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Supporting information

Regioselective Synthesis of Indenones *via* Nickel-Catalyzed Larock Annulations

Feipeng Liu,[‡a] Yongjie Li,[‡a,b] Xuchao Wang,[a] Qing Qiang,[a] Zijuan Yan,[a] Yao Zhang,[b] and Zi-Qiang Rong*[a,c]

[a]Frontiers Science Center for Flexible Electronics (FSCFE), Shaanxi Institute of Flexible Electronics (SIFE) & Shaanxi Institute of Biomedical Materials and Engineering (SIBME), Northwestern Polytechnical University (NPU), 127 West Youyi Road, Xi'an 710072, P. R. China

[b]College of Chemistry, Liaoning University, Shenyang, 110036, P. R. China

[c]Chongqing Key Laboratory of Natural Product Synthesis and Drug Research, Chongqing 401331, P. R. China

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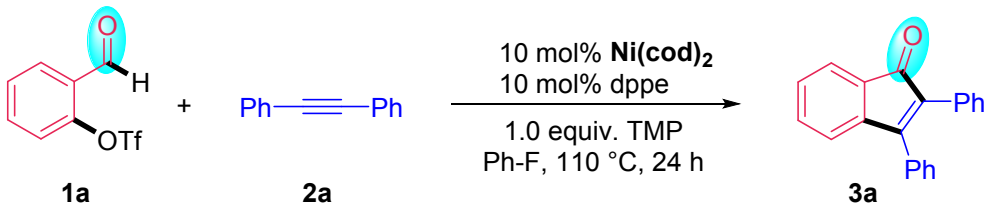
1. General Information

Unless noted otherwise, all solvents were dried by filtration through a Pure-Solv MD-5 Solvent Purification System (Innovative Technology). Florobenzene(Ph-F) was carefully freeze-pump-thawed and dried by 4A molecular sieves(activated at 350 ^{o}C for 8h). Reaction temperatures were reported as the temperatures of the bath surrounding vial. Sensitive reagents and solvents were transferred under nitrogen into a nitrogen-filled glovebox with standard techniques. Analytical thin-layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates (silica gel 60, F254, Leyan chemical). Vial (26 x 109 mm (15 mL) with PTFE lined cap attached) were purchased from Synthware. High resolution mass spectra (HR-MS) were recorded on an Agilent 6530 LC Q-TOF mass spectrometer using electrospray ionization with fragmentation voltage set at 115 V and processed with an Agilent MassHunter Operating System. Nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded with a Bruker DMX 400 (400 MHz, ^{1}H at 400 MHz, ^{13}C at 101 MHz) or Bruker Model DMX 500 (500 MHz, ^{1}H at 500 MHz, ^{13}C at 126 MHz,). Chemical shifts were reported in parts per million (ppm, δ), downfield from tetramethylsilane (TMS, δ=0.00ppm) and were referenced to residual solvent ($CDCl_3$, δ=7.26 ppm (^{1}H) and 77.00 ppm (^{13}C)). All the ^{19}F chemical shifts were not referenced. Coupling constants were reported in Hertz (Hz). Data for ^{1}H NMR spectra were reported as follows: chemical shift (ppm, referenced to protium, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration). All other materials were obtained from Rhawn Corporation, Aladdin Bio-Chem Technology or Energy chemical and were used as received.

2. Optimization of Ni-catalyzed Indenone synthesis

Table S1 Optimization of Ni-catalyzed annulation reaction between **1a** and **2a**[a]



1a **2a** **3a**

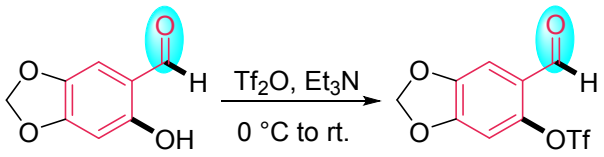
entry	Variation from standard conditions	yield (%)[b]
1	**None**	**89**
2	w/o [Ni]	< 5%
3	w/o ligand	< 5%
4	w/o TMP	10
5	5 mol% $Ni(cod)_2$	79%
6	$NiBr_2$ instead of $Ni(cod)_2$	< 5%
7	$Ni(OTf)_2$ instead of $Ni(cod)_2$	6
8	$Ni(acac)_2$ instead of $Ni(cod)_2$	< 5%
9	$NiCl_2$. glyme instead of $Ni(cod)_2$	11
10	IPr instead of dppe	< 5%
11	IMes instead of dppe	< 5%
12	2,2'-bipyridine instead of dppe	< 5%
13	PCy_3 instead of dppe	< 5%
14	dppp instead of dppe	64
15	dppb instead of dppe	75
16	dcype instead of dppe	49
17	Xantphos instead of dppe	8
18	1,2,2,6,6-pentamethylpiperidine instead of TMP	86
19	1-methylpiperidine instead of TMP	18
20	K_2CO_3 instead of TMP	32
21	toluene instead of Ph-F	61
22	chlorobenzene instead Ph-F	57
23	THF instead of Ph-F	5
24	2-Bromobenzaldehyde instead of **1a**	29[c]
25	2-Iodo benzaldehyde instead of **1a**	54[c]
26	1,4-dioxane instead of Ph-F	6
27	0.05 M instead of 0.1 M	80%
28	0.2 M instead of 0.1 M	86%

[a]Reaction condition: **1a**(0.2mmol), **2a** (0.4 mmol), TMP (1.0 equiv.), $Ni(cod)_2$ catalyst (10 mol%), in Ph-F (2.0 mL) at 110 °C under N_2 for 24 h. [b]Yields was isolated. [c]2-(1,2-diphenylvinyl)benzaldehyde byproduct was founded.

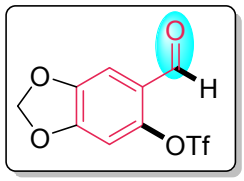
3. Experimental Procedures and Characterization Data

3.1. Preparation of aryl triflates (1):

Aryl triflates **1a-1k** and **4** were known compounds and were synthesized according to the reported procedures.[1]



To a solution of salicylaldehyde (830.7 mg, 5.0 mmol) in CH_2Cl_2 (15 mL), Et_3N (2.0 mL, 15 mmol) and Tf_2O (1.4 mL, 7.5 mmol) were successively added at 0 °C. After being stirred for 3 h at room temperature, the recation was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude product was extracted with CH_2Cl_2 and the combined organic extracts were washed with 1 M aqueous HCl, brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography (silica gel, PE/EtOAc = 10/1) to give **1l** (1.4 g, 91%) as a colorless oil.

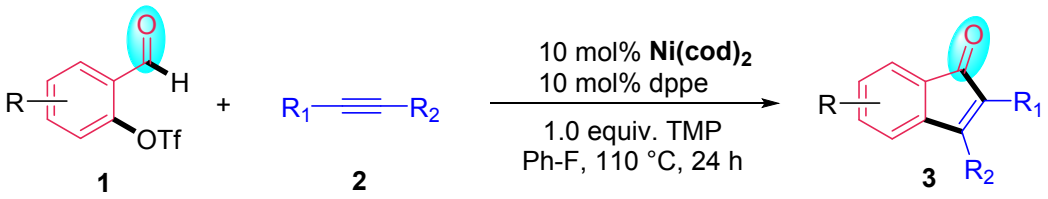


1l: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.11 (s, 1H), 7.36 (s, 1H), 6.85 (s, 1H), 6.17 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.8, 153.5, 148.1, 146.6, 123.4, 118.6(q, J = 320.8 Hz), 106.9, 103.6, 103.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -72.7. **HRMS** (ESI): Calculated for $C_9H_6F_3O_6S$ ($M+H^+$): 298.9832, found: 298.9825.

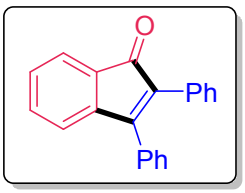
3.2. Preparation of alkyne (2):

Alkenes **2** are commercially available from Rhawn Corporation, Aladdin Bio-Chem Technology and Energy chemical, or synthesized according to the reported procedures.[2]

3.3 General Procedure of Ni-Catalyzed Annulation Reaction

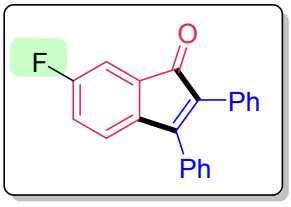


A flame-dried 15.0 mL vial were charged with 2-formylphenyl trifluoromethanesulfonate **1** (0.3 mmol, 1.0 equiv.) and substituted alkyne **2** (0.6 mmol, 2.0 equiv). The vial was directly transferred into a nitrogen-filled glovebox without caps. Then, $Ni(cod)_2$ (8.3 mg, 0.03 mmol, 10 mol%), dppe (12.0 mg, 0.03 mmol, 10 mol%), TMP (42.4 mg, 0.3 mmol, 1.0 equiv.) and 3.0 mL dry Ph-F were added. The vial was tightly sealed, transferred out of glovebox and stirred at 100 °C for 24 hours. After completion of the reaction, the mixture was filtered through a thin pad of silica gel and washed with EtOAc. The solvent was removed *in vacuo* and the residue was purified by flash column chromatography on silica gel to give the desired indenone product.



CAS: 1801-42-9

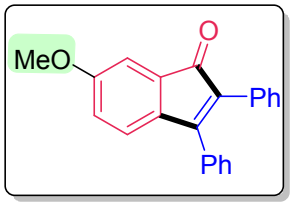
3a: Red solid (0.3 mmol scale, 75.3 mg, 89%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 6.8 Hz, 1H), 7.45 – 7.34 (m, 6H), 7.31 – 7.23 (m, 6H), 7.15 (d, *J* = 7.3 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 196.5, 155.3, 145.2, 133.4, 132.7, 132.4, 130.7, 130.7, 130.0, 129.3, 128.9, 128.8, 128.5, 128.1, 127.7, 123.0, 121.2. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



CAS: 1632479-36-7

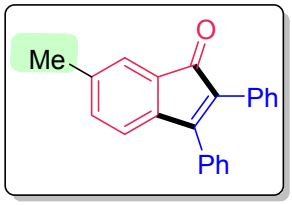
3b: Orange solid (0.3 mmol scale, 87.4 mg, 97%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) 7.40 (m, 3H), 7.36 (m, 2H), 7.28 (dd, *J* = 7.0, 2.4 Hz, 1H), 7.24 (m, 4H), 7.09 (dd, *J* = 8.0, 4.5 Hz, 1H), 7.01 (td, *J* = 8.5, 2.4 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.9, 163.7(d, *J* = 250.4 Hz), 155.4, 140.6(d, *J* = 3.4 Hz), 133.2(d, *J* = 7.3 Hz), 132.7(d, *J* = 5.4 Hz), 132.5, 130.5, 129.9, 129.6, 128.9, 128.4, 128.2, 127.9, 122.4(d, *J* = 8.0

Hz), 118.6 (d, J = 23.0 Hz), 111.6(d, J = 24.8 Hz). Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



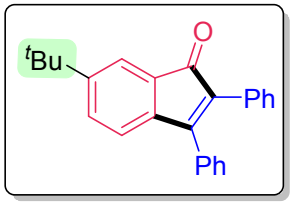
CAS: 70603-19-9

3c: Red solid (0.3 mmol scale, 66.5 mg, 71%). R_f = 0.30 (hexane/ethyl acetate = 5:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38 (m, 6H), 7.26 – 7.18 (m, 5H), 7.02 (d, J = 8.0 Hz, 1H), 6.78 (dd, J = 8.0, 2.5 Hz, 1H), 3.83 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.2, 161.1, 156.4, 137.0, 133.0, 132.9, 131.4, 131.0, 129.9, 129.4, 128.8, 128.5, 128.1, 127.5, 122.3, 116.3, 110.7, 55.8. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[4]

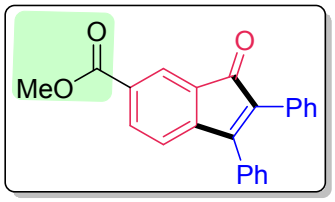


CAS: 34665-58-2

3d: Orange solid (0.3 mmol scale, 53.8 mg, 77.3%). R_f = 0.40 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.56 – 7.32 (m, 6H), 7.28 (d, J = 3.9 Hz, 5H), 7.18 (d, J = 7.4 Hz, 1H), 7.05 (d, J = 7.4 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.8, 155.6, 142.4, 139.3, 133.3, 132.9, 131.8, 131.1, 130.9, 129.9, 129.2, 128.7, 128.5, 128.0, 127.6, 124.1, 121.1, 21.4. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]

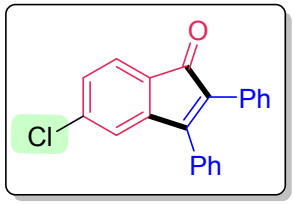


3e: Orange solid (0.3 mmol scale, 88.4 mg, 87%). Melting point: 141-143 ℃. R_f = 0.40 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.42 (m, 6H), 7.29 (m, 5H), 7.10 (d, J = 7.7 Hz, 1H), 1.37 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.9, 155.4, 152.9, 142.4, 132.9, 132.3, 131.0, 130.9, 129.9, 129.5, 129.2, 128.7, 128.5, 128.1, 127.6, 121.0, 120.8, 35.1, 31.1. **HRMS** (ESI): Calculated for $C_{25}H_{23}O$ ($M+H^+$): 339.1743, found: 339.1740.



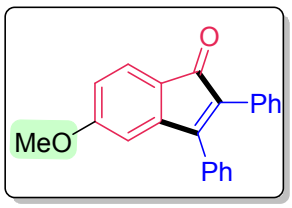
CAS: 2324882-81-5

3f: Orange solid (0.3 mmol scale, 67.3 mg, 66%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.12 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.35 (m, 6H), 7.28 (s, 4H), 7.23 (d, *J* = 7.6 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.1, 166.1, 154.4, 149.6, 135.6, 134.6, 132.2, 130.9, 130.8, 130.2, 130.0, 129.6, 128.9, 128.5, 128.2, 128.2, 123.6, 121.0, 52.3. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



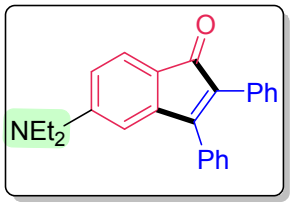
CAS: 855612-26-9

3g: Orange solid (0.3 mmol scale, 91.1 mg, 96%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.46 – 7.41 (m, 3H), 7.36 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.26 (s, 6H), 7.11 (d, *J* = 1.6 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 195.0, 154.0, 147.2, 139.7, 133.5, 132.2, 130.3, 130.0, 129.6, 129.0, 128.9, 128.5, 128.4, 128.13, 128.06, 123.9, 122.0. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



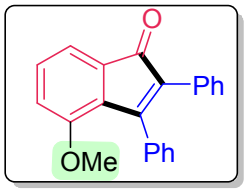
CAS: 65908-33-0

3h: Orange solid (0.3 mmol scale, 62.9 mg, 67%). R_f = 0.30 (hexane/ethyl acetate = 5:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.43 (dt, *J* = 6.0, 2.6 Hz, 3H), 7.39 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.28 (mz, 5H), 6.73 (d, *J* = 2.1 Hz, 1H), 6.70 (dd, *J* = 7.9, 2.2 Hz, 1H), 3.86 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.0, 164.4, 153.1, 147.9, 133.8, 132.7, 130.8, 130.0, 129.1, 128.8, 128.5, 128.0, 127.7, 124.9, 123.4, 110.4, 110.3, 55.7. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[5]



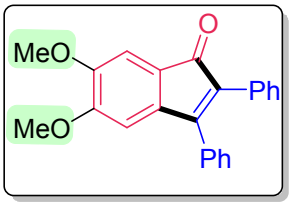
CAS: 1924649-77-3

3i: Red solid (0.3 mmol scale, 76.3 mg, 72%). R_f = 0.25 (hexane/ethyl acetate = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.3 Hz, 1H), 7.47 – 7.34 (m, 5H), 7.34 – 7.21 (m, 5H), 6.47 (d, *J* = 2.3 Hz, 1H), 6.38 (dd, *J* = 8.3, 2.3 Hz, 1H), 3.42 (q, *J* = 7.1 Hz, 4H), 1.21 (t, *J* = 7.1 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.4, 152.0, 151.7, 148.5, 134.3, 133.2, 131.5, 130.0, 128.6, 128.6, 127.8, 127.3, 125.6, 117.1, 107.5, 106.2, 44.9, 12.6. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[5]



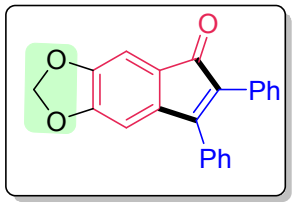
CAS: 70603-18-8

3j: Orange solid (0.3 mmol scale, 74.0 mg, 79%). R_f = 0.35 (hexane/ethyl acetate = 5:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36 (m, 5H), 7.32 – 7.27 (m, 2H), 7.22 (m, 3H), 7.18 (m, 2H), 7.01 (dd, *J* = 7.0, 2.3 Hz, 1H), 3.61 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.5, 157.0, 154.0, 134.9, 132.6, 132.2, 131.0, 130.9, 130.1, 128.6, 128.3, 127.8, 127.5, 127.3, 119.6, 116.0, 55.7. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[6]



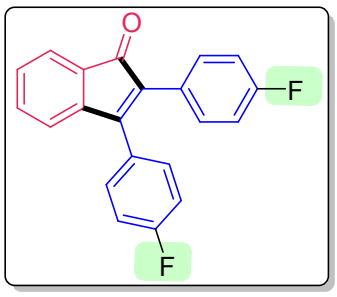
CAS: 1629016-39-2

3k: Red solid (0.3 mmol scale, 72.9 mg, 71%). R_f = 0.25 (hexane/ethyl acetate = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.46 – 7.34 (m, 5H), 7.26 – 7.20 (m, 6H), 6.68 (s, 1H), 3.93 (s, 3H), 3.87 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.0, 154.0, 152.7, 149.1, 139.6, 132.9, 131.3, 130.9, 129.8, 129.2, 128.8, 128.3, 128.0, 127.4, 123.0, 107.6, 105.9, 56.4, 56.3. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[7]



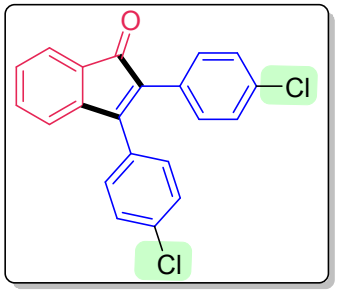
CAS: 1300636-00-3

3l: Red solid (0.3 mmol scale, 75.4 mg, 77%). R_f = 0.35 (hexane/ethyl acetate = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.4 (m, 3H), 7.33 (m, 2H), 7.23 (m, 5H), 7.08 (s, 1H), 6.64 (s, 1H), 6.01 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.1, 153.7, 151.6, 147.7, 141.8, 132.7, 131.4, 130.8, 129.8, 129.2, 128.8, 128.4, 128.0, 127.5, 124.7, 105.2, 104.0, 102.1. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[7]



CAS: 1264166-21-3

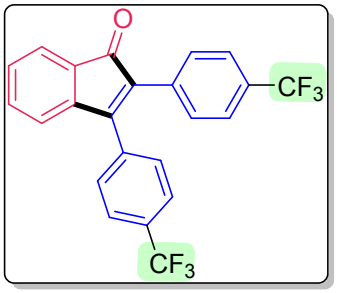
3m: Orange solid (0.3 mmol scale, 83.1 mg, 87%). R_f = 0.30 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.58 (d, J = 7.0 Hz, 1H), 7.42 – 7.34 (m, 3H), 7.30 (t, J = 7.4 Hz, 1H), 7.12 (t, J = 8.8 Hz, 3H), 7.01 – 6.93 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.2, 163.1 (d, J = 250.6 Hz), 162.4(d, J = 248.7 Hz), 154.1, 144.9, 133.6, 131.7 (d, J = 8.2 Hz), 131.5, 130.5 (d, J = 8.2 Hz), 129.1, 128.5 (d, J = 3.6 Hz), 126.5 (d, J = 3.6 Hz), 123.1, 121.1, 116.2 (d, J = 21.6 Hz), 115.4, 115.3 (d, J = 21.9 Hz). Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[4]



CAS: 96286-65-6

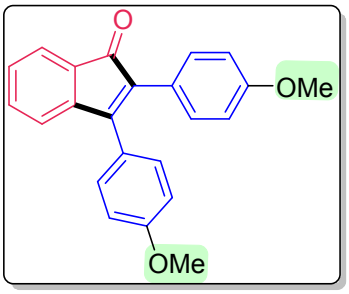
3n: Orange solid (0.3 mmol scale, 100.8 mg, 96%). R_f = 0.15 (hexane/ethyl acetate = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (d, J = 7.0 Hz, 1H), 7.50 – 7.39 (m, 3H), 7.39 – 7.31 (m, 3H), 7.30 – 7.27 (m, 2H), 7.25 – 7.20 (m,

2H), 7.14 (d, J = 7.3 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.8, 154.3, 144.6, 135.5, 134.0, 133.7, 131.5, 131.2, 130.8, 130.5, 129.8, 129.3, 128.5, 123.3, 121.2. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[8]



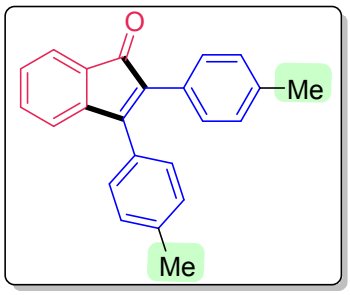
CAS: 1198576-71-4

3o: Yellow solid (0.3 mmol scale, 101.6 mg, 81%). R_f = 0.30 (hexane/ethyl acetate = 5:1).**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (d, J = 7.7 Hz, 1H), 7.64 (d, J = 6.8 Hz, 1H), 7.53 (dd, J = 18.5, 8.0 Hz, 4H), 7.43 (td, J = 7.5, 2.4 Hz, 1H), 7.36 (d, J = 7.8 Hz, 3H), 7.12 (d, J = 7.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.3, 155.0, 144.3, 136.0, 133.9, 133.8, 131.7(q, J = 21.6Hz), 130.2, 130.19(q, J = 21.6Hz), 130.15, 129.9, 129.8, 128.8, 126.1 (q, J = 3.9 Hz), 125.2 (q, J = 3.7 Hz), 124.0 (q, J = 272.6 Hz), 123.7(q, J = 272.9 Hz),123.6, 121.4. Both the ^{1}H NMR, ^{13}C NMR and ^{19}F NMR match the literature reported data.[4]



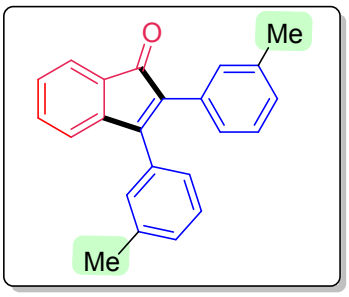
CAS: 41099-25-6

3p: Red solid (0.3 mmol scale, 80.3 mg, 78%). R_f = 0.20 (hexane/ethyl acetate = 5:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.57 (d, J = 7.0 Hz, 1H), 7.37 (m, 3H), 7.28 (m, 3H), 7.19 (d, J = 7.2 Hz, 1H), 6.96 (d, J = 8.2 Hz, 2H), 6.84 (d, J = 8.3 Hz, 2H), 3.88 (s, 3H), 3.82 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.8, 154.8 145.4, 139.3, 137.5, 133.3, 132.0, 130.9, 129.8, 129.4, 128.8, 128.7, 128.5, 127.9, 122.7, 121.1, 21.5, 21.3. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



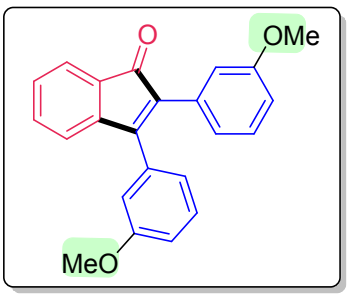
CAS: 41099-26-7

3q: Orange solid (0.3 mmol scale, 66.4 mg, 71%). R_f = 0.30 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.0 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.23 – 7.16 (m, 3H), 7.11 (d, *J* = 7.8 Hz, 2H), 2.43 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 196.8, 154.8, 145.4, 139.3, 137.5, 133.3, 132.0, 130.9, 129.8, 129.4, 128.8, 128.7, 128.6, 127.9, 122.8, 121.1, 21.5, 21.3. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



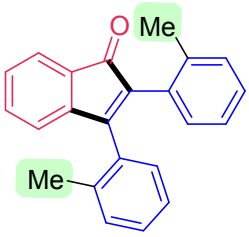
CAS: 112818-89-0

3r: Orange solid (0.3 mmol scale, 68.0 mg, 73%). R_f = 0.30 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.0 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.35 – 7.15 (m, 8H), 7.07 (m, 2H), 2.39 (s, 3H), 2.32 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.6, 155.4, 145.4, 138.3, 137.5, 133.3, 132.7, 132.3, 130.8, 130.7, 130.6, 130.0, 128.8, 128.6, 128.5, 127.8, 127.0, 125.6, 122.8, 121.2, 21.4 (s). Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[7]



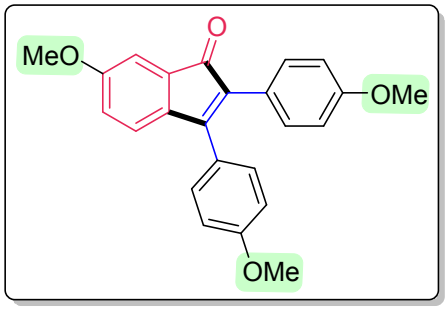
CAS: 1264166-23-5

3s: Red solid (0.3 mmol scale, 78.1 mg, 76%). R_f = 0.30 (hexane/ethyl acetate = 5:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 6.8 Hz, 1H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.36 – 7.14 (m, 8H), 7.09 (d, *J* = 7.3 Hz, 1H), 7.05 (d, *J* = 7.4 Hz, 1H), 2.39 (s, 3H), 2.32 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.3, 159.7, 159.1, 155.4, 145.1, 134.0, 133.5, 132.2, 131.9, 130.7, 129.9, 129.01, 128.96, 122.9, 122.4, 121.3, 120.8, 115.1, 114.9, 114.0, 113.7, 55.2, 55.0. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



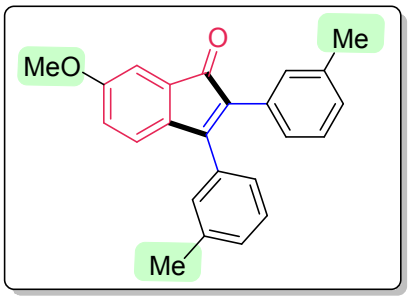
CAS: 1380243-16-2

3t: Orange oil (0.3 mmol scale, 36.4 mg, 39%). R_f = 0.30 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 6.9 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.32-7.25 (m, 2H), 7.27 – 7.12 (m, 5H), 7.07 (t, *J* = 6.8 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 7.1 Hz, 1H), 2.17 (s, 3H), 2.11 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.3, 157.6, 145.9, 137.1, 135.9, 135.8, 133.5, 131.0, 130.7, 130.6, 130.3, 128.9, 128.9 128.2, 125.8, 125.4, 122.9, 121.5, 20.7, 20.2. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[9]



CAS: 114095-38-4

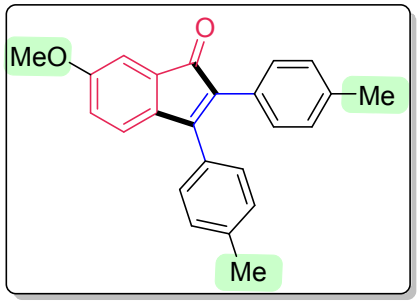
3u: Orange solid (0.3 mmol scale, 83.8 mg, 75%). R_f = 0.15 (hexane/ethyl acetate = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.15 (s, 1H), 7.05 (d, *J* = 7.9 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 2H), 6.81 (d, *J* = 8.1 Hz, 2H), 6.77 (d, *J* = 8.1 Hz, 1H), 3.84 (s, 6H), 3.78 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.5, 160.8, 160.3, 158.8, 154.8, 137.1, 133.2, 131.1, 130.2, 130.1, 125.3, 123.7, 121.9, 116.1, 114.1, 113.6, 110.3, 55.8, 55.3, 55.1. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[7]



CAS: 2241766-18-5

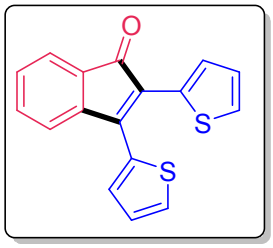
3v: Orange solid (0.3 mmol scale, 87.8 mg, 86%). R_f = 0.35 (hexane/ethyl acetate = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 1H), 7.26 – 7.23 (m, 2H), 7.21 (d, *J* = 2.5 Hz, 1H), 7.19 – 7.16 (m, 2H), 7.14 (d, *J* = 7.6 Hz, 1H), 7.07 (dd, *J* = 7.8, 4.3 Hz, 2H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.82 (dd, *J* = 8.0, 2.5 Hz, 1H), 3.87 (s, 3H), 2.38 (s, 3H), 2.31 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.3, 160.9, 156.4, 138.2, 137.4, 137.0, 132.9, 132.9, 131.3, 130.9, 130.4, 130.0, 128.7, 128.5, 128.2, 127.8, 126.8, 125.6, 122.2, 116.1, 110.5, 55.7, 21.4. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[7]

^{13}C NMR (126 MHz, $CDCl_3$)



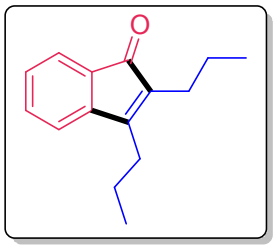
CAS: 2241766-17-4

3w: Red solid (0.3 mmol scale, 79.7 mg, 71%). R_f = 0.35 (hexane/ethyl acetate = 5:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 – 7.30 (m, 2H), 7.27 – 7.17 (m, 5H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 1H), 6.81 (dd, *J* = 8.0, 2.5 Hz, 1H), 3.87 (s, 3H), 2.43 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.4, 160.8, 155.8, 139.3, 137.1, 137.1, 133.1, 131.0, 130.0, 129.6, 129.6, 128.8, 128.4, 128.2, 122.0, 116.1, 110.4, 55.7, 21.5, 21.3. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[7]



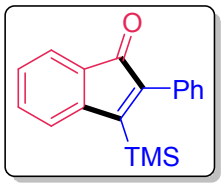
CAS: 131269-31-3

3x: Red solid (0.3 mmol scale, 60.0 mg, 68%). R_f = 0.25 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.54 (d, *J* = 7.1 Hz, 1H), 7.48 (dd, *J* = 3.7, 1.1 Hz, 1H), 7.41 – 7.32 (m, 3H), 7.28 – 7.19 (m, 3H), 7.02 (dd, *J* = 5.1, 3.7 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.0, 146.0, 145.6, 133.9, 133.1, 132.0, 130.1, 129.3, 129.1, 128.9, 128.8, 127.9, 127.7, 127.3, 127.0, 123.0, 121.3. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[8]



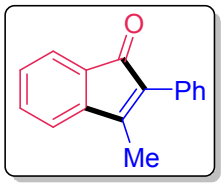
CAS: 147730-15-2

3y: Yellow oil (0.3 mmol scale, 34.7 mg, 54%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.1 Hz, 1H), 7.36 – 7.30 (m, 1H), 7.20 – 7.14 (m, 1H), 7.05 (d, *J* = 7.4 Hz, 1H), 2.54 (t, *J* = 7.6 Hz, 3H), 2.26 (t, *J* = 7.6 Hz, 3H), 1.67 (q, *J* = 7.1 Hz, 2H), 1.52 (q, *J* = 7.3 Hz, 2H), 1.06 (t, *J* = 7.3 Hz, 3H), 0.96 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 198.6, 157.7, 145.7, 134.8, 133.1, 131.1, 127.9, 121.7, 119.0, 28.3, 24.9, 22.5, 21.2, 14.4, 14.2. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[3]



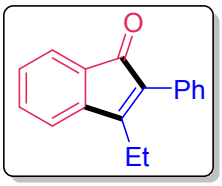
CAS: 182224-30-2

3z: Orange solid (0.3 mmol scale, 56.1 mg, 67%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.1 Hz, 1H), 7.50 – 7.43 (m, 4H), 7.37 – 7.27 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 197.7, 156.8, 148.6, 147.9, 134.0, 133.3, 130.0, 129.7, 128.2, 129.0, 128.0, 123.14, 123.11. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[8]



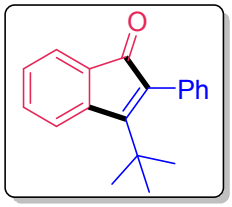
CAS: 10408-73-8

3aa: Orange oil (0.3 mmol scale, 45.0 mg, 68%). R_f = 0.30 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.1 Hz, 1H), 7.47 – 7.38 (m, 5H), 7.36 – 7.32 (m, 1H), 7.28 – 7.24 (m, 1H), 7.16 (d, *J* = 7.2 Hz, 1H), 2.32 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.4, 154.6, 145.9, 133.6, 133.4, 131.2, 130.4, 129.5, 128.9, 128.3, 127.7, 122.1, 119.4, 12.6 (major:minor 5.8:1). Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[10]

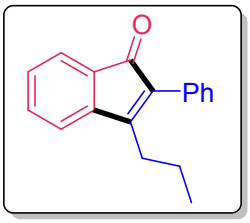


CAS: 13304-50-2

3ab: Orange solid (0.3 mmol scale, 42.7 mg, 61%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.1 Hz, 1H), 7.43 (m, 6H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 7.3 Hz, 1H), 2.76 (q, *J* = 7.4 Hz, 2H), 1.36 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.8, 159.9, 144.9, 133.5, 132.8, 131.2, 130.8, 129.3, 128.7, 128.3, 127.7, 122.3, 119.8, 20.0, 12.8 (major:minor 14:1). Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[11]

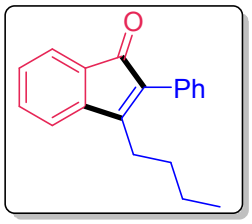


3ac: Yellow solid (0.3 mmol scale, 42.5 mg, 54%). Melting point: 124-126 ℃. R_f = 0.30 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.57 – 7.53 (m, 2H), 7.43 (td, *J* = 7.7, 1.3 Hz, 1H), 7.41 – 7.34 (m, 3H), 7.29 – 7.24 (m, 1H), 7.21 – 7.17 (m, 2H), 1.33 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 198.0, 164.3, 145.1, 134.2, 133.9, 133.2, 131.4, 130.2, 128.0, 127.5, 127.4, 123.9, 122.4, 36.2, 30.4. **HRMS** (ESI): Calculated for $C_{19}H_{19}O$ ($M+H^+$): 263.1430, found: 263.1429.



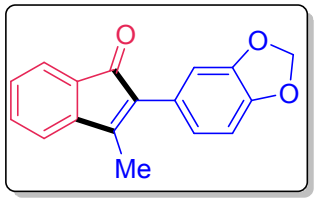
CAS: 13304-58-0

3ad: Yellow oil (0.3 mmol scale, 52.9 mg, 71%). R_f = 0.40 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.1 Hz, 1H), 7.46 – 7.32 (m, 6H), 7.28 – 7.22 (m, 1H), 7.18 (d, *J* = 7.2 Hz, 1H), 2.73 – 2.63 (m, 2H), 1.77 – 1.68 (m, 2H), 1.02 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.7, 158.6, 145.2, 133.49, 133.46, 131.3, 130.7, 129.4, 128.7, 128.3, 127.7, 122.3, 119.9, 28.8, 21.6, 14.5. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[12]

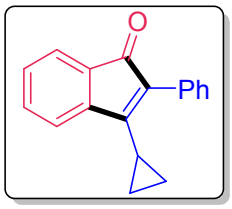


CAS: 5041-48-5

3ae: Orange oil (0.3 mmol scale, 61.4 mg, 78%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.0 Hz, 1H), 7.49 – 7.35 (m, 6H), 7.28 (td, *J* = 7.3, 0.9 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 1H), 2.74 (t, *J* = 7.9 Hz,, 2H), 1.78 – 1.67 (m, 2H), 1.48 (dt, *J* = 14.9, 7.4 Hz, 2H), 0.96 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.7, 158.9, 145.2, 133.5, 133.3, 131.3, 130.7, 129.4, 128.7, 128.3, 127.7, 122.3, 119.9, 30.3, 26.5, 23.0, 13.8.Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[13]



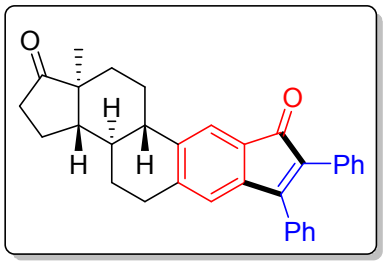
3af: Red solid (0.3 mmol scale, 57.9 mg, 73%). Melting point: 121-123 ℃. R_f = 0.35 (hexane/ethyl acetate = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.0 Hz, 1H), 7.43 (td, *J* = 7.5, 1.2 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.16 (d, *J* = 7.2 Hz, 1H), 6.95 (t, *J* = 1.0 Hz, 1H), 6.92 (t, *J* = 1.3 Hz, 2H), 6.01 (s, 2H), 2.32 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.5, 153.7, 147.5, 147.2, 145.9, 133.6, 133.0, 130.3, 128.7, 124.9, 123.5, 122.1, 119.3, 109.9, 108.3, 101.1, 12.6.**HRMS** (ESI): Calculated for $C_{17}H_{13}O_3$ ($M+H^+$): 265.0859, found: 265.0859.



CAS: 2139334-97-5

3ag: Orange oil (0.3 mmol scale, 48.0 mg, 65%). R_f = 0.35 (hexane/ethyl acetate = 10:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.67 – 7.42 (m, 5H), 7.38 (m, 2H), 7.27 (td, *J* = 7.6, 2.6 Hz, 1H), 7.18 (dd, *J* = 7.4, 2.7 Hz, 1H), 2.18 – 2.12 (m, 1H), 1.21 – 0.97 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.3, 159.6, 144.1, 133.8, 133.4, 131.2, 131.1, 129.9, 128.7, 128.0, 127.6, 122.2, 120.5, 11.3, 8.1. Both the ^{1}H NMR and ^{13}C NMR match the literature reported data.[14]

3.4 *Sythesis of Estrone-derived indenone*



A flame-dried 15.0 mL vial were charged with **4** which was prepared from estrone according to the reported procedure (0.3 mmol, 120.6 mg, 1.0 equiv.) and diphenylacetylene **2a** (0.6 mmol, 106.8mg, 2.0 equiv). The vial was directly transferred into a nitrogen-filled glovebox without caps. Then, $Ni(cod)_2$ (8.3 mg, 0.03 mmol, 10 mol%), dppe (12.0 mg, 0.03 mmol, 10 mol%), TMP (42.4 mg, 0.3 mmol, 1.0 equiv.) and 3.0 mL dry Ph-F were added. The vial was tightly sealed, transferred out of glovebox and stirred at 100 °C for 24 hours. After completion of the reaction, the mixture was filtered through a thin pad of silica gel and washed with EtOAc. The solvent was removed *in vacuo* and the residue was purified by flash column chromatography on silica gel to give the desired indenone **5**.

5: Red solid (0.3 mmol scale, 114.0 mg, 83%). R_f = 0.30 (hexane/ethyl acetate = 3:1). Melting point: 231-233 ℃. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.41 (m, 5H), 7.32 – 7.22 (m, 5H), 6.87 (s, 1H), 2.90 (dd, *J* = 9.2, 4.2 Hz, 2H), 2.59 – 2.48 (m, 2H), 2.32 (t, *J* = 8.9 Hz, 1H), 2.25 – 2.13 (m, 1H), 2.12 – 1.98 (m, 3H), 1.73 – 1.47 (m, 6H), 0.95 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 196.4, 155.0, 142.7, 142.4, 140.4, 132.9, 132.6, 130.91, 129.88, 129.1,

128.8, 128.7, 128.4, 128.0, 127.6, 122.3, 120.7, 50.3, 47.9, 44.5, 38.0, 35.8, 31.5, 30.3, 26.1, 25.8, 21.5, 13.8. **HRMS** (ESI): Calculated for $C_{33}H_{31}O_2$ ($M+H^+$): 459.2319, found: 459.2319.

4. References

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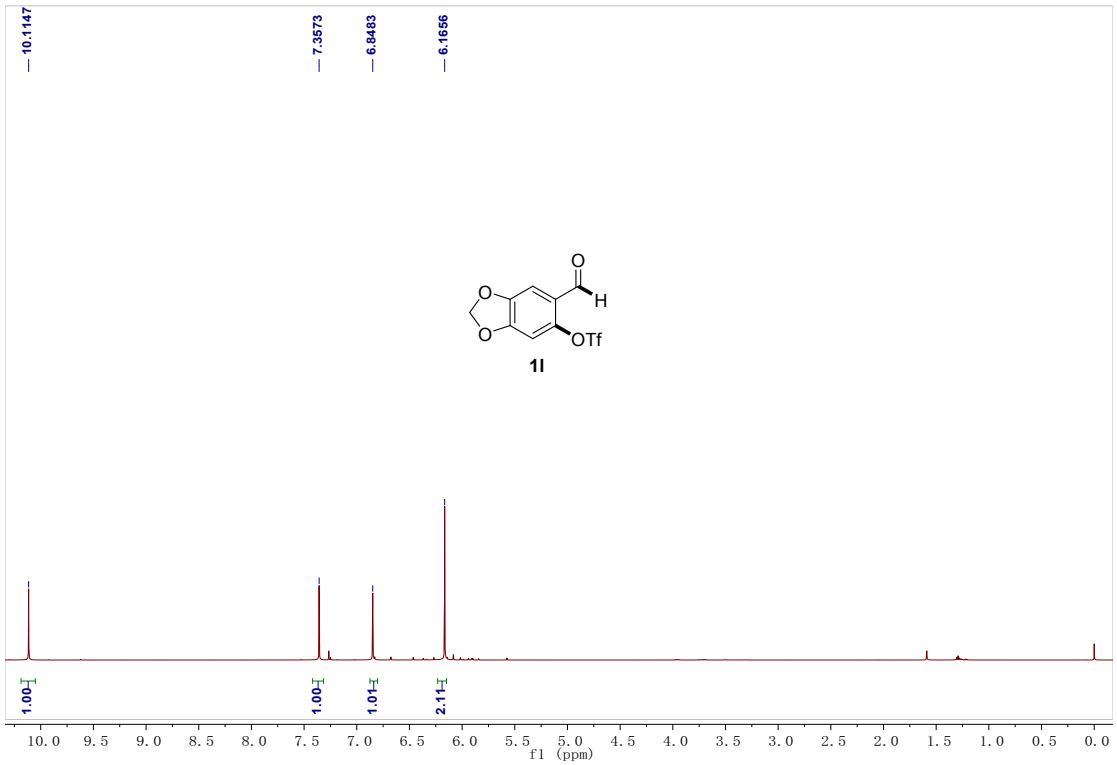
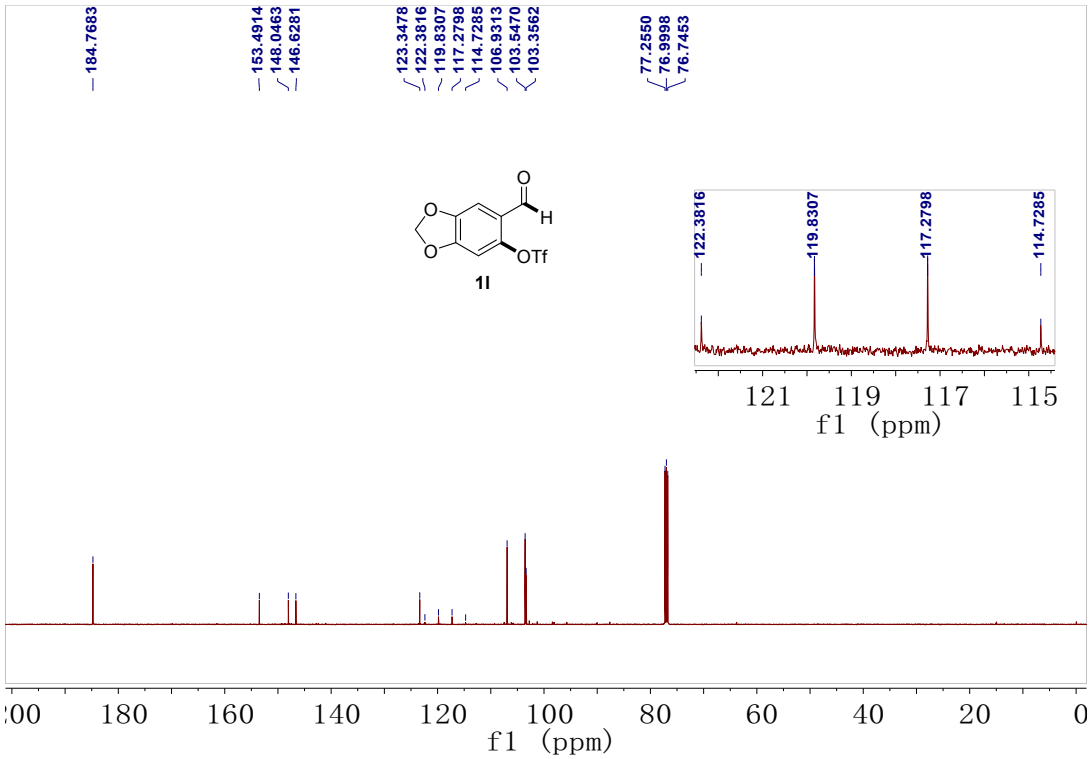
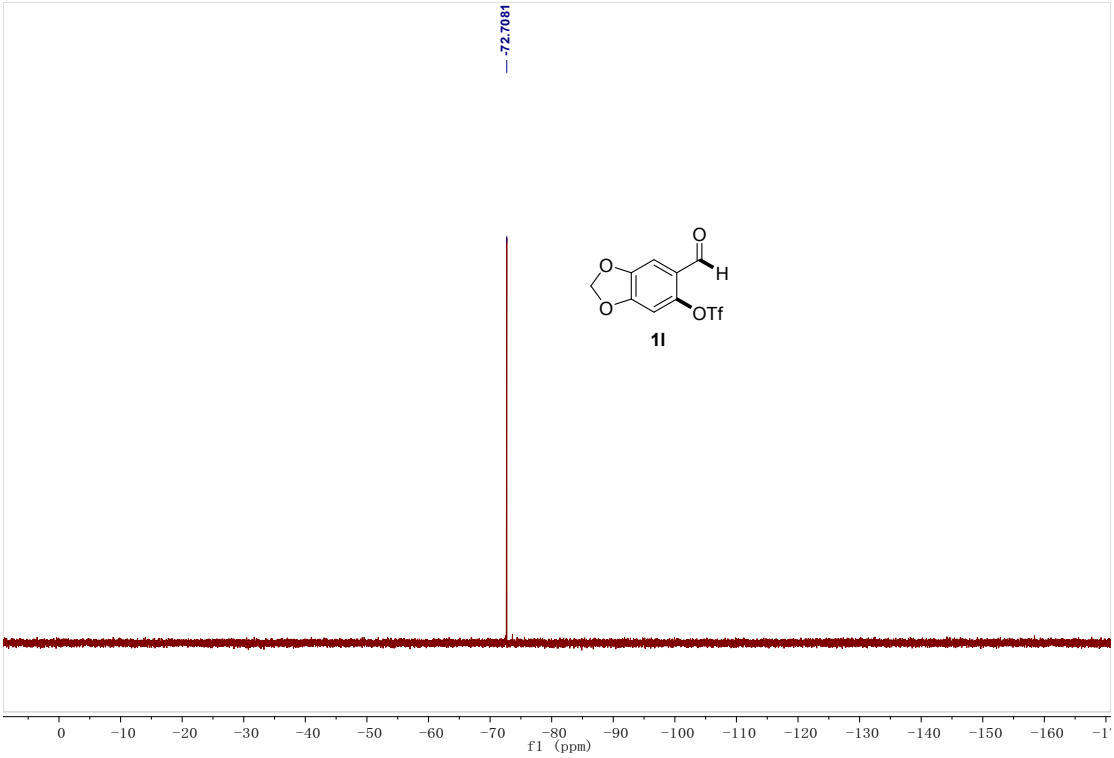
5. NMR Spectra



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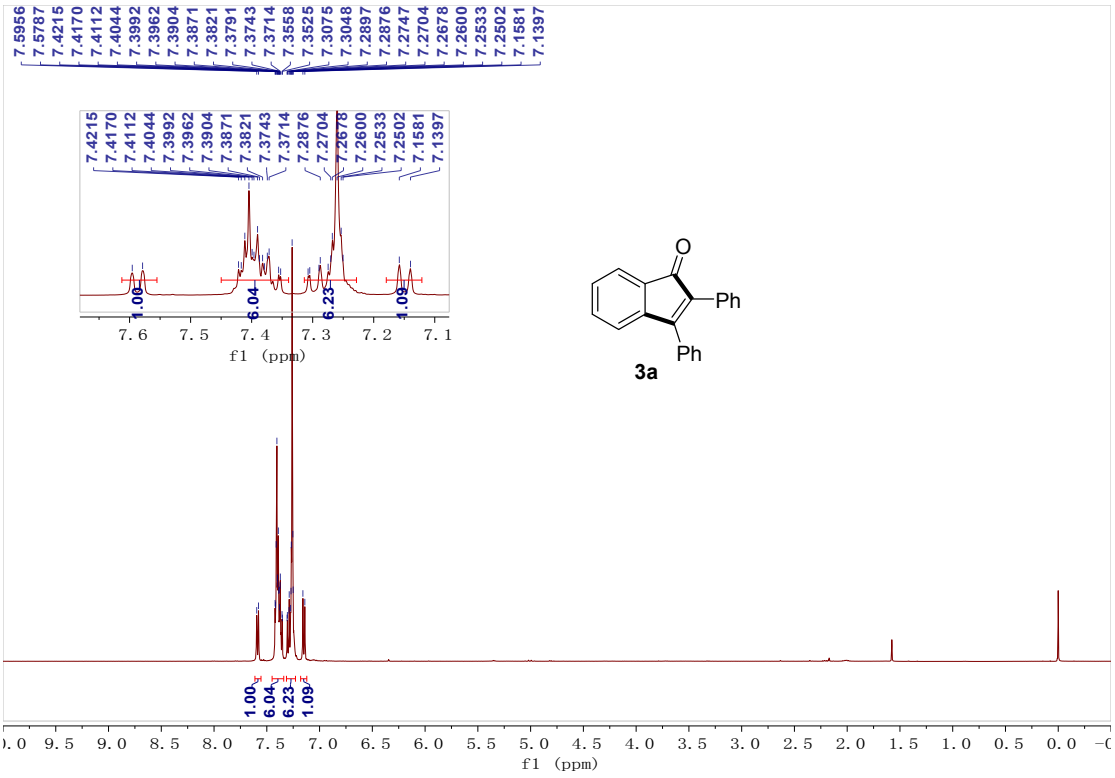
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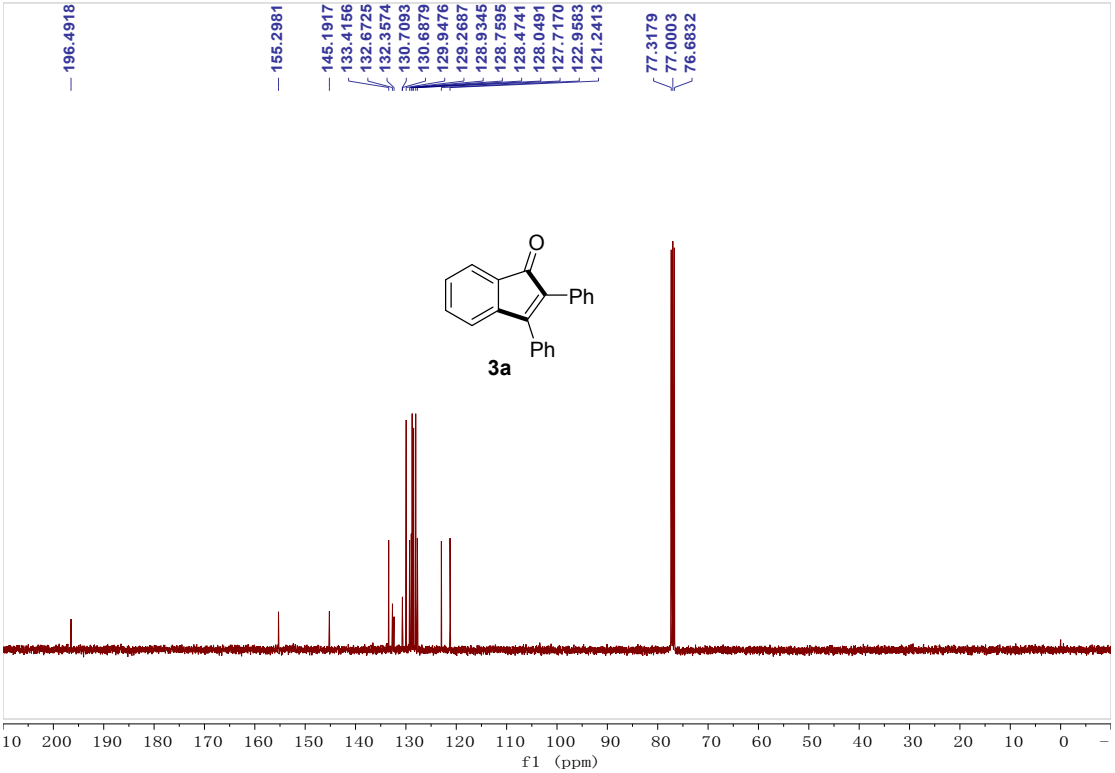
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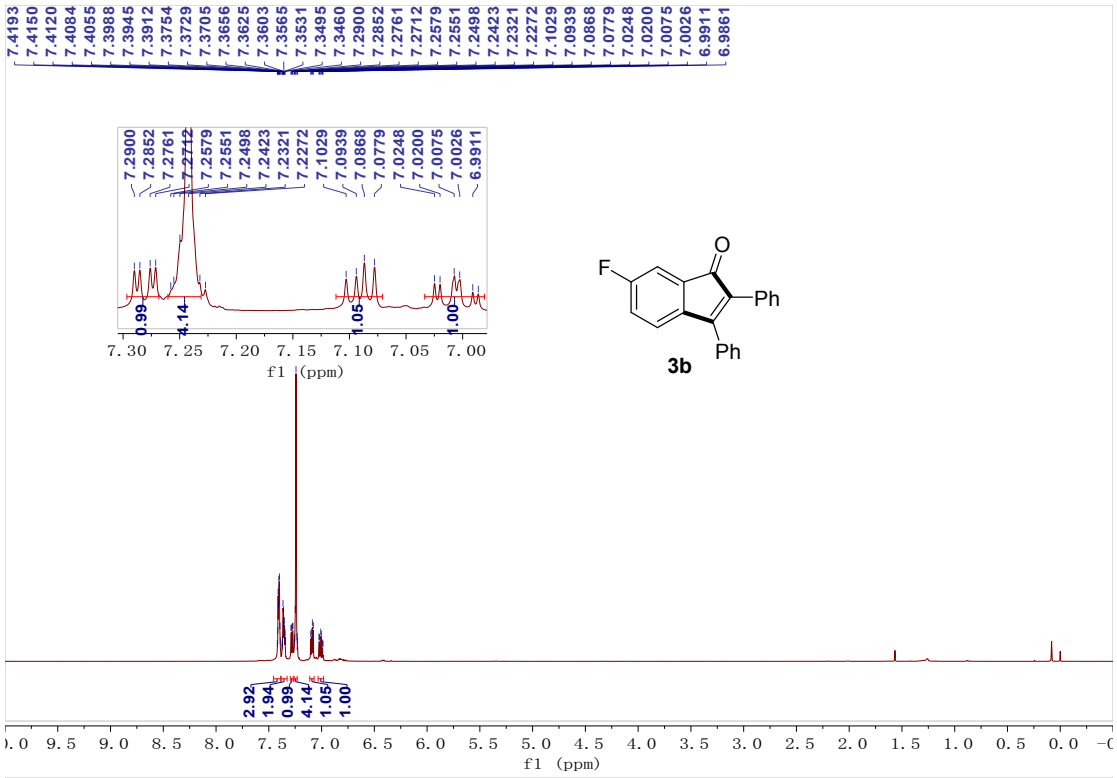
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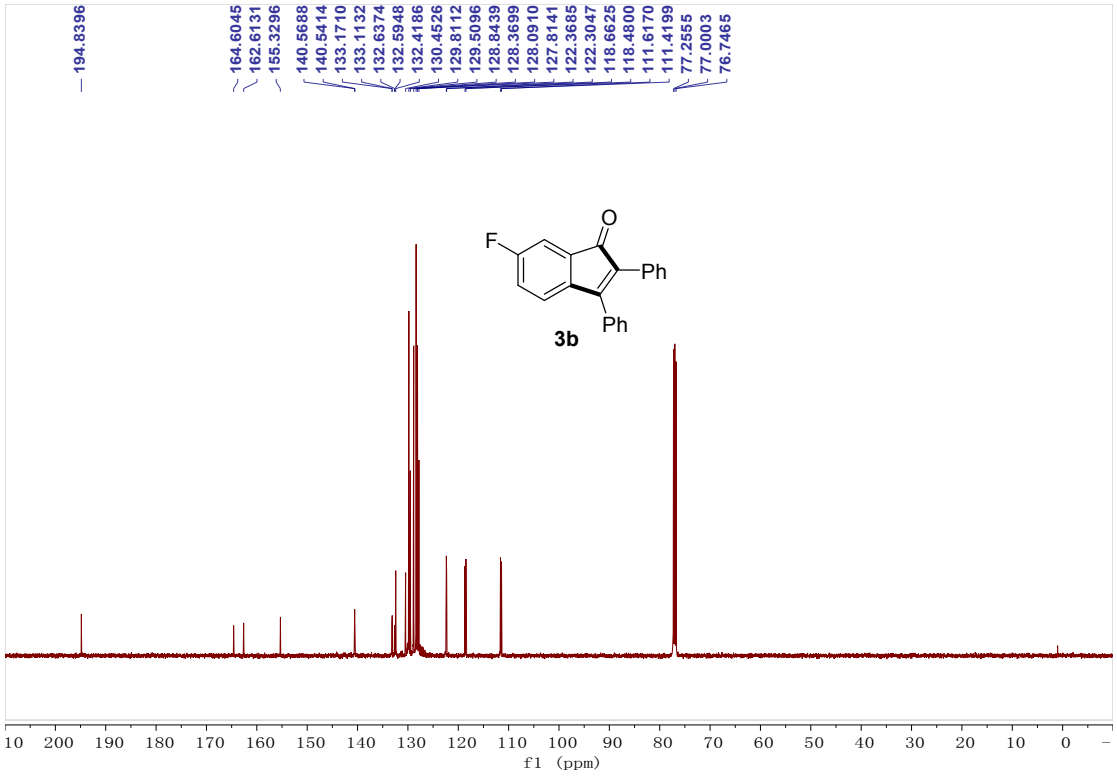
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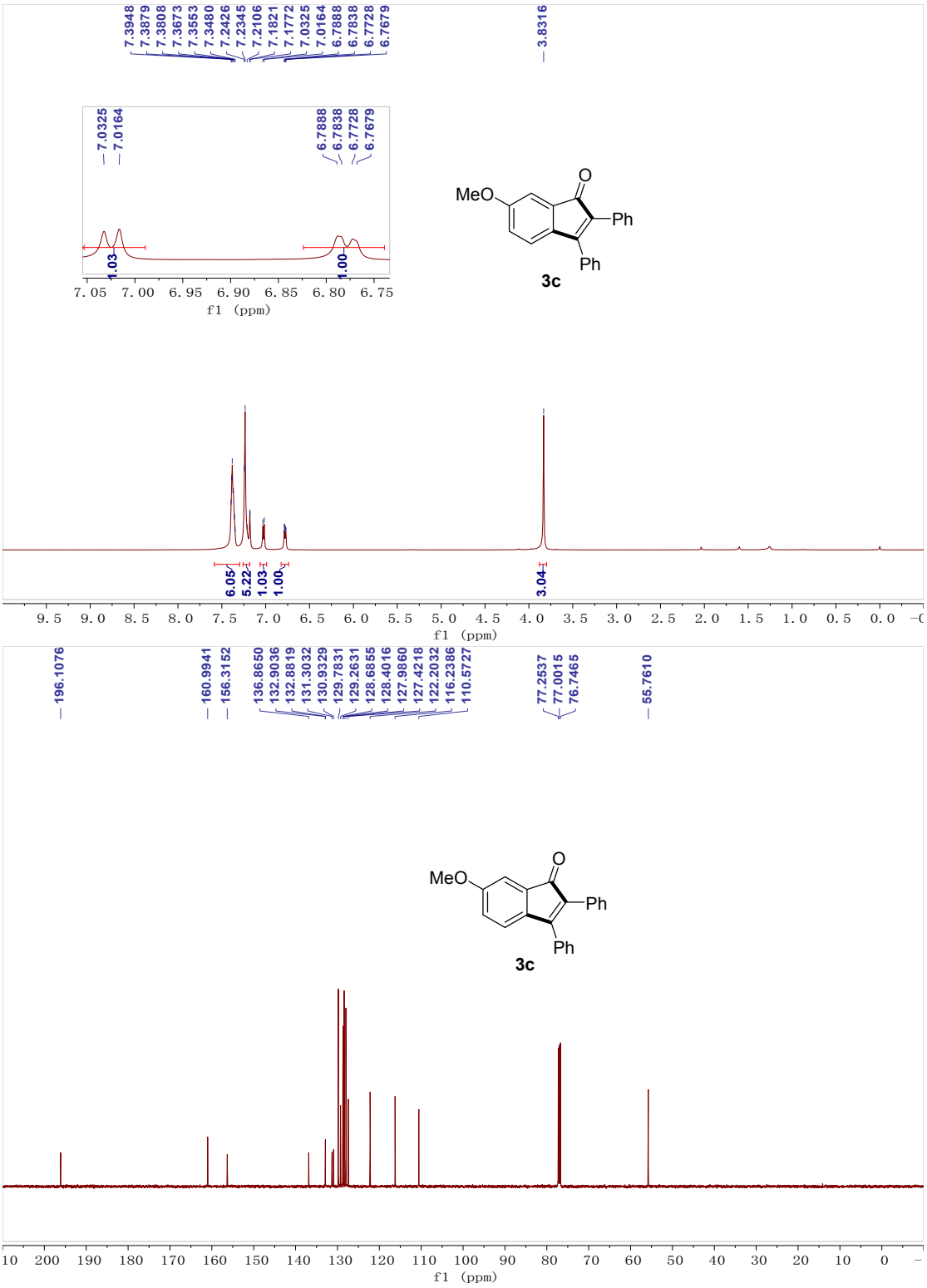
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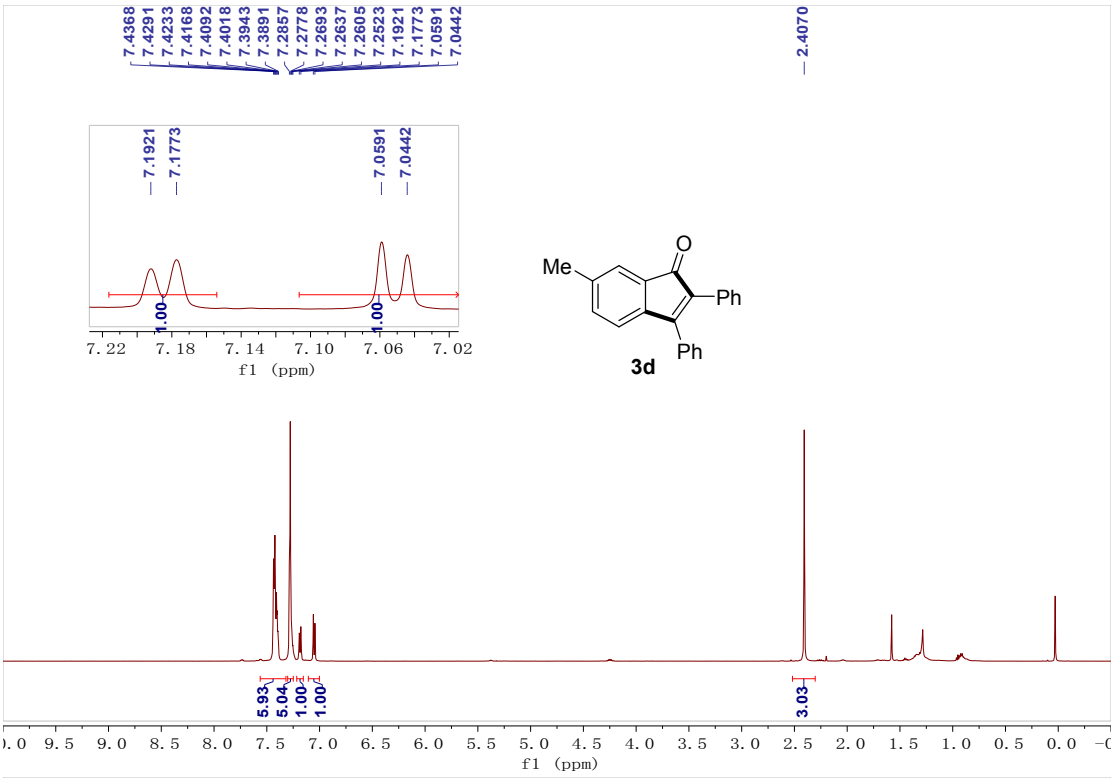
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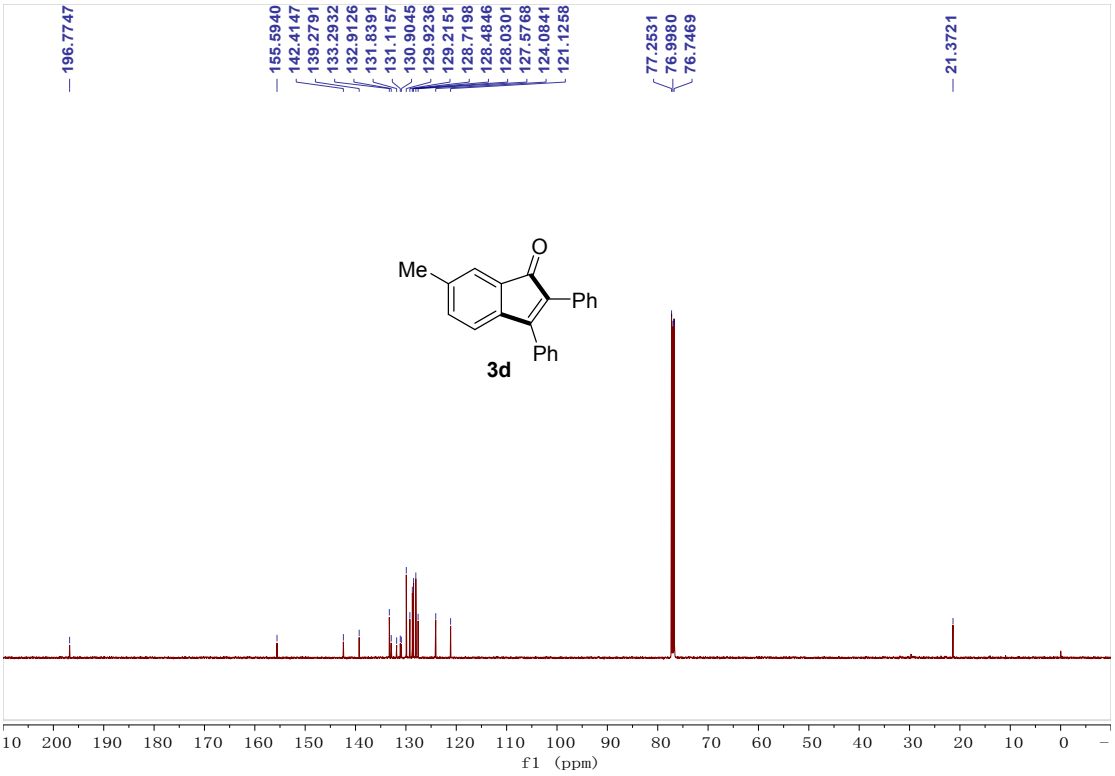
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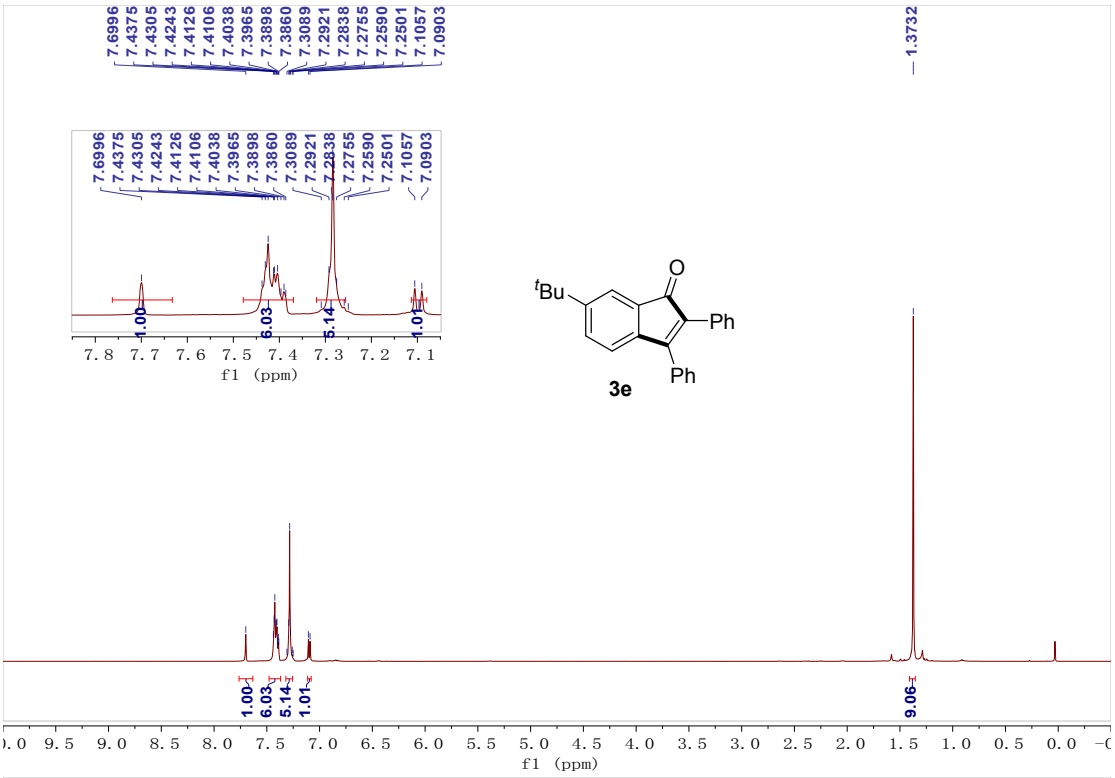
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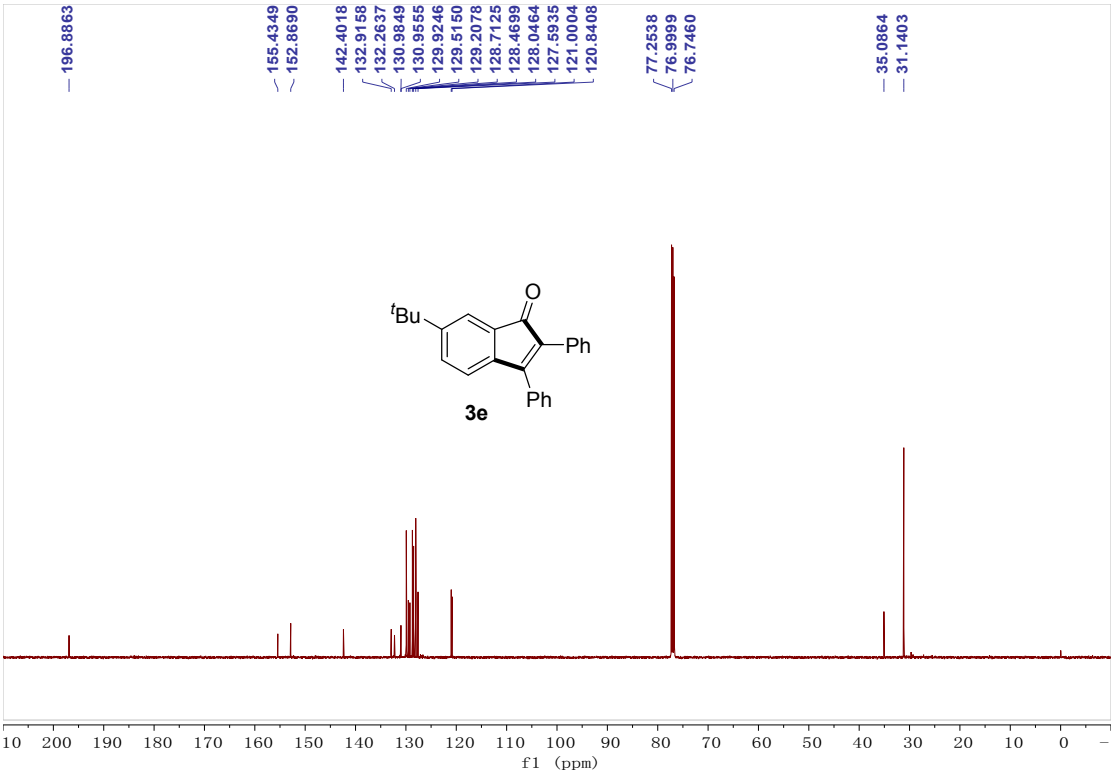
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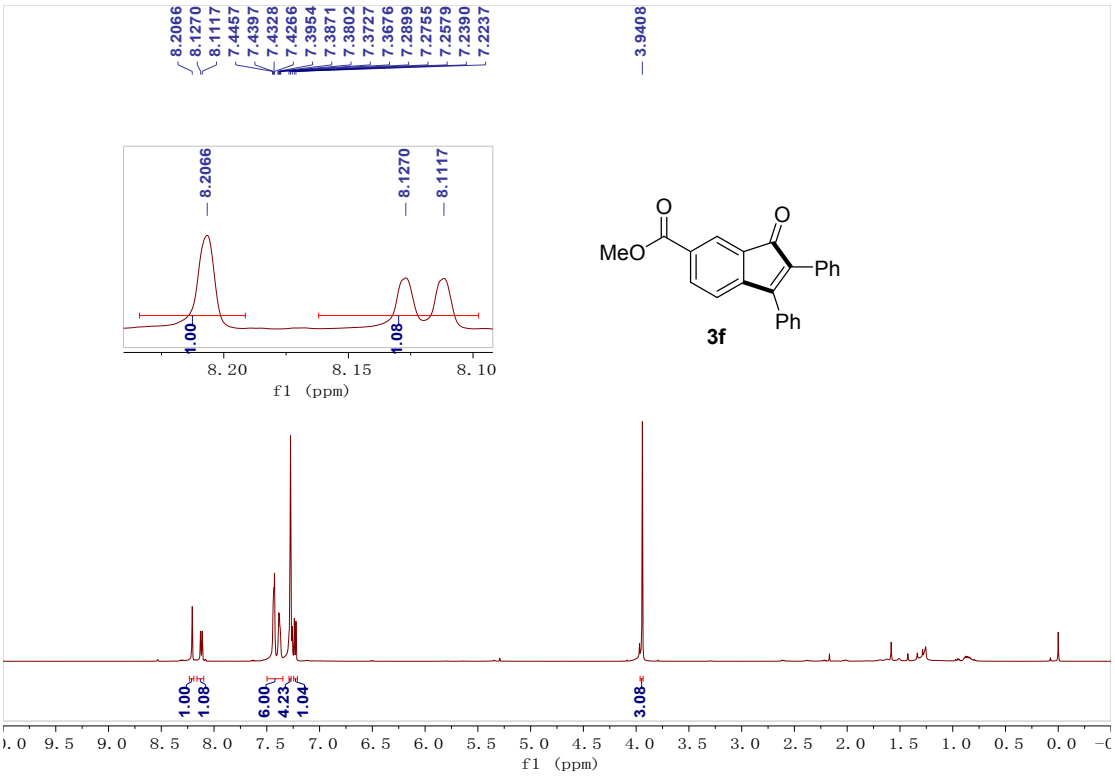
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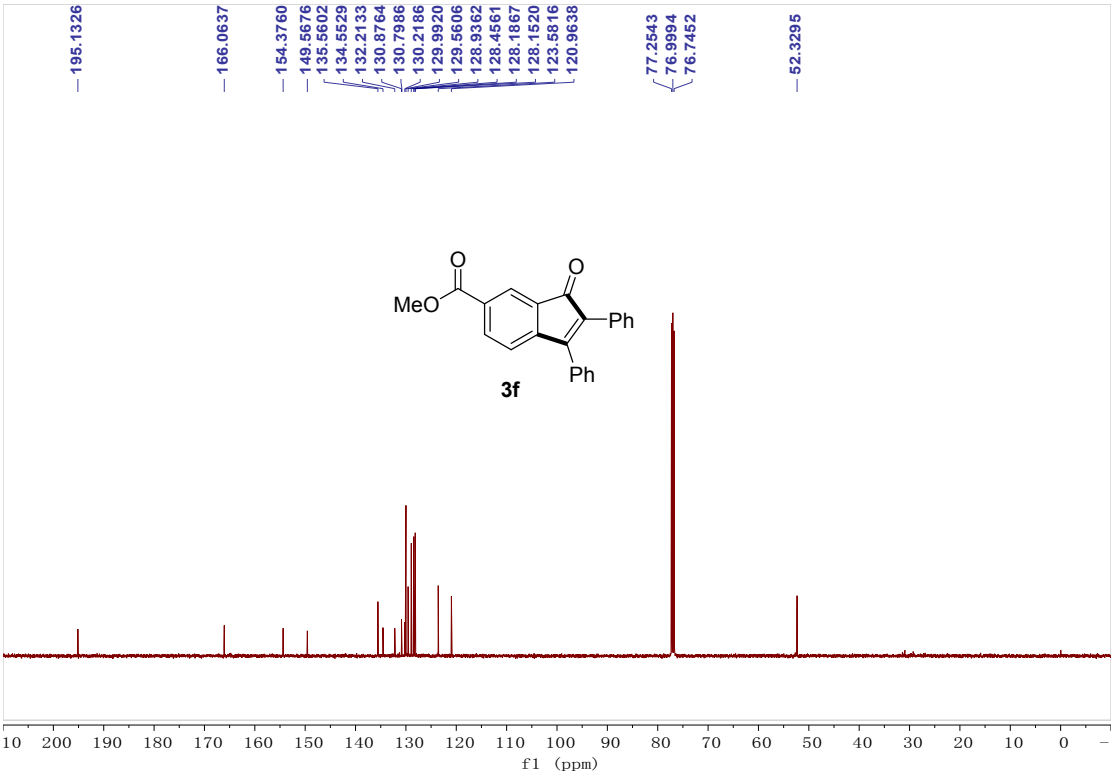
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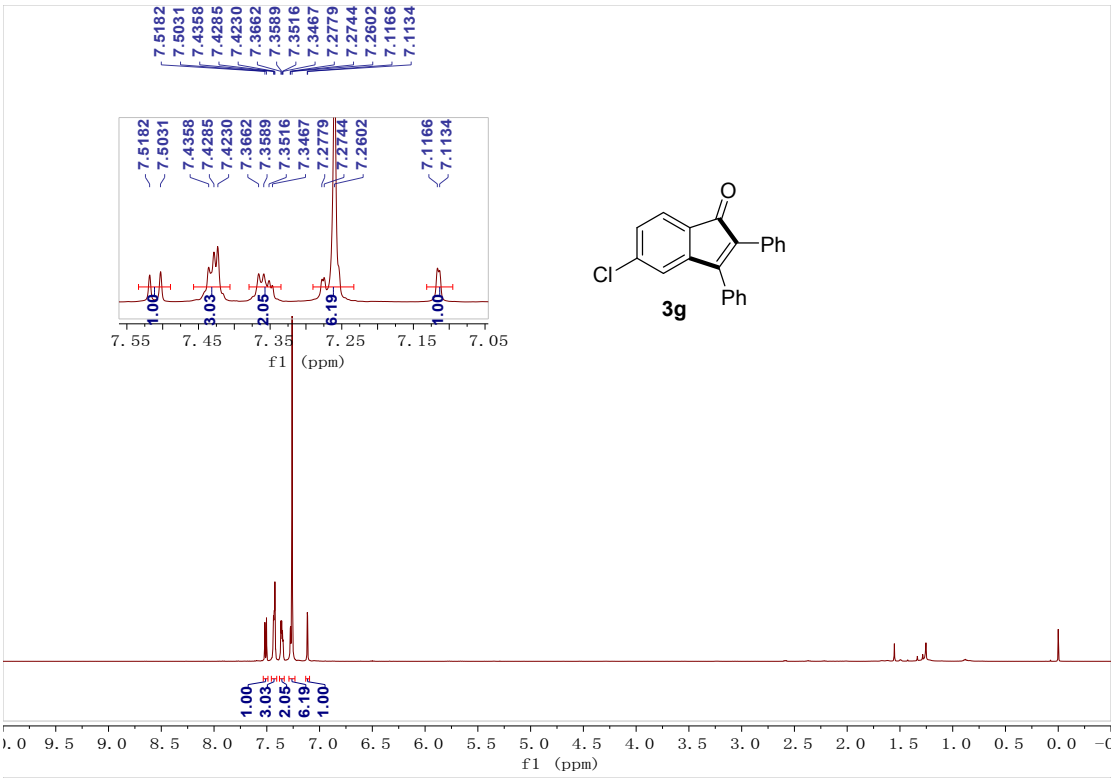
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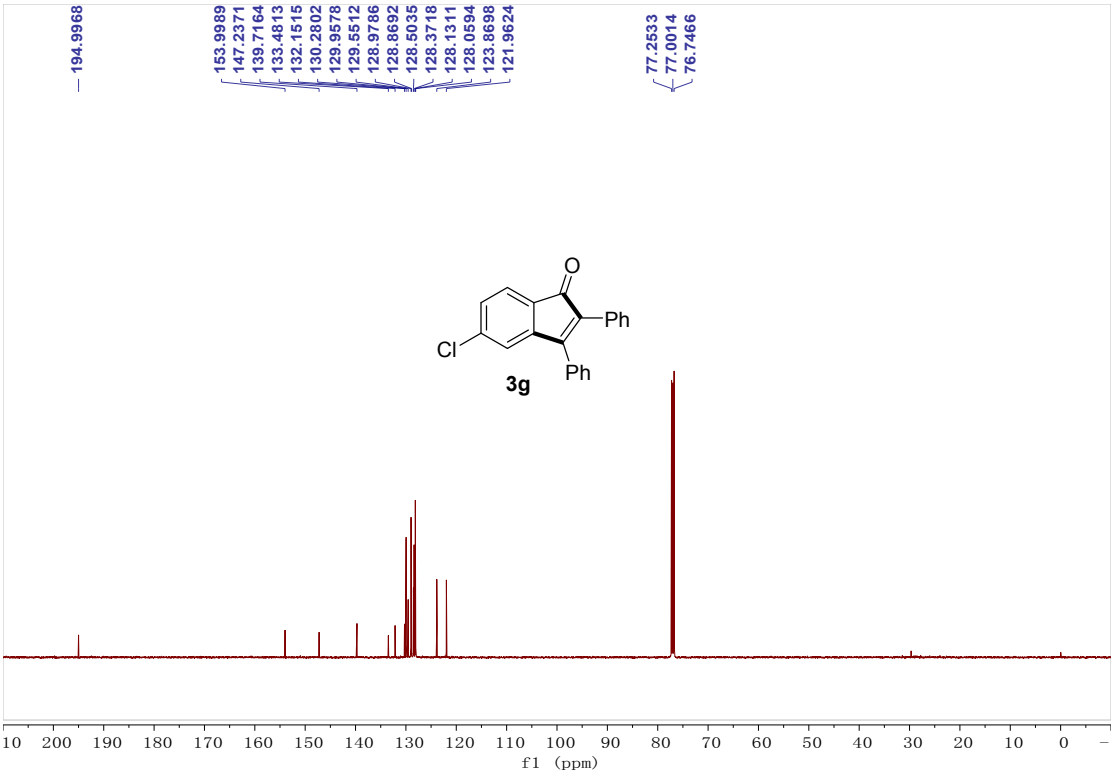
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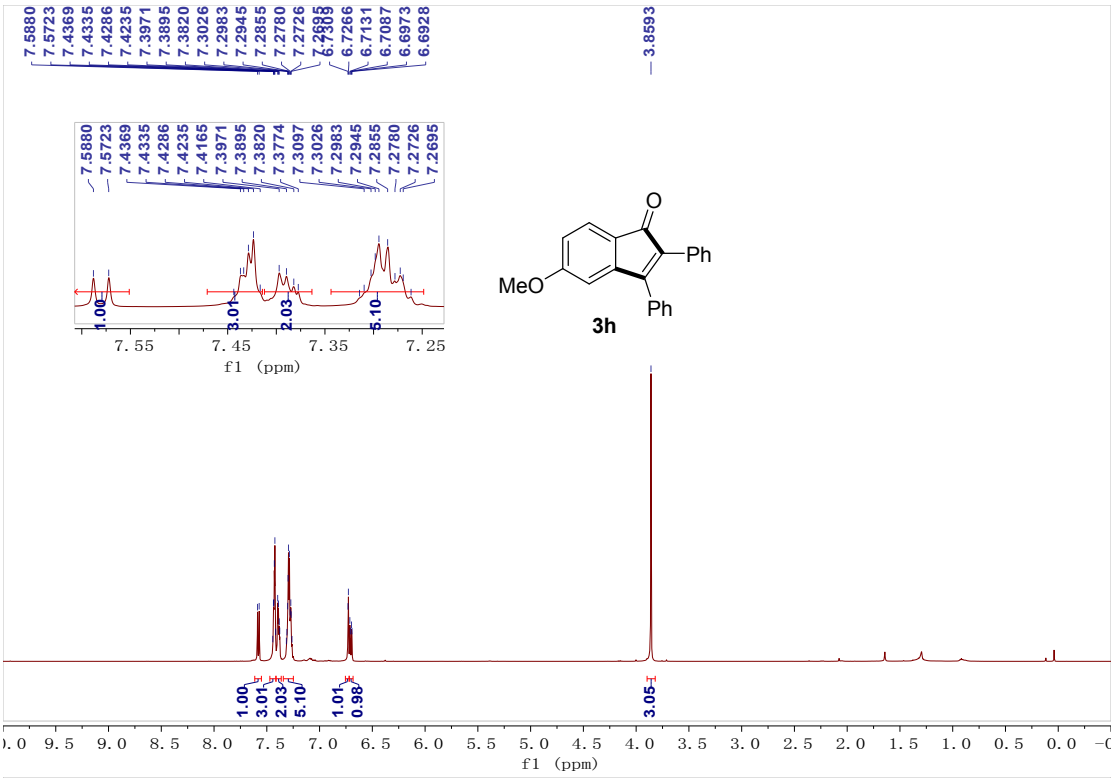
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Ph
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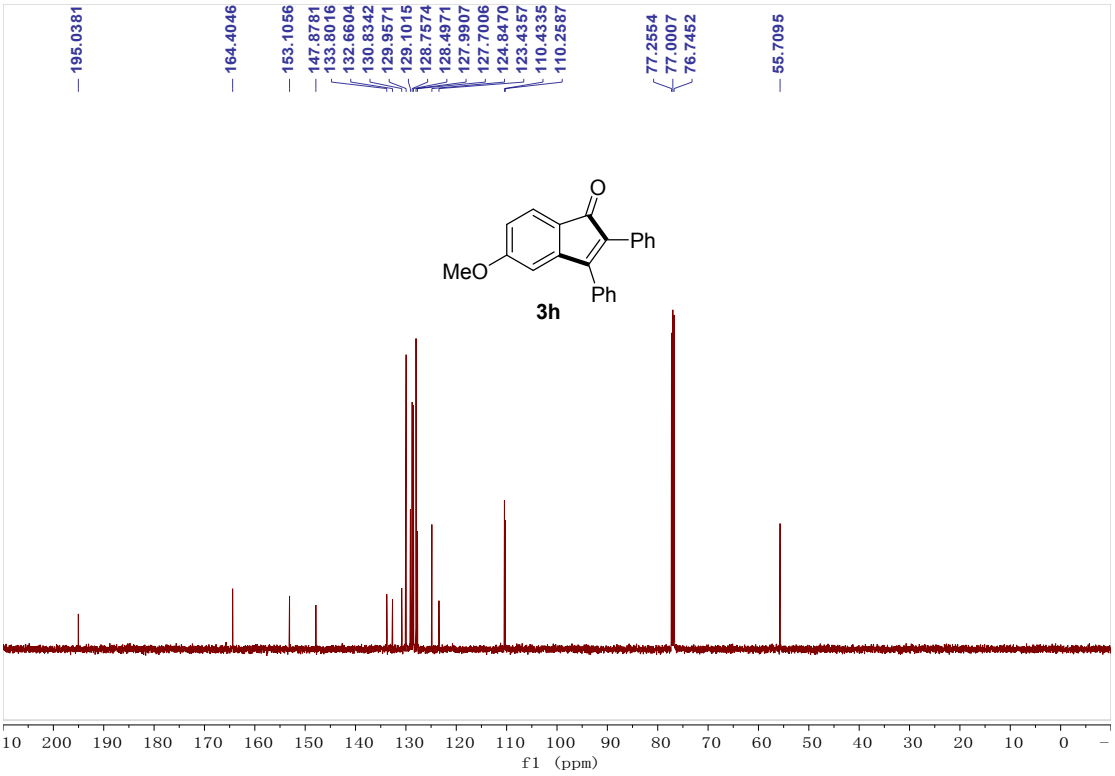
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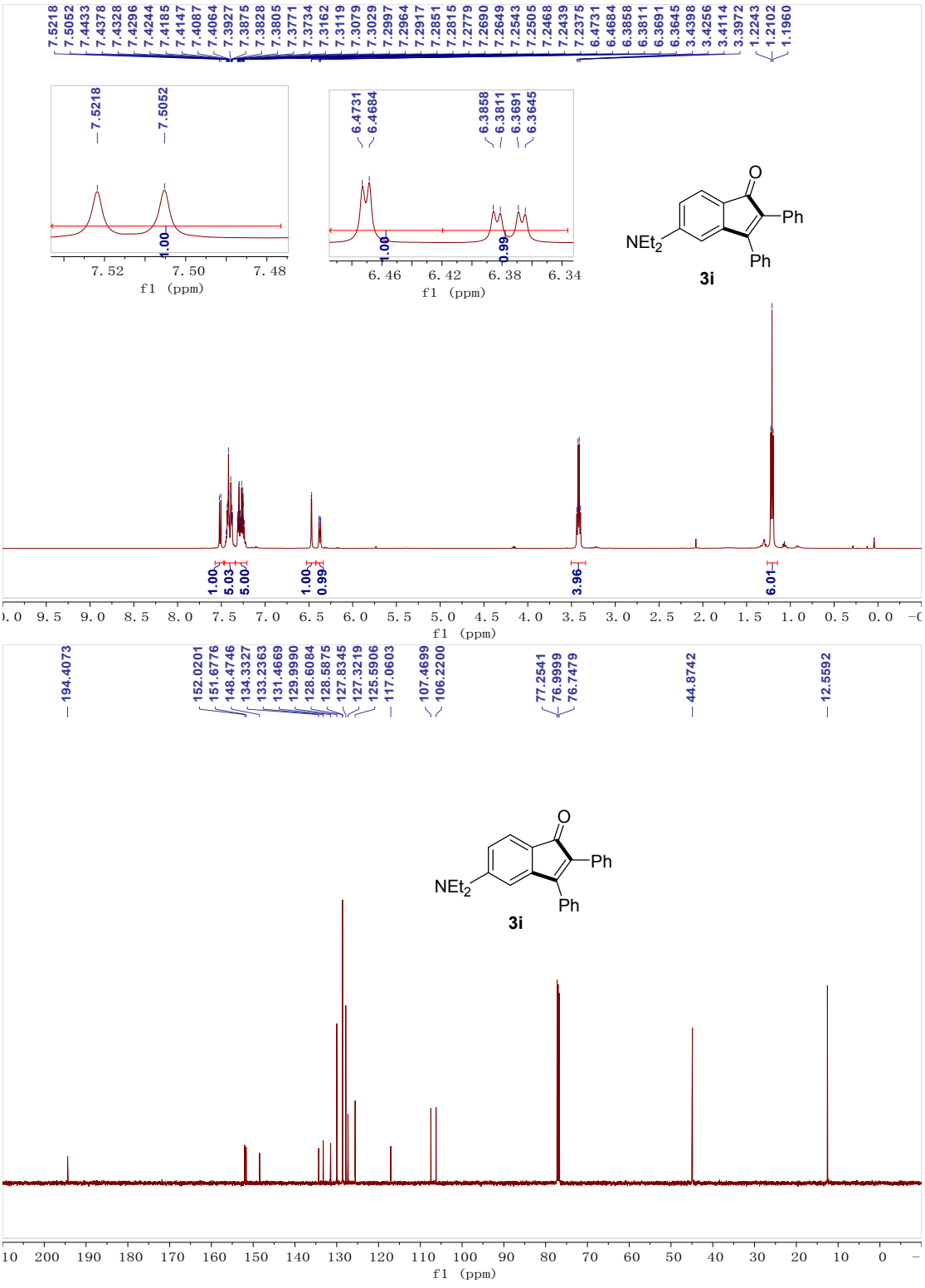
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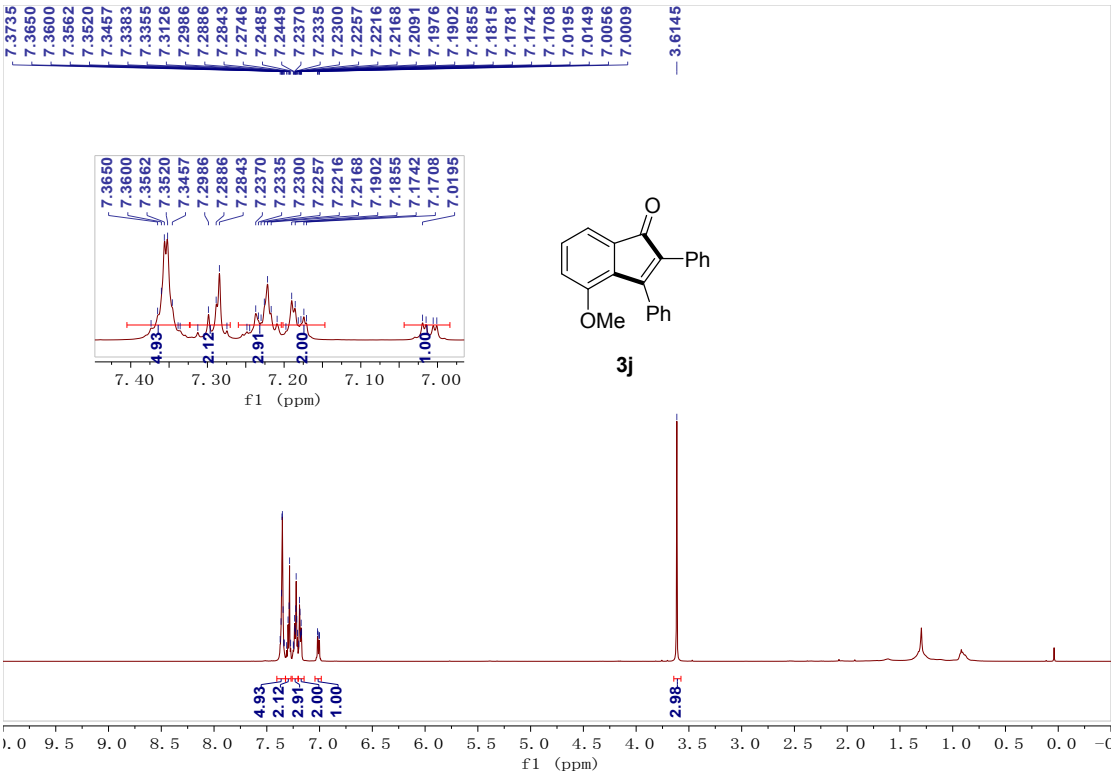
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2.12
2.91
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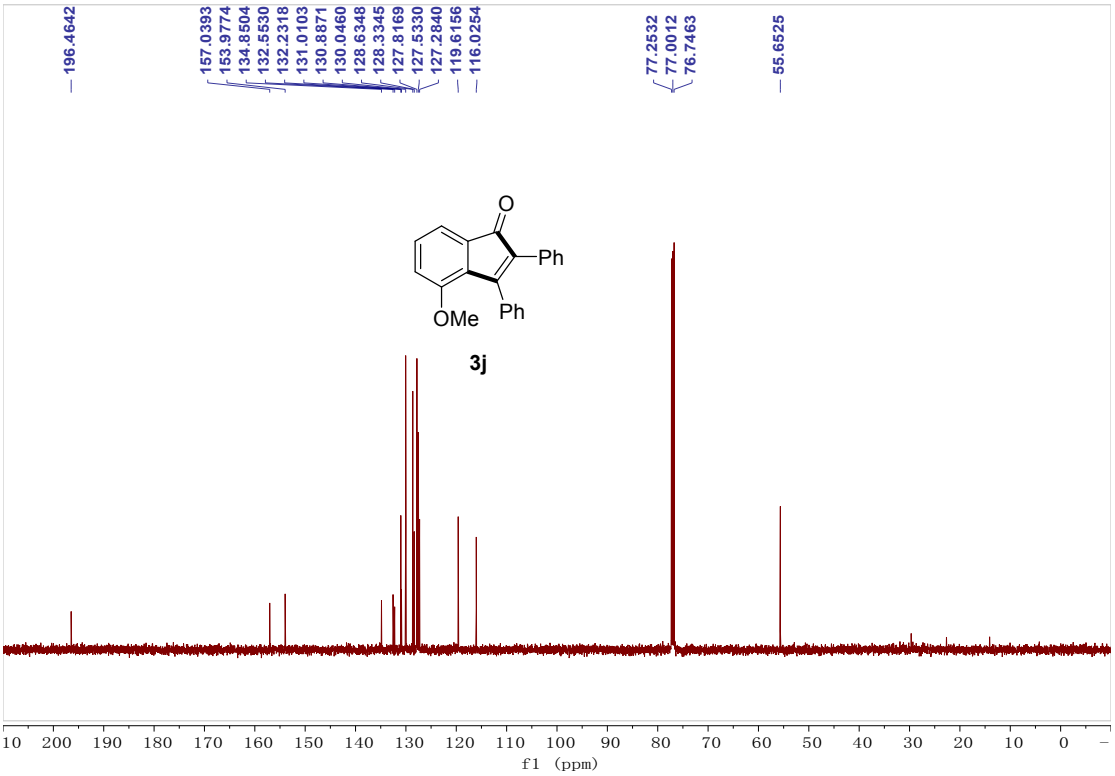
1.00
2.98
f1 (ppm)
O
Ph
Ph
OMe
3j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127.2840
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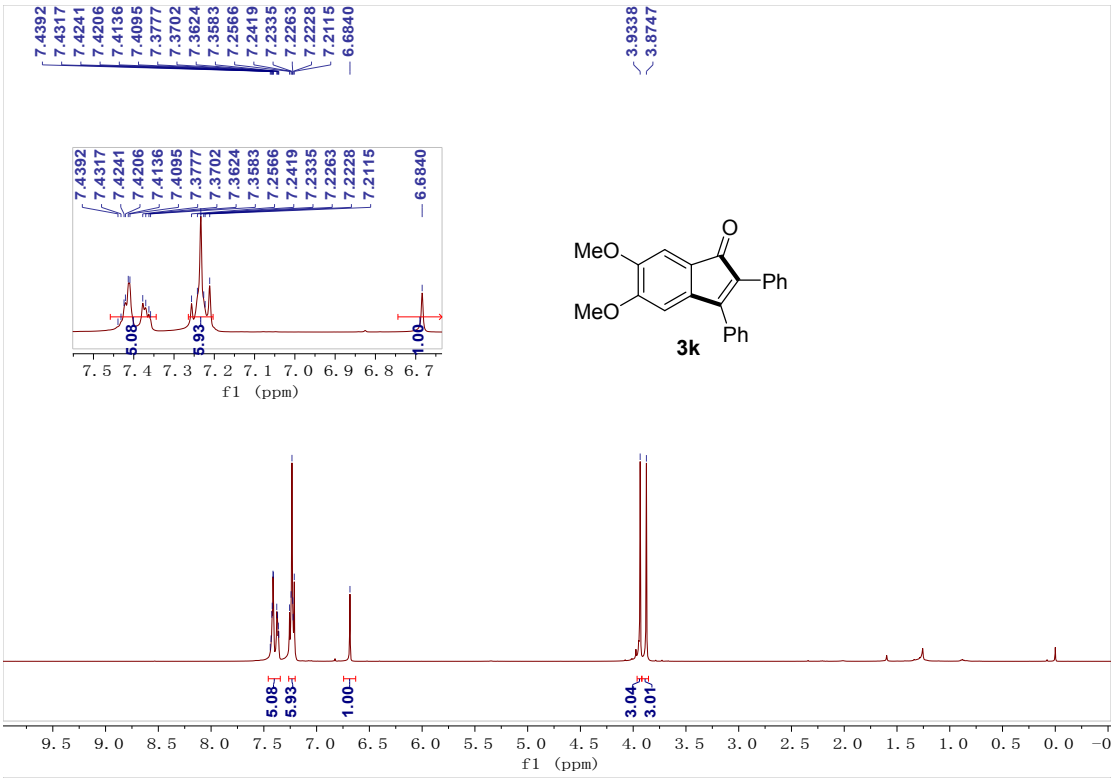
O
Ph
Ph
OMe
3j
f1 (ppm)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7.2335
7.2263
7.2228
7.2115
6.6840
3.9338
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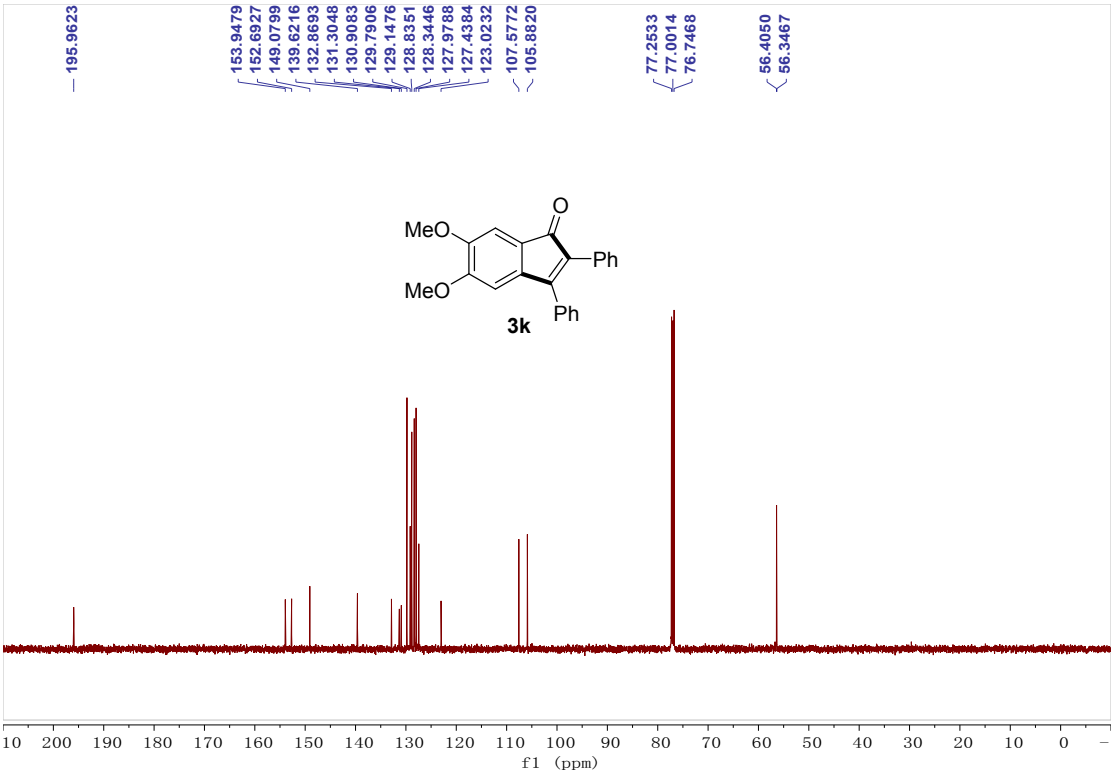
5.93
1.00
3.04
3.01
MeO
MeO
O
Ph
Ph
3k
f1 (ppm)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127.4384
123.0232
107.5772
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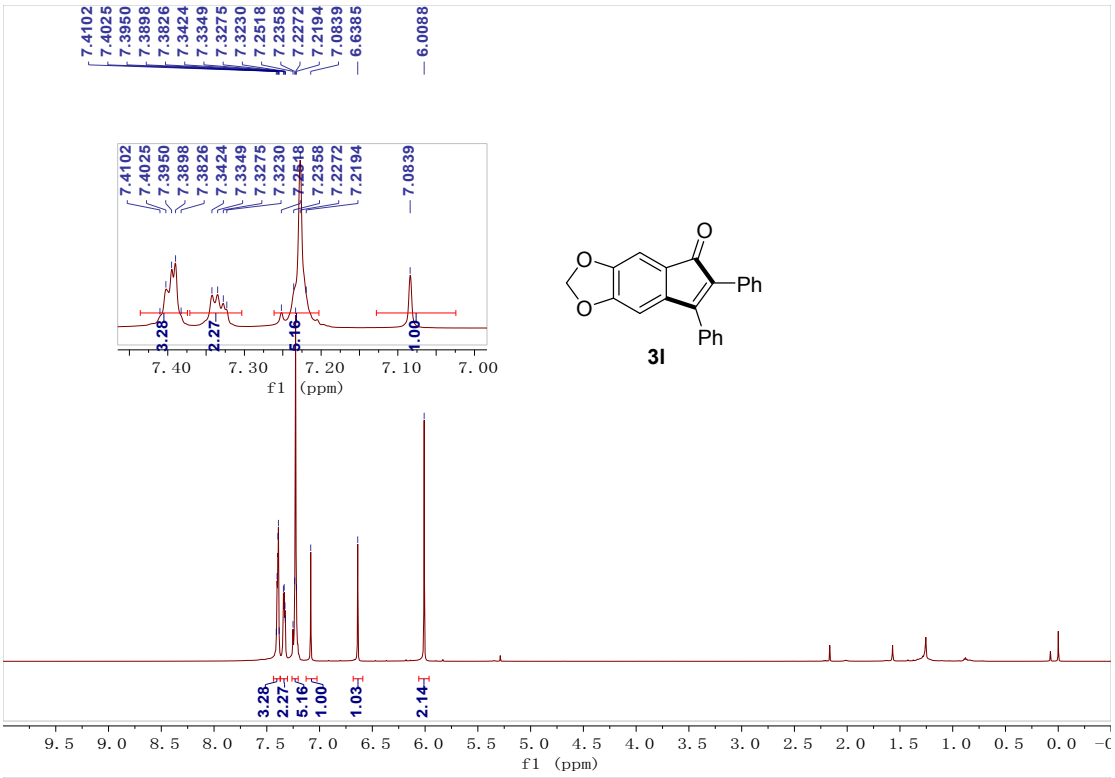
56.3467
MeO
MeO
O
Ph
Ph
3k
f1 (ppm)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7.2272
7.2194
7.0839
6.6385
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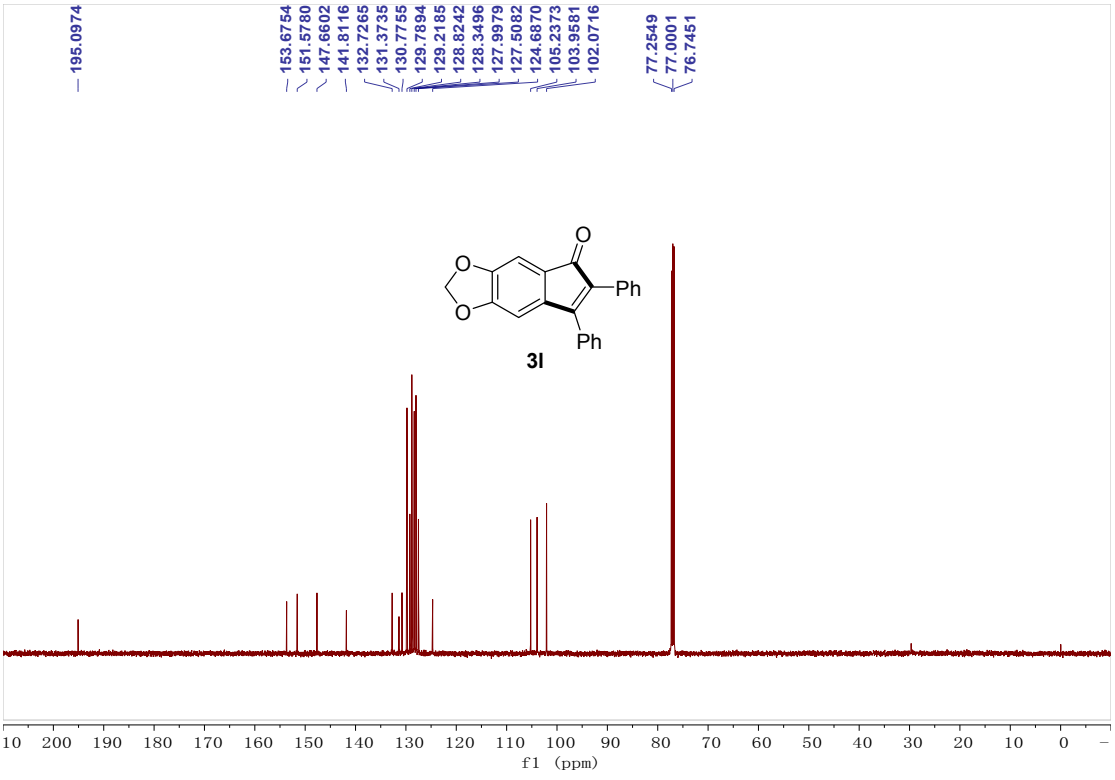
5.16
1.00
1.03
2.14
f1 (ppm)
O
O
O
Ph
Ph
3l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127.5082
124.6870
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77.0001
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f1 (ppm)
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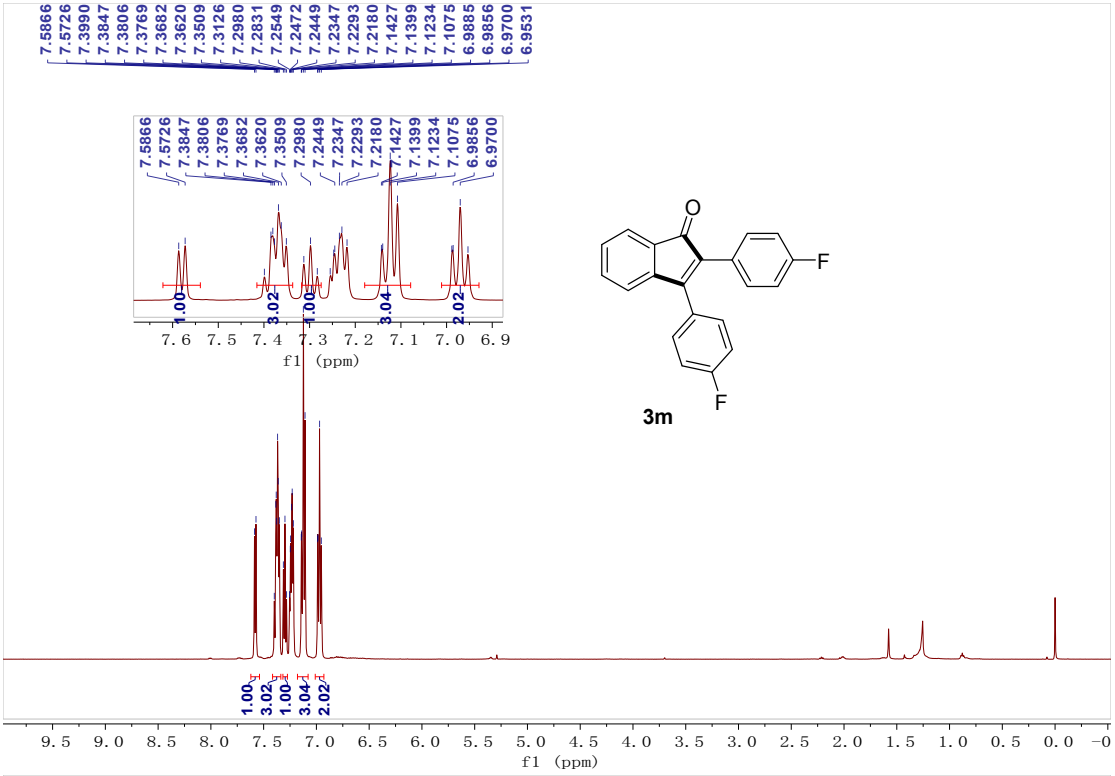
O
O
Ph
Ph
3l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7.1234
7.1075
6.9885
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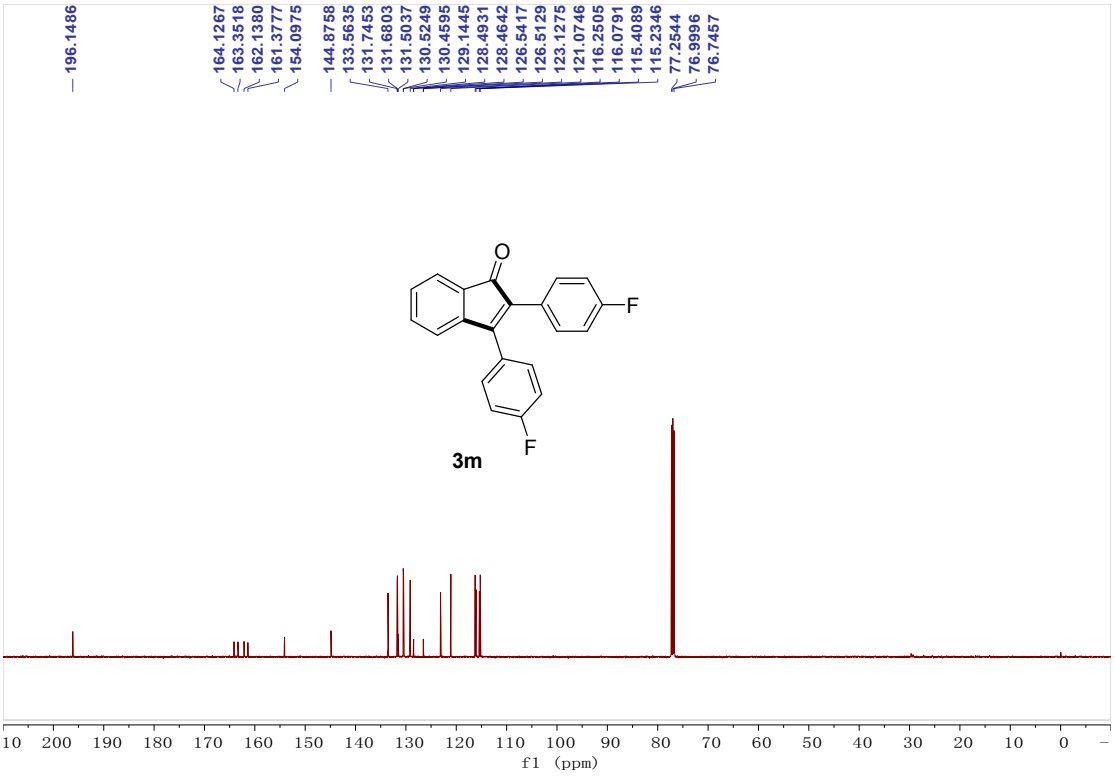
1.00
3.02
1.00
3.04
2.02
f1 (ppm)
O
F
F
3m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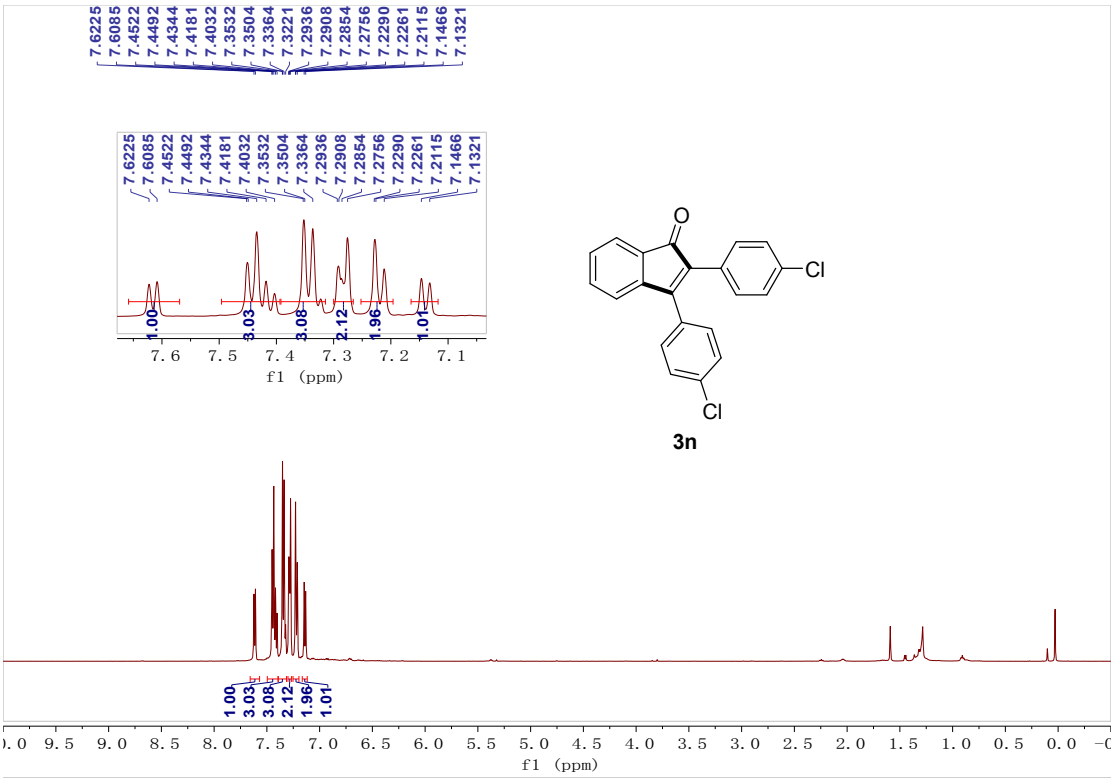
76.7457
O
F
F
3m
f1 (ppm)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7.2936
7.2908
7.2854
7.2756
7.2290
7.2261
7.2115
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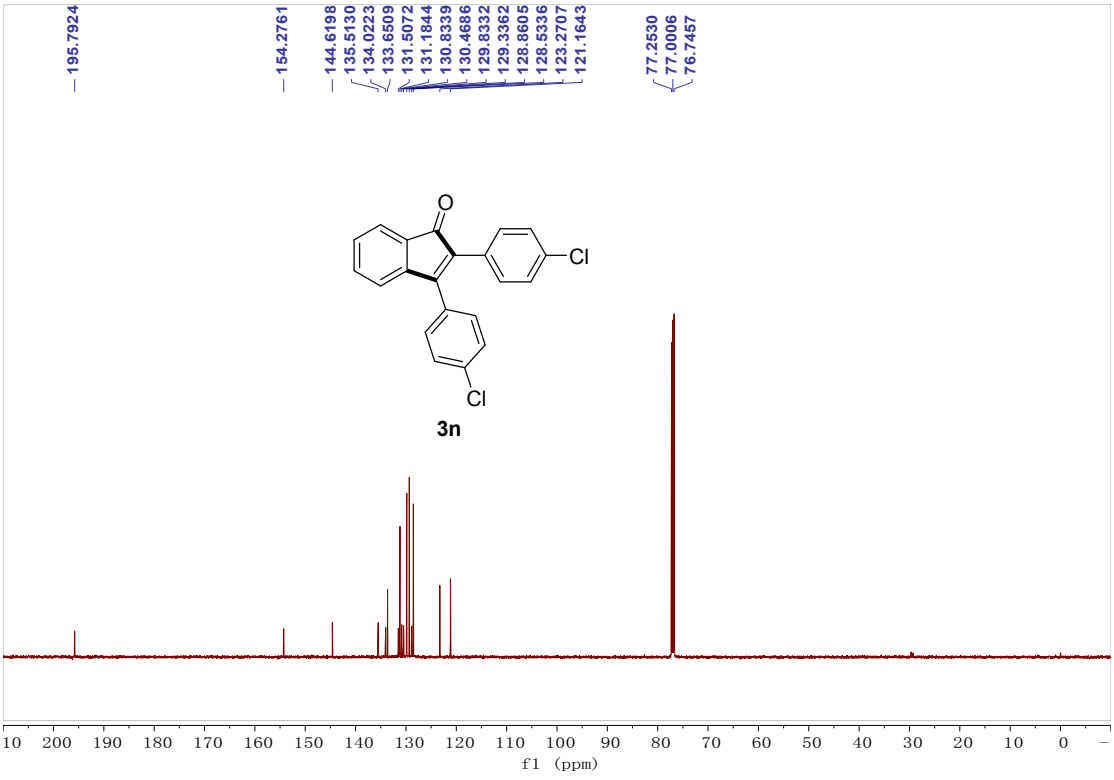
7.1321
1.00
3.03
3.08
2.12
1.96
1.01
f1 (ppm)
O
Cl
Cl
3n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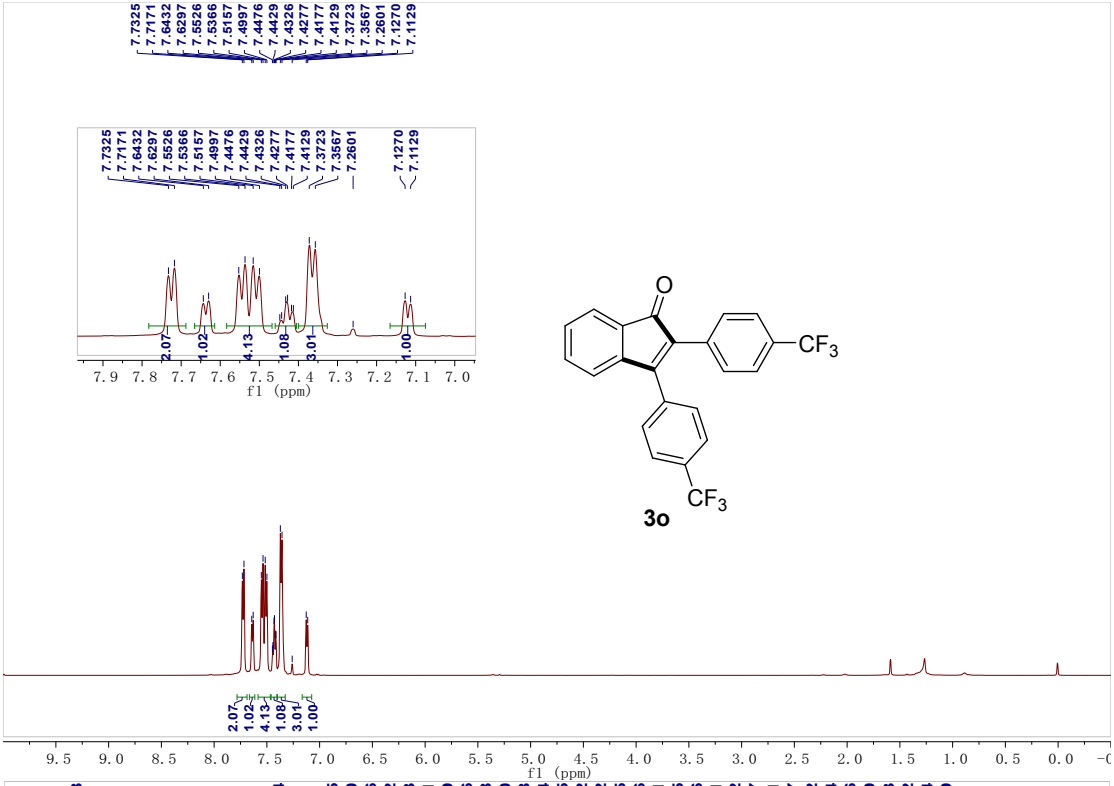
76.7457
O
Cl
Cl
3n
f1 (ppm)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7.4277
7.4177
7.4129
7.3723
7.3567
7.2601
7.1270
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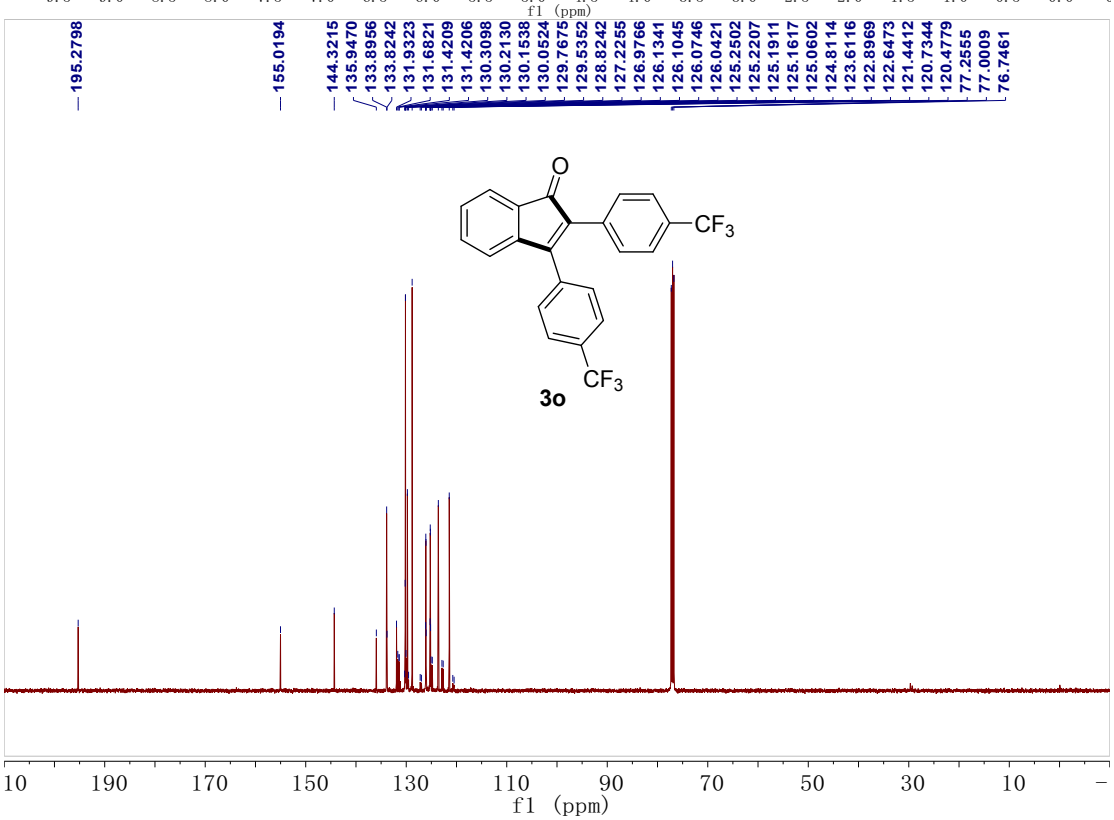
1.02
4.13
1.08
3.01
1.00
f1 (ppm)
O
CF3
CF3
3o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130.1538
130.0524
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129.5352
128.8242
127.2255
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126.1341
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125.0602
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123.6116
122.8969
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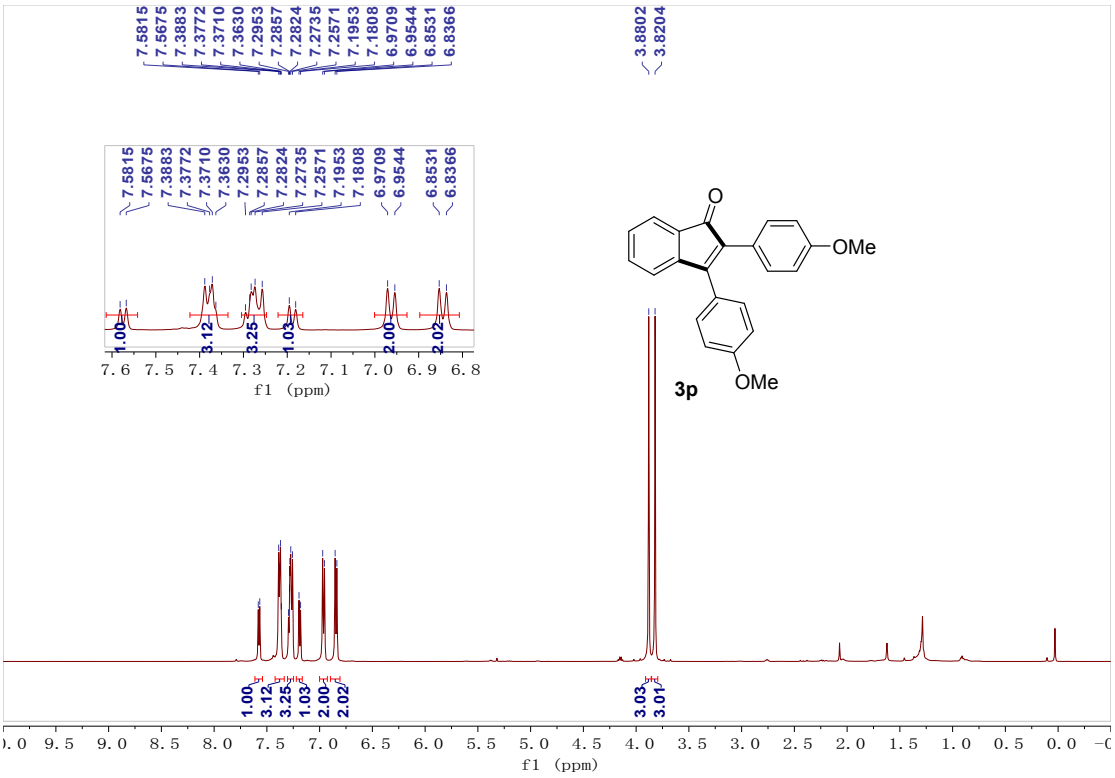
77.0009
76.7461
f1 (ppm)
O
CF3
CF3
3o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7.1808
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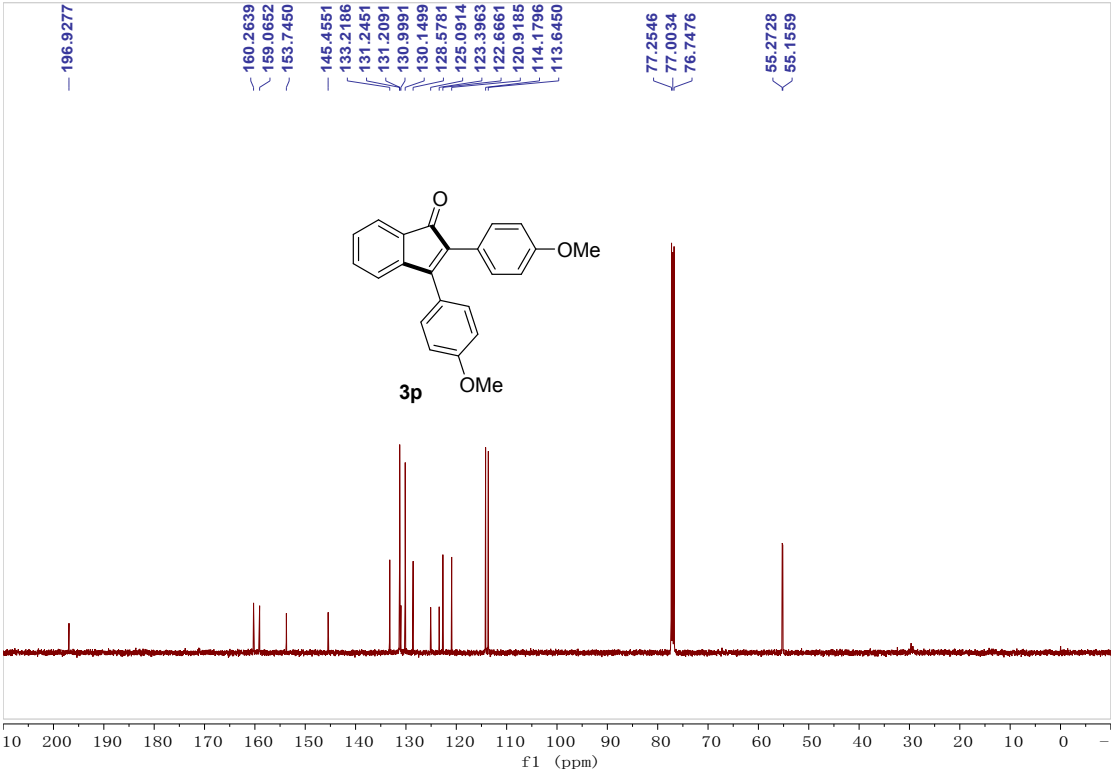
6.9544
6.8531
6.8366
3.8802
3.8204
1.00
3.12
3.25
1.03
2.00
2.02
f1 (ppm)
O
OMe
OMe
3p
3.03
3.01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128.5781
125.0914
123.3963
122.6661
120.9185
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77.2546
77.0034
76.7476
55.2728
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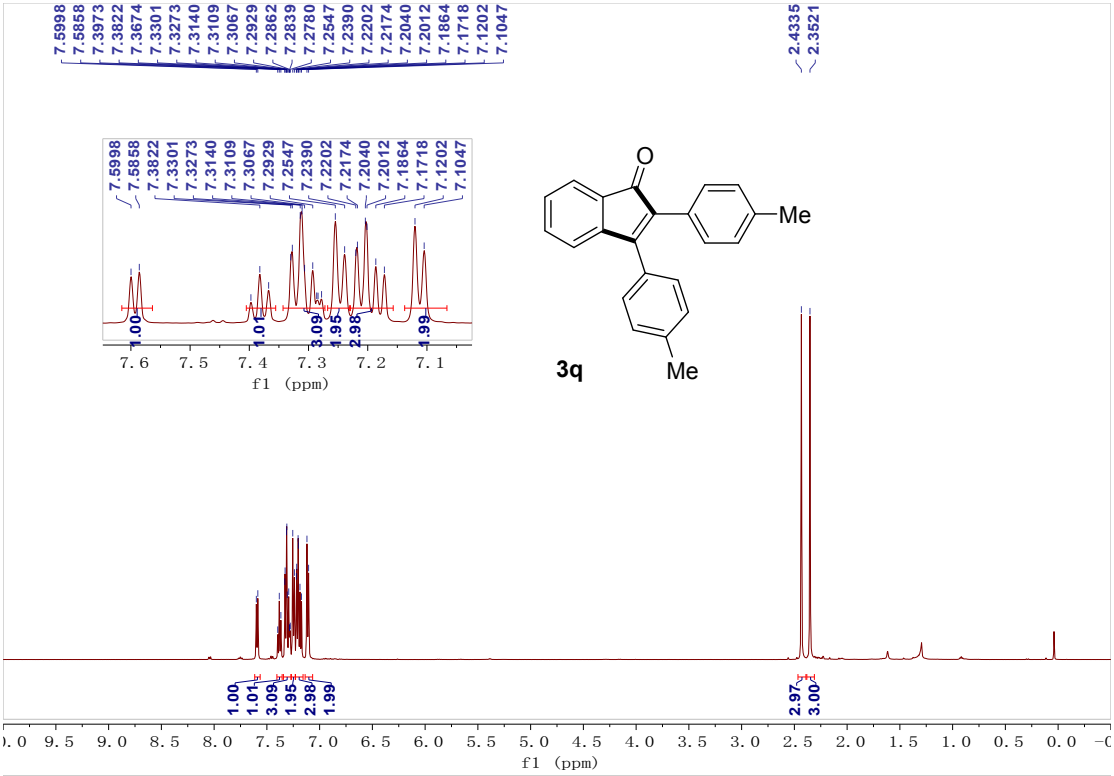
O
OMe
OMe
3p
f1 (ppm)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7.2862
7.2839
7.2780
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7.2390
7.2202
7.2174
7.2040
7.2012
7.1864
7.1718
7.1202
7.1047
2.4335
2.3521
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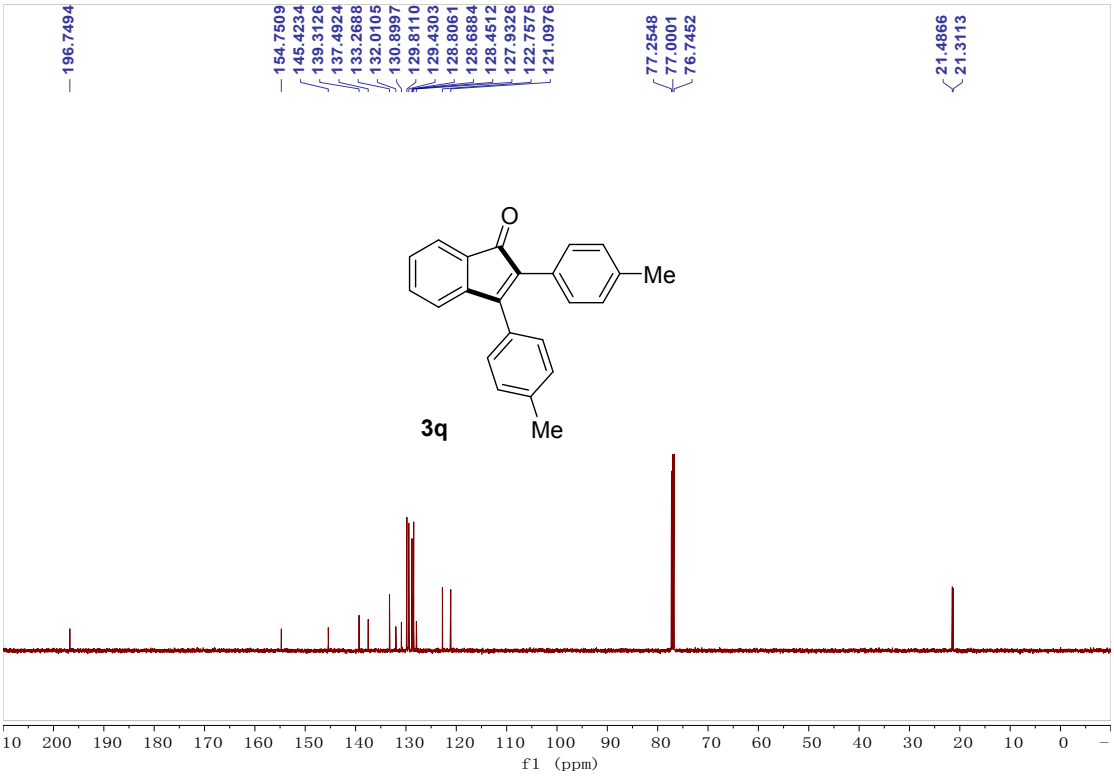
1.01
3.09
1.95
2.98
1.99
2.97
3.00
O
Me
3q
Me
f1 (ppm)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128.6884
128.4512
127.9326
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77.0001
76.7452
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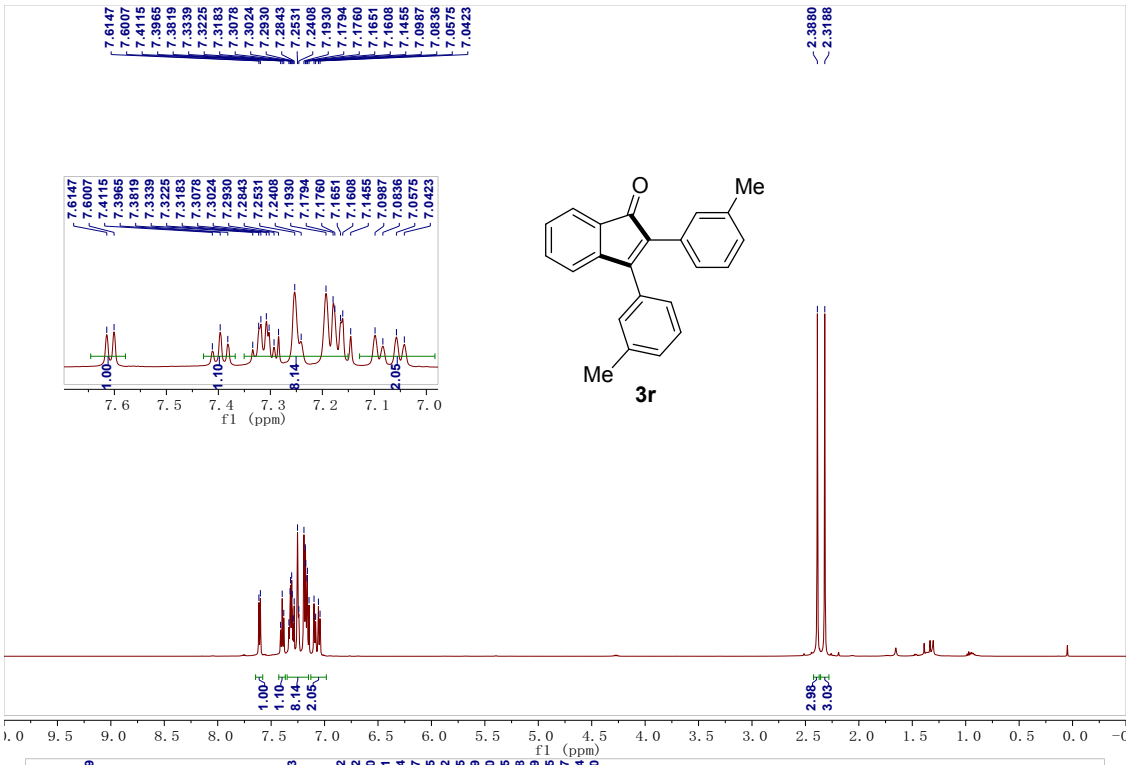
21.3113
O
Me
3q
Me
f1 (ppm)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7.1608
7.1455
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7.0836
7.0575
7.0423
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1.10
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3.03
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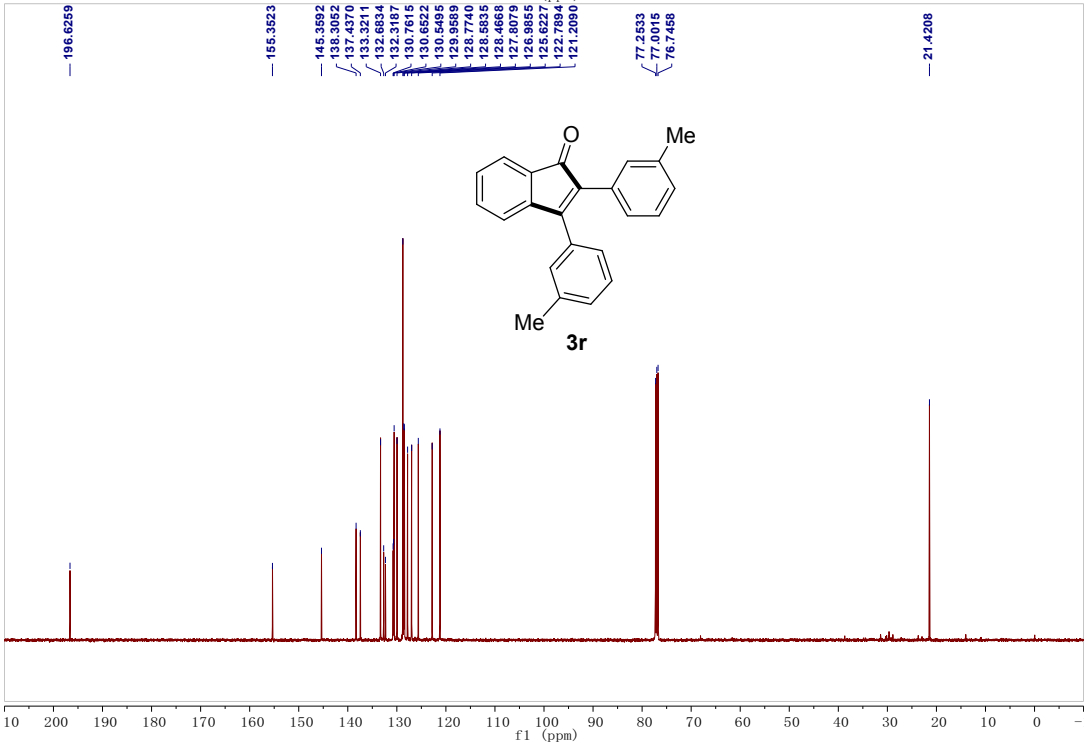
Me
Me
3r
f1 (ppm)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126.9855
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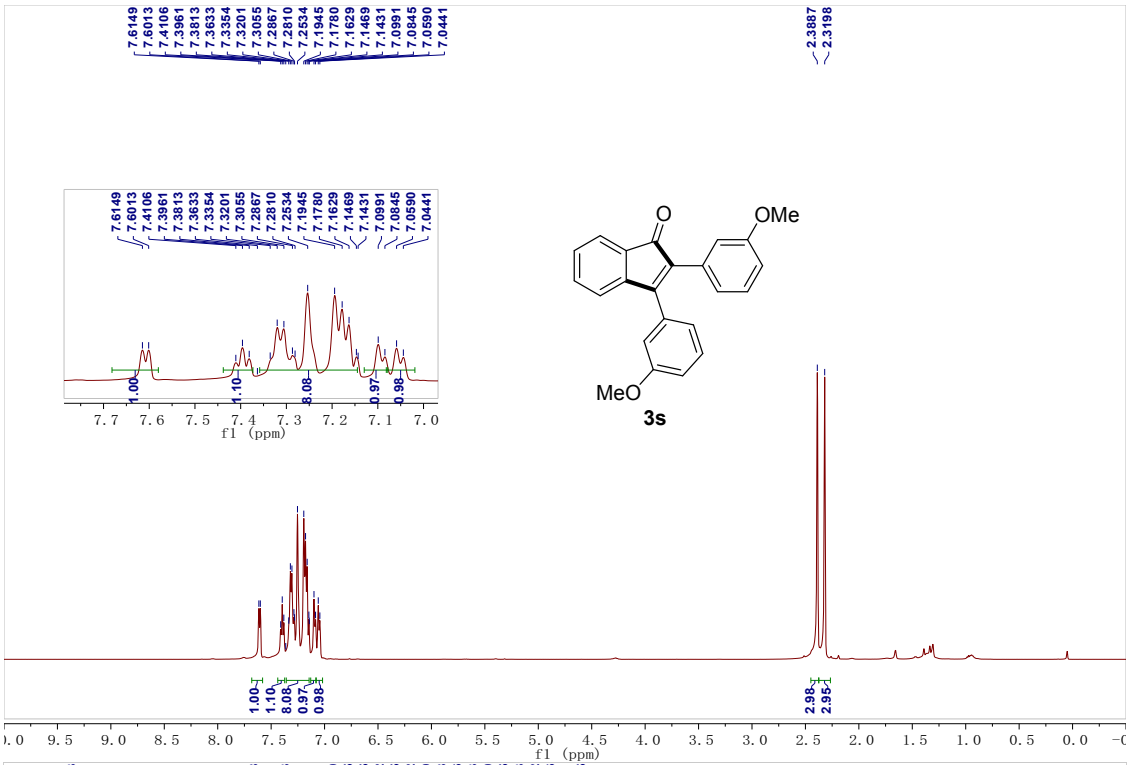
Me
Me
3r
f1 (ppm)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7.0845
7.0590
7.0441
2.3887
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8.08
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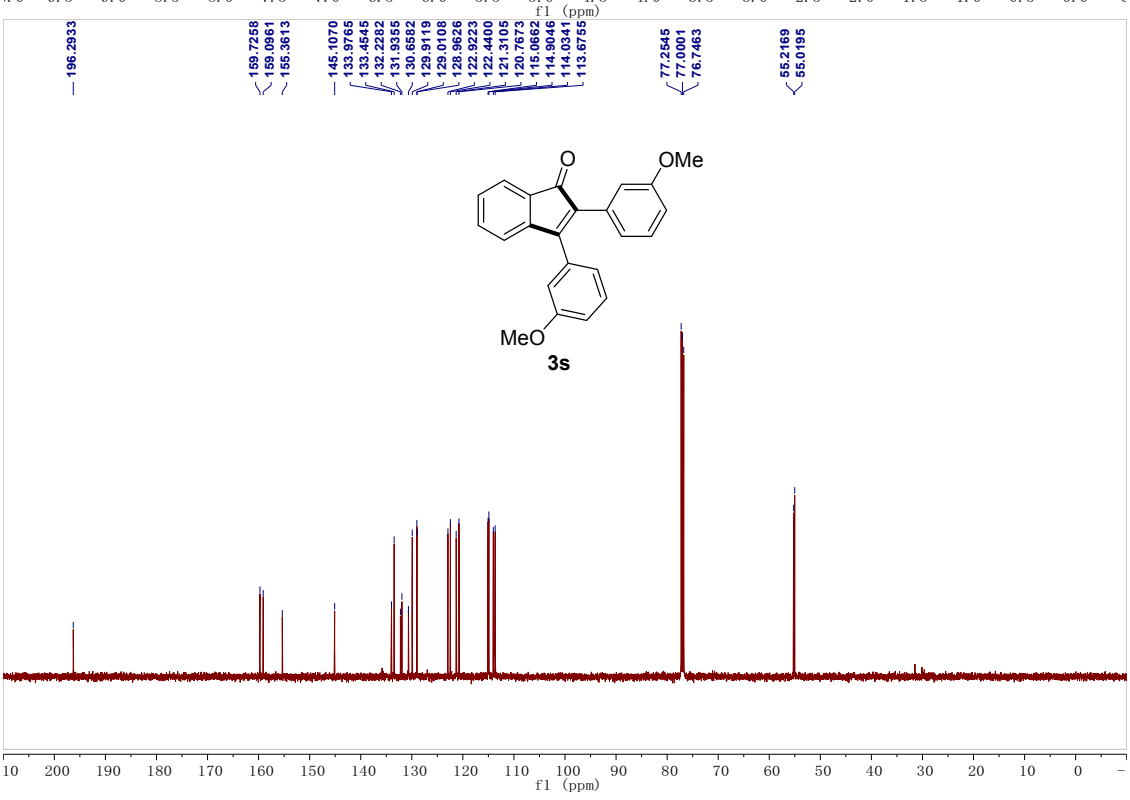
2.95
f1 (ppm)
O
OMe
MeO
3s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122.4400
121.3105
120.7673
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114.0341
113.6755
77.2545
77.0001
76.7463
55.2169
55.0195
f1 (ppm)
O
OMe
MeO
3s


7.6132
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7.3874
7.3725
7.3579
7.3226
7.3080
7.2931
7.2841
7.2690
7.2309
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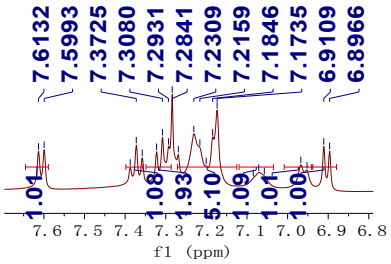
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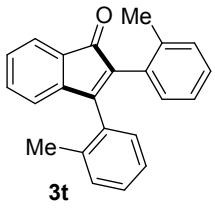
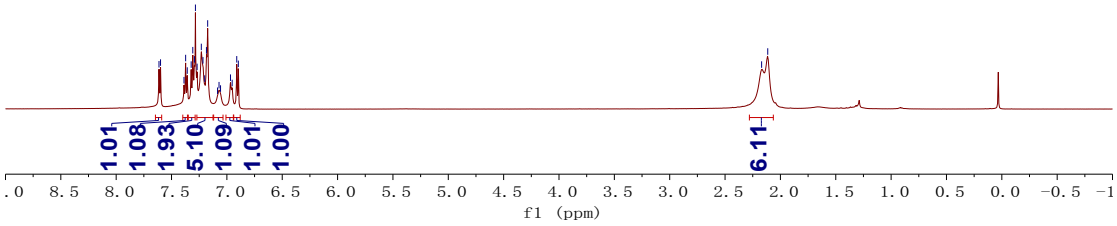
6.9109
6.8966
1.01
1.08
1.93
5.10
1.09
1.01
1.00
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)


O
Me
Me

3t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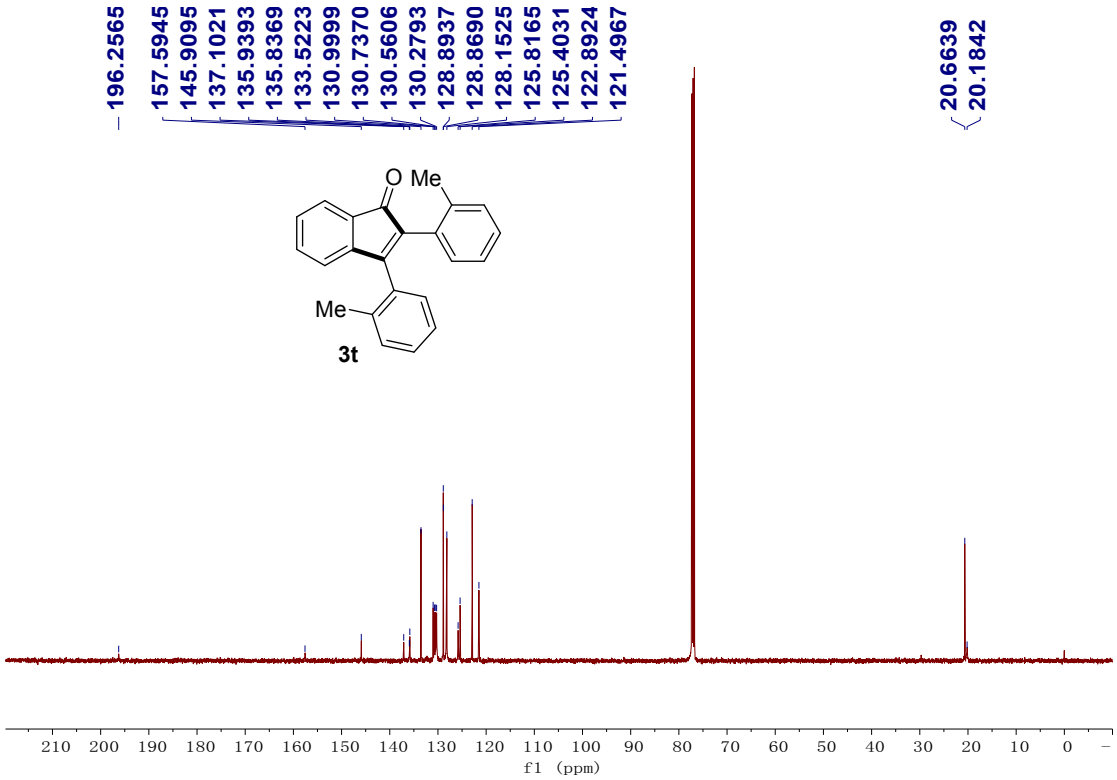
1.01
1.00
6.11
f1 (ppm)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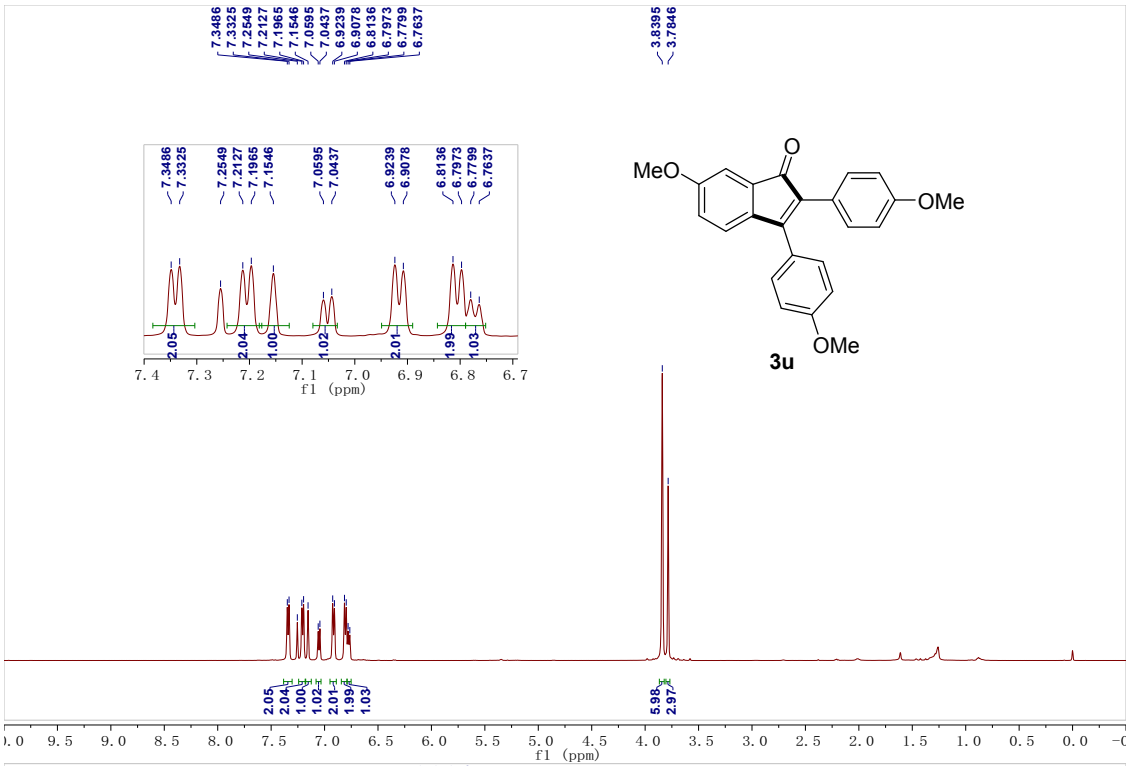
O
Me
Me
3t
f1 (ppm)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6.7973
6.7799
6.7637
3.8395
3.7846
MeO
OMe
OMe
O
3u
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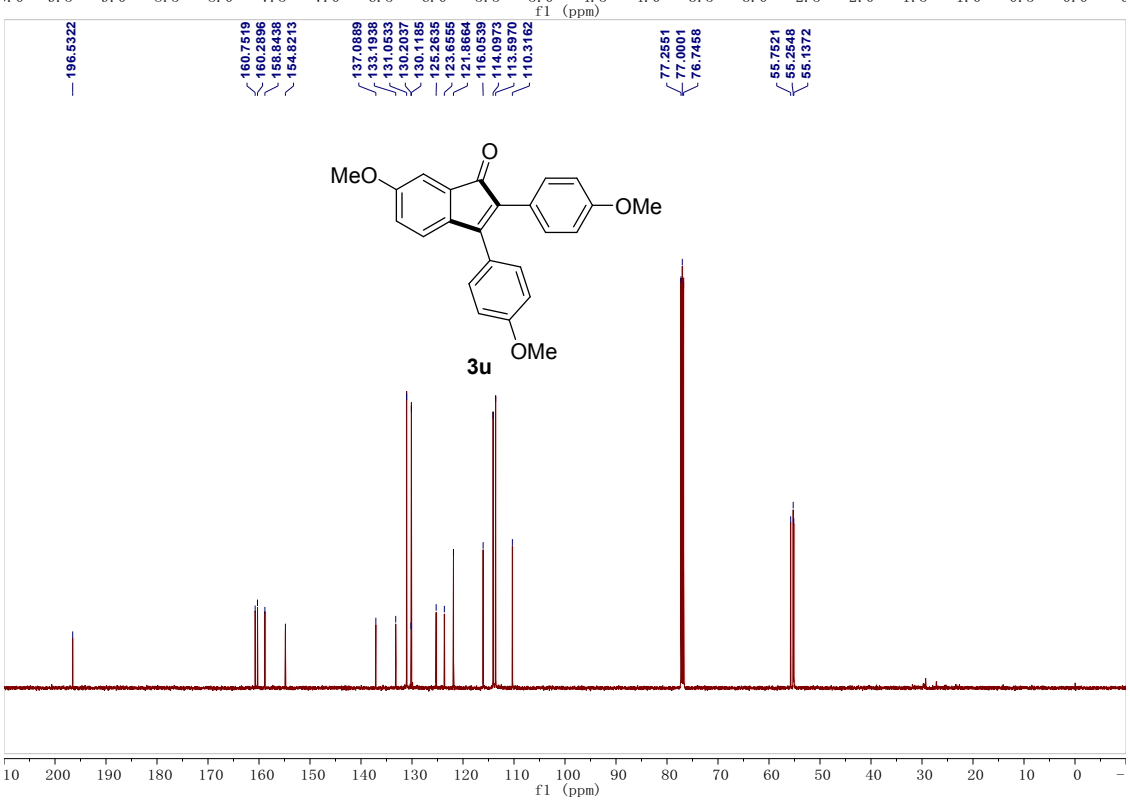
2.04
1.00
1.02
2.01
1.99
1.03
5.98
2.97
f1 (ppm)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123.6555
121.8664
116.0539
114.0973
113.5970
110.3162
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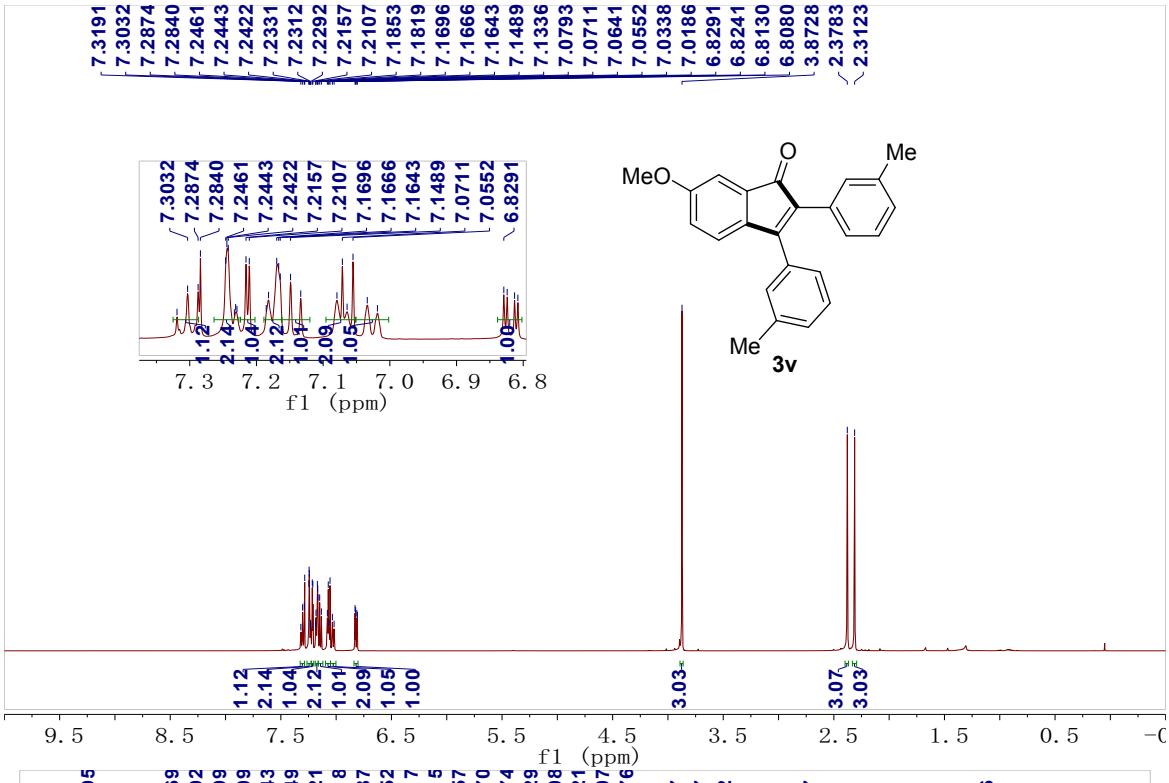
55.7521
55.2548
55.1372
MeO
OMe
OMe
O
3u
f1 (ppm)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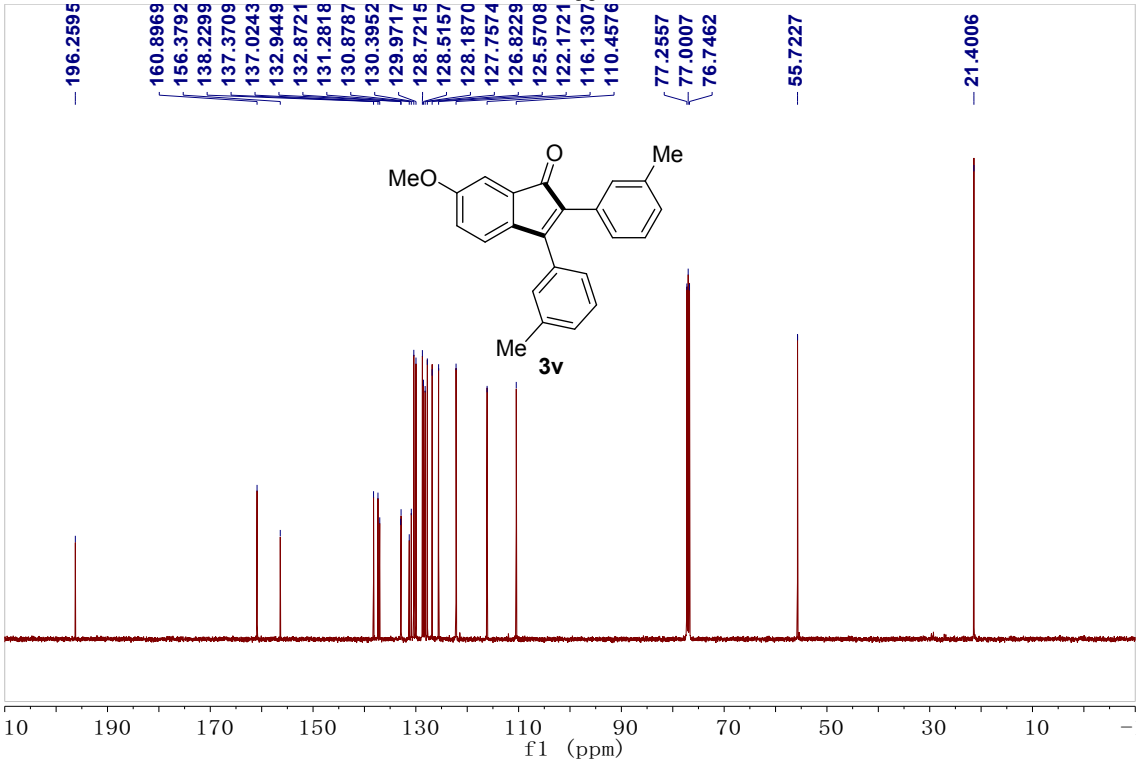
1.12 2.14 1.04 2.12 1.01 2.09 1.05 1.00 3.03 3.07 3.03
f1 (ppm)
MeO
O
Me
Me
3v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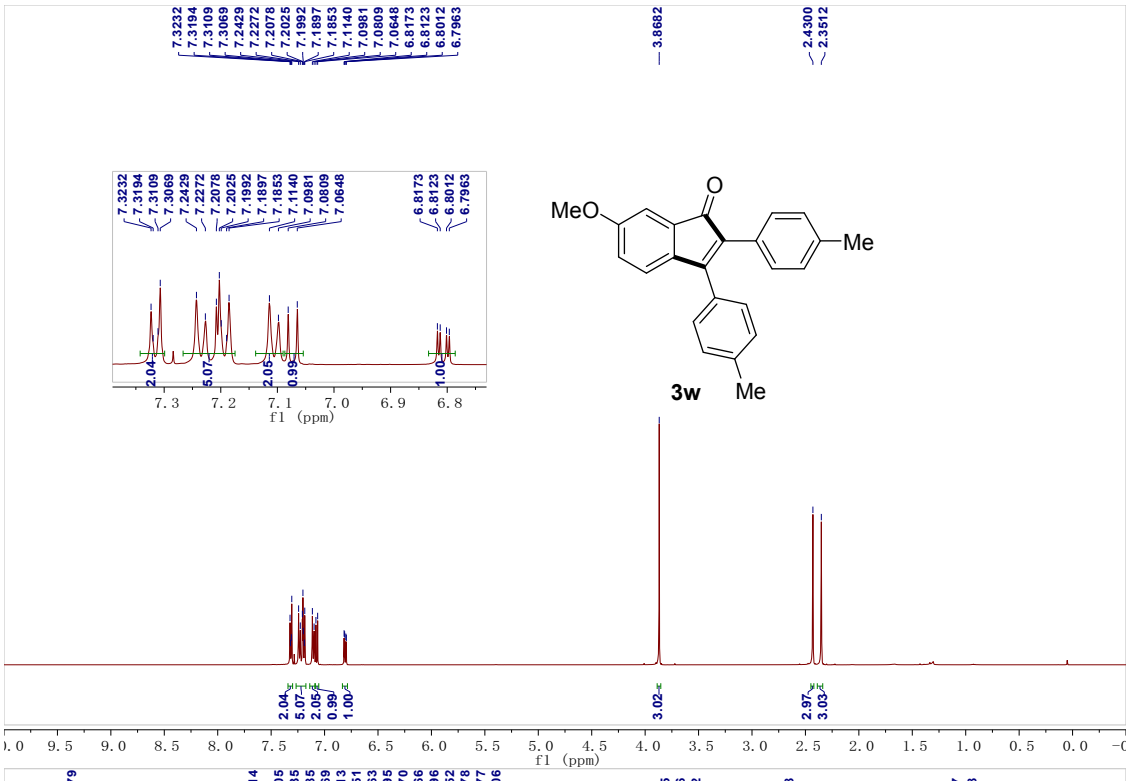
f1 (ppm)
MeO
O
Me
Me
3v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7.3109
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7.2429
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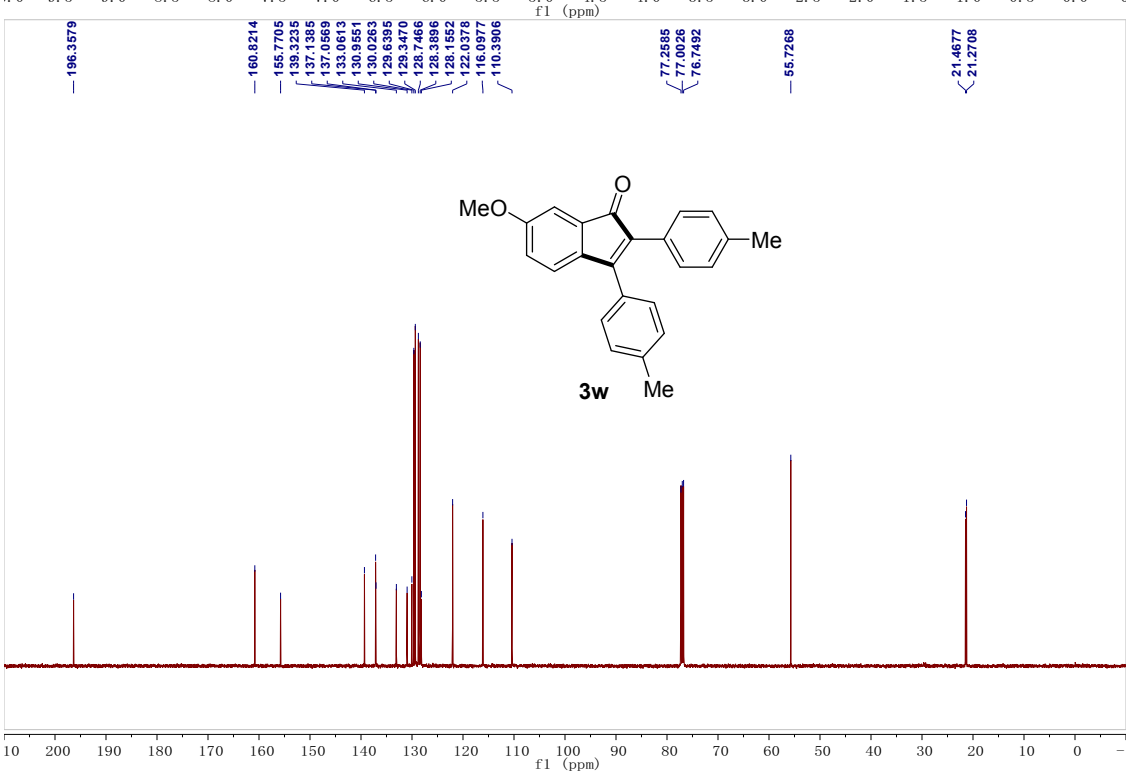
7.2078
7.2025
7.1992
7.1897
7.1853
7.1140
7.0981
7.0809
7.0648
6.8173
6.8123
6.8012
6.7963
3.8682
2.4300
2.3512
MeO
O
Me
3w
Me
f1 (ppm)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128.7466
128.3896
128.1552
122.0378
116.0977
110.3906
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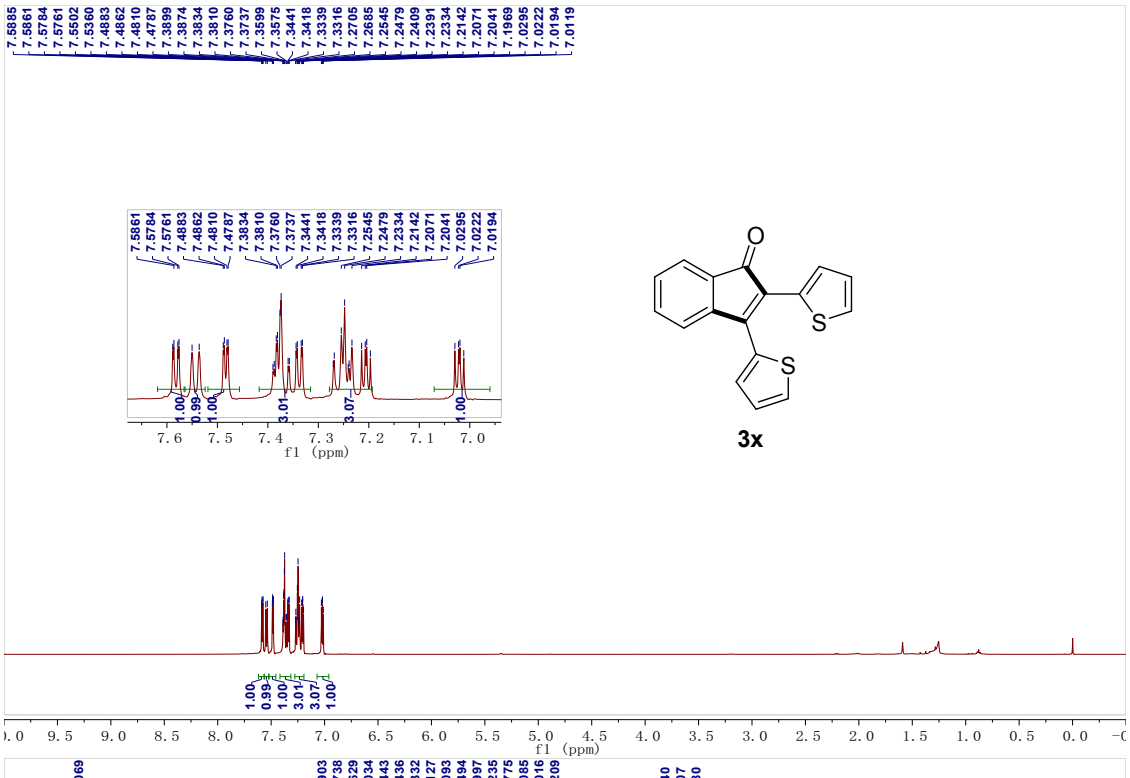
76.7492
55.7268
21.4677
21.2708
MeO
O
Me
3w
Me
f1 (ppm)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7.4810
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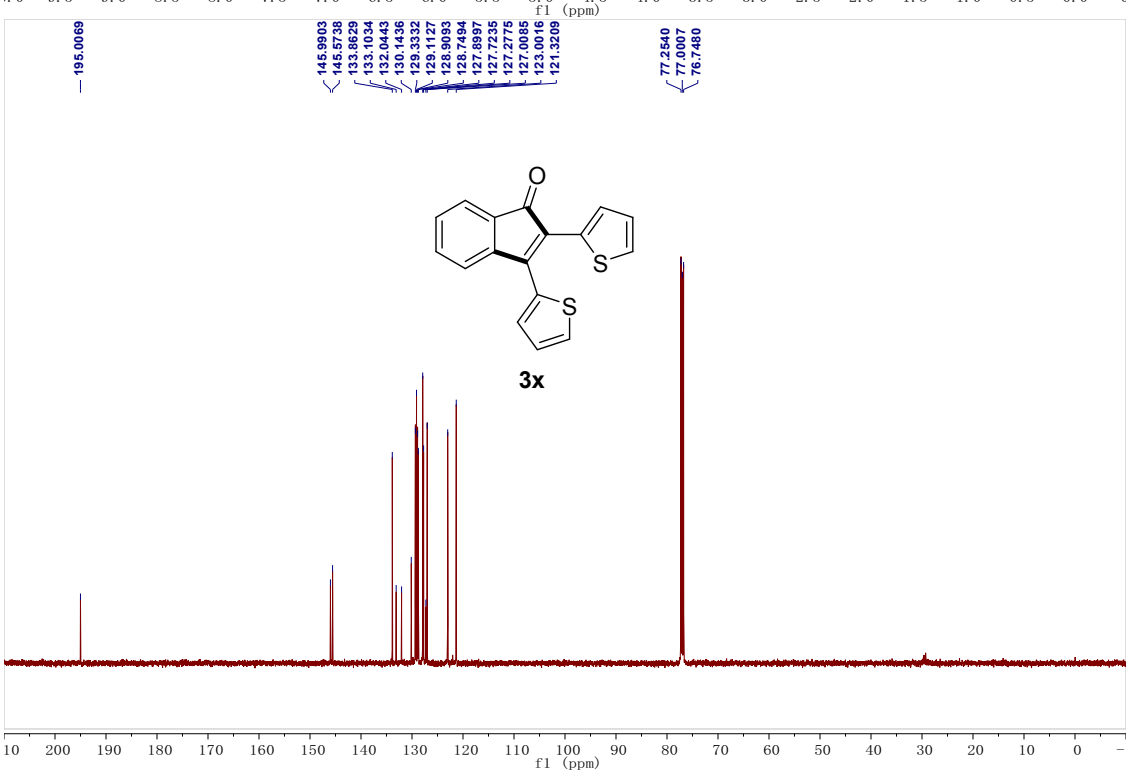
7.3874
7.3834
7.3810
7.3760
7.3737
7.3599
7.3575
7.3441
7.3418
7.3339
7.3316
7.2705
7.2685
7.2545
7.2479
7.2409
7.2391
7.2334
7.2142
7.2071
7.2041
7.1969
7.0295
7.0222
7.0194
7.0119
1.00
0.99
1.00
3.01
3.07
1.00
7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
O
S
S
3x
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.7494
127.8997
127.7235
127.2775
127.0085
123.0016
121.3209
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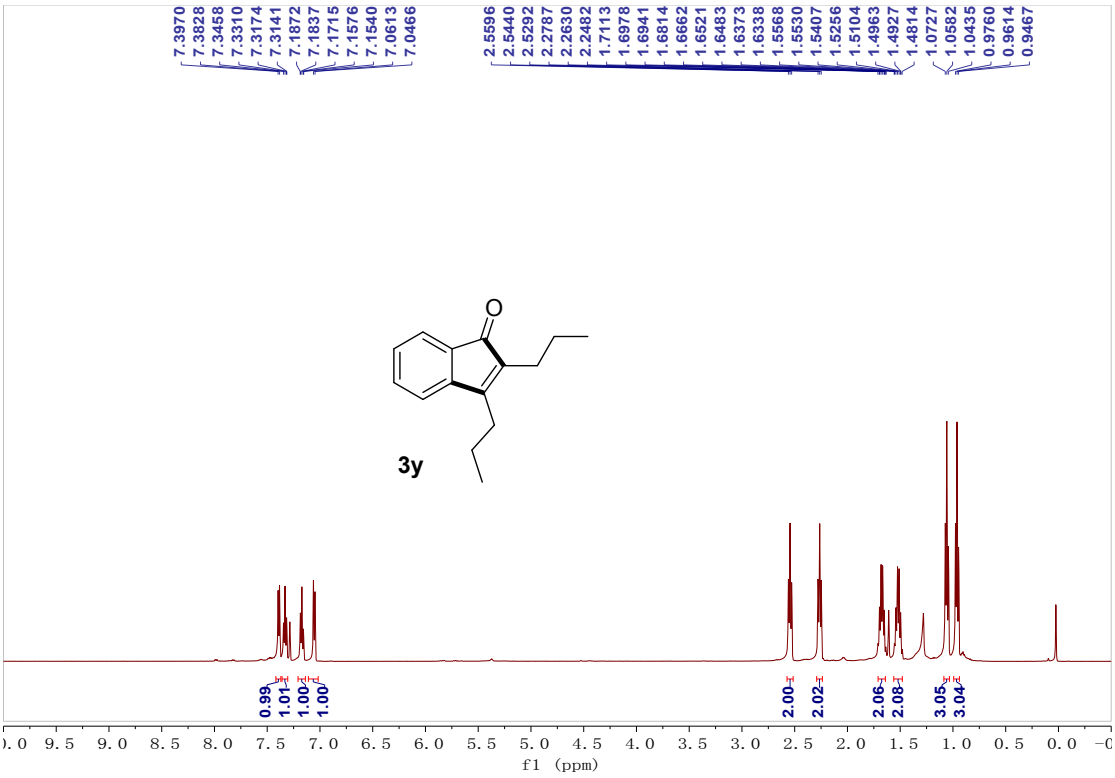
76.7480
O
S
S
3x
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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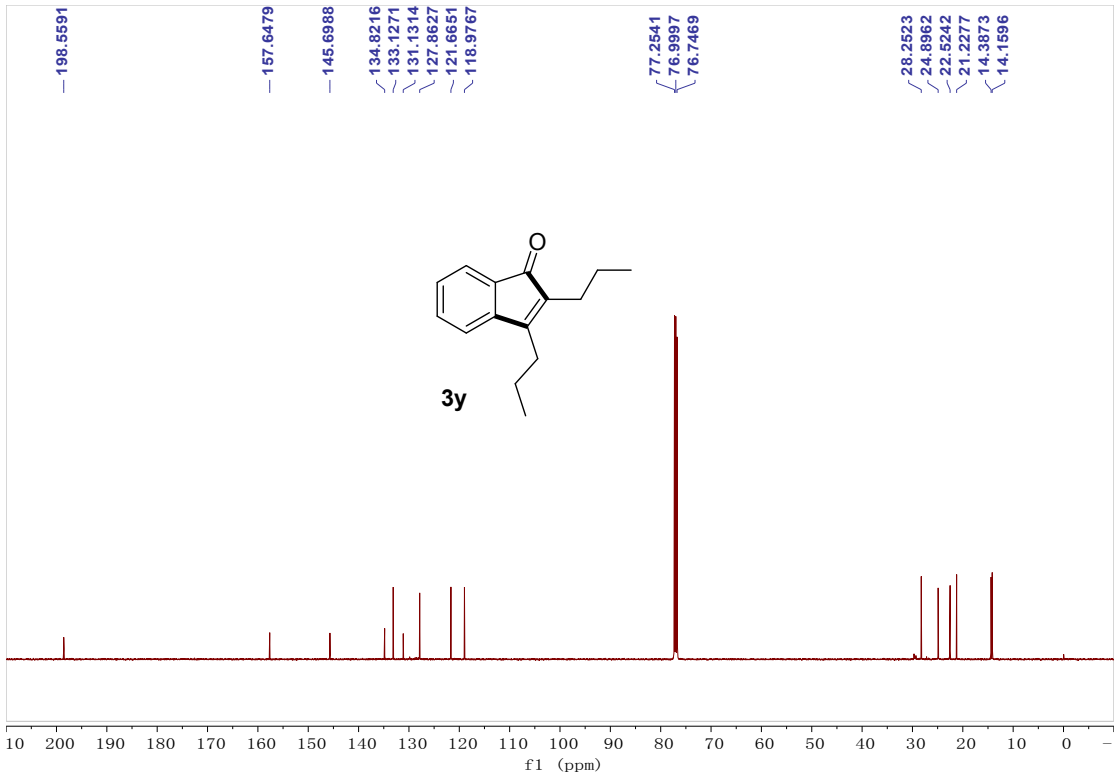
7.0613
7.0466
2.5596
2.5440
2.5292
2.2787
2.2630
2.2482
1.7113
1.6978
1.6941
1.6814
1.6662
1.6521
1.6483
1.6373
1.6338
1.5568
1.5530
1.5407
1.5256
1.5104
1.4963
1.4927
1.4814
1.0727
1.0582
1.0435
0.9760
0.9614
0.9467
O
3y
0.99
1.01
1.00
1.00
2.00
2.02
2.06
2.08
3.05
3.04
f1 (ppm)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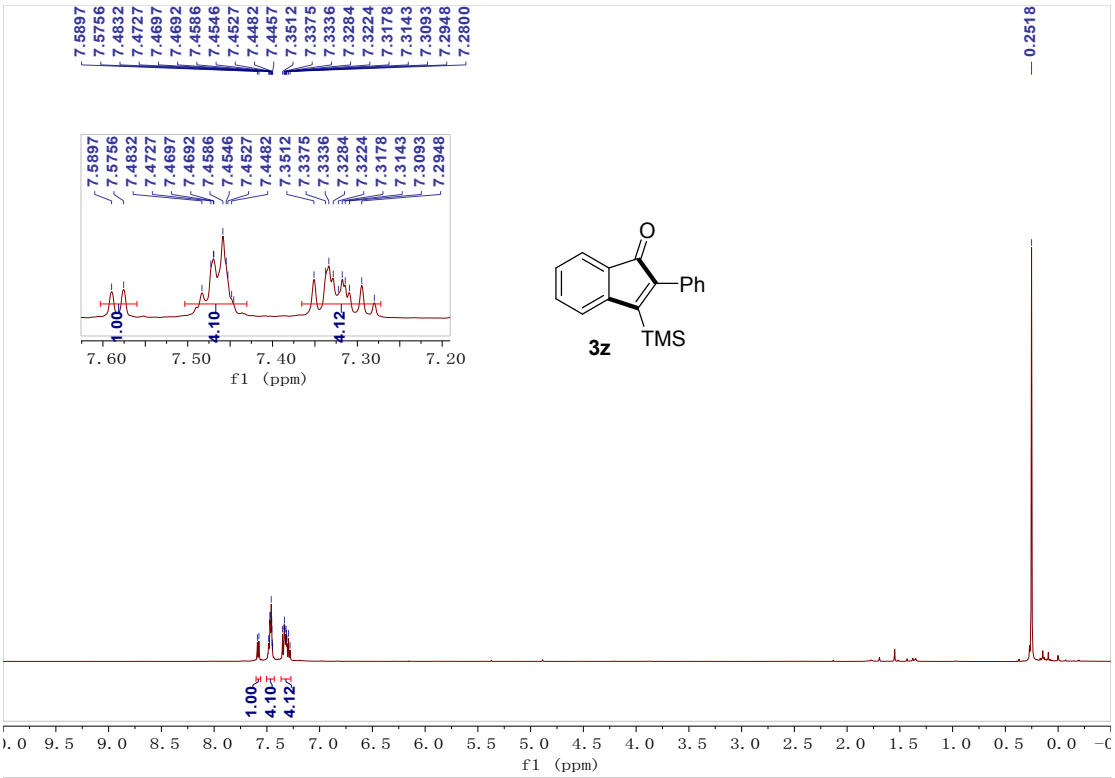
28.2523
24.8962
22.5242
21.2277
14.3873
14.1596
O
3y
f1 (ppm)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7.4727
7.4697
7.4692
7.4586
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7.4527
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7.4457
7.3512
7.3375
7.3336
7.3284
7.3224
7.3178
7.3143
7.3093
7.2948
7.2800
0.2518
1.00
4.10
4.12
7.60
7.50
7.40
7.30
7.20
f1 (ppm)
O
Ph
TMS
3z
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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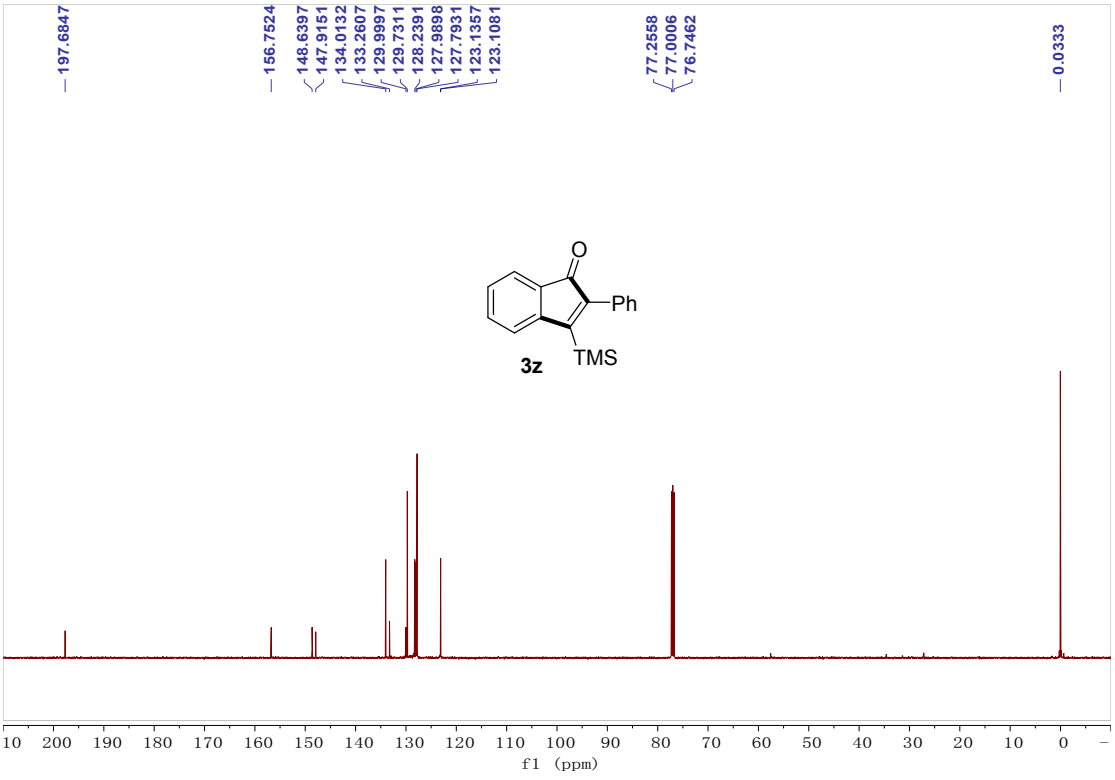
2.0
1.5
1.0
0.5
0.0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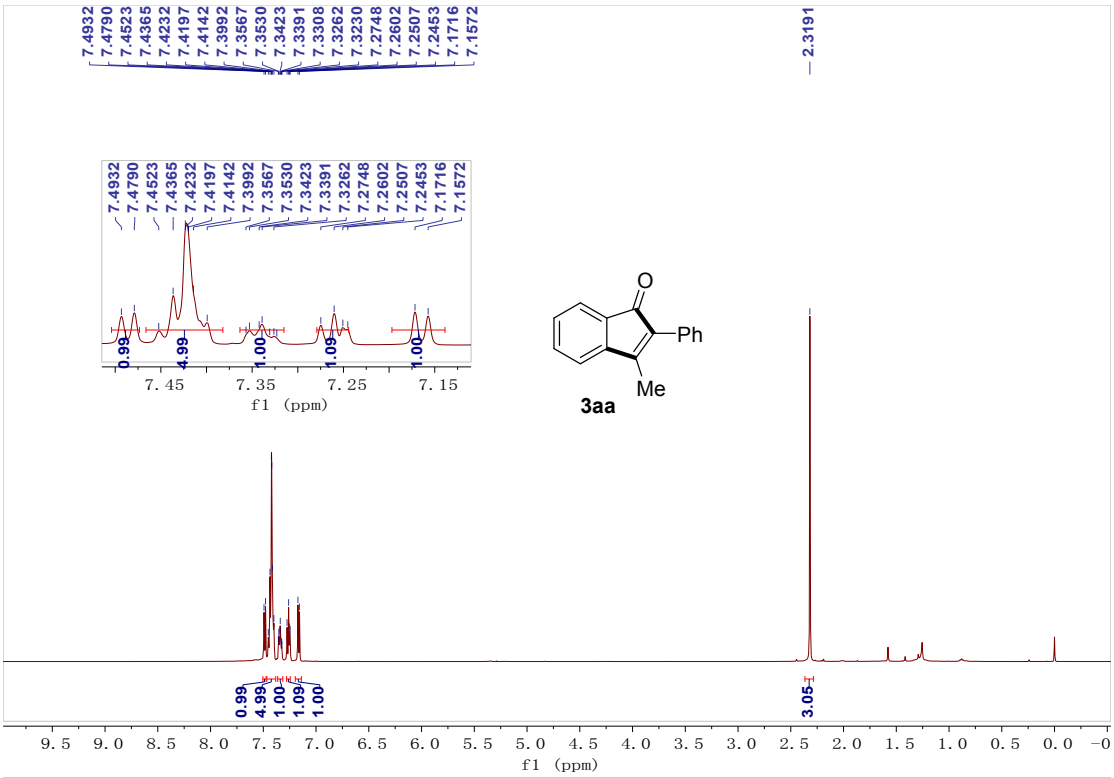
133.2607
129.9997
129.7311
128.2391
127.9898
127.7931
123.1357
123.1081
77.2558
77.0006
76.7462
0.0333
O
Ph
TMS
3z
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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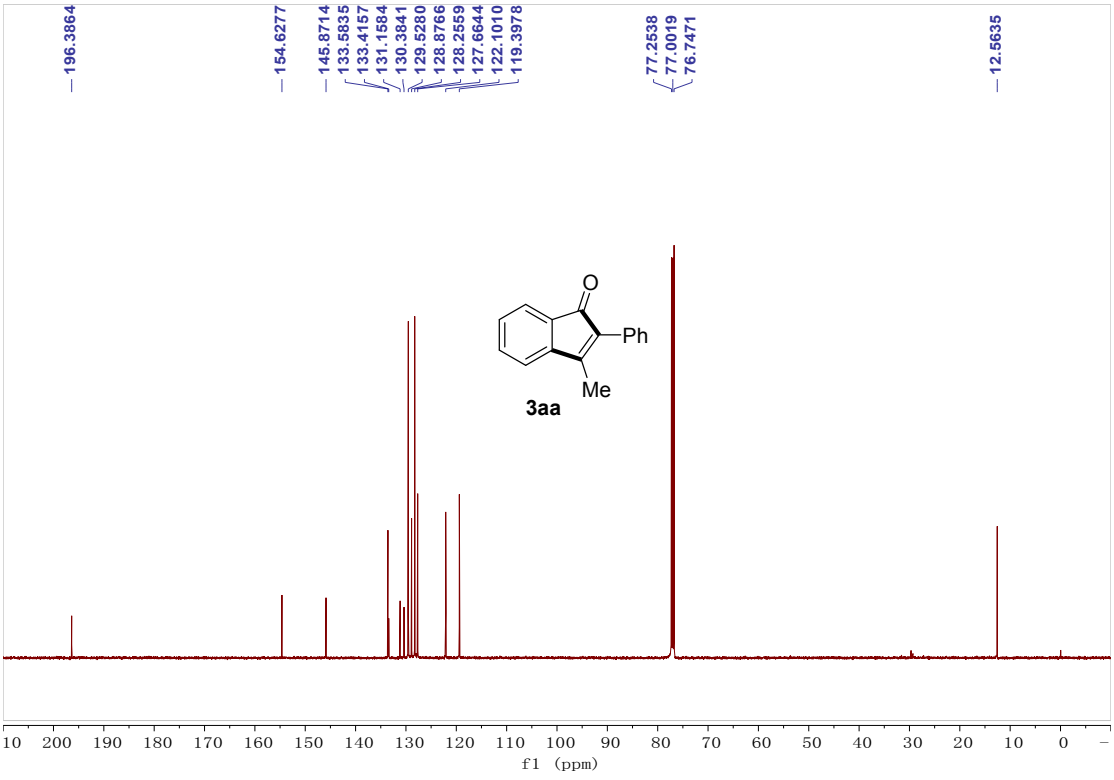
7.4232
7.4197
7.4142
7.3992
7.3567
7.3530
7.3423
7.3391
7.3308
7.3262
7.3230
7.2748
7.2602
7.2507
7.2453
7.1716
7.1572
2.3191
0.99
4.99
1.00
1.09
1.00
3.05
f1 (ppm)
O
Ph
Me
3aa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130.3841
129.5280
128.8766
128.2559
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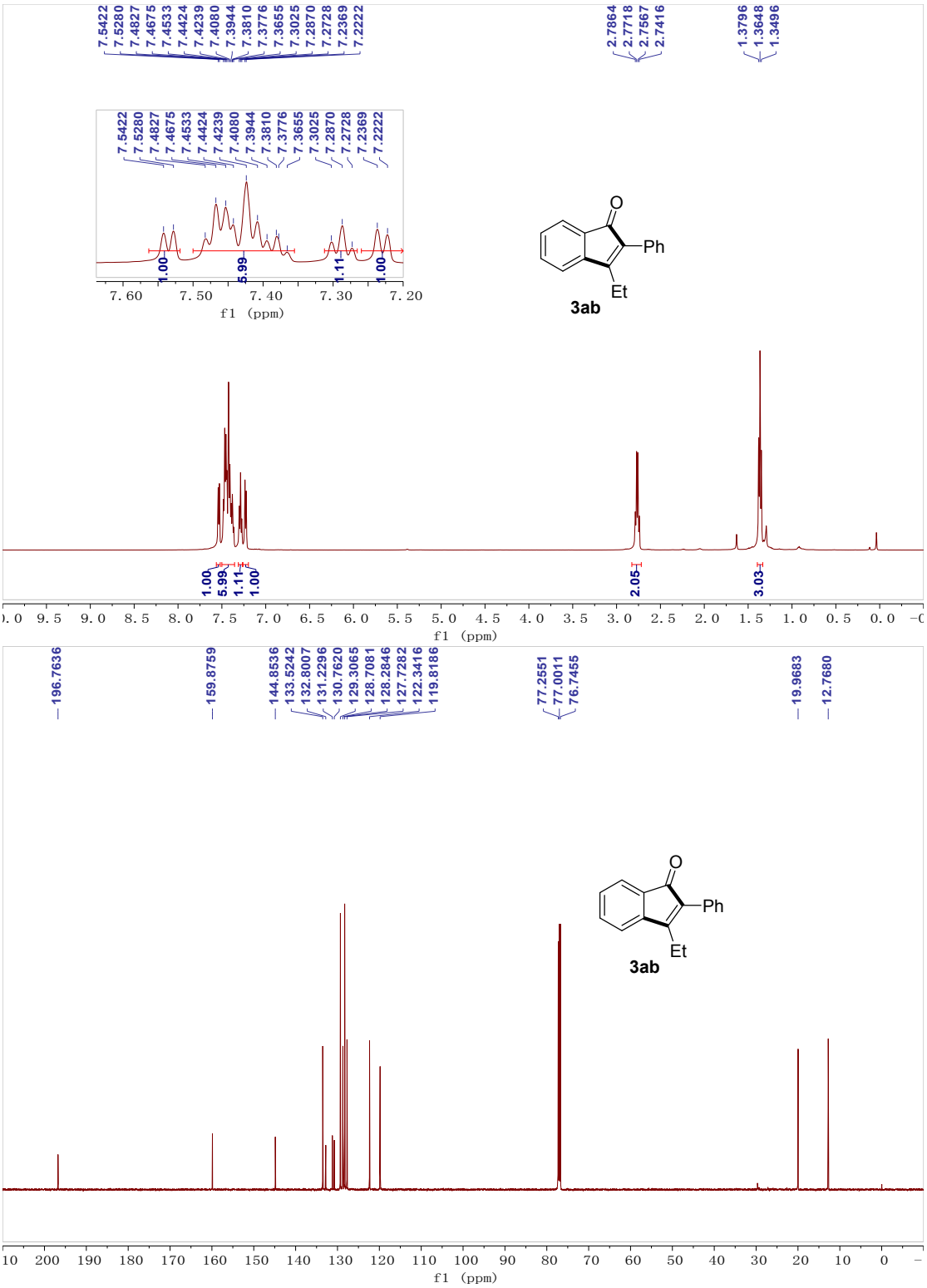
119.3978
77.2538
77.0019
76.7471
12.5635
f1 (ppm)
O
Ph
Me
3aa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7.4827
7.4675
7.4533
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7.4239
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7.3944
7.3810
7.3776
7.3655
7.3025
7.2870
7.2728
7.2369
7.2222
2.7864
2.7718
2.7567
2.7416
1.3796
1.3648
1.3496
1.00
5.99
1.11
1.00
7.60
7.50
7.40
7.30
7.20
f1 (ppm)
O
Ph
Et
3ab
1.00
5.99
1.11
1.00
2.05
3.03
f1 (ppm)
196.7636
159.8759
144.8536
133.5242
132.8007
131.2296
130.7620
129.3065
128.7081
128.2846
127.7282
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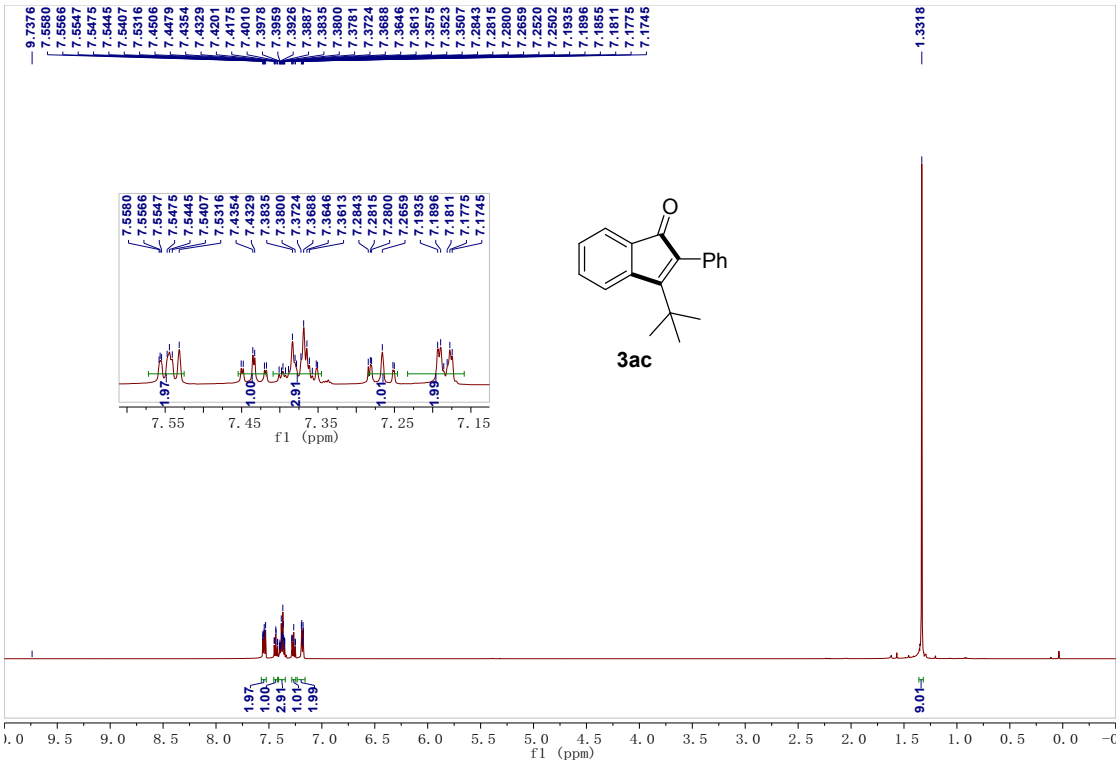
O
Ph
Et
3ab
f1 (ppm)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7.5407
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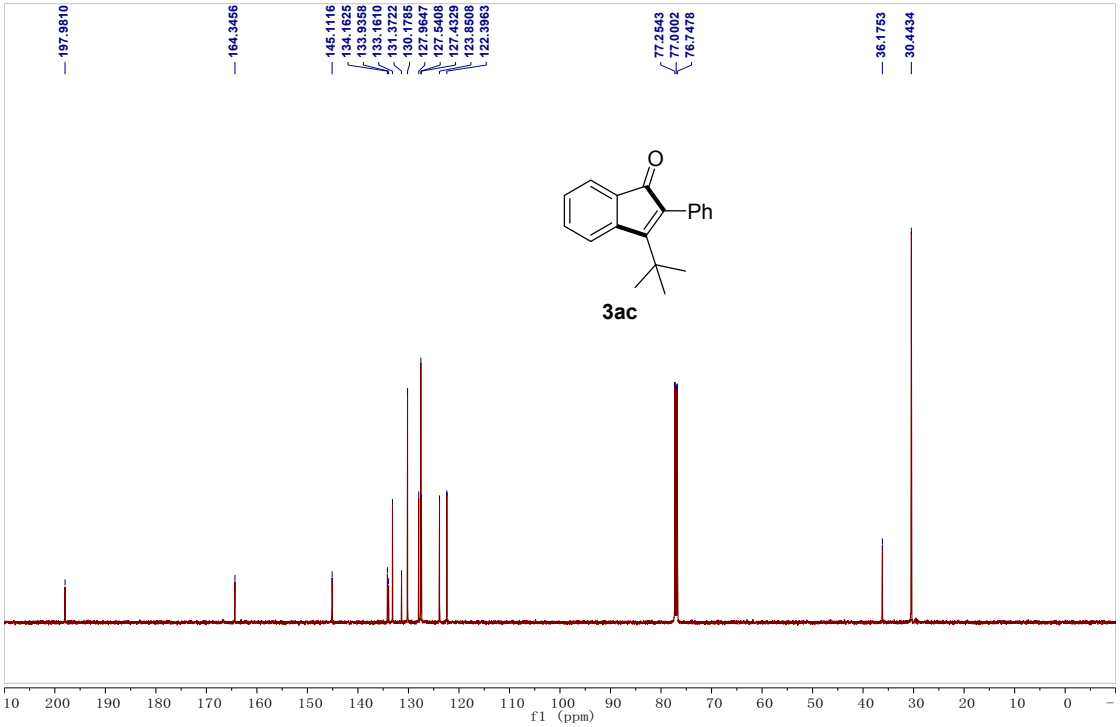
7.4354
7.4329
7.4201
7.4175
7.4010
7.3978
7.3959
7.3926
7.3887
7.3835
7.3800
7.3781
7.3724
7.3688
7.3646
7.3613
7.3575
7.3523
7.3507
7.2843
7.2815
7.2800
7.2659
7.2520
7.2502
7.1935
7.1896
7.1855
7.1811
7.1775
7.1745
1.3318
1.97
1.00
2.91
1.01
1.99
9.01
f1 (ppm)
O
Ph
3ac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127.4329
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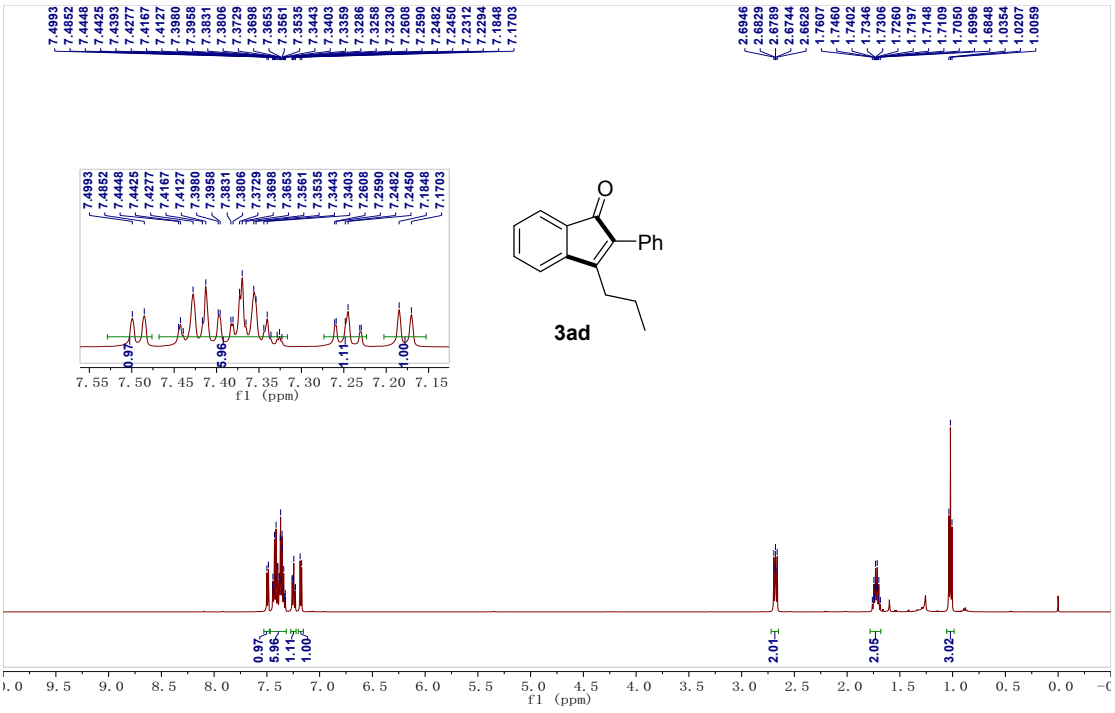
77.2543
77.0002
76.7478
36.1753
30.4434
f1 (ppm)
O
Ph
3ac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7.4277
7.4167
7.4127
7.3980
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7.3831
7.3806
7.3729
7.3698
7.3653
7.3561
7.3535
7.3443
7.3403
7.3359
7.3286
7.3258
7.3230
7.2608
7.2590
7.2482
7.2450
7.2312
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7.1848
7.1703
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2.6829
2.6789
2.6744
2.6628
1.7607
1.7460
1.7402
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1.7260
1.7197
1.7148
1.7109
1.7050
1.6996
1.6848
1.0354
1.0207
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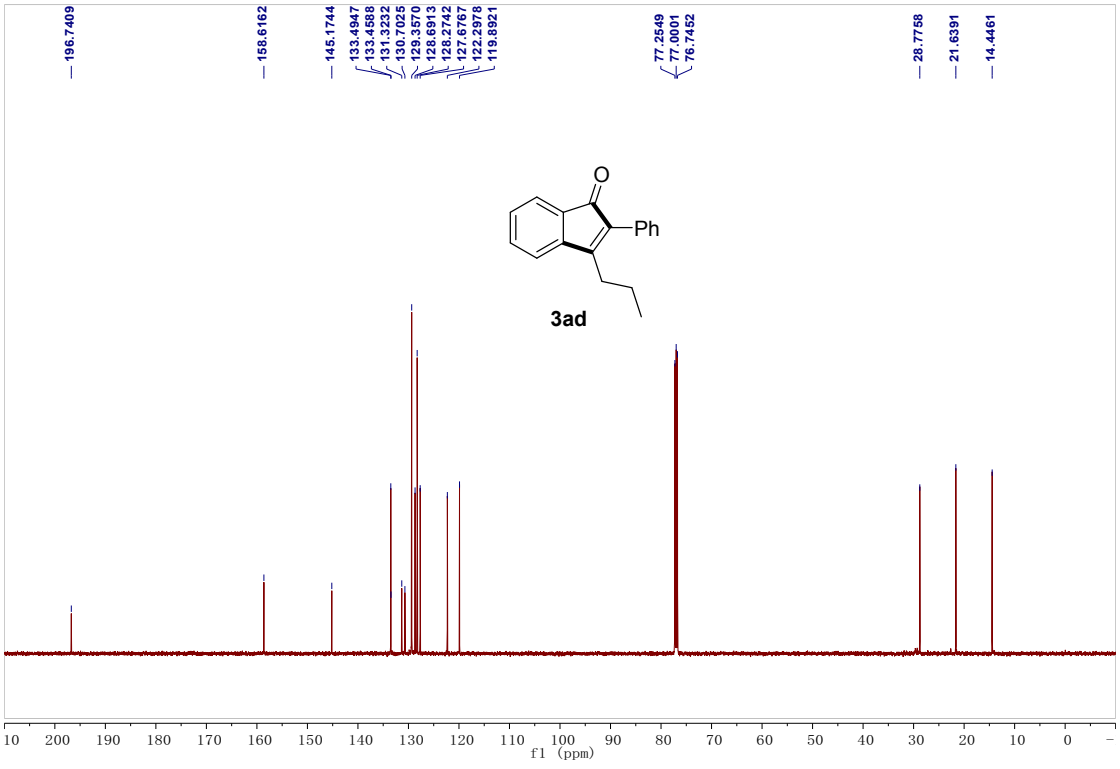
5.96
1.11
1.00
2.01
2.05
3.02
f1 (ppm)
Ph
O
3ad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122.2978
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77.0001
76.7452
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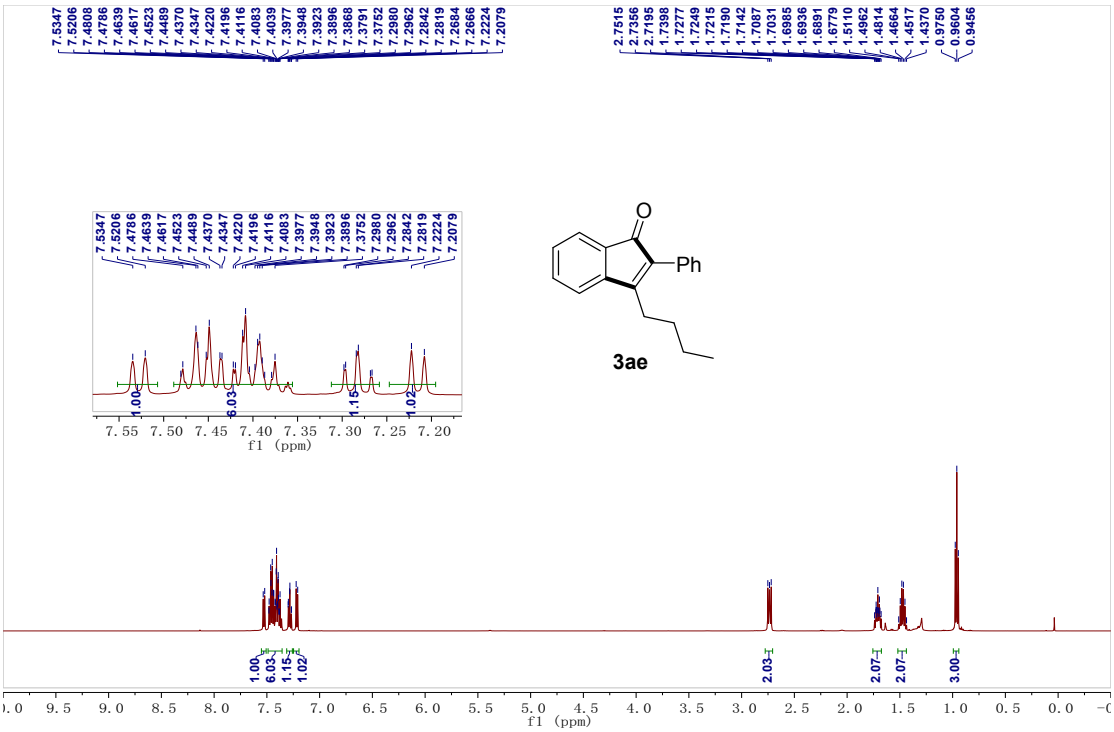
14.4461
f1 (ppm)
Ph
O
3ad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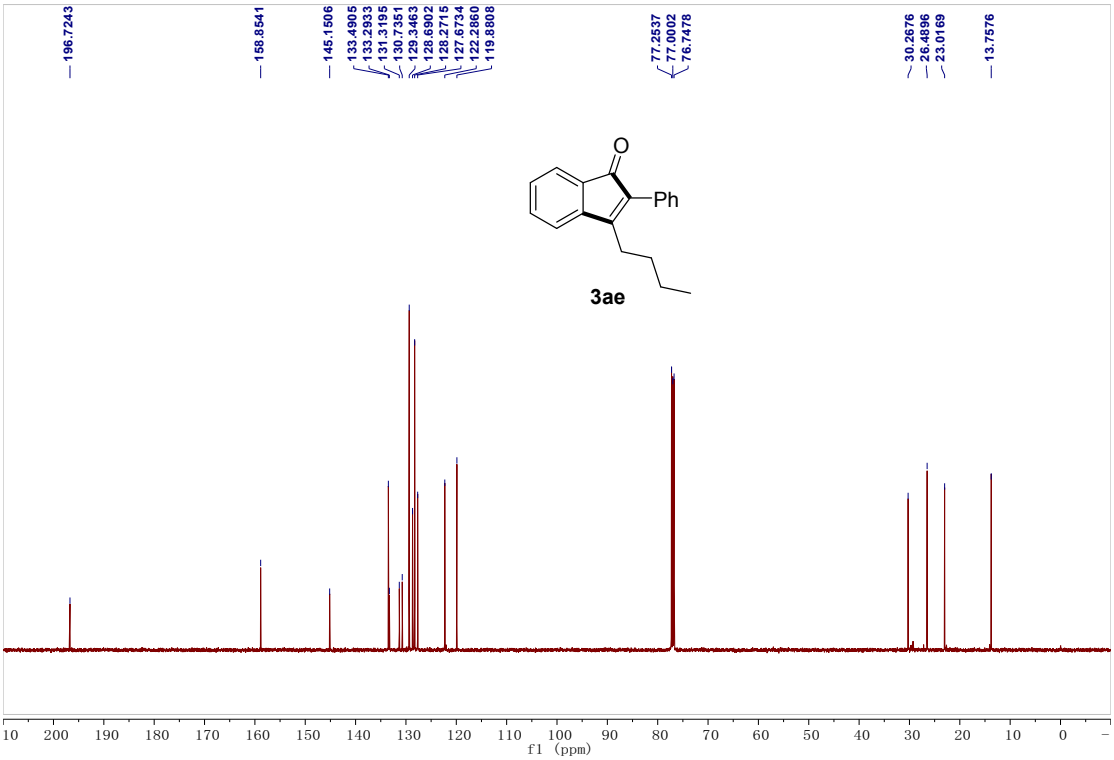
2.7515 2.7356 2.7195 1.7398 1.7277 1.7249 1.7215 1.7190 1.7142 1.7087 1.7031 1.6985 1.6936 1.6891 1.6779 1.5110 1.4962 1.4814 1.4664 1.4517 1.4370 0.9750 0.9604 0.9456
1.00 6.03 1.15 1.02
7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20
f1 (ppm)
O
Ph
3ae
1.00 6.03 1.15 1.02 2.03 2.07 2.07 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.6902
128.2715
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122.2860
119.8808
77.2537
77.0002
76.7478
30.2676
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O
Ph
3ae
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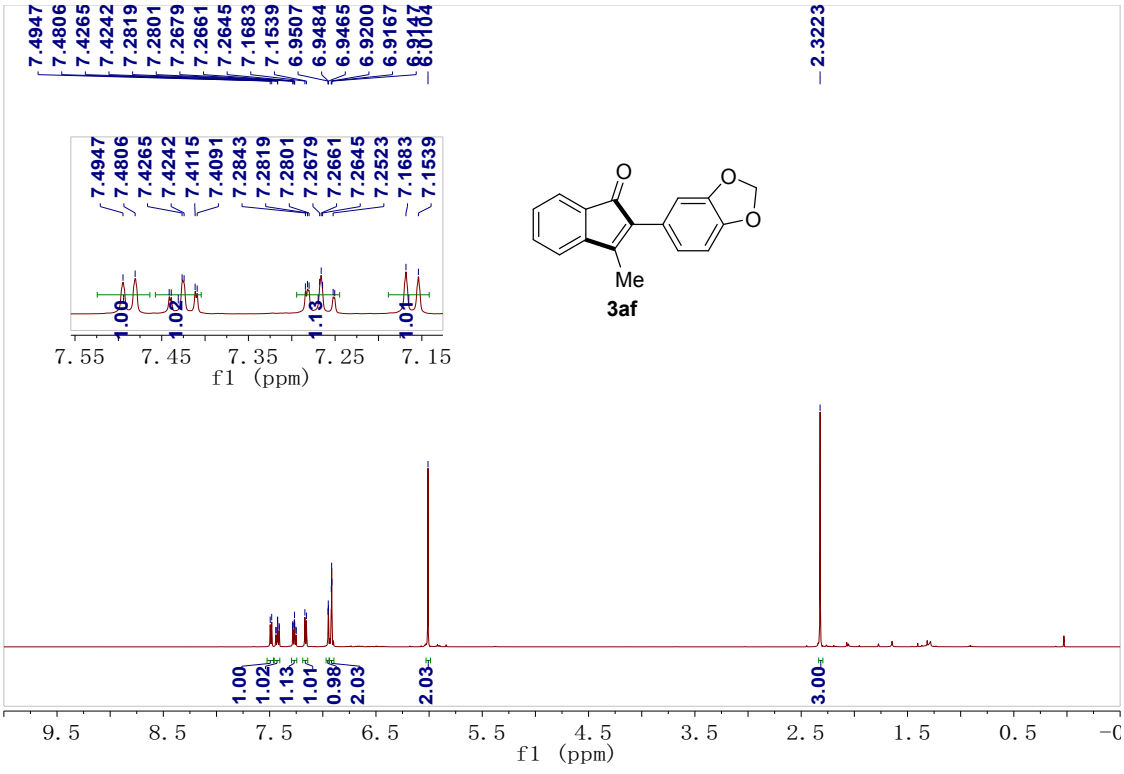
f1 (ppm)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6.9507
6.9484
6.9465
6.9200
6.9167
6.9147
6.9104
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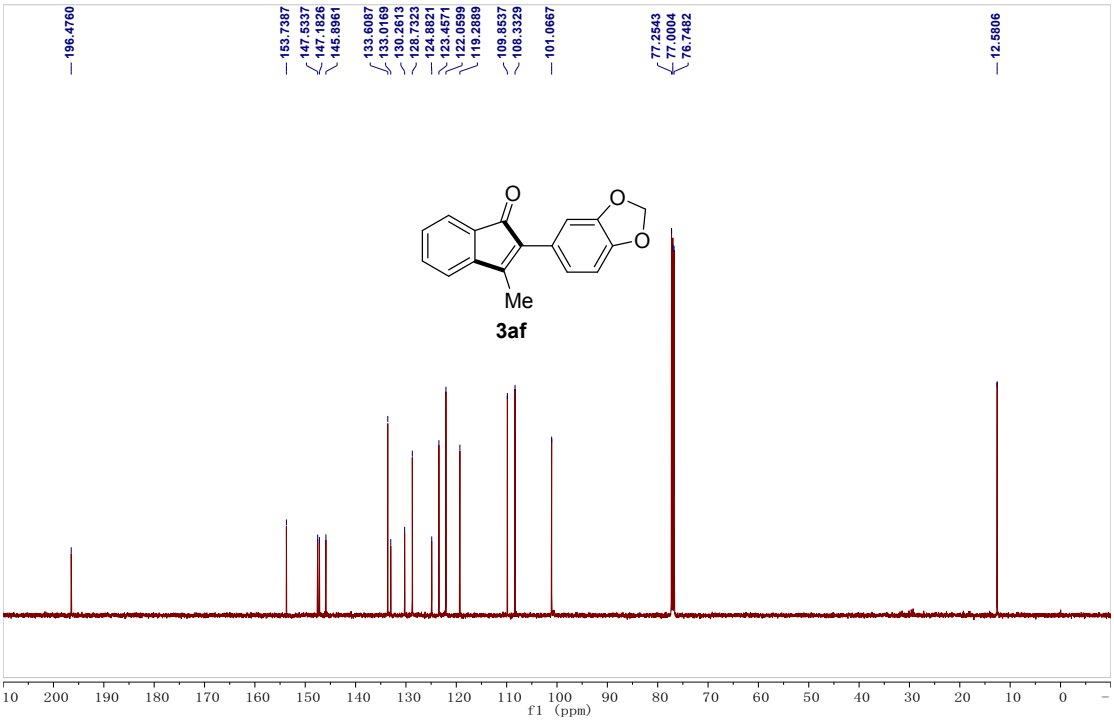
7.2801
7.2679
7.2661
7.2645
7.2523
7.1683
7.1539
1.00
1.02
1.13
1.01
7.55
7.45
7.35
7.25
7.15
f1 (ppm)
O
O
O
Me
3af
1.00
1.02
1.13
1.01
0.98
2.03
2.03
3.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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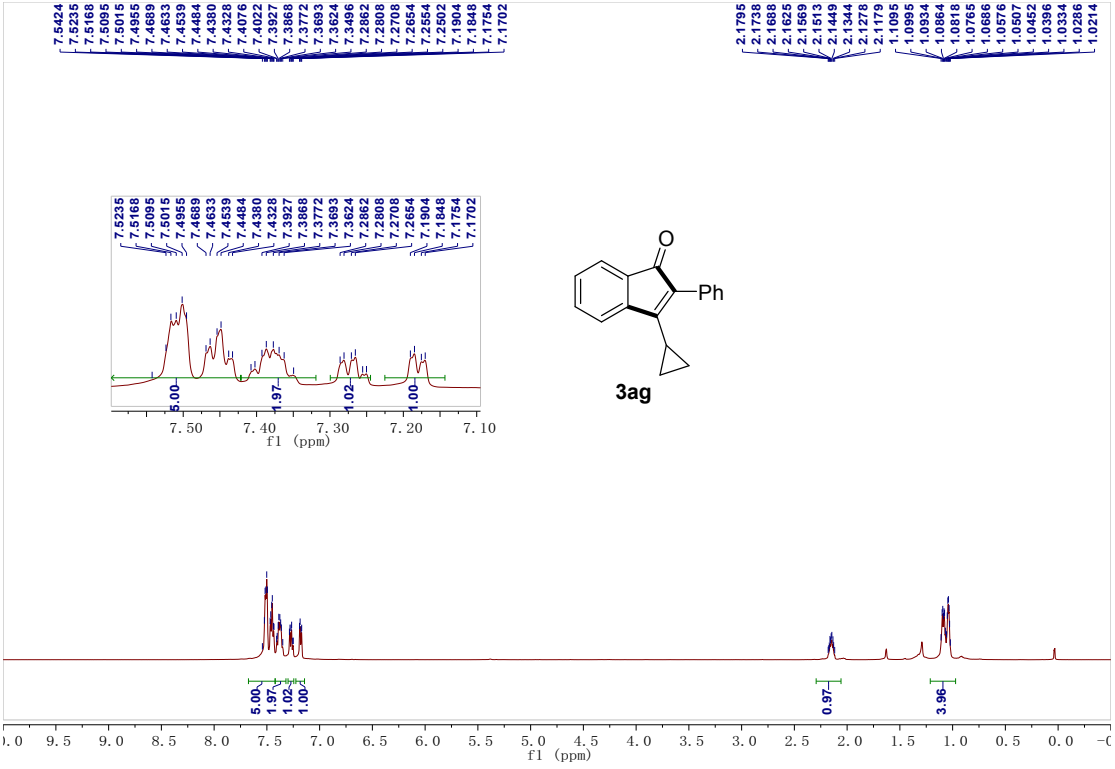
119.2889
109.8537
108.3329
101.0667
77.2543
77.0004
76.7482
12.5806
O
O
O
Me
3af
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4328
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7.4022
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7.3868
7.3772
7.3693
7.3624
7.3496
7.2862
7.2808
7.2708
7.2654
7.2554
7.2502
7.1904
7.1848
7.1754
7.1702
2.1795
2.1738
2.1688
2.1625
2.1569
2.1513
2.1449
2.1344
2.1278
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1.1095
1.0995
1.0934
1.0864
1.0818
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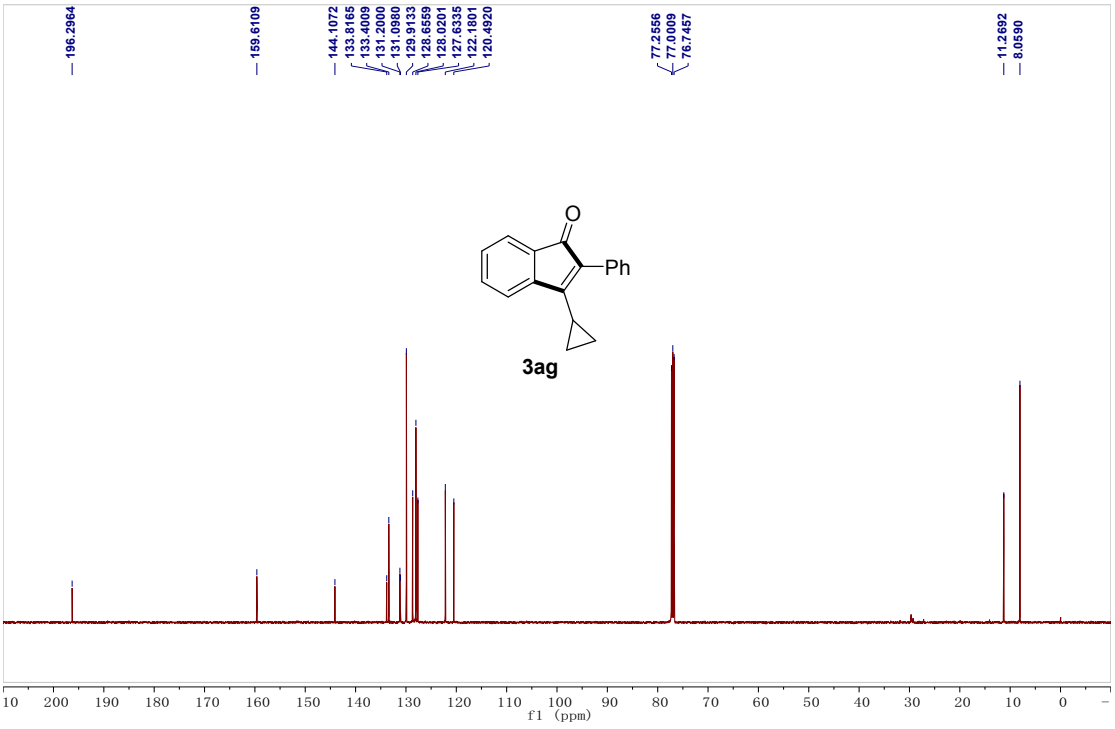
1.0452
1.0396
1.0334
1.0286
1.0214
5.00
1.97
1.02
1.00
7.50
7.40
7.30
7.20
7.10
f1 (ppm)
O
Ph
3ag
0.97
3.96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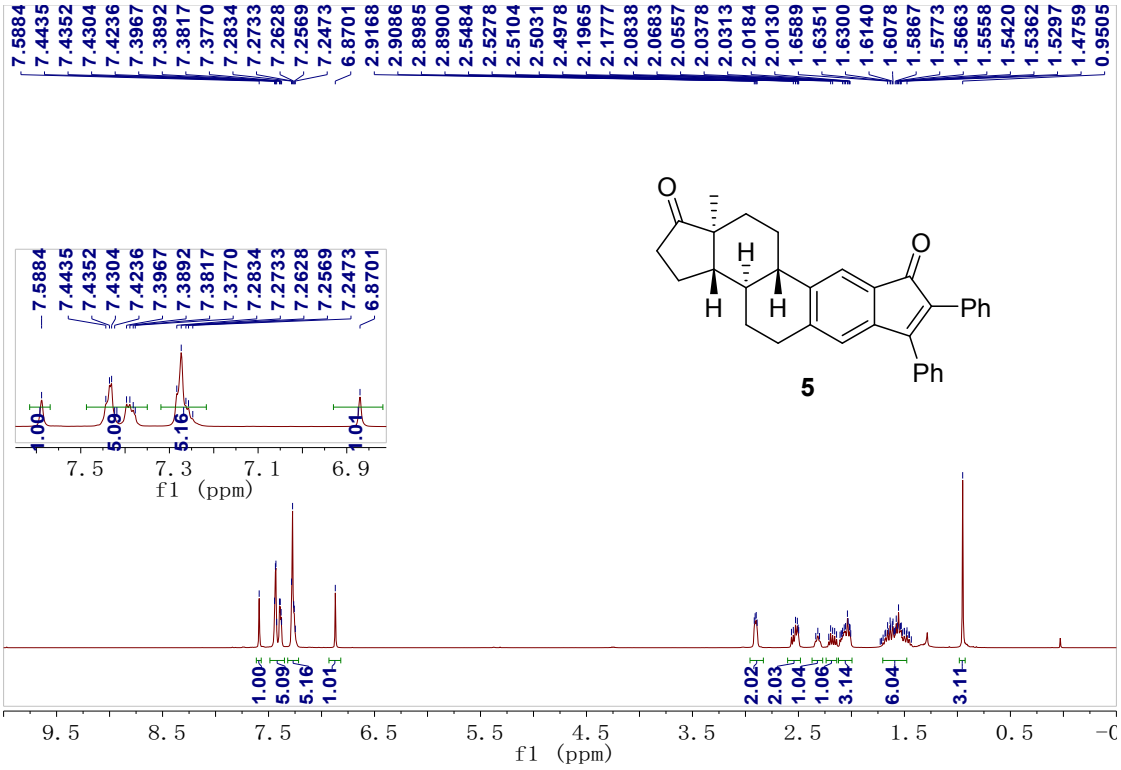
8.0590
O
Ph
3ag
f1 (ppm)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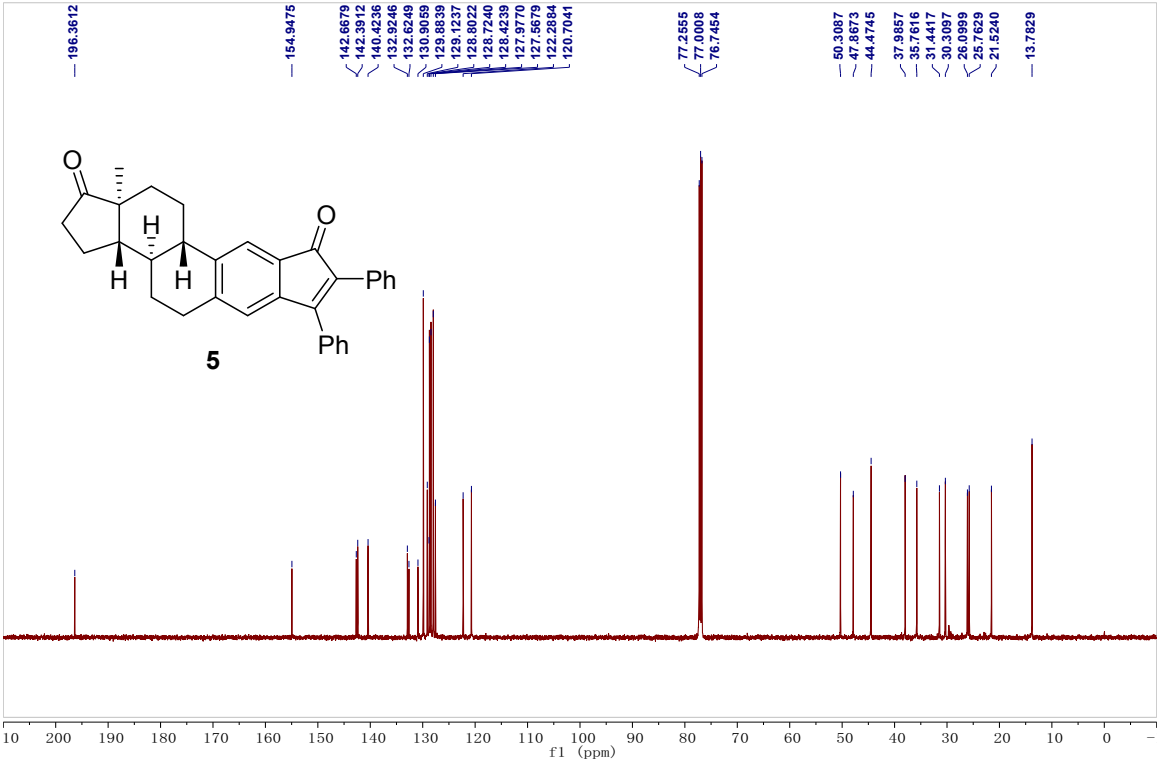
1.00 5.09 5.16 1.01 2.02 2.03 1.04 1.06 3.14 6.04 3.11
9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)
O
H
H
H
O
Ph
Ph
5


196.3612 154.9475 142.6679 142.3912 140.4236 132.9246 132.6249 130.9059 129.8839 129.1237 128.8022 128.7240 128.4239 127.9770 127.5679 122.2884 120.7041 77.2555 77.0008 76.7454 50.3087 47.8673 44.4745 37.9857 35.7616 31.4417 30.3097 26.0999 25.7629 21.5240 13.7829
O
H
H
H
O
Ph
Ph
5
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)