

Supporting Information

Direct C-H Arylation of Aldehydes by Merging Photocatalyzed Hydrogen-atom Transfer with Palladium Catalysis

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General Information

NMR spectra were obtained on the 400 MHz spectrometer using CDCl_3 as deuterated solvents, with proton, carbon and fluorine resonances at 400 MHz, 100 MHz and 376 MHz, respectively. ^1H NMR and ^{13}C NMR chemical shifts were determined relative to internal standard TMS at δ 0.0 ppm and ^{19}F NMR chemical shifts were determined related to CFCl_3 as inter standard. Chemical shifts (δ) are reported in ppm, and coupling constants (J) are in hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. The NMR yield was determined by ^{19}F NMR using fluorobenzene (^{19}F NMR δ : -114.0 ppm) as an internal standard before working up the reaction. HRMS (ESI) data were tested on a Thermo Scientific LTQ Orbitrap XL. Unless otherwise noted, solvents were freshly dried and degassed according to the purification handbook Purification of Laboratory Chemicals before using. Flash column chromatography was carried out using 300-400 mesh silica gel.

Equipment for palladium-photocatalysis reaction: The reaction mixture was irradiated with a 34 W Kessil PR160 390 nm lamps in a photoredox box.

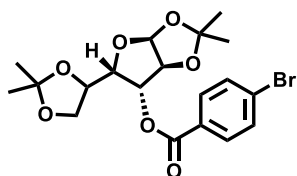


Preparation of Substrates

1. Synthesis of Aryl bromide



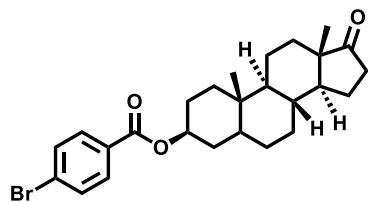
4-bromobenzoyl chloride was synthesized according to the published literature.¹ To a solution of alcohol (5.0 mmol, 1.0 equiv.), DMAP (0.5 mmol, 0.1 equiv.) and Et₃N (10.0 mmol, 2.0 equiv.) in DCM (10.0 mL) was added the solution of 4-bromobenzoyl chloride (1.0 equiv.) in DCM (10.0 mL) dropwise using syringe at 0 °C. After stirring for 30 min, the mixture was allowed to stir at room temperature overnight. Then the mixture was diluted with saturated NH₄Cl solution (20.0 mL), and extracted with DCM (10.0 mL × 3). The organic layer was washed with brine, dried over MgSO₄ and evaporated. The residue was purified with flash column chromatography to give the desired aryl bromide.



Substrate **S34** was obtained in 62% yield as a white solid, and matched previously published spectroscopic data.^[1]

¹H NMR (400 MHz, CHCl₃) δ 7.79-7.70 (m, 2H), 7.47-7.40 (m, 2H), 5.85 (d, *J* = 3.7 Hz, 1H), 5.37 (d, *J* = 2.6 Hz, 1H), 4.57 (d, *J* = 3.7 Hz, 1H), 4.30-4.13 (m, 2H), 3.98 (m, 2H), 1.41 (s, 3H), 1.27 (s, 3H), 1.20 (s, 3H), 1.12 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 163.5, 130.9, 130.2, 127.7, 127.4, 111.4, 108.5, 104.1, 82.3, 78.9, 71.5, 66.3, 25.8, 25.7, 25.2, 24.2.

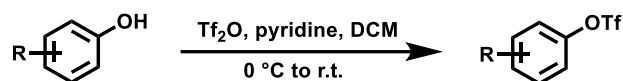


Substrate **S35** was obtained in 55% yield as a white solid, and matched previously published spectroscopic data.^[1]

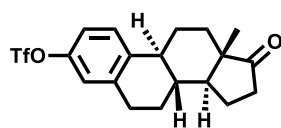
¹H NMR (400 MHz, CHCl₃) δ 7.94-7.80 (m, 2H), 7.60-7.47 (m, 2H), 4.90 (tt, *J* = 11.2, 4.9 Hz, 1H), 2.41 (dd, *J* = 19.2, 8.7 Hz, 1H), 2.05 (m, 1H), 1.92 (m, 2H), 1.84-1.70 (m, 4H), 1.66-1.63 (m, 2H), 1.60-1.43 (m, 3H), 1.41-1.20 (m, 6H), 1.15-0.90 (m, 2H), 0.85 (d, *J* = 11.8 Hz, 6H), 0.75 (td, *J* = 11.6, 3.8 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 220.2, 164.3, 130.6, 130.1, 128.7, 126.8, 73.5, 53.3, 50.4, 46.8, 43.7, 35.7, 34.8, 34.7, 34.0, 33.0, 30.5, 29.8, 27.3, 26.5, 20.8, 19.5, 12.8, 11.3.

2. Synthesis of Aryl triflates



To a solution of the aryl phenol (1.0 equiv.) and pyridine (2.0 equiv.) in DCM (5.0 mL) was added a solution of trifluoromethanesulfonic anhydride (1.2 equiv) in DCM (5.0 mL) dropwise at 0 °C. The mixture was stirred for 30 min, then allowed to warm to room temperature and stir for another 2 hours. The mixture was then quenched with saturated NH₄Cl solution (15.0 mL), and extracted with DCM (10.0 mL × 3). The organic layer was washed with brine, dried over MgSO₄ and evaporated. The residue was purified with flash column chromatography to give the desired aryl triflates.

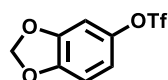


Substrate **S39** was obtained in 91% yield as a white solid, and matched previously published spectroscopic data.^[2]

¹H NMR (400 MHz, CHCl₃) δ 7.33 (d, *J* = 8.7 Hz, 1H), 7.01 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.97 (d, *J* = 2.3 Hz, 1H), 2.92 (dd, *J* = 8.5, 3.8 Hz, 2H), 2.50 (m, 1H), 2.43-2.36 (m, 1H), 2.33-2.24 (m, 1H), 2.20-2.00 (m, 3H), 2.01-1.91 (m, 1H), 1.70-1.40 (m, 6H), 0.91 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 219.3, 146.6, 139.3, 138.3, 126.2, 120.2, 117.7 (q, *J* = 320.7 Hz), 117.3, 49.4, 46.8, 43.1, 36.7, 34.8, 30.5, 28.4, 25.1, 24.7, 20.6, 12.8.

¹⁹F NMR (376 MHz, CHCl₃) δ -71.99.

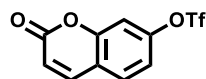


Substrate **S40** was obtained in 75% yield as a white solid, and matched previously published spectroscopic data.^[2]

¹H NMR (400 MHz, CHCl₃) δ 6.78 (m, 1H), 6.76-6.70 (m, 2H), 6.02 (s, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 147.6, 146.5, 142.6, 117.8 (q, *J* = 320.9 Hz), 113.4, 107.6, 102.4, 101.5.

¹⁹F NMR (376 MHz, CHCl₃) δ -71.59.



Substrate **S41** was obtained in 82% yield as a white solid, and matched previously published spectroscopic data.^[3]

¹H NMR (400 MHz, CHCl₃) δ 7.72 (d, *J* = 9.6 Hz, 1H), 7.58 (d, *J* = 8.6 Hz, 1H), 7.30-7.23 (m, 1H), 7.21 (m, 1H), 6.47 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 158.2, 153.6, 149.8, 141.1, 128.4, 117.8, 117.7 (q, *J* = 321.0 Hz), 116.8, 116.7, 109.5.

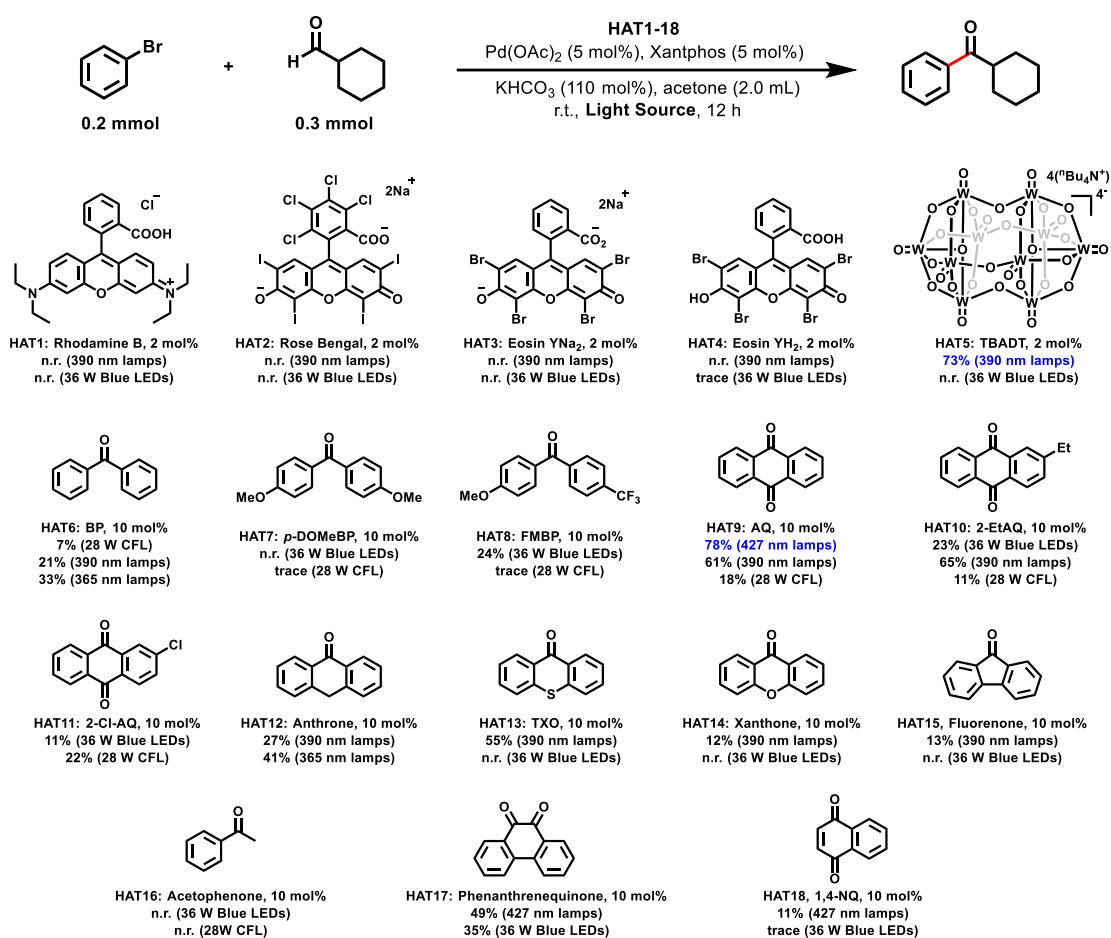
¹⁹F NMR (376 MHz, CHCl₃) δ -71.73.

References:

- [1] Shen, Y.; Gu, Y.; Martin, R. *sp*³ C-H Arylation and Alkylation Enabled by the Synergy of Triplet Excited Ketones and Nickel Catalysts. *J. Am. Chem. Soc.* **2018**, *140*, 12200-12209.
- [2] Yu, P.; Morandi, B. Nickel-Catalyzed Cyanation of Aryl Chlorides and Triflates Using Butyronitrile: Merging Retro-hydrocyanation with Cross-Coupling. *Angew. Chem. Int. Ed.* **2017**, *56*, 15693-15697.
- [3] Wang, H.; Li, W.-G.; Zeng, K.; Wu, Y.-J.; Zhang, Y.; Xu, T.-L.; Chen, Y. Photocatalysis Enables Visible-Light Uncaging of Bioactive Molecules in Live Cells. *Angew. Chem. Int. Ed.* **2019**, *58*, 561-565.

Optimization of Parameters for the Palladium-Photocatalyzed catalyzed C-H arylation

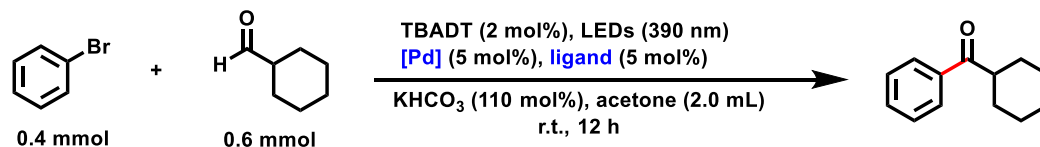
Scheme S1. Screening of hydrogen atom transfer (HAT) catalysts^a



^aThe yields were obtained by ¹H NMR with diphenylmethane as an internal standard.

2. Using TBADT as the HAT catalyst

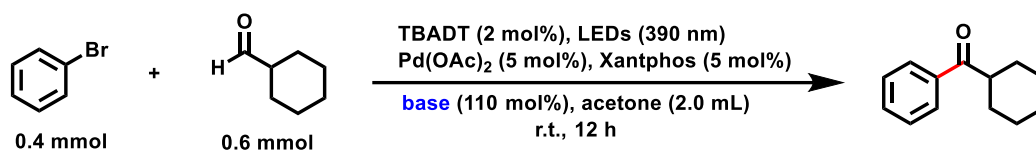
2.1 Investigation of palladium catalysts and ligands^a



entry	[Pd]	ligand	yield (%)
1	Pd ₂ (dba) ₃	Xantphos	trace
2	Pd(PPh ₃) ₄	Xantphos	n.r.
3	Pd(PPh ₃) ₂ Cl ₂	Xantphos	n.r.
4	Pd(TFA) ₂	Xantphos	61
5	PdCl ₂	Xantphos	34
6	Pd(PhCN) ₂ Cl ₂	Xantphos	18
7 ^b	Pd(OAc) ₂	PtBu ₃ HBF ₄	29
8 ^b	Pd(OAc) ₂	Cy-JohnPhos	25
9 ^b	Pd(OAc) ₂	PPh ₃	n.r.
10	Pd(OAc) ₂	Xantphos	71
11	Pd(OAc) ₂	dppe	n.r.
12	Pd(OAc) ₂	dpph	trace
13	Pd(OAc) ₂	dppbz	n.r.
14	Pd(OAc) ₂	BINAP	13
15	Pd(OAc) ₂	dppp	trace
16	Pd(OAc) ₂	Triphos	n.r.
17	Pd(OAc) ₂	Ni-Xantphos	56
18	Pd(OAc) ₂	dppf	11
19	Pd(OAc) ₂	Phenanthroline	n.r.
20	Pd(OAc) ₂	DPE-Phos	54

^aReaction conditions: Aryl bromide (0.4 mmol), Aldehyde (0.6 mmol), TBADT (2 mol%, 0.008 mmol), [Pd] (5 mol%, 0.02 mmol), Ligand (5 mol%, 0.02 mmol), K₂CO₃ (110 mol%, 0.44 mmol) in Acetone (2.0 mL), irradiated by 390 nm Kessil lamp in the PhotoRedOx Box equipped with a fan for 12 h at room temperature under Ar atmosphere, the results were obtained by ¹H NMR with diphenylmethane as an internal standard. ^bLigand was 10 mol%. Xantphos = (9,9-dimethyl-4,5-bis(diphenylphosphino)xanthene), Cy-JohnPhos = (2-(Dicyclohexylphosphino)biphenyl), dppe = (1,2-Bis(diphenylphosphino)ethane), dpph = (1,6-Bis(diphenylphosphino)hexane), dppbz = (1,2-Bis(diphenylphosphino)benzene), BINAP = (2,2-bis(diphenylphosphino)-1,1-binaphthyl), dppp = (1,3-bis(diphenylphosphino)propane), Triphos = Bis(2-diphenylphosphinoethyl)phenylphosphine, Ni-Xantphos = (4,6-bis(diphenylphosphino)phenoxazine), dppf = (1,1'-Bisdiphenylphosphinoferrocene), DPE-Phos = ((oxybis(2,1-phenylene))bis(diphenylphosphane)).

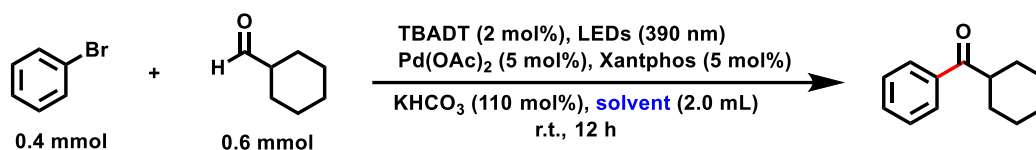
2.2 Investigation of base effect^a



entry	base	yield (%)
1	K ₂ CO ₃	trace
2	Na ₂ CO ₃	7
3	Cs ₂ CO ₃	n.r.
4	KHCO ₃	71
5	NaHCO ₃	51
6	K ₂ HPO ₄	37
7	Na ₂ HPO ₄	22
8	KH ₂ PO ₄	trace
9	K ₃ PO ₄	5
10	KOAc	11
11	NaOAc	trace
12	CsOAc	trace
13	Et ₃ N	trace
14	DBU	n.r.
15	DABCO	n.r.

^aReaction conditions: Aryl bromide (0.4 mmol), Aldehyde (0.6 mmol), TBADT (2 mol%, 0.008 mmol), Pd(OAc)₂ (5 mol%, 0.02 mmol), Xantphos (5 mol%, 0.02 mmol), base (110 mol%, 0.44 mmol) in Acetone (2.0 mL), irradiated by 390nm Kessil lamp in the PhotoRedOx Box equipped with a fan for 12 h at room temperature under Ar atmosphere, the results were obtained by ¹H NMR with diphenylmethane as an internal standard. DBU = (1,8-diazabicyclo[5.4.0]undec-7-ene), DABCO = 1,4-Diazabicyclo[2.2.2]octane.

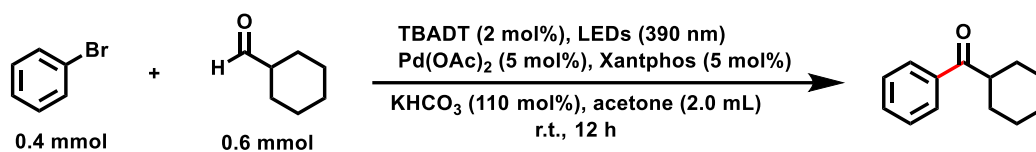
2.3 Investigation of solvent effect^a



entry	solvent	yield (%)
1	acetone	71
2	benzotrifluoride	n.r.
3	CH ₃ CN	18
4	DMA	43
5	2,3-butanedione	trace
6	2-butanone	27
7	toluene	n.r.
8	DMSO	trace
9	<i>t</i> BuOH	n.r.
10	CH ₂ Cl ₂	trace

^aReaction conditions: Aryl bromide (0.4 mmol), Aldehyde (0.6 mmol), TBADT (2 mol%, 0.008 mmol), Pd(OAc)₂ (5 mol%, 0.02 mmol), Xantphos (5 mol%, 0.02 mmol), K₂CO₃ (110 mol%, 0.44 mmol) in solvent (2.0 mL), irradiated by 390 nm Kessil lamp in the PhotoRedOx Box equipped with a fan for 12 h at room temperature under Ar atmosphere, the results were obtained by ¹H NMR with diphenylmethane as an internal standard.

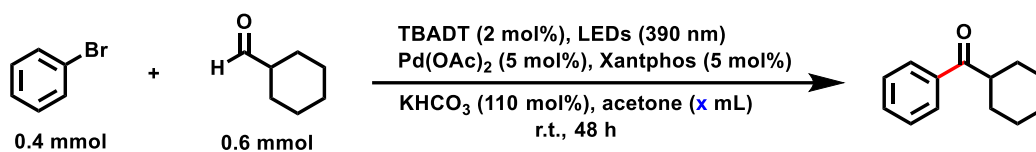
2.4 Control experiments for C-H arylation of aldehyde^a



entry	conditions	yield (%)
1	identical	71
2	t = 48 h	82
3	t = 24 h	76
4	1.0 equiv. aldehyde	68
5	0.5 equiv. KHCO ₃	53
6	without KHCO ₃	6
7	36 W blue LEDs	n.r.
8	28 W 365 nm lamps	51
9	without TBADT	n.r.
10	without light	n.r.
11	without Pd(OAc) ₂	n.r.
12	without Xantphos	11
13	with Air	n.r.
14	add 10 equiv. H ₂ O	9

^aReaction conditions: Aryl bromide (0.4 mmol), Aldehyde (0.6 mmol), TBADT (2 mol%, 0.008 mmol), Pd(OAc)₂ (5 mol%, 0.02 mmol), Xantphos (5 mol%, 0.02 mmol), KHCO₃ (110 mol%, 0.44 mmol) in acetone (2.0 mL) with or without some variations, irradiated in the Photo RedOx Box equipped with a fan for indicated time at room temperature under Ar atmosphere, the results were obtained by ¹H NMR with diphenylmethane as an internal standard.

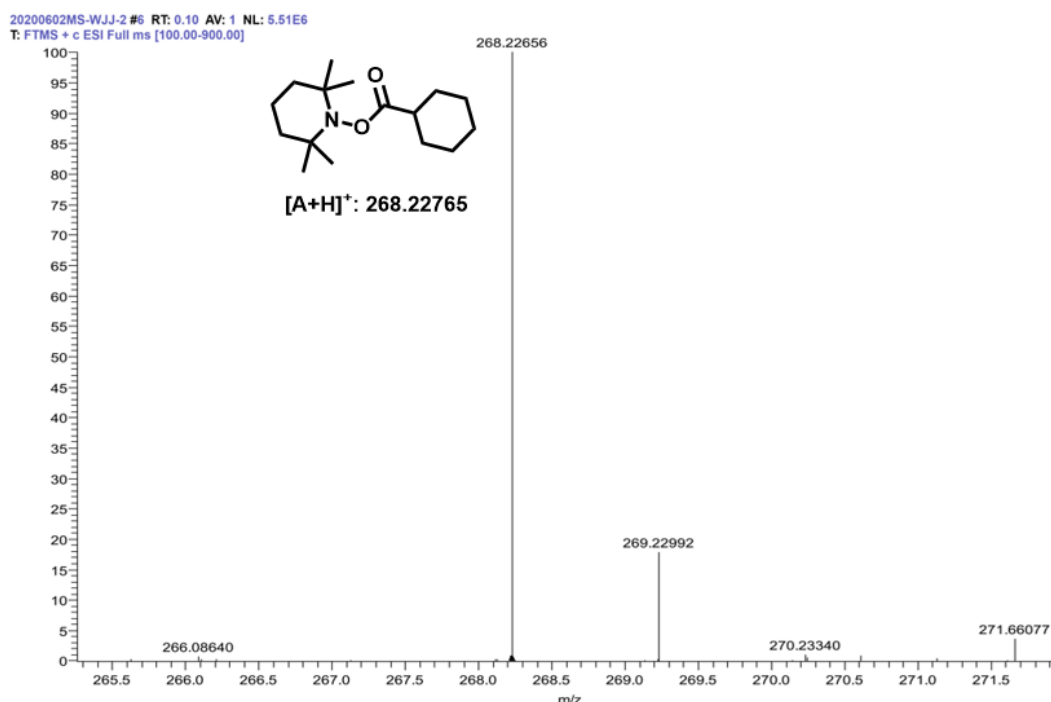
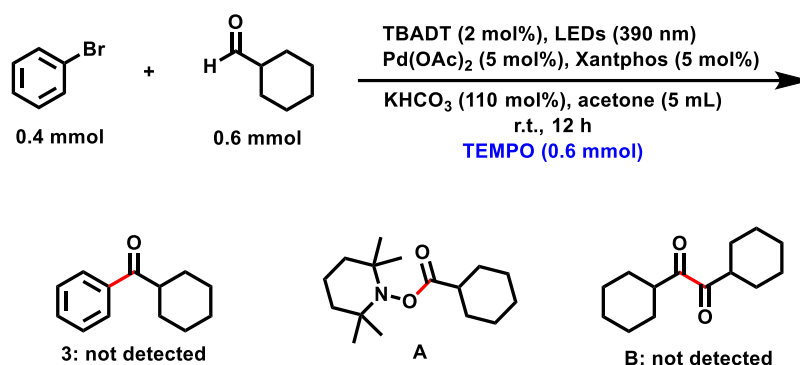
2.5 Investigation of reaction concentrations^a



entry	acetone (x mL)	yield (%)
1	1	64
2	2	82
3	5	88
4	10	52
5	15	43
6	20	31

^aReaction conditions: Aryl bromide (0.4 mmol), Aldehyde (0.6 mmol), TBADT (2 mol%, 0.008 mmol), Pd(OAc)₂ (5 mol%, 0.02 mmol), Xantphos (5 mol%, 0.02 mmol), KHCO₃ (110 mol%, 0.44 mmol) in acetone (x mL), irradiated by 390 nm Kessil lamp in the PhotoRedOx Box equipped with a fan for 48 h at room temperature under Ar atmosphere, the results were obtained by ¹H NMR with diphenylmethane as an internal standard.

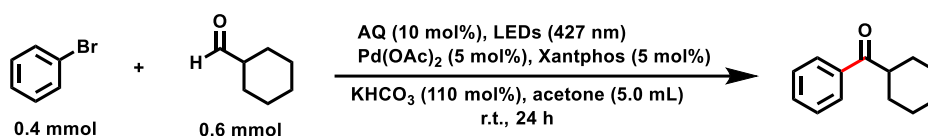
2.6 Radical trapping experiment



Conclusion

When using TBADT as the catalyst, the standard reaction conditions (**Condition A**) are aryl bromide (0.4 mmol), aldehyde (0.6 mmol), TBADT (2 mol%, 0.008 mmol), Pd(OAc)₂ (5 mol%, 0.02 mmol), Xantphos (5 mol%, 0.02 mmol), K₂CO₃ (110 mol%, 0.44 mmol) and acetone (5.0 mL). The mixture is irradiated by 390 nm Kessil lamp in the PhotoRedOx Box equipped with a fan for 48 h at room temperature under Ar atmosphere.

3. Using AQ as the HAT catalyst^a



entry	conditions	yield (%)
1	identical	90
2	CH ₃ CN instead of acetone	45
3	DMF instead of acetone	tracer
4	CH ₂ Cl ₂ instead of acetone	n.r.
5	5 mol% AQ	73
6	K ₂ HPO ₄ instead of KHCO ₃	61
7	KOAc instead of KHCO ₃	64
8	K ₃ PO ₄ instead of KHCO ₃	55
9	without KHCO ₃	7
10	without AQ	n.r
11	Ni-xantphos instead of xantphos	58
12	DPE-phos instead of cantphos	61
13	390 nM LEDs	81

^aReaction conditions: Aryl bromide (0.4 mmol), Aldehyde (0.6 mmol), AQ (10 mol%, 0.04 mmol), Pd(OAc)₂ (5 mol%, 0.02 mmol), Xantphos (5 mol%, 0.02 mmol), KHCO₃ (110 mol%, 0.44 mmol) in acetone (5 mL), irradiated by 427 nm Kessil lamp in the PhotoRedOx Box equipped with a fan for 24 h at room temperature under Ar atmosphere, the results were obtained by ¹H NMR with diphenylmethane as an internal standard.

Conclusion

When using AQ as the catalyst, the standard reaction conditions (**Condition B**) are aryl bromide (0.4 mmol), aldehyde (0.6 mmol), AQ (10 mol%, 0.04 mmol), Pd(OAc)₂ (5 mol%, 0.02 mmol), Xantphos (5 mol%, 0.02 mmol), KHCO₃ (110 mol%, 0.44 mmol) and acetone (5.0 mL). The mixture is irradiated by 427 nm Kessil lamp in the PhotoRedOx Box equipped with a fan for 24 h at room temperature under Ar

atmosphere.

General Experimental Procedures for the Palladium-Photocatalyzed C-H arylation

Procedure A:

If both substrates are solid, aryl bromide (0.4 mmol, 1.0 equiv), aldehyde (0.6 mmol, 1.5 equiv), KHCO_3 (0.44 mmol, 1.1 equiv, 44 mg), TBADT (0.008 mmol, 2.0 mol%, 26.4 mg), $\text{Pd}(\text{OAc})_2$ (0.02 mmol, 5 mol%, 4.5 mg) and Xantphos (0.02 mmol, 5 mol%, 11.6 mg) are placed in a Schlenk tube equipped with a stirring bar. The tube is evacuated and filled with argon (repeat 3 times). Acetone (5.0 mL) is finally added via a syringe under Ar atmosphere.

If either or both of the substrates is/are liquid, the solid substrate (if there is), KHCO_3 (0.44 mmol, 1.1 equiv, 44 mg), TBADT (0.008 mmol, 2.0 mol%, 26.4 mg), $\text{Pd}(\text{OAc})_2$ (0.02 mmol, 5 mol%, 4.5 mg) and Xantphos (0.02 mmol, 5 mol%, 11.6 mg) are placed in a Schlenk tube equipped with a stirring bar. The tube is evacuated and filled with argon (repeat 3 times). The liquid substrate(s) should be dissolved in acetone (5.0 mL), then the mixture was added into the Schlenk tube via a syringe under Ar atmosphere.

The mixture was stirred under the irradiation of a 34W Kessil® PR160 390 nm lamps at room temperature for 48 h. Then the mixture was quenched with saturated NaCl solution (10 mL) and extracted with ethyl acetate (3 x 10 mL). The organic layers were combined, washed with brine (1 x 30 mL), and concentrated under vacuo. The product was purified by flash column chromatography on silica gel with hexane/ethyl acetate.

Procedure B:

If both substrates are solid, aryl bromide (0.4 mmol, 1.0 equiv), aldehyde (0.6 mmol, 1.5 equiv), KHCO_3 (0.44 mmol, 1.1 equiv, 44 mg), AQ (0.04 mmol, 10 mol%, 8.4 mg), $\text{Pd}(\text{OAc})_2$ (0.02 mmol, 5 mol%, 4.5 mg) and Xantphos (0.02 mmol, 5 mol%,

11.6 mg) are placed in a Schlenk tube equipped with a stirring bar. The tube is evacuated and filled with argon (repeat 3 times). Acetone (5.0 mL) is finally added via a syringe under Ar atmosphere.

If either or both of the substrates is/are liquid, the solid substrate (if there is), KHCO_3 (0.44 mmol, 1.1 equiv, 44 mg), AQ (0.04 mmol, 10 mol%, 8.4 mg), $\text{Pd}(\text{OAc})_2$ (0.02 mmol, 5 mol%, 4.5 mg) and Xantphos (0.02 mmol, 5 mol%, 11.6 mg) are placed in a Schlenk tube equipped with a stirring bar. The tube is evacuated and filled with argon (repeat 3 times). The liquid substrate(s) should be dissolved in acetone (5.0 mL), then the mixture was added into the Schlenk tube via a syringe under Ar atmosphere.

The mixture was stirred under the irradiation of a 34W Kessil® PR160 427 nm lamps at room temperature for 24 h. Then the mixture was quenched with saturated NaCl solution (10 mL) and extracted with ethyl acetate (3 x 10 mL). The organic layers were combined, washed with brine (1 x 30 mL), and concentrated under vacuo. The product was purified by flash column chromatography on silica gel with hexane/ethyl acetate.

Procedure C:

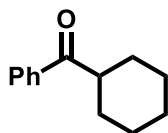
If both substrates are solid, aryl iodide or aryl triflate (0.4 mmol, 1.0 equiv), aldehyde (0.6 mmol, 1.5 equiv), KHCO_3 (0.44 mmol, 1.1 equiv, 44 mg), TBAB (0.48 mmol, 1.2 equiv, 154.7 mg), TBADT (0.008 mmol, 2.0 mol%, 26.4 mg) for *condition A* or AQ (0.04 mmol, 10 mol%, 8.4 mg) for *condition B*, $\text{Pd}(\text{OAc})_2$ (0.02 mmol, 5 mol%, 4.5 mg) and Xantphos (0.02 mmol, 5 mol%, 11.6 mg) are placed in a Schlenk tube equipped with a stirring bar. The tube is evacuated and filled with argon (repeat 3 times). Acetone (5.0 mL) is finally added via a syringe under Ar atmosphere.

If either or both of the substrates is/are liquid, the solid substrate (if there is), KHCO_3 (0.44 mmol, 1.1 equiv, 44 mg), TBAB (0.48 mmol, 1.2 equiv, 154.7 mg), TBADT (0.008 mmol, 2.0 mol%, 26.4 mg), $\text{Pd}(\text{OAc})_2$ (0.02 mmol, 5 mol%, 4.5 mg) and Xantphos (0.02 mmol, 5 mol%, 11.6 mg) are placed in a Schlenk tube equipped with a stirring bar. The tube is evacuated and filled with argon (repeat 3 times). The

liquid substrate(s) should be dissolved in acetone (5.0 mL), then the mixture was added into the Schlenk tube via a syringe under Ar atmosphere.

The mixture was stirred under the irradiation of a 34W Kessil® PR160 lamps (390 nm for *condition A* or 427 nm for *condition B*) at room temperature for 24 h. Then the mixture was quenched with saturated NaCl solution (10 mL) and extracted with ethyl acetate (3 x 10 mL). The organic layers were combined, washed with brine (1 x 30 mL), and concentrated under vacuo. The product was purified by flash column chromatography on silica gel with hexane/ethyl acetate.

Characterization of the Products in the Palladium-Photocatalyzed C-H arylation

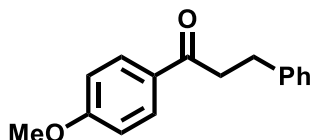


cyclohexyl(phenyl)methanone (3): Prepared following procedure A or procedure B.

The pure product was a colorless liquid, and matched previously published spectroscopic data (*J. Org. Chem.* **2016**, *81*, 6409-6423).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.94-7.86 (m, 2H), 7.53-7.47 (m, 1H), 7.41 (m, 2H), 3.21 (tt, $J = 11.4, 3.2$ Hz, 1H), 1.91-1.76 (m, 4H), 1.71 (m, 1H), 1.51-1.30 (m, 4H), 1.23 (m, 1H).

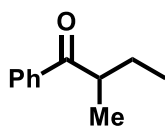
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 203.9, 136.4, 132.7, 128.5, 128.2, 45.6, 29.4, 26.0, 25.9.



1-(4-methoxyphenyl)-3-phenylpropan-1-one (4): Prepared following procedure A or procedure B. The pure product was a white solid, and matched previously published spectroscopic data (*Chem. Eur. J.* **2018**, *24*, 8774-8778).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98-7.89 (m, 2H), 7.31-7.21 (m, 4H), 7.20-7.15 (m, 1H), 6.94-6.83 (m, 2H), 3.82 (s, 3H), 3.30-3.20 (m, 2H), 3.05 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 197.8, 163.5, 141.5, 130.3, 130.0, 128.5, 128.4, 126.1, 113.7, 55.5, 40.1, 30.4.

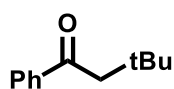


2-methyl-1-phenylbutan-1-one (5): Prepared following procedure A or procedure B.

The pure product was a colorless liquid, and matched previously published spectroscopic data (*Angew. Chem. Int. Ed.* **2001**, *40*, 3458-3460).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.00-7.88 (m, 2H), 7.57-7.49 (m, 1H), 7.45 (m, 2H), 3.36 (q, $J = 6.7$ Hz, 1H), 1.83 (m, 1H), 1.46 (m, 1H), 1.15 (d, $J = 6.9$, 3H), 0.87 (t, $J = 7.4$ Hz, 3H).

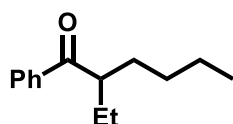
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 204.4, 136.9, 132.7, 128.6, 128.2, 42.1, 26.7, 16.7, 11.7.



3,3-dimethyl-1-phenylbutan-1-one (6): Prepared following procedure A or procedure B. The pure product was a colorless liquid, and matched previously published spectroscopic data (*J. Am. Chem. Soc.* **1992**, *114*, 255-261).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98-7.88 (m, 2H), 7.54-7.46 (m, 1H), 7.41 (m, 2H), 2.82 (s, 2H), 1.02 (s, 9H).

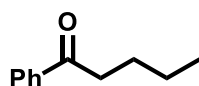
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 200.4, 138.6, 132.6, 128.4, 128.2, 50.0, 31.3, 30.0.



2-ethyl-1-phenylhexan-1-one (7): Prepared following procedure A or procedure B. The pure product was a colorless liquid, and matched previously published spectroscopic data (*Chem. Eur. J.* **2018**, *24*, 8774-8778).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.92-7.83 (m, 2H), 7.48 (m, 1H), 7.39 (m, 2H), 3.27 (tt, $J = 7.5, 5.5$ Hz, 1H), 1.70 (m, 2H), 1.54-1.36 (m, 2H), 1.15 (m, 4H), 0.77 (m, 6H).

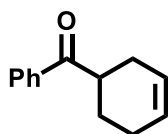
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 204.7, 137.8, 132.8, 128.6, 128.2, 47.7, 31.7, 29.8, 25.4, 22.9, 13.9, 11.9.



1-phenylpentan-1-one (8): Prepared following procedure A or procedure B. The pure product was a colorless liquid, and matched previously published spectroscopic data (*Eur. J. Org. Chem.* **2013**, 2445-2452).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.95 (m, 2H), 7.56-7.50 (m, 1H), 7.43 (m, 2H), 2.97-2.93 (t, $J = 7.5$ Hz, 2H), 1.71 (m, 2H), 1.40 (m, 2H), 0.93 (t, $J = 7.4$ Hz, 3H).

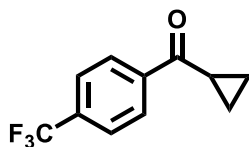
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 200.5, 137.1, 132.8, 128.5, 128.0, 38.3, 26.5, 22.5, 13.9.



cyclohex-3-en-1-yl(phenyl)methanone (9): Prepared following procedure A or procedure B in which thioxanthone (10 mol%) was used instead of AQ. The pure product was a colorless liquid, and matched previously published spectroscopic data (*J. Am. Chem. Soc.* **2015**, 137, 3454-3457).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.95 (m, 2H), 7.61-7.53 (m, 1H), 7.53-7.41 (m, 2H), 5.74 (d, $J = 2.0$ Hz, 2H), 3.51 (m, 1H), 2.45-2.29 (m, 1H), 2.26-2.12 (m, 3H), 1.97 (m, 1H), 1.80-1.59 (m, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 203.4, 136.3, 132.8, 128.6, 128.3, 126.6, 125.7, 41.5, 27.9, 25.7, 24.9.

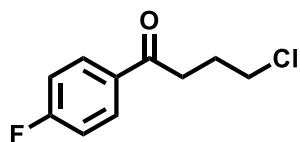


cyclopropyl(4-(trifluoromethyl)phenyl)methanone (10): Prepared following procedure A or procedure B. *Note:* 2.0 equiv of aldehyde was used. The pure product was a white solid, and matched previously published spectroscopic data (*Angew. Chem. Int. Ed.* **2014**, 53, 8416-8420).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.11 (d, $J = 8.0$ Hz, 2H), 7.71 (d, $J = 8.2$ Hz, 2H), 2.63 (tt, $J = 7.6, 4.4$ Hz, 1H), 1.27 (dt, $J = 4.7, 3.4$ Hz, 2H), 1.10 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 199.7, 140.7, 133.9 (q, $J = 32.7$ Hz), 128.3, 125.5, 123.7 (q, $J = 271.0$ Hz), 17.6, 12.2.

^{19}F NMR (376 MHz, CDCl_3) δ -63.03.

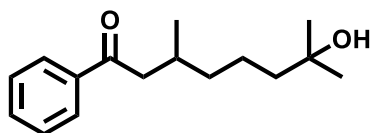


4-chloro-1-(4-fluorophenyl)butan-1-one (11): Prepared following procedure A or procedure B. The pure product was a colorless liquid, and matched previously published spectroscopic data (*J. Am. Chem. Soc.* **2017**, *139*, 11353-11356).

^1H NMR (400 MHz, CDCl_3) δ 8.07-7.95 (m, 2H), 7.20-7.09 (m, 2H), 3.67 (t, $J = 6.3$ Hz, 2H), 3.16 (t, $J = 7.0$ Hz, 2H), 2.21 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ 197.3, 165.7 (d, $J = 253.0$ Hz), 133.2 (d, $J = 3.0$ Hz), 130.6 (d, $J = 9.0$ Hz), 115.7 (d, $J = 22.0$ Hz), 44.6, 35.2, 26.7.

^{19}F NMR (376 MHz, CDCl_3) δ -105.04

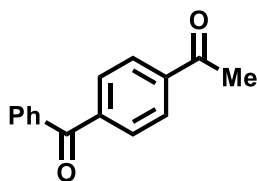


7-hydroxy-3,7-dimethyl-1-phenyloctan-1-one (12): Prepared following procedure A or procedure B. *Note:* 2.0 equiv of aldehyde was used. The pure product was a colorless liquid.

^1H NMR (400 MHz, CDCl_3) δ 7.97-7.90 (m, 2H), 7.57-7.50 (m, 1H), 7.44 (m, 2H), 2.93 (dd, $J = 15.9, 5.8$ Hz, 1H), 2.76 (dd, $J = 15.9, 7.8$ Hz, 1H), 2.18 (m, 1H), 1.57 (s, 1H), 1.50-1.32 (m, 5H), 1.25 (m, 1H), 1.19 (s, 6H), 0.96 (d, $J = 6.7$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 200.4, 137.3, 132.9, 128.5, 128.0, 70.9, 45.9, 43.9, 37.5, 29.7, 29.3, 29.1, 21.7, 20.0.

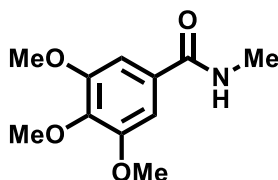
HRMS (ESI) Calcd for $\text{C}_{16}\text{H}_{25}\text{O}_2^+$ $[\text{M}+\text{H}]^+$: 249.1849, found: 249.1850



1-(4-benzoylphenyl)ethan-1-one (13): Prepared following procedure A or procedure B. *Note:* 2.0 equiv of aldehyde was used. The pure product was a white solid, and matched previously published spectroscopic data (*Synlett.* **2005**, 2309-2312).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12-8.05 (m, 2H), 7.93-7.87 (m, 2H), 7.82 (m, 2H), 7.69-7.63 (m, 1H), 7.59-7.48 (m, 2H), 2.69 (s, 3H).

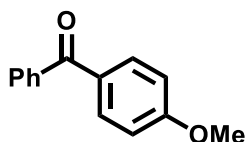
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 197.5, 195.9, 141.3, 139.6, 136.9, 133.0, 130.1, 130.0, 128.5, 128.2, 26.9.



3,4,5-trimethoxy-N-methylbenzamide (14): Prepared following procedure A or procedure B. *Note:* 2.0 equiv of aldehyde was used. The pure product was a white solid, and matched previously published spectroscopic data (*Angew. Chem. Int. Ed.* **2013**, 52, 13086-13090).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.02 (s, 2H), 6.33 (br s, 1H), 3.91 (s, 6H), 3.88 (s, 3H), 3.00 (d, $J = 4.6$ Hz, 3H).

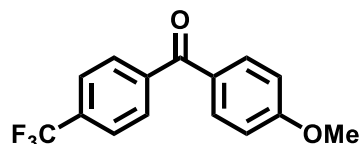
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.0, 153.2, 140.8, 130.1, 104.4, 60.9, 56.3, 26.9.



(4-methoxyphenyl)(phenyl)methanone (15): Prepared following procedure A or procedure B. *Note:* DPE-Phos was used instead of Xantphos, while Na_2CO_3 was used instead of KHCO_3 . The pure product was a white solid, and matched previously published spectroscopic data (*Synlett.* **2005**, 2309-2312).

¹H NMR (400 MHz, CDCl₃) δ 7.89-7.81 (m, 2H), 7.81-7.74 (m, 2H), 7.58 (m, 1H), 7.49 (m, 2H), 7.03-6.94 (m, 2H), 3.85 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 195.5, 163.2, 138.3, 132.6, 131.9, 130.1, 129.7, 128.2, 113.6, 55.5.

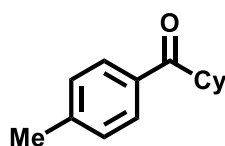


(4-methoxyphenyl)(4-(trifluoromethyl)phenyl)methanone (16): Prepared following procedure A or procedure B. *Note*: DPE-Phos was used instead of Xantphos, while Na₂CO₃ was used instead of KHCO₃. The pure product was a white solid, and matched previously published spectroscopic data (*J. Am. Chem. Soc.* **2018**, *140*, 12200-12209).

¹H NMR (400 MHz, CDCl₃) δ 7.85 (m, 4H), 7.76 (m, 2H), 6.70 (m, 2H), 3.92 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 194.2, 163.7, 141.5, 133.3 (q, *J* = 32.3 Hz), 132.6, 129.8, 129.4, 125.2 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 271.0 Hz), 113.8, 55.6.

¹⁹F NMR (376 MHz, CDCl₃) δ -62.93.

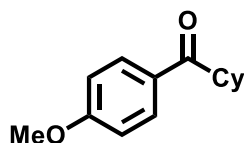


cyclohexyl(p-tolyl)methanone (17): Prepared following procedure A, or procedure B, or procedure C with *condition A*. The pure product was a colorless liquid, and matched previously published spectroscopic data (*J. Org. Chem.* **2015**, *80*, 10660-10667).

¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 3.27 (tt, *J* = 11.3, 3.0 Hz, 1H), 2.44 (s, 3H), 1.97-1.83 (m, 4H), 1.80-1.71 (m, 1H), 1.58-1.35 (m, 4H), 1.34-1.24 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 203.5, 143.4, 133.8, 129.2, 128.4, 45.5, 29.5, 26.0,

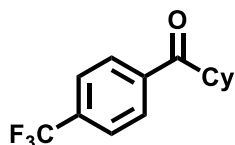
25.9, 21.6.



cyclohexyl(4-methoxyphenyl)methanone (18): Prepared following procedure A or procedure B. The pure product was a white solid, and matched previously published spectroscopic data (*J. Org. Chem.* **2015**, *80*, 10660-10667).

¹H NMR (400 MHz, CDCl₃) δ 8.00-7.83 (m, 2H), 6.94-6.86 (m, 2H), 3.83 (s, 3H), 3.21 (tt, *J* = 11.3, 3.0 Hz, 1H), 1.87-1.80 (m, 4H), 1.70 (m, 1H), 1.54-1.30 (m, 4H), 1.24 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 202.4, 163.2, 130.5, 129.3, 113.7, 55.4, 45.3, 29.6, 26.0, 25.9.

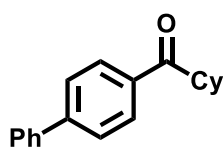


cyclohexyl(4-(trifluoromethyl)phenyl)methanone (19): Prepared following procedure A or procedure B. The pure product was a white solid, and matched previously published spectroscopic data (*J. Org. Chem.* **2015**, *80*, 10660-10667).

¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, *J* = 8.2 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 3.25 (tt, *J* = 11.2, 3.0 Hz, 1H), 1.85 (m, 4H), 1.75 (m, 1H), 1.52-1.31 (m, 4H), 1.24 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 202.8, 139.2, 134.0 (q, *J* = 32.3 Hz), 128.5, 125.6 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 270.7 Hz), 46.0, 29.2, 25.9, 25.7.

¹⁹F NMR (376 MHz, CDCl₃) δ -63.08.

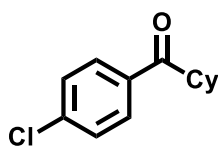


[1,1'-biphenyl]-4-yl(cyclohexyl)methanone (20): Prepared following procedure A or

procedure B. The pure product was a white solid, and matched previously published spectroscopic data (*Bioorg. Med. Chem.* **2002**, *10*, 437–448).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.05-7.95 (m, 2H), δ 7.70-7.64 (m, 2H), 7.63-7.57 (m, 2H), 7.50-7.41 (m, 2H), 7.40-7.33 (m, 1H), 3.30 (tt, $J = 11.2, 3.1$ Hz, 1H), 1.89 (m, 4H), 1.73 (m, 1H), 1.57-1.32 (m, 4H), 1.32-1.21 (m, 1H).

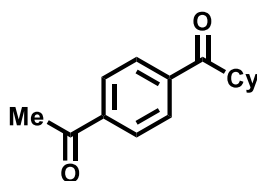
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 203.5, 145.4, 140.0, 135.1, 129.0, 128.9, 128.2, 127.3, 45.7, 29.5, 26.0, 25.9. (one carbon signal is overlapped)



(4-chlorophenyl)(cyclohexyl)methanone (21): Prepared following procedure A, or procedure B, or procedure C with *condition B*. The pure product was a white solid, and matched previously published spectroscopic data (*J. Org. Chem.* **1990**, *55*, 1286-1291).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.88 (d, $J = 6.9$ Hz, 2H), 7.42 (d, $J = 8.5$ Hz, 2H), 3.20 (tt, $J = 11.3, 3.2$ Hz, 1H), 1.91-1.78 (m, 4H), 1.73 (m, 1H), 1.54-1.32 (m, 4H), 1.31-1.22 (m, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 202.5, 139.1, 134.7, 129.7, 128.9, 45.6, 29.4, 25.9, 25.8.

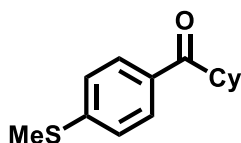


1-(4-(cyclohexanecarbonyl)phenyl)ethan-1-one (22): Prepared following procedure A. The pure product was a white solid, and matched previously published spectroscopic data (*J. Org. Chem.* **1990**, *55*, 1286-1291).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.09-7.99 (m, 4H), 3.28 (tt, $J = 11.2, 3.2$ Hz, 1H), 2.66 (s, 3H), 1.97-1.85 (m, 4H), 1.80-1.74 (m, 1H), 1.55-1.32 (m, 4H), 1.31-1.22 (m, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 203.3, 197.5, 139.9, 139.7, 128.5, 128.4, 46.0, 29.3,

26.8, 25.9, 25.8.



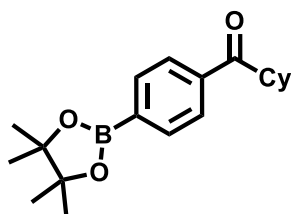
cyclohexyl(4-(methylthio)phenyl)methanone (23): Prepared following procedure A.

The pure product was a colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.96-7.75 (m, 2H), 7.26-7.22 (m, 2H), 3.20 (tt, *J* = 11.2, 3.2 Hz, 1H), 2.53 (s, 3H), 1.94-1.81 (m, 4H), 1.78-1.67 (m, 1H), 1.58-1.30 (m, 4H), 1.30-1.23 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 202.8, 145.3, 132.6, 128.7, 125.1, 45.4, 29.5, 26.0, 25.9, 14.8.

HRMS (ESI) Calcd for C₁₄H₁₉OS⁺ [M+H]⁺: 235.1151, found: 235.1146.



cyclohexyl(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanone (24):

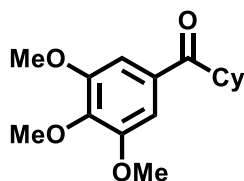
Prepared following procedure A, or procedure B, or procedure C with *condition A*.

The pure product was a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.98-7.87 (m, 4H), 3.29 (tt, *J* = 11.2, 3.2 Hz, 1H), 1.92-1.76 (m, 4H), 1.71 (m, 1H), 1.52-1.37 (m, 4H), 1.33 (s, 12H), 1.30-1.16 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 204.1, 138.4, 134.9, 127.2, 84.1, 45.7, 29.3, 26.0, 25.8, 24.9 (the carbon directly attached to the boron atom was not detected due to quadrupolar broadening).

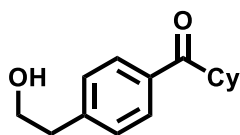
HRMS (ESI) Calcd for C₁₉H₂₈BO₃⁺ [M+H]⁺: 315.2126, found: 315.2124.



cyclohexyl(3,4,5-trimethoxyphenyl)methanone (25): Prepared following procedure A, or procedure B, or procedure C with *condition A*. The pure product was a white solid, and matched previously published spectroscopic data (*Org. Lett.* **2010**, *12*, 4042-4045).

¹H NMR (400 MHz, CDCl₃) δ 7.12 (s, 2H), 3.83 (s, 6H), 3.81 (s, 3H), 3.12 (tt, *J* = 11.4, 3.2 Hz, 1H), 1.85-1.72 (m, 4H), 1.70-1.63 (m, 1H), 1.47-1.23 (m, 4H), 1.22-1.11 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 202.6, 153.1, 142.4, 131.6, 105.9, 60.9, 56.3, 45.4, 29.6, 25.9, 25.8.

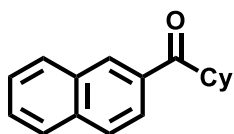


cyclohexyl(4-(2-hydroxyethyl)phenyl)methanone (26): Prepared following procedure A. The pure product was a white solid.

¹H NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 3.87 (t, *J* = 6.6 Hz, 2H), 3.22 (tt, *J* = 11.4, 3.2 Hz, 1H), 2.90 (t, *J* = 6.5 Hz, 2H), 1.90-1.76 (m, 5H), 1.74-1.66 (m, 1H), 1.53-1.30 (m, 4H), 1.25 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 203.6, 144.1, 134.7, 129.2, 128.6, 63.2, 45.6, 39.1, 29.4, 26.0, 25.9.

HRMS (ESI) Calcd for C₁₅H₂₁O₂⁺ [M+H]⁺: 233.1536, found: 233.1534.

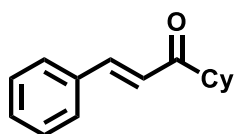


cyclohexyl(naphthalen-2-yl)methanone (27): Prepared following procedure A or procedure B. The pure product was a white solid, and matched previously published

spectroscopic data (*J. Org. Chem.* **1990**, *55*, 1286-1291).

¹H NMR (400 MHz, CDCl₃) δ 8.43 (s, 1H), 8.03-7.92 (m, 2H), 7.86 (t, *J* = 8.6 Hz, 2H), 7.62-7.50 (m, 2H), 3.41 (tt, *J* = 11.4, 3.2 Hz, 1H), 2.00-1.85 (m, 4H), 1.75 (m, 1H), 1.64-1.36 (m, 4H), 1.29 (m, 1H).

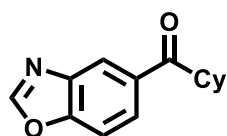
¹³C NMR (100 MHz, CDCl₃) δ 203.8, 135.5, 133.7, 132.6, 129.5, 128.4, 128.2, 127.7, 126.6, 124.3, 45.7, 29.6, 26.0, 25.9 (one carbon signal is overlapped).



(E)-1-cyclohexyl-3-phenylprop-2-en-1-one (28): Prepared following procedure A. The pure product was a white solid, and matched previously published spectroscopic data (*Chem. Eur. J.* **2014**, *20*, 14604-14607).

¹H NMR (400 MHz, CDCl₃) δ 7.64-7.53 (m, 3H), 7.42-7.33 (m, 3H), 6.81 (d, *J* = 16.0 Hz, 1H), 2.64 (tt, *J* = 11.4, 3.2 Hz, 1H), 1.93-1.77 (m, 4H), 1.74-1.63 (m, 1H), 1.51-1.32 (m, 4H), 1.30-1.21 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 203.1, 142.2, 134.8, 130.2, 128.9, 128.2, 124.7, 49.4, 28.7, 25.9, 25.8.

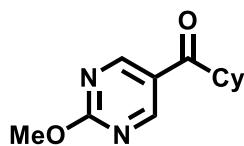


benzo[d]oxazol-2-yl(cyclohexyl)methanone (29): Prepared following procedure A or procedure B. *Note*: 2.0 equiv of aldehyde was used. The pure product was a white solid.

¹H NMR (400 MHz, CDCl₃) δ 8.38 (s, 1H), 8.16 (s, 1H), 8.06 (d, *J* = 8.6 Hz, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 3.30 (tt, *J* = 11.4, 3.2 Hz, 1H), 1.87 (m, 4H), 1.72 (m, 1H), 1.60-1.36 (m, 4H), 1.26 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 202.7, 153.7, 152.7, 140.3, 133.6, 126.4, 121.3, 111.1, 45.9, 29.6, 25.9, 25.8.

HRMS (ESI) Calcd for $C_{14}H_{16}NO_2^+$ $[M+H]^+$: 230.1176, found: 230.1172.

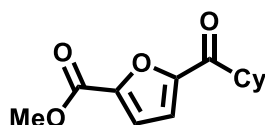


cyclohexyl(2-methoxypyrimidin-5-yl)methanone (30): Prepared following procedure A or procedure B. The pure product was a white solid.

1H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 2H), 4.10 (s, 3H), 3.10 (tt, $J = 11.4, 3.2$ Hz, 1H), 1.98-1.85 (m, 4H), 1.80-1.73 (m, 1H), 1.56-1.32 (m, 4H), 1.27 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0, 167.0, 160.3, 123.7, 55.6, 46.1, 29.0, 25.8, 25.6.

HRMS (ESI) Calcd for $C_{12}H_{17}N_2O_2^+$ $[M+H]^+$: 221.1285, found: 221.1280.

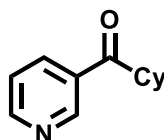


methyl 5-(cyclohexanecarbonyl)furan-2-carboxylate (31): Prepared following procedure A. *Note:* 2.0 equiv of aldehyde was used. The pure product was a white solid.

1H NMR (400 MHz, $CDCl_3$) δ 7.25-7.13 (m, 2H), 3.94 (s, 3H), 3.15 (tt, $J = 11.4, 3.2$ Hz, 1H), 1.94-1.76 (m, 4H), 1.75-1.68 (m, 1H), 1.61-1.33 (m, 4H), 1.32-1.19 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.5, 158.7, 153.8, 146.0, 118.7, 116.8, 52.4, 46.2, 28.6, 25.8, 25.6.

HRMS (ESI) Calcd for $C_{13}H_{17}O_4^+$ $[M+H]^+$: 237.1121, found: 237.1119.

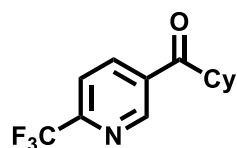


cyclohexyl(pyridin-3-yl)methanone (32): Prepared following procedure A, or procedure B, or procedure C with *condition* A. The pure product was a white solid, and matched previously published spectroscopic data (*J. Am. Chem. Soc.* **2006**, *128*,

14800-14801).

¹H NMR (400 MHz, CDCl₃) δ 9.12 (d, *J* = 2.2 Hz, 1H), 8.73 (dd, *J* = 4.8, 1.8 Hz, 1H), 8.21 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.40 (dd, *J* = 8.0, 4.8 Hz, 1H), 3.23 (tt, *J* = 11.4, 3.2 Hz, 1H), 1.86 (m, 4H), 1.75 (m, 1H), 1.56-1.32 (m, 4H), 1.31-1.17 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 202.5, 153.0, 149.6, 135.8, 131.5, 123.7, 46.1, 29.1, 25.8, 25.7.

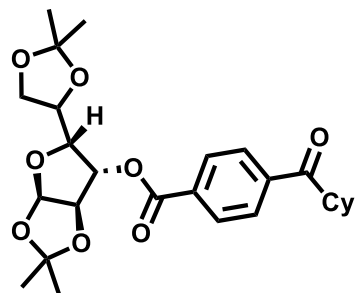


cyclohexyl(6-(trifluoromethyl)pyridin-3-yl)methanone (33): Prepared following procedure A or procedure B. The pure product was a white solid, and matched previously published spectroscopic data (*J. Am. Chem. Soc.* **2017**, *139*, 11353-11356).

¹H NMR (400 MHz, CDCl₃) δ 9.18 (d, *J* = 2.0 Hz, 1H), 8.35 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 3.20 (tt, *J* = 11.4, 3.2 Hz, 1H), 1.86 (m, 4H), 1.82-1.70 (m, 1H), 1.56-1.32 (m, 4H), 1.27 (m, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 201.3, 150.9 (q, *J* = 35.0 Hz), 149.7, 137.3, 133.6, 121.1 (q, *J* = 273.0 Hz), 120.5 (q, *J* = 2.7 Hz), 46.5, 29.0, 25.7, 25.6.

¹⁹F NMR (376 MHz, CDCl₃) δ -68.26.



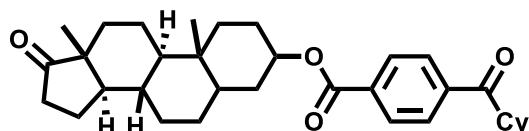
(3a*S*,5*S*,6*R*,6a*S*)-5-(2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl 4-(cyclohexanecarbonyl)benzoate (34): Prepared following procedure B. The pure product was a white solid.

¹H NMR (400 MHz, CDCl₃) δ 8.07 (d, *J* = 8.4 Hz, 2H), 7.96 (d, *J* = 8.4 Hz, 2H), 5.93 (d, *J* = 3.7 Hz, 1H), 5.50 (d, *J* = 2.6 Hz, 1H), 4.61 (d, *J* = 3.7 Hz, 1H), 4.42-4.23 (m,

2H), 4.07 (m, 2H), 3.22 (tt, $J = 11.4, 3.2$ Hz, 1H), 1.84 (m, 4H), 1.76-1.67 (m, 1H), 1.53 (s, 3H), 1.51-1.34 (m, 7H), 1.29 (s, 3H), 1.23 (m, 4H).

^{13}C NMR (100 MHz, CDCl_3) δ 203.2, 164.4, 140.1, 132.9, 130.0, 128.3, 112.4, 109.5, 105.1, 83.3, 80.0, 72.5, 67.4, 46.0, 29.2, 26.9, 26.7, 26.2, 25.9, 25.7, 25.2.

HRMS (ESI) Calcd for $\text{C}_{26}\text{H}_{35}\text{O}_8^+$ $[\text{M}+\text{H}]^+$: 475.2326, found: 475.2323.

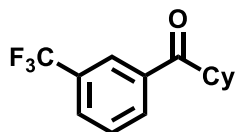


(3S,8R,9S,10S,13S,14S)-10,13-dimethyl-17-oxohexadecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-(cyclohexanecarbonyl)benzoate (35): Prepared following procedure B. The pure product was a white solid.

^1H NMR (400 MHz, CHCl_3) δ 8.09 (d, $J = 8.3$ Hz, 2H), 7.94 (d, $J = 8.4$ Hz, 2H), 4.95 (m, 1H), 3.24 (m, 1H), 2.42 (dd, $J = 19.2, 8.6$ Hz, 1H), 2.05 (m, 1H), 2.02-1.72 (m, 10H), 1.72-1.63 (m, 3H), 1.59-1.22 (m, 14H), 1.13 (td, $J = 13.5, 3.7$ Hz, 1H), 1.04 (td, $J = 12.1, 4.9$ Hz, 1H), 0.87 (d, $J = 15.4$ Hz, 6H), 0.74 (td, $J = 11.5, 3.8$ Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 221.2, 203.5, 165.3, 139.6, 134.3, 129.8, 128.1, 74.7, 54.3, 51.4, 47.8, 46.0, 44.7, 36.7, 35.9, 35.7, 35.1, 34.0, 31.5, 30.8, 29.3, 28.3, 27.5, 25.9, 25.8, 21.8, 20.5, 13.8, 12.3.

HRMS (ESI) Calcd for $\text{C}_{33}\text{H}_{44}\text{NaO}_4^+$ $[\text{M}+\text{Na}]^+$: 527.3132, found: 527.3127.



cyclohexyl(3-(trifluoromethyl)phenyl)methanone (36): Prepared following procedure C with *condition A*. The pure product was a colorless liquid.

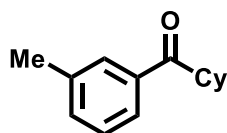
^1H NMR (400 MHz, CDCl_3) δ 8.17 (s, 1H), 8.11 (d, $J = 7.8$ Hz, 1H), 7.79 (d, $J = 7.8$ Hz, 1H), 7.60 (t, $J = 7.8$ Hz, 1H), 3.25 (tt, $J = 11.4, 3.3$ Hz, 1H), 1.94-1.79 (m, 4H), 1.74 (m, 1H), 1.60-1.33 (m, 4H), 1.27 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 202.3, 136.9, 131.7, 131.2 (q, $J = 32.7$ Hz), 129.2, 129.1 (q, $J = 3.7$ Hz), 125.0 (q, $J = 3.3$ Hz), 123.7 (q, $J = 270.7$ Hz), 45.7, 29.3, 25.8,

25.7.

^{19}F NMR (376 MHz, CDCl_3) δ -62.76.

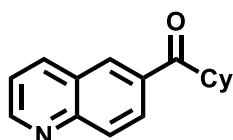
HRMS (ESI) Calcd for $\text{C}_{14}\text{H}_{16}\text{F}_3\text{O}^+$ $[\text{M}+\text{H}]^+$: 257.1148, found: 257.1142.



cyclohexyl(m-tolyl)methanone (37): Prepared following procedure C with *condition B*. The pure product was a colorless liquid, and matched previously published spectroscopic data (*J. Org. Chem.* **2016**, *81*, 6409-6423).

^1H NMR (400 MHz, CDCl_3) δ 7.72 (d, $J = 6.2$ Hz, 2H), 7.36-7.30 (m, 2H), 3.25 (tt, $J = 11.5, 3.2$ Hz, 1H), 2.39 (s, 3H), 1.92-1.77 (m, 4H), 1.75-1.67 (m, 1H), 1.55-1.33 (m, 4H), 1.24 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 204.0, 138.3, 136.4, 133.4, 128.7, 128.4, 125.4, 45.6, 29.4, 26.0, 25.8, 21.4.

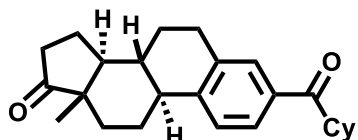


cyclohexyl(quinolin-6-yl)methanone (38): Prepared following procedure C with *condition A*. The pure product was a white solid.

^1H NMR (400 MHz, CDCl_3) δ 8.99 (dd, $J = 4.2, 1.6$ Hz, 1H), 8.42 (d, $J = 1.6$ Hz, 1H), 8.28 (d, $J = 8.2$ Hz, 1H), 8.24 (dd, $J = 8.9, 1.9$ Hz, 1H), 8.16 (d, $J = 8.9$ Hz, 1H), 7.46 (dd, $J = 8.3, 4.2$ Hz, 1H), 3.39 (tt, $J = 11.3, 3.3$ Hz, 1H), 2.01-1.82 (m, 4H), 1.75 (m, 1H), 1.63-1.37 (m, 4H), 1.35-1.22 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 203.1, 152.3, 149.8, 137.6, 134.2, 129.9, 129.3, 128.0, 127.5, 121.8, 45.8, 29.4, 25.9, 25.8.

HRMS (ESI) Calcd for $\text{C}_{16}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$: 240.1383, found: 240.1380.

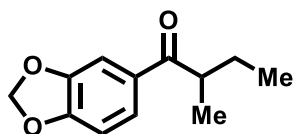


(8R,9S,13S,14S)-3-(cyclohexanecarbonyl)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[*a*]phenanthren-17-one (39): Prepared following procedure C with *condition A*. The pure product was a white solid.

¹H NMR (400 MHz, CHCl₃) δ 7.76-7.64 (m, 2H), 7.36 (d, *J* = 8.2 Hz, 1H), 3.22 (tt, *J* = 11.2, 8.2, 3.1, 0.3 Hz, 1H), 3.03-2.92 (m, 2H), 2.57-2.40 (m, 2H), 2.32 (dt, *J* = 11.0, 5.7 Hz, 1H), 2.11 (m, 3H), 2.00-1.93 (m, 1H), 1.84 (t, *J* = 12.0 Hz, 4H), 1.72 (m, 1H), 1.51 (m, 10H), 1.32-1.20 (m, 1H), 0.91 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 220.5, 203.7, 145.0, 136.9, 134.0, 128.9, 125.7, 125.5, 50.5, 47.9, 45.5, 44.7, 37.8, 35.8, 31.5, 29.5, 29.4, 26.3, 26.0, 25.9, 25.6, 21.6, 13.8.

HRMS (ESI) Calcd for C₂₅H₃₂NaO₂⁺ [M+Na]⁺: 387.2295, found: 387.2288.

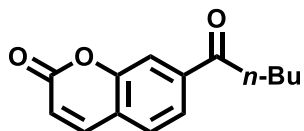


1-(benzo[*d*][1,3]dioxol-5-yl)-2-methylbutan-1-one (40): Prepared following procedure C with *condition A*. The pure product was a white solid.

¹H NMR (400 MHz, CHCl₃) δ 7.57 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.45 (d, *J* = 1.7 Hz, 1H), 6.85 (d, *J* = 8.2 Hz, 1H), 6.04 (s, 2H), 3.31 (m, 1H), 1.90-1.71 (m, 1H), 1.48 (m, 1H), 1.17 (d, *J* = 6.9 Hz, 3H), 0.90 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 202.5, 151.5, 148.2, 131.7, 124.3, 108.2, 107.9, 101.8, 41.9, 26.9, 17.0, 11.8.

HRMS (ESI) Calcd for C₁₂H₁₄NaO₃⁺ [M+Na]⁺: 229.0385, found: 229.0380.



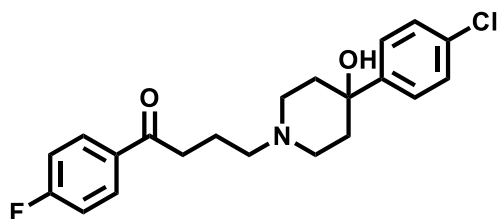
7-pentanoyl-2H-chromen-2-one (41): Prepared following procedure C with *condition A*. The pure product was a white solid.

¹H NMR (400 MHz, CHCl₃) δ 7.70 (d, *J* = 9.6 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.11

(d, $J = 2.0$ Hz, 1H), 7.05 (dd, $J = 8.4, 2.1$ Hz, 1H), 6.40 (d, $J = 9.6$ Hz, 1H), 2.60 (t, $J = 7.5$ Hz, 2H), 1.76 (m, 2H), 1.46 (m, 2H), 0.98 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.6, 160.4, 154.7, 153.3, 142.9, 128.5, 118.4, 116.6, 116.0, 110.4, 34.1, 26.8, 22.2, 13.7.

HRMS (ESI) Calcd for $\text{C}_{14}\text{H}_{15}\text{O}_4^+$ $[\text{M}+\text{H}]^+$: 247.0965, found: 247.0968.



Haloperidol (42): To a 10 mL vial equipped with a stir bar was added 4-chloro-1-(4-fluorophenyl)butan-1-one **11** (54 mg, 0.27 mmol, 1.0 equiv), 4-(4-chlorophenyl)-4-hydroxypiperidine (114 mg, 0.54 mmol, 2.0 equiv), and anhydrous potassium iodide (1.3 mg, 8.0 μmol , 0.03 equiv). Then 2 mL of anhydrous toluene was added, and the vial was sealed. The mixture was stirred at 130 $^\circ\text{C}$ for 45 h. After cooling to room temperature, the reaction mixture was diluted with EtOAc (3 mL), and quenched with aq. NaHCO_3 (3 mL). The aqueous layer was extracted with three portions of EtOAc (3 x 3 mL). The combined organic layers were washed with brine, dried over MgSO_4 , filtered, and concentrated. The residue was purified by flash chromatography (10% $\text{MeOH}/\text{CH}_2\text{Cl}_2 = 1:10$ with 1% Et_3N) provided the pure compound **42** (87 mg, 81 % yield) as a white solid, which matched previously published spectroscopic data (*J. Am. Chem. Soc.* **2017**, *139*, 11353-11356).

^1H NMR (400 MHz, CDCl_3) δ 8.05-7.98 (m, 2H), 7.41-7.35 (m, 2H), 7.33-7.27 (m, 2H), 7.18-7.09 (m, 2H), 2.99 (t, $J = 7.0$ Hz, 2H), 2.80 (d, $J = 11.3$ Hz, 2H), 2.54-2.37 (m, 4H), 2.00 (m, 4H), 1.68 (m, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 198.3, 165.6 (d, $J = 253.0$ Hz), 146.9, 133.7 (d, $J = 3.0$ Hz), 132.7, 130.7 (d, $J = 10.0$ Hz), 128.3, 126.1, 115.6 (d, $J = 22.0$ Hz), 71.1, 57.8, 49.3, 38.3, 36.2, 21.9.

^{19}F NMR (376 MHz, CDCl_3) δ -105.59.

Density Functional Theory (DFT) Calculations

1.1 Computational Methods

All the calculations were performed with Gaussian 09 package.¹ Geometries were optimized in the gas phase using unrestricted B3LYP-D3²⁻⁵ and def2-SVP basis set⁶⁻¹⁰ for all atoms. Optimized geometries were verified by frequency computations as minima (zero imaginary frequencies) or transition structures (a single imaginary frequency) at the same level of theory. In addition, the correctness of the imaginary frequency of transition states were confirmed by viewing normal mode vibrational vector. Solvent effect was included by single-point energy calculation using SMD model¹¹ and B3LYP-D3 method with the def2-TZVP basis set⁶⁻¹⁰. All the computational data (relative Gibbs free energies and electronic energies) were reported in kcal/mol in solvent (Acetone) at 298.15 K and 1 atm.

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1.2 Computational Details

Table S1. Corrections to zero point energies, enthalpies, free energies and electronic potential energies (in Hartree) and imaginary frequencies (IF) (cm^{-1}) of optimized structures which were calculated at uB3LYP-D3/def2-TZVP//uB3LYP-D3/def2-SVP level in solvent (Acetone) at 298.15 K and 1 atm.

Geometry	cZPE _{298, gas}	cH _{298, gas}	cG _{298, gas}	E _{0, sol}	IF
AQ-H_radical	0.191293	0.203798	0.153055	-689.65799	1
AQ	0.181297	0.193215	0.144027	-689.072068	1
acyl_radical	0.166855	0.17546	0.133804	-348.706787	1
PhBr	0.090536	0.097164	0.059663	-2805.934496	1
KHCO ₃	0.028355	0.034525	-0.001293	-864.558199	1
KBr_H ₂ CO ₃	0.040824	0.04936	0.005652	-3439.399411	1
LPd ⁰	0.596921	0.635097	0.52542	-2392.140893	1
Product	0.261511	0.274371	0.222594	-580.518345	1
INT1A	0.689352	0.734657	0.610103	-5198.130795	1
INT1B	0.766071	0.813186	0.682648	-2740.89753	1
INT2	0.860444	0.913956	0.773677	-5546.871202	1
INT4	0.598634	0.638929	0.52295	-4966.388942	1
INT5	0.628217	0.675598	0.542313	-5830.961736	1
INT6	0.82155	0.881102	0.722565	-6520.667404	1
INT7	0.82196	0.881351	0.724622	-6520.665842	1
INT8	0.822651	0.882111	0.725483	-6520.677053	1
INT9	0.823051	0.882672	0.727291	-6520.678178	1
TS1A	0.687484	0.732825	0.606436	-5198.079196	-179.537
TS1B	0.765061	0.812067	0.680978	-2740.859388	-22.519
TS2A	0.858863	0.91259	0.768586	-5546.842986	-38.348
TS2B	0.857246	0.911341	0.766164	-5546.822422	-194.349
TS3	0.859321	0.912899	0.770551	-5546.852135	-223.248
TS4	0.627614	0.674352	0.543434	-5830.959415	-19.26
TS5	0.818104	0.87707	0.721863	-6520.663549	-669.896
TS6	0.819594	0.878703	0.722823	-6520.650592	-53.123
TS7	0.822226	0.881435	0.725316	-6520.672359	-49.422

Cartesian coordinates (in Å) of related structures which were calculated at the uB3LYP-D3/def2-SVP level of theory.

AQ-H_radical			H	4.647082	1.247264	0.000065	
C	-3.690049	0.664419	-0.000118	H	2.465059	2.491566	-0.000067
C	-2.495860	1.366838	0.000402	H	2.465060	-2.491565	0.000099
C	-1.246049	0.689301	0.000330	H	4.647082	-1.247263	0.000161
C	-1.254088	-0.739872	-0.000040	H	-4.647082	1.247262	0.000067
C	-2.477075	-1.429539	-0.000556	H	-4.647081	-1.247264	0.000163
C	-3.686714	-0.744635	-0.000743	H	-2.465059	-2.491566	0.000098
C	1.264513	-0.740145	0.000117	C	-0.000001	1.484260	-0.000133
C	1.252003	0.685907	0.000139	C	0.000001	-1.484260	0.000098
C	2.488840	1.383246	-0.000189	O	-0.000002	2.704194	-0.000124
H	2.480600	2.473707	-0.000216	O	0.000002	-2.704194	-0.000371
C	3.686320	0.685738	-0.000406				
C	3.693984	-0.724018	-0.000362	acyl_radical			
C	2.492338	-1.422621	-0.000072	C	-2.135648	0.262494	0.357807
H	-4.637791	1.208531	-0.000038	C	-1.261338	1.379886	-0.226230
H	-2.541769	2.460784	0.001088	C	0.224318	1.147264	0.075396
H	-2.436346	-2.520653	-0.000747	C	0.679188	-0.240396	-0.411498
H	-4.631424	-1.293231	-0.001358	C	-0.197841	-1.366926	0.167241
H	4.631728	1.234375	-0.000651	C	-1.681017	-1.117505	-0.135350
H	4.643463	-1.264895	-0.000542	H	0.851842	1.927490	-0.383409
H	2.462793	-2.513995	-0.000016	H	-1.407430	1.420071	-1.321668
C	0.004253	1.385026	0.000304	H	-1.575431	2.361626	0.165937
C	0.006662	-1.519598	0.000408	H	-2.071302	0.291741	1.461306
O	0.072438	2.733041	0.000141	H	-3.195029	0.430112	0.101928
H	-0.812609	3.119151	-0.000391	H	0.598709	-0.285824	-1.515864
O	0.003422	-2.751047	0.000808	H	0.129793	-2.340382	-0.231201
				H	-0.048061	-1.405310	1.261553
AQ			H	-1.841885	-1.184299	-1.227356	
C	3.700466	0.701080	0.000059	H	-2.294913	-1.912110	0.320069
C	2.494071	1.400298	0.000006	H	0.398660	1.208731	1.164309
C	1.276165	0.705371	-0.000008	C	2.155312	-0.498349	-0.140578
C	1.276165	-0.705370	0.000058	O	2.969651	0.261169	0.260459
C	2.494072	-1.400296	0.000083				
C	3.700466	-0.701079	0.000107	PhBr			
C	-1.276165	-0.705371	0.000058	C	-0.097272	-0.000050	-0.000005
C	-1.276166	0.705371	-0.000009	C	-0.785376	1.217545	-0.000033
C	-2.494072	1.400296	0.000006	C	-2.183616	1.209397	0.000034
H	-2.465061	2.491565	-0.000067	C	-2.885854	0.000001	-0.000003
C	-3.700466	0.701079	0.000060	C	-2.183704	-1.209347	-0.000027
C	-3.700466	-0.701080	0.000107	C	-0.785382	-1.217548	0.000023
C	-2.494071	-1.400298	0.000081	H	-0.233039	2.158718	-0.000036

H	-2.724690	2.158886	0.000040	C	-2.072412	-1.188512	1.207124
H	-3.978311	0.000096	0.000005	C	1.963831	-1.142710	1.249591
H	-2.724702	-2.158879	-0.000015	C	3.655534	-1.318314	-1.099807
H	-0.233190	-2.158805	0.000035	C	-4.865659	-1.089056	-0.242556
Br	1.812033	0.000000	0.000001	C	-2.269608	-2.572160	1.371149
				C	2.506046	-0.326057	2.255191
KHCO₃				C	4.717170	-1.613108	-0.228668
C	0.993582	0.042116	-0.000038	C	-3.937760	-1.196262	-2.476154
O	0.404396	1.146638	-0.000014	C	-1.839631	-0.400501	2.343399
O	2.360876	0.083042	0.000020	C	1.345142	-2.349484	1.614684
H	2.641190	-0.844091	0.000085	C	3.836012	-1.504849	-2.480634
O	0.457809	-1.104312	0.000143	C	-6.124020	-1.420098	-0.751473
K	-1.809859	-0.021661	-0.000055	C	-2.264269	-3.146698	2.642207
				C	2.435994	-0.713292	3.597236
				C	5.936274	-2.076789	-0.732572
KBr_H₂CO₃				C	-5.199115	-1.518095	-2.986765
Br	1.662243	-0.770494	0.000219	C	-1.814301	-0.982158	3.615589
K	0.586535	2.012936	-0.000612	C	1.287231	-2.740767	2.953235
O	-1.703130	0.867262	0.002030	C	5.058812	-1.955582	-2.984536
C	-2.117210	-0.291447	0.000080	C	-6.293784	-1.632751	-2.124544
O	-3.426337	-0.568235	-0.000293	C	-2.034278	-2.351924	3.771376
H	-3.891539	0.281820	-0.000136	C	1.830486	-1.922990	3.948729
O	-1.410238	-1.377797	-0.001245	C	6.111772	-2.244728	-2.110037
H	-0.410234	-1.181482	-0.000323	H	-0.586900	4.461365	2.689109
				H	0.254301	2.899416	2.493928
LPd⁰				H	1.201525	4.404900	2.610822
P	-2.057043	-0.528849	-0.522847	H	1.173068	6.092270	0.721923
P	2.004568	-0.689763	-0.546847	H	0.208834	5.803067	-0.752378
O	0.092950	1.385481	0.376890	H	-0.586729	6.160516	0.805512
C	0.211918	4.135893	0.670600	H	-2.297011	5.223319	-0.110706
C	-1.071072	3.462688	0.167326	H	2.725774	5.027217	-0.334435
C	1.392045	3.369643	0.061801	H	-4.269964	1.487858	-0.894029
C	-1.068261	2.061674	0.082075	H	4.342400	1.135921	-1.201261
C	1.275369	1.974653	-0.008184	H	-4.317483	3.955696	-0.773258
C	0.273435	3.963302	2.214423	H	4.582285	3.602903	-1.139763
C	0.253500	5.630909	0.333624	H	-4.740520	-0.921426	0.829799
C	-2.198672	1.310768	-0.294947	H	-2.435700	-3.202822	0.493264
C	2.314119	1.136764	-0.454188	H	2.981401	0.621730	1.992676
C	-2.255191	4.134548	-0.156182	H	4.592369	-1.483118	0.848512
C	2.595804	3.944752	-0.364190	H	-3.074067	-1.122970	-3.143935
C	-3.371030	2.026259	-0.592017	H	-1.675977	0.673300	2.245471
C	3.511565	1.751089	-0.851866	H	0.881334	-2.970016	0.843808
C	-3.396879	3.420363	-0.528701	H	3.004033	-1.297443	-3.160675
C	3.646054	3.141357	-0.816648	H	-6.976929	-1.512008	-0.073617
C	-3.759514	-0.972234	-1.102267				

H	-2.431242	-4.221642	2.751890			
H	2.856485	-0.064698	4.370596	INT1A		
H	6.753939	-2.307650	-0.044422	C	3.472058	2.230430 -0.326246
H	-5.324762	-1.689302	-4.059075	C	2.296483	1.466553 -0.392121
H	-1.620382	-0.355305	4.489684	C	1.181730	2.034552 -1.043766
H	0.790360	-3.675424	3.221288	C	1.232917	3.307777 -1.635045
H	5.186602	-2.091742	-4.061671	C	2.418575	4.041939 -1.529413
H	-7.278857	-1.893396	-2.520493	C	3.532520	3.508707 -0.878762
H	-2.016591	-2.802320	4.767098	H	4.347865	1.826178 0.183085
H	1.770099	-2.222351	4.998359	H	2.482562	5.038525 -1.966582
H	7.066006	-2.607405	-2.501150	H	4.453208	4.091506 -0.802581
Pd	-0.057176	-1.096225	-1.470590	C	0.000049	3.766337 -2.419418
				C	-1.232835	3.307791 -1.635064
				C	-1.181673	2.034566 -1.043780
Product				C	-2.418484	4.041970 -1.529455
C	3.895590	0.604297	-0.304846	C	-2.296441	1.466586 -0.392145
C	2.723694	1.519091	-0.680237	C	-3.532445	3.508756 -0.878820
C	1.440407	0.717862	-0.931888	H	-2.482447	5.038555 -1.966630
C	1.083861	-0.175883	0.281972	C	-3.472007	2.230482 -0.326293
C	2.264536	-1.088626	0.643151	H	-4.453127	4.091567 -0.802658
C	3.544004	-0.283181	0.895612	H	-4.347829	1.826243 0.183022
H	0.604366	1.393953	-1.172586	O	0.000025	1.326569 -1.118135
H	2.544843	2.237940	0.141148	C	0.000052	5.279631 -2.669888
H	2.971061	2.119493	-1.571868	H	0.000065	5.846576 -1.726810
H	4.141188	-0.039457	-1.169510	H	0.880716	5.577717 -3.256695
H	4.797244	1.203052	-0.092891	H	-0.880625	5.577723 -3.256673
H	0.883028	0.489720	1.140098	C	0.000053	3.031906 -3.790108
H	2.005936	-1.700163	1.522863	H	-0.895212	3.306724 -4.370253
H	2.419557	-1.799904	-0.184692	H	0.895314	3.306735 -4.370253
H	3.407066	0.354011	1.789456	H	0.000059	1.940170 -3.655357
H	4.379111	-0.965416	1.126282	P	-2.245930	-0.224567 0.361133
H	1.578528	0.063914	-1.811596	P	2.245926	-0.224604 0.361135
C	-0.177684	-0.980514	-0.023983	C	2.919168	-1.299840 -0.968658
O	-0.099541	-2.147359	-0.362123	C	3.185498	-2.645180 -0.656706
C	-1.522338	-0.304023	0.049301	C	3.060762	-0.863395 -2.292910
C	-2.647902	-1.043845	-0.357067	C	3.588555	-3.533624 -1.650981
C	-1.705650	1.014520	0.501792	H	3.050688	-3.005004 0.365650
C	-3.922287	-0.481499	-0.315505	C	3.461501	-1.759685 -3.290411
H	-2.490086	-2.066965	-0.703589	H	2.853367	0.176463 -2.552890
C	-2.983234	1.578906	0.543778	C	3.723955	-3.093854 -2.973284
H	-0.853257	1.612097	0.828208	H	3.777830	-4.579111 -1.396875
C	-4.092974	0.833354	0.135202	H	3.565797	-1.409474 -4.320646
H	-4.788179	-1.067154	-0.634759	H	4.029224	-3.793986 -3.755108
H	-3.112437	2.604620	0.898169	C	3.580238	-0.234268 1.630070
H	-5.091787	1.276381	0.168566			

C	4.915083	-0.534324	1.302026	Pd	-0.000001	-0.580480	0.930323
C	3.248299	0.058887	2.963594				
C	5.900955	-0.536769	2.292243	INT1B			
H	5.186689	-0.772755	0.271747	P	-1.471288	-1.630431	-0.250865
C	4.240415	0.058695	3.947943	P	0.946893	1.437896	-0.104661
H	2.216099	0.304212	3.223719	O	-1.945672	1.252382	0.127548
C	5.565742	-0.239398	3.617056	C	-4.075057	2.967339	-0.390741
H	6.934430	-0.773566	2.026152	C	-4.184926	1.467738	-0.695313
H	3.971188	0.291448	4.981308	C	-2.635873	3.390096	-0.709709
H	6.337694	-0.243006	4.391132	C	-3.083321	0.662753	-0.371586
C	-2.919165	-1.299832	-0.968637	C	-1.617200	2.490093	-0.373095
C	-3.185445	-2.645175	-0.656649	C	-4.305682	3.167013	1.133373
C	-3.060843	-0.863410	-2.292886	C	-5.108031	3.793311	-1.166811
C	-3.588541	-3.533644	-1.650886	C	-3.065111	-0.731869	-0.539231
H	-3.050550	-3.004986	0.365699	C	-0.250414	2.776145	-0.518728
C	-3.461606	-1.759730	-3.290353	C	-5.316535	0.831631	-1.218758
H	-2.853485	0.176448	-2.552892	C	-2.250844	4.626314	-1.244511
C	-3.724016	-3.093899	-2.973190	C	-4.226336	-1.331227	-1.054228
H	-3.777779	-4.579130	-1.396750	C	0.096029	4.033881	-1.036612
H	-3.565957	-1.409540	-4.320590	C	-5.337475	-0.555561	-1.391356
H	-4.029311	-3.794050	-3.754987	C	-0.898101	4.943952	-1.404727
C	-3.580270	-0.234172	1.630036	C	-1.885838	-3.351867	-0.776368
C	-3.248384	0.059215	2.963524	C	-1.360798	-1.802758	1.585120
C	-4.915076	-0.534420	1.302013	C	0.874502	1.376970	1.737179
C	-4.240521	0.059089	3.947849	C	2.574463	2.241898	-0.432045
H	-2.216210	0.304669	3.223634	C	-2.690214	-4.212215	-0.008221
C	-5.900969	-0.536805	2.292210	C	-0.464316	-2.763000	2.090470
H	-5.186635	-0.773043	0.271765	C	0.274596	2.376350	2.519204
C	-5.565814	-0.239184	3.616981	C	3.384993	2.788856	0.575621
H	-3.971340	0.292032	4.981183	C	-1.368700	-3.807941	-1.998784
H	-6.934413	-0.773750	2.026135	C	-2.051323	-0.979560	2.485838
H	-6.337782	-0.242746	4.391042	C	1.467090	0.274811	2.376701
C	-0.000021	-2.322939	-0.090695	C	3.044943	2.230347	-1.758019
C	-0.000074	-3.525725	0.631522	C	-2.976758	-5.501848	-0.461699
C	-0.000001	-2.381581	-1.493090	C	-0.288281	-2.915740	3.466083
C	-0.000099	-4.759093	-0.036636	C	0.274983	2.277205	3.914188
H	-0.000101	-3.513295	1.725918	C	4.644779	3.309958	0.262310
C	-0.000021	-3.609141	-2.159722	C	-1.662470	-5.097067	-2.455040
H	0.000030	-1.458017	-2.076632	C	-1.861269	-1.125275	3.863742
C	-0.000072	-4.805086	-1.433664	C	1.479833	0.185793	3.768988
H	-0.000143	-5.687478	0.542703	C	4.297058	2.763679	-2.069070
H	0.000000	-3.630048	-3.252843	C	-2.465554	-5.945334	-1.687314
H	-0.000089	-5.766826	-1.953667	C	-0.988231	-2.096458	4.358579
Br	0.000040	1.581864	2.373324	C	0.882547	1.186324	4.542234

C	5.103295	3.299667	-1.058326	H	2.486767	-2.384631	0.505751
H	-5.315931	2.829774	1.414420	H	3.480461	-3.283593	-0.645065
H	-3.574056	2.592720	1.721249	C	5.982923	-2.458544	0.374480
H	-4.200046	4.230531	1.400293	H	6.124684	-0.310143	0.133010
H	-5.020356	4.860625	-0.917376	H	7.120709	-1.220302	-1.011504
H	-4.984475	3.678210	-2.254245	H	4.516845	-1.661474	1.756565
H	-6.130758	3.491456	-0.898256	H	4.490865	-3.428006	1.635648
H	-6.195907	1.416589	-1.490957	H	6.106187	-3.361014	-0.252805
H	-3.007688	5.357509	-1.531099	H	6.780436	-2.495605	1.136090
H	-4.255734	-2.409922	-1.212498				
H	1.148095	4.295654	-1.161627				
H	-6.229494	-1.037909	-1.798033	INT2			
H	-0.615470	5.916052	-1.815728	C	2.732613	-0.053374	-3.038273
H	-3.089196	-3.871978	0.950511	C	1.973514	0.505792	-2.001057
H	0.091735	-3.402333	1.399399	C	0.899973	1.335448	-2.357144
H	-0.192528	3.239454	2.039879	C	0.574090	1.662164	-3.675020
H	3.037827	2.800097	1.610703	C	1.355196	1.086386	-4.684683
H	-0.720294	-3.149804	-2.585413	C	2.419182	0.235378	-4.368776
H	-2.739029	-0.217044	2.118690	H	3.553088	-0.733659	-2.806654
H	1.908229	-0.524438	1.777636	H	1.134896	1.295203	-5.732206
H	2.440541	1.772549	-2.544657	H	3.010482	-0.211275	-5.171328
H	-3.600337	-6.164844	0.143953	C	-0.586282	2.642397	-3.888263
H	0.403321	-3.674163	3.842469	C	-1.665145	2.301170	-2.851190
H	-0.198874	3.060339	4.512165	C	-1.234688	1.918015	-1.573543
H	5.270809	3.725131	1.056574	C	-3.045689	2.386320	-3.064061
H	-1.253672	-5.440986	-3.408550	C	-2.109688	1.617689	-0.516092
H	-2.399746	-0.470205	4.553077	C	-3.946542	2.109490	-2.031174
H	1.937615	-0.681511	4.249349	H	-3.430069	2.671372	-4.043911
H	4.651747	2.741773	-3.102522	C	-3.486092	1.727811	-0.769364
H	-2.688874	-6.955887	-2.039450	H	-5.020998	2.177309	-2.215487
H	-0.844383	-2.208289	5.436216	H	-4.204912	1.483548	0.012966
H	0.880702	1.109424	5.632558	O	0.110766	1.794558	-1.325191
H	6.090332	3.702483	-1.299578	C	-1.127794	2.590770	-5.321738
Pd	0.587023	-0.706201	-1.066986	H	-1.507703	1.589068	-5.572913
C	2.464059	-0.972157	-1.846243	H	-0.342187	2.857194	-6.043482
C	3.638445	-1.134197	-0.855497	H	-1.940397	3.318647	-5.460249
O	2.653088	-0.937750	-3.041947	C	-0.067998	4.076041	-3.587872
C	5.010791	-1.106125	-1.540006	H	-0.885534	4.807779	-3.685317
C	3.473100	-2.395112	0.012211	H	0.735118	4.345996	-4.291620
H	3.570574	-0.261164	-0.182331	H	0.335037	4.143754	-2.566153
C	6.139189	-1.211885	-0.507271	P	-1.377498	0.889644	1.022622
H	5.105316	-0.183362	-2.133185	P	2.102493	0.085920	-0.226001
H	5.068302	-1.943791	-2.256779	C	2.525667	1.686258	0.582765
C	4.602417	-2.503346	1.043806	C	2.591143	1.711377	1.985447
				C	2.873192	2.835679	-0.145665

C	3.020246	2.865080	2.643150	C	1.947500	-4.469000	-1.582585
H	2.296987	0.830714	2.562251	H	1.490668	-2.416108	-2.033710
C	3.295993	3.988767	0.520768	C	1.166558	-5.294030	0.546030
H	2.829474	2.833740	-1.236207	H	0.151532	-3.873201	1.809349
C	3.375962	4.004383	1.915672	C	1.831748	-5.516011	-0.663868
H	3.060329	2.875368	3.734388	H	2.460851	-4.627992	-2.535544
H	3.568223	4.876798	-0.056041	H	1.066996	-6.104466	1.274344
H	3.704809	4.907458	2.436276	H	2.255276	-6.498574	-0.889137
C	3.687771	-0.821092	-0.008735	Br	0.627007	-1.309560	3.036916
C	4.878749	-0.306449	-0.554382	Pd	-0.004063	-1.112096	0.466567
C	3.734691	-1.974948	0.786209	C	-1.008337	-1.331623	-1.305815
C	6.090841	-0.965114	-0.344586	C	-2.474469	-1.776623	-1.145157
H	4.859625	0.618647	-1.135488	O	-0.537484	-1.109915	-2.385386
C	4.953764	-2.626311	0.999733	C	-3.255915	-1.575094	-2.452667
H	2.826450	-2.357487	1.250105	C	-2.593417	-3.228475	-0.641774
C	6.128479	-2.131445	0.429168	H	-2.923275	-1.129571	-0.374873
H	7.009849	-0.562091	-0.778080	C	-4.727045	-1.960738	-2.270558
H	4.976939	-3.526597	1.618250	H	-3.160707	-0.529599	-2.781549
H	7.078457	-2.646478	0.594930	H	-2.792175	-2.194584	-3.238810
C	-0.734929	2.329034	1.968707	C	-4.067131	-3.618405	-0.473231
C	-0.542302	2.170164	3.353215	H	-2.050633	-3.354141	0.306151
C	-0.451717	3.565714	1.370990	H	-2.097371	-3.899836	-1.363816
C	-0.106150	3.246512	4.126567	C	-4.869401	-3.401109	-1.762483
H	-0.725574	1.200870	3.820213	H	-5.194673	-1.269037	-1.545025
C	-0.006451	4.636045	2.151134	H	-5.272390	-1.830468	-3.220704
H	-0.579104	3.704813	0.297300	H	-4.506208	-3.005231	0.335558
C	0.157090	4.483403	3.529879	H	-4.139403	-4.669068	-0.145960
H	0.034094	3.113586	5.202299	H	-4.497921	-4.094421	-2.539500
H	0.216127	5.593297	1.673780	H	-5.931488	-3.651058	-1.600308
H	0.501766	5.324245	4.137260				
C	-2.846268	0.414550	2.031461	INT3			
C	-3.082147	-0.936946	2.324329	P	-1.881971	-0.256797	0.136581
C	-3.731751	1.387028	2.531290	P	1.825161	-0.400695	0.175086
C	-4.201575	-1.314243	3.072881	O	0.097379	1.883491	-0.105828
H	-2.374784	-1.697955	1.991490	C	0.211331	4.306232	-1.455286
C	-4.848766	1.008835	3.278213	C	-1.077865	3.470836	-1.455922
H	-3.541447	2.445987	2.340535	C	1.383647	3.317216	-1.528671
C	-5.089022	-0.344347	3.545184	C	-1.062002	2.270011	-0.734600
H	-4.369189	-2.370744	3.295403	C	1.261628	2.134280	-0.792579
H	-5.530953	1.773168	3.659078	C	0.301187	5.062653	-0.101183
H	-5.961772	-0.639461	4.133386	C	0.241144	5.322112	-2.603198
C	0.753121	-2.973333	-0.072339	C	-2.156447	1.399883	-0.638872
C	1.406131	-3.211783	-1.290902	C	2.254375	1.149504	-0.722451
C	0.634210	-4.033048	0.843519	C	-2.276297	3.816649	-2.091098

C	2.581429	3.506663	-2.230258	H	4.389169	-0.309817	1.707471
C	-3.343813	1.787630	-1.280997	H	-2.673637	-2.357663	-1.747053
C	3.446409	1.378903	-1.425167	H	-1.508701	2.165739	1.911462
C	-3.399513	2.987927	-1.993395	H	0.929312	-1.798205	2.515307
C	3.601733	2.550100	-2.172767	H	2.683394	-2.612024	-1.537463
C	-3.490138	-1.114208	-0.164571	H	-6.743612	-1.192692	0.888391
C	-1.932707	0.039910	1.952737	H	-2.407904	-1.786524	4.804986
C	1.759590	0.116311	1.938653	H	2.470229	2.663505	4.102686
C	3.397426	-1.361036	0.085906	H	6.510261	-1.570644	1.484578
C	-4.644077	-0.800043	0.577453	H	-4.825495	-3.482160	-2.232057
C	-2.168643	-1.069755	2.785177	H	-1.545433	2.419978	4.369590
C	2.181494	1.374586	2.394169	H	0.881181	-1.261453	4.937657
C	4.479624	-1.082013	0.940123	H	4.815209	-3.854013	-1.766671
C	-3.566458	-2.084236	-1.176901	H	-6.870283	-2.911555	-0.916951
C	-1.704966	1.294162	2.536588	H	-2.017699	0.456650	5.832856
C	1.285208	-0.825673	2.865720	H	1.650677	0.970982	5.742513
C	3.526386	-2.365960	-0.886315	H	6.738211	-3.344515	-0.256475
C	-5.853273	-1.442591	0.305398	Pd	-0.064348	-1.480306	-0.723163
C	-2.210441	-0.918160	4.171127	Br	0.094356	-3.411228	-2.286352
C	2.140056	1.679949	3.758032				
C	5.675283	-1.792753	0.814831	INT4			
C	-4.780983	-2.724474	-1.445908	P	-1.708423	0.837495	0.483101
C	-1.731514	1.438371	3.927013	P	1.755896	-1.089849	0.458445
C	1.257272	-0.522500	4.227052	O	1.119242	1.756566	0.446959
C	4.727810	-3.071481	-1.008829	C	2.386463	4.041719	-0.527614
C	-5.923806	-2.405939	-0.708176	C	0.863720	3.882323	-0.622288
C	-1.993325	0.338343	4.746661	C	3.006884	2.653311	-0.723426
C	1.684155	0.731098	4.676753	C	0.299801	2.712158	-0.092687
C	5.802488	-2.787156	-0.161938	C	2.325210	1.560483	-0.174491
H	-0.551752	5.750618	0.010083	C	2.731516	4.525952	0.907805
H	0.290297	4.359970	0.745305	C	2.921063	5.057164	-1.545808
H	1.234499	5.645424	-0.051319	C	-1.077179	2.460570	-0.095983
H	1.165123	5.917689	-2.571419	C	2.800838	0.247273	-0.243299
H	0.179354	4.826722	-3.583846	C	-0.010437	4.838159	-1.147722
H	-0.594222	6.032405	-2.518301	C	4.223816	2.394879	-1.362339
H	-2.343053	4.738873	-2.669724	C	-1.926165	3.459384	-0.601772
H	2.728819	4.407591	-2.827292	C	4.038265	0.028693	-0.865934
H	-4.219548	1.138499	-1.245094	C	-1.395062	4.637724	-1.123809
H	4.243627	0.633842	-1.400483	C	4.740859	1.096930	-1.424458
H	-4.327733	3.274668	-2.493059	C	-3.220623	0.584263	-0.538553
H	4.529428	2.717638	-2.724853	C	-2.282674	1.162201	2.207005
H	-4.595794	-0.053417	1.373588	C	2.426181	-1.261107	2.171776
H	-2.334363	-2.055896	2.343290	C	2.325682	-2.600973	-0.429329
H	2.550666	2.119193	1.685886	C	-4.391205	0.032724	0.003511

C	-2.692714	0.072164	3.001648	H	-2.613449	3.649755	4.529167
C	3.806900	-1.368471	2.414089	H	1.319148	-1.381498	5.403805
C	2.566760	-3.805127	0.253068	H	2.677856	-3.738009	-3.635442
C	-3.134175	0.785949	-1.931340	H	-6.194870	-0.417207	-2.862824
C	-2.255887	2.448281	2.772574	H	-3.361688	1.718066	5.920758
C	1.537907	-1.265641	3.258635	H	3.771970	-1.589428	5.819654
C	2.363075	-2.587302	-1.839377	H	3.087085	-5.879226	-2.411269
C	-5.451596	-0.329916	-0.832086	Pd	-0.558166	-1.283598	0.453641
C	-3.087027	0.278497	4.325998	Br	0.462595	0.497016	-2.931962
C	4.286658	-1.490817	3.718968	K	-1.188406	-2.056049	-2.869928
C	2.838575	-4.977526	-0.459898	O	-2.840602	-3.049514	-1.240011
C	-4.204285	0.433406	-2.757311	C	-3.128288	-2.852865	-0.046232
C	-2.641566	2.643735	4.102249	O	-2.423184	-2.279843	0.837218
C	2.021272	-1.383059	4.566379	O	-4.336059	-3.277789	0.413950
C	2.638138	-3.762530	-2.542629	H	-4.778805	-3.682602	-0.346336
C	-5.363292	-0.133405	-2.212389				
C	-3.060348	1.562034	4.881597	INT5			
C	3.393954	-1.498044	4.798019	P	0.663249	0.943163	1.208035
C	2.872679	-4.961760	-1.857152	P	-0.594461	-2.111735	-0.544920
H	2.272021	5.508597	1.100401	O	1.615613	-1.847562	1.336309
H	2.358822	3.817896	1.662764	C	4.109931	-3.025970	1.619826
H	3.822796	4.614951	1.029205	C	3.952812	-1.503862	1.744036
H	4.010373	5.171577	-1.447995	C	3.171558	-3.457596	0.484738
H	2.691327	4.749159	-2.576828	C	2.656470	-0.985177	1.620954
H	2.486783	6.052195	-1.371218	C	1.911135	-2.844702	0.438881
H	0.384042	5.760307	-1.576194	C	3.620620	-3.687350	2.937748
H	4.785966	3.211714	-1.816414	C	5.562926	-3.439936	1.360268
H	-3.005714	3.299152	-0.610087	C	2.355368	0.384379	1.690563
H	4.438043	-0.983469	-0.948471	C	0.934540	-3.149579	-0.520895
H	-2.062317	5.403226	-1.526455	C	4.991353	-0.588510	1.966736
H	5.695772	0.916504	-1.923387	C	3.450359	-4.424390	-0.491383
H	-4.473991	-0.147031	1.075174	C	3.422347	1.266126	1.931666
H	-2.710763	-0.936201	2.579758	C	1.240323	-4.140986	-1.466991
H	4.511288	-1.352244	1.579253	C	4.724245	0.779656	2.067169
H	2.541045	-3.830490	1.344914	C	2.491093	-4.765876	-1.452223
H	-2.217893	1.192616	-2.369967	C	0.808273	2.773049	1.247333
H	-1.929858	3.303240	2.177788	C	-0.457731	0.500392	2.580910
H	0.462780	-1.170443	3.080490	C	-1.540725	-2.655390	0.923276
H	2.167403	-1.653504	-2.378350	C	-1.514745	-2.818673	-1.972993
H	-6.348155	-0.775497	-0.394416	C	0.295816	3.570902	2.283682
H	-3.411152	-0.574369	4.928096	C	-1.762357	1.021681	2.528098
H	5.361907	-1.575999	3.896300	C	-1.177236	-3.760285	1.709304
H	3.025051	-5.907876	0.082746	C	-2.400687	-3.898201	-1.833727
H	-4.127698	0.602371	-3.835302	C	1.519887	3.378369	0.196770

C	-0.093171	-0.336090	3.645885	H	-3.025409	-0.311098	5.396885
C	-2.702648	-1.933936	1.234131	H	-3.762145	-3.720656	3.938369
C	-1.307576	-2.254817	-3.243053	H	-3.389417	-4.232746	-5.084948
C	0.493719	4.953999	2.258600	Pd	0.062210	0.085740	-0.934851
C	-2.679827	0.747709	3.542437	C	-5.093156	-1.532229	-1.677939
C	-1.975666	-4.138450	2.792075	C	-4.153463	-0.575383	-2.023828
C	-3.068077	-4.405398	-2.951771	C	-3.968095	0.582807	-1.223972
C	1.726250	4.757668	0.184936	C	-4.784705	0.745801	-0.065647
C	-1.021270	-0.628065	4.649845	C	-5.729453	-0.243298	0.268016
C	-3.502648	-2.322650	2.308598	C	-5.885578	-1.373833	-0.521504
C	-1.975471	-2.764563	-4.358737	C	-3.692907	2.957294	0.358763
C	1.208189	5.549658	1.214037	C	-2.864525	2.775530	-0.796378
C	-2.307007	-0.080951	4.606094	C	-1.957348	3.815343	-1.139921
C	-3.140176	-3.423285	3.090299	H	-1.318031	3.714974	-2.015422
C	-2.858503	-3.840030	-4.214149	C	-1.876926	4.967164	-0.376004
H	4.247044	-3.358999	3.781547	C	-2.687105	5.133681	0.764463
H	2.577675	-3.415306	3.156884	C	-3.581233	4.135195	1.120810
H	3.681289	-4.784198	2.859550	H	-5.213070	-2.416964	-2.306926
H	5.649113	-4.533731	1.285877	H	-3.543215	-0.697923	-2.916478
H	5.957290	-2.996258	0.433041	H	-6.327360	-0.081426	1.167229
H	6.209742	-3.127613	2.192518	H	-6.620560	-2.136470	-0.252306
H	6.020581	-0.938046	2.054219	H	-1.166135	5.745749	-0.659310
H	4.418668	-4.926325	-0.501566	H	-2.606741	6.042920	1.364986
H	3.246719	2.341055	1.961661	H	-4.222656	4.225566	1.999538
H	0.505127	-4.408555	-2.227715	C	-2.965709	1.560413	-1.560559
H	5.544466	1.483878	2.215937	C	-4.640653	1.921291	0.808427
H	2.721775	-5.529577	-2.198540	O	-2.176259	1.252494	-2.582180
H	-0.256114	3.122737	3.110608	O	-5.265748	2.021518	1.874954
H	-2.060152	1.658961	1.695033	H	-1.395737	1.870933	-2.849665
H	-0.274712	-4.329752	1.477784	C	0.967823	2.299427	-2.980151
H	-2.581611	-4.334330	-0.849065	O	-0.182815	2.584344	-3.358717
H	1.960088	2.776412	-0.595873	O	1.949460	3.139557	-3.285674
H	0.911961	-0.756845	3.701840	H	2.802925	2.880016	-2.842637
H	-2.985710	-1.066507	0.637036	O	1.285175	1.244385	-2.307256
H	-0.643450	-1.393246	-3.359529	Br	4.683186	2.462208	-1.620069
H	0.085679	5.568522	3.064914	K	3.377853	-0.240392	-1.769690
H	-3.686052	1.168470	3.475102				
H	-1.687134	-4.997309	3.403579	INT6			
H	-3.761743	-5.241818	-2.834384	P	0.320177	1.027983	1.242392
H	2.298845	5.195251	-0.635542	P	0.055410	-2.187695	-0.610356
H	-0.733325	-1.286066	5.473561	O	1.968809	-1.418966	1.430604
H	-4.402168	-1.747750	2.535896	C	4.655264	-1.904161	1.905079
H	-1.816974	-2.309528	-5.339303	C	4.092854	-0.480918	2.028017
H	1.361044	6.631963	1.203772	C	3.959260	-2.524402	0.686679

C	2.719641	-0.318479	1.797852	H	2.377150	3.032972	2.198293
C	2.587732	-2.265877	0.544803	H	1.864214	-4.010130	-2.277562
C	4.249638	-2.713844	3.167465	H	4.793074	2.803748	2.653827
C	6.181856	-1.915558	1.769129	H	4.293137	-4.493896	-2.089080
C	2.063983	0.919882	1.838084	H	-1.186283	3.026653	2.966110
C	1.803769	-2.771153	-0.502734	H	-2.517948	1.125633	1.598425
C	4.830367	0.668017	2.341560	H	0.806734	-4.435117	1.245669
C	4.562769	-3.329083	-0.289471	H	-1.253755	-4.840332	-1.104133
C	2.836246	2.044819	2.174559	H	1.272410	3.013773	-0.603058
C	2.439180	-3.593051	-1.449058	H	0.825868	-0.529832	3.785951
C	4.203239	1.914678	2.423534	H	-2.511314	-1.728158	0.620510
C	3.808028	-3.860082	-1.343123	H	0.055305	-1.419884	-3.405759
C	0.041244	2.841214	1.183880	H	-1.409681	5.483189	2.778849
C	-0.738647	0.374405	2.582963	H	-4.081368	0.239702	3.281281
C	-0.773679	-3.013642	0.798339	H	-0.424360	-5.499421	3.115053
C	-0.526595	-3.069199	-2.116667	H	-1.990195	-5.958781	-3.196771
C	-0.700576	3.550196	2.141491	H	1.036365	5.441014	-0.790541
C	-2.125346	0.571678	2.451810	H	-0.746362	-1.453956	5.461770
C	-0.189894	-4.074926	1.509864	H	-3.744497	-2.811511	2.455735
C	-1.111191	-4.343169	-2.065896	H	-0.664235	-2.549387	-5.492398
C	0.654419	3.537965	0.126498	H	-0.304425	6.712323	0.912730
C	-0.245965	-0.358720	3.671777	H	-3.196992	-1.062283	5.241683
C	-2.053891	-2.561421	1.153826	H	-2.707826	-4.702702	3.727126
C	-0.366546	-2.428737	-3.358246	H	-1.700069	-4.818737	-5.395741
C	-0.822099	4.938136	2.036270	Pd	-0.281818	0.116722	-0.832895
C	-3.008597	0.072597	3.409321	C	-4.216348	-2.606063	-1.719907
C	-0.885062	-4.676864	2.561867	C	-3.536577	-1.424375	-1.962446
C	-1.528255	-4.969381	-3.244025	C	-3.795294	-0.264061	-1.188858
C	0.538155	4.924264	0.032426	C	-4.785097	-0.333827	-0.163986
C	-1.134692	-0.875717	4.619624	C	-5.450288	-1.552724	0.077655
C	-2.749167	-3.175688	2.196194	C	-5.174588	-2.678779	-0.685243
C	-0.781761	-3.059284	-4.533219	C	-4.461813	2.106976	0.277087
C	-0.204158	5.626460	0.987256	C	-3.442900	2.152986	-0.726095
C	-2.509742	-0.655726	4.495407	C	-2.820607	3.399662	-0.999271
C	-2.166184	-4.230577	2.903521	H	-2.033110	3.453586	-1.748343
C	-1.364803	-4.330194	-4.477490	C	-3.213133	4.548152	-0.334044
H	4.694939	-2.259645	4.066082	C	-4.218826	4.497478	0.654458
H	3.157584	-2.732798	3.296120	C	-4.822475	3.286541	0.958167
H	4.605259	-3.752844	3.084837	H	-4.000715	-3.486141	-2.329981
H	6.557293	-2.945973	1.686473	H	-2.791905	-1.361051	-2.754264
H	6.519544	-1.349675	0.887296	H	-6.188983	-1.569318	0.881890
H	6.653046	-1.477169	2.660428	H	-5.699644	-3.617450	-0.490778
H	5.904755	0.599966	2.515590	H	-2.726735	5.496874	-0.569667
H	5.628426	-3.553658	-0.229829	H	-4.514969	5.408436	1.181053

H	-5.592526	3.204999	1.727984	C	0.060774	-2.126569	-3.634375
C	-3.033653	0.945767	-1.407553	C	-0.974891	4.925688	2.316758
C	-5.107418	0.839543	0.665722	C	-3.446212	0.036055	3.664040
O	-1.965475	0.905365	-2.165999	C	-0.513780	-5.408634	1.641201
O	-5.864039	0.759991	1.647216	C	-1.081168	-4.658210	-3.962759
H	-1.212026	1.933842	-3.033048	C	0.401745	4.820991	0.327788
C	0.629002	2.456471	-3.112014	C	-1.632689	-1.231288	4.646238
O	-0.617458	2.655010	-3.445664	C	-2.185026	-3.719340	2.101867
O	1.389536	3.501305	-3.323586	C	-0.258439	-2.588820	-4.912614
H	2.296040	3.373103	-2.901852	C	-0.281707	5.573091	1.288164
O	1.050887	1.388644	-2.632399	C	-2.990630	-0.898374	4.601247
Br	4.047251	3.218749	-1.608944	C	-1.635368	-4.977248	2.360106
K	3.215372	0.313697	-1.658456	C	-0.833413	-3.853893	-5.079497
				H	4.225046	-2.471640	4.257374
INT7				H	2.859719	-2.943090	3.210118
P	-0.109919	0.936431	1.468781	H	4.417118	-3.799453	3.073338
P	0.220623	-2.190366	-0.875239	H	6.443919	-2.643360	2.094038
O	1.804585	-1.449729	1.409768	H	6.361576	-0.948466	1.542170
C	4.439024	-1.795019	2.183921	H	6.271082	-1.346474	3.277833
C	3.728724	-0.456196	2.425727	H	5.356288	0.645882	3.330368
C	3.974507	-2.274166	0.804432	H	5.846460	-3.000630	-0.009074
C	2.381750	-0.361952	2.026988	H	1.680034	2.829757	2.935615
C	2.611917	-2.118531	0.515730	H	2.417968	-3.514692	-2.573128
C	3.951458	-2.816997	3.248292	H	4.029087	2.707426	3.676801
C	5.964435	-1.670029	2.272822	H	4.855681	-3.766141	-2.143794
C	1.611167	0.803904	2.176098	H	-1.485031	3.040777	3.234129
C	2.014007	-2.560981	-0.675443	H	-2.901937	1.357857	2.059485
C	4.312419	0.670050	3.015974	H	0.931253	-4.926454	0.113989
C	4.777856	-2.866676	-0.181226	H	-0.952522	-4.840063	-1.815362
C	2.233983	1.900759	2.800514	H	0.903636	2.865514	-0.382651
C	2.846088	-3.164463	-1.631572	H	0.324610	-0.929932	3.793627
C	3.564723	1.834800	3.212761	H	-2.045213	-1.905102	0.946684
C	4.217086	-3.302244	-1.388314	H	0.472779	-1.122430	-3.501107
C	-0.294436	2.769065	1.438411	H	-1.512070	5.510217	3.068253
C	-1.177687	0.294039	2.814524	H	-4.501808	0.309919	3.595512
C	-0.501590	-3.320107	0.394237	H	-0.076699	-6.390161	1.842914
C	-0.170904	-2.939127	-2.508185	H	-1.537389	-5.643762	-4.087778
C	-0.970924	3.529865	2.404826	H	0.973246	5.296314	-0.472696
C	-2.542585	0.625779	2.780172	H	-1.272922	-1.964467	5.372608
C	0.051847	-4.584557	0.665581	H	-3.049900	-3.362209	2.664424
C	-0.748992	-4.206880	-2.681133	H	-0.076534	-1.948217	-5.779155
C	0.372250	3.428101	0.388930	H	-0.273051	6.664952	1.237547
C	-0.727793	-0.643060	3.757685	H	-3.693078	-1.368339	5.294403
C	-1.619557	-2.893206	1.126703	H	-2.074514	-5.621635	3.126297

H	-1.097725	-4.208152	-6.079113	C	1.946929	-5.414759	0.753038
Pd	-0.613580	0.040209	-0.608469	C	3.570268	-5.402302	-1.166764
C	-4.249360	-2.802047	-1.044439	C	2.738307	-1.090531	1.232490
C	-3.461031	-1.771718	-1.545337	C	-0.544819	-2.547236	-1.423785
C	-3.585569	-0.466219	-1.030461	C	4.553200	-3.104184	0.427923
C	-4.545321	-0.207650	-0.027307	C	1.066171	-4.592764	-2.534775
C	-5.326226	-1.260142	0.477273	C	4.119711	-0.946455	1.450527
C	-5.178175	-2.551618	-0.021500	C	-0.863183	-3.123272	-2.665920
C	-3.972378	2.257919	-0.148016	C	5.014265	-1.939297	1.048105
C	-2.991668	1.997268	-1.141927	C	-0.056706	-4.120488	-3.220942
C	-2.322272	3.084364	-1.735469	C	2.619055	1.627614	2.070285
H	-1.588932	2.901465	-2.517083	C	0.700019	-0.315324	3.139707
C	-2.586408	4.385788	-1.326648	C	-2.211583	-2.039394	0.842302
C	-3.526814	4.640749	-0.315926	C	-2.921761	-1.063213	-1.802055
C	-4.216147	3.580520	0.260474	C	2.778140	2.089076	3.385564
H	-4.132690	-3.812329	-1.444220	C	-0.190833	0.573542	3.766347
H	-2.730131	-1.955214	-2.332429	C	-2.404618	-3.430740	0.880025
H	-6.050955	-1.027461	1.259679	C	-4.176931	-1.647744	-1.570108
H	-5.787187	-3.366808	0.376806	C	3.332447	2.254227	1.032672
H	-2.043341	5.211999	-1.790662	C	0.869728	-1.598308	3.681298
H	-3.715707	5.665045	0.012790	C	-2.574108	-1.271069	1.958442
H	-4.962776	3.740134	1.040692	C	-2.700252	-0.355097	-2.996980
C	-2.696922	0.604516	-1.535088	C	3.636553	3.161964	3.654239
C	-4.751738	1.168144	0.495662	C	-0.884292	0.198636	4.916692
O	-1.839035	0.280532	-2.435513	C	-2.952378	-4.036788	2.013744
O	-5.526025	1.388197	1.423745	C	-5.192412	-1.531802	-2.523733
H	-0.846187	1.085619	-3.501246	C	4.209319	3.303668	1.307808
C	0.852093	1.932636	-3.379184	C	0.164367	-1.977452	4.827998
O	-0.300516	1.755243	-4.000567	C	-3.132539	-1.876105	3.086157
O	1.409101	3.070813	-3.694989	C	-3.716479	-0.248289	-3.949375
H	2.204787	3.258213	-3.099450	C	4.358074	3.767277	2.620266
O	1.327276	1.105323	-2.595129	C	-0.708811	-1.082035	5.451514
Br	3.638186	3.774909	-1.586024	C	-3.320427	-3.260223	3.117897
K	3.359912	0.797968	-1.028531	C	-4.965642	-0.832914	-3.714385
				H	2.741696	-5.744055	1.440550
INT8				H	1.205351	-4.843856	1.330968
P	1.500198	0.248019	1.576325	H	1.447957	-6.304755	0.338479
P	-1.506801	-1.167710	-0.625472	H	3.092551	-6.299568	-1.586088
O	0.955577	-2.438624	0.417365	H	4.030907	-4.836065	-1.990737
C	2.552316	-4.556607	-0.393002	H	4.369955	-5.754262	-0.499353
C	3.183427	-3.302838	0.219550	H	5.270509	-3.863326	0.114480
C	1.405004	-4.066440	-1.282024	H	1.669999	-5.385841	-2.976870
C	2.307998	-2.286722	0.634693	H	4.500741	-0.038206	1.917547
C	0.600368	-3.035342	-0.770570	H	-1.744565	-2.782346	-3.209006

H	6.084804	-1.799583	1.213644	C	-2.480230	2.667495	2.031932
H	-0.316192	-4.543900	-4.193997	O	-2.458035	2.408331	-2.164160
H	2.236015	1.615910	4.206211	O	-2.486550	2.715590	3.256709
H	-0.354850	1.567703	3.354835	H	-1.470289	2.596256	-3.509483
H	-2.126926	-4.046059	0.021140	C	0.310316	2.178683	-4.025182
H	-4.367614	-2.189120	-0.641762	O	-0.789804	2.894410	-4.171669
H	3.213637	1.941203	-0.009029	O	1.355427	2.782853	-4.535884
H	1.551040	-2.310971	3.214022	H	2.199869	2.416614	-4.132669
H	-2.407907	-0.194058	1.952258	O	0.333877	1.084082	-3.458770
H	-1.730754	0.114587	-3.178731	Br	3.849691	2.018317	-2.730165
H	3.747032	3.518688	4.681704	K	2.077118	-0.429463	-2.298735
H	-1.576682	0.911165	5.370834				
H	-3.093671	-5.120694	2.033918	TS1A			
H	-6.167700	-1.987382	-2.332599	C	-4.144156	0.027428	-1.321161
H	4.758982	3.761171	0.481358	C	-2.920460	0.271382	-0.681321
H	0.300648	-2.982683	5.234989	C	-2.479588	1.602333	-0.606917
H	-3.400093	-1.260168	3.946627	C	-3.209342	2.686332	-1.108553
H	-3.532714	0.312405	-4.869193	C	-4.418698	2.401732	-1.756735
H	5.033129	4.599359	2.836884	C	-4.878582	1.085428	-1.864658
H	-1.258692	-1.385655	6.346063	H	-4.517707	-0.995218	-1.400535
H	-3.746465	-3.736309	4.004858	H	-5.018866	3.211311	-2.173955
H	-5.763013	-0.741032	-4.456457	H	-5.825591	0.882942	-2.370622
Pd	-0.261922	0.718544	0.041117	C	-2.659987	4.088588	-0.821972
C	-5.856368	1.109508	-0.101426	C	-1.132785	4.015621	-0.948266
C	-4.729052	1.518310	-0.813327	C	-0.499557	2.853289	-0.481125
C	-3.606168	2.012394	-0.137017	C	-0.319009	5.045194	-1.434271
C	-3.637287	2.119977	1.271513	C	0.895526	2.679814	-0.485011
C	-4.774992	1.707145	1.977508	C	1.072988	4.916643	-1.429625
C	-5.880344	1.198649	1.295950	H	-0.768241	5.964409	-1.811882
C	-1.311328	3.140105	1.241897	C	1.675014	3.749436	-0.957221
C	-1.238451	2.923142	-0.169140	H	1.695144	5.734279	-1.801221
C	-0.070713	3.353824	-0.844273	H	2.761914	3.659344	-0.971503
H	-0.013826	3.238826	-1.920131	O	-1.265914	1.821756	0.001332
C	0.950409	4.020564	-0.166265	C	-3.268832	5.149597	-1.746694
C	0.832367	4.289696	1.202112	H	-3.045650	4.941064	-2.803943
C	-0.286737	3.839520	1.898554	H	-4.360614	5.192961	-1.623267
H	-6.717215	0.708026	-0.641043	H	-2.885788	6.150390	-1.500082
H	-4.689966	1.442616	-1.899678	C	-3.002237	4.440711	0.653043
H	-4.765563	1.797550	3.065216	H	-2.587592	5.426798	0.916084
H	-6.763255	0.873695	1.851886	H	-4.094200	4.465444	0.796434
H	1.841946	4.319195	-0.721052	H	-2.582281	3.694114	1.343750
H	1.632886	4.811721	1.728981	P	1.613192	1.041452	-0.001010
H	-0.393204	4.013497	2.970662	P	-1.796575	-1.018667	0.002506
C	-2.407547	2.420325	-0.927931	C	-1.928291	-0.706934	1.820550

C	-0.927540	-1.240039	2.648987	Br	1.181572	-2.605871	-2.654780
C	-2.964397	0.042916	2.401150	C	1.971873	-2.454531	-0.578153
C	-0.974037	-1.045113	4.030667	C	3.346761	-2.167855	-0.496798
H	-0.094580	-1.791490	2.207386	C	1.373813	-3.345022	0.336210
C	-3.001858	0.247335	3.783803	C	4.080260	-2.656898	0.583442
H	-3.745478	0.476567	1.772369	H	3.818973	-1.540044	-1.250587
C	-2.009179	-0.299566	4.602219	C	2.125926	-3.812246	1.421982
H	-0.181539	-1.456904	4.658560	H	0.338710	-3.662896	0.199177
H	-3.811160	0.837653	4.222044	C	3.473801	-3.467207	1.556337
H	-2.036114	-0.135671	5.682642	H	5.137562	-2.391893	0.669068
C	-2.770886	-2.569634	-0.226465	H	1.649699	-4.471382	2.153152
C	-3.831012	-2.948307	0.615268	H	4.058673	-3.848403	2.396746
C	-2.413929	-3.405371	-1.298109				
C	-4.526964	-4.136974	0.380796	TS1B			
H	-4.110053	-2.314291	1.459889	P	-1.130853	1.275715	-0.082262
C	-3.116660	-4.591423	-1.533486	P	1.726288	-1.576873	-0.317238
H	-1.572900	-3.131847	-1.940346	O	1.864162	1.371354	0.069126
C	-4.173404	-4.959119	-0.695437	C	3.754990	3.311029	-0.499651
H	-5.348127	-4.424301	1.042950	C	2.261416	3.602476	-0.692165
H	-2.828182	-5.233522	-2.369678	C	3.988550	1.853673	-0.917309
H	-4.717875	-5.889964	-0.874909	C	1.361975	2.582645	-0.347389
C	1.672983	1.107621	1.839943	C	3.007941	0.921742	-0.550163
C	2.290853	0.030062	2.501710	C	4.080552	3.433441	1.015468
C	1.088026	2.129781	2.600505	C	4.641326	4.288690	-1.280555
C	2.353795	-0.001160	3.894377	C	-0.036395	2.735477	-0.408925
H	2.723649	-0.789215	1.924476	C	3.132113	-0.460574	-0.784734
C	1.130436	2.081263	3.998315	C	1.728646	4.820871	-1.128720
H	0.596787	2.969660	2.105255	C	5.128838	1.374763	-1.574328
C	1.770728	1.023865	4.648586	C	-0.527919	3.980492	-0.834907
H	2.846657	-0.840974	4.391331	C	4.299859	-0.901200	-1.427093
H	0.661552	2.879071	4.580085	C	0.345182	5.008512	-1.195085
H	1.806075	0.991846	5.740617	C	5.282341	0.008640	-1.825841
C	3.376451	1.260586	-0.499469	C	-2.823729	1.933871	-0.433400
C	3.687124	0.995739	-1.845290	C	-1.144669	1.144183	1.765360
C	4.404399	1.641773	0.375475	C	1.826589	-1.553402	1.533238
C	4.997345	1.122425	-2.309729	C	2.409985	-3.243906	-0.742615
H	2.894481	0.663886	-2.522919	C	-3.566053	2.728062	0.458662
C	5.720193	1.752862	-0.087946	C	-2.159957	0.372775	2.359708
H	4.181384	1.848477	1.424134	C	2.968608	-1.134561	2.234433
C	6.019475	1.497248	-1.429193	C	3.271516	-3.976936	0.090483
H	5.224424	0.912805	-3.358141	C	-3.401891	1.564654	-1.657795
H	6.514606	2.043790	0.604535	C	-0.154638	1.698196	2.590191
H	7.048304	1.583998	-1.788079	C	0.696325	-1.962865	2.260419
Pd	0.520841	-0.916539	-0.763986	C	2.028333	-3.791253	-1.978531

C	-4.859693	3.139297	0.126627	Pd	-0.271246	-0.656261	-0.957178
C	-2.199237	0.178825	3.740209	C	-3.906119	-1.827626	-2.753704
C	2.981299	-1.133408	3.633263	C	-4.465174	-2.308278	-1.423493
C	3.745562	-5.229226	-0.311116	O	-4.328717	-0.986627	-3.473652
C	-4.694494	1.978773	-1.992497	C	-5.734335	-1.544889	-1.001980
C	-0.186671	1.491605	3.973354	C	-3.377407	-2.245564	-0.334197
C	0.714277	-1.972428	3.655609	H	-4.712144	-3.374434	-1.595168
C	2.512387	-5.037860	-2.385002	C	-6.258998	-2.053827	0.345687
C	-5.426288	2.765713	-1.098559	H	-6.502710	-1.632576	-1.786771
C	-1.208477	0.738361	4.554936	H	-5.485892	-0.473171	-0.924327
C	1.856548	-1.556167	4.346689	C	-3.910649	-2.725755	1.019766
C	3.370701	-5.760535	-1.549959	H	-2.494846	-2.829245	-0.640403
H	3.877603	4.456931	1.368608	H	-3.034967	-1.201193	-0.246282
H	3.470590	2.735518	1.608032	C	-5.180164	-1.968872	1.432947
H	5.141606	3.199802	1.197151	H	-6.586753	-3.104704	0.239027
H	5.705591	4.072658	-1.107900	H	-7.151199	-1.477205	0.642384
H	4.446324	4.237973	-2.362443	H	-4.135660	-3.806661	0.961488
H	4.472093	5.321912	-0.944215	H	-3.124705	-2.609511	1.784714
H	2.392477	5.638058	-1.412941	H	-4.933539	-0.905212	1.605138
H	5.912011	2.066967	-1.885327	H	-5.565173	-2.359095	2.389947
H	-1.604983	4.140145	-0.903578				
H	4.435932	-1.965239	-1.627602	TS2A			
H	-0.057311	5.966564	-1.532733	C	2.581669	1.502012	2.669902
H	6.179767	-0.352424	-2.333955	C	1.996180	0.479073	1.910323
H	-3.134541	3.016935	1.419899	C	1.036574	-0.325136	2.534906
H	-2.935650	-0.071805	1.735386	C	0.675884	-0.209125	3.878411
H	3.854218	-0.801737	1.688266	C	1.289477	0.812736	4.611415
H	3.572182	-3.569560	1.058295	C	2.222698	1.663895	4.010382
H	-2.842630	0.925806	-2.345990	H	3.289927	2.189546	2.206677
H	0.650976	2.294335	2.161631	H	1.030956	0.963887	5.659916
H	-0.212036	-2.250898	1.725063	H	2.672600	2.470038	4.594139
H	1.340257	-3.231405	-2.619513	C	-0.337730	-1.224476	4.419021
H	-5.430934	3.752076	0.829241	C	-1.372855	-1.470709	3.311779
H	-3.004794	-0.416284	4.179086	C	-0.920091	-1.480769	1.983904
H	3.875512	-0.798824	4.166177	C	-2.732821	-1.717172	3.526984
H	4.411668	-5.793253	0.347398	C	-1.755117	-1.686182	0.875278
H	-5.130382	1.654145	-2.939817	C	-3.587266	-1.980828	2.452129
H	0.598892	1.923529	4.598435	H	-3.135660	-1.710731	4.540202
H	-0.177880	-2.280174	4.205173	C	-3.107622	-1.964557	1.141269
H	2.210436	-5.450232	-3.351331	H	-4.644261	-2.185963	2.636271
H	-6.442072	3.081894	-1.350237	H	-3.799266	-2.140925	0.318301
H	-1.229140	0.580111	5.636149	O	0.405352	-1.245371	1.729403
H	1.864209	-1.548350	5.439750	C	-0.993941	-0.738286	5.717002
H	3.742441	-6.740403	-1.861037	H	-1.538527	0.204509	5.557796

H	-0.237331	-0.577839	6.498641	C	-4.788258	-0.579339	-2.523918
H	-1.694593	-1.489358	6.109421	H	-3.202523	0.528663	-1.586217
C	0.411029	-2.559165	4.685341	C	-4.373208	-2.931848	-2.882526
H	-0.292549	-3.329382	5.039104	H	-2.489021	-3.688467	-2.171187
H	1.190823	-2.413909	5.449693	C	-5.211989	-1.820553	-3.007161
H	0.893629	-2.929663	3.768224	H	-5.428892	0.300554	-2.623971
P	-1.102386	-1.373921	-0.841452	H	-4.694488	-3.907790	-3.255634
P	2.199601	0.191086	0.112148	H	-6.191085	-1.921403	-3.482728
C	2.791716	-1.557167	-0.016178	C	1.000165	2.684013	-1.017975
C	2.991640	-2.063376	-1.309141	C	1.002794	3.335138	0.225554
C	3.174390	-2.331644	1.088239	C	1.421416	3.403386	-2.148121
C	3.580053	-3.314356	-1.494881	C	1.426917	4.668004	0.337515
H	2.691316	-1.471705	-2.177602	H	0.679828	2.821381	1.130421
C	3.752575	-3.590264	0.899319	C	1.852410	4.728515	-2.032622
H	3.036652	-1.955165	2.103188	H	1.396106	2.936526	-3.133782
C	3.962806	-4.081959	-0.391163	C	1.859881	5.368894	-0.788581
H	3.725044	-3.696721	-2.507043	H	1.417528	5.150328	1.319673
H	4.046237	-4.184776	1.768523	H	2.176507	5.266884	-2.928286
H	4.417633	-5.064832	-0.537807	H	2.195415	6.405864	-0.701814
C	3.796721	0.984588	-0.362289	Br	-1.125213	1.486726	-3.073559
C	4.914456	0.938184	0.489952	Pd	0.267503	0.771418	-1.089519
C	3.954828	1.478233	-1.664224	C	-1.589286	1.600593	1.589413
C	6.149558	1.428955	0.062559	C	-2.992777	1.763051	1.057991
H	4.829811	0.500507	1.486433	O	-1.153618	1.951332	2.635917
C	5.194748	1.959264	-2.094032	C	-4.031160	1.931462	2.180320
H	3.106240	1.485138	-2.346198	C	-3.011223	2.953515	0.070711
C	6.291114	1.948115	-1.228949	H	-3.220596	0.847218	0.491775
H	7.007715	1.396197	0.738768	C	-5.432142	2.126741	1.588999
H	5.297958	2.348715	-3.109771	H	-4.004135	1.052943	2.845193
H	7.258497	2.332593	-1.562292	H	-3.749740	2.805786	2.792619
C	-0.226559	-2.915180	-1.323787	C	-4.421787	3.154231	-0.496308
C	0.133576	-3.032390	-2.678927	H	-2.285784	2.787204	-0.739673
C	0.057115	-3.965306	-0.442319	H	-2.691827	3.863475	0.609004
C	0.722811	-4.205327	-3.150246	C	-5.469677	3.310372	0.612989
H	-0.072215	-2.207225	-3.367366	H	-5.729032	1.204704	1.055143
C	0.668813	-5.130841	-0.915609	H	-6.167275	2.269514	2.399151
H	-0.206458	-3.881591	0.613692	H	-4.684292	2.284774	-1.125365
C	0.987355	-5.260241	-2.269383	H	-4.427113	4.030401	-1.164841
H	0.981714	-4.294583	-4.208405	H	-5.269075	4.243349	1.171615
H	0.892851	-5.943006	-0.219739	H	-6.477579	3.416393	0.177584
H	1.454885	-6.177288	-2.636794				
C	-2.684469	-1.559506	-1.790141	TS2B			
C	-3.532968	-0.449175	-1.926308	C	-2.460009	2.572106	2.143633
C	-3.120311	-2.804854	-2.274355	C	-1.740820	2.026476	1.070521

C	-0.584989	2.708071	0.652983	C	-4.747658	-1.080109	3.028585
C	-0.145952	3.905723	1.232479	H	-2.619496	-0.752270	2.807302
C	-0.879657	4.404961	2.316109	C	-6.009789	-0.965598	2.433577
C	-2.023030	3.741953	2.769353	H	-7.108377	-0.310755	0.688562
H	-3.360585	2.070599	2.500435	H	-4.647113	-1.522463	4.023336
H	-0.565992	5.325780	2.808358	H	-6.900033	-1.318511	2.960788
H	-2.585669	4.146289	3.613984	C	0.767569	-0.019530	-3.009785
C	1.046904	4.614392	0.580781	C	0.424334	-1.143260	-3.785746
C	2.031270	3.534965	0.117925	C	0.484414	1.261577	-3.511081
C	1.496275	2.341113	-0.387072	C	-0.154061	-0.984321	-5.046175
C	3.423506	3.678071	0.099519	H	0.618061	-2.147970	-3.404955
C	2.286824	1.300814	-0.905559	C	-0.107026	1.414673	-4.767330
C	4.238894	2.669960	-0.422870	H	0.723861	2.148127	-2.923455
H	3.883405	4.586039	0.490522	C	-0.419806	0.295655	-5.543200
C	3.678018	1.493926	-0.922823	H	-0.403123	-1.867792	-5.639934
H	5.323396	2.800830	-0.435271	H	-0.327635	2.418398	-5.138598
H	4.328274	0.708786	-1.310183	H	-0.880377	0.419822	-6.526549
O	0.137352	2.146063	-0.375590	C	2.936227	-1.376876	-1.661392
C	1.705796	5.626447	1.527179	C	3.427294	-2.135082	-0.586089
H	2.094379	5.137687	2.433602	C	3.599967	-1.441779	-2.898043
H	0.988072	6.402374	1.829411	C	4.562483	-2.935572	-0.736681
H	2.535836	6.146998	1.028228	H	2.909875	-2.097901	0.373873
C	0.525352	5.358176	-0.680249	C	4.727413	-2.254007	-3.052299
H	1.358696	5.847050	-1.209416	H	3.235070	-0.856350	-3.744565
H	-0.211919	6.124614	-0.393279	C	5.212788	-3.000422	-1.973104
H	0.037821	4.658514	-1.375987	H	4.932489	-3.516638	0.111955
P	1.470299	-0.303838	-1.331990	H	5.231720	-2.301021	-4.021113
P	-2.160396	0.436835	0.231419	H	6.094780	-3.633983	-2.097297
C	-2.725893	0.998119	-1.429723	C	-0.538819	-3.287612	0.858241
C	-2.812872	0.032697	-2.447116	C	-1.616100	-3.373883	1.760859
C	-3.074615	2.327840	-1.717098	C	0.686955	-3.924988	1.143013
C	-3.263038	0.388008	-3.719769	C	-1.400291	-3.933159	3.018821
H	-2.515363	-0.998349	-2.244964	H	-2.587422	-2.960132	1.490093
C	-3.509294	2.682779	-2.997593	C	0.878603	-4.487048	2.405482
H	-3.011012	3.090199	-0.937568	H	1.477054	-3.945841	0.391649
C	-3.610349	1.713015	-3.999490	C	-0.152728	-4.477309	3.355346
H	-3.318760	-0.371622	-4.502216	H	-2.217443	-3.940481	3.745326
H	-3.775724	3.721676	-3.210340	H	1.845530	-4.935883	2.650079
H	-3.949697	1.991604	-5.000583	H	0.006636	-4.916867	4.342701
C	-3.721034	-0.065606	1.071907	Br	-1.091543	-3.267663	-1.231208
C	-4.989582	0.052499	0.482239	Pd	-0.243953	-1.134873	0.280678
C	-3.607140	-0.643285	2.351736	C	0.372919	-0.535016	2.144928
C	-6.126250	-0.401465	1.160242	C	1.815223	-0.049781	2.354780
H	-5.093615	0.495655	-0.510058	O	-0.393081	-0.560071	3.077395

C	1.855478	1.259418	3.162356	H	0.869709	6.121814	0.839017
C	2.623787	-1.150469	3.069173	H	1.693065	4.549985	0.999672
H	2.277868	0.132700	1.376776	P	2.106141	-0.259323	-0.437117
C	3.302032	1.715949	3.381812	P	-1.290207	0.346965	1.378223
H	1.279698	2.039591	2.641732	C	-0.229501	0.510583	2.879217
H	1.350588	1.087471	4.127833	C	0.561142	-0.578086	3.278924
C	4.073378	-0.698924	3.281791	C	-0.225983	1.685826	3.650377
H	2.581272	-2.088805	2.494732	C	1.328015	-0.494623	4.444287
H	2.141796	-1.365066	4.038637	H	0.594452	-1.492599	2.680980
C	4.142096	0.623877	4.057473	C	0.555400	1.767649	4.804433
H	3.748307	1.970658	2.404303	H	-0.835724	2.541022	3.352698
H	3.319376	2.641445	3.983126	C	1.331380	0.675501	5.206049
H	4.556678	-0.570299	2.295389	H	1.942962	-1.347146	4.738754
H	4.641199	-1.483934	3.809773	H	0.555656	2.688632	5.393474
H	3.760837	0.457441	5.081915	H	1.946127	0.741774	6.107419
H	5.189906	0.953148	4.161802	C	-2.901286	-0.230789	2.077339
				C	-2.934728	-0.980442	3.264867
				C	-4.104041	-0.056104	1.362774
TS3				C	-4.133999	-1.530085	3.727471
C	-2.818089	2.825677	1.197083	H	-2.019116	-1.144185	3.834944
C	-1.627852	2.120480	0.957976	C	-5.302863	-0.594176	1.834090
C	-0.590552	2.816408	0.317956	H	-4.111884	0.493487	0.419366
C	-0.719520	4.118280	-0.182423	C	-5.322411	-1.336603	3.019181
C	-1.943911	4.764129	0.026172	H	-4.134708	-2.114277	4.651062
C	-2.972676	4.133436	0.731166	H	-6.222859	-0.441689	1.264058
H	-3.632140	2.355421	1.747355	H	-6.258539	-1.765829	3.384655
H	-2.096682	5.778250	-0.344688	C	3.076509	0.065299	1.099321
H	-3.908927	4.665034	0.915908	C	3.616243	-1.043676	1.778195
C	0.507234	4.757791	-0.842737	C	3.280191	1.349577	1.627485
C	1.296907	3.646678	-1.547077	C	4.360638	-0.862411	2.944439
C	1.361871	2.395538	-0.921798	H	3.443157	-2.050456	1.394877
C	2.034717	3.804835	-2.726897	C	4.013399	1.522836	2.804798
C	2.166508	1.338585	-1.366613	H	2.876383	2.227553	1.125752
C	2.818983	2.759733	-3.224736	C	4.561228	0.419991	3.463790
H	2.009444	4.753613	-3.263819	H	4.778631	-1.734415	3.454084
C	2.898926	1.541155	-2.546242	H	4.157458	2.529749	3.204638
H	3.384089	2.900236	-4.148959	H	5.138126	0.559153	4.381748
H	3.522115	0.738945	-2.942807	C	3.256633	-1.304944	-1.429637
O	0.597321	2.147417	0.193252	C	2.731100	-2.199669	-2.374438
C	0.115435	5.884564	-1.808145	C	4.651487	-1.184006	-1.301511
H	-0.529501	5.513164	-2.618994	C	3.587120	-2.963330	-3.172718
H	-0.416574	6.688310	-1.279607	H	1.652914	-2.291379	-2.501975
H	1.008760	6.343900	-2.254837	C	5.503304	-1.953425	-2.097605
C	1.406899	5.336067	0.284551	H	5.077864	-0.489724	-0.574909
H	2.326594	5.766721	-0.141772				

C	4.972786	-2.847122	-3.033703	C	-0.799912	-2.508263	-0.854029
H	3.163481	-3.657874	-3.902311	C	-2.509486	-0.931193	-1.018997
H	6.586027	-1.854586	-1.983874	C	-3.703533	-3.849451	-0.822011
H	5.640078	-3.452385	-3.652965	C	-3.380822	-3.834409	-3.318947
C	-1.678782	-2.635272	-1.019969	C	0.567131	-2.558046	-0.553124
C	-2.961647	-2.655523	-0.460401	C	-2.730965	0.429818	-0.786905
C	-1.245428	-3.760358	-1.744185	C	-0.640406	-4.403224	-2.305098
C	-3.785111	-3.781030	-0.588509	C	-4.159010	-1.006883	-2.738664
H	-3.336116	-1.799962	0.091926	C	1.314563	-3.613007	-1.105015
C	-2.061555	-4.883327	-1.875483	C	-3.700622	1.073698	-1.564666
H	-0.263163	-3.748336	-2.219752	C	0.712735	-4.529626	-1.966987
C	-3.335837	-4.899709	-1.293280	C	-4.400227	0.356975	-2.540361
H	-4.777892	-3.775917	-0.129823	C	3.027711	-1.144094	-0.303767
H	-1.702504	-5.750932	-2.435666	C	1.470373	-1.820116	2.122163
H	-3.975563	-5.780392	-1.395964	C	-2.335579	0.421695	2.045254
Br	1.060588	-3.407656	0.803384	C	-2.273064	2.946243	0.544764
Pd	-0.117688	-1.323523	-0.290870	C	4.188964	-1.107902	0.480208
C	-1.042284	-0.949718	-2.103718	C	1.999080	-0.963878	3.109705
C	-2.184922	0.057609	-2.189530	C	-3.678124	0.025541	2.169214
O	-0.364368	-1.232673	-3.060177	C	-3.056005	3.471413	1.585057
C	-3.314553	-0.438437	-3.112125	C	3.140157	-1.014232	-1.703439
C	-1.632653	1.399530	-2.702235	C	0.957347	-3.071205	2.500427
H	-2.600713	0.202384	-1.183484	C	-1.447039	0.170230	3.101760
C	-4.431644	0.610103	-3.189792	C	-1.865133	3.788491	-0.509067
H	-3.705245	-1.399371	-2.745906	C	5.440815	-0.936108	-0.119831
H	-2.890718	-0.621842	-4.114343	C	2.029069	-1.372036	4.444832
C	-2.740088	2.453176	-2.774862	C	-4.119774	-0.610939	3.332009
H	-0.813802	1.738072	-2.057185	C	-3.433031	4.818298	1.569072
H	-1.191907	1.233125	-3.699339	C	4.396169	-0.875242	-2.299041
C	-3.905330	1.976209	-3.651273	C	0.974978	-3.464158	3.842485
H	-4.893084	0.716873	-2.189559	C	-1.888396	-0.472767	4.261459
H	-5.231345	0.257961	-3.862658	C	-2.256301	5.128753	-0.522823
H	-3.102749	2.664746	-1.753822	C	5.552158	-0.825258	-1.507628
H	-2.329523	3.403109	-3.156866	C	1.512376	-2.619020	4.816982
H	-3.557615	1.890225	-4.697089	C	-3.224951	-0.864611	4.378270
H	-4.718939	2.721141	-3.650842	C	-3.038085	5.648063	0.515877
				H	-3.500281	-4.931626	-0.784981
TS4				H	-3.403782	-3.408116	0.140222
P	1.325517	-1.175594	0.407028	H	-4.787260	-3.696538	-0.946745
P	-1.680270	1.205260	0.508880	H	-4.461615	-3.696089	-3.467580
O	-1.537031	-1.527234	-0.253419	H	-2.851800	-3.399529	-4.180311
C	-2.929351	-3.194740	-1.999901	H	-3.202364	-4.919550	-3.310107
C	-1.427003	-3.389778	-1.749289	H	-1.082017	-5.113130	-3.005645
C	-3.209433	-1.685931	-1.964285	H	-4.726687	-1.542259	-3.501065

H	2.379748	-3.694950	-0.881516	C	-2.095136	-0.899180	1.769573
H	-3.897209	2.137154	-1.419764	C	-1.709516	2.841512	-0.508835
H	1.305567	-5.340456	-2.396756	C	-4.866724	-0.603597	2.217126
H	-5.145384	0.867907	-3.154534	C	-4.465954	3.430680	-0.364683
H	4.125166	-1.184626	1.565684	C	-2.891724	-2.011510	2.088805
H	2.371862	0.025450	2.826939	C	-2.304466	3.697082	-1.450418
H	-4.378104	0.206064	1.349680	C	-4.261472	-1.859821	2.309604
H	-3.372542	2.830905	2.410807	C	-3.672783	3.978028	-1.380691
H	2.240242	-1.003163	-2.324231	C	-0.060213	-2.841206	1.176180
H	0.533055	-3.740197	1.748898	C	0.704513	-0.351850	2.519346
H	-0.397310	0.456318	3.005065	C	0.837039	3.001145	0.873689
H	-1.243807	3.386356	-1.316481	C	0.689504	3.183604	-2.021240
H	6.333596	-0.891148	0.508871	C	0.738574	-3.510773	2.117211
H	2.448016	-0.702980	5.201025	C	2.092479	-0.541929	2.396962
H	-5.165647	-0.917352	3.418789	C	0.234393	4.012576	1.639393
H	-4.040260	5.218937	2.385103	C	1.272394	4.452310	-1.882363
H	4.471516	-0.807902	-3.389094	C	-0.724696	-3.581677	0.181744
H	0.564981	-4.437304	4.125297	C	0.201175	0.359756	3.618009
H	-1.175887	-0.681904	5.062985	C	2.132709	2.568035	1.192468
H	-1.941918	5.773129	-1.348067	C	0.585263	2.608821	-3.299272
H	6.533937	-0.705249	-1.973327	C	0.868506	-4.900337	2.054788
H	1.525660	-2.928852	5.865304	C	2.965103	-0.067764	3.376637
H	-3.570447	-1.374637	5.281438	C	0.928073	4.586975	2.707643
H	-3.335945	6.699876	0.505693	C	1.744442	5.134181	-3.007546
Pd	0.634917	1.144273	0.364444	C	-0.597022	-4.969326	0.129939
Br	0.358333	1.490081	-2.730992	C	1.079427	0.856955	4.585404
K	3.214114	2.491345	-2.479482	C	2.826840	3.156442	2.250240
O	4.114634	2.489378	-0.167588	C	1.056119	3.293057	-4.422172
C	3.743916	1.997708	0.916667	C	0.204272	-5.631375	1.065300
O	2.590783	1.634144	1.263097	C	2.455259	0.635373	4.473445
O	4.694079	1.799298	1.882572	C	2.226473	4.163665	3.010574
H	5.524762	2.115958	1.498923	C	1.638717	4.556921	-4.277295
				H	-4.735267	2.300367	3.962072
TS5				H	-3.170865	2.758412	3.238890
P	-0.348289	-1.027399	1.186314	H	-4.597080	3.802655	2.999980
P	0.035141	2.236891	-0.583289	H	-6.521953	3.039074	1.538170
O	-1.950888	1.439788	1.381224	H	-6.484223	1.450441	0.723930
C	-4.641375	1.967483	1.798824	H	-6.665719	1.562263	2.493657
C	-4.104202	0.534789	1.923515	H	-5.943552	-0.519242	2.367264
C	-3.902688	2.593756	0.608667	H	-5.529619	3.669407	-0.330227
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C	-4.259316	2.757539	3.080833	H	-4.870007	-2.740466	2.522270
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H	1.260763	-2.958615	2.898889	O	5.768153	-0.914724	1.691149
H	2.493594	-1.077509	1.536315	H	1.426128	-1.868580	-2.786921
H	-0.774540	4.357736	1.403843	C	-0.543074	-2.533711	-2.927275
H	1.370203	4.903569	-0.892939	O	0.669132	-2.696861	-3.261724
H	-1.390426	-3.089573	-0.526370	O	-1.363327	-3.523699	-3.216787
H	-0.871802	0.525920	3.726394	H	-2.260803	-3.382828	-2.794692
H	2.602641	1.770648	0.616790	O	-0.990798	-1.498767	-2.341281
H	0.158284	1.607913	-3.416465	Br	-4.115508	-3.209317	-1.569454
H	1.500449	-5.411998	2.784448	K	-3.253605	-0.325730	-1.710969
H	4.038426	-0.237293	3.259094				
H	0.453137	5.371184	3.302849	TS6			
H	2.203760	6.118925	-2.890115	P	-0.539355	-1.203166	-1.107279
H	-1.133210	-5.518783	-0.646721	P	1.543468	1.673251	0.176737
H	0.682142	1.417836	5.435049	O	2.330615	-0.501270	-1.509327
H	3.835400	2.809148	2.480817	C	4.670136	-1.967990	-1.879327
H	0.980953	2.831243	-5.409540	C	3.306281	-2.666900	-1.778686
H	0.313011	-6.718162	1.022960	C	4.639624	-0.781224	-0.909383
H	3.134346	1.022296	5.237375	C	2.169350	-1.851397	-1.642010
H	2.767987	4.615348	3.845602	C	3.438568	-0.075686	-0.806360
H	2.016731	5.088568	-5.154065	C	4.816106	-1.412418	-3.323188
Pd	0.071779	-0.063820	-0.950435	C	5.833733	-2.922900	-1.587144
C	4.267189	2.481608	-1.709484	C	0.853754	-2.345678	-1.598335
C	3.585957	1.307073	-1.981489	C	3.259968	1.042475	0.013438
C	3.801843	0.142032	-1.201200	C	3.100569	-4.048388	-1.875087
C	4.750951	0.201800	-0.139157	C	5.719135	-0.312648	-0.148030
C	5.421184	1.411653	0.129757	C	0.691788	-3.737539	-1.748803
C	5.186572	2.542473	-0.640088	C	4.362381	1.494636	0.748721
C	4.388829	-2.238247	0.275980	C	1.803654	-4.577056	-1.872892
C	3.414819	-2.278639	-0.774307	C	5.582729	0.818755	0.663031
C	2.813202	-3.529198	-1.082509	C	-1.919347	-2.432528	-1.076618
H	2.070309	-3.595095	-1.874887	C	-0.949131	-0.205901	-2.587960
C	3.173924	-4.677402	-0.398883	C	1.194538	2.484337	-1.427488
C	4.128920	-4.629413	0.637306	C	1.735230	3.104740	1.325199
C	4.717407	-3.418861	0.969899	C	-2.641216	-2.793066	-2.227701
H	4.082414	3.364797	-2.325022	C	-2.191322	0.450406	-2.550416
H	2.878583	1.253621	-2.806789	C	2.180144	2.741746	-2.393038
H	6.131194	1.417253	0.959471	C	1.996479	4.397853	0.841117
H	5.713821	3.475065	-0.424007	C	-2.160586	-3.121714	0.119450
H	2.701005	-5.625877	-0.661929	C	-0.121902	-0.058822	-3.708518
H	4.399847	-5.540943	1.176190	C	-0.118611	2.929628	-1.640426
H	5.453311	-3.338345	1.772369	C	1.610270	2.901726	2.709625
C	3.060285	-1.067046	-1.471743	C	-3.567067	-3.838541	-2.177176
C	5.036647	-0.980039	0.690528	C	-2.624707	1.216721	-3.630958
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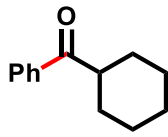
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H	4.796610	-2.234585	-4.055931	C	-5.603070	-1.902187	0.754463
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H	5.768554	-0.869141	-3.424953	C	-5.935188	-0.020366	-0.726903
H	6.795998	-2.399354	-1.679337	H	-0.716663	4.679213	2.091913
H	5.766662	-3.346022	-0.573179	H	-1.163442	2.297253	2.637475
H	5.856405	-3.749923	-2.311695	H	-3.774401	4.522791	-0.973791
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H	-0.308464	-4.171250	-1.747750	H	-7.160718	-1.793691	-0.760791
H	4.256477	2.357801	1.407839	H	-6.462319	0.493009	-1.533771
H	1.656330	-5.654257	-1.984619	C	-2.951632	0.668749	1.488863
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H	-2.478885	-2.262933	-3.167613	O	-2.104994	0.063086	2.270673
H	-2.832607	0.348703	-1.674357	O	-5.045492	2.496300	-1.6282+8
H	3.205370	2.399540	-2.236439	K	1.121525	-3.632341	1.839576
H	2.086883	4.575622	-0.231721	O	-0.235771	-3.424514	4.066678
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H	-0.894493	2.712342	-0.906067	H	-2.041793	-1.184222	2.798893
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H	-4.127485	-4.105071	-3.076900	H	-0.049307	-1.553422	5.399260
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H	-1.460865	3.999054	-2.934545	C	-3.830924	-2.927835	-2.008971
H	1.634208	3.806633	4.666007	C	-3.732018	-1.397639	-1.991795
H	-4.502304	-5.359689	-0.953444	C	-2.991019	-3.419174	-0.826005
H	-2.129838	1.952159	-5.605369	C	-2.470257	-0.842386	-1.720905
H	0.298321	4.481663	-4.647843	C	-1.757163	-2.779661	-0.619697
H	2.087347	6.104496	3.797213	C	-3.185738	-3.454225	-3.321079
Pd	0.096242	-0.064050	0.904378	C	-5.281431	-3.418597	-1.936680
Br	1.838670	-0.761247	2.862252	C	-2.224904	0.544772	-1.712162
C	-1.485154	4.129553	1.544725	C	-0.854192	-3.159191	0.393538

C	-4.793338	-0.519103	-2.241457	H	0.919674	-4.798135	-0.840702
C	-3.341955	-4.458718	0.045966	H	2.655368	-4.490594	1.059564
C	-3.317202	1.385390	-1.985952	H	-1.766389	2.787627	0.853181
C	-1.236660	-4.219953	1.232400	H	-0.825336	-0.423358	-3.754522
C	-4.584653	0.861122	-2.238447	H	2.544378	-0.811022	-1.178496
C	-2.471668	-4.853844	1.067277	H	0.443230	-1.584823	3.370268
C	-0.907074	3.022521	-1.129694	H	-0.684772	5.998870	-2.791051
C	0.471978	0.966387	-2.707273	H	3.603877	1.861978	-3.749593
C	1.668497	-2.760652	-0.851786	H	2.223097	-5.496107	-2.830610
C	1.454203	-3.000643	2.076097	H	3.649026	-5.392878	3.146761
C	-0.613119	3.937462	-2.152334	H	-2.363214	5.154308	1.105658
C	1.727136	1.599235	-2.734117	H	0.776411	-0.849118	-5.584313
C	1.574696	-4.077463	-1.336779	H	3.843762	-1.504679	-3.163038
C	2.368173	-4.064126	2.022547	H	1.395235	-2.530242	5.464807
C	-1.518387	3.483930	0.049639	H	-1.808825	6.796153	-0.711663
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C	2.490109	-1.844216	-1.524159	H	3.694530	-3.856619	-4.003360
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C	-0.923766	5.291973	-1.991930	Pd	0.348240	0.128567	0.598246
C	2.631632	1.363840	-3.769815	C	4.834754	-1.594764	1.122264
C	2.304661	-4.470286	-2.461434	C	3.897141	-0.715403	1.660383
C	2.930931	-4.570067	3.199651	C	3.690950	0.543750	1.076489
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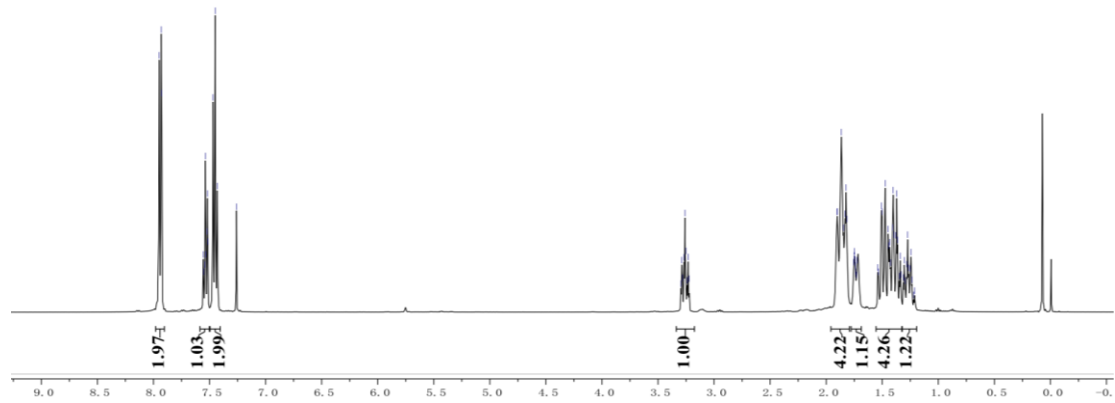
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O	-1.273040	0.617164	3.097394
Br	-4.538251	1.938065	1.821123
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NMR Spectra

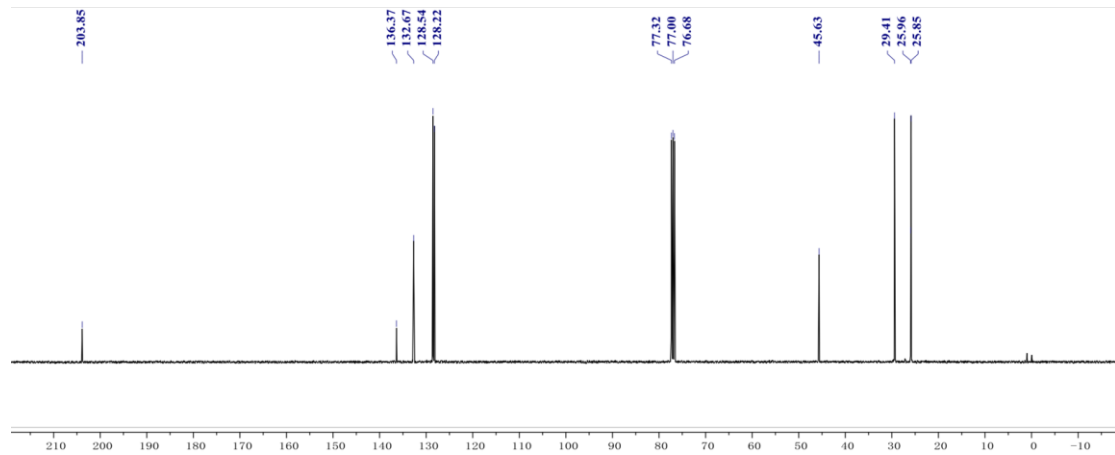
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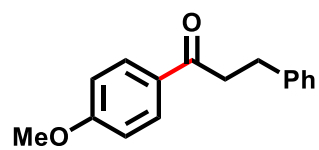
^1H NMR



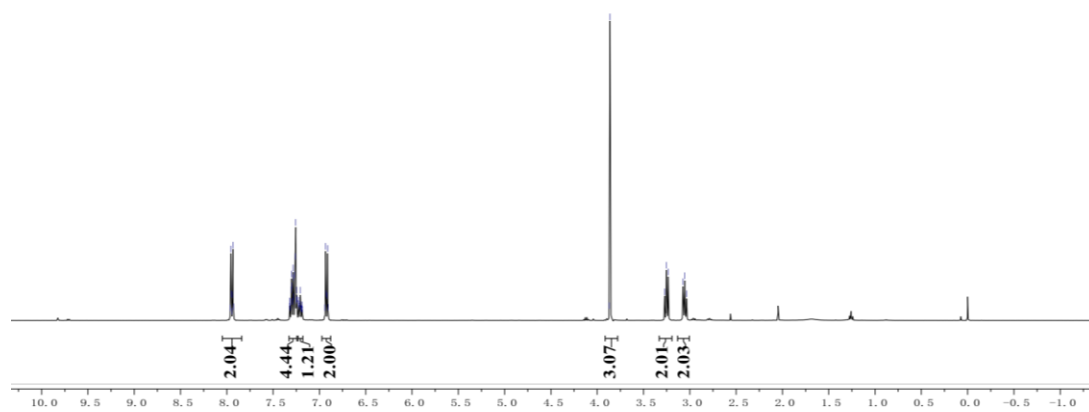
^{13}C NMR



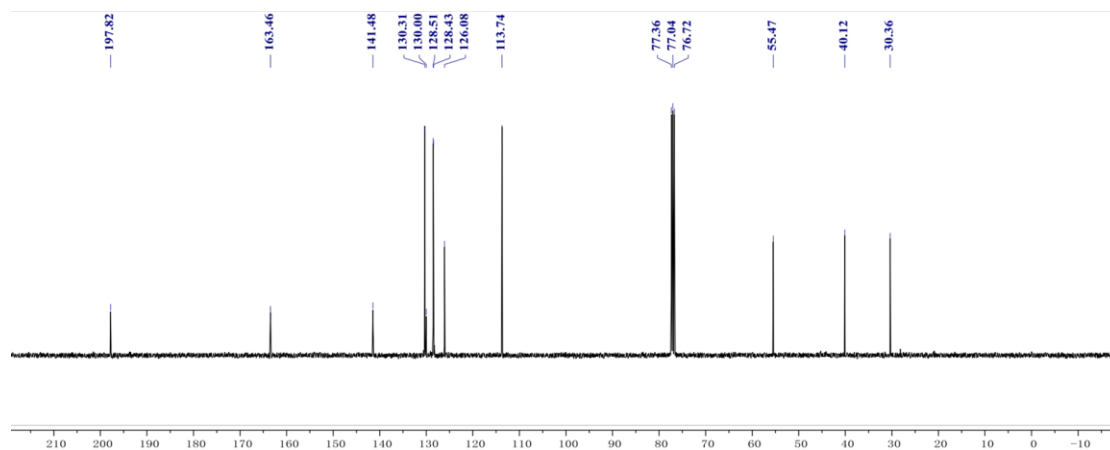
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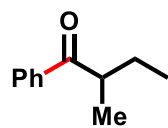
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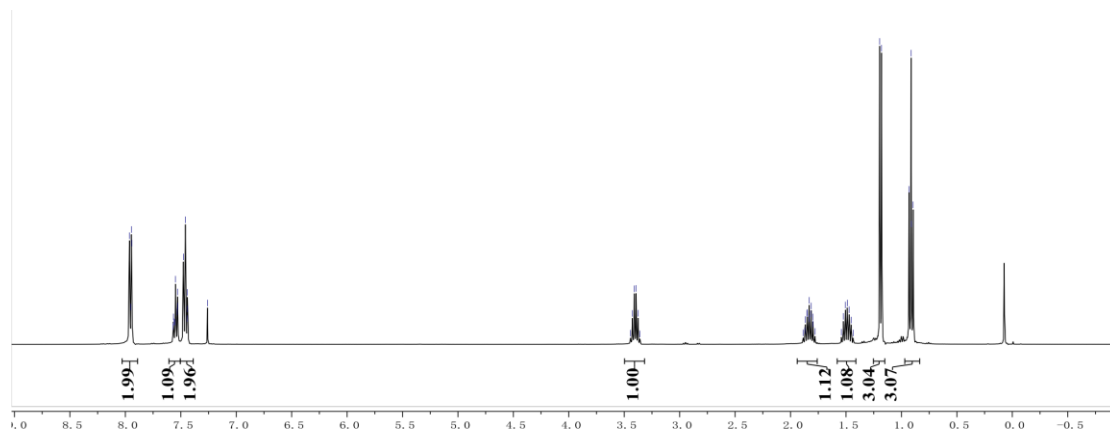
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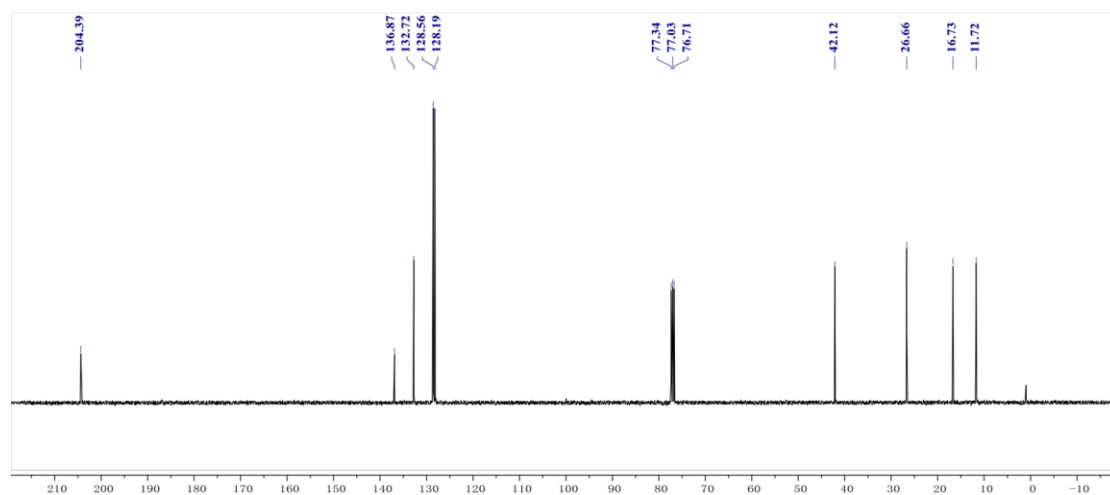
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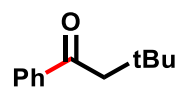
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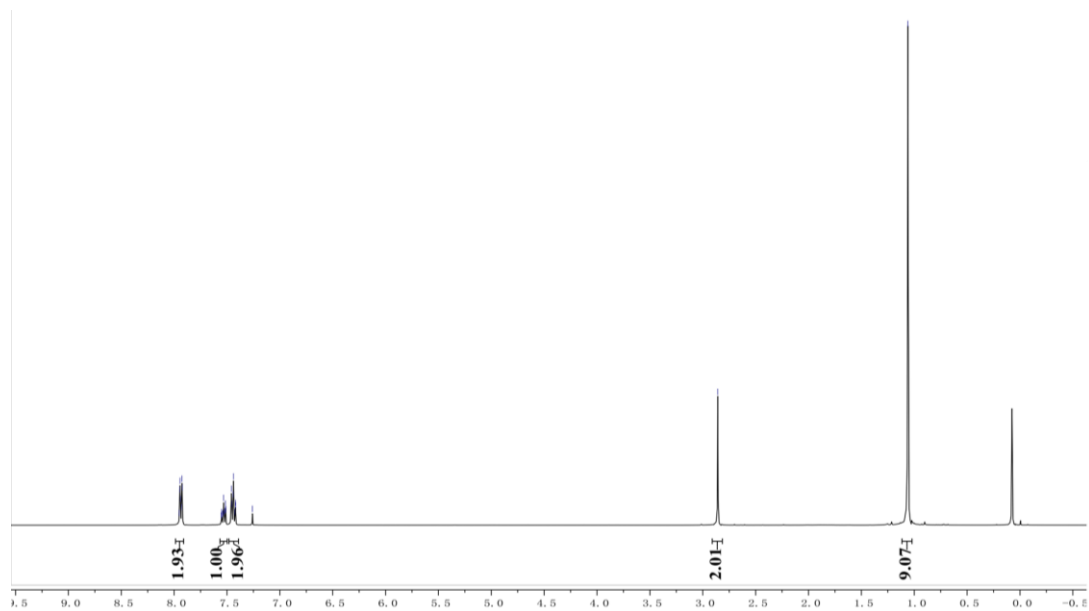
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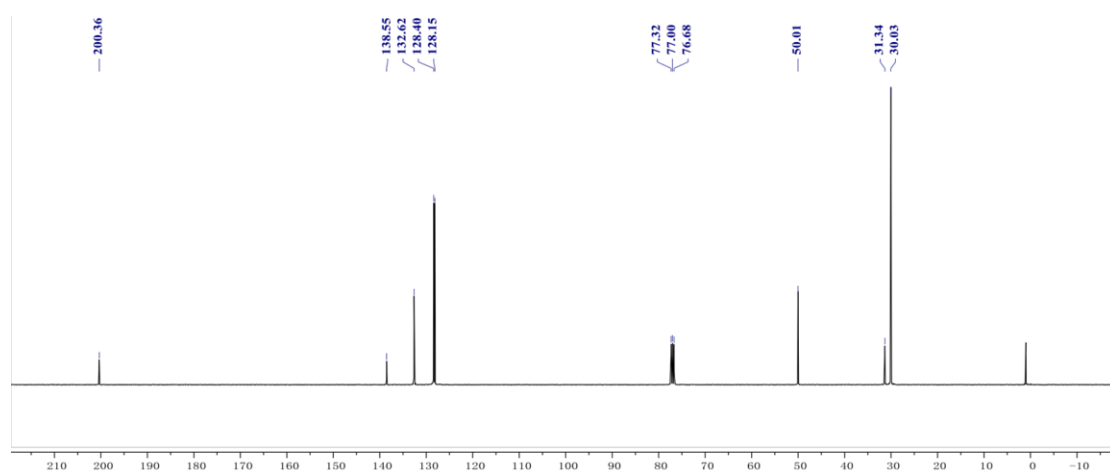
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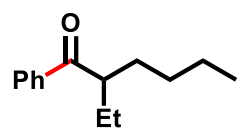
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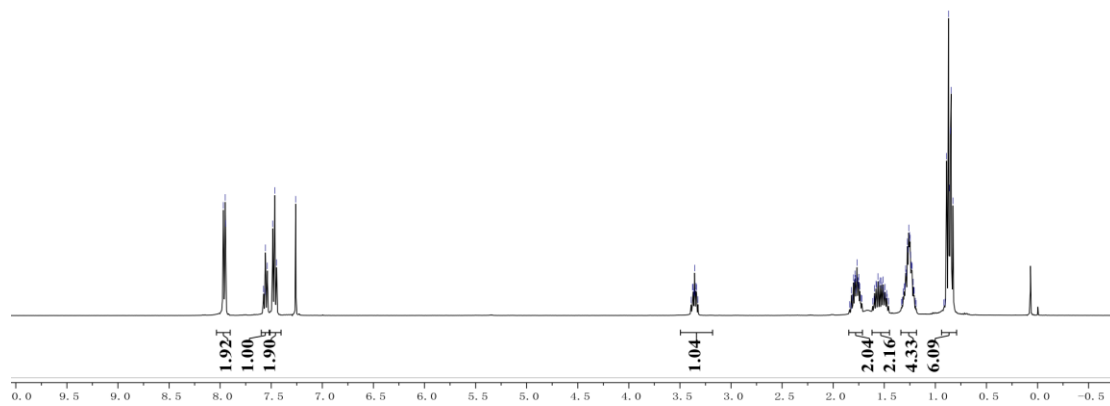
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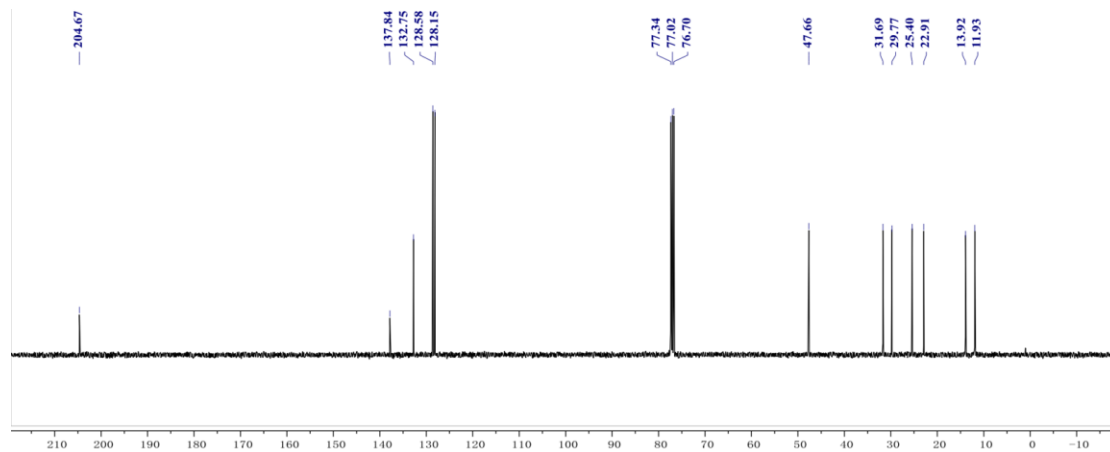
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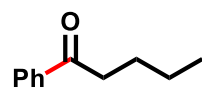
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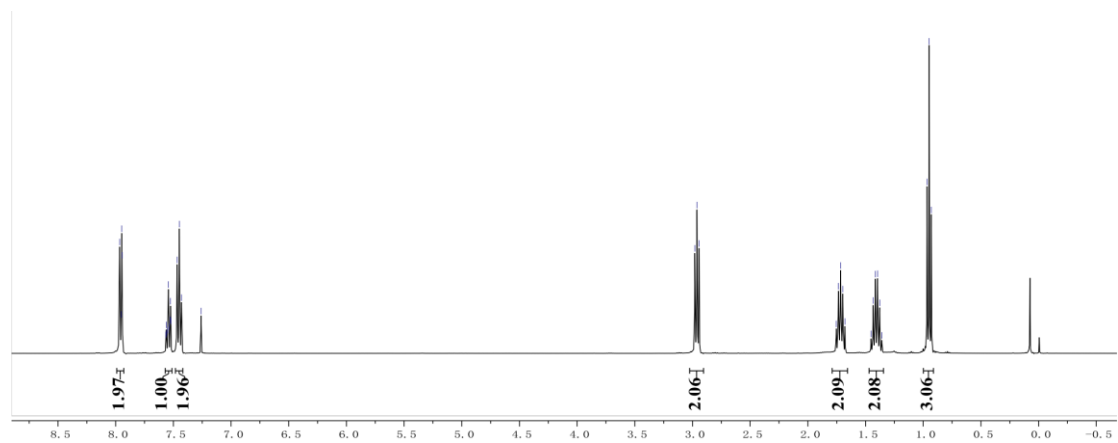
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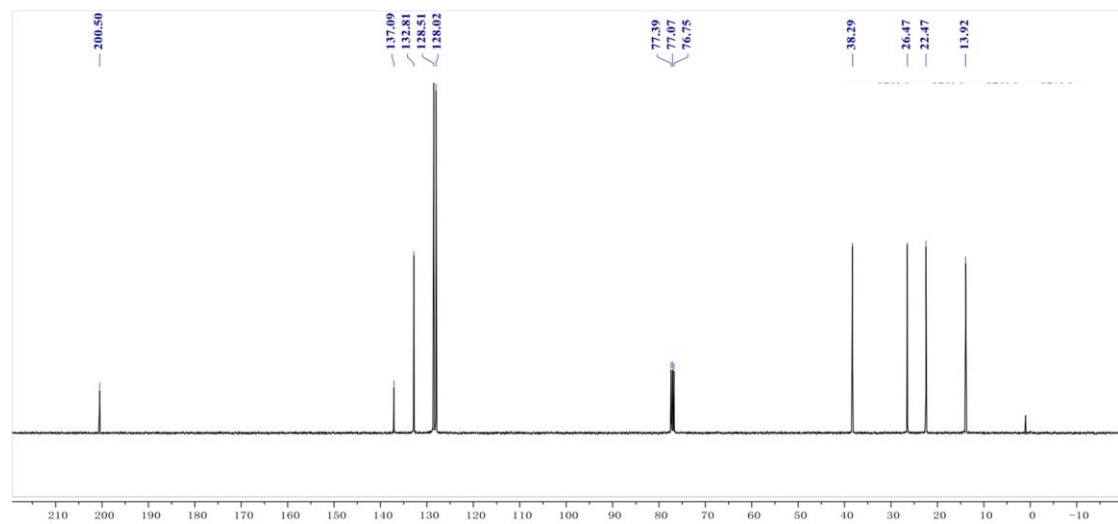
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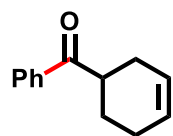
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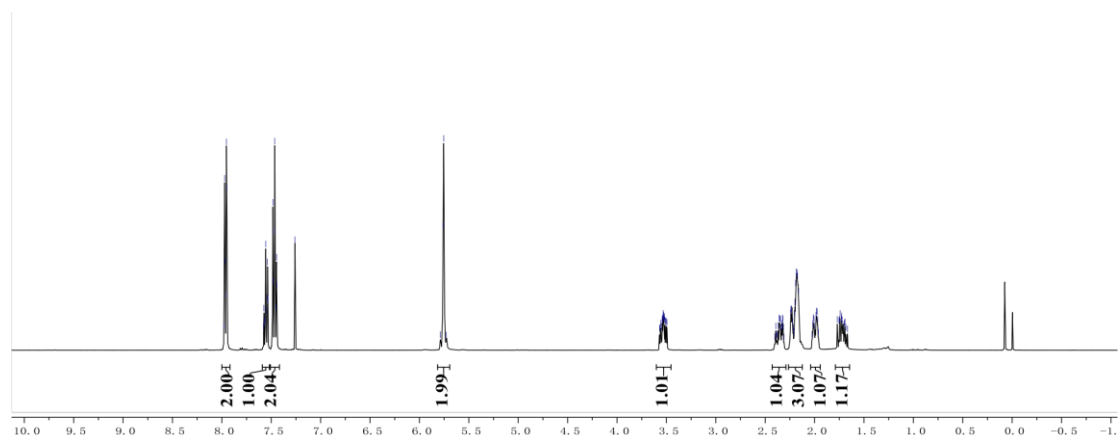
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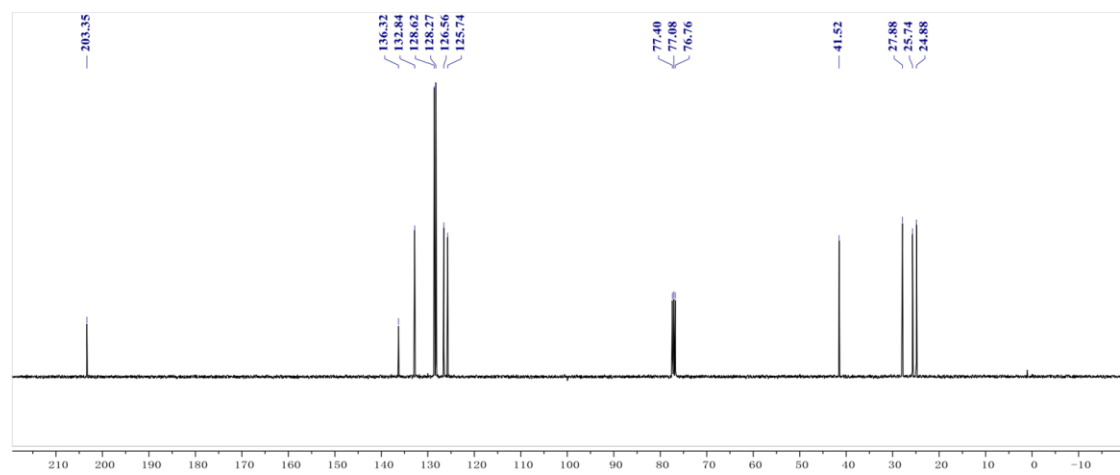
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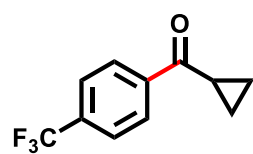
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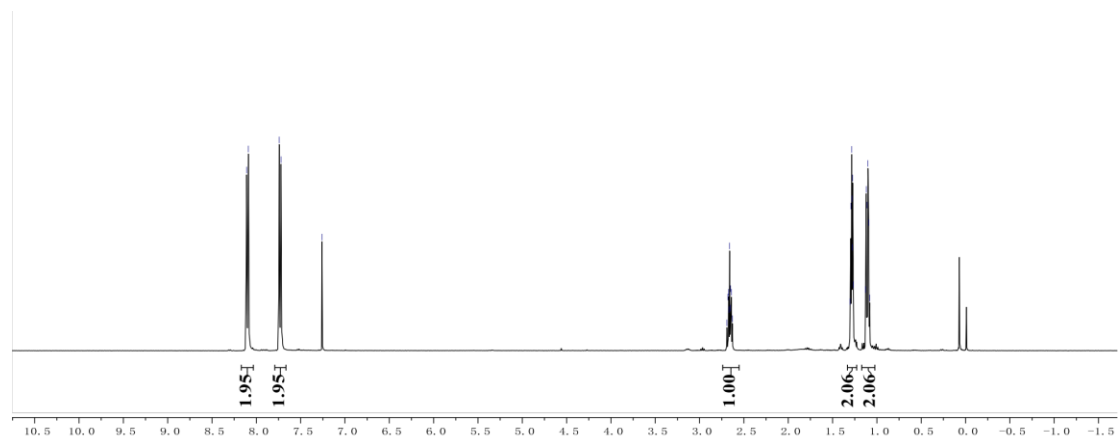
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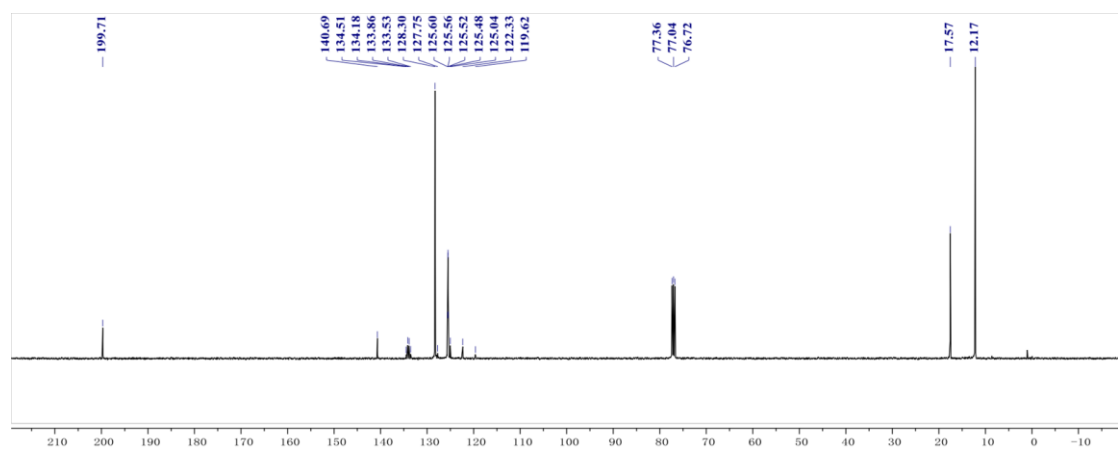
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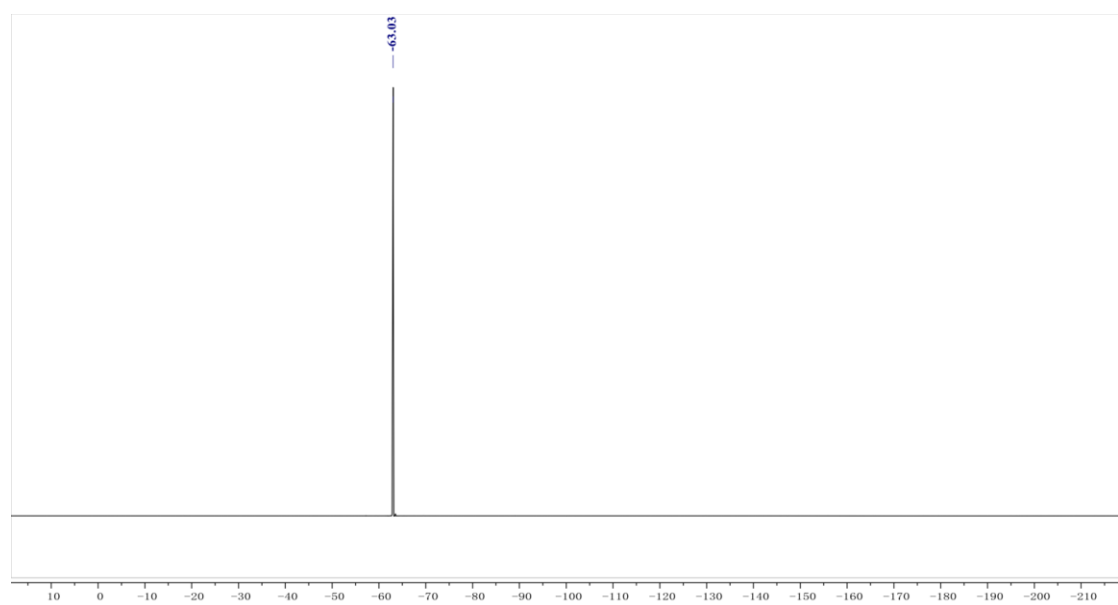
^1H NMR



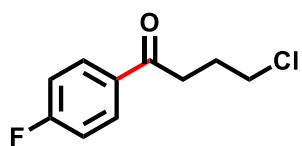
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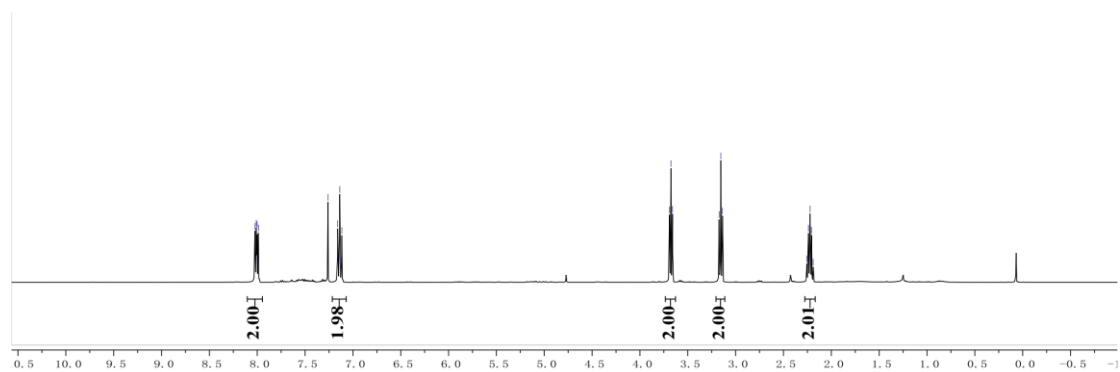
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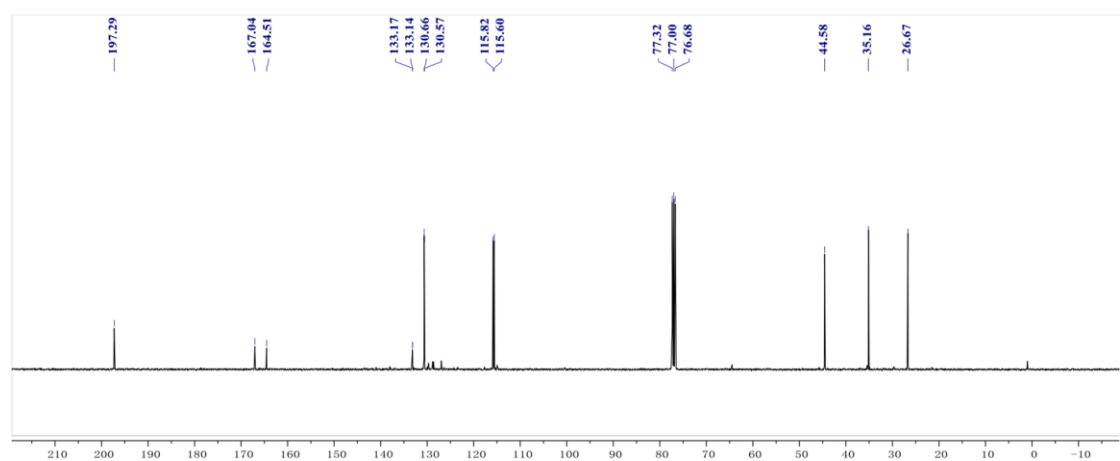
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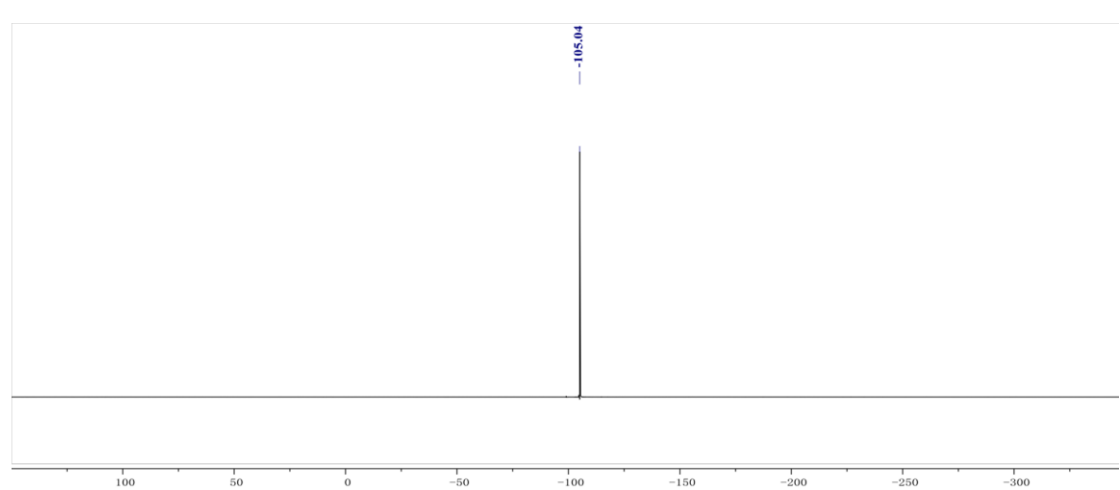
¹H NMR



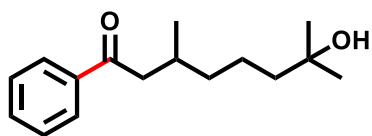
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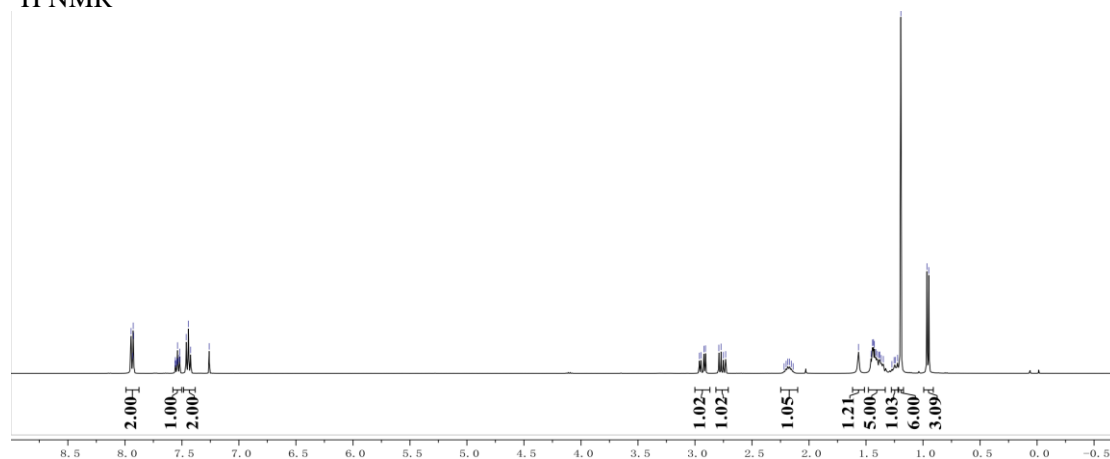
¹⁹F NMR



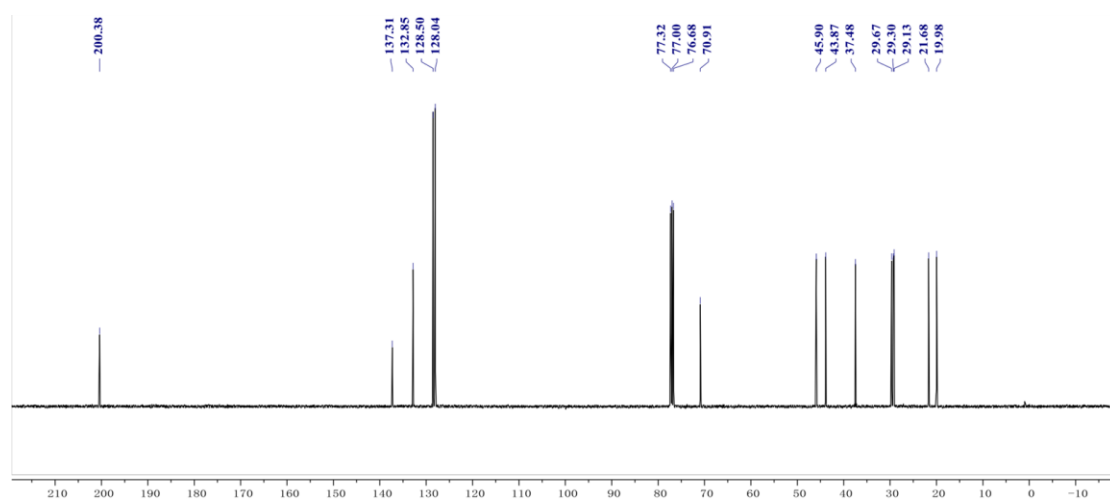
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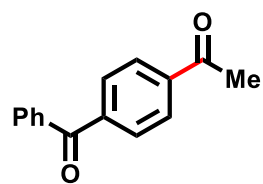
^1H NMR



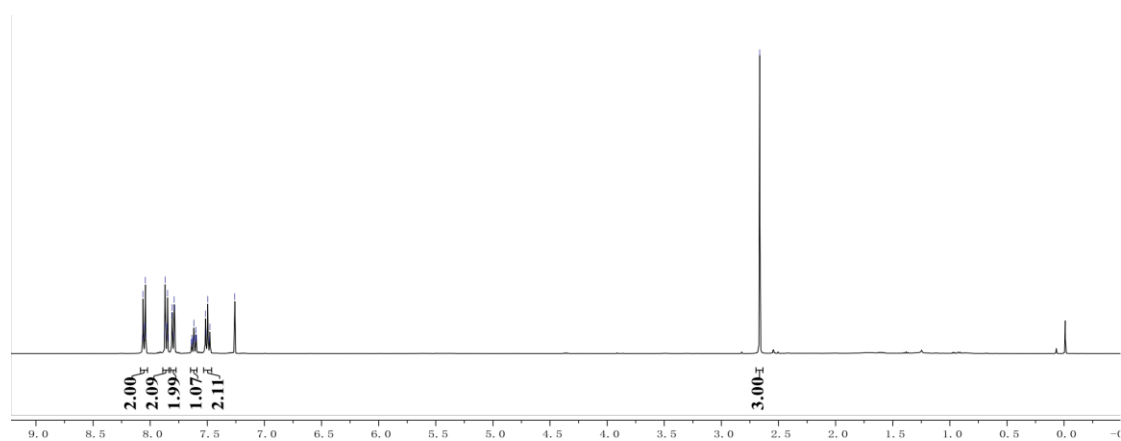
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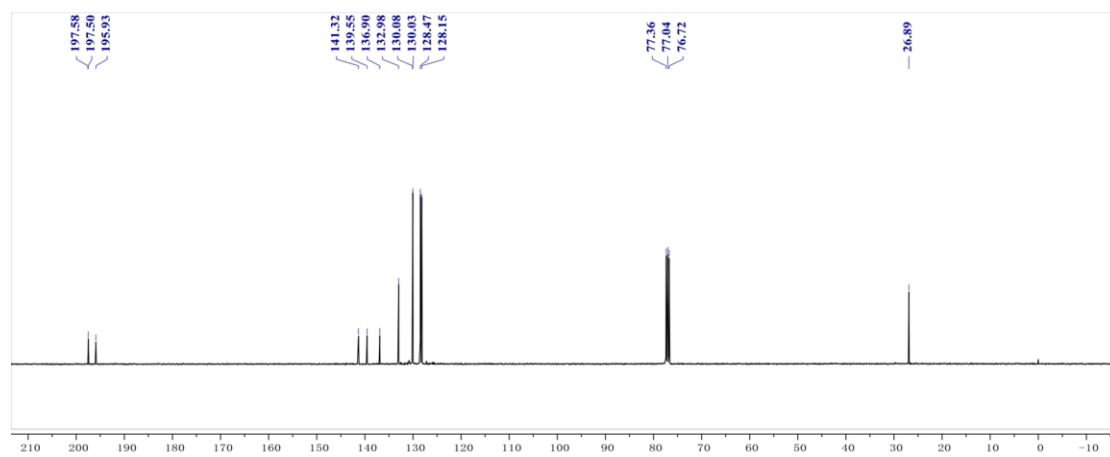
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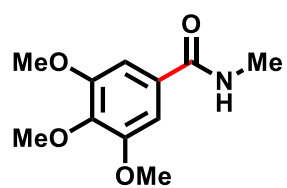
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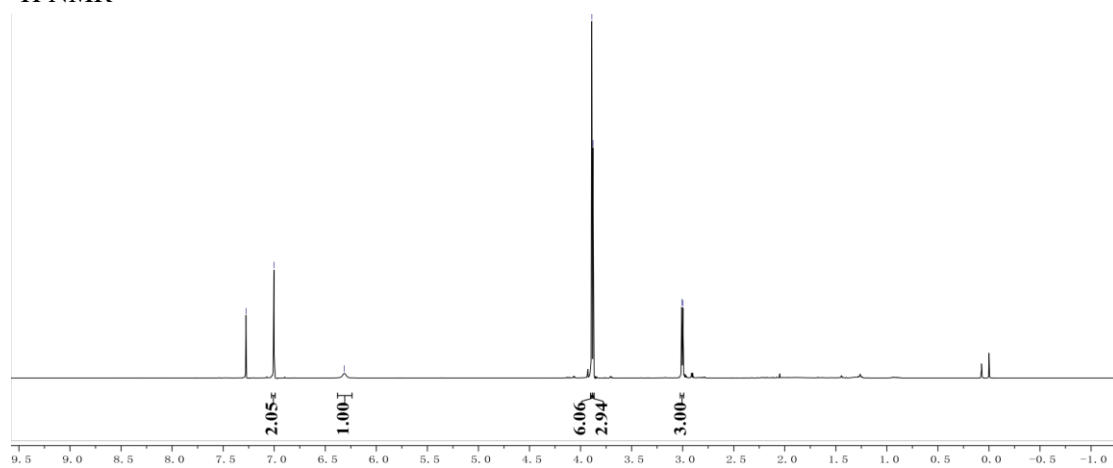
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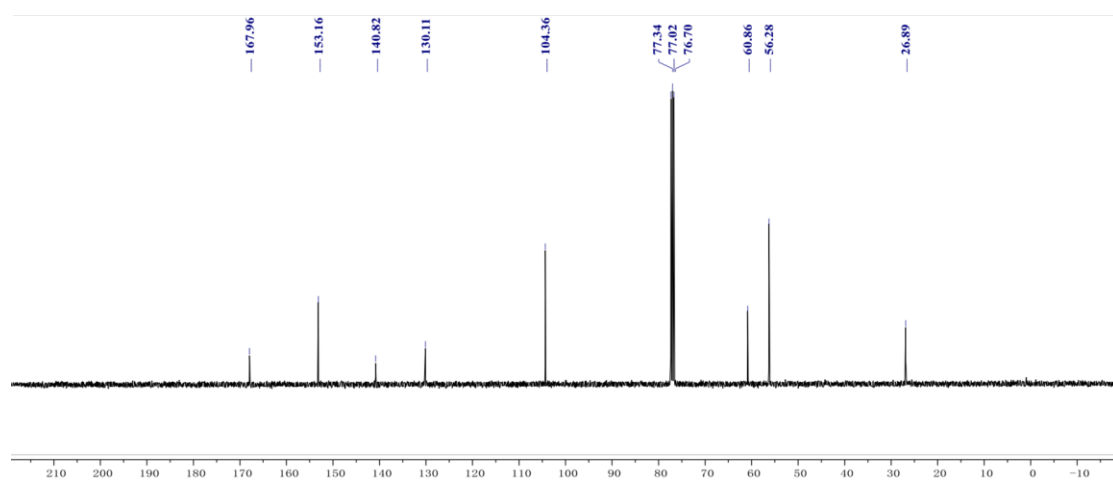
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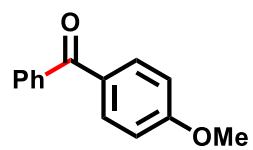
¹H NMR



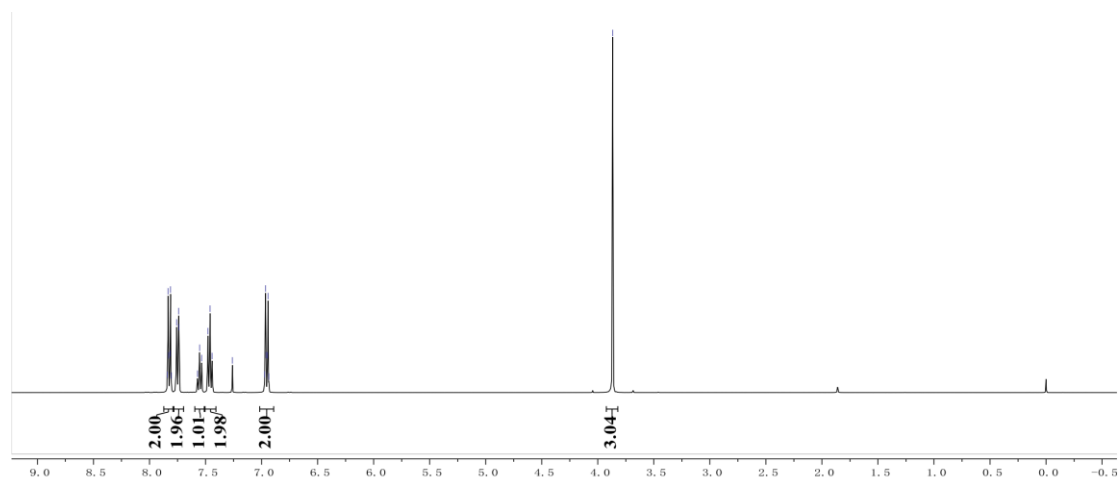
¹³C NMR



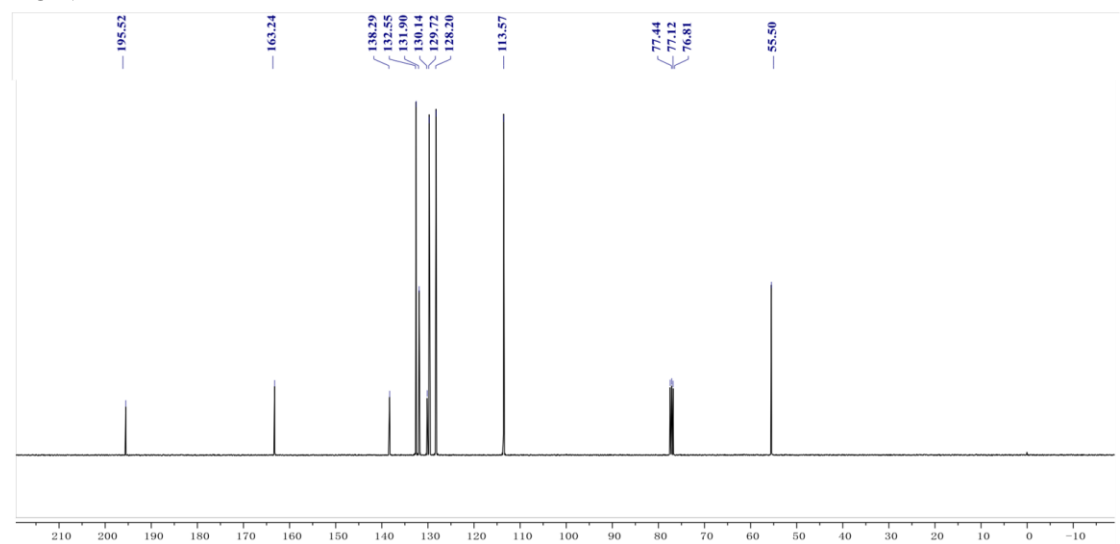
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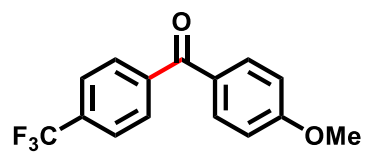
^1H NMR



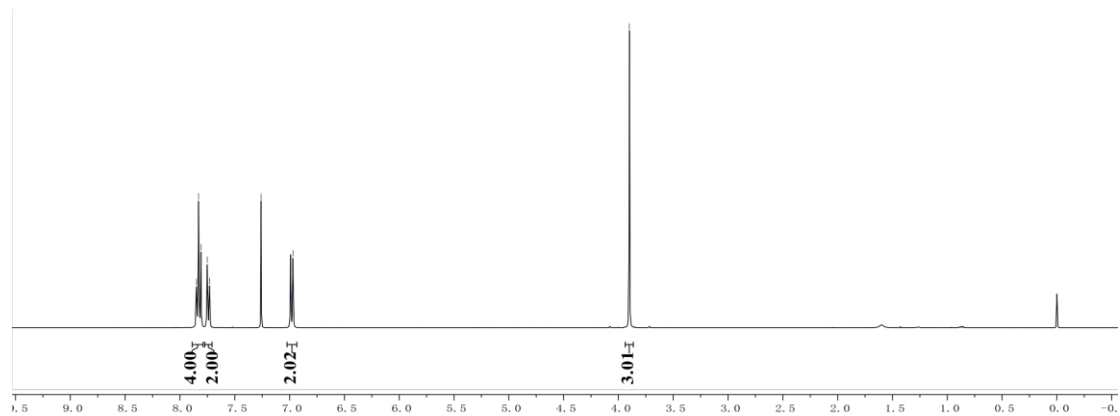
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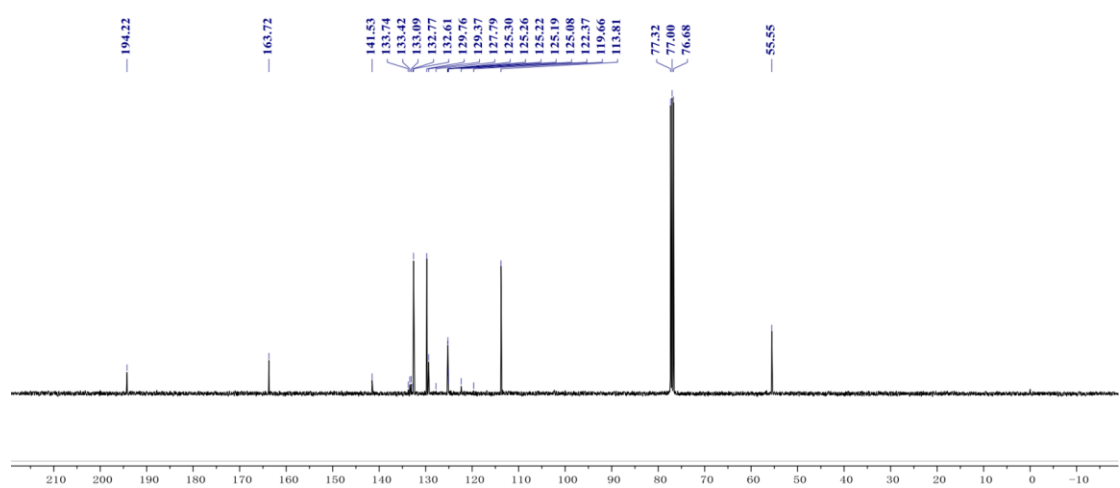
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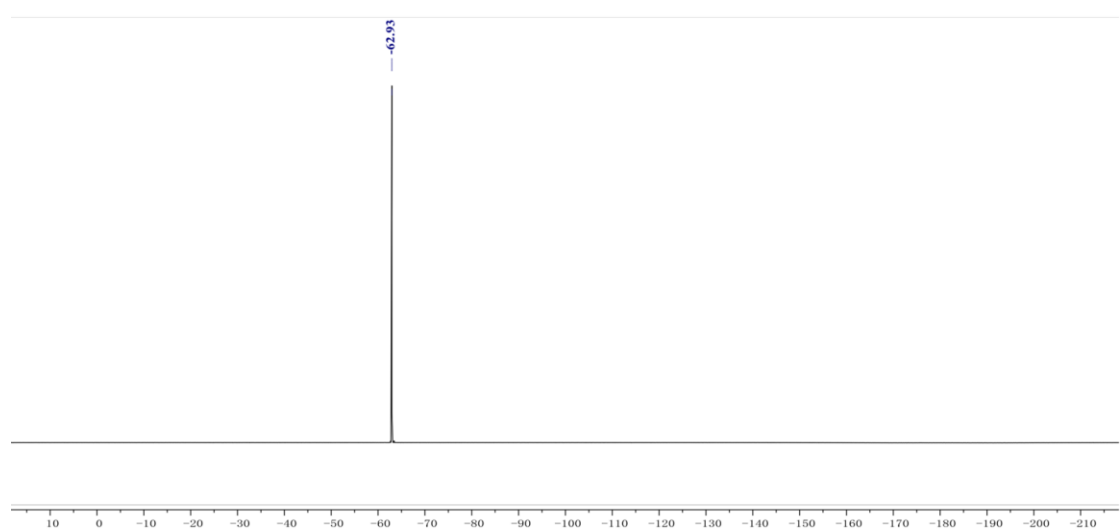
¹H NMR



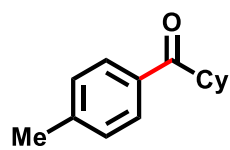
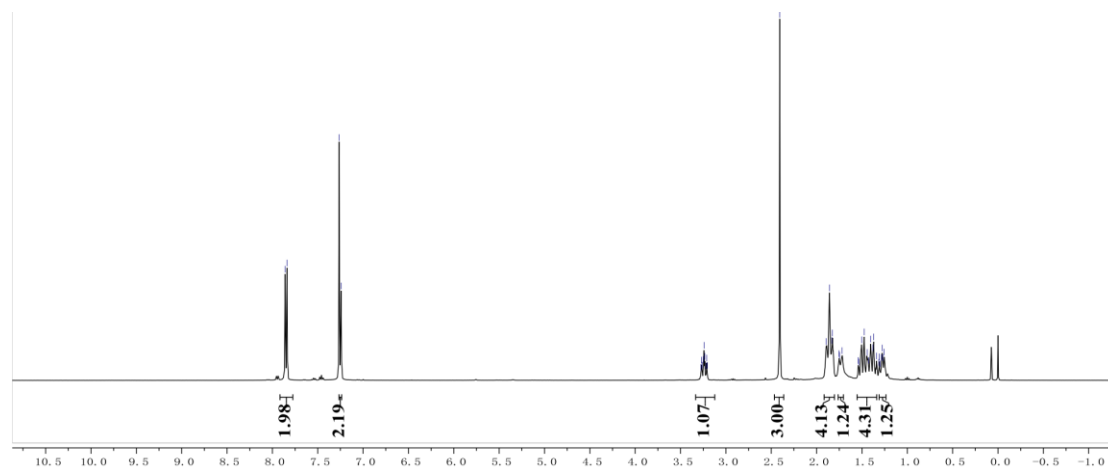
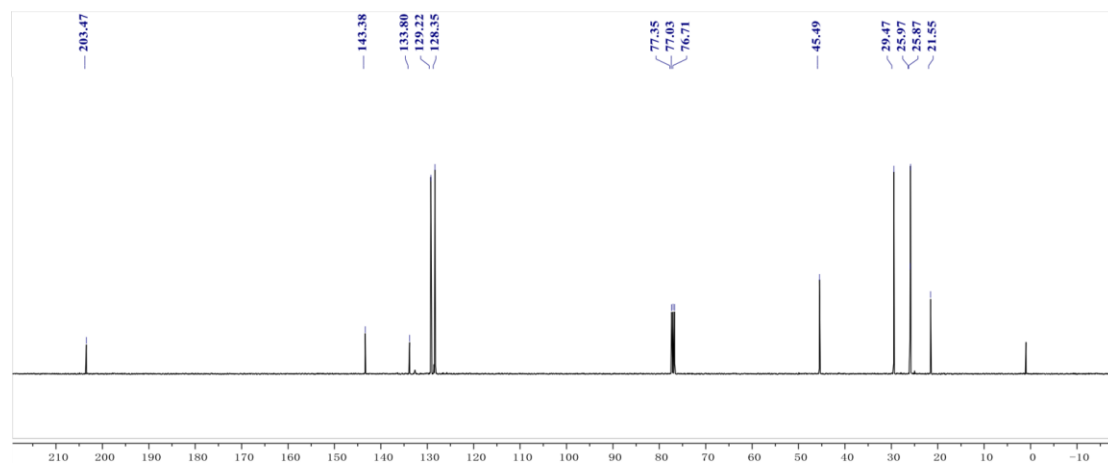
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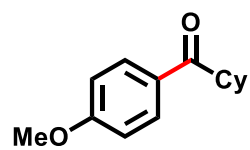
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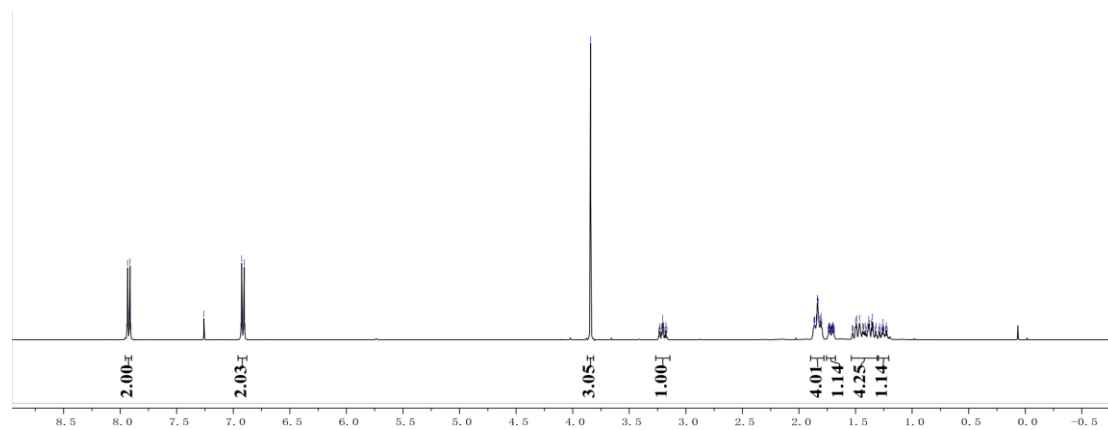
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 $^1\text{H NMR}$  $^{13}\text{C NMR}$ 

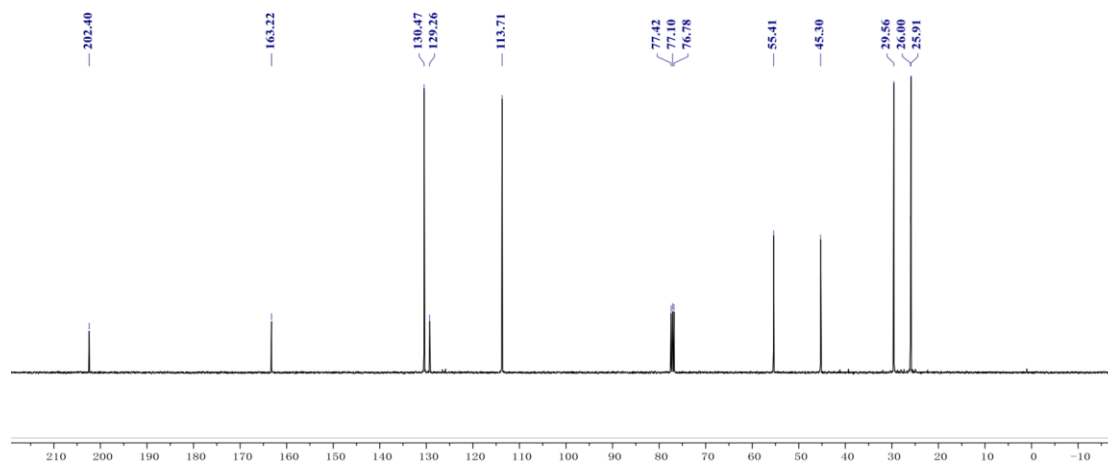
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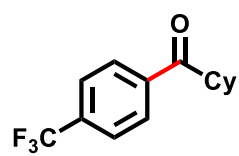
^1H NMR



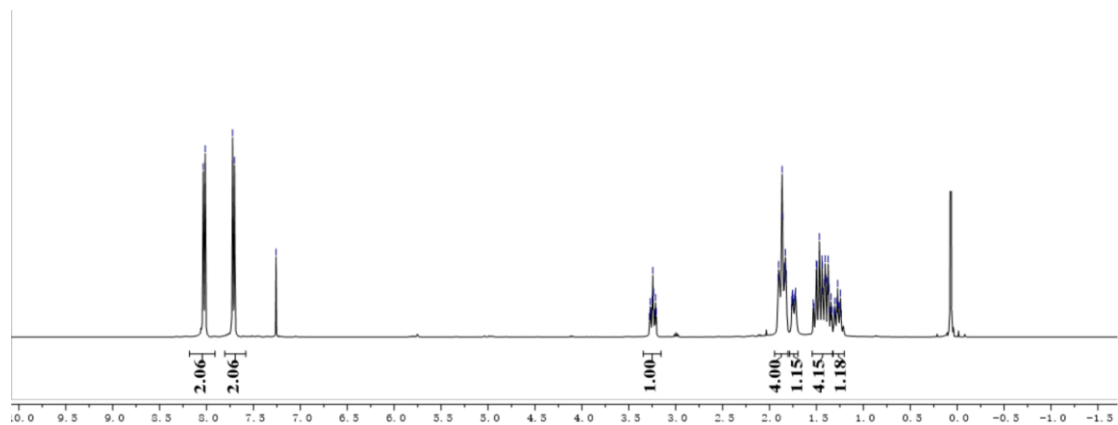
^{13}C NMR



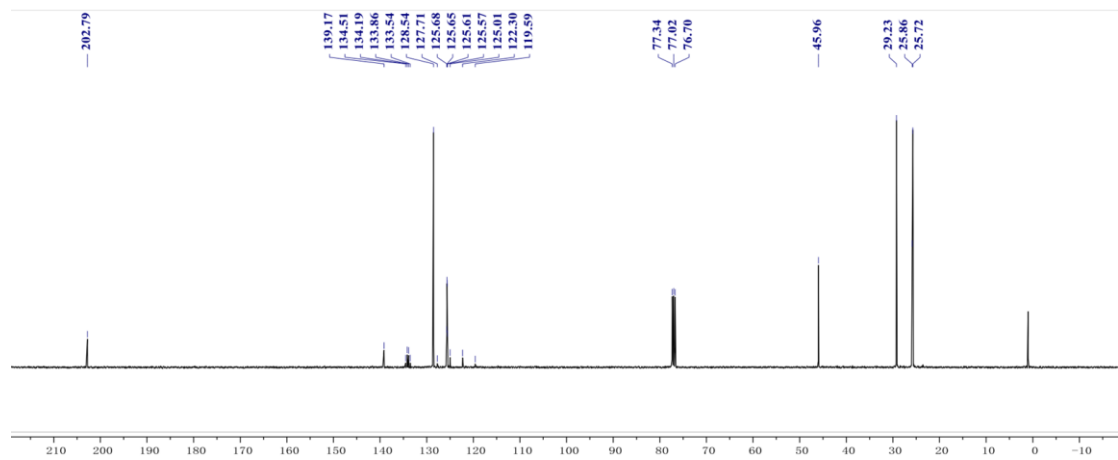
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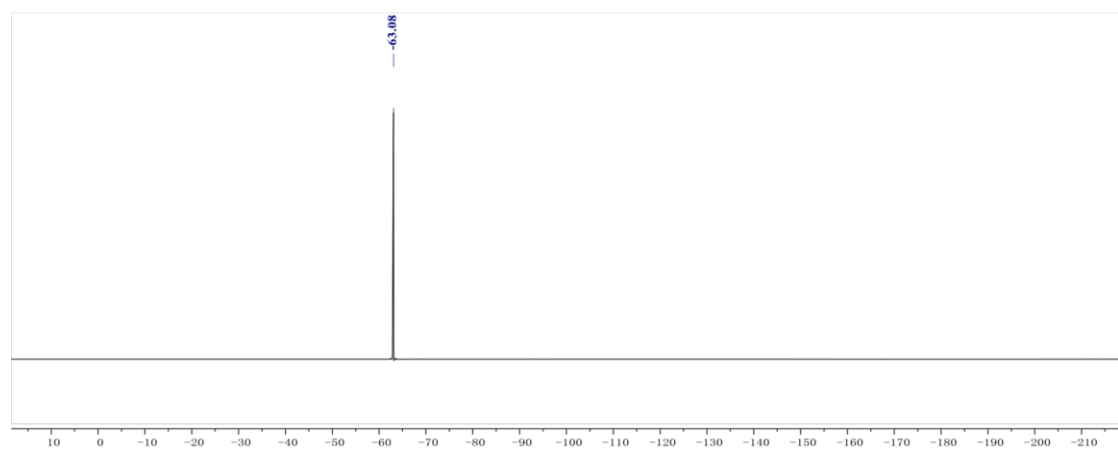
^1H NMR



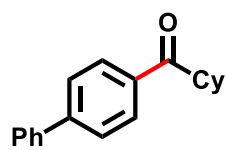
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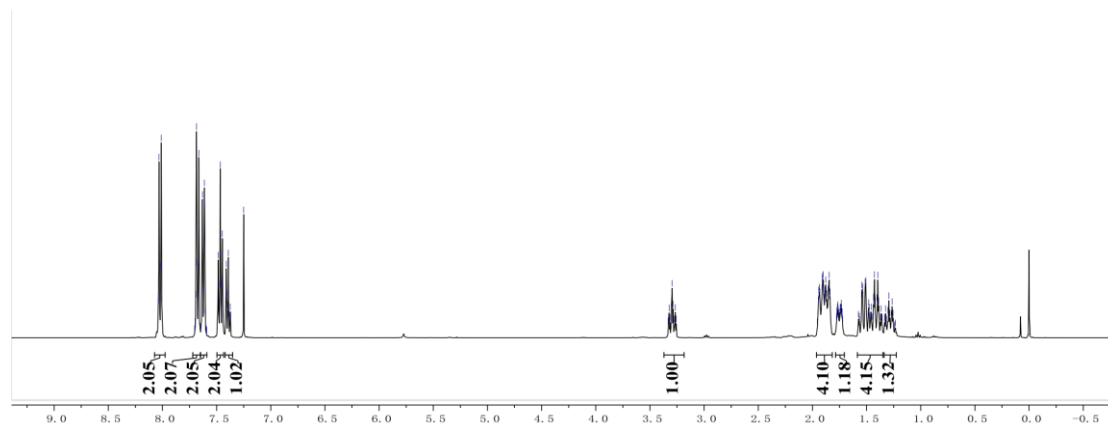
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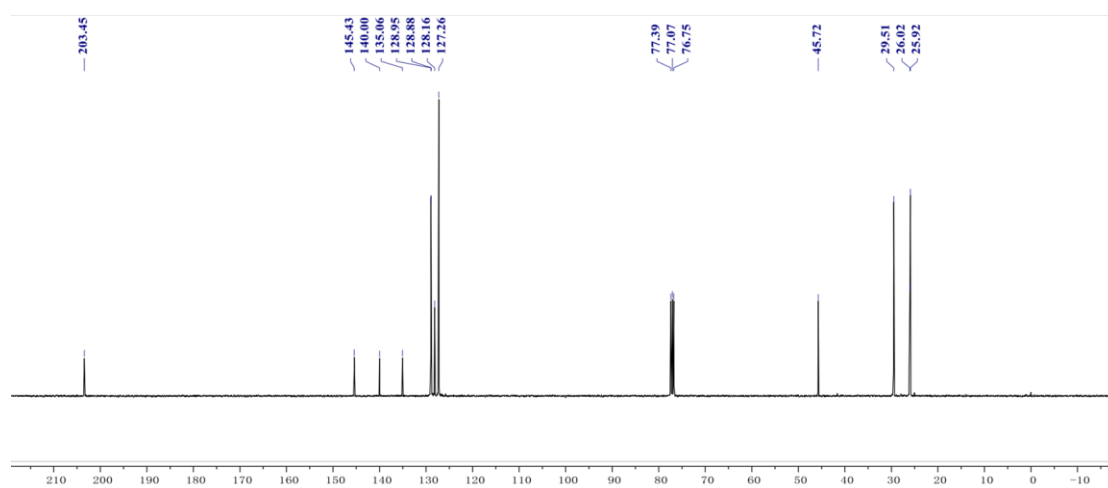
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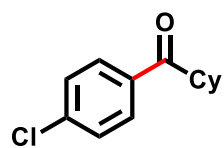
^1H NMR



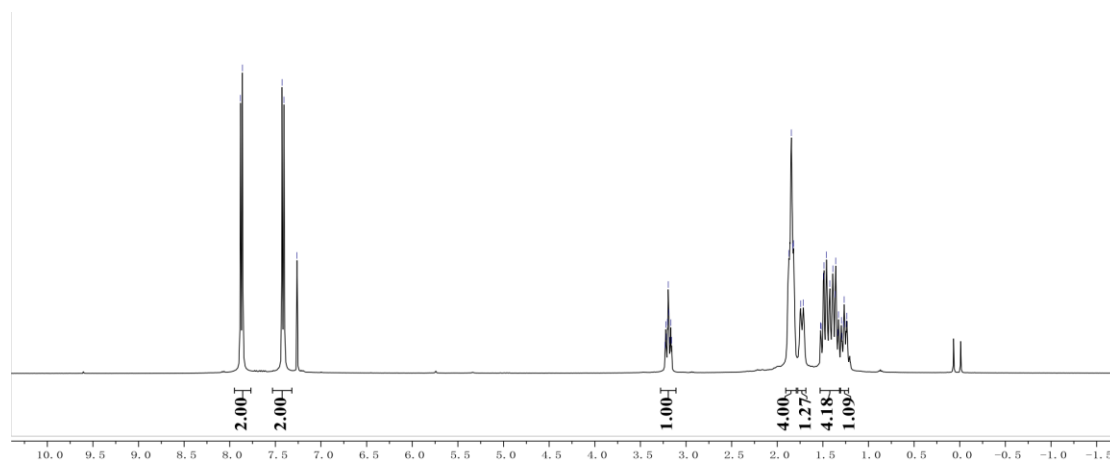
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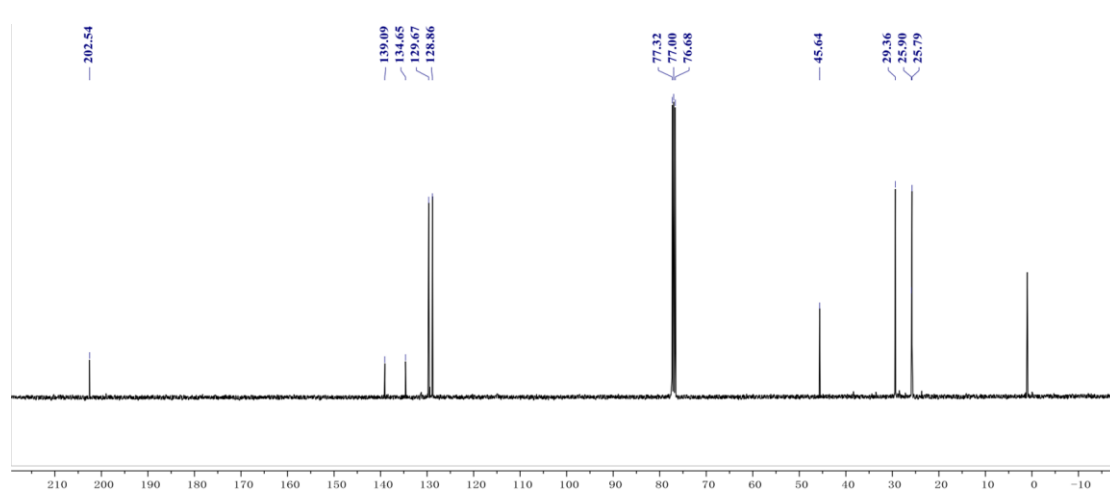
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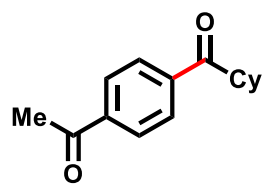
^1H NMR



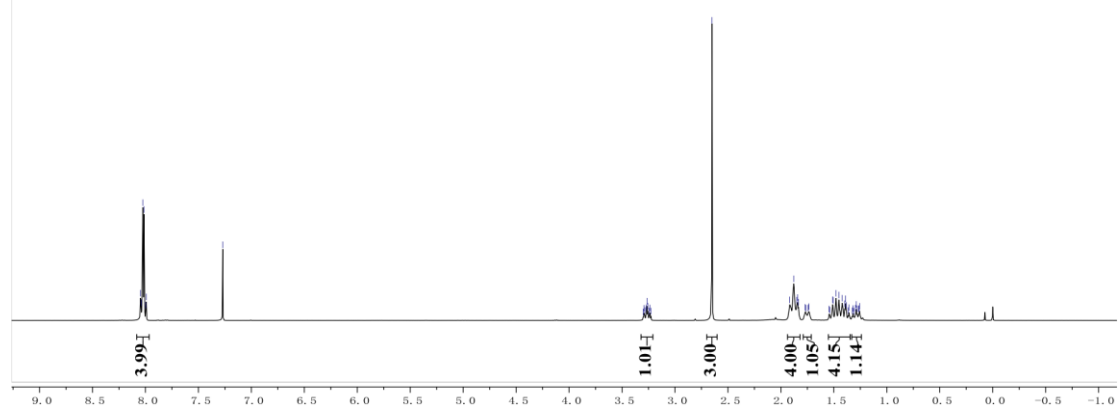
^{13}C NMR



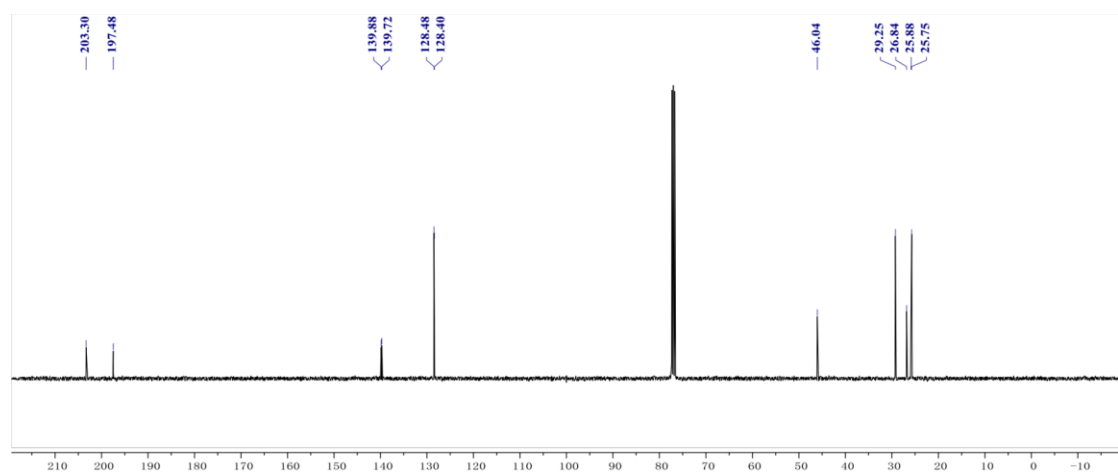
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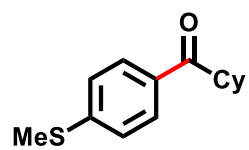
$^1\text{H NMR}$



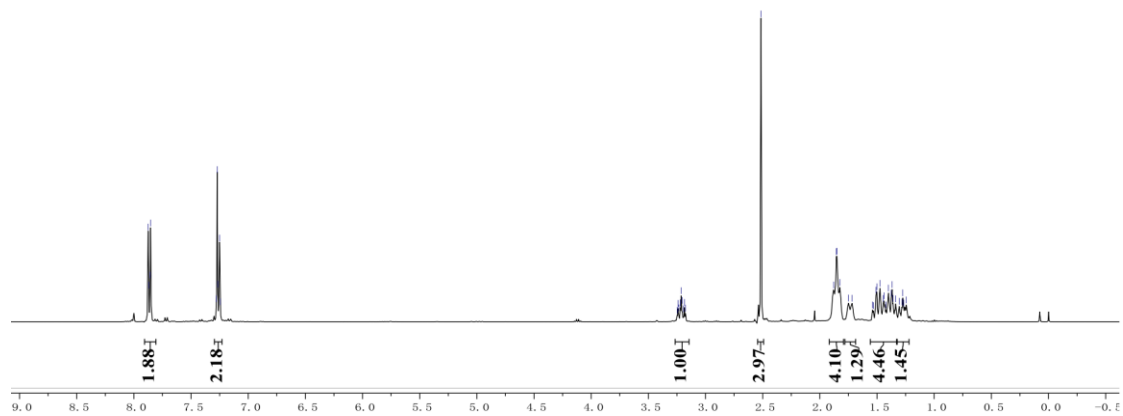
$^{13}\text{C NMR}$



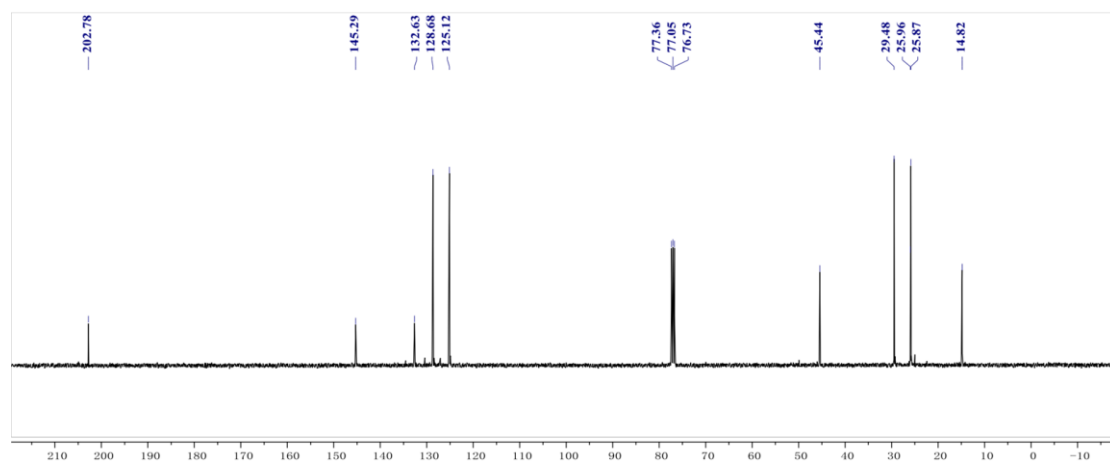
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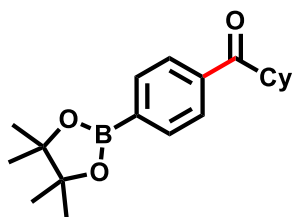
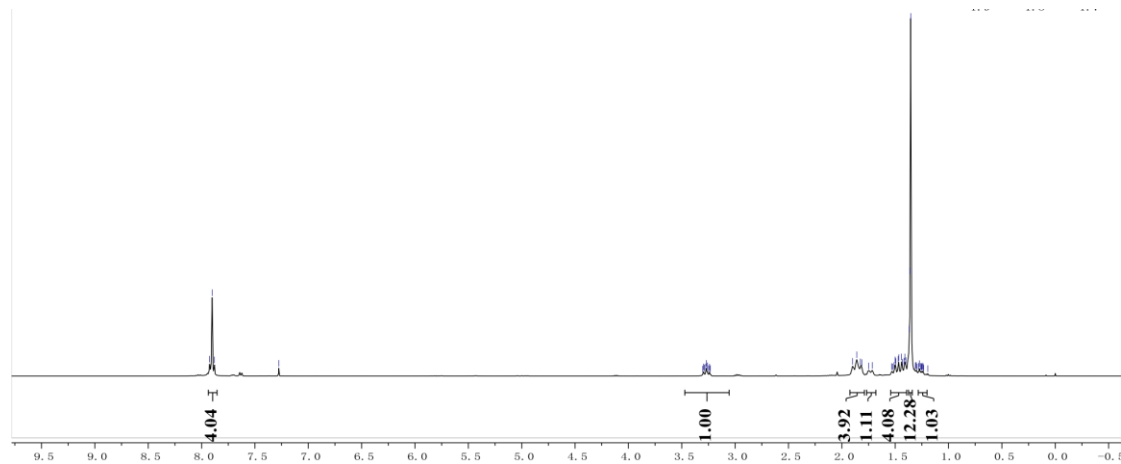
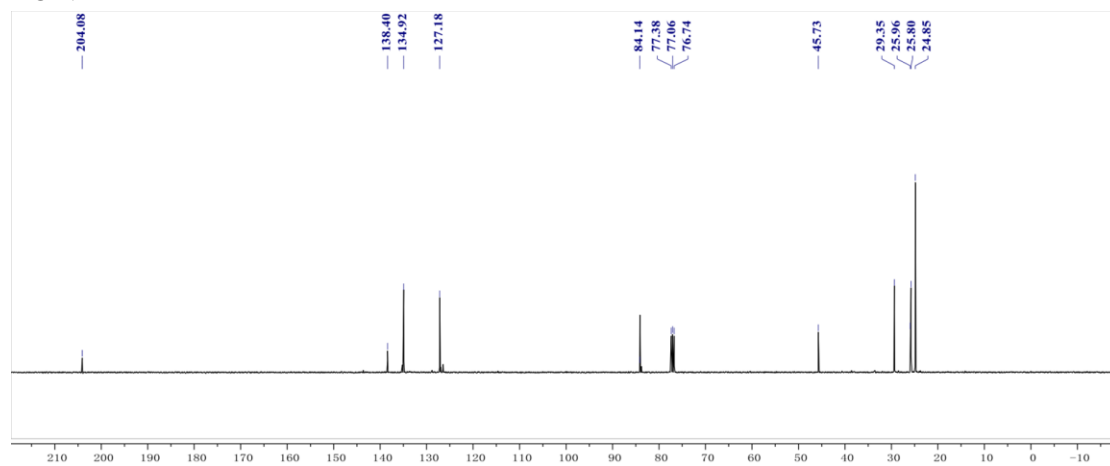


^1H NMR

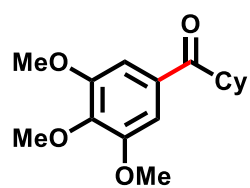


^{13}C NMR

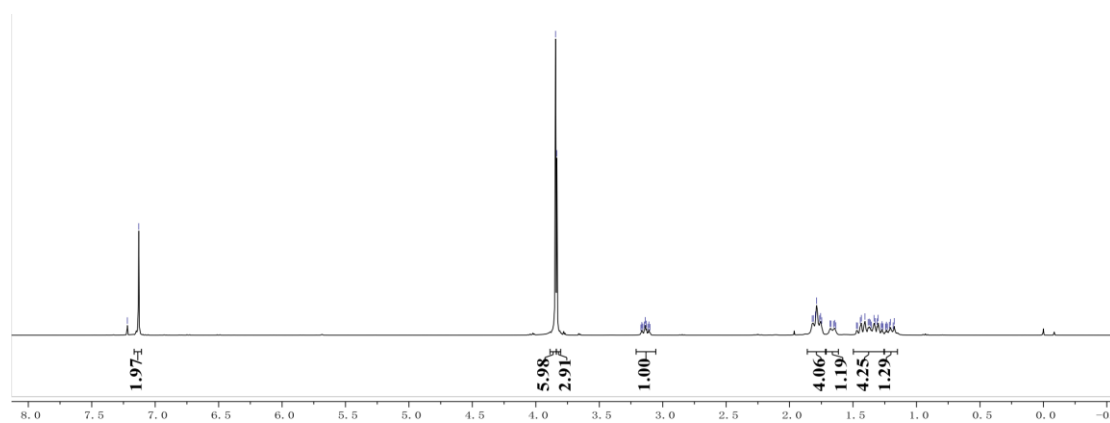


 $^1\text{H NMR}$  $^{13}\text{C NMR}$ 

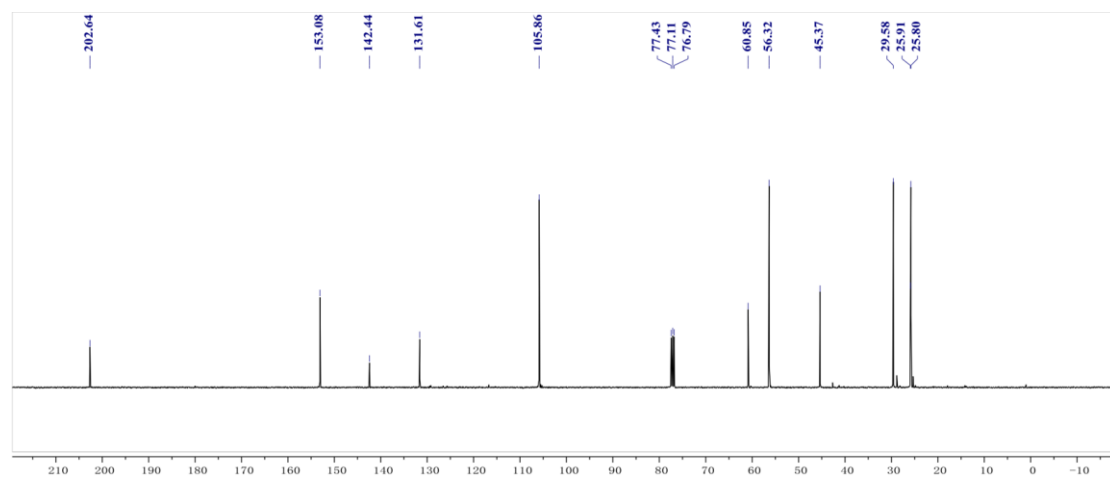
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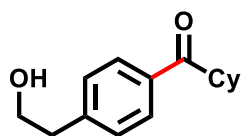
^1H NMR



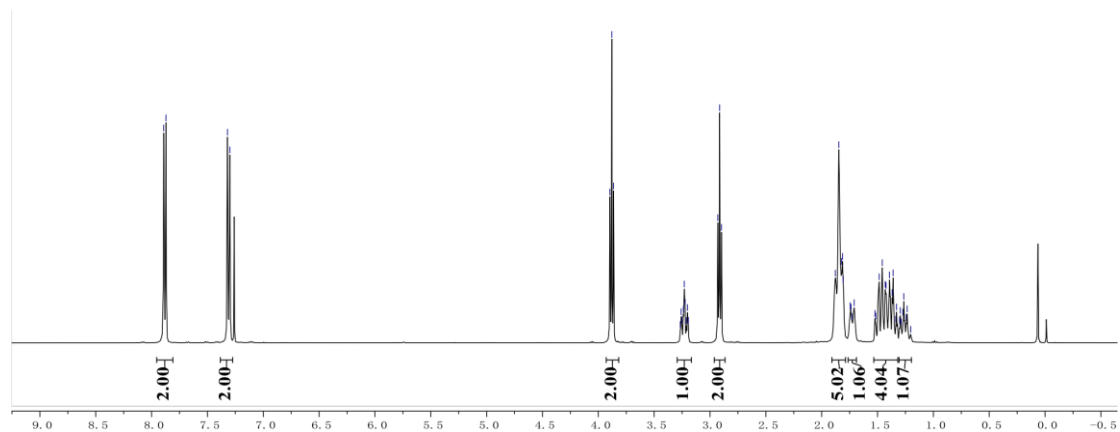
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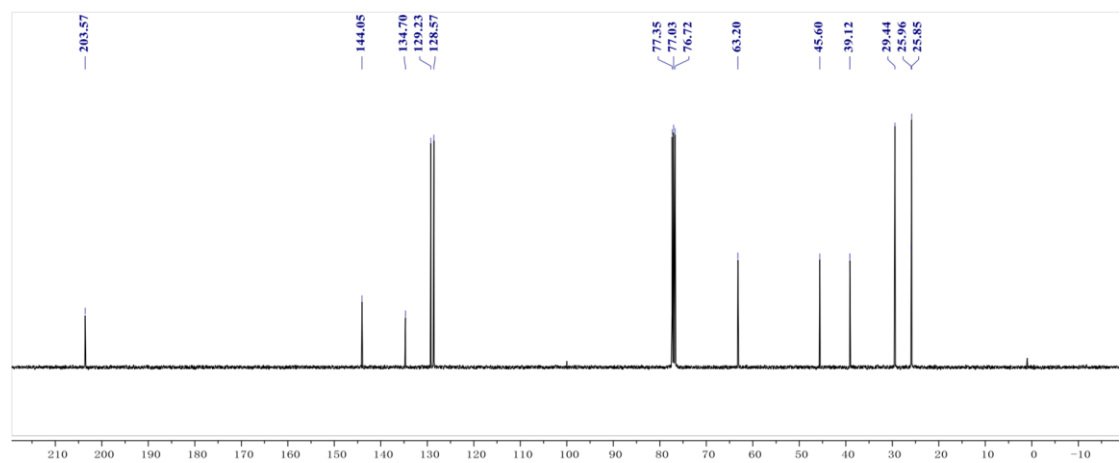
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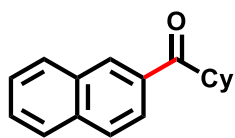
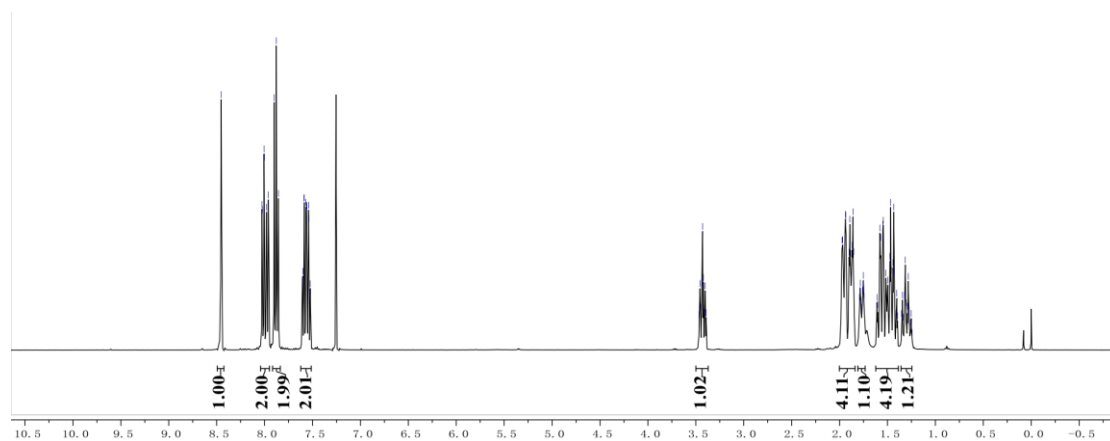
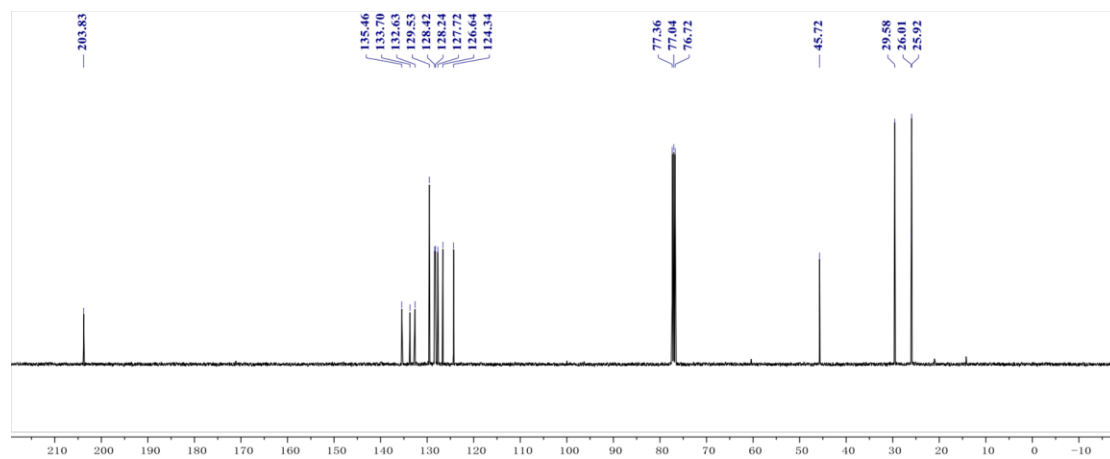
¹H NMR



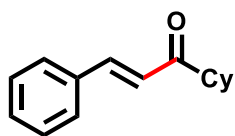
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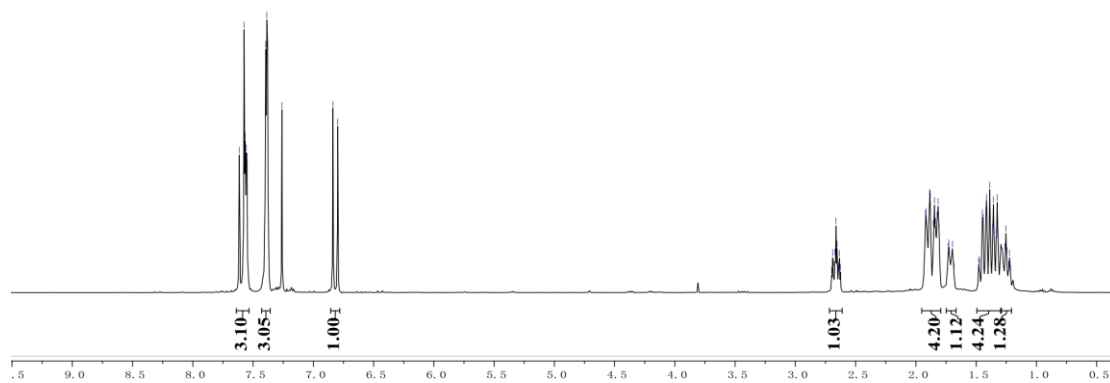
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 ^1H NMR ^{13}C NMR

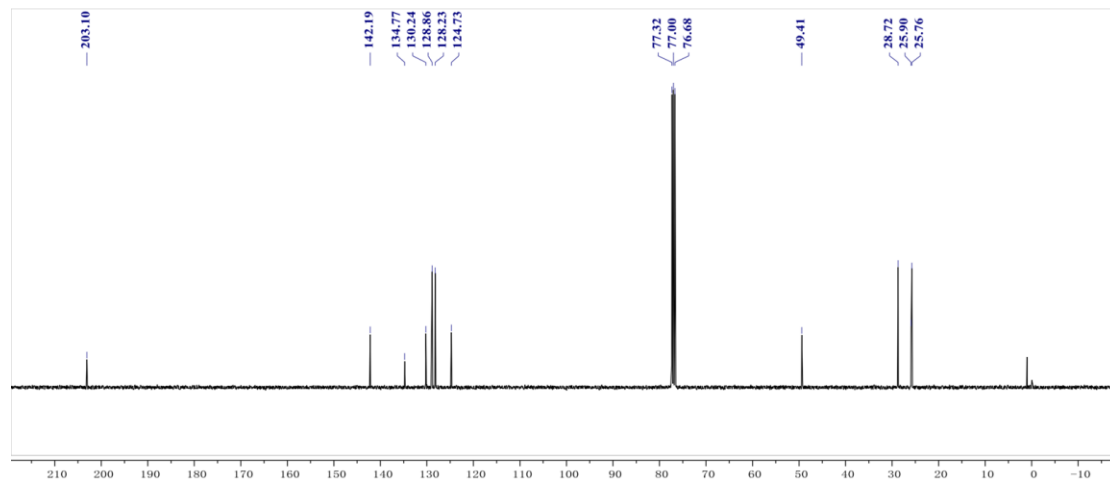
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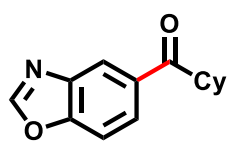
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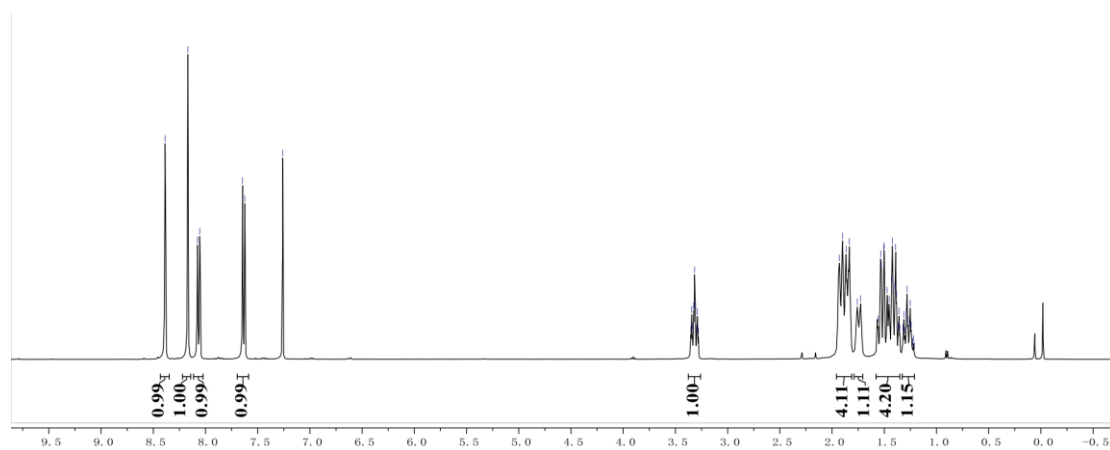
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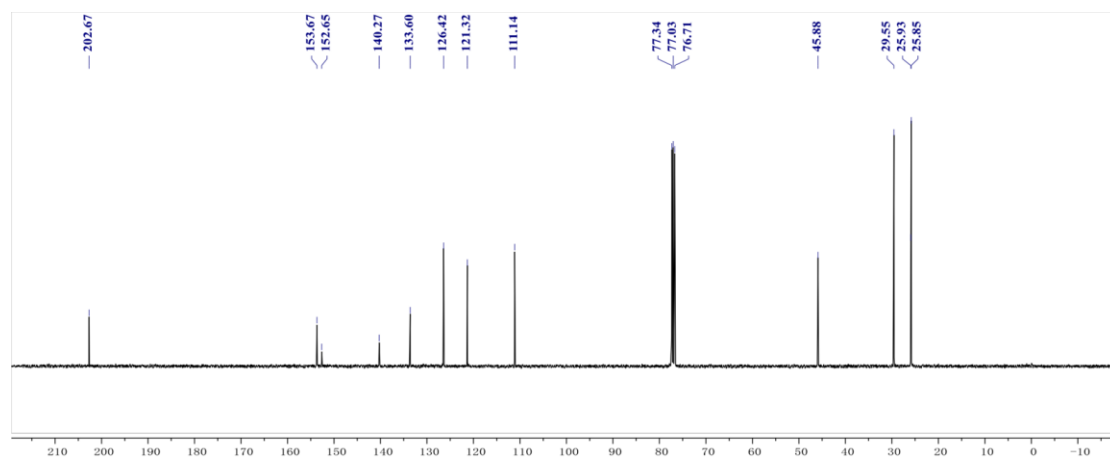
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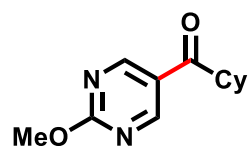
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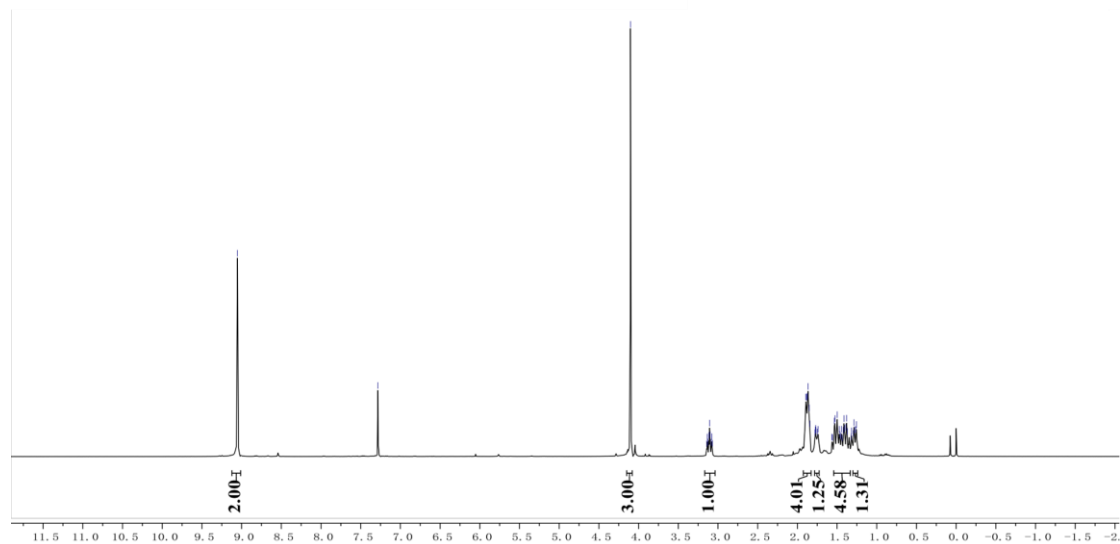
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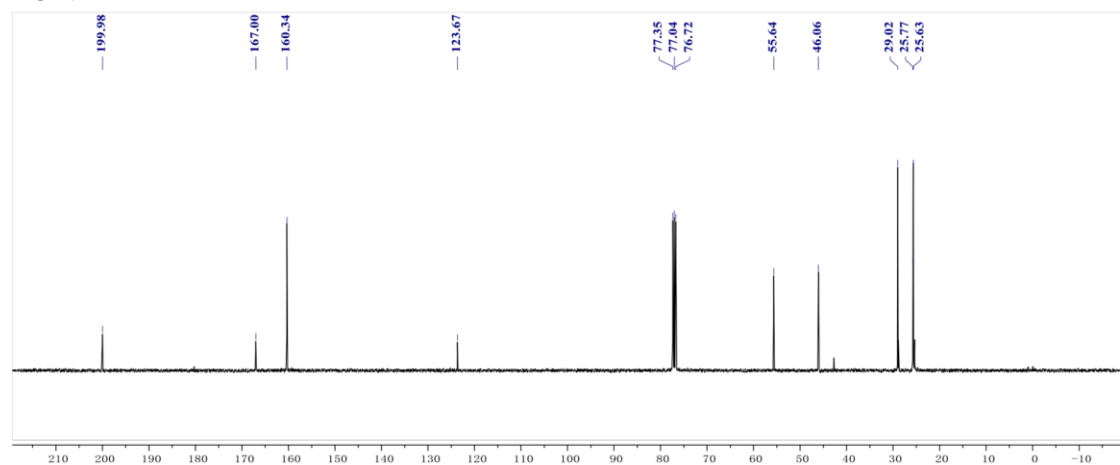
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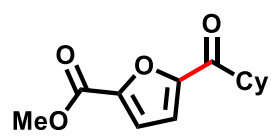
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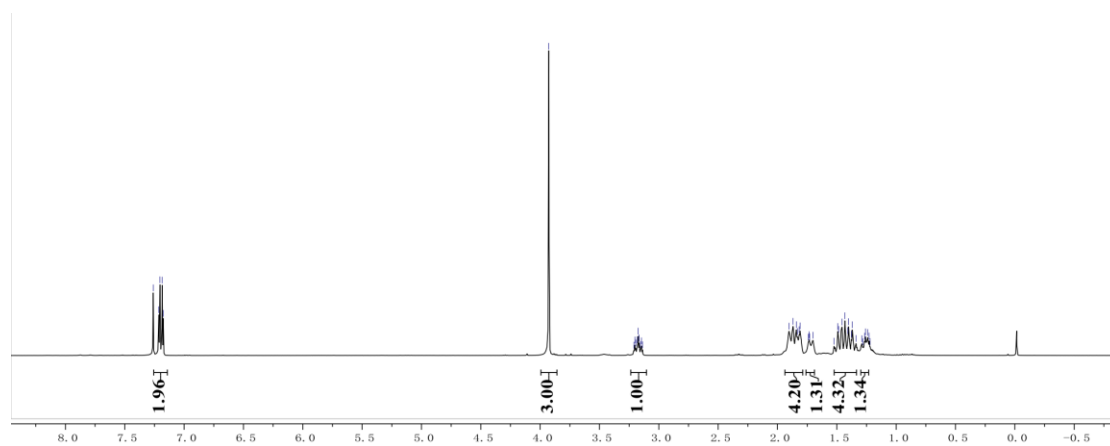
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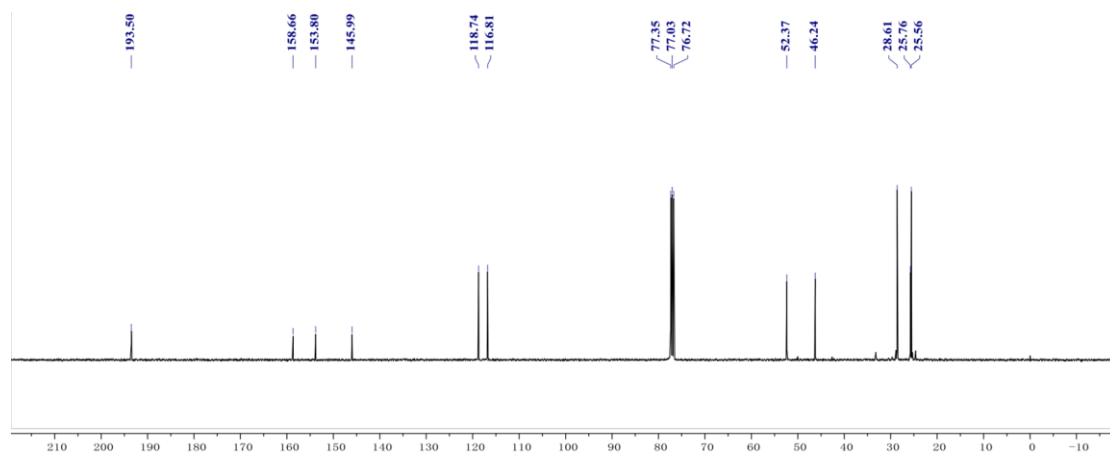
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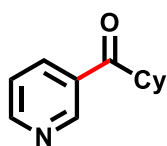
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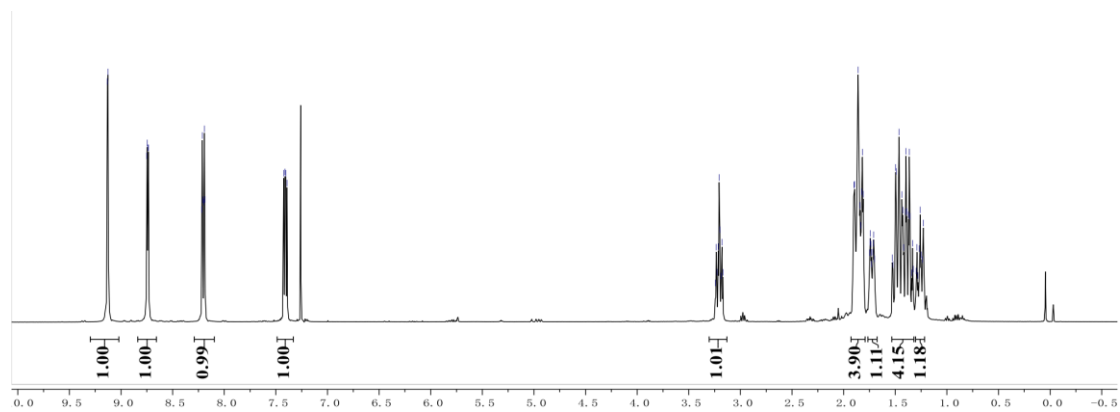
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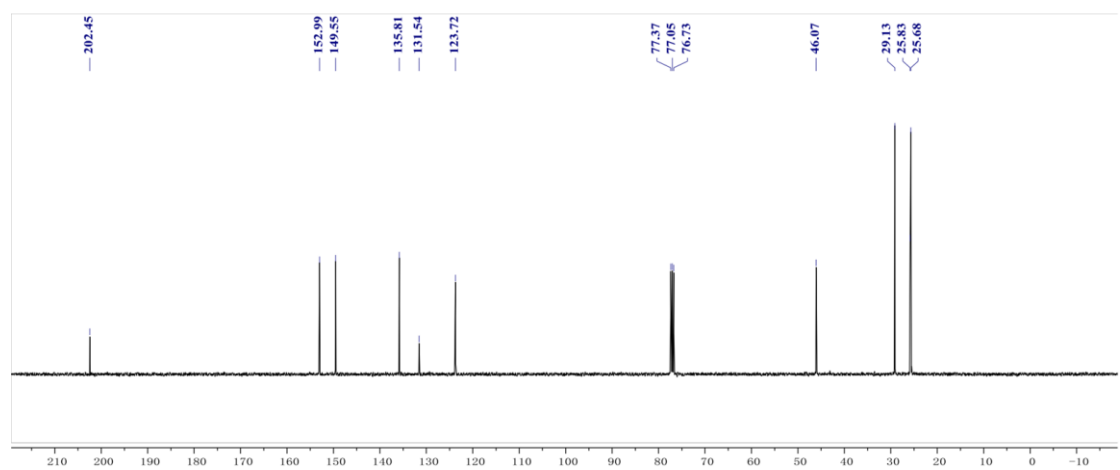
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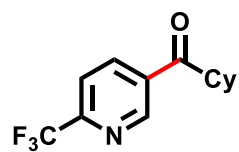
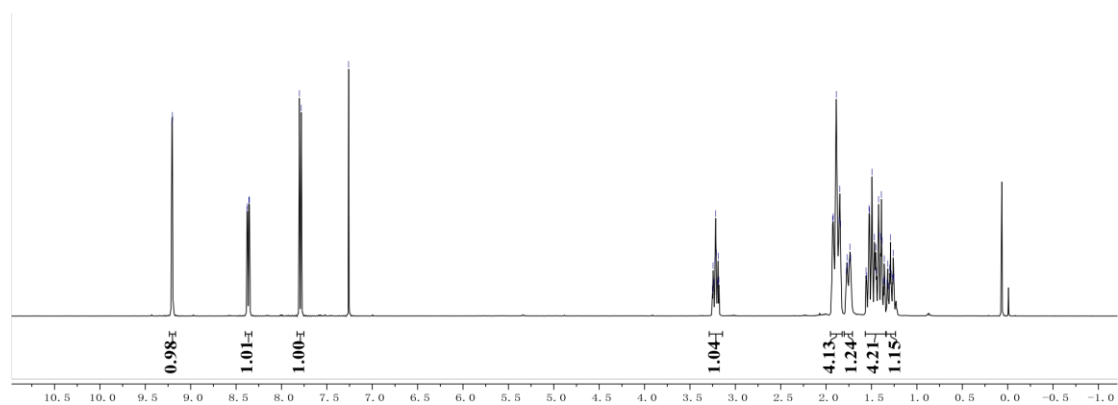
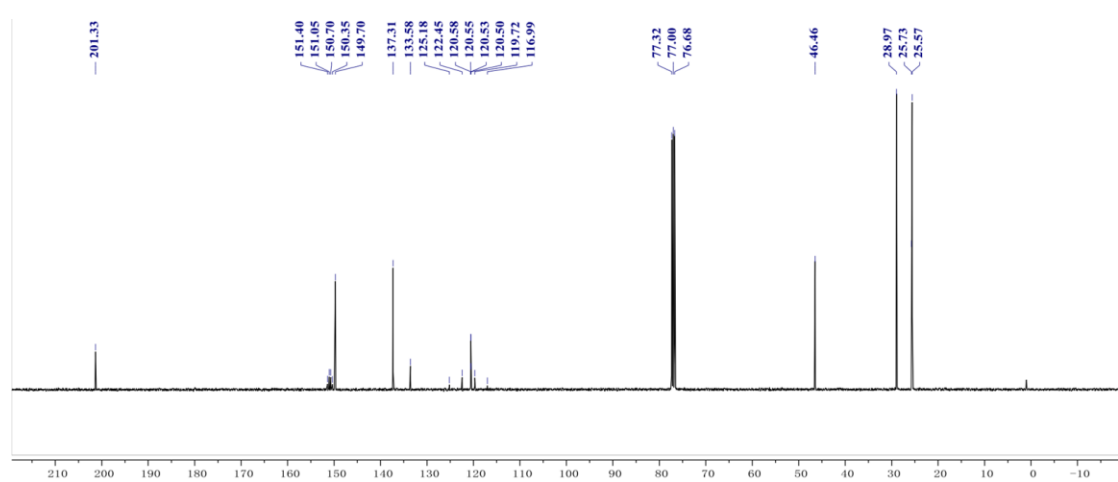
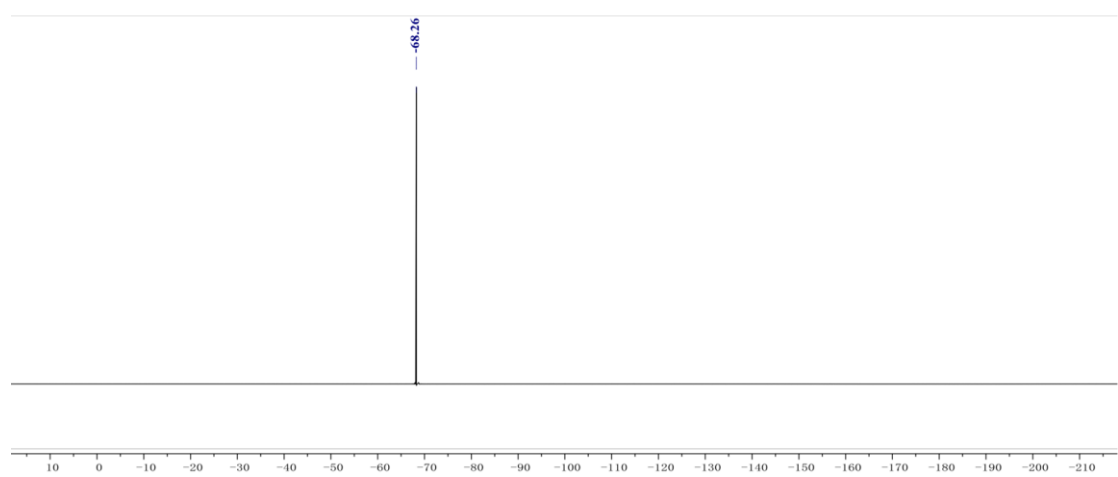


^1H NMR

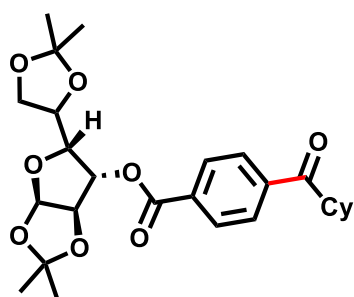


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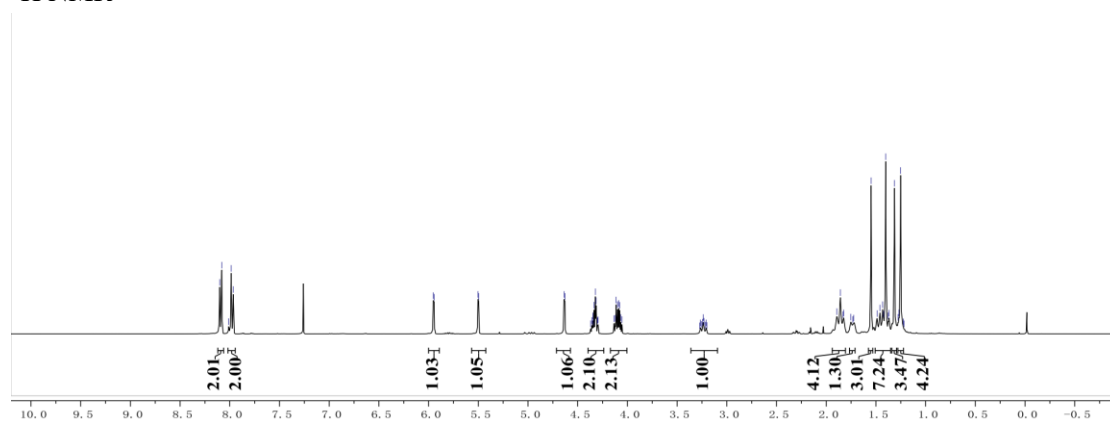


¹H NMR¹³C NMR¹⁹F NMR

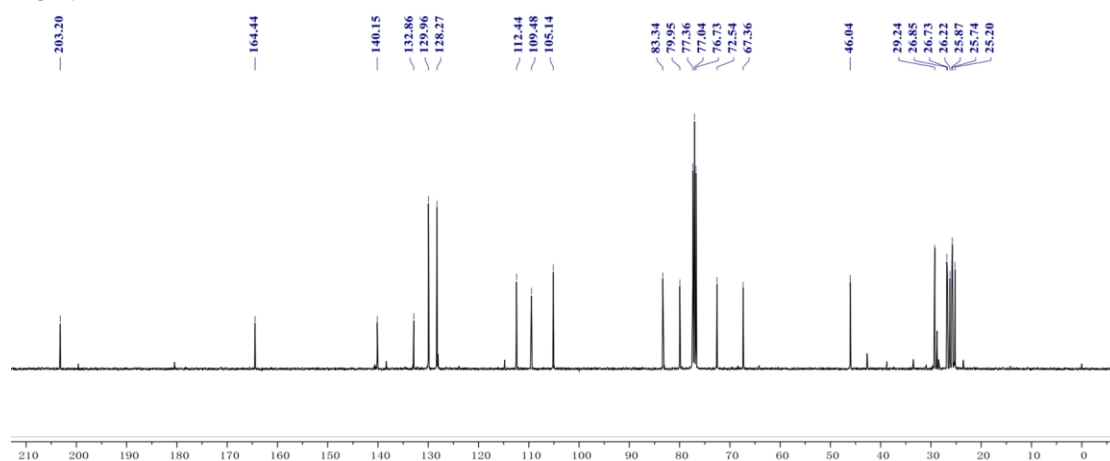
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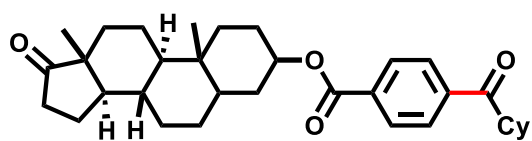
^1H NMR



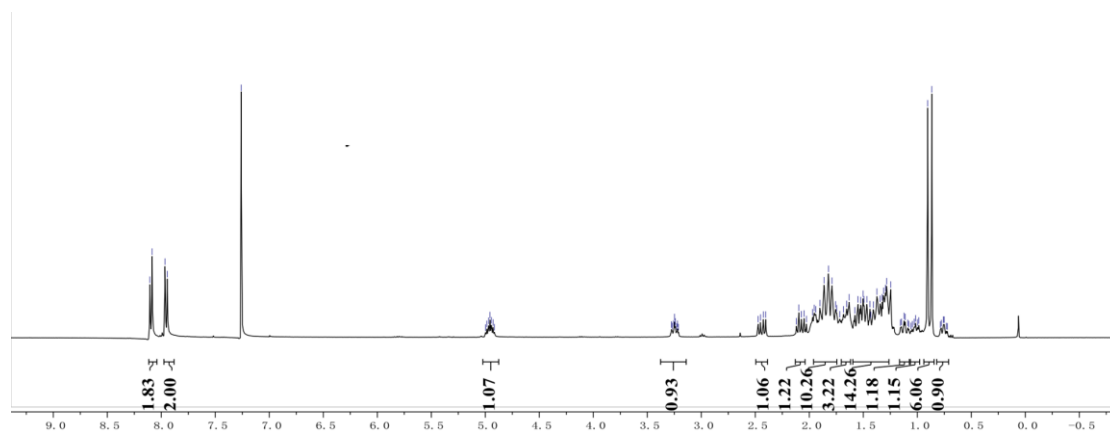
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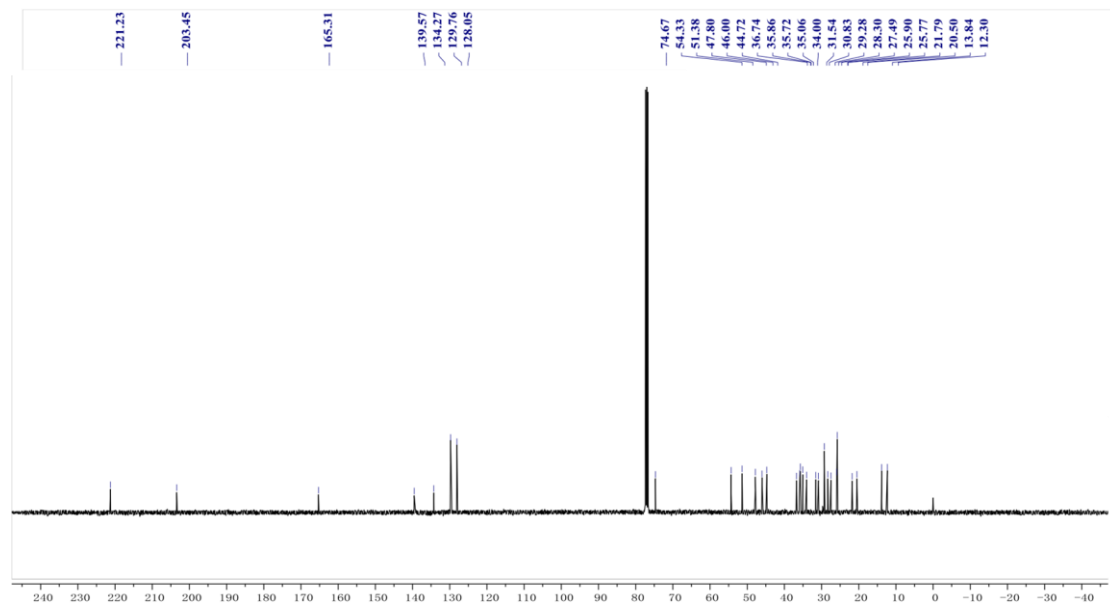
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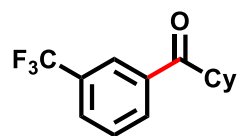
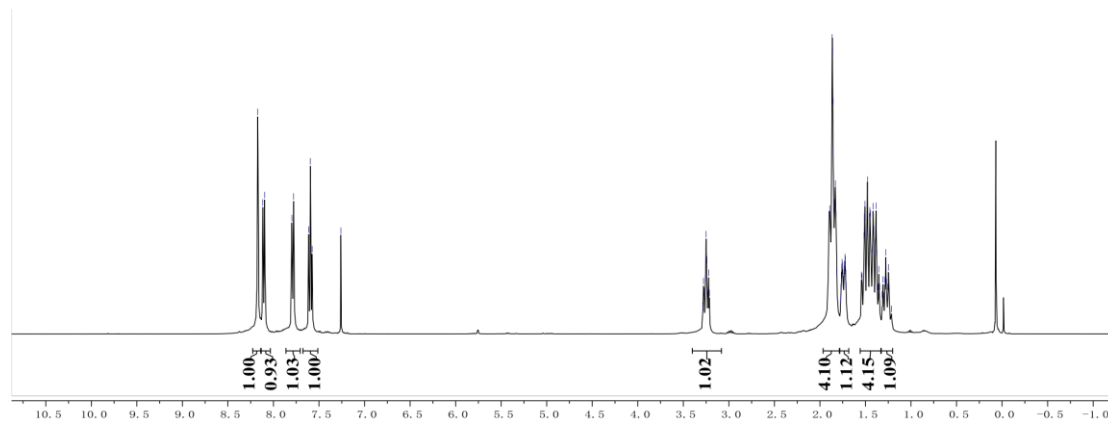
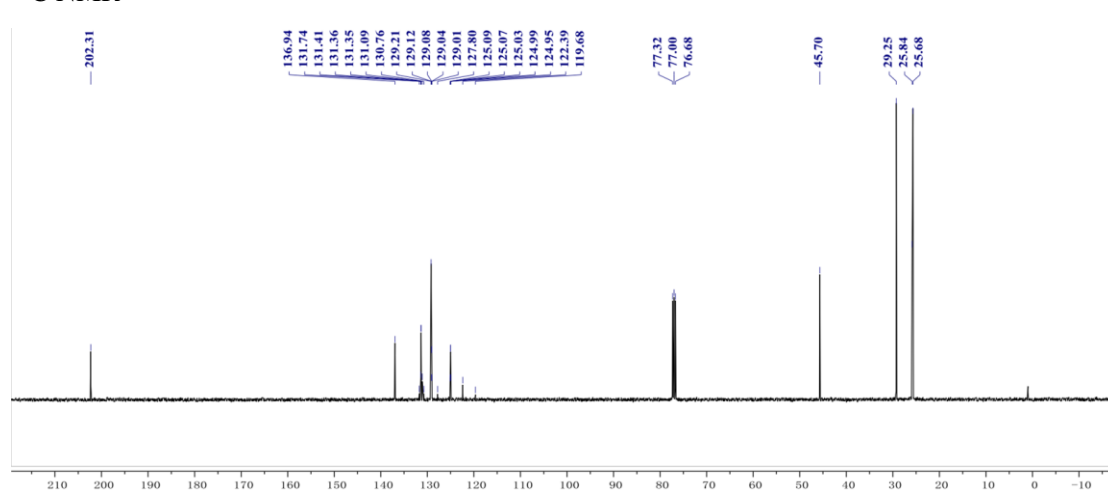
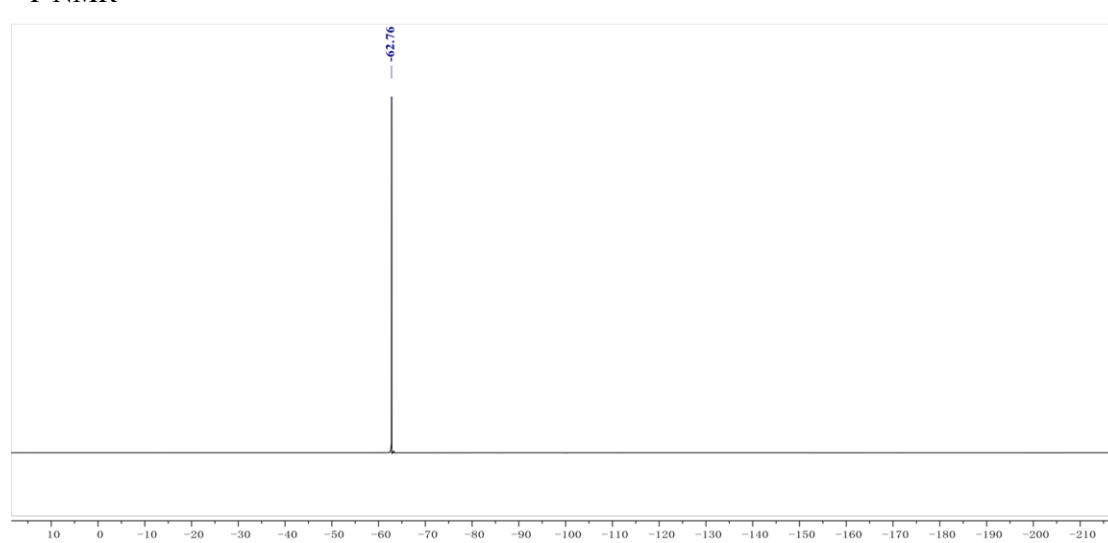
^1H NMR



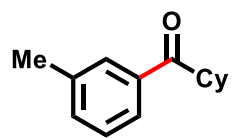
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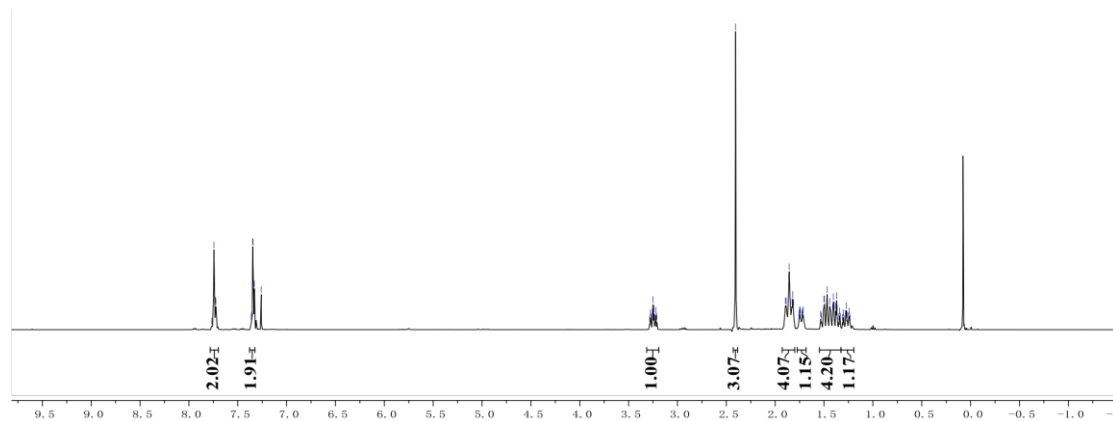
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¹H NMR¹³C NMR¹⁹F NMR

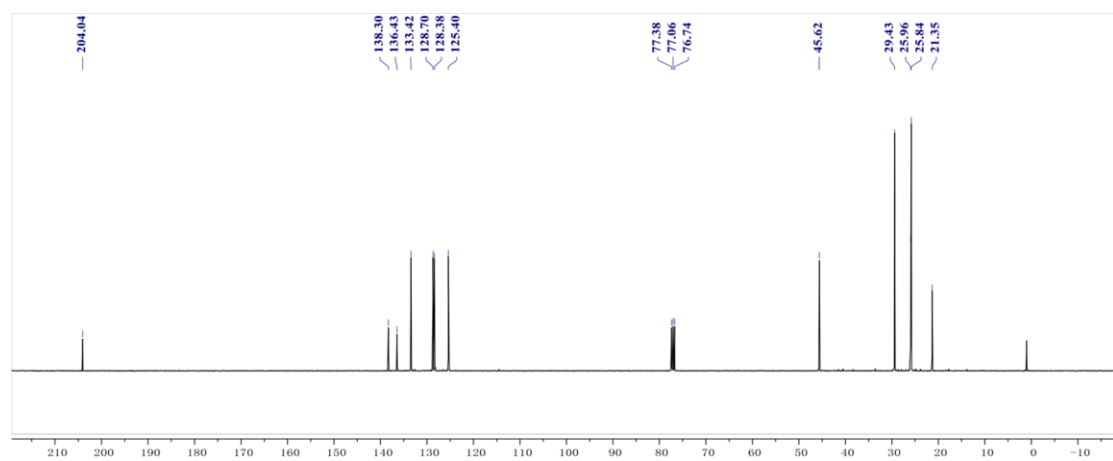
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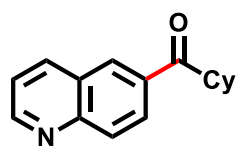
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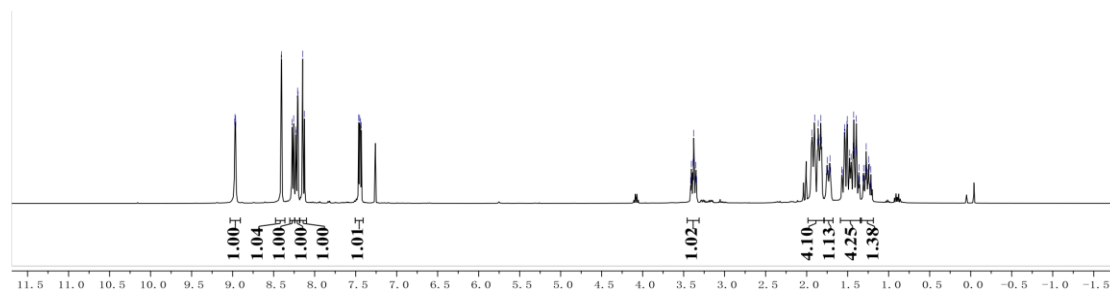
^{13}C NMR



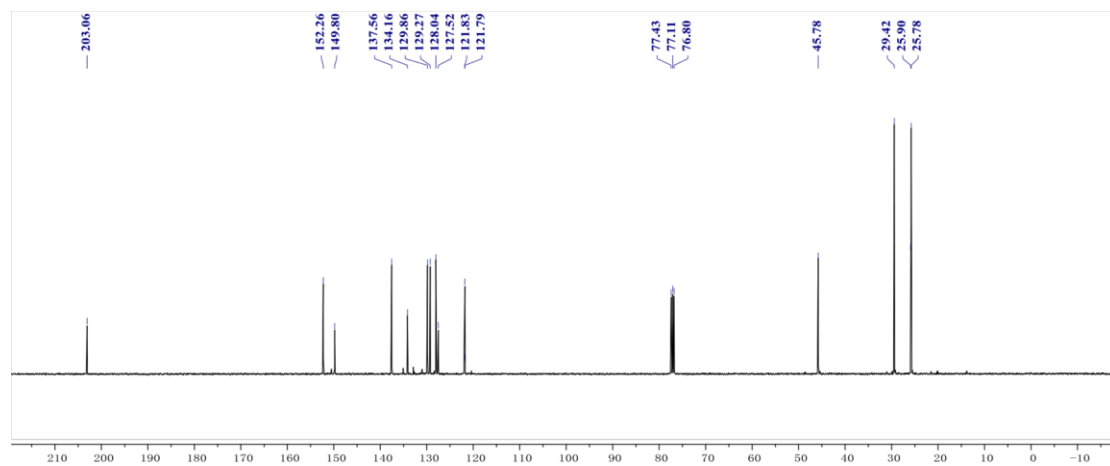
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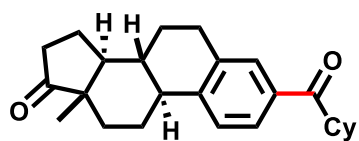
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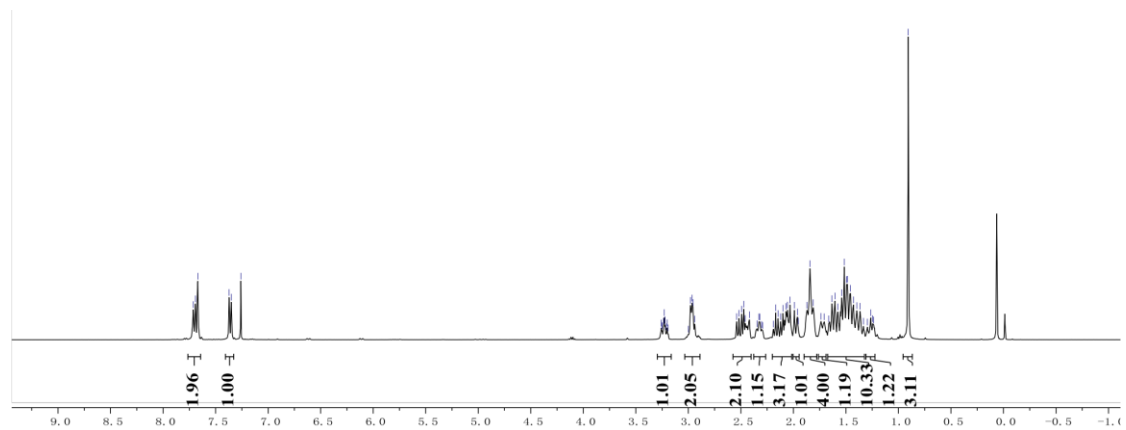
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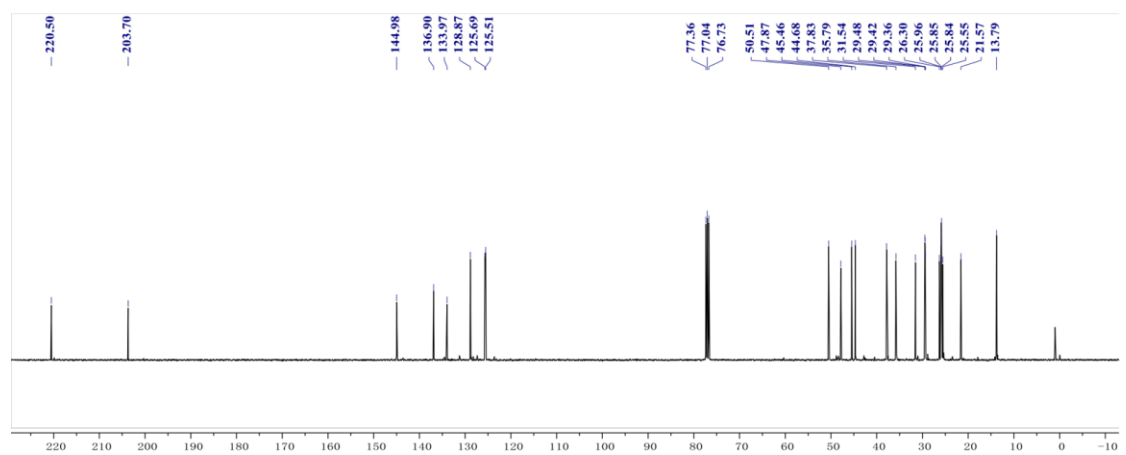
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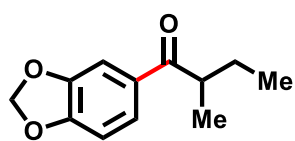
^1H NMR



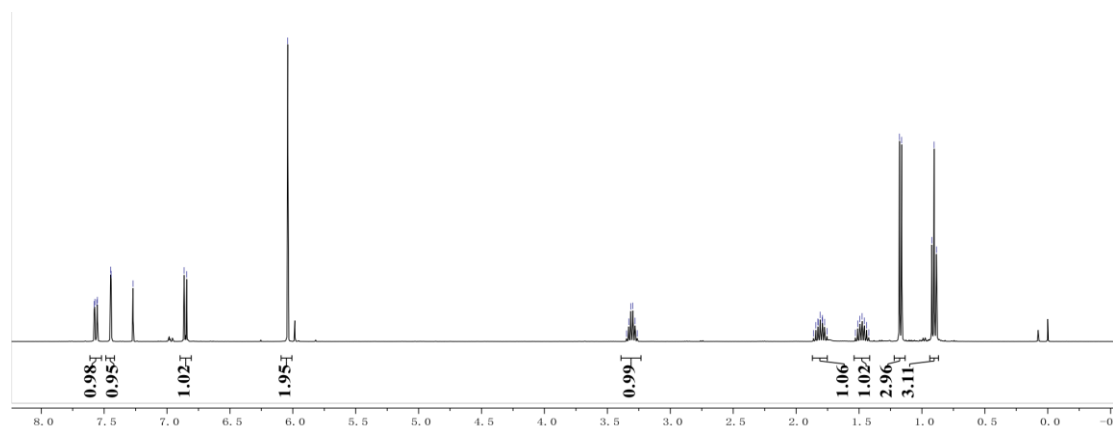
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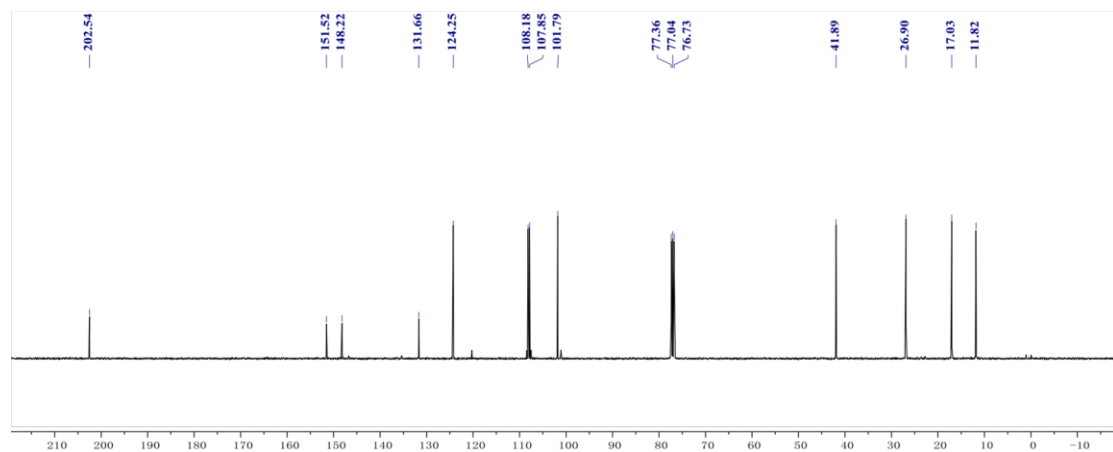
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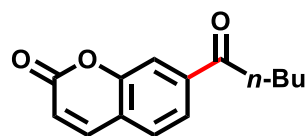
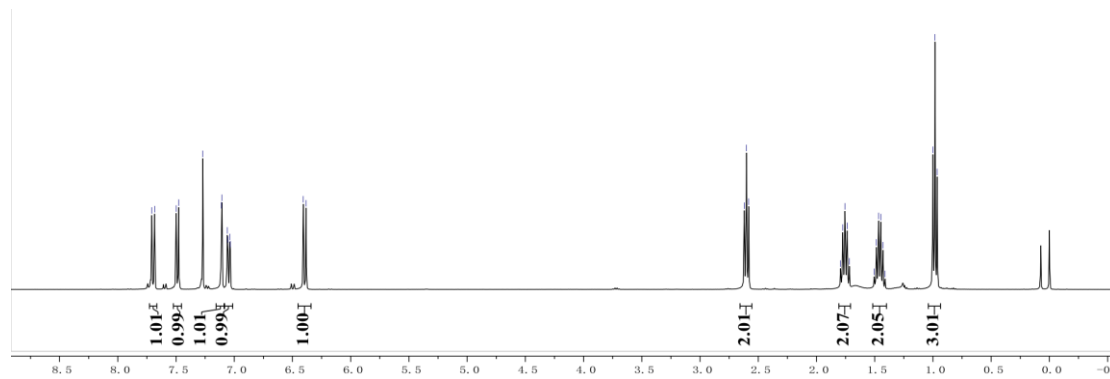
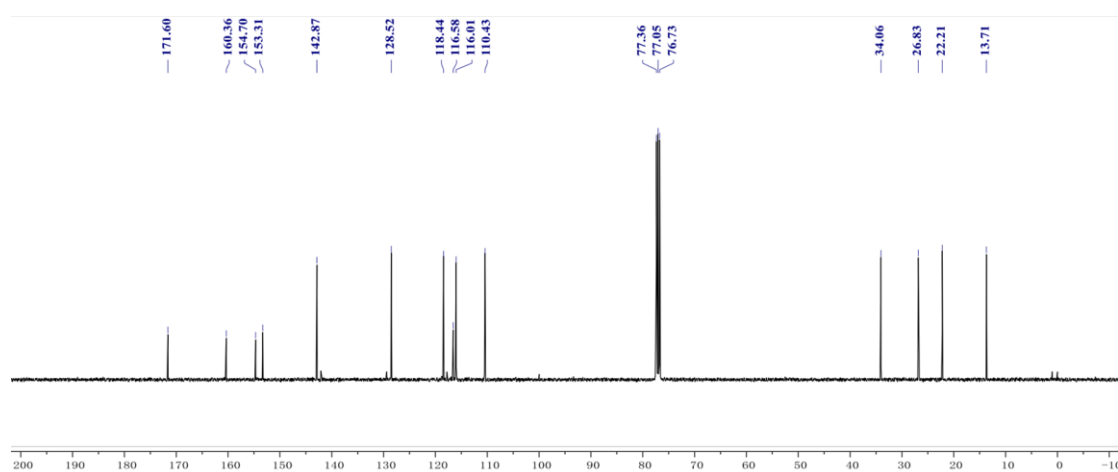
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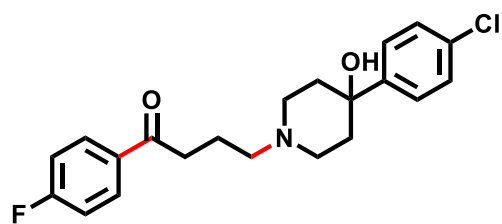
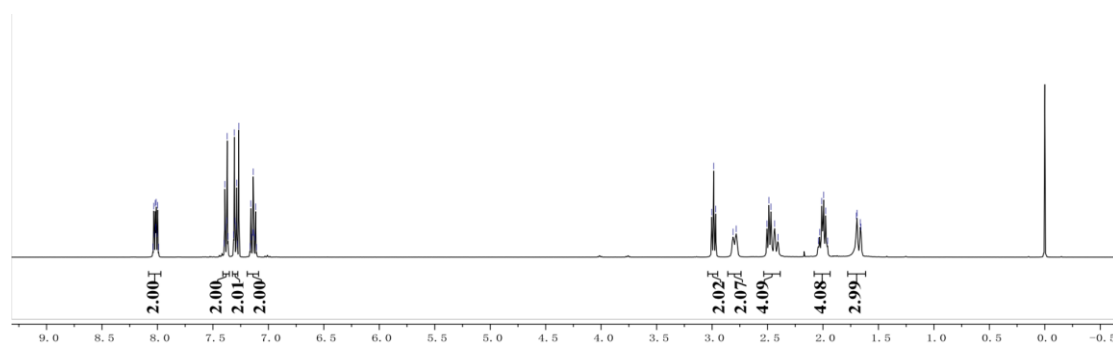
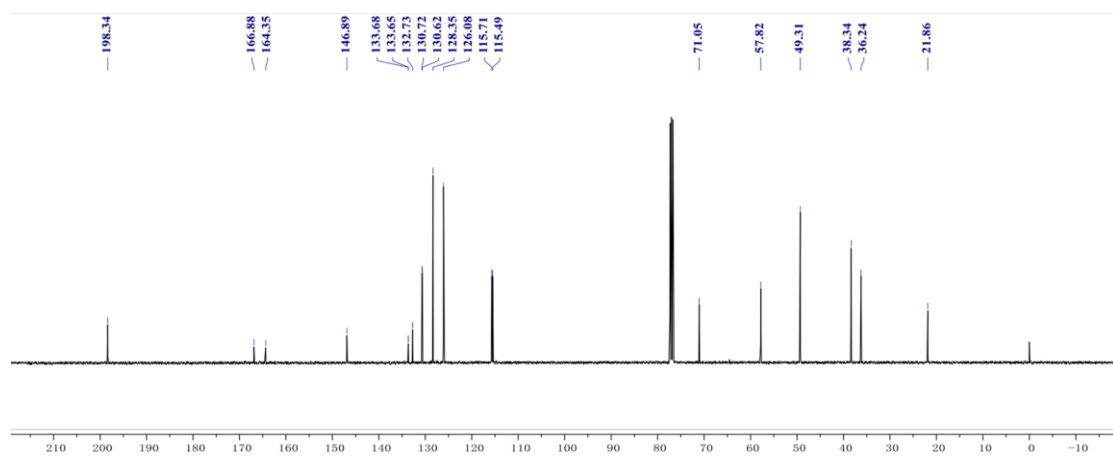


¹³C NMR



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 ^1H NMR ^{13}C NMR

 $^1\text{H NMR}$  $^{13}\text{C NMR}$  $^{19}\text{F NMR}$ 