A Diversity-Oriented Synthesis of Cyclopenta[*b*]pyrroles and Related Compounds through a Calcium(II)/Copper(II) Catalytic Sequence

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Supporting Information

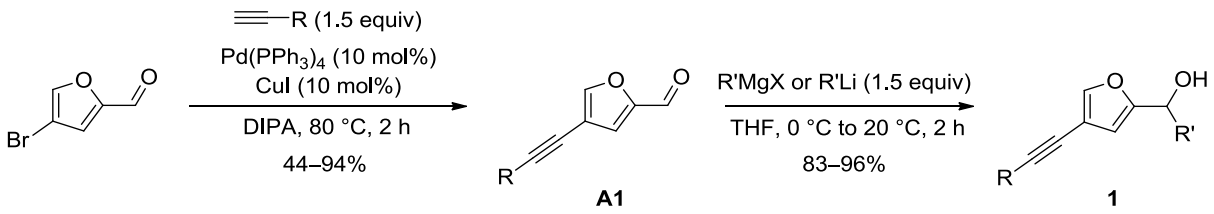
General Information

Unless otherwise stated, reactions were carried out in oven-dried flasks. Analytical thin layer chromatography was carried out using TLC-aluminum sheets with 0.2 mm of silica gel (Merck GF234) using UV light as the visualizing agent and a solution of phosphomolybdic acid in ethanol as the developing agent. Chromatography purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60 mm). Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator. NMR spectra were recorded at 298 K on AM250, AV300 or AV360 MHz Bruker spectrometer. Mass spectra were recorded on MicrOTOFq Bruker spectrometer by electrospray ionization. Melting points were determined using a Reichert melting point apparatus. Infrared spectra were recorded on a FTIR spectrometer (Perkin-Elmer spectrum one, NaCl pellets or Bruker Vertex 70 ATR Pike Germanium) and are reported in cm^{-1}.

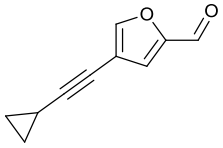
Experimental Part

The following compounds (**1a, 1b, 1e, 1f, 1g, 1h, 1i, 1j, 1k, 1n, 1o, 1p, 1q, 1r, 1s, 1u, 1v, 1w, 1y, 3aa, 3ba, 3ea, 3fa, 3ga, 3ha, 3ia, 3ab, 3ja, 3ka, 3na, 3ae, 3oe, 3og, 3oh, 3pa, 3qa, 3ra, 3sa, 3ua, 3va, 3wa, 3aj, 3oa**) were characterized in: L. Marin, V. Gandon, E. Schulz, D. Leboeuf, *Adv. Synth. Catal.* **2017**, *359*, 1157.

Characterization data



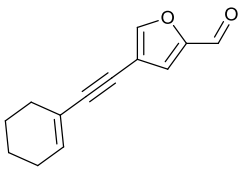
4-(cyclopropylethynyl)furan-2-carbaldehyde (A1c)



To a Schlenk flask (under argon) was added 4-bromofuran-2-carbaldehyde (250 mg, 1.43 mmol, 1 equiv), $Pd(PPh_3)_4$ (166 mg, 0.143 mmol, 10 mol%), CuI (27 mg, 0.143 mmol, 10 mol%) and DIPA (4.2 mL, 0.35 M). Ethynylcyclopropane (0.18 mL, 2.14 mmol, 1.5 equiv) was then added to the reaction mixture. The mixture was stirred at 80 °C for 2 h. After completion of the reaction, the mixture was passed through a short pad of celite and rinsed with AcOEt. The filtrate was washed with saturated NH_4Cl aqueous solution, brine, dried over anhydrous $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 95:5 as eluent to give **A1c** (180 mg, 79%).

A1c: brown solid, 79%; ^{1}H NMR (250 MHz, $CDCl_3$) δ 9.60 (s, 1H), 7.72 (s, 1H), 7.18 (s, 1H), 1.48–1.33 (m, 1H), 0.94–0.72 (m, 4H).

4-(cyclohex-1-en-1-ylethynyl)furan-2-carbaldehyde (A1d)

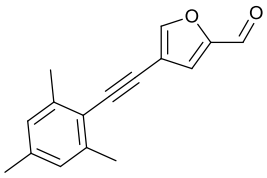


To a Schlenk flask (under argon) was added 4-bromofuran-2-carbaldehyde (200 mg, 1.14 mmol, 1 equiv), $PdCl_2(PPh_3)_2$ (80 mg, 0.114 mmol, 10 mol%), CuI (22 mg, 0.114 mmol, 10 mol%) and DIPA (3.3 mL, 0.35 M). 1-Ethynylcyclohex-1-ene (0.18 mL, 1.71 mmol, 1.5 equiv) was then added to the reaction mixture. The mixture was stirred at 80 °C for 2 h. After completion of the reaction, the mixture was passed through a short pad of celite and rinsed with AcOEt. The filtrate was washed with saturated NH_4Cl aqueous solution, brine, dried over

anhydrous $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 95:5 as eluent to give **A1d** (100 mg, 44%).

A1d: brown solid, 44%; ^{1}H NMR (360 MHz, C_6D_6) δ 9.03 (s, 1H), 6.99 (s, 1H), 6.56 (s, 1H), 6.23–6.15 (m, 1H), 2.21–2.13 (m, 2H), 1.86–1.78 (m, 2H), 1.44–1.25 (m, 4H).

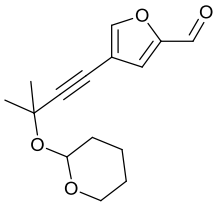
4-(mesitylethynyl)furan-2-carbaldehyde (A1l)



To a Schlenk flask (under argon) was added 4-bromofuran-2-carbaldehyde (250 mg, 1.43 mmol, 1 equiv), $Pd(PPh_3)_4$ (166 mg, 0.143 mmol, 10 mol%), CuI (27 mg, 0.143 mmol, 10 mol%) and DIPA (4.2 mL, 0.35 M). 2-Ethynyl-1,3,5-trimethylbenzene (0.34 mL, 2.14 mmol, 1.5 equiv) was then added to the reaction mixture. The mixture was stirred at 80 °C for 2 h. After completion of the reaction, the mixture was passed through a short pad of celite and rinsed with AcOEt. The filtrate was washed with saturated NH_4Cl aqueous solution, brine, dried over anhydrous $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 95:5 as eluent to give **A1l** (320 mg, 94%).

A1l: brown solid, 94%; ^{1}H NMR (360 MHz, $CDCl_3$) δ 9.66 (s, 1H), 7.87 (s, 1H), 7.32 (s, 1H), 6.90 (s, 2H), 2.43 (s, 6H), 2.30 (s, 3H).

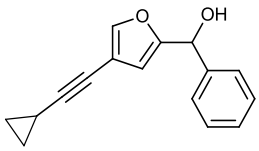
4-(3-methyl-3-((tetrahydro-2H-pyran-2-yl)oxy)but-1-yn-1-yl)furan-2-carbaldehyde (A1z)



To a Schlenk flask (under argon) was added 4-bromofuran-2-carbaldehyde (264 mg, 1.51 mmol, 1 equiv), $Pd(PPh_3)_4$ (175 mg, 0.151 mmol, 10 mol%), CuI (29 mg, 0.151 mmol, 10 mol%) and DIPA (4.5 mL, 0.35 M). 2-[(2-methylbut-3-yn-2-yl)oxy]oxane (380 mg, 2.3 mmol, 1.5 equiv) was then added to the reaction mixture. The mixture was stirred at 80 °C for 2 h. After completion of the reaction, the mixture was passed through a short pad of celite and rinsed with AcOEt. The filtrate was washed with saturated NH_4Cl aqueous solution, brine, dried over anhydrous $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 95:5 as eluent to give **A1z** (370 mg, 94%).

A1z: brown solid, 94%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.65 (s, 1H), 7.81 (s, 1H), 7.24 (s, 1H), 5.14–5.03 (m, 1H), 4.06–3.89 (m, 1H), 3.62–3.42 (m, 1H), 1.93–1.66 (m, 2H), 1.64–1.52 (m, 10H).

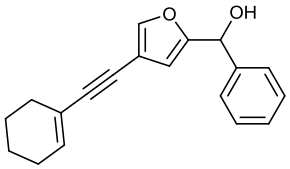
(4-(cyclopropylethynyl)furan-2-yl)(phenyl)methanol (1c)



A solution of phenylmagnesium bromide (2.7 mL, 0.6 M in THF) was added slowly to a solution 4-(cyclopropylethynyl)furan-2-carbaldehyde (160 mg, 1.0 mmol) in THF (2.0 mL) at 0 °C. The cold bath was then removed and the reaction mixture was stirred at room temperature for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 9:1 as eluent to give **1c** (200 mg, 56%).

1c: colorless oil, 56%; ^{1}H NMR (300 MHz, C_6D_6) δ 7.22–7.11 (m, 2H), 7.11–6.90 (m, 4H), 6.04 (s, 1H), 5.32 (s, 1H), 2.38 (bs, 1H), 1.07 (tt, J = 8.3, 5.0 Hz, 1H), 0.54 (td, J = 6.6, 4.1 Hz, 2H), 0.34 (ddd, J = 10.9, 6.7, 4.1 Hz, 2H). ^{13}C NMR (75 MHz, C_6D_6) δ 157.2, 145.2, 141.2, 128.6, 127.0, 110.6, 109.3, 95.2, 70.0, 67.4, 8.6, 0.6, one carbon hidden. IR (neat) 3354, 3091, 3064, 3029, 3011, 2961, 2918, 2850, 17.04, 1603, 1548, 1494, 1364, 1261, 1189, 1078 cm^{-1}. HRMS-ESI: m/z calculated for $C_{16}H_{14}NaO_2$ $[M+Na]^+$: 261.0886, found: 261.0881.

(4–(cyclohex–1–en–1–ylethynyl)furan–2–yl)(phenyl)methanol (1d)

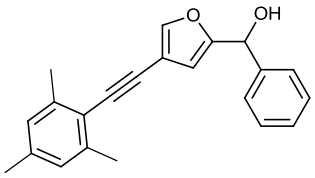


A solution of phenylmagnesium bromide (1.1 mL, 0.6 M in THF) was added slowly to a solution 4-(cyclohex-1-en-1-ylethynyl)furan-2-carbaldehyde (90 mg, 0.450 mmol) in THF (0.9 mL) at 0 °C. The cold bath was then removed and the reaction mixture was stirred at room temperature for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 9:1 as eluent to give **1d** (105 mg, 84%).

1d: orange oil, 84%; ^{1}H NMR (250 MHz, C_6D_6) δ 7.31–7.21 (m, 3H), 7.15–7.01 (m, 3H), 6.24–6.14 (m, 2H), 5.41 (s, 1H), 2.44 (bs, 1H), 2.24–2.14 (m, 2H), 1.89–1.78 (m, 2H), 1.46–1.22 (m, 4H); ^{13}C NMR (63 MHz, C_6D_6) δ 157.4,

145.0, 141.2, 134.8, 128.6, 128.1, 127.0, 121.4, 110.4, 109.3, 93.6, 78.6, 70.0, 29.5, 25.9, 22.6, 21.8. IR (neat) 3391, 3029, 2931, 2858, 2185, 1597, 1493 ,1452, 1348, 1133 cm^{-1}. HRMS-ESI: m/z calculated for $C_{19}H_{17}O$ [*M*-OH]$^+$: 261.1279, found: 261.1318.

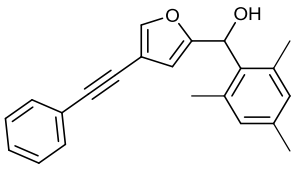
(4-(mesitylethynyl)furan-2-yl)(phenyl)methanol (1l)



A solution of phenylmagnesium bromide (2.0 mL, 0.9 M in THF) was added slowly to a 4-(mesitylethynyl)furan-2-carbaldehyde (290 mg, 1.2 mmol) in THF (4.0 mL) at 0 °C. The cold bath was then removed and the reaction mixture was stirred at room temperature for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 9:1 as eluent to give **1l** (320 mg, 83%).

1l: brown solid, 83%; mp = 69–73 °C. ^{1}H NMR (300 MHz, C_6D_6) δ 7.38–7.31 (m, 3H), 7.21–7.06 (m, 3H), 6.74 (s, 2H), 6.30 (s, 1H), 5.53 (s, 1H), 3.02 (bs, 1H), 2.48 (s, 6H), 2.12 (s, 3H). ^{13}C NMR (75 MHz, C_6D_6) δ 157.4, 145.0, 141.1, 140.2, 137.8, 128.6, 128.2, 127.0, 120.5, 110.4, 109.3, 89.6, 88.5, 70.1, 21.3, 21.2, one carbon hidden. IR (neat) 3303, 3144, 3090, 3061, 3029, 3004, 2972, 2946, 2853, 1721, 1604, 1552, 1527, 1494, 1377, 1269, 1136, 1118 cm^{-1}. HRMS-ESI: m/z calculated for $C_{22}H_{20}NaO_2$ [M+Na]$^+$: 339.1356, found: 339.1349.

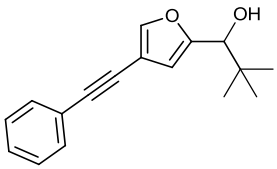
Mesityl(4-(phenylethynyl)furan-2-yl)methanol (1m)



A solution of 2-mesitylmagnesium bromide (0.9 mL, 1 M in THF) was added slowly to of 4-(phenylethynyl)furan-2-carbaldehyde (120 mg, 0.61 mmol) in THF (1.2 mL) at 0 °C. The cold bath was then removed and the reaction mixture was stirred at room temperature for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 85:15 as eluent to give **1m** (160 mg, 83%).

1m: yellow oil, 83%; ^{1}H NMR (250 MHz, C_6D_6) δ 7.52–7.42 (m, 2H), 7.31 (s, 1H), 7.02–6.90 (m, 3H), 6.70 (s, 2H), 6.28 (s, 1H), 5.94 (s, 1H), 2.23 (s, 6H), 2.11 (s, 3H), 1.95 (bs, 1H); ^{13}C NMR (63 MHz, C_6D_6) δ 157.0, 145.2, 137.4, 137.2, 133.8, 131.8, 130.3, 128.7, 124.0, 109.7, 108.9, 91.7, 81.6, 67.1, 20.9, 20.5, one carbon hidden. IR (neat) 3378, 2967, 2920, 2867, 1724, 1610, 1487, 1443, 1377, 1132, 1044 cm^{-1}. HRMS-ESI: m/z calculated for $C_{22}H_{20}NaO_2$ $[M+Na]^+$: 339.1356, found: 339.1345.

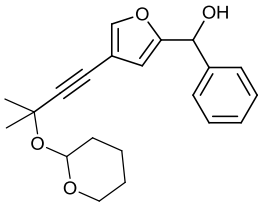
2,2-dimethyl-1-(4-(phenylethynyl)furan-2-yl)propan-1-ol (1x)



A solution of tert-butylmagnesium chloride (1.1 mL, 0.7 M in THF) was added slowly to of 4-(phenylethynyl)furan-2-carbaldehyde (100 mg, 0.51 mmol) in THF (1.0 mL) at 0 °C. The cold bath was then removed and the reaction mixture was stirred at room temperature for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 85:15 as eluent to give **1x** (90 mg, 69%).

1x: yellow oil, 69%; ^{1}H NMR (300 MHz, C_6D_6) δ 7.60–7.45 (m, 2H), 7.31 (d, J = 0.8 Hz, 1H), 7.04–6.94 (m, 3H), 6.25 (s, 1H), 4.01 (s, 1H), 0.91 (s, 9H), OH unobserved; ^{13}C NMR (75 MHz, C_6D_6) δ 157.5, 144.5, 131.8, 128.7, 128.4, 124.0, 110.0, 108.7, 91.7, 81.6, 76.1, 35.8, 25.8. IR (film) 3426, 2957, 2901, 2870, 1751, 1736, 1668, 1606, 1487, 1443, 1365, 1238 cm^{-1}. HRMS-ES: m/z calculated for $C_{17}H_{17}O_2$ $[M-H]^-$: 253.1229, found: 253.1239.

(4-(3-methyl-3-((tetrahydro-2H-pyran-2-yl)oxy)but-1-yn-1-yl)furan-2-yl)(phenyl)methanol (1z)

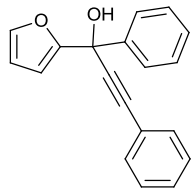


A solution of phenylmagnesium bromide (3.4 mL, 0.6 M in THF) was added slowly to a 4-(3-methyl-3-((tetrahydro-2H-pyran-2-yl)oxy)but-1-yn-1-yl)furan-2-carbaldehyde (355 mg, 1.35 mmol) in THF (2.6 mL) at 0 °C. The cold bath was then removed and the reaction mixture was stirred at room temperature for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary

evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 75:25 as eluent to give **1z** (425 mg, 92%).

1z: colorless oil, 92%; ^{1}H NMR (300 MHz, C_6D_6) δ 7.29–7.19 (m, 2H), 7.20–7.14 (m, 2H), 7.14–7.00 (m, 3H), 6.12 (s, 1H), 5.47 (t, *J* = 3.4 Hz, 1H), 5.36 (s, 1H), 4.03–3.80 (m, 1H), 3.43 (dd, *J* = 11.1, 5.6 Hz, 1H), 1.74 (s, 3H), 1.72–1.64 (m, 3H), 1.63 (s, 3H), 1.35–1.23 (m, 3H); ^{13}C NMR (75 MHz, C_6D_6) *δ* 157.7, 145.6, 141.3, 128.6, 128.1, 127.0, 110.3, 108.3, 95.9, 94.0, 76.1, 71.8, 70.0, 62.3, 32.1, 31.1, 30.3, 25.8, 20.0. IR (neat) 3375, 3063, 3031, 2983, 2942, 2868, 2230, 1690, 1603, 1494, 1453, 1381, 1125, 1074 cm^{-1}. HRMS-ESI: m/z calculated for $C_{21}H_{24}NaO_4$ $[M+Na]^+$: 363.1567, found: 363.1552.

Diphenyl(4-(phenylethynyl)furan-2-yl)methanol (11)



A solution of *n*-butyllithium (0.7 mL, 2.5 M in THF) was added slowly to a solution of phenylacetylene (0.191 mL, 1.7 mmol) in THF (2.3 mL) at −78 °C. After 30 minutes, furan-2-yl(phenyl)methanone (200 mg, 1.2 mmol) was added to the solution. The cold bath was then removed and the reaction mixture was stirred at room temperature for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using PE/EtOAc 9:1 as eluent to give **11** (150 mg, 47%).

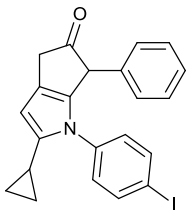
11: brown oil, 47%; ^{1}H NMR (360 MHz, C_6D_6) *δ* 7.95–7.78 (m, 2H), 7.36–7.26 (m, 2H), 7.15–7.08 (m, 2H), 7.07–7.01 (m, 1H), 6.97–6.94 (m, 1H), 6.93–6.86 (m, 3H), 6.29 (dd, *J* = 3.2, 0.7 Hz, 1H), 5.94 (dd, *J* = 3.2, 1.8 Hz, 1H), 2.76 (s, 1H); ^{13}C NMR (91 MHz, C_6D_6) *δ* 156.8, 143.1, 142.9, 132.2, 129.4, 128.8, 128.6, 128.5, 126.8, 122.8, 110.4, 107.8, 90.7, 86.5, 70.8. IR (neat) 3401, 3121, 3061, 3032, 2963, 1705, 1598, 1550, 1490, 1449, 1262, 1225, 1178, 1148 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{19}H_{14}NaO_2$ $[M+Na]^+$: 297.0886, found: 297.0891.

General procedure for the cyclization reaction

To a solution of 2-furancarbinol **1** (0.07 mmol, 1 equiv) and aniline **2** (0.091 mmol, 1.3 equiv) in 1,2-DCE or HFIP (0.25 mL, 0.3 M) were added $Ca(NTf_2)_2$ (2.1 mg, 5 mol%) and nBu_4NPF_6 (1.4 mg, 5 mol%). The reaction mixture was stirred at the indicated temperature until TLC showed full conversion (t_1). After t_1, $Cu(OTf)_2$ (2.5 mg, 10 mol%) was added and the reaction mixture was stirred at the indicated temperature until TLC showed full

conversion (t_2). Then, the crude product was purified by flash column chromatography using gradients of Pentane/EtOAc to give the desired products.

2-cyclopropyl-1-(4-iodophenyl)-6-phenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (3ca)

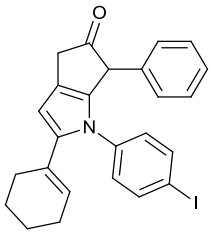


Starting from 2-furylcarbinol **1c** (25 mg, 0.11 mmol, 1 equiv), aniline **2a** (30 mg, 0.14 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (3.1 mg, 0.0052 mmol, 5 mol%), $n$$Bu_4NPF_6$ (2.0 mg, 0.0052 mmol, 5 mol%) and $Cu(OTf)_2$ (3.8 mg, 0.011 mmol, 10 mol%), 27 mg of cyclopenta[*b*]pyrrole **3ca** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

3ca: brown solid, 59% (1,2-DCE, t_1 = 1.25 h at 80 °C, t_2 = 0.15 h at 40 °C); mp = 38–43 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 (d, J = 8.6 Hz, 2H), 7.23–7.12 (m, 3H), 6.97–6.89 (m, 2H), 6.84 (d, J = 8.6 Hz, 2H), 5.91 (s, 1H), 4.40 (s, 1H), 3.45 (dd, J = 21.5, 0.9 Hz, 1H), 3.37 (d, J = 21.6 Hz, 1H), 1.64–1.49 (m, 1H), 0.88–0.55 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 213.5, 139.5, 138.4, 138.0, 133.5, 128.7, 128.4, 127.7, 127.4, 120.6, 100.8, 92.3, 55.8, 39.3, 8.4, 8.2, 8.1, one carbon hidden. IR (neat) 3084, 3063, 3026, 3008, 2892, 1749, 1681, 1589, 1548, 1491, 14441, 1416, 1378, 1334, 1246, 1219, 1093, 1058 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{22}H_{19}INO$ $[M+H]^+$: 440.0505, found: 440.0488.

2-(cyclohex-1-en-1-yl)-1-(4-iodophenyl)-6-phenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (3da)



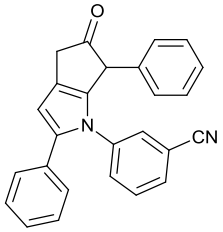
Starting from 2-furylcarbinol **1d** (25 mg, 0.090 mmol, 1 equiv), aniline **2a** (26 mg, 0.12 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.7 mg, 0.0045 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.7 mg, 0.0045 mmol, 5 mol%) and $Cu(OTf)_2$ (3.2 mg, 0.0090 mmol, 10 mol%), 18 mg of cyclopenta[*b*]pyrrole **3da** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

3da: red solid, 42% (1,2-DCE, t_1 = 0.15 h at 80 °C, t_2 = 0.15 h at 40 °C); mp = 70–73 °C. ^{1}H NMR (360 MHz, C_6D_6) δ 7.13 (d, J = 8.6 Hz, 2H), 7.00–6.81 (m, 5H), 6.49 (d, J = 8.6 Hz, 2H), 6.21 (s, 1H), 5.69–5.60 (m, 1H), 4.16 (s, 1H), 3.26 (d, J = 21.4 Hz, 1H), 3.19 (d, J = 21.1 Hz, 1H), 2.12–1.98 (m, 2H), 1.89–1.79 (m, 2H), 1.47–1.27 (m, 4H); ^{13}C

NMR (75 MHz, C_6D_6) δ 210.8, 140.0, 139.3, 138.7, 138.1, 135.8, 130.1, 128.8, 127.6, 127.3, 121.7, 105.1, 91.6, 56.1, 39.0, 28.9, 25.8, 23.1, 22.3, two carbons hidden. IR (neat) 3057, 3025, 2926, 2855, 1750, 1681, 1585, 1489, 1446, 1393, 1263, 1229, 1058 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{22}INNaO$ $[M+Na]^+$: 502.0638, found: 502.0631.

3-(5-oxo-2,6-diphenyl-5,6-dihydrocyclopenta[*b*]pyrrol-1(4H)-yl)benzonitrile (3ac)

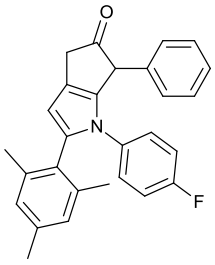


Starting from 2-furylcarbinol **1a** (15 mg, 0.055 mmol, 1 equiv), aniline **2c** (8.4 mg, 0.071 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.6 mg, 0.0027 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.1 mg, 0.0027 mmol, 5 mol%) and $Cu(OTf)_2$ (2.0 mg, 0.0055 mmol, 10 mol%), 14 mg of cyclopenta[*b*]pyrrole **3ab** were obtained.

Flash column chromatography using Pentane/EtOAc 87.5:12.5 as eluent.

3ac: yellow solid, 67% (1,2-DCE, t_1 = 0.15 h at 80 °C, t_2 = 0.33 h at 80 °C); mp = 53–56 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.7 Hz, 1H), 7.24–7.04 (m, 11H), 7.00–6.89 (m, 2H), 6.50 (s, 1H), 4.49 (s, 1H), 3.57 (d, *J* = 21.6 Hz, 1H), 3.49 (d, *J* = 21.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.5, 139.9, 137.5, 137.2, 136.6, 132.1, 130.9, 130.4, 129.9, 129.7, 129.0, 128.7, 128.3, 127.8, 127.7, 127.2, 122.6, 117.7, 113.1, 106.9, 56.1, 39.3. IR (neat) 3063, 3030, 2900, 1753, 1688, 1601, 1583, 1555, 1512, 1468, 1360, 1259 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{26}H_{18}N_2NaO$ $[M+Na]^+$: 397.1311, found: 397.1237.

1-(4-fluorophenyl)-2-mesityl-6-phenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (3ld)

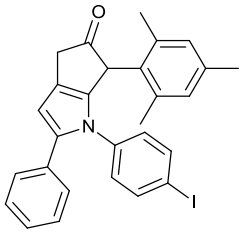


Starting from 2-furylcarbinol **1l** (25 mg, 0.079 mmol, 1 equiv), aniline **2d** (11 mg, 0.14 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.4 mg, 0.0040 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.5 mg, 0.0040 mmol, 5 mol%) and $Cu(OTf)_2$ (2.9 mg, 0.0079 mmol, 10 mol%), 11 mg of cyclopenta[*b*]pyrrole **3ld** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

3ld: brown oil, 34% (HFIP, t_1 = 0.5 h at 40 °C, t_2 = 1 h at 80 °C). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.19–6.76 (m, 9H), 6.76–6.60 (m, 2H), 6.20 (s, 1H), 4.58 (s, 1H), 3.59 (d, *J* = 22.2 Hz, 1H), 3.51 (d, *J* = 20.5 Hz, 1H), 2.34 (s, 3H), 2.22 (s, 3H), 1.89 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.0, 156.7 (d, *J* = 249.4 Hz), 137.9, 137.7, 137.3, 129.1, 128.6 (d, *J* = 7.7 Hz), 128.4, 128.3, 127.9, 127.8, 127.5, 126.2 (d, *J* = 11.7 Hz), 123.7 (d, *J* = 3.7 Hz), 121.0, 116.0 (d, *J* = 20.4 Hz), 106.0, 55.9, 39.7, 21.1, 19.9. IR (film) 3025, 2920, 2845, 1751, 1641, 1612, 1508, 1457, 1377, 1347, 1265, 1154, 1065 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{28}H_{24}FNNaO$ $[M+Na]^+$: 432.1734, found: 432.1730.

1-(4-iodophenyl)-6-mesityl-2-phenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (3ma)

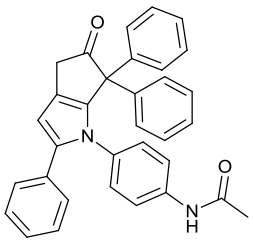


Starting from 2-furylcarbinol **1m** (25 mg, 0.079 mmol, 1 equiv), aniline **2a** (22.5 mg, 0.10 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.4 mg, 0.0040 mmol, 5 mol%), nBu$_4$NPF$_6$ (1.5 mg, 0.0040 mmol, 5 mol%) and $Cu(OTf)_2$ (2.9 mg, 0.0079 mmol, 10 mol%), 36 mg of cyclopenta[*b*]pyrrole **3ma** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

3ma: brown solid, 88% (HFIP, t_1 = 0.15 h at 60 °C, t_2 = 0.15 h at 20 °C); mp = 42–45 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.6 Hz, 2H), 7.21–7.08 (m, 5H), 6.69 (d, *J* = 6.2 Hz, 2H), 6.43 (s, 1H), 6.40 (d, *J* = 8.6 Hz, 2H), 4.91 (s, 1H), 3.57 (t, *J* = 1.2 Hz, 2H), 2.23 (s, 3H), 1.94 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 216.2, 138.4, 138.1, 137.7, 137.2, 136.8, 136.5, 136.3, 132.6, 132.0, 130.5, 129.1, 128.8, 128.4, 128.0, 126.5, 120.2, 106.0, 92.1, 51.8, 40.6, 20.9, 20.9, 19.7. IR (neat) 3061, 2964, 2916, 1750, 1679, 1645, 1598, 1570, 1545, 1488, 1353, 1256, 1231 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{28}H_{24}INNaO$ $[M+Na]^+$: 540.0795, found: 540.0812.

N-(4-(5-oxo-2,6,6-triphenyl-5,6-dihydrocyclopenta[*b*]pyrrol-1(4H)-yl)phenyl)acetamide (3of)

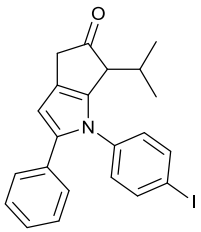


Starting from 2-furylcarbinol **1o** (25 mg, 0.071 mmol, 1 equiv), aniline **2f** (14 mg, 0.093 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.1 mg, 0.0036 mmol, 5 mol%), nBu$_4$NPF$_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0071 mmol, 10 mol%), 28 mg of cyclopenta[*b*]pyrrole **3of** were obtained.

Flash column chromatography using Pentane/EtOAc 92.5:7.5 as eluent.

3of: white solid, 81%; (HFIP, t_1 = 0.08 h at 60°C, t_2 = 0.15 h at 20°C); mp = 105–109 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.21–6.96 (m, 17H), 6.56–6.39 (m, 3H), 3.54 (s, 2H), 2.07 (s, 3H), NH unobserved; ^{13}C NMR (91 MHz, $CDCl_3$) δ 215.2, 168.3, 140.8, 139.5, 138.0, 137.2, 134.3, 132.8, 129.5, 129.2, 128.2, 128.2, 128.0, 127.1, 126.5, 119.7, 119.1, 105.0, 67.1, 38.6, 24.7. IR (neat) 3384, 3261, 3201, 3063, 3026, 2928, 1744, 1693, 1671, 1642, 1604, 1516, 1464, 1409, 1371, 1295, 1265 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{33}H_{26}N_2NaO_2$ [*M*+Na]$^+$: 505.1886, found: 505.1860.

1-(4-iodophenyl)-6-isopropyl-2-phenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (3ta)

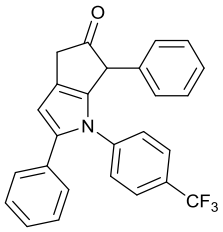


Starting from 2-furylcarbinol **1t** (20 mg, 0.083 mmol, 1 equiv), aniline **2a** (27 mg, 0.13 mmol, 1.5 equiv), $Ca(NTf_2)_2$ (2.5 mg, 0.0042 mmol, 5 mol%), nBu$_4$NPF$_6$ (1.6 mg, 0.0042 mmol, 5 mol%) and $Cu(OTf)_2$ (2.9 mg, 0.017 mmol, 20 mol%), 21 mg of cyclopenta[*b*]pyrrole **3ta** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

3ta: orange oil, 58% ($MeNO_2$, t_1 = 0.5 h at 90 °C). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.6 Hz, 2H), 7.24–7.04 (m, 5H), 6.87 (d, *J* = 8.6 Hz, 2H), 6.34 (s, 1H), 3.41 (d, *J* = 3.4 Hz, 1H), 3.35 (d, *J* = 21.5 Hz, 1H), 3.23 (dd, *J* = 21.4, 1.0 Hz, 1H), 1.72–1.51 (m, 1H), 0.91 (d, *J* = 6.9 Hz, 3H), 0.51 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 217.1, 139.3, 138.6, 136.6, 136.4, 132.8, 128.5, 128.4, 126.7, 121.7, 106.2, 92.3, 55.8, 40.9, 31.4, 19.9, 18.3, one carbon hidden. IR (neat) 3092, 3063, 3029, 2963, 2930, 2903, 2872, 1745, 1679, 1585, 1563, 1489, 1464, 1391, 1261, 1179 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{22}H_{20}INNaO$ [*M*+Na]$^+$: 464.0482, found: 464.0467.

2-cyclopropyl-1-(4-iodophenyl)-6-phenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (3ah)

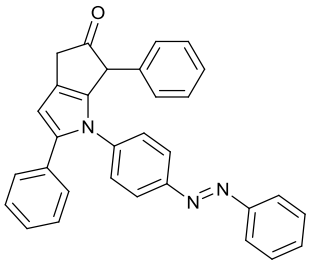


Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **2i** (15 mg, 0.094 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.073 mmol, 10 mol%), 22 mg of cyclopenta[*b*]pyrrole **3ah** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

3ah: yellow solid, 72% ($MeNO_2$, t_1 = 0.5 h at 90 °C); mp = 53–56 °C. ^{1}H NMR (300 MHz, C_6D_6) δ 7.14–7.12 (m, 2H), 7.00–6.81 (m, 10H), 6.62 (d, J = 8.3 Hz, 2H), 6.36 (s, 1H), 4.18 (s, 1H), 3.23 (s, 2H); ^{13}C NMR (75 MHz, C_6D_6) δ 210.3, 142.4, 138.1, 137.1, 137.0, 133.1, 128.9, 128.8, 127.9, 127.5, 127.1, 126.6, 126.1 (q, J = 3.1 Hz), 123.0, 122.6, 107.5, 56.2, 38.9, two carbons hidden. ^{19}F NMR (235 MHz, $CDCl_3$) δ –62.14. IR (neat) 3058, 3025, 2957, 2890, 1754, 1681, 1614, 1597, 1522, 1493, 1465, 1358, 1324, 1166, 1125, 1066, 1017 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{26}H_{18}F_3NNaO$ [M+Na]$^+$: 440.1227, found: 440.1222.

(*E*)-2,6-diphenyl-1-(4-(phenyldiazenyl)phenyl)-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (3ak)

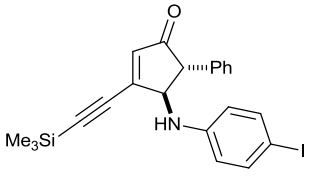


Starting from 2-furylcarbinol **1a** (15 mg, 0.055 mmol, 1 equiv), aniline **2k** (14 mg, 0.071 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.6 mg, 0.0027 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.1 mg, 0.0027 mmol, 5 mol%) and $Cu(OTf)_2$ (2.0 mg, 0.0071 mmol, 10 mol%), 18 mg of cyclopenta[*b*]pyrrole **3ak** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

3ak: orange solid, 73% (HFIP, t_1 = 2 h at 60 °C, t_2 = 1 h at 20 °C); mp = 173–175 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.89–7.79 (m, 2H), 7.67 (d, J = 8.6 Hz, 2H), 7.53–7.43 (m, 3H), 7.25–7.12 (m, 8H), 7.07–6.95 (m, 4H), 6.52 (s, 1H), 4.57 (s, 1H), 3.59 (d, J = 21.4 Hz, 1H), 3.49 (d, J = 21.5 Hz, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 213.0, 152.7, 150.7, 141.2, 137.8, 137.3, 136.5, 132.7, 131.4, 129.3, 128.9, 128.5, 128.3, 127.8, 127.5, 126.9, 126.8, 123.5, 123.0, 122.3, 106.5, 56.2, 39.2. IR (neat) 3052, 3036, 2961, 2927, 2895, 1754, 1598, 1504, 1465, 1409, 1394, 1300, 1236 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{31}H_{23}N_3NaO$ [M+Na]$^+$: 476.1733, found: 476.1740.

4-((4-iodophenyl)amino)-5-phenyl-3-((trimethylsilyl)ethynyl)cyclopent-2-enone (4ya)

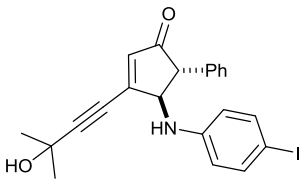


Starting from 2-furylcarbinol **1y** (20 mg, 0.073 mmol, 1 equiv), aniline **2a** (21 mg, 0.096 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0073 mmol, 10 mol%), 26 mg of **4ya** were obtained.

Flash column chromatography using Pentane/EtOAc 9:1 as eluent.

4ya: orange solid, 73% (1,2-DCE, t_1 = 0.5 h at 80 °C, t_2 = 2 h at 80 °C); mp = 55–59 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42–7.28 (m, 5H), 7.18–7.10 (m, 2H), 6.45 (s, 1H), 6.32 (d, J = 8.5 Hz, 2H), 4.66 (s, 1H), 4.45–3.95 (m, 1H), 3.47–3.41 (m, 1H), 0.18 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 205.3, 155.1, 146.5, 137.9, 137.6, 136.4, 129.3, 128.1, 127.8, 116.3, 98.0, 79.7, 65.6, 60.9, -0.6, one carbon hidden. IR (neat) 3062, 3030, 2962, 2921, 2899, 2853, 1706, 1589, 1486, 1451, 1314, 1250, 1166 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{22}H_{23}INOSi$ [M+H]$^+$: 472.0588, found: 472.0567.

2-(2-hydroxypropan-2-yl)-1-(4-iodophenyl)-6-phenyl-4,6-dihydrocyclopenta[b]pyrrol-5(1H)-one (4za)

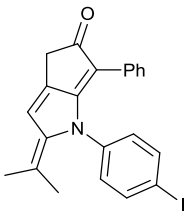


Starting from 2-furylcarbinol **1z** (20 mg, 0.059 mmol, 1 equiv), aniline **2a** (17 mg, 0.076 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.8 mg, 0.0029 mmol, 5 mol%) and $n$$Bu_4NPF_6$ (0.8 mg, 0.0029 mmol, 5 mol%), 22 mg of 4-aminocyclopentenone **4za** were obtained.

Flash column chromatography using Pentane/EtOAc 85:15 as eluent.

4za: yellow solid, 70% (1,2-DCE, t_1 = 0.5 h at 80 °C); mp = 43–46 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.42–7.29 (m, 5H), 7.18–7.11 (m, 2H), 6.42 (d, J = 1.5 Hz, 1H), 6.35 (d, J = 8.8 Hz, 2H), 4.68 (s, 1H), 4.13 (s, 1H), 3.46 (d, J = 3.0 Hz, 1H), 1.95 (s, 1H), 1.48 (s, 3H), 1.46 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 205.0, 155.2, 146.5, 138.0, 137.5, 135.9, 129.3, 128.1, 127.8, 116.4, 113.0, 79.7, 77.4, 65.9, 65.6, 60.6, 30.8. IR (neat) 3092, 3019, 2981, 2929, 2857, 1702, 1590, 1486, 1452, 1395, 1375, 1314, 1290, 1244, 1170 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{22}H_{20}INNaO_2$ [M+Na]$^+$: 480.0431, found: 480.0403.

2-acetyl-1-(4-iodophenyl)-2-methyl-6-phenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (5)

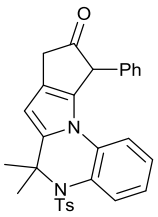


Starting from 2-furylcarbinol **1z** (35 mg, 0.10 mmol, 1 equiv), aniline **2a** (29 mg, 0.134 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (3.1 mg, 0.0051 mmol, 5 mol%), $n$$Bu_4NPF_6$ (2.0 mg, 0.0051 mmol, 5 mol%) and $Cu(OTf)_2$ (5.6 mg, 0.015 mmol, 15 mol%), 24 mg of cyclopenta[*b*]pyrrole **5** were obtained.

Flash column chromatography using Pentane/EtOAc 85:15 as eluent.

5: yellow solid, 53% (1,2-DCE, t_1 = 0.2 h at 80 °C); mp = 165–168 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.42 (d, J = 8.5 Hz, 2H), 7.12–6.93 (m, 3H), 6.73 (d, J = 8.5 Hz, 2H), 6.70–6.60 (m, 3H), 3.18 (d, J = 0.7 Hz, 2H), 2.01 (s, 3H), 1.38 (s, 3H). ^{13}C NMR (91 MHz, $CDCl_3$) δ 200.4, 168.9, 143.9, 139.6, 138, 136.4, 130.8, 130.1, 129.6, 127.4, 126.3, 117.4, 117.2, 111.7, 92.8, 34.7, 23.5, 20.7. IR (neat) 3056, 3029, 2929, 2855, 1710, 1668, 1601, 1576, 1535, 1486, 1411, 1370, 1288, 1189 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{22}H_{19}INO$ $[M+H]^+$: 440.0505, found: 440.0481.

6,6-dimethyl-10-phenyl-5-tosyl-8,10-dihydro-5H-cyclopenta[4,5]pyrrolo[1,2-a]quinoxalin-9(6H)-one (6)

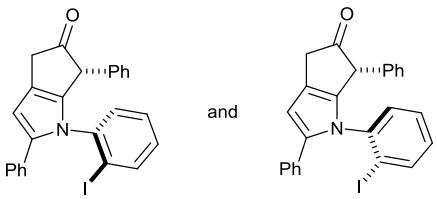


Starting from 2-furylcarbinol **1z** (25 mg, 0.073 mmol, 1 equiv), aniline **2l** (25 mg, 0.095 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0037 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0037 mmol, 5 mol%) and $Cu(OTf)_2$ (2.7 mg, 0.0073 mmol, 10 mol%), 19 mg of cyclopenta[*b*]pyrrole **6** were obtained.

Flash column chromatography using Pentane/EtOAc 85:15 as eluent.

6: orange oil, 54% (1,2-DCE, t_1 = 0.5 h at 80 °C, t_2 = 1.5 h at 80 °C); ^{1}H NMR (250 MHz, $CDCl_3$) δ ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.71 (d, J = 7.9 Hz, 1H), 7.39–7.30 (m, 3H), 7.17–7.08 (m, 3H), 7.05–6.91 (m, 5H), 6.57 (d, J = 8.1 Hz, 1H), 5.87 (s, 1H), 3.99 (s, 1H), 3.30 (d, J = 21.3 Hz, 1H), 3.01 (d, J = 21.2 Hz, 1H), 2.26 (s, 3H), 2.08 (s, 3H), 1.41 (s, 3H).^{13}C NMR (91 MHz, $CDCl_3$) δ 211.1, 143.0, 137.6, 136.7, 134.8, 132.7, 131.6, 129.3, 128.9, 128.4, 128.2, 127.9, 127.4, 127.3, 124.5, 122.8, 116.1, 100.3, 57.9, 56.1, 37.7, 30.3, 26.2, 21.3, one carbon hidden. HRMS-ESI: *m/z* calculated for $C_{29}H_{27}N_2O_3S$ $[M+H]^+$: 483.1737, found: 483.1753.

1-(2-iodophenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8aa and 8'aa)



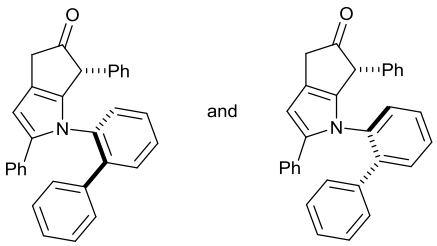
8aa **8'aa**

Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7a** (21 mg, 0.95 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0073 mmol, 10 mol%), 21 mg of cyclopenta[*b*]pyrrole **8aa** and **8'aa** were obtained (34% and 27%, respectively) (1,2-DCE, t_1 = 0.15 h at 80 °C, t_2 = 1 h at 40 °C).
Flash column chromatography using Pentane/EtOAc 98:2 as eluent.

8aa: orange solid, 34%; mp = 145–150 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (dd, J = 7.5, 1.8 Hz, 1H), 7.17–7.07 (m, 8H), 6.92–6.82 (m, 4H), 6.62 (dd, J = 7.4, 2.0 Hz, 1H), 6.50 (s, 1H), 4.56 (s, 1H), 3.56 (s, 2H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 214.1, 141.7, 139.4, 137.9, 137.4, 137.1, 132.7, 130.2, 129.6, 128.6, 128.5, 128.3, 128.0, 127.2, 126.7, 121.2, 105.2, 98.6, 56.5, 39.8, one carbon hidden. IR (neat) 3062, 3029, 2954, 2923, 2853, 1751, 1602, 1581, 1511, 1464, 1378, 1354, 1149 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{18}INNaO$ [*M*+Na]$^+$: 498.0325, found: 498.0303.

8'aa: orange solid, 27%; mp = 63–67 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 (dd, J = 7.8, 1.6 Hz, 1H), 7.45 (dd, J = 8.0, 1.2 Hz, 1H), 7.39 (td, J = 7.7, 1.4 Hz, 1H), 7.18–7.14 (m, 5H), 7.11–7.04 (m, 3H), 6.94–6.85 (m, 3H), 6.48 (s, 1H), 4.45 (s, 1H), 3.63 (dd, J = 21.4, 1.2 Hz, 1H), 3.53 (d, J = 21.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.1, 141.7, 140.15, 137.6, 137.2, 136.6, 133.4, 129.6, 129.0, 128.8, 128.4, 128.4, 128.3, 127.7, 127.2, 126.7, 121.1, 105.0, 98.8, 55.8, 40.0. IR (neat) 3062, 3028, 2965, 2894, 1751, 1643, 1601, 1584, 1567, 1547, 1482, 1451, 1359, 1260, 1235, 1180, 1074 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{18}INNaO$ [*M*+Na]$^+$: 498.0325, found: 498.0308.

1-([1,1'-biphenyl]-2-yl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8ab and 8'ab)



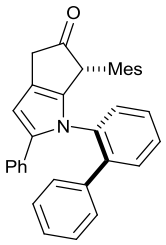
8ab **8'ab**

Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **2b** (16 mg, 0.095 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (3.6 mg, 0.0073 mmol, 10 mol%), 18 mg of cyclopenta[*b*]pyrrole **8ab** and **8'ab** were obtained (39% and 19%, respectively) (DCE, t_1 = 0.75 h at 80 °C, t_2 = 0.75 h at 40 °C).
Flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent.

8ab: orange solid, 39%; mp = 59–62°C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.31 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.26–7.08 (m, 9H), 7.06–7.01 (m, 2H), 7.00–6.96 (m, 2H), 6.94 (dd, *J* = 7.6, 1.4 Hz, 1H), 6.87 (dd, *J* = 7.5, 1.9 Hz, 2H), 6.70 (dd, *J* = 7.9, 1.0 Hz, 1H), 6.40 (s, 1H), 3.65 (s, 1H), 3.45 (dd, *J* = 21.5, 1.1 Hz, 1H), 3.36 (d, *J* = 21.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.0, 138.6, 138.4, 137.9, 137.1, 136.9, 136.4, 132.9, 130.8, 129.4, 128.5, 128.4, 128.3, 128.1, 127.9, 127.8, 127.6, 127.4, 127.2, 126.3, 121.0, 105.3, 56.0, 39.3, one carbon hidden. IR (neat) 3060, 3025, 2923, 2851, 1751, 1600, 1505, 1484, 1466, 1436, 1355, 1267, 1074 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{31}H_{23}NNaO$ $[M+Na]^+$: 448.1672, found: 448.1656.

8'ab: orange solid, 19%; mp = 56–60°C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.45 (td, *J* = 7.6, 1.5 Hz, 1H), 7.30 (td, *J* = 7.5, 1.3 Hz, 1H), 7.11–6.98 (m, 6H), 6.95–6.85 (m, 6H), 6.51 (dd, *J* = 8.3, 1.2 Hz, 2H), 6.13 (s, 1H), 6.05 (dd, *J* = 8.3, 1.1 Hz, 2H), 4.74 (s, 1H), 3.69 (dd, *J* = 21.6, 1.2 Hz, 1H), 3.57 (d, *J* = 21.9 Hz, 1H); ^{13}C NMR (91 MHz, C_6D_6) δ 212.8, 139.3, 139.2, 138.8, 137.5, 137.4, 136.7, 133.7, 131.3, 128.6, 128.5, 128.2, 128.0, 127.6, 127.2, 126.7, 126.1, 121.3, 105.2, 56.3, 40.2, four carbons hidden. IR (neat) 3060, 3030, 2923, 1751, 1601, 1505, 1484, 1436, 1356, 1256, 1265, 1152, 1074 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{31}H_{23}NNaO$ $[M+Na]^+$: 448.1672, found: 448.1659.

1-([1,1'-biphenyl]-2-yl)-6-mesityl-2-phenyl-4,6-dihydrocyclopenta[b]pyrrol-5(1H)-one (8mb)

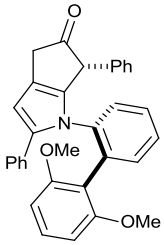


Starting from 2-furylcarbinol **1m** (20 mg, 0.063 mmol, 1 equiv), aniline **2b** (14 mg, 0.082 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.9 mg, 0.0032 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.2 mg, 0.0032 mmol, 5 mol%) and $Cu(OTf)_2$ (2.3 mg, 0.0063 mmol, 10 mol%), 22 mg of cyclopenta[*b*]pyrrole **8mb** were obtained.

Flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent.

8mb: yellow solid, 76% (HFIP, t_1 = 1 h at 60 °C, t_2 = 0.5 h at 20 °C); mp = 93–97 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.47–7.32 (m, 4H), 7.15–7.03 (m, 4H), 6.96 (t, *J* = 7.6 Hz, 2H), 6.86 (dd, *J* = 6.6, 3.2 Hz, 2H), 6.57 (s, 1H), 6.46 (s, 1H), 6.44–6.37 (m, 2H), 6.34 (s, 1H), 4.95 (s, 1H), 3.53 (d, *J* = 1.2 Hz, 2H), 2.13 (s, 3H), 1.91 (s, 3H), 1.70 (s, 3H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 217.1, 139.4, 137.8, 137.7, 137.4, 136.8, 136.4, 136.1, 133.3, 131.4, 131.1, 131.0, 129.5, 129.3, 129.0, 128.9, 128.7, 128.2, 128.1, 128.0, 127.7, 127.3, 126.8, 126.1, 120.5, 104.8, 51.8, 40.7, 20.9, 20.7 19.4. IR (neat) 3061, 3023, 2963, 2924, 2854, 1747, 1600, 1566, 1462, 1434, 1351, 1263 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{34}H_{29}NNaO$ $[M+Na]^+$: 490.2141, found: 490.2121.

1-(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8ac)

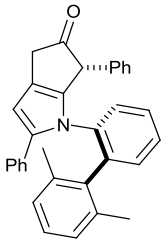


Starting from 2-furylcarbinol **1a** (30 mg, 0.109 mmol, 1 equiv), aniline **2c** (38 mg, 0.164 mmol, 1.5 equiv), $Ca(NTf_2)_2$ (3.3 mg, 0.0055 mmol, 5 mol%), $n$$Bu_4NPF_6$ (2.1 mg, 0.0055 mmol, 5 mol%) and $Cu(OTf)_2$ (3.9 mg, 0.011 mmol, 10 mol%), 29 mg of cyclopenta[*b*]pyrrole **8ac** were obtained.

Flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent.

8ac: red solid, 55% ($MeNO_2$, t_1 = 3 h at 90 °C); mp = 86–89 °C. ^{1}H NMR (300 MHz, C_6D_6) δ 7.34–7.24 (m, 3H), 7.12–6.84 (m, 11H), 6.71 (td, J = 7.7, 1.5 Hz, 1H), 6.29 (s, 1H), 6.21 (d, J = 8.4 Hz, 1H), 6.06 (d, J = 8.3 Hz, 1H), 4.25 (s, 1H), 3.30 (d, J = 20.9 Hz, 1H), 3.22–3.07 (m, 4H), 2.85 (s, 3H); ^{13}C NMR (75 MHz, C_6D_6) δ 211.4, 157.8, 157.7, 139.3, 138.7, 137.8, 137.4, 133.9, 133.4, 132.1, 129.2, 128.6, 128.4, 127.7, 127.3, 127.2, 126.9, 126.7, 125.5, 120.3, 115.2, 104.8, 103.2, 102.7, 56.3, 54.5, 54.2, 38.6. IR (neat) 3059, 2932, 2835, 1749, 1591, 1591, 1505, 1470, 1431, 1355, 1249, 1150, 1109, 1038 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{33}H_{27}NNaO_3$ $[M+Na]^+$: 508.1883, found: 508.1866.

1-(2',6'-dimethyl-[1,1'-biphenyl]-2-yl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8ad)



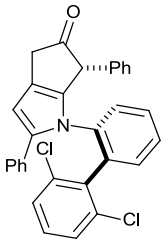
Starting from 2-furylcarbinol **1a** (10 mg, 0.036 mmol, 1 equiv), aniline **2d** (9 mg, 0.047 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.1 mg, 0.0018 mmol, 5 mol%), $n$$Bu_4NPF_6$ (0.7 mg, 0.0018 mmol, 5 mol%) and $Cu(OTf)_2$ (1.3 mg, 0.0036 mmol, 10 mol%), 9.5 mg of cyclopenta[*b*]pyrrole **8ad** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

8ad: brown solid, 57% (HFIP, t_1 = 0.75 h at 60 °C, t_2 = 2 h at 20 °C); mp = 148–152 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.40–7.28 (m, 3H), 7.23 (dd, J = 7.5, 1.2 Hz, 1H), 7.12–6.96 (m, 8H), 6.91 (d, J = 7.4 Hz, 1H), 6.84–6.74 (m, 3H), 6.70 (d, J = 7.5 Hz, 1H), 6.09 (s, 1H), 4.07 (s, 1H), 3.48 (dd, J = 21.5, 0.9 Hz, 1H), 3.35 (d, J = 21.5 Hz, 1H), 1.75 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 213.3, 139.3, 138.6, 138.2, 137.8, 137.7, 137.1, 136.7, 136.0, 133.6, 132.7, 129.3, 129.0, 128.2, 128.1, 127.7, 127.6, 127.4, 126.8, 126.5, 121.6, 105.9, 57.0, 38.9, 20.8, 19.9,

two carbons hidden. IR (neat) 3062, 3028, 2962, 2931, 2909, 1750, 1691, 1601, 1493, 1463, 1445, 1357, 1261, 1180, 1114 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{33}H_{27}NNaO$ $[M+Na]^+$: 476.1985, found: 476.1978.

1-(2',6'-dichloro-[1,1'-biphenyl]-2-yl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8ae)

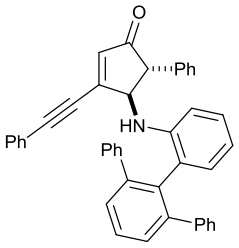


Starting from 2-furylcarbinol **1a** (13 mg, 0.048 mmol, 1 equiv), aniline **2e** *(*mg, 0.063 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.5 mg, 0.0024 mmol, 5 mol%), $n$$Bu_4NPF_6$ (0.9 mg, 0.0024 mmol, 5 mol%) and $Cu(OTf)_2$ (1.7 mg, 0.0048 mmol, 10 mol%), 12 mg of cyclopenta[*b*]pyrrole **8ae** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

8ae: orange solid, 48% (HFIP, t_1 = 0.33 h at 60 °C, t_2 = 7 h at 20 °C); mp = 46–50 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42–7.23 (m, 4H), 7.23–6.96 (m, 10H), 6.89–6.70 (m, 3H), 6.10 (s, 1H), 4.30 (s, 1H), 3.52 (d, *J* = 21.4 Hz, 1H), 3.37 (d, *J* = 21.3 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 213.4, 139.7, 138.5, 138.4, 138.0, 137.3, 135.3, 134.1, 133.9, 133.0, 132.7, 129.4, 129.1, 129.1, 128.4, 128.3, 128.2, 127.8, 127.6, 127.5, 127.5, 126.6, 121.5, 105.9, 57.2, 39.0. IR (neat) 3062, 3028, 2963, 2906, 1751, 1601, 1499, 1462, 1453, 1426, 1356, 1261, 1098 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{31}H_{21}Cl_2NNaO$ $[M+Na]^+$: 516.0892, found: 516.0866.

5-phenyl-4-((6'-phenyl-[1,1':2',1''-terphenyl]-2-yl)amino)-3-(phenylethynyl)cyclopent-2-enone



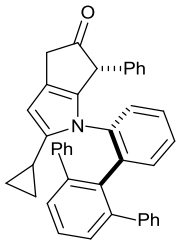
Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7f** (30 mg, 0.095 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (3.6 mg, 0.0073 mmol, 10 mol%), 36 mg of aza-Piancatelli product were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

Orange solid, 85% ($MeNO_2$, t_1 = 0.5 h at 90 °C); mp = 69–74 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.52–7.42 (m, 3H), 7.40–6.94 (m, 18H), 6.90–6.84 (m, 2H), 6.76 (d, *J* = 7.6 Hz, 2H), 6.52–6.39 (m, 2H), 6.05 (d, *J* = 8.0 Hz, 1H), 4.74 (d, *J* = 9.2 Hz, 1H), 3.92 (d, *J* = 9.3 Hz, 1H), 2.24 (d, *J* = 1.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 206.0, 155.7,

143.7, 143.4, 142.0, 141.8, 141.2, 138.9, 135.7, 135.1, 132.7, 132.3, 130.3, 130.1, 129.8, 129.4, 129.2, 129.0, 128.6, 128.4, 128.1, 127.9, 127.8, 127.7, 127.3, 127.1, 126.6, 125.6, 121.4, 117.5, 111.1, 107.5, 84.0, 64.1, 60.3. IR (neat) 3057, 3028, 2962, 2922, 2852, 1704, 1602, 1582, 1511, 1495, 1442, 1311, 1264, 1162 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{43}H_{31}NNaO$ $[M+Na]^+$: 600.2298, found: 600.2291.

2-cyclopropyl-6-phenyl-1-(6'-phenyl-[1,1':2',1''-terphenyl]-2-yl)-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8cf)

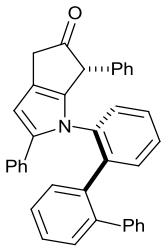


Starting from 2-furylcarbinol **1c** (15 mg, 0.063 mmol, 1 equiv), aniline **2f** (26 mg, 0.082 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.9 mg, 0.0031 mmol, 5 mol%), $n Bu_4NPF_6$ (1.2 mg, 0.0031 mmol, 5 mol%) and $Cu(OTf)_2$ (2.3 mg, 0.0063 mmol, 10 mol%), 15 mg of cyclopenta[*b*]pyrrole **8cf** were obtained.

Flash column chromatography using Pentane/EtOAc 97:3 as eluent.

8cf: yellow solid, 44% (DCE, t_1 = 0.33 h at 80 °C, t_2 = 8 h at 80 °C); mp = 151–155 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50–7.39 (m, 2H), 7.28 (d, *J* = 1.7 Hz, 1H), 7.13–6.84 (m, 15H), 6.73–6.63 (m, 2H), 6.61–6.49 (m, 2H), 5.56 (s, 1H), 3.22 (d, *J* = 21.2 Hz, 1H), 3.14 (dd, *J* = 21.3, 0.9 Hz, 1H), 2.91 (s, 1H), 0.66–0.40 (m, 2H), 0.40–0.23 (m, 2H), 0.07– -0.00 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.0, 142.7, 142.4, 141.0, 140.8, 138.7, 137.9, 135.4, 134.7, 133.8, 133.2, 130.5, 130.3, 130.3, 130.0, 130.0, 128.6, 128.4, 127.9, 127.9, 127.4, 127.1, 127.0, 126.7, 126.5, 126.1, 120.2, 99.2, 55.6, 38.4, 11.6, 8.7, 6.7, 1.2. IR (neat) 3054, 3027, 2964, 2883, 1751, 1723, 1582, 1530, 1494, 1441, 1415, 1262, 1098, 1074 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{40}H_{31}NNaO$ $[M+Na]^+$: 564.2298, found: 5642287.

1-([1,1':2',1''-terphenyl]-2-yl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8ag)

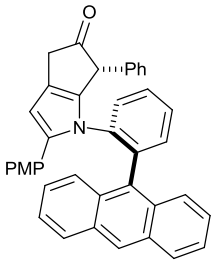


Starting from 2-furylcarbinol **1a** (17 mg, 0.062 mmol, 1 equiv), aniline **2g** (20 mg, 0.081 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.9 mg, 0.0031 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.2 mg, 0.0031 mmol, 5 mol%) and $Cu(OTf)_2$ (2.2 mg, 0.0062 mmol, 10 mol%), 14 mg of cyclopenta[*b*]pyrrole **8ag** were obtained.

Flash column chromatography using Pentane/EtOAc 97:3 as eluent.

8ag: brown solid, 45% ($MeNO_2$, t_1 = 1 h at 90 °C); mp = 180–185 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.30 (d, J = 6.1 Hz, 2H), 7.25–6.73 (m, 17H), 6.65–6.54 (m, 2H), 6.36 (d, J = 7.8 Hz, 1H), 6.07 (s, 1H), 5.99 (d, J = 7.5 Hz, 1H), 3.39 (d, J = 21.4 Hz, 1H), 3.25 (d, J = 21.4 Hz, 1H), 2.29 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.3, 141.2, 140.1, 139.7, 139.4, 137.7, 137.3, 136.8, 136.6, 133.5, 132.8, 132.1, 130.0, 129.5, 128.8, 128.7, 128.3, 128.1, 128.0, 127.8, 127.7, 127.3, 127.2, 126.8, 125.9, 120.3, 104.7, 54.6, 39.1, two carbons hidden. IR (neat) 3061, 3026, 2961, 2924, 2854, 1750, 1603, 1550, 1493, 1477, 1463, 1445, 1354, 1262, 1230 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{37}H_{27}NNaO$ $[M+Na]^+$: 524.1985, found: 524.2010.

1-(2-(anthracen-9-yl)phenyl)-2-(4-methoxyphenyl)-6-phenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8fh)

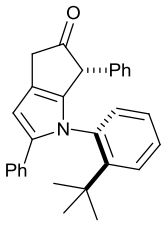


Starting from 2-furylcarbinol **1f** (25 mg, 0.082 mmol, 1 equiv), aniline **7h** (29 mg, 0.11 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.5 mg, 0.0041 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.6 mg, 0.0041 mmol, 5 mol%) and $Cu(OTf)_2$ (3.0 mg, 0.0082 mmol, 10 mol%), 20 mg of cyclopenta[*b*]pyrrole **8fh** were obtained.

Flash column chromatography using Pentane/EtOAc 95:5 as eluent.

8fh: yellow solid, 44% (1,2-DCE, t_1 = 0.75 h at 80 °C, t_2 = 6 h at 80 °C); mp = 101–106 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.88 (dd, J = 19.2, 8.4 Hz, 2H), 7.54–7.11 (m, 12H), 6.94 (d, J = 7.4 Hz, 1H), 6.81–6.66 (m, 2H), 6.22 (d, J = 8.8 Hz, 2H), 6.12 (d, J = 8.8 Hz, 2H), 5.39 (s, 1H), 4.54 (s, 1H), 3.69 (s, 3H), 3.22 (d, J = 20.8 Hz, 1H), 2.80 (d, J = 21.3 Hz, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 213.4, 158.0, 139.9, 139.5, 138.6, 136.9, 136.6, 133.7, 132.0, 131.2, 130.6, 130.4, 129.2, 129.1, 128.8, 128.6, 128.2, 128.2, 127.8, 127.6, 127.6, 127.0, 126.8, 126.0, 125.8, 125.0, 124.6, 124.3, 122.9, 121.1, 113.4, 104.0, 57.3, 55.2, 38.6, one carbon hidden. IR (neat) 3053, 3019, 2924, 2851, 1749, 1524, 1492, 1461, 1450, 1354, 1292, 1246, 1176, 1030 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{40}H_{29}NNaO_2$ $[M+Na]^+$: 578.2091, found: 578.2065.

1-(2-(tert-butyl)phenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[b]pyrrol-5(1H)-one (8ai)

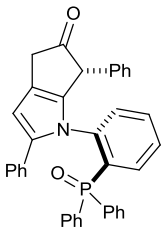


Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7i** (14 mg, 0.073 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (5.3 mg, 0.0146 mmol, 20 mol%), 17.5 mg of cyclopenta[*b*]pyrrole **8ai** were obtained.

Flash column chromatography using Pentane/EtOAc 98:2 as eluent.

8ai: brown solid, 59% ($MeNO_2$, t_1 = 1.5 h at 90 °C); mp = 85–89 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.34–7.28 (m, 3H), 7.21–6.97 (m, 9H), 6.74–6.57 (m, 2H), 6.38 (s, 1H), 4.51 (s, 1H), 3.70 (dd, J = 21.7, 1.2 Hz, 1H), 3.56 (d, J = 21.7 Hz, 1H), 0.38 (s, 9H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 216.0, 146.9, 138.6, 138.3, 135.7, 133.6, 130.8, 130.7, 128.9, 128.6, 128.3, 128.1, 127.1, 126.5, 126.4, 119.5, 104.0, 56.1, 40.7, 35.7, 30.7, two carbons hidden. IR (neat) 3062, 3027, 2964, 2908, 2873, 1749, 1631, 1601, 1584, 1494, 1441, 1361, 1262 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{29}H_{27}NNaO$ $[M+Na]^+$: 428.1985, found: 428.1967.

1-(2-(diphenylphosphoryl)phenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[b]pyrrol-5(1H)-one (8aj)

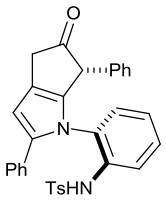


Starting from 2-furylcarbinol **1a** (40 mg, 0.15 mmol, 2 equiv), aniline **7j** (21 mg, 0.073 mmol, 1 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (5.3 mg, 0.0146 mmol, 10 mol%), 26 mg of cyclopenta[*b*]pyrrole **8aj** were obtained.

Flash column chromatography using Pentane/EtOAc 7:3 as eluent.

8aj: brown solid, 65% (1,2-DCE, t_1 = 1.5 h at 80 °C, t_2 = 0.16 h at 80 °C); mp = 95–99 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59–7.42 (m, 7H), 7.41–7.34 (m, 3H), 7.34–7.27 (m, 2H), 7.10–6.95 (m, 9H), 6.80–6.74 (m, 2H), 6.69 (ddd, J = 7.9, 4.4, 0.8 Hz, 1H), 6.23 (s, 1H), 4.18 (s, 1H), 3.38 (dd, J = 21.4, 1.2 Hz, 1H), 3.27 (d, J = 21.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.3, 141.7 (d, J = 3.8 Hz), 138.6, 138.1, 137.3, 134.7 (d, J = 9.5 Hz), 133.4, 132.9, 133.2 (d, J = 7.8 Hz), 132.1 (d, J = 11.4 Hz), 131.9, 131.8, 131.8, 131.7, 131.6, 131.6 (d, J = 2.9 Hz), 130.6 (d, J = 14.0 Hz), 128.5, 128.3, 128.3, 128.2, 128.0, 128.0, 128.0, 127.9 (d, J = 11.6 Hz), 127.8, 127.4, 126.9, 126.0, 120.2, 105.4, 55.9, 39.3. IR (neat) 3058, 3025, 2924, 2890, 1749, 1680, 1602, 1585, 1483, 1438, 1387, 1355, 1179, 1117 cm^{-1}. HRMS-ES+: *m/z* calculated for $C_{39}H_{28}NO_2P$ $[M+H]^+$: 550.1936, found: 550.1934.

4-methyl-N-(2-(5-oxo-2,6-diphenyl-5,6-dihydrocyclopenta[*b*]pyrrol-1(4H)-yl)phenyl)benzenesulfonamide (3al)

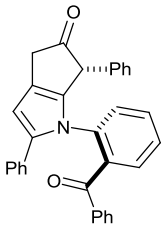


Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **2l** (25 mg, 0.095 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0073 mmol, 10 mol%), 21 mg of cyclopenta[*b*]pyrrole **3al** were obtained (dr 6:1).

Flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent.

3al: brown solid, 56% ($MeNO_2$, t_1 = 0.5 h at 90°C). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (dd, J = 8.2, 1.0 Hz, 1H), 7.46 (d, J = 8.3 Hz, 2H), 7.21–7.12 (m, 10H), 7.08–7.04 (m, 2H), 6.74–6.69 (m, 2H), 6.56 (s, 1H), 6.43 (dd, J = 7.9, 1.3 Hz, 1H), 6.22 (s, 1H), 3.52 (d, J = 21.7 Hz, 1H), 3.42 (d, J = 21.5 Hz, 1H), 3.12 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.8, 144.9, 138.1, 137.8, 137.0, 136.2, 133.2, 131.4, 130.0, 129.5, 129.2, 129.1, 128.8, 128.7, 127.8, 127.5, 127.3, 127.2, 127.1, 124.7, 122.1, 121.1, 106.2, 54.9, 39.4, 21.7. IR (neat) 3058, 3025, 2922, 2857, 1751, 1599, 1502, 1463, 1401, 1339, 1267, 1166, 1091 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{32}H_{26}N_2NaO_3S$ $[M+H]^+$: 541.1556, found: 541.1566.

1-(2-benzoylphenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8ak)



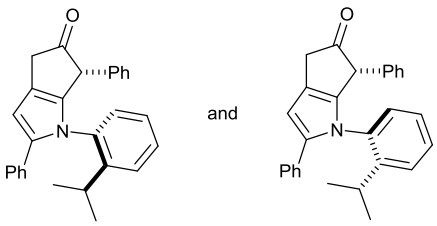
Starting from 2-furylcarbinol **1a** (25 mg, 0.091 mmol, 1 equiv), aniline **7k** (23 mg, 0.12 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.7 mg, 0.0046 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.8 mg, 0.0046 mmol, 5 mol%) and $Cu(OTf)_2$ (3.3 mg, 0.0091 mmol, 10 mol%), 25 mg of cyclopenta[*b*]pyrrole **8ak** were obtained (dr 4:1).

Flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent.

8ak: brown solid, 60% (1,2-DCE, t_1 = 0.2 h at 80 °C, t_2 = 0.2 h at 80 °C); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51–7.44 (m, 2H), 7.36–7.22 (m, 9H), 7.08–7.04 (m, 4H), 7.00–6.96 (m, 2H), 6.90–6.87 (m, J = 1.8 Hz, 1H), 6.82–6.76 (m, 1H), 6.24 (s, 1H), 4.33 (s, 1H), 3.45 (dd, J = 21.4, 1.2 Hz, 1H), 3.30 (d, J = 21.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 213.3, 194.6, 138.6, 138.2, 138.0, 137.9, 137.2, 136.4, 132.9, 132.4, 131.1, 130.1, 129.7, 129.5, 128.9, 128.3, 128.2, 128.0, 128.9, 127.5, 127.4, 126.5, 121.4, 105.7, 56.2, 39.2. IR (neat) 3062, 3028, 2916, 2893, 1751, 1665,

1598, 1580, 1511, 1493, 1415, 1316, 1290, 1180 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{32}H_{23}NNaO_2$ $[M+Na]^+$: 476.1621, found: 476.1599.

1-(2-isopropylphenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[b]pyrrol-5(1H)-one (8al and 8'al)



8al **8'al**

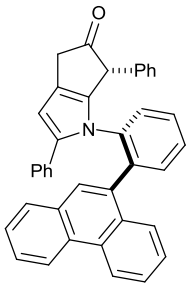
Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7l** (13 mg, 0.95 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0073 mmol, 10 mol%), 14 mg of cyclopenta[*b*]pyrrole **8al** and **8'al** were obtained (30% and 20%, respectively) ($MeNO_2$, t_1 = 1.5 h at 90°C).

Flash column chromatography using Pentane/EtOAc 98:2 as eluent.

8al: yellow solid, 30%, mp = 91–94 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25–7.06 (m, 10H), 6.97–6.90 (m, 2H), 6.85–6.70 (m, 1H), 6.60 (d, *J* = 7.8 Hz, 1H), 6.52 (s, 1H), 4.22 (s, 1H), 3.61 (dd, *J* = 21.4, 1.1 Hz, 1H), 3.52 (d, *J* = 21.3 Hz, 1H), 2.49 (hept, *J* = 6.7 Hz, 1H), 1.07 (d, *J* = 6.9 Hz, 3H), 0.69 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 214.1, 146.4, 138.4, 138.2, 137.4, 136.2, 132.9, 129.3, 128.9, 128.7, 128.2, 128.1, 127.6, 127.4, 126.5, 126.4, 125.7, 120.6, 104.0, 56.0, 39.6, 27.5, 24.7, 22.9. IR (neat) 3063, 3029, 2967, 2926, 2887, 2869, 1750, 1601, 1511, 1493, 1464, 1450, 1357, 1261, 1152, 1029 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{28}H_{25}NNaO$ $[M+Na]^+$: 414.1828, found: 414.1812.

8'al: brown solid, 20%, mp = 172–176 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43–7.36 (m, 1H), 7.32–7.23 (m, 2H), 7.14–6.98 (m, 8H), 6.98–6.91 (m, 1H), 6.83–6.70 (m, 2H), 6.43 (s, 1H), 4.51 (s, 1H), 3.64 (dd, *J* = 21.4, 1.1 Hz, 1H), 3.54 (d, *J* = 21.4 Hz, 1H), 2.28 (h, *J* = 6.8 Hz, 1H), 0.21–0.12 (m, 6H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 214.6, 145.9, 138.3, 137.8, 137.6, 136.2, 133.3, 128.8, 128.7, 128.3, 128.0, 127.9, 127.7, 127.2, 127.1, 126.6, 126.4, 120.4, 104.3, 55.9, 40.0, 27.5, 23.7, 22.3. IR (neat) 3064, 3030, 2957, 2887, 2867, 1749, 1602, 1550, 1496, 1451, 1359, 1262, 1157, 1098 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{28}H_{25}NNaO$ $[M+Na]^+$: 414.1828, found: 414.1822.

1-(2-(phenanthren-9-yl)phenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8am)

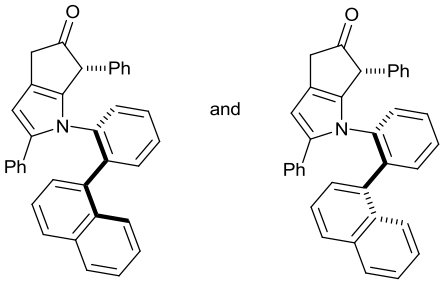


Starting from 2-furylcarbinol **1a** (18 mg, 0.066 mmol, 1 equiv), aniline **7m** (23 mg, 0.085 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.0 mg, 0.0033 mmol, 5 mol%), $n Bu_4NPF_6$ (1.3 mg, 0.0033 mmol, 5 mol%) and $Cu(OTf)_2$ (2.4 mg, 0.0066 mmol, 10 mol%), 18 mg of cyclopenta[*b*]pyrrole **8am** were obtained (dr 2.5:1).

Flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent.

8am: brown solid, 52% ($MeNO_2$, t_1 = 0.5 h at 90 °C); ^{1}H NMR (360 MHz, $CDCl_3$) δ 8.69–8.62 (m, 2H), 7.68–7.49 (m, 4H), 7.48–7.29 (m, 9H), 7.15 (ddd, *J* = 7.3, 3.5, 1.6 Hz, 2H), 7.10–7.05 (m, 3H), 6.76–6.71 (m, 2H), 6.57 (s, 1H), 5.90 (s, 1H), 4.16 (s, 1H), 3.26 (d, *J* = 21.4 Hz, 1H), 2.93 (d, *J* = 21.4 Hz, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 213.5, 138.8, 138.4, 138.1, 136.7, 134.3, 133.6, 132.4, 131.4, 130.4, 130.0, 129.9, 129.5, 129.3, 129.3, 128.9, 128.4, 128.3, 128.2, 128.1, 127.7, 127.5, 127.2, 127.1, 126.7, 126.5, 126.2, 126.1, 125.4, 122.9, 122.4, 121.0, 104.7, 56.5, 38.8. IR (neat) 3061, 3028, 2925, 2853, 1749, 1601, 1492, 1463, 1451, 1357, 1232 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{39}H_{27}NNaO$ $[M+Na]^+$: 548.1985, found: 548.2004.

1-(2-(naphthalen-1-yl)phenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[b]pyrrol-5(1H)-one (8an and 8'an)



8an **8'an**

Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7n** (24 mg, 0.11 mmol, 1.5 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (4.0 mg, 0.011 mmol, 15 mol%), 28 mg of cyclopenta[*b*]pyrroles **8an** and **8'an** were obtained (47% and 34%, respectively) (1,2-DCE, t_1 = 0.5 h at 80 °C, t_2 = 1.5 h at 80 °C).

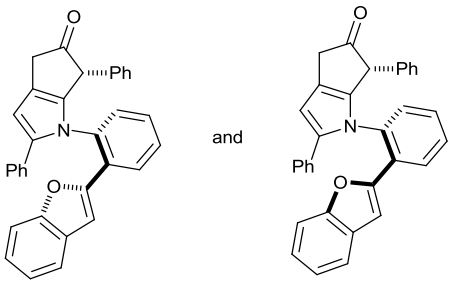
Flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent.

8an: yellow solid, 47%; mp = 72–75 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.84–7.76 (m, 1H), 7.73–7.59 (m, 2H), 7.53–7.32 (m, 4H), 7.24–6.81 (m, 13H), 6.73 (d, *J* = 7.9 Hz, 1H), 6.36 (s, 1H), 3.70 (s, 1H), 3.43 (d, *J* = 21.5 Hz, 1H), 3.31 (d, *J* = 21.5 Hz, 1H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 213.8, 138.5, 138.1, 137.3, 136.9, 136.6, 136.1, 133.5, 133.0,

132.6, 131.1, 129.4, 128.6, 128.3, 128.2, 127.9, 127.7, 127.6, 127.2, 126.3, 126.0, 121.2, 105.3, 56.1, 39.3, six carbons hidden. IR (neat) 3058, 3025, 2890, 1752, 1600, 1493, 1468, 1448, 1354, 1269, 1144, 1038 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{35}H_{25}NNaO$ $[M+Na]^+$: 498.1828, found: 498.1822.

8'an: yellow solid, 34%; mp = 82–86 °C. ^1H NMR (250 MHz, $CDCl_3$) δ 7.73–7.65 (m, 1H), 7.61 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.50 (td, *J* = 7.6, 1.5 Hz, 1H), 7.42–7.32 (m, 5H), 7.15–7.01 (m, 4H), 7.00–6.90 (m, 3H), 6.78 (t, *J* = 7.6 Hz, 2H), 6.48 (s, 1H), 6.41–6.28 (m, 2H), 6.14 (dd, *J* = 8.5, 1.7 Hz, 1H), 6.05 (s, 1H), 4.77 (s, 1H), 3.71 (d, *J* = 21.7 Hz, 1H), 3.57 (d, *J* = 21.5 Hz, 1H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 215.2, 139.0, 138.5, 137.7, 137.0, 136.5, 135.9, 133.1, 133.0, 132.1, 131.5, 128.7, 128.7, 128.3, 128.3, 128.2, 128.1, 127.9, 127.7, 127.6, 127.5, 127.4, 127.3, 126.8, 126.1, 125.8, 125.6, 120.7, 104.6, 56.3, 40.4. IR (neat) 3057, 2928, 2879, 1751, 1601, 1577, 1494, 1468, 1450, 1356, 1265 cm^{-1} HRMS-ESI: *m/z* calculated for $C_{35}H_{25}NNaO$ $[M+Na]^+$: 498.1828, found: 498.1811.

1-(2-(benzofuran-2-yl)phenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[*b*]pyrrol-5(1H)-one (8ao and 8'ao)



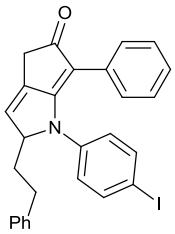
8ao **8'ao**

Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7o** (20 mg, 0.11 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.073 mmol, 10 mol%), 30 mg of cyclopenta[*b*]pyrrole **8ao** and **8'ao** were obtained (51% and 37%, respectively) (1,2-DCE, t_1 = 0.75 h at 80 °C, t_2 = 0.5 h at 40 °C).
Flash column chromatography using Pentane/EtOAc 92.5:7.5 as eluent.

8ao: orange solid, 51%, mp = 53–56 °C. ^1H NMR (360 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.50 (dd, *J* = 15.7, 7.9 Hz, 2H), 7.34–7.19 (m, 2H), 7.16–7.05 (m, 9H), 6.88 (td, *J* = 7.6, 1.4 Hz, 1H), 6.80 (dd, *J* = 6.5, 2.9 Hz, 2H), 6.70–6.53 (m, 2H), 5.85 (s, 1H), 4.05 (s, 1H), 3.57 (s, 2H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 214.0, 154.4, 151.6, 137.8, 136.2, 136.0, 135.1, 132.5, 130.2, 129.4, 128.6, 128.5, 128.4, 128.3, 127.9, 127.7, 127.2, 127.1, 126.7, 125.2, 123.2, 121.7, 121.7, 111.2, 105.3, 104.9, 55.6, 39.8, one carbon hidden. IR (neat) 3064, 3029, 2895, 1752, 1602, 1582, 1495, 1476, 1465, 1454, 1417, 1357, 1258, 1178, 1147, 1075 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{33}H_{23}NNaO_2$ $[M+Na]^+$: 488.1621, found: 488.1614.

8'ao: orange solid, 37%, mp = 58–63 °C ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.78–7.61 (m, 1H), 7.45–7.42 (m, 1H), 7.37–7.29 (m, 4H), 7.20–7.13 (m, 4H), 7.10–6.98 (m, 5H), 6.85–6.71 (m, 1H), 6.67–6.51 (m, 5H), 5.74 (d, *J* = 0.7 Hz, 1H), 4.39 (s, 1H), 3.69 (dd, *J* = 21.5, 1.2 Hz, 1H), 3.56 (d, *J* = 20.8 Hz, 1H). ^{13}C NMR (91 MHz, $CDCl_3$) δ 214.6, 154.1, 151.1, 137.0, 136.7, 136.2, 135.4, 132.5, 129.4, 129.4, 129.3, 128.9, 128.9, 128.3, 128.1, 127.8, 127.6, 127.5, 126.7, 126.7, 124.7, 122.7, 121.4, 121.2, 111.0, 105.4, 105.0, 56.0, 40.2. IR (neat) 3064, 3029, 2967, 2899, 2886, 1752, 1601, 1582, 1494, 1453, 1357, 1259, 1178, 1075 cm^{-1} HRMS-ESI: *m/z* calculated $C_{33}H_{23}NNaO_2$ $[M+Na]^+$: 488.1621, found: 488.1607.

1-(4-iodophenyl)-2-phenethyl-6-phenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (9ba)

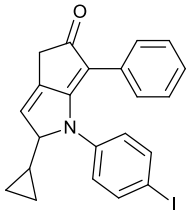


Starting from 2-furylcarbinol **1b** (12.5 mg, 0.041 mmol, 1 equiv), aniline **2a** (12 mg, 0.054 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.2 mg, 0.0021 mmol, 5 mol%), $n$$Bu_4NPF_6$ (0.8 mg, 0.0021 mmol, 5 mol%) and $Cu(OTf)_2$ (1.5 mg, 0.0041 mmol, 10 mol%), 16 mg of **9ba** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

9ba: red oil, 77% (HFIP, t_1 = 1 h at 40 °C, t_2 = 2 h at 20 °C); ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.6 Hz, 2H), 7.21–7.07 (m, 3H), 7.05–6.96 (m, 3H), 6.95–6.88 (m, 2H), 6.88–6.78 (m, 2H), 6.41 (d, *J* = 8.7 Hz, 2H), 6.17 (d, *J* = 1.8 Hz, 1H), 5.27–5.18 (m, 1H), 3.12 (d, *J* = 20.7 Hz, 1H), 3.04 (d, *J* = 20.9 Hz, 1H), 2.53–2.34 (m, 2H), 2.07–1.96 (m, 1H), 1.85–1.69 (m, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 201.1, 169.1, 140.7, 139.2, 137.6, 137.2, 131.2, 129.5, 128.7, 128.3, 127.4, 126.5, 126.4, 126.3, 124.5, 109.9, 90.0, 75.1, 34.7, 33.5, 30.7. IR (neat) 3088, 3061, 3028, 2958, 2924, 2853, 1679, 1630, 1549, 1487, 1452, 1397, 1262, 1177, 1099 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{27}H_{23}INO$ $[M+H]^+$: 504.0819, found: 504.0815.

2-cyclopropyl-1-(4-iodophenyl)-6-phenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (9ca)

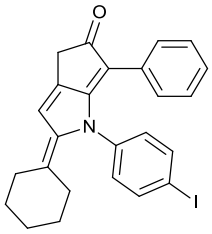


Starting from 2-furylcarbinol **1c** (25 mg, 0.11 mmol, 1 equiv), aniline **2a** (30 mg, 0.14 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (3.1 mg, 0.0052 mmol, 5 mol%), $n$$Bu_4NPF_6$ (2.0 mg, 0.0052 mmol, 5 mol%) and $Cu(OTf)_2$ (3.8 mg, 0.011 mmol, 10 mol%), 23 mg of **9ca** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

9ca: brown solid, 50% (HFIP, t_1 = 0.75 h at 40 °C, t_2 = 1.25 h at 20 °C); mp = 165–170 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 (d, J = 8.7 Hz, 2H), 7.10–6.96 (m, 3H), 6.96–6.86 (m, 2H), 6.64 (d, J = 8.7 Hz, 2H), 6.10 (d, J = 1.8 Hz, 1H), 4.64 (dd, J = 8.4, 1.8 Hz, 1H), 3.16 (d, J = 20.9 Hz, 1H), 3.08 (d, J = 20.8 Hz, 1H), 0.93–0.76 (m, 1H), 0.58–0.40 (m, 2H), 0.40–0.21 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.0, 169.8, 138.8, 138.3, 137.4, 131.0, 129.2, 127.4, 127.3, 126.2, 124.5, 109.7, 90.5, 80.7, 34.7, 13.8, 5.7, 0.6. IR (neat) 3081, 3002, 2918, 2845, 1675, 1607, 1578, 1492, 1415, 1395, 1326, 1265, 1179 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{22}H_{18}INNaO$ [M+Na]$^+$: 462.0325, found: 462.0328.

2-cyclohexylidene-1-(4-iodophenyl)-6-phenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (9da)

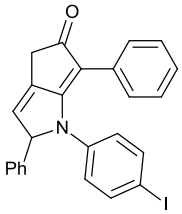


Starting from 2-furylcarbinol **1d** (25 mg, 0.090 mmol, 1 equiv), aniline **2a** (26 mg, 0.12 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.7 mg, 0.0045 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.7 mg, 0.0045 mmol, 5 mol%) and $Cu(OTf)_2$ (3.2 mg, 0.0090 mmol, 10 mol%), 20 mg of **9da** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

9da: brown solid, 46% (HFIP, t_1 = 1 h at 40 °C, t_2 = 0.15 h at 20 °C); mp = 159–162 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.04 (d, J = 8.6 Hz, 2H), 6.97–6.91 (m, 3H), 6.90–6.84 (m, 2H), 6.18 (d, J = 8.6 Hz, 2H), 6.03–5.96 (m, 1H), 2.97 (d, J = 1.1 Hz, 2H), 2.15–2.00 (m, 2H), 1.59–1.50 (m, 2H), 1.49–1.38 (m, 2H), 1.32–1.23 (m, 2H), 1.10–0.99 (m, 2H). ^{13}C NMR (91 MHz, C_6D_6) δ 198.9, 168.2, 142.2, 140.7, 138.1, 136.9, 131.7, 130.3, 129.8, 127.4, 126.3, 124.4, 116.4, 112.3, 92.6, 34.7, 33.4, 29.5, 29.0, 27.5, 26.5. IR (neat) 2933, 2853, 2835, 1675, 1609, 1590, 1551, 1485, 1403, 1339, 1279, 1222, 1141 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{23}INO$ [M+H]$^+$: 480.0819, found: 480.0787.

1-(4-iodophenyl)-2,6-diphenyl-1,2-dihydrocyclopenta[b]pyrrol-5(4H)-one (9aa)

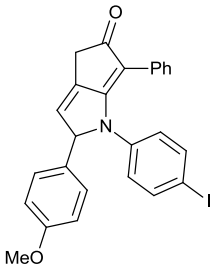


Starting from 2-furylcarbinol **1a** (20 mg, 0.072 mmol, 1 equiv), aniline **2a** (21 mg, 0.095 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0073 mmol, 10 mol%), 23 mg of **9aa** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

9aa: orange solid, 66% (HFIP, t_1 = 1 h at 40 °C, t_2 = 16 h at 20 °C); mp = 180–182 °C. ^{1}H NMR (360 MHz, C_6D_6) δ 7.44–7.33 (m, 2H), 7.04–6.90 (m, 8H), 6.84–6.77 (m, 2H), 6.11 (d, J = 8.7 Hz, 2H), 5.34–5.28 (m, 2H), 2.95 (d, J = 20.8 Hz, 1H), 2.86 (d, J = 20.8 Hz, 1H); ^{13}C NMR (91 MHz, C_6D_6) δ 199.4, 168.4, 138.7, 138.5, 137.3, 137.2, 131.8, 129.8, 129.2, 128.7, 127.5, 127.4, 126.7, 125.5, 111.2, 89.2, 80.3, 34.7, one carbon hidden. IR (neat) 3075, 3053, 3019, 2922, 2840, 1678, 1608, 1579, 1491, 1411, 1321, 1262, 1176, 1060 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{18}INNaO$ $[M+Na]^+$: 498.0325, found: 498.0316.

1-(4-iodophenyl)-2-(4-methoxyphenyl)-6-phenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (9la)

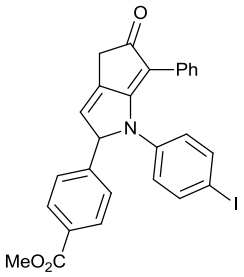


Starting from 2-furylcarbinol **1l** (30 mg, 0.099 mmol, 1 equiv), aniline **2a** (28 mg, 0.128 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (3.0 mg, 0.0049 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.9 mg, 0.0049 mmol, 5 mol%) and $Cu(OTf)_2$ (3.6 mg, 0.0099 mmol, 10 mol%), 22 mg of **9la** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

9la: brown solid, 44% (HFIP, t_1 = 2 h at 40 °C, t_2 = 16 h at 20 °C); mp = 47–51 °C. ^{1}H NMR (360 MHz, C_6D_6) δ 7.42–7.35 (m, 2H), 7.04–6.88 (m, 5H), 6.76 (d, J = 8.7 Hz, 2H), 6.64 (d, J = 8.7 Hz, 2H), 6.16 (d, J = 8.7 Hz, 2H), 5.40 (dd, J = 8.5, 1.7 Hz, 2H), 3.16 (s, 3H), 3.00 (d, J = 20.7 Hz, 1H), 2.90 (d, J = 20.6 Hz, 1H); ^{13}C NMR (91 MHz, C_6D_6) δ 199.5, 168.4, 160.2, 138.7, 138.3, 137.3, 131.9, 129.9, 128.9, 128.8, 127.5, 126.7, 125.8, 125.7, 114.6, 110.9, 89.4, 79.8, 54.7, 34.8. IR (neat) 3080, 3031, 3000, 2960, 2909, 2836, 1679, 1608, 1580, 1512, 1491, 1412, 1395, 1322, 1249, 1118 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{26}H_{20}INNaO_2$ $[M+Na]^+$: 528.0431, found: 528.0416.

Methyl 4-(1-(4-iodophenyl)-5-oxo-6-phenyl-1,2,4,5-tetrahydrocyclopenta[*b*]pyrrol-2-yl)benzoate (9ja)

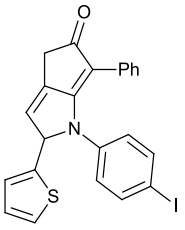


Starting from 2-furylcarbinol **1j** (30 mg, 0.090 mmol, 1 equiv), aniline **2a** (26 mg, 0.117 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.7 mg, 0.0045 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.7 mg, 0.0045 mmol, 5 mol%) and $Cu(OTf)_2$ (3.3 mg, 0.0090 mmol, 10 mol%), 32 mg of **9ja** were obtained.

Flash column chromatography using Et_2O as eluent.

9ja: brown solid, 66% (HFIP, t_1 = 0.75 h at 40 °C, t_2 = 16 h at 20 °C); mp = 177–180 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, J = 8.3 Hz, 2H), 7.40–7.32 (m, 2H), 7.05–6.92 (m, 5H), 6.75 (d, J = 8.3 Hz, 2H), 6.06 (d, J = 8.8 Hz, 2H), 5.31–5.25 (m, 1H), 5.23 (d, J = 2.1 Hz, 1H), 3.44 (s, 3H), 2.94 (d, J = 20.8 Hz, 1H), 2.85 (d, J = 20.8 Hz, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 199.4, 168.2, 166.0, 142.0, 139.1, 138.4, 137.4, 131.6, 131.0, 130.6, 129.9, 127.6, 127.5, 126.9, 125.5, 124.7, 111.4, 89.5, 79.5, 51.8, 34.8. IR (neat) 3053, 2952, 2924, 2854, 1720, 1620, 1608, 1579, 1491, 1434, 1395, 1320, 1280, 1178, 1111, 1061 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{27}H_{20}INNaO_3$ [*M*+Na]$^+$: 556.0380, found: 556.0382.

1-(4-iodophenyl)-6-phenyl-2-(thiophen-2-yl)-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (9wa)

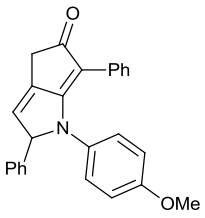


Starting from 2-furylcarbinol **1w** (30 mg, 0.107 mmol, 1 equiv), aniline **2a** (30 mg, 0.139 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (3.2 mg, 0.0054 mmol, 5 mol%), $n$$Bu_4NPF_6$ (2.1 mg, 0.0054 mmol, 5 mol%) and $Cu(OTf)_2$ (3.9 mg, 0.011 mmol, 10 mol%), 21 mg of **9wa** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

9wa: brown solid, 40% (HFIP, t_1 = 1.25 h at 40 °C, t_2 = 4 h at 40 °C); mp = 85–88 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.38–7.31 (m, 2H), 7.03–6.88 (m, 5H), 6.66 (dd, J = 5.0, 3.0 Hz, 1H), 6.51 (dd, J = 2.9, 1.1 Hz, 1H), 6.40 (dd, J = 5.0, 1.0 Hz, 1H), 6.09 (d, J = 8.6 Hz, 2H), 5.38–5.34 (m, 1H), 5.32–5.29 (m, 1H), 2.94 (d, J = 20.7 Hz, 1H), 2.86 (d, J = 20.6 Hz, 1H). ^{13}C NMR (91 MHz, $CDCl_3$) δ 199.4, 168.0, 138.7, 138.6, 138.1, 137.3, 131.7, 129.8, 127.5, 127.1, 126.7, 125.9, 125.8, 124.5, 123.7, 111.1, 89.5, 75.5, 34.8. IR (neat) 2924, 2854, 1674, 1607, 1579, 1492, 1413, 1396, 1268, 1237, 1178 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{23}H_{16}INNaOS$ [*M*+Na]$^+$: 503.9890, found: 503.9881.

1-(4-methoxyphenyl)-2,6-diphenyl-1,2-dihydrocyclopenta[b]pyrrol-5(4H)-one (9ae)

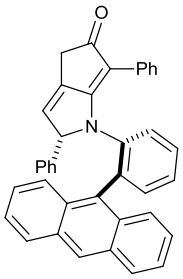


Starting from 2-furylcarbinol **1a** (70 mg, 0.26 mmol, 1 equiv), aniline **2e** (47 mg, 0.382 mmol, 1.5 equiv), $Ca(NTf_2)_2$ (7.7 mg, 0.013 mmol, 5 mol%), $n$$Bu_4NPF_6$ (4.9 mg, 0.013 mmol, 5 mol%) and $Cu(OTf)_2$ (9.2 mg, 0.026 mmol, 10 mol%), 49 mg of **9ae** were obtained.

Flash column chromatography using Pentane/EtOAc 1:1 as eluent.

9ae: orange solid, 51% (HFIP, t_1 = 2 h at 60 °C, t_2 = 16 h at 20 °C); mp = 83–85 °C. ^{1}H NMR (250 MHz, C_6D_6) δ 7.58–7.38 (m, 2H), 7.06–6.89 (m, 8H), 6.49 (d, J = 8.9 Hz, 2H), 6.25 (d, J = 9.0 Hz, 2H), 5.50–5.38 (m, 2H), 3.06–2.94 (m, 5H). ^{13}C NMR (63 MHz, C_6D_6) δ 199.14, 169.30, 157.53, 138.67, 137.32, 131.94, 129.58, 128.77, 127.09, 125.81, 125.53, 125.36, 113.45, 109.84, 80.85, 54.49, 34.63, three carbons hidden. IR (neat) 3061, 3031, 3001, 2961, 2911, 2835, 1677, 1607, 1582, 1511, 1415, 1297, 1248, 1177 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{26}H_{21}NNaO_2$ $[M+Na]^+$: 402.1465, found: 402.1474.

1-((r)-2-(anthracen-9-yl)phenyl)-2,6-diphenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (10ah)



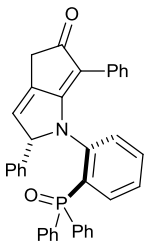
Starting from 2-furylcarbinol **1a** (15 mg, 0.055 mmol, 1 equiv), aniline **7h** (19 mg, 0.071 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (1.6 mg, 0.0027 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.1 mg, 0.0027 mmol, 5 mol%) and $Cu(OTf)_2$ (2.0 mg, 0.0055 mmol, 10 mol%), 19.5 mg of **10ah** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

10ah: red solid, 68% (HFIP, t_1 = 0.3 h at 60 °C, t_2 = 2 h at 60 °C then 10 h at 40 °C); mp = 136–140 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.09 (t, J = 7.9 Hz, 2H), 7.69 (d, J = 8.9 Hz, 1H), 7.53–7.41 (m, 3H), 7.31–7.27 (m, 4H), 7.25–7.03 (m, 6H), 7.01–6.94 (m, 2H), 6.90–6.83 (m, 2H), 6.29–6.19 (m, 2H), 5.44 (d, J = 2.2 Hz, 1H), 4.17 (d, J = 2.1 Hz, 1H), 2.98 (d, J = 20.8 Hz, 1H), 2.84 (d, J = 20.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.9, 171.2, 136.9, 136.5, 135.7, 133.5, 133.3, 133.1, 132.6, 131.8, 131.2, 130.6, 130.4, 129.6, 129.4, 128.6, 128.5, 128.4, 127.9, 127.8, 127.8, 127.5, 127.2, 127.0, 126.9, 126.6, 126.4, 125.9, 125.8, 125.6, 125.4, 111.1, 78.4, 34.2, obe

carbon hidden. IR (neat) 3042, 2923, 2845, 1678, 1610, 1580, 1493, 1446, 1404, 1317, 1257, 1178 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{39}H_{27}NNaO$ $[M+Na]^+$: 548.1985, found: 548.1982.

1-(2-(diphenylphosphoryl)phenyl)-2,6-diphenyl-1,2-dihydrocyclopenta[b]pyrrol-5(4H)-one (10aj)

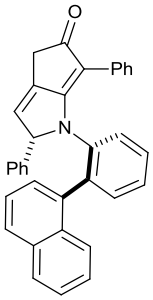


Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7j** (28 mg, 0.095 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0073 mmol, 10 mol%), 28 mg of **10aj** were obtained.

Flash column chromatography using DCM/MeOH 95:5 as eluent.

10aj: brown solid, 70% (HFIP, t_1 = 0.5 h at 40 °C, t_2 = 1 h at 40 °C); mp = 62–65 °C. ^{1}H NMR (300 MHz, C_6D_6) δ 7.91–7.78 (m, 4H), 7.32–7.22 (m, 3H), 7.12–7.03 (m, 6H), 7.03–6.97 (m, 4H), 6.97–6.93 (m, 2H), 6.92–6.88 (m, 3H), 6.46–6.24 (m, 3H), 5.55 (s, 1H), 2.96 (d, *J* = 20.5 Hz, 1H), 2.75 (d, *J* = 20.6 Hz, 1H); ^{13}C NMR (75 MHz, C_6D_6) δ 199.7, 171.0, 142.7 (d, *J* = 3.3 Hz), 138.6, 137.0, 134.4 (d, *J* = 10.9 Hz), 133.8, 133.7 (d, *J* = 105.0 Hz), 132.5 (d, *J* = 9.32 Hz), 132.5, 132.4 (d, *J* = 3.2 Hz), 132.0 (d, *J* = 2.8 Hz), 131.9, 131.9, 131.8 (d, *J* = 2.4 Hz), 131.7, 130.0 (d, *J* = 97.5 Hz), 129.8, 128.9, 128.9, 128.9, 128.8, 128.7, 128.7, 128.5, 127.2, 126.5 (d, *J* = 12.1 Hz), 126.1, 125.7, 110.5, 82.0, 34.8, 30.2. IR (neat) 3081, 3056, 3025, 2923, 2845, 1677, 1610, 1581, 1492, 1438, 1412, 1322, 1261, 1182, 1117 cm^{-1}. HRMS-ES+: *m/z* calculated for $C_{39}H_{28}NO_2P$ $[M+H]^+$: 550.1936, found: 550.1930.

1-(2-(naphthalen-1-yl)phenyl)-2,6-diphenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (10an)

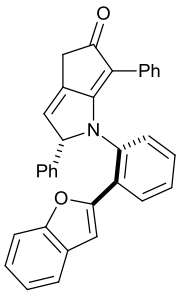


Starting from 2-furylcarbinol **1a** (30 mg, 0.11 mmol, 1 equiv), aniline **7n** (30 mg, 0.14 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (3.3 mg, 0.0055 mmol, 5 mol%), $n$$Bu_4NPF_6$ (2.1 mg, 0.0055 mmol, 5 mol%) and $Cu(OTf)_2$ (4.0 mg, 0.011 mmol, 10 mol%), 36 mg of **10an** were obtained.

Flash column chromatography using Pentane/EtOAc 6.5:3.5 as eluent.

10an: brown solid, 69% (HFIP, t_1 = 0.3 h at 60 °C, t_2 = 20 h at 20 °C); mp = 68–71 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.78–7.66 (m, 4H), 7.57 (d, J = 7.8 Hz, 2H), 7.33–7.28 (m, 2H), 7.08–7.02 (m, 3H), 7.00–6.82 (m, 5H), 6.73 (t, J = 7.4 Hz, 1H), 6.66 (d, J = 7.0 Hz, 2H), 6.53–6.41 (m, 2H), 5.19 (s, 1H), 5.08 (s, 1H), 2.97 (d, J = 20.7 Hz, 1H), 2.85 (d, J = 20.7 Hz, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 199.7, 170.6, 138.8, 137.5, 137.4, 136.6, 136.3, 134.1, 133.1, 132.1, 131.1, 129.8, 129.1, 128.9, 128.7, 128.6, 128.5, 128.2, 127.4, 127.0, 126.9, 126.2, 125.6, 110.5, 79.3, 34.8, five carbons hidden. IR (neat) 3055, 3031, 2968, 2911, 1710, 1609, 1584, 1178, 1257, 1321, 1409, 1451 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{35}H_{25}NNaO$ [*M*+Na]$^+$: 498.1828, found: 498.1807.

1-(2-(benzofuran-2-yl)phenyl)-2,6-diphenyl-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (10ao)

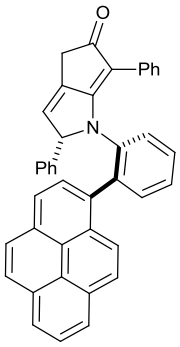


Starting from 2-furylcarbinol **1a** (20 mg, 0.073 mmol, 1 equiv), aniline **7o** (20 mg, 0.095 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (2.2 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.0073 mmol, 10 mol%), 24 mg of **10o** were obtained.

Flash column chromatography using Pentane/EtOAc 6:4 as eluent.

10ao: orange solid, 69% (HFIP, t_1 = 1.25 h at 40 °C, t_2 = 16 h at 20 °C); mp = 64–67 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56 (d, J = 7.8 Hz, 1H), 7.51–7.35 (m, 4H), 7.14–7.07 (m, 2H), 6.93–6.65 (m, 10H), 6.35 (s, 2H), 5.73 (s, 1H), 5.47 (s, 1H), 3.07 (d, J = 20.6 Hz, 1H), 2.94 (d, J = 20.6 Hz, 1H); ^{13}C NMR (91 MHz, C_6D_6) δ 199.3, 170.5, 155.3, 153.7, 139.6, 136.1, 131.7, 130.1, 129.5, 129.4, 128.7, 128.7, 128.6, 128.4, 128.2, 128.0, 127.6, 127.3, 126.1, 125.4, 125.2, 123.7, 121.7, 111.5, 110.8, 105.6, 78.8, 35.0, one carbon hidden. IR (neat) 3082, 3064, 3031, 2918, 2851, 1753, 1680, 1611, 1585, 1494, 1454, 1415, 1347, 1258, 1176 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{33}H_{23}NNaO_2$ [*M*+Na]$^+$: 488.1621, found: 488.1609.

2,6-diphenyl-1-(2-(pyren-1-yl)phenyl)-1,2-dihydrocyclopenta[*b*]pyrrol-5(4H)-one (10aq)



Starting from 2-furylcarbinol **1a** (30 mg, 0.11 mmol, 1 equiv), aniline **7q** (42 mg, 0.14 mmol, 1.3 equiv), $Ca(NTf_2)_2$ (3.3 mg, 0.0055 mmol, 5 mol%), $n$$Bu_4NPF_6$ (2.1 mg, 0.0055 mmol, 5 mol%) and $Cu(OTf)_2$ (4.0 mg, 0.011 mmol, 10 mol%), 44 mg of **10aq** were obtained.

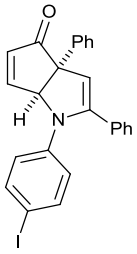
Flash column chromatography using Pentane/EtOAc 6.5/3.5 as eluent.

10aq: brown solid, 73% (HFIP, t_1 = 0.3 h at 60 °C, t_2 = 16 h at 20 °C); mp = 142–144 °C. ^{1}H NMR (300 MHz, C_6D_6) δ 8.18 (d, J = 7.9 Hz, 1H), 8.03–7.61 (m, 12H), 7.13–7.07 (m, 1H), 7.06–6.99 (m, 1H), 6.88–6.81 (m, 3H), 6.77 (td, J = 7.5, 1.3 Hz, 1H), 6.68 (dd, J = 8.0, 1.1 Hz, 1H), 6.57–6.49 (m, 1H), 6.43–6.30 (m, 2H), 4.95 (d, J = 2.1 Hz, 1H), 4.61 (d, J = 2.1 Hz, 1H), 2.96 (d, J = 20.8 Hz, 1H), 2.84 (d, J = 20.7 Hz, 1H); ^{13}C NMR (91 MHz, C_6D_6) δ 199.6, 170.7, 138.1, 137.4, 136.2, 136.0, 134.4, 132.9, 132.4, 132.0, 131.5, 131.5, 130.7, 130.0, 130.0, 129.3, 128.8, 128.5, 128.2, 127.9, 127.6, 127.6, 126.7, 126.6, 126.3, 126.1, 126.0, 125.8, 125.5, 125.5, 125.4, 110.4, 78.9, 34.8, three carbons hidden. IR (neat) 3081, 3039, 2958, 2927, 2879, 1680, 1586, 1494, 1405, 1254, 1176, 1128, 1056 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{41}H_{27}NNaO$ $[M+Na]^+$: 572.1985, found: 572.1997.

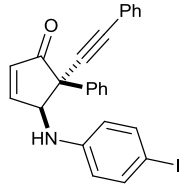
1-(4-iodophenyl)-2,3a-diphenyl-1,6a-dihydrocyclopenta[*b*]pyrrol-4(3aH)-one (12) and 4-((4-iodophenyl)amino)-5-phenyl-5-(phenylethynyl)cyclopent-2-enone (13)

Starting from 2-furylcarbinol **11** (30 mg, 0.073 mmol, 1 equiv), aniline **2a** (21 mg, 0.095 mmol, 1.5 equiv), $Ca(NTf_2)_2$ (2.1 mg, 0.0036 mmol, 5 mol%), $n$$Bu_4NPF_6$ (1.4 mg, 0.0036 mmol, 5 mol%) and $Cu(OTf)_2$ (2.6 mg, 0.012 mmol, 10 mol%), 17 mg of **12** and 10 mg of **13** were obtained (49% and 35%, respectively) (HFIP, t_1 = 1.75 h at 20 °C, t_2 = 0.75 h at 20 °C).

Flash column chromatography using Pentane/EtOAc 9:1 then 8:2 as eluent.

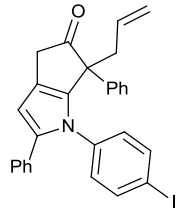


12: orange solid, 49%; mp = 65–69°C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.80 (dd, J = 5.7, 2.3 Hz, 1H), 7.44–7.38 (m, 4H), 7.35–7.28 (m, 5H), 7.25–7.21 (m, 3H), 6.64–6.49 (m, 3H), 5.46 (s, 1H), 4.83 (s, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 206.4, 157.5, 146.7, 146.2, 140.5, 137.9, 135.2, 132.2, 129.0, 129.0, 128.8, 127.6, 127.2, 127.0, 122.9, 108.6, 85.4, 80.0, 65.3. IR (neat) 3082, 3060, 3027, 2965, 1710, 1620, 1583, 1486, 1446, 1366, 1288, 1174, 1073 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{18}INNaO$ $[M+Na]^+$: 498.0325, found: 498.0325.



13: red solid, 35%; mp = 59–63°C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.69 (dd, J = 5.9, 2.3 Hz, 1H), 7.53–7.49 (m, 2H), 7.37–7.30 (m, 6H), 7.23–7.20 (m, 4H), 6.64 (dd, J = 5.9, 2.2 Hz, 1H), 6.32 (d, J = 8.8 Hz, 2H), 5.32 (s, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 203.4, 161.7, 145.5, 137.8, 136.4, 135.0, 132.0, 128.8, 128.5, 128.5, 128.1, 122.7, 116.3, 88.6, 86.3, 79.9, 67.0, 57.5, one carbon hidden. IR (neat) 3081, 3053, 2957, 2924, 1854, 1715, 1588, 1488, 1446, 1398, 1342, 1314, 1292, 1241, 1183, 1157 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{19}NNaO$ $[M+Na]^+$: 498.0325, found: 498.0318.

6-allyl-1-(4-iodophenyl)-2,6-diphenyl-4,6-dihydrocyclopenta[b]pyrrol-5(1H)-one (14)

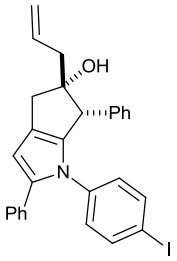


A solution of LDA (0.10 mL, 0.057 mmol, 1.1 equiv, 0.6M in THF) was added dropwise to a solution of **3aa** (25 mg, 0.053 mmol) in THF (1 mL) at −78 °C. After 1 h at 0 °C, allyl bromide (6.5 mg, 0.53 mmol, 1 equiv) was added dropwise at −78°C, and the reaction mixture was stirred at −78 °C for 2 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using Pentane/EtOAc 97.5:2.5 as eluent to give **14** (15 mg, 55%).

14: yellow solid, 55%.; mp = 59−64 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.45–7.27 (m, 5H), 7.24–7.08 (m, 7H), 6.52–6.38 (m, 3H), 5.34–5.13 (m, 1H), 4.87 (dd, J = 10.2, 1.5 Hz, 1H), 4.78 (dd, J = 16.9, 1.4 Hz, 1H), 3.53 (d, J = 21.5 Hz, 1H), 3.27 (d, J = 21.5 Hz, 1H), 3.15 (dd, J = 13.5, 7.6 Hz, 1H), 2.15 (dd, J = 13.4, 6.6 Hz, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 215.5, 141.9, 139.0, 138.8, 138.0, 137.4, 133.2, 132.6, 129.3, 129.0, 128.4, 128.3, 127.5, 126.8, 126.7,

121.6, 118.8, 106.0, 92.5, 60.8, 39.0, 37.9. IR (neat) 3064, 2924, 2854, 1753, 1681, 1639, 1600, 1488, 1443, 1261, 1058 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{28}H_{22}NNaO$ [*M*+Na]$^+$: 538.0638, found: 538.0624.

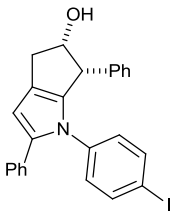
5-allyl-1-(4-iodophenyl)-2,6-diphenyl-1,4,5,6-tetrahydrocyclopenta[*b*]pyrrol-5-ol (15)



A solution of allylmagnesium bromide (70 µL, 1 M in THF) was added slowly to a solution of **3aa** (22 mg, 0.046 mmol) in THF (0.25 mL) at 0 °C. The cold bath was then removed and the reaction mixture was stirred at room temperature for 1 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using Pentane/EtOAc 9:1 as eluent to give **15** (20 mg, 84%).

15: yellow solid, 84%; mp = 44–48 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.6 Hz, 2H), 7.26–7.03 (m, 8H), 6.93 (dd, *J* = 7.6, 1.6 Hz, 2H), 6.52 (d, *J* = 8.6 Hz, 2H), 6.31 (s, 1H), 6.10–5.88 (m, 1H), 5.24–5.09 (m, 2H), 4.09 (s, 1H), 3.00 (d, *J* = 15.1 Hz, 1H), 2.80 (d, *J* = 15.0 Hz, 1H), 2.62 (d, *J* = 7.2 Hz, 2H), OH unobserved; ^{13}C NMR (91 MHz, $CDCl_3$) δ 139.1, 138.8, 138.1, 137.8, 137.2, 134.3, 133.1, 129.2, 128.8, 128.3, 128.3, 128.0, 127.5, 126.3, 124.8, 118.6, 106.4, 91.3, 86.7, 55.0, 46.6, 40.0. IR (neat) 3535, 3062, 3025, 2924, 2852, 1638, 1600, 1489, 1458, 1388, 1355, 1265, 1179, 1073 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{28}H_{24}NNaO$ [*M*+Na]$^+$: 540.0795, found: 540.0781.

1-(4-iodophenyl)-2,6-diphenyl-1,4,5,6-tetrahydrocyclopenta[b]pyrrol-5-ol (16)

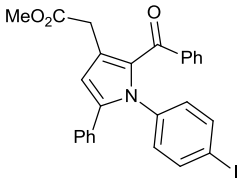


To a solution of **3aa** (22 mg, 0.046 mmol, 1 equiv) in a mixture MeOH/THF (1 mL, 1:1) at 0 °C was added $NaBH_4$ (2 mg, 0.051 mmol, 1.1 equiv). The reaction mixture was stirred at 0 °C for 1 h. The reaction was then quenched with saturated NH_4Cl aqueous solution and extracted with AcOEt. The combined organic layers were

washed with brine, dried over MgSO4 and filtered. The solvent was removed by rotary evaporation to give **16** (21 mg, 98%).

16: orange solid, 98%; mp = 55–59 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.41 (d, J = 8.6 Hz, 2H), 7.34–7.24 (m, 3H), 7.22–7.08 (m, 5H), 7.01–6.94 (m, 2H), 6.54 (d, J = 8.6 Hz, 2H), 6.34 (s, 1H), 5.13–4.93 (m, 1H), 4.24 (d, J = 7.4 Hz, 1H), 3.17 (dd, J = 14.4, 7.2 Hz, 1H), 2.62 (dd, J = 14.4, 7.5 Hz, 1H), OH unobserved; ^{13}C NMR (91 MHz, $CDCl_3$) δ 139.2, 138.8, 137.96, 137.4, 137.2, 133.0, 129.1, 129.0, 128.4, 128.2, 128.1, 127.7, 126.4, 124.2, 106.4, 91.5, 78.6, 50.1, 34.6. IR (neat) 3400, 3060, 3027, 2963, 2921, 2852, 1510, 1489, 1390, 1355, 1261, 1172, 1076 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{20}INNaO$ $[M+Na]^+$: 500.0482, found: 500.0451.

Methyl 2-(2-benzoyl-1-(4-iodophenyl)-5-phenyl-1H-pyrrol-3-yl)acetate (17)

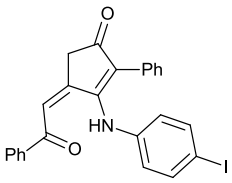


To a solution of **3aa** (20 mg, 0.042 mmol, 1 equiv) in 0.2 mL of DMF was added NaH (2.5 mg, 0.063 mmol, 1.5 equiv) at 0 °C (open flask). After 1 h at 20 °C, the reaction was quenched with saturated NH_4Cl aqueous solution and extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was engaged in the next step without further purification.

To a solution of the latter compound in a mixture MeOH/DCM (2.5 mL, 1:4) was added a solution of (trimethylsilyl)diazomethane (40 µL, 2 M in hexanes, 2 equiv) at 0 °C under argon. After 10 min, the reaction was quenched with water and extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using Pentane/EtOAc 85:15 as eluent to give **17** (12 mg, 54% over two steps).

17: yellow solid, 54%; mp = 33–38 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.78–7.63 (m, 2H), 7.55–7.44 (m, 3H), 7.36 (t, J = 7.6 Hz, 2H), 7.25–7.16 (m, 3H), 7.09 (dd, J = 6.5, 3.0 Hz, 2H), 6.84 (d, J = 8.5 Hz, 2H), 6.44 (s, 1H), 3.63 (s, 3H), 3.44 (s, 2H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 187.7, 171.6, 139.6, 139.5, 138.6, 137.8, 132.5, 131.9, 131.3, 129.9, 129.2, 128.9, 128.4, 128.2, 127.7, 124.6, 112.8, 92.9, 52.0, 33.0. IR (neat) 3061, 3031, 2951, 2923, 2853, 1739, 1633, 1597, 1487, 1451, 1370, 1345, 1263, 1220, 1195, 1173 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{26}H_{20}INNaO_3$ $[M+Na]^+$: 544.0380, found: 544.0395.

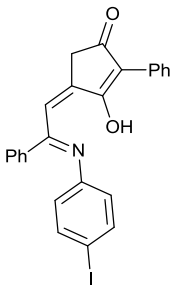
(*Z*)-3-((4-iodophenyl)amino)-4-(2-oxo-2-phenylethylidene)-2-phenylcyclopent-2-enone (18)



To a solution of **3aa** (20 mg, 0.042 mmol, 1 equiv) in 0.2 mL of DMF was added K_2CO_3 (8.7 mg, 0.063 mmol, 1.5 equiv) at 20 °C (open flask). After 0.5 h, the reaction was quenched with saturated NH_4Cl aqueous solution and extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using Pentane/EtOAc 7:3 as eluent to give **18** (12 mg, 60%).

18: red solid, 60%; mp = 79–82 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.45 (d, J = 8.7 Hz, 2H), 7.27–7.14 (m, 8H), 7.10–7.03 (m, 2H), 6.76 (d, J = 8.6 Hz, 2H), 6.50 (s, 1H), 3.60 (d, J = 0.7 Hz, 2H), 3.22 (s, 1H); ^{13}C NMR (91 MHz, $CDCl_3$) δ 196.8, 191.9, 156.1, 153.1, 138.4, 137.7, 136.8, 134.1, 131.3, 129.1, 129.0, 129.0, 127.6, 123.5, 123.1, 119.2, 86.9, 43.1, one carbon hidden. IR (neat) 3053, 3025, 2952, 2925, 2851, 1680, 1644, 1597, 1577, 1566, 1545, 1487, 1445, 1362, 1255, 1232, 1181 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{18}INNaO_2$ $[M+Na]^+$: 514.0274, found: 514.0272.

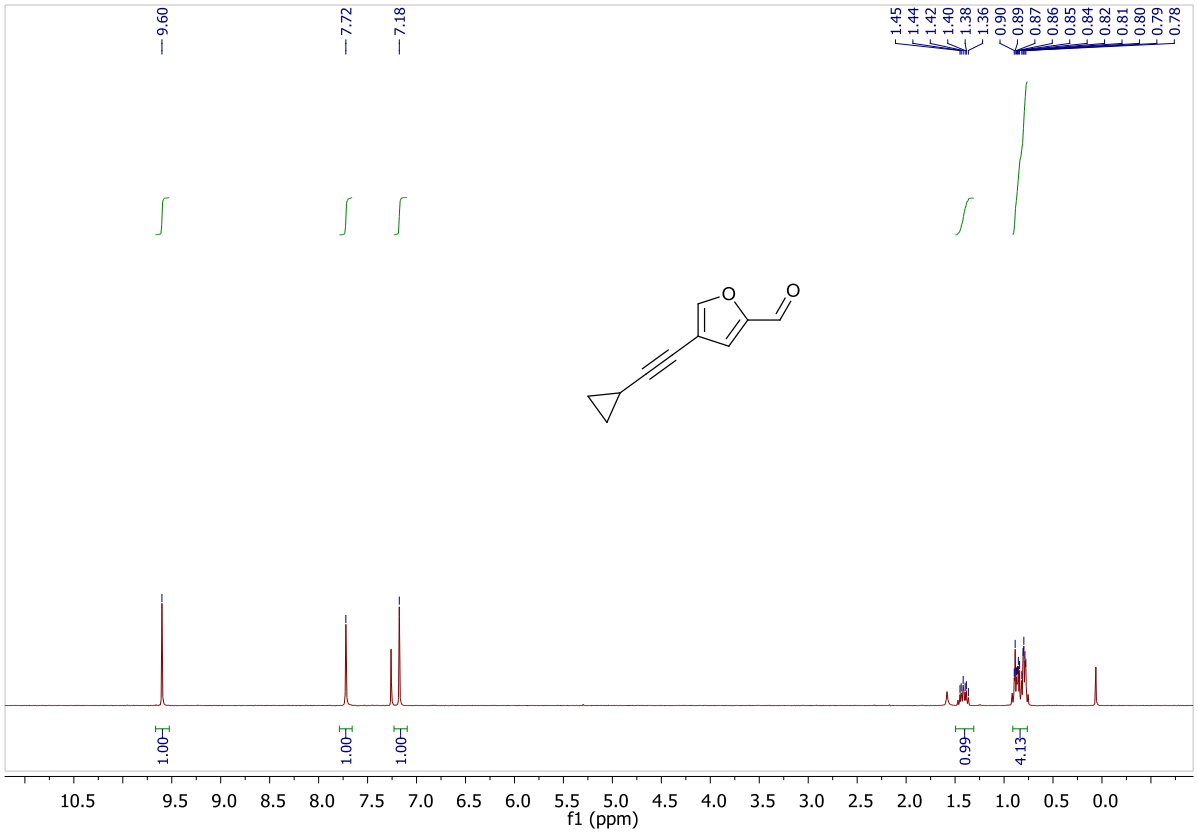
(*Z*)-3-hydroxy-4-((Z)-2-((4-iodophenyl)imino)-2-phenylethylidene)-2-phenylcyclopent-2-en-1-one (19)



To a solution of **3aa** (23 mg, 0.048 mmol, 1 equiv) in 1 mL of DCM was added MCPBA (28 mg, 0.12 mmol, 2.5 equiv) at 0 °C. After 20 min at 20 °C, the reaction was quenched with saturated $NaHCO_3$ aqueous solution and extracted with DCM. The combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. The crude product was purified by flash column chromatography using Pentane/EtOAc 55:45 as eluent to give **19** (15 mg, 63%).

19: red solid, 61%; mp = 64-69 °C. ^{1}H NMR (300 MHz, C_6D_6) δ 16.90 (s, 1H), 8.88 (dd, J = 8.4, 1.3 Hz, 2H), 7.45–7.35 (m, 2H), 7.20–7.11 (m, 3H), 6.89–6.75 (m, 3H), 6.71–6.62 (m, 2H), 6.19 (d, J = 8.7 Hz, 2H), 5.59 (s, 1H), 2.84 (d, J = 1.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 174.9, 168.3, 149.4, 144.1, 138.4, 135.9, 131.4, 130.7, 129.2, 128.7, 128.2, 128.1, 127.9, 125.0, 124.5, 123.6, 91.2, 42.0. IR (neat) 3240, 3055, 3026, 2963, 2223, 2853,

1678, 1640, 1621, 1583, 1535, 1481, 1443, 1368, 1304, 1262, 1178 cm^{-1}. HRMS-ESI: *m/z* calculated for $C_{25}H_{18}INNaO_2$ $[M+Na]^+$: 514.0274, found: 514.0248.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0.86
0.85
0.84
0.82
0.81
0.80
0.79
0.78
O
O
1.00
1.00
1.00
0.99
4.13
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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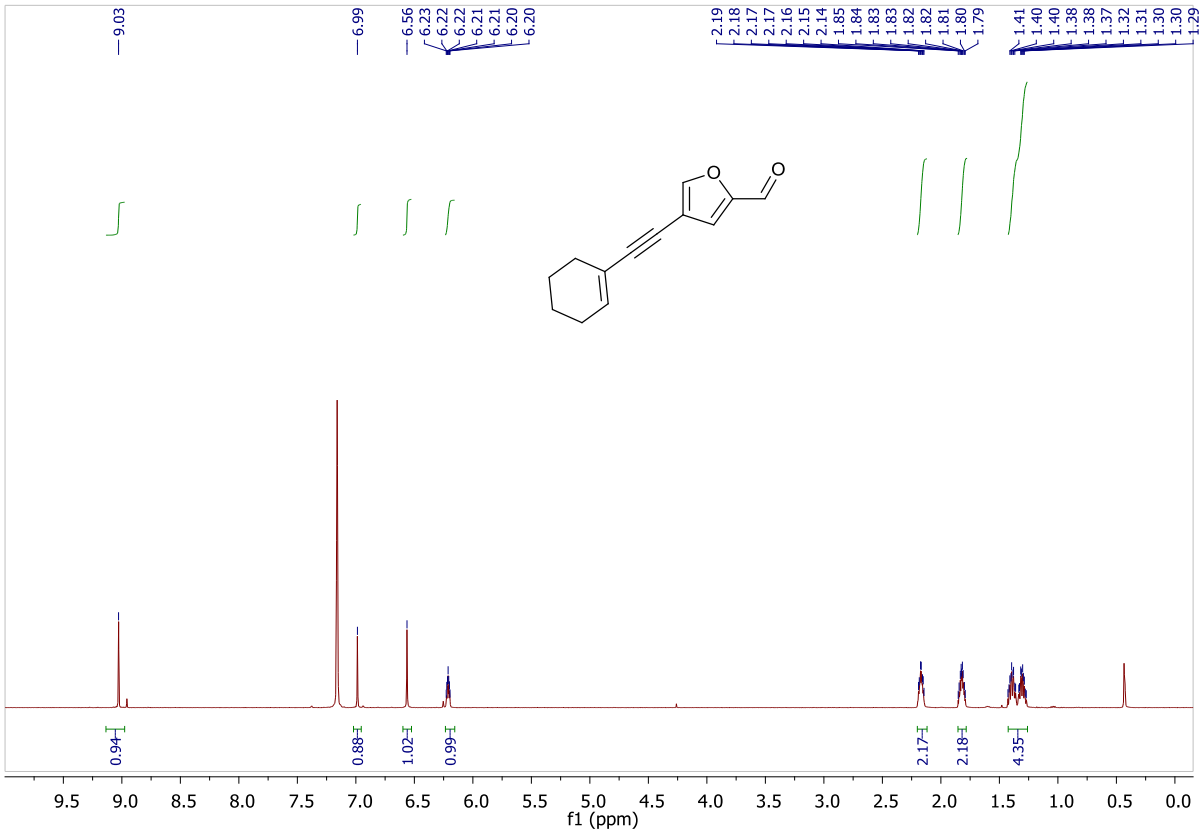
f1 (ppm)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2.17
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2.15
2.14
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1.83
1.83
1.82
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1.30
1.29
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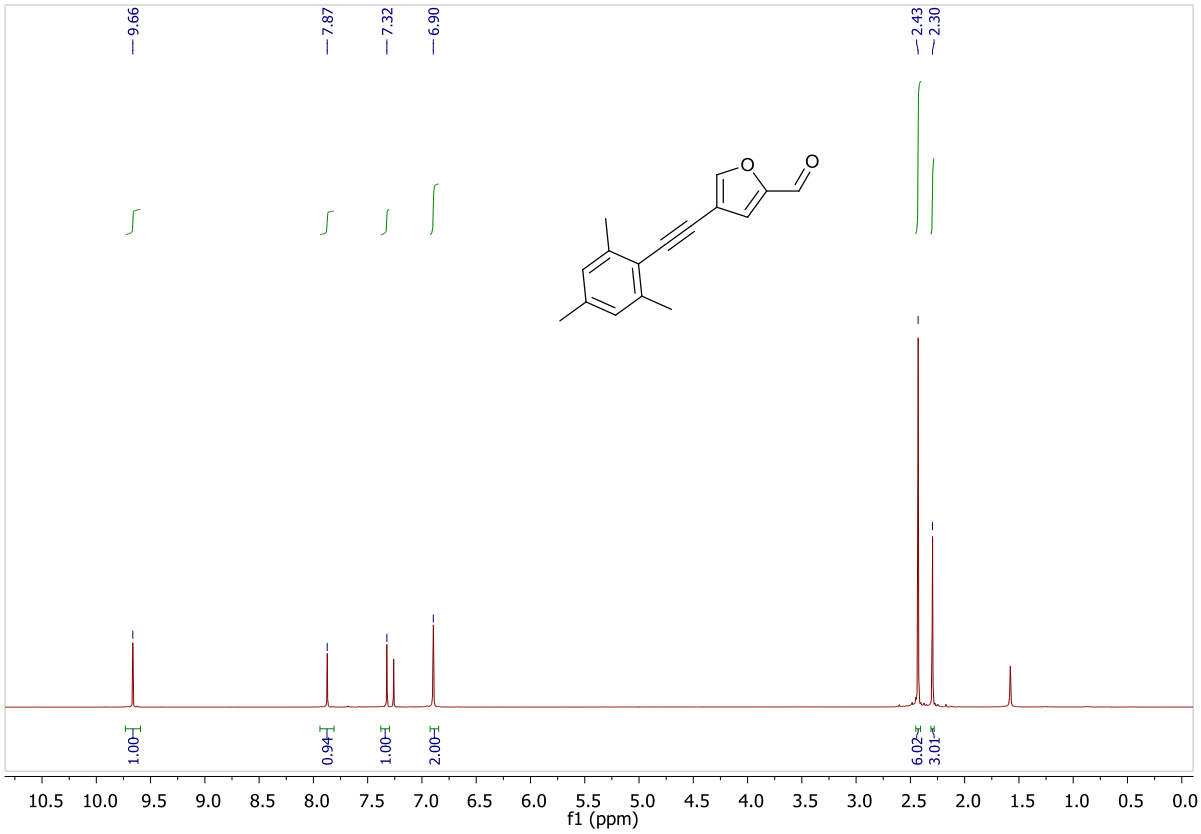
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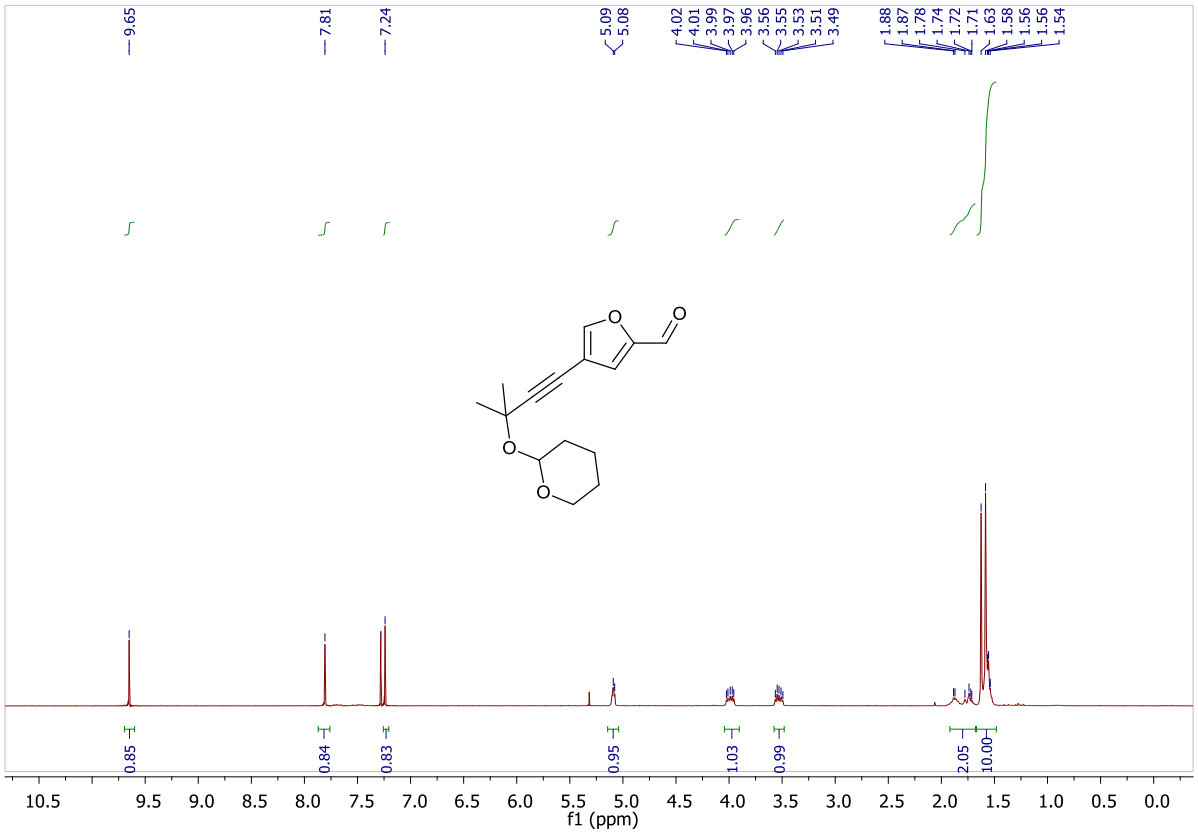
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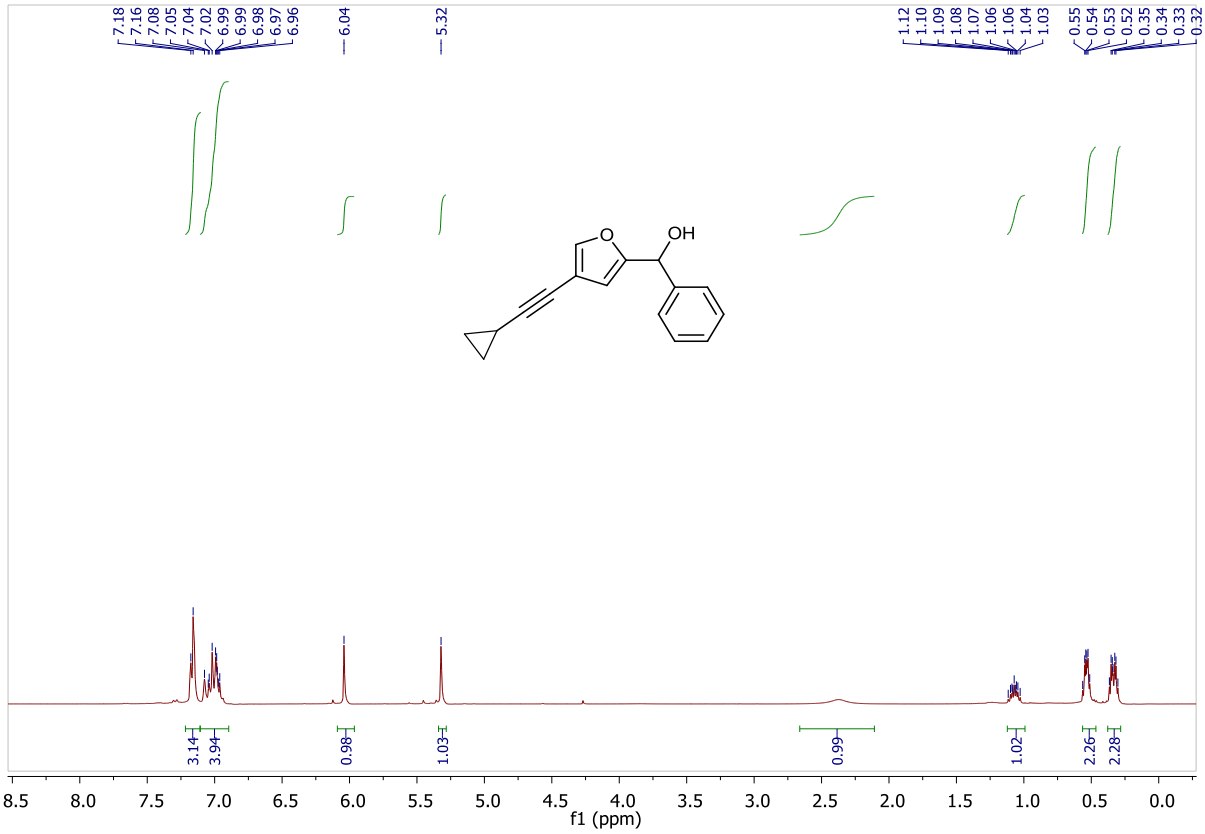
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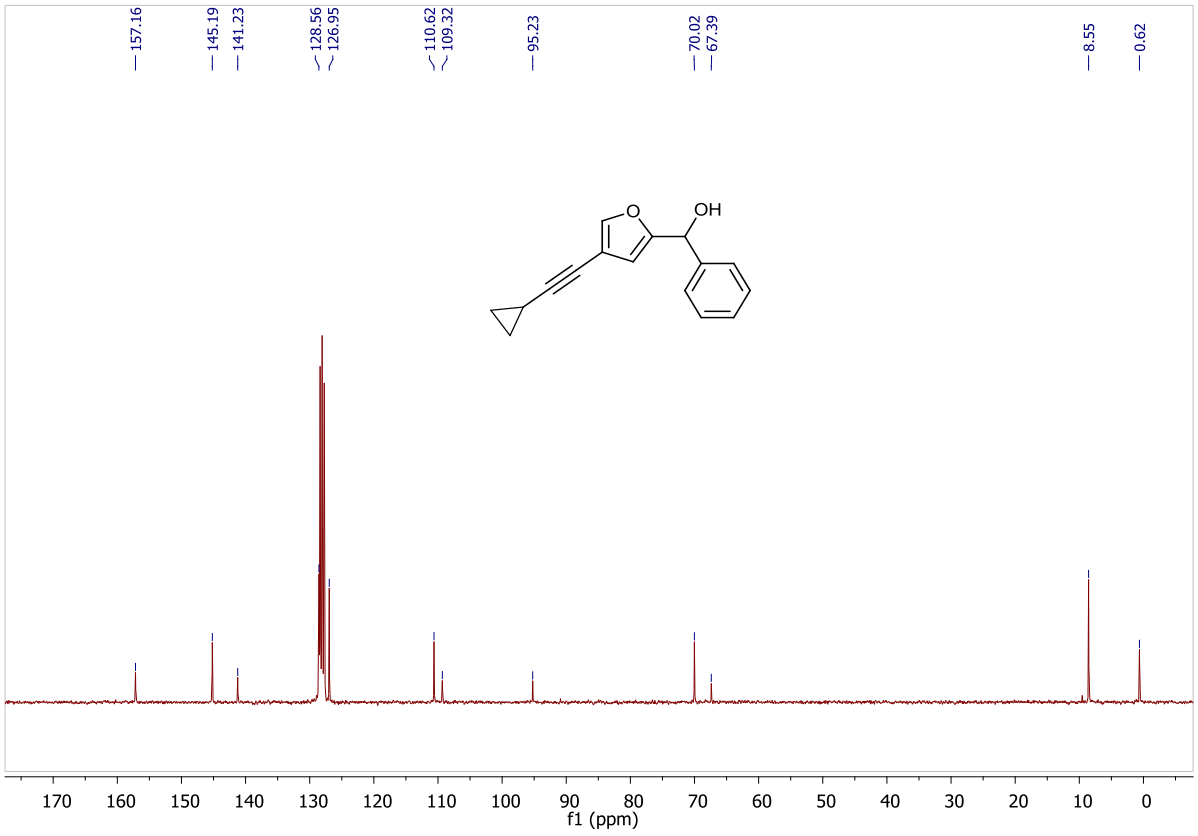
f1 (ppm)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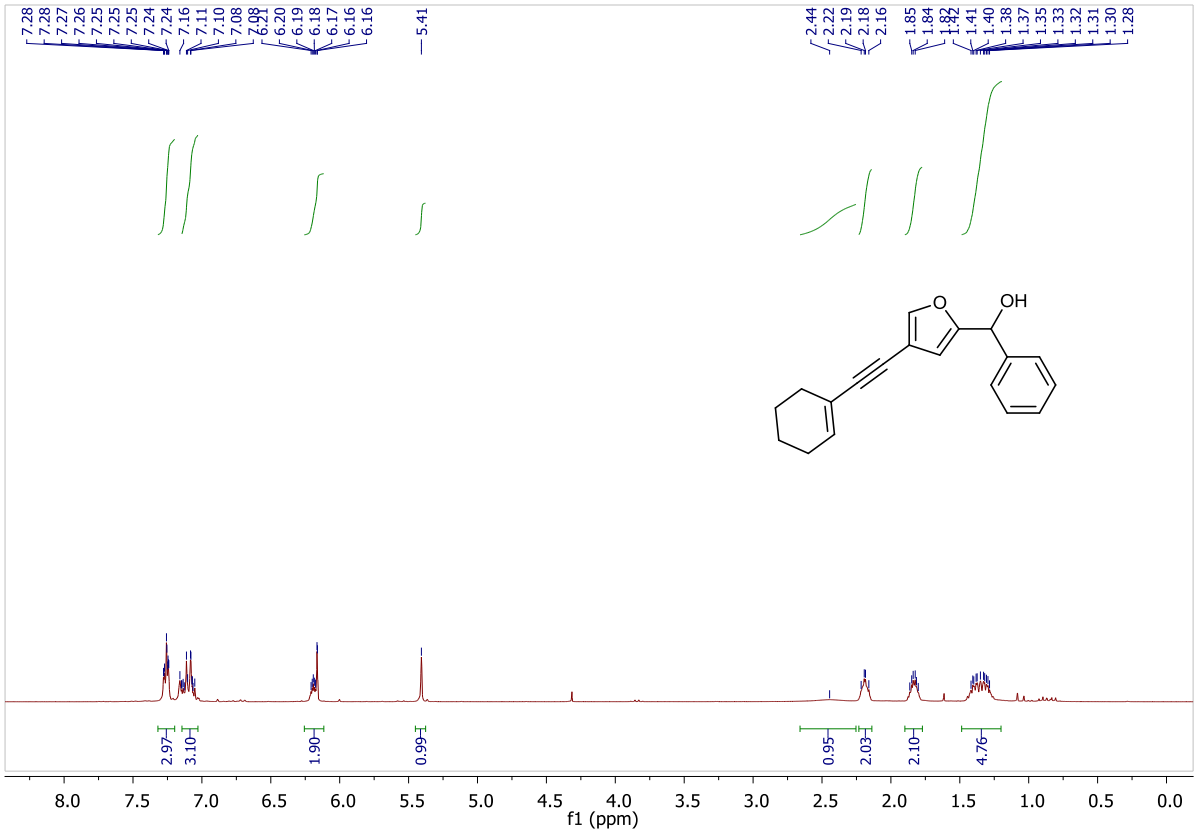
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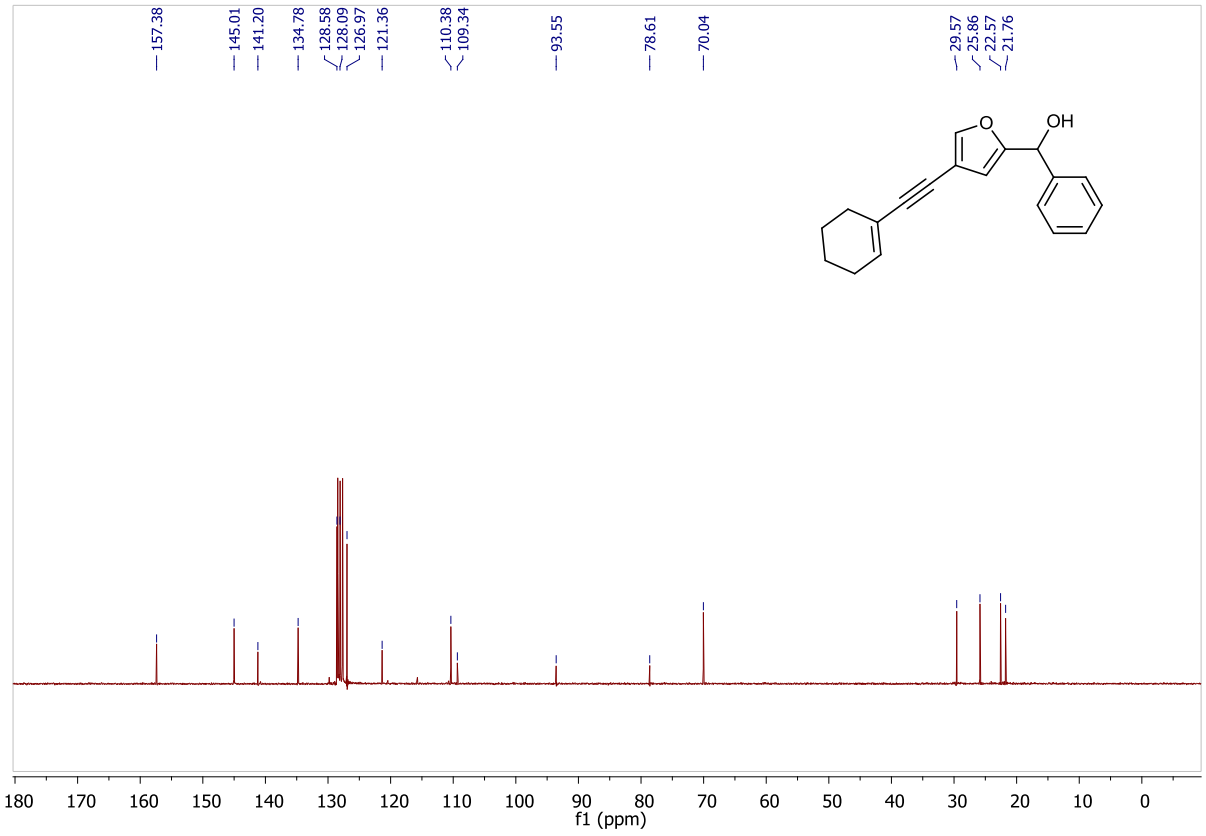
f1 (ppm)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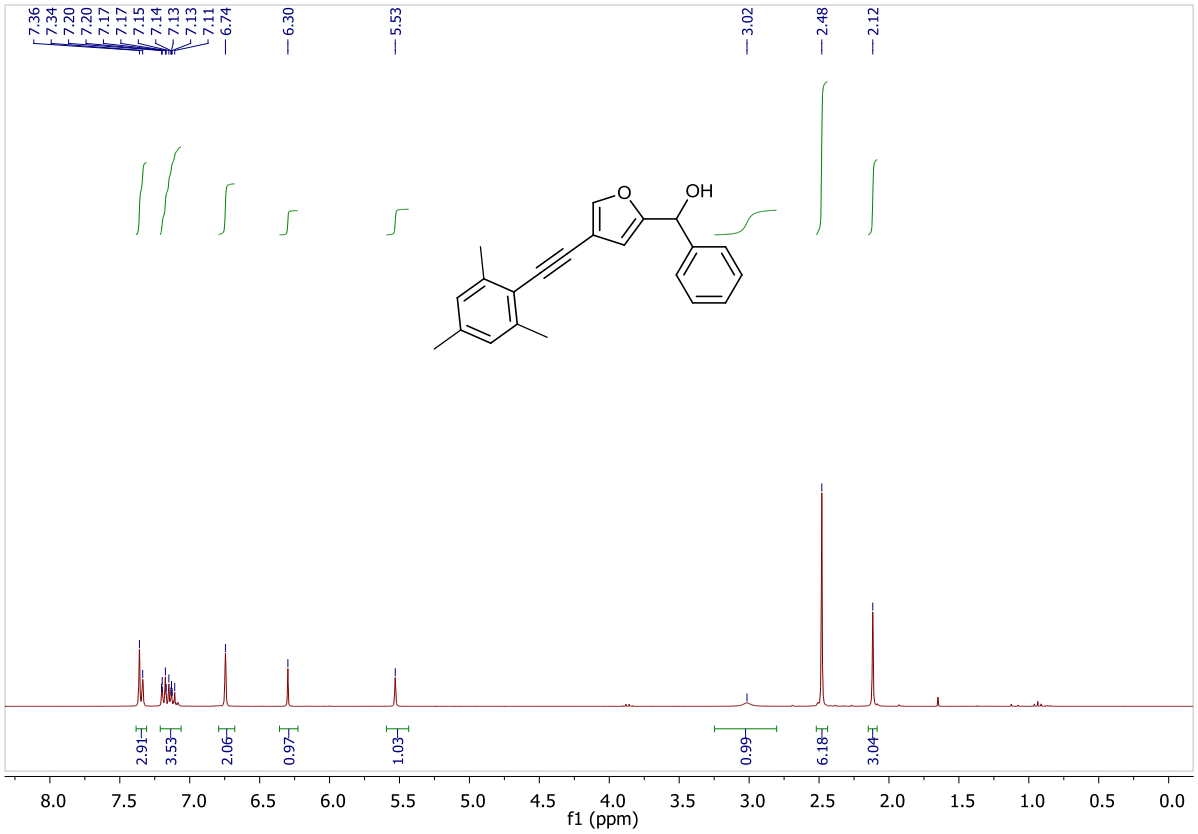
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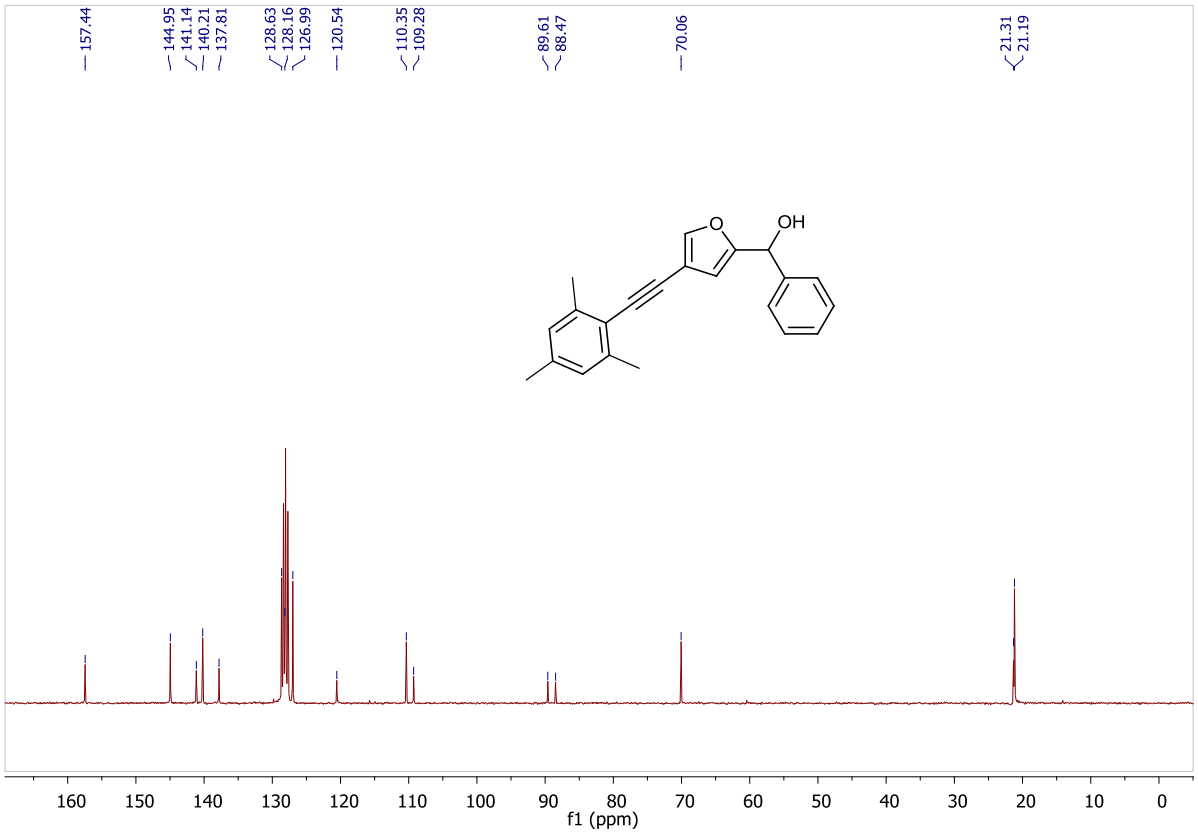
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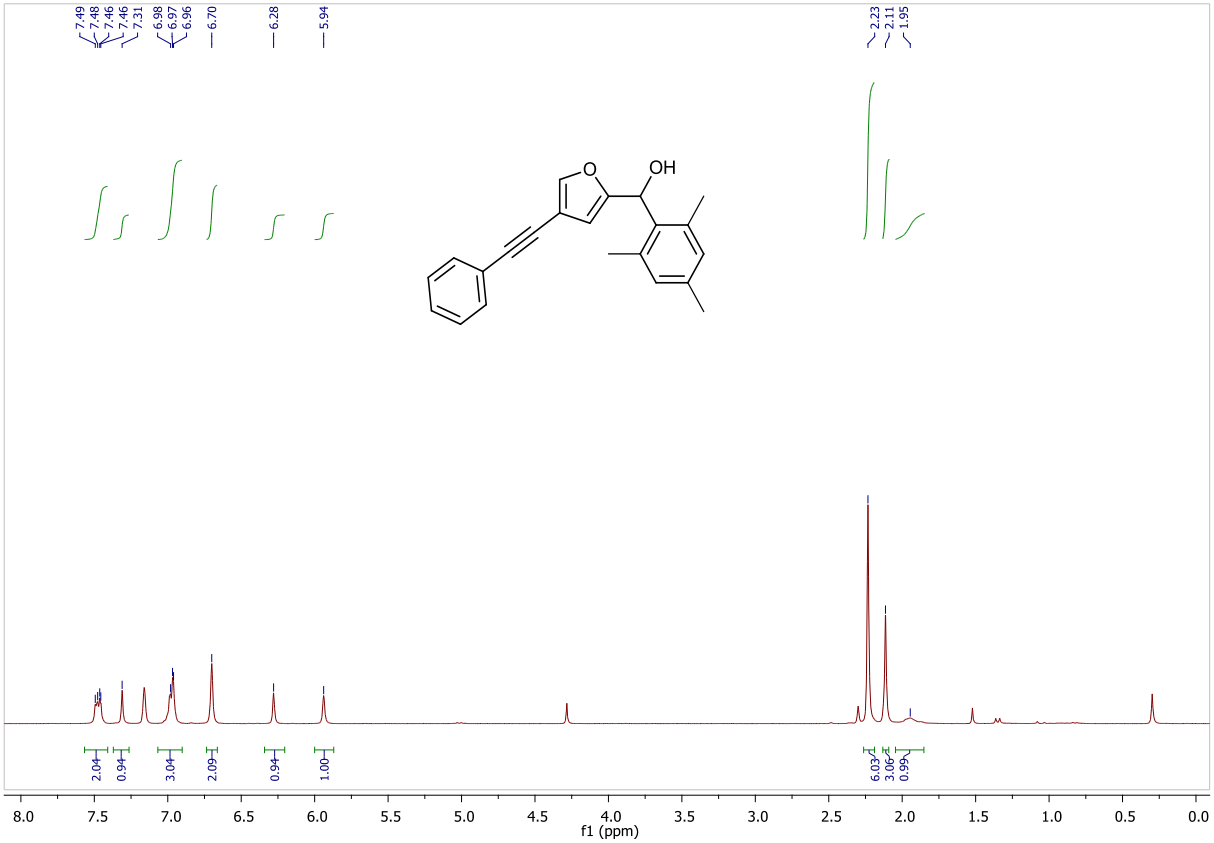
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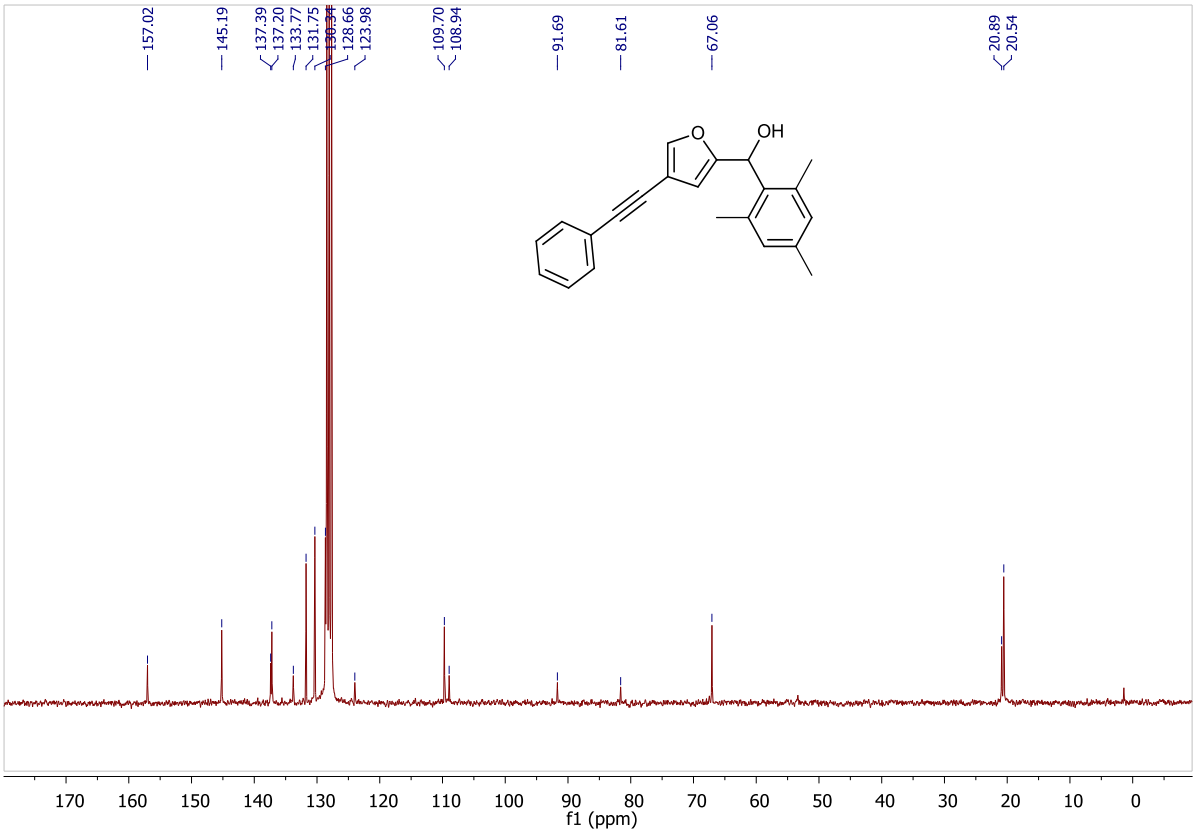
f1 (ppm)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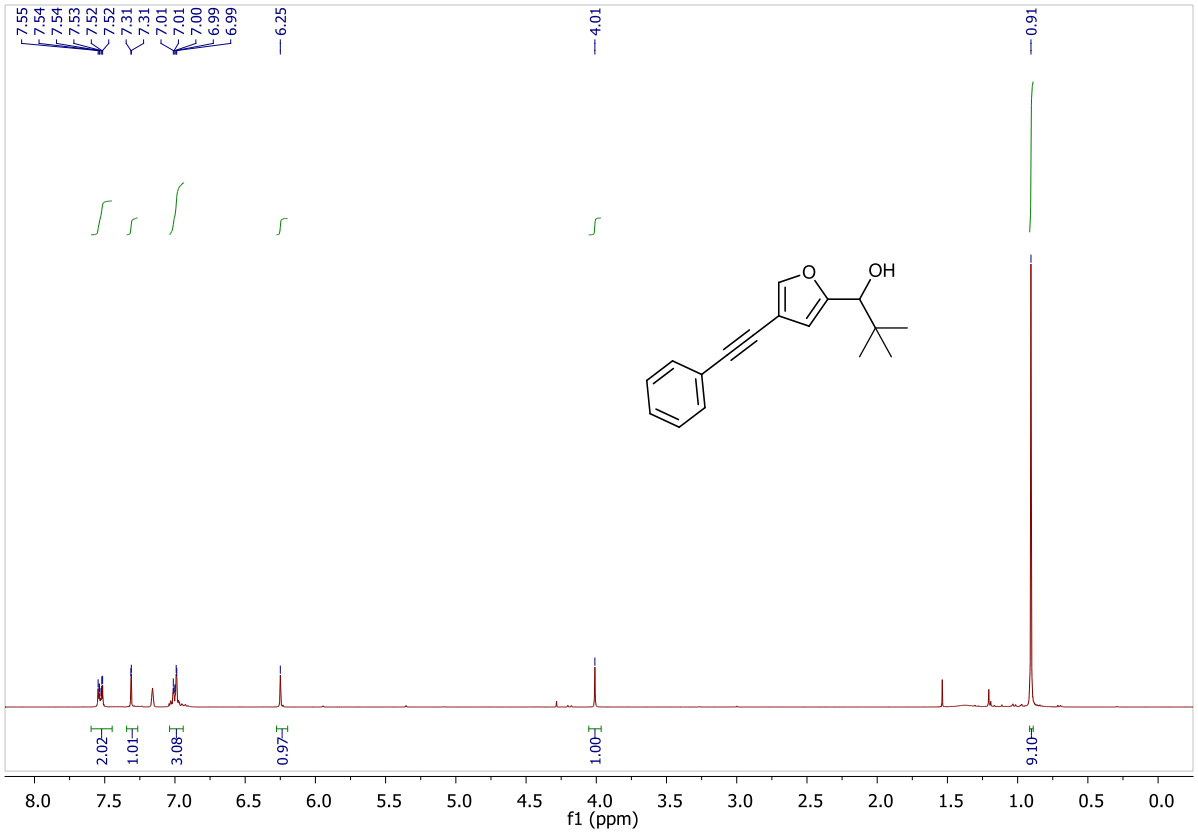
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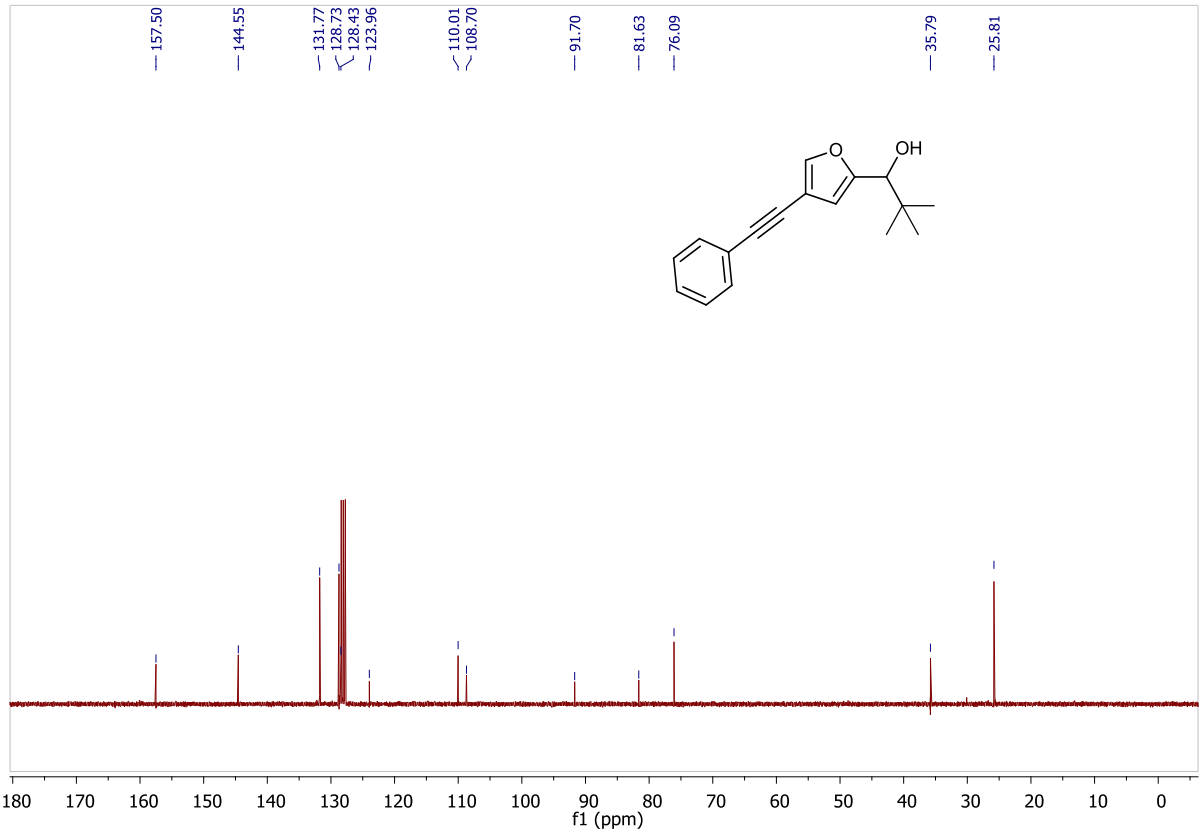
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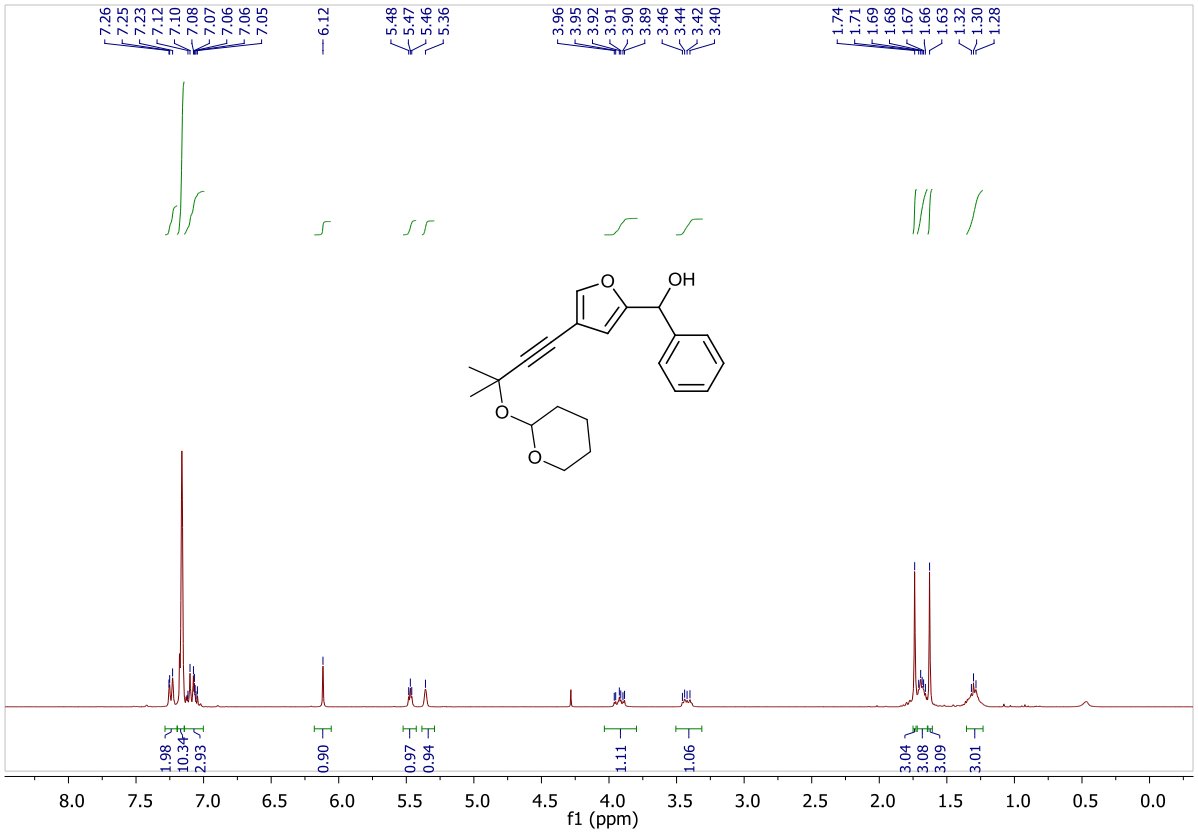
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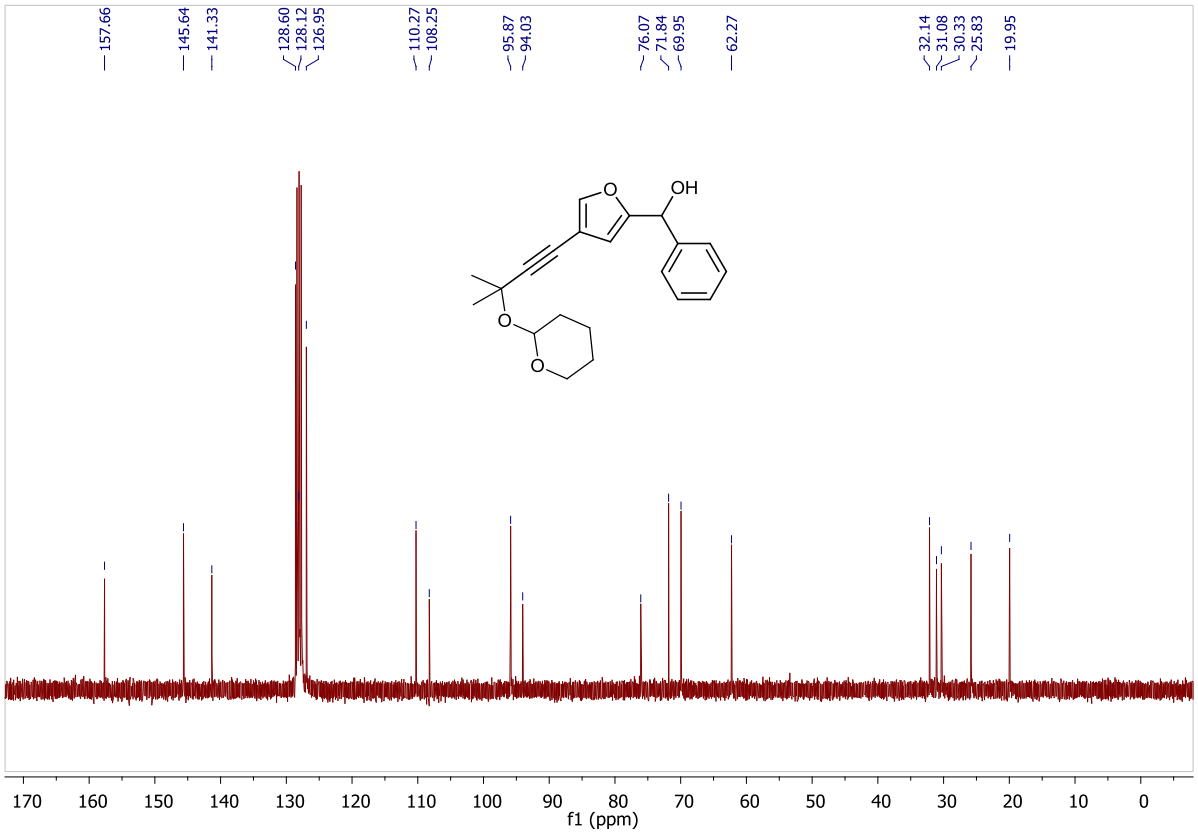
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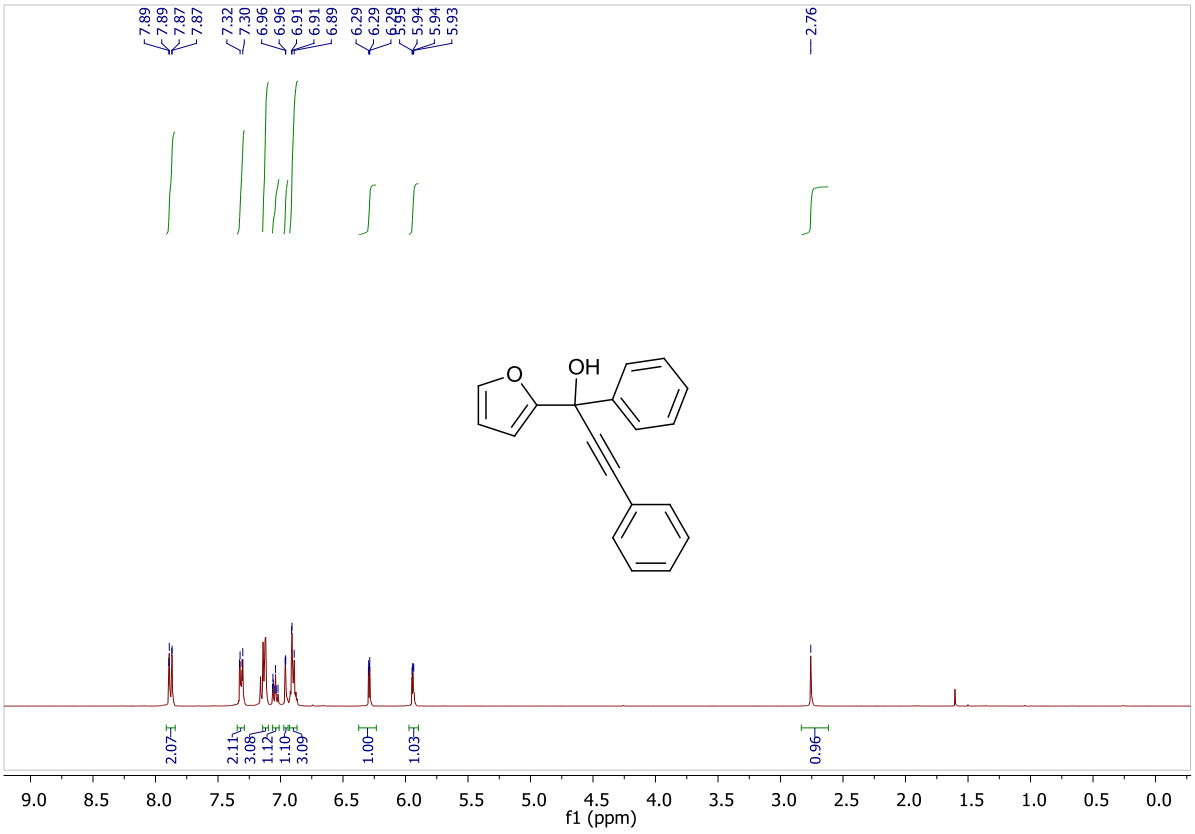
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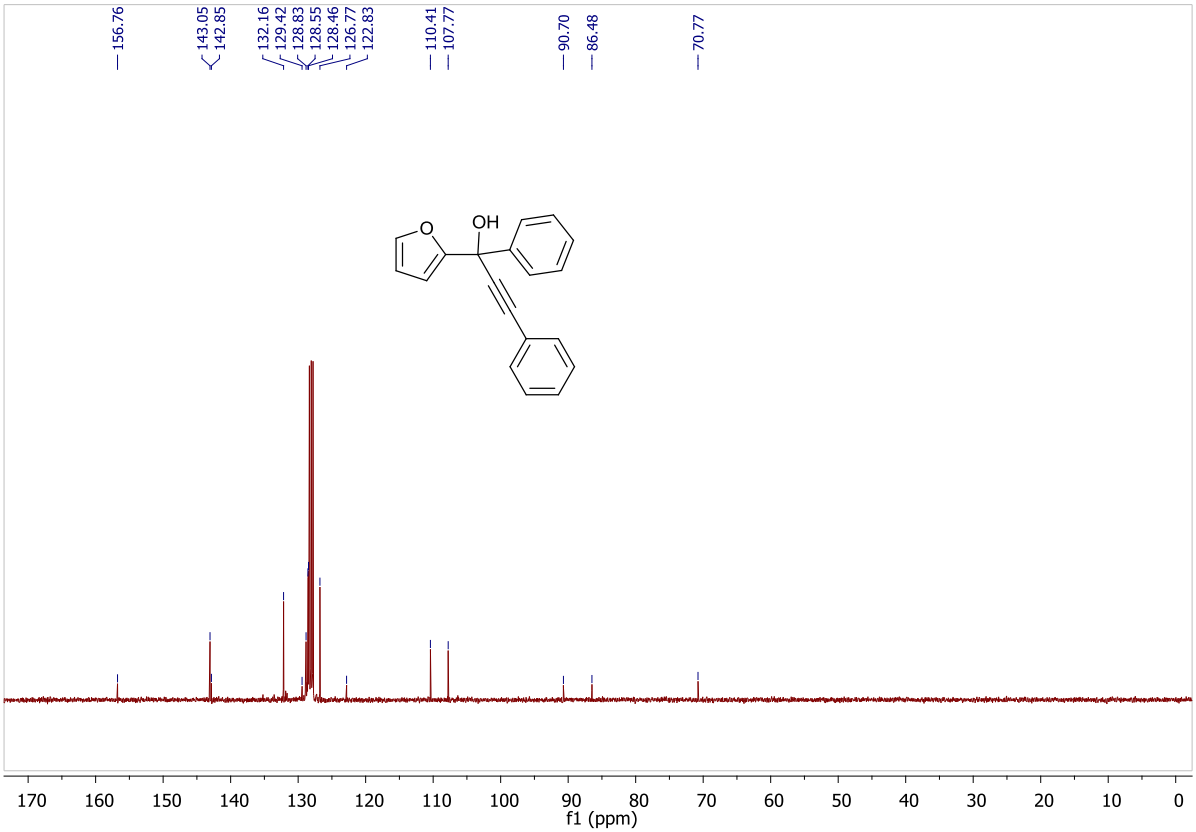
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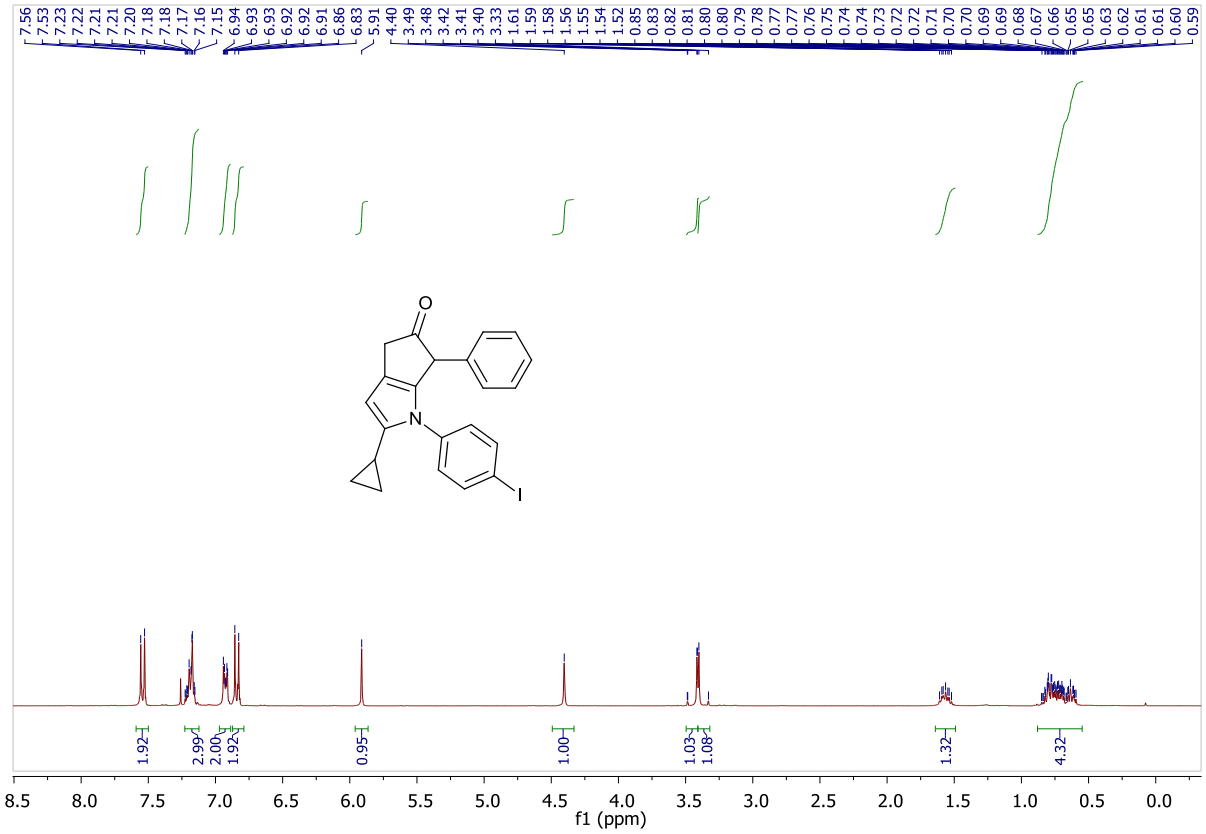
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O
N
I
1.92 2.99 2.00 1.92 0.95 1.00 1.03 1.08 1.32 4.32
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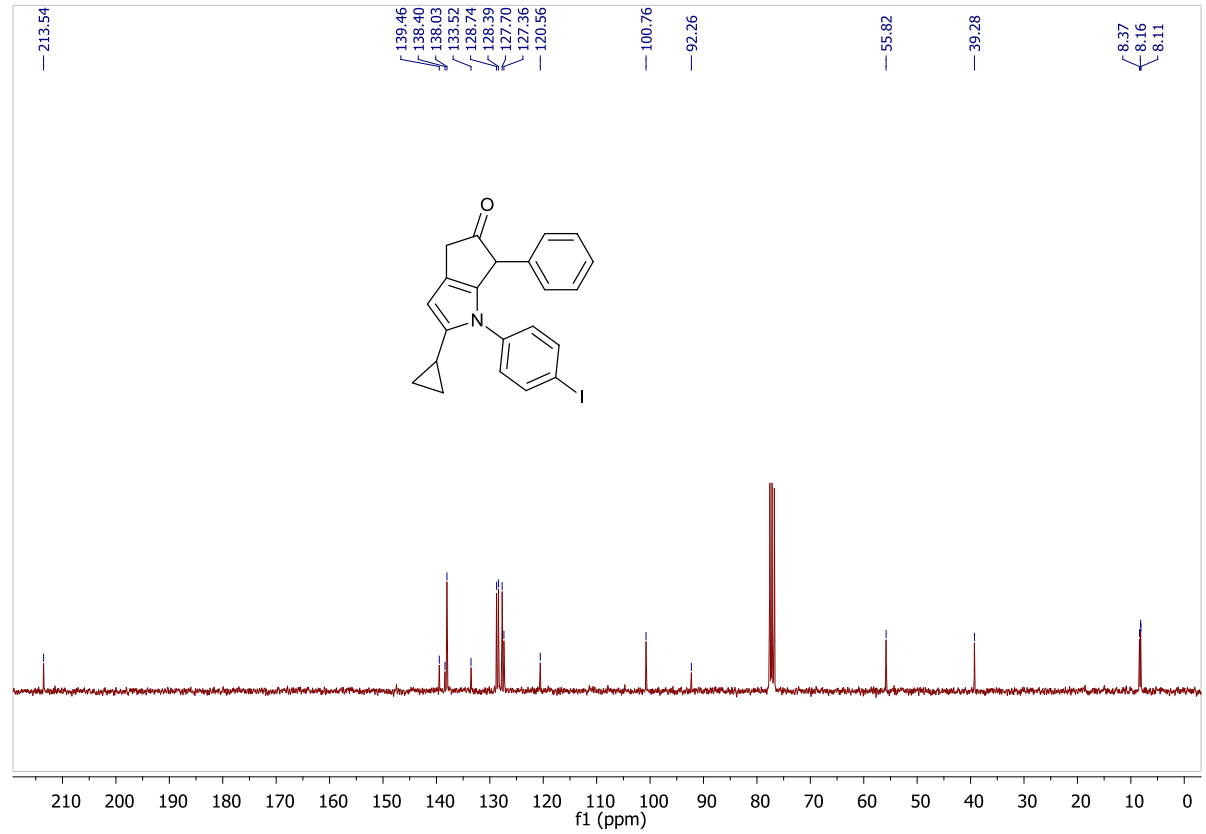
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N
I
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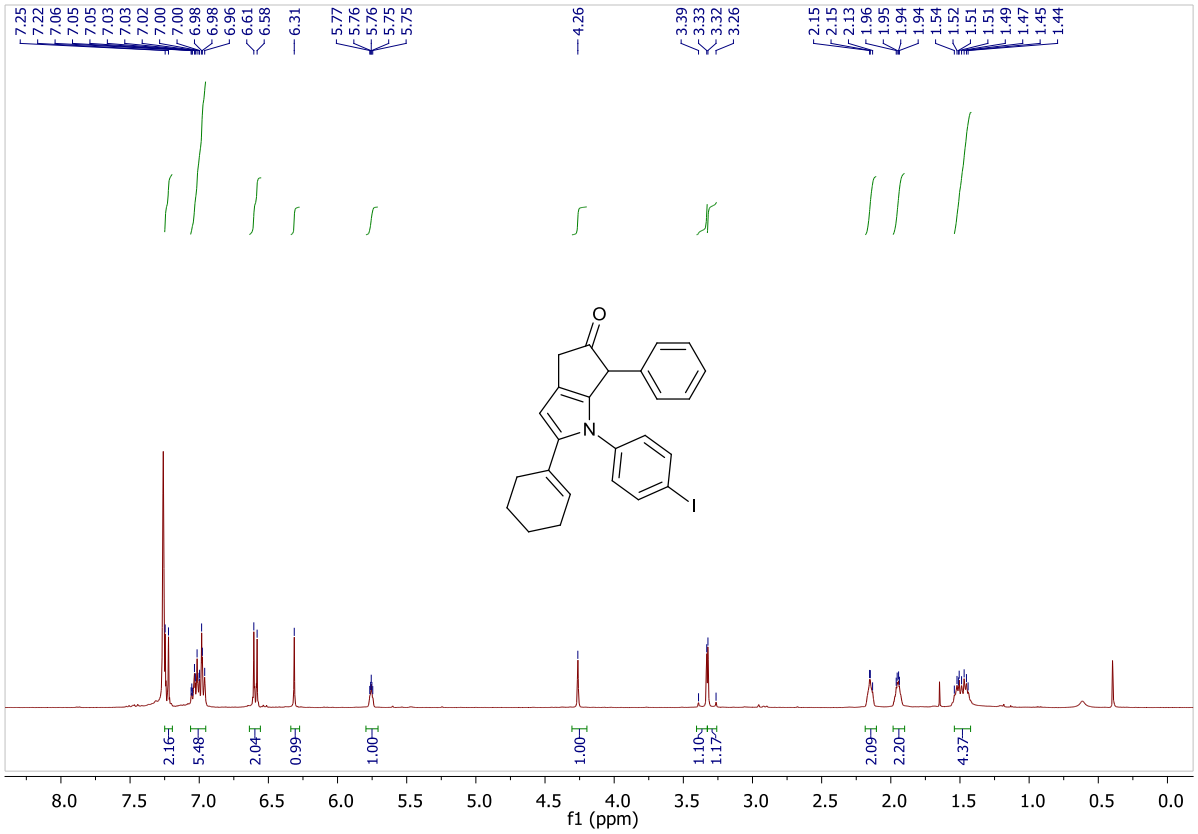
f1 (ppm)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6.31
5.77
5.76
5.76
5.75
5.75
4.26
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3.33
3.32
3.26
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2.15
2.13
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1.95
1.94
1.94
1.54
1.52
1.51
1.51
1.49
1.47
1.45
1.44
O
N
I
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1.00
1.00
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1.17
2.09
2.20
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7.0
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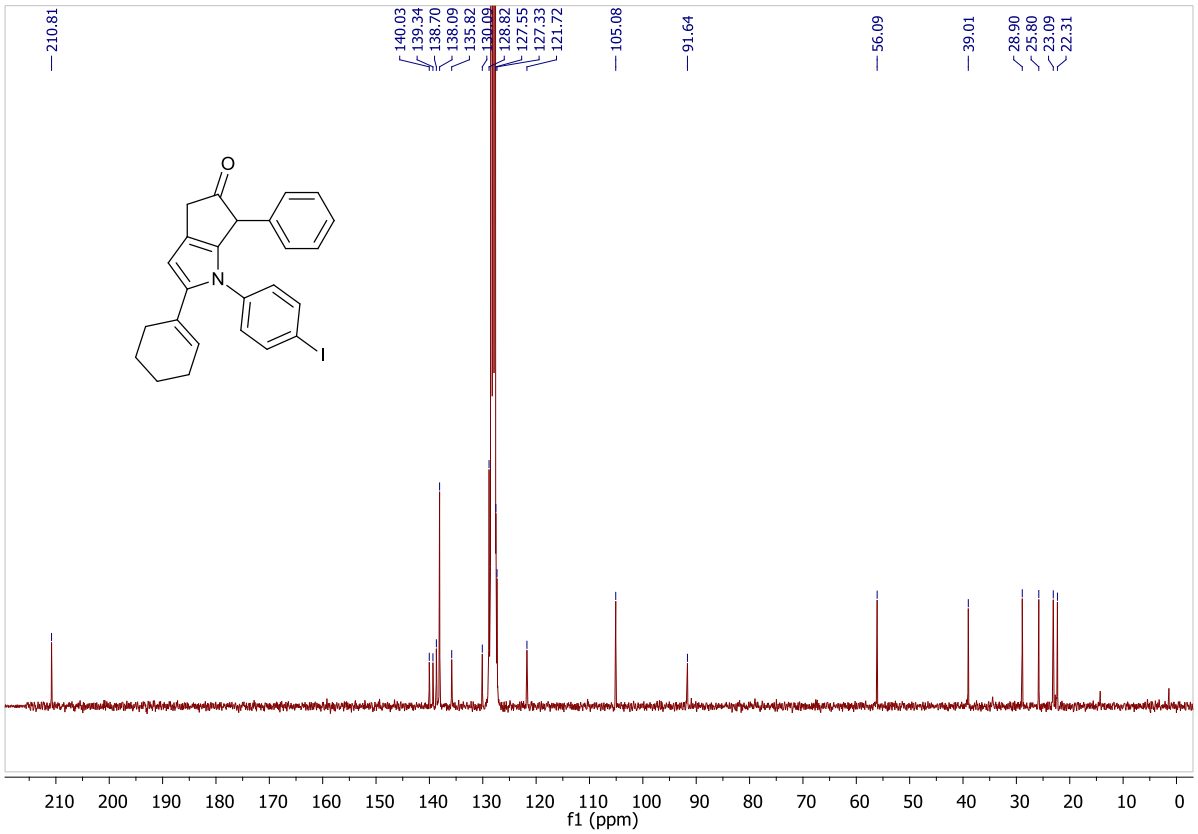
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91.64
56.09
39.01
28.90
25.80
23.09
22.31
O
N
I
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190
180
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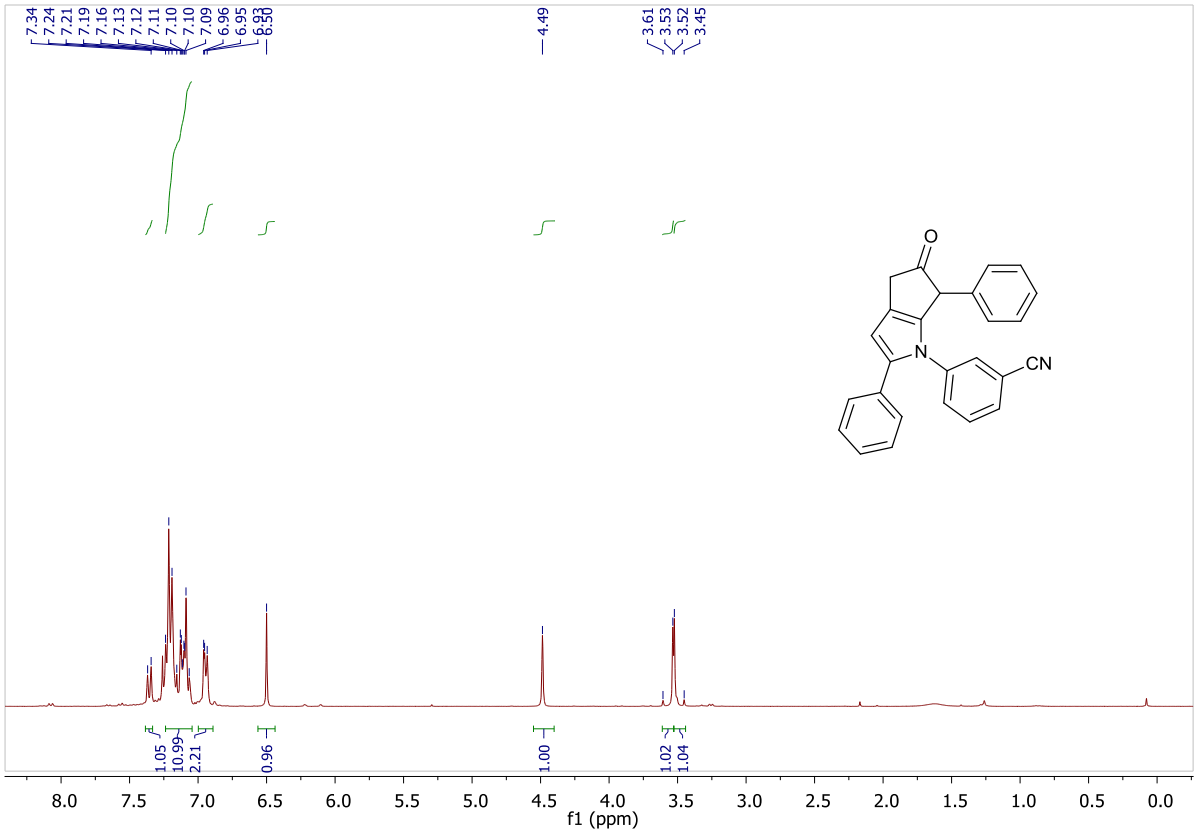
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6.95
6.93
6.90
4.49
3.61
3.53
3.52
3.45
O
N
CN
1.05
10.99
2.21
0.96
1.00
1.02
1.04
8.0
7.5
7.0
6.5
6.0
5.5
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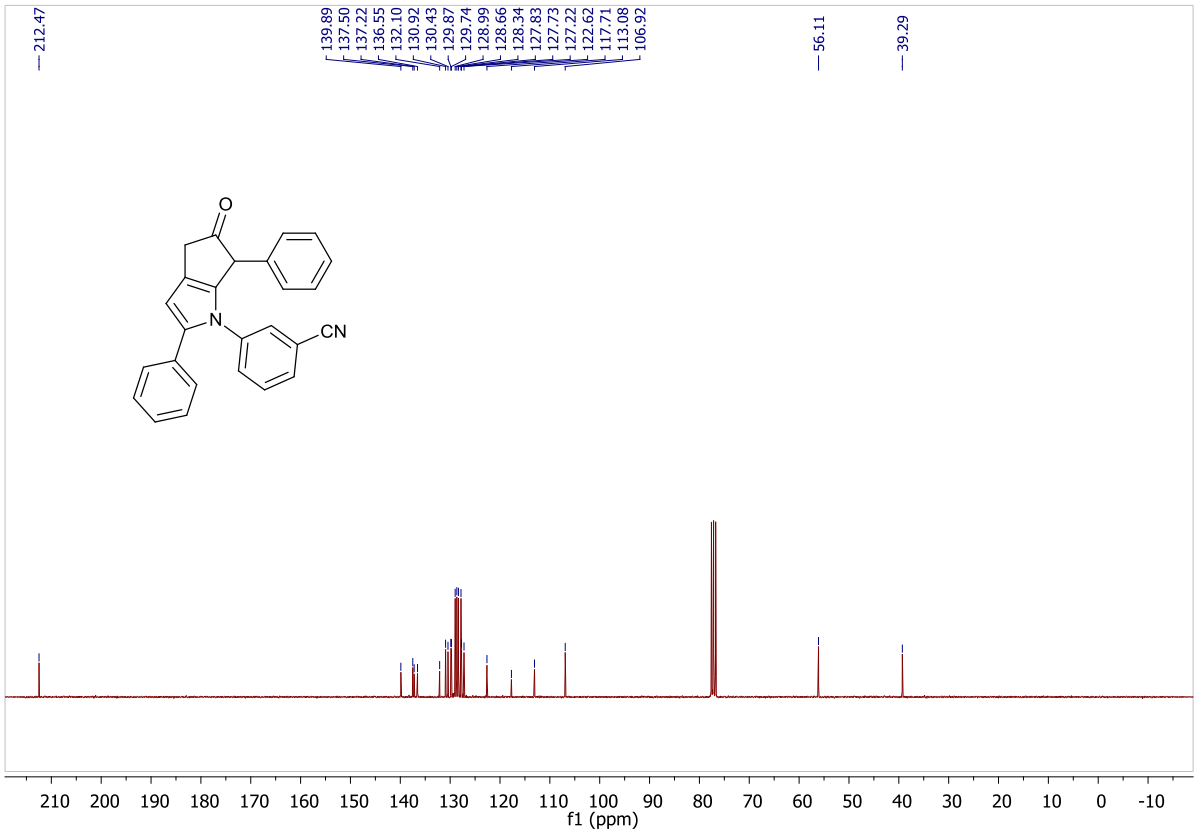
0.0
f1 (ppm)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127.73
127.22
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117.71
113.08
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CN
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180
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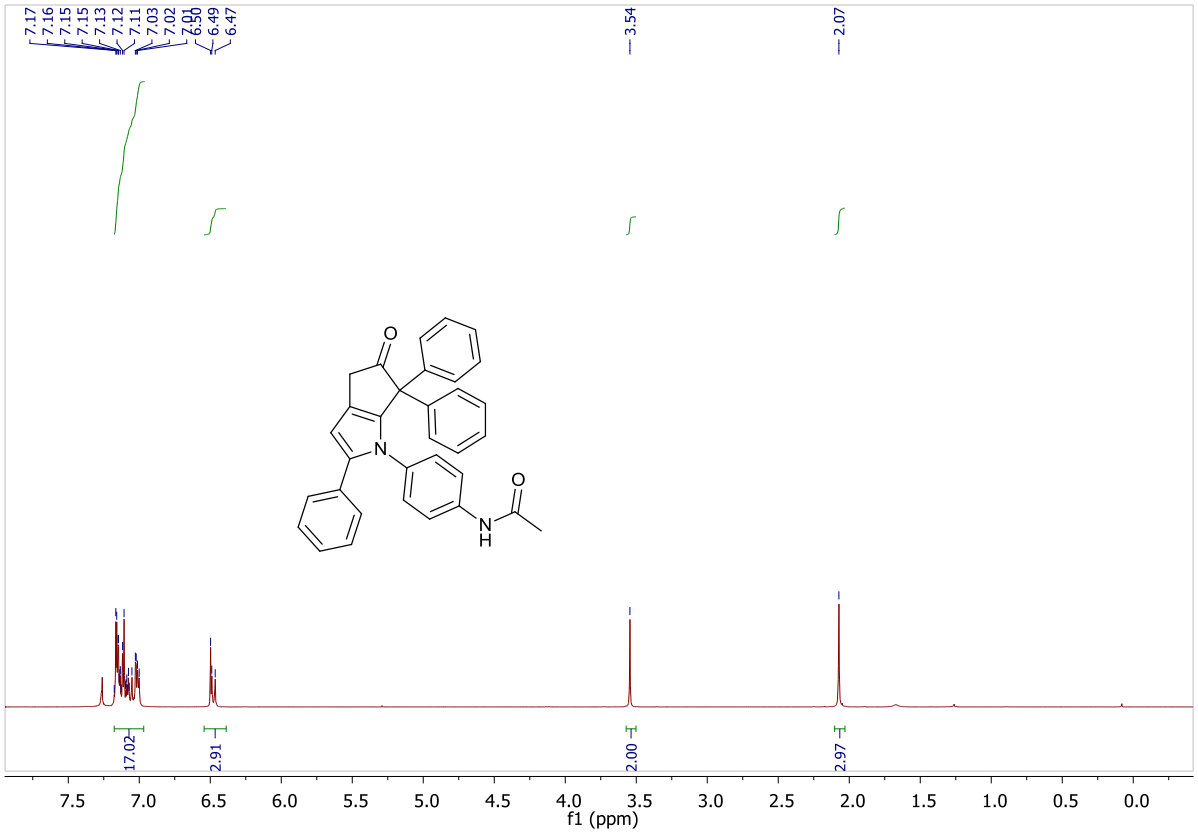
f1 (ppm)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N
O
N
H
17.02
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6.5
6.0
5.5
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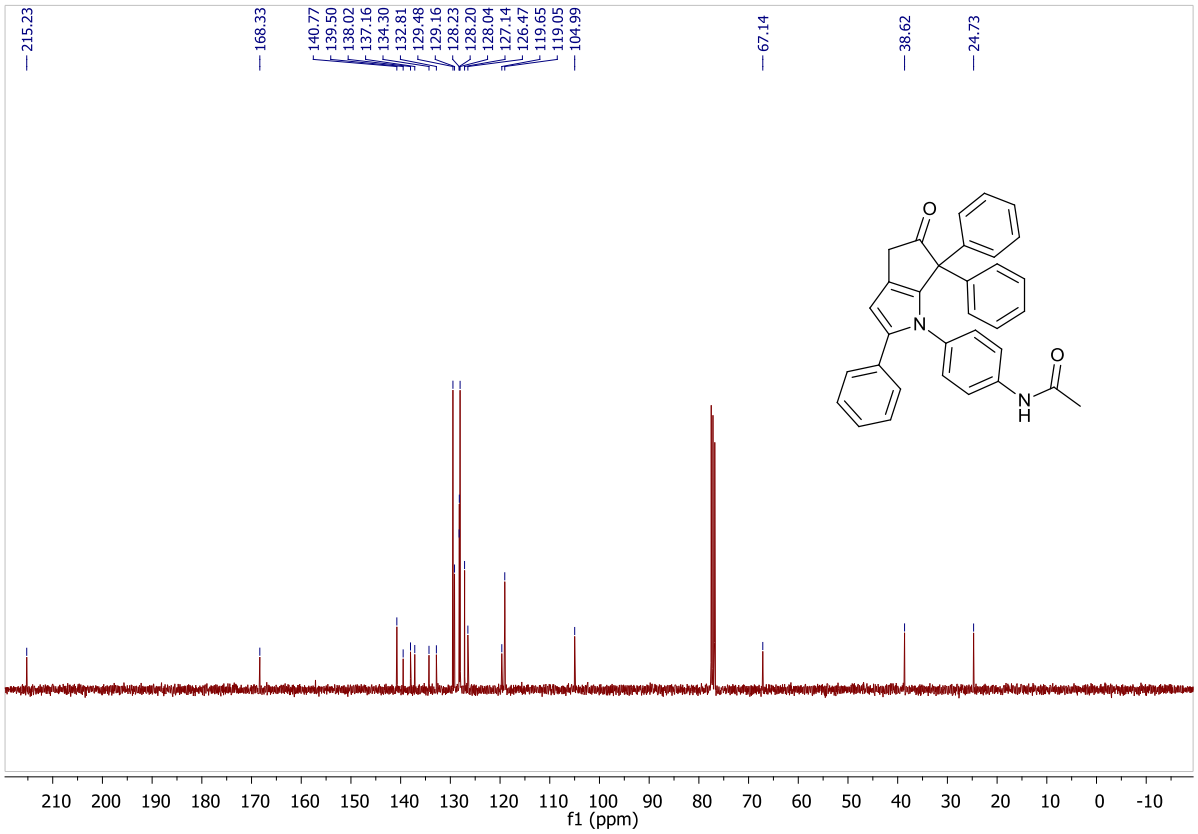
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128.23
128.20
128.04
127.14
126.47
119.65
119.05
104.99
67.14
38.62
24.73
O
N
O
N
H
210
200
190
180
170
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30
20
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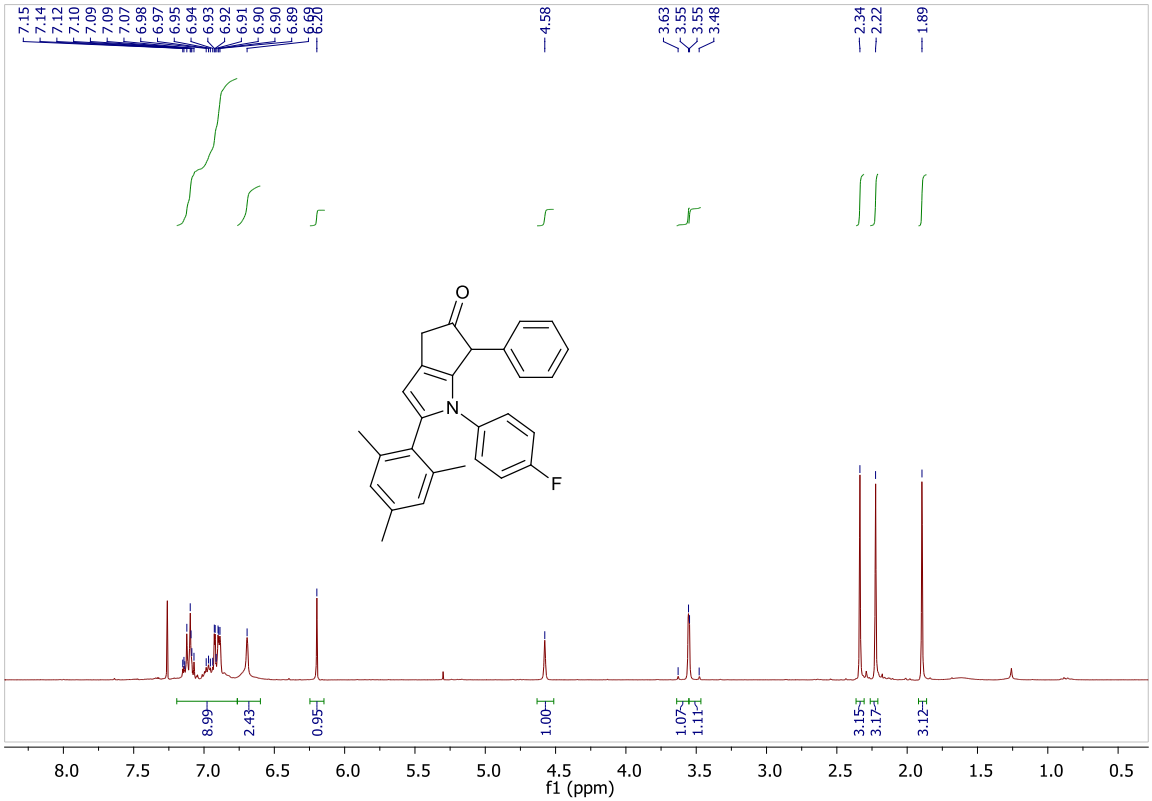
f1 (ppm)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7.09
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6.94
6.93
6.92
6.91
6.90
6.90
6.89
6.69
6.68
4.58
3.63
3.55
3.55
3.48
2.34
2.22
1.89
O
N
F
8.99
2.43
0.95
1.00
1.07
1.11
3.15
3.17
3.12
8.0
7.5
7.0
6.5
6.0
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5.0
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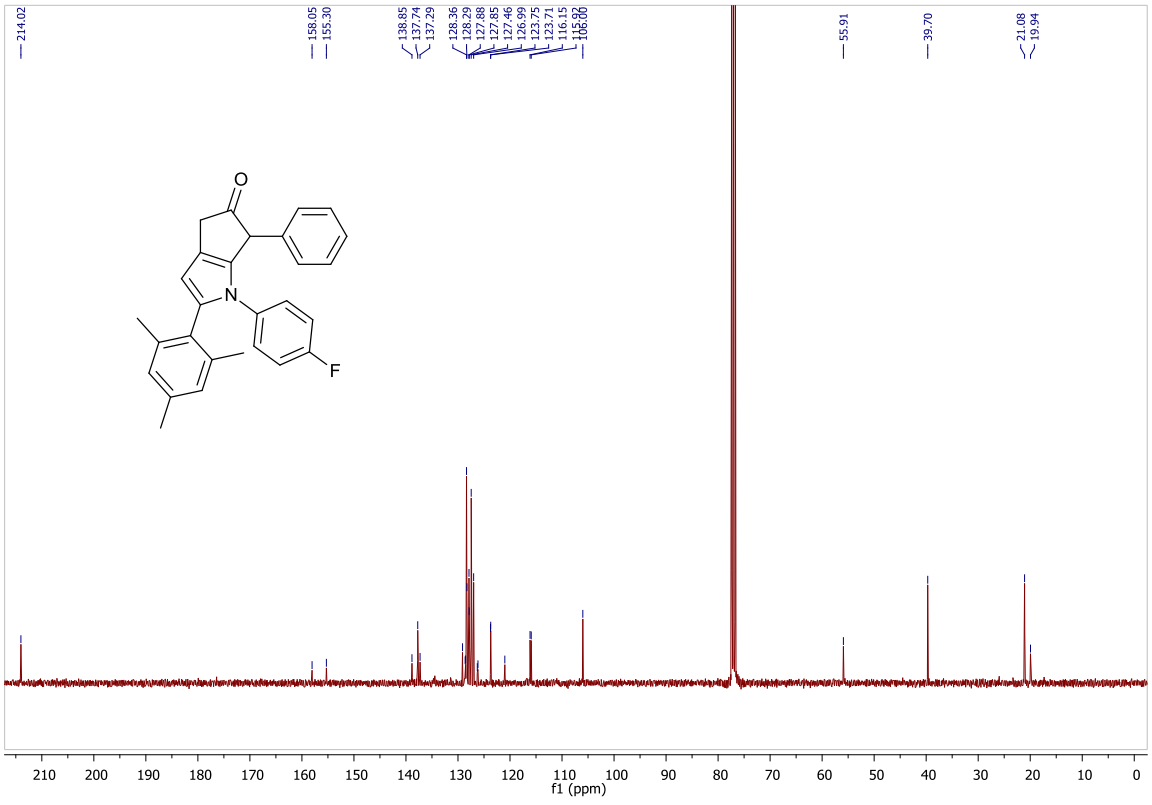
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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127.85
127.46
126.99
123.75
123.71
116.15
115.93
115.80
55.91
39.70
21.08
19.94
O
N
F
210
200
190
180
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130
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110
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50
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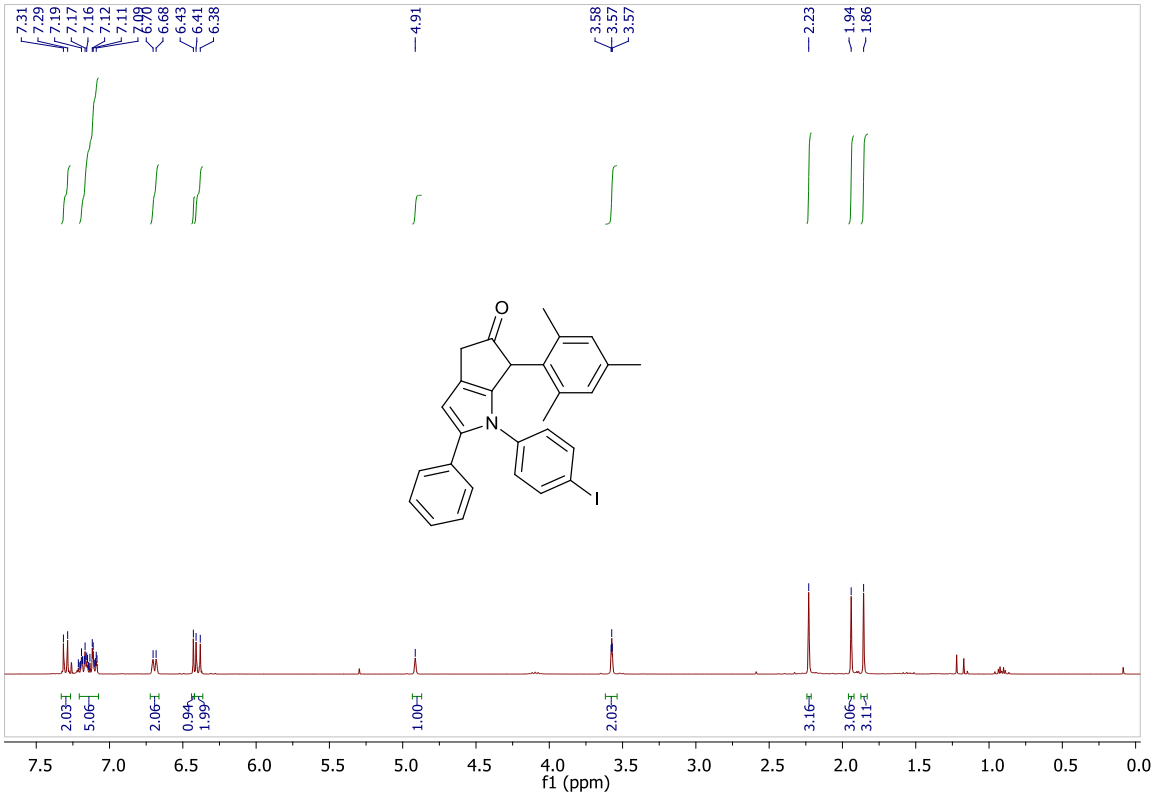
f1 (ppm)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7.09
6.70
6.68
6.43
6.41
6.38
4.91
3.58
3.57
3.57
2.23
1.94
1.86
O
N
I
2.03
5.06
2.06
0.94
1.99
1.00
2.03
3.16
3.06
3.11
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
2.0
1.5
1.0
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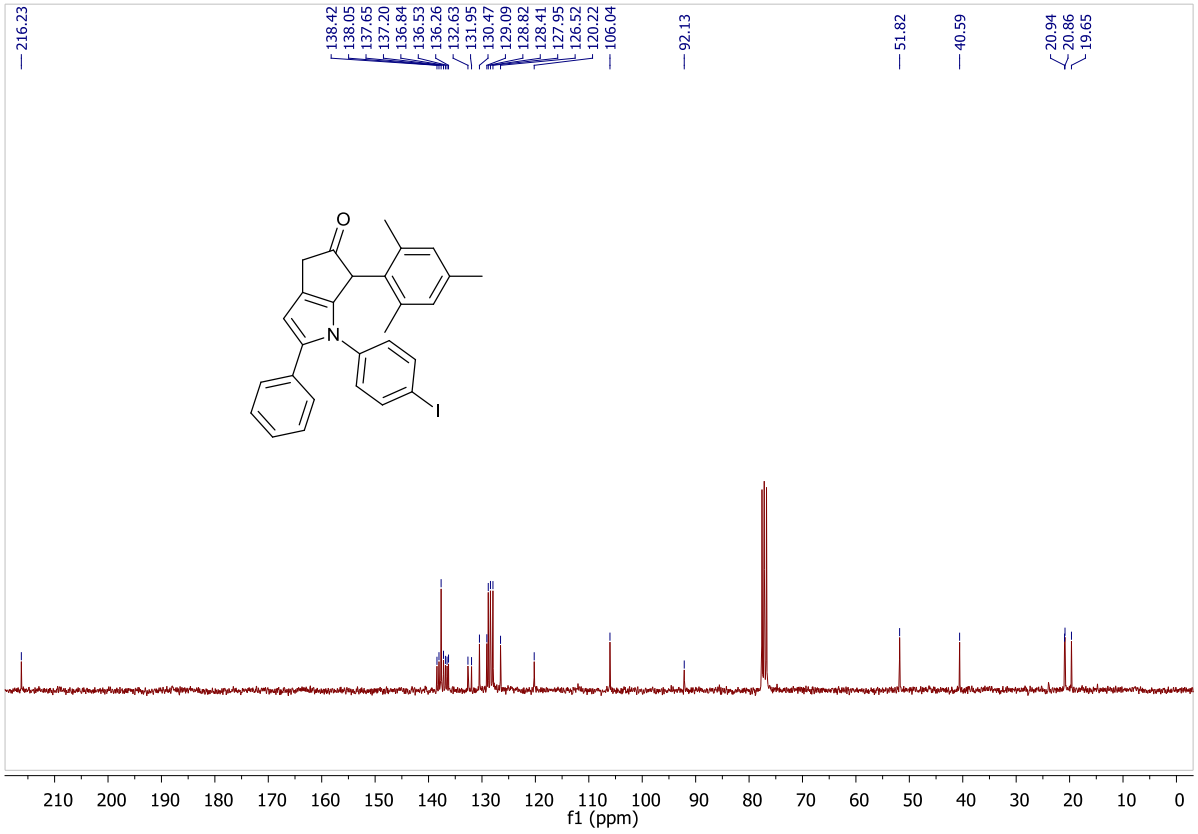
0.0
f1 (ppm)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128.41
127.95
126.52
120.22
106.04
92.13
51.82
40.59
20.94
20.86
19.65
O
N
I
210
200
190
180
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130
120
110
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90
80
70
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50
40
30
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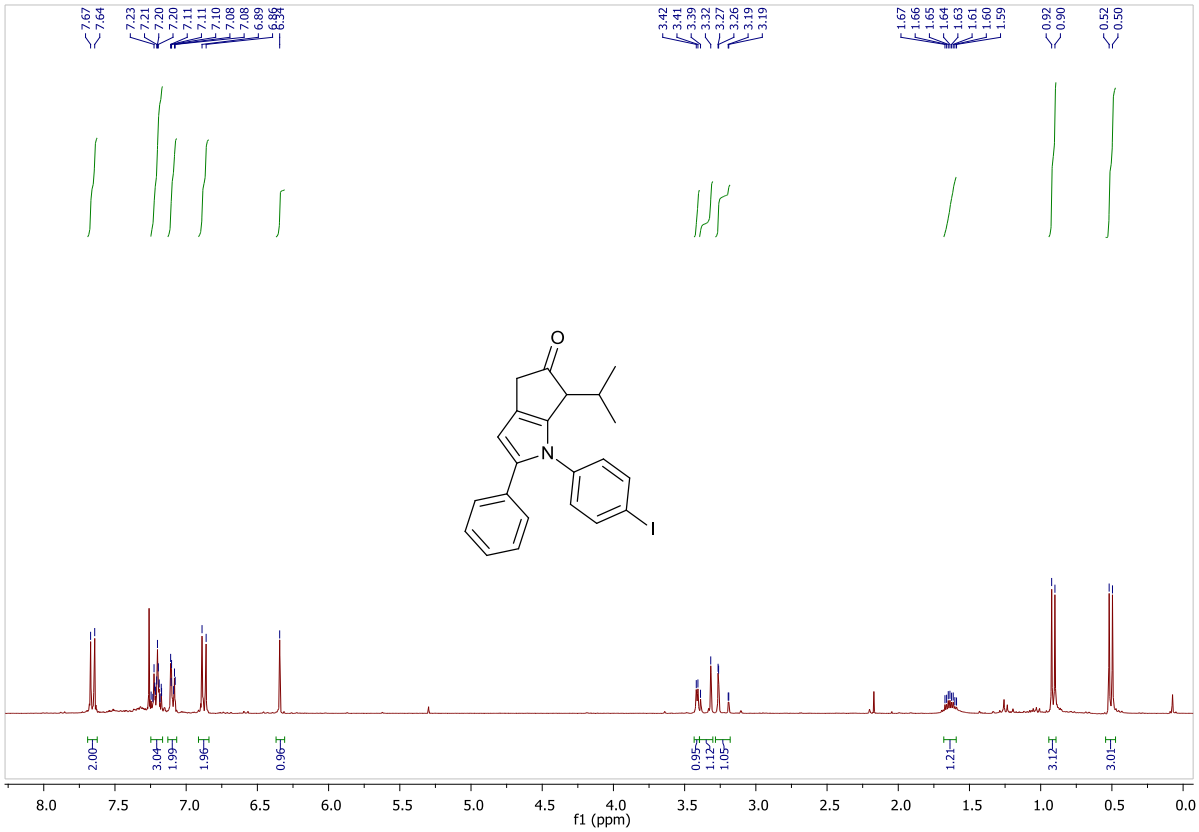
f1 (ppm)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7.11
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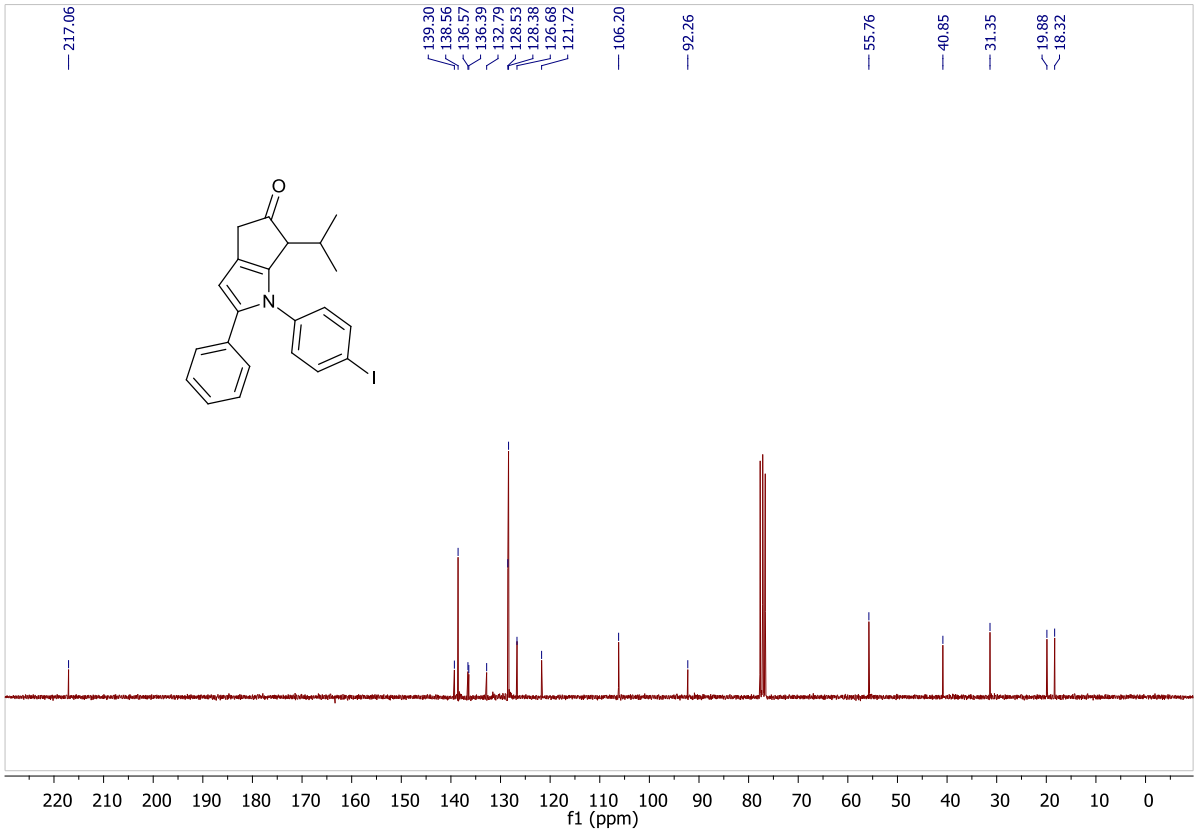
7.08
7.08
6.89
6.86
6.84
3.42
3.41
3.39
3.32
3.27
3.26
3.19
3.19
1.67
1.66
1.65
1.64
1.63
1.61
1.60
1.59
0.92
0.90
0.52
0.50
O
N
I
2.00
3.04
1.99
1.96
0.96
0.95
1.12
1.05
1.21
3.12
3.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.38
126.68
121.72
106.20
92.26
55.76
40.85
31.35
19.88
18.32
O
N
I
220
210
200
190
180
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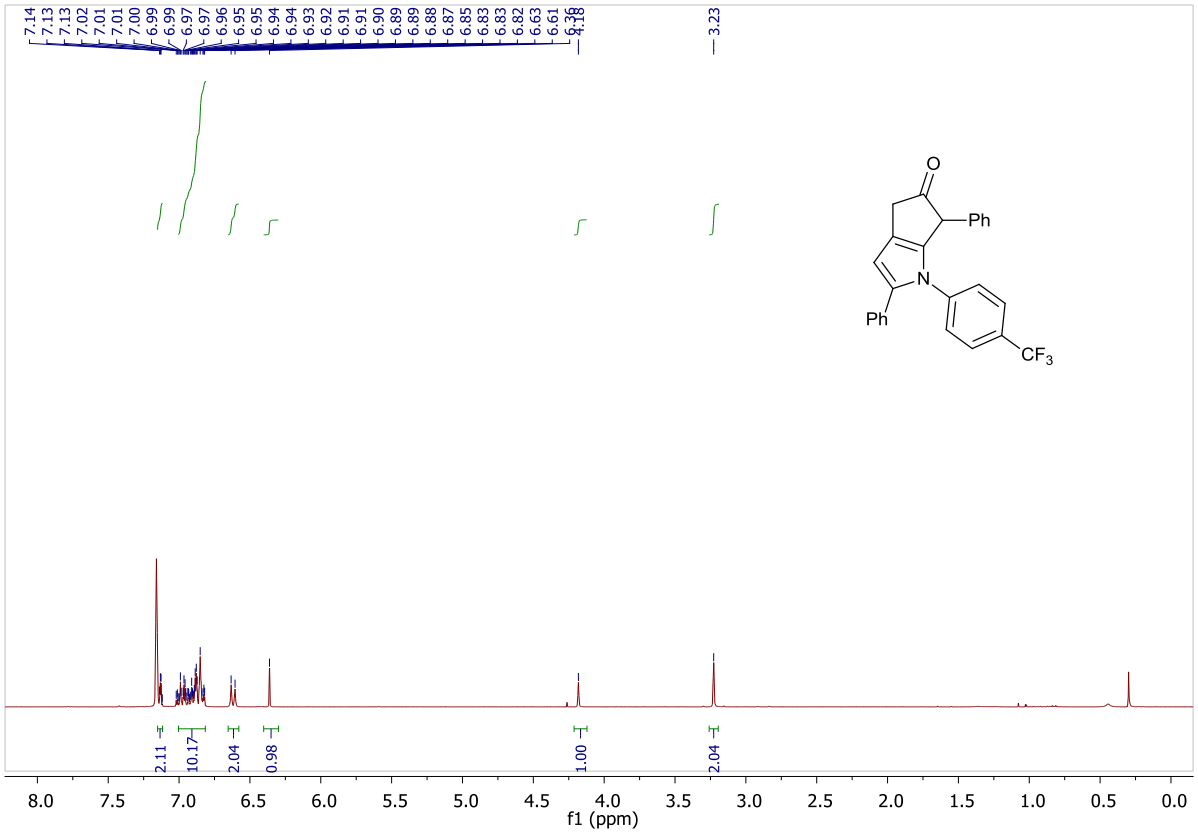
f1 (ppm)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6.97
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6.96
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6.95
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6.93
6.92
6.91
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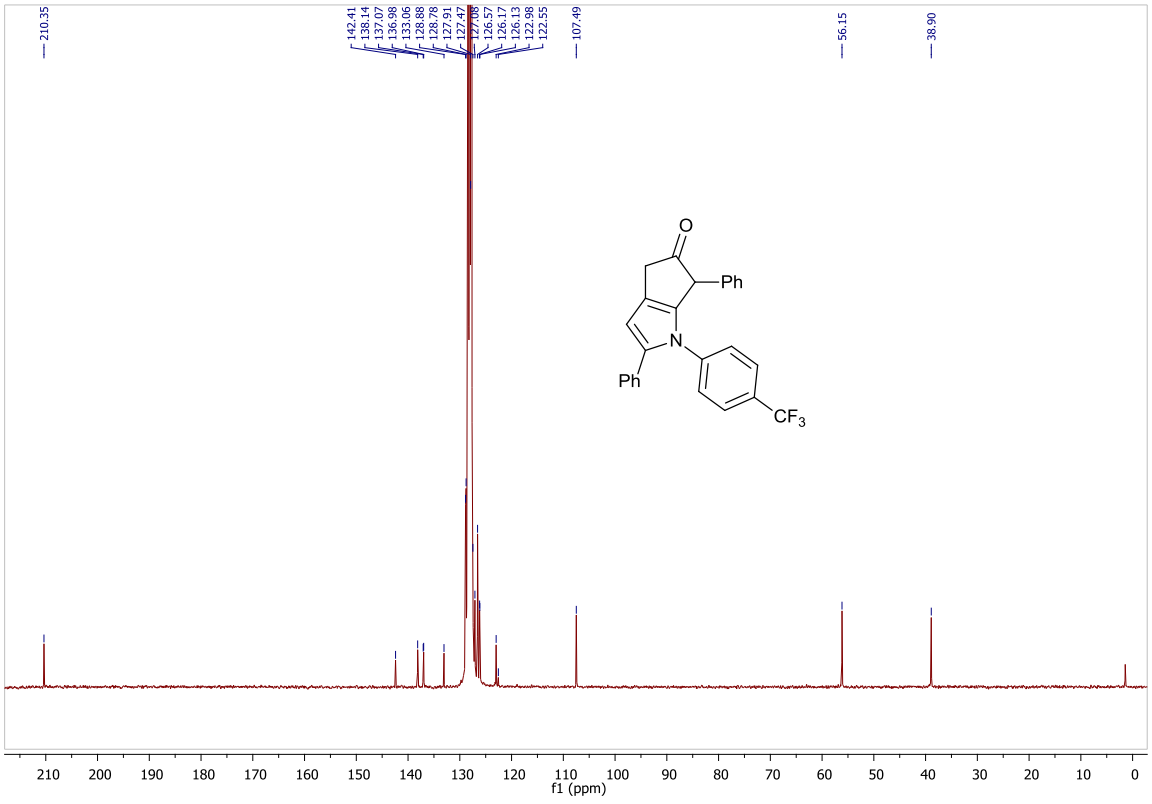
6.90
6.89
6.89
6.88
6.87
6.85
6.83
6.83
6.82
6.63
6.61
6.36
4.18
3.23
O
Ph
N
Ph
CF3
2.11
10.17
2.04
0.98
1.00
2.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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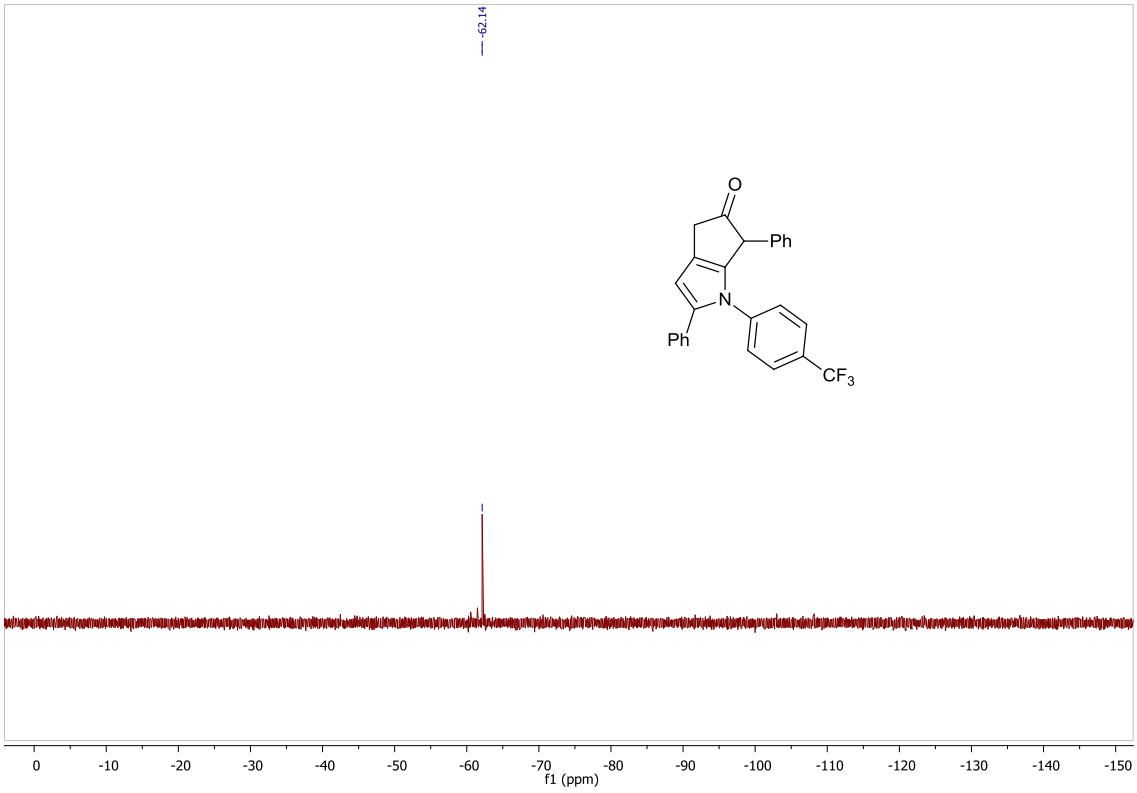
127.08
126.57
126.17
126.13
122.98
122.55
107.49
56.15
38.90
O
Ph
N
Ph
CF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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Ph
N
Ph
CF3
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-10
-20
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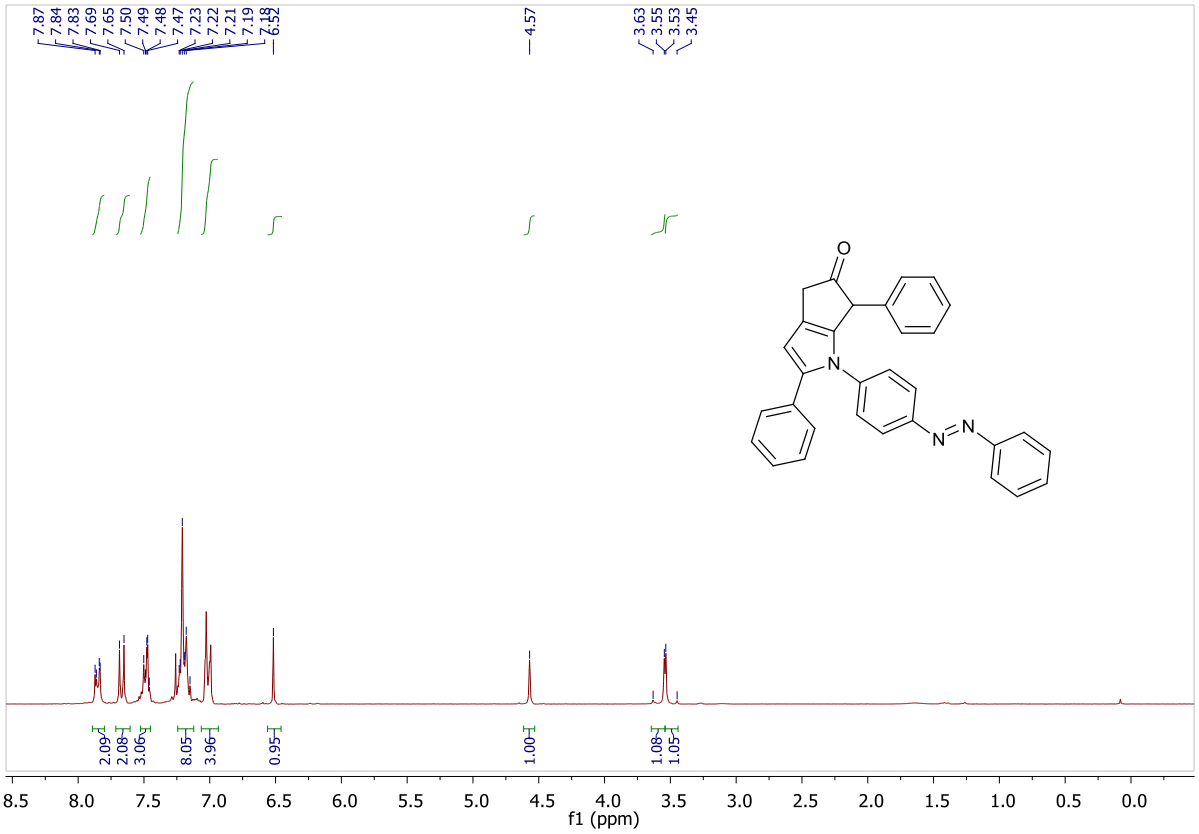
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)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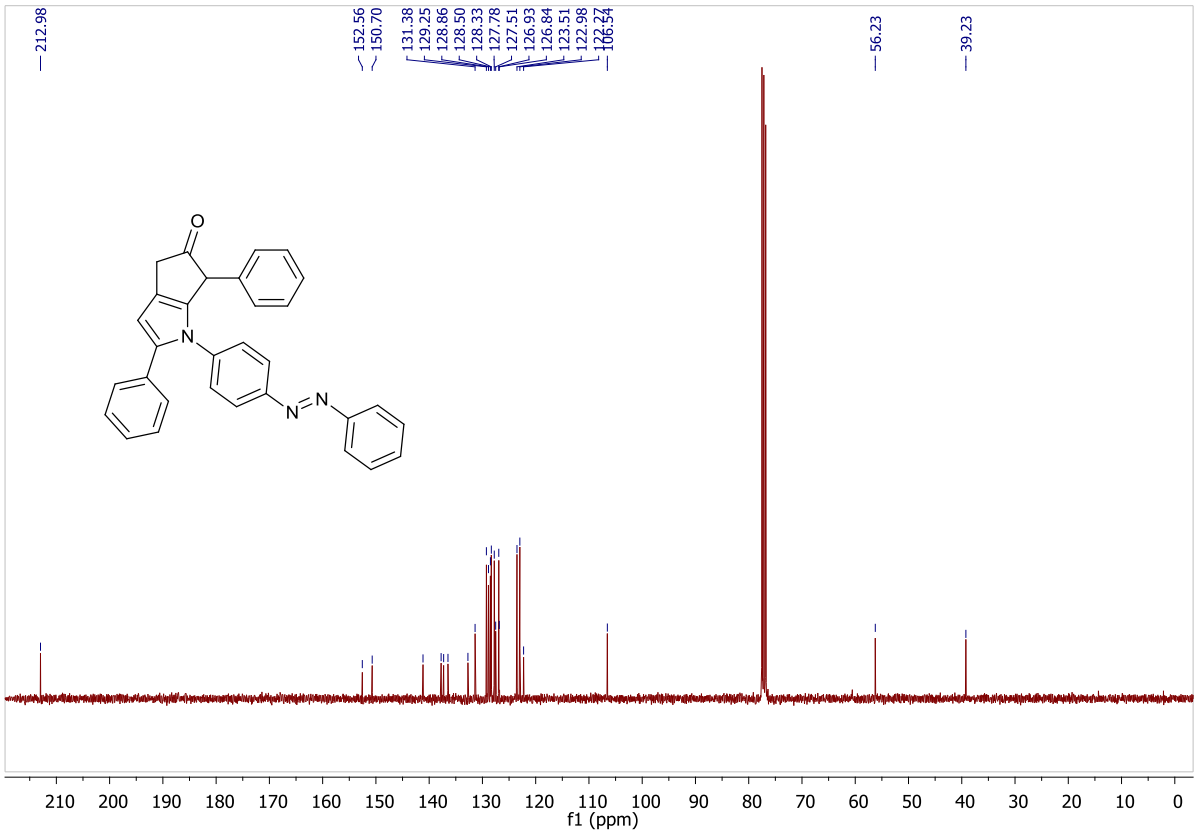
7.48
7.47
7.23
7.22
7.21
7.19
7.18
6.52
4.57
3.63
3.55
3.53
3.45
O
N
N=N
2.09
2.08
3.06
8.05
3.96
0.95
1.00
1.08
1.05
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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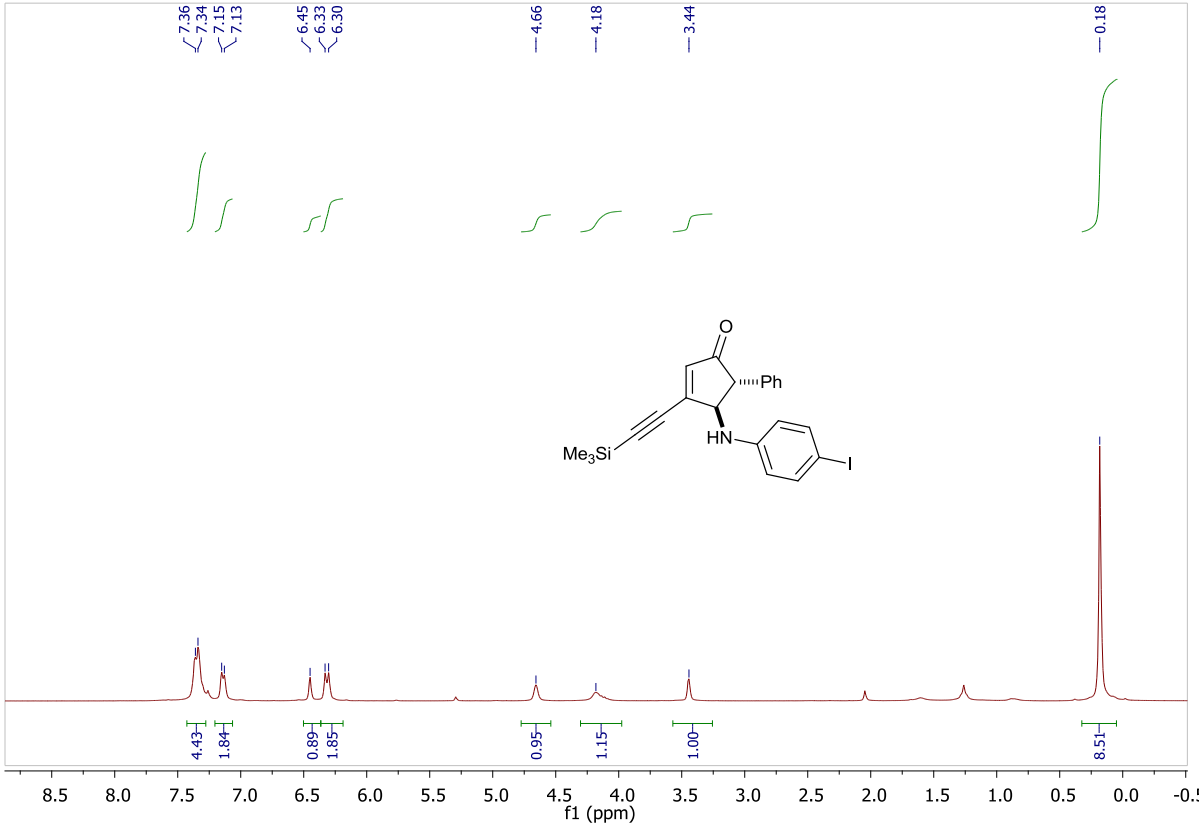
128.50
128.33
127.78
127.51
126.93
126.84
123.51
122.98
122.27
106.54
56.23
39.23
O
N
N=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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6.45
6.33
6.30
4.66
4.18
3.44
0.18
O
Ph
HN
Me3Si
I
4.43
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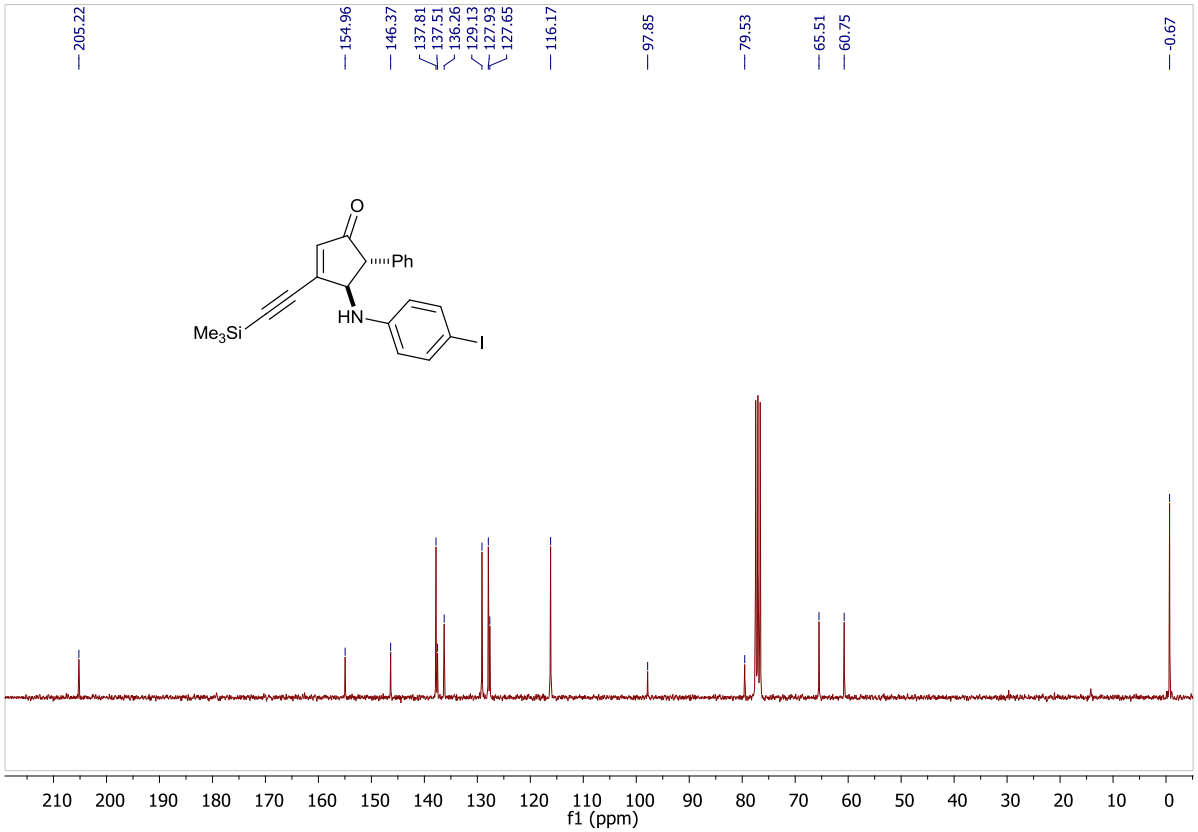
0.89
1.85
0.95
1.15
1.00
8.51
f1 (ppm)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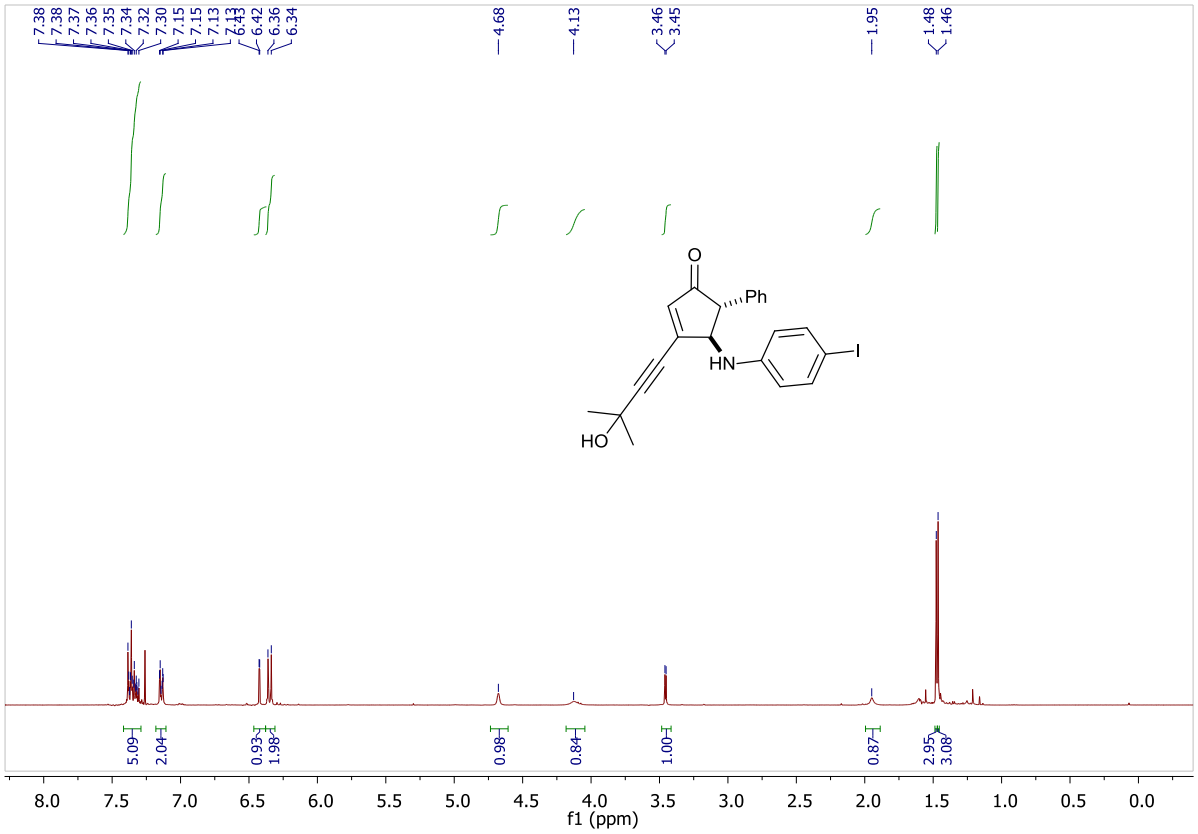
Ph
HN
Me3Si
I
f1 (ppm)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7.15
7.13
6.43
6.42
6.36
6.34
4.68
4.13
3.46
3.45
1.95
1.48
1.46
O
Ph
HN
I
HO
5.09
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0.93
1.98
0.98
0.84
1.00
0.87
2.95
3.08
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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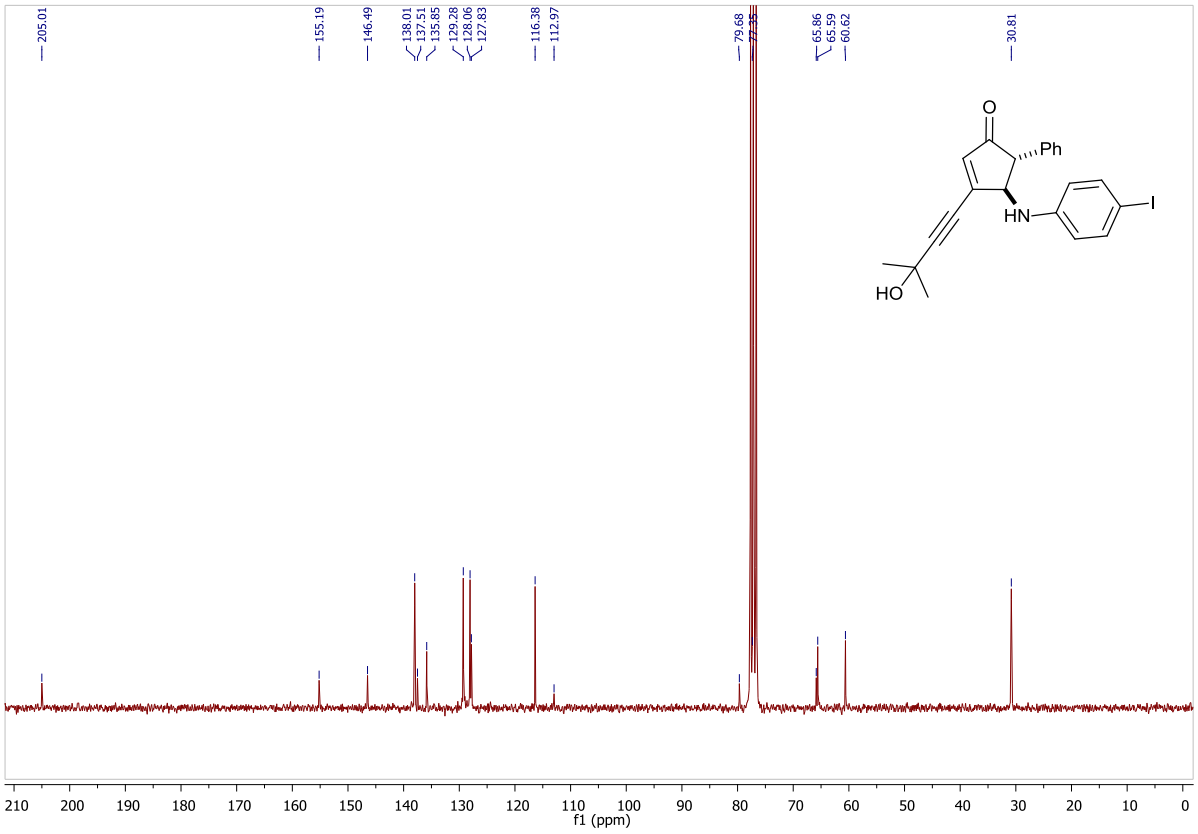
0.0
f1 (ppm)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128.06
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116.38
112.97
79.68
77.35
65.86
65.59
60.62
30.81
O
Ph
HN
I
HO
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
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50
40
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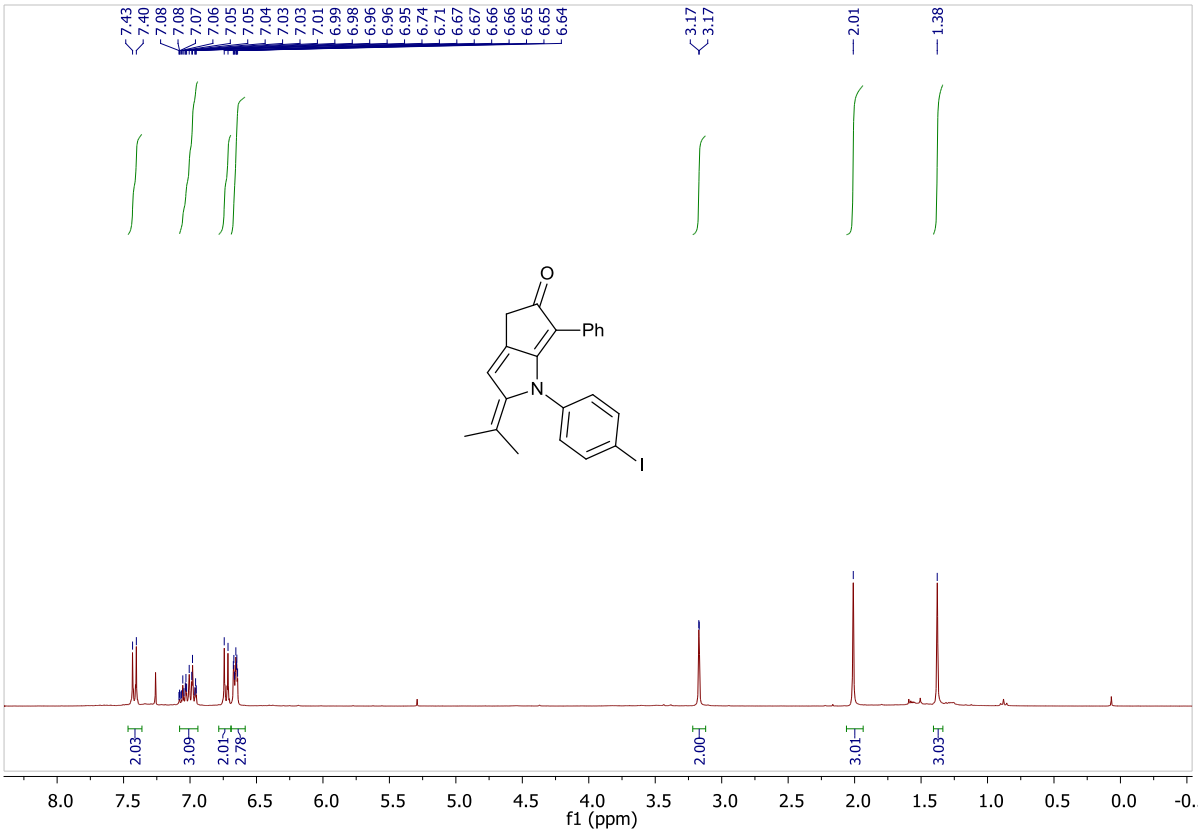
f1 (ppm)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7.06
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7.05
7.04
7.03
7.03
7.01
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6.96
6.95
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6.71
6.67
6.67
6.66
6.66
6.65
6.65
6.64
3.17
3.17
2.01
1.38
O
Ph
N
I
2.03
3.09
2.01
2.78
2.00
3.01
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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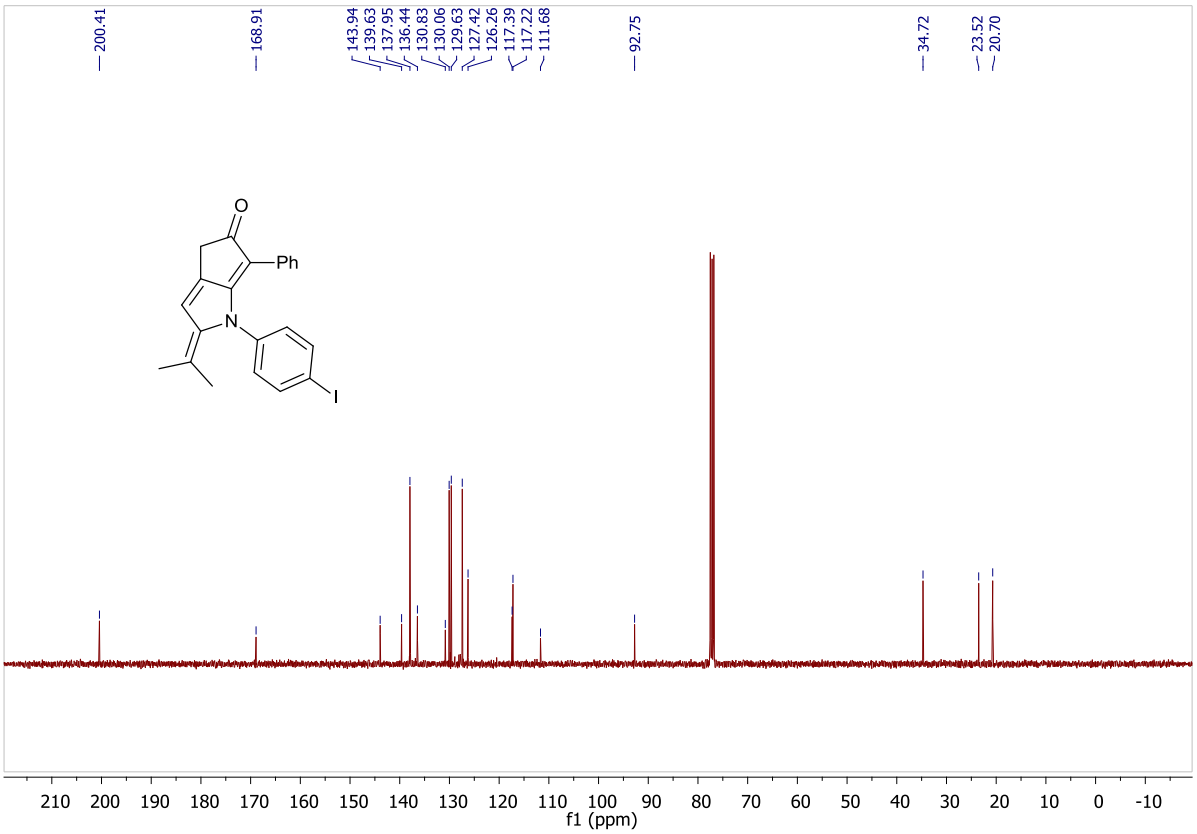
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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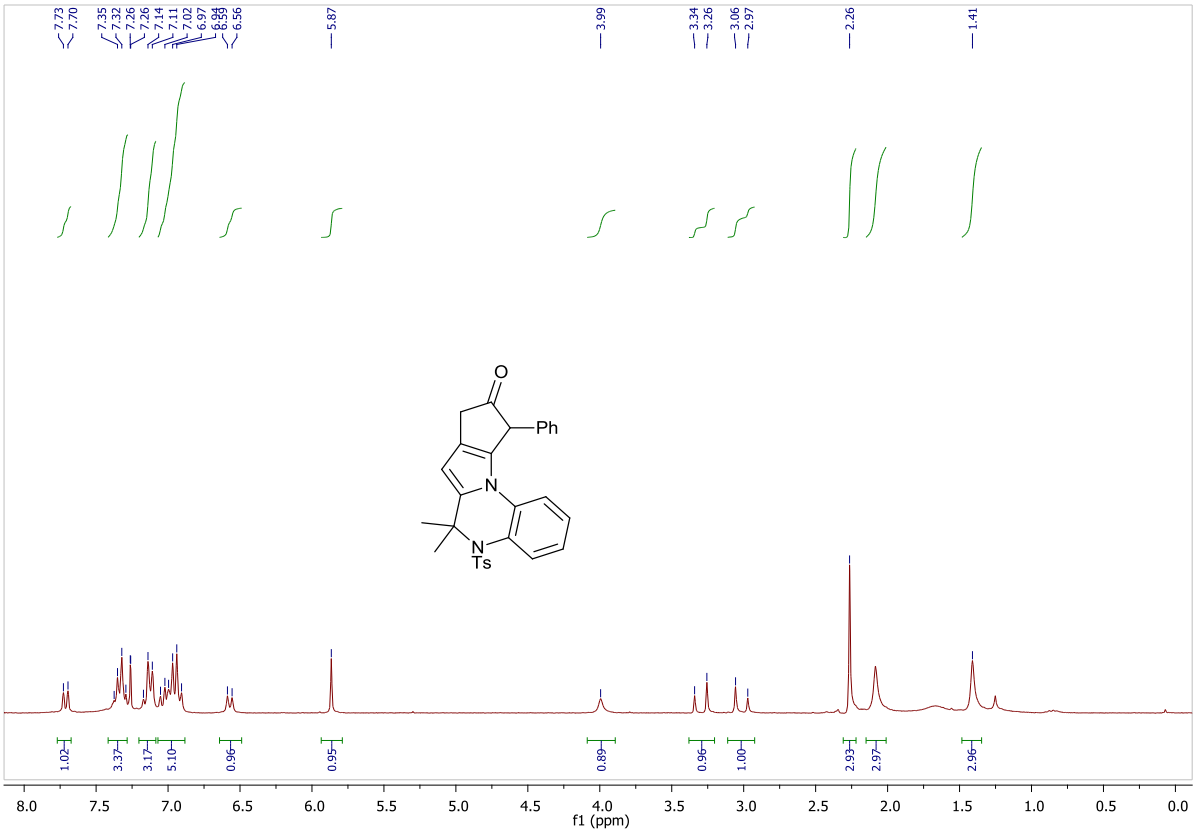
130.06
129.63
127.42
126.26
117.39
117.22
111.68
92.75
34.72
23.52
20.70
O
Ph
N
I
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.11
7.02
6.97
6.94
6.93
6.56
5.87
3.99
3.34
3.26
3.06
2.97
2.26
1.41
O
Ph
N
N
Ts
1.02
3.37
3.17
5.10
0.96
0.95
0.89
0.96
1.00
2.93
2.97
2.96
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
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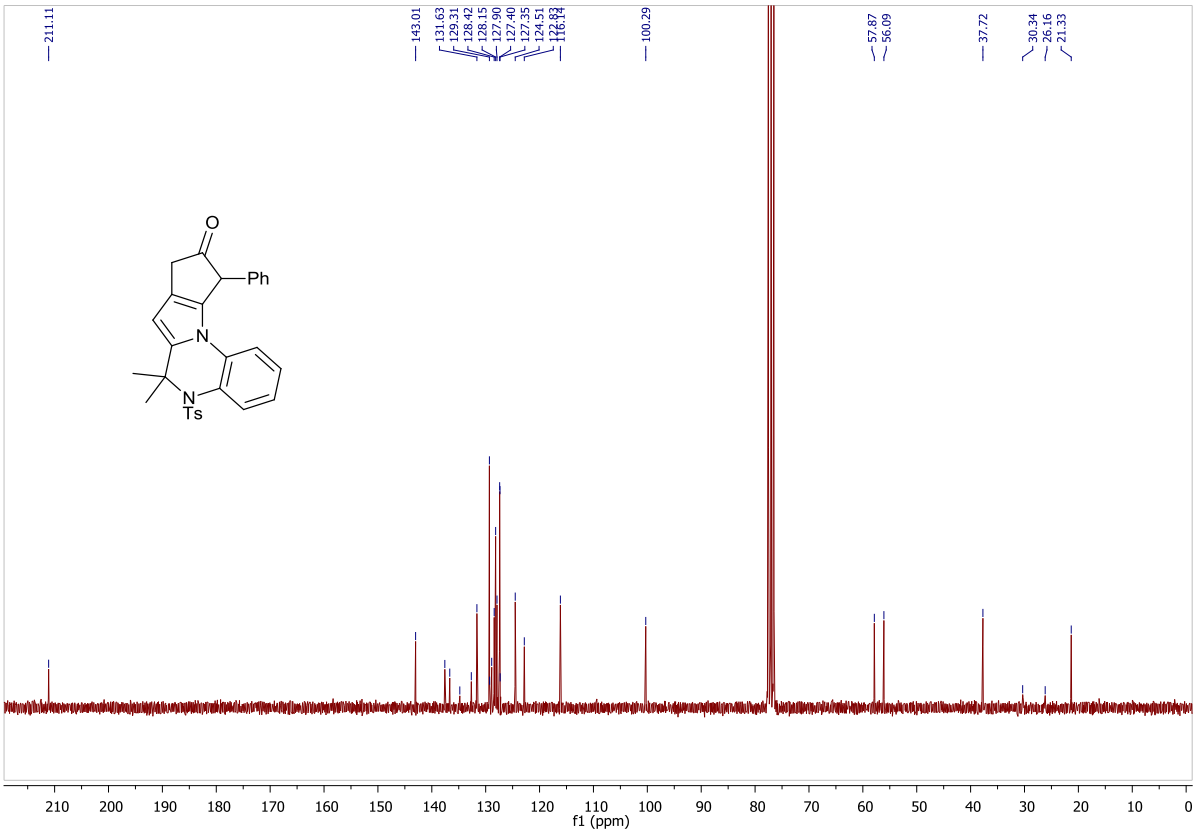
0.0
f1 (ppm)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122.83
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37.72
30.34
26.16
21.33
O
Ph
N
N
Ts
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200
190
180
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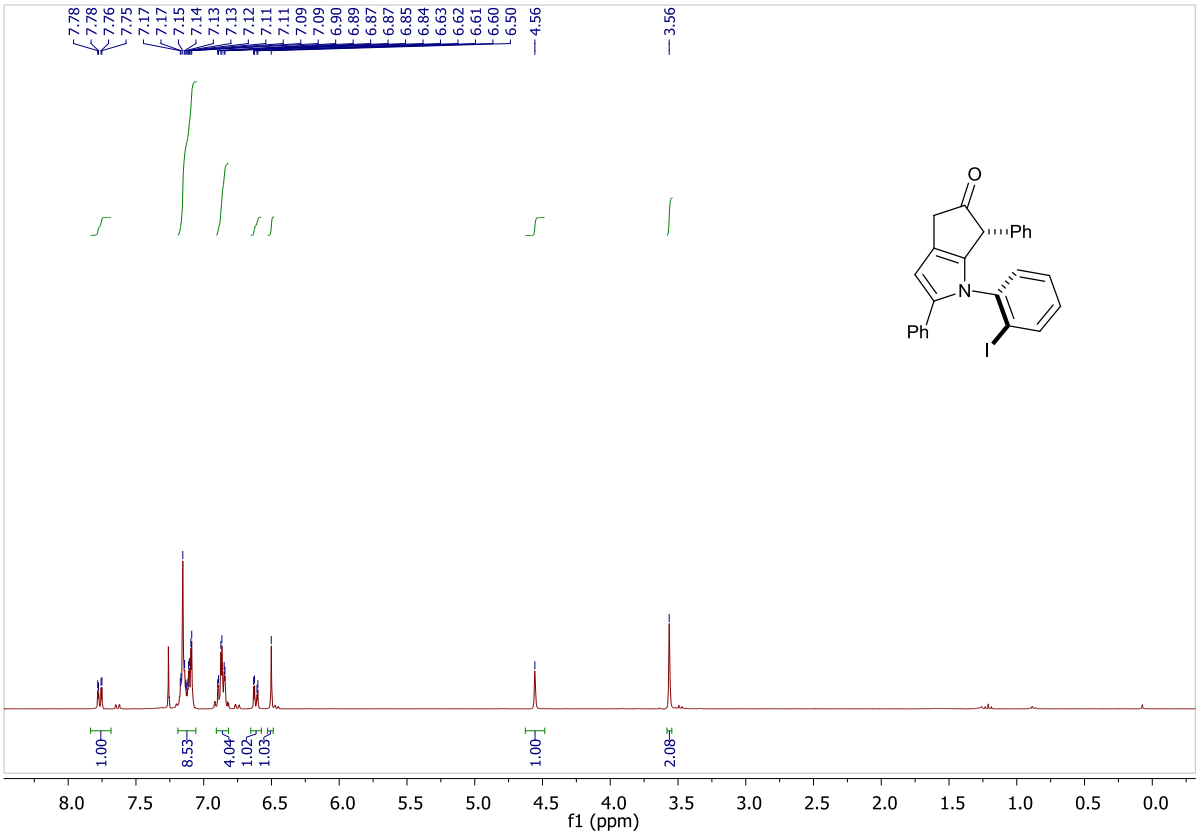
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7.09
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6.87
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6.62
6.61
6.60
6.50
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3.56
O
Ph
N
Ph
I
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1.02
1.03
1.00
2.08
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7.0
6.5
6.0
5.5
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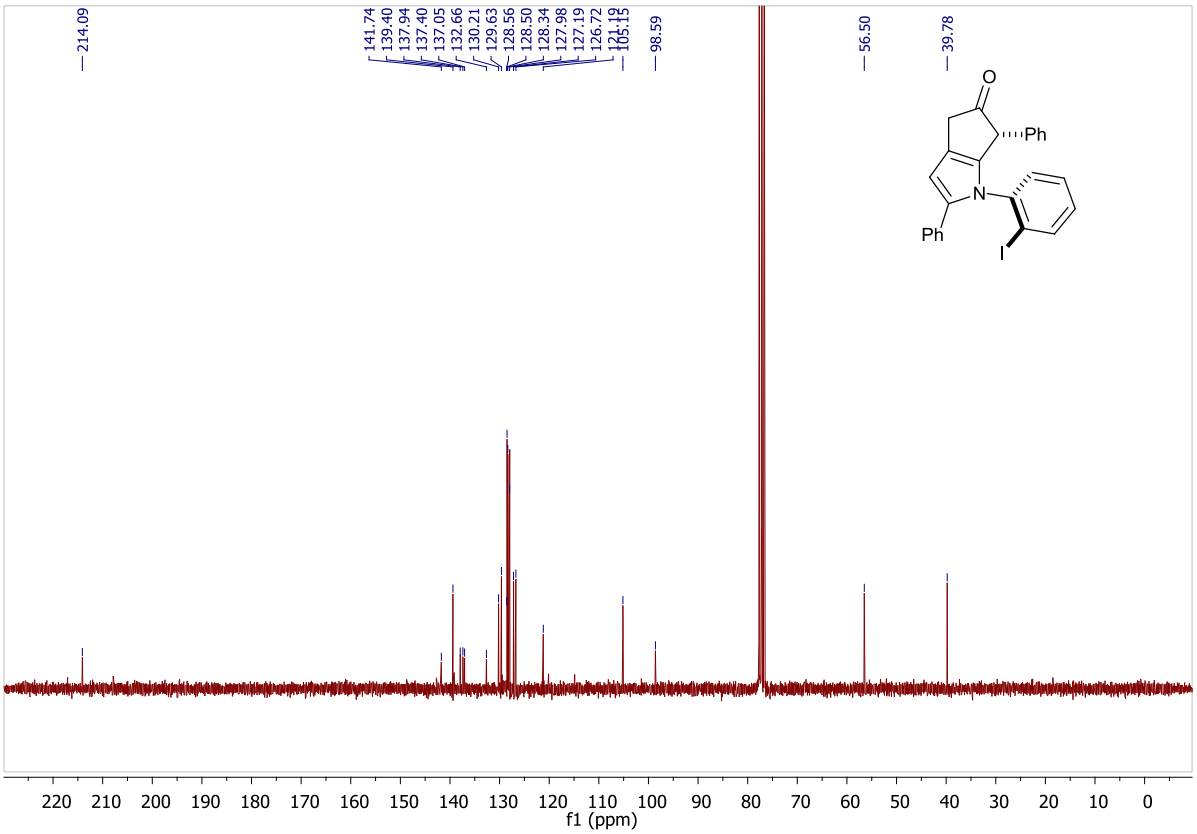
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127.19
126.72
121.19
105.15
98.59
56.50
39.78
O
Ph
N
Ph
I
220
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200
190
180
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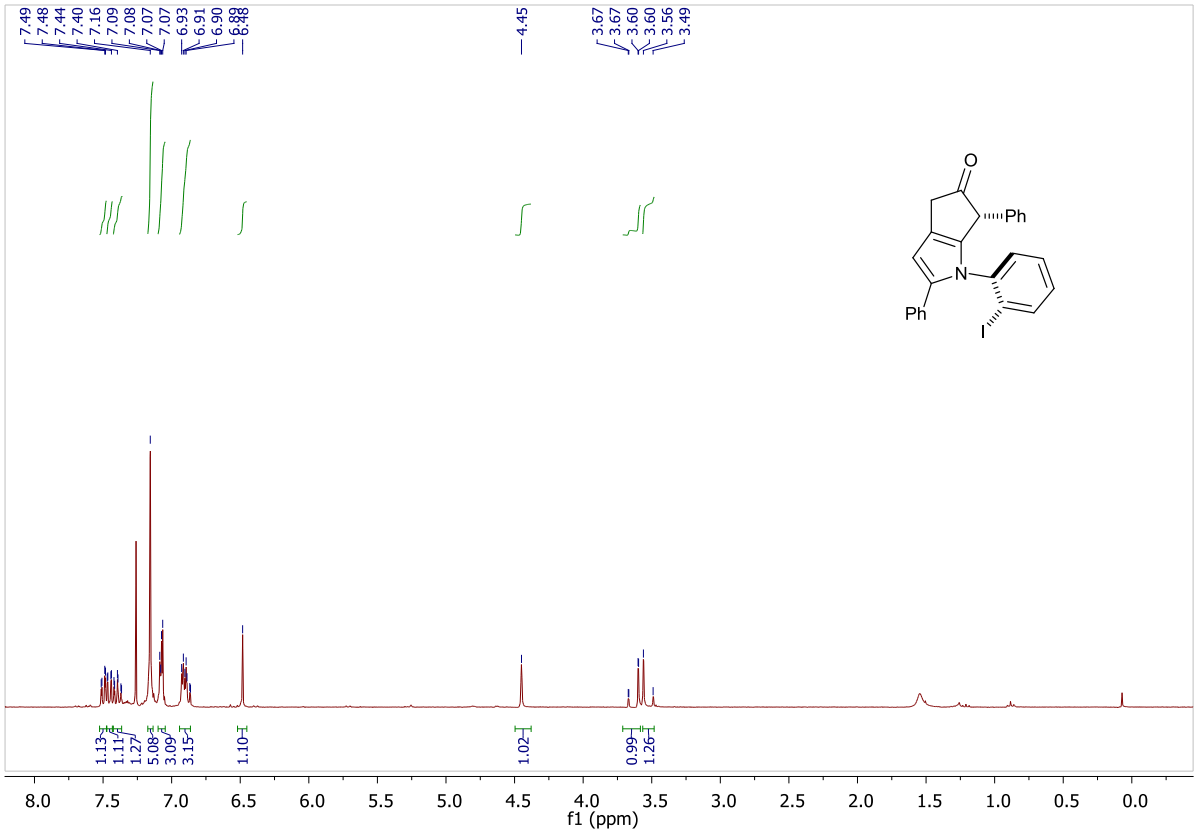
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3.60
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3.49
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Ph
N
Ph
I
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1.11
1.27
5.08
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3.15
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1.02
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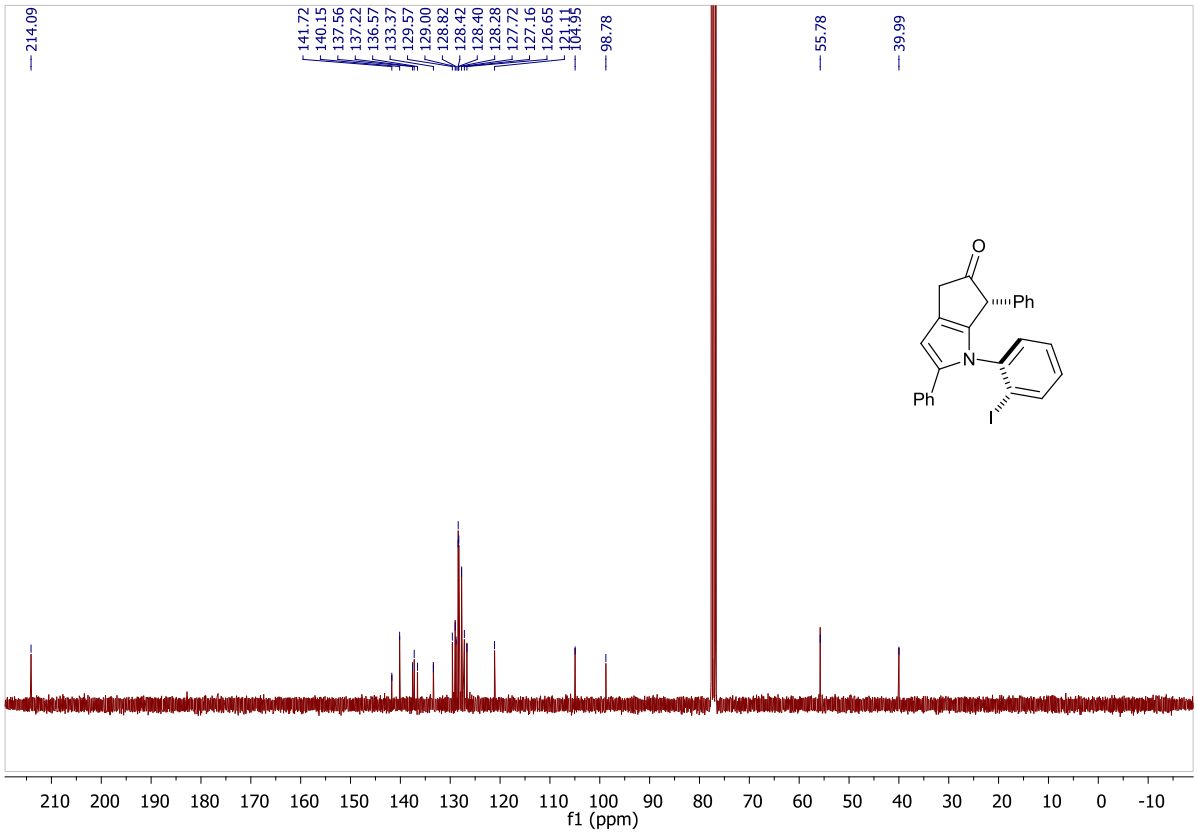
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127.16
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55.78
39.99
O
Ph
N
Ph
I
210
200
190
180
170
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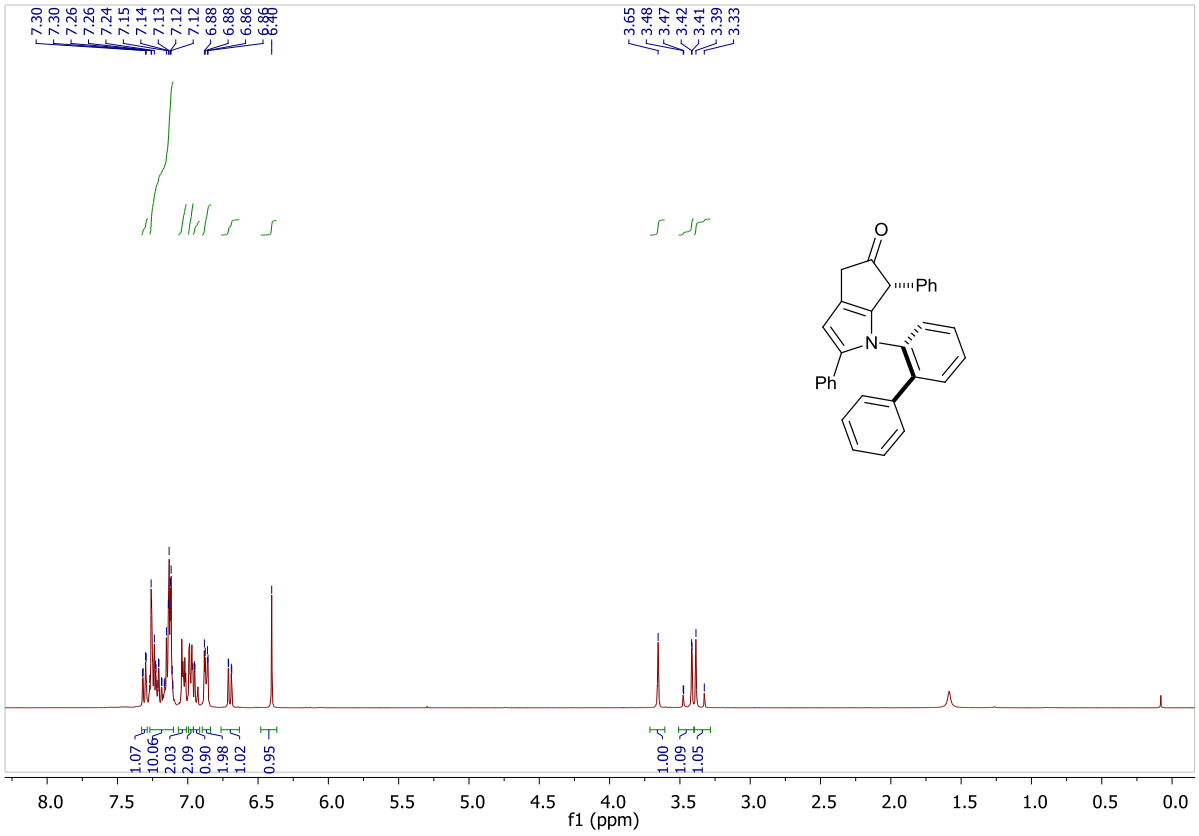
f1 (ppm)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3.41
3.39
3.33
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Ph
N
Ph
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10.06
2.03
2.09
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1.02
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1.00
1.09
1.05
8.0
7.5
7.0
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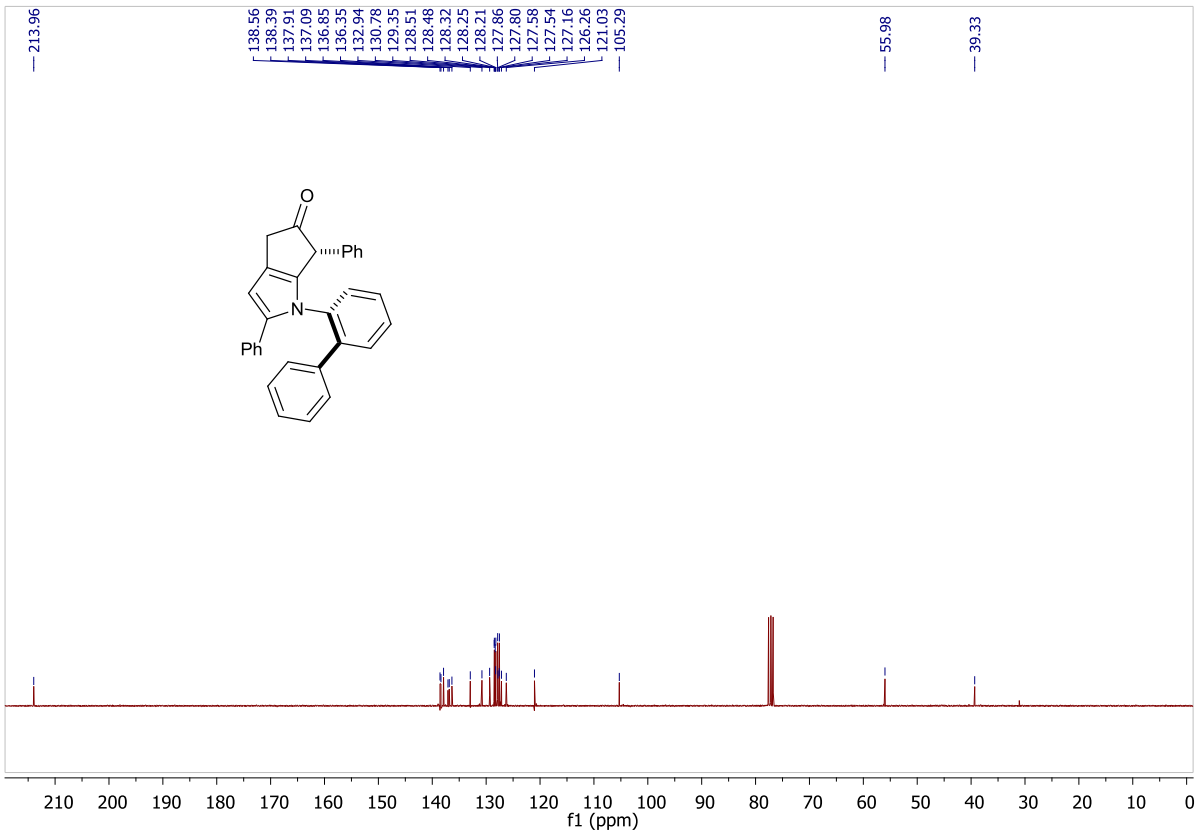
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128.21
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127.58
127.54
127.16
126.26
121.03
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39.33
O
Ph
N
Ph
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200
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180
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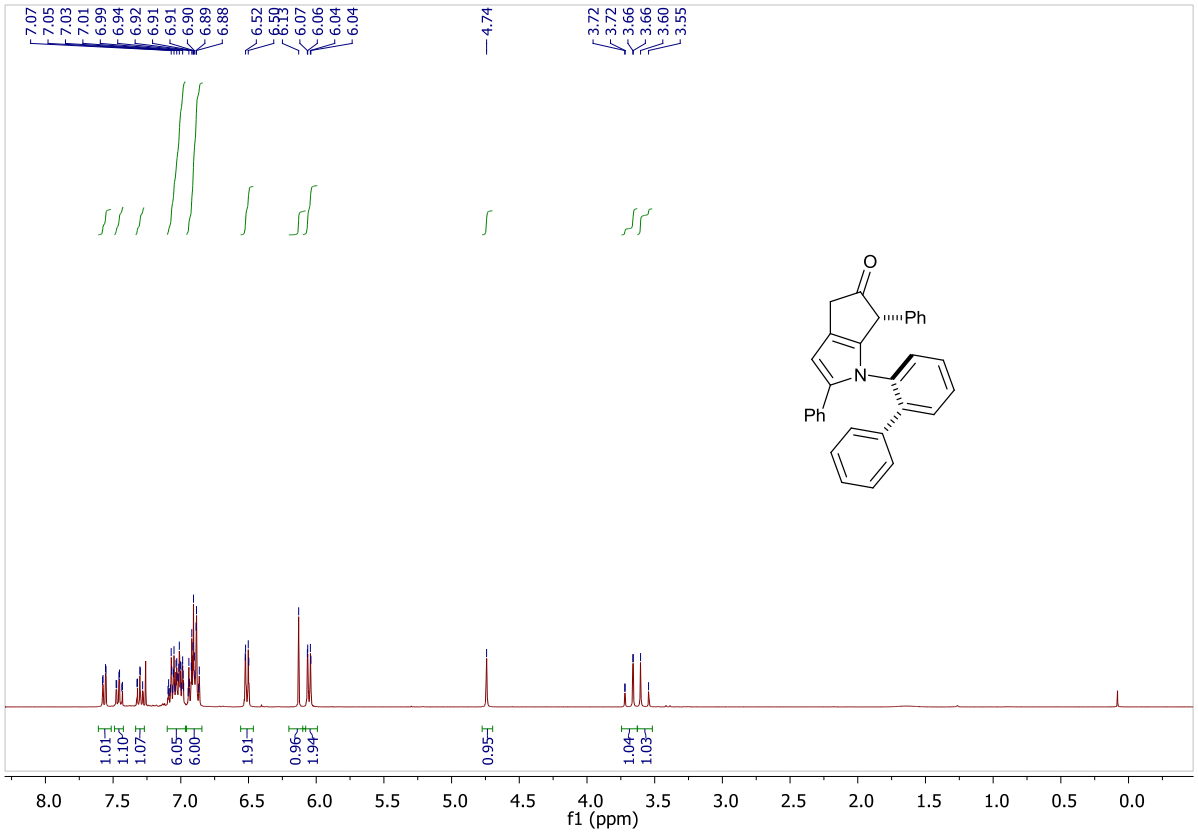
f1 (ppm)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6.52
6.50
6.13
6.07
6.06
6.04
6.04
4.74
3.72
3.72
3.66
3.66
3.60
3.55
O
Ph
N
Ph
1.01
1.10
1.07
6.05
6.00
1.91
0.96
1.94
0.95
1.04
1.03
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
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1.0
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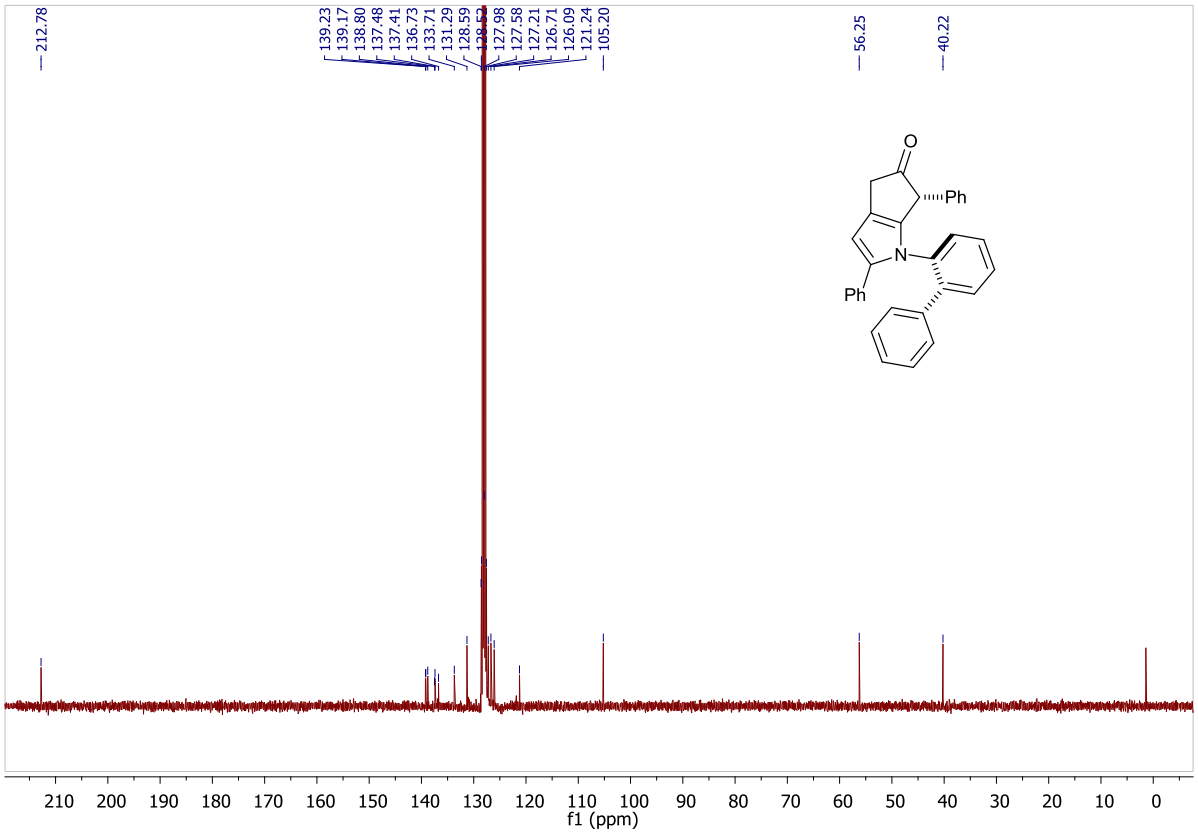
0.0
f1 (ppm)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127.21
126.71
126.09
121.24
105.20
56.25
40.22
O
Ph
N
Ph
210
200
190
180
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50
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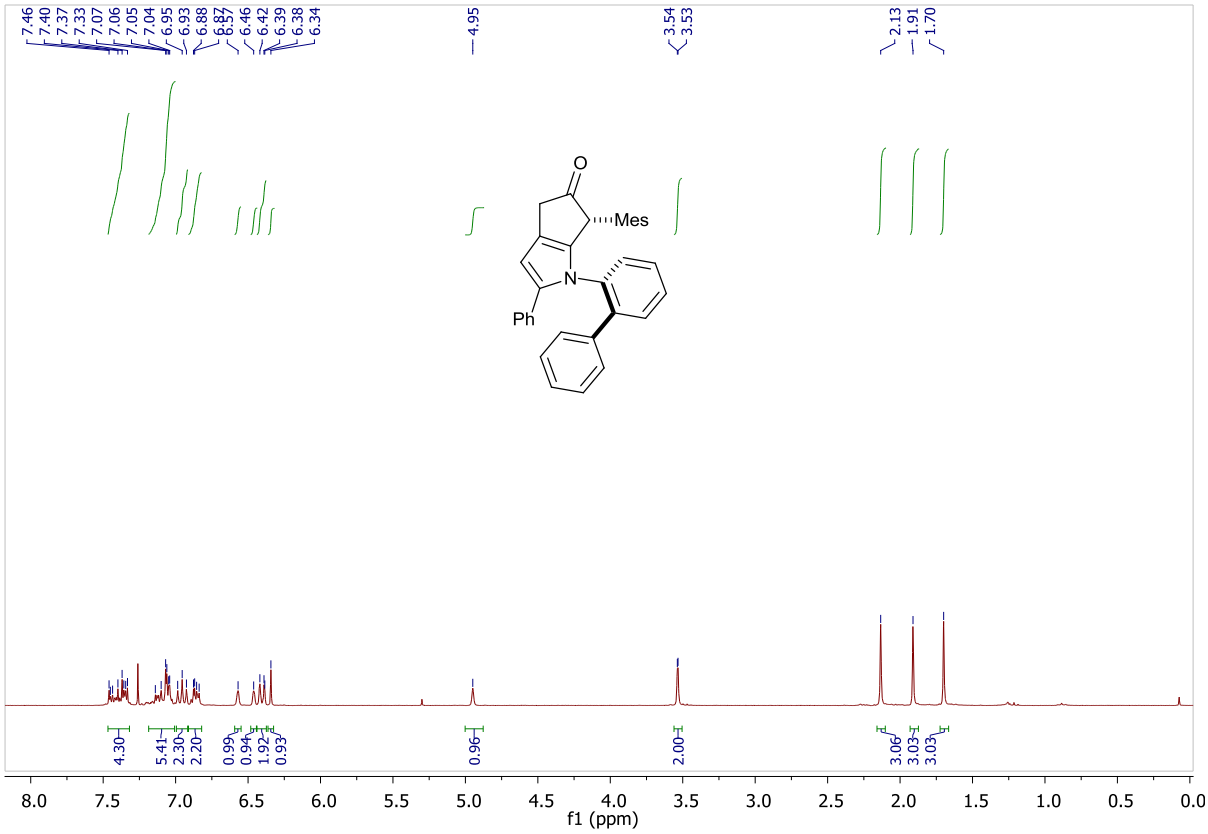
f1 (ppm)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6.46
6.42
6.39
6.38
6.34
4.95
3.54
3.53
2.13
1.91
1.70
O
Mes
N
Ph
4.30
5.41
2.30
2.20
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1.92
0.93
0.96
2.00
3.06
3.03
3.03
8.0
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7.0
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6.0
5.5
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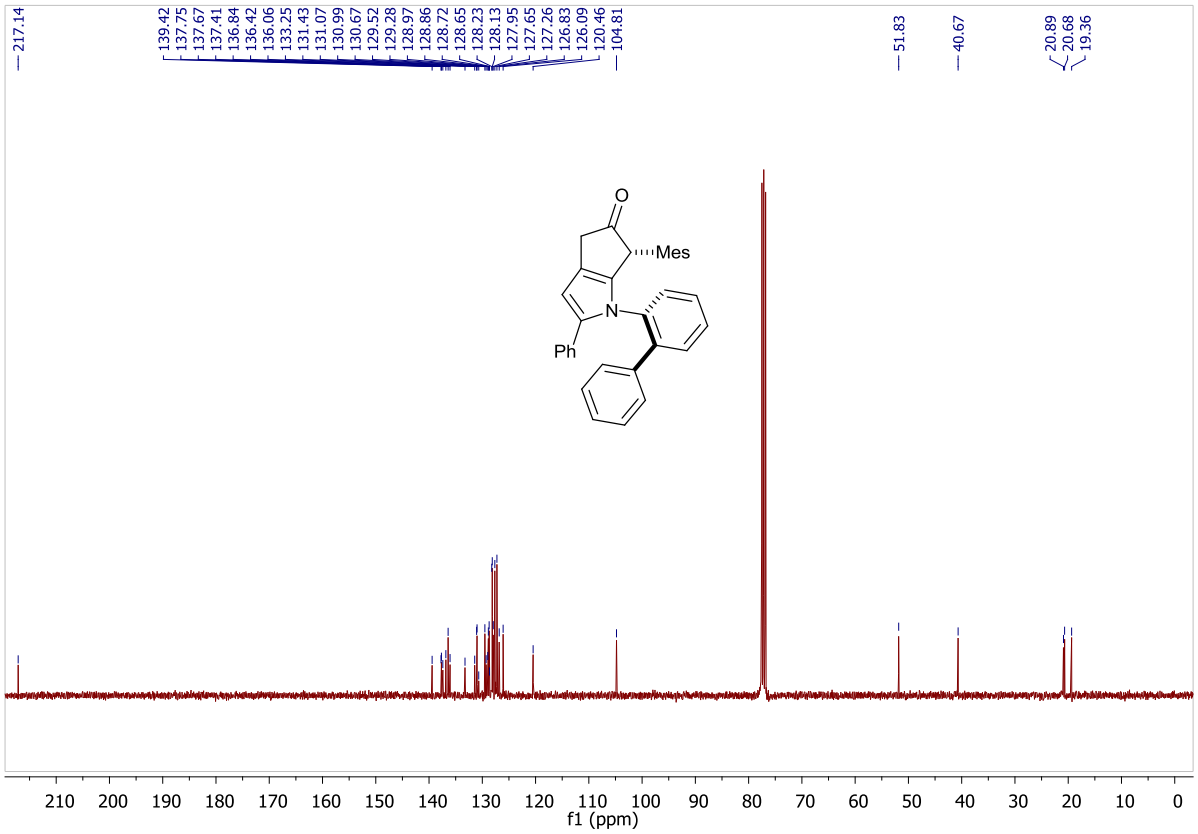
f1 (ppm)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128.13
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127.65
127.26
126.83
126.09
120.46
104.81
51.83
40.67
20.89
20.68
19.36
O
Mes
N
Ph
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200
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180
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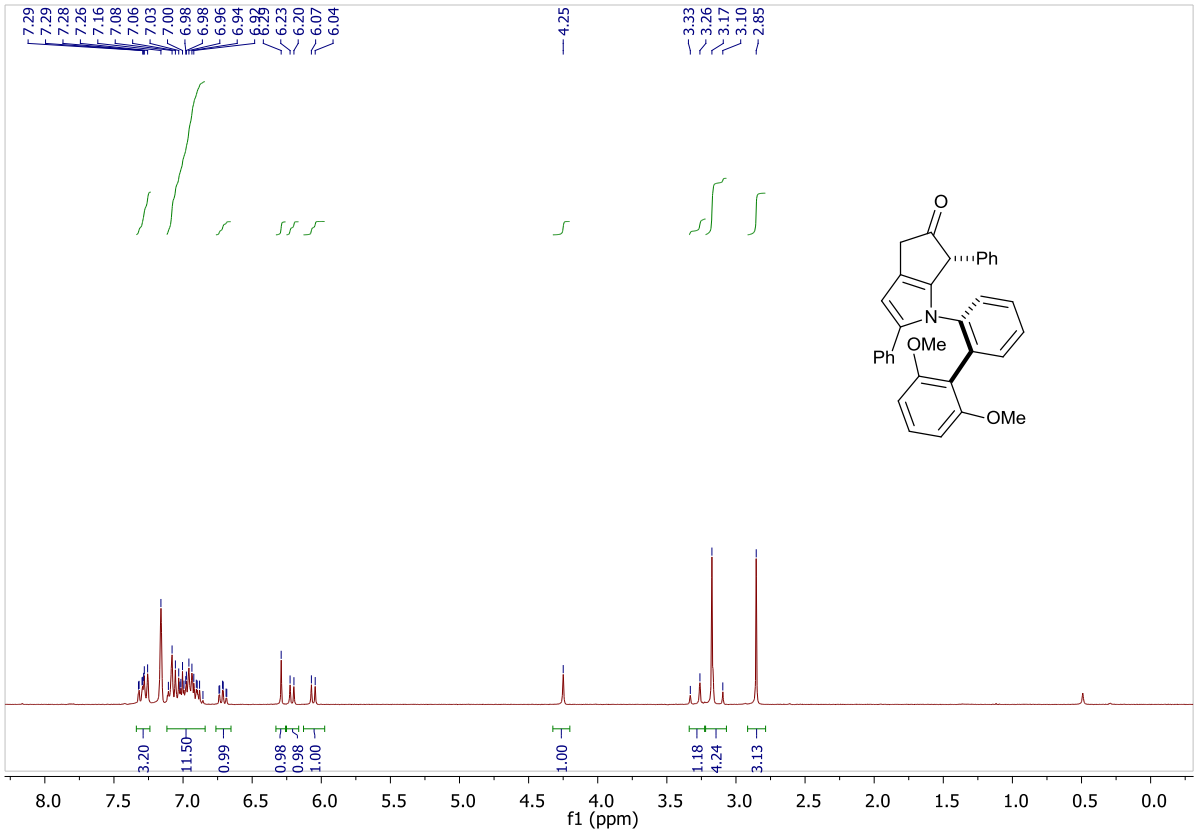
f1 (ppm)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6.94
6.23
6.20
6.07
6.04
4.25
3.33
3.26
3.17
3.10
2.85
O
Ph
N
Ph
OMe
OMe
3.20
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0.99
0.98
0.98
1.00
1.00
1.18
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3.13
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7.0
6.5
6.0
5.5
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1.0
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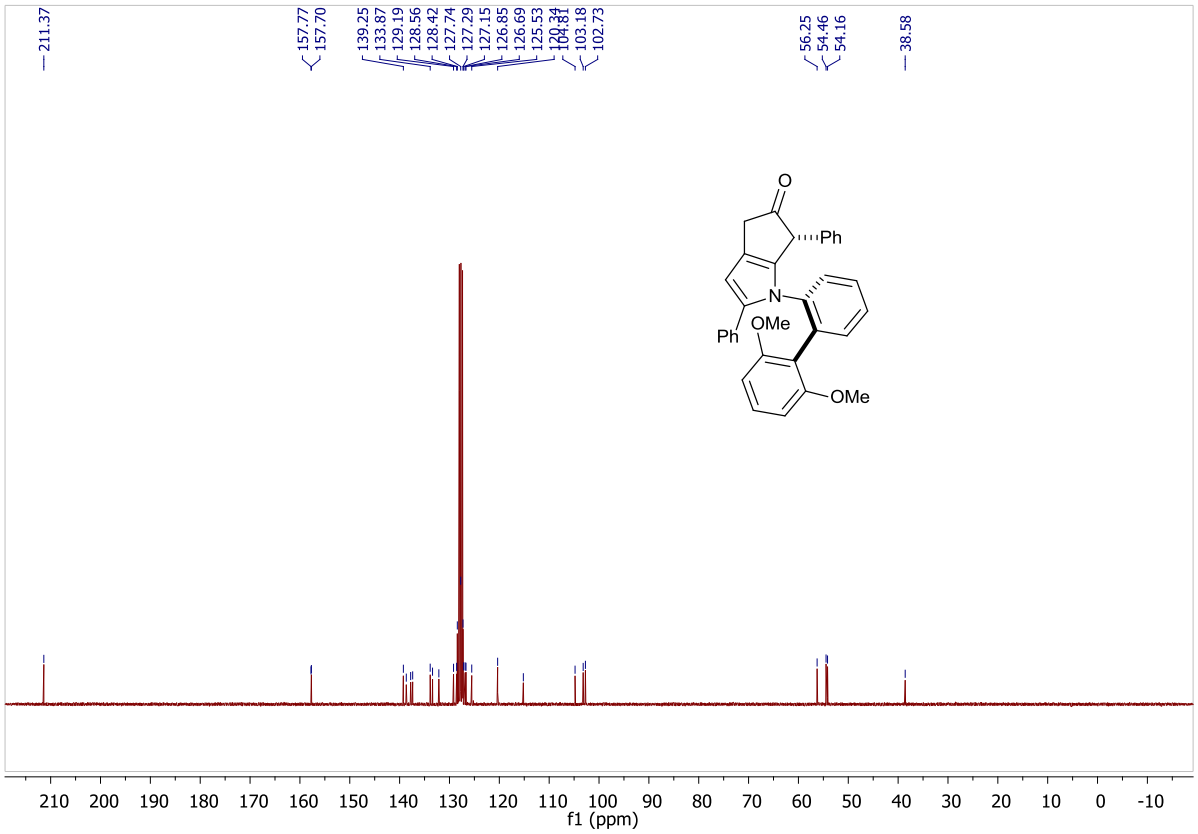
0.0
f1 (ppm)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120.34
104.81
103.18
102.73
56.25
54.46
54.16
38.58
O
Ph
N
Ph
OMe
OMe
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200
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180
170
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100
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30
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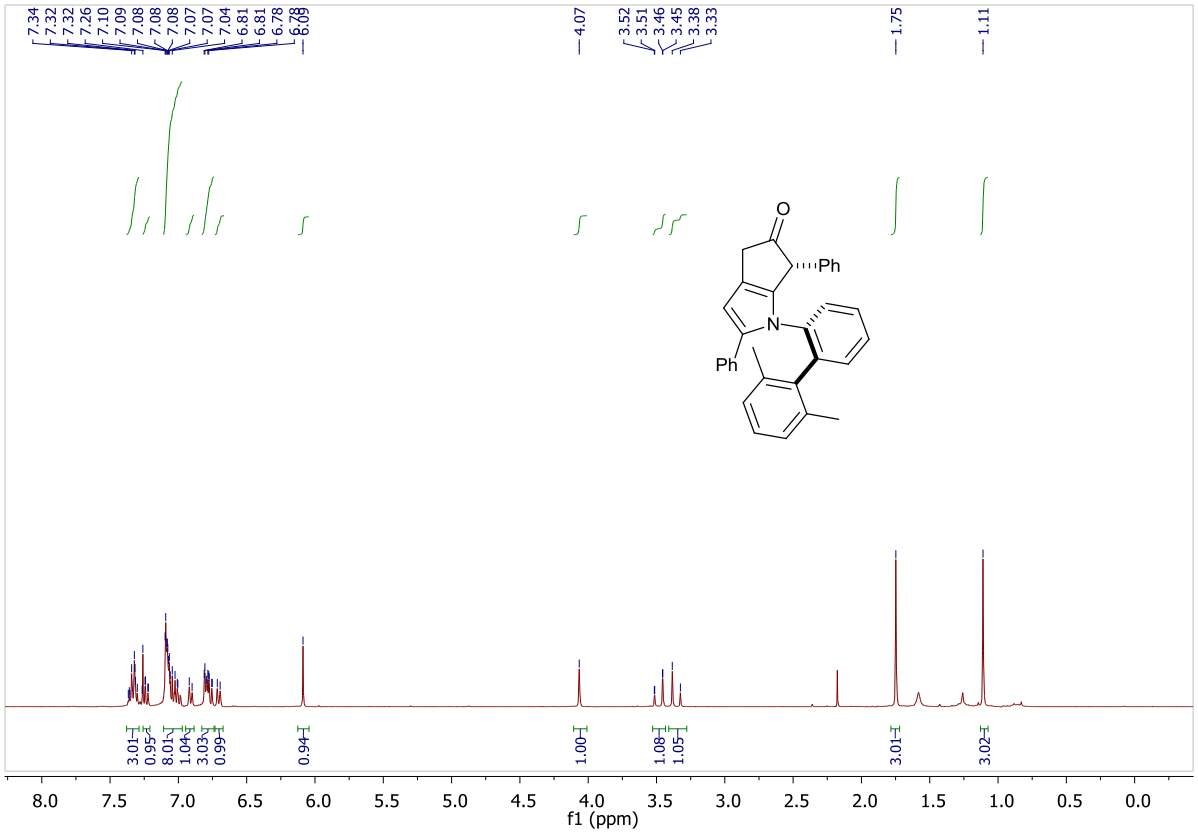
-10
f1 (ppm)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7.07
7.04
6.81
6.78
6.08
4.07
3.52
3.51
3.46
3.45
3.38
3.33
1.75
1.11
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Ph
N
Ph
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0.95
8.01
1.04
3.03
0.99
0.94
1.00
1.08
1.05
3.01
3.02
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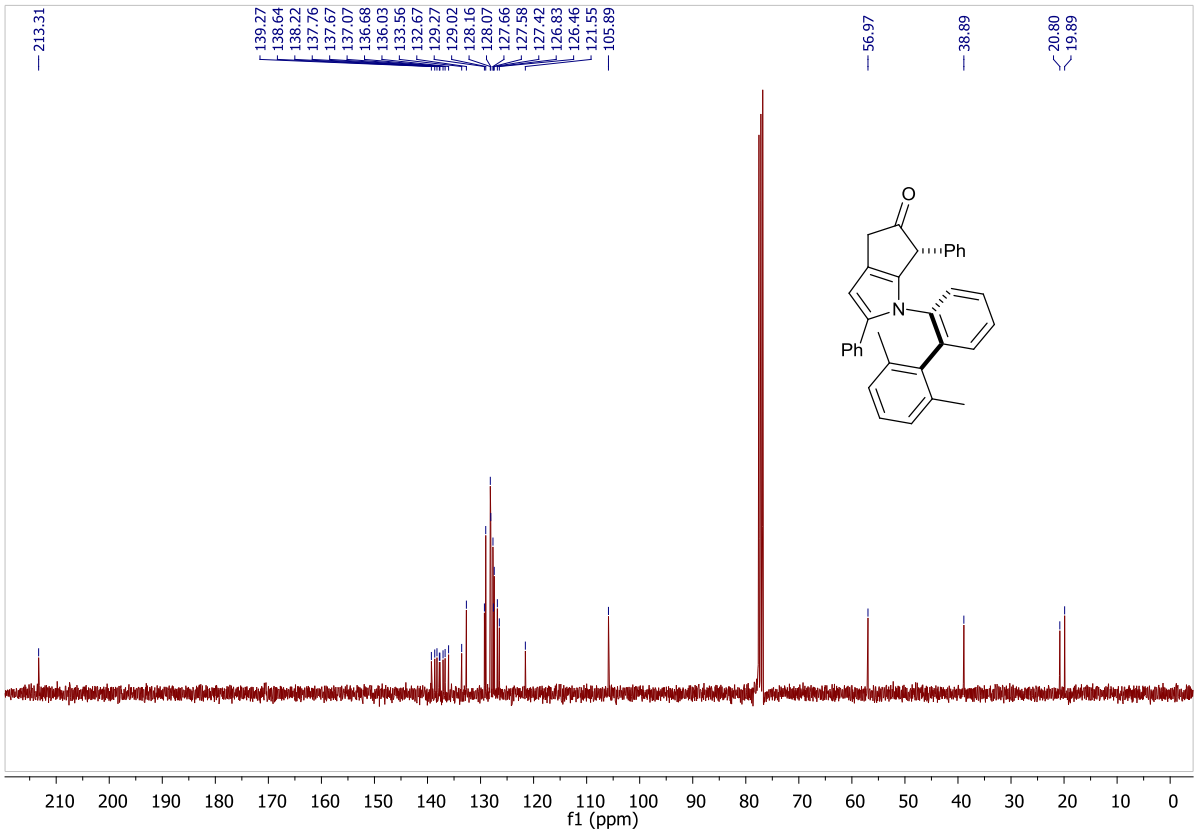
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127.42
126.83
126.46
121.55
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N
Ph
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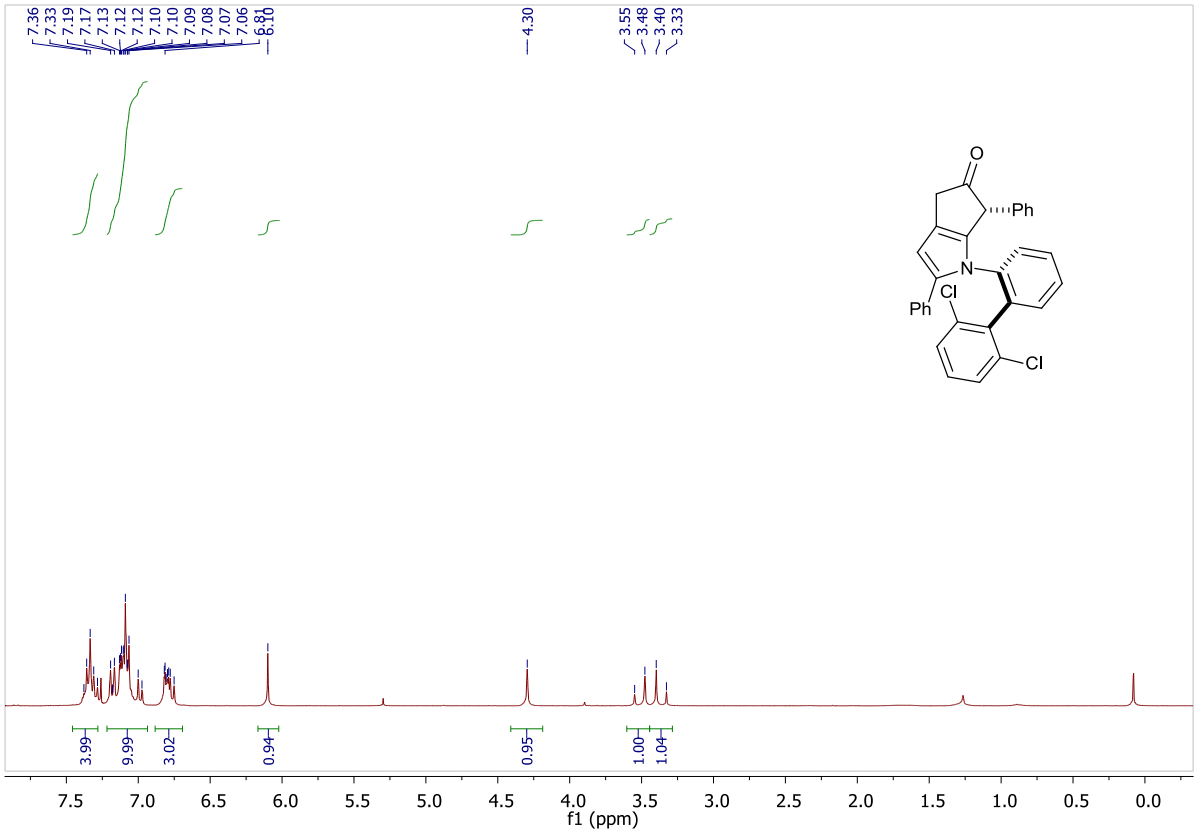
f1 (ppm)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6.81
6.10
4.30
3.55
3.48
3.40
3.33
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Ph
N
Cl
Ph
Cl
3.99
9.99
3.02
0.94
0.95
1.00
1.04
7.5
7.0
6.5
6.0
5.5
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1.0
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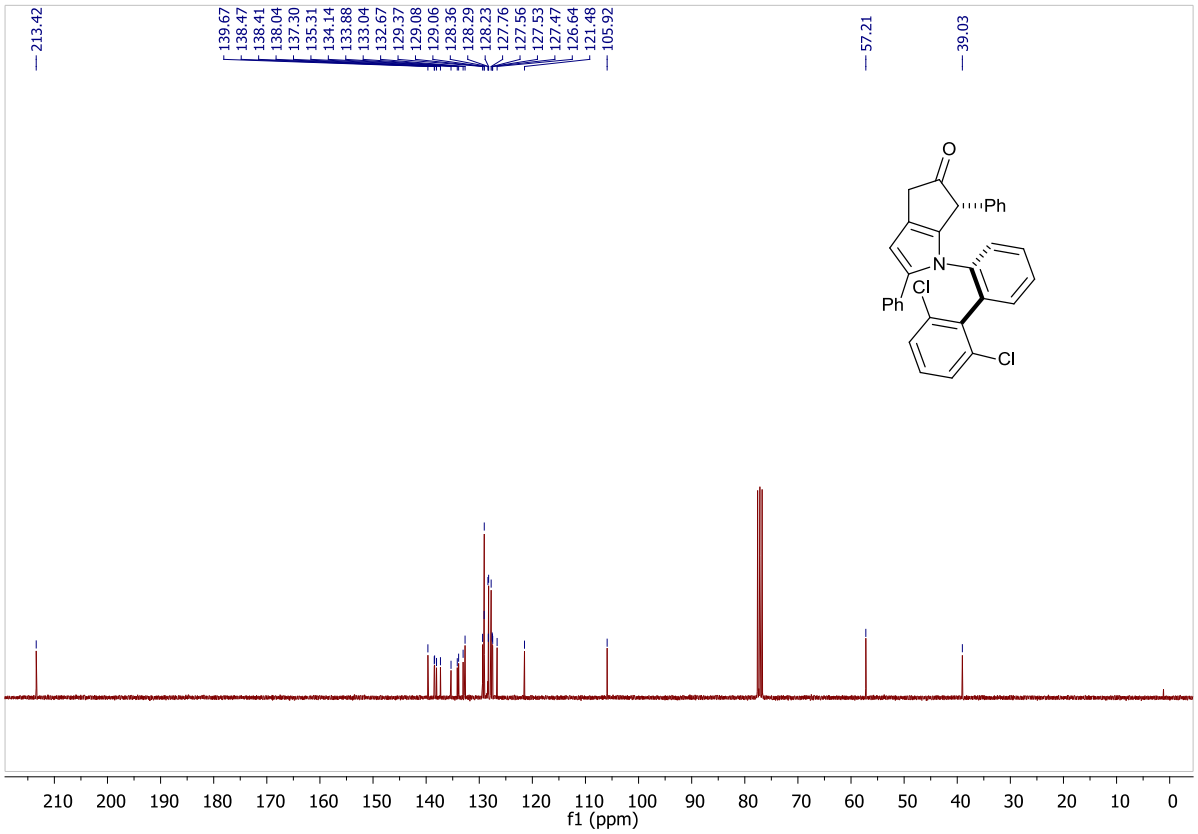
f1 (ppm)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129.08
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128.36
128.29
128.23
127.76
127.56
127.53
127.47
126.64
121.48
105.92
57.21
39.03
O
Ph
N
Cl
Ph
Cl
210
200
190
180
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130
120
110
100
90
80
70
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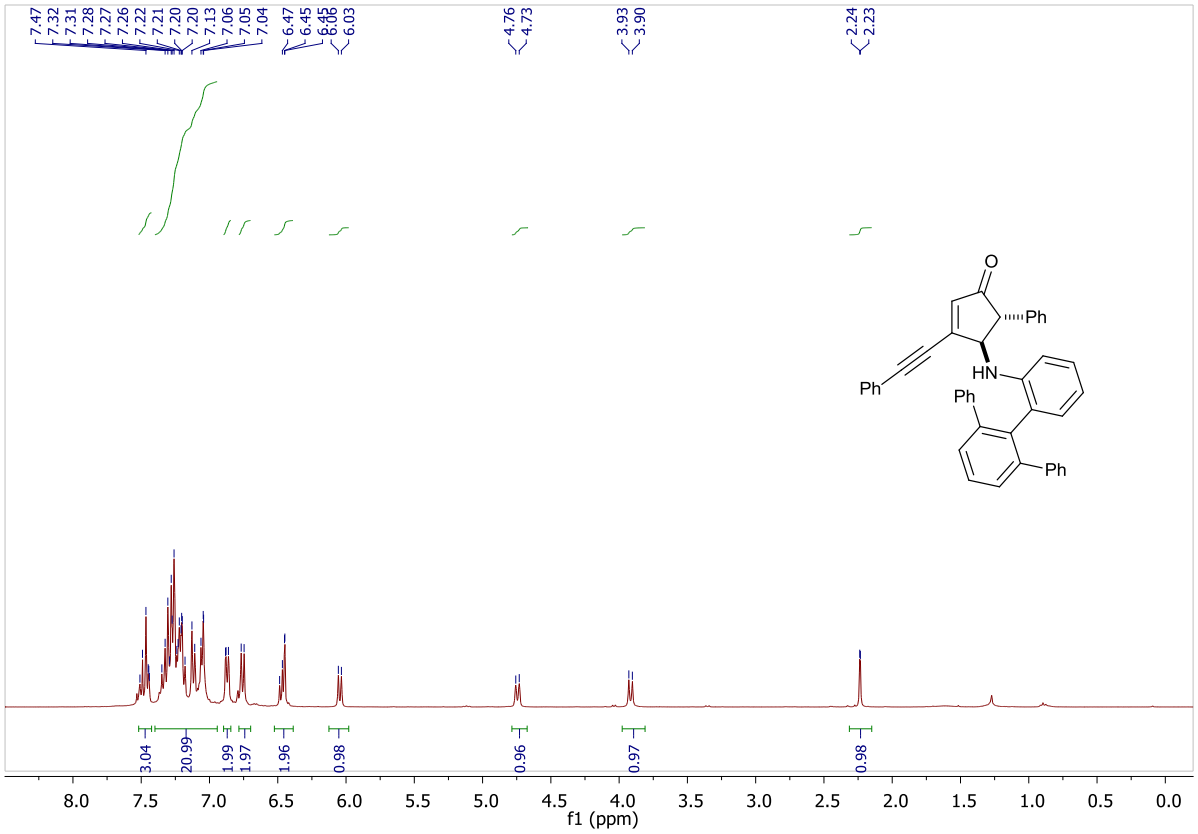
50
40
30
20
10
0
f1 (ppm)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7.20
7.13
7.06
7.05
7.04
6.47
6.45
6.06
6.03
4.76
4.73
3.93
3.90
2.24
2.23
O
Ph
HN
Ph
Ph
Ph
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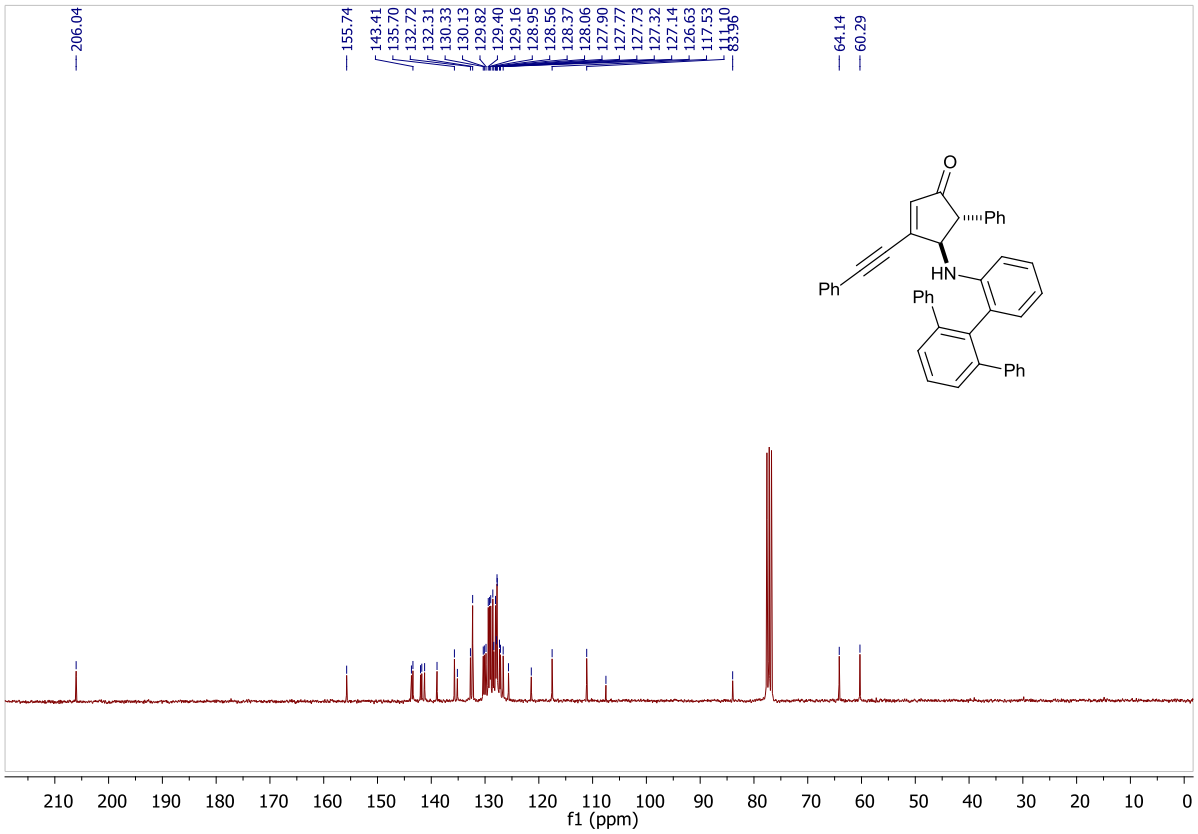
20.99
1.99
1.97
1.96
0.98
0.96
0.97
0.98
f1 (ppm)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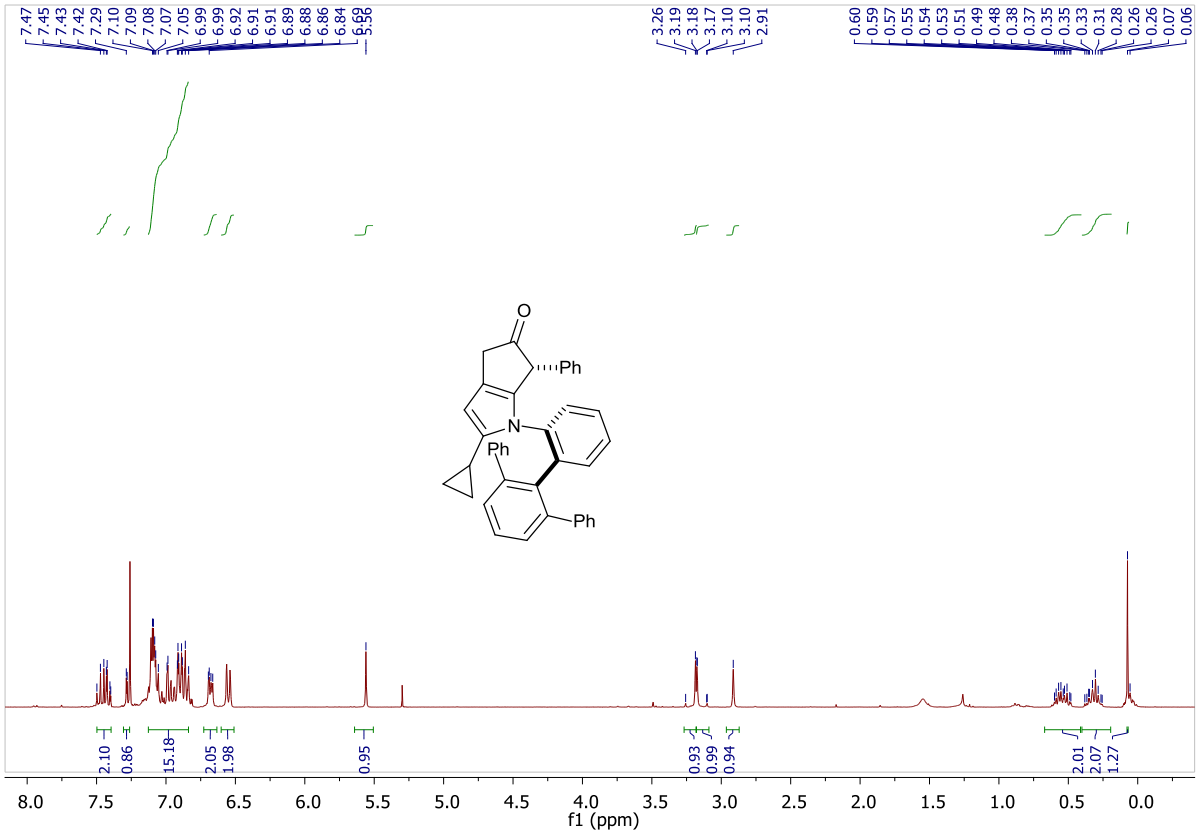
64.14
60.29
O
Ph
HN
Ph
Ph
Ph
f1 (ppm)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6.84
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3.19
3.18
3.17
3.10
3.10
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0.38
0.37
0.35
0.35
0.33
0.31
0.28
0.26
0.26
0.07
0.06
O
Ph
N
Ph
Ph
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15.18
2.05
1.98
0.95
0.93
0.99
0.94
2.01
2.07
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7.0
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6.0
5.5
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2.5
2.0
1.5
1.0
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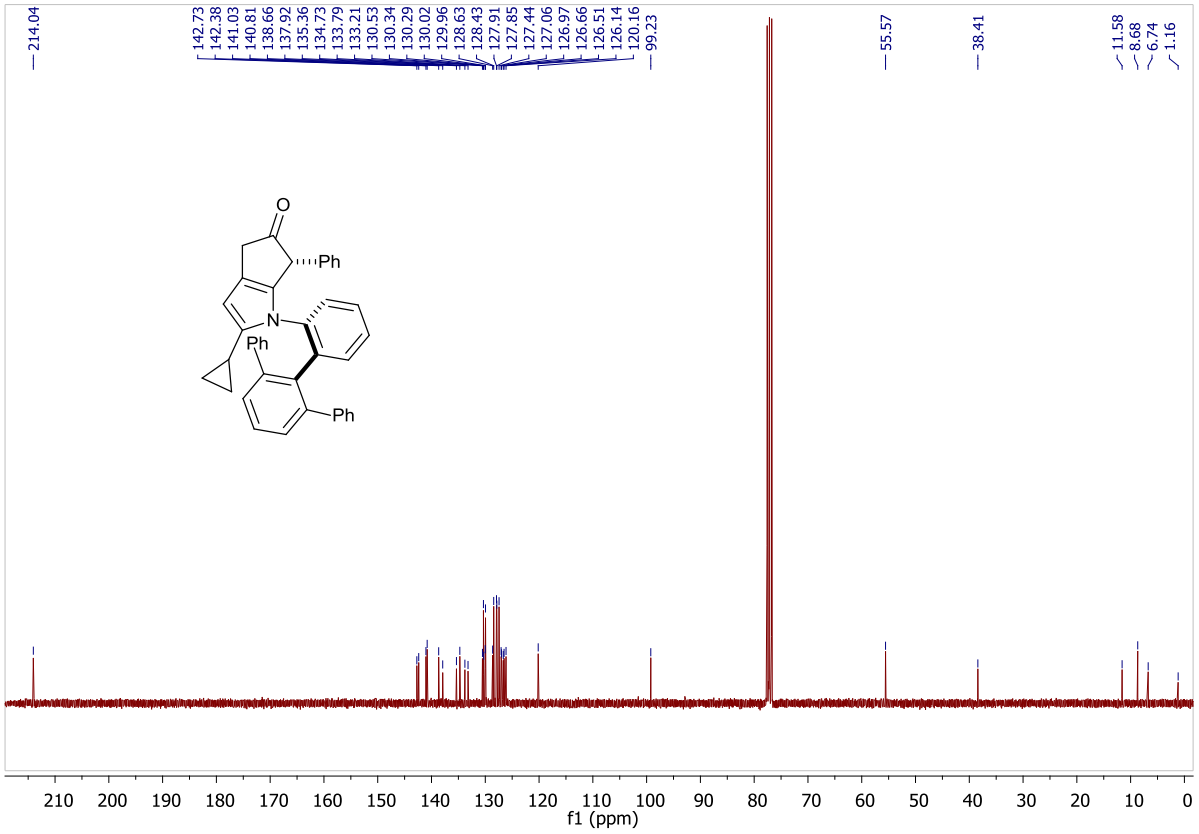
0.0
f1 (ppm)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130.02
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126.51
126.14
120.16
99.23
55.57
38.41
11.58
8.68
6.74
1.16
O
Ph
N
Ph
Ph
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200
190
180
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110
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90
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70
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50
40
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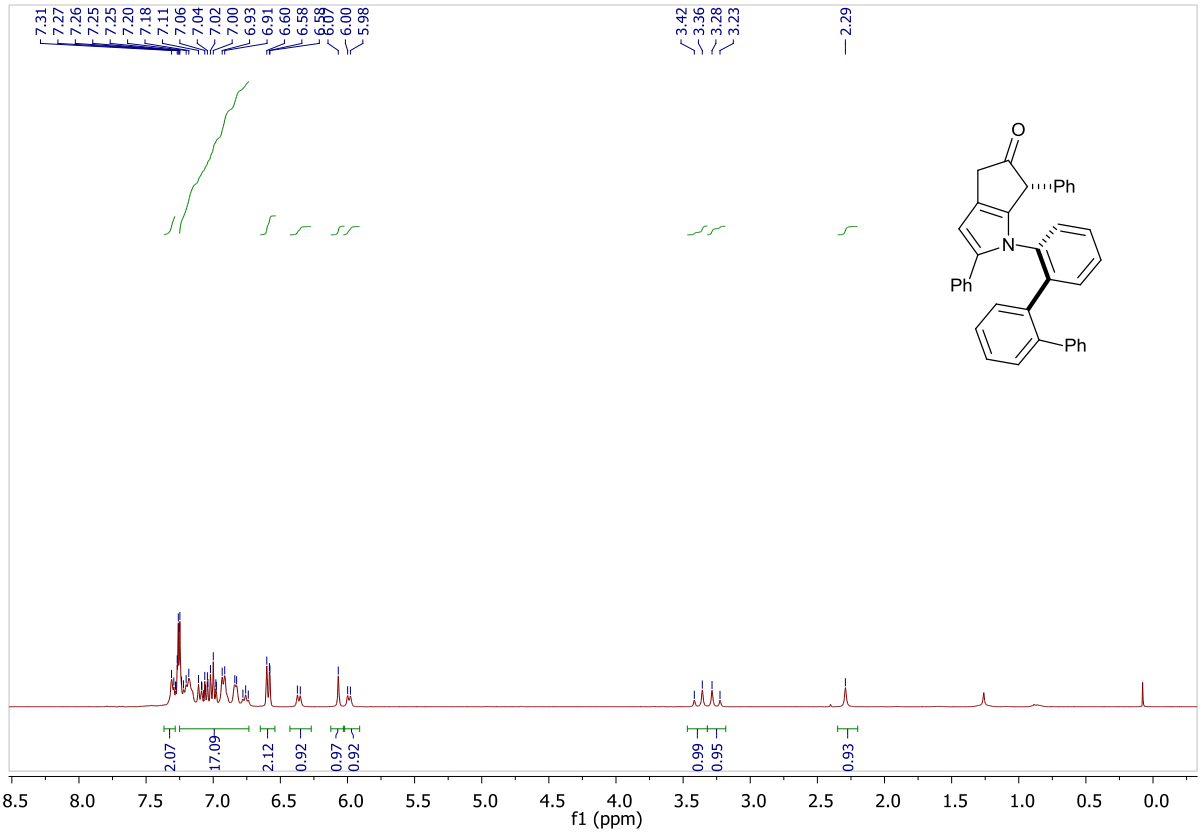
10
0
f1 (ppm)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6.91
6.60
6.58
6.58
6.07
6.00
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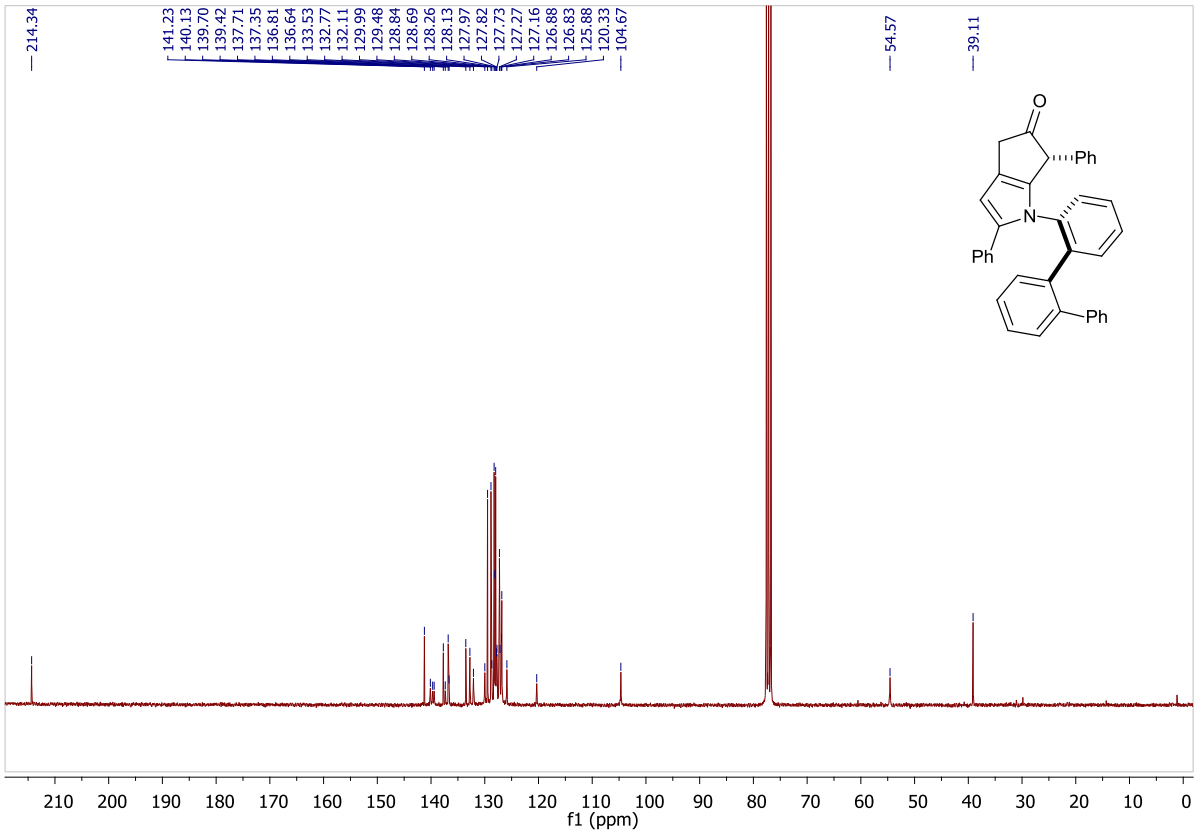
3.42
3.36
3.28
3.23
2.29
O
Ph
N
Ph
Ph
2.07
17.09
2.12
0.92
0.97
0.92
0.99
0.95
0.93
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.16
126.88
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39.11
O
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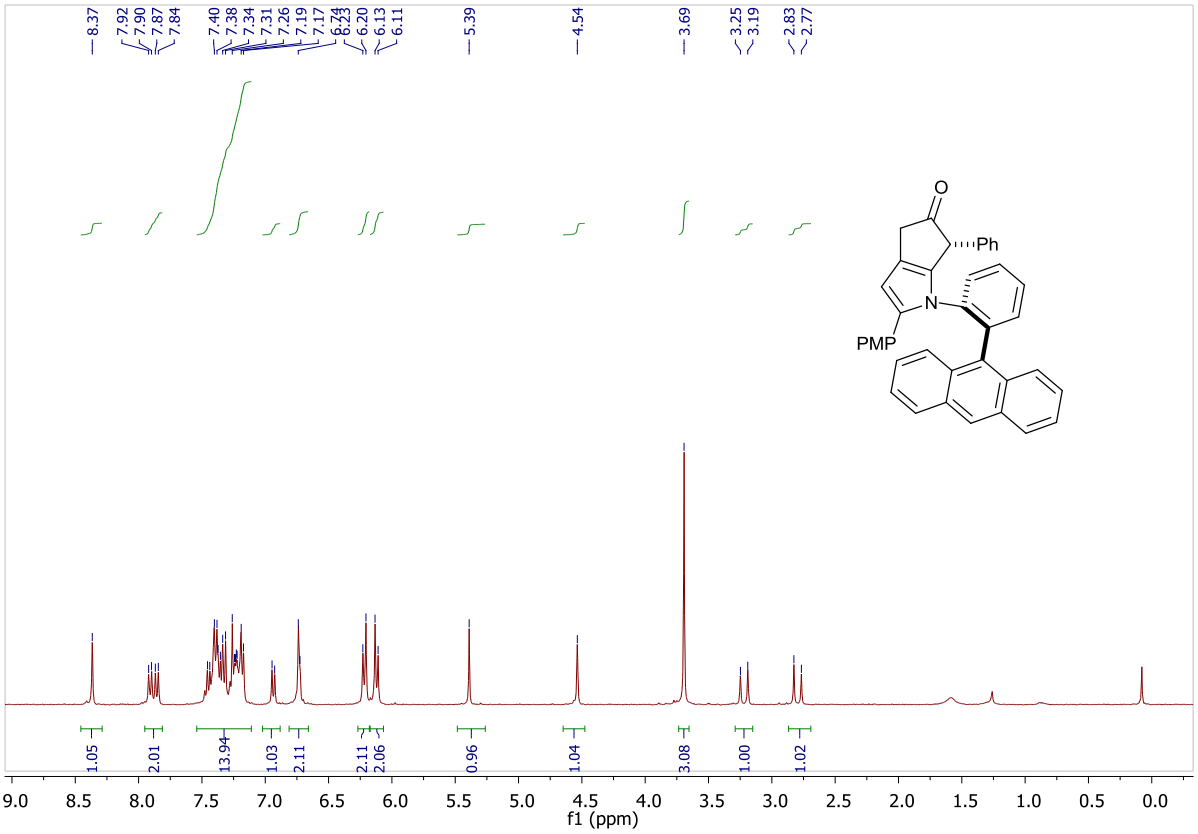
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6.11
5.39
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3.69
3.25
3.19
2.83
2.77
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Ph
N
PMP
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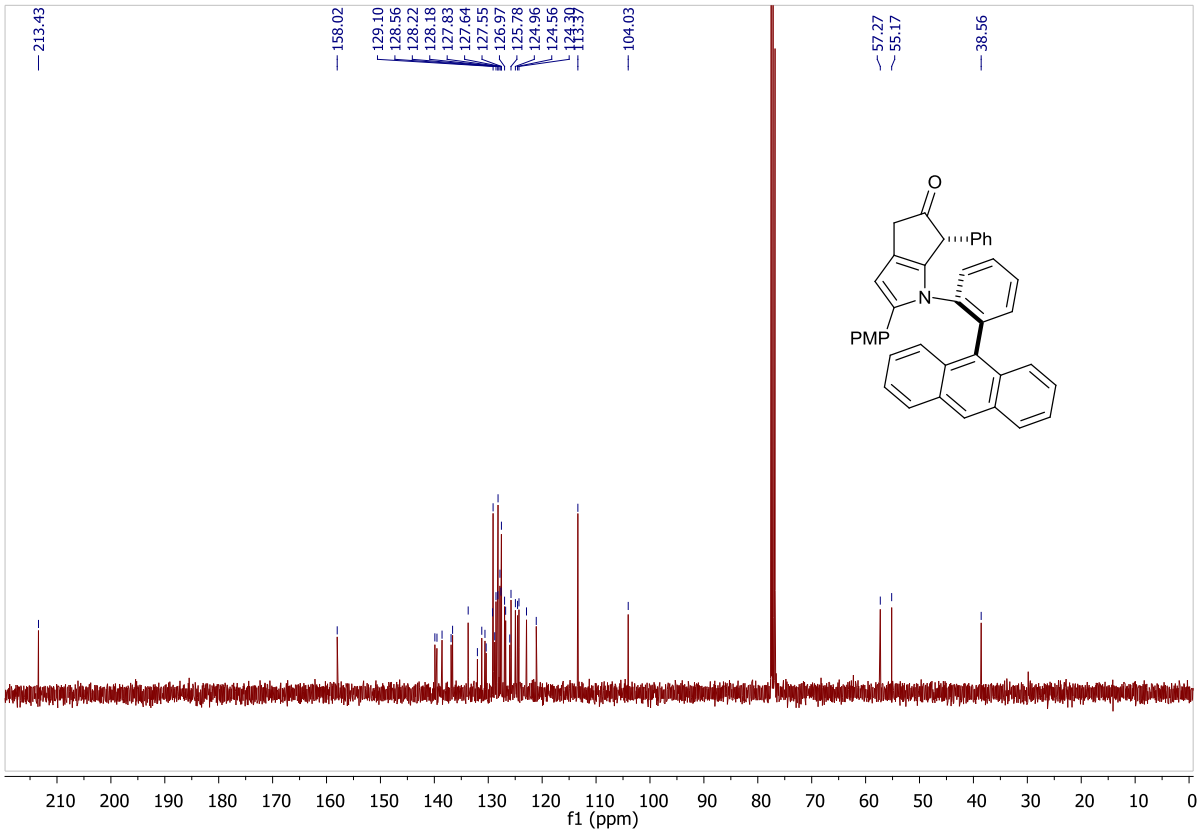
1.04
3.08
1.00
1.02
f1 (ppm)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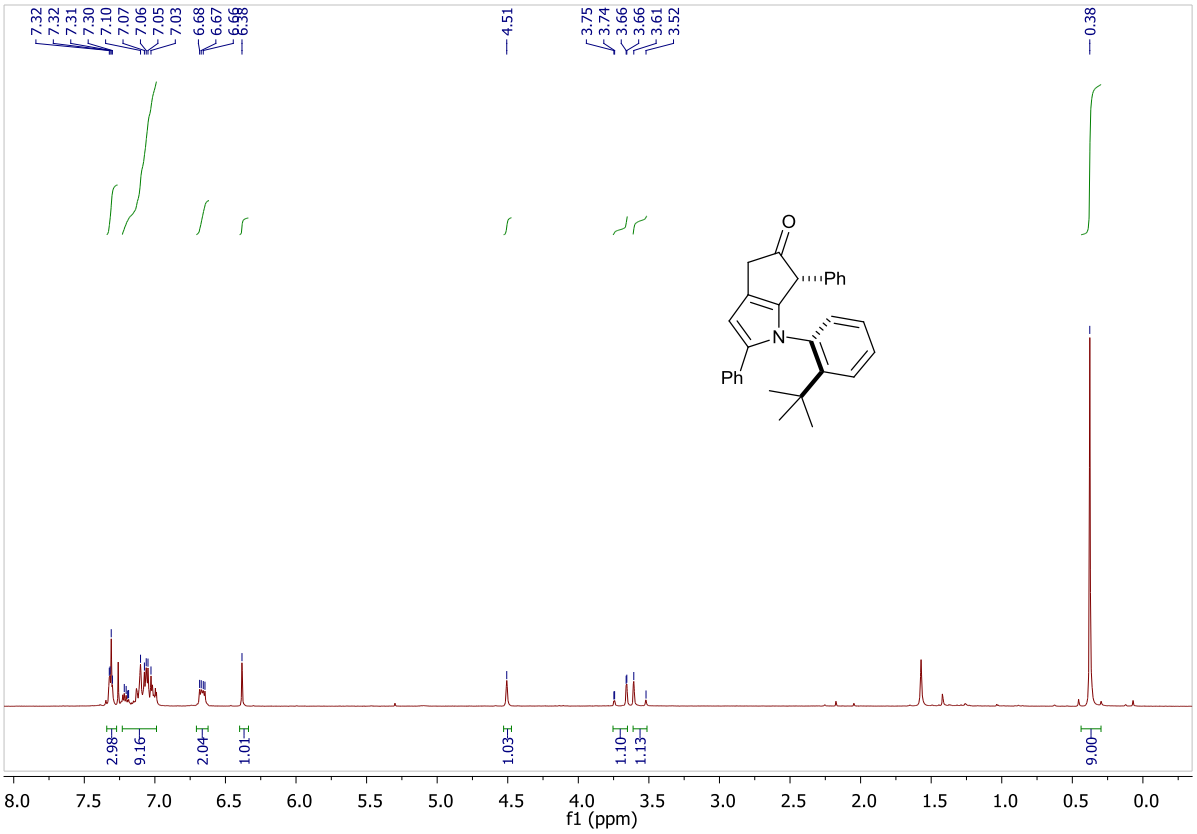
PMP
f1 (ppm)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3.61
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Ph
N
Ph
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9.16
2.04
1.01
1.03
1.10
1.13
9.00
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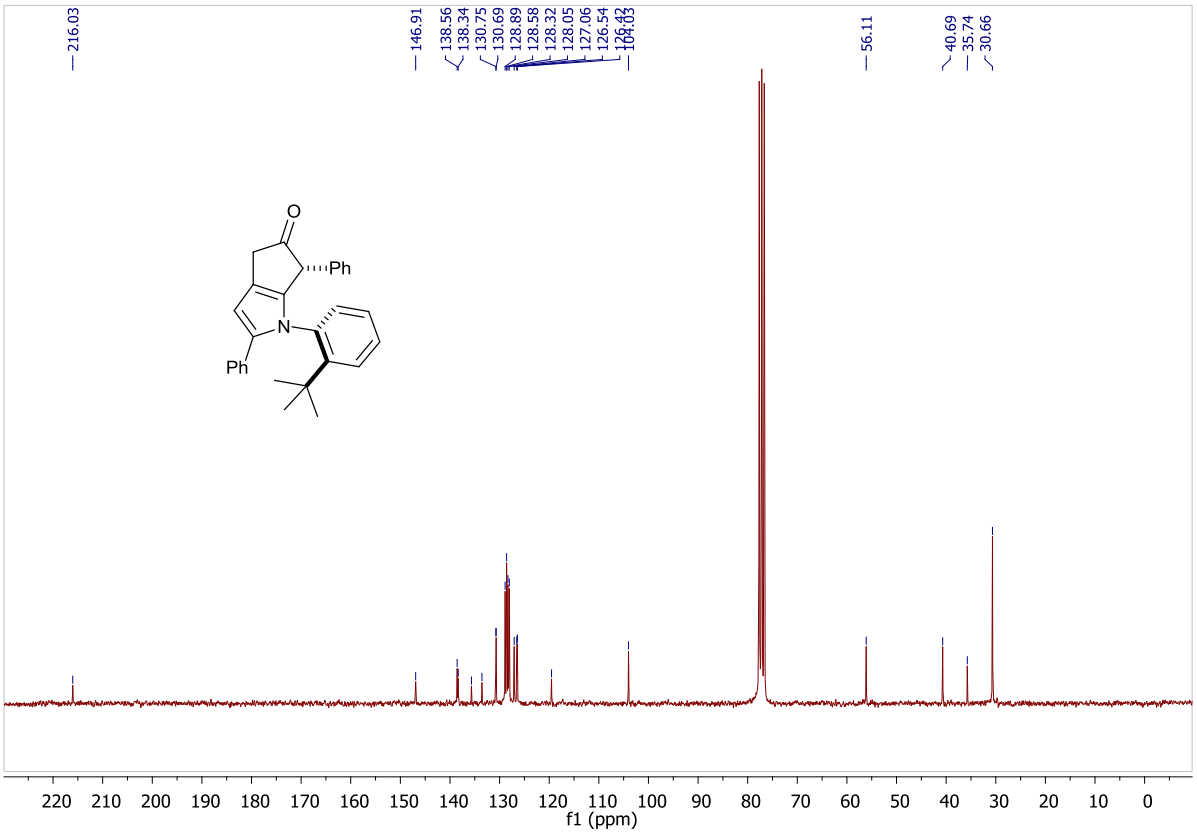
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N
Ph
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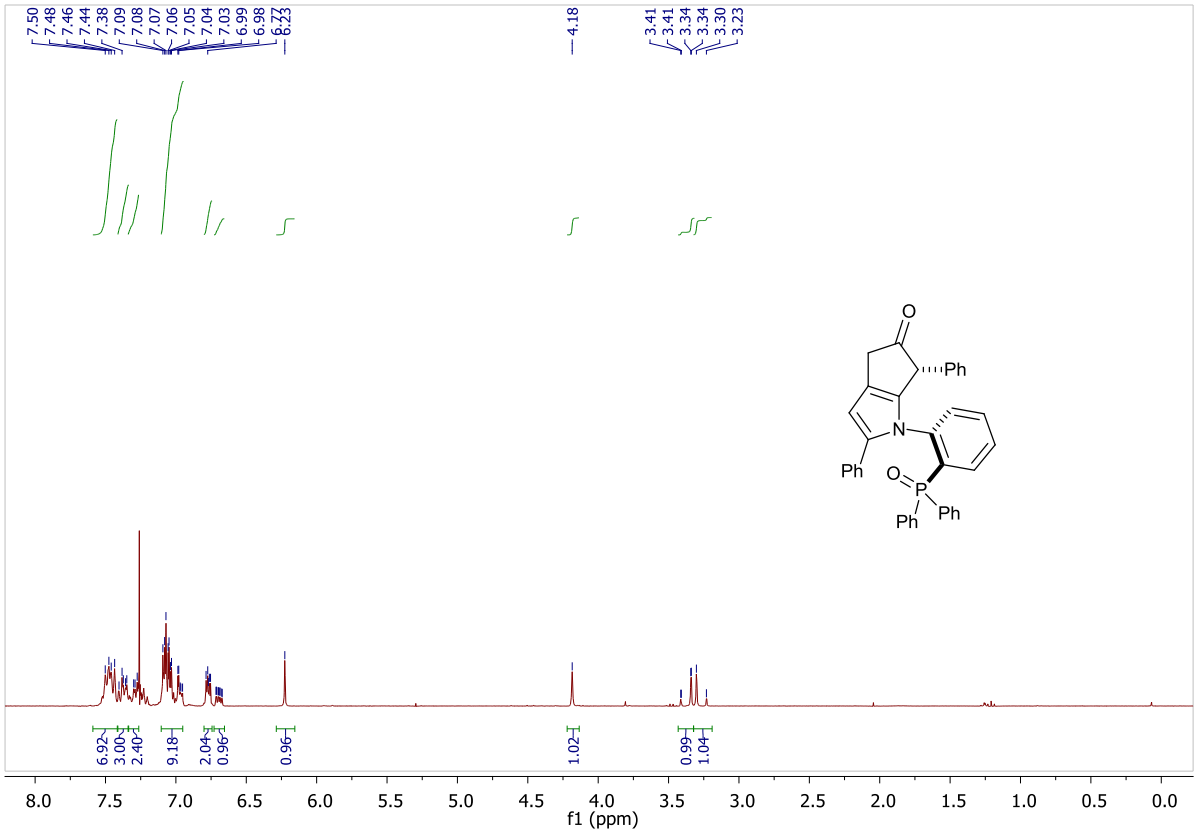
f1 (ppm)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3.34
3.34
3.30
3.23
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Ph
N
Ph
O
P
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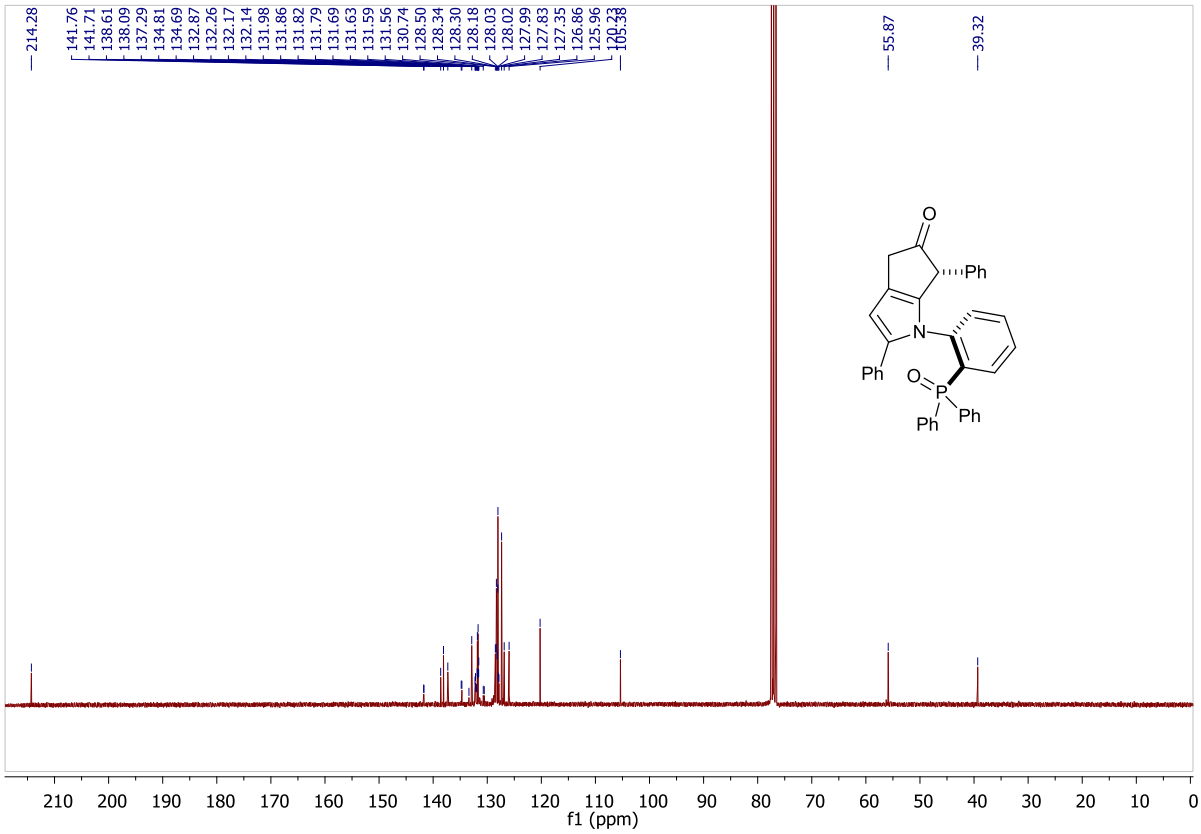
1.04
f1 (ppm)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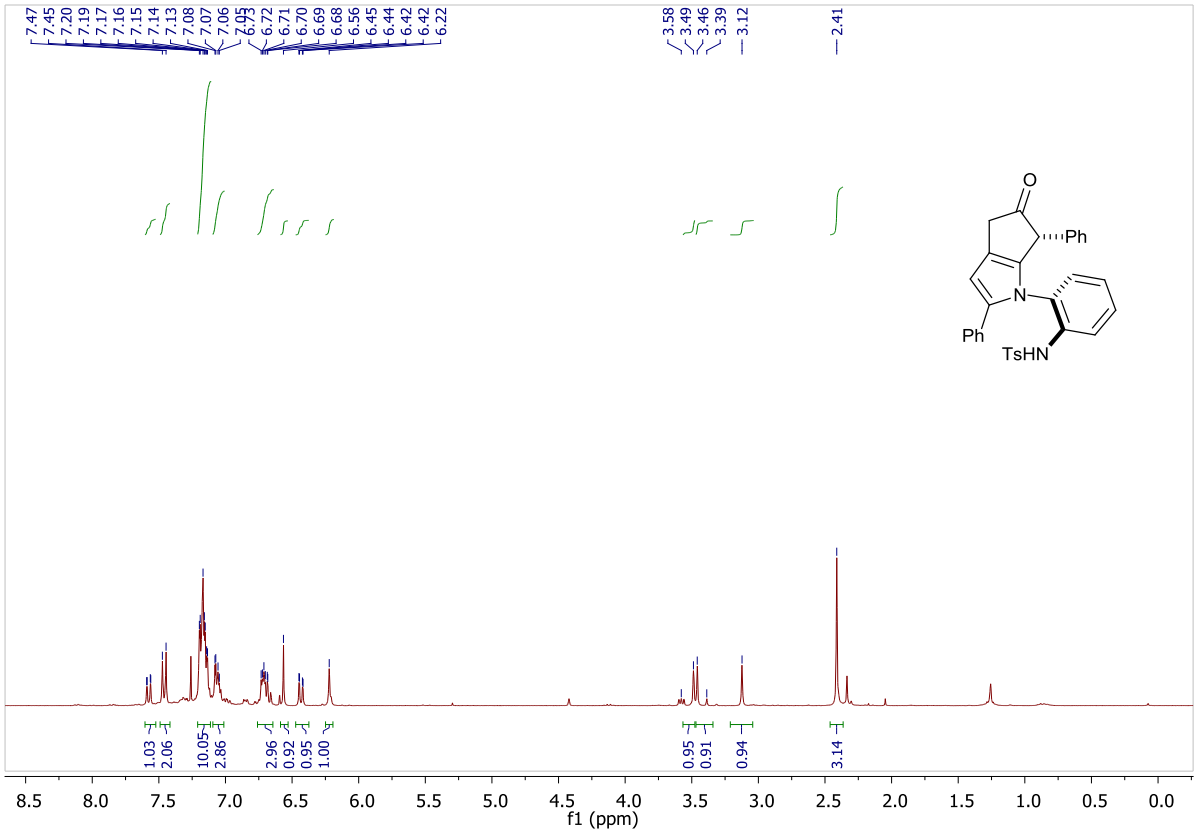
N
Ph
O
P
Ph
Ph
f1 (ppm)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Ph
N
Ph
TsHN
1.03
2.06
10.05
2.86
2.96
0.92
0.95
1.00
0.95
0.91
0.94
3.14
8.5
8.0
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7.0
6.5
6.0
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1.0
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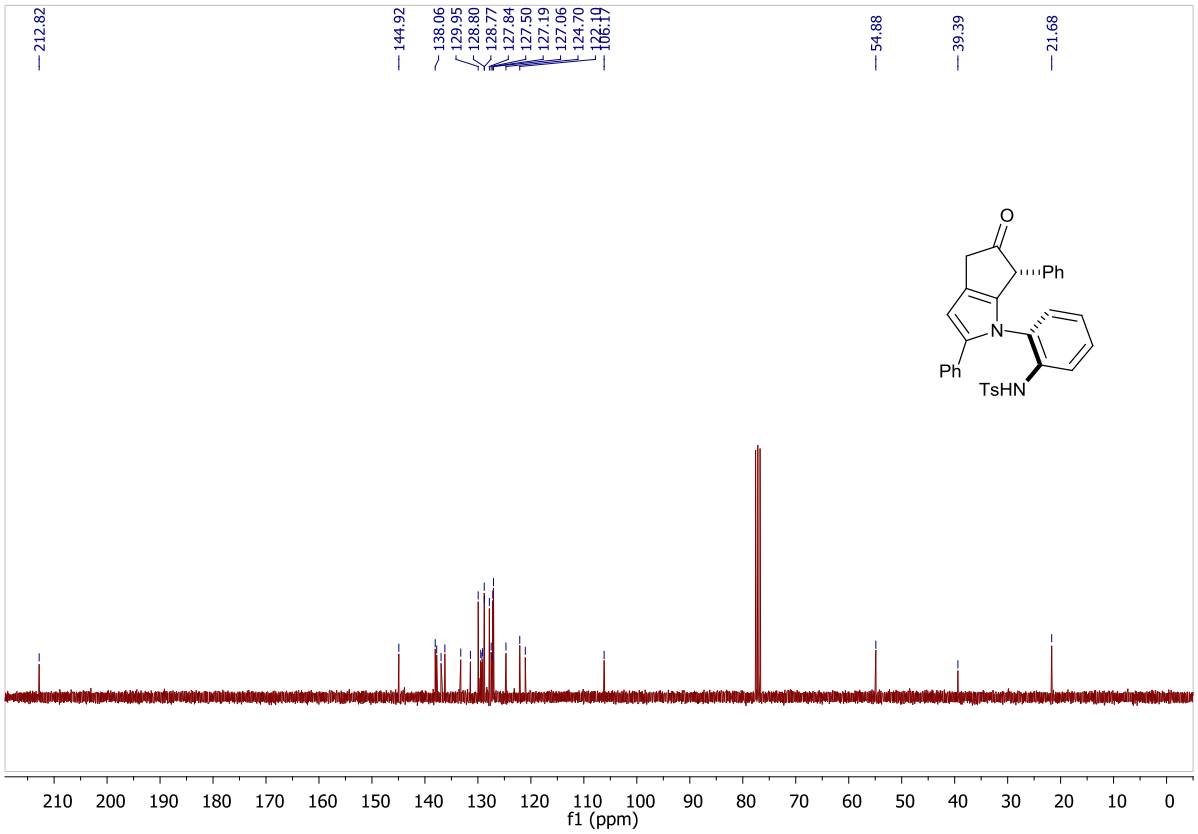
0.0
f1 (ppm)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O
Ph
N
Ph
TsHN
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200
190
180
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130
120
110
100
90
80
70
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50
40
30
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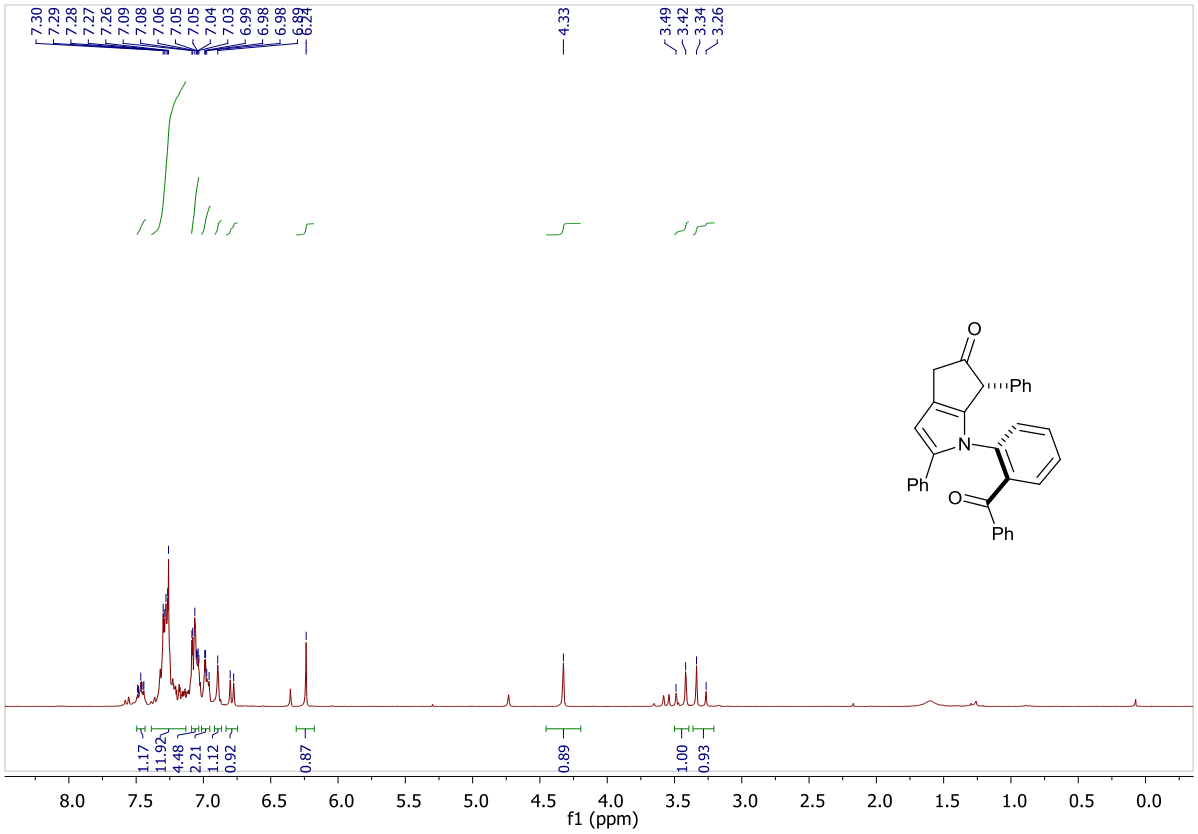
10
0
f1 (ppm)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3.42
3.34
3.26
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Ph
N
Ph
O
Ph
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1.00
0.93
8.0
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6.0
5.5
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3.5
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1.0
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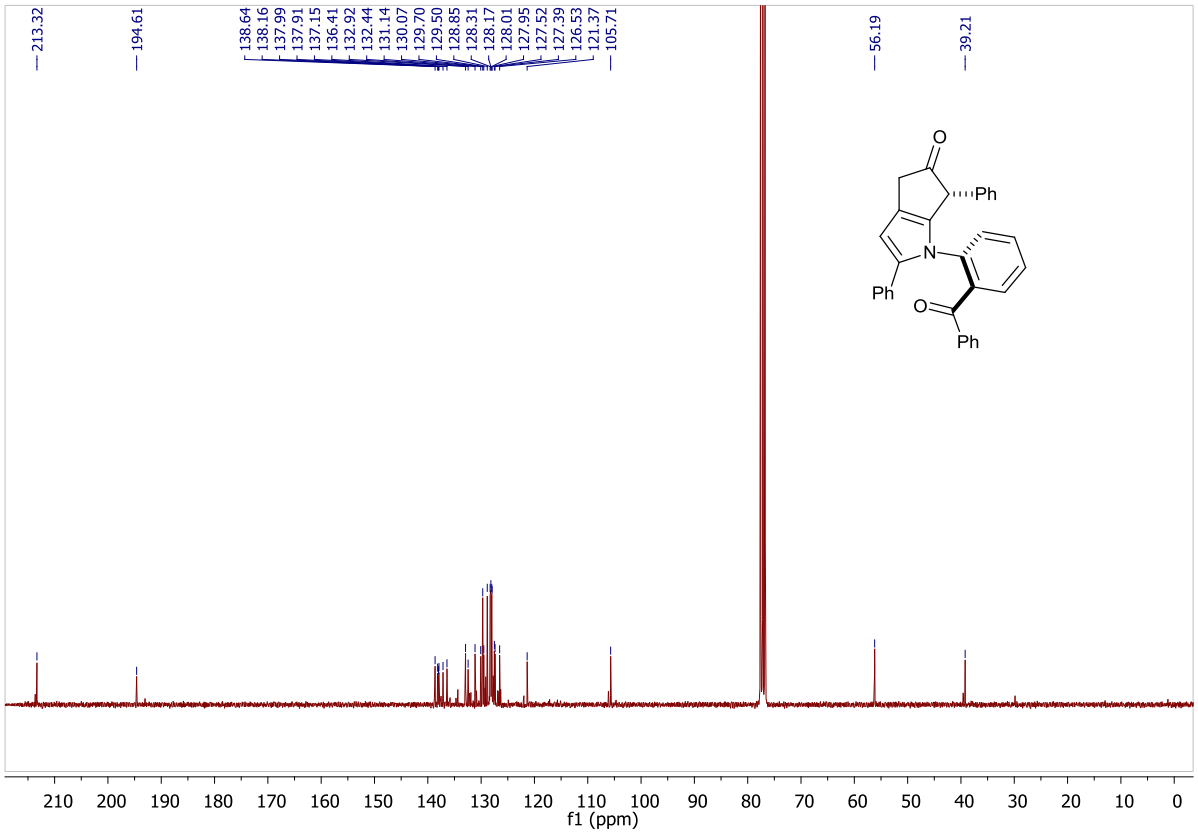
0.0
f1 (ppm)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O
Ph
N
Ph
O
Ph
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200
190
180
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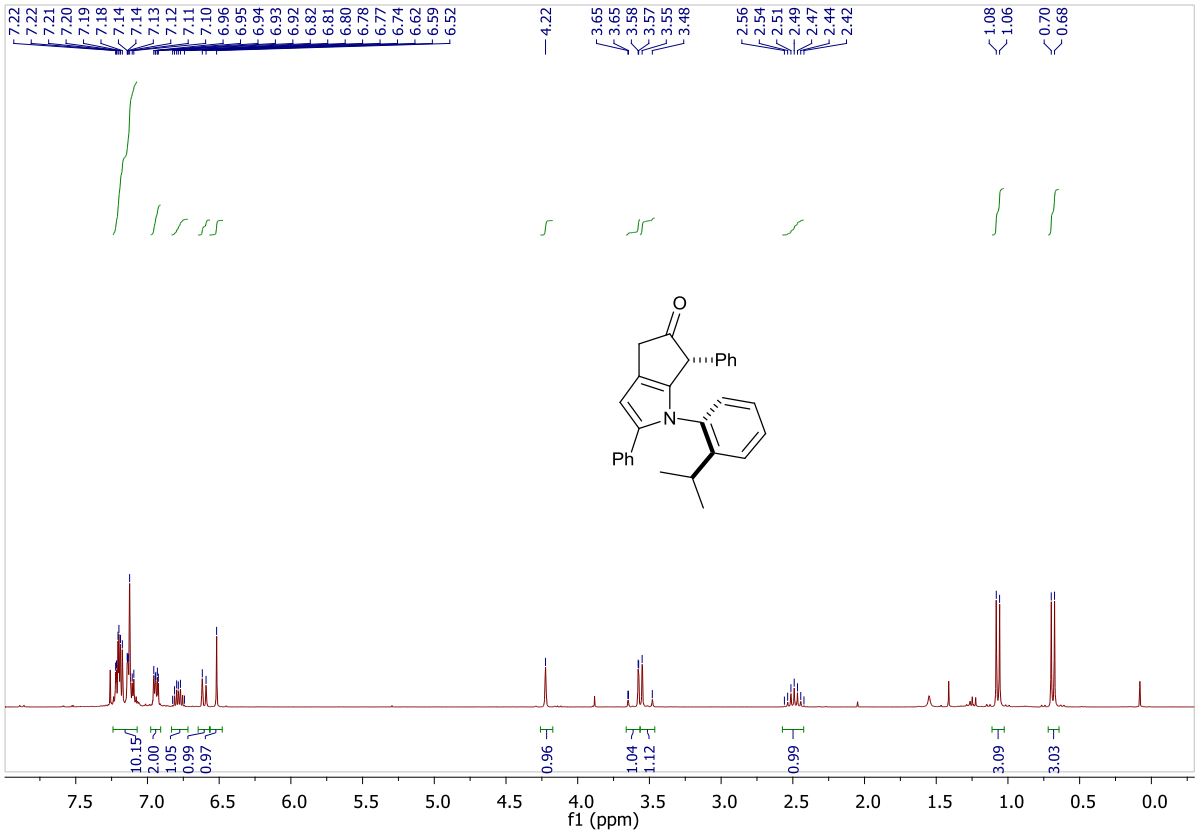
f1 (ppm)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3.57
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2.42
1.08
1.06
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O
Ph
N
Ph
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2.00
1.05
0.99
0.97
0.96
1.04
1.12
0.99
3.09
3.03
7.5
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6.0
5.5
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1.0
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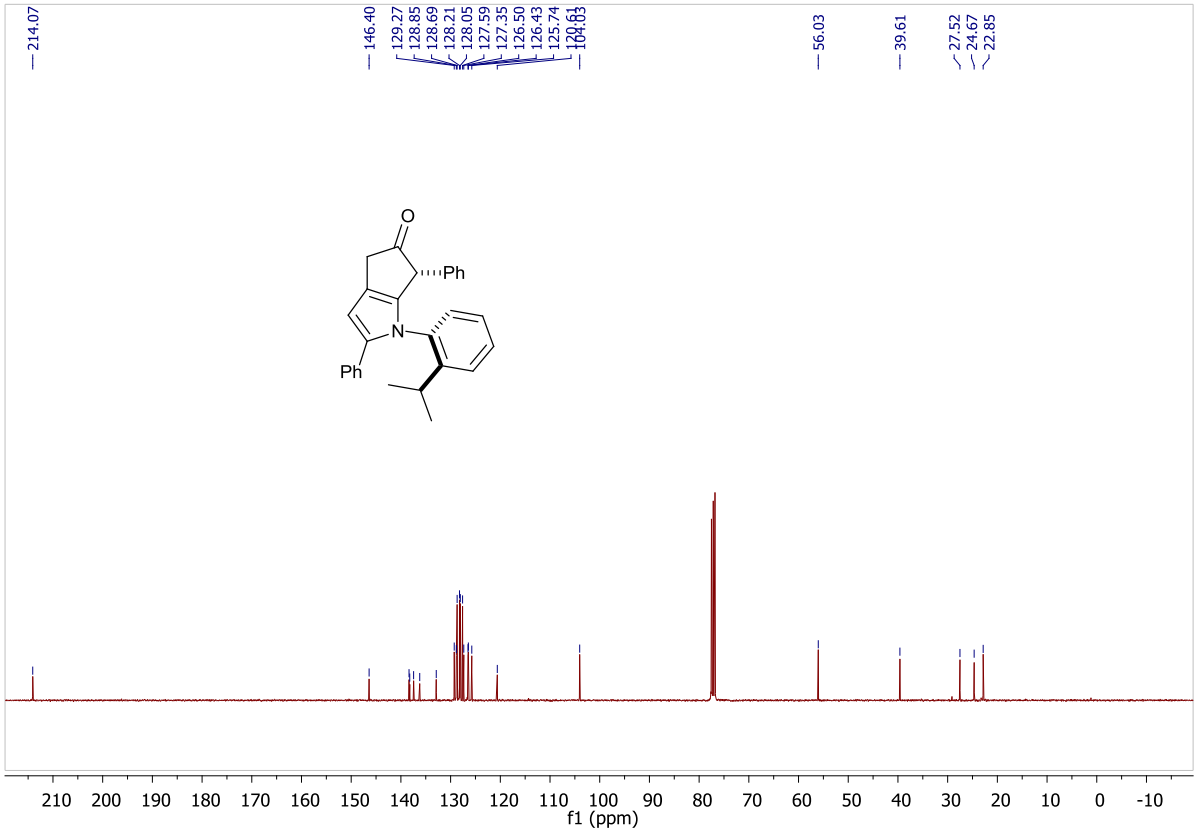
f1 (ppm)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125.74
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56.03
39.61
27.52
24.67
22.85
O
Ph
N
Ph
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200
190
180
170
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100
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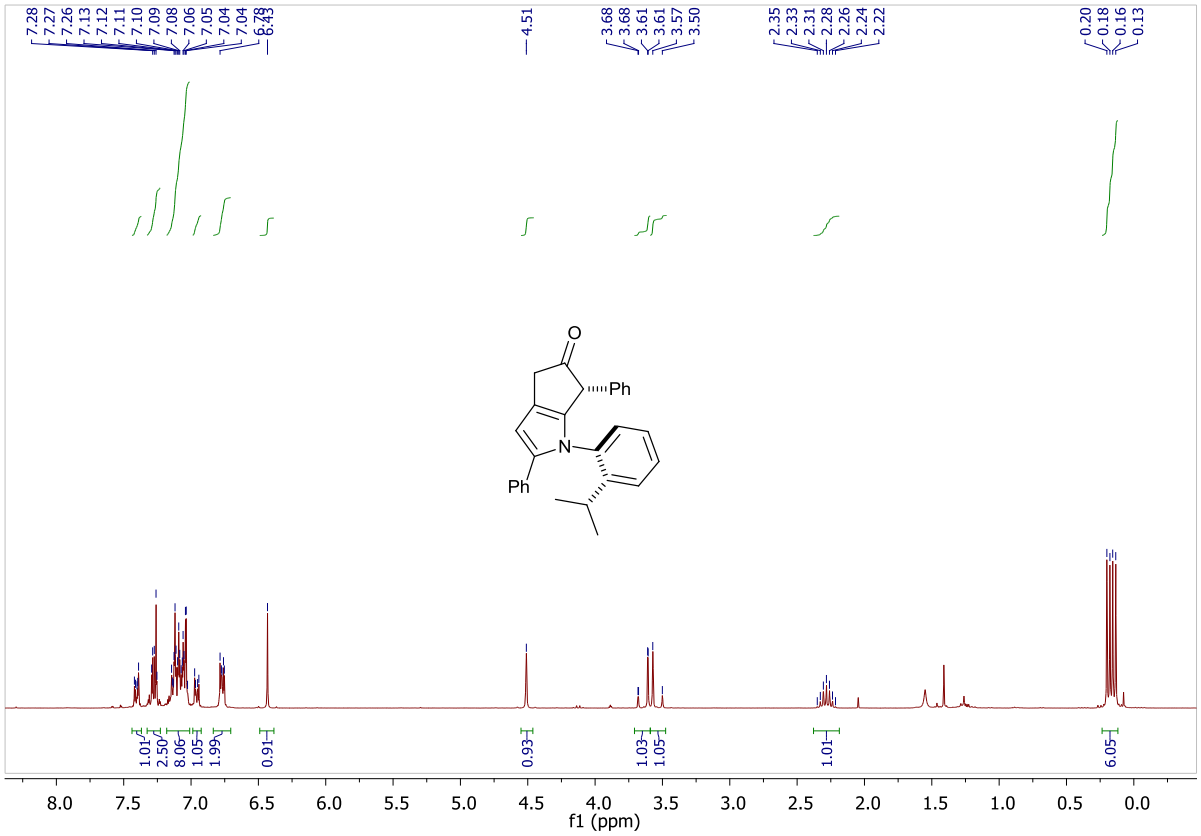
f1 (ppm)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3.68
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2.26
2.24
2.22
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0.18
0.16
0.13
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Ph
N
Ph
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1.05
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0.93
1.03
1.05
1.01
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7.0
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2.0
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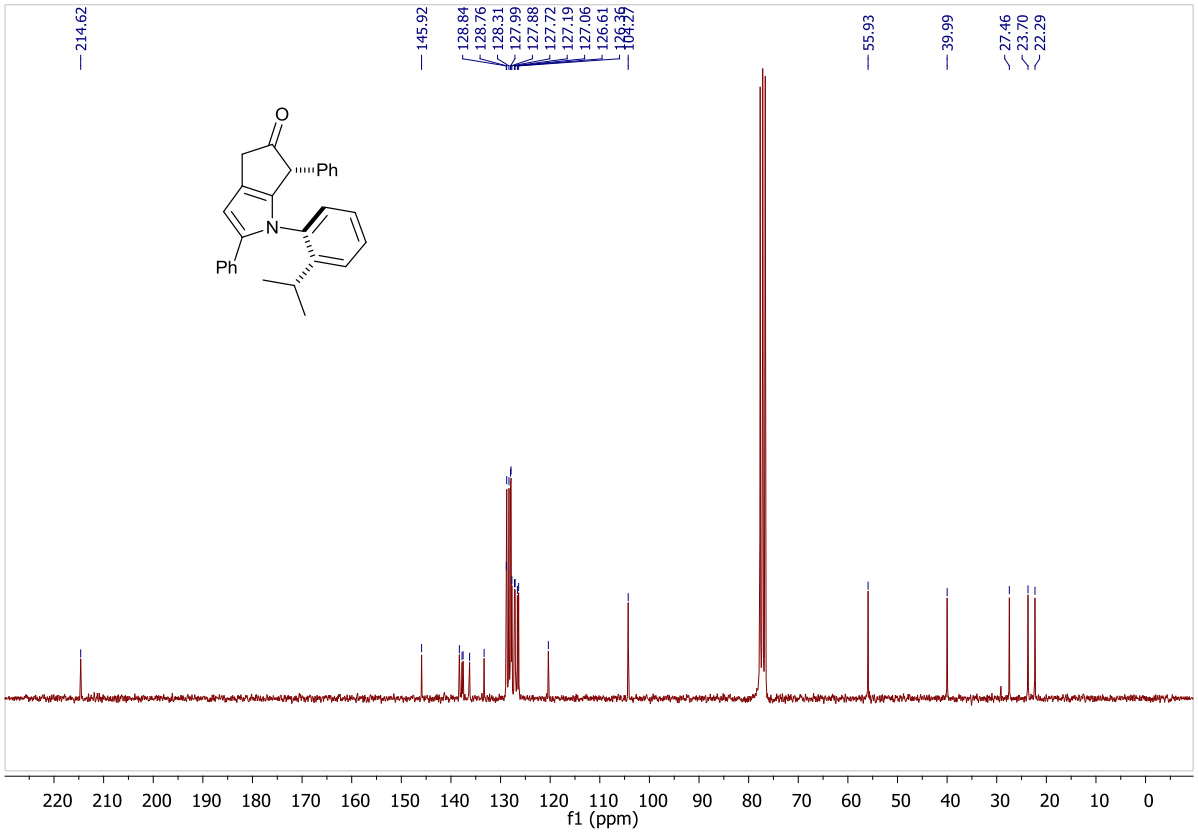
f1 (ppm)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22.29
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Ph
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180
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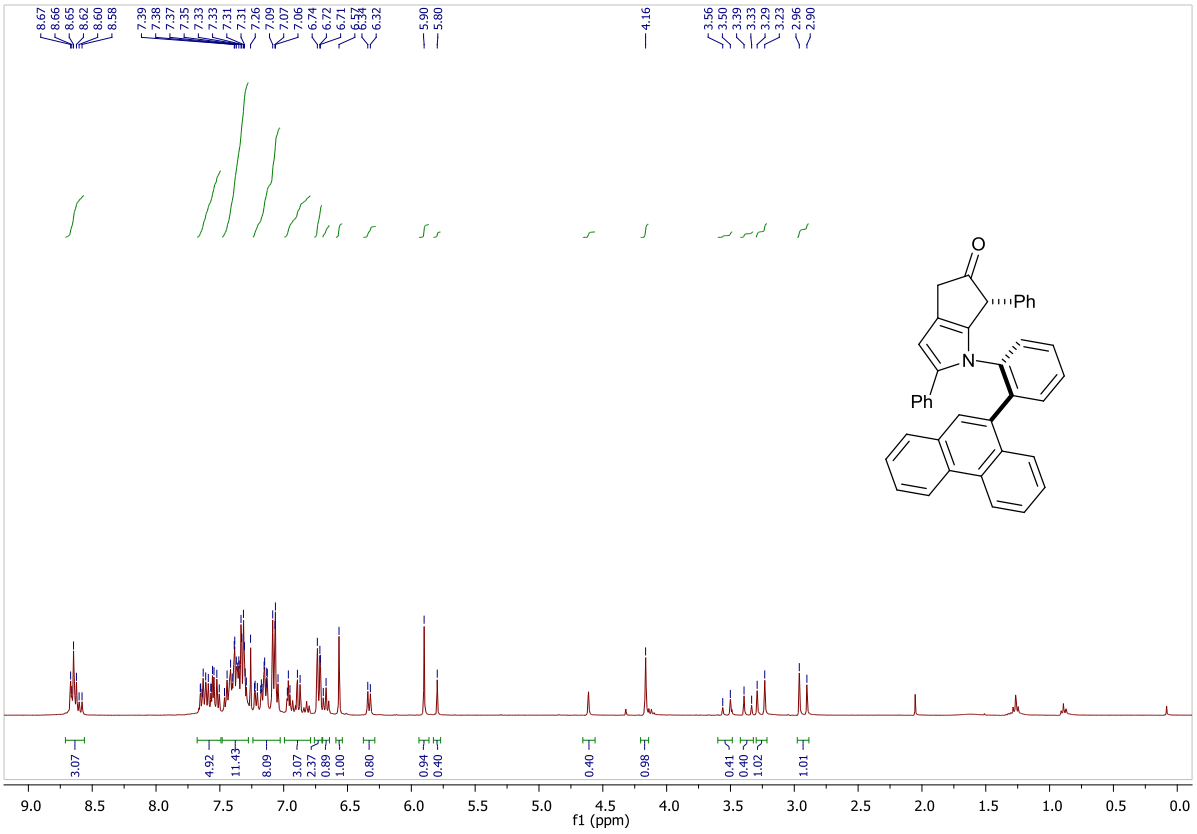
f1 (ppm)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0.40
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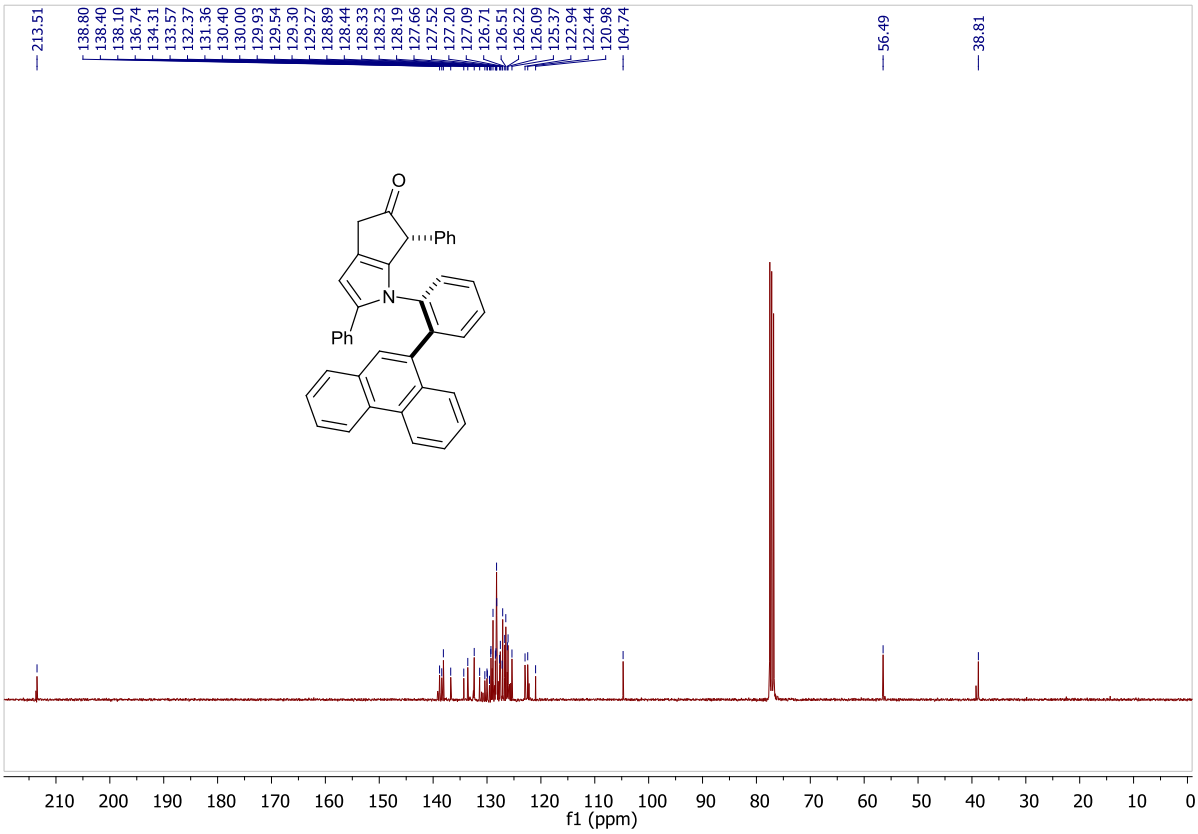
1.01
f1 (ppm)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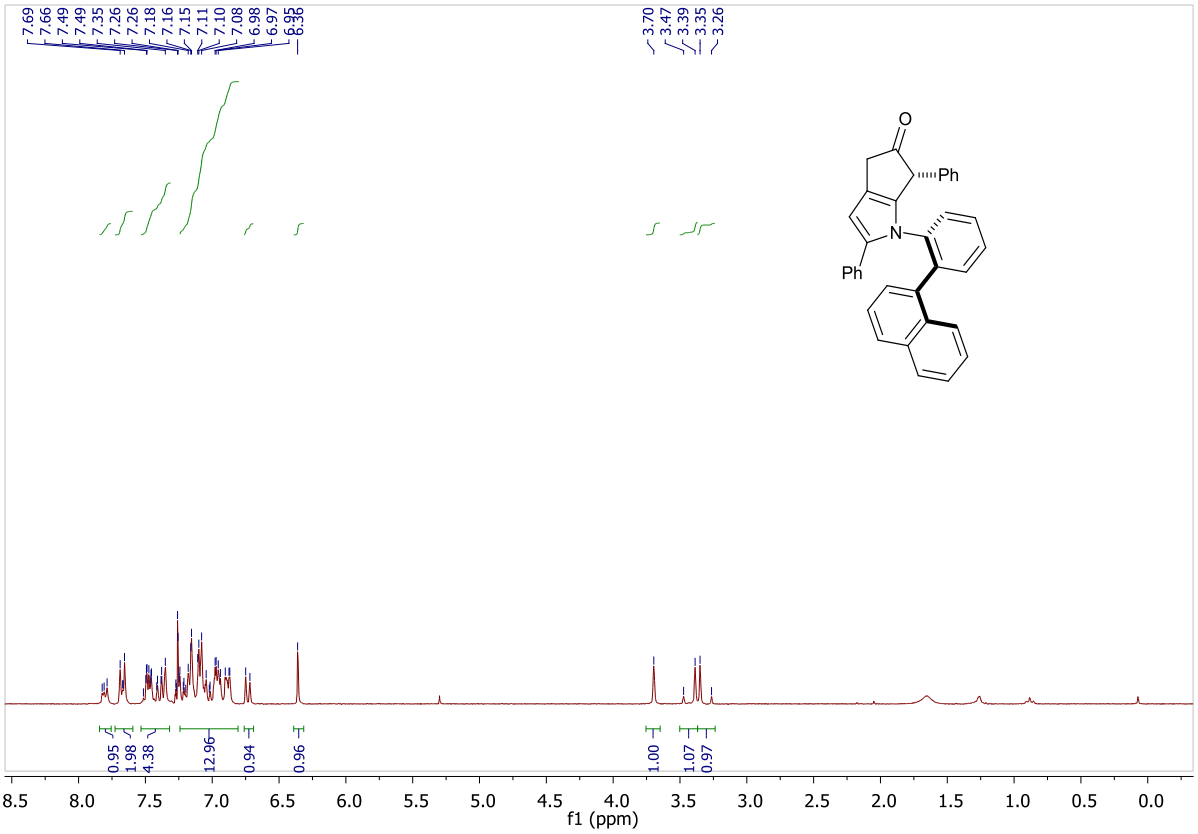
N
Ph
f1 (ppm)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6.97
6.95
6.36
3.70
3.47
3.39
3.35
3.26
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Ph
N
Ph
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1.98
4.38
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0.94
0.96
1.00
1.07
0.97
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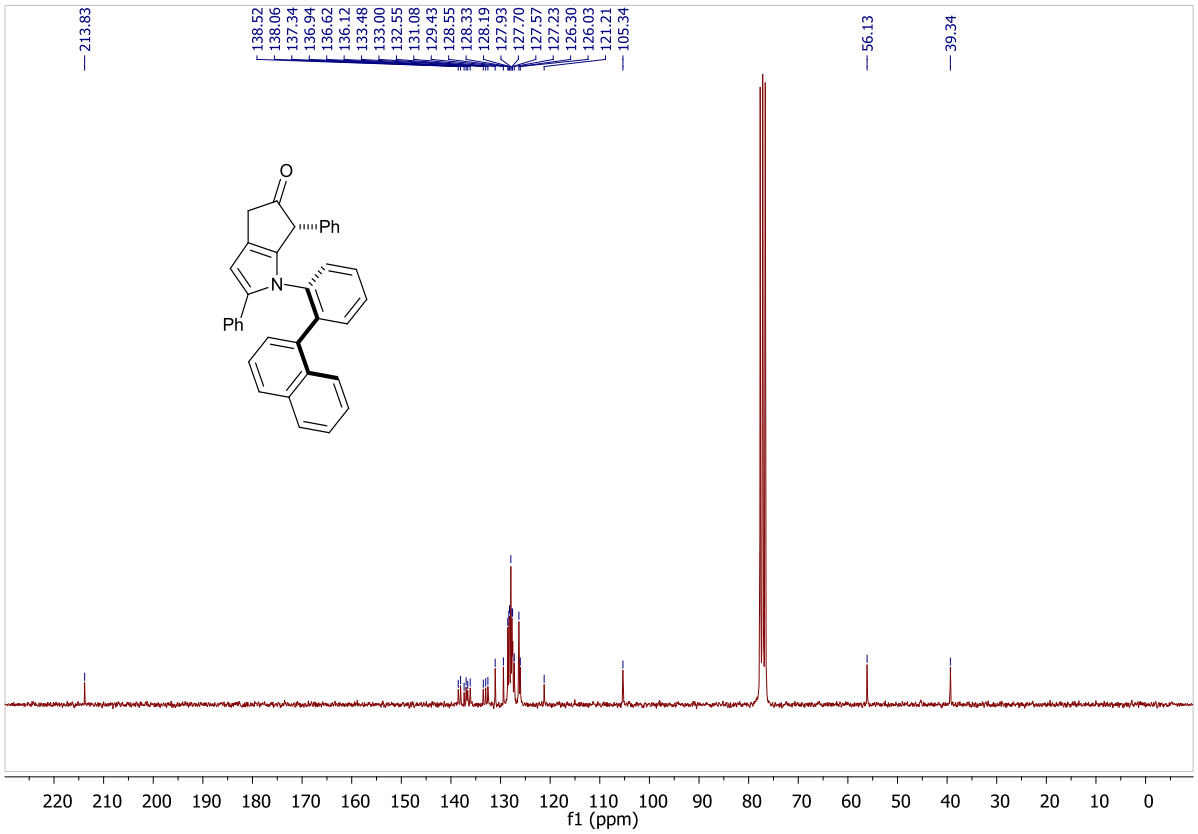
f1 (ppm)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127.70
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127.23
126.30
126.03
121.21
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N
Ph
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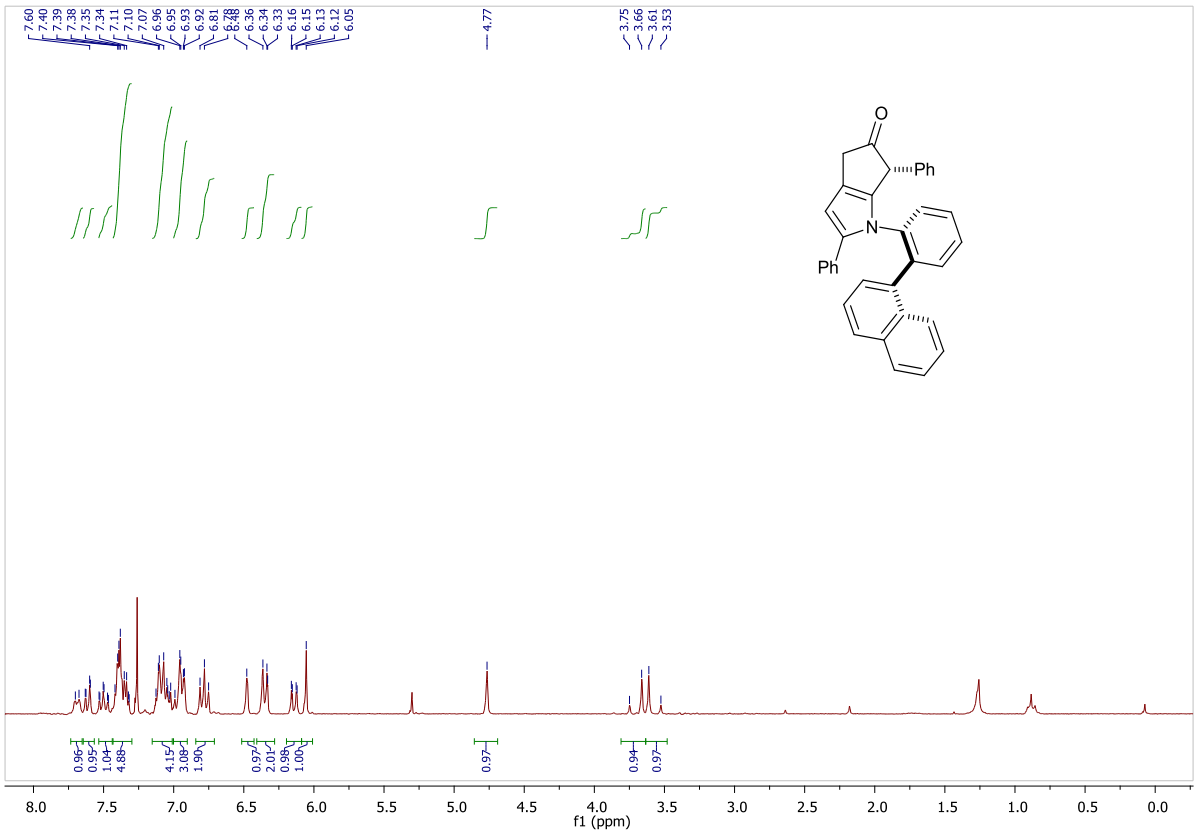
f1 (ppm)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6.12
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Ph
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3.08
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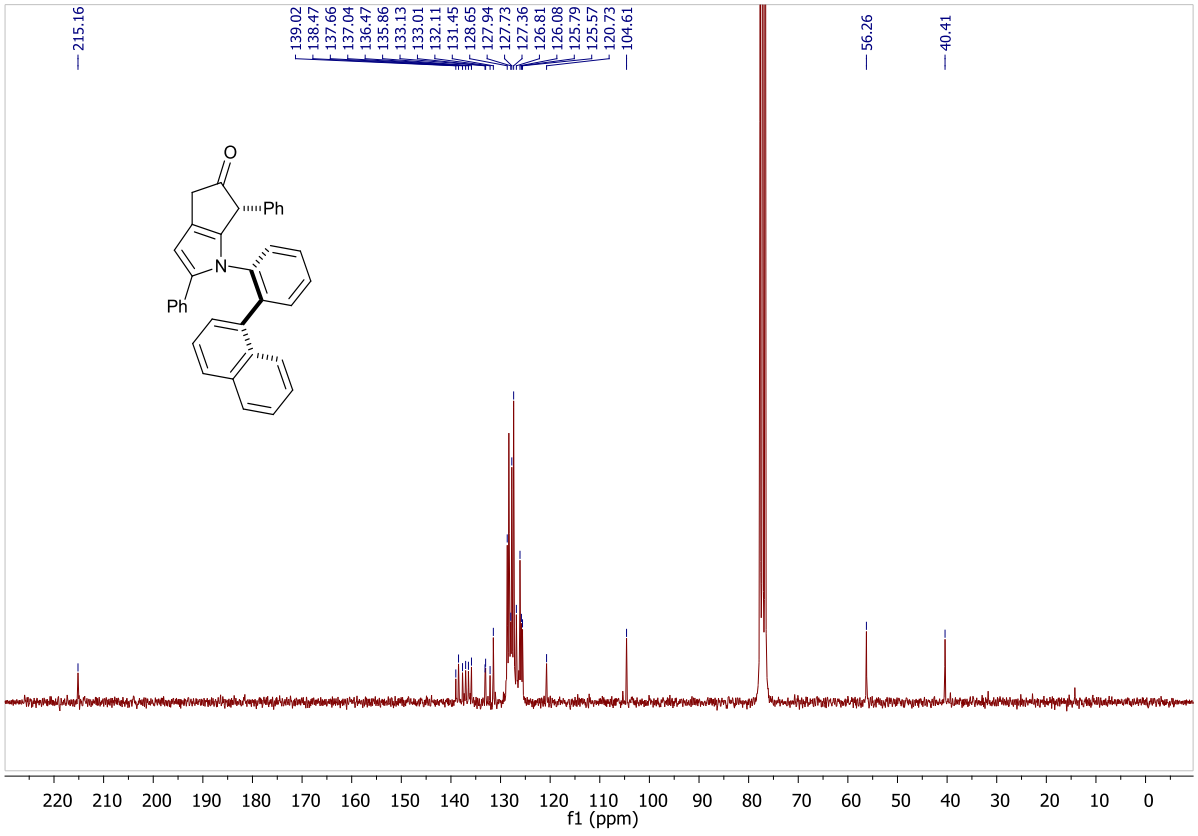
f1 (ppm)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120.73
104.61
56.26
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O
Ph
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Ph
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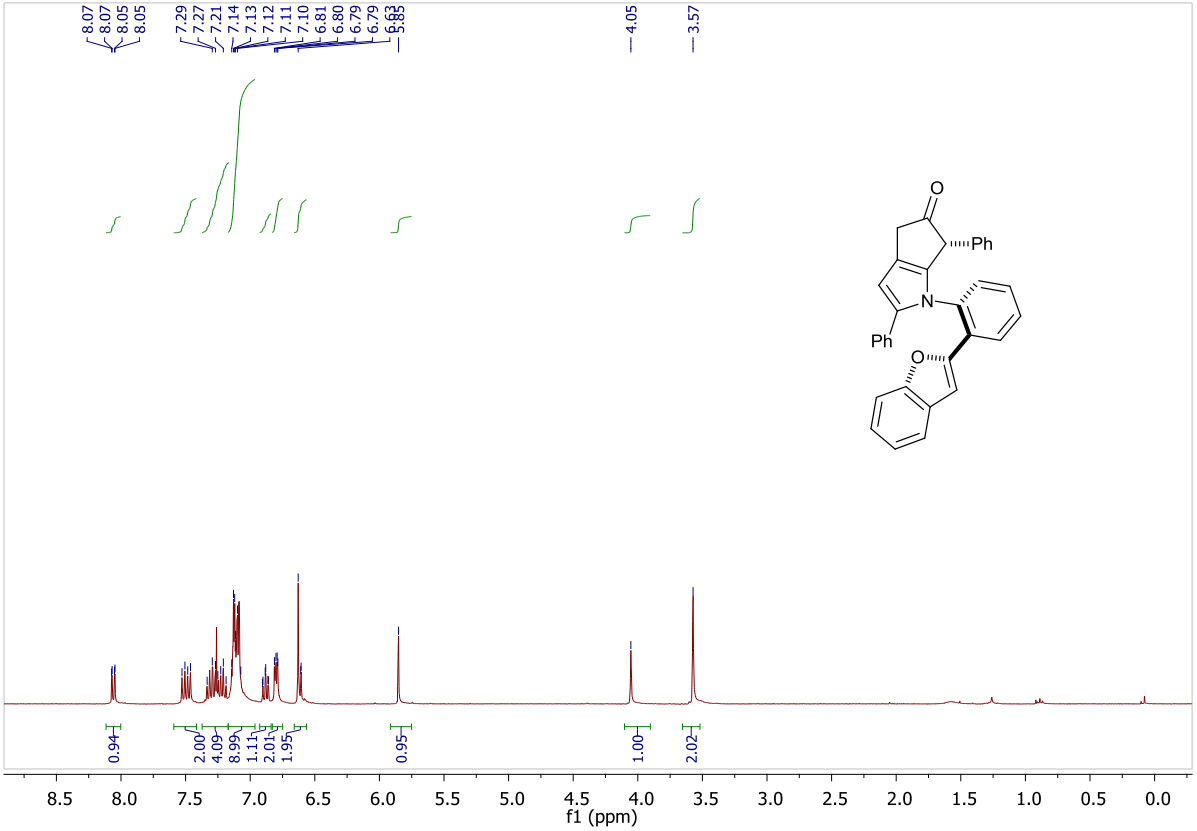
f1 (ppm)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3.57
O
Ph
N
Ph
O
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2.00
4.09
8.99
1.11
2.01
1.95
0.95
1.00
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7.0
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6.0
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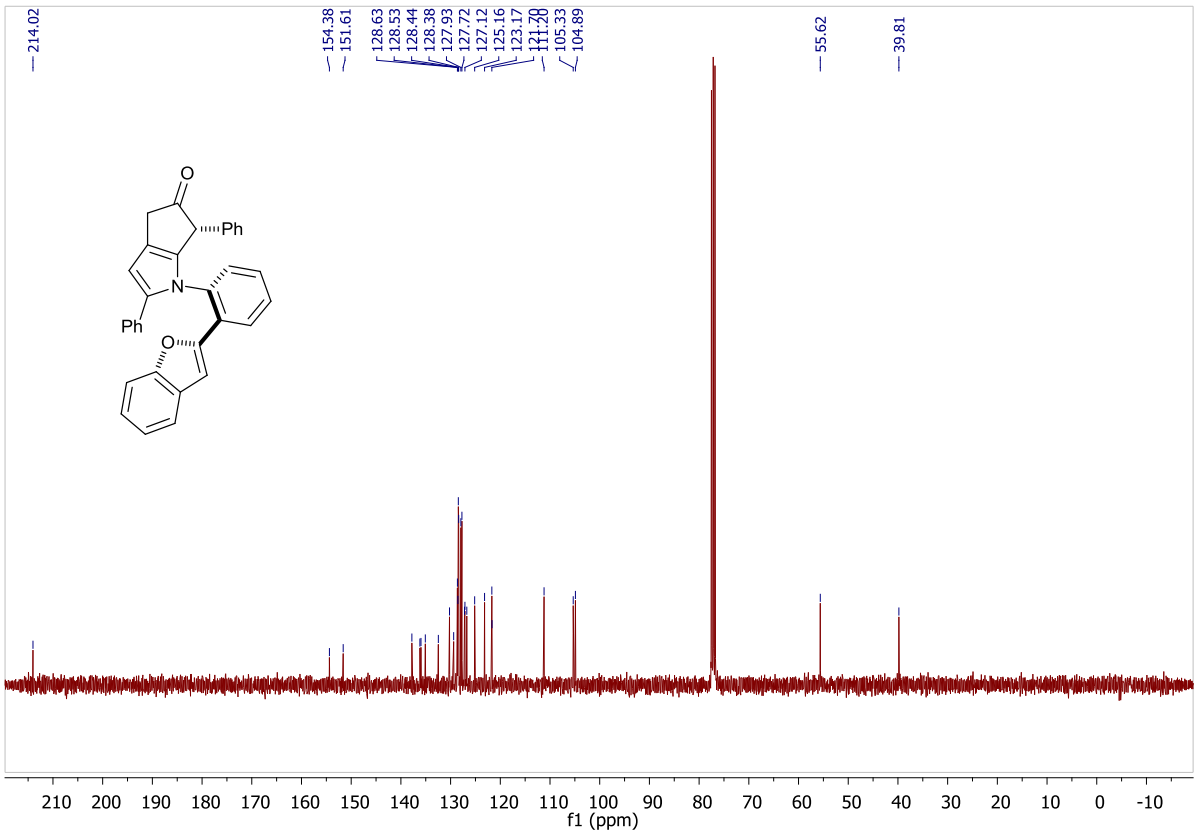
f1 (ppm)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105.33
104.89
55.62
39.81
O
Ph
N
Ph
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210
200
190
180
170
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100
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80
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60
50
40
30
20
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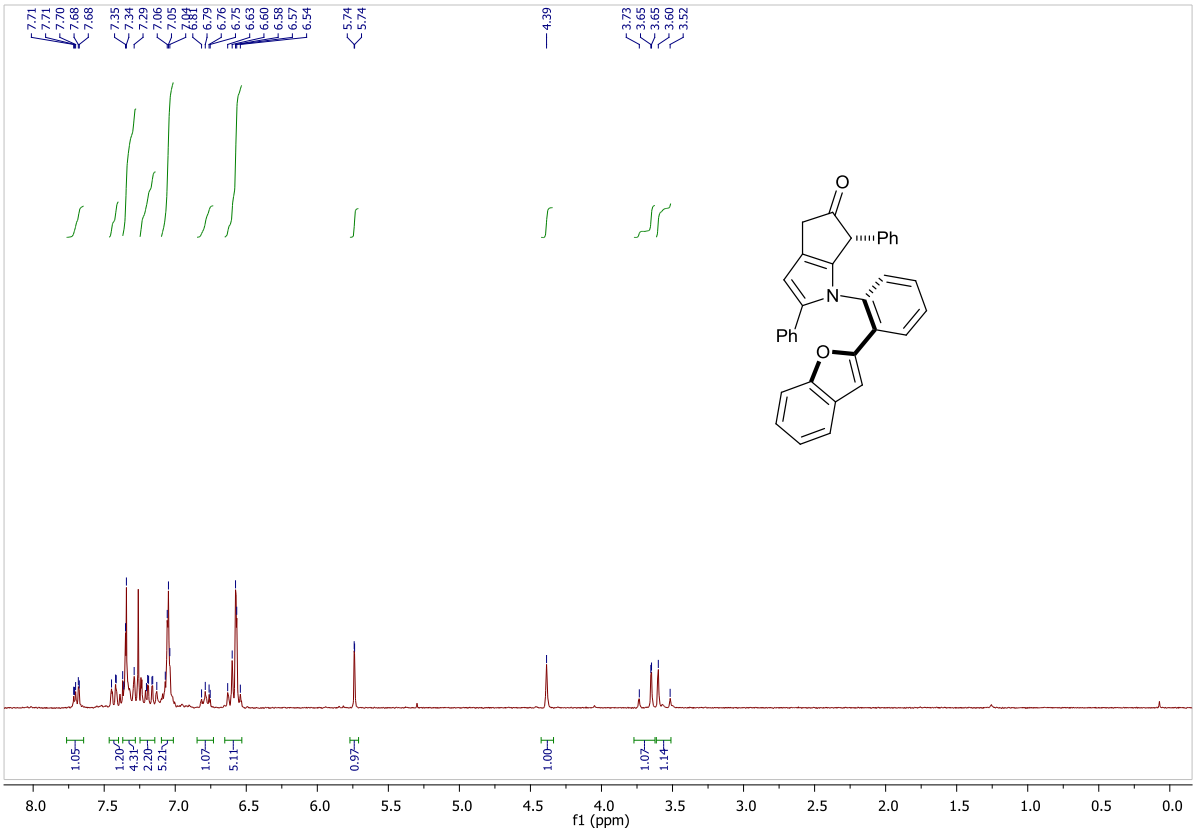
-10
f1 (ppm)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3.60
3.52
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Ph
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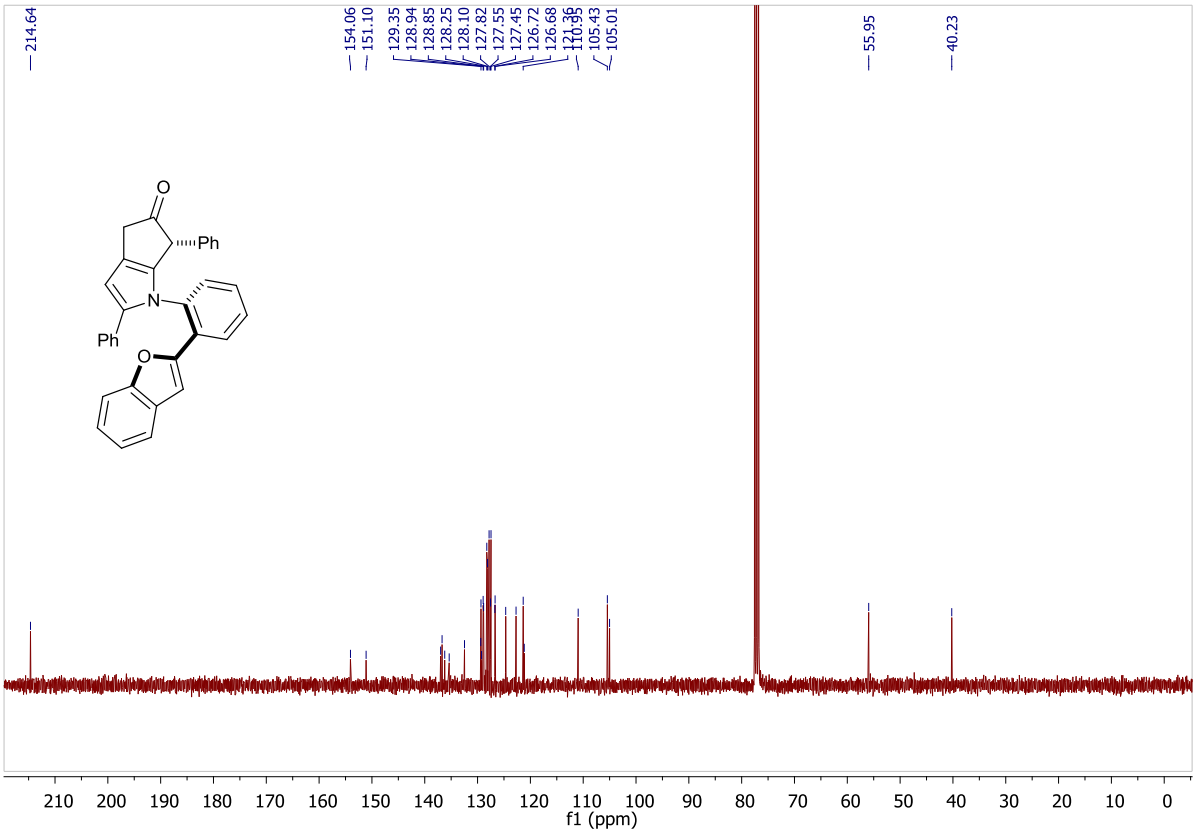
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127.45
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126.68
121.36
110.95
105.43
105.01
55.95
40.23
O
Ph
N
Ph
O
210
200
190
180
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90
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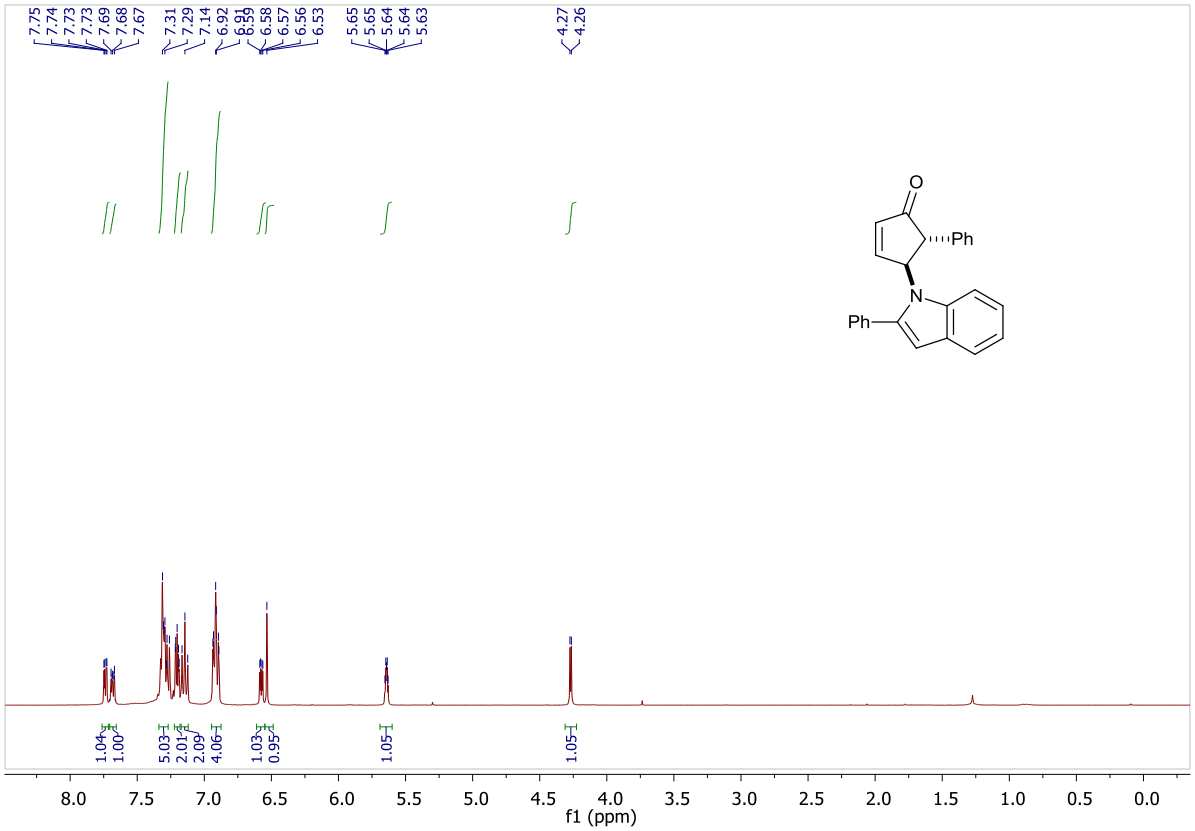
f1 (ppm)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6.59
6.58
6.57
6.56
6.53
5.65
5.65
5.64
5.64
5.63
4.27
4.26
O
Ph
N
Ph
1.04
1.00
5.03
2.01
2.09
4.06
1.03
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1.05
1.05
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7.0
6.5
6.0
5.5
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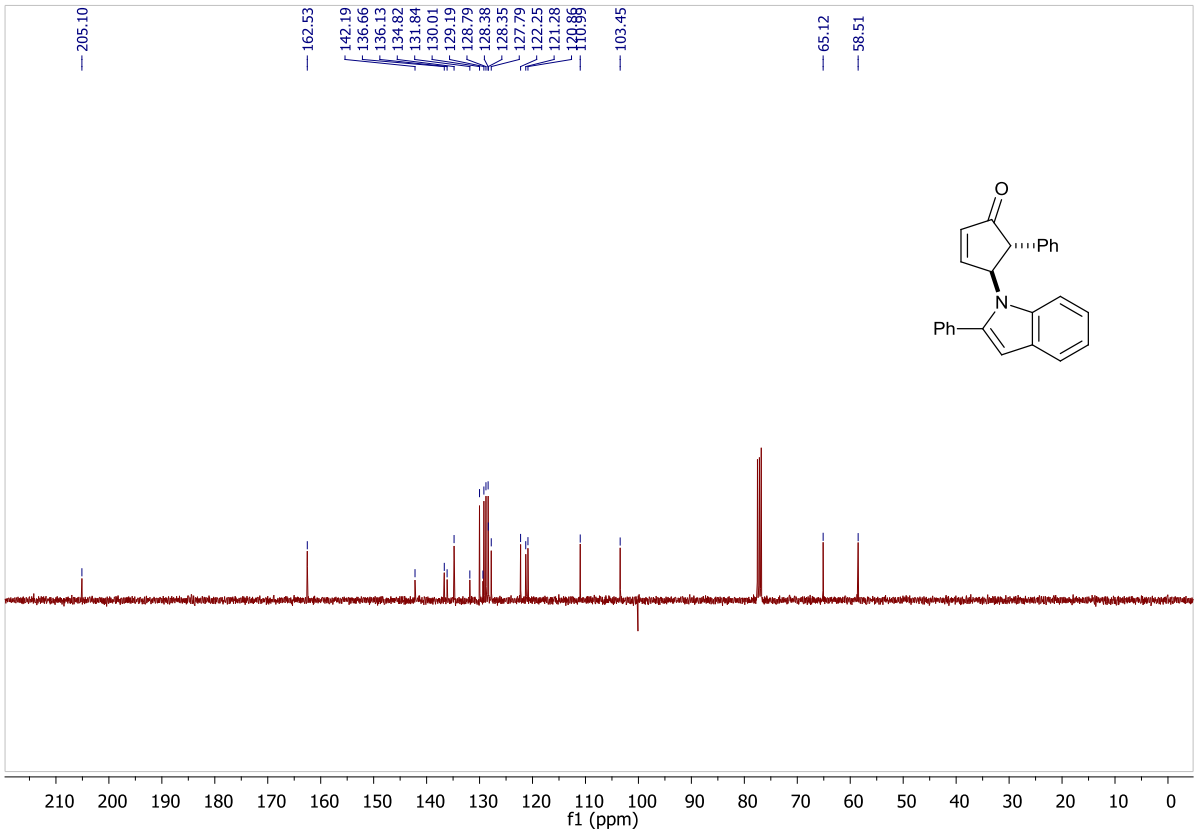
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127.79
122.25
121.28
120.86
110.99
103.45
65.12
58.51
O
Ph
N
Ph
210
200
190
180
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50
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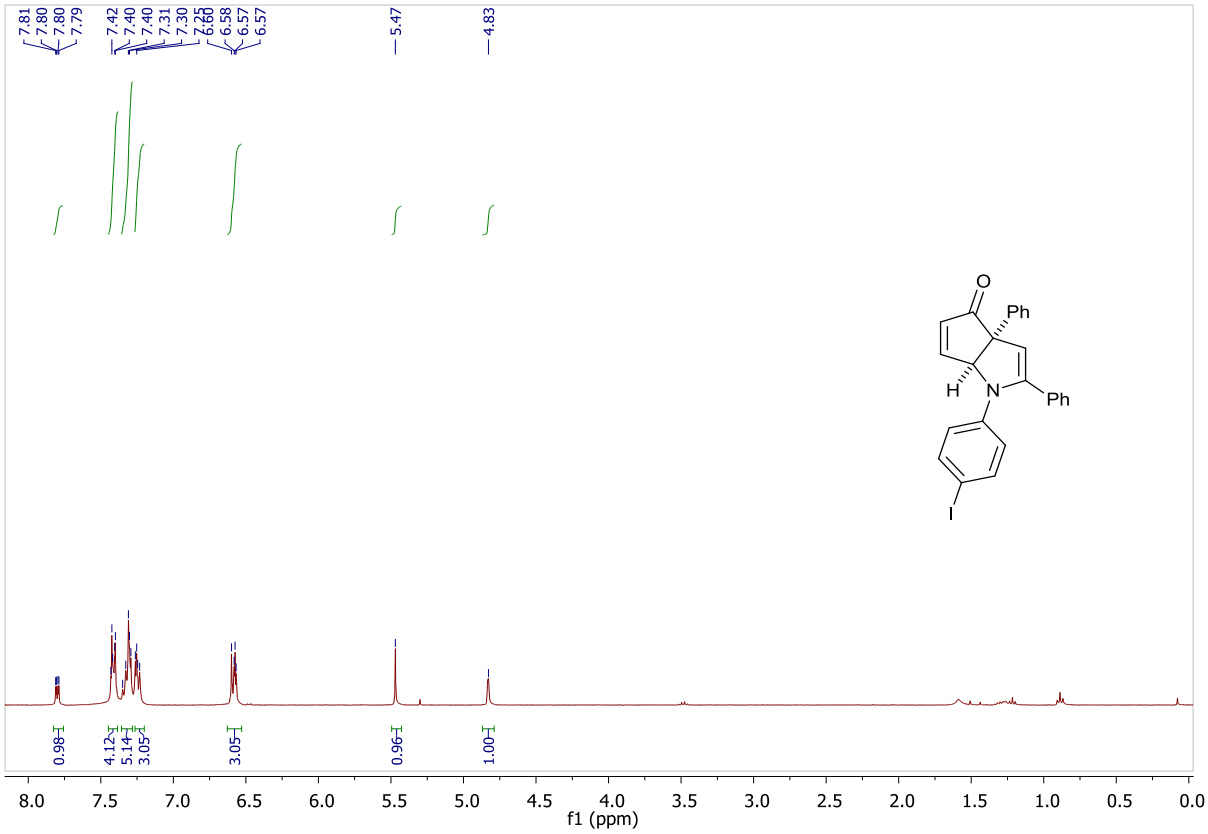
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O
Ph
H
N
Ph
I
0.98
4.12
5.14
3.05
3.05
0.96
1.00
8.0
7.5
7.0
6.5
6.0
5.5
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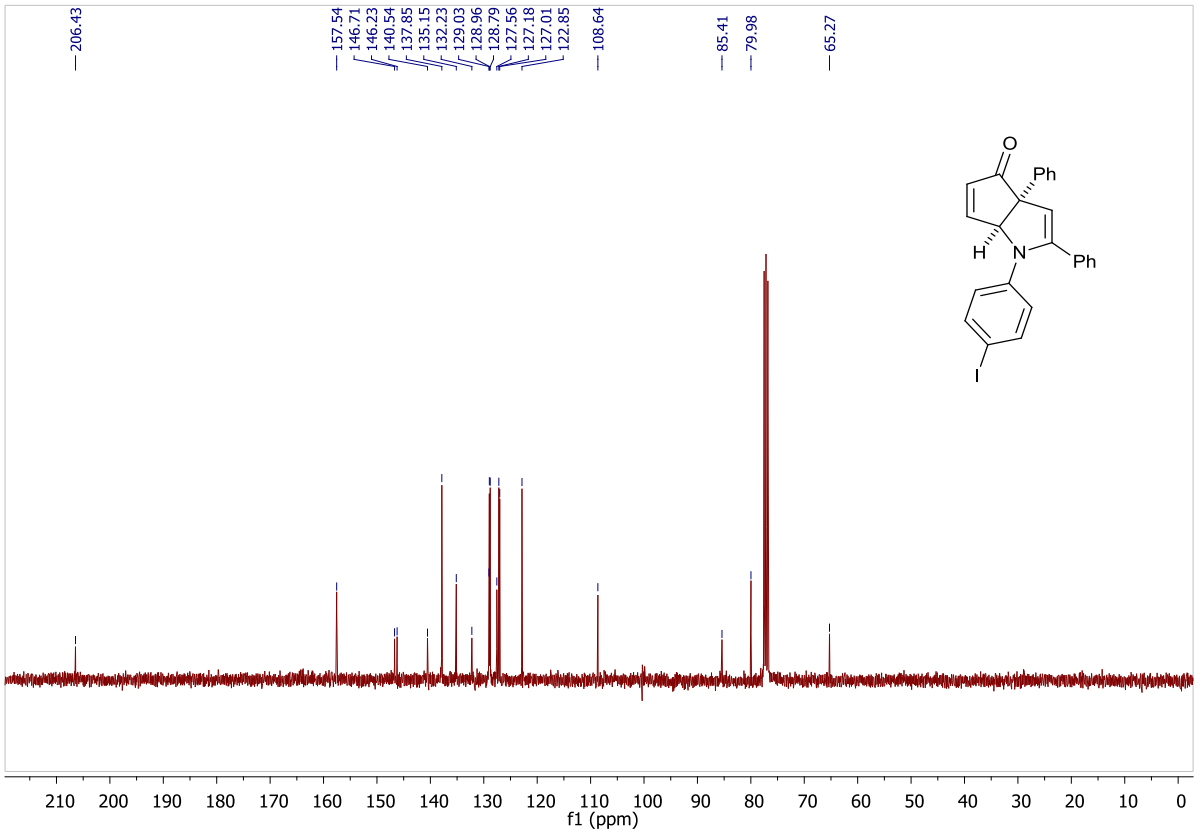
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127.18
127.01
122.85
108.64
85.41
79.98
65.27
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Ph
H
N
Ph
I
210
200
190
180
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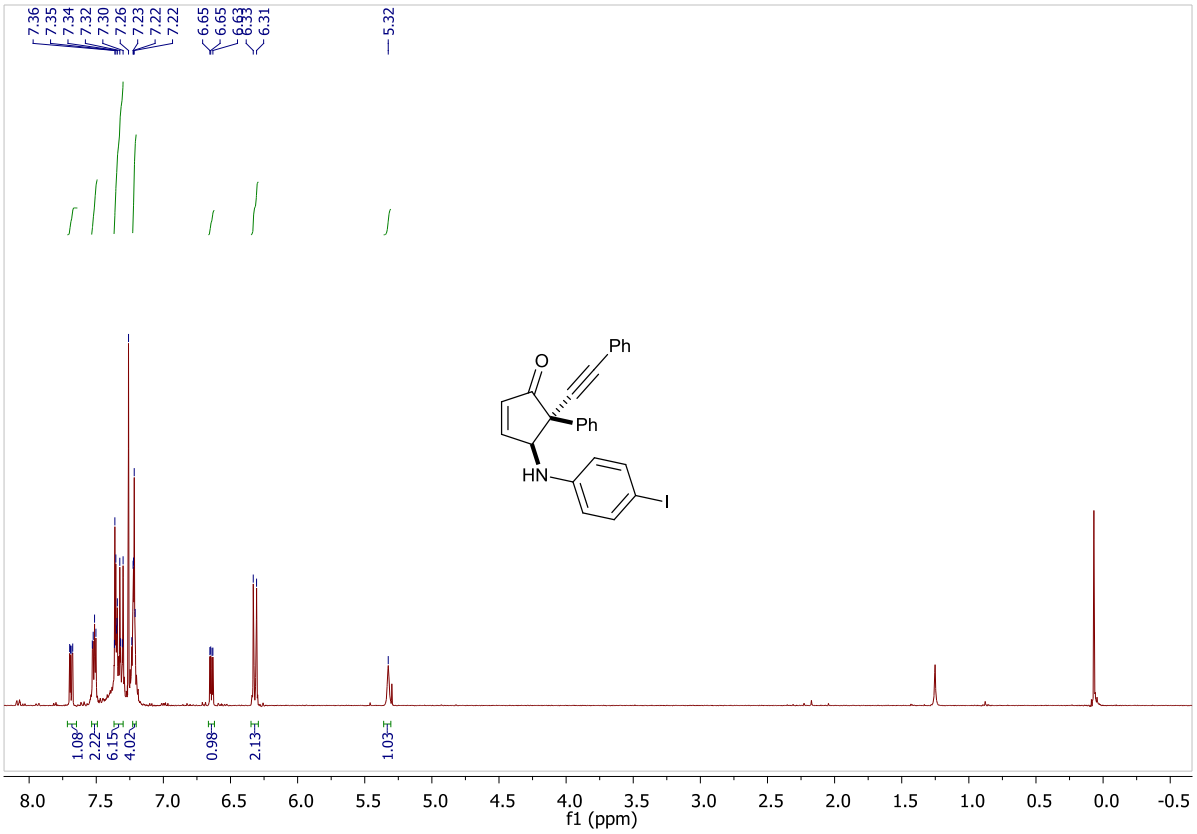
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6.63
6.33
6.31
5.32
1.08
2.22
6.15
4.02
0.98
2.13
1.03
O
Ph
Ph
HN
I
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
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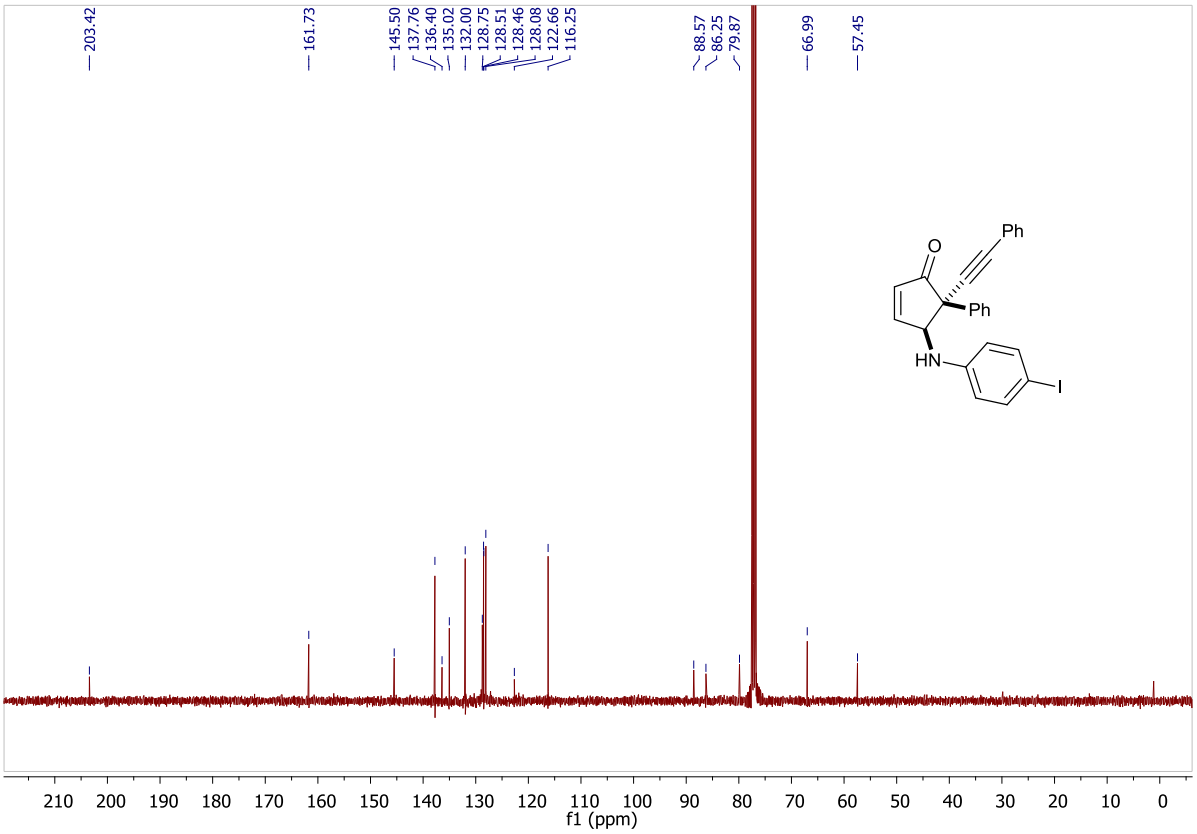
f1 (ppm)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116.25
88.57
86.25
79.87
66.99
57.45
O
Ph
Ph
HN
I
210
200
190
180
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110
100
90
80
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50
40
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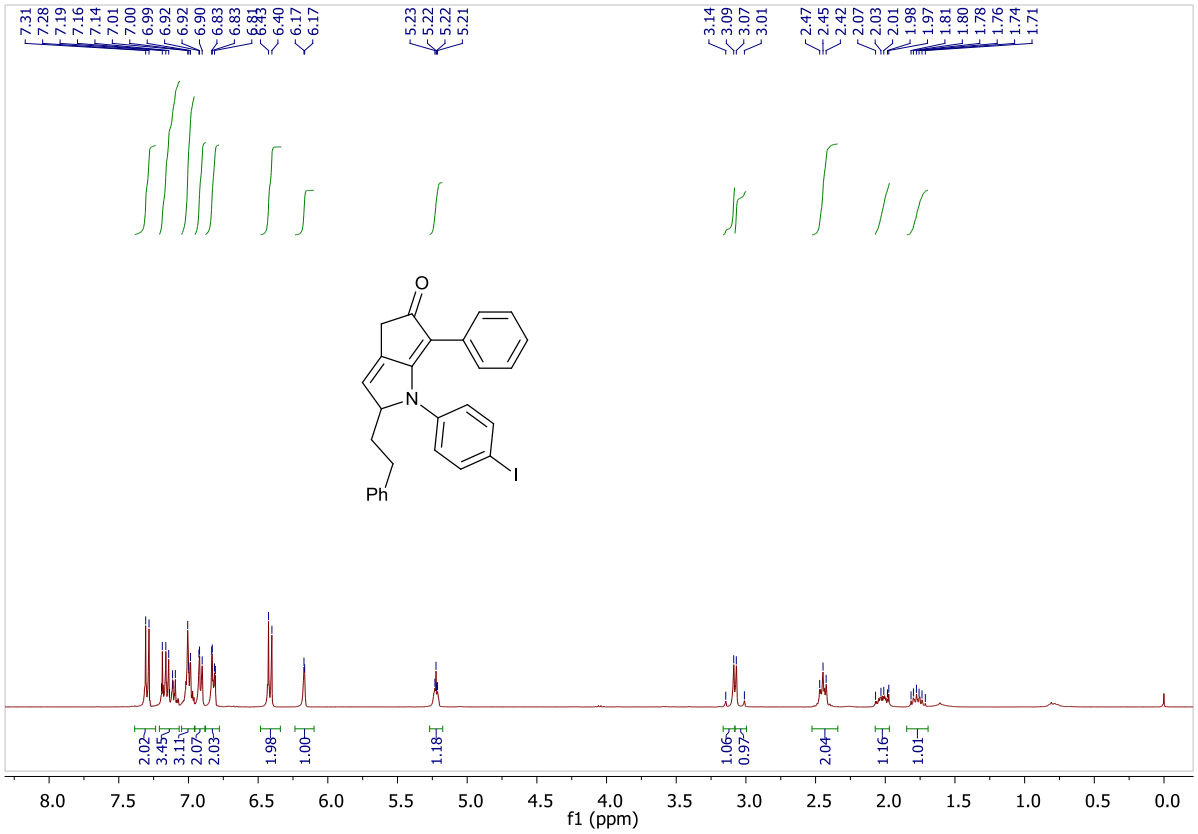
f1 (ppm)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6.83
6.81
6.43
6.40
6.17
6.17
5.23
5.22
5.22
5.21
3.14
3.09
3.07
3.01
2.47
2.45
2.42
2.07
2.03
2.01
1.98
1.97
1.81
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1.78
1.76
1.74
1.71
O
N
Ph
I
2.02
3.45
3.11
2.07
2.03
1.98
1.00
1.18
1.06
0.97
2.04
1.16
1.01
8.0
7.5
7.0
6.5
6.0
5.5
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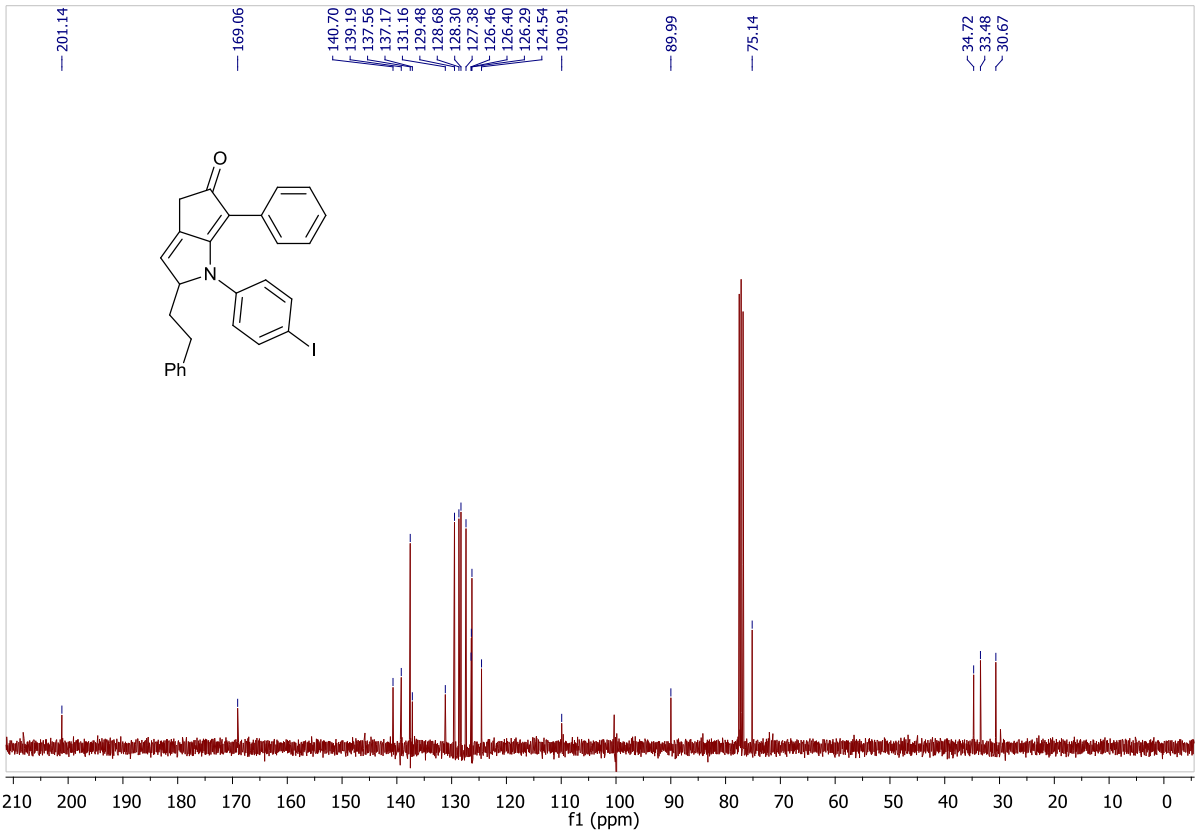
f1 (ppm)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124.54
109.91
89.99
75.14
34.72
33.48
30.67
O
N
Ph
I
210
200
190
180
170
160
150
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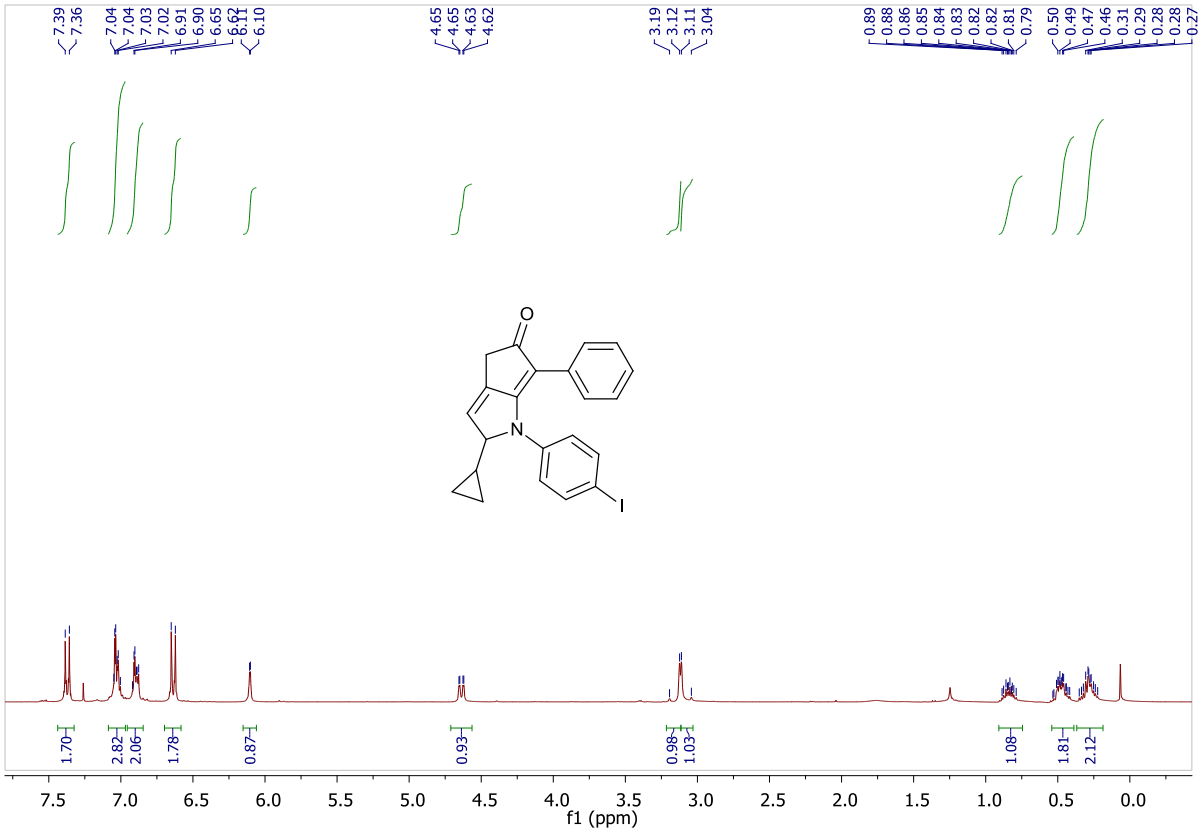
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.62
6.11
6.10
4.65
4.65
4.63
4.62
3.19
3.12
3.11
3.04
0.89
0.88
0.86
0.85
0.84
0.83
0.82
0.82
0.81
0.79
0.50
0.49
0.47
0.46
0.31
0.29
0.28
0.28
0.27
O
N
I
1.70
2.82
2.06
1.78
0.87
0.93
0.98
1.03
1.08
1.81
2.12
7.5
7.0
6.5
6.0
5.5
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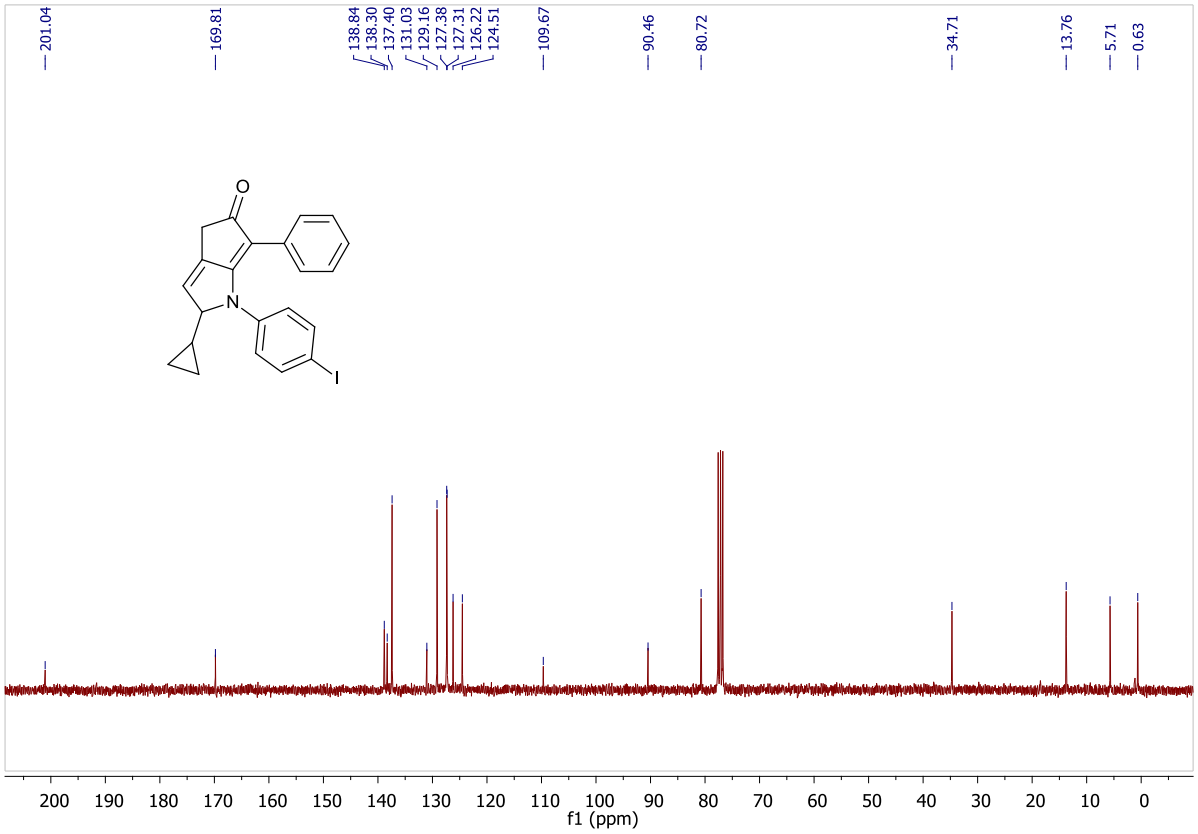
0.0
f1 (ppm)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127.31
126.22
124.51
109.67
90.46
80.72
34.71
13.76
5.71
0.63
O
N
I
200
190
180
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130
120
110
100
90
80
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50
40
30
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10
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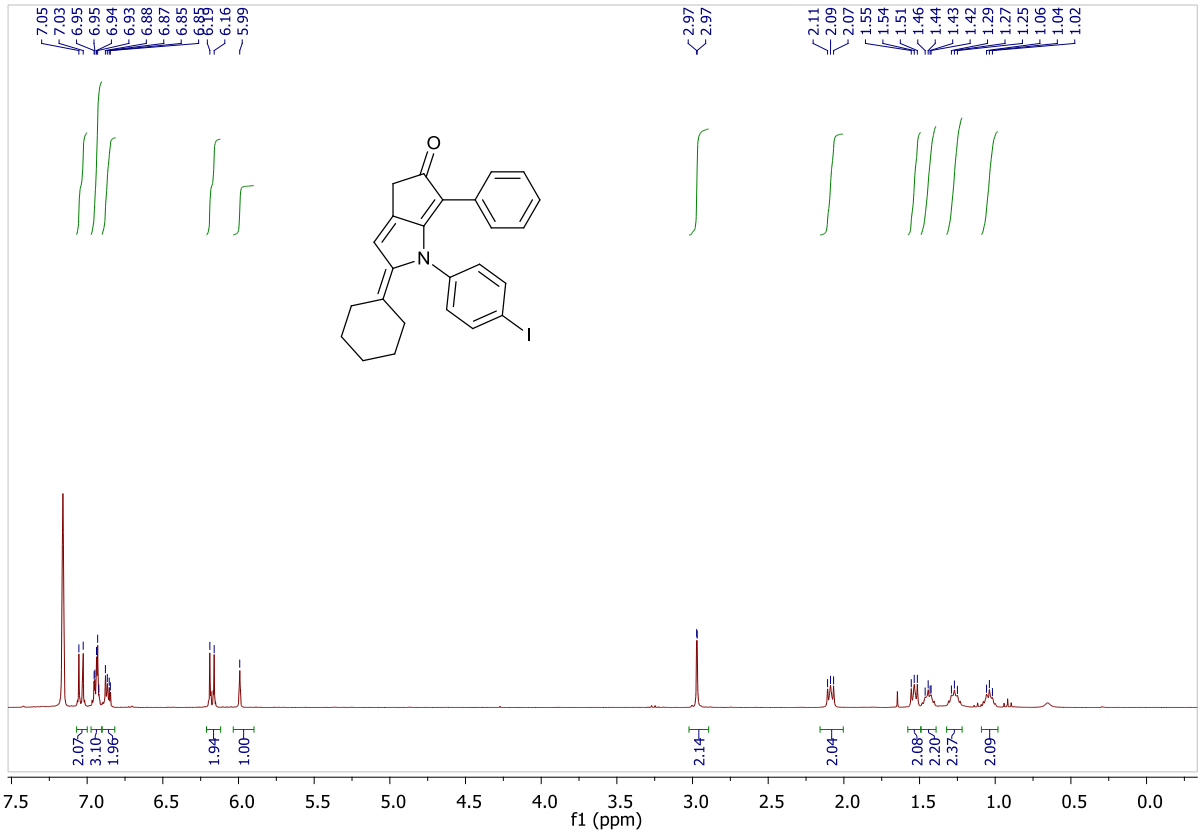
f1 (ppm)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6.19
6.16
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2.97
2.97
2.11
2.09
2.07
1.55
1.54
1.51
1.46
1.44
1.43
1.42
1.29
1.27
1.25
1.06
1.04
1.02
O
N
I
2.07
3.10
1.96
1.94
1.00
2.14
2.04
2.08
2.20
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6.5
6.0
5.5
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3.0
2.5
2.0
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1.0
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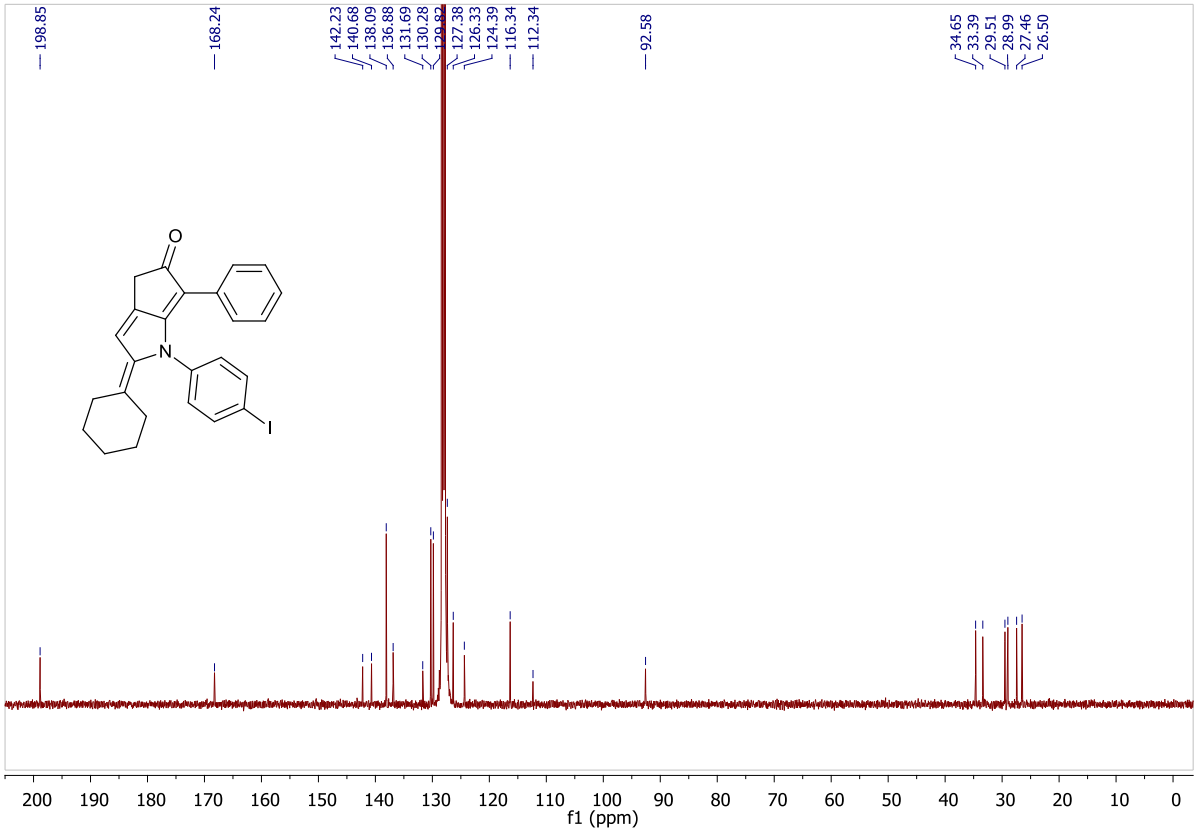
0.0
f1 (ppm)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116.34
112.34
92.58
34.65
33.39
29.51
28.99
27.46
26.50
O
N
I
200
190
180
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110
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50
40
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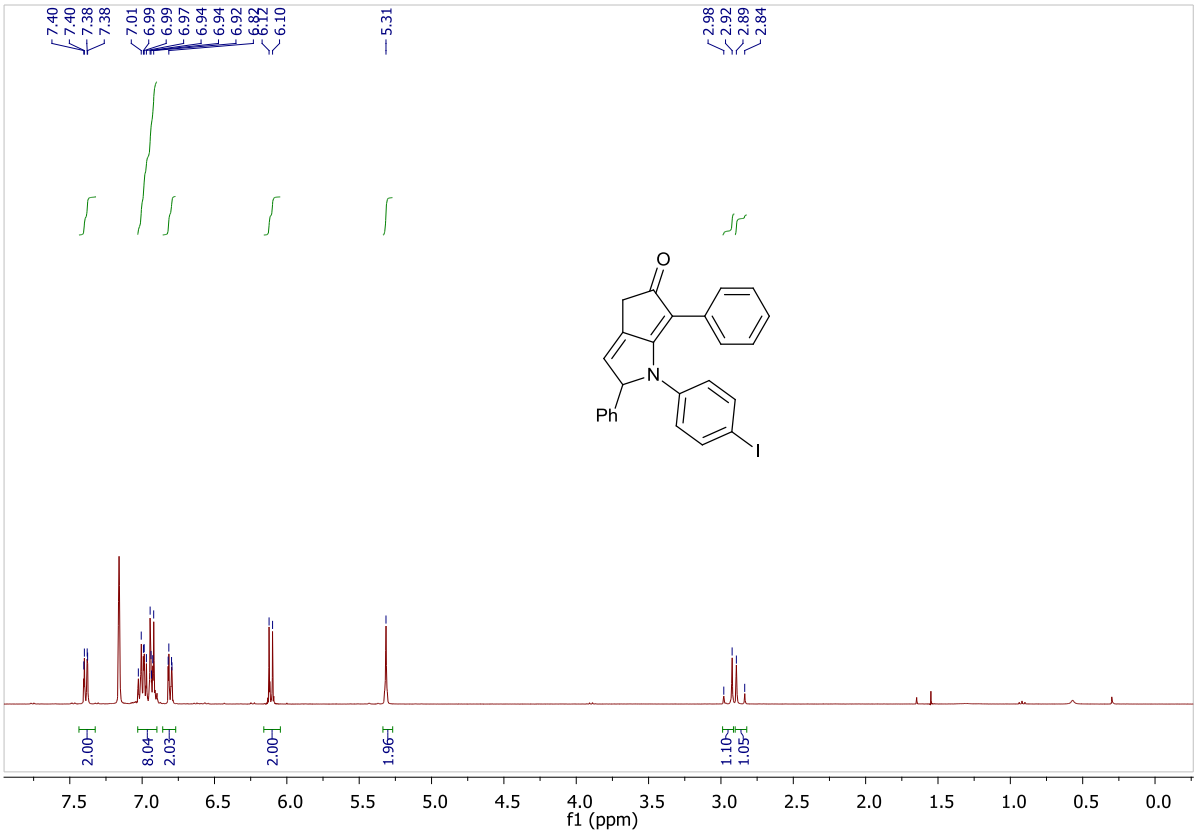
0
f1 (ppm)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6.94
6.92
6.82
6.10
5.31
2.98
2.92
2.89
2.84
O
N
Ph
I
2.00
8.04
2.03
2.00
1.96
1.10
1.05
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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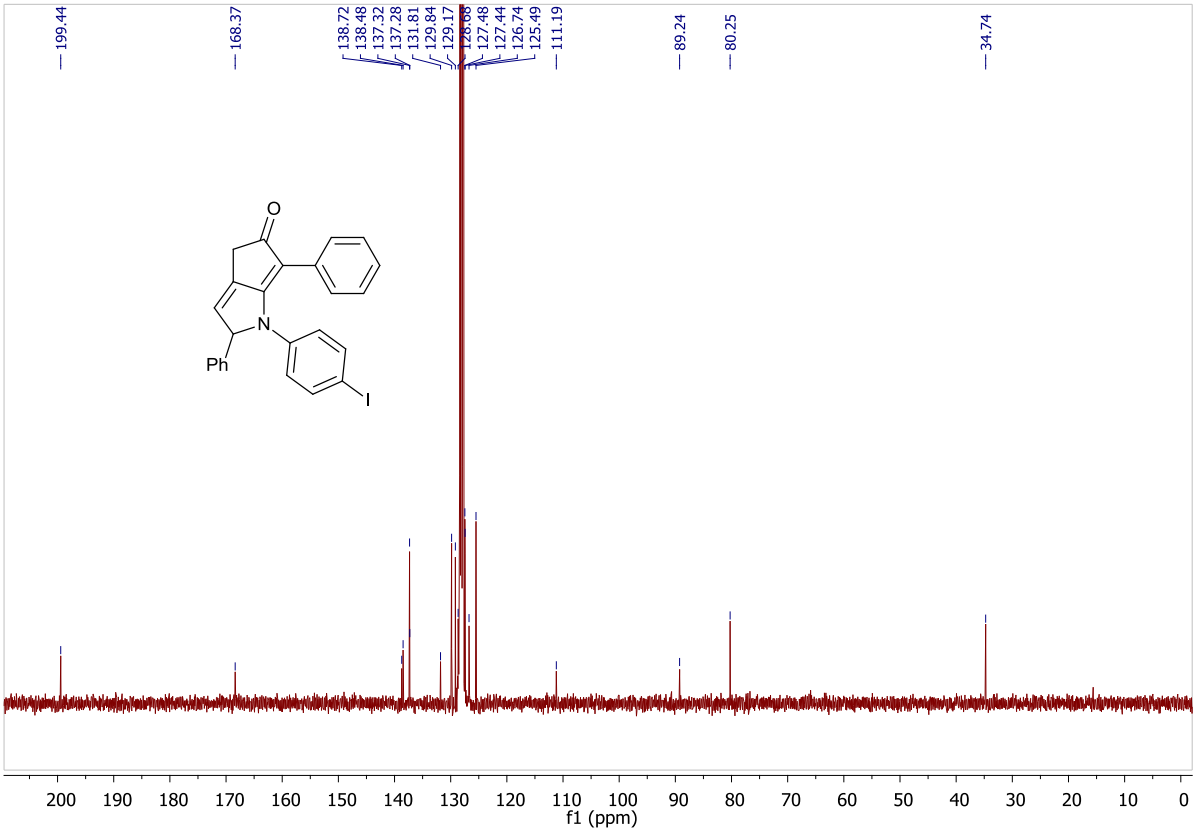
0.0
f1 (ppm)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34.74
O
N
Ph
I
200
190
180
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50
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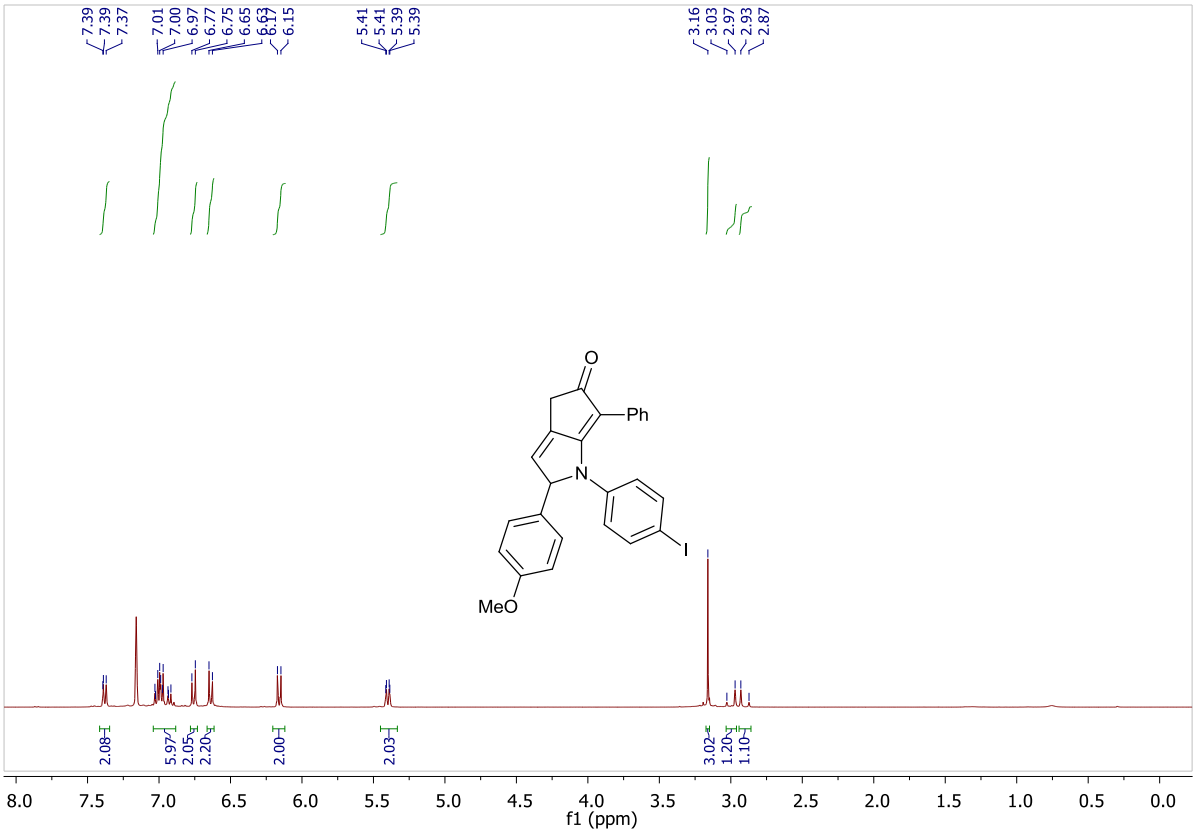
f1 (ppm)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6.63
6.17
6.15
5.41
5.41
5.39
5.39
3.16
3.03
2.97
2.93
2.87
O
Ph
N
I
MeO
2.08
5.97
2.05
2.20
2.00
2.03
3.02
1.20
1.10
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
2.0
1.5
1.0
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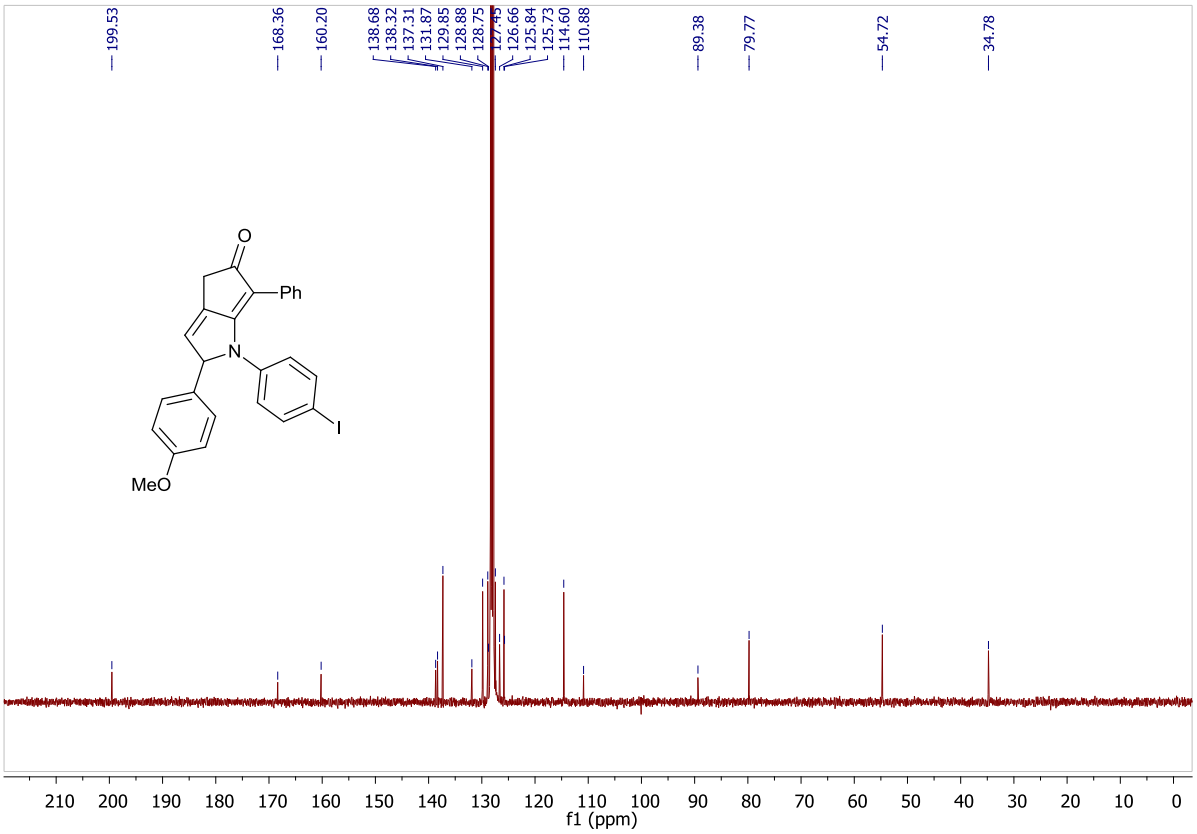
0.0
f1 (ppm)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125.84
125.73
114.60
110.88
89.38
79.77
54.72
34.78
O
Ph
N
I
MeO
210
200
190
180
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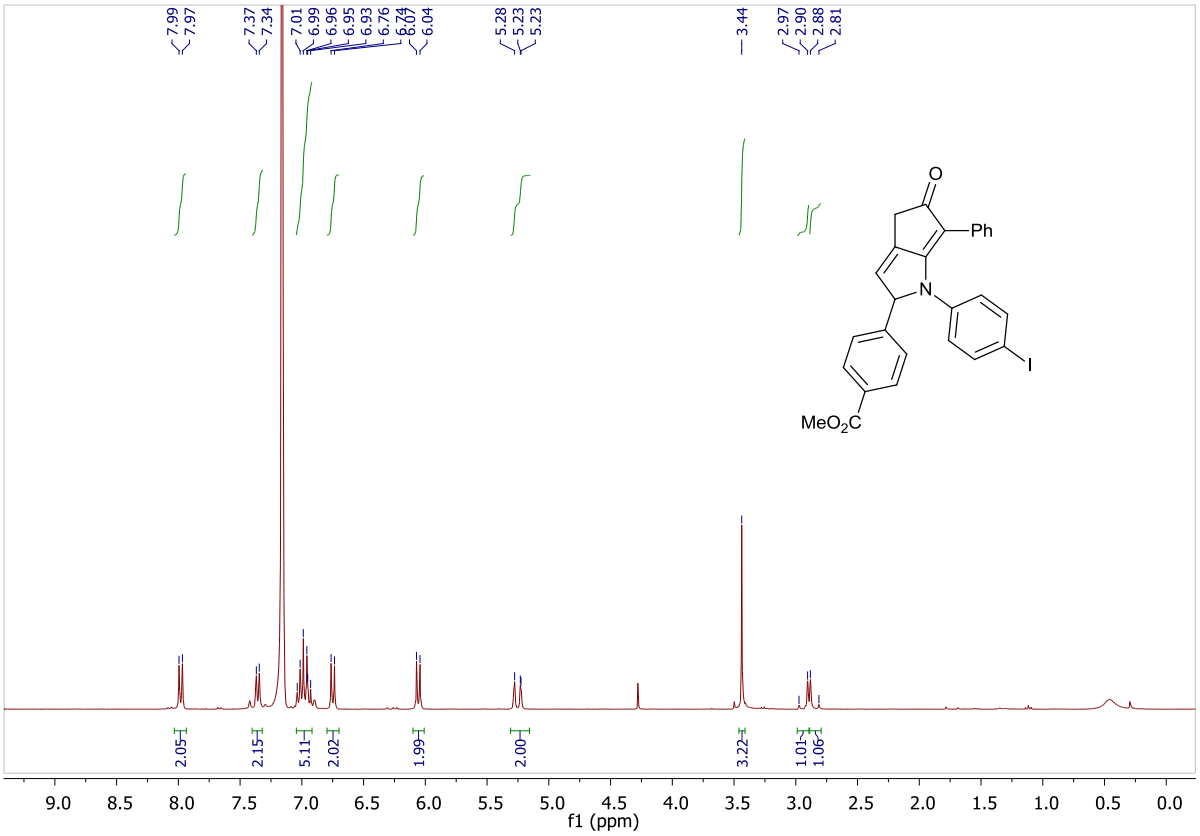
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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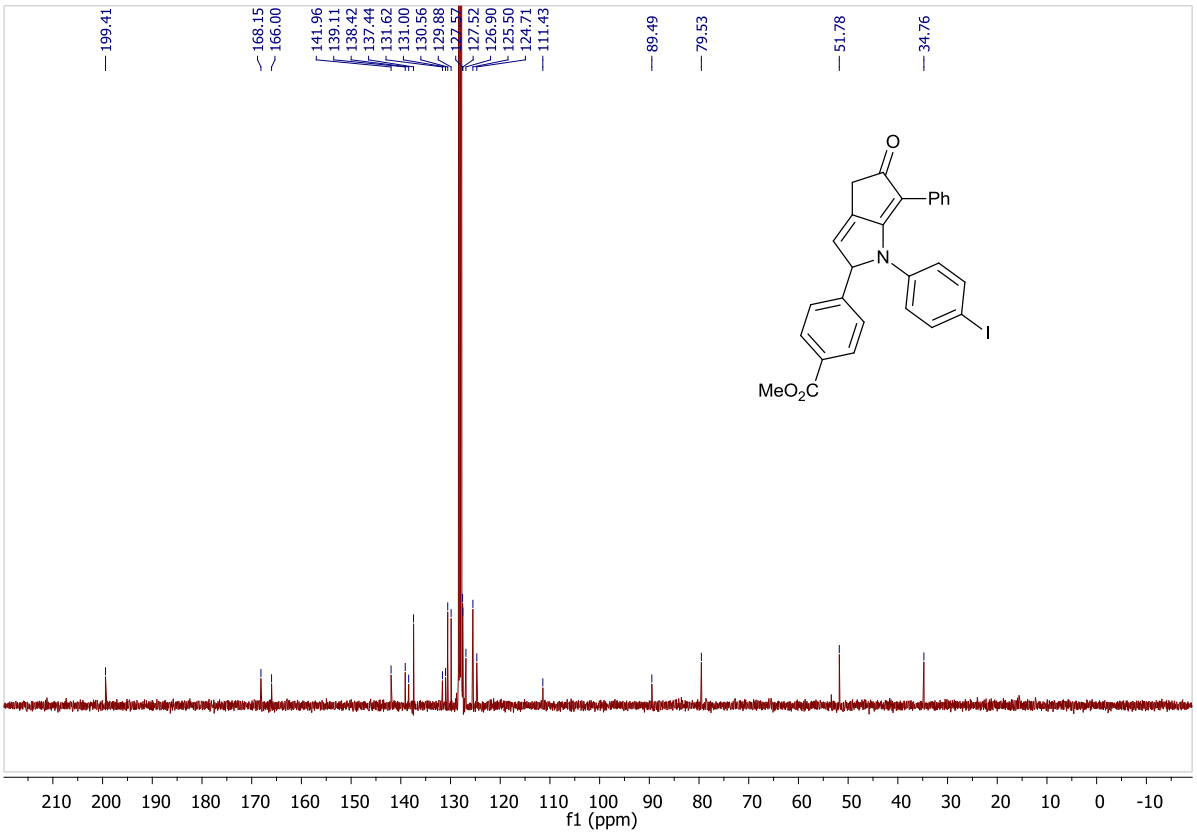
6.04
5.28
5.23
5.23
3.44
2.97
2.90
2.88
2.81
2.05
2.15
5.11
2.02
1.99
2.00
3.22
1.01
1.06
O
Ph
N
I
MeO2C
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.90
125.50
124.71
111.43
89.49
79.53
51.78
34.76
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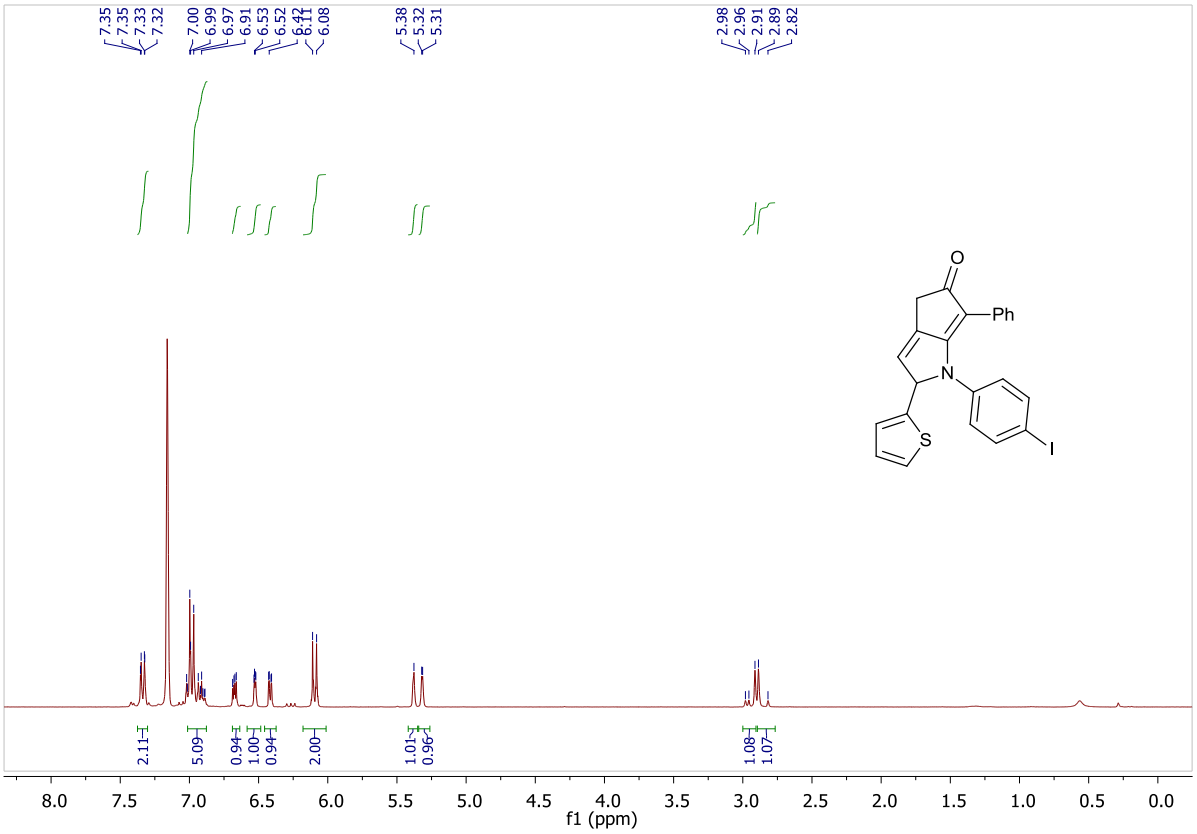
Ph
N
I
MeO2C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.52
6.42
6.41
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5.32
5.31
2.98
2.96
2.91
2.89
2.82
O
Ph
N
S
I
2.11
5.09
0.94
1.00
0.94
2.00
1.01
0.96
1.08
1.07
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
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1.0
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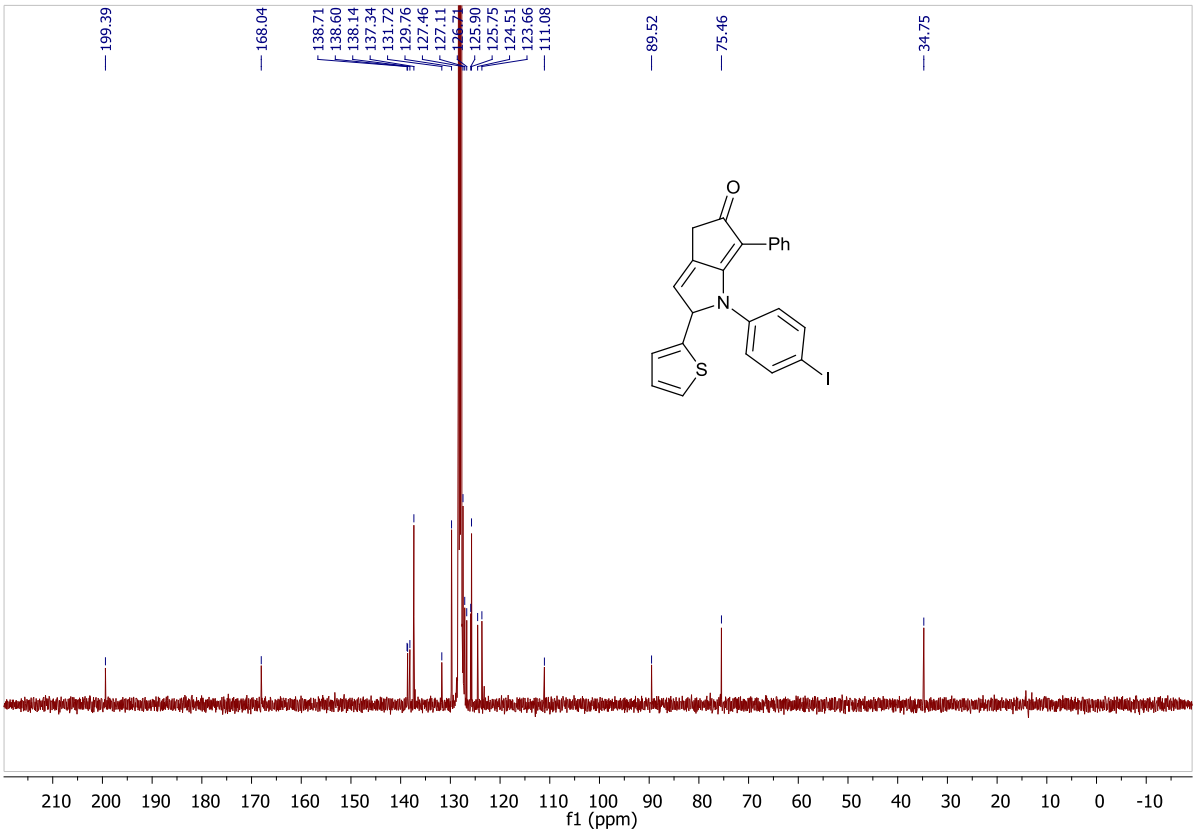
0.0
f1 (ppm)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125.90
125.75
124.51
123.66
111.08
89.52
75.46
34.75
O
Ph
N
S
I
210
200
190
180
170
160
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140
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120
110
100
90
80
70
60
50
40
30
20
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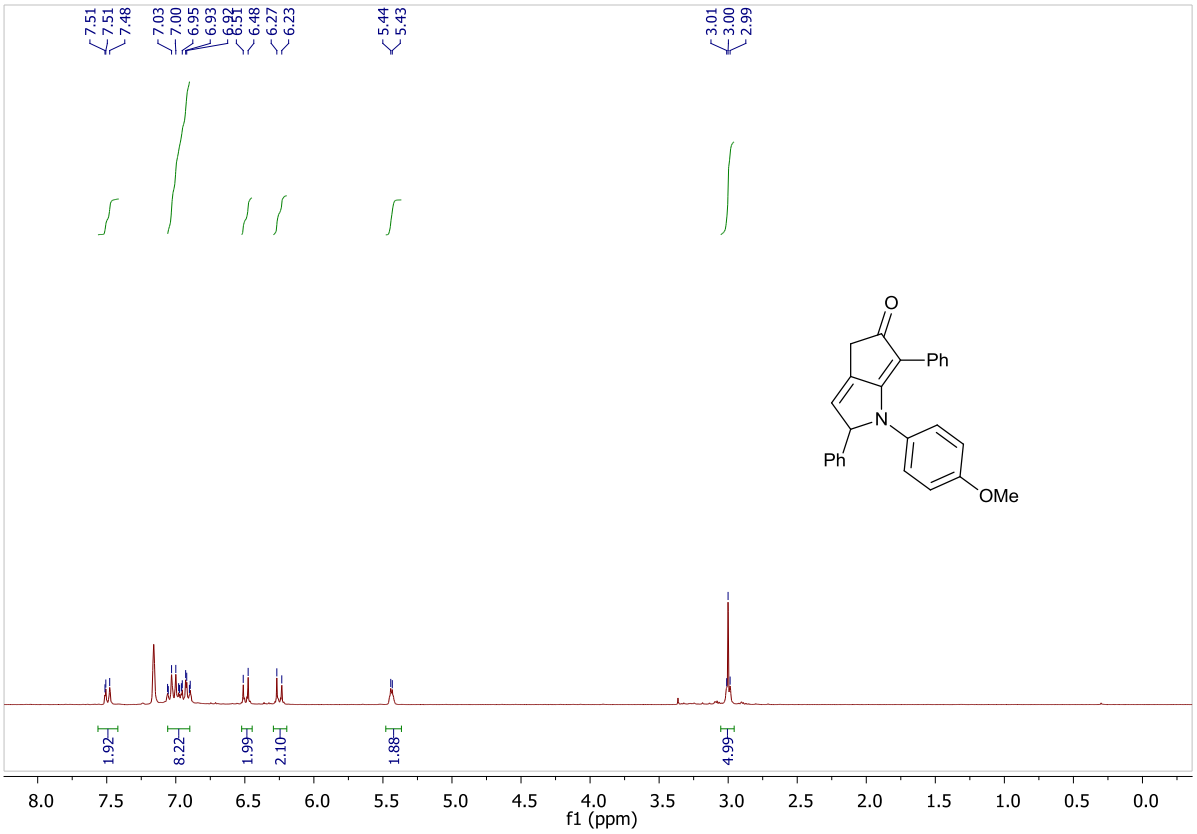
-10
f1 (ppm)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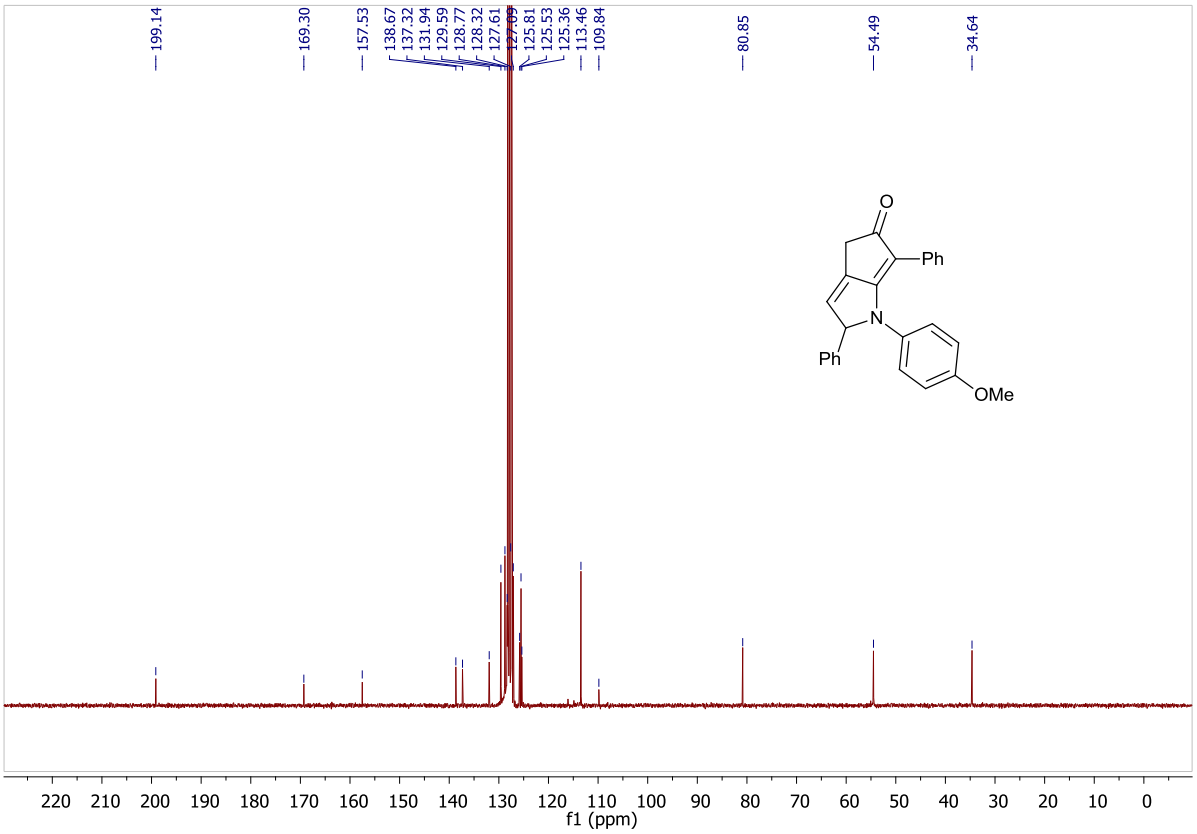
6.93
6.51
6.48
6.27
6.23
5.44
5.43
3.01
3.00
2.99
O
Ph
N
Ph
OMe
1.92
8.22
1.99
2.10
1.88
4.99
f1 (ppm)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80.85
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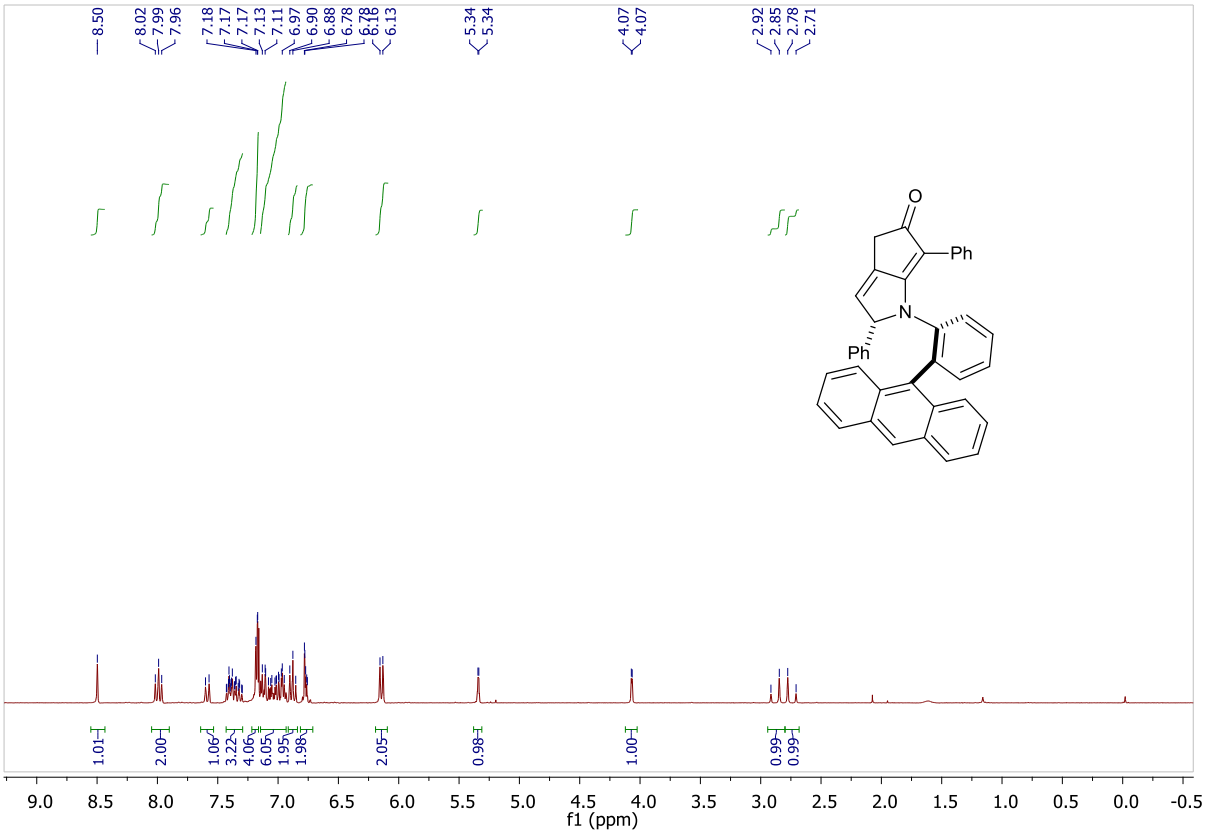
O
Ph
N
Ph
OMe
f1 (ppm)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5.34
4.07
4.07
2.92
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2.78
2.71
O
Ph
N
Ph
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2.00
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1.00
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0.99
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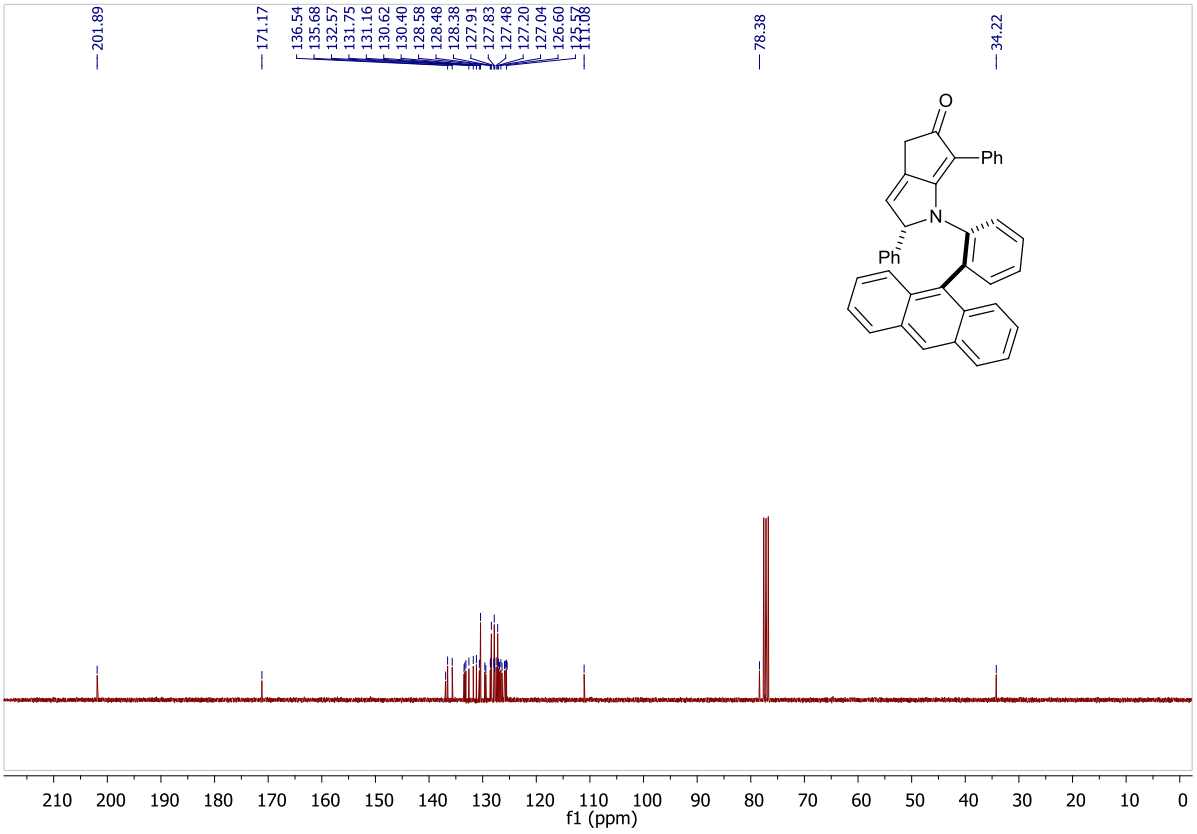
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34.22
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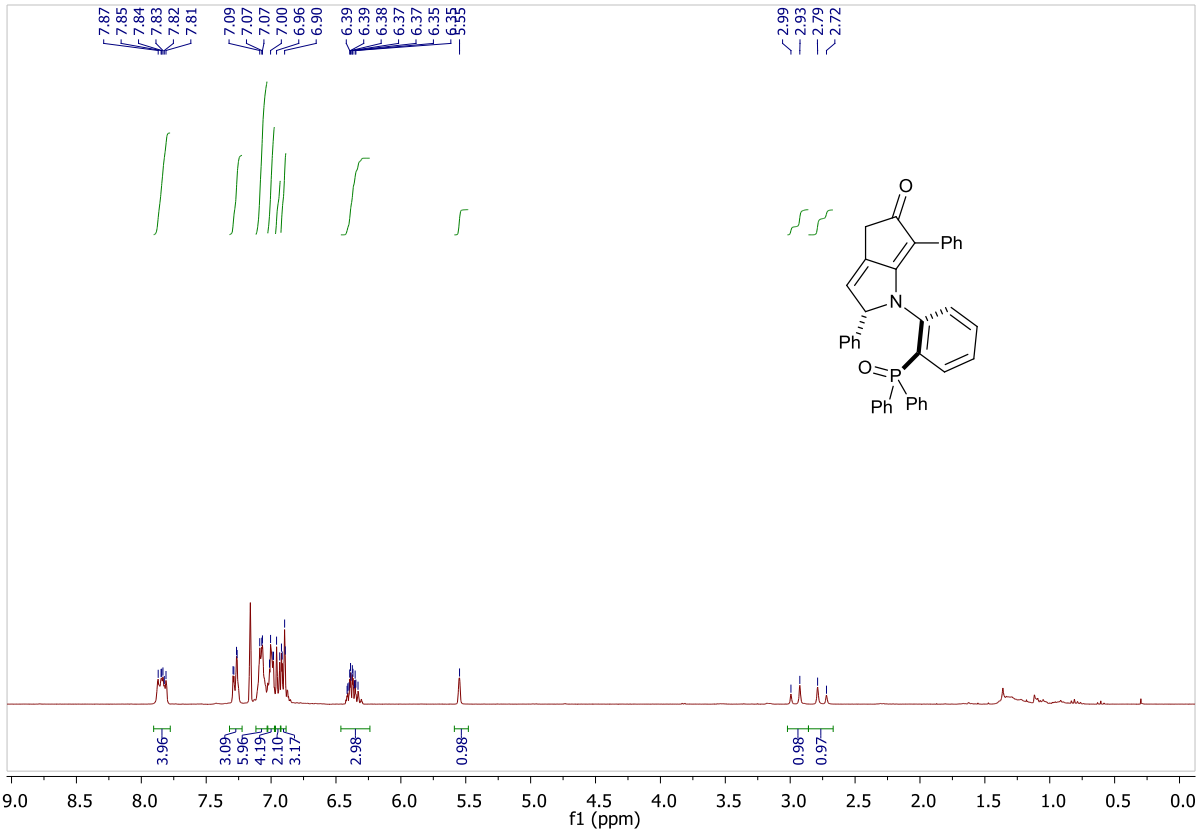
Ph
N
Ph
f1 (ppm)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7.07
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6.90
6.39
6.39
6.38
6.37
6.37
6.35
5.55
2.99
2.93
2.79
2.72
O
Ph
N
Ph
O=P
Ph
Ph
3.96
3.09
5.96
4.19
2.10
3.17
2.98
0.98
0.98
0.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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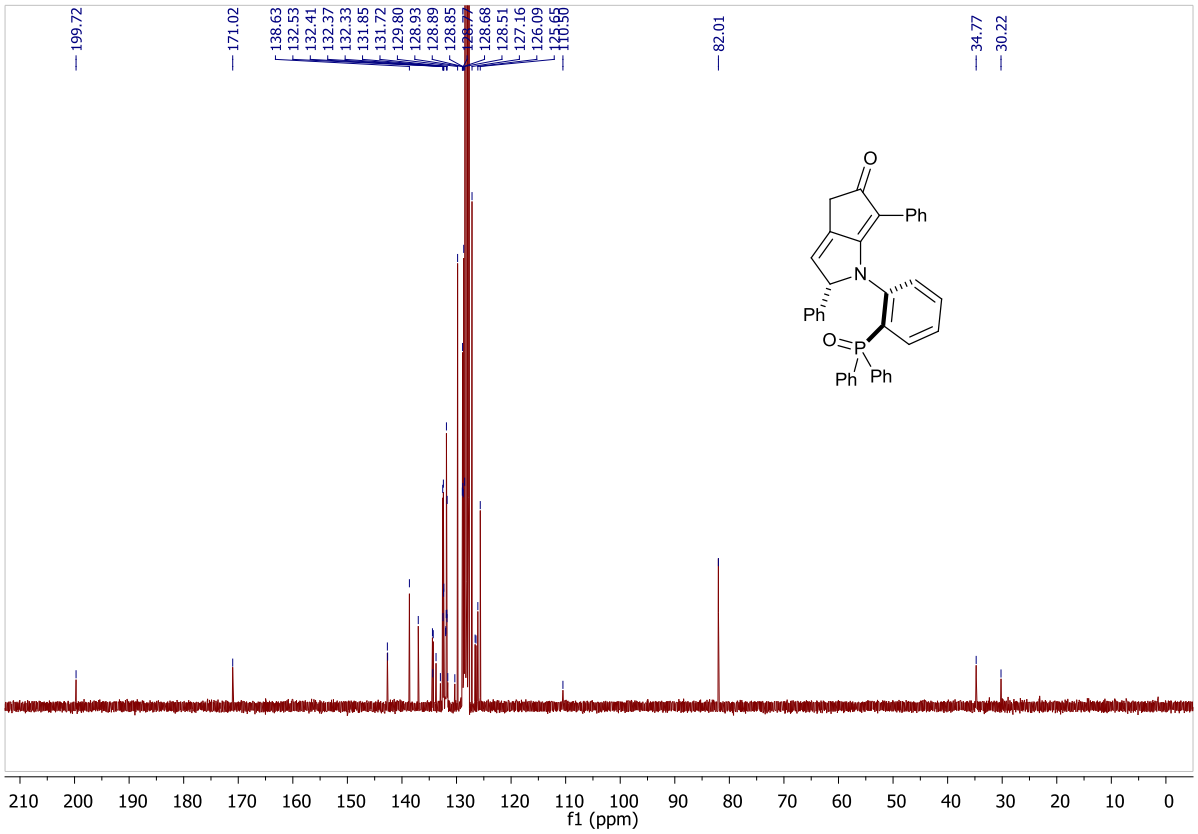
f1 (ppm)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128.89
128.85
128.77
128.68
128.51
127.16
126.09
125.65
110.50
82.01
34.77
30.22
O
Ph
N
Ph
O=P
Ph
Ph
210
200
190
180
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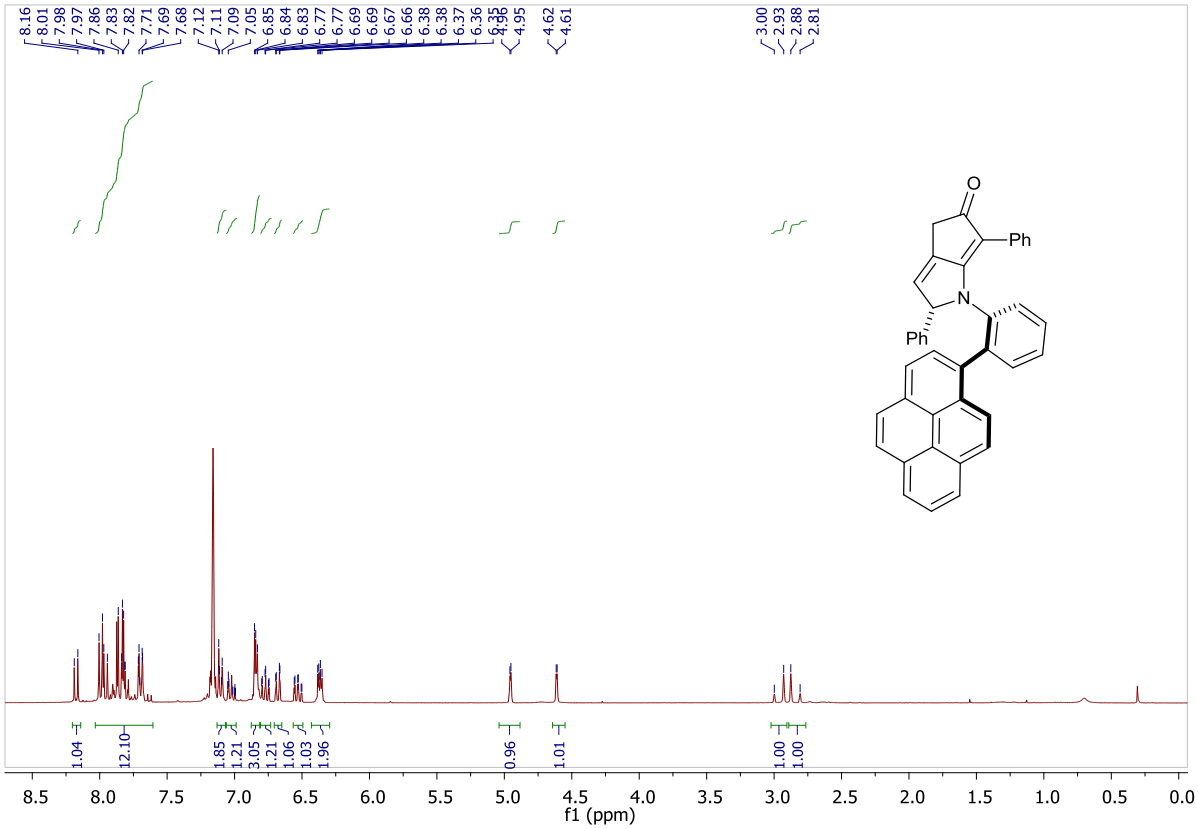
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7.09
7.05
6.85
6.84
6.83
6.77
6.77
6.69
6.69
6.67
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6.37
6.36
4.95
4.62
4.61
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2.88
2.81
1.04
12.10
1.85
1.21
3.05
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1.00
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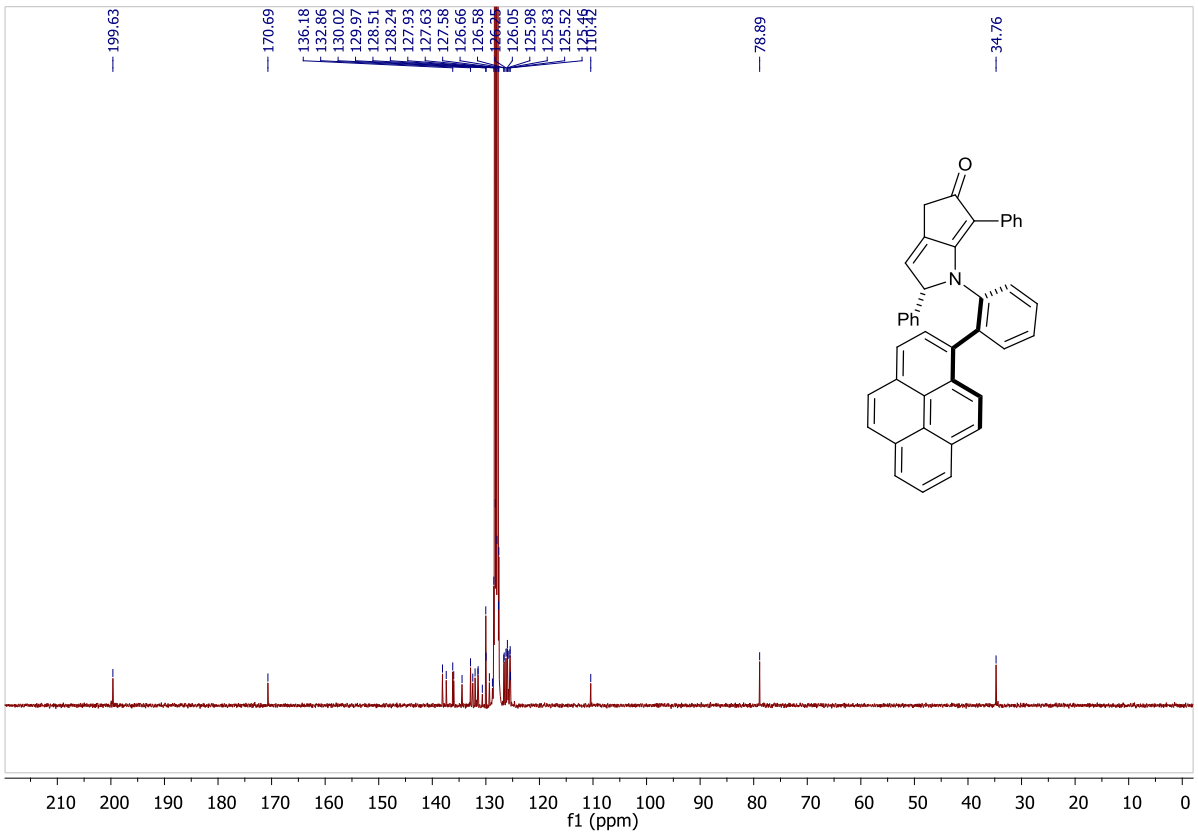
Ph
N
Ph
f1 (ppm)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128.51
128.24
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127.58
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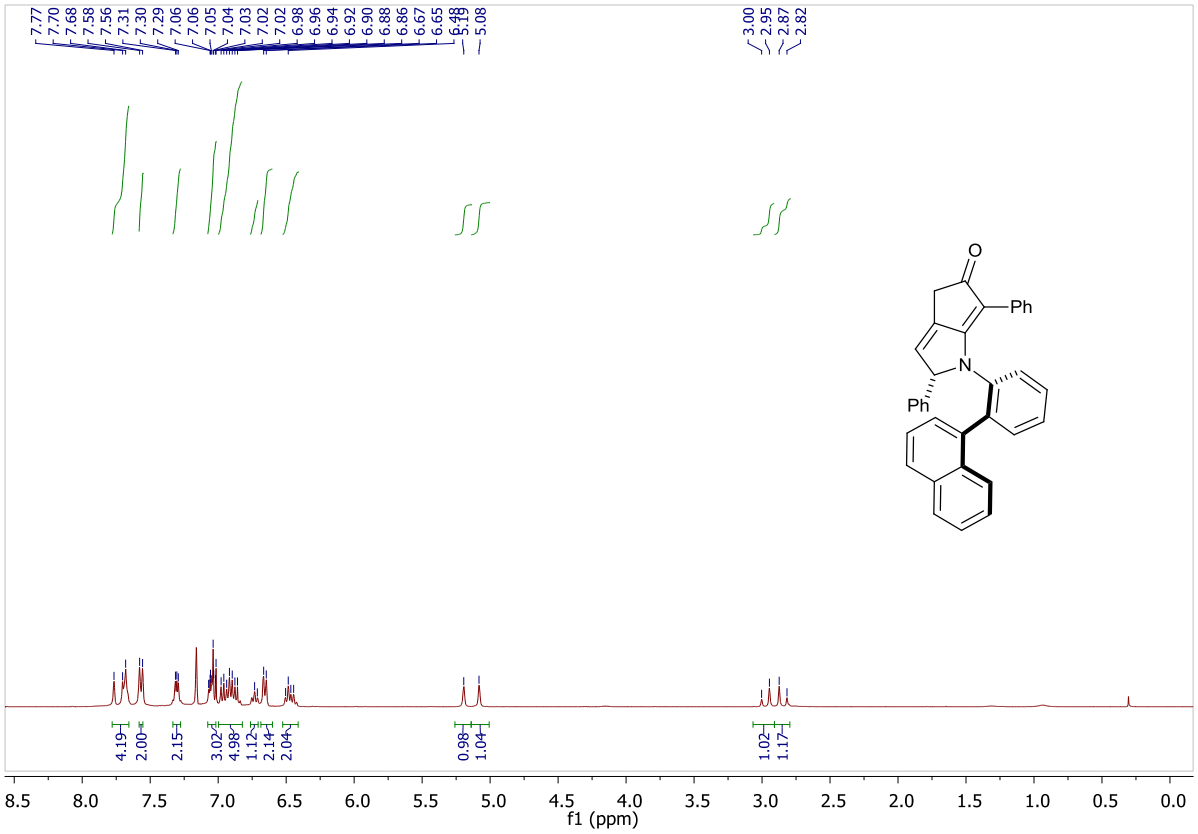
N
Ph
f1 (ppm)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7.31
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7.29
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7.06
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7.04
7.03
7.02
7.02
6.98
6.96
6.94
6.92
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6.88
6.86
6.67
6.65
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5.08
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2.82
O
Ph
N
Ph
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2.00
2.15
3.02
4.98
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2.14
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1.04
1.02
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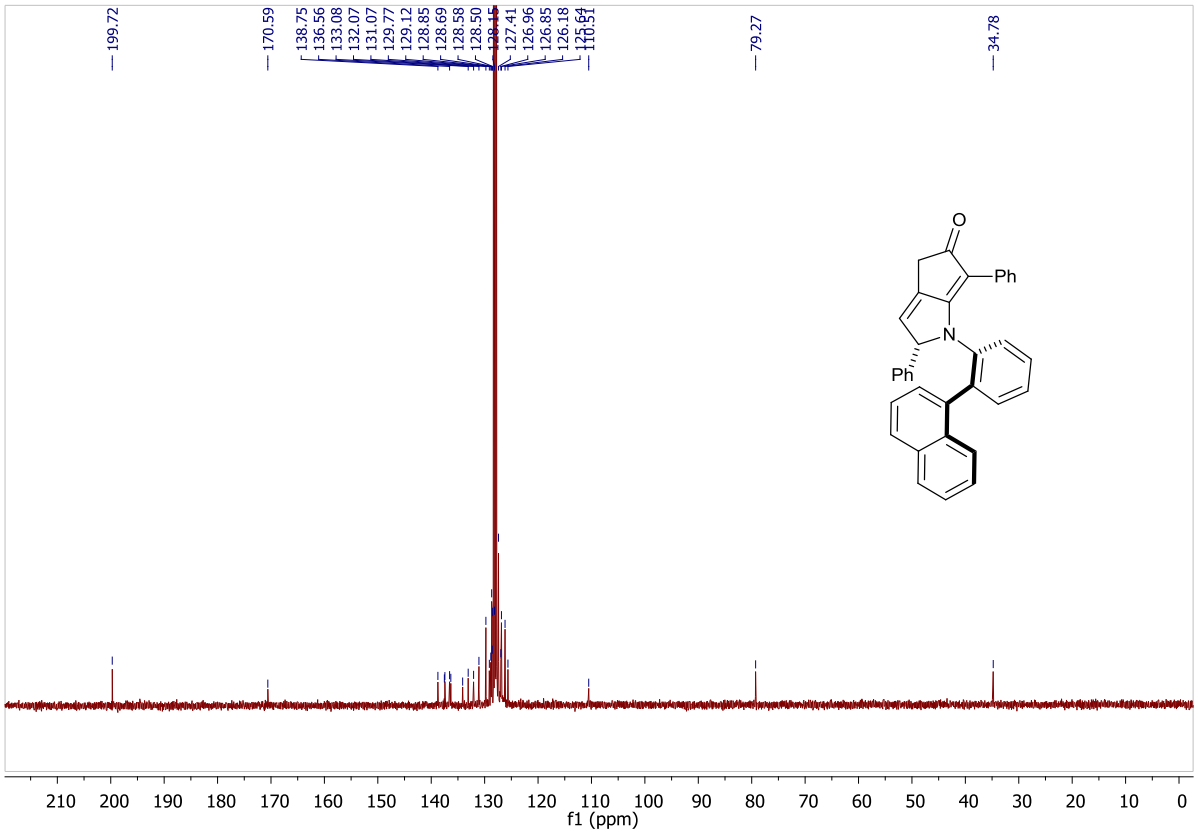
f1 (ppm)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128.58
128.50
127.41
126.96
126.85
126.18
110.51
79.27
34.78
O
Ph
N
Ph
210
200
190
180
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130
120
110
100
90
80
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50
40
30
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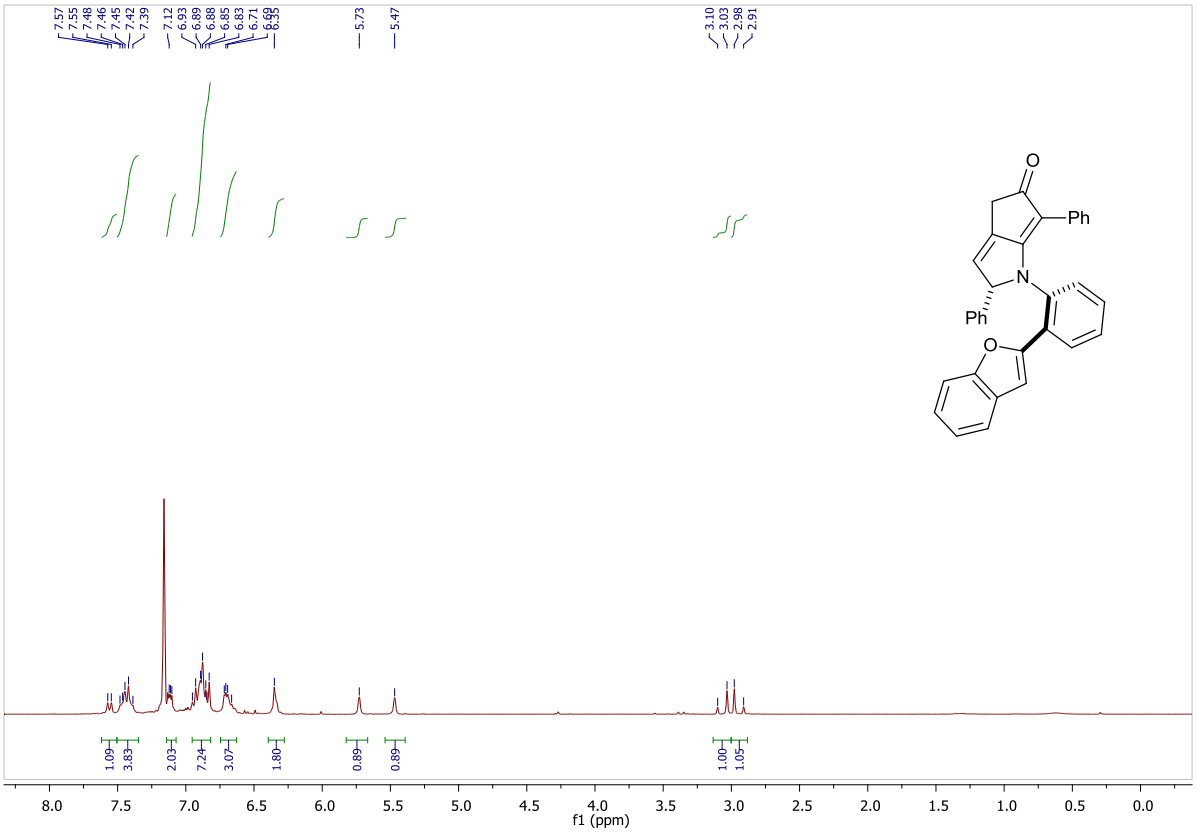
f1 (ppm)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7.39
7.12
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6.89
6.88
6.85
6.83
6.71
6.69
6.39
5.73
5.47
3.10
3.03
2.98
2.91
O
Ph
N
Ph
O
1.09
3.83
2.03
7.24
3.07
1.80
0.89
0.89
1.00
1.05
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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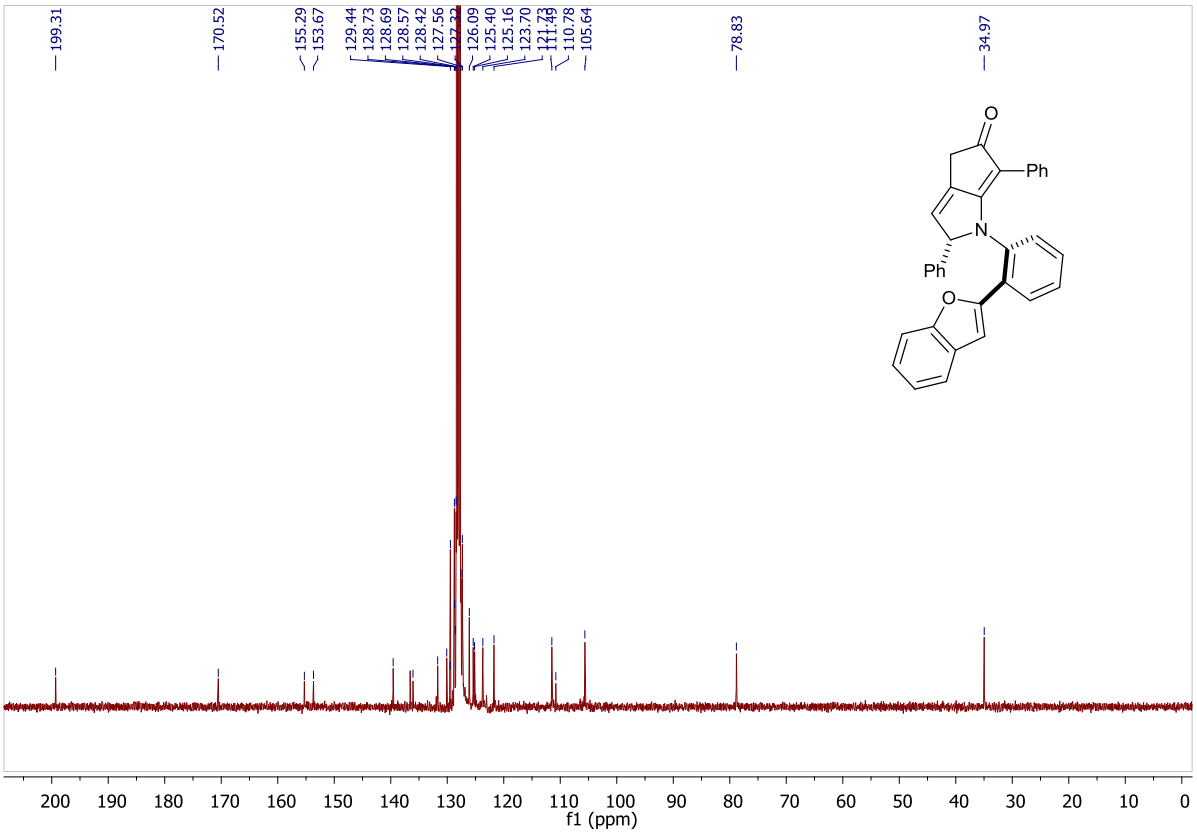
f1 (ppm)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128.57
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127.32
126.09
125.40
125.16
123.70
111.73
111.49
110.78
105.64
78.83
34.97
O
Ph
N
Ph
O
200
190
180
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110
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80
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50
40
30
20
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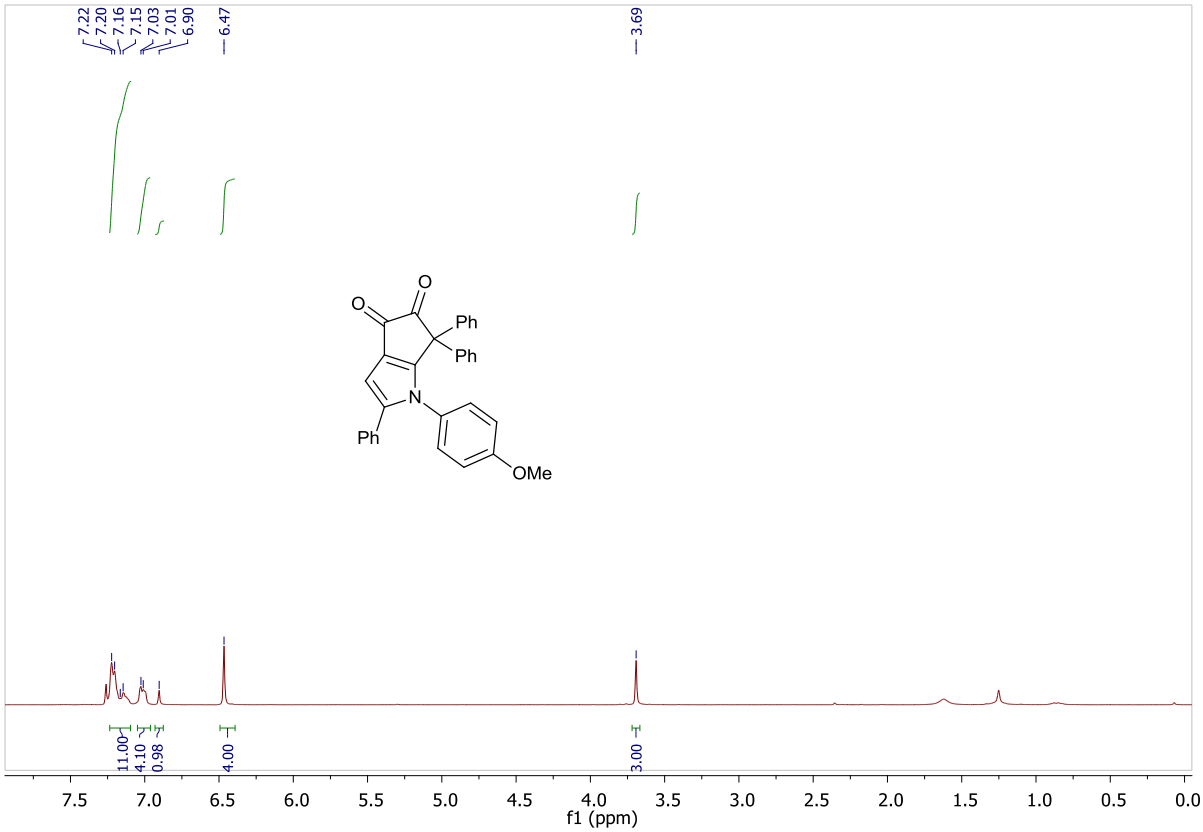
0
f1 (ppm)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O
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Ph
N
Ph
OMe
11.00
4.10
0.98
4.00
3.00
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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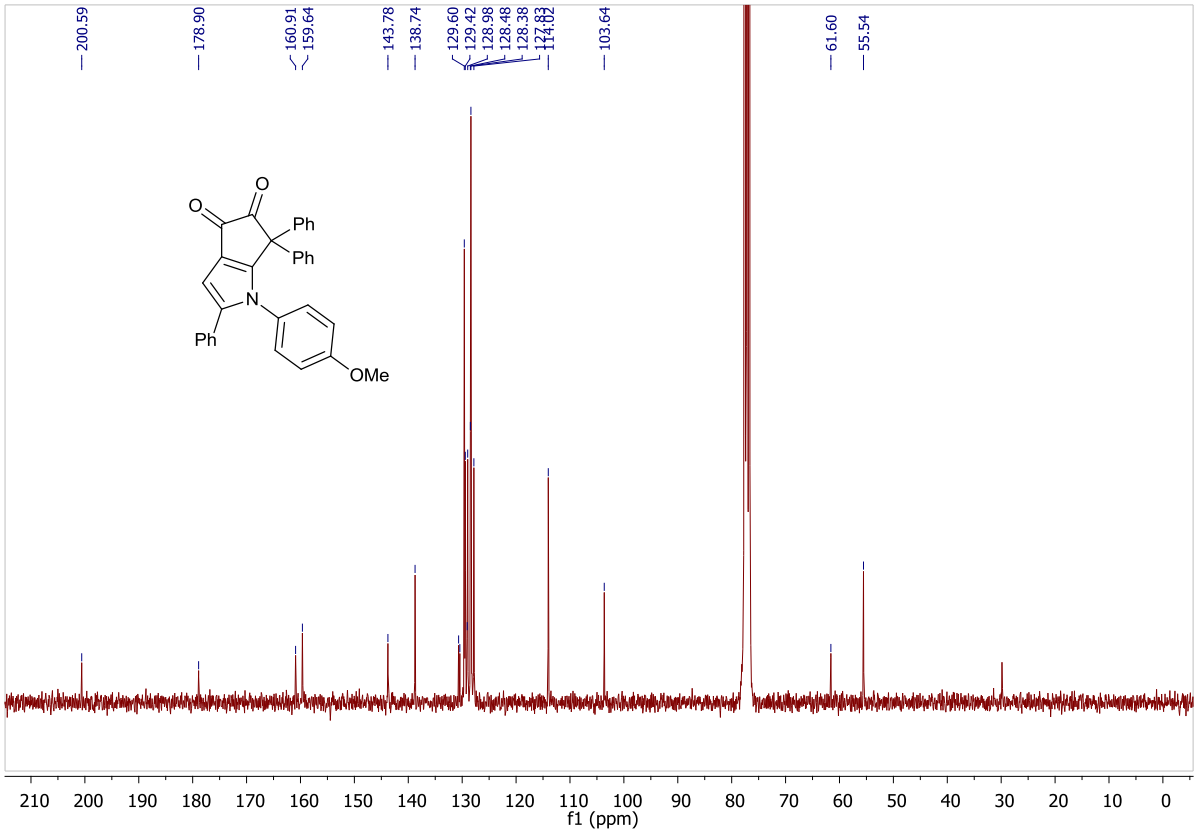
f1 (ppm)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128.38
127.83
114.02
103.64
61.60
55.54
O
O
Ph
Ph
N
Ph
OMe
210
200
190
180
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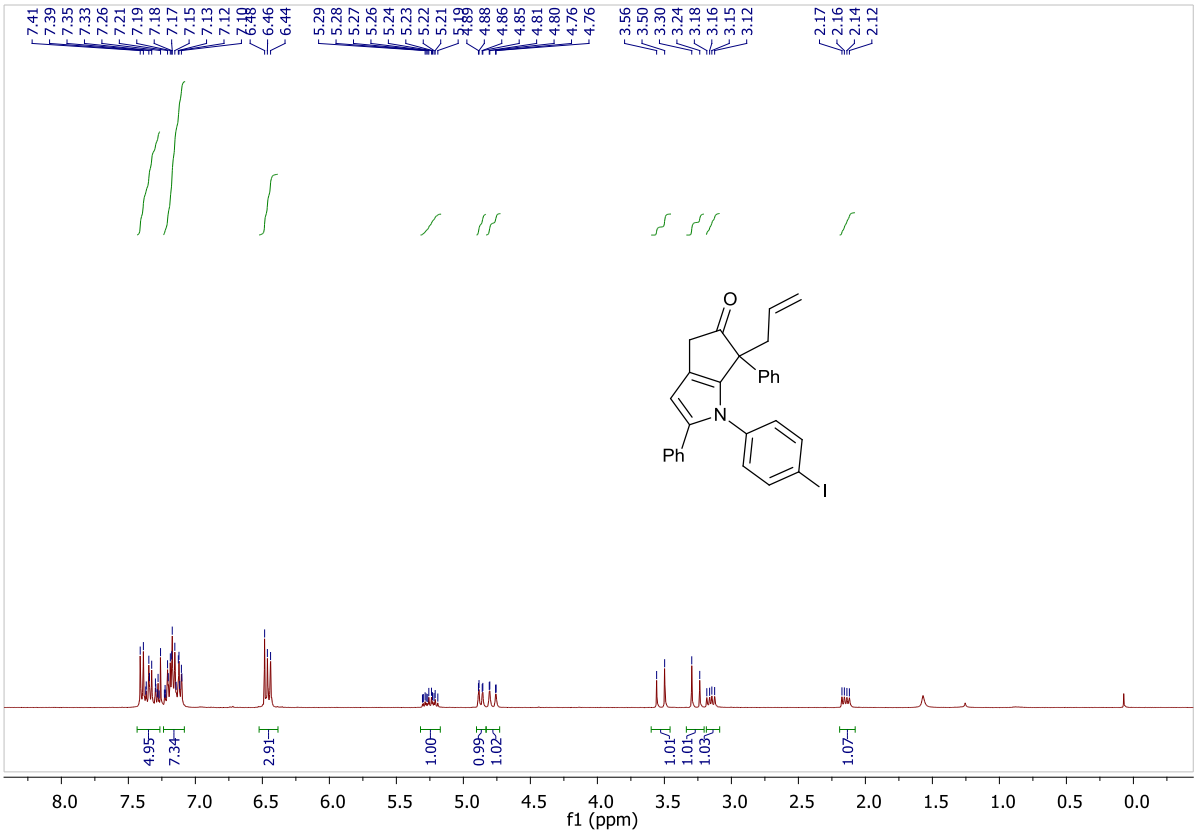
f1 (ppm)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7.13
7.12
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6.44
5.29
5.28
5.27
5.26
5.24
5.23
5.22
5.21
4.88
4.86
4.85
4.81
4.80
4.76
3.56
3.50
3.30
3.24
3.18
3.16
3.15
3.12
2.17
2.16
2.14
2.12
O
Ph
N
Ph
I
4.95
7.34
2.91
1.00
0.99
1.02
1.01
1.01
1.03
1.07
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
2.0
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1.0
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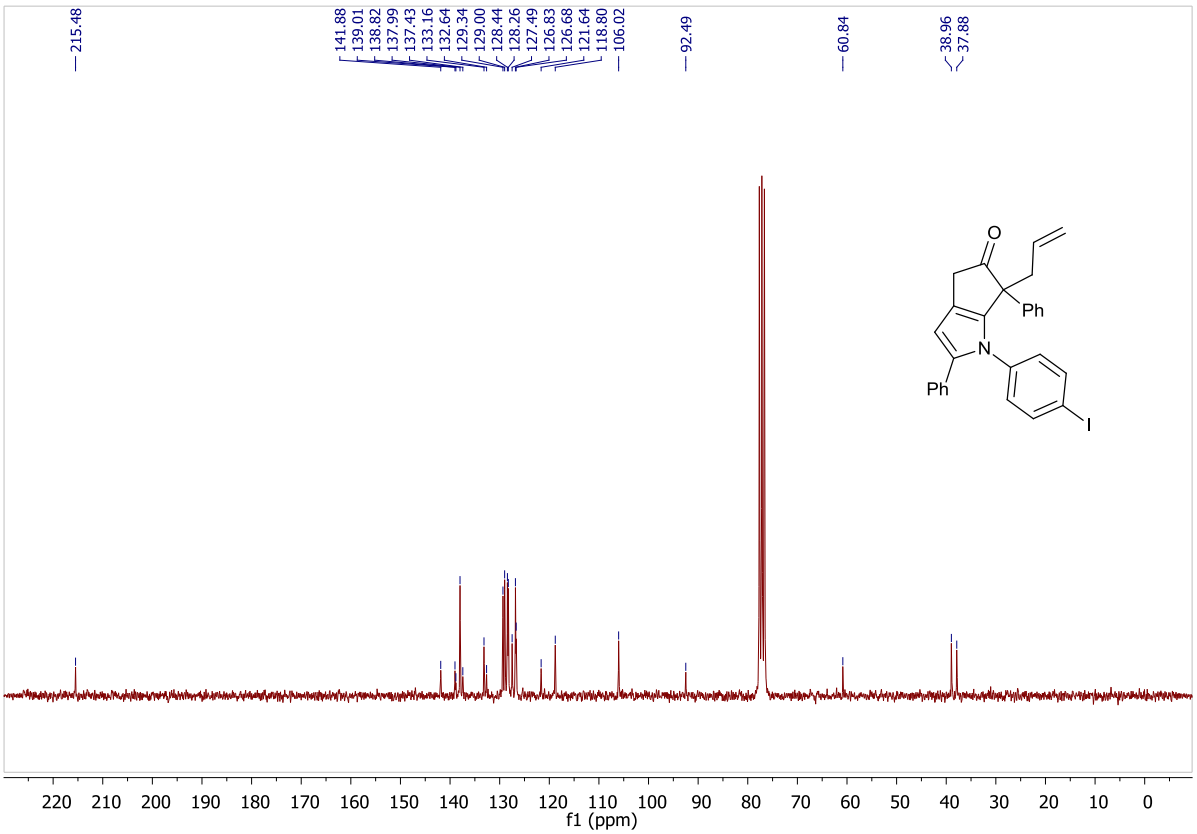
0.0
f1 (ppm)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126.83
126.68
121.64
118.80
106.02
92.49
60.84
38.96
37.88
O
Ph
N
Ph
I
220
210
200
190
180
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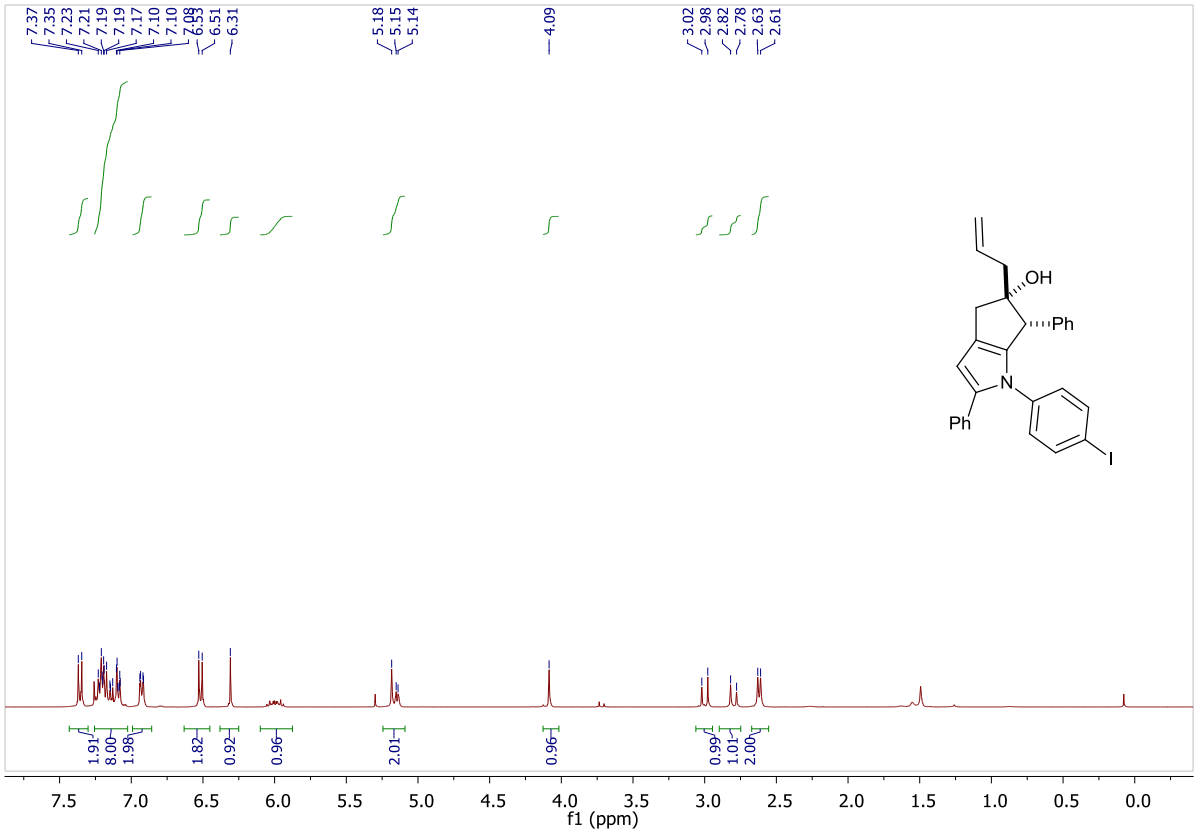
f1 (ppm)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5.18
5.15
5.14
4.09
3.02
2.98
2.82
2.78
2.63
2.61
OH
Ph
N
Ph
I
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8.00
1.98
1.82
0.92
0.96
2.01
0.96
0.99
1.01
2.00
7.5
7.0
6.5
6.0
5.5
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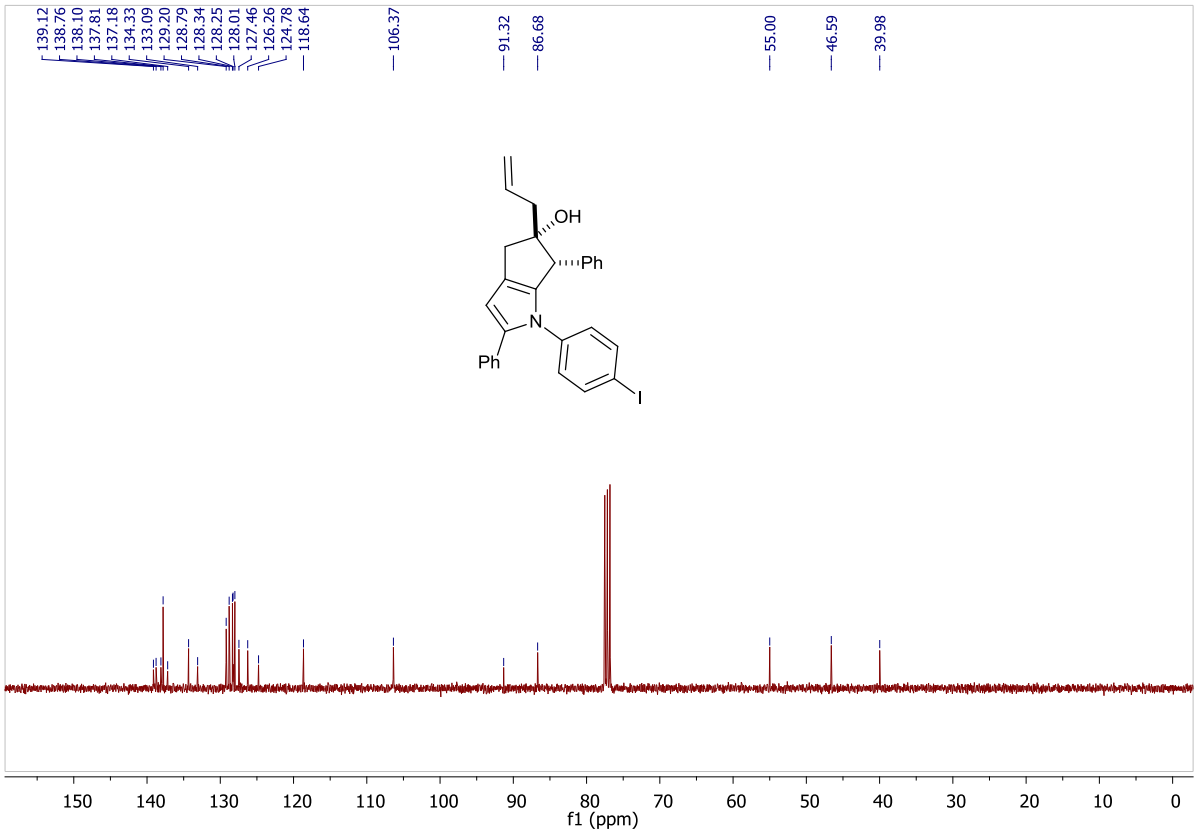
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128.25
128.01
127.46
126.26
124.78
118.64
106.37
91.32
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55.00
46.59
39.98
OH
Ph
N
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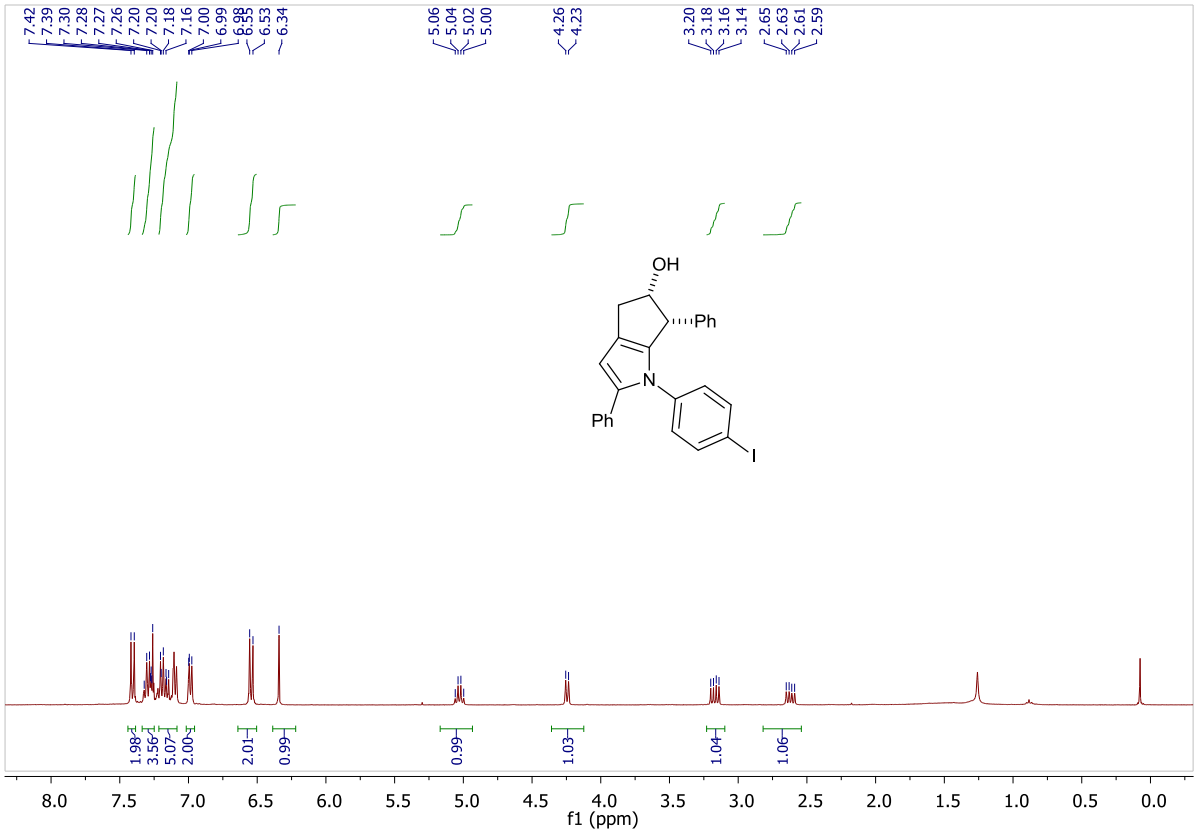
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5.04
5.02
5.00
4.26
4.23
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3.18
3.16
3.14
2.65
2.63
2.61
2.59
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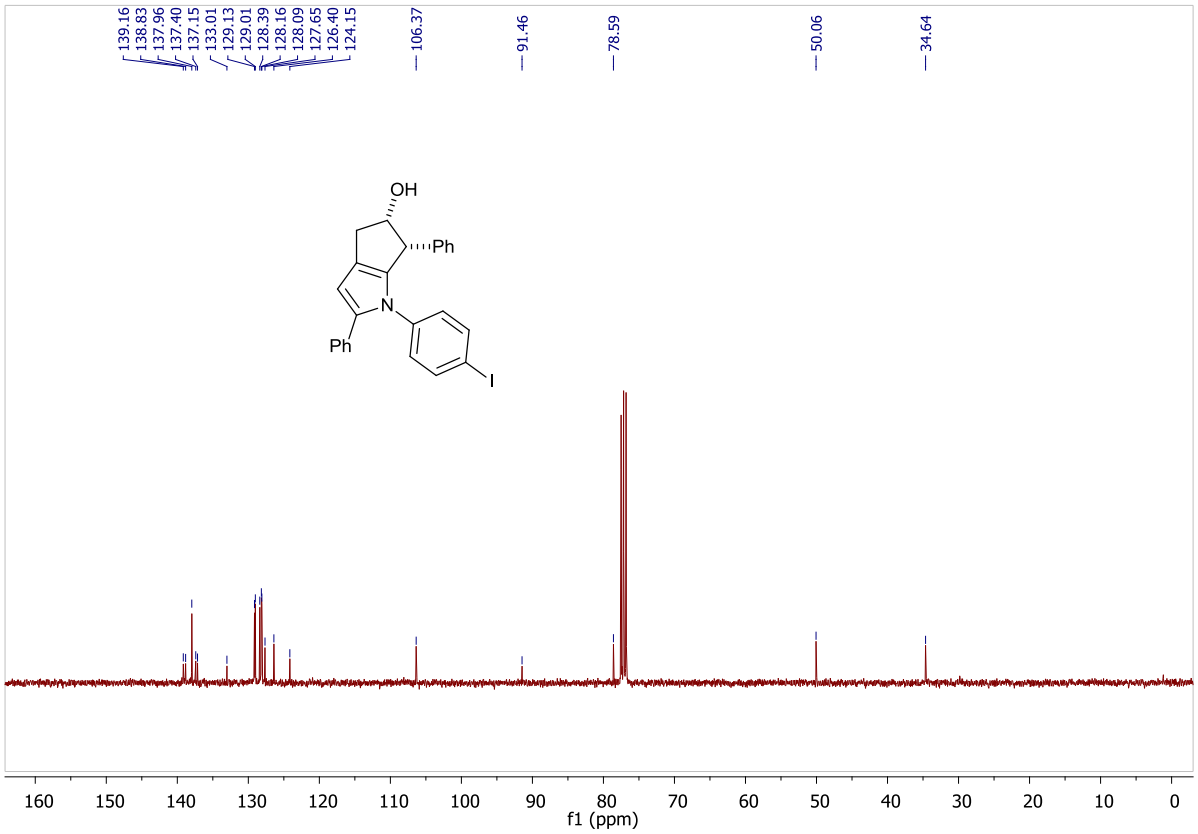
0.99
0.99
1.03
1.04
1.06
f1 (ppm)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128.09
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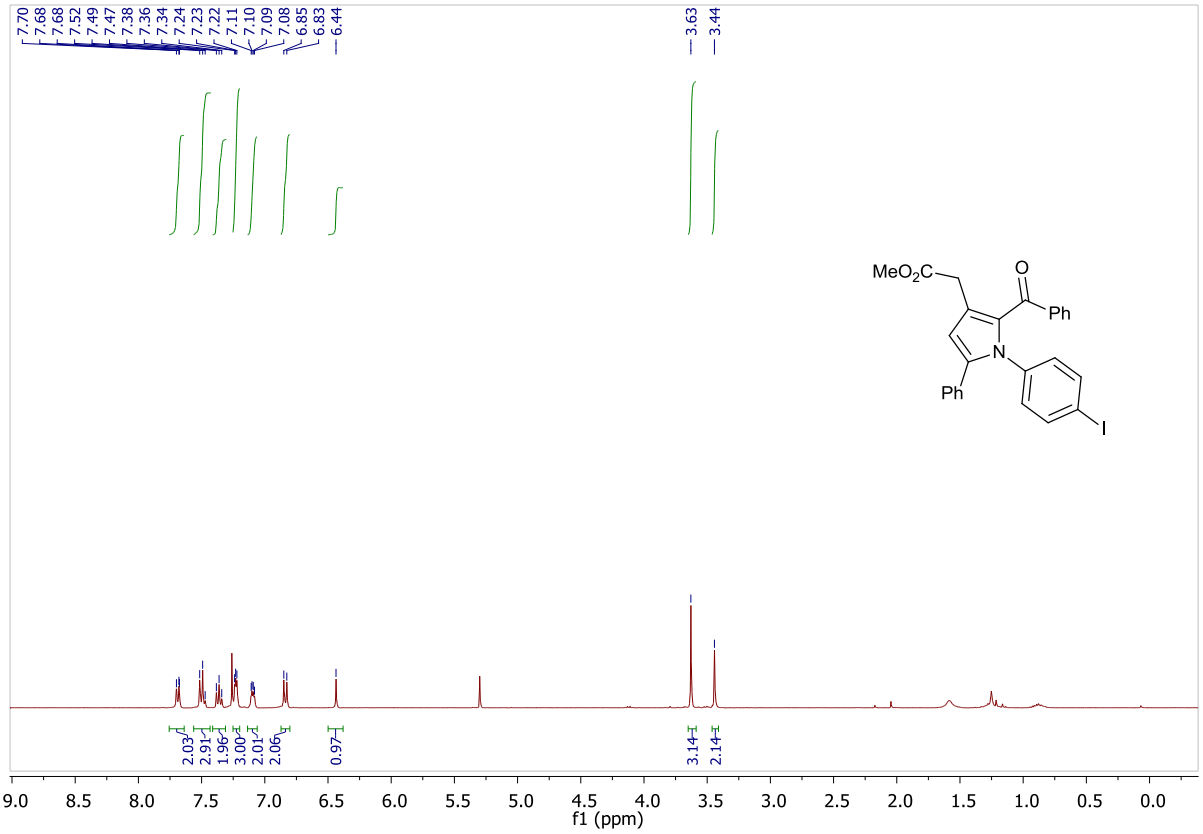
106.37
91.46
78.59
50.06
34.64
OH
Ph
N
Ph
I
f1 (ppm)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7.11
7.10
7.09
7.08
6.85
6.83
6.44
3.63
3.44
MeO2C
O
Ph
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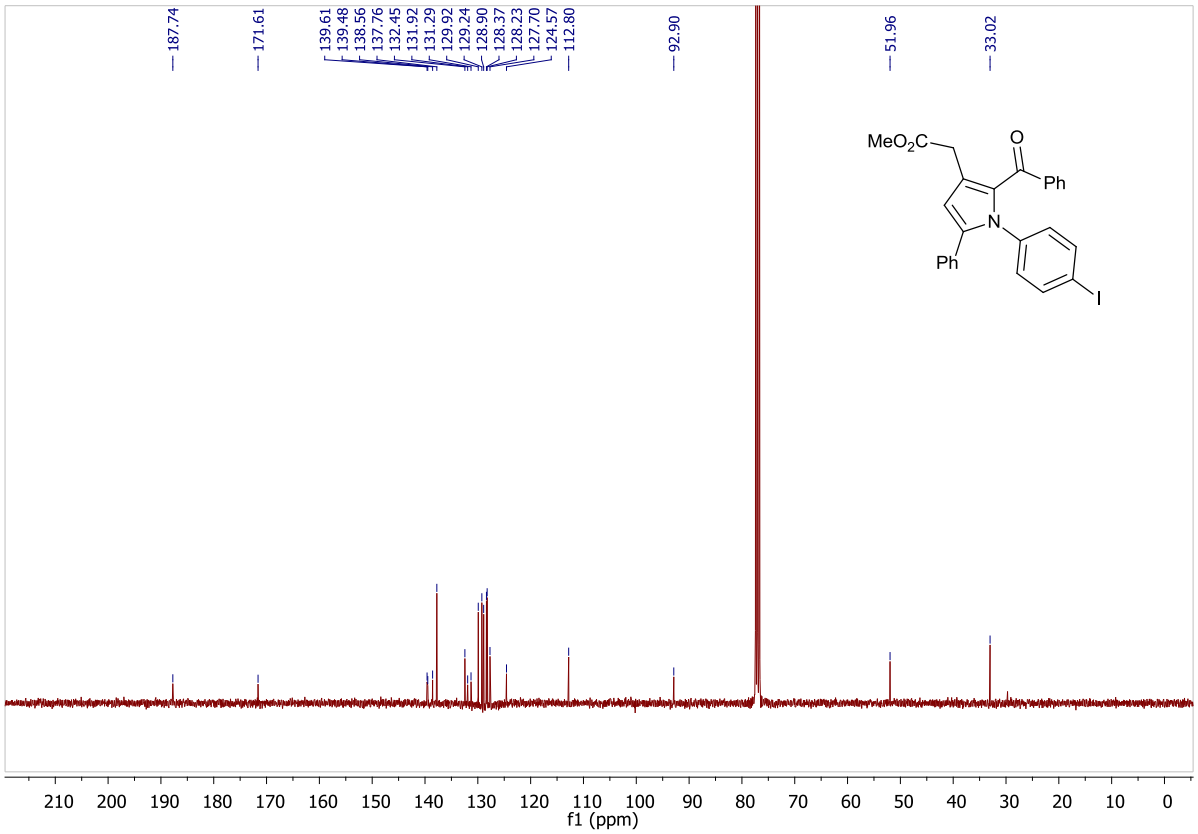
2.14
f1 (ppm)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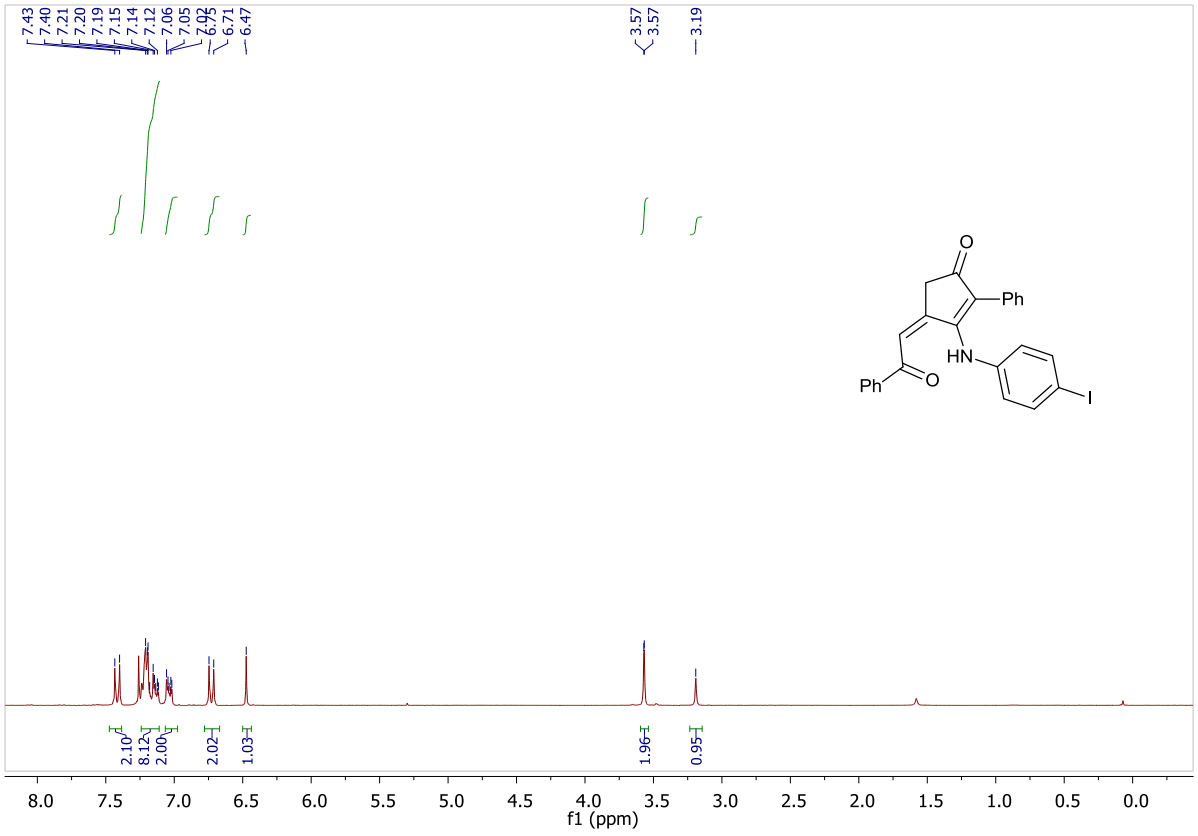
MeO2C
O
Ph
N
Ph
I
f1 (ppm)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7.05
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3.57
3.19
O
Ph
HN
Ph
O
I
2.10
8.12
2.00
2.02
1.03
1.96
0.95
8.0
7.5
7.0
6.5
6.0
5.5
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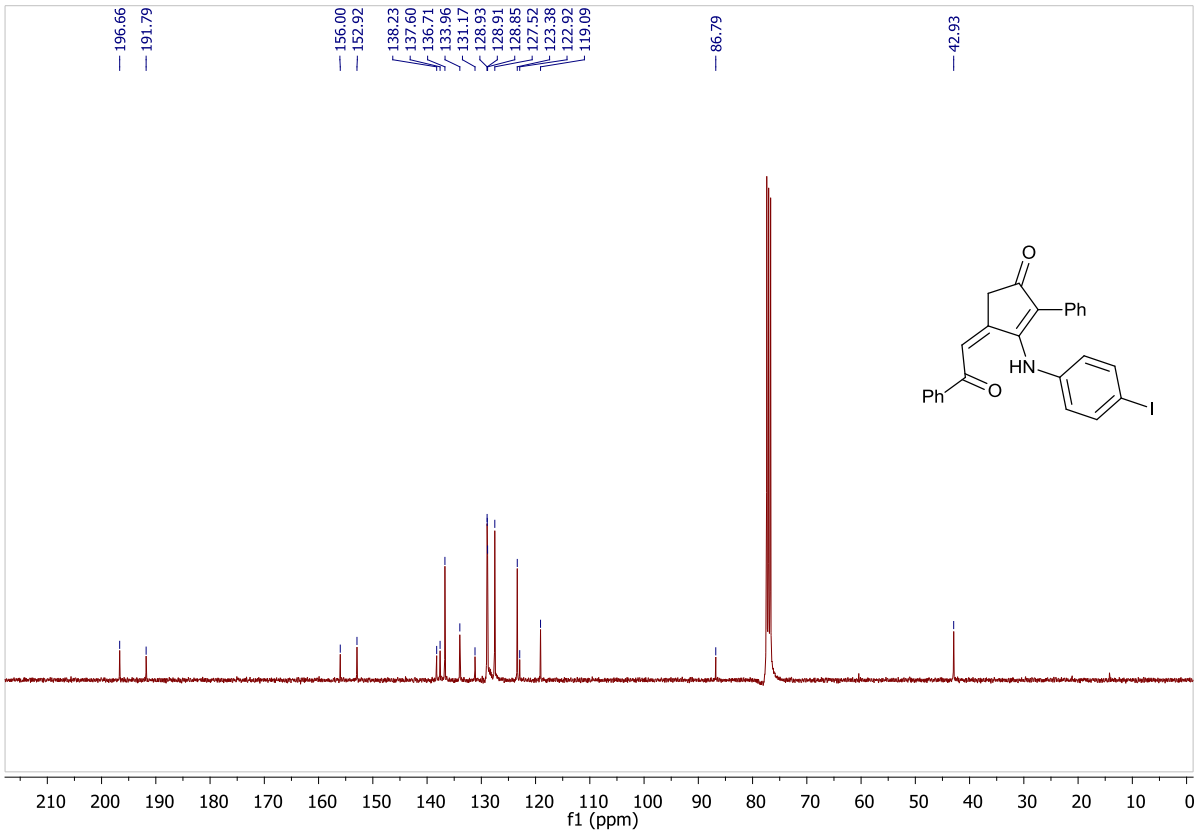
f1 (ppm)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128.91
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127.52
123.38
122.92
119.09
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42.93
O
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HN
Ph
O
I
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200
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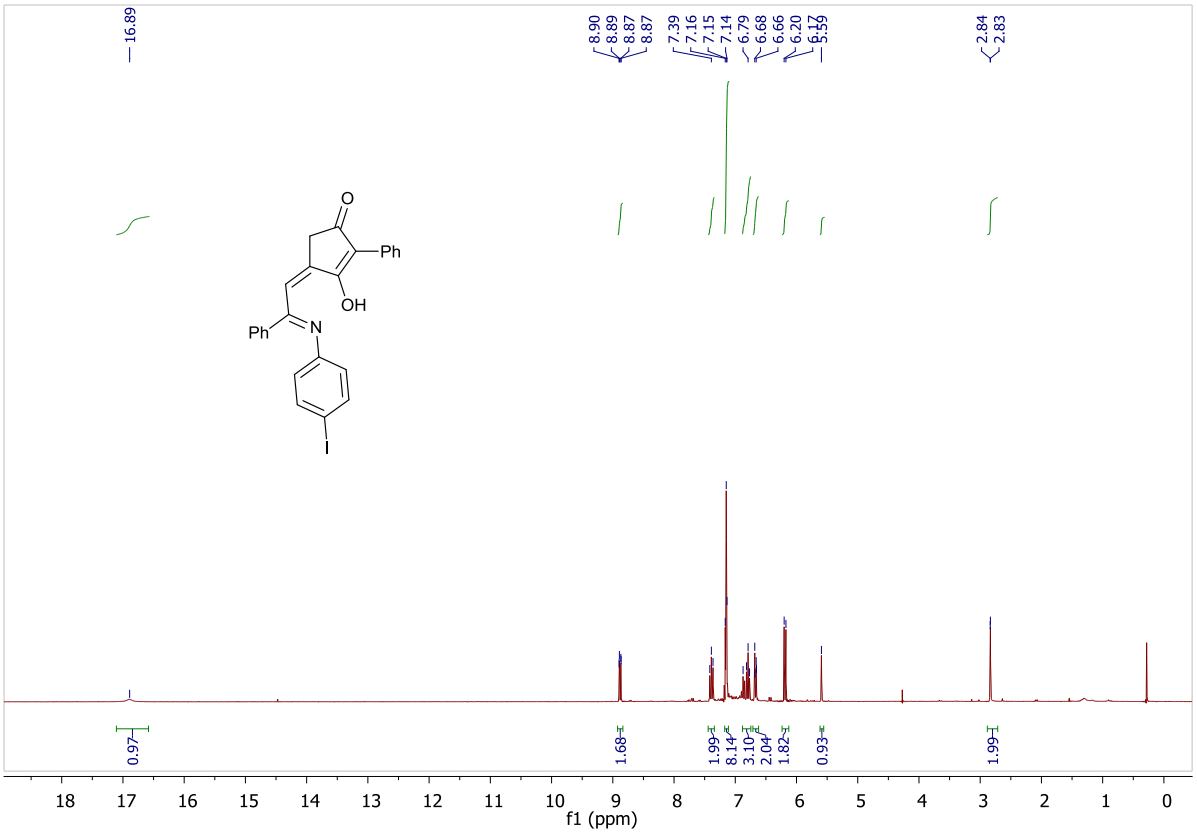
f1 (ppm)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6.68
6.66
6.20
5.59
2.84
2.83
O
Ph
OH
Ph
N
I
0.97
1.68
1.99
8.14
3.10
2.04
1.82
0.93
1.99
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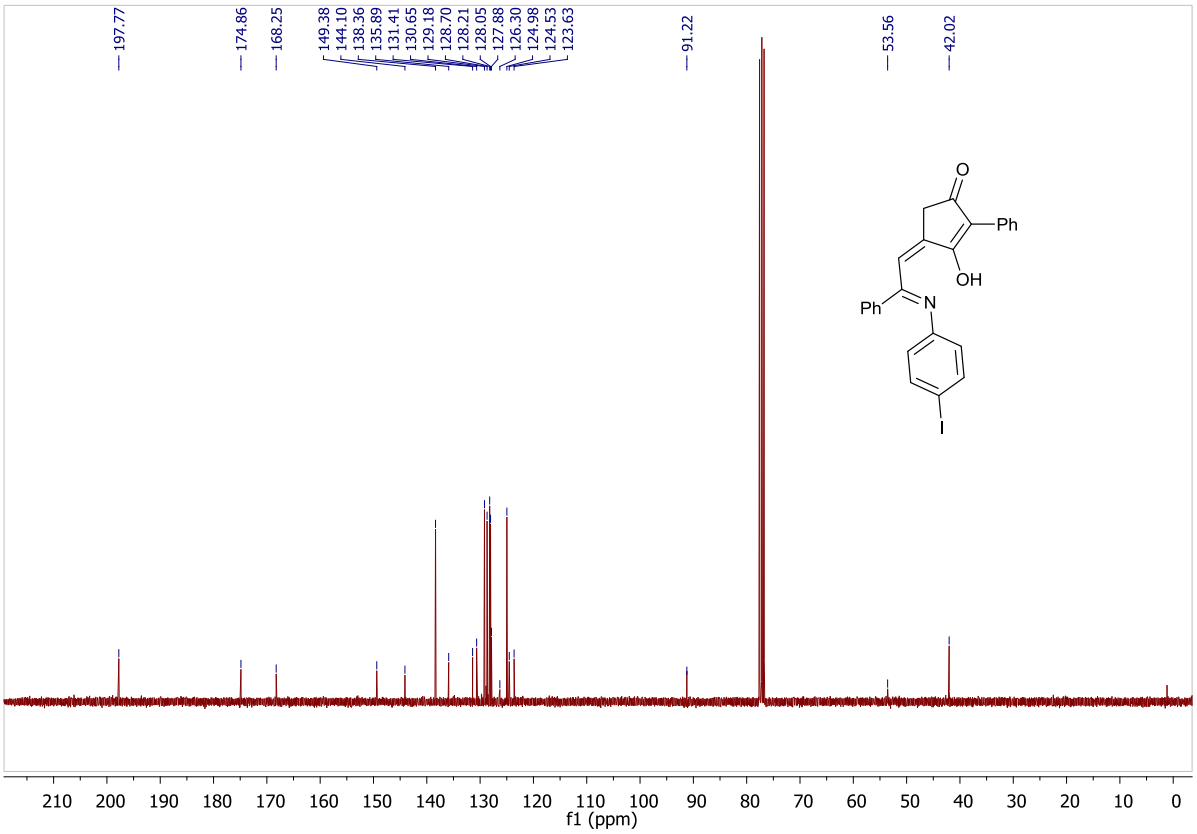
f1 (ppm)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128.05
127.88
126.30
124.98
124.53
123.63
91.22
53.56
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O
Ph
OH
Ph
N
I
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

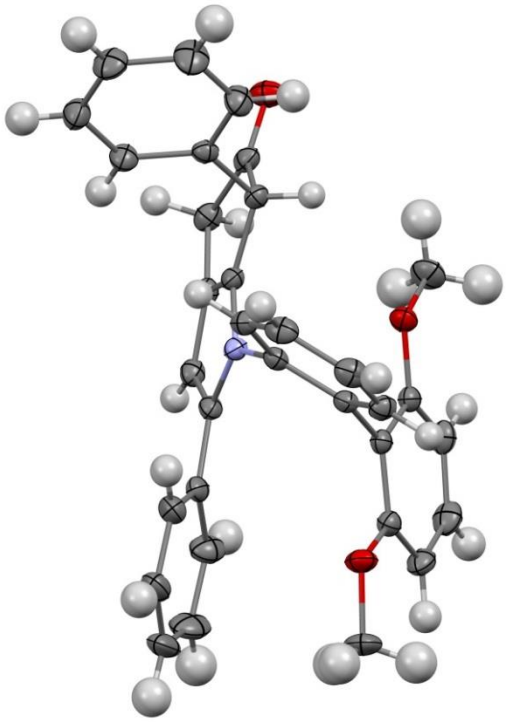

Fig. 1. ORTEP diagram of compound **8ac**, showing 50% probability ellipsoids. Solvent is omitted for clarity.

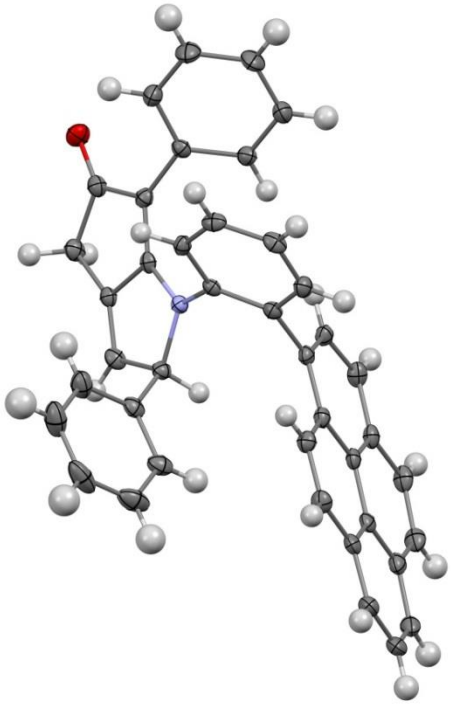

Fig. 2. ORTEP diagram of compound **10aq**, showing 50% probability ellipsoids. Solvent is omitted for clarity.

X-ray diffraction data for the two compounds **8ac** & **10aq** were collected by using a X8 APEXII CCD Bruker diffractometer with graphite-monochromated MoKα radiation. X-ray diffraction Crystals were mounted on a CryoLoop (Hampton Research) with Paratone-N (Hampton Research) as cryoprotectant and then flashfrozen in a nitrogen-gas stream at 100 K. For compounds, the temperature of the crystal was maintained at the selected value (100K) by means of a 700 series Cryostream cooling device to within an accuracy of ±1 K. The data were corrected for Lorentz polarization, and absorption effects. The structures were solved by direct methods using SHELXS-97[1] and refined against F^2 by full-matrix least-squares techniques using SHELXL-2014[2] with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were located on a difference Fourier map and introduced into the calculations as a riding model with isotropic thermal parameters. All calculations were performed by using the Crystal Structure crystallographic software package WINGX.[3]

The crystal data collection and refinement parameters are given in Table X1.

CCDC 1555744 & 1555745 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/Community/Requestastructure.

1) Sheldrick, G. M. SHELXS-97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, Germany, **1997**.
2) G. M. Sheldrick, Acta Crystallogr., Sect. A: Found. Crystallogr., **2008**, 64, 112-122
3) Farrugia, L. J. *J. Appl. Cryst*., **1999**, *32*, 837.

Table X1. Crystallographic data and structure refinement details for **8ac** & **10aq**.

Compounds	**8ac**	**10aq**
Empirical Formula	$C_{33}\ H_{27}\ N\ O_3$, $C\ H_2\ Cl_2$	$2(C_{41}\ H_{27}\ N\ O)$, $C\ Cl_2$
M_r	570.48	1182.18
Crystal size, mm^3	0.27 x 0.24 x 0.04	0.26 x 0.21 x 0.09
Crystal system	monoclinic	triclinic
Space group	*P* $2_1/c$	*P -1*
a, Å	14.1223(5)	9.6948(2)
b, Å	10.4359(3)	10.6078(3)
c, Å	19.4476(6)	14.8224(4)
α, °	90	105.2660(10)
β, °	97.282(2)	103.770(2)
γ, °	90	93.623(2)
Cell volume, $Å^3$	2843.05(16)	1415.34(6)
Z ; Z’	4 ; 1	2 ; 1
T, K	100(1)	100(1)
Radiation type ; wavelength Å	MoKα ; 0.71073	MoKα ; 0.71073
F_{000}	1192	616
μ, mm^{-1}	0.265	0.173
θ range, °	2.111 - 30.566	1.477 - 24.997
Reflection collected	36 151	24 994
Reflections unique	8 452	4 993
R_{int}	0.0515	0.0373
GOF	1.022	1.043
Refl. obs. (I>2σ(I))	5 090	4 092
Parameters	391	403
wR_2 (all data)	0.1434	0.2508
R value (I>2σ(I))	0.0556	0.0850
Largest diff. peak and hole (e-.$Å^{-3}$)	0.739 ; -0.519	0.834 ; -1.694

Coordinates (x,y,z) of the computed species

8ad				8'ad			
C	1.291756	0.889272	0.565742	C	-1.474032	1.412971	0.580751
C	1.087567	1.745502	1.611884	C	-1.360367	2.625779	-0.040053
C	-0.171427	1.423686	2.184272	C	0.018366	2.852565	-0.280812
C	-0.684026	0.367556	1.45674	C	0.702079	1.761646	0.219882
C	-1.137249	-1.510246	-2.654716	C	0.650331	-2.735894	1.185344
C	2.567463	1.076622	-0.180186	C	-2.880805	0.962162	0.839568
C	3.080252	2.381279	0.517233	C	-3.640349	2.268102	0.450515
C	2.222235	2.712307	1.755365	C	-2.693147	3.281292	-0.221108
C	-1.04925	-0.634199	-1.568275	C	0.677217	-1.458798	0.613487
C	3.598458	-0.024423	-0.018387	C	-3.32711	-0.221547	-0.002292
C	4.448449	-0.348364	-1.072961	C	-3.299091	-1.509726	0.528155
C	5.402809	-1.350649	-0.927926	C	-3.616951	-2.60926	-0.263927
C	5.52007	-2.03417	0.277473	C	-3.983536	-2.429953	-1.592852
C	4.680951	-1.706934	1.339288	C	-4.036827	-1.144169	-2.123367
C	3.726297	-0.706921	1.19274	C	-3.70815	-0.049567	-1.333525
C	-1.869892	-0.448608	1.75543	C	2.157439	1.614665	0.348494
C	-1.770154	-1.841266	1.846129	C	2.743239	1.221751	1.555709
C	-2.874157	-2.604155	2.209285	C	4.126175	1.159055	1.675963
C	-4.090612	-1.98609	2.483008	C	4.940121	1.48753	0.595872
C	-4.198529	-0.601171	2.387794	C	4.361851	1.883302	-0.606884
C	-3.096091	0.163371	2.024982	C	2.980401	1.94474	-0.731461
C	0.004056	-0.834281	-0.661089	C	-0.018553	-0.441425	1.288512
C	0.919804	-1.869258	-0.843673	C	-0.609816	-0.690617	2.528797
C	0.814437	-2.717016	-1.936819	C	-0.594678	-1.960535	3.084919
C	-0.220461	-2.53557	-2.847416	C	0.016311	-2.999368	2.39129
H	-0.638583	1.8436	3.061451	H	0.493424	3.727245	-0.697086
H	2.438127	1.295109	-1.244799	H	-3.098276	0.752494	1.891297
H	2.829655	2.565528	2.654856	H	-2.996705	3.410306	-1.265481
H	1.940056	3.767595	1.720136	H	-2.800151	4.252142	0.269798
H	4.357202	0.183119	-2.013987	H	-3.012414	-1.658233	1.563066
H	6.053212	-1.598116	-1.758697	H	-3.578751	-3.605389	0.161251
H	6.261523	-2.816122	0.390885	H	-4.23338	-3.2848	-2.210006
H	4.768728	-2.23312	2.282723	H	-4.331442	-0.993236	-3.155288
H	3.059759	-0.46339	2.015161	H	-3.741531	0.946242	-1.764982
H	-0.818219	-2.321751	1.648038	H	2.112838	0.980104	2.40504
H	-2.782459	-3.681608	2.282956	H	4.569619	0.854324	2.617257
H	-4.951327	-2.580779	2.76607	H	6.018508	1.437447	0.692144
H	-5.146734	-0.115138	2.58714	H	4.988572	2.130095	-1.456204

H	-3.180981	1.239298	1.916183	H	2.525019	2.218143	-1.676454
H	1.714162	-1.99974	-0.118256	H	-1.084899	0.134018	3.047875
H	1.536597	-3.512989	-2.071765	H	-1.061156	-2.135555	4.047114
H	-1.93602	-1.358052	-3.372053	H	1.151999	-3.537904	0.655518
N	0.214975	0.045364	0.447489	N	-0.221891	0.863511	0.744348
O	4.002834	3.027145	0.118312	O	-4.803339	2.447919	0.662143
H	-0.311707	-3.186724	-3.708533	H	0.017601	-4.004535	2.795094
C	-2.060945	0.461933	-1.439041	C	1.499296	-1.253679	-0.619765
C	-1.687065	1.807215	-1.584495	C	2.884811	-1.509584	-0.543826
C	-3.409525	0.123286	-1.211994	C	0.923198	-0.834922	-1.829422
C	-2.660625	2.800089	-1.458247	C	3.671631	-1.303566	-1.674897
C	-4.353639	1.141098	-1.097369	C	1.746197	-0.64119	-2.939704
C	-3.984798	2.475237	-1.209551	C	3.112438	-0.864822	-2.866739
H	-2.367385	3.838831	-1.569852	H	4.740222	-1.479011	-1.610092
H	-5.388676	0.879195	-0.904442	H	1.296978	-0.320223	-3.873953
H	-4.72931	3.25707	-1.111416	H	3.73913	-0.705093	-3.736846
C	-0.276353	2.233871	-1.906529	C	3.564066	-1.999625	0.714568
H	0.326705	1.404926	-2.277684	H	3.093682	-1.609298	1.616505
H	-0.28953	3.013255	-2.67117	H	3.539814	-3.091986	0.774045
H	0.211537	2.646188	-1.019286	H	4.609521	-1.687321	0.713893
C	-3.8599	-1.309185	-1.067208	C	-0.557071	-0.605868	-1.973771
H	-3.941962	-1.801378	-2.040517	H	-0.881463	-0.851049	-2.986926
H	-3.162369	-1.890408	-0.462622	H	-1.133578	-1.218656	-1.27913
H	-4.838933	-1.348004	-0.588329	H	-0.81134	0.443123	-1.78957
		A				**3aa**	
C	1.269227	-0.736176	0.116278	C	2.336334	0.338114	-0.693602
C	0.513187	-1.875804	0.800233	C	3.351728	1.238018	-0.856714
C	-0.800632	-2.197394	0.362885	C	2.842073	2.519962	-0.522788
C	-1.930792	-2.346288	-0.019116	C	1.518705	2.348409	-0.16711
C	0.119125	3.790215	-1.295239	C	-2.391889	0.471376	-0.996056
C	2.6129	-0.664052	0.889204	C	2.679733	-1.07885	-0.999207
C	2.443822	-1.655547	2.057352	C	4.10693	-0.867893	-1.605523
C	1.171162	-2.387334	1.845425	C	4.599325	0.570414	-1.346805
C	-0.135414	2.658802	-0.521149	C	-1.119336	1.025517	-0.991934
C	3.837487	-1.030062	0.075685	C	2.793238	-2.006442	0.197459
C	4.96821	-0.213735	0.091655	C	2.587306	-3.375714	0.03725
C	6.095963	-0.552731	-0.651931	C	2.718407	-4.238859	1.11984
C	6.093916	-1.705268	-1.431184	C	3.060732	-3.741516	2.373261
C	4.976923	-2.53106	-1.444254	C	3.275483	-2.376494	2.537361
C	3.854272	-2.192668	-0.693871	C	3.14344	-1.512982	1.454966
C	-3.284504	-2.505841	-0.4319	C	0.568756	3.355289	0.326517
C	-3.77398	-1.770352	-1.5172	C	-0.295564	3.083803	1.393285

C	-5.097925	-1.903488	-1.909687
C	-5.948023	-2.77181	-1.223496
C	-5.46409	-3.508487	-0.142578
C	-4.140679	-3.372786	0.260232
C	0.766171	1.584588	-0.546237
C	1.927206	1.682508	-1.329638
C	2.166478	2.829091	-2.083565
C	1.263156	3.883836	-2.077107
H	2.728209	0.334876	1.30708
H	0.833087	-3.176507	2.499324
H	4.964251	0.683527	0.691207
H	6.962033	0.091507	-0.633934
H	6.972692	-1.969396	-2.008614
H	4.975644	-3.428598	-2.046633
H	2.988387	-2.844079	-0.71254
H	-3.111992	-1.093948	-2.04147
H	-5.473397	-1.337042	-2.753353
H	-6.979534	-2.88309	-1.530855
H	-6.120696	-4.181821	0.396626
H	-3.752736	-3.936463	1.101298
H	2.656803	0.880686	-1.348306
H	3.068941	2.890812	-2.675989
H	-0.596663	4.605107	-1.263297
N	0.490903	0.468969	0.230205
O	3.221546	-1.813277	2.957323
H	1.453484	4.775498	-2.662802
C	-1.351826	2.564634	0.348175
C	-1.216015	2.711828	1.736492
C	-2.596341	2.257224	-0.220338
C	-2.345615	2.591276	2.538193
C	-3.709125	2.13494	0.6105
C	-3.583958	2.3023	1.98376
H	-2.249133	2.721662	3.615132
H	-4.675639	1.88953	0.181944
H	-4.459155	2.199129	2.629027
C	0.134258	2.977976	2.376902
H	0.781696	3.568455	1.727001
H	0.008737	3.503265	3.321055
H	0.640453	2.031485	2.574785
C	-2.742736	2.044121	-1.708497
H	-2.652714	2.991927	-2.248337
H	-1.960008	1.38343	-2.094705
C	-1.167324	4.059136	1.859047
C	-1.183677	5.323005	1.275921
C	-0.321667	5.604846	0.221287
C	0.543833	4.626529	-0.254623
C	-0.098949	0.423483	-0.259422
C	-0.348147	-0.740445	0.461075
C	-1.617457	-1.309756	0.442954
C	-2.631982	-0.696728	-0.280801
H	3.368067	3.461282	-0.48399
H	2.048761	-1.543363	-1.762985
H	5.410709	0.537836	-0.611985
H	5.010043	0.977764	-2.273451
H	2.323083	-3.76416	-0.94032
H	2.551392	-5.300931	0.983848
H	3.159463	-4.413973	3.21695
H	3.544486	-1.982115	3.510275
H	3.299947	-0.446302	1.586327
H	-0.276064	2.10714	1.863575
H	-1.830157	3.833876	2.686132
H	-1.863832	6.08255	1.642348
H	-0.330182	6.585165	-0.240392
H	1.199167	4.837628	-1.092291
H	0.443571	-1.198589	1.042055
H	-1.808166	-2.217715	1.00043
H	-3.18492	0.944265	-1.560556
H	-0.915285	1.929248	-1.553384
I	-4.565583	-1.545516	-0.301154
N	1.206815	0.993312	-0.266262
O	4.709737	-1.715472	-2.192679

H	-3.720444	1.614317	-1.944691				
H	1.439386	-0.99962	-0.934894				
H	-0.481229	0.35404	0.510021				
3aa·HFIP				**3aa**·(HFIP)$_2$			
C	0.443535	0.83702	1.270253	C	-0.901515	-0.021868	1.370784
C	1.273761	1.88959	1.533891	C	0.199889	0.658136	1.807861
C	0.565412	3.078236	1.223886	C	-0.085593	2.043151	1.71053
C	-0.685174	2.696498	0.776851	C	-1.368856	2.153082	1.211932
C	-3.147776	-0.073429	-1.668792	C	-4.454128	0.804272	-1.659252
C	1.037587	-0.514327	1.477618	C	-0.773802	-1.508099	1.372345
C	2.508499	-0.093668	1.742579	C	0.743753	-1.609867	1.659582
C	2.623531	1.417432	1.980477	C	1.30422	-0.283809	2.178217
C	-2.177751	0.731195	-1.086038	C	-3.314143	1.142941	-0.943034
C	0.518748	-1.304163	2.667813	C	-1.527253	-2.246294	2.470034
C	0.516247	-2.696949	2.632292	C	-1.889112	-3.579601	2.286622
C	0.057427	-3.427241	3.723453	C	-2.550889	-4.272799	3.294473
C	-0.397528	-2.770159	4.862057	C	-2.851696	-3.639394	4.496377
C	-0.389117	-1.379245	4.905792	C	-2.48626	-2.310792	4.686344
C	0.067666	-0.648682	3.814132	C	-1.825209	-1.61613	3.678431
C	-1.811849	3.553939	0.381855	C	-2.153572	3.374626	0.980619
C	-3.125852	3.270444	0.770848	C	-3.50509	3.456965	1.333985
C	-4.166074	4.113232	0.40123	C	-4.216392	4.630871	1.124292
C	-3.911128	5.256064	-0.351403	C	-3.588294	5.742382	0.56927
C	-2.60675	5.550659	-0.73428	C	-2.242648	5.671897	0.223763
C	-1.565383	4.702855	-0.375915	C	-1.530938	4.494854	0.422327
C	-1.767489	0.488343	0.222103	C	-3.050444	0.525889	0.277363
C	-2.319577	-0.561833	0.948089	C	-3.917948	-0.440391	0.776546
C	-3.279198	-1.380527	0.361928	C	-5.051604	-0.795719	0.052018
C	-3.68964	-1.127281	-0.940779	C	-5.31511	-0.166187	-1.157577
H	0.885119	4.101234	1.346016	H	0.532734	2.877414	2.00308
H	1.02608	-1.14937	0.585826	H	-0.972368	-1.983486	0.406859
H	2.835488	1.59355	3.041148	H	1.475467	-0.371222	3.257951
H	3.465825	1.806558	1.402077	H	2.266689	-0.079093	1.703186
H	0.867295	-3.210123	1.743465	H	-1.656079	-4.073693	1.349527
H	0.05295	-4.509991	3.682776	H	-2.833446	-5.307302	3.139513
H	-0.756906	-3.338942	5.711242	H	-3.3697	-4.178095	5.280818
H	-0.741586	-0.861408	5.790081	H	-2.71722	-1.811351	5.619774
H	0.058873	0.436997	3.840764	H	-1.550319	-0.575498	3.822366
H	-3.331852	2.391856	1.371861	H	-3.995896	2.599945	1.78173
H	-5.178618	3.880958	0.709419	H	-5.262443	4.680516	1.402771
H	-4.724667	5.912013	-0.636834	H	-4.144355	6.657794	0.406766
H	-2.398768	6.436644	-1.322526	H	-1.747903	6.531573	-0.212389

H	-0.551779	4.918202	-0.69492	H	-0.488431	4.430798	0.131108
H	-2.007396	-0.735738	1.971245	H	-3.717477	-0.90754	1.733951
H	-3.70693	-2.199249	0.926525	H	-5.725757	-1.547757	0.441844
H	-3.468299	0.116258	-2.685061	H	-4.659738	1.288623	-2.605194
H	-1.737798	1.550742	-1.641895	H	-2.629167	1.888924	-1.327758
I	-5.152722	-2.363698	-1.830337	I	-7.043284	-0.68977	-2.252243
N	-0.76145	1.305994	0.813102	N	-1.877025	0.871064	1.006639
O	3.430609	-0.868649	1.721808	O	1.394877	-2.605434	1.447863
H	4.988825	-0.163619	0.967824	H	3.036566	-2.221107	0.969059
O	5.459876	0.161838	0.185072	O	3.719513	-1.962664	0.315912
C	5.021887	-0.566869	-0.911474	C	3.34137	-2.465756	-0.925549
H	4.519002	-1.499157	-0.630592	H	2.691025	-3.342437	-0.837732
C	6.24886	-0.951405	-1.738583	C	4.620287	-2.903101	-1.638069
F	7.004649	0.101402	-2.03382	F	5.547657	-1.940689	-1.594264
F	5.895923	-1.543854	-2.885296	F	4.391598	-3.201544	-2.917048
F	6.997196	-1.815783	-1.048632	F	5.124173	-3.98079	-1.041133
F	3.458052	-0.473557	-2.697549	F	1.993752	-1.95259	-2.80302
C	4.006994	0.249891	-1.718481	C	2.568042	-1.411753	-1.728606
F	4.536877	1.344635	-2.255495	F	3.357738	-0.413933	-2.139457
F	3.008021	0.639756	-0.90651	F	1.603107	-0.881472	-0.970664
				H	4.95745	-0.644871	0.694515
				O	5.484545	0.142243	0.898457
				C	5.497925	0.982462	-0.20392
				H	5.39834	0.451585	-1.156077
				C	6.855912	1.679686	-0.232376
				F	7.164168	2.236346	0.935083
				F	6.882886	2.636634	-1.16823
				F	7.808273	0.792432	-0.528914
				F	4.181727	2.640879	-1.284411
				C	4.335651	1.9798	-0.134868
				F	4.478167	2.875247	0.842252
				F	3.195026	1.310233	0.098263
		3aa·$(HFIP)_3$				**9aa**	
C	1.546049	0.247817	-0.729811	C	2.276913	-0.914864	-0.529993
C	0.654618	0.944466	-1.495712	C	3.620935	-0.704901	-1.068832
C	1.392006	1.856737	-2.28931	C	3.759892	0.572337	-1.421573
C	2.724422	1.681871	-1.965134	C	2.483317	1.331053	-1.113665
C	5.817825	0.964293	1.157595	C	-1.760779	1.631266	0.197754
C	0.944997	-0.750671	0.200406	C	2.056693	-2.206355	-0.137051
C	-0.544053	-0.399069	0.00047	C	3.284256	-2.96764	-0.462644
C	-0.753605	0.521122	-1.201442	C	4.350001	-2.0048	-1.037767
C	4.721329	1.316321	0.382072	C	-0.377477	1.50839	0.135831

C	1.101008	-2.213133	-0.184043	C	0.87923	-2.792844	0.514574
C	1.267796	-3.187764	0.798225	C	0.440378	-4.076082	0.170588
C	1.350156	-4.531645	0.445802	C	-0.706212	-4.60526	0.75178
C	1.25141	-4.908419	-0.889746	C	-1.425099	-3.869302	1.688911
C	1.082402	-3.940049	-1.872223	C	-0.982168	-2.601871	2.056209
C	1.007235	-2.597187	-1.523926	C	0.163054	-2.071337	1.477445
C	3.897467	2.357361	-2.540072	C	2.719717	2.481394	-0.150497
C	5.067115	1.657283	-2.858566	C	2.556578	3.797648	-0.568139
C	6.148484	2.320787	-3.423156	C	2.78815	4.850013	0.315642
C	6.077189	3.685648	-3.685871	C	3.178648	4.585827	1.622124
C	4.918359	4.386318	-3.376478	C	3.342503	3.266991	2.044142
C	3.835982	3.728813	-2.802638	C	3.118434	2.220189	1.160645
C	3.964138	0.324266	-0.234685	C	0.198127	0.419223	-0.517783
C	4.297668	-1.01775	-0.082062	C	-0.619334	-0.536774	-1.120291
C	5.387797	-1.372345	0.710707	C	-2.001261	-0.42664	-1.044841
C	6.142364	-0.378396	1.320239	C	-2.563903	0.65706	-0.382077
H	1.028127	2.535856	-3.041047	H	4.62848	1.070374	-1.829322
H	1.207595	-0.615102	1.25378	H	2.024476	1.725354	-2.02885
H	-1.224282	-0.053014	-2.012138	H	4.667361	-2.349324	-2.02357
H	-1.445703	1.329797	-0.946401	H	5.223561	-2.002017	-0.382669
H	1.335893	-2.893331	1.841979	H	1.004771	-4.653205	-0.550988
H	1.485044	-5.283469	1.216741	H	-1.039146	-5.597447	0.470408
H	1.30684	-5.957216	-1.160294	H	-2.321235	-4.283406	2.135681
H	0.993491	-4.231943	-2.911598	H	-1.530088	-2.025165	2.792186
H	0.882852	-1.840333	-2.291086	H	0.506966	-1.084539	1.76961
H	5.122286	0.589702	-2.673513	H	2.236219	4.002964	-1.584602
H	7.046498	1.764564	-3.667866	H	2.656017	5.872578	-0.017251
H	6.924656	4.197143	-4.127478	H	3.353496	5.401629	2.313226
H	4.857461	5.451697	-3.575178	H	3.645408	3.057726	3.063295
H	2.938264	4.279324	-2.538201	H	3.239581	1.190994	1.484871
H	3.716543	-1.781058	-0.578918	H	-0.172293	-1.382464	-1.629428
H	5.642892	-2.416029	0.83534	H	-2.62798	-1.185213	-1.496019
H	6.408063	1.734294	1.637867	H	-2.204507	2.474351	0.711454
H	4.451401	2.357112	0.256207	H	0.250434	2.248541	0.616234
I	7.790626	-0.91219	2.524956	I	-4.664775	0.821889	-0.243372
N	2.818783	0.675602	-1.006727	N	1.607188	0.272708	-0.559906
O	-1.416018	-0.868596	0.696646	O	3.469709	-4.150892	-0.309893
H	-2.972889	-0.442064	0.760957				
O	-3.932029	-0.193164	0.665344				
C	-4.672734	-0.517771	1.803924				
H	-4.602178	-1.576992	2.065155				
C	-6.126655	-0.216764	1.447323				

F	-6.283309	1.060715	1.094328				
F	-6.945754	-0.480485	2.457554				
F	-6.478534	-0.972213	0.404974				
F	-4.847928	-0.024484	4.115066				
C	-4.168886	0.275878	3.009003				
F	-4.25485	1.600394	2.817624				
F	-2.884497	-0.022843	3.212216				
H	-3.921171	1.495081	-0.119678				
O	-3.653355	2.312438	-0.568534				
C	-3.519714	3.339885	0.352906				
H	-4.25888	3.300556	1.159688				
C	-3.744089	4.650605	-0.399957				
F	-3.043189	4.705114	-1.526819				
F	-3.399054	5.697264	0.35898				
F	-5.035802	4.775466	-0.711482				
F	-2.07223	4.069183	2.092332				
C	-2.134614	3.29355	1.013662				
F	-1.157555	3.65695	0.178034				
F	-1.871827	2.032042	1.402364				
H	-4.379431	-1.243604	-1.00737				
O	-4.274219	-1.864564	-1.741071				
C	-3.11072	-2.599906	-1.57589				
H	-2.260517	-2.014112	-1.212286				
C	-2.723426	-3.119968	-2.961268				
F	-3.747929	-3.671958	-3.597771				
F	-1.743039	-4.022477	-2.886056				
F	-2.277178	-2.097295	-3.701118				
F	-2.141667	-4.24399	-0.1784				
C	-3.305993	-3.724464	-0.55609				
F	-4.0856	-4.701313	-1.00098				
F	-3.893672	-3.207321	0.544175				
9aa·(HFIP)				**9aa**·$(HFIP)_2$			
C	0.127582	1.51757	-1.474256	C	2.00925	-2.053306	-1.455967
C	0.715762	2.738521	-2.022161	C	2.200275	-3.464137	-1.790958
C	-0.176242	3.725073	-1.936393	C	3.450091	-3.815444	-1.490701
C	-1.447391	3.212472	-1.284844	C	4.183064	-2.632823	-0.886288
C	-3.765841	-0.110919	0.754555	C	4.115937	1.605719	0.739783
C	0.98066	0.445433	-1.528176	C	0.736487	-1.612342	-1.723418
C	2.22405	0.927125	-2.119379	C	-0.003908	-2.75877	-2.225977
C	2.103256	2.421772	-2.474859	C	0.911714	-3.990975	-2.332339
C	-2.87866	0.908878	0.425891	C	3.945357	0.245404	0.50744
C	0.79261	-0.920632	-1.016668	C	0.121625	-0.298827	-1.478279

C	1.083987	-2.024569	-1.822222	C	-0.620386	0.324899	-2.487535
C	0.881056	-3.314957	-1.345556	C	-1.193547	1.571942	-2.269653
C	0.386215	-3.515488	-0.061109	C	-1.031425	2.211045	-1.044275
C	0.104013	-2.420825	0.751404	C	-0.302803	1.593889	-0.032639
C	0.312329	-1.132518	0.279083	C	0.262934	0.342519	-0.244863
C	-1.802057	3.966448	-0.016339	C	4.664451	-2.910222	0.526888
C	-3.004553	4.657189	0.082189	C	6.013467	-2.819847	0.84945
C	-3.327332	5.342295	1.252147	C	6.439138	-3.052758	2.156074
C	-2.447581	5.332374	2.326701	C	5.513629	-3.372412	3.141045
C	-1.240643	4.639975	2.23111	C	4.159671	-3.466075	2.819618
C	-0.917706	3.963211	1.063252	C	3.738001	-3.239746	1.517296
C	-2.095151	0.801321	-0.72105	C	3.423594	-0.188423	-0.709676
C	-2.218236	-0.314931	-1.54657	C	3.095485	0.737762	-1.697476
C	-3.086452	-1.343846	-1.211106	C	3.248768	2.097216	-1.462614
C	-3.852633	-1.235893	-0.056876	C	3.753145	2.522515	-0.23959
H	-0.070222	4.761044	-2.226794	H	3.92312	-4.782864	-1.587509
H	-2.295508	3.266066	-1.978579	H	5.038381	-2.334157	-1.503884
H	2.255185	2.565817	-3.546585	H	0.97875	-4.318144	-3.372306
H	2.876512	2.981538	-1.944595	H	0.49005	-4.809902	-1.745979
H	1.469781	-1.865592	-2.823706	H	-0.743462	-0.173284	-3.443469
H	1.114222	-4.164484	-1.976523	H	-1.781066	2.040924	-3.049728
H	0.229772	-4.521162	0.310322	H	-1.497101	3.17356	-0.870889
H	-0.27243	-2.571831	1.756207	H	-0.191463	2.079748	0.929604
H	0.103676	-0.27817	0.914843	H	0.815794	-0.146718	0.550585
H	-3.69776	4.651188	-0.752577	H	6.733418	-2.552051	0.083001
H	-4.267472	5.87614	1.322861	H	7.491529	-2.976252	2.401852
H	-2.698168	5.861008	3.238539	H	5.8423	-3.547528	4.15842
H	-0.55327	4.630375	3.068528	H	3.435489	-3.713214	3.586686
H	0.017918	3.417002	0.985778	H	2.683526	-3.300321	1.263736
H	-1.60468	-0.393236	-2.436585	H	2.684498	0.392432	-2.63935
H	-3.150033	-2.223563	-1.838421	H	2.962806	2.813045	-2.222218
H	-4.363406	-0.035065	1.654012	H	4.505783	1.944311	1.691112
H	-2.777432	1.767777	1.078058	H	4.187389	-0.468258	1.285029
I	-5.137792	-2.819993	0.487104	I	3.939776	4.588468	0.146865
N	-1.1243	1.788051	-1.040755	N	3.157797	-1.565414	-0.942253
O	3.248963	0.283937	-2.287875	O	-1.20065	-2.793791	-2.488118
H	3.552328	-1.167564	-1.179112	H	-2.241094	-1.622594	-1.593793
O	3.967505	-1.585222	-0.403274	O	-2.882944	-1.43303	-0.876763
C	4.812234	-0.651222	0.168355	C	-3.196669	-2.636904	-0.26132
H	5.174986	0.093089	-0.550714	H	-3.096615	-3.48728	-0.944445
C	6.038164	-1.393621	0.695231	C	-4.659343	-2.556597	0.165815
F	5.716624	-2.368031	1.542931	F	-4.916004	-1.405653	0.80315

F	6.878597	-0.562075	1.325946	F	-4.998197	-3.558223	0.978042
F	6.703935	-1.939476	-0.324989	F	-5.451327	-2.604752	-0.904931
F	4.840485	1.089502	1.796555	F	-2.401412	-4.170009	1.359046
C	4.077779	0.125195	1.266236	C	-2.263806	-2.911076	0.925394
F	3.65158	-0.653743	2.256692	F	-2.477183	-2.094128	1.95321
F	3.000112	0.726111	0.733026	F	-0.989976	-2.760164	0.540029
				H	-3.632202	0.267324	-0.688427
				O	-4.00861	1.157674	-0.798604
				C	-4.656717	1.568931	0.351053
				H	-5.43112	0.87246	0.694026
				C	-5.366113	2.874826	0.004377
				F	-4.551068	3.759263	-0.566895
				F	-5.88922	3.441763	1.098568
				F	-6.366958	2.635579	-0.846341
				F	-4.328693	1.859347	2.683973
				C	-3.680205	1.738306	1.521356
				F	-2.88298	2.802943	1.387806
				F	-2.902622	0.65462	1.601637
		9aa·$(HFIP)_3$					
C	2.628615	-1.990327	-1.426906				
C	2.803969	-3.365597	-1.885134				
C	4.108832	-3.619137	-1.991102				
C	4.904719	-2.390581	-1.587576				
C	4.826866	1.779692	0.351799				
C	1.307612	-1.633285	-1.287181				
C	0.527985	-2.800753	-1.633988				
C	1.444204	-3.960311	-2.065308				
C	4.755736	0.416012	0.085328				
C	0.779996	-0.334467	-0.824714				
C	-0.022452	0.446849	-1.661331				
C	-0.393453	1.731543	-1.27839				
C	0.031174	2.247905	-0.058161				
C	0.807592	1.466265	0.792142				
C	1.172402	0.1794	0.414546				
C	5.856511	-2.631603	-0.431476				
C	7.208554	-2.332584	-0.552673				
C	8.069342	-2.524721	0.526418				
C	7.57591	-3.013604	1.729147				
C	6.220263	-3.316628	1.853615				
C	5.365257	-3.129449	0.776819				
C	4.03588	-0.033366	-1.017845				
C	3.41611	0.87805	-1.86971				

C	3.468598	2.237278	-1.597391
C	4.166688	2.677377	-0.478646
H	4.599733	-4.536089	-2.286559
H	5.472286	-1.998658	-2.440705
H	1.227699	-4.240733	-3.098546
H	1.25302	-4.829018	-1.431969
H	-0.332168	0.05199	-2.622465
H	-1.017896	2.329245	-1.932818
H	-0.263257	3.246556	0.241138
H	1.12749	1.85877	1.750395
H	1.787315	-0.428432	1.070389
H	7.590455	-1.936187	-1.48788
H	9.121251	-2.285736	0.426398
H	8.243306	-3.159174	2.570004
H	5.833383	-3.698314	2.791074
H	4.307171	-3.355869	0.87021
H	2.852343	0.516262	-2.721988
H	2.953335	2.939403	-2.239947
H	5.3698	2.130512	1.220129
H	5.226266	-0.294152	0.754818
I	4.191459	4.736999	-0.024707
N	3.835112	-1.424112	-1.24761
O	-0.693792	-2.92287	-1.567932
H	-1.565534	-2.042056	-0.534765
O	-2.106456	-1.825049	0.28075
C	-2.169556	-2.972667	1.065964
H	-2.217945	-3.882723	0.458019
C	-3.459199	-2.881792	1.878911
F	-3.574827	-1.674533	2.453499
F	-3.510829	-3.801957	2.839586
F	-4.510633	-3.046165	1.080989
F	-0.887119	-4.321469	2.524801
C	-0.937865	-3.106083	1.971139
F	-0.91943	-2.20294	2.948209
F	0.17711	-2.946444	1.248334
H	-2.260049	-0.035556	0.840788
O	-2.654914	0.841559	0.696159
C	-3.231378	1.334571	1.857197
H	-4.004936	0.676623	2.270953
C	-3.920245	2.639271	1.468238
F	-3.099692	3.474616	0.831857
F	-4.403797	3.26684	2.542508

F	-4.941055	2.376031	0.647448
F	-2.782088	1.706821	4.150467
C	-2.191306	1.544929	2.964041
F	-1.404392	2.601803	2.751348
F	-1.408828	0.463805	3.040432
H	-3.876417	-1.093321	-0.44258
O	-4.727573	-0.876705	-0.850631
C	-4.552133	0.189495	-1.721296
H	-4.05917	1.047057	-1.249896
C	-5.941581	0.64104	-2.160626
F	-6.667236	-0.357037	-2.658429
F	-5.845334	1.591183	-3.101127
F	-6.610271	1.15294	-1.128559
F	-3.206608	0.856794	-3.562365
C	-3.681475	-0.215055	-2.91654
F	-4.312952	-0.981617	-3.802699
F	-2.624435	-0.909117	-2.465641