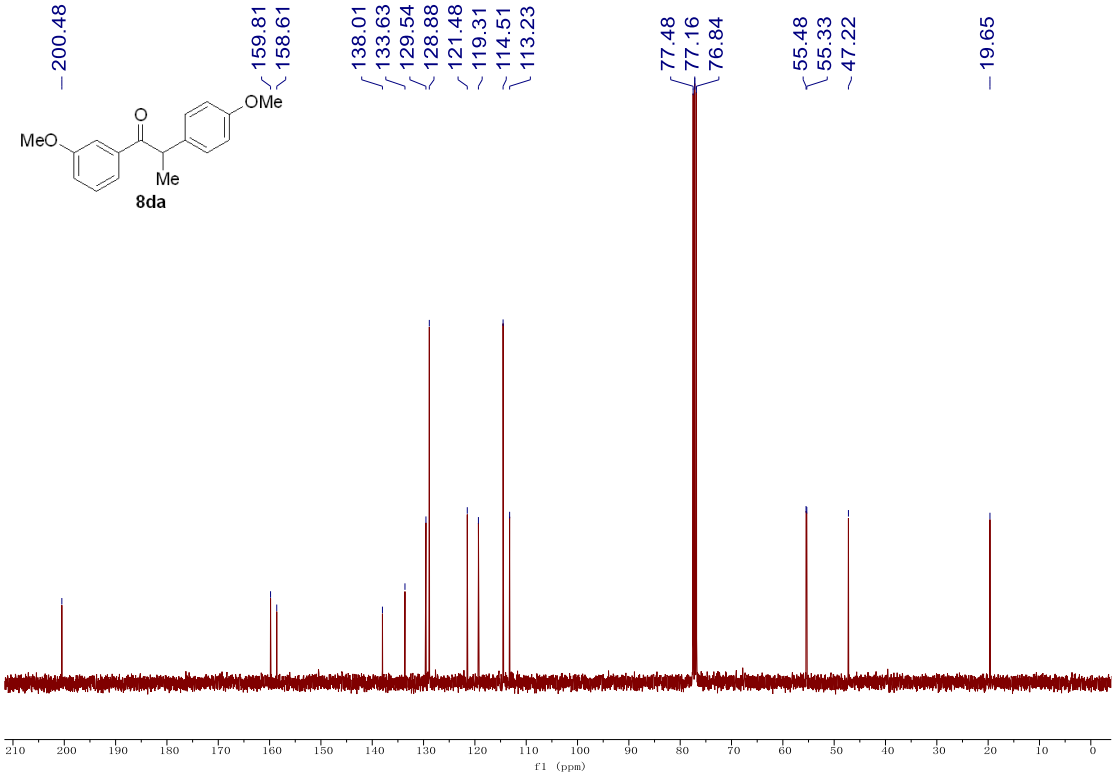
0.97
1.94
1.00
3.05
2.96
2.97
f1 (ppm)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113.23
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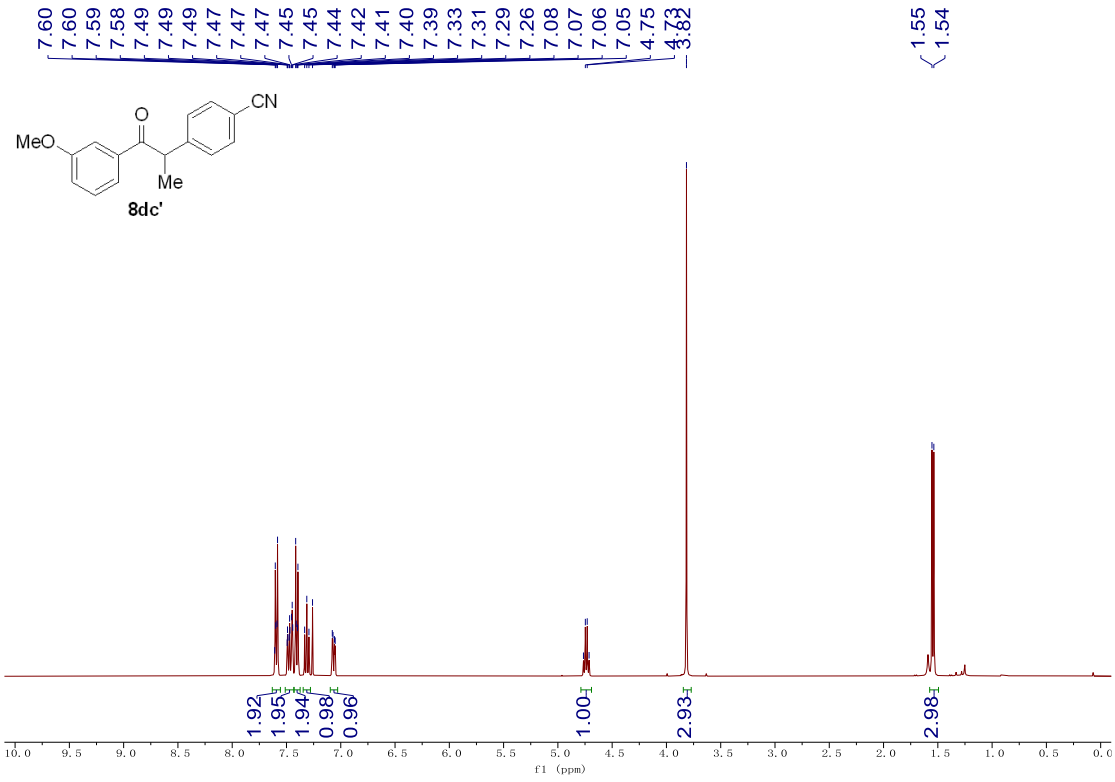
76.84
55.48
55.33
47.22
19.65
OMe
O
MeO
Me
8da
f1 (ppm)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7.44
7.42
7.41
7.40
7.39
7.33
7.31
7.29
7.26
7.08
7.07
7.06
7.05
4.75
4.73
3.82
1.55
1.54
MeO
O
CN
Me
8dc'
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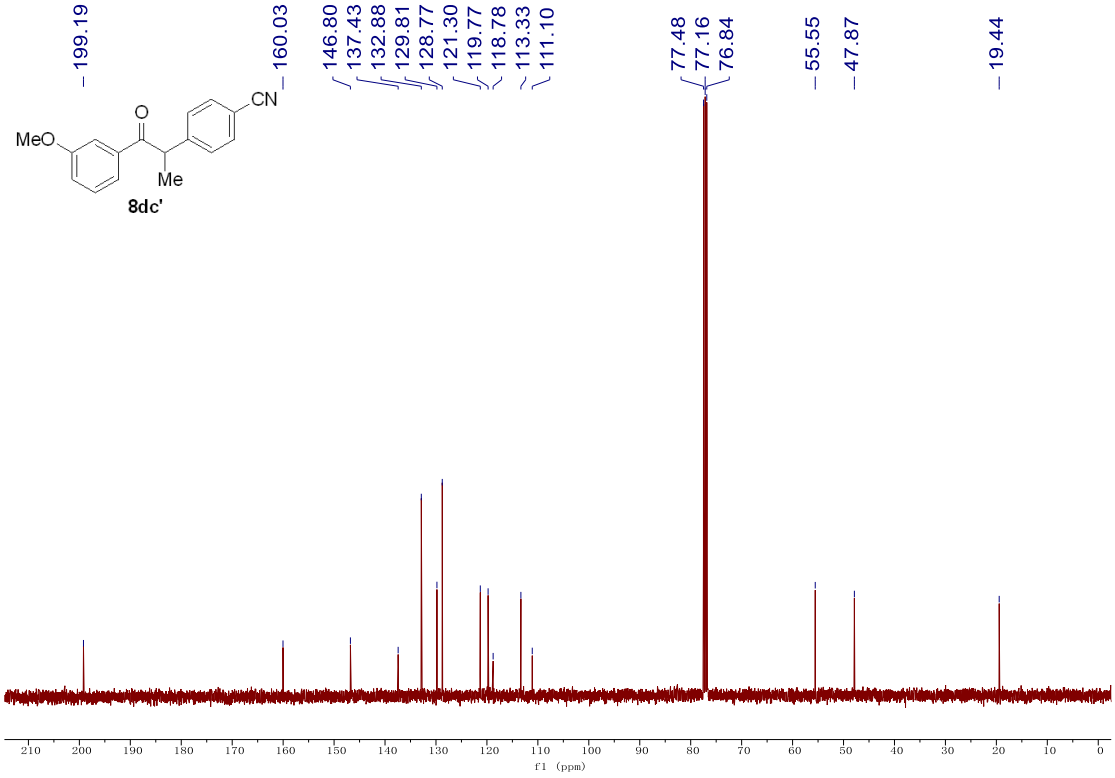
1.95
1.94
0.98
0.96
1.00
2.93
2.98
f1 (ppm)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113.33
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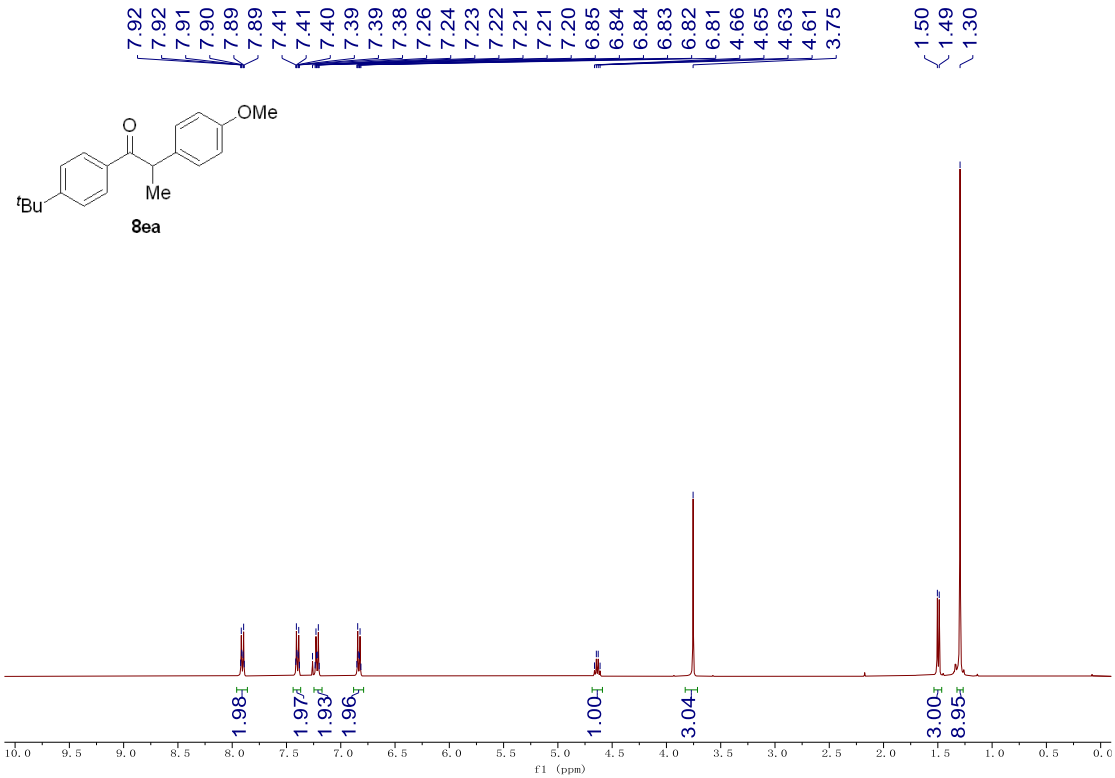
77.16
76.84
55.55
47.87
19.44
MeO
O
CN
Me
8dc'
f1 (ppm)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7.41
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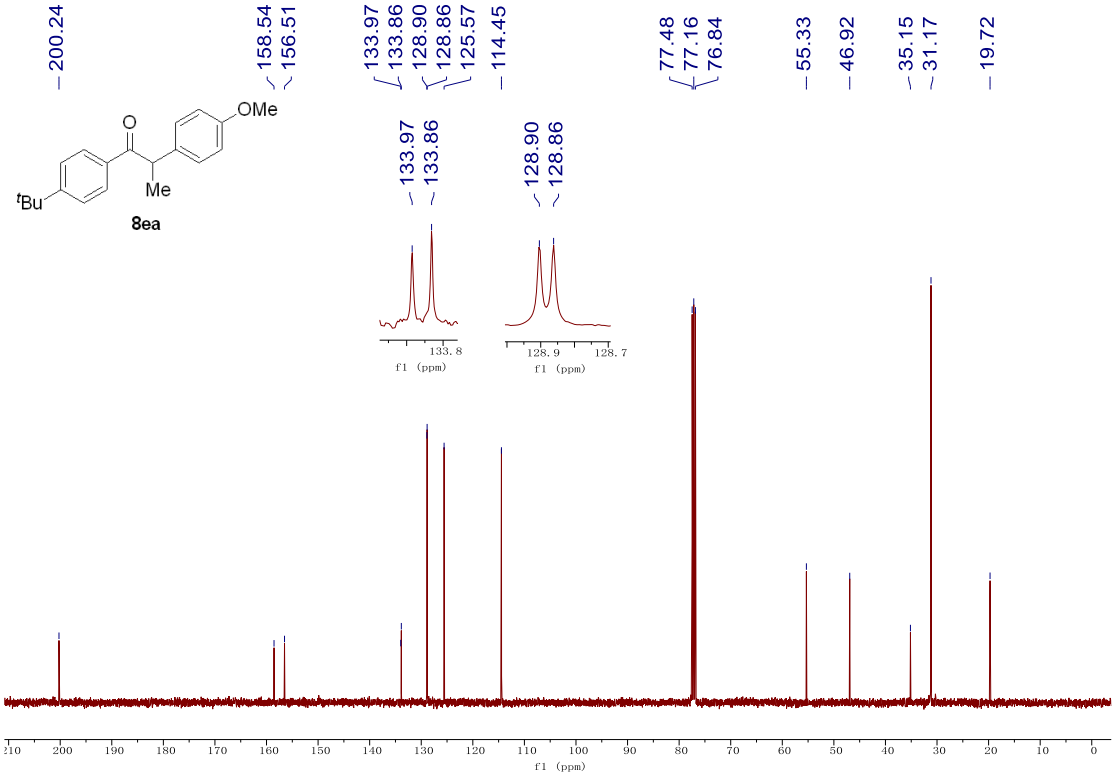
7.39
7.39
7.38
7.26
7.24
7.23
7.22
7.21
7.21
7.20
6.85
6.84
6.84
6.83
6.82
6.81
4.66
4.65
4.63
4.61
3.75
1.50
1.49
1.30
O
OMe
Me
tBu
8ea
1.98
1.97
1.93
1.96
1.00
3.04
3.00
8.95
f1 (ppm)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77.16
76.84
55.33
46.92
35.15
31.17
19.72
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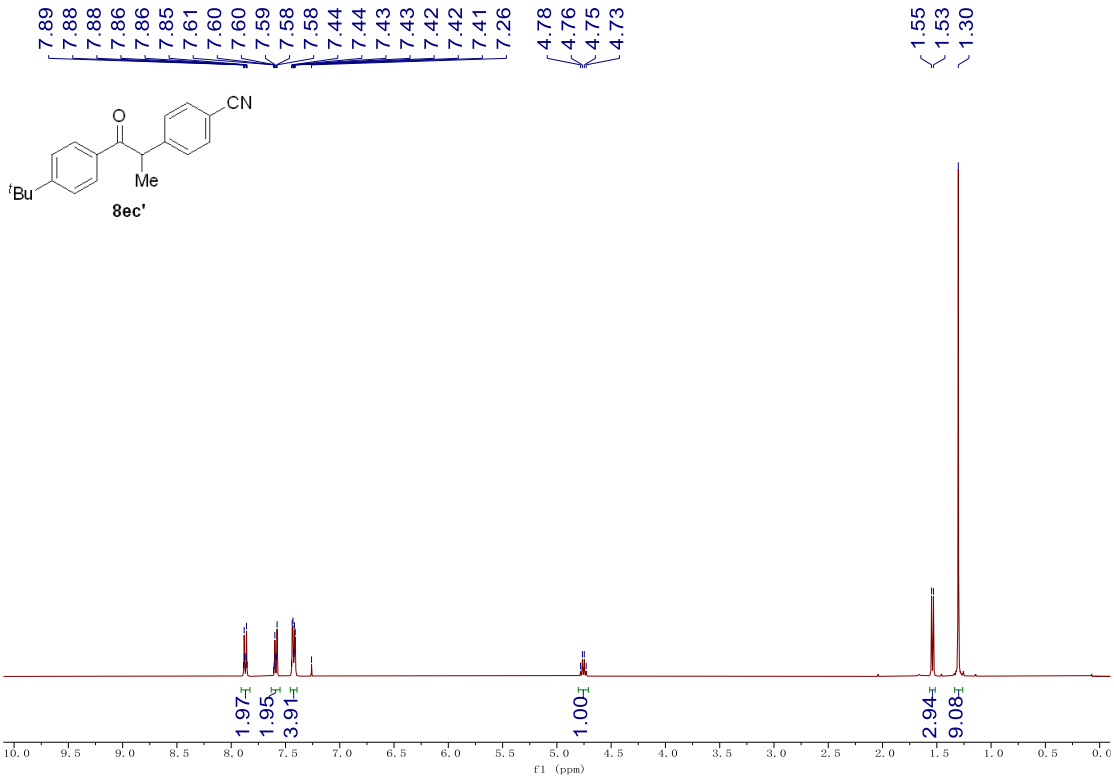
OMe
Me
tBu
8ea
133.97
133.86
128.90
128.86
f1 (ppm)
f1 (ppm)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7.43
7.43
7.42
7.42
7.41
7.26
4.78
4.76
4.75
4.73
1.55
1.53
1.30
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Me
tBu
8ec'
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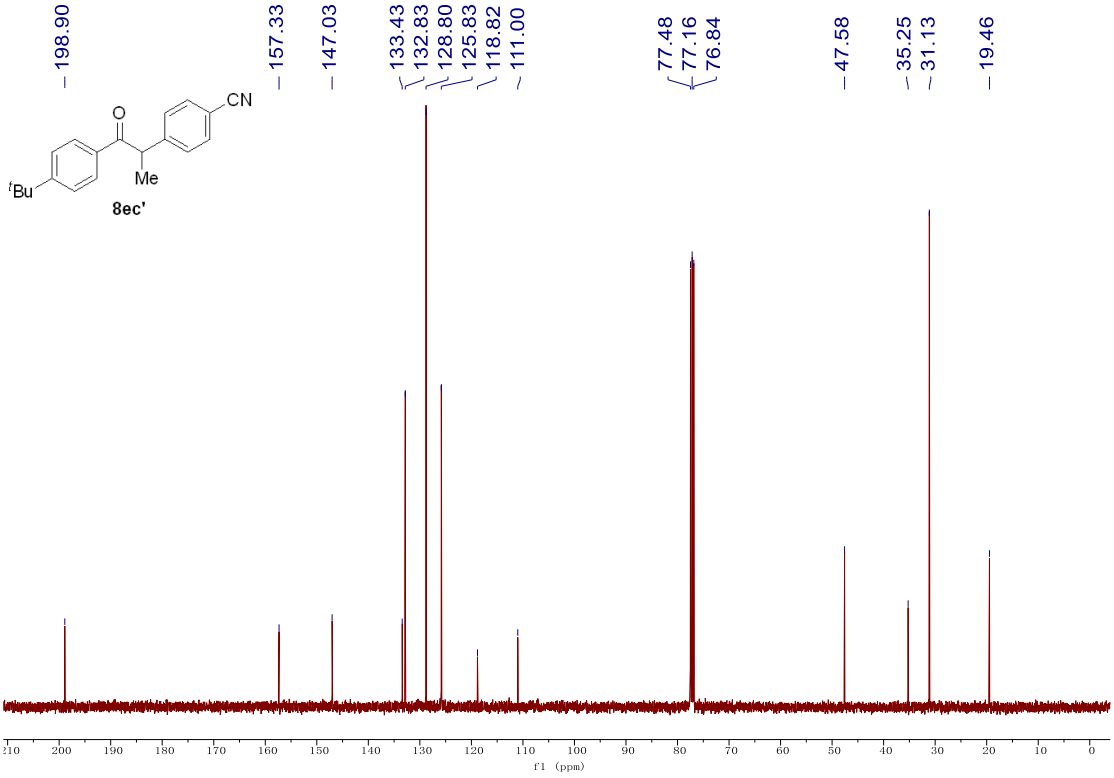
1.95
3.91
1.00
2.94
9.08
f1 (ppm)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125.83
118.82
111.00
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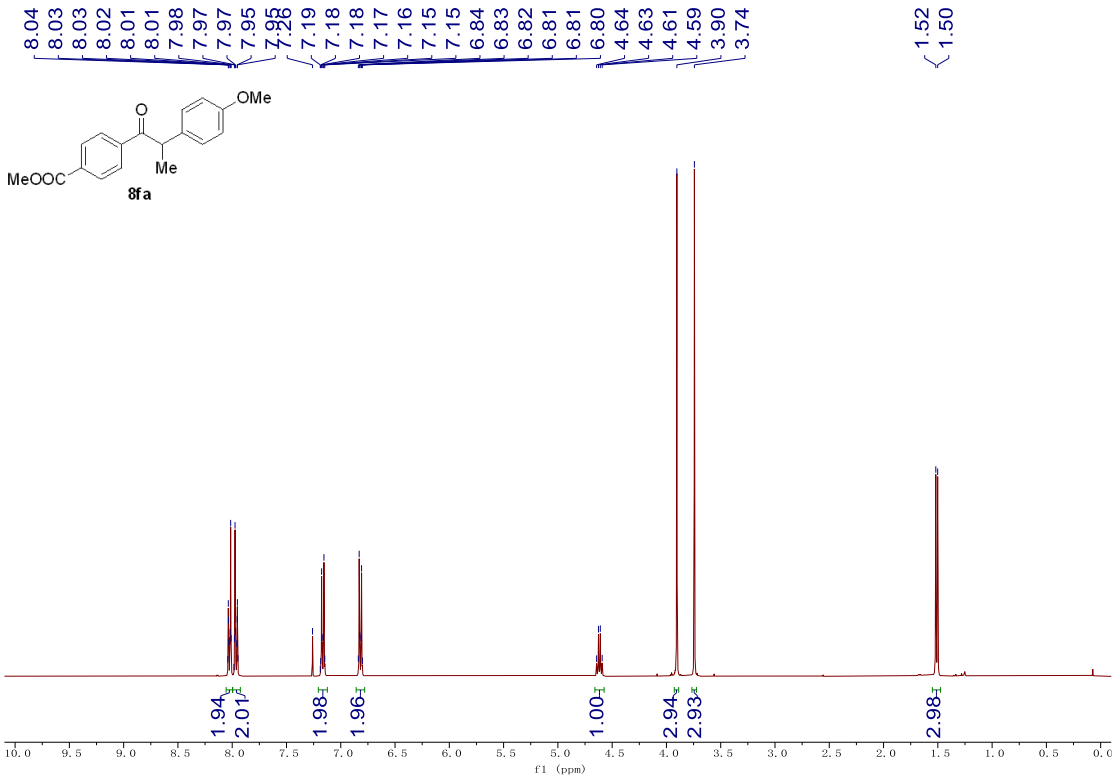
76.84
47.58
35.25
31.13
19.46
O
CN
Me
tBu
8ec'
f1 (ppm)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7.19
7.18
7.18
7.17
7.16
7.15
7.15
6.84
6.83
6.82
6.81
6.81
6.80
4.64
4.63
4.61
4.59
3.90
3.74
1.52
1.50
OMe
O
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MeOOC
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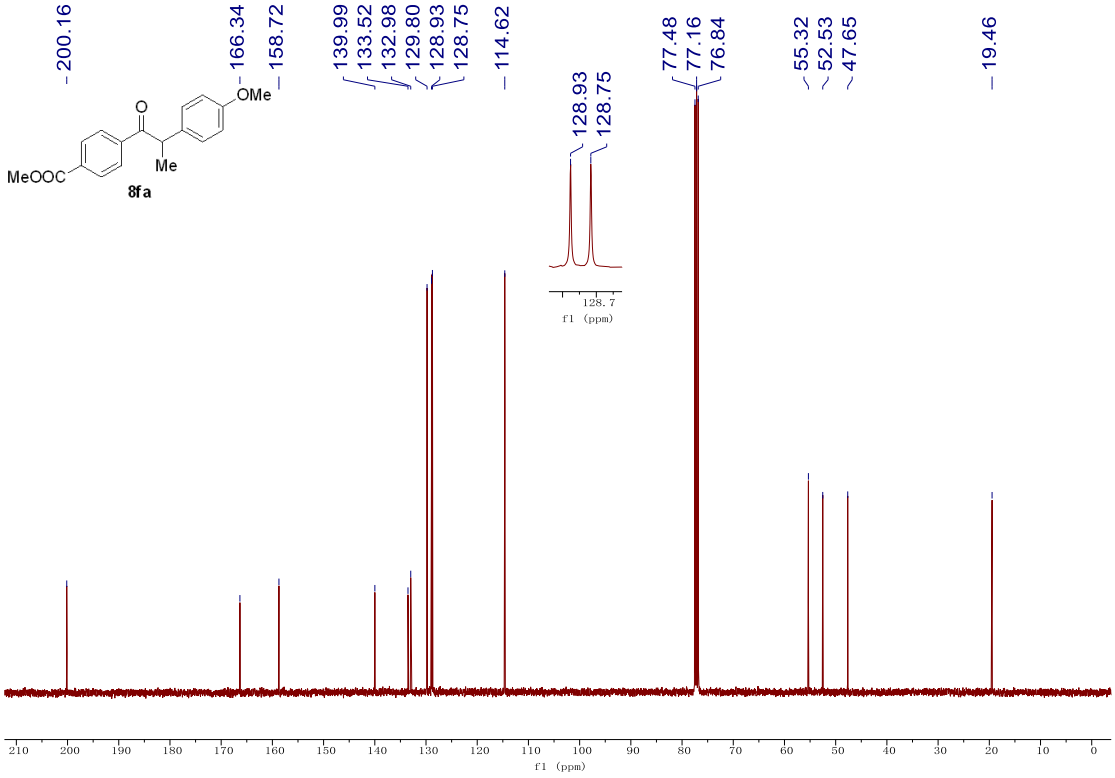
1.00
2.94
2.93
2.98
f1 (ppm)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77.48
77.16
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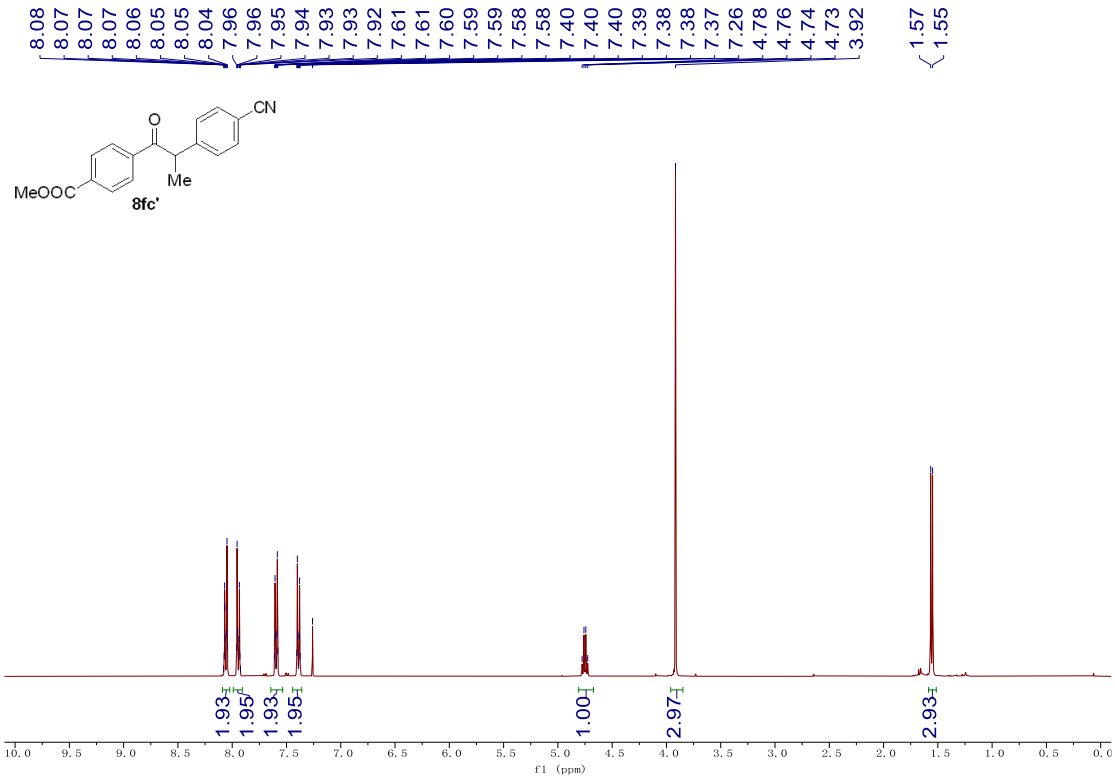
47.65
19.46
128.93
128.75
OMe
O
Me
MeOOC
8fa
f1 (ppm)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8.05
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8.04
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7.94
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7.38
7.38
7.37
7.26
4.78
4.76
4.74
4.73
3.92
1.57
1.55
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Me
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8fc'
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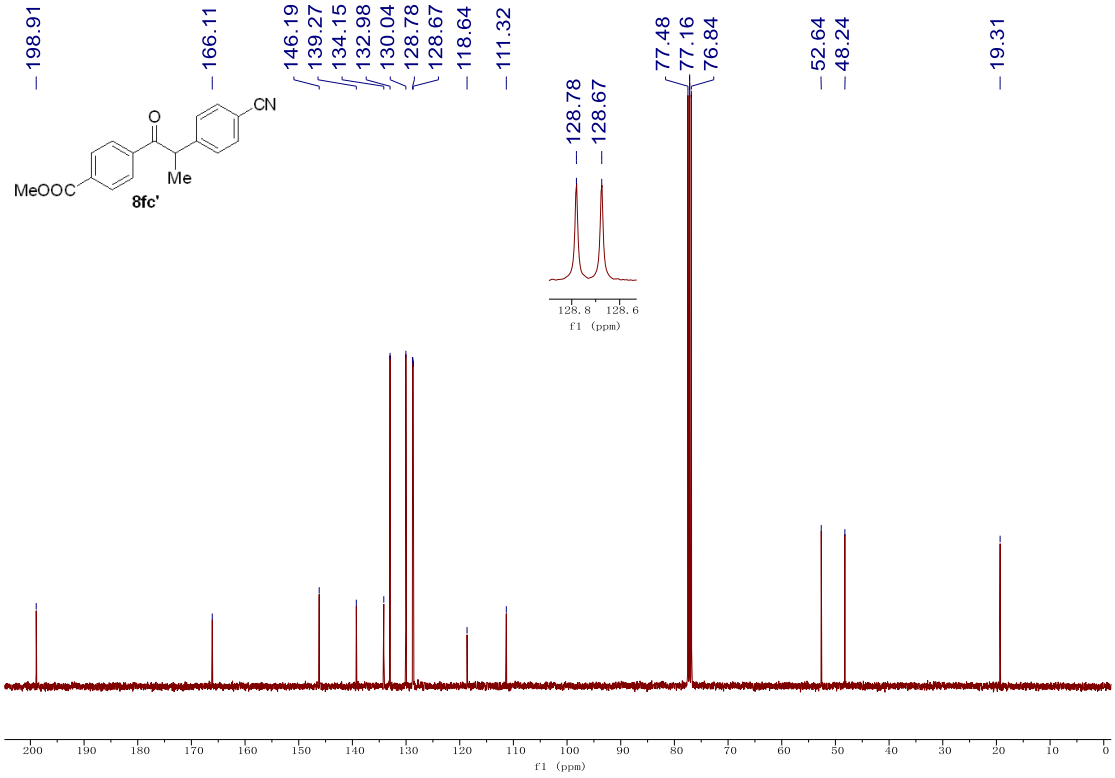
1.95
1.93
1.95
1.00
2.97
2.93
f1 (ppm)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111.32
77.48
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76.84
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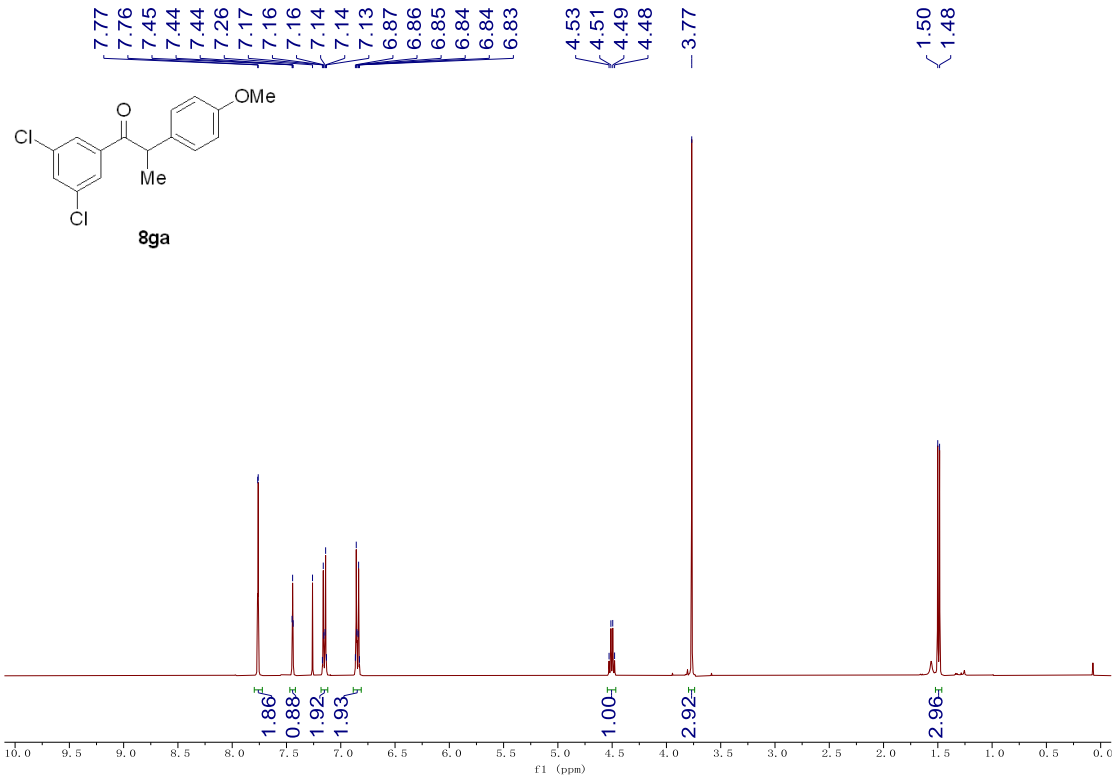
48.24
19.31
128.78
128.67
CN
O
Me
MeOOC
8fc'
f1 (ppm)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7.13
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6.84
6.83
4.53
4.51
4.49
4.48
3.77
1.50
1.48
O
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1.00
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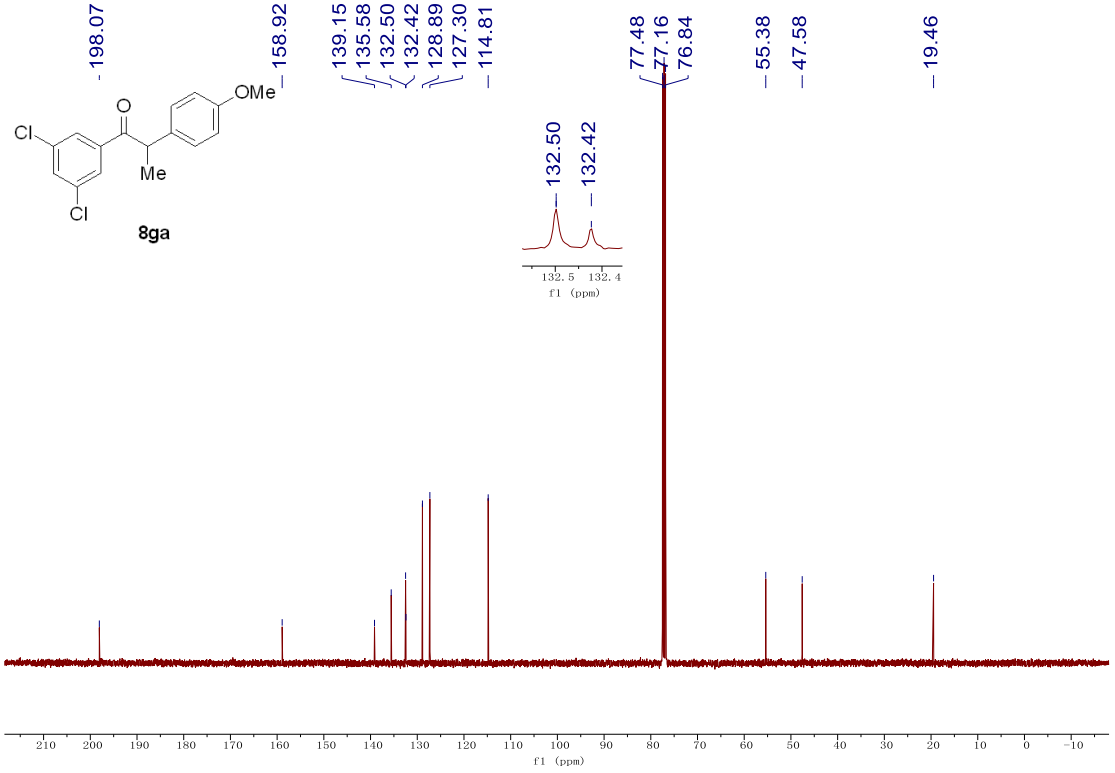
2.96
f1 (ppm)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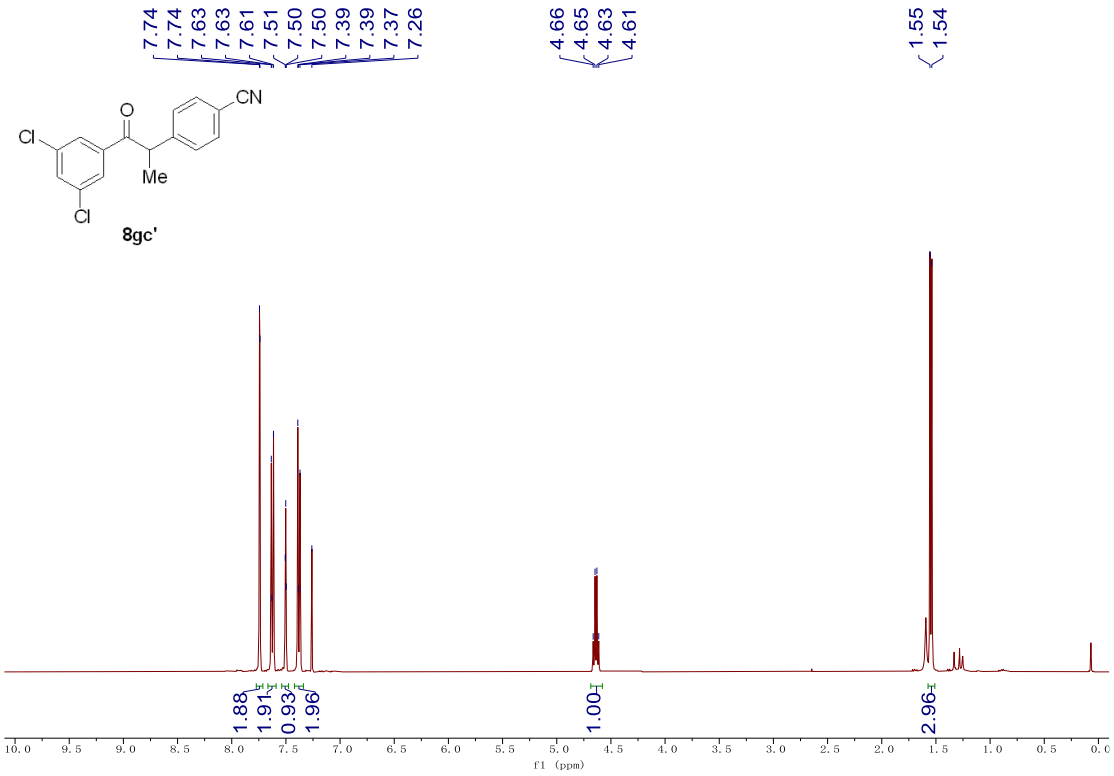
132.50
132.42
O
OMe
Cl
Me
Cl
8ga
f1 (ppm)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7.39
7.37
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4.66
4.65
4.63
4.61
1.55
1.54
Cl
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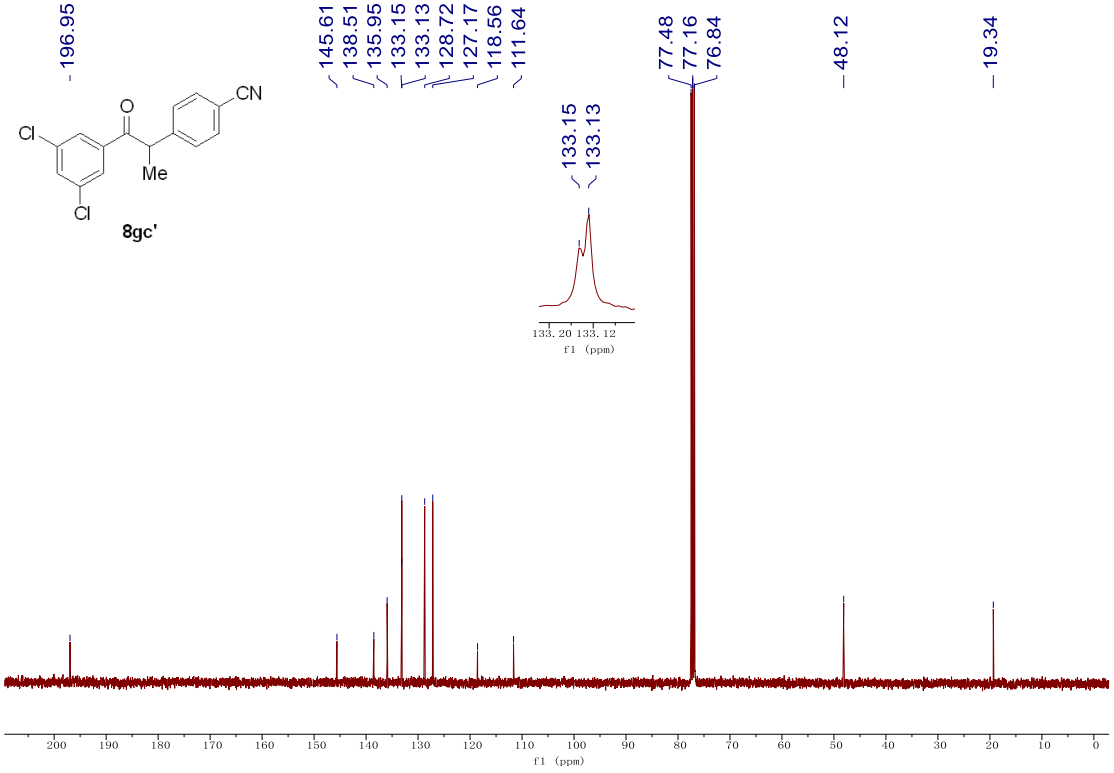
CN
Me
Cl
8gc'
1.88
1.91
0.93
1.96
1.00
2.96
f1 (ppm)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118.56
111.64
77.48
77.16
76.84
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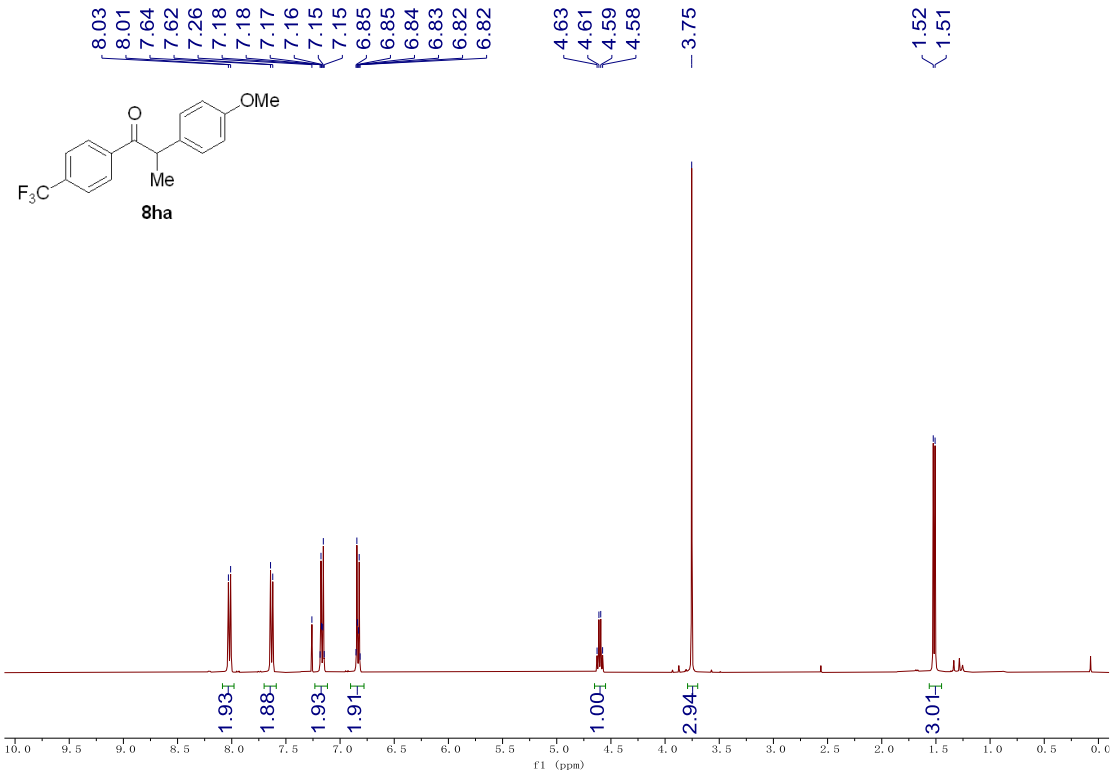
133.15
133.13
133.20 133.12
f1 (ppm)
Cl
O
CN
Me
Cl
8gc'
f1 (ppm)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7.15
7.15
6.85
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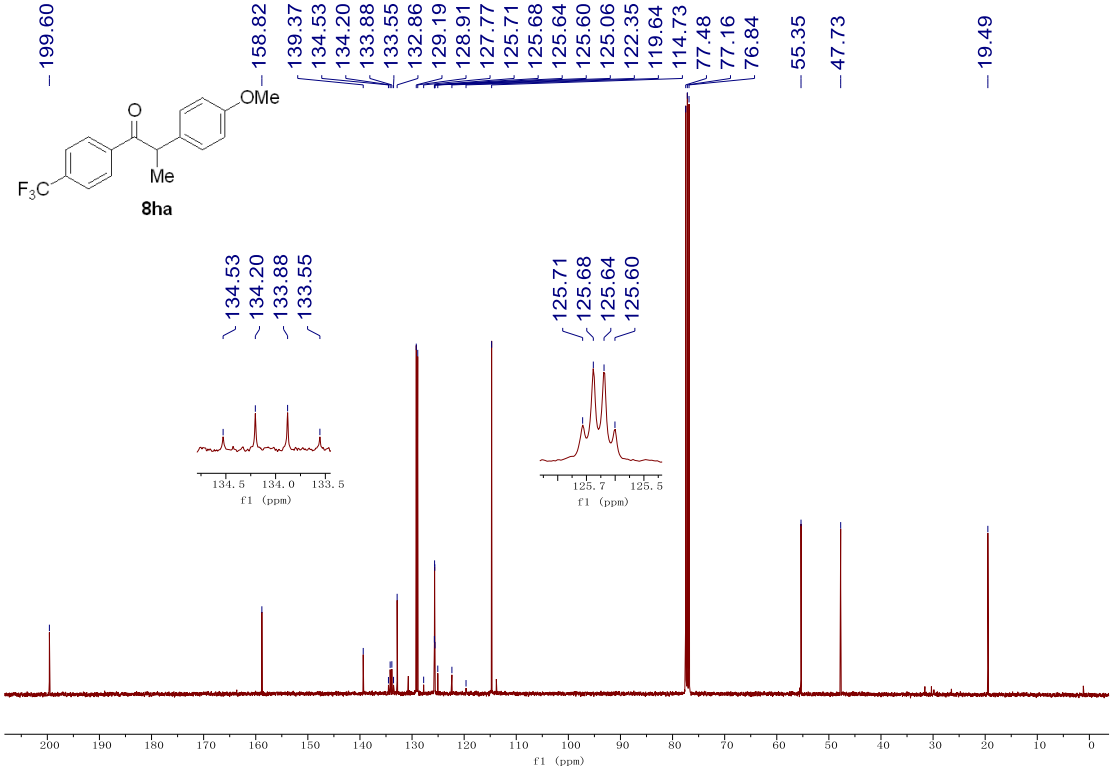
6.84
6.83
6.82
6.82
4.63
4.61
4.59
4.58
3.75
1.52
1.51
OMe
O
Me
F3C
8ha
1.93
1.88
1.93
1.91
1.00
2.94
3.01
f1 (ppm)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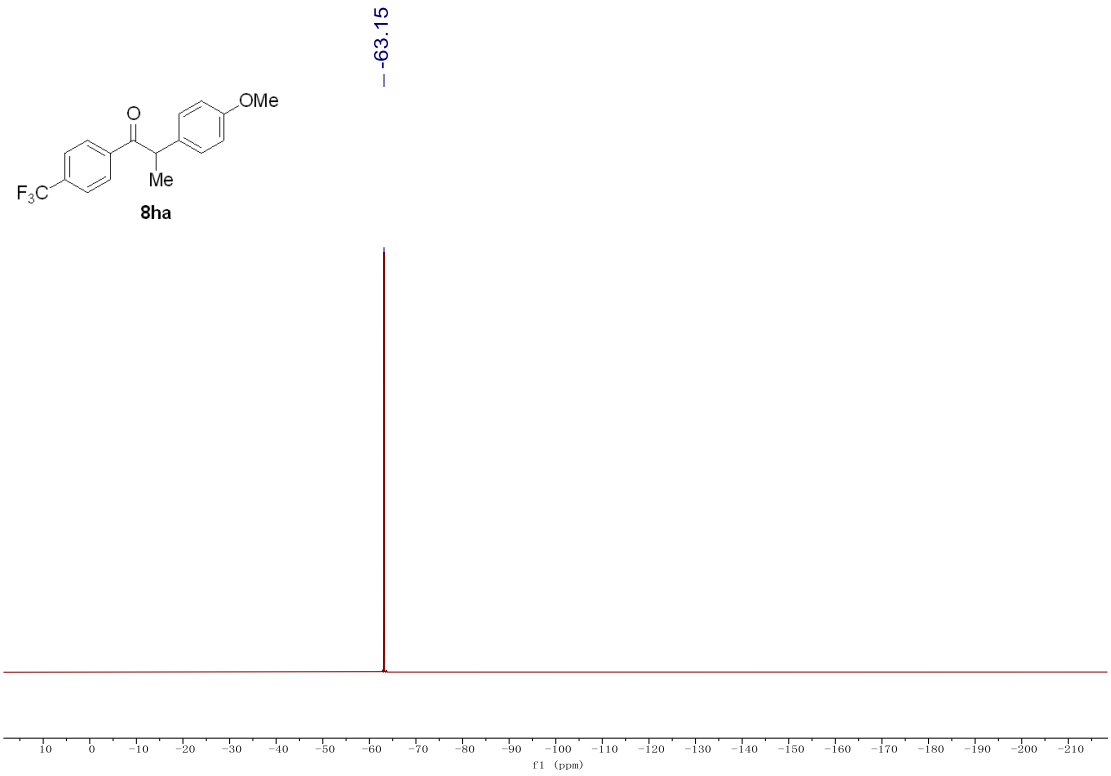
125.71
125.68
125.64
125.60
125.06
122.35
119.64
114.73
77.48
77.16
76.84
55.35
47.73
19.49
OMe
O
Me
F3C
8ha
134.53
134.20
133.88
133.55
125.71
125.68
125.64
125.60
f1 (ppm)
f1 (ppm)
f1 (ppm)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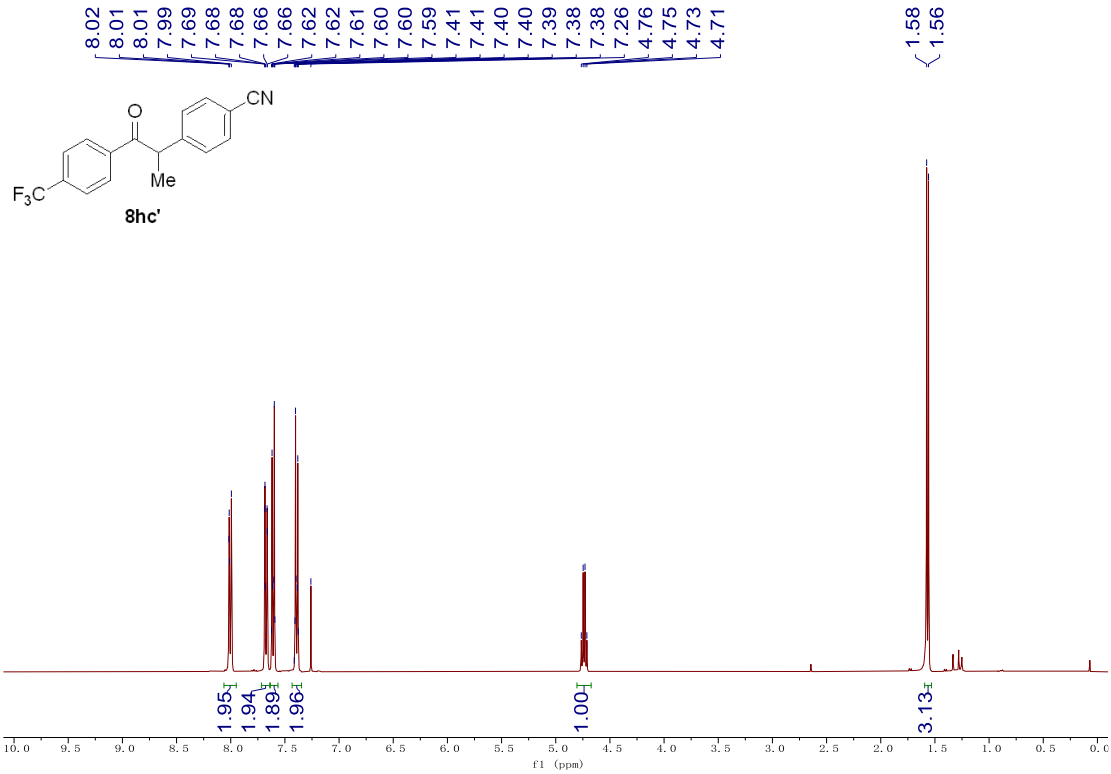
Me
F3C
8ha
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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7.60
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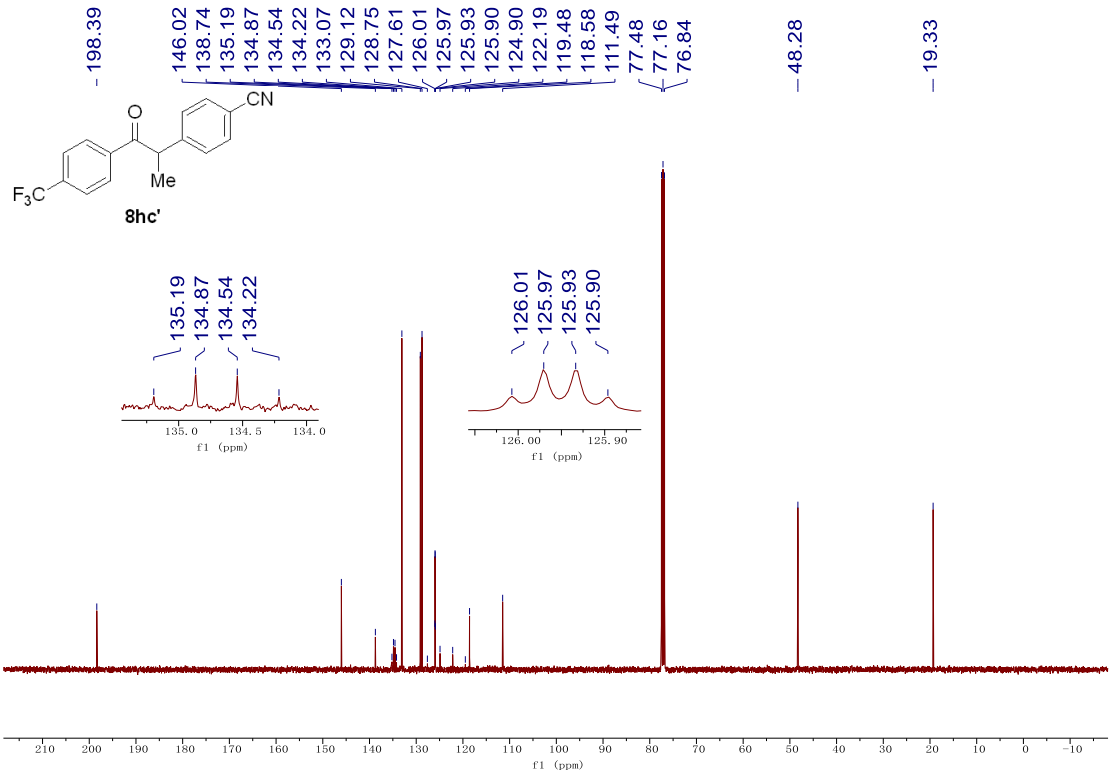
7.40
7.40
7.39
7.38
7.38
7.26
4.76
4.75
4.73
4.71
1.58
1.56
CN
O
Me
F3C
8hc'
1.95
1.94
1.89
1.96
1.00
3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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127.61
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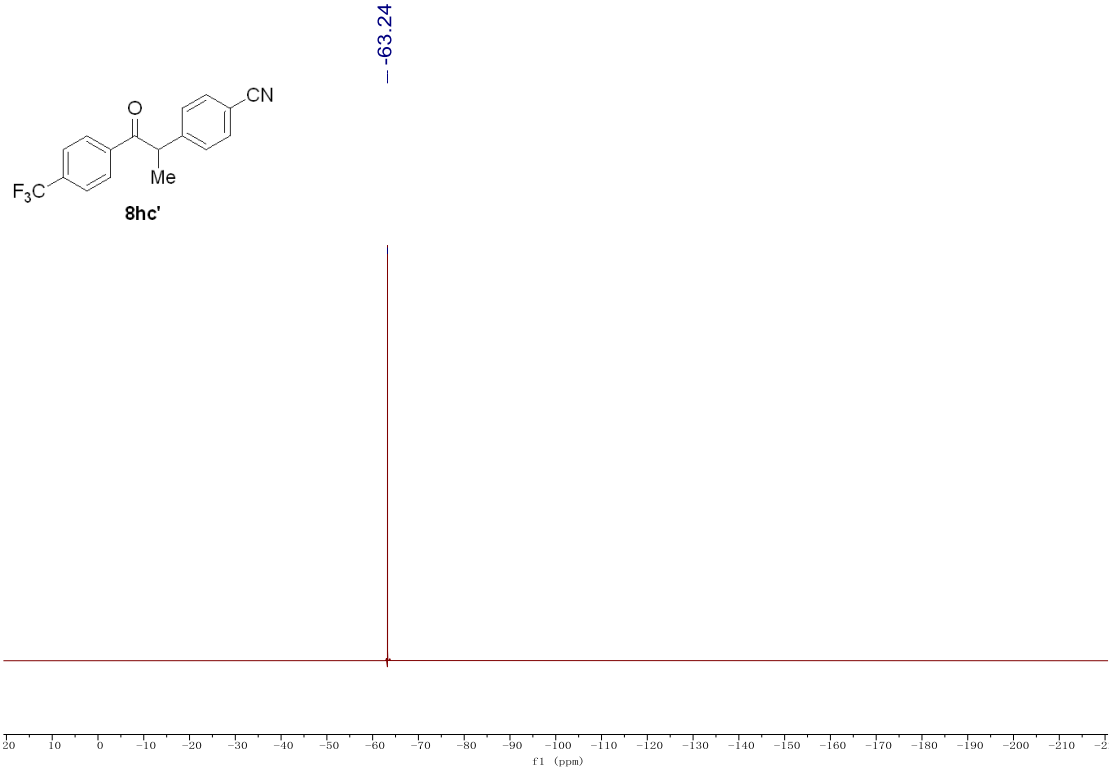
125.93
125.90
124.90
122.19
119.48
118.58
111.49
77.48
77.16
76.84
48.28
19.33
O
CN
Me
F3C
8hc'
135.19
134.87
134.54
134.22
126.01
125.97
125.93
125.90
f1 (ppm)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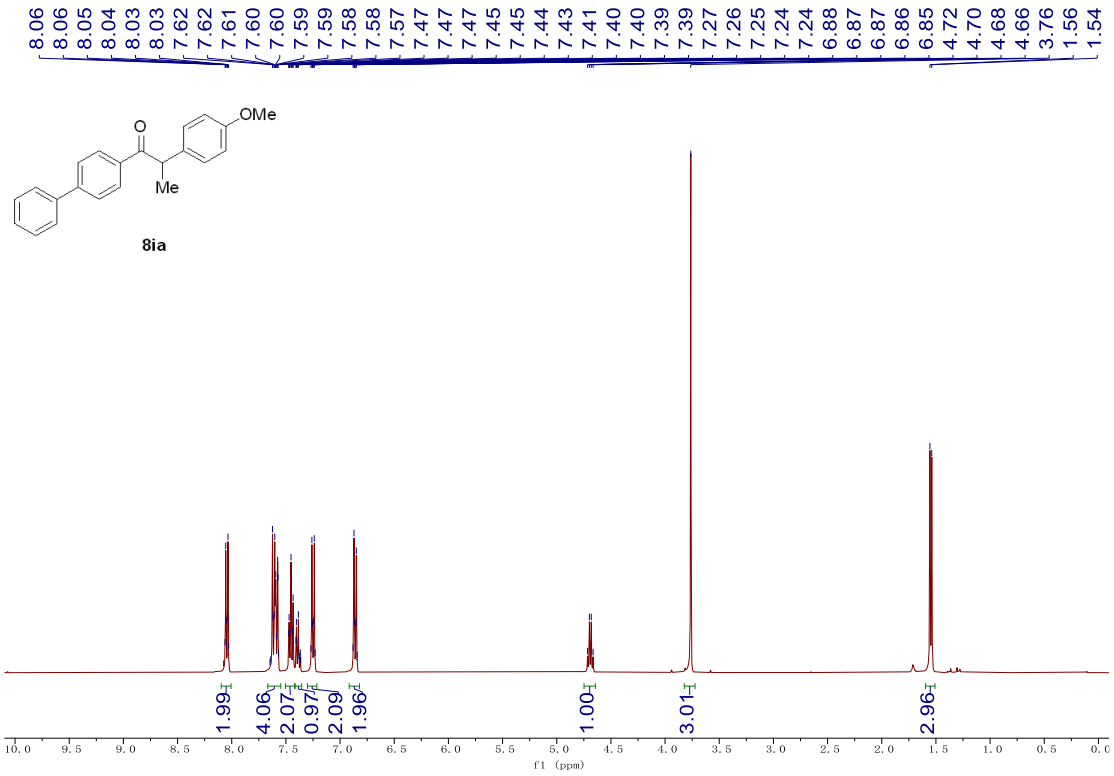
CN
Me
F3C
8hc'
f1 (ppm)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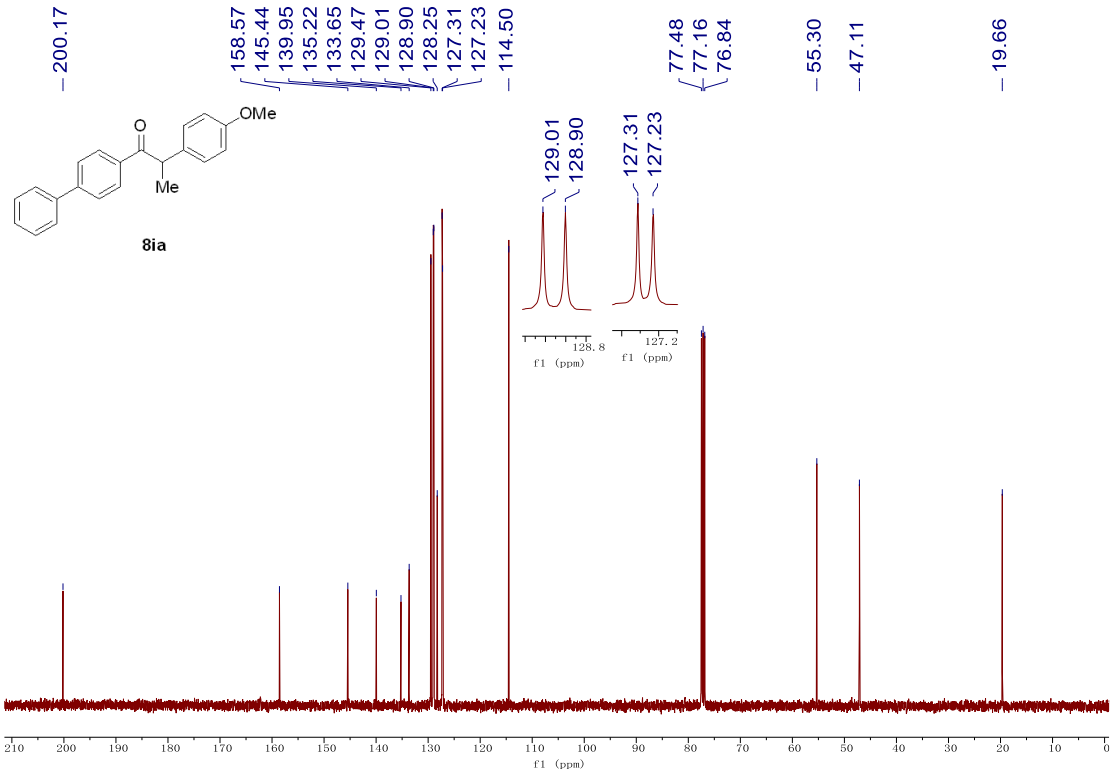
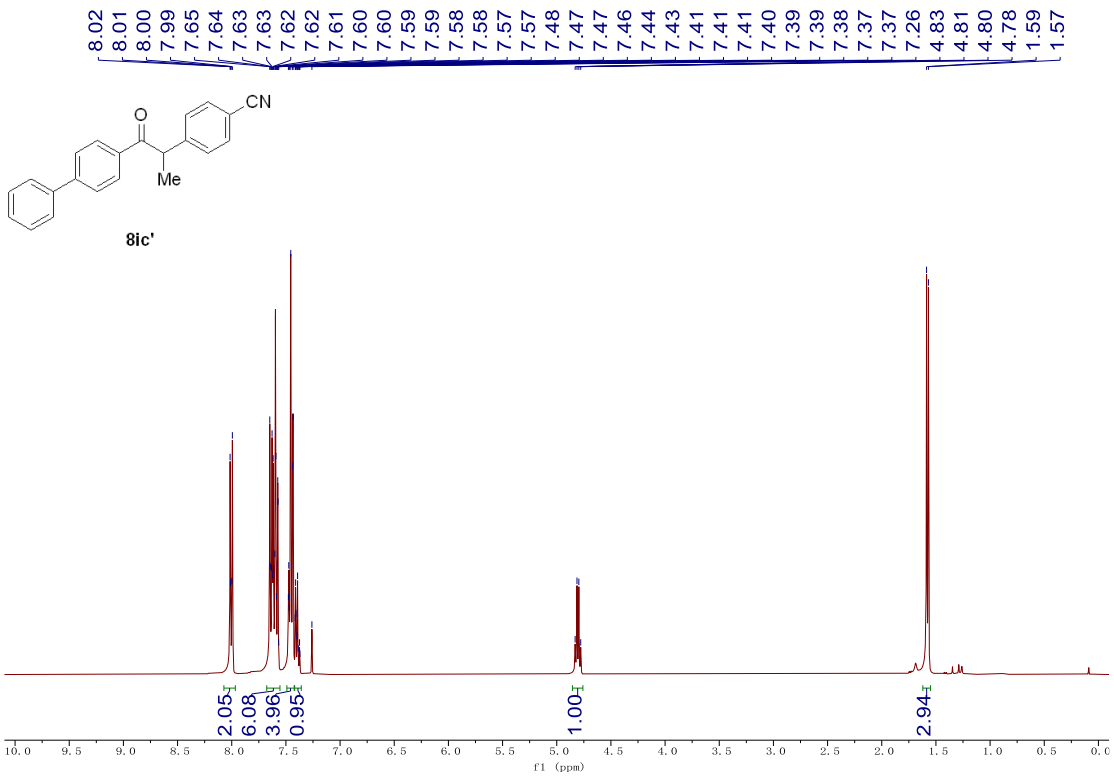
OMe
O
Me
8ia
1.99 4.06 2.07 0.97 2.09 1.96 1.00 3.01 2.96
f1 (ppm)


200.17 158.57 145.44 139.95 135.22 133.65 129.47 129.01 128.90 128.25 127.31 127.23 114.50 77.48 77.16 76.84 55.30 47.11 19.66
OMe
O
Me
8ia
129.01 128.90 127.31 127.23
f1 (ppm)
f1 (ppm)
f1 (ppm)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7.47
7.47
7.46
7.44
7.43
7.41
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
7.26
4.83
4.81
4.80
4.78
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CN
Me
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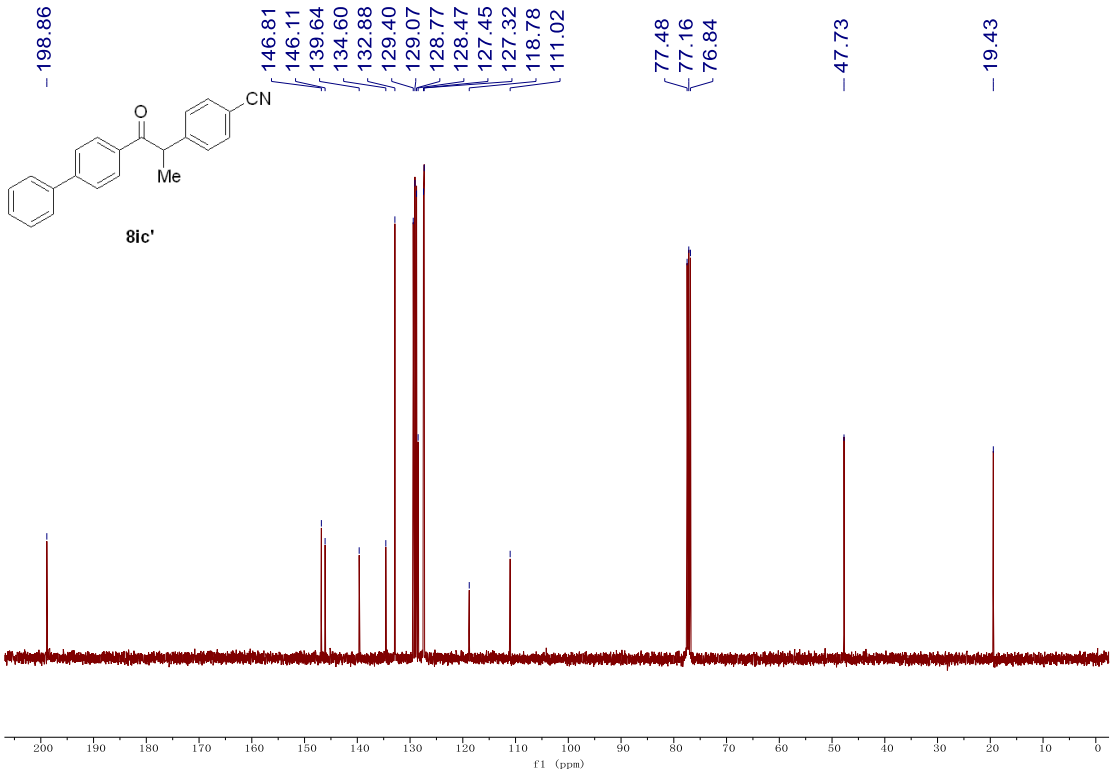
1.00
2.94
f1 (ppm)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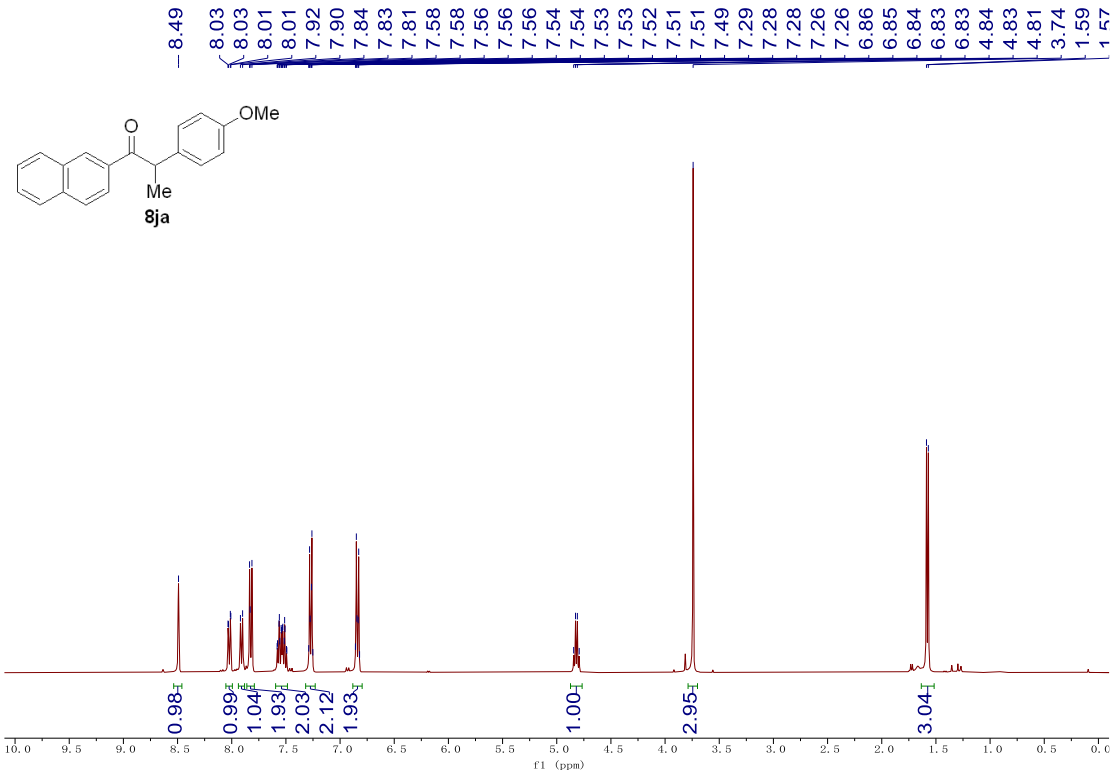
47.73
19.43
O
CN
Me
8ic'
f1 (ppm)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7.53
7.52
7.51
7.51
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7.29
7.28
7.28
7.26
7.26
6.86
6.85
6.84
6.83
6.83
4.84
4.83
4.81
3.74
1.59
O
OMe
Me
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2.03
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1.00
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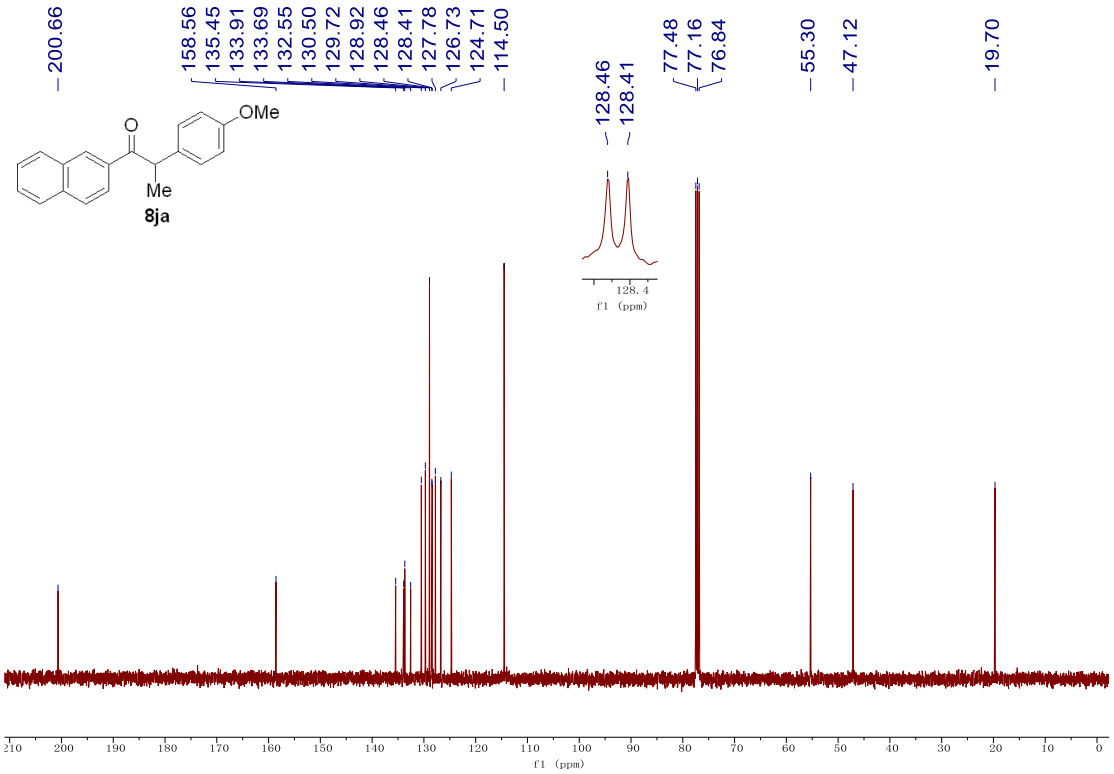
3.04
f1 (ppm)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126.73
124.71
114.50
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55.30
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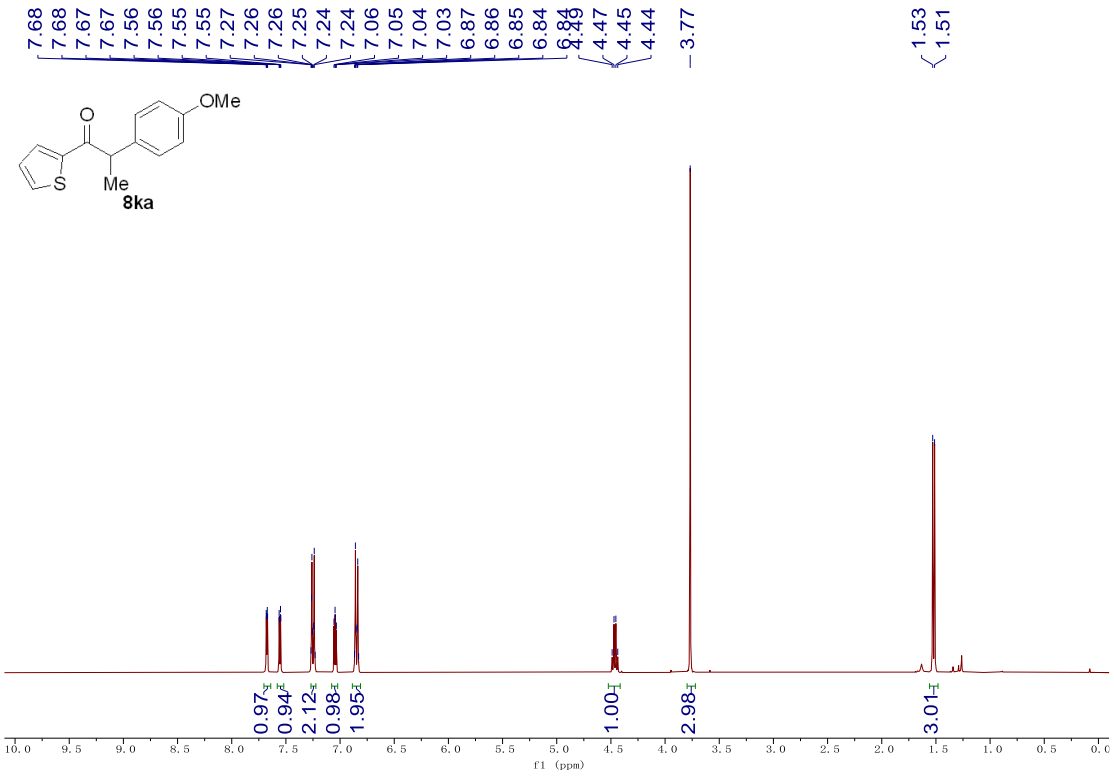
128.41
O
OMe
Me
8ja
f1 (ppm)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7.24
7.24
7.06
7.05
7.04
7.03
6.87
6.86
6.85
6.84
6.84
4.49
4.47
4.45
4.44
3.77
1.53
1.51
O
OMe
S
Me
8ka
0.97
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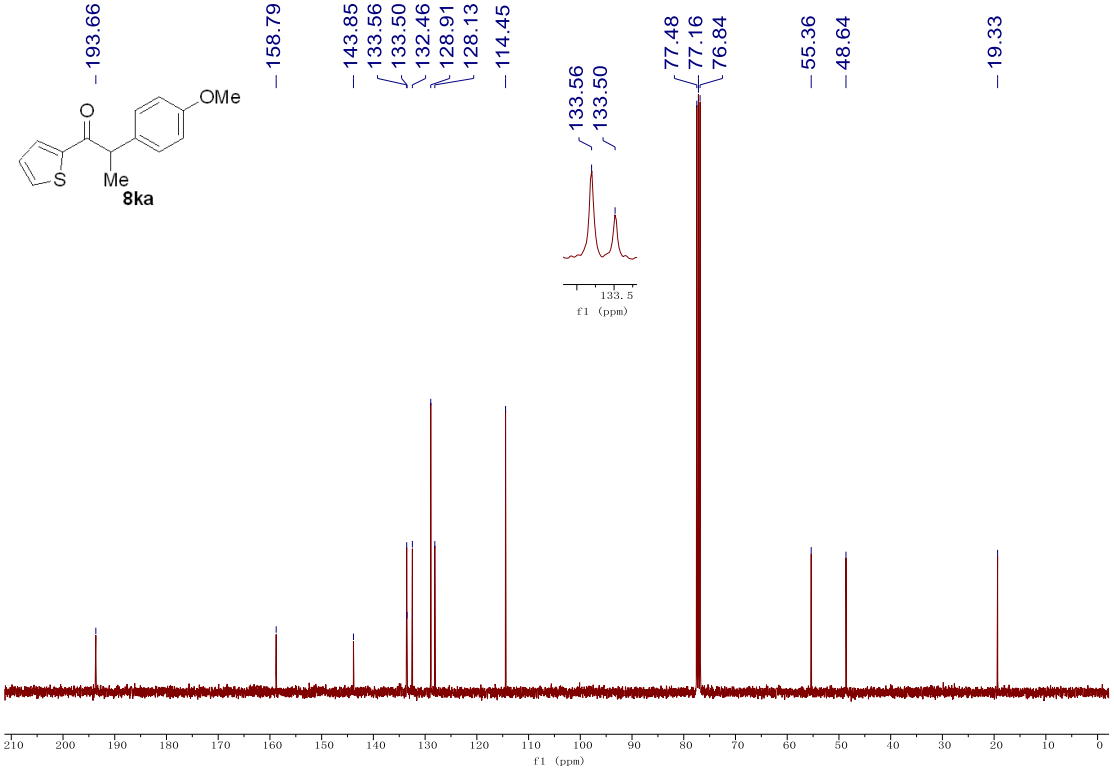
2.12
0.98
1.95
1.00
2.98
3.01
f1 (ppm)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132.46
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128.13
114.45
77.48
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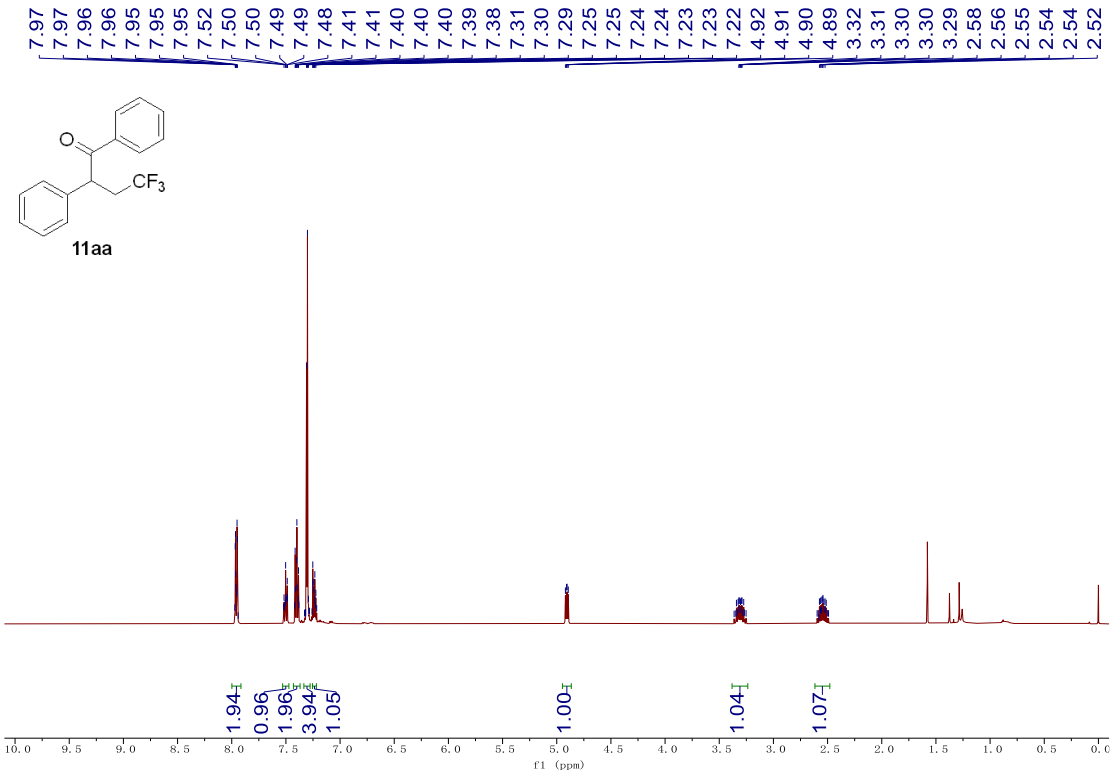
55.36
48.64
19.33
133.56
133.50
O
OMe
S
Me
8ka
f1 (ppm)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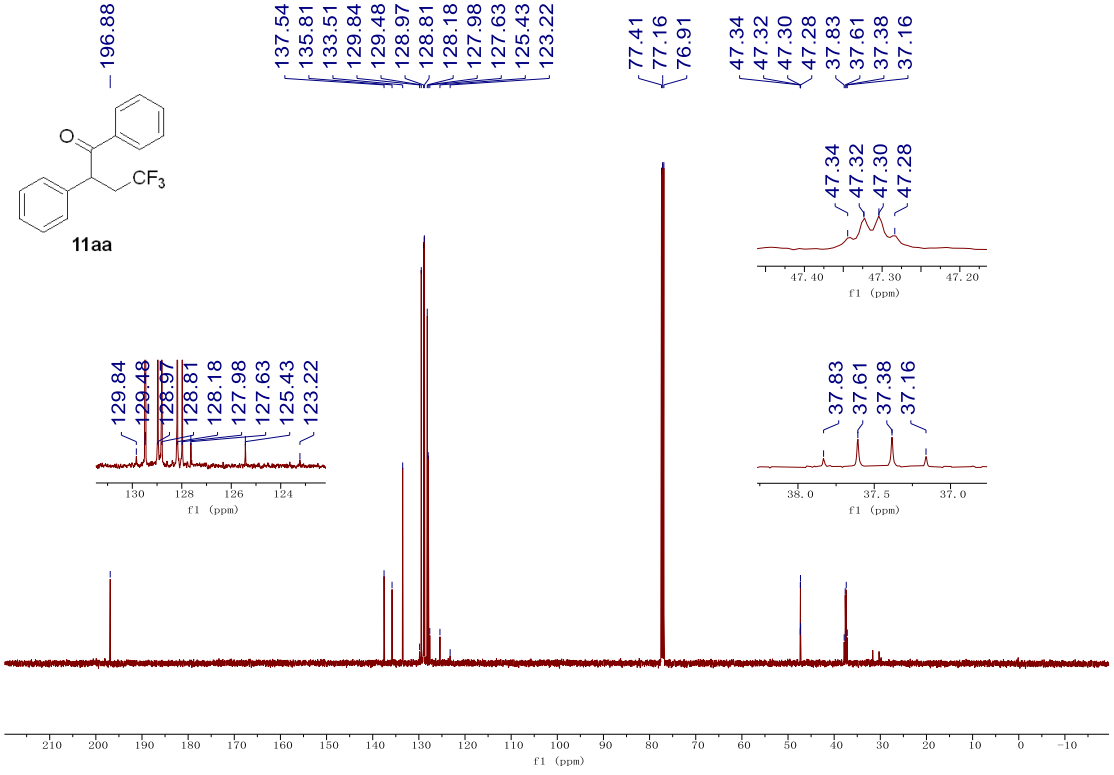
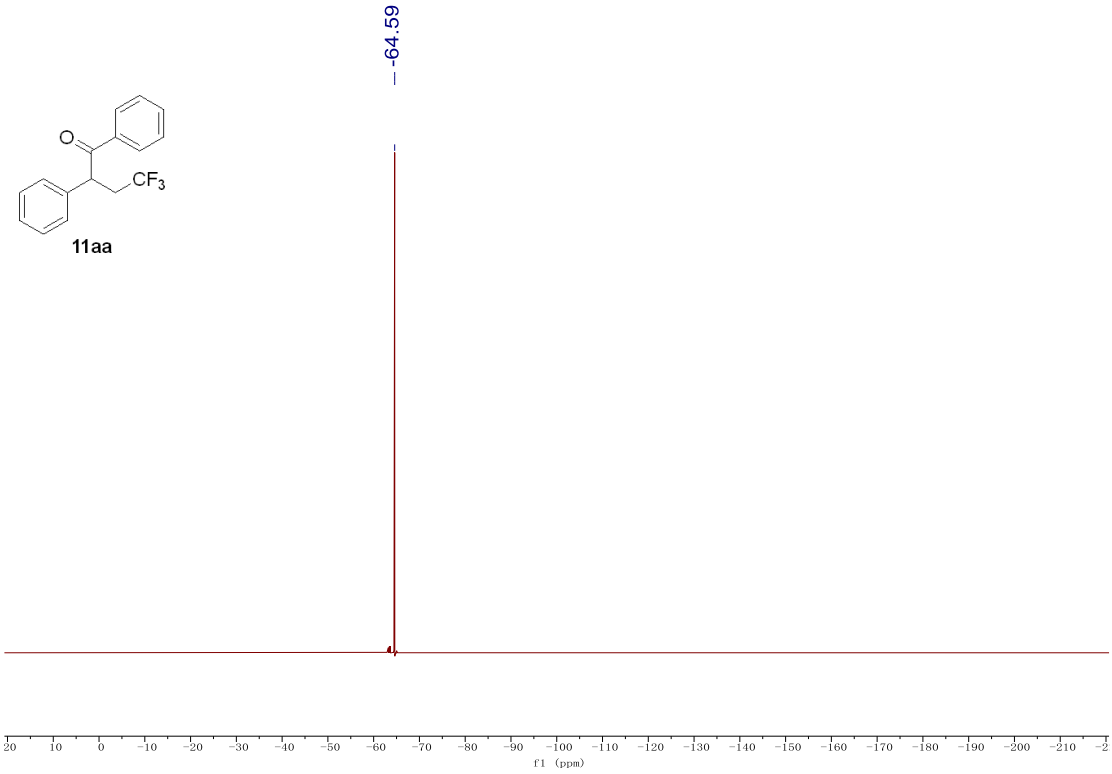
O
CF3
11aa
1.94 0.96 1.96 3.94 1.05 1.00 1.04 1.07
f1 (ppm)


196.88
137.54 135.81 133.51 129.84 129.48 128.97 128.81 128.18 127.98 127.63 125.43 123.22
77.41 77.16 76.91
47.34 47.32 47.30 47.28 37.83 37.61 37.38 37.16
O
CF3
11aa
47.34 47.32 47.30 47.28
129.84 129.48 128.97 128.81 128.18 127.98 127.63 125.43 123.22
37.83 37.61 37.38 37.16
f1 (ppm)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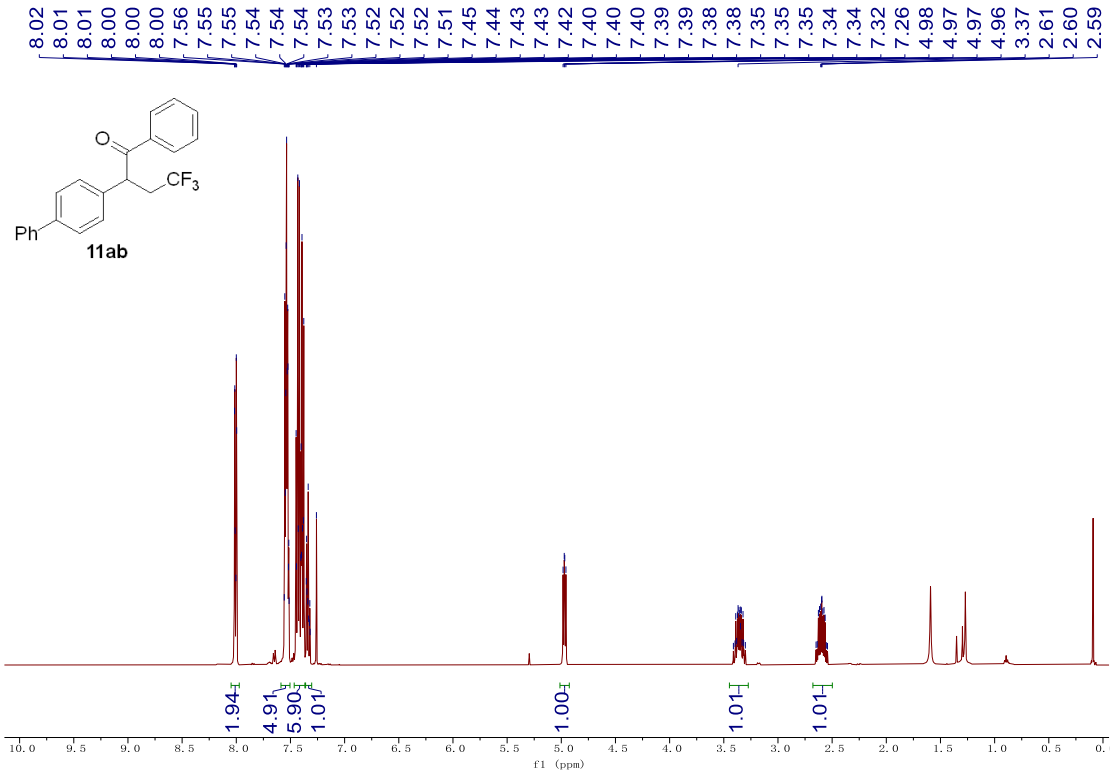
CF3
11aa
f1 (ppm)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8.01
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7.34
7.34
7.32
7.26
4.98
4.97
4.97
4.96
3.37
2.61
2.60
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Ph
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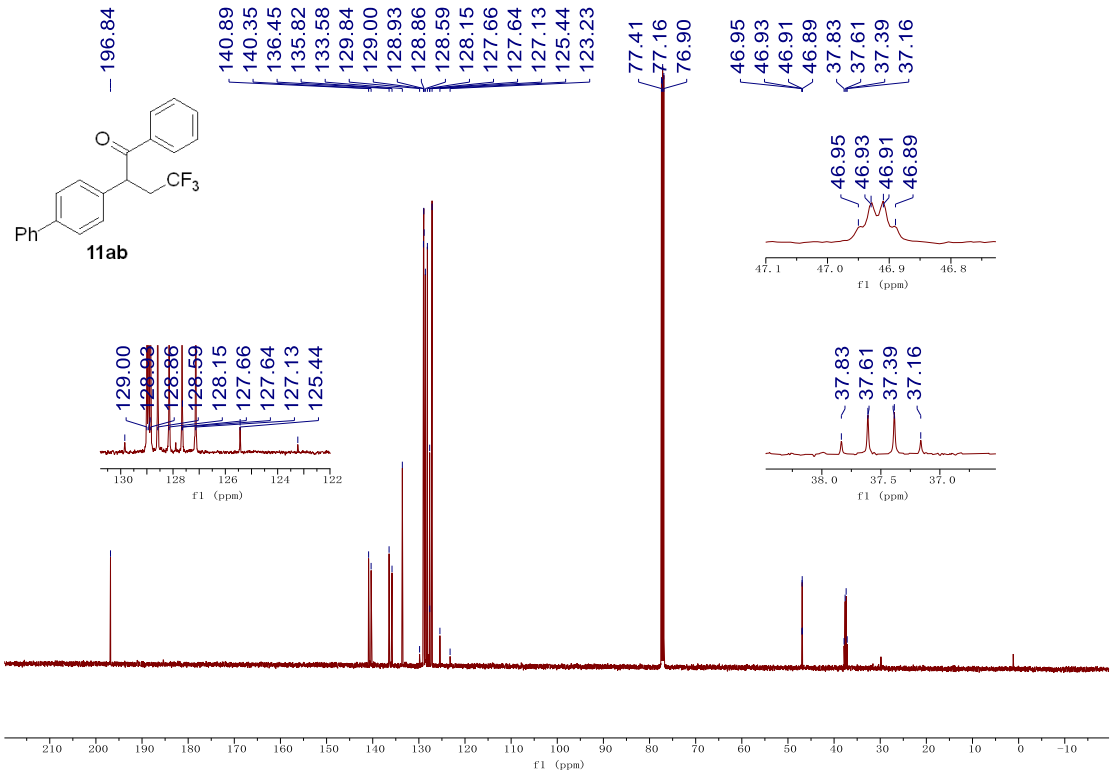
4.91
5.90
1.01
1.00
1.01
1.01
f1 (ppm)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129.00
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128.86
128.59
128.15
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127.64
127.13
125.44
123.23
77.41
77.16
76.90
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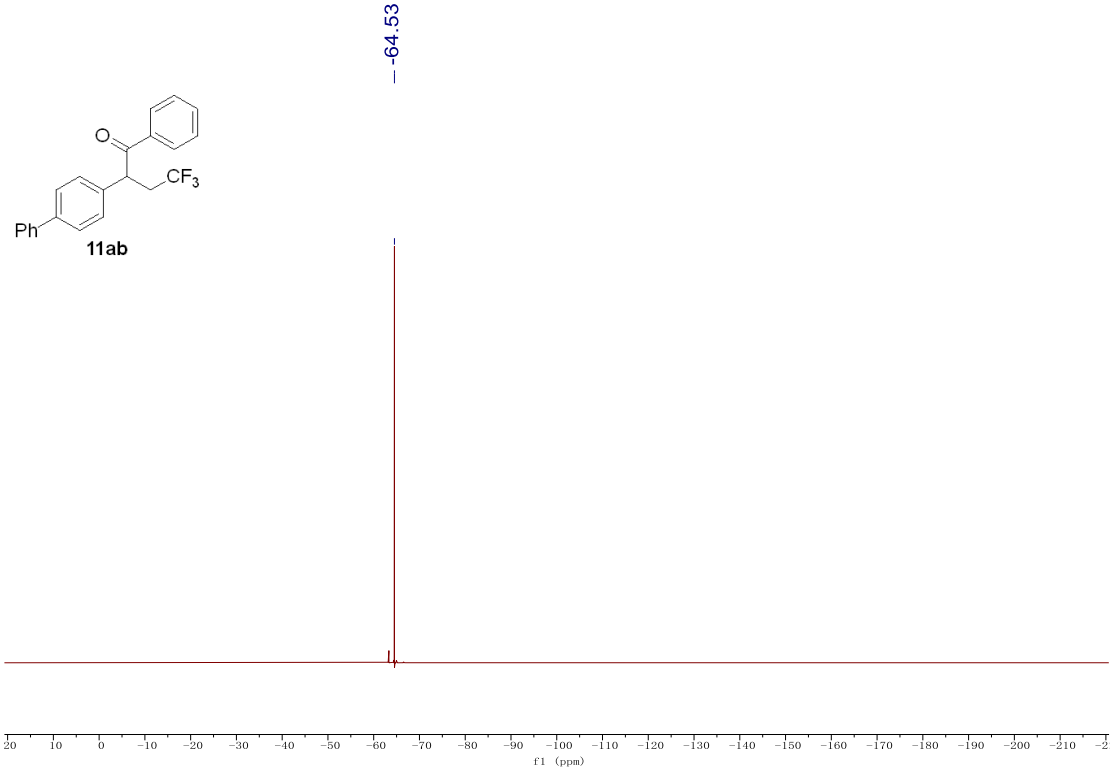
37.61
37.39
37.16
O
CF3
Ph
11ab
f1 (ppm)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Ph
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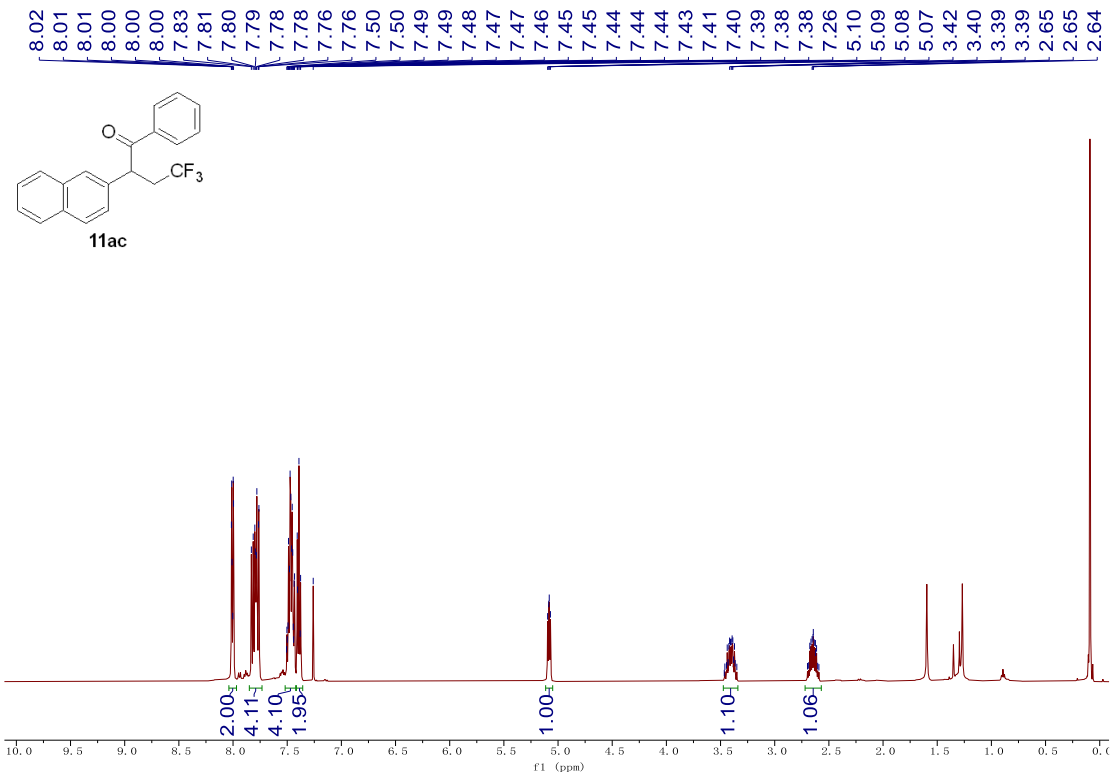
f1 (ppm)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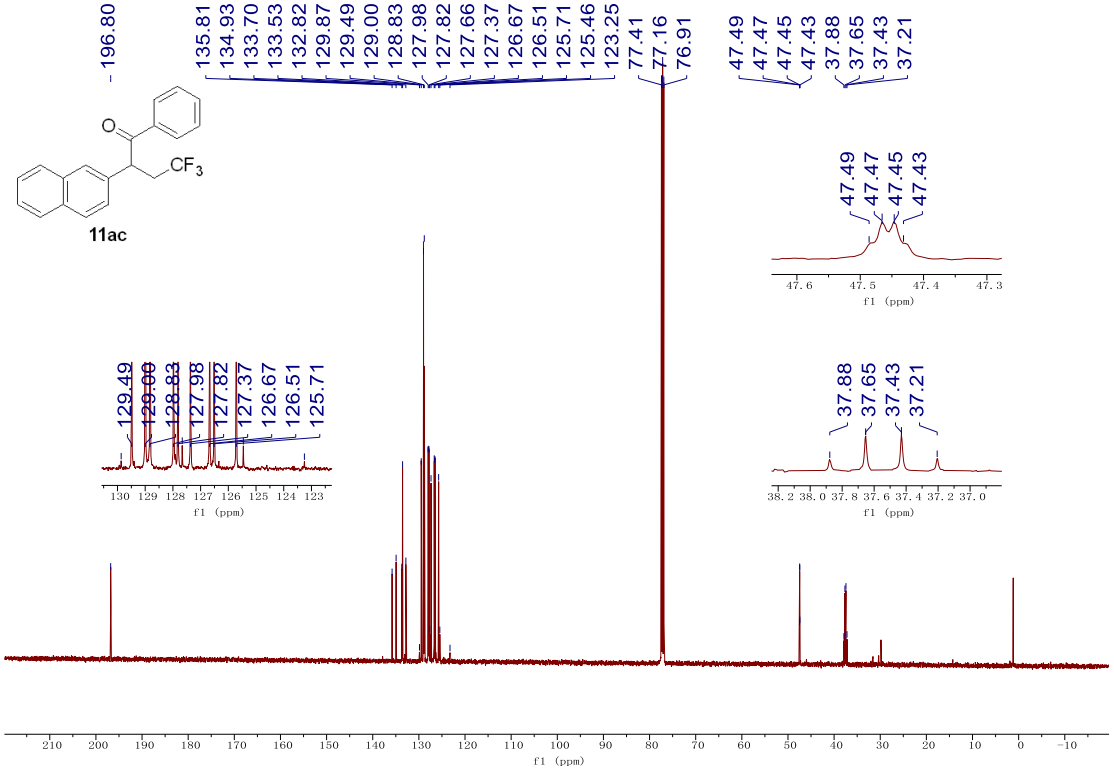
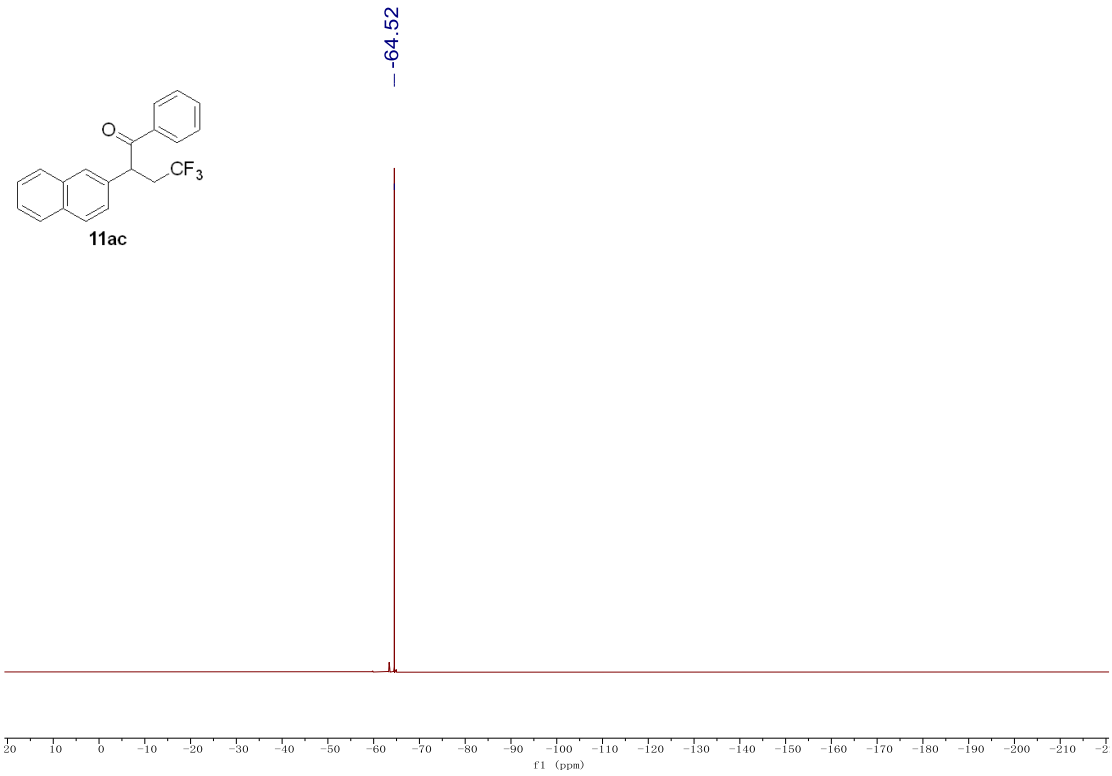
CF3
11ac
2.00 4.11 4.10 1.95 1.00 1.10 1.06
f1 (ppm)


196.80
135.81 134.93 133.70 133.53 132.82 129.87 129.49 129.00 128.83 127.98 127.82 127.66 127.37 126.67 126.51 125.71 125.46 123.25 77.41 77.16 76.91 47.49 47.47 47.45 47.43 37.88 37.65 37.43 37.21
O
CF3
11ac
47.49 47.47 47.45 47.43
129.49 129.00 128.83 127.98 127.82 127.37 126.67 126.51 125.71
37.88 37.65 37.43 37.21
f1 (ppm)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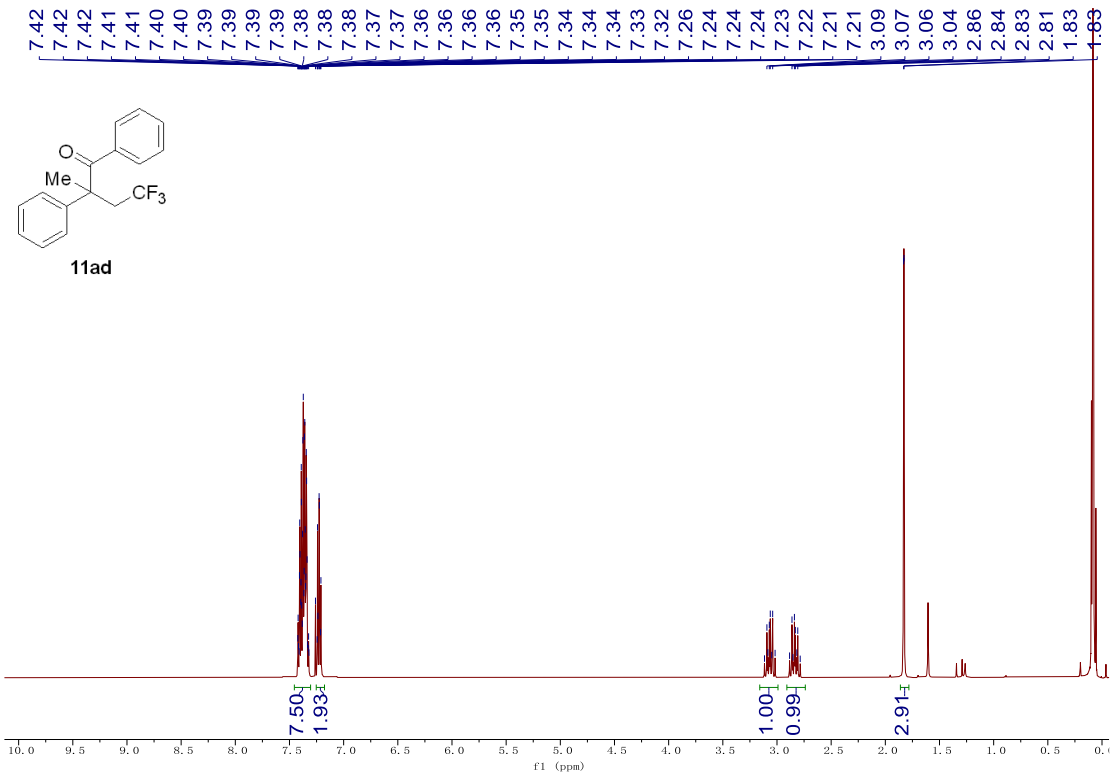
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7.21
7.21
3.09
3.07
3.06
3.04
2.86
2.84
2.83
2.81
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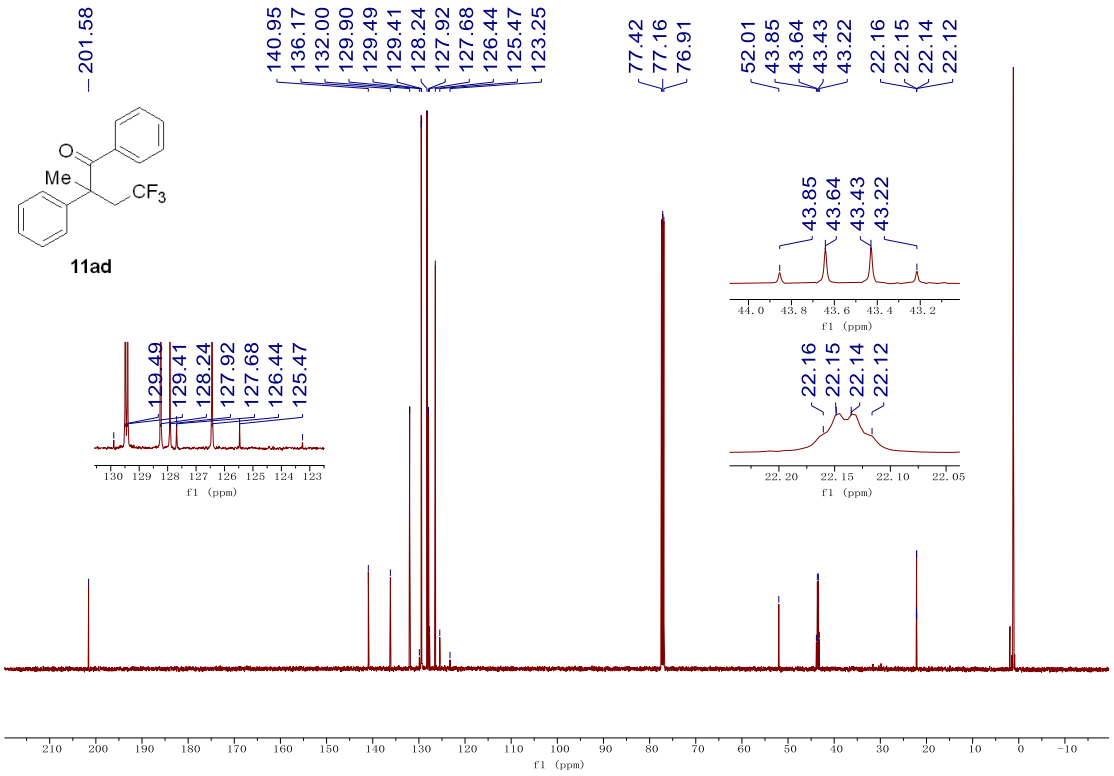
Me
CF3
11ad
7.50H
1.93H
1.00H
0.99H
2.91H
f1 (ppm)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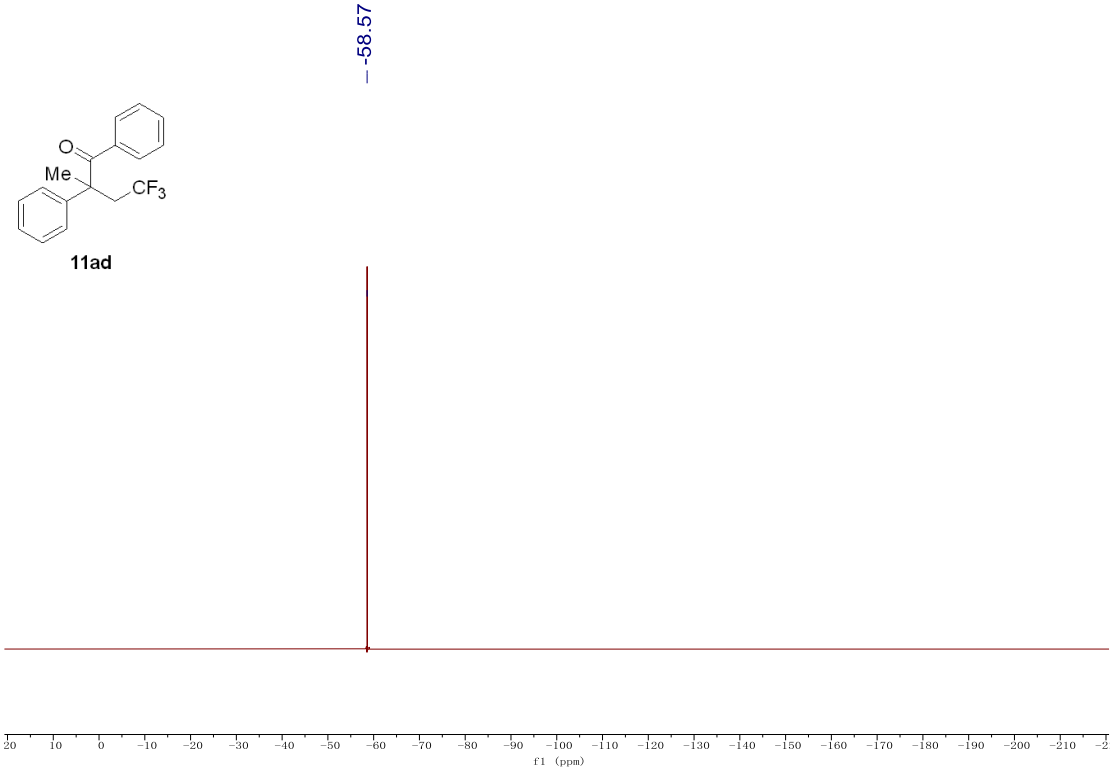
127.68
126.44
125.47
123.25
77.42
77.16
76.91
52.01
43.85
43.64
43.43
43.22
22.16
22.15
22.14
22.12
O
Me
CF3
11ad
f1 (ppm)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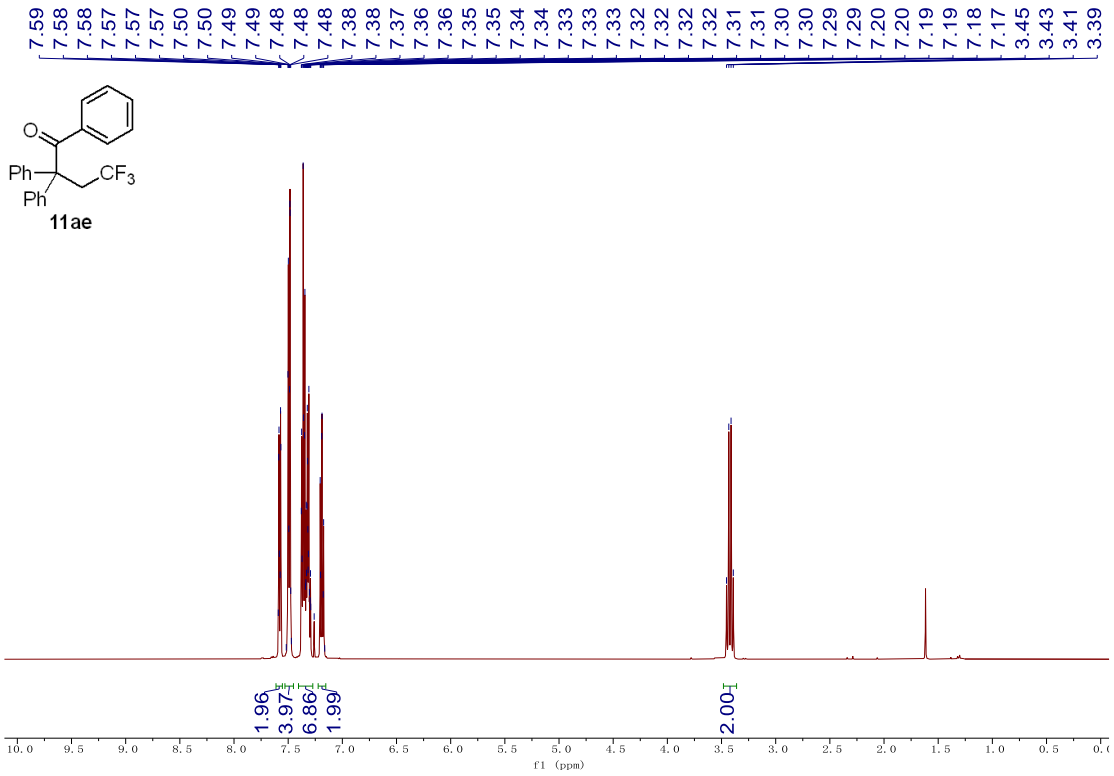
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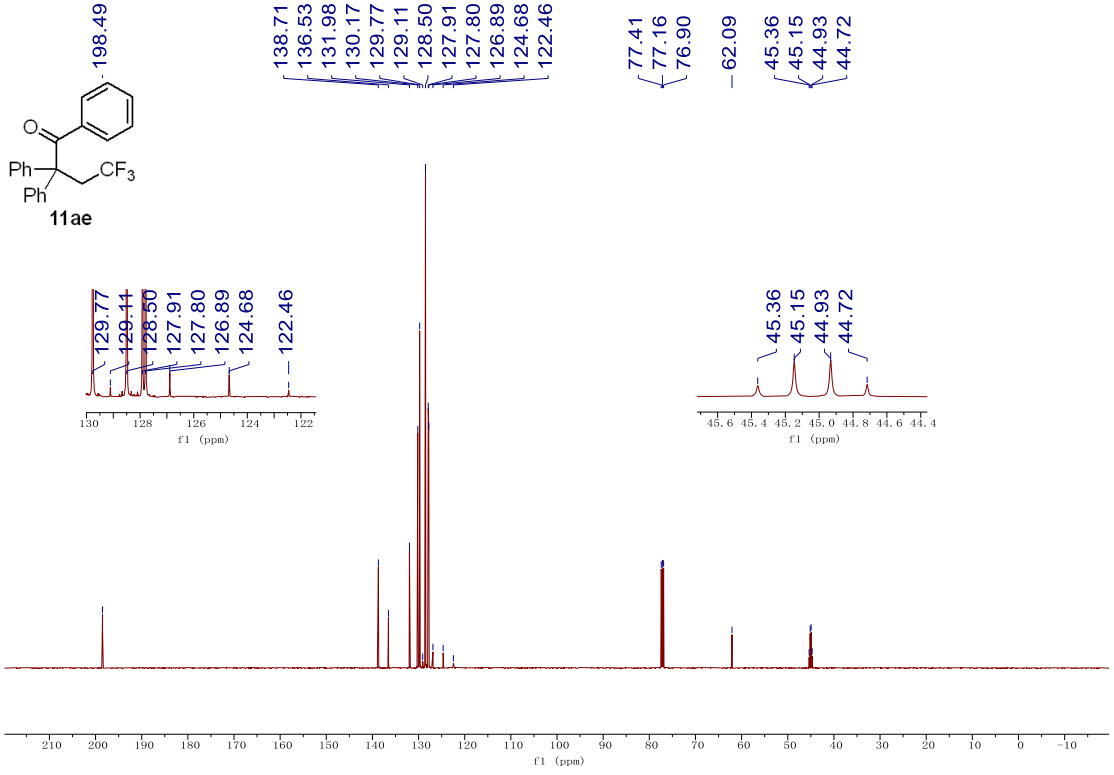
O
Ph
CF3
Ph
11ae
1.96 3.97 6.86 1.99 2.00
f1 (ppm)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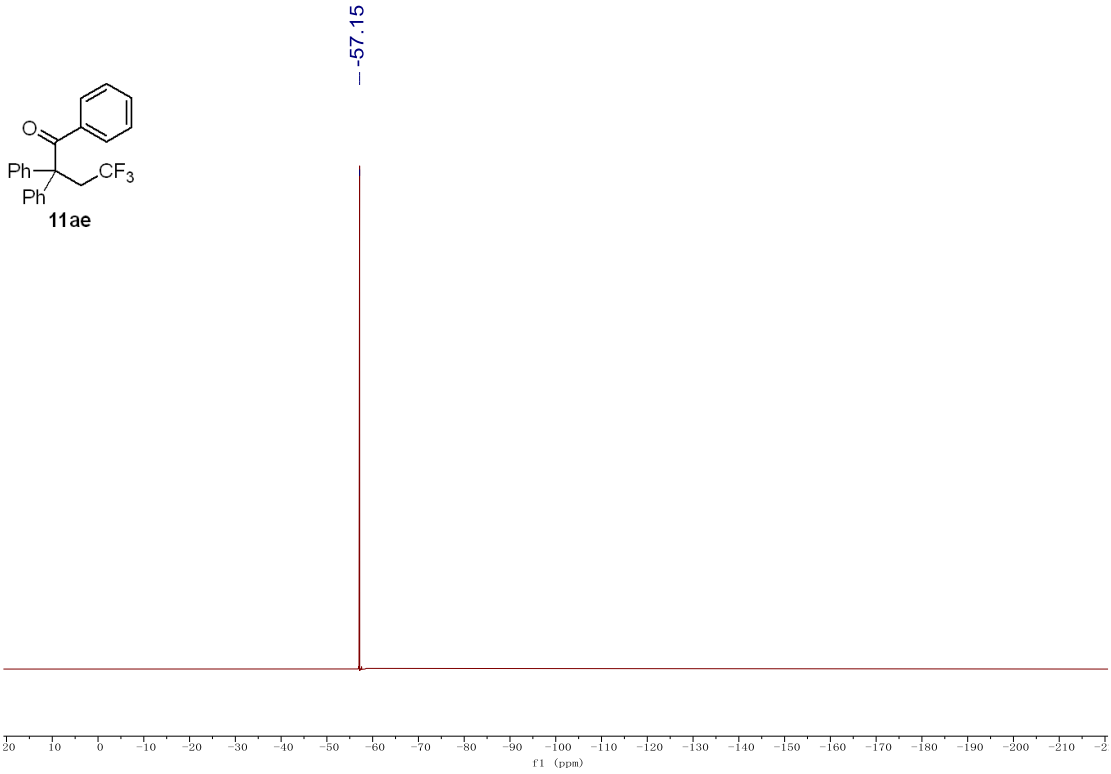
77.41 77.16 76.90
62.09
45.36 45.15 44.93 44.72
O
Ph
CF3
Ph
11ae
129.77 129.11 128.50 127.91 127.80 126.89 124.68 122.46
45.36 45.15 44.93 44.72
f1 (ppm)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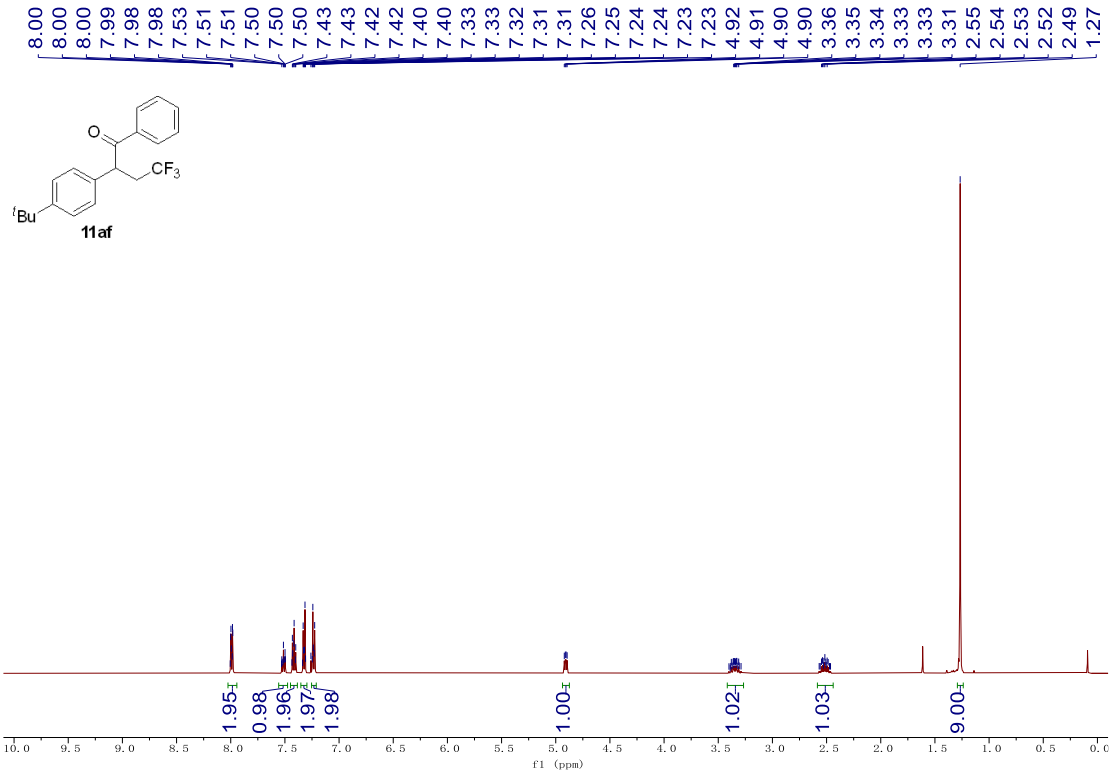
11ae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4.90
4.90
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3.33
3.31
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2.54
2.53
2.52
2.49
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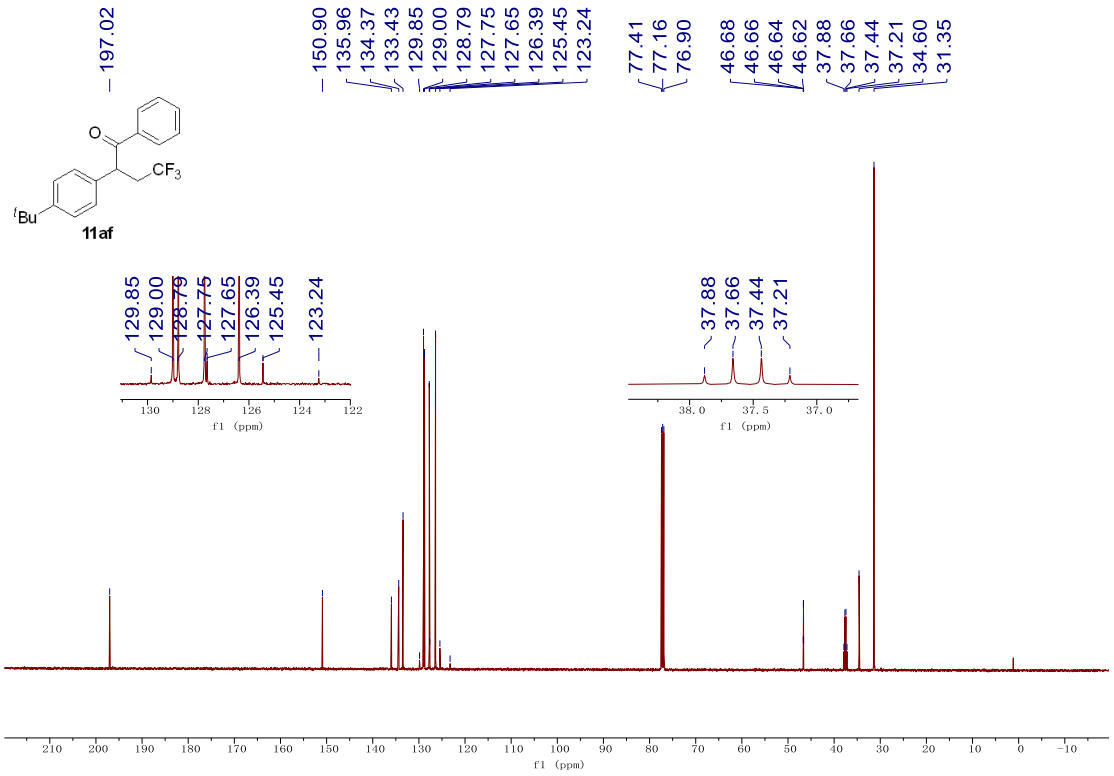
1.96
1.97
1.98
1.00
1.02
1.03
9.00
f1 (ppm)

11af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126.39
125.45
123.24
77.41
77.16
76.90
46.68
46.66
46.64
46.62
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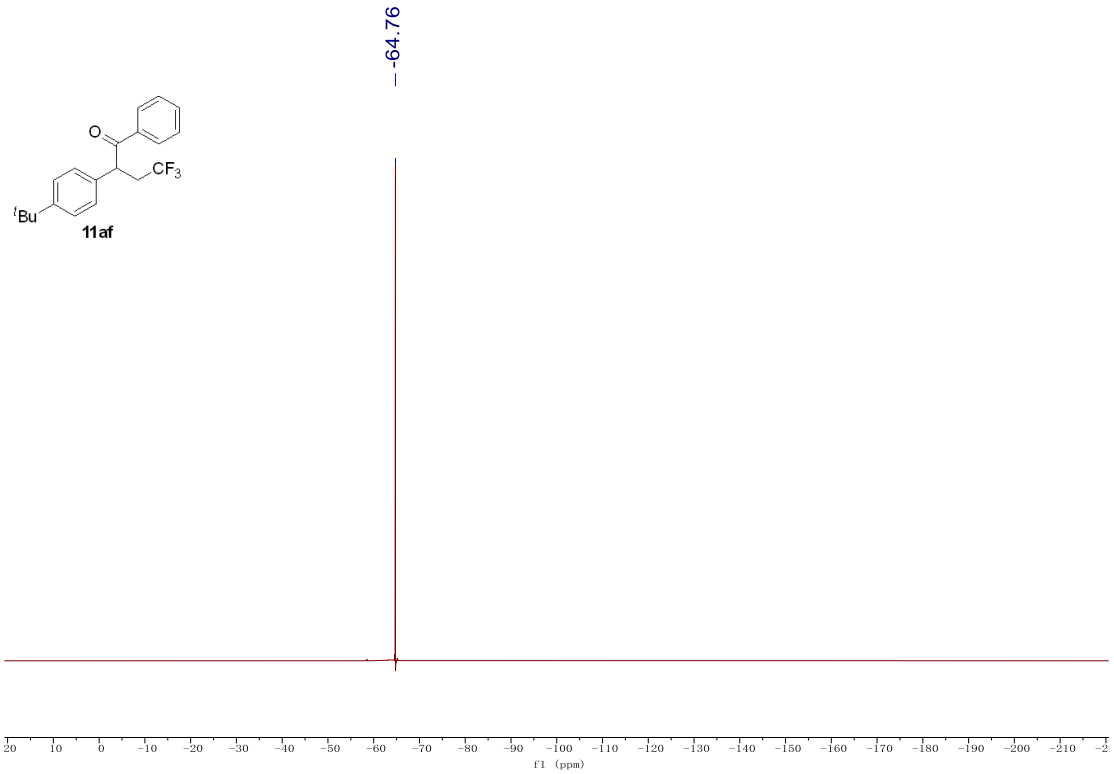
37.66
37.44
37.21
34.60
31.35
O
CF3
tBu
11af
f1 (ppm)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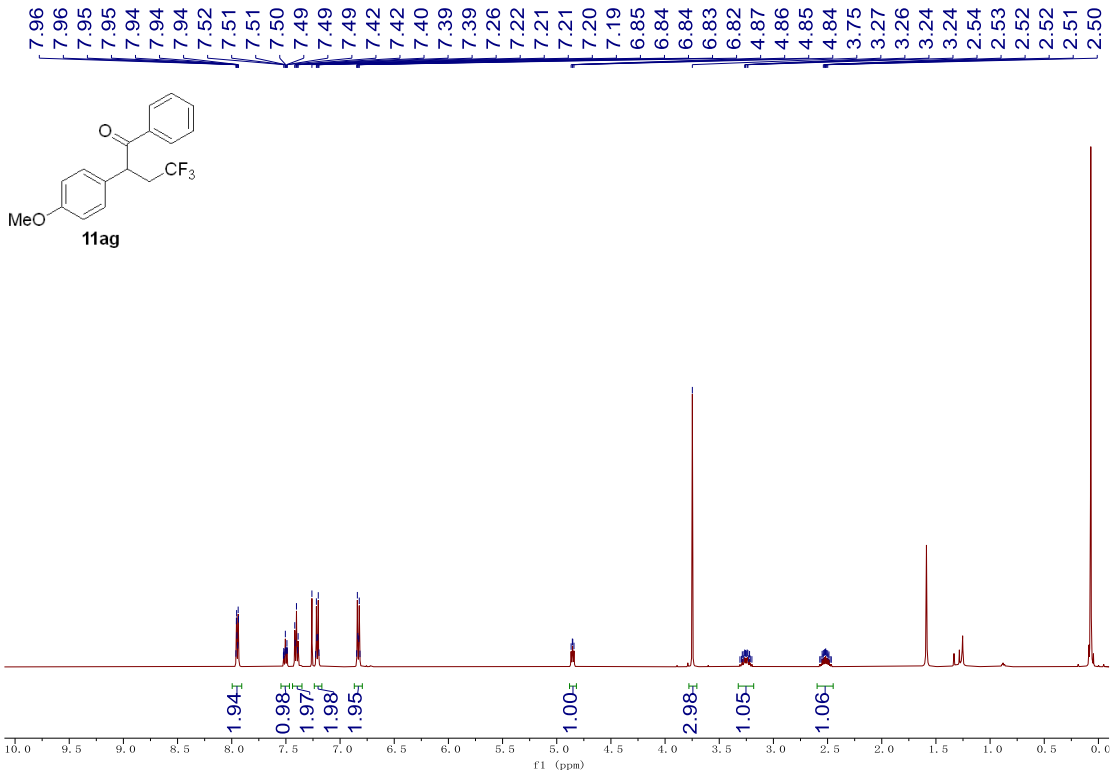
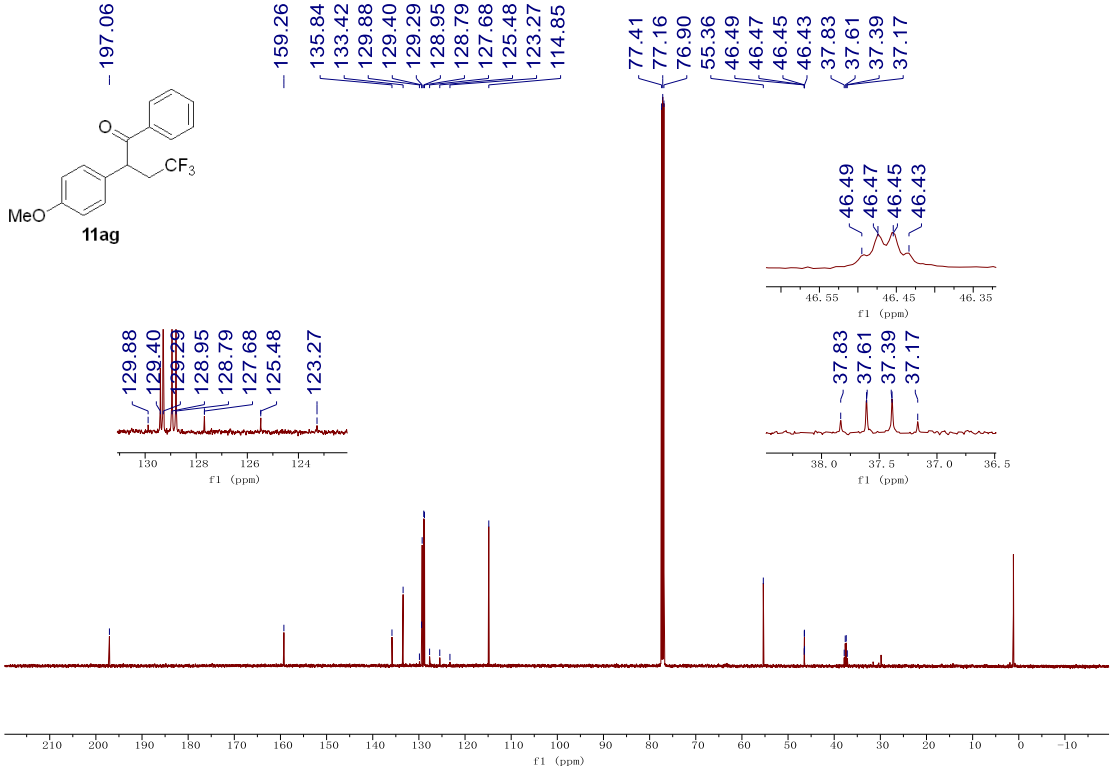

7.96 7.96 7.95 7.95 7.94 7.94 7.94 7.52 7.51 7.51 7.50 7.49 7.49 7.49 7.42 7.42 7.40 7.39 7.39 7.26 7.22 7.21 7.21 7.20 7.19 6.85 6.84 6.84 6.83 6.82 4.87 4.86 4.85 4.84 3.75 3.27 3.26 3.24 3.24 2.54 2.53 2.52 2.52 2.51 2.50
O
CF3
MeO
11ag
1.94 0.98 1.97 1.98 1.95 1.00 2.98 1.05 1.06
f1 (ppm)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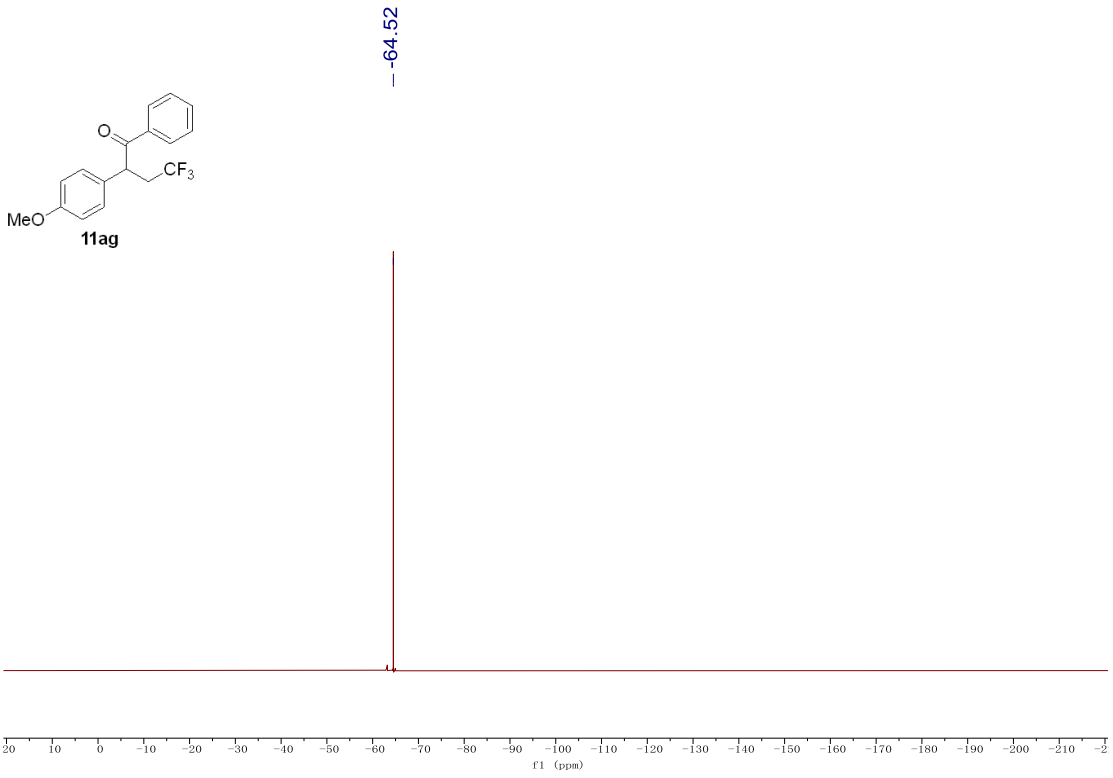
77.41 77.16 76.90 55.36 46.49 46.47 46.45 46.43 37.83 37.61 37.39 37.17
O
CF3
MeO
11ag
46.49 46.47 46.45 46.43
37.83 37.61 37.39 37.17
129.88 129.40 129.29 128.95 128.79 127.68 125.48 123.27
f1 (ppm)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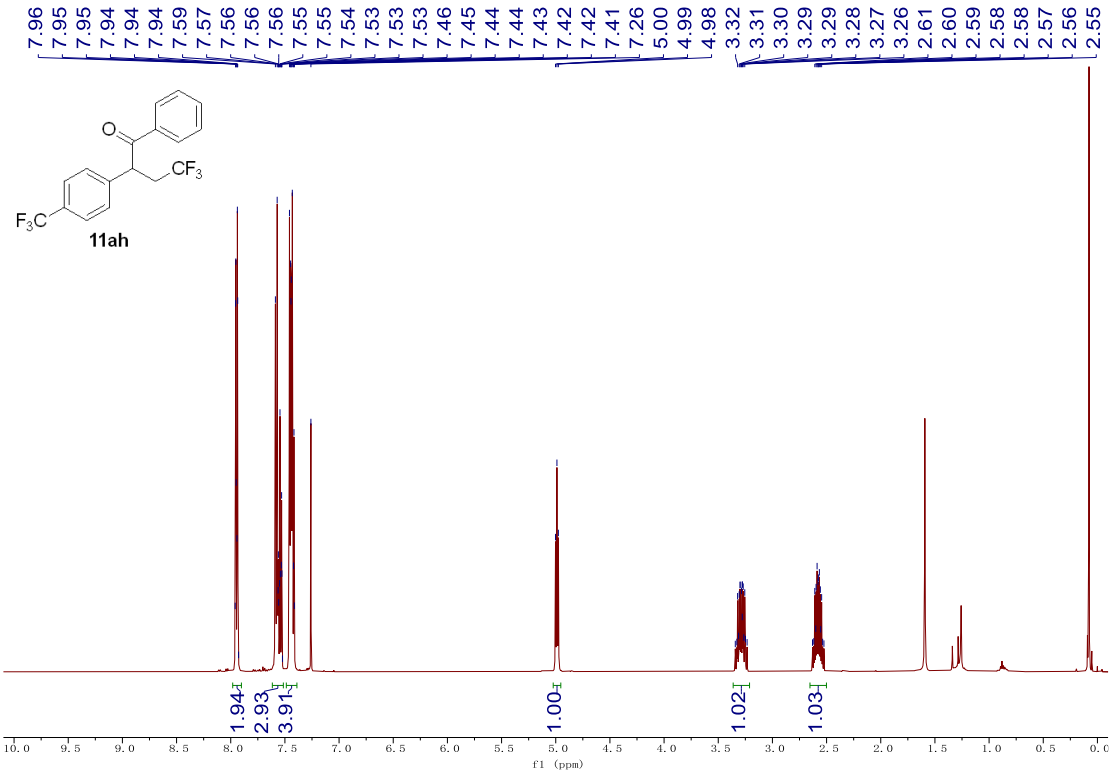
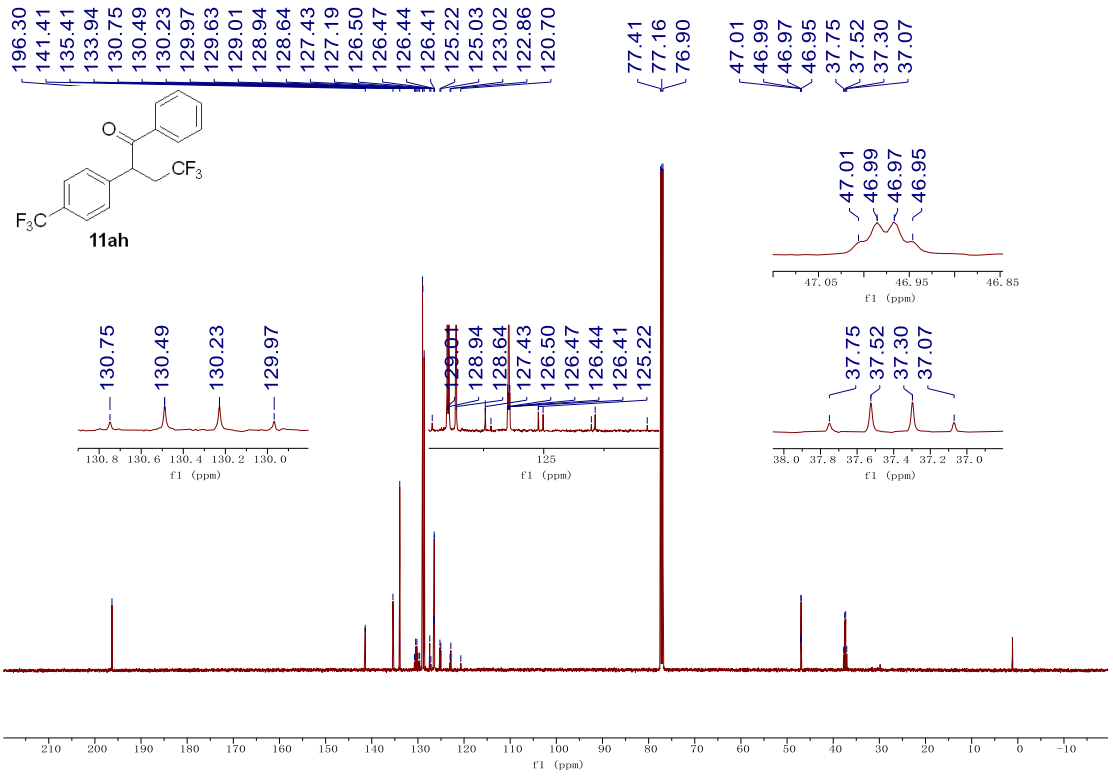
O
CF3
MeO
11ag
f1 (ppm)


7.96 7.95 7.95 7.94 7.94 7.94 7.59 7.57 7.56 7.56 7.56 7.55 7.55 7.54 7.53 7.53 7.53 7.46 7.45 7.44 7.44 7.43 7.42 7.42 7.41 7.26 5.00 4.99 4.98 3.32 3.31 3.30 3.29 3.29 3.28 3.27 3.26 2.61 2.60 2.59 2.58 2.58 2.57 2.56 2.55
O
CF3
F3C
11ah
1.94 2.93 3.91 1.00 1.02 1.03
f1 (ppm)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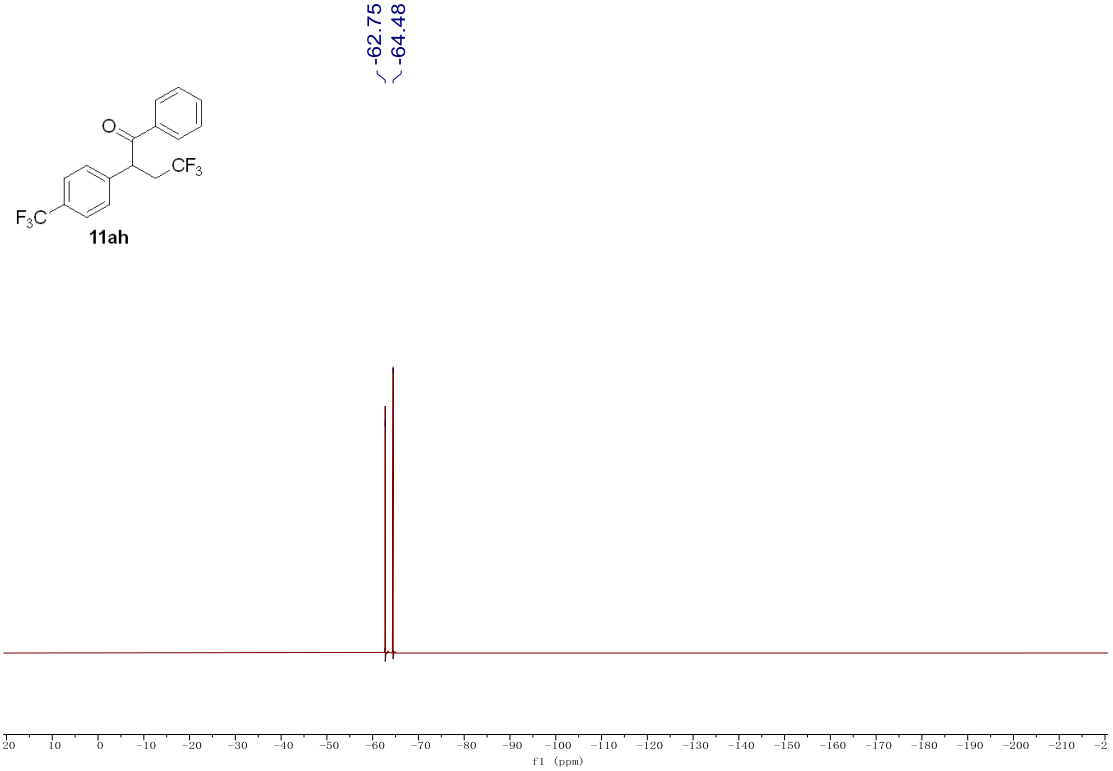
127.43
127.19
126.50
126.47
126.44
126.41
125.22
125.03
123.02
122.86
120.70
77.41
77.16
76.90
47.01
46.99
46.97
46.95
37.75
37.52
37.30
37.07
O
CF3
F3C
11ah
f1 (ppm)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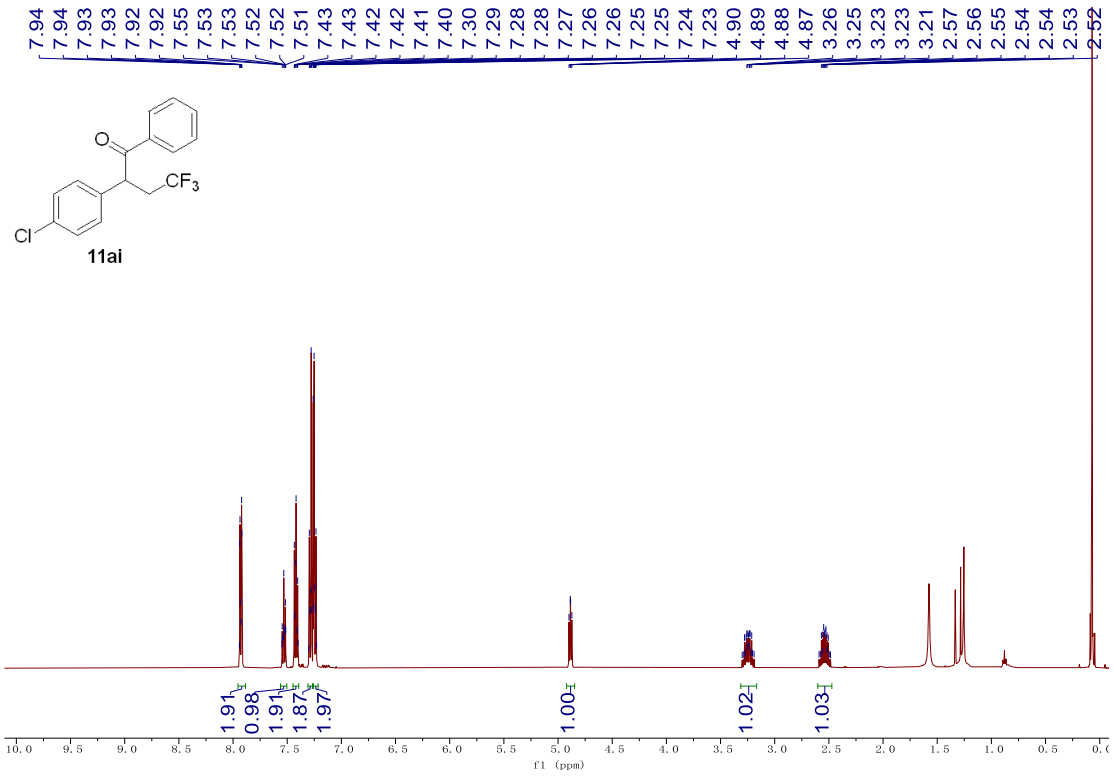
O
CF3
F3C
11ah
f1 (ppm)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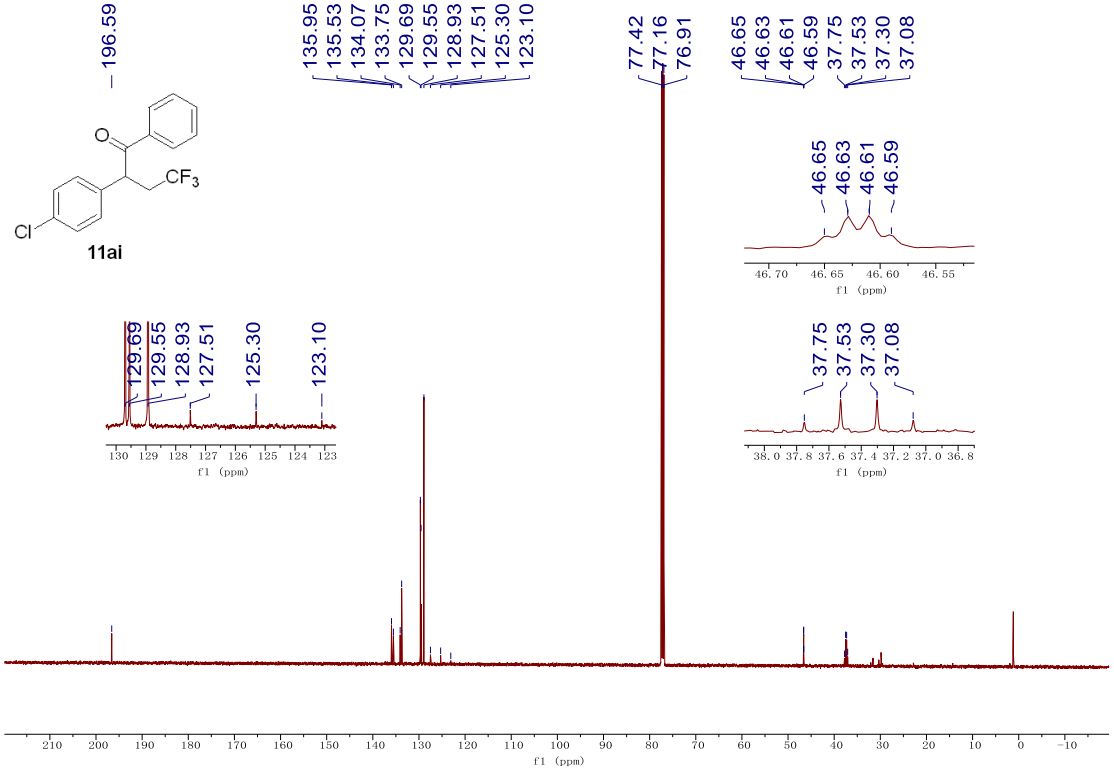
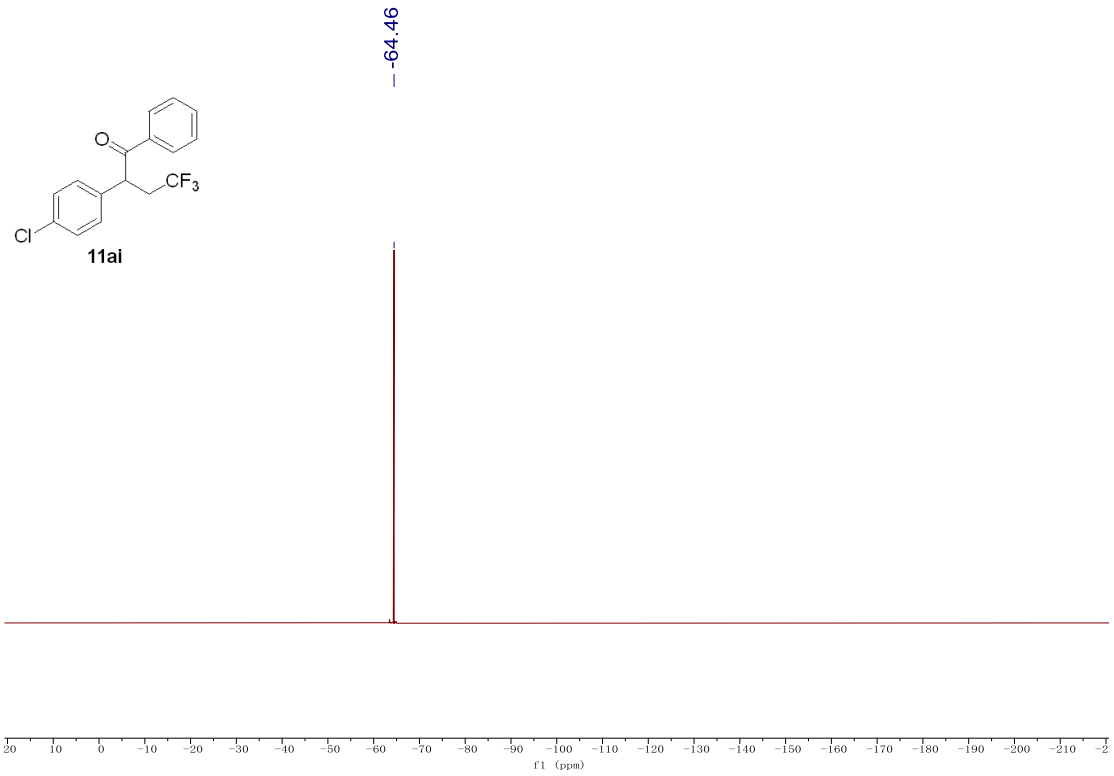
O
CF3
Cl
11ai
1.91 0.98 1.91 1.87 1.97 1.00 1.02 1.03
f1 (ppm)


196.59
135.95 135.53 134.07 133.75 129.69 129.55 128.93 127.51 125.30 123.10
77.42 77.16 76.91
46.65 46.63 46.61 46.59 37.75 37.53 37.30 37.08
O
CF3
Cl
11ai
f1 (ppm)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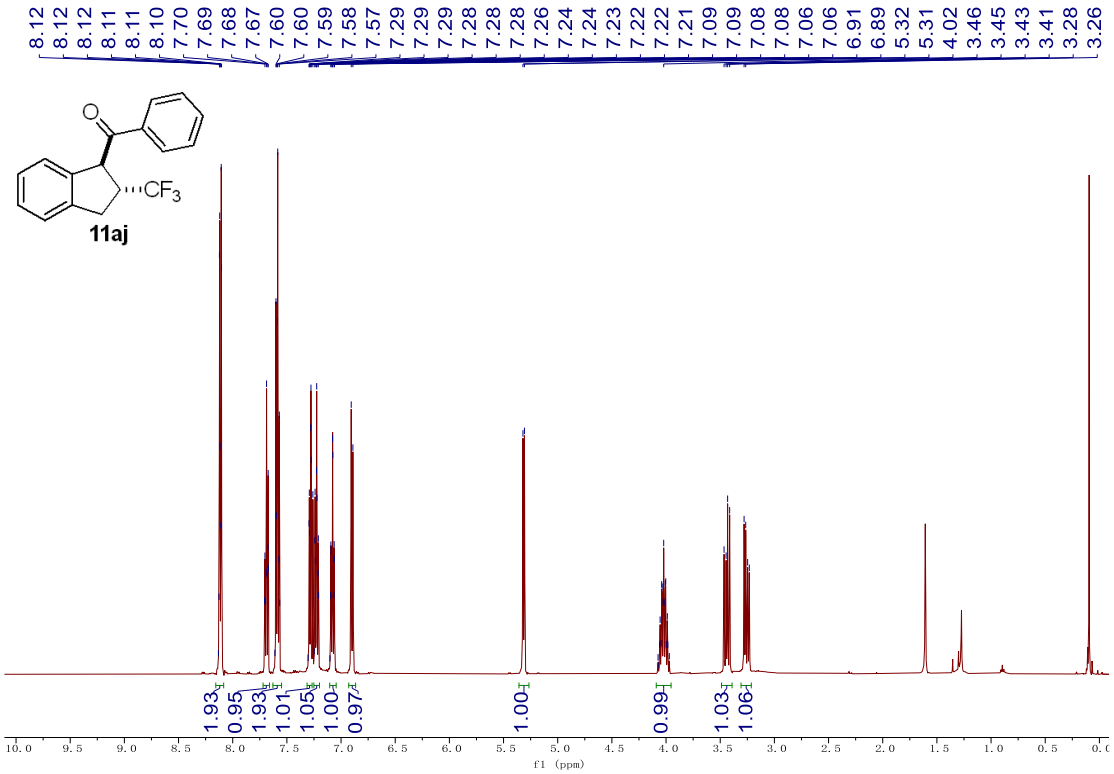
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7.57
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7.29
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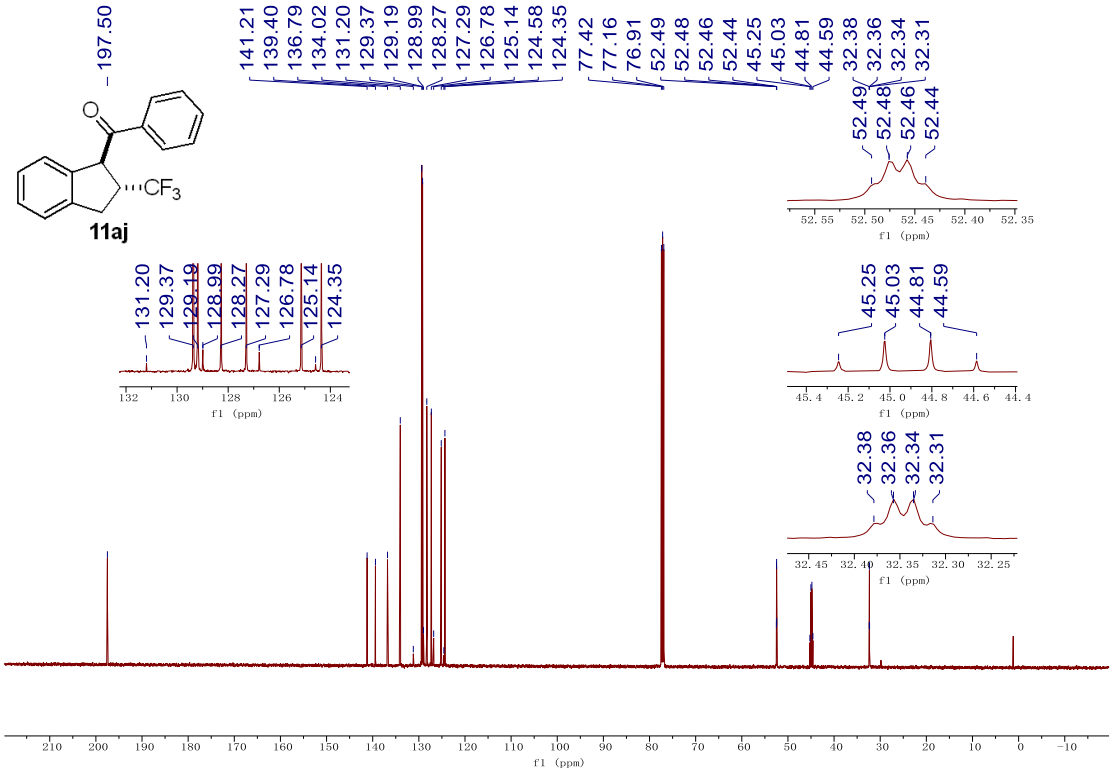
7.23
7.22
7.22
7.21
7.09
7.09
7.08
7.08
7.06
7.06
6.91
6.89
5.32
5.31
4.02
3.46
3.45
3.43
3.41
3.28
3.26
O
CF3
11aj
1.93
0.95
1.93
1.01
1.05
1.00
0.97
1.00
0.99
1.03
1.06
f1 (ppm)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129.19
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128.27
127.29
126.78
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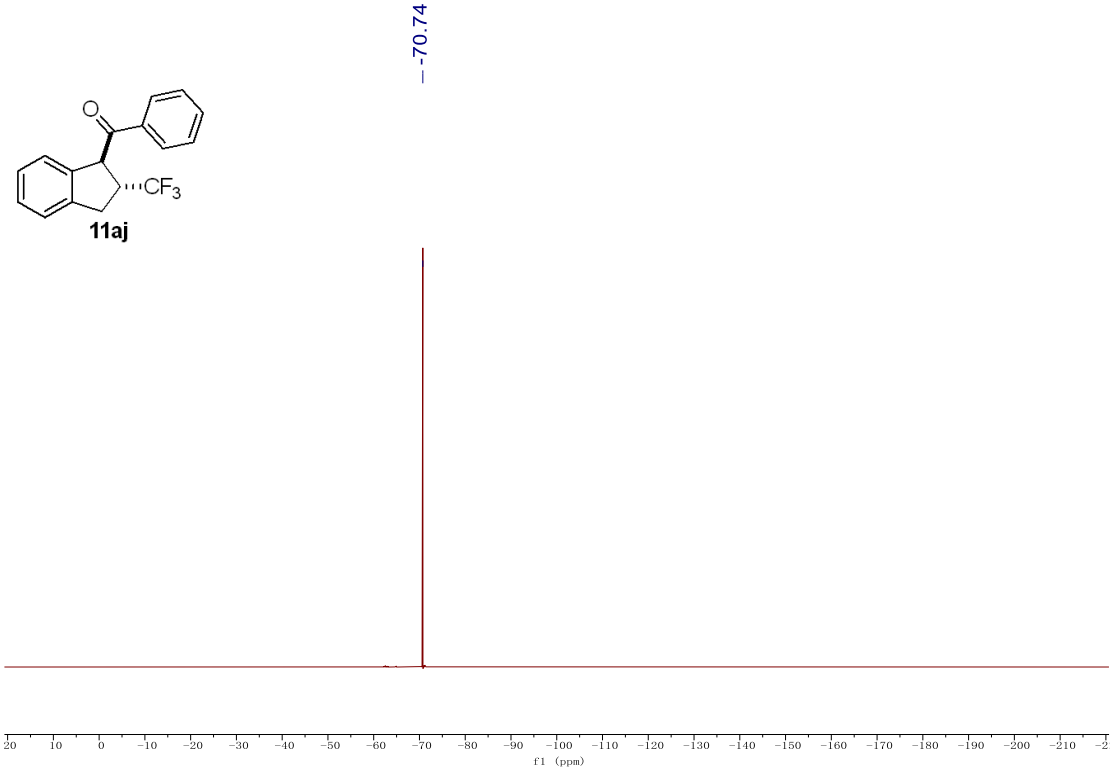
124.58
124.35
77.42
77.16
76.91
52.49
52.48
52.46
52.44
45.25
45.03
44.81
44.59
32.38
32.36
32.34
32.31
CF3
11aj
f1 (ppm)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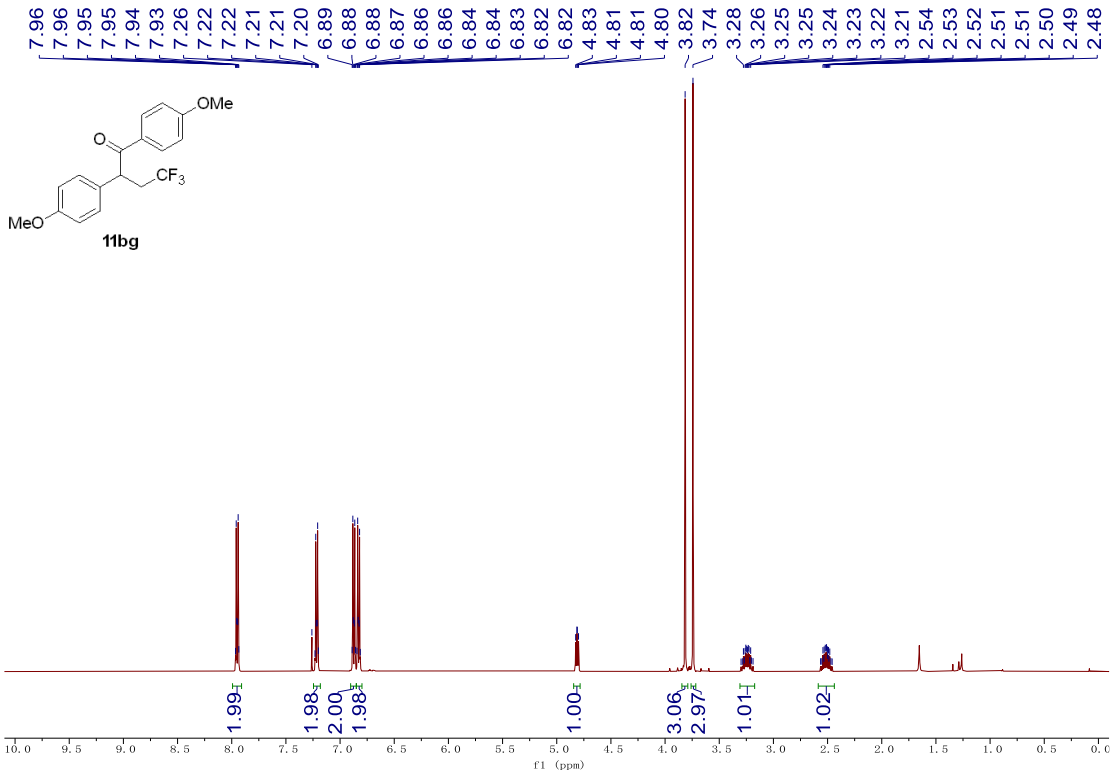
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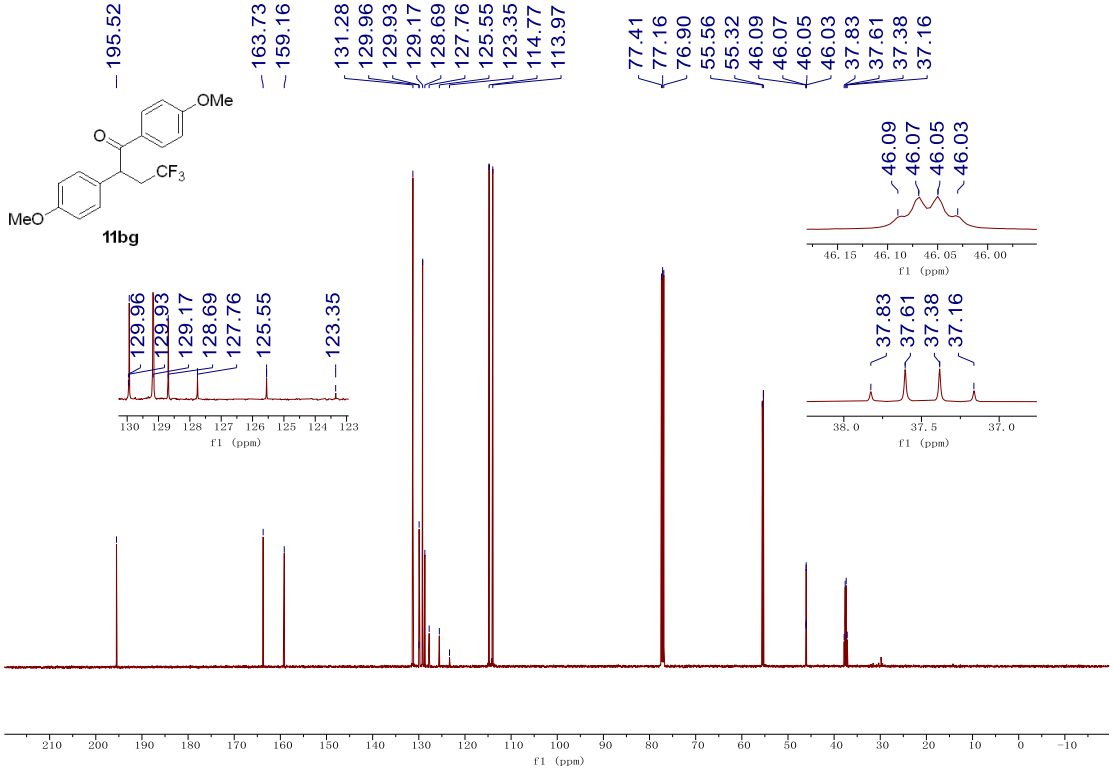
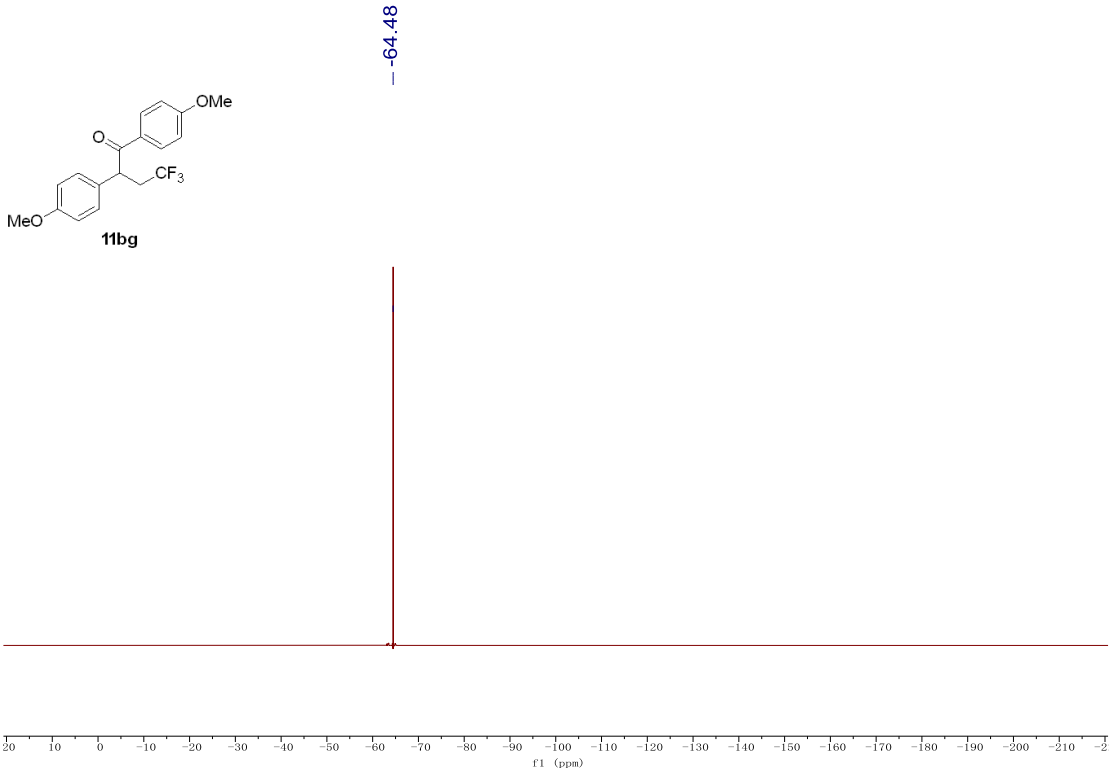
OMe
O
CF3
MeO
11bg
1.99 1.98 2.00 1.98 1.00 3.06 2.97 1.01 1.02
f1 (ppm)


195.52
163.73 159.16
131.28 129.96 129.93 129.17 128.69 127.76 125.55 123.35 114.77 113.97
77.41 77.16 76.90 55.56 55.32 46.09 46.07 46.05 46.03 37.83 37.61 37.38 37.16
OMe
O
CF3
MeO
11bg
46.09 46.07 46.05 46.03
37.83 37.61 37.38 37.16
129.96 129.93 129.17 128.69 127.76 125.55 123.35
f1 (ppm)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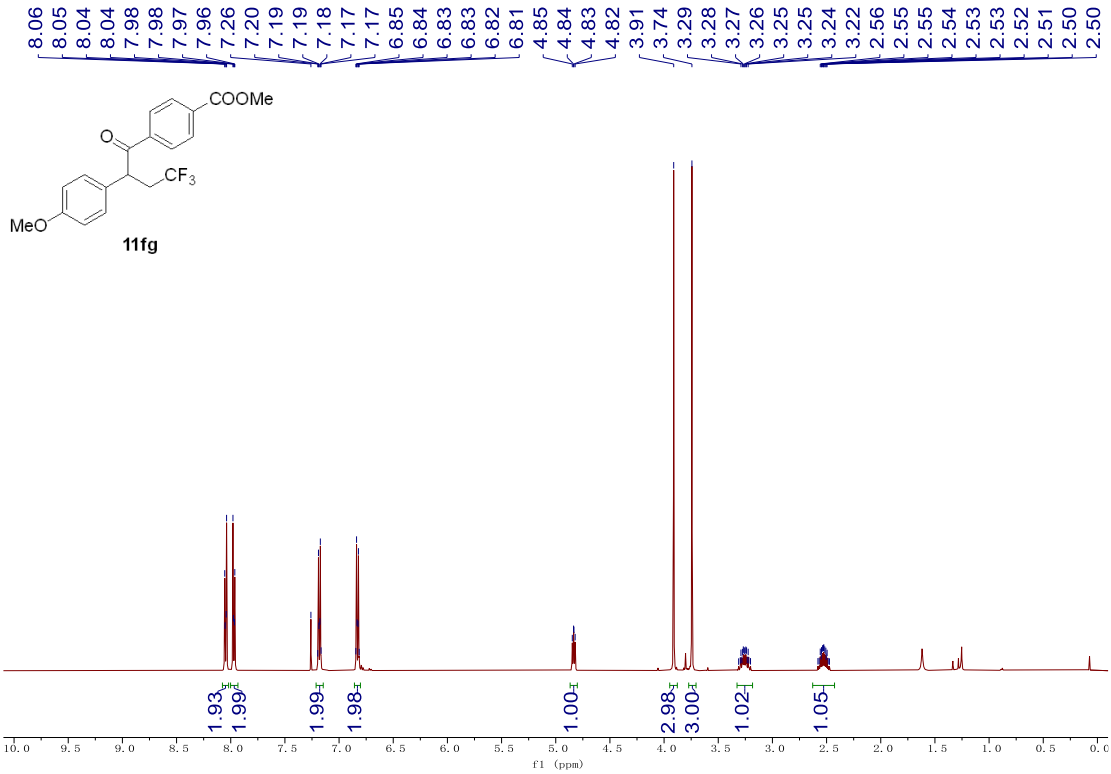
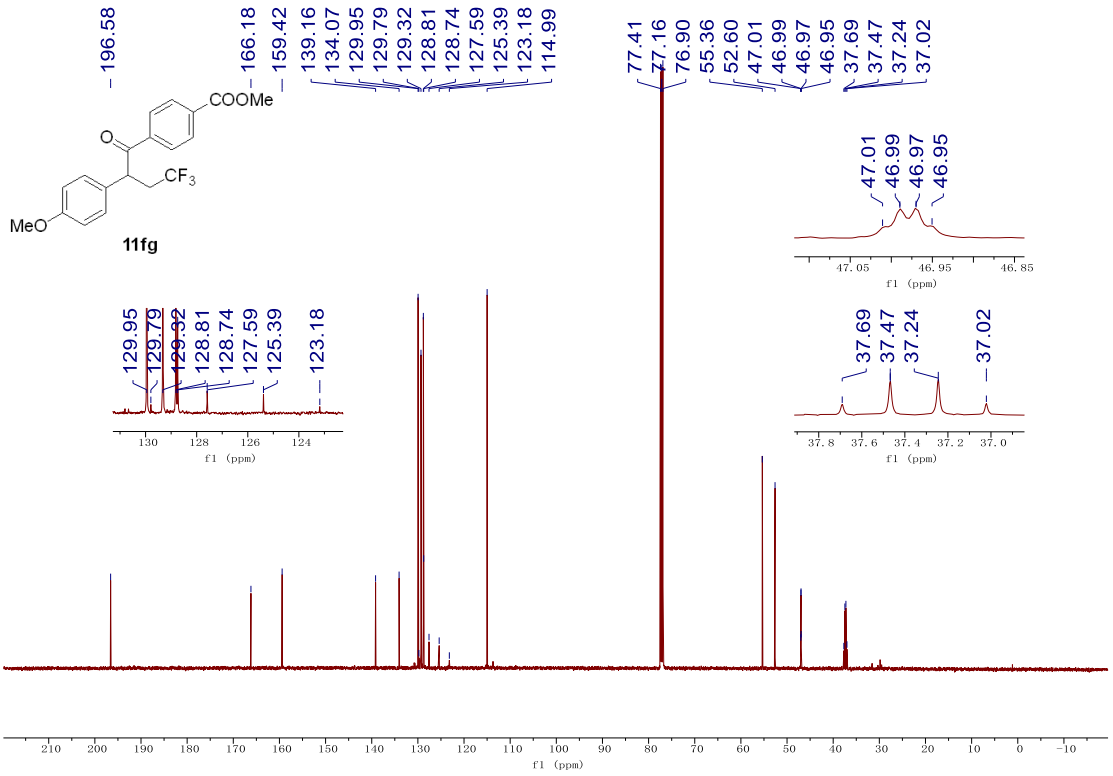
O
CF3
MeO
11bg
f1 (ppm)


8.06 8.05 8.04 8.04 7.98 7.98 7.97 7.96 7.26 7.20 7.19 7.19 7.18 7.17 7.17 6.85 6.84 6.83 6.83 6.82 6.81
4.85 4.84 4.83 4.82
3.91 3.74 3.29 3.28 3.27 3.26 3.25 3.25 3.24 3.22
2.56 2.55 2.55 2.54 2.53 2.53 2.52 2.51 2.50 2.50
COOMe
O
CF3
MeO
11fg
1.93 1.99 1.99 1.98 1.00 2.98 3.00 1.02 1.05
f1 (ppm)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166.18
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139.16
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129.95
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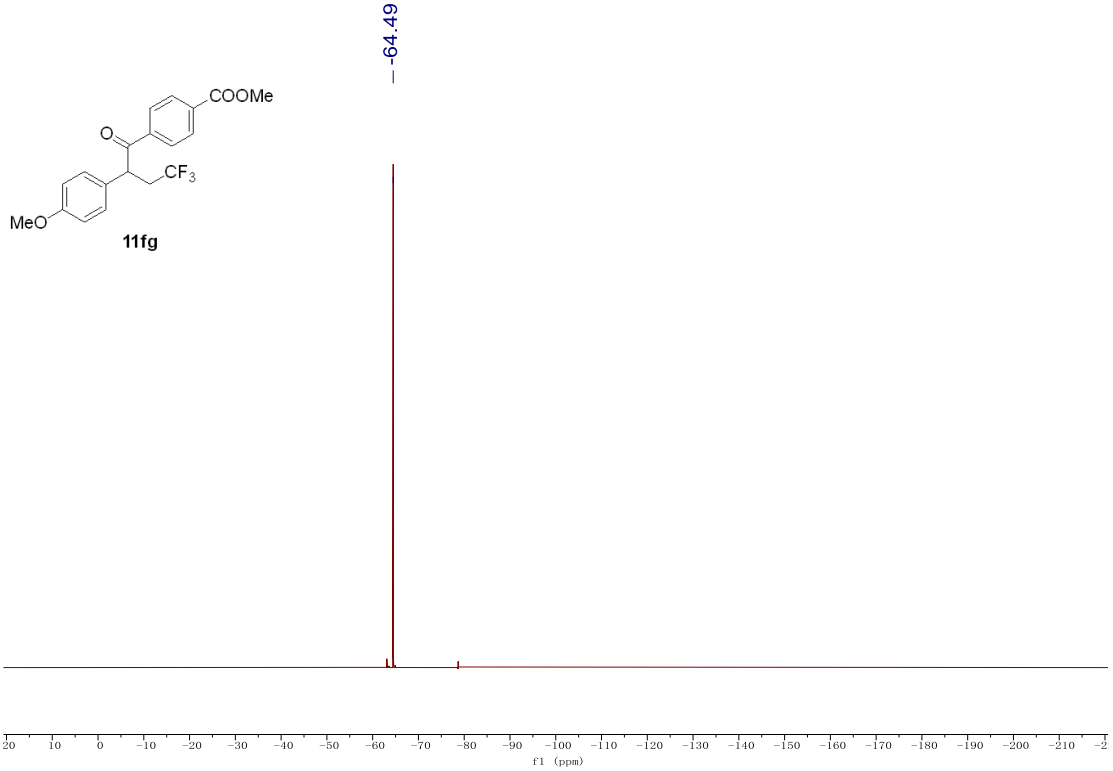
129.32
128.81
128.74
127.59
125.39
123.18
114.99
77.41
77.16
76.90
55.36
52.60
47.01
46.99
46.97
46.95
37.69
37.47
37.24
37.02
COOMe
O
CF3
MeO
11fg
f1 (ppm)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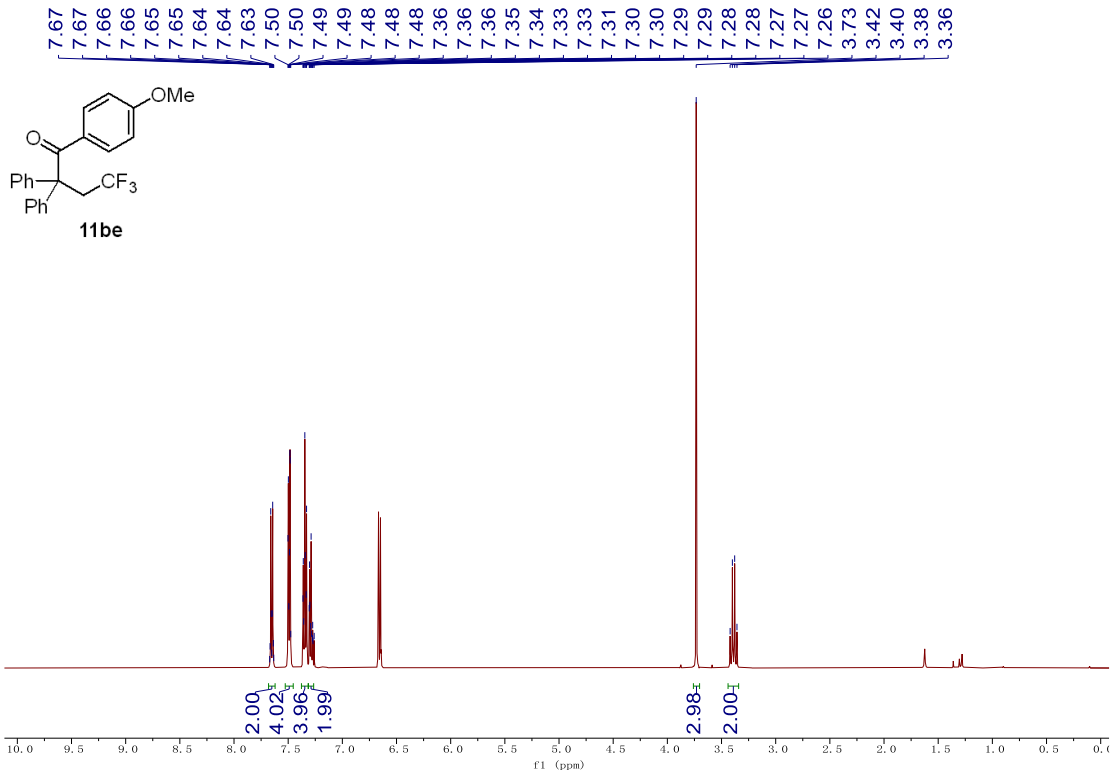
COOMe
O
CF3
MeO
11fg
f1 (ppm)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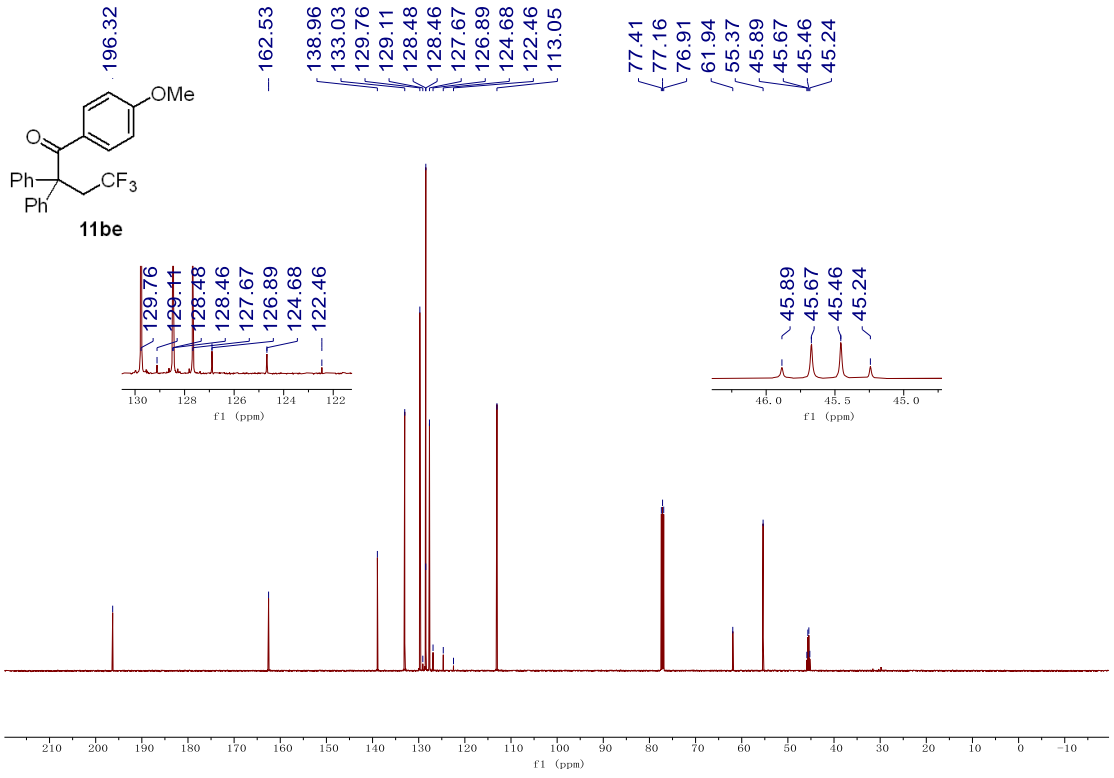
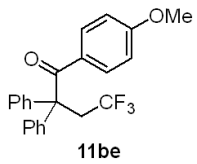
OMe
O
Ph
Ph
CF3
11be
2.00 4.02 3.96 1.99 2.98 2.00
f1 (ppm)


196.32
162.53
138.96 133.03 129.76 129.11 128.48 128.46 127.67 126.89 124.68 122.46 113.05
77.41 77.16 76.91 61.94 55.37 45.89 45.67 45.46 45.24
OMe
O
Ph
Ph
CF3
11be
129.76 129.11 128.48 128.46 127.67 126.89 124.68 122.46
45.89 45.67 45.46 45.24
f1 (ppm)


OMe
O
Ph
CF3
Ph

11be

-57.14
f1 (ppm)


7.30
7.30
7.30
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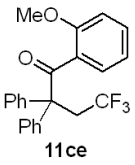
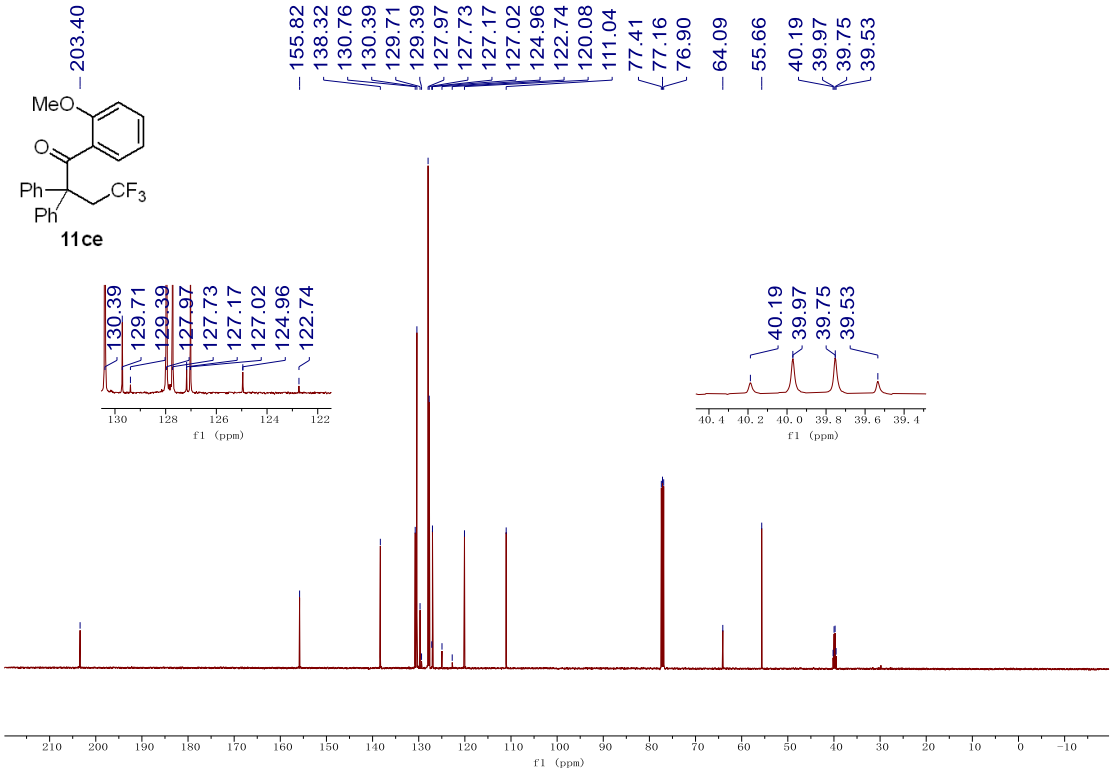
6.17
3.55
3.30
3.28
3.26
3.24


MeO
O
Ph
CF3
Ph

11ce

9.89
1.14
0.99
0.99
0.98
3.00
2.00
f1 (ppm)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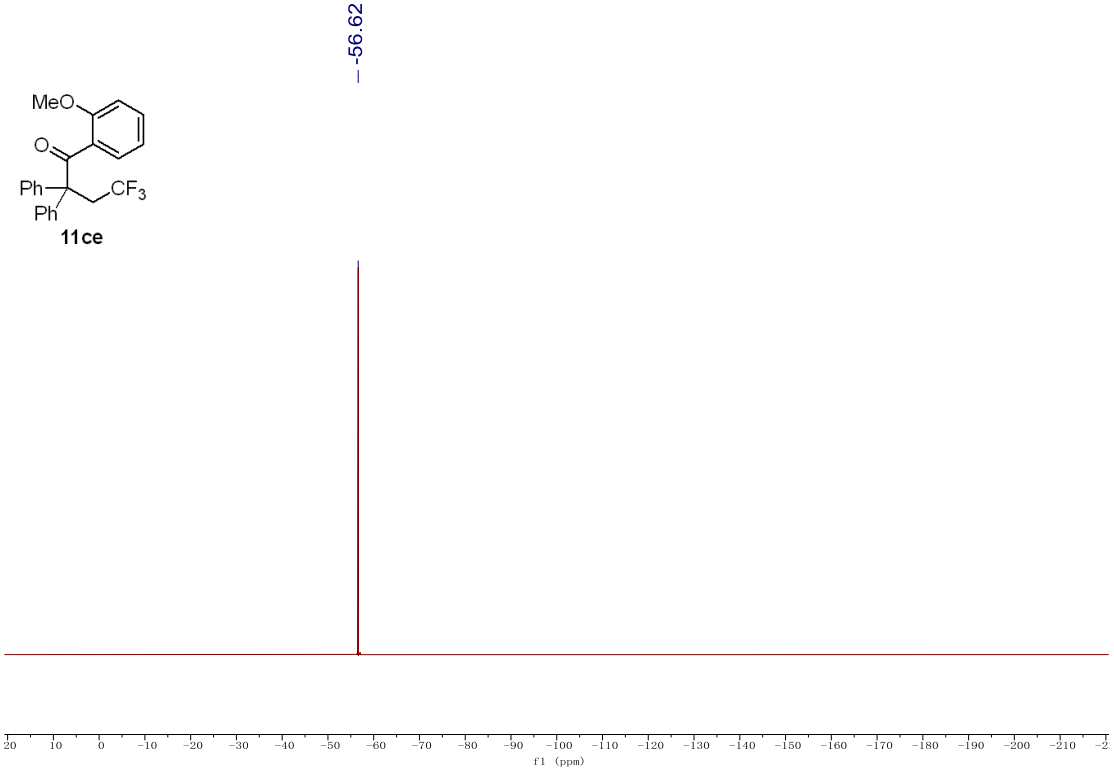
129.71
129.39
127.97
127.73
127.17
127.02
124.96
122.74
120.08
111.04
77.41
77.16
76.90
64.09
55.66
40.19
39.97
39.75
39.53
MeO
O
Ph
Ph
CF3
11ce
130.39
129.71
129.39
127.97
127.73
127.17
127.02
124.96
122.74
40.19
39.97
39.75
39.53
f1 (ppm)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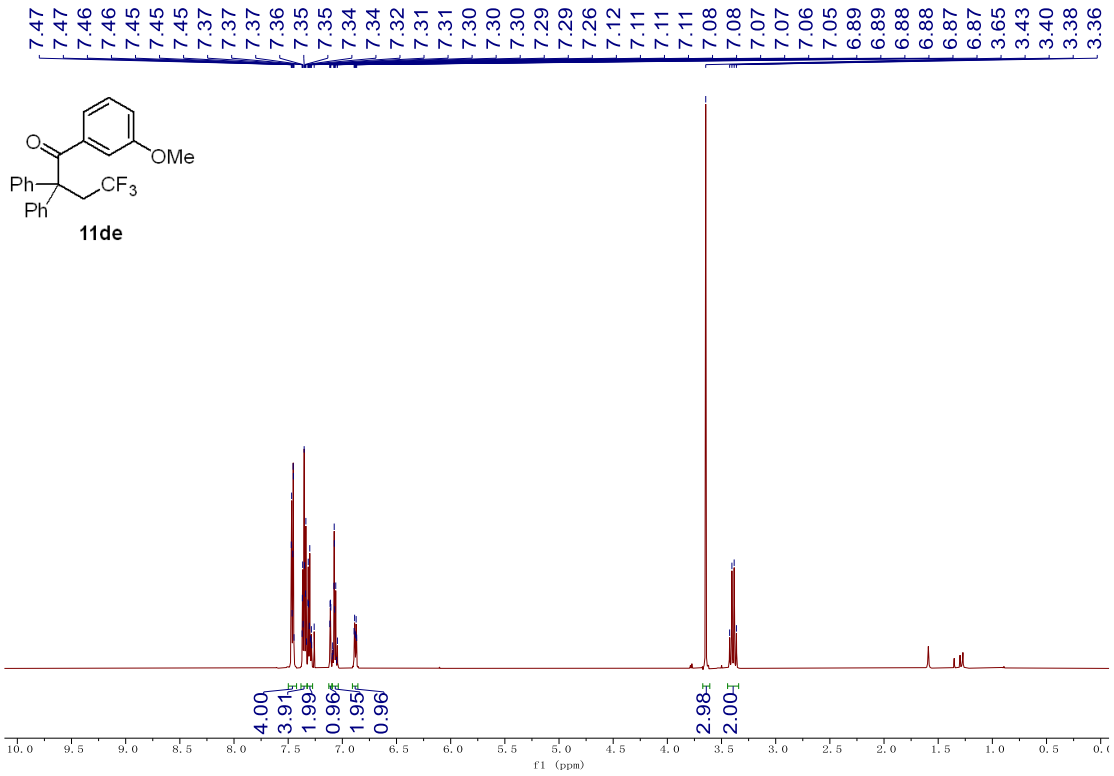
MeO
O
Ph
Ph
CF3
11ce
f1 (ppm)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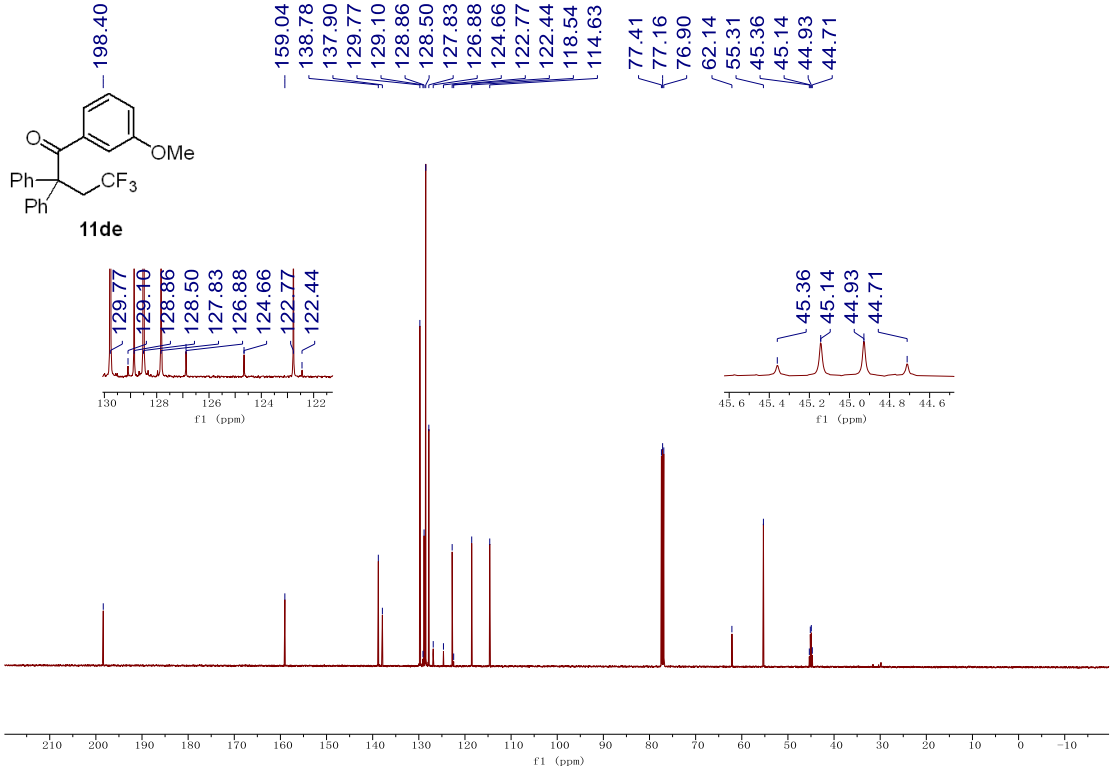
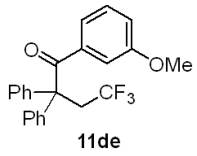
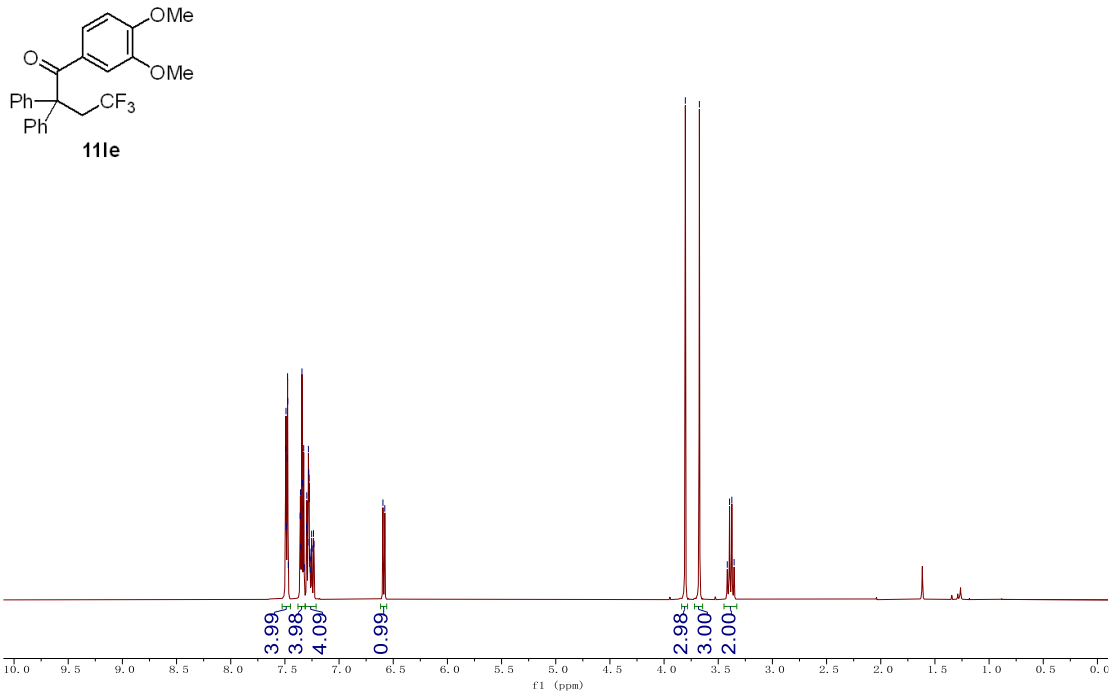
O
OMe
Ph
CF3
Ph
11de
4.00 3.91 1.99 0.96 1.95 0.96 2.98 2.00
f1 (ppm)


198.40
159.04 138.78 137.90 129.77 129.10 128.86 128.50 127.83 126.88 124.66 122.77 122.44 118.54 114.63
77.41 77.16 76.90 62.14 55.31 45.36 45.14 44.93 44.71
O
OMe
Ph
CF3
Ph
11de
129.77 129.10 128.86 128.50 127.83 126.88 124.66 122.77 122.44
45.36 45.14 44.93 44.71
f1 (ppm)


O
OMe
Ph
CF3
Ph

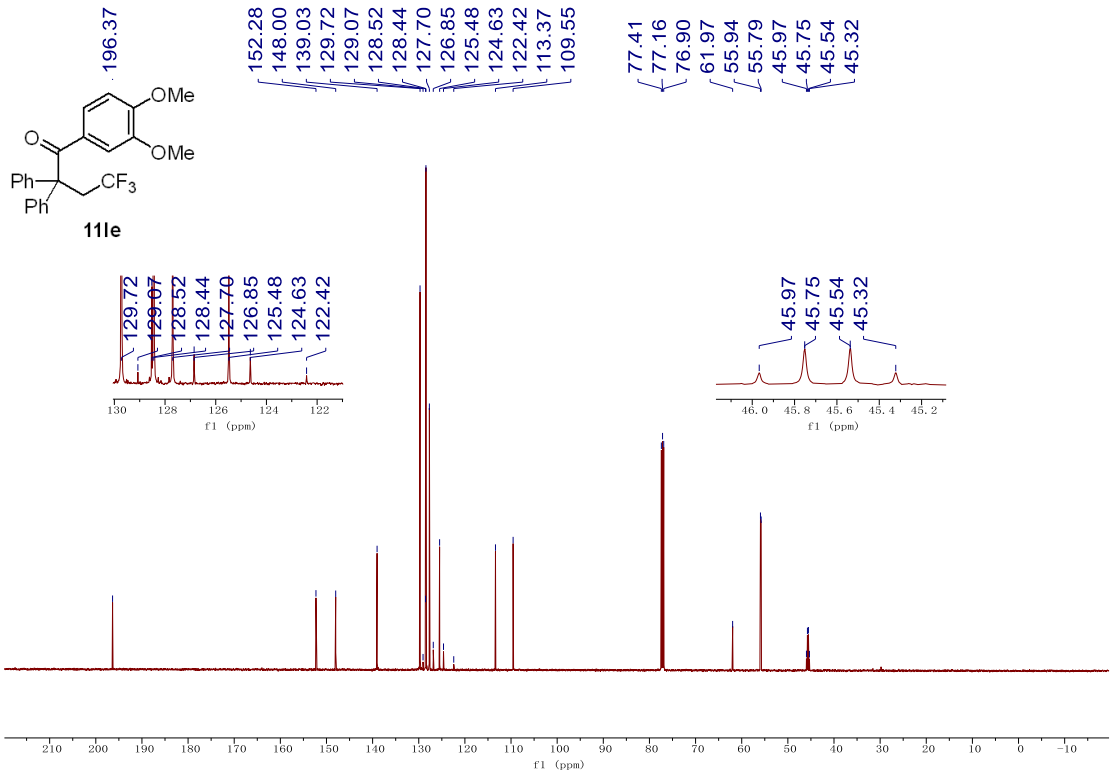
11de

-57.17
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.49 7.49 7.49 7.48 7.48 7.47 7.47 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.30 7.30 7.30 7.29 7.28 7.28 7.28 7.27 7.27 7.27 7.26 7.25 7.25 7.24 7.23 6.60 6.58 3.80 3.67 3.42 3.40 3.37 3.35
3.99 3.98 4.09 0.99 2.98 3.00 2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

OMe
O
OMe
Ph
CF3
Ph

11le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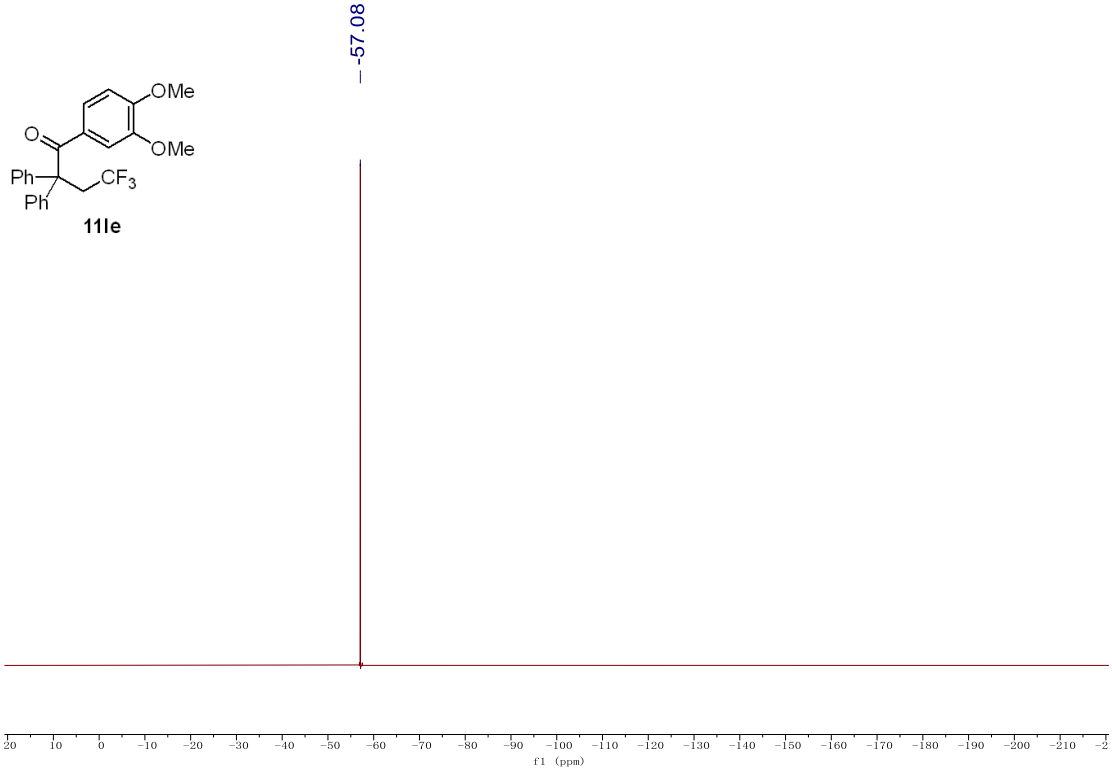
127.70
126.85
125.48
124.63
122.42
113.37
109.55
77.41
77.16
76.90
61.97
55.94
55.79
45.97
45.75
45.54
45.32
OMe
OMe
O
Ph
Ph
CF3
11le
f1 (ppm)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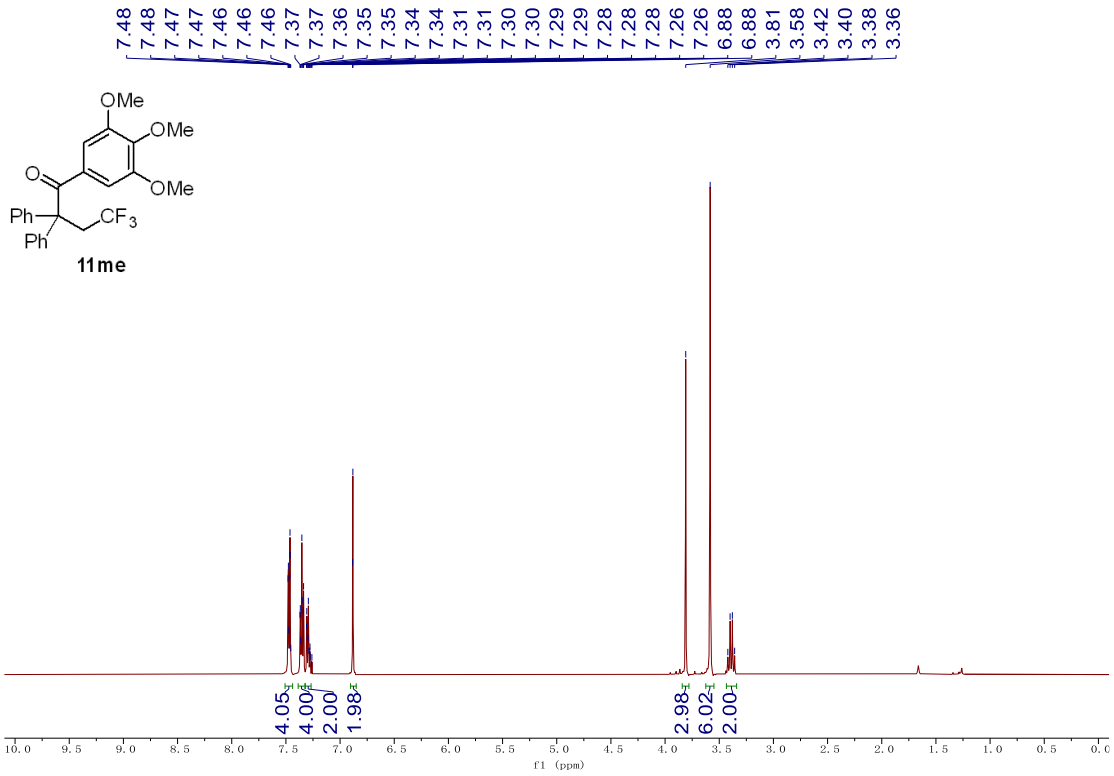
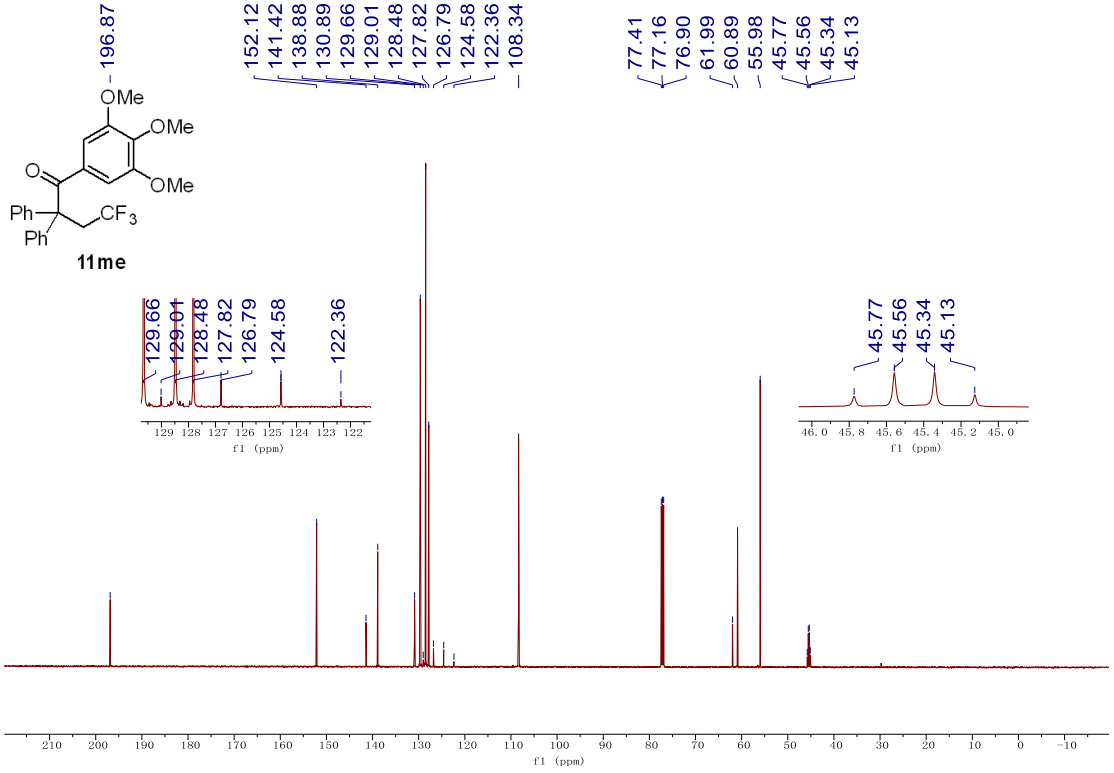
OMe
O
Ph
Ph
CF3
11le
f1 (ppm)


7.48 7.48 7.47 7.47 7.46 7.46 7.46 7.37 7.37 7.36 7.35 7.35 7.34 7.34 7.31 7.31 7.30 7.30 7.29 7.29 7.28 7.28 7.28 7.26 7.26 6.88 6.88 3.81 3.58 3.42 3.40 3.38 3.36
OMe
OMe
OMe
O
Ph
Ph
CF3
11me
4.05 4.00 2.00 1.98 2.98 6.02 2.00
f1 (ppm)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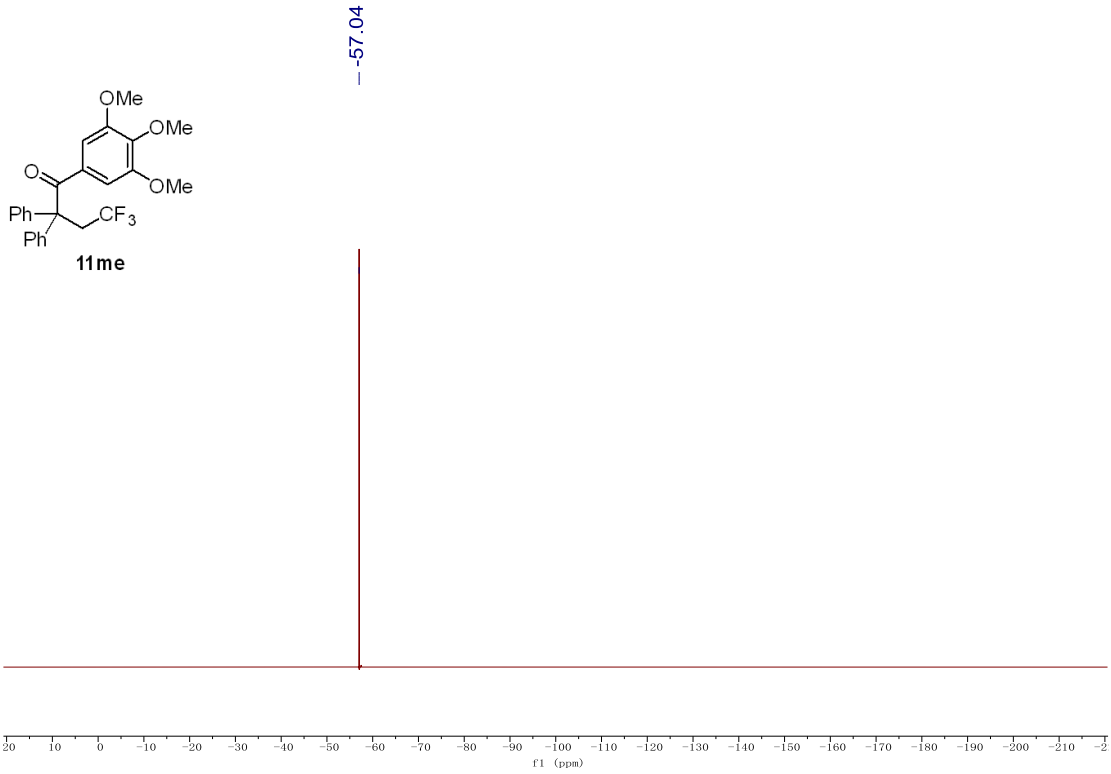
77.41 77.16 76.90 61.99 60.89 55.98 45.77 45.56 45.34 45.13
OMe
OMe
OMe
O
Ph
Ph
CF3
11me
129.66 129.01 128.48 127.82 126.79 124.58 122.36
45.77 45.56 45.34 45.13
f1 (ppm)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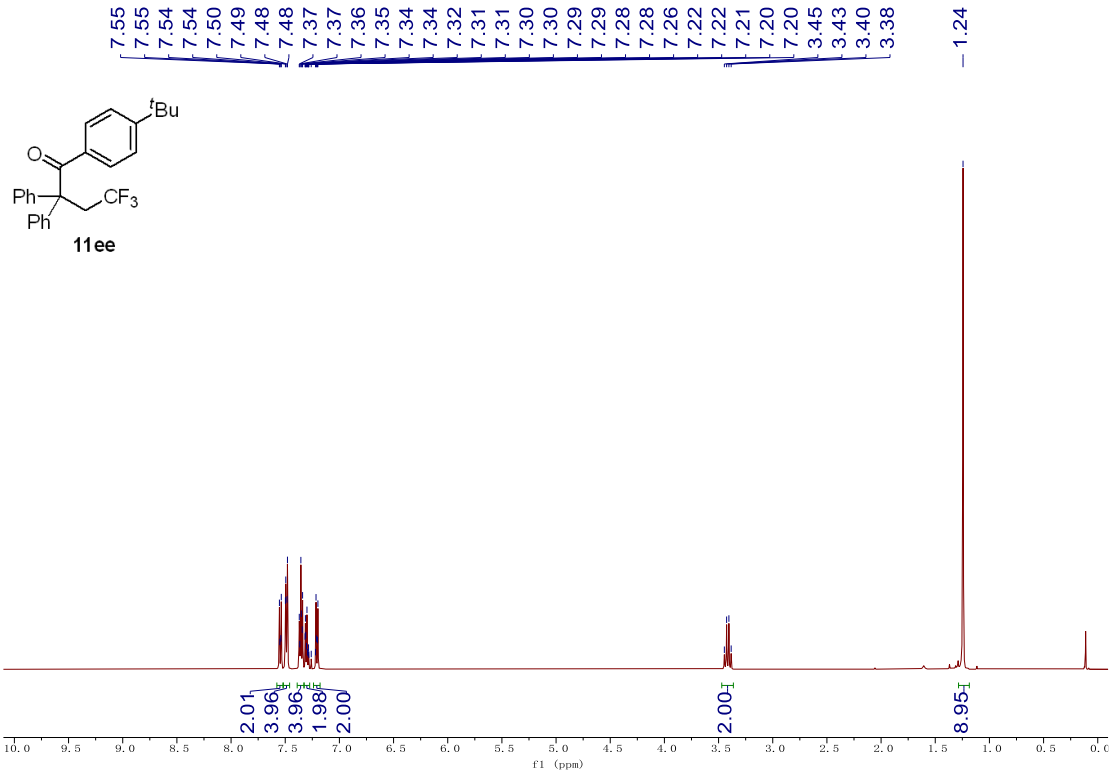
OMe
OMe
OMe
O
Ph
Ph
CF3
11me
f1 (ppm)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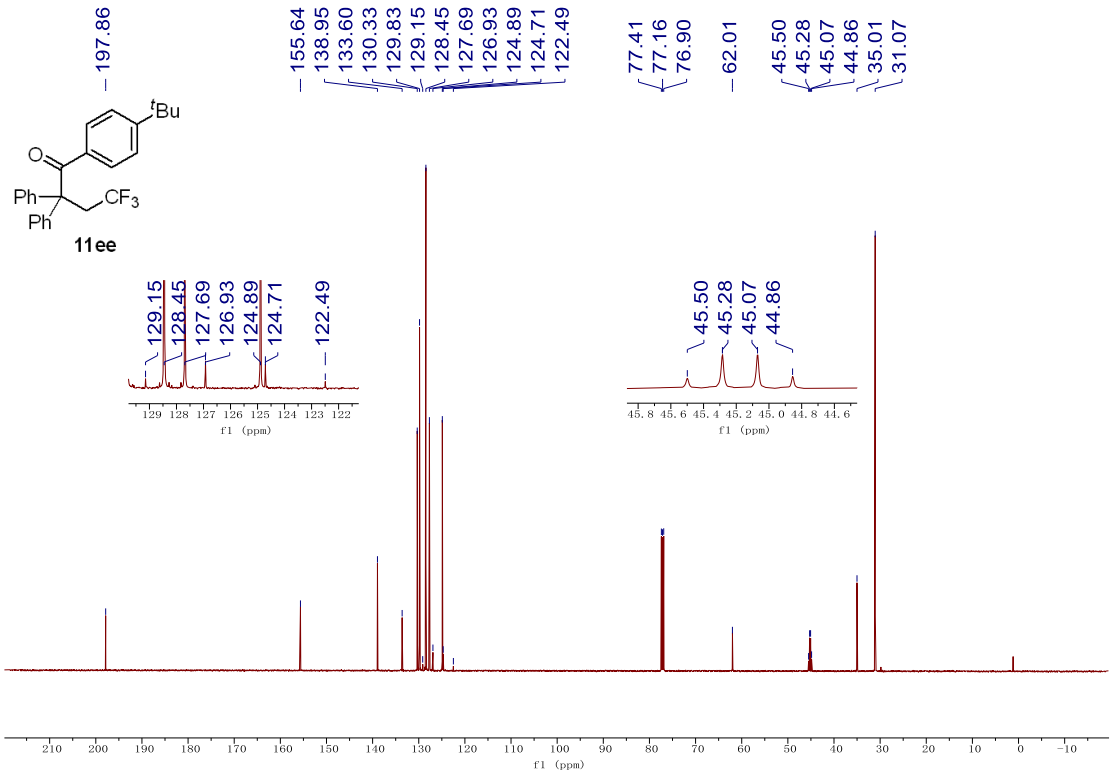
7.26
7.22
7.22
7.21
7.20
7.20
3.45
3.43
3.40
3.38
1.24
tBu
O
Ph
Ph
CF3
11ee
2.01
3.96
3.96
1.98
2.00
2.00
8.95
f1 (ppm)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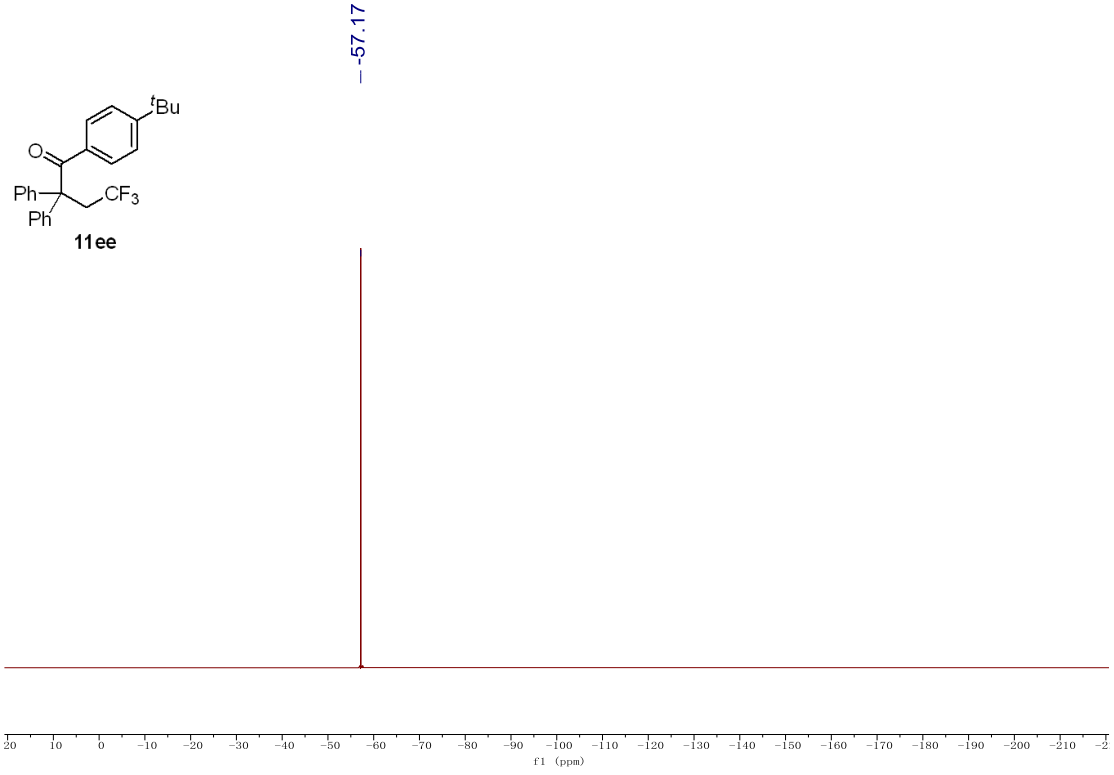
122.49
77.41
77.16
76.90
62.01
45.50
45.28
45.07
44.86
35.01
31.07
tBu
O
Ph
CF3
Ph
11ee
f1 (ppm)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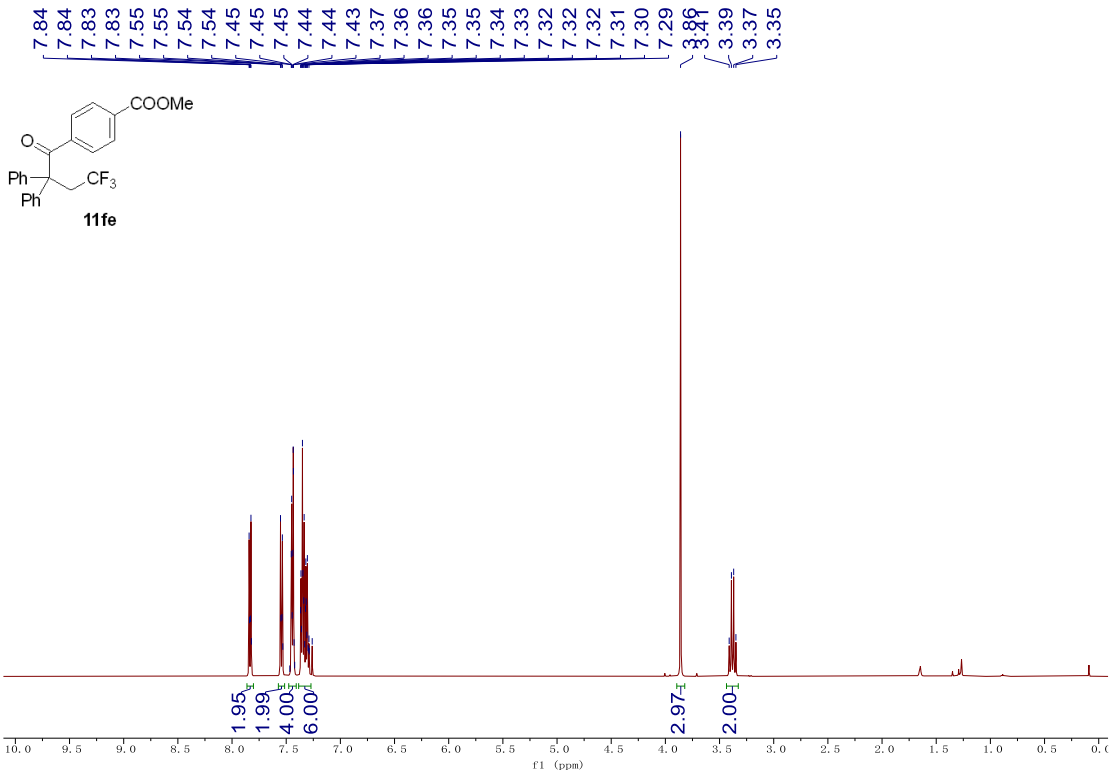
tBu
O
Ph
CF3
Ph
11ee
f1 (ppm)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7.54
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3.37
3.35
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CF3
Ph
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2.00
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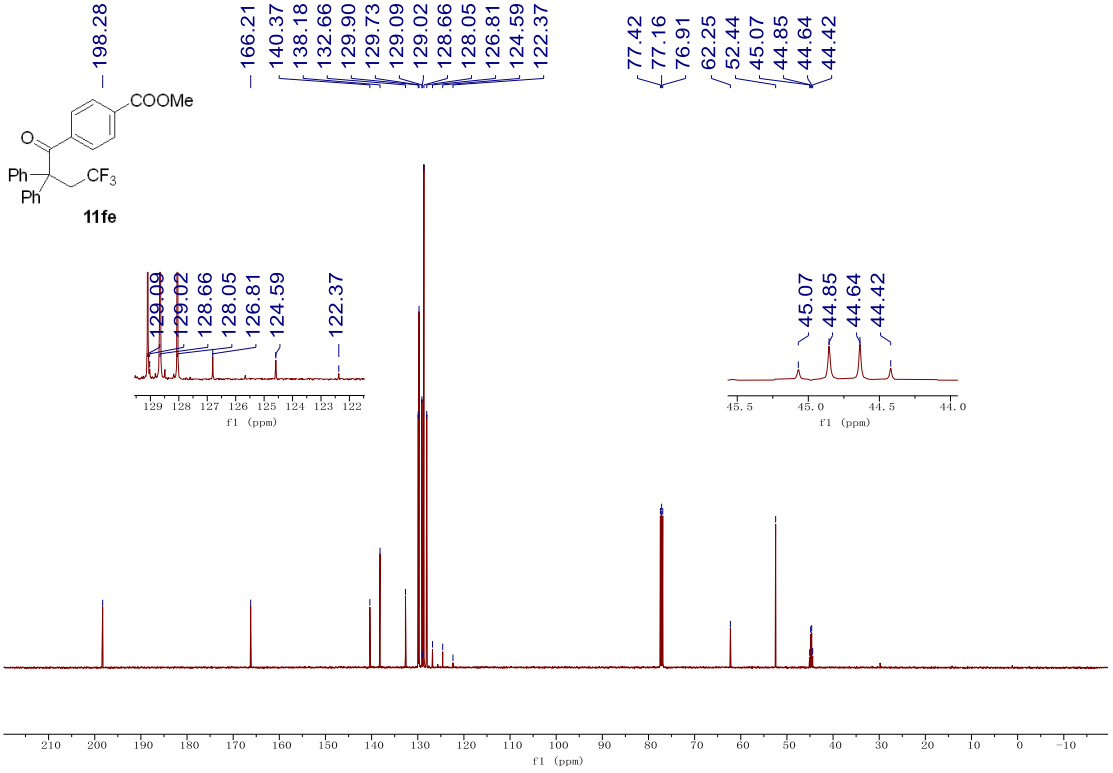
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77.16
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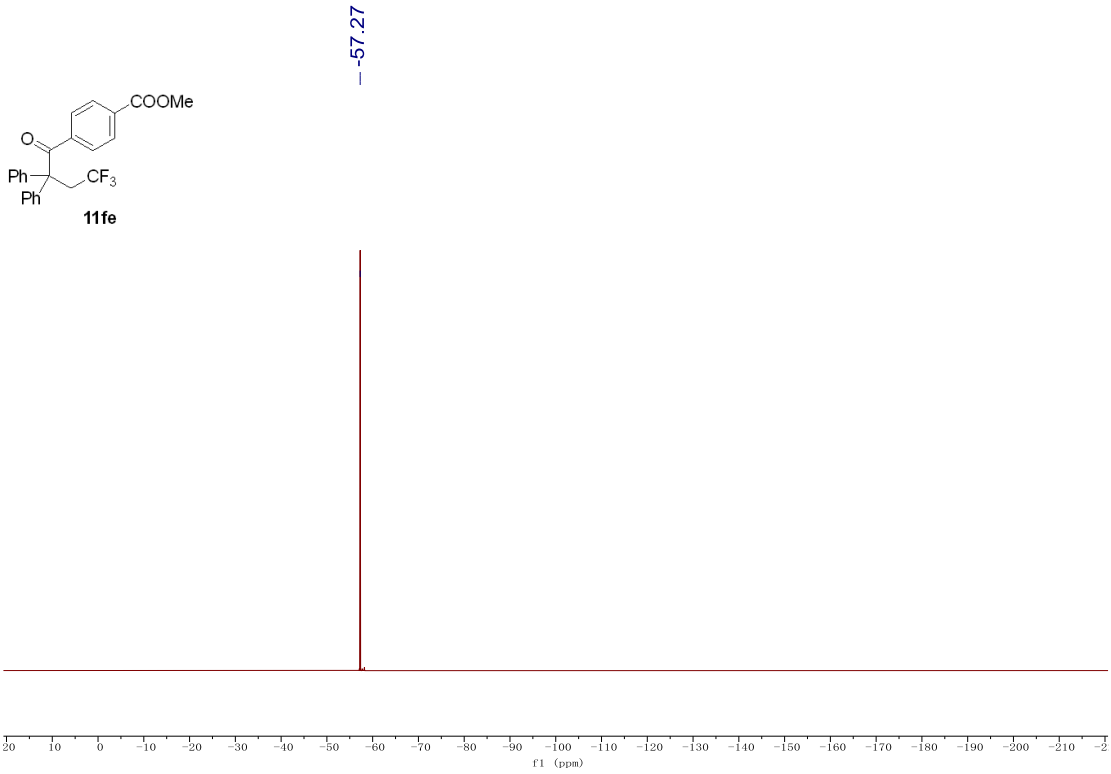
f1 (ppm)
f1 (ppm)
f1 (ppm)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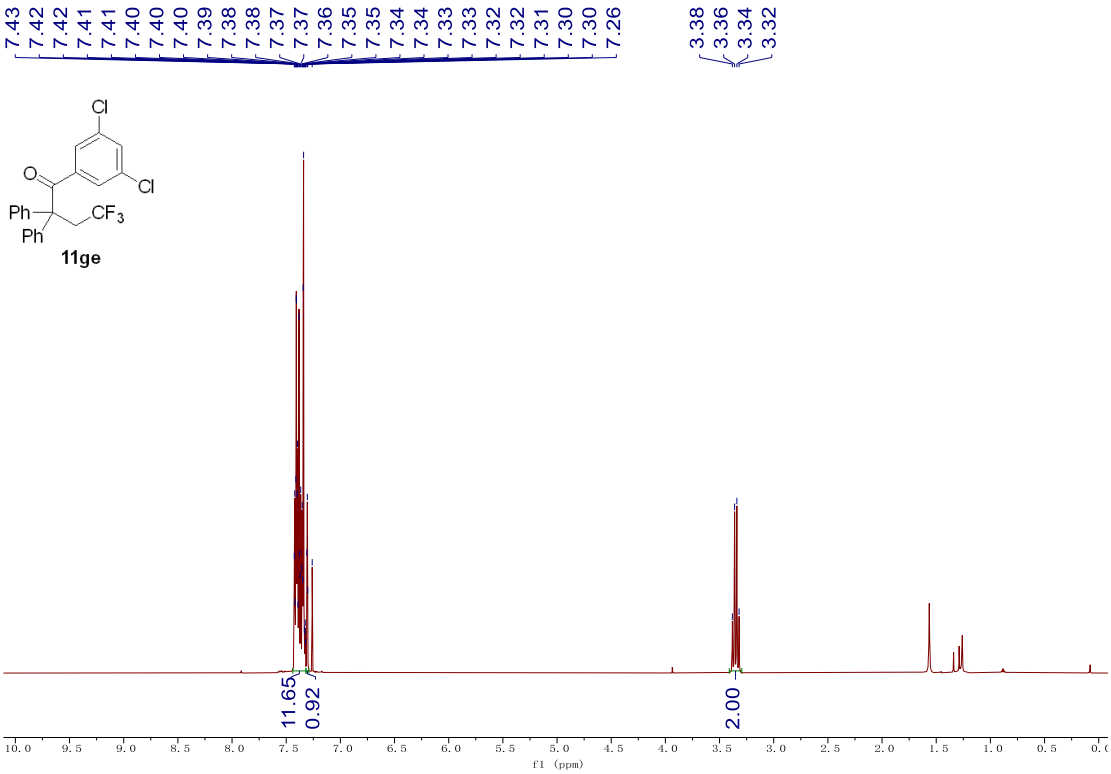
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7.30
7.30
7.26
3.38
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Cl
Ph
Ph
CF3
11ge
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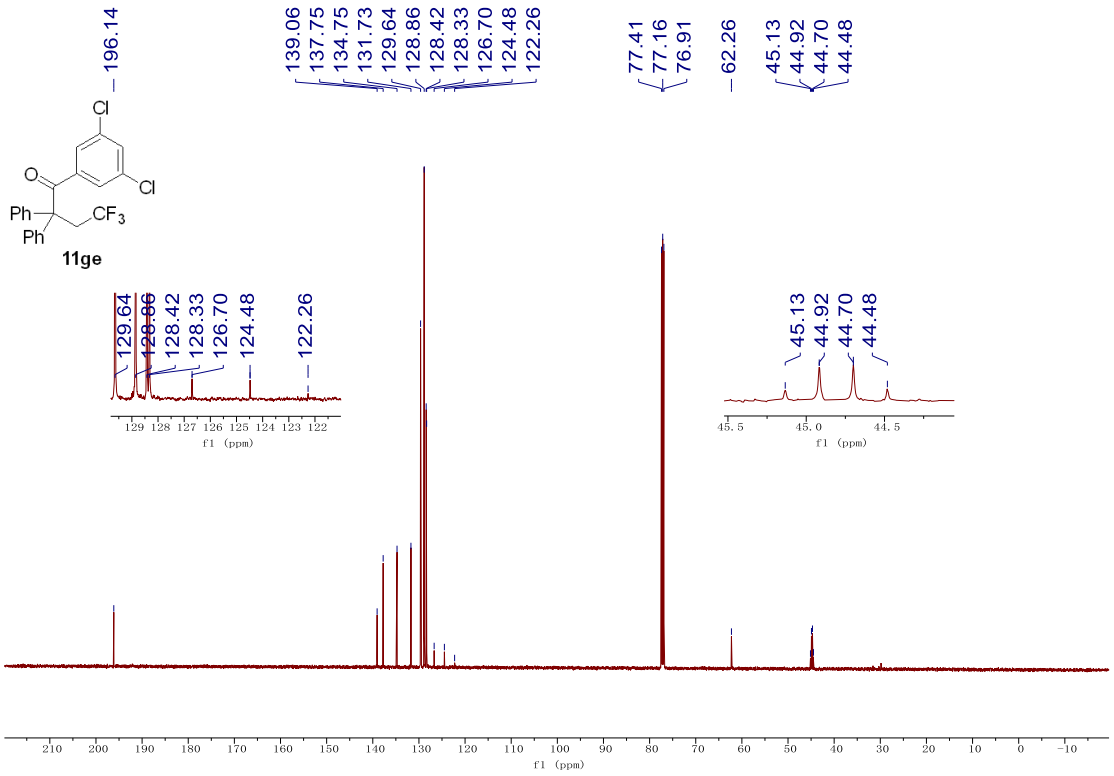
f1 (ppm)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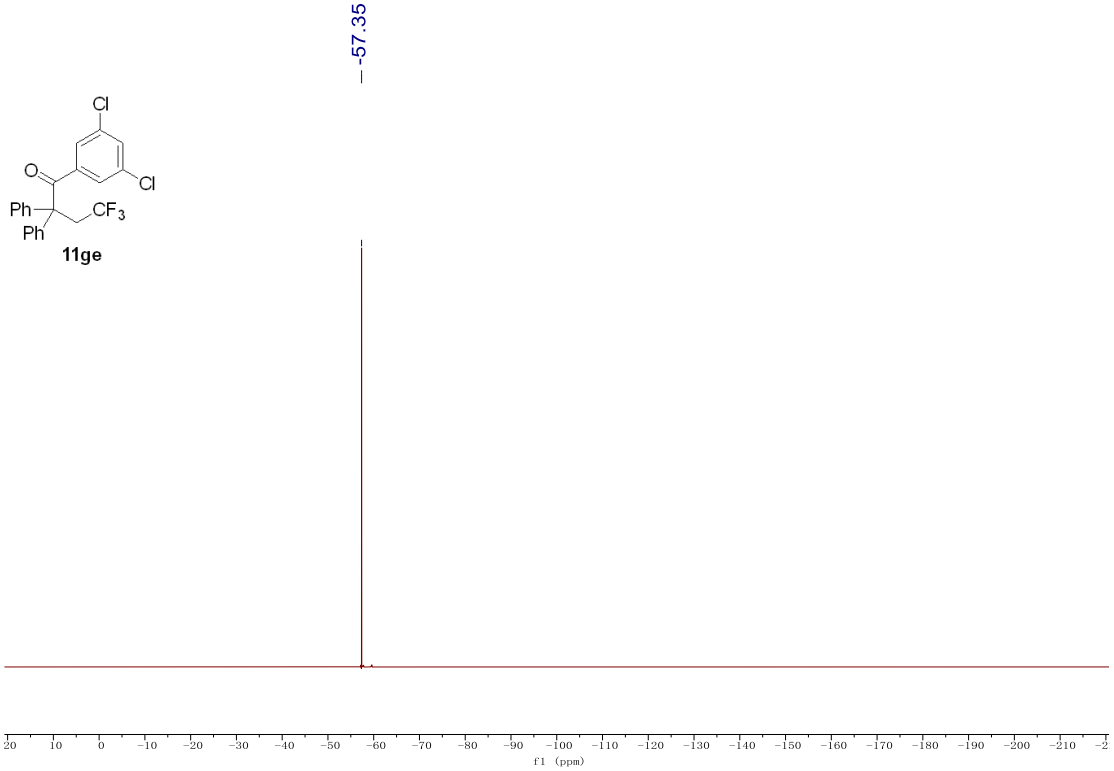
Cl
Ph
CF3
Ph
11ge
f1 (ppm)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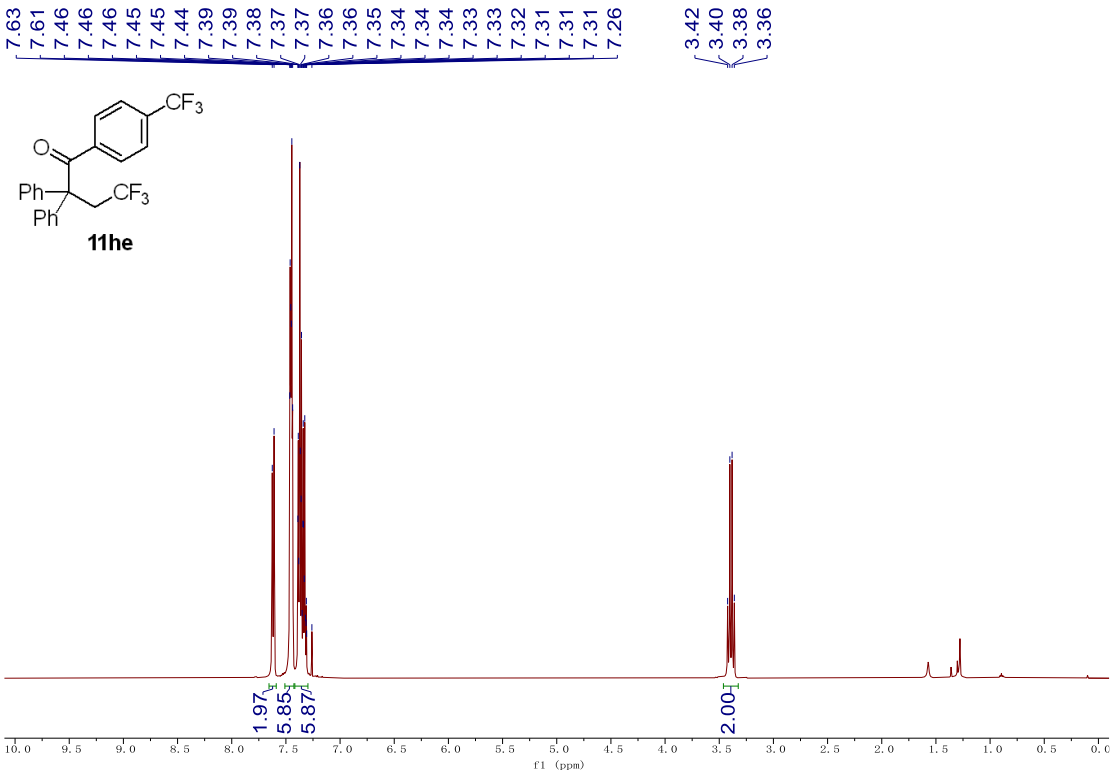
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CF3
Ph
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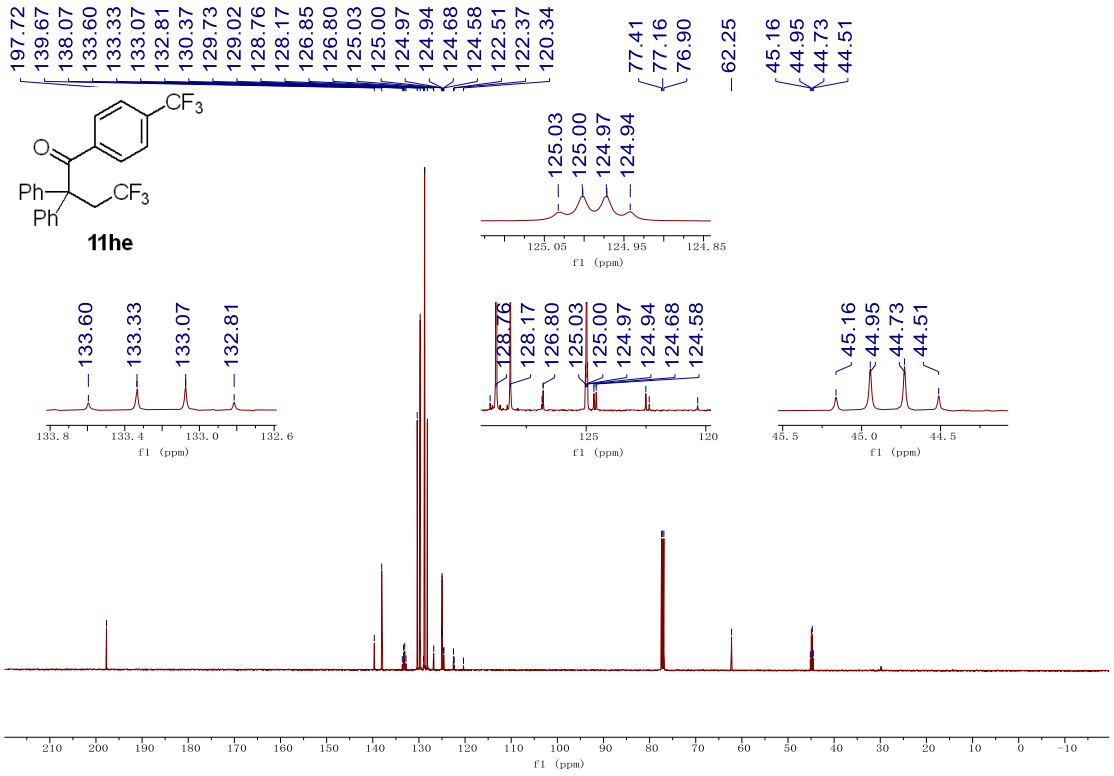
2.00
f1 (ppm)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125.00
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122.37
120.34
77.41
77.16
76.90
62.25
45.16
44.95
44.73
44.51
CF3
O
Ph
CF3
Ph
11he
125.03
125.00
124.97
124.94
133.60
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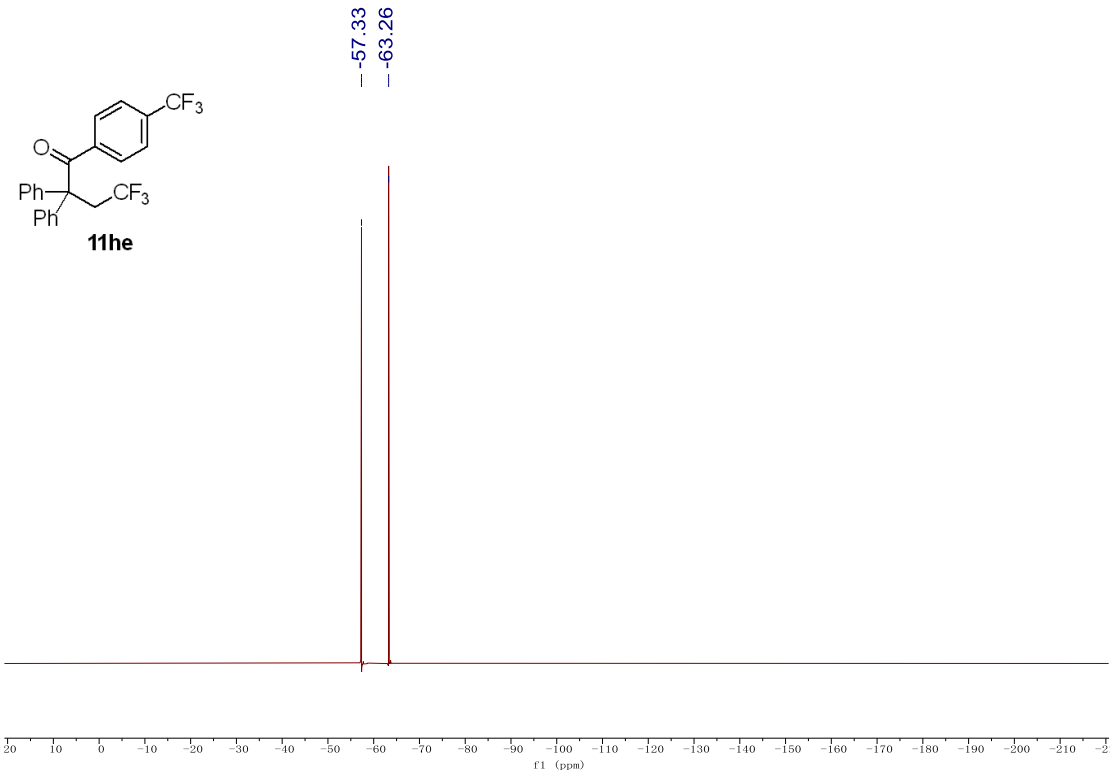
f1 (ppm)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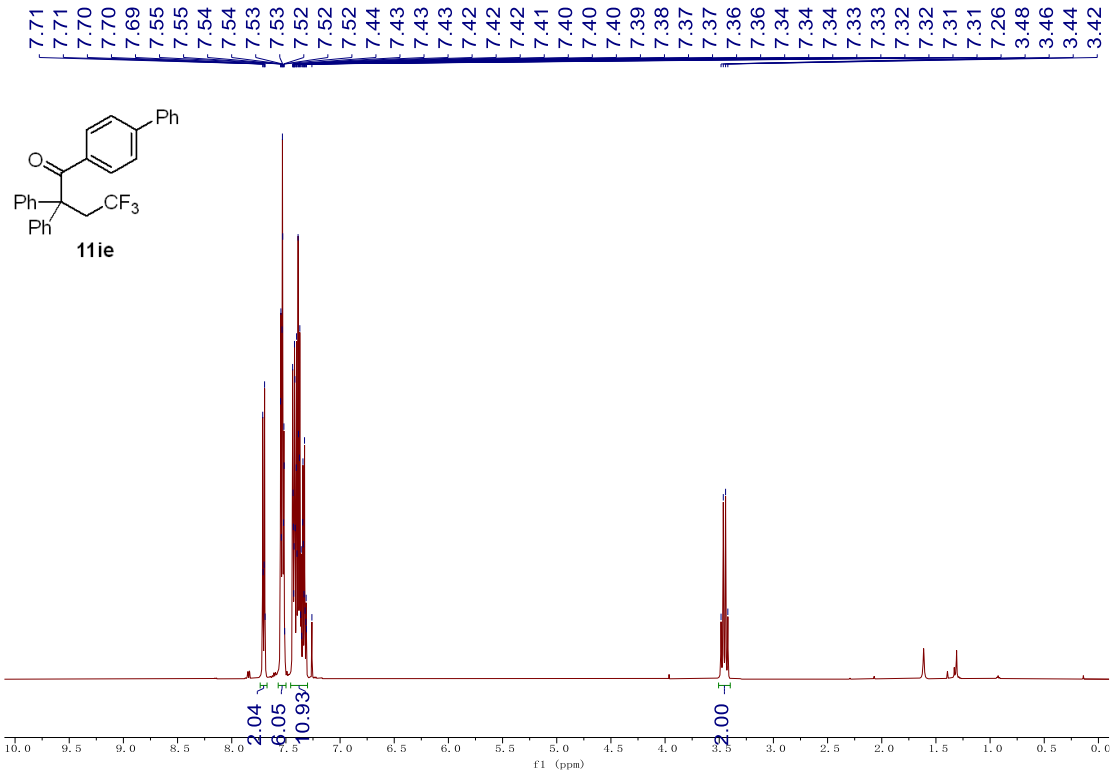
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7.33
7.33
7.32
7.32
7.31
7.31
7.26
3.48
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Ph
O
Ph
CF3
Ph
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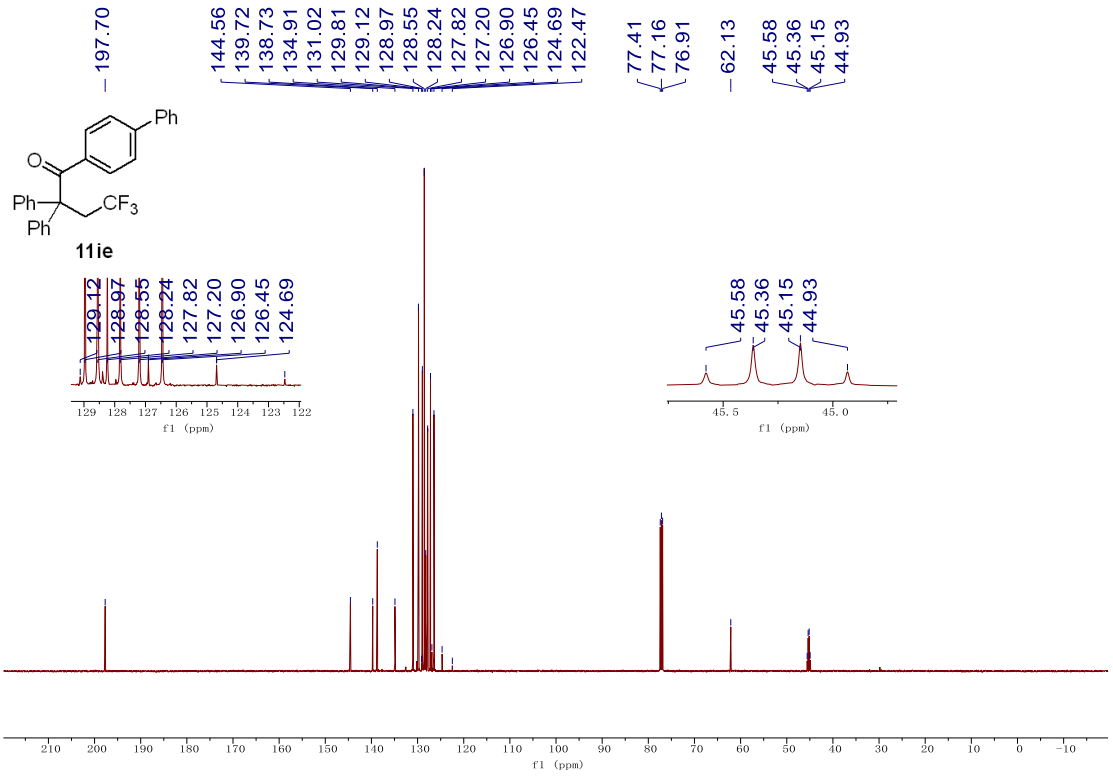
6.05
10.93
2.00
f1 (ppm)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127.20
126.90
126.45
124.69
122.47
77.41
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76.91
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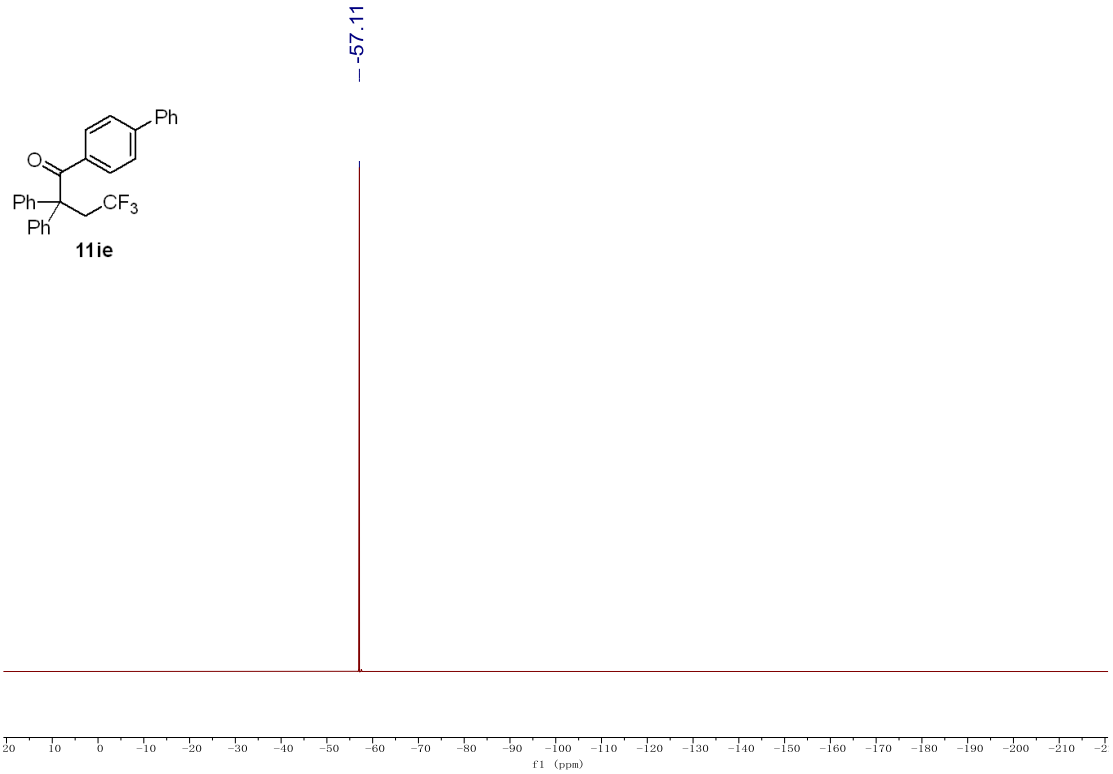
45.58
45.36
45.15
44.93
Ph
O
Ph
CF3
Ph
11ie
f1 (ppm)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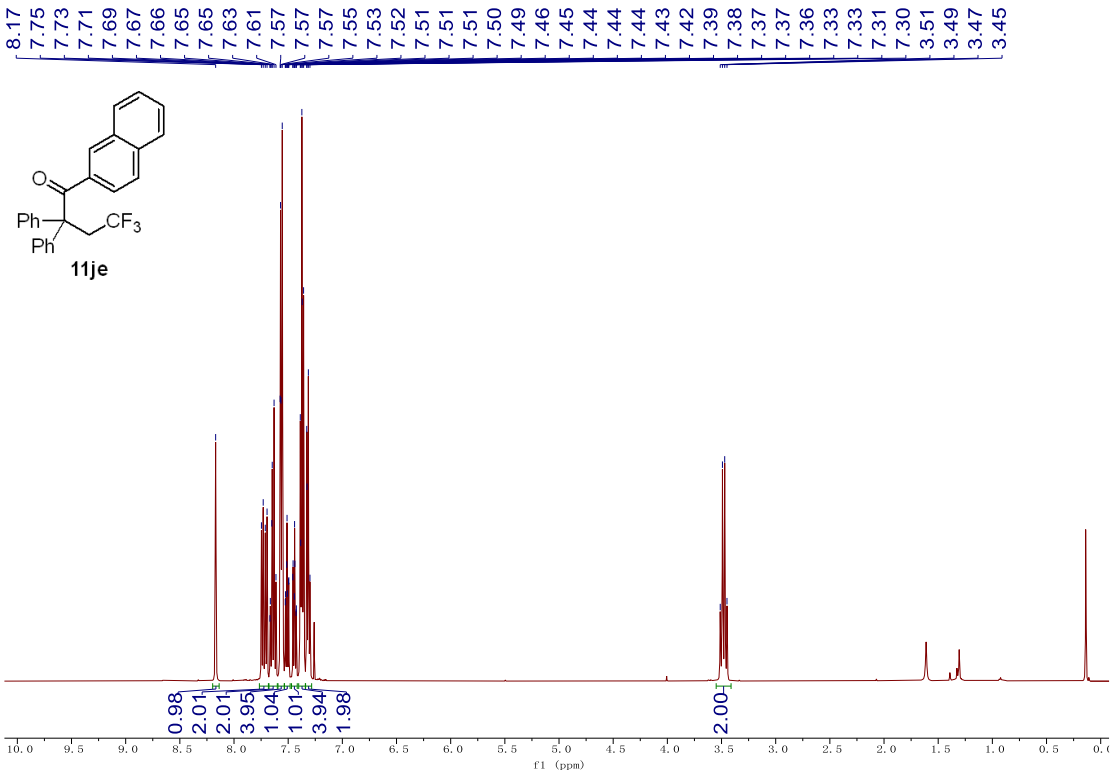
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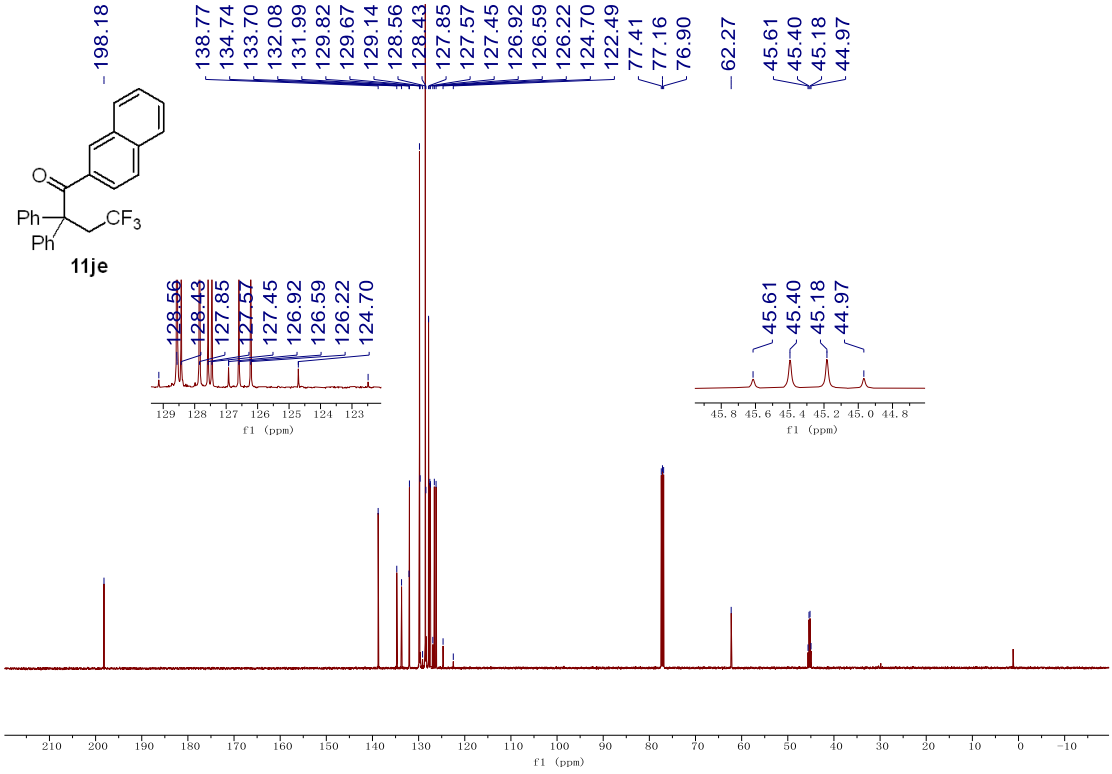
Ph
Ph
CF3
11je
0.98 2.01 2.01 3.95 1.04 1.01 3.94 1.98 2.00
f1 (ppm)


198.18
138.77 134.74 133.70 132.08 131.99 129.82 129.67 129.14 128.56 128.43 127.85 127.57 127.45 126.92 126.59 126.22 124.70 122.49
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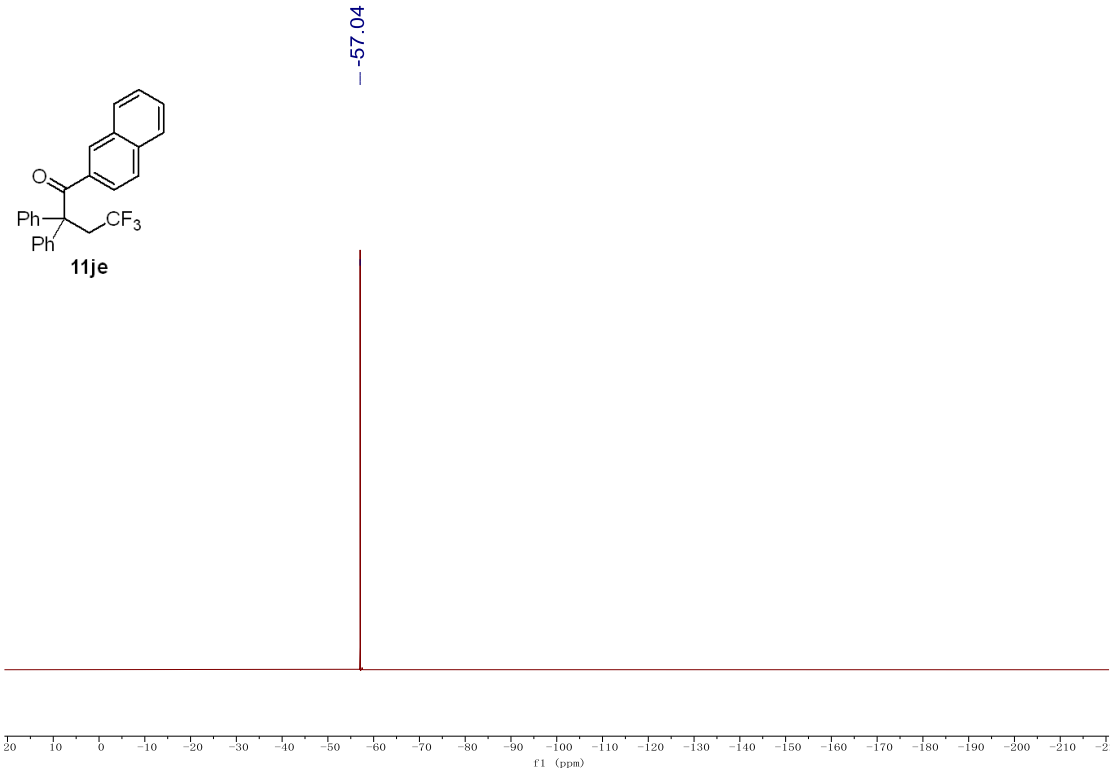
62.27
45.61 45.40 45.18 44.97
O
Ph
Ph
CF3
11je
f1 (ppm)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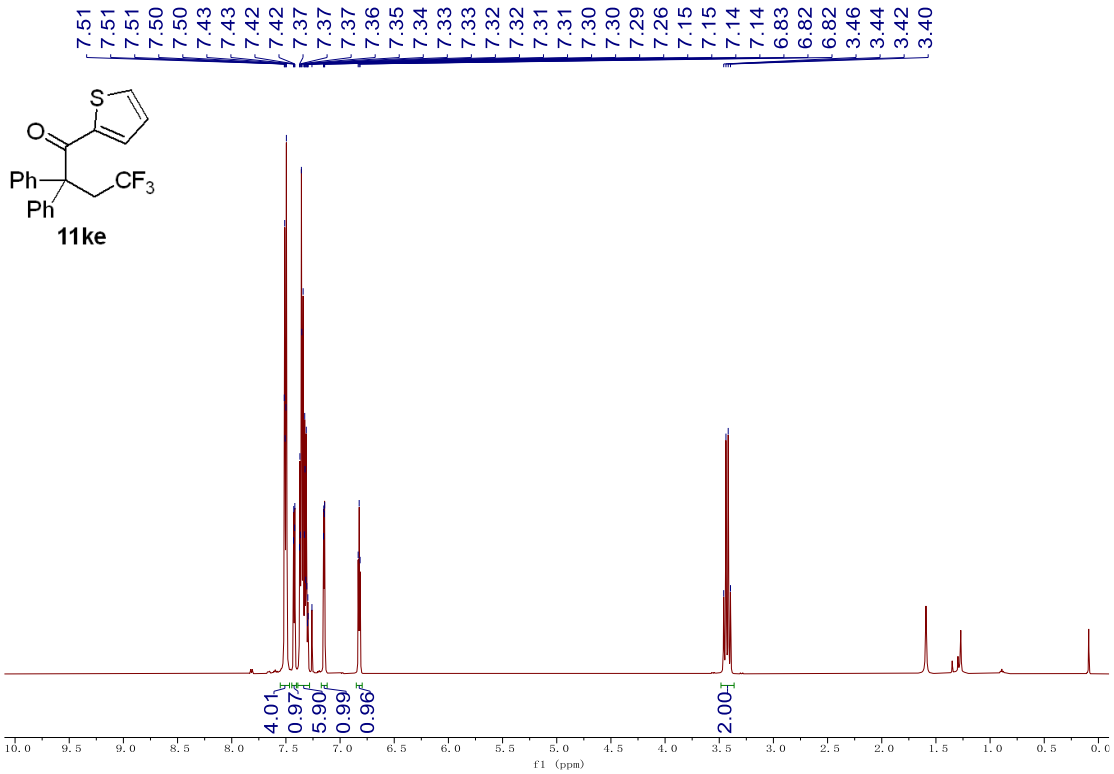
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7.32
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7.31
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7.30
7.29
7.26
7.15
7.15
7.14
7.14
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6.82
6.82
3.46
3.44
3.42
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Ph
Ph
CF3
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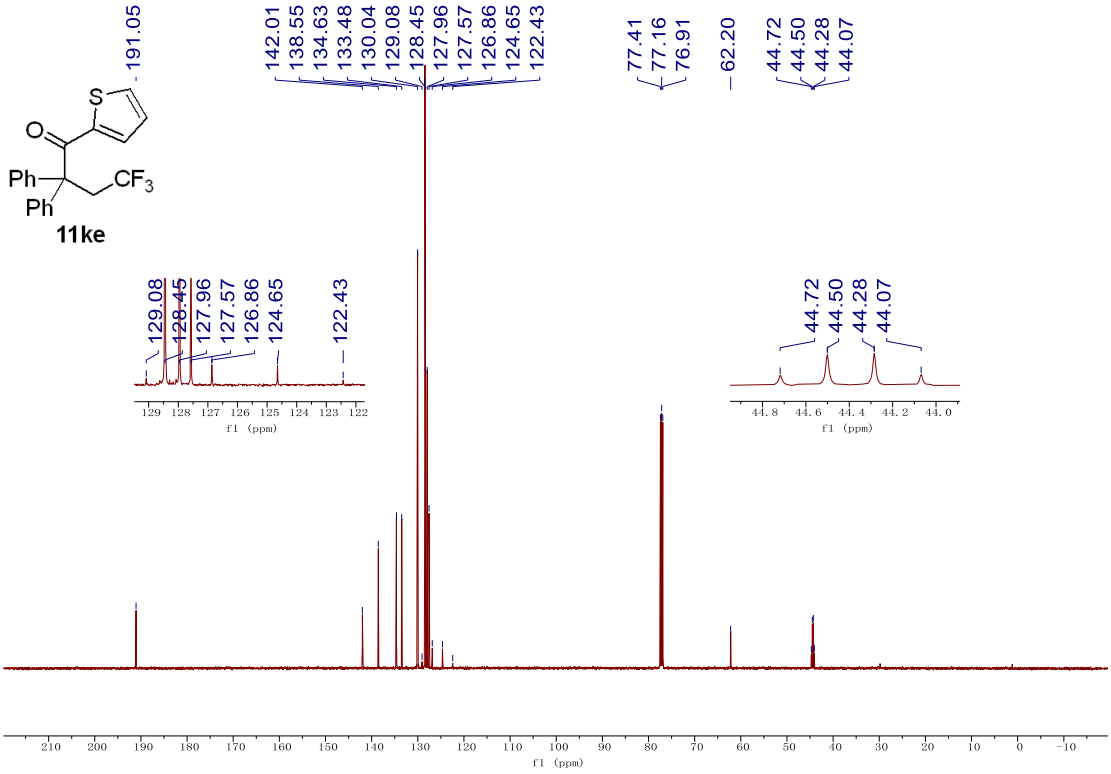
0.99
0.96
2.00
f1 (ppm)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77.41
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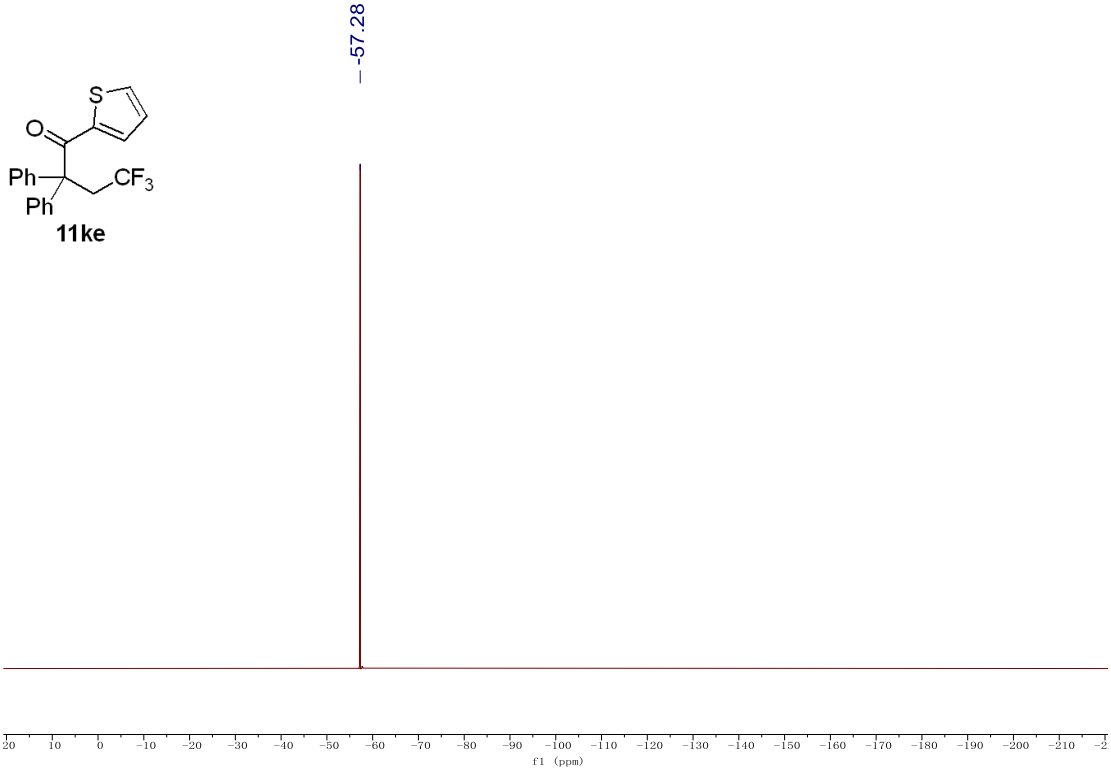
S
O
Ph
CF3
Ph
11ke
f1 (ppm)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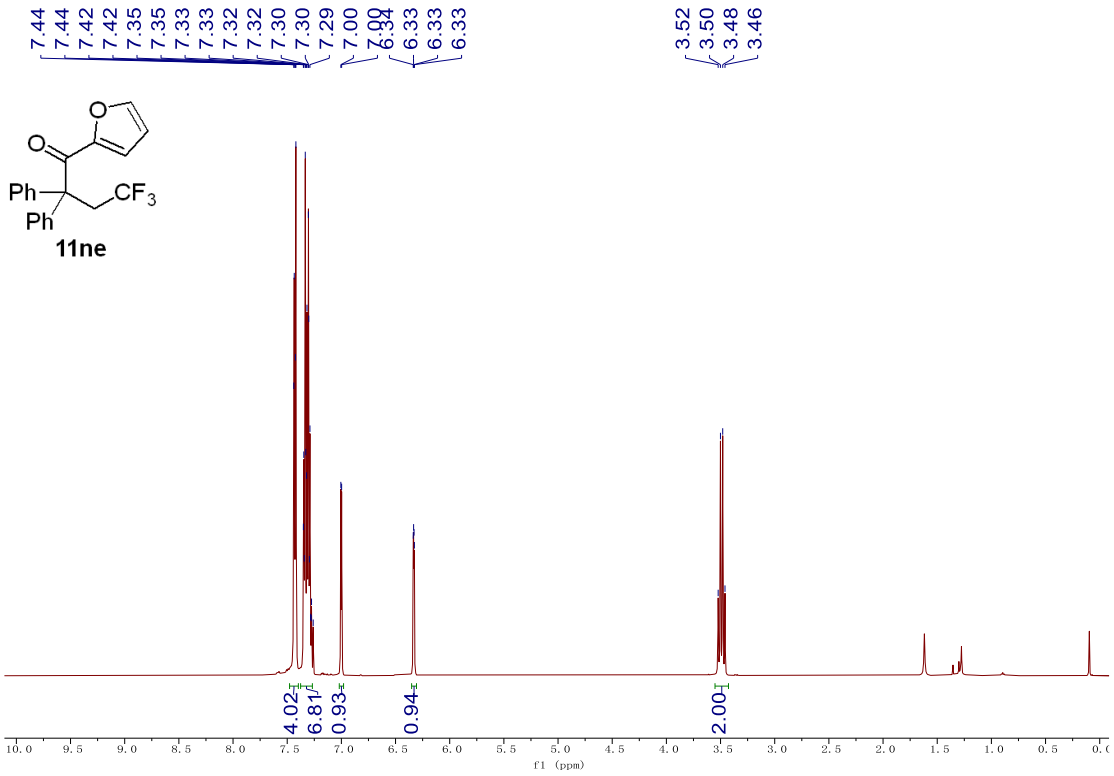
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6.33
6.33
3.52
3.50
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O
Ph
Ph
CF3
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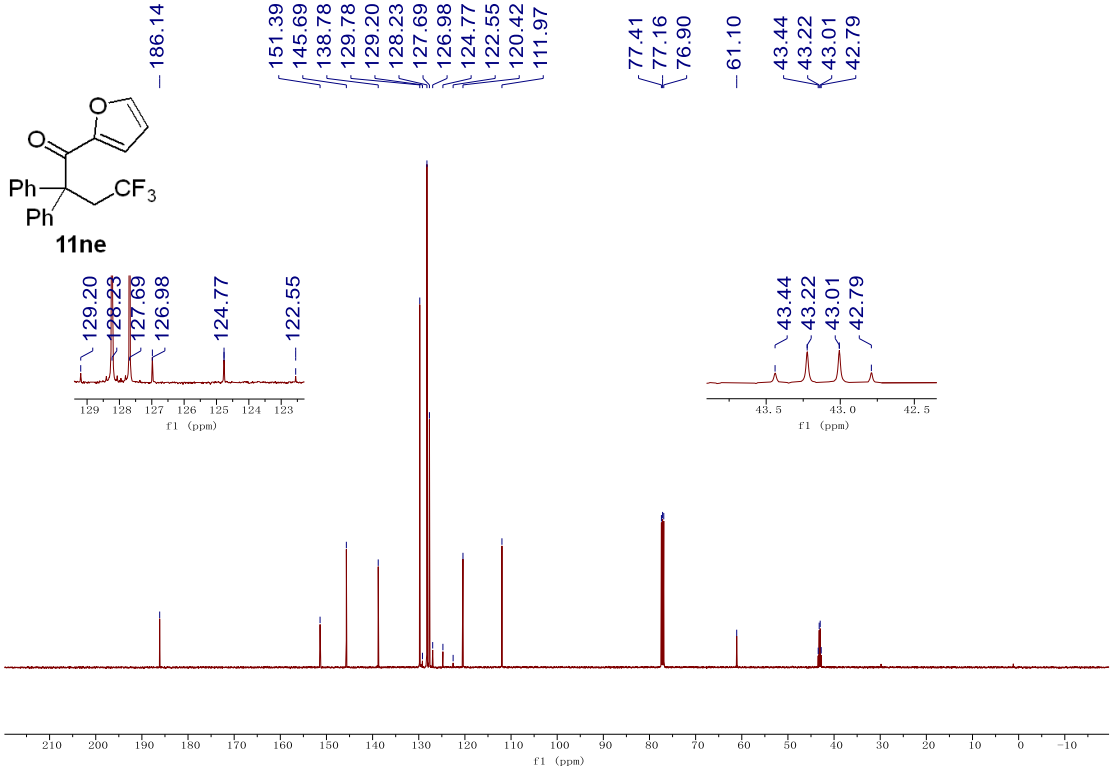
2.00
f1 (ppm)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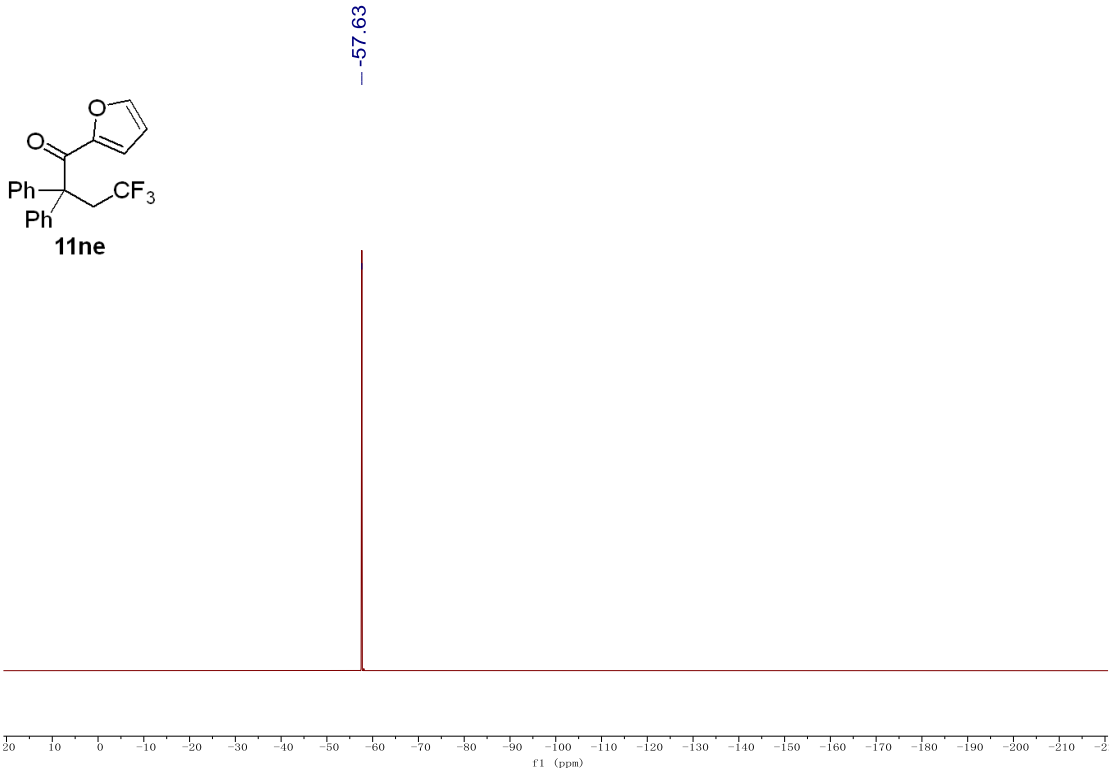
111.97
77.41
77.16
76.90
61.10
43.44
43.22
43.01
42.79
O
O
Ph
Ph
CF3
11ne
129.20
128.23
127.69
126.98
124.77
122.55
f1 (ppm)
43.44
43.22
43.01
42.79
f1 (ppm)
f1 (ppm)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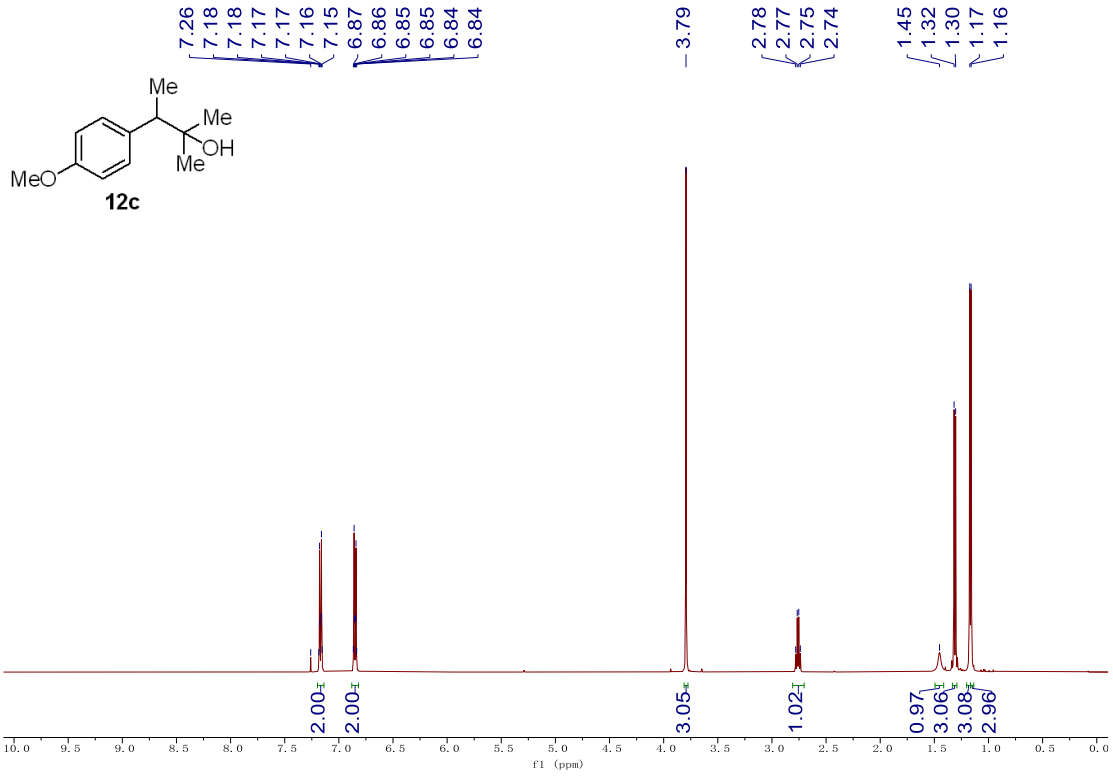
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6.84
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2.78
2.77
2.75
2.74
1.45
1.32
1.30
1.17
1.16
Me
Me
OH
Me
MeO
12c
2.00
2.00
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1.02
0.97
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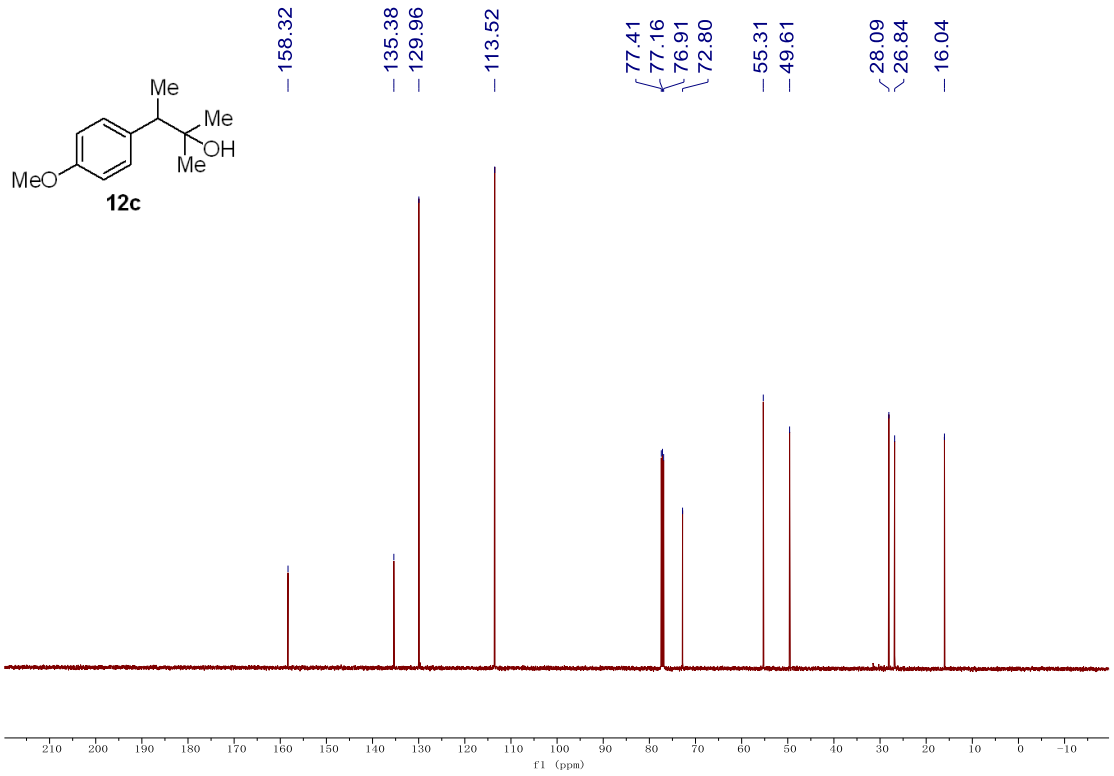
3.08
2.96
f1 (ppm)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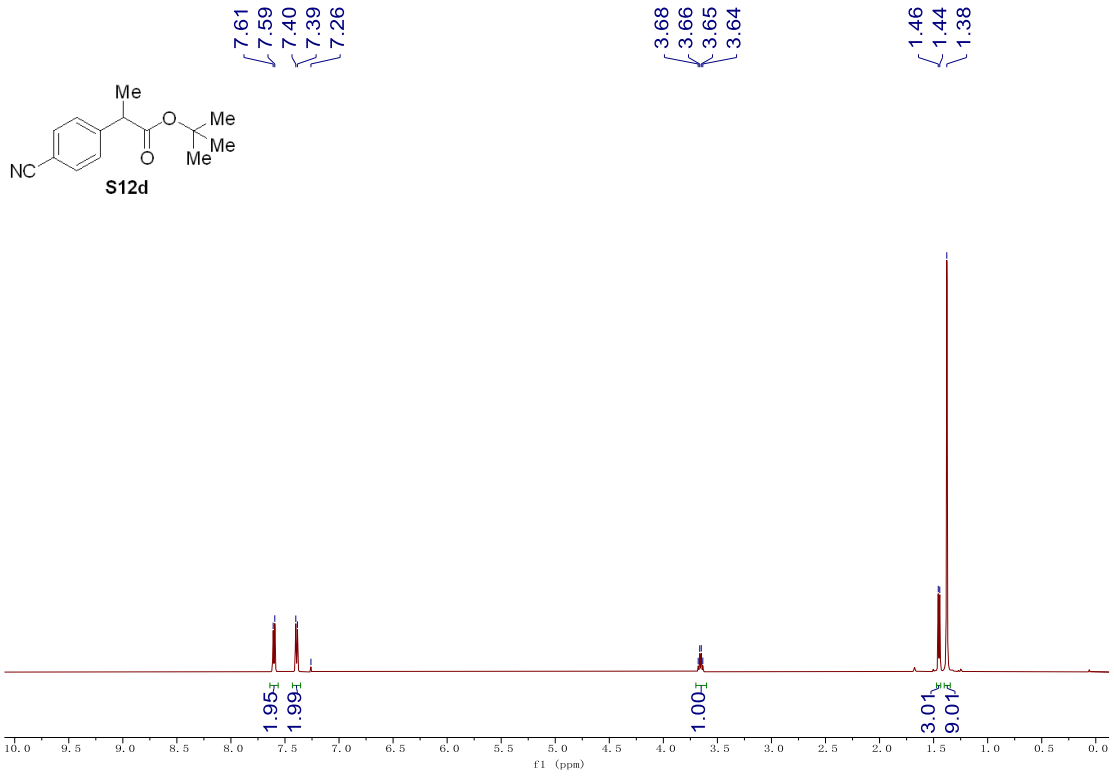
28.09
26.84
16.04
Me
Me
OH
Me
MeO
12c
f1 (ppm)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3.65
3.64
1.46
1.44
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Me
Me
O
NC
S12d
1.95
1.99
1.00
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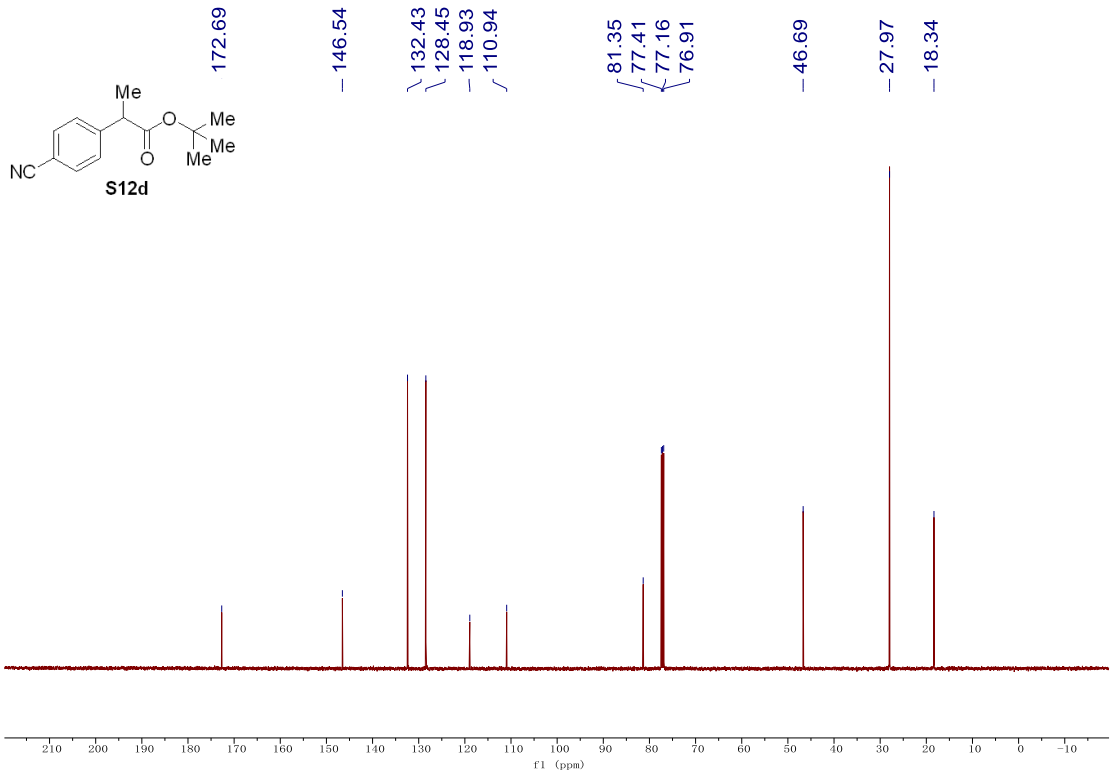
9.01
f1 (ppm)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46.69
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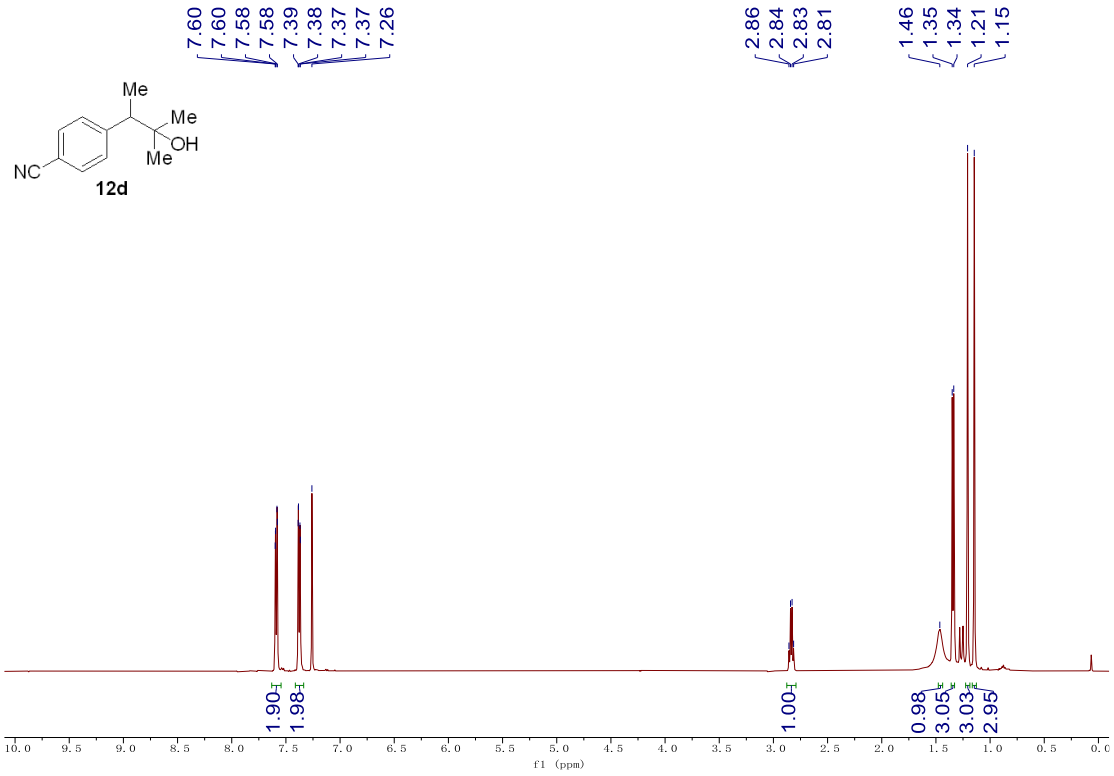
Me
Me
O
O
NC
S12d
f1 (ppm)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1.46
1.35
1.34
1.21
1.15
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NC
12d
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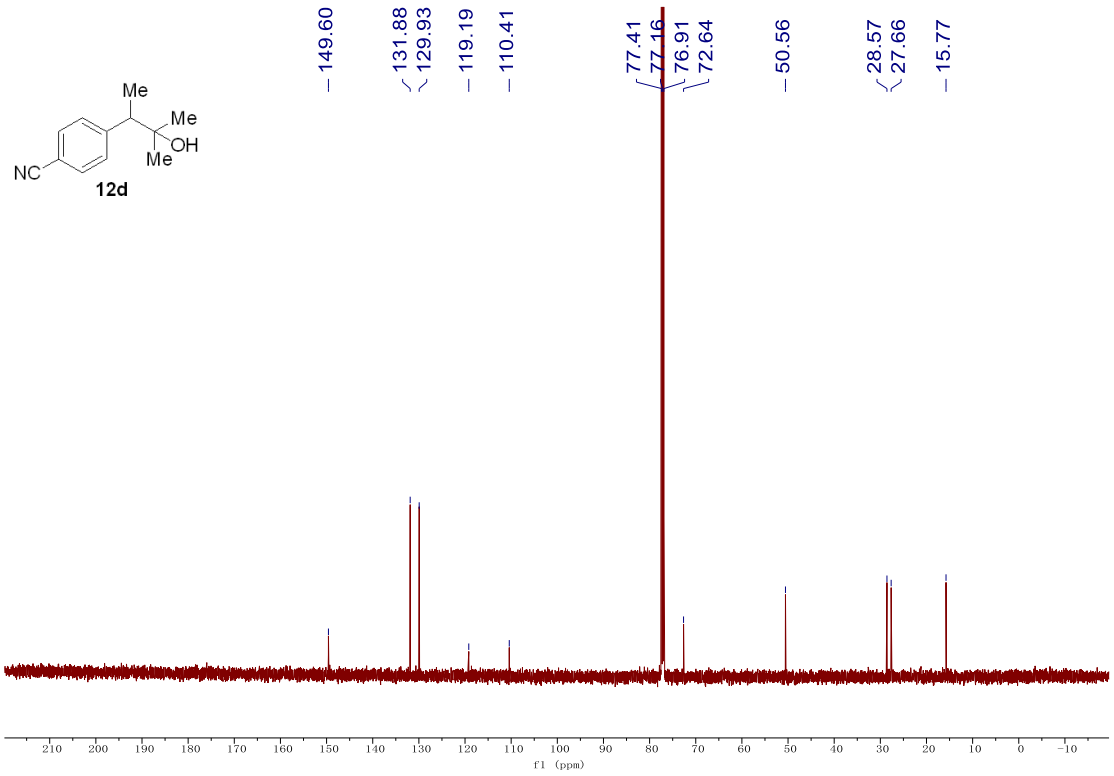
2.95
f1 (ppm)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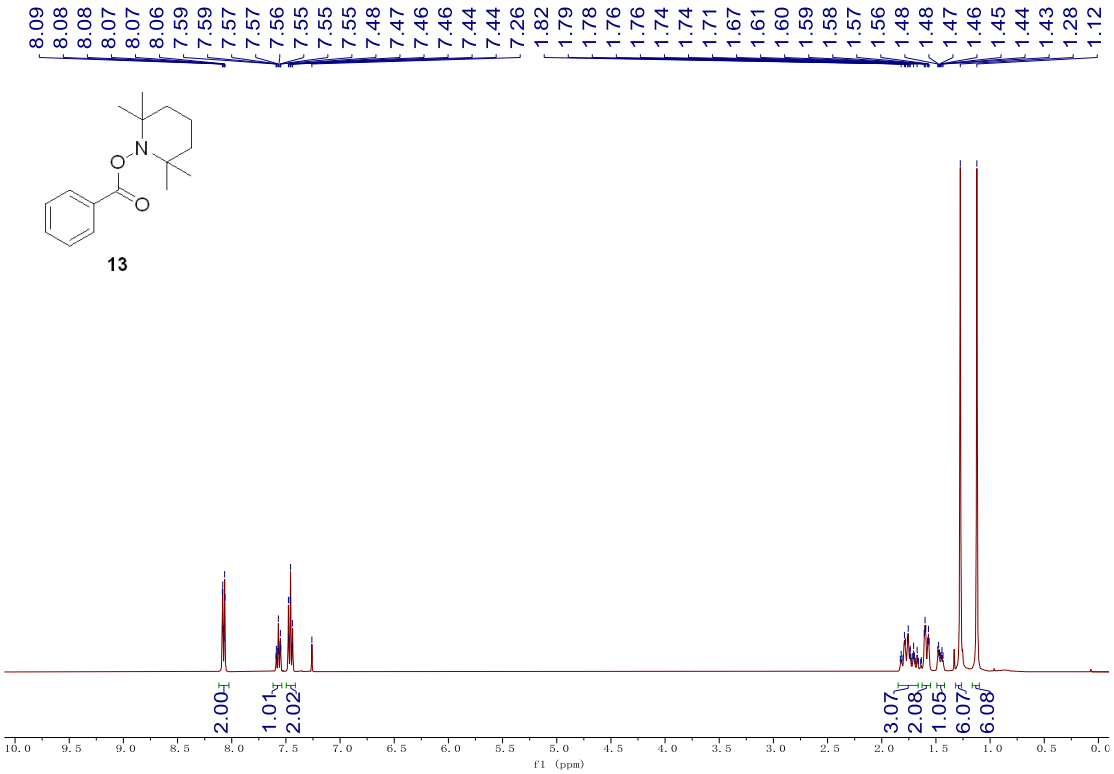
Me
OH
Me
NC
12d
f1 (ppm)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7.44
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1.05
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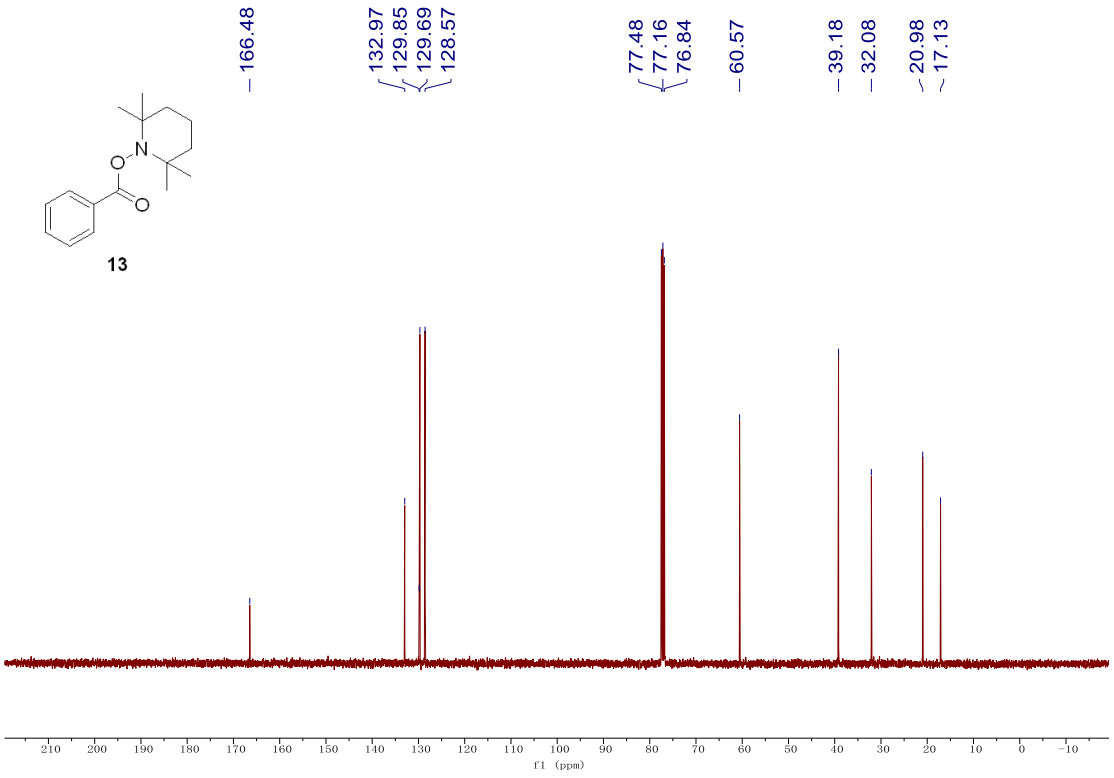
6.08
f1 (ppm)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32.08
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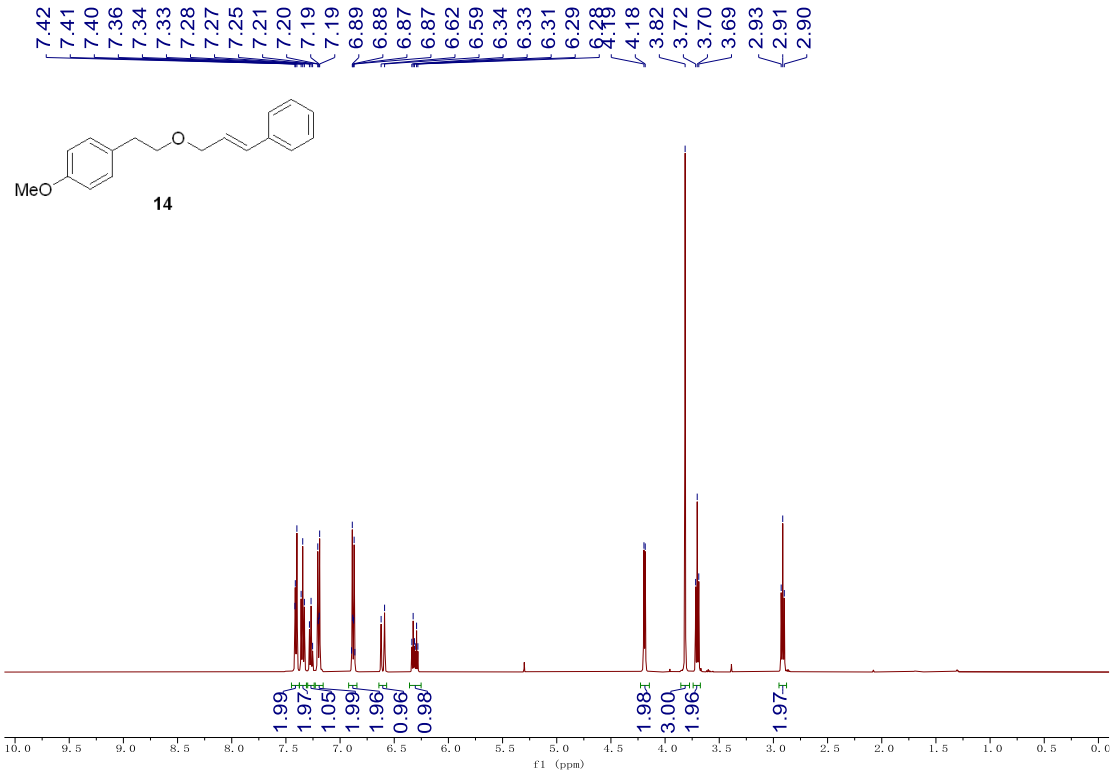
13
f1 (ppm)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6.88
6.87
6.87
6.62
6.59
6.34
6.33
6.31
6.29
4.18
3.82
3.72
3.70
3.69
2.93
2.91
2.90
MeO
14
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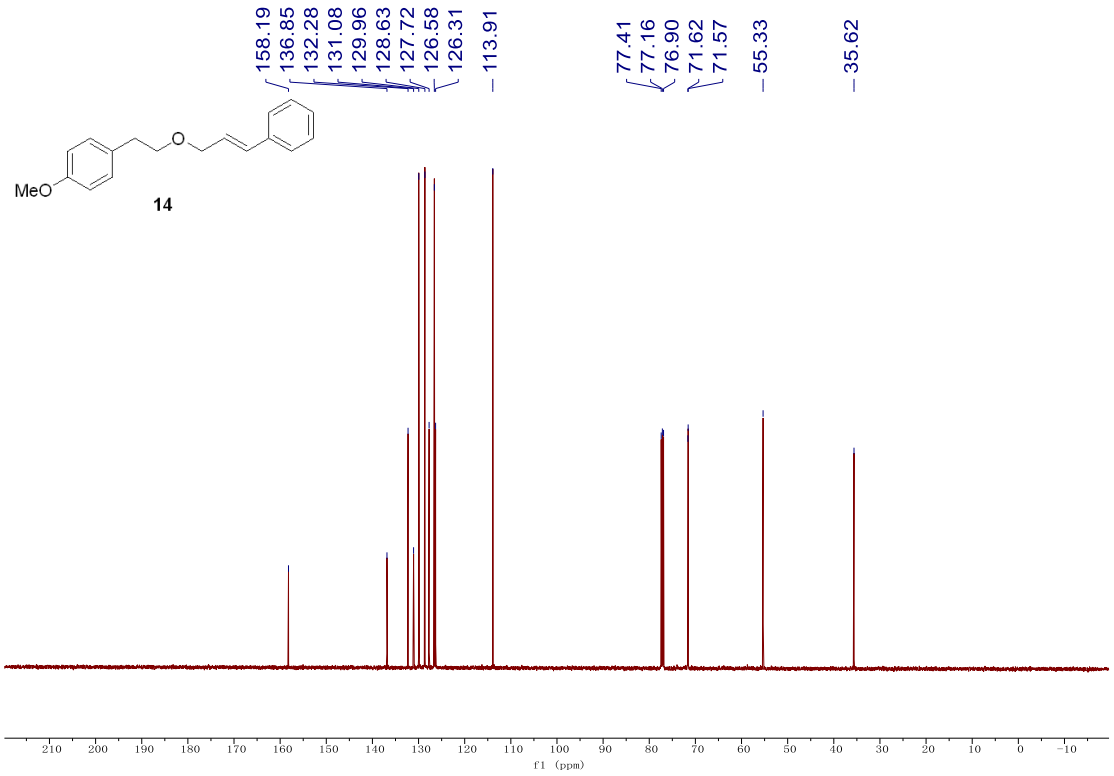
f1 (ppm)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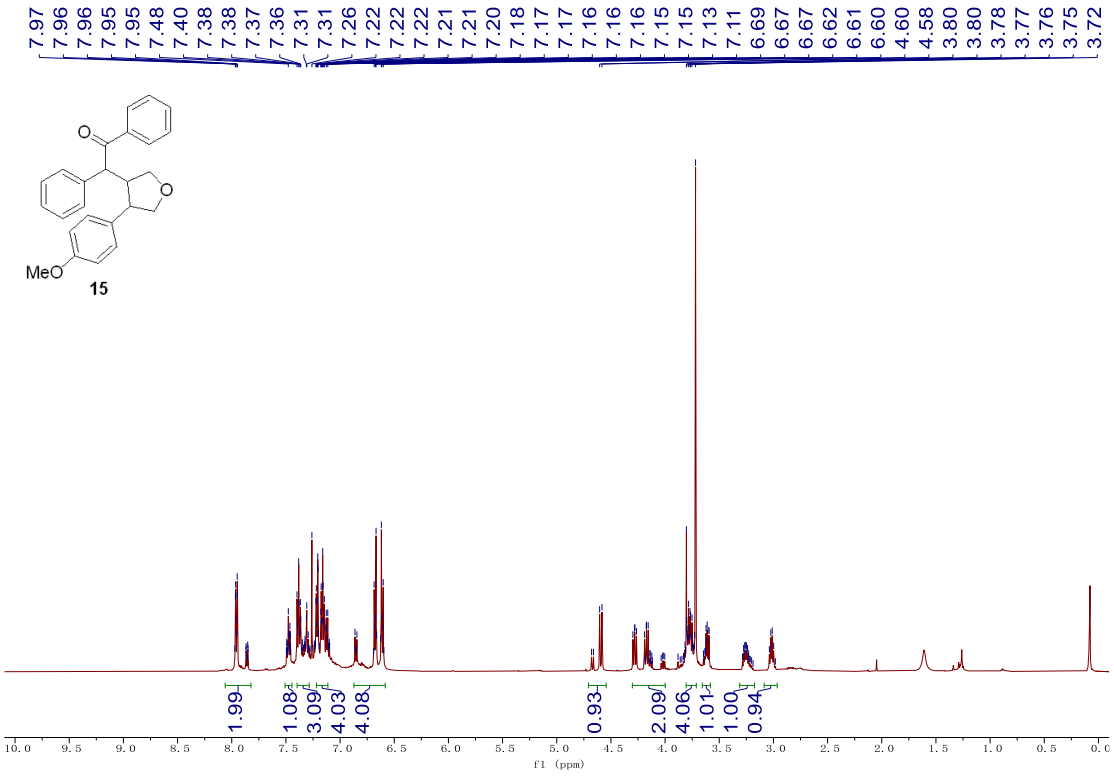
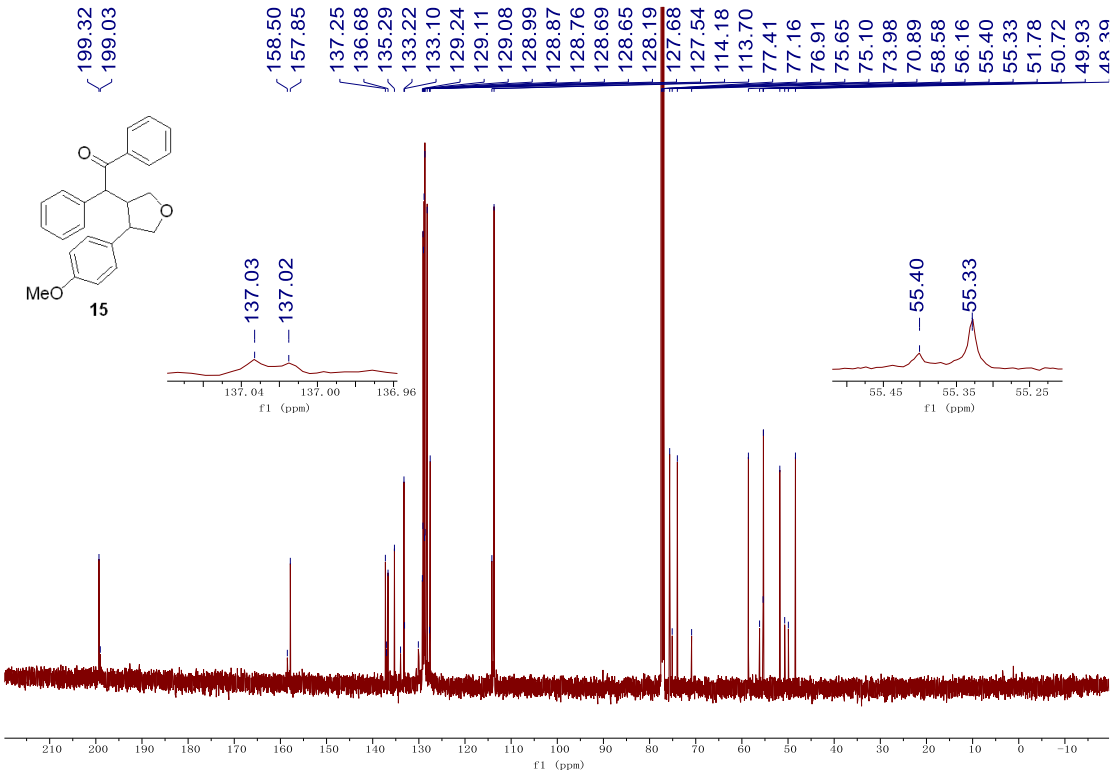
77.16
76.90
71.62
71.57
55.33
35.62
MeO
O
14
f1 (ppm)


7.97
7.96
7.96
7.95
7.95
7.48
7.40
7.38
7.38
7.37
7.36
7.31
7.31
7.26
7.22
7.22
7.22
7.21
7.21
7.20
7.18
7.17
7.17
7.16
7.16
7.16
7.15
7.15
7.13
7.11
6.69
6.67
6.67
6.62
6.61
6.60
4.60
4.58
3.80
3.80
3.78
3.77
3.76
3.75
3.72
O
O
MeO
15
1.99
1.08
3.09
4.03
4.08
0.93
2.09
4.06
1.01
1.00
0.94
f1 (ppm)


199.32
199.03
158.50
157.85
137.25
136.68
135.29
133.22
133.10
129.24
129.11
129.08
128.99
128.87
128.76
128.69
128.65
128.19
127.68
127.54
114.18
113.70
77.41
77.16
76.91
75.65
75.10
73.98
70.89
58.58
56.16
55.40
55.33
51.78
50.72
49.93
O
O
MeO
15
137.03
137.02
137.04
137.00
136.96
f1 (ppm)
55.40
55.33
55.45
55.35
55.25
f1 (ppm)
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)