Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

(47 pages including the cover page)

Palladium Complexes with an Annellated Mesoionic Carbene (MIC) Ligand: Catalytic Sequential Sonogashira Coupling/Cyclization Reaction for One–Pot Synthesis of Benzofuran, Indole, Isocoumarin and Isoquinolone Derivatives

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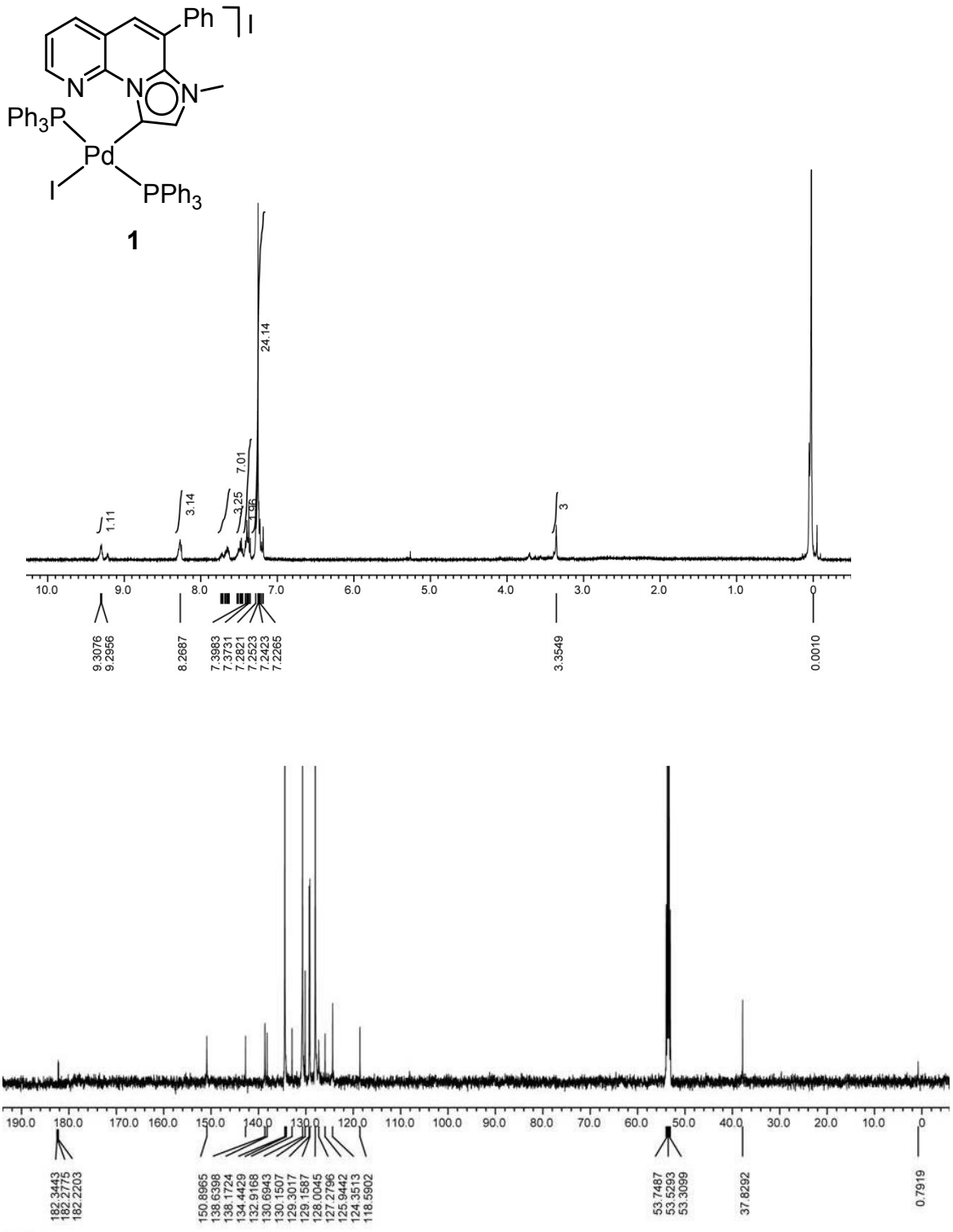


Figure S1. ^{1}H NMR (top) and ^{13}C NMR (below) spectra of **1**.

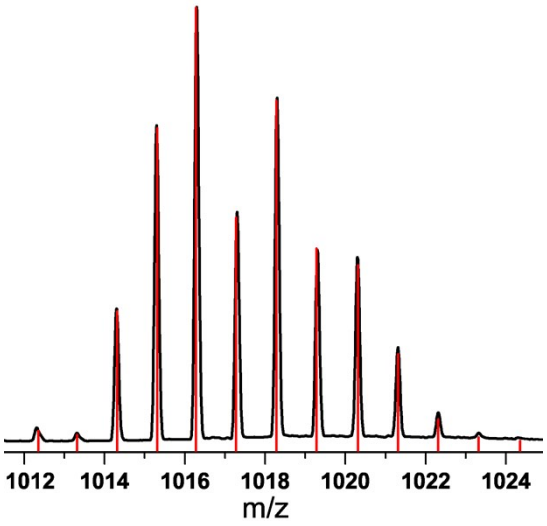


Figure S2. Simulated (red line) and experimental (black line) mass distributions for molecular ion at *m/z* 1016.0917 (*z* = 1) in complex **1**.

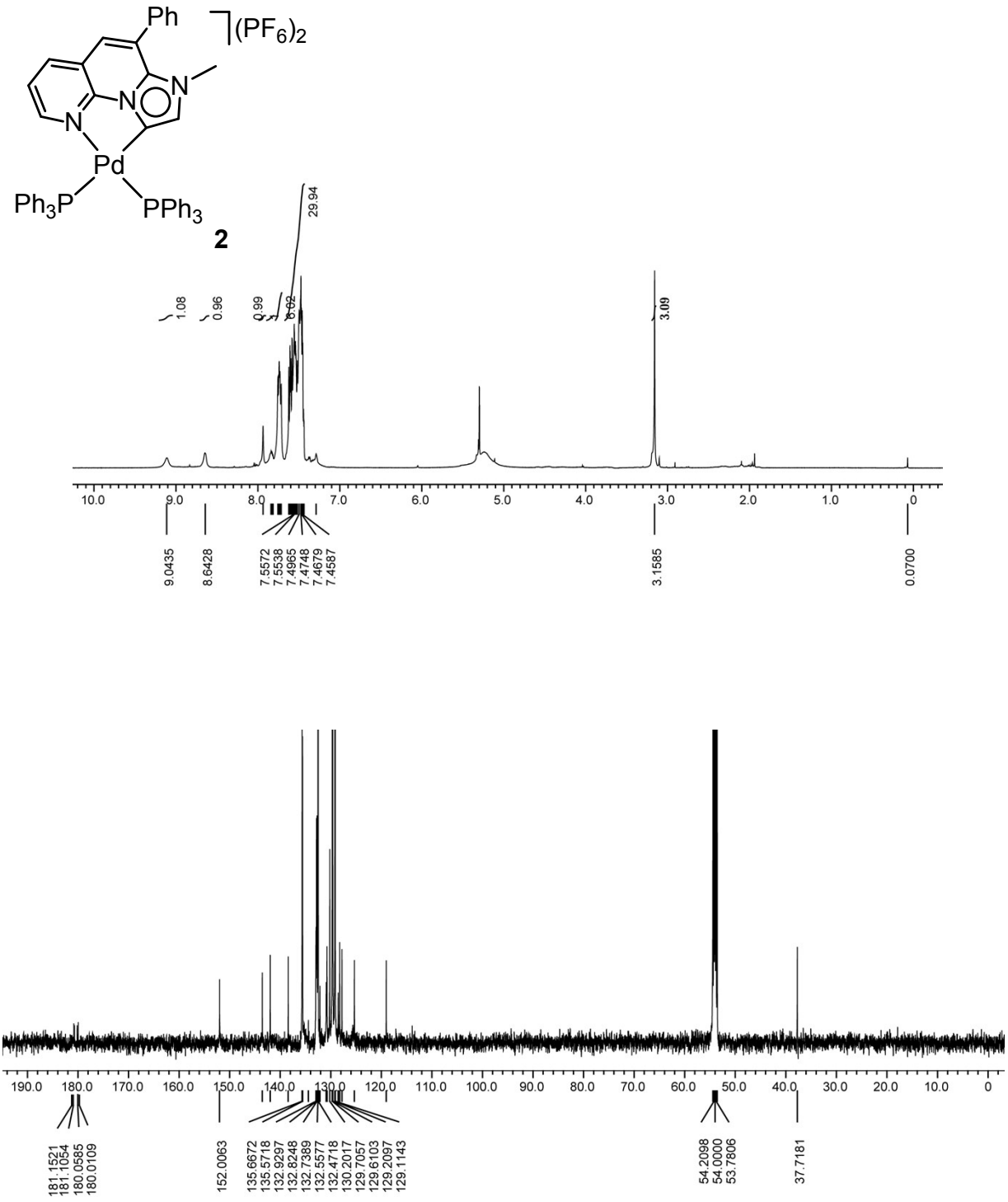


Figure S3. ^{1}H NMR (top) and ^{13}C NMR (below) spectra of **2**.

X–Ray Data Collection and Refinements:

Single–crystal X–ray studies were performed on a CCD Bruker SMART APEX diffractometer equipped with an Oxford Instruments low–temperature attachment. The data were collected at 100(2) K using graphite–monochromated Mo–K (λ_α = 0.71073 Å). The frames were indexed, integrated, and scaled using the SMART and SAINT software packages[1], and the data were corrected for absorption using the SADABS program[2]. The structures of **1** and **2** were solved and refined with the SHELX suite of programs[3]. The hydrogen atoms were included into geometrically calculated positions in the final stages of the refinement and were refined according to 'riding model'. All non-hydrogen atoms were refined with anisotropic thermal parameters unless mentioned otherwise. The Olex–2 program has been used to discard for minor disorder modeling for compound **2**. Diamond 3.1e software was used to produce the diagrams[5]. CCDC numbers 2014440 and 2014441 contain the supplementary crystallographic data for compounds **1** and **2** respectively. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

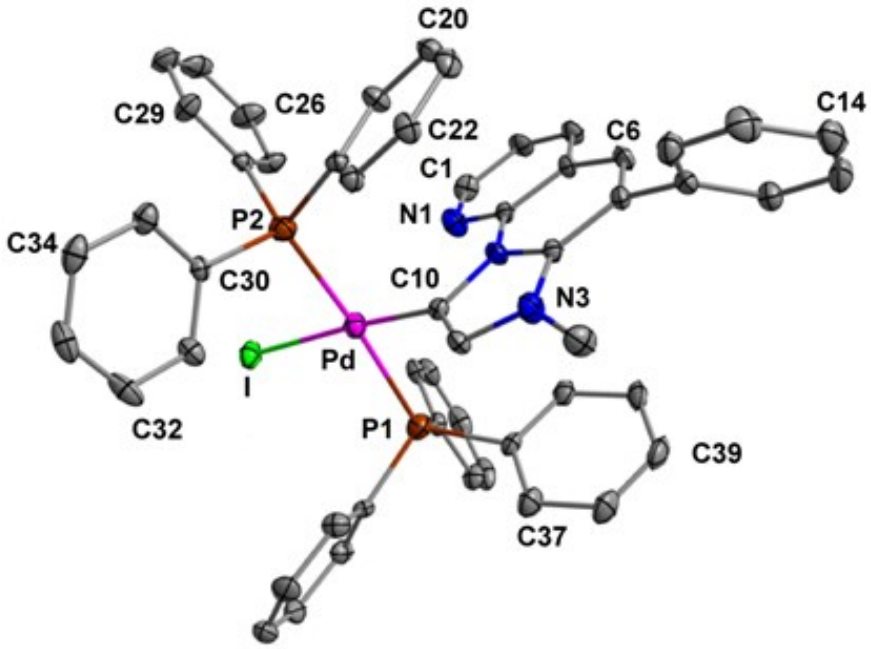


Figure S4. Molecular structure of the cationic unit in **1** with important atoms labelled. All hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 40% probability level. Selected bond lengths (Å) and angles (deg): Pd–C10 2.003(6), Pd–P1 2.3334(16), Pd–P2 2.3452(16), Pd–I1 2.6625(6), C10–Pd–P1 88.81(17), C10–Pd–P2 88.18(17), C10–Pd–I1 174.51(17), P1–Pd–P2 171.07(6), P1–Pd–I 90.20(4), P2–Pd–I 91.99(4).

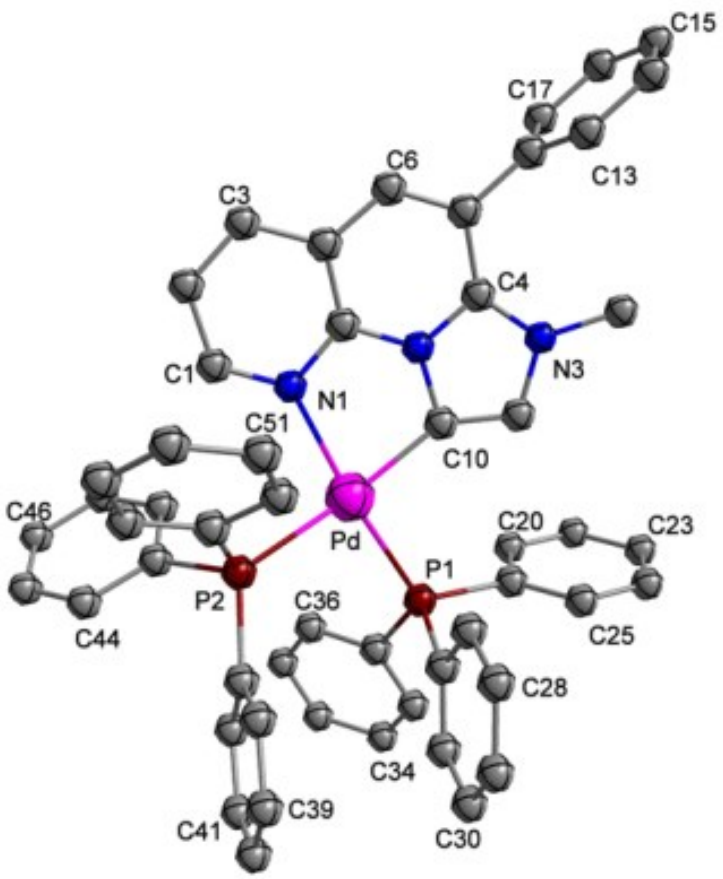


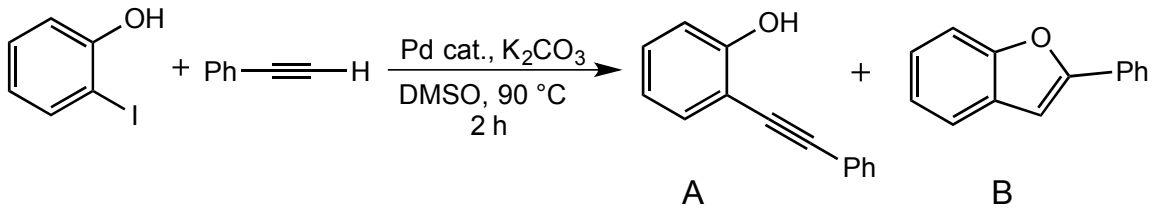
Figure S5. Molecular structure of the cationic unit in **2** with important atoms labelled. All hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 40% probability level. Selected bond lengths (Å) and angles (deg): Pd–C10 2.037(3), Pd–P1 2.2543(8), Pd–P2 2.3659(8), Pd–N1 2.169(2), C10–Pd–P1 92.97(8), C10–Pd–P2 165.85(8), C10–Pd–N1 80.58(10), P1–Pd–P2 94.74(3), P1–Pd–N1 173.02(7), P2–P–N1 92.12(7).

Table S1. Crystallographic Data and Pertinent Refinement Parameters for **1** and **2**.

	1	**2**
Empirical formula	$C_{53}H_{43}I_2N_3P_2Pd$	$C_{56}H_{49}N_3PdP_4F_{12}Cl_6O$
Formula Weight	1144.04	1450.96
Crystal System	Monoclinic	Monoclinic
Space Group	$P2_1/c$	$P2_1/c_1$
a (Å)	17.0016(14)	13.1613(12)
b (Å)	17.0493(14)	14.5225(12)
c (Å)	16.9889(14)	31.355(3)
α (deg)	90	90
β (deg)	102.567(1)	97.944(2)
γ (deg)	90	90
V (Å^3)	4806.5(7)	5935.5(9)
Z	4	4
ρ_{calcd} (g cm^{-3})	1.581	1.624
μ (mm^{-1})	1.776	0.772
F(000)	2256.0	2920
Reflections		
Collected	30117	59486
Independent	11790	14796
Observed [I >2σ (I)]	6510	10484
No. of variables	551	713
GOF	1.017	1.018
R_{int}	0.0930	0.0600
Final R indices	R1 = 0.0625	R1 = 0.0495
[I > 2σ(I)][a]	wR2 = 0.1193	wR2 = 0.1000
R indices (all data)[a]	R1 = 0.1455	R1 = 0.0831
	wR2 = 0.1470	wR2 = 0.1111

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ with $F_o^2 > 2\sigma(F_o^2)$. $wR_2 = [\Sigma w(|F_o^2| - |F_c^2|)^2/\Sigma|F_o^2|^2]^{1/2}$

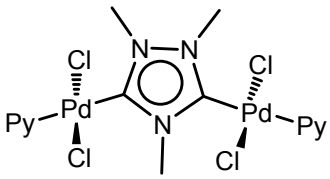
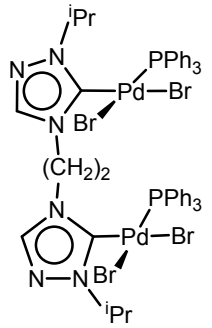
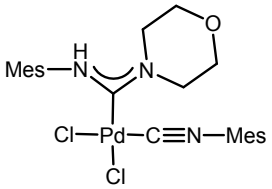
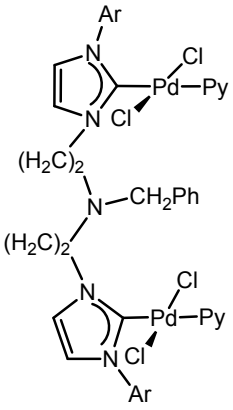
Table S2. Catalyst screening.[a]



Entry	Catalyst	% Yield[b]	
		A	B
1	**1**	nd[c]	100
2	**2**	nd[c]	100
3	$Pd(OAc)_2$	48	10
4	$Pd(PPh_3)_2Cl_2$	57	12
5	$PdCl_2$	38	nd[c]
6	PdI_2	36	nd[c]
7	$PdCl_2(CH_3CN)_2$	23	nd[c]

[a]Reaction conditions: 2–iodophenol/phenylacetylene/base/catalyst = 1/1.2/1/0.02 mmol), DMSO (2 mL). [b]Determined by GC–MS using *p*–xylene as an internal standard. [c]not detected.

Table S3. Pd–carbene complexes employed in C–C coupling/cyclization reaction of 2–iodophenol with alkynes.

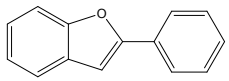
S.N.	Catalyst	Reaction Condition	Yield%	Ref.[a]
1		Cat. (1 mol%), Cs_2CO_3 (3 equiv), DMSO, 80 ^{0}C, 8h [Substrate: 2-iodophenol, phenylacetylene]	93	**7c**
2		Cat. (1 mol%), Cs_2CO_3 (3 equiv), DMSO, 80 ^{0}C, 4h [Substrate: 2-iodophenol, phenylacetylene]	81	**7d**
3		Cat. (2 mol%), NaOH (3 equiv), 1-4dioxane/H2O 80 ^{0}C, 4h [Substrate: 2-iodophenol, triethoxy(phenylethynyl)silane]	57	**7e**
4		Cat. (0.2 mol%), K_3PO_4 (2equiv), DMSO, 90 ^{0}C, 16h [Substrate: 2-iodophenol, phenylacetylene]	97[b]	**7f**
5	Catalyst **1** **[Pd(aPmic)(PPh_3)$_2$I]I**	Cat. (2 mol%), K_2CO_3 (1equiv), DMSO, 90 ^{0}C, 2h Substrate: 2-iodophenol, phenylacetylene	100	This work

[a] Cited in manuscript. [b] High yield was reported at a very low catalyst loading.

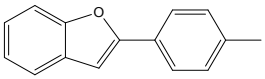
General Procedure for Reaction profile

A mixture of catalyst (0.02 mmol), phenylacetylene (1.2 mmol), 2–iodophenol (1 mmol), K_2CO_3 (1 mmol) and *p*–xylene (1 mmol) in 3 mL of DMSO was heated 90 °C. After stipulated time intervals, small aliquots (0.1 mL) were taken out from the reaction mixture, diluted with EtOAc and passed through a short silica column for GC–MS analysis.

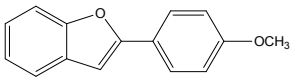
Spectroscopic Characterizations of Products



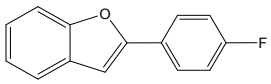
2-Phenylbenzofuran (entry 1, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.86 (d, *J* = 7.3 Hz, 2H), 7.58 (d, *J* = 7.3 Hz, 1H), 7.52 (d, *J* = 7.7, 1H), 7.44 (t, *J* = 7.3 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 2H), 7.29-7.20 (m, 1H), 7.02(s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 156.0, 155.0, 132.6, 129.3, 128.9, 128.7, 125.1, 124.4, 123.1, 121.0, 111.3, 101.4.



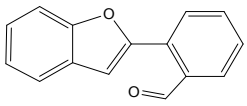
2-(4-Methylphenyl)benzofuran (entry 2, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.50-7.28 (m, 2h), 7.26-7.06 (m, 4H), 6.84 (d, *J* = 8.0 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 156.3, 154.9, 138.7, 129.6, 129.5, 125.0, 124.1, 122.9, 120.9, 111.4, 111.2, 103.8, 100.7, 21.5.



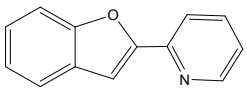
2-(4-Methoxyphenyl)benzofuran (entry 3, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.54 (d, *J* = 7.6, 1H), 7.49 (d, *J* = 7.6, 1H), 7.26-7.19 (m, 2H), 6.97 (d, *J* = 8.6, 2H), 6.88 (s, 1H), 3.85 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.0, 156.1, 154.7, 129.5, 126.5, 126.5, 123.8, 123.4, 122.9, 120.6, 114.3, 111.0, 99.7, 55.4.



2-(4-flurophenyl)benzofuran (entry 4, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.83 (q, *J* = 8.6 Hz, 2H), 7.57 (d, *J* = 7.4, 1H), 7.51 (d, *J* = 7.4, 1H), 7.29-7.21 (m, 2H), 7.14 (t, *J* = 8.6, 2H), 6.95 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.9, 161.9, 155.1, 154.9, 129.2, 126.9, 126.8, 124.3, 123.1, 120.9, 116.0, 115.8, 111.2, 101.0.

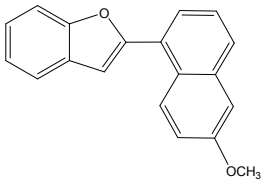


2-(2-aldehyde-phenyl)benzofuran (entry 5, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 10.48 (s, 1H), 7.45 (d, *J* = 8.0, 1H), 7.84 (d, *J* = 8.0, 1H), 7.67 (dd, *J* = 16.6, 7.4, 2H), 7.54 (dd, *J* = 16.6, 8.0, 2H), 7.36 (t, *J* = 7.4, 1H), 7.29 (t, *J* = 7.4, 1H), 6.98 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 192.0, 155.5, 152.8, 133.9, 133.5, 129.2, 128.2, 128.5, 125.2, 123.3, 121.3, 111.4, 107.8.

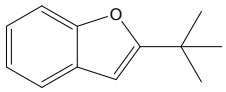


2-pyridine-benzofuran (entry 6, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.67 (d, *J* = 5.9 Hz, 1H), 7.89 (d, *J* = 7.8, 1H), 7.77 (t, *J* =

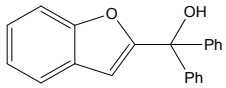
7.8, 1H), 7.63 (d, *J* = 7.8, 1H), 7.55 (d, *J* = 8.0, 1H), 7.42 (s, 1H), 7.32 (t, *J* = 7.3, 1H), 7.26-7.21 (m, 2H).



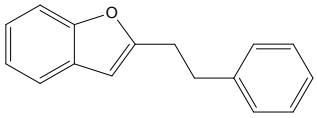
2-(4-methoxy napthyl-benzofuran (entry 7, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.29 (s, 1H), 7.88 (d, *J* = 8.6, 1H), 7.80 (dd, *J* = 16.6, 9.2, 2H), 7.59 (d, *J* = 8.0, 1H), 7.30-7.22 (m, 2H), 7.19-7.14 (m, 2H), 7.07 (s, 1H), 3.94 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.2, 156.2, 154.9, 134.5, 129.9, 129.4, 129.8, 127.2, 125.7, 124.1, 123.7, 123.3, 122.9, 120.7, 119.4, 111.0, 105.9,101.0, 55.3.



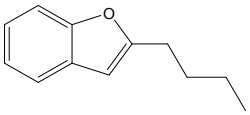
2-(tert-butyl)-benzofuran (entry 8, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.47 (d, *J* = 6.8, 1H), 7.41 (d, *J* = 8.0, 1H),7.21-7.14 (m, 2H), 6.34 (s, 1H), 1.37 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): 165.7, 152.5, 129.9, 121.4, 120.8, 118.8, 109.1, 97.23, 32.0, 27.2.



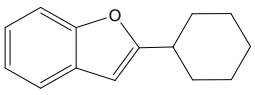
α,α-Diphenyl-2-benzofuranmethanol (entry 9, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.51 (d, *J* = 6.8 Hz, 1H), 7.46 (d, *J* = 8, 1H), 7.42-7.40 (m, 4H), 7.38-7.33 (m, 6H), 7.29 (t, *J* = 6.8, 1H), 7.23 (t, *J* = 7.4, 1H), 6.34 (s, 1H), 3.30 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.2, 155.1, 144.0, 128.0, 127.8, 127.3, 124.4, 122.9, 121.2, 111.4, 106.5, 78.3.



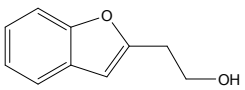
2-(phenylethyl)-benzofuran (entry 10, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.45 (dd, *J* = 19.4, 7.4, 2H), 7.31-7.16 (m, 7H), 6.36 (s, 1H), 3.08 (s, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.5, 154.7, 140.9, 128.9, 128.5, 128.4, 126.2, 123.3, 122.5, 120.4, 110.8, 102.4, 34.0, 30.4.



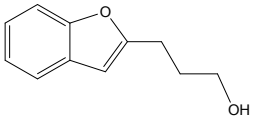
2-(butyl)-benzofuran (entry 11, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.4, 1H), 7.39 (d, *J* = 8.0, 1H),7.20-7.14 (m, 2H), 6.36 (s, 1H), 2.76 (t, *J* = 7.4, 2H), 1.75-1.69 (m, 2H), 1.45-1.39 (m, 2H), 0.94(t, *J* = 7.4, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 157.4, 154.7, 129.2, 123.0, 122.4, 120.2, 110.7, 101.8, 29.7, 28.2, 22.3, 13.8.



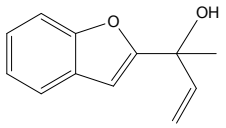
2-cyclohexylbenzofuran (entry 12, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.47 (d, *J* = 8.6, 1H), 7.40 (d, *J* = 7.8, 1H),7.20-7.18 (m, 2H), 6.34 (s, 1H), 2.75(tt, *J* = 11.0, 3.2, 1H), 2.11(d, *J* = 12.8, 2H), 1.83(dt, *J* = 12.3, 3.2, 2H), 1.73(d, *J* = 12.8, 1H), 1.50-1.28 (m, 5H) ; ^{13}C NMR (125 MHz, $CDCl_3$): 154.4, 154.1, 128.4, 123.0, 122.3, 120.3, 110.8, 99.8, 37.6, 31.4, 26.1, 26.0.



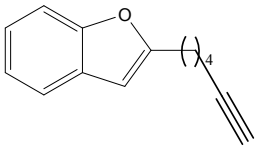
2-(benzofuran-2-yl)ethanol (entry 13, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.49 (d, *J* = 7.4, 1H), 7.42 (d, *J* = 8.0, 1H),7.24-7.17 (m, 2H), 6.49 (s, 1H), 3.96 (t, *J* = 6.2, 2H) 3.02 (t, *J* = 6.3, 2H) 2.00 (br, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 155.9, 154.7, 128.6, 123.4, 122.5, 120.3, 110.7, 103.5, 60.6, 31.9.



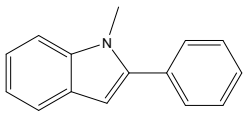
3-(benzofuran-2-yl)propan-1-ol (entry 14, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.47 (d, *J* = 6.8, 1H), 7.40 (d, *J* = 7.4, 1H),7.22-7.16 (m, 2H), 6.40 (s, 1H), 3.72 (t, *J* = 6.3, 2H), 2.87(t, *J* = 7.4, 2H), 2.04-1.97(m, 2H), 1.75(br, 1H) ; ^{13}C NMR (125 MHz, $CDCl_3$): 158.7, 154.6, 128.8, 123.1, 122.4, 120.2, 110.6, 102.1, 61.8, 30.5, 24.7.



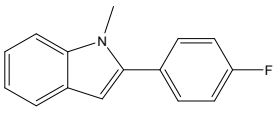
2-(benzofuran-2-yl)but-3-en-2-ol (entry 15, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.53 (d, *J* = 7.4, 1H), 7.45 (d, *J* = 8.5, 1H),7.22-7.19 (m, 2H) 6.61 (s, 1H), 6.23 (dd, *J* = 17.2,10.9, 1H), 5.39 (d, *J* = 17.2, 1H), 5.23 (d, *J* = 10.9, 1H), 2.30 (s, 1H), 1.73 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.8, 154.9, 141.8, 128.2, 124.2, 122.8, 121.1, 113.8, 111.3, 101.9, 71.9, 27.0.



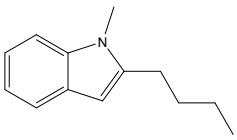
2-(hex-5-yn-1-yl)benzofuran (entry 16, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.47 (d, *J* = 6.85, 1H), 7.39 (d, *J* = 7.4, 1H),7.21-7.14 (m, 2H) 6.38 (s, 1H), 3.73 (s, 1H), 2.79 (t, *J* = 7.4, 2H), 2.26-2.22 (m, 2H), 1.90-1.84 (m,2H), 1.66-1.62 (m,2H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.0, 152.5, 123.2, 122.4, 120.28, 110.7, 102.1, 84.1, 68.6, 29.7, 28.0, 27.9, 26.7, 18.2.



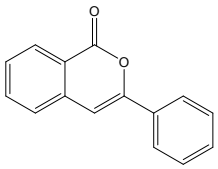
1-methyl-2-phenyl-1H-indole (entry 17, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8.0, 1H), 7.65 (d, *J* = 7.6, 2H), 7.42 (t, *J* = 7.4, 2H), 7.37-7.33 (m, 2H), 7.29-7.27 (m, 1H), 7.23 (s, 1H), 7.18 (t, *J* = 7.4, 1H), 3.84 (s, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): 146.7, 135.7, 130.0, 128.8, 127.4, 126.6, 125.7, 122.0, 120.0, 119.9, 109.5, 104.5, 33.0.



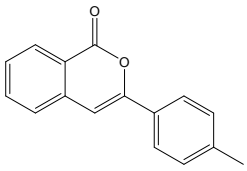
2-(4-fluorophenyl)-1-methyl-1H-indole (entry 19, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.63 (d, *J* = 8.0, 1H), 7.47 (dd, *J* = 8.6, 5.1, 2H), 7.36 (d, J = 8.0, 1H), 7.25 (t, J = 8.0, 1H), 7.18-7.12 (m, 3H), 6.53 (s, 1H), 3.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.6, 161.7, 140.5, 138.3, 131.1(d), 129.0,128.2, 127.9, 127.7, 121.8, 120.5, 120.0, 115.6 (d), 109.6, 101.8, 31.1.



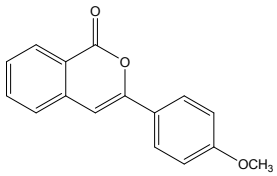
2-butyl-1-methyl-1H-indole (entry 20, Table 2): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.51 (d, *J* = 7.4, 1H), 7.17-7.11 (m, 2H), 7.05 (t, *J* = 6.9, 1H), 6.24 (s, 1H), 3.66 (s, 3H), 2.73 (t, *J* = 7.4, 2H), 1.73-1.67 (m, 2H), 1.49-1.43 (m,2H), 0.97 (t, *J* = 7.4, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 141.7,137.4, 130.1, 128.1, 119.7, 119.2, 106.7, 96.7, 30.8, 29.4, 26.6, 22.7, 14.0.



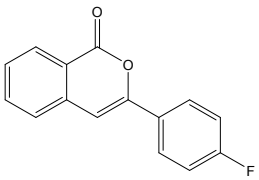
3-phenyl-1H-isochromen-1-one (entry 1, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ, 8.29 (d, *J* = 8.0, 1H), 7.86 (d, *J* = 8.0, 2H), 7.69 (t, *J* = 8.0, 1H), 7.48-7.41 (m, 5H), 6.93 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.3, 153.7, 136.6, 134.9, 132.0, 130.0, 129.7, 128.9, 128.2, 126.0, 125.3, 120.6, 101.8.



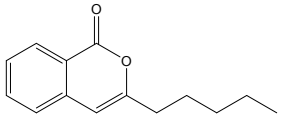
3-(p-tolyl)-1H-isochromen-1-one (entry 2, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.30(d, *J* = 8.0, 1H), 7.77(d, *J* = 8.0, 2H), 7.70(t, *J* = 8.0, 1H), 7.49-7.46 (m, 2H), 7.27-7.25 (m, 2H), 6.90 (s, 1H), 2.40(s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.5, 153.9, 140.3, 137.8, 134.9,129.7, 129.6, 129.3, 127.9, 125.9, 125.2, 120.5, 101.1, 21.4.



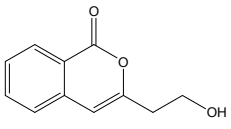
3-(4-methoxyphenyl)-1H-isochromen-1-one (entry 3, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.29(d, *J* = 8.0, 1H), 7.82 (d, *J* = 8.5, 2H), 7.69 (t, *J* = 7.4, 1H), 7.47-7.44 (m, 2H), 6.97 (d, *J* = 8.6, 2H), 6.83 (s, 1H), 3.86 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.1, 161.1, 153.1, 137.9, 134.9, 129.7, 126.9, 125.7, 124.6, 118.2, 114.3, 100.3, 53.4.



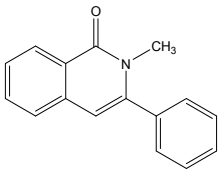
3-(4-fluorophenyl)-1H-isochromen-1-one (entry 4, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.29 8.27 (m, 1H), 8.26-8.24 (m, 2H), 7.87-7.80 (m, 1H), 7.72-7.45 (m, 2H), 7.16-7.08 (m, 2H) 6.86 (s, 1H);^{13}C NMR (125 MHz, $CDCl_3$): 164.8, 162.8, 162.2, 152.8, 137.5, 135.0, 129.8, 128.3, 127.3, 126.0, 120.5, 115.9, 101.6.



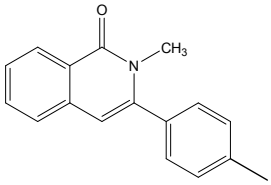
3-pentyl-1H-isochromen-1-one (entry 7, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.24 (d, *J* = 8.0, 1H), 7.66 (t, *J* = 7.4, 1H), 7.43 (t, *J* = 8.0, 1H), 7.34 (d, *J* = 7.4, 1H), 6.24 (s, 1H), 2.51 (t, *J* = 7.4, 2H), 1.73-1.68 (m, 2H), 1.37-1.32 (m, 4H), 0.90 (t, *J* = 7.4, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.1, 154.4, 137.7, 134.7, 129.6, 127.5, 125.0, 120.2, 102.9, 33.5, 31.2, 26.6, 24.4, 14.0.



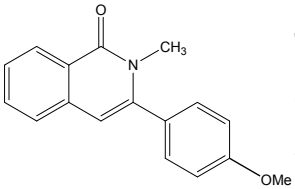
3-(2-hydroxyethyl)-1H-isochromen-1-one (entry 8, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.0, 1H), 7.67 (t, *J* = 8.0, 1H), 7.45 (t, *J* = 8.0, 1H), 7.36 (d, *J* = 8.0, 1H), 6.37 (s, 1H), 3.99 (t, *J* = 6.3, 2H), 2.78 (t, *J* = 6.3, 2H),1.77 (br, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.9, 154.8, 137.3, 134.9, 129.6, 128.0, 125.2, 120.3, 104.9, 59.7, 36.9.



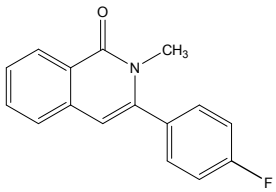
2-methyl-3-phenylisoquinolin-1(2H)-one (entry 9, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.84 (d, *J* = 7.4, 1H), 7.73 (d, *J* = 8.0 , 1H), 7.58 (t, *J* = 7.4, 1H), 7.39-7.29 (m, 5H), 6.77 (s, 1H), 3.02 (s, 3H), , ^{13}C NMR (125 MHz, $CDCl_3$): 168.9, 138.1, 136.2, 134.8, 131.9, 129.7, 129.0, 128.5, 128.1, 127.5, 123.2, 119.3, 106.5, 30.5.



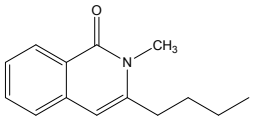
2-methyl-3-(p-tolyl)isoquinolin-1(2H)-one (entry 10, Table 3): ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 7.9, 1H), 7.72 (d, *J* = 7.9 , 1H), 7.57 (t, *J* = 7.3, 1H), 7.46 (t, *J* = 7.3, 1H), 7.23-7.17 (m, 4H), 6.74 (s, 1H), 3.40 (s, 3H), 2.37 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): 169.1, 163.2, 16.4, 1382., 136.8, 132.2, 131.7, 131.6, 129.4, 128.4, 119.5, 115.6, 115.4, 105.5, 30.84, 25.7.



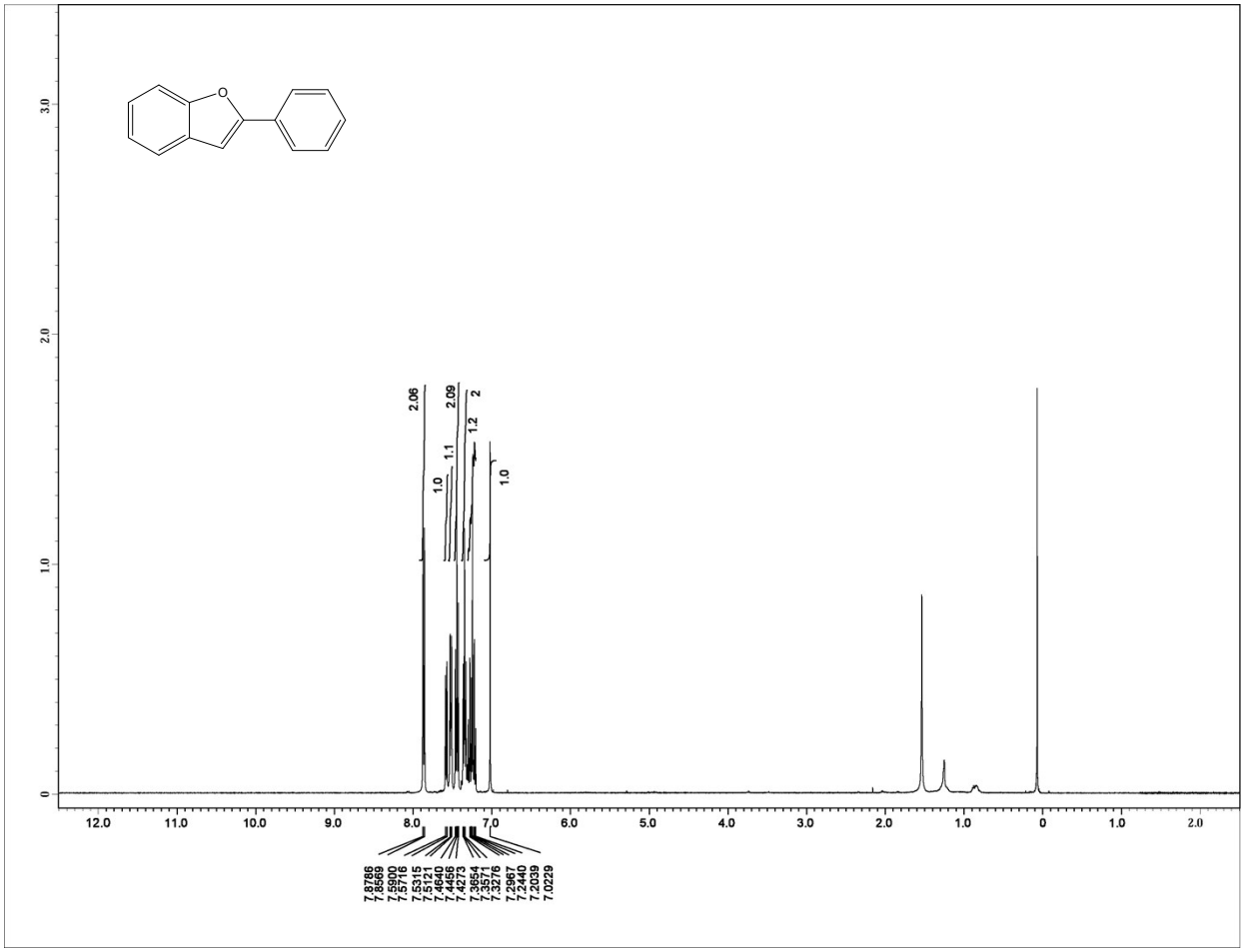
3-(4-methoxyphenyl)-2-methylisoquinolin-1(2H)-one (entry 11, Table 3): ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 7.3, 1H), 7.71 (d, *J* = 7.9 , 1H), 7.57 (t, *J* = 7.3, 1H), 7.46 (t, *J* = 7.3, 1H), 7.23-7.24 (m, 2H), 6.91 (d, *J* = 7.9 , 1H), 6.72 (s, 1H), 3.83 (s, 3H), 3.06 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): 169.3, 159.4, 138.4, 135.9, 132.1, 131.2, 129.1, 128.7, 119.4, 113.9, 106.9, 55.6, 30.0.

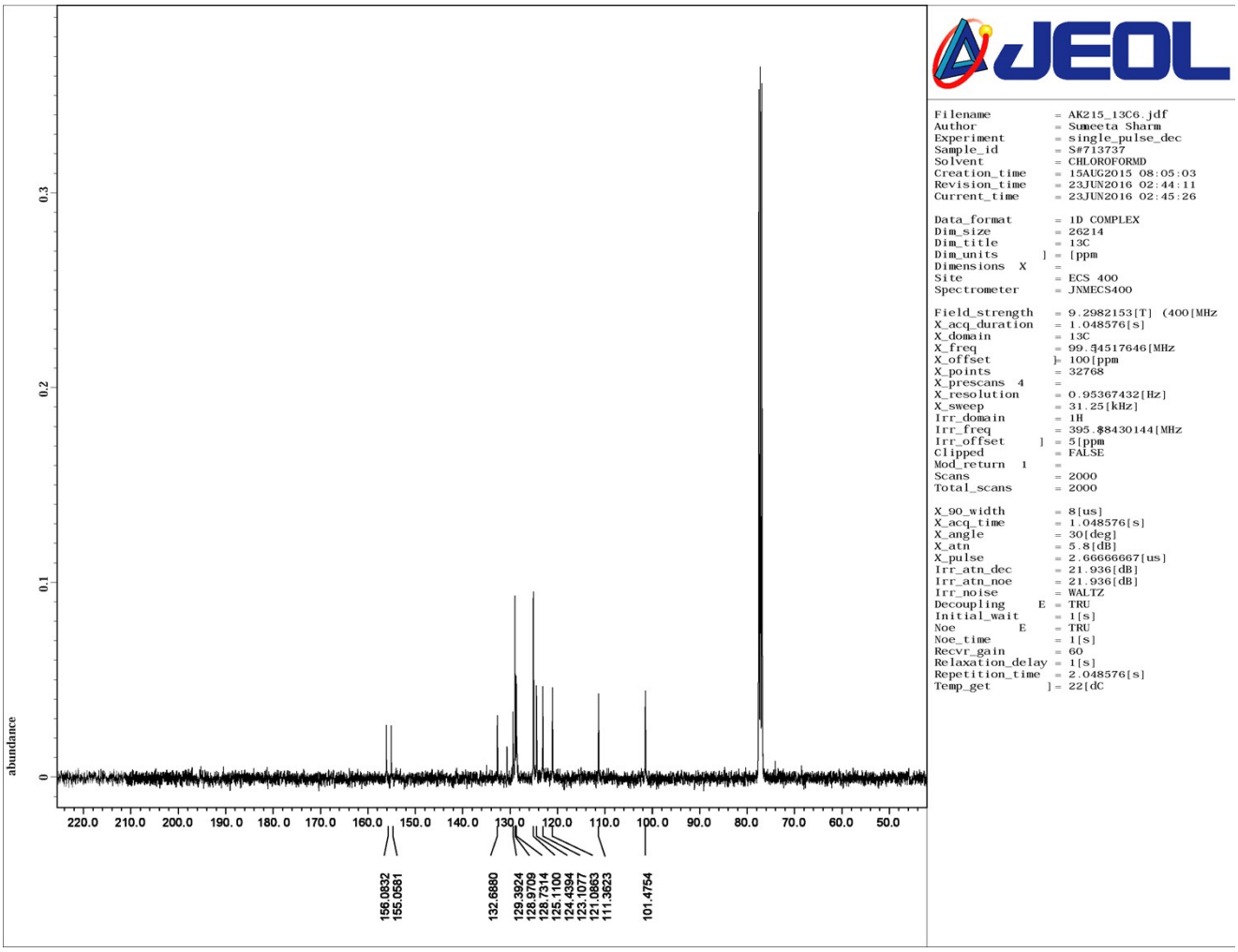


3-(4-fluorophenyl)-2-methylisoquinolin-1(2H)-one (entry 12, Table 3): ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 7.9, 1H), 7.71 (d, *J* = 7.9 , 1H), 7.58 (t, *J* = 7.3, 1H), 7.48 (t, *J* = 7.3, 1H), 7.31-7.28 (m, 2H), 7.07 (t, *J* = 8.5, 1H), 6.69 (s, 1H), 3.01 (s, 3H), , ^{13}C NMR (125 MHz, $CDCl_3$): 169.2, 163.4, 161.5, 138.2, 136.8, 132.2, 131.7, 131.6, 130.0, 129.4, 128.2, 123.5, 119.5, 115.6, 115.4, 105.5, 30.8.



3-butyl-2-methylisoquinolin-1(2H)-one (entry 13, Table 3): ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.24 (d, *J* = 8.0, 1H), 7.66 (t, *J* = 8.0, 1H), 7.43(t, *J* = 7.4, 1H), 7.34 (d, *J* = 7.4, 1H), 6.24 (s, 1H), 2.52 (t, *J* = 7.4, 2H), 1.72-1.66 (m, 2H), 1.42-1.36 (m,2H), 0.94 (t, *J* = 7.4, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.2, 158.4, 144.2, 137.7, 134.7, 129.6, 127.6, 125.0, 120.2, 102.9, 33.3, 29.0, 22.2, 13.8.



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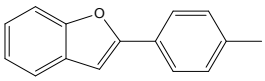

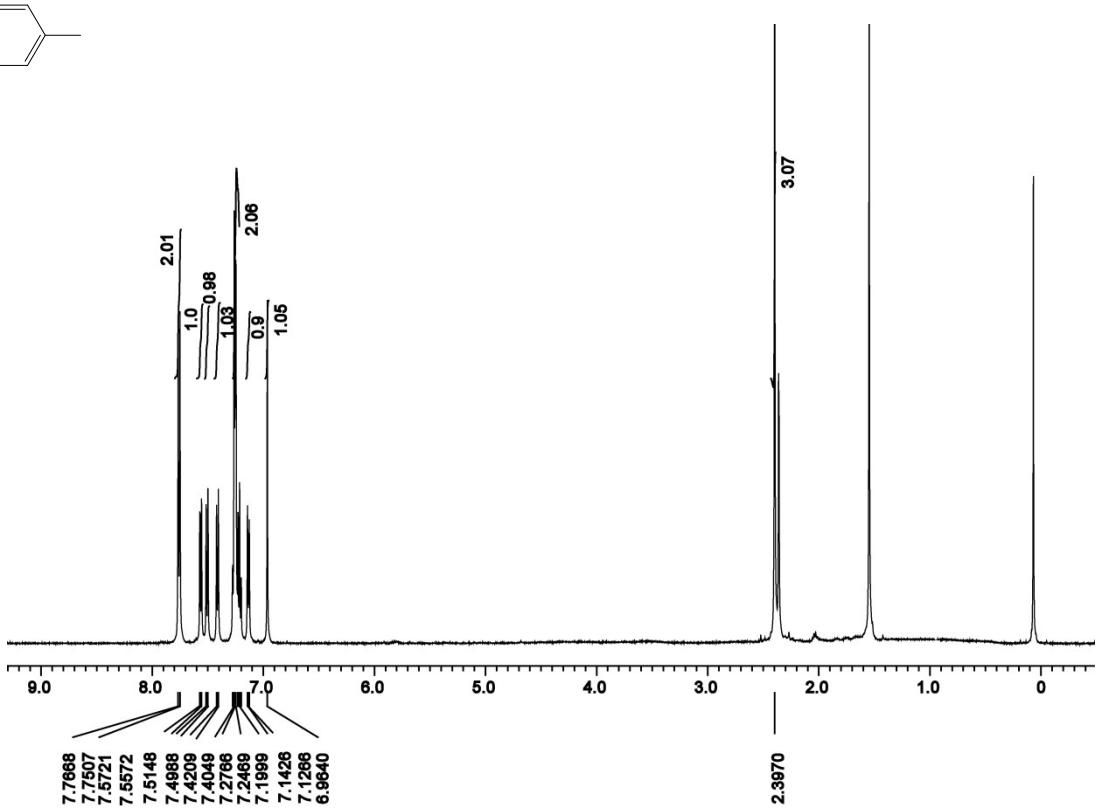
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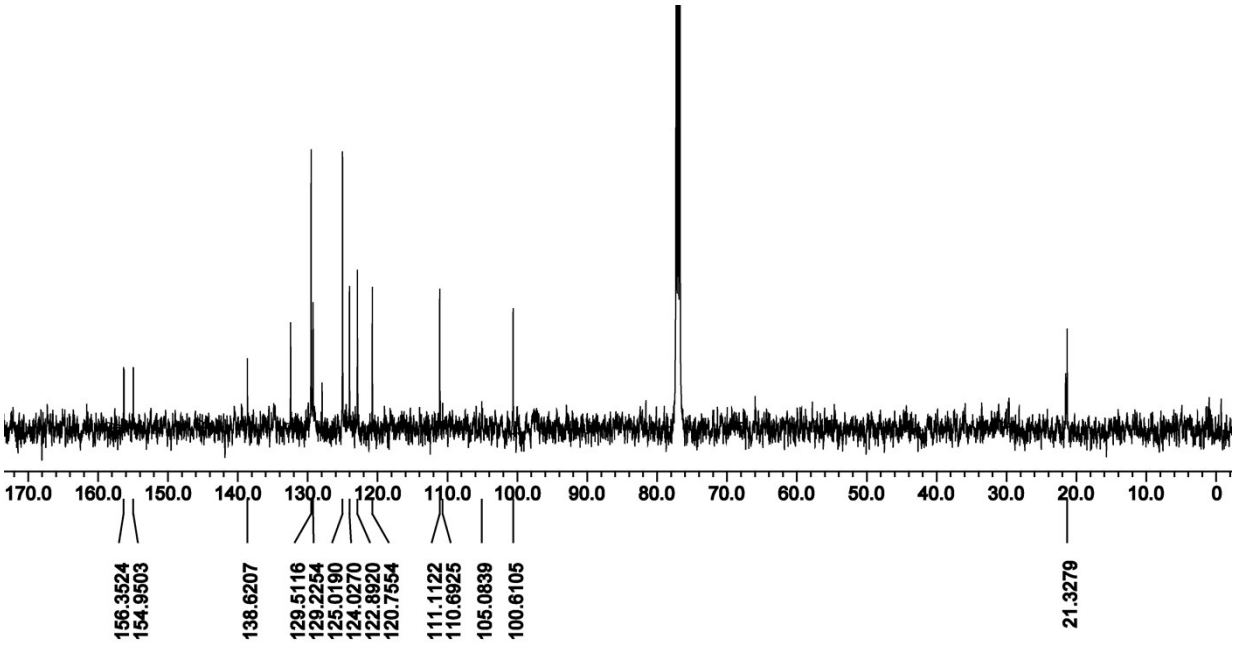
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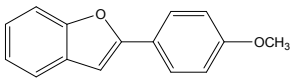
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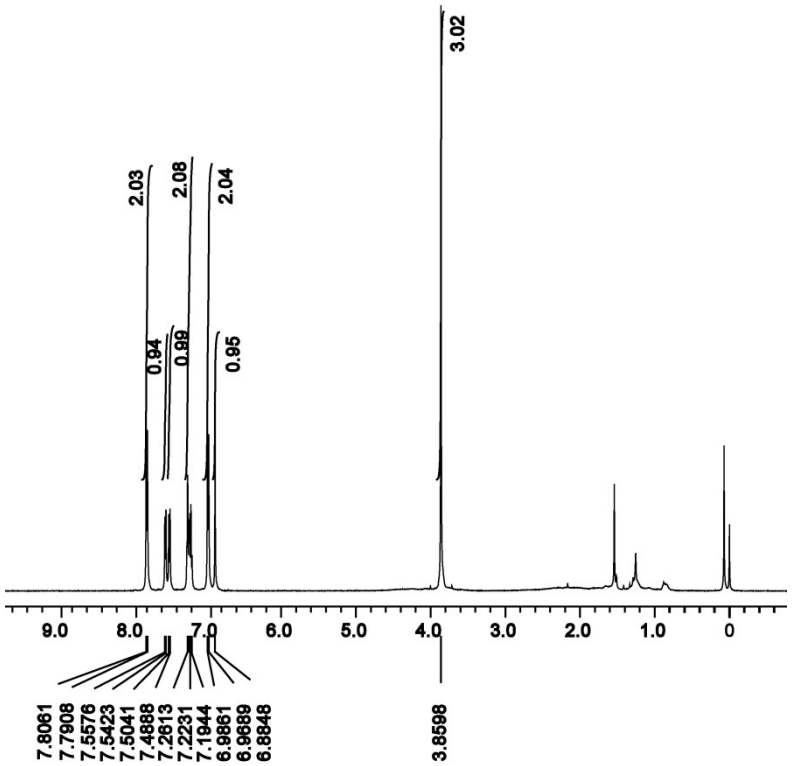
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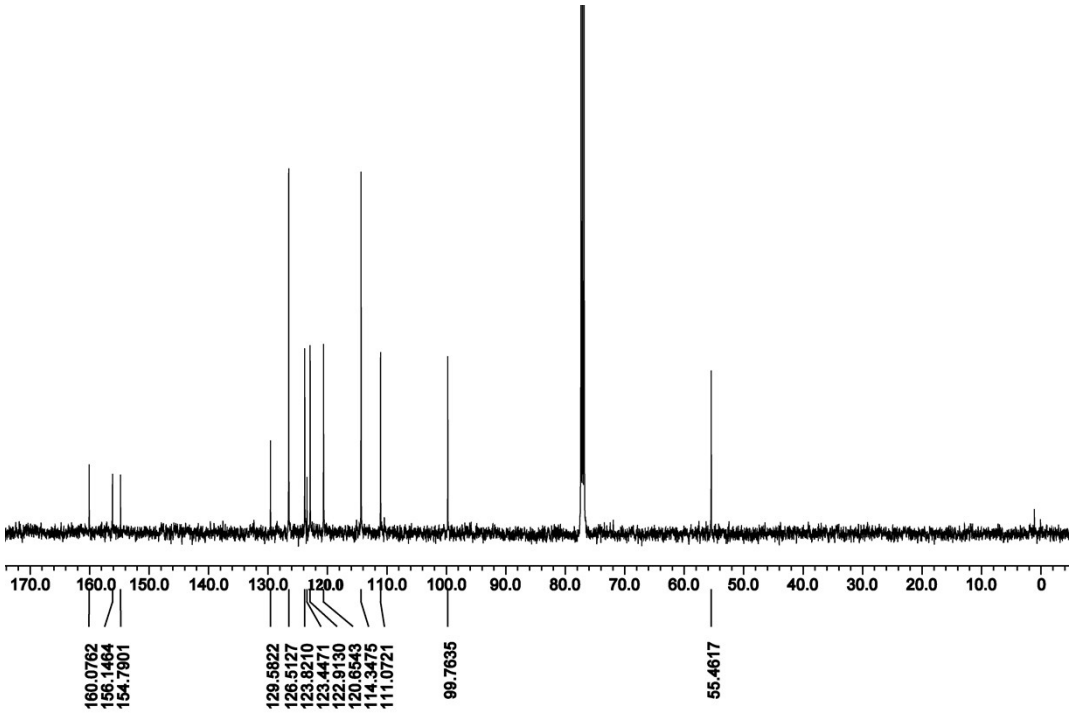
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10.0
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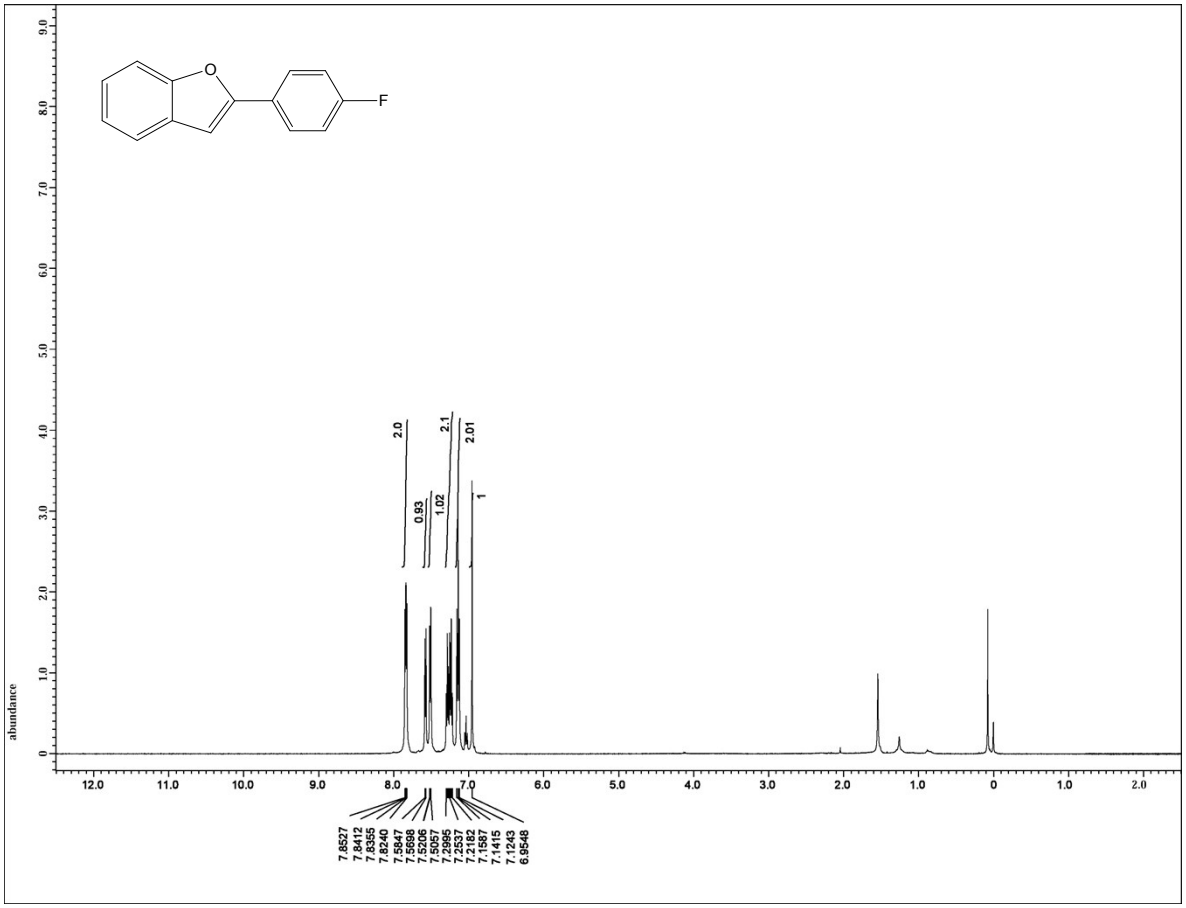
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F
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1
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7.8240
7.5847
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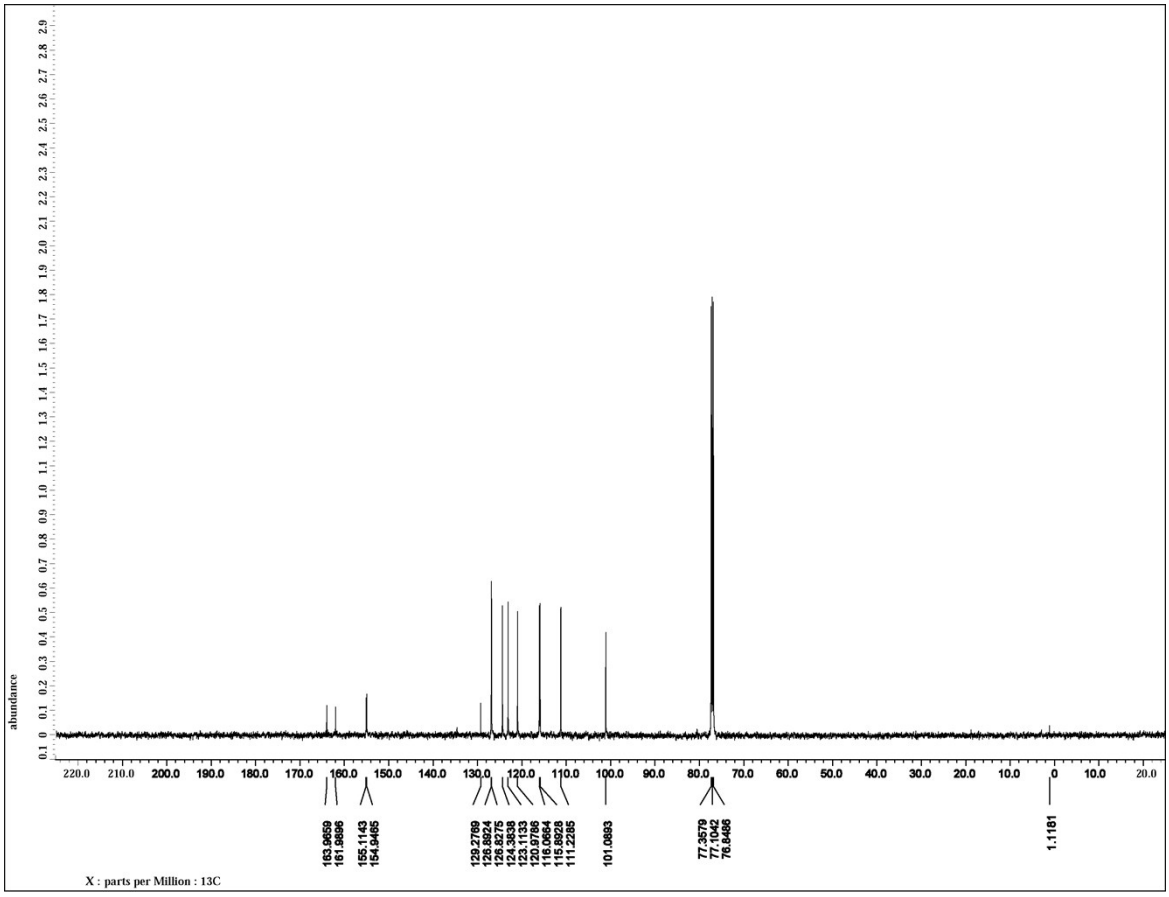
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126.8824
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124.3838
123.1733
120.0795
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111.2285
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77.3579
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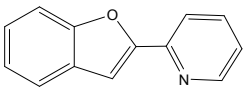
76.8486
1.1181
X : parts per Million : 13C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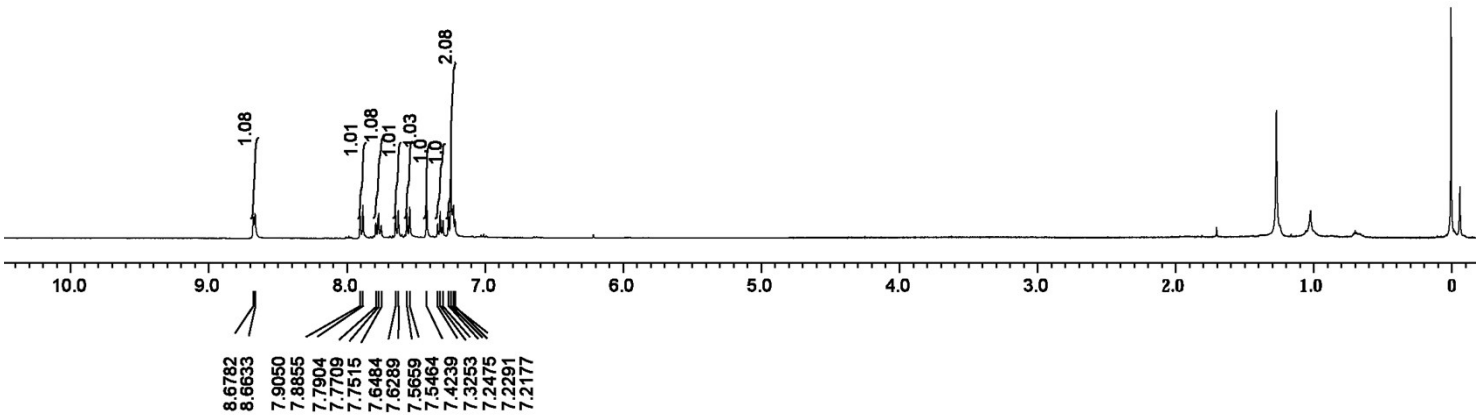
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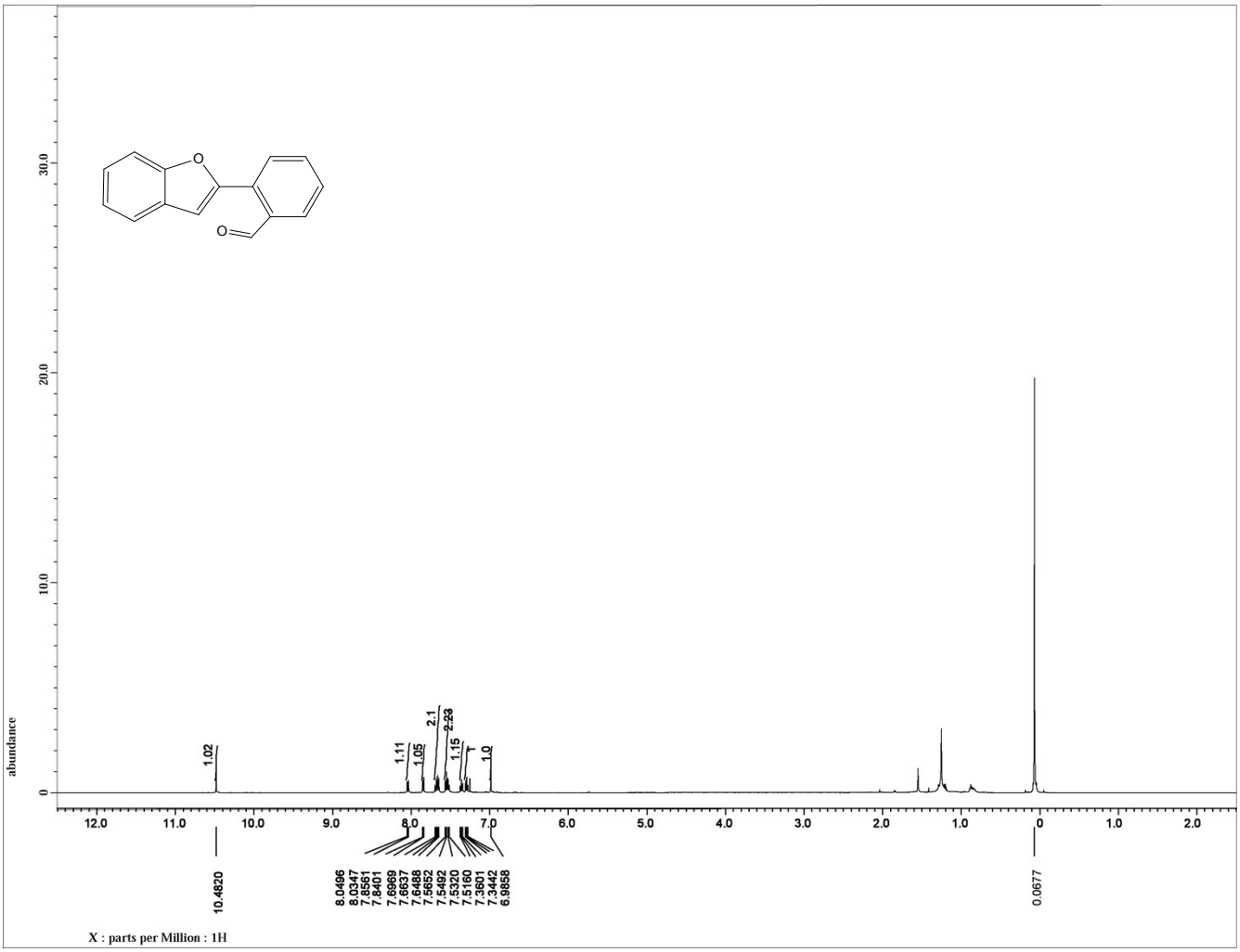
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O
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1.11
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2.1
2.23
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1.0
12.0
11.0
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.0
2.0
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8.0347
7.8561
7.8401
7.6969
7.6637
7.6488
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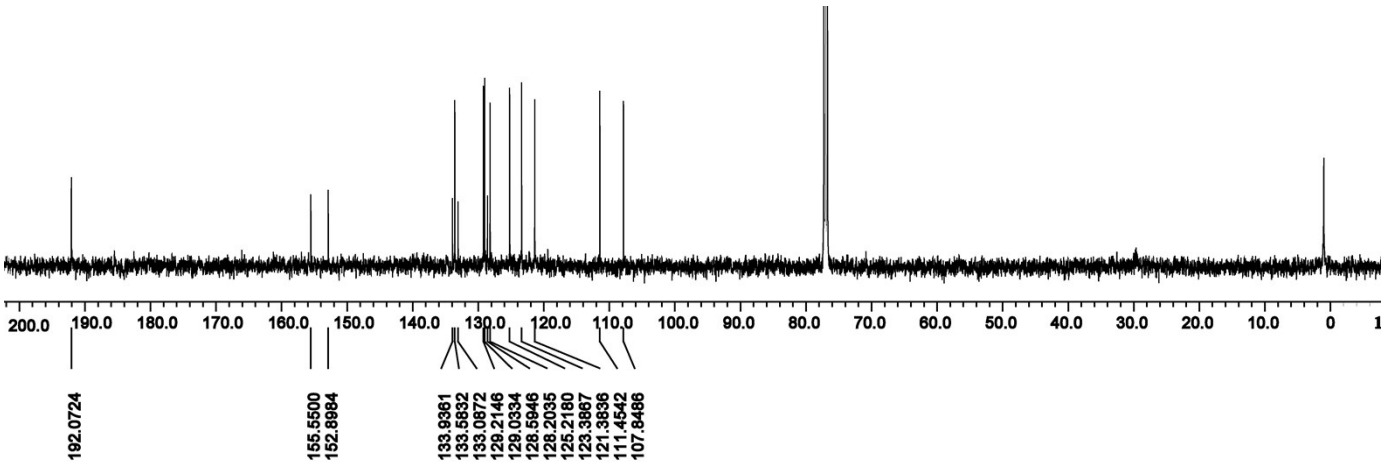
X : parts per Million : 1H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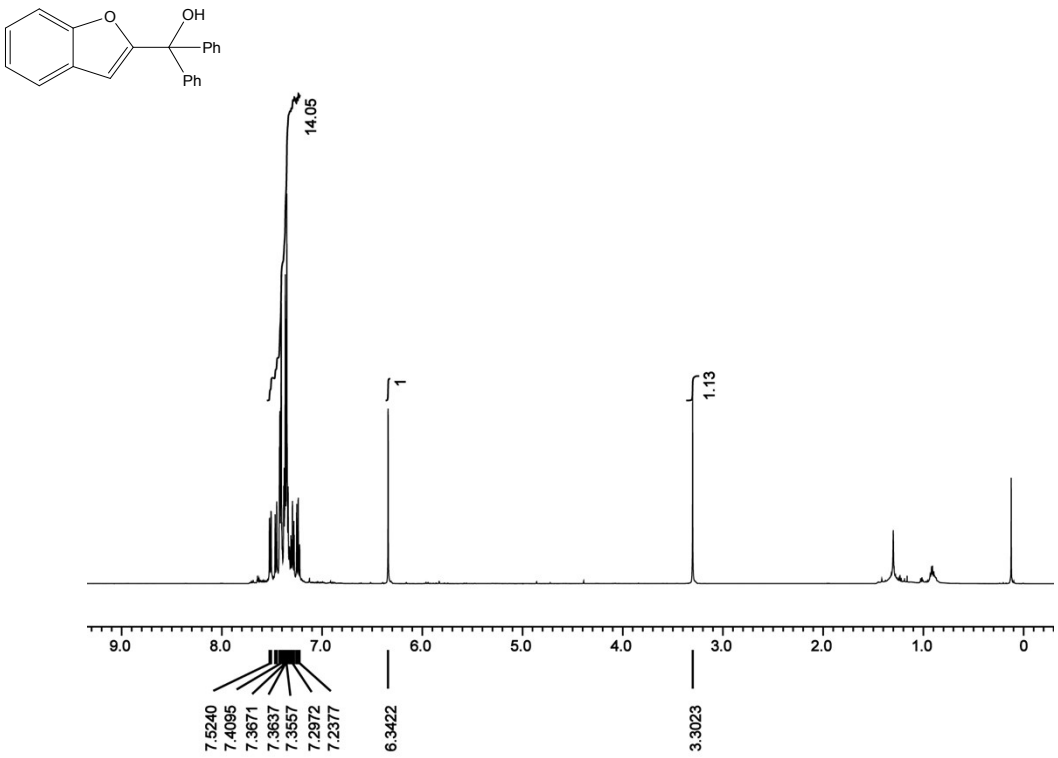
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OH
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Ph
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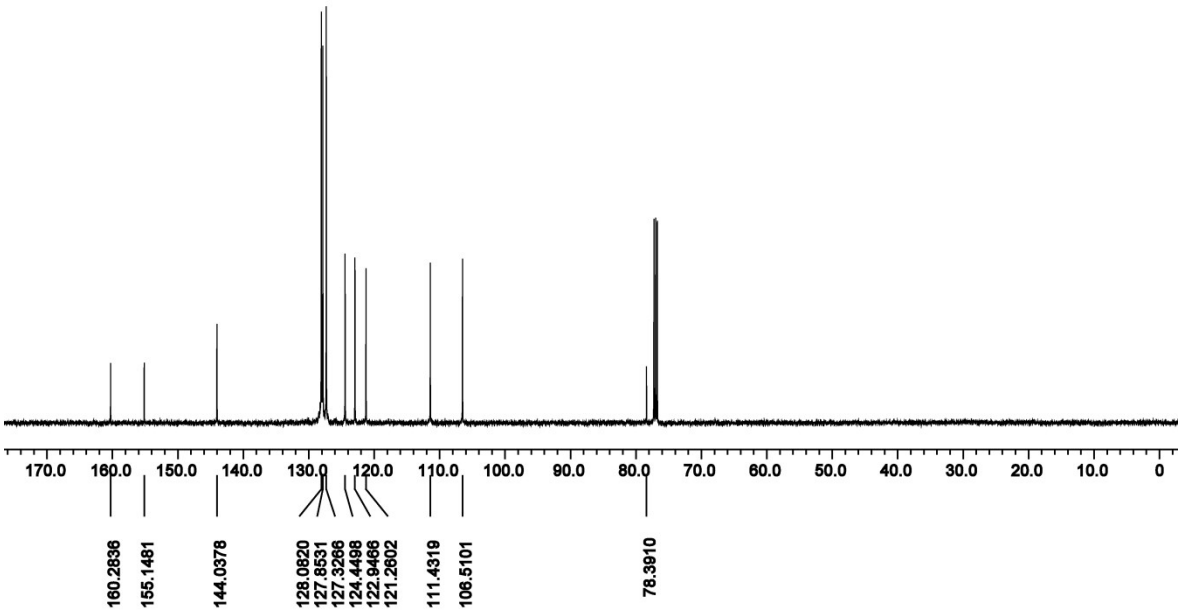
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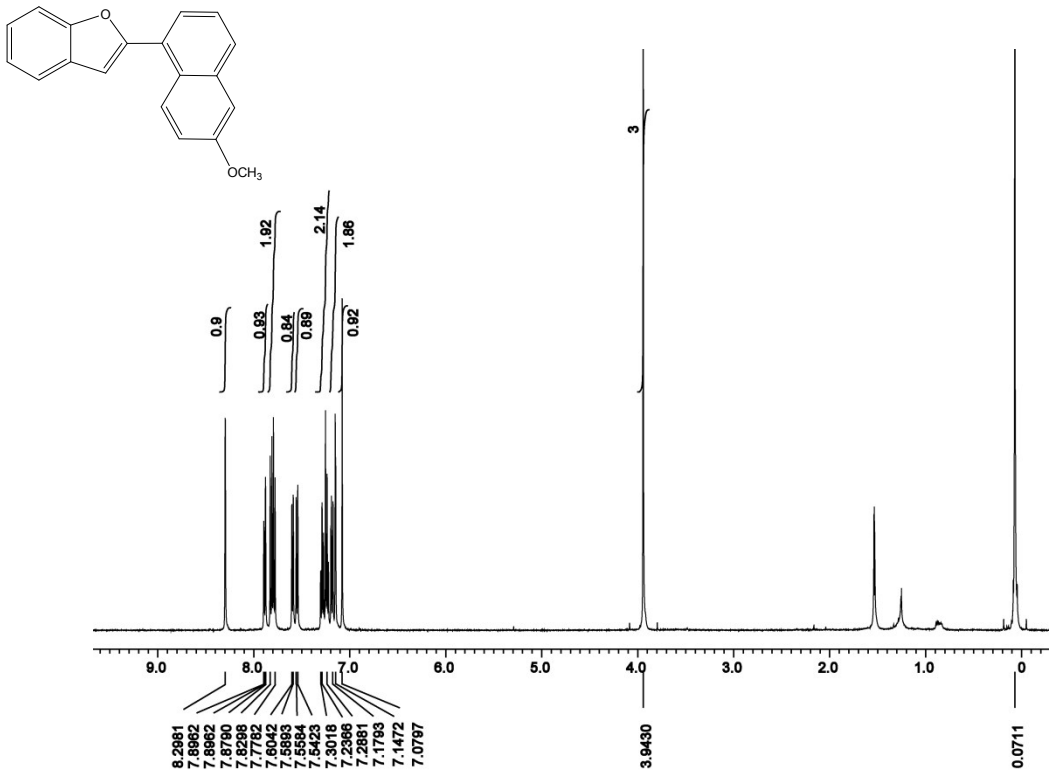
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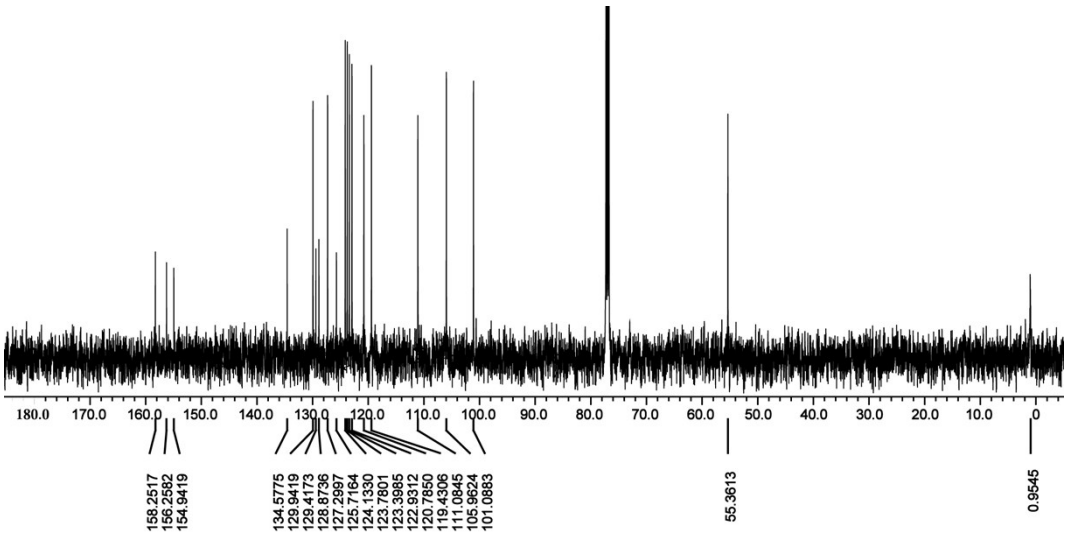
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10.0
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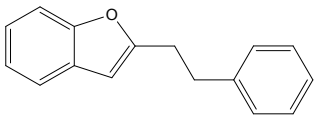

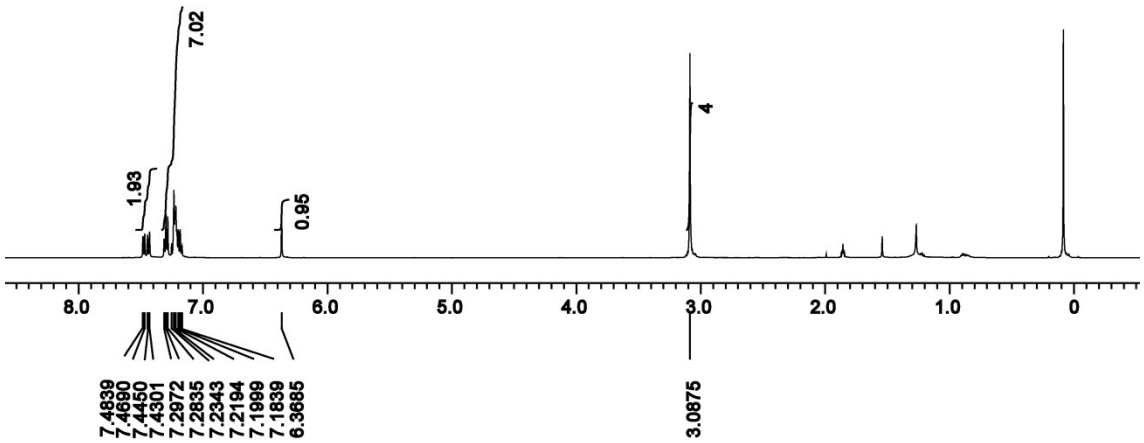
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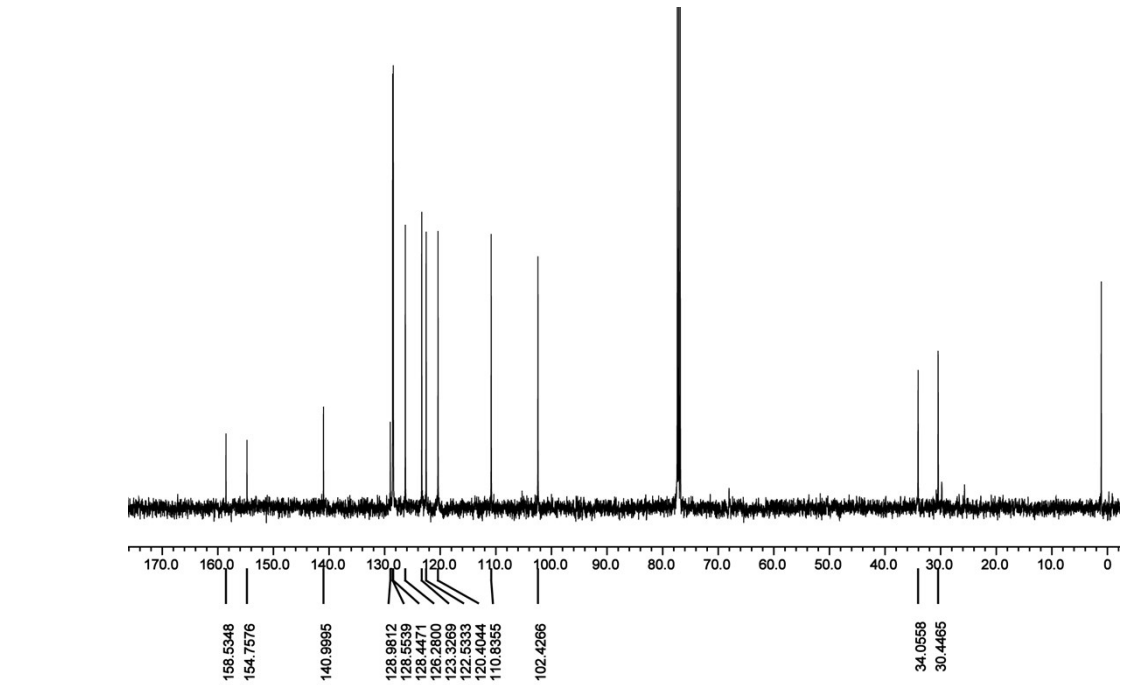
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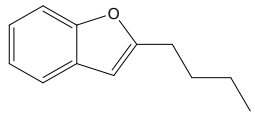

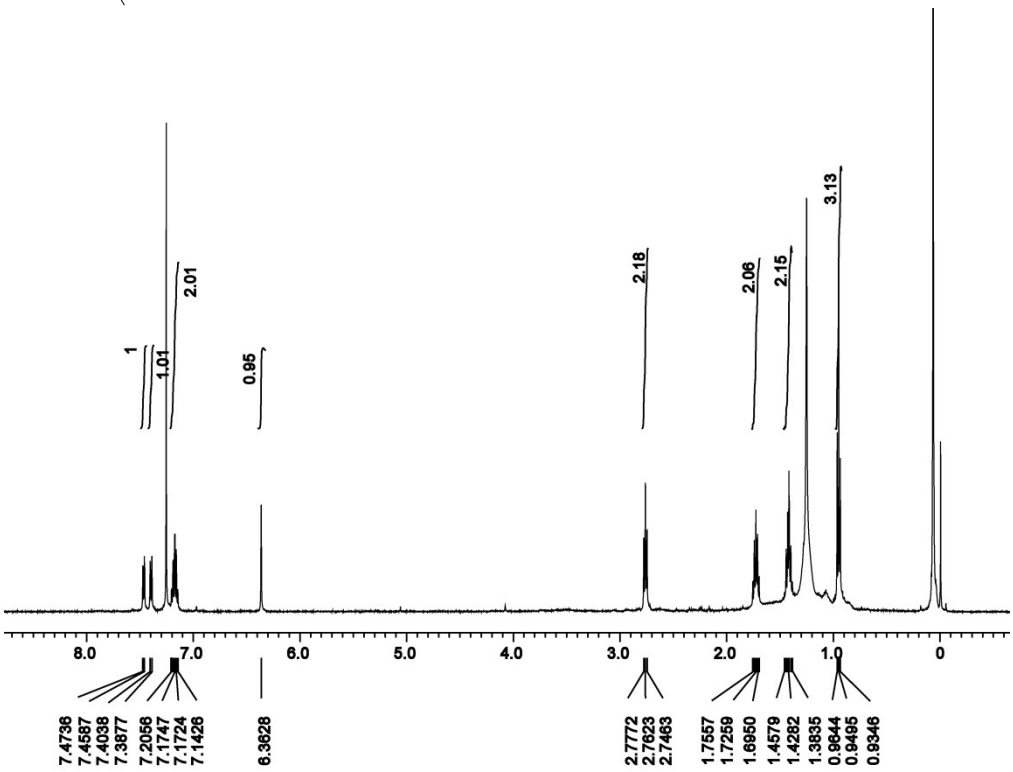
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3.0
2.0
1.0
0
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7.1724
7.1428
6.3628
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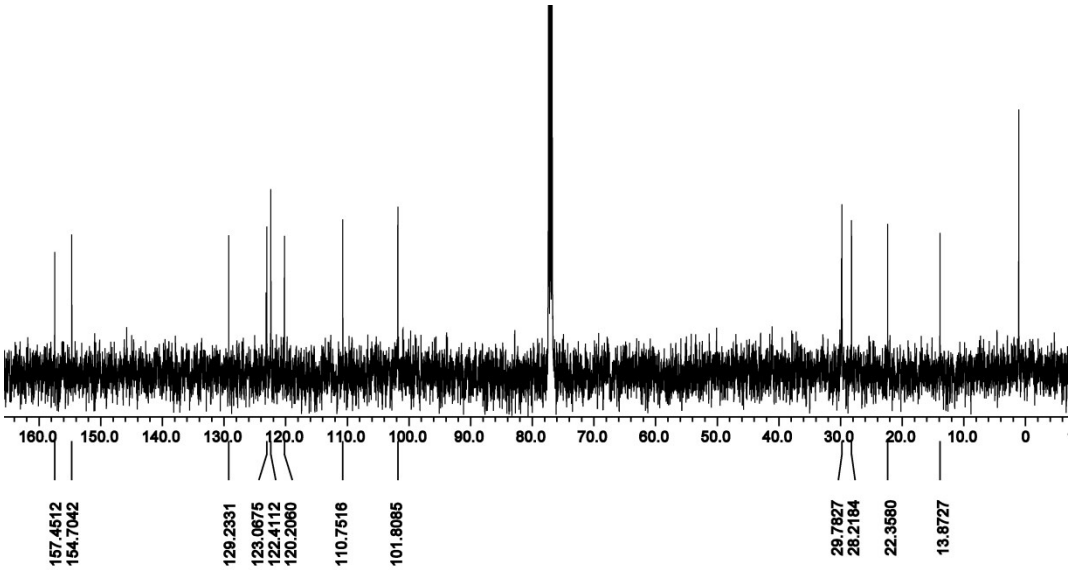
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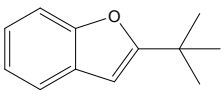

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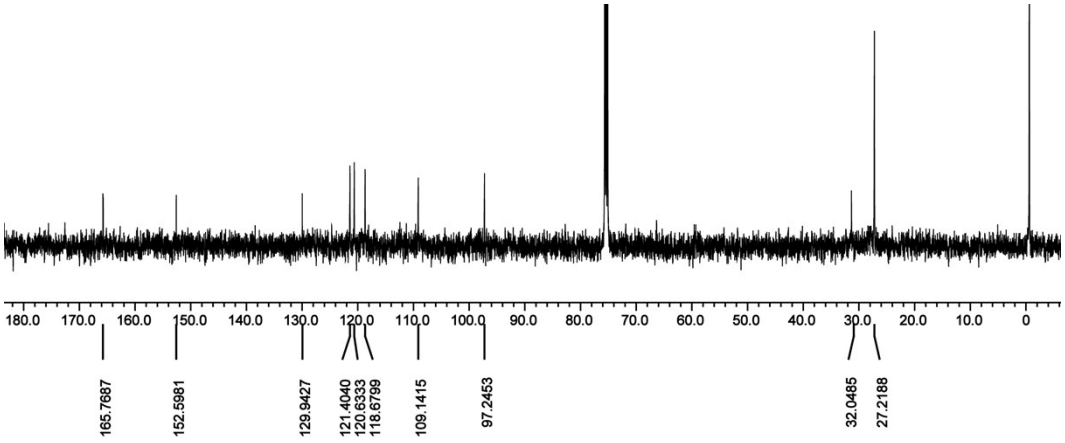
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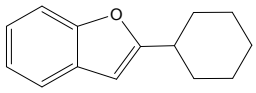

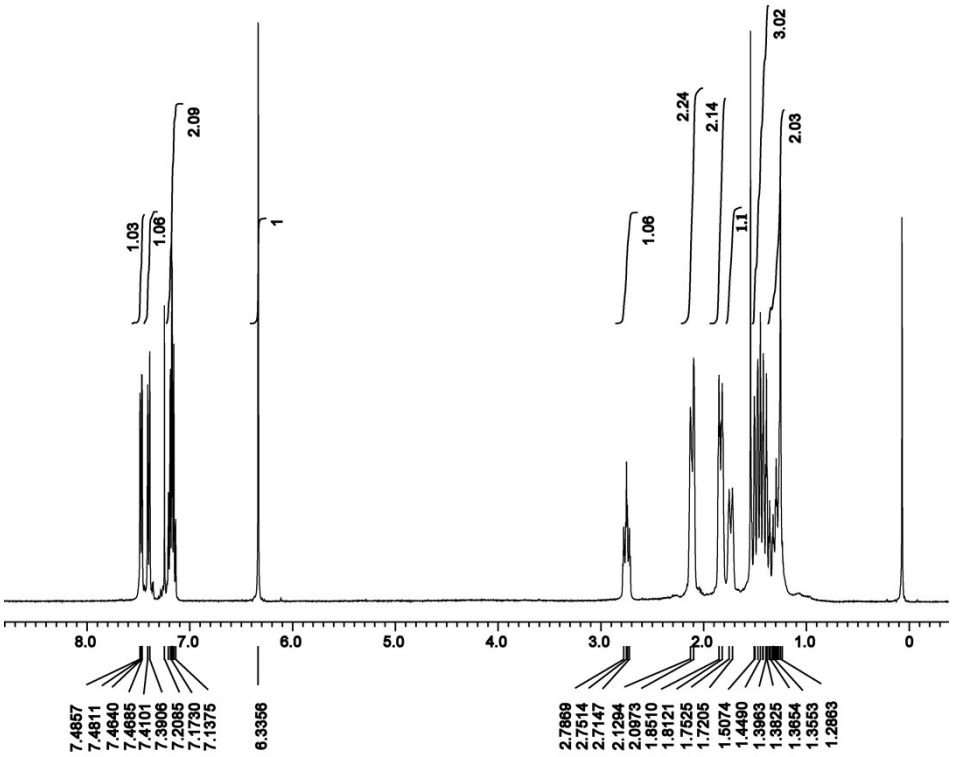
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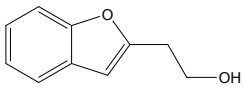
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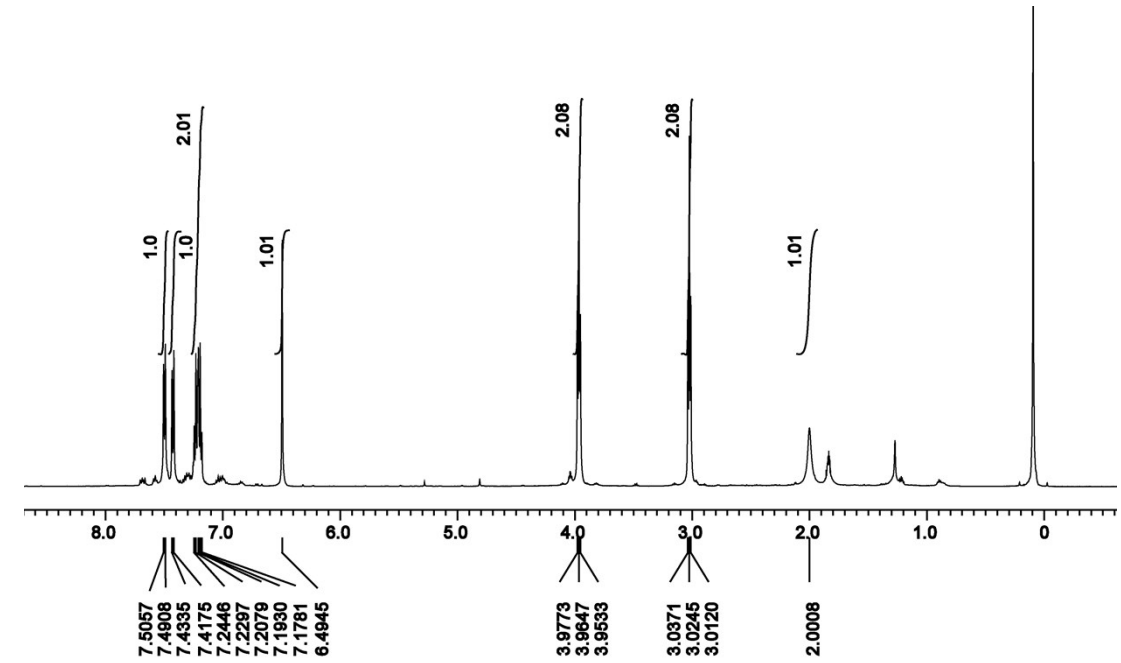
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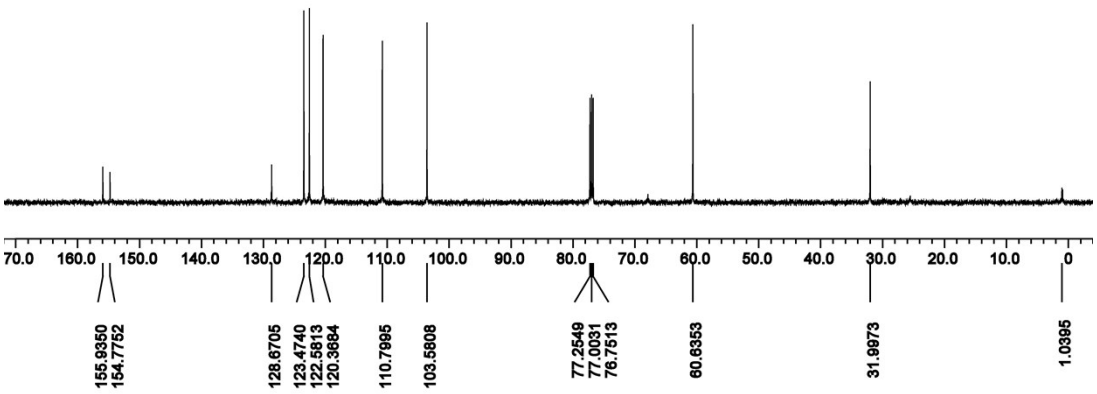
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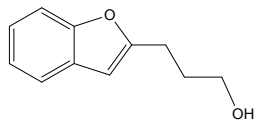
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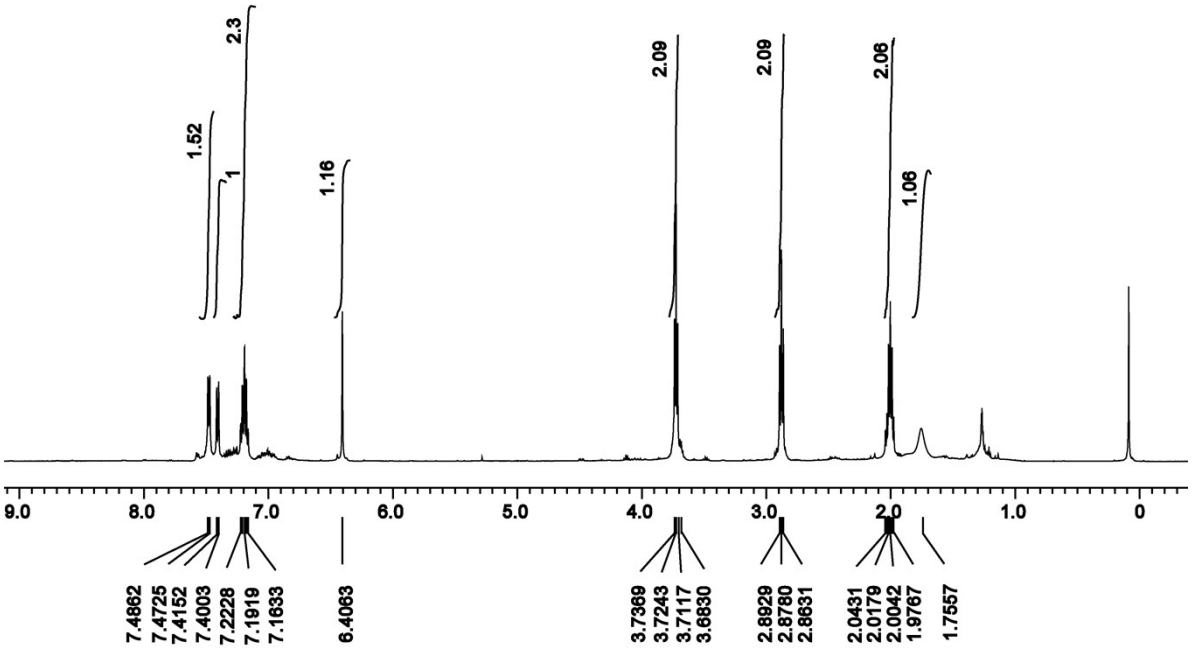
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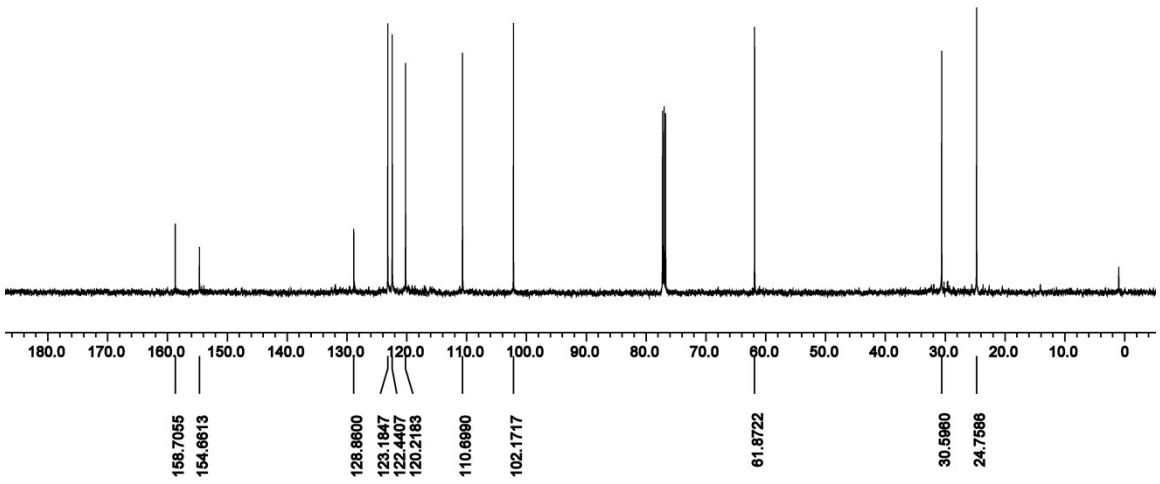
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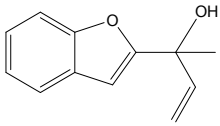
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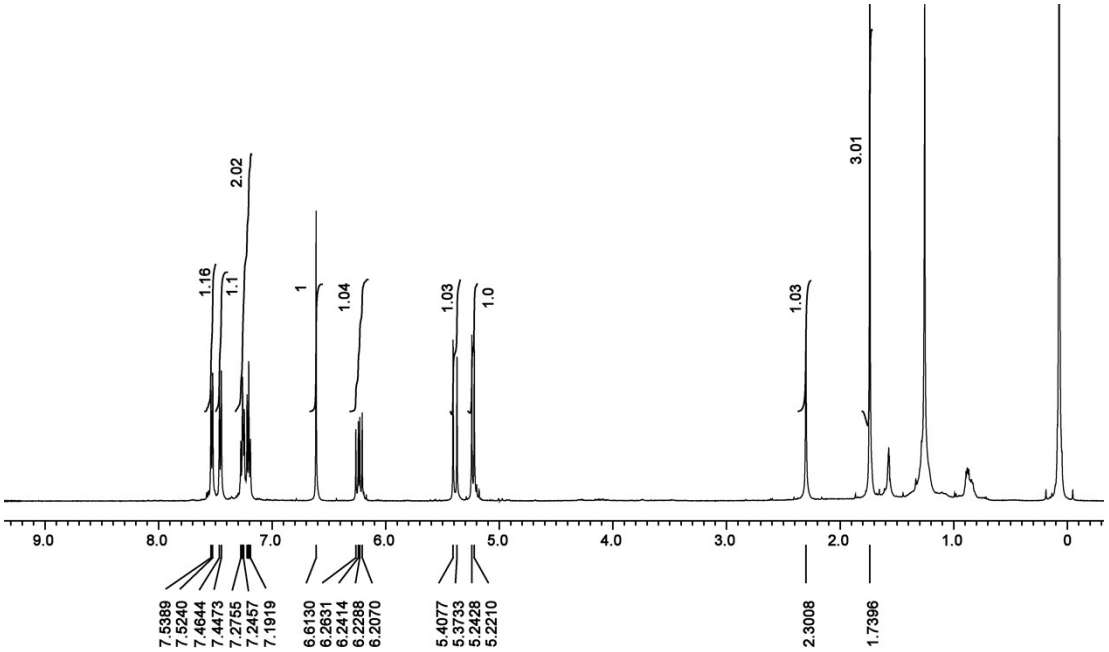
OH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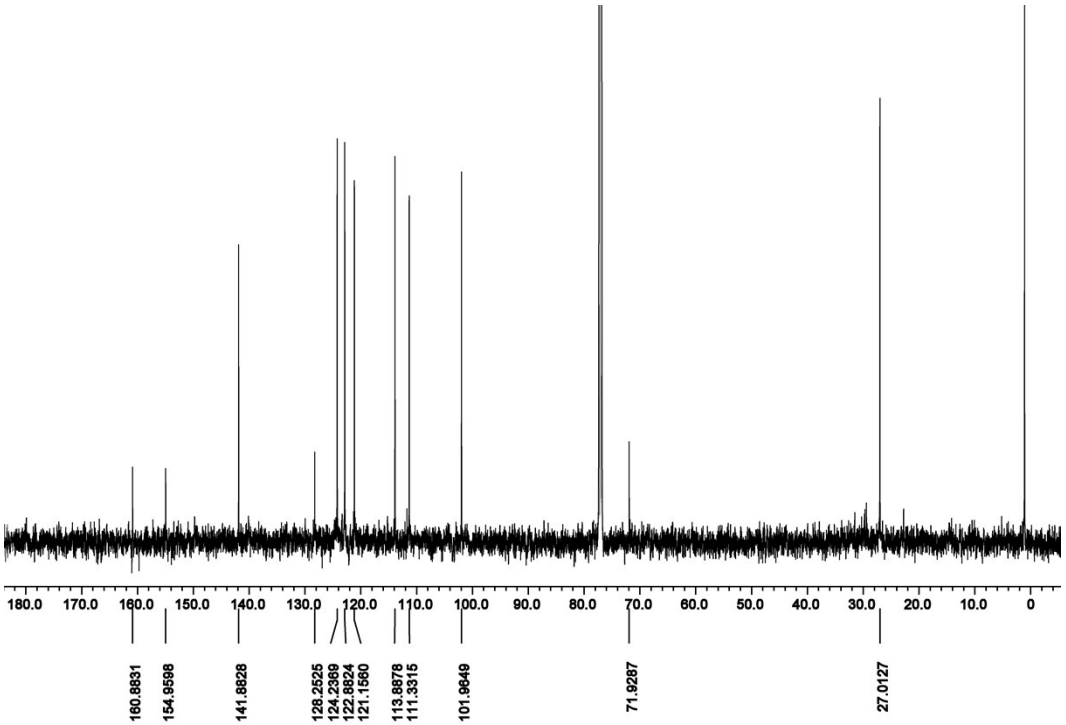
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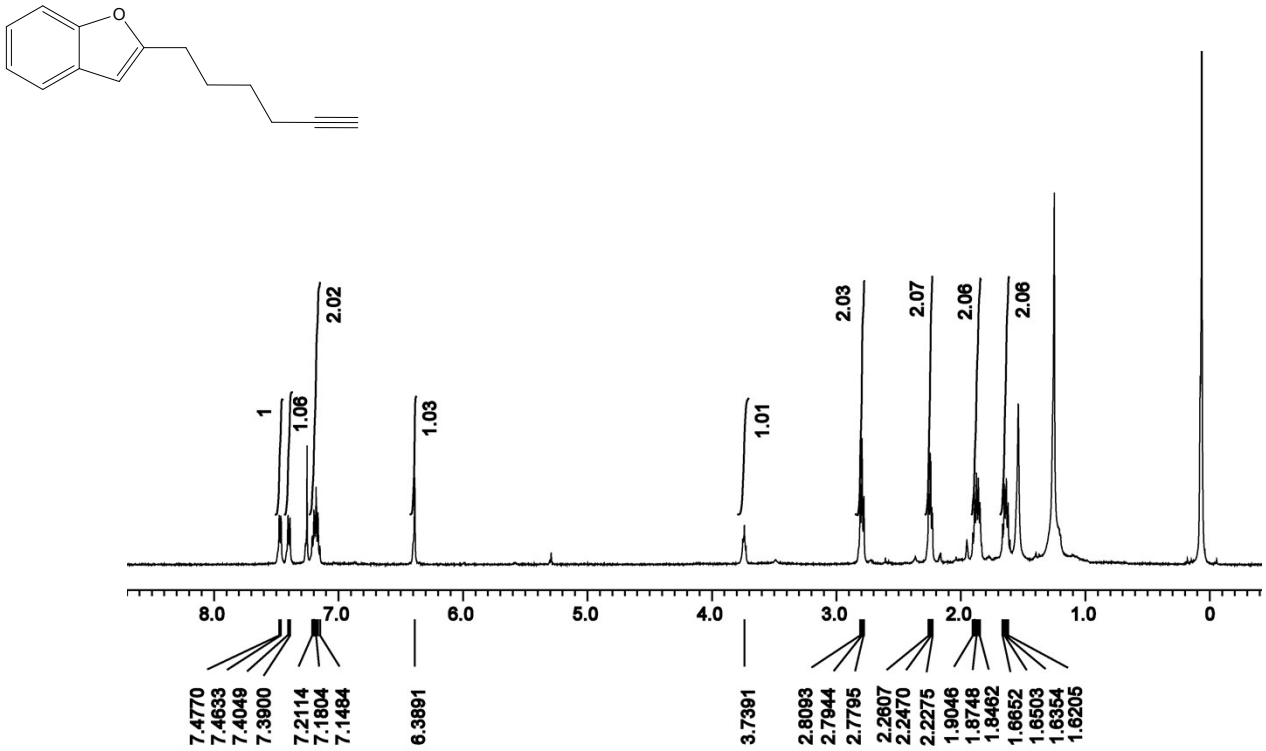
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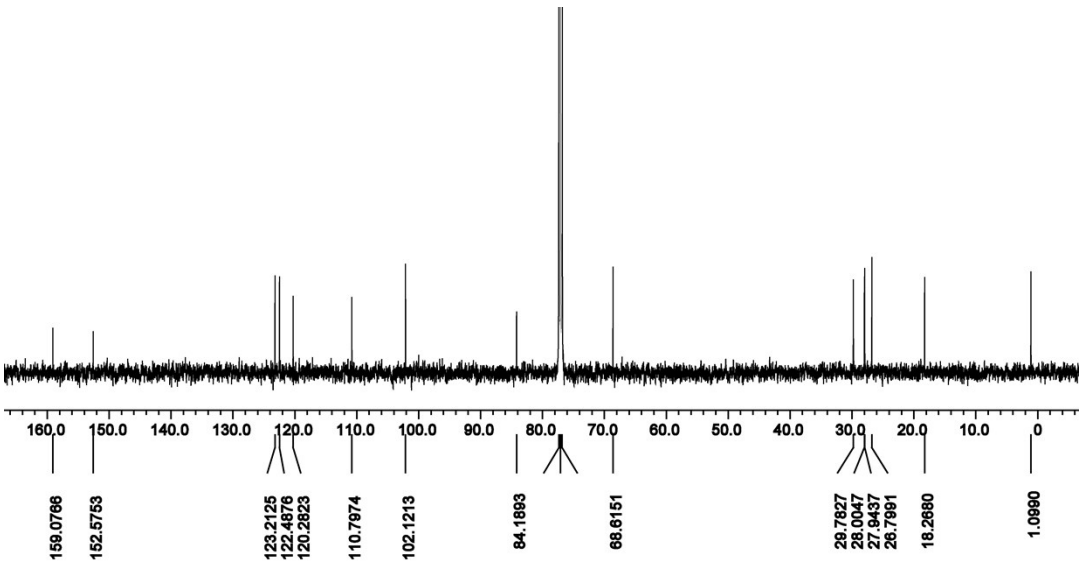
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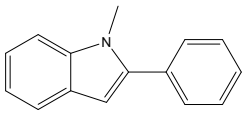

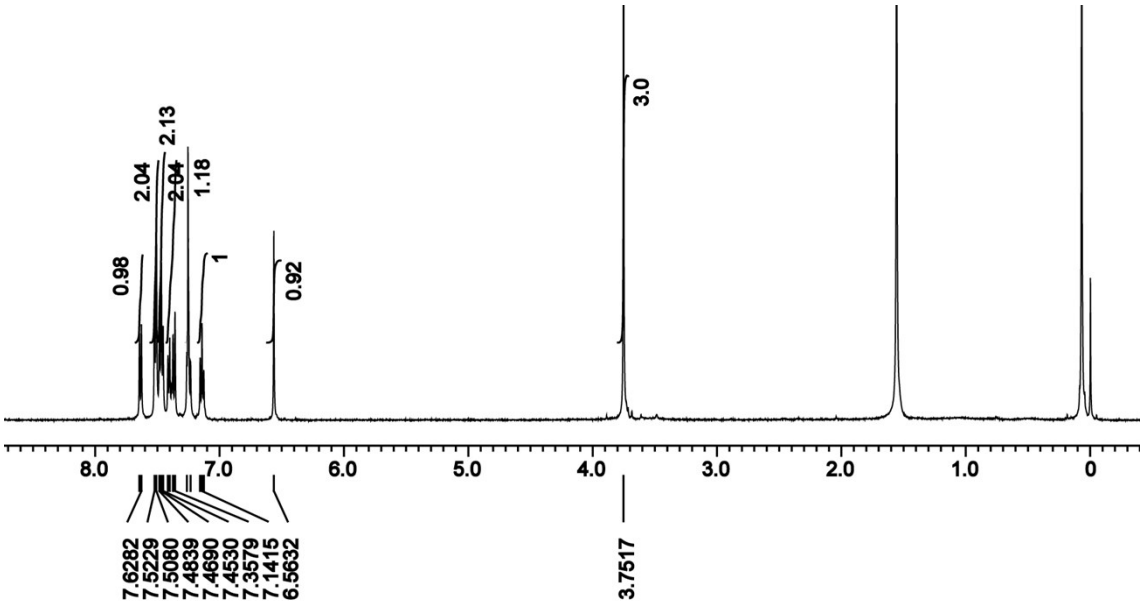
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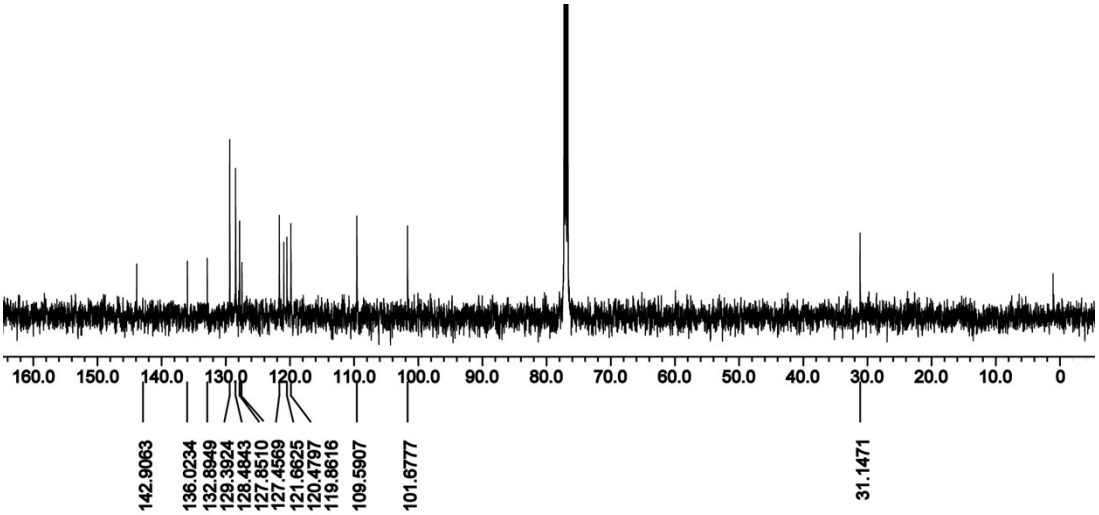
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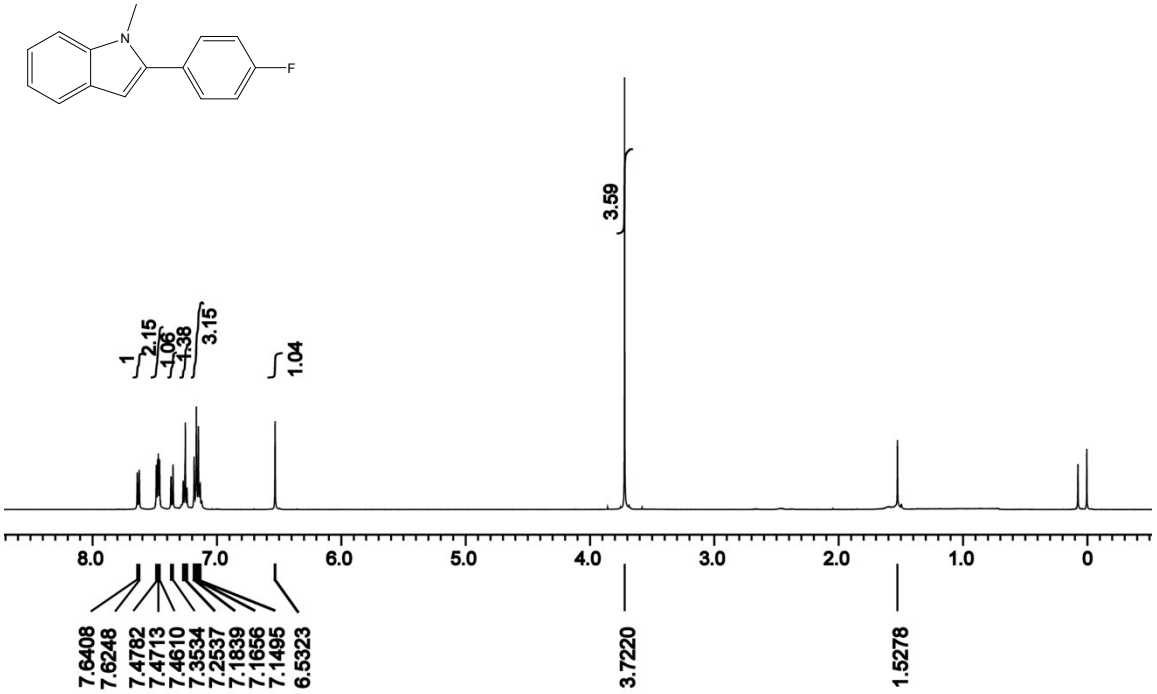
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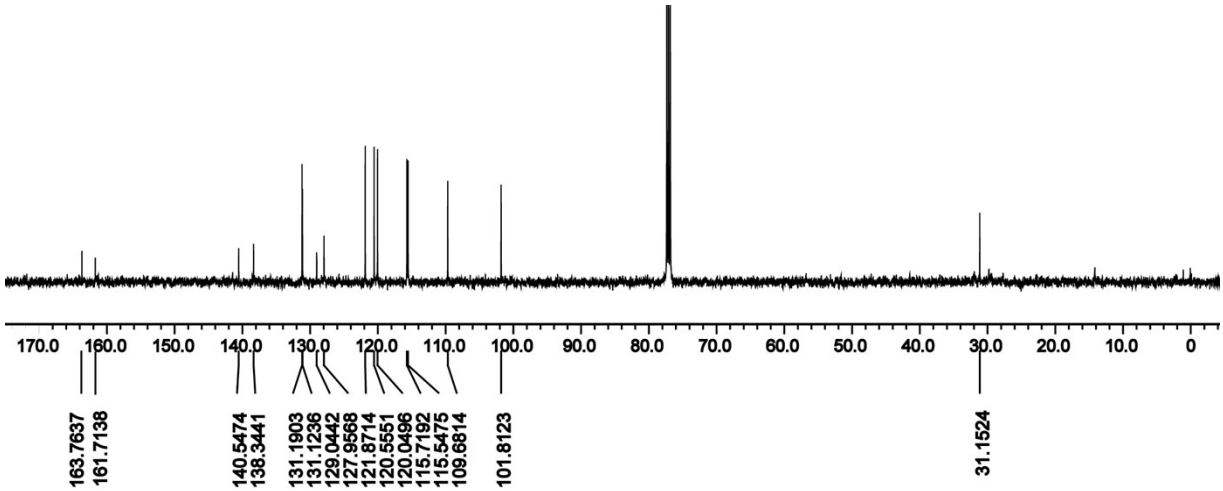
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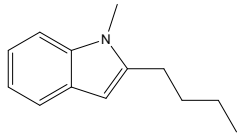

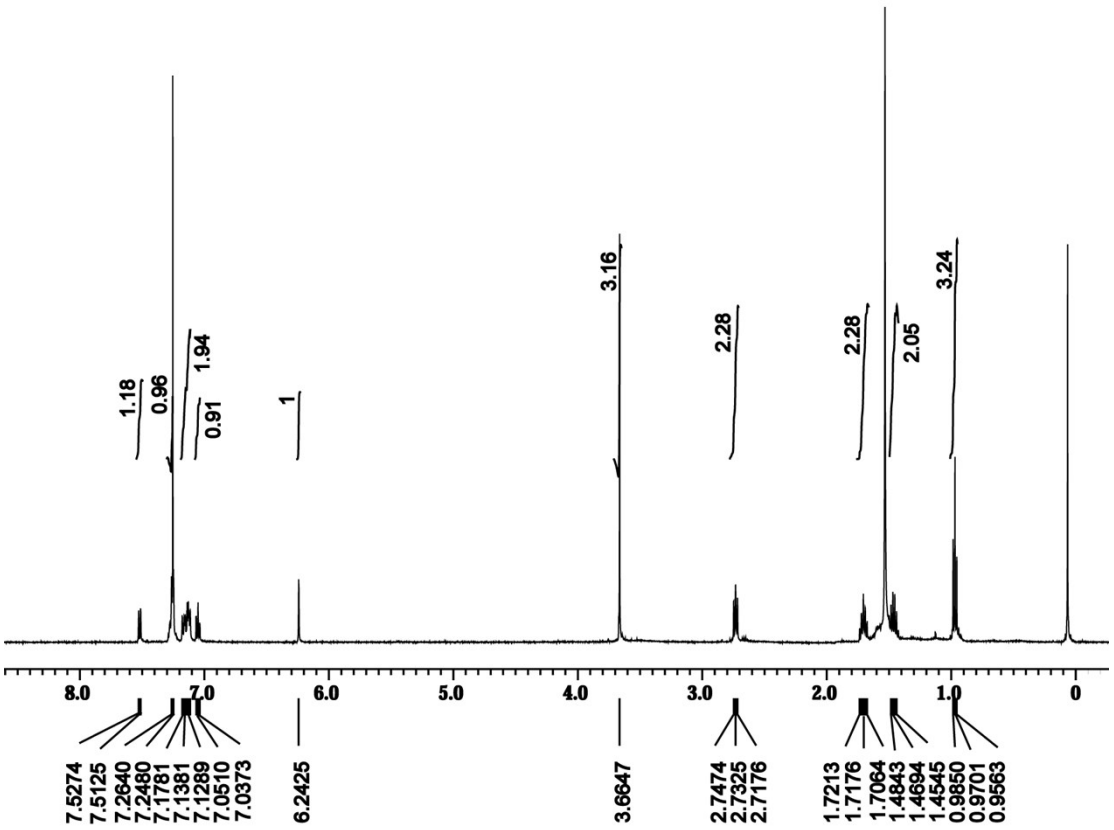
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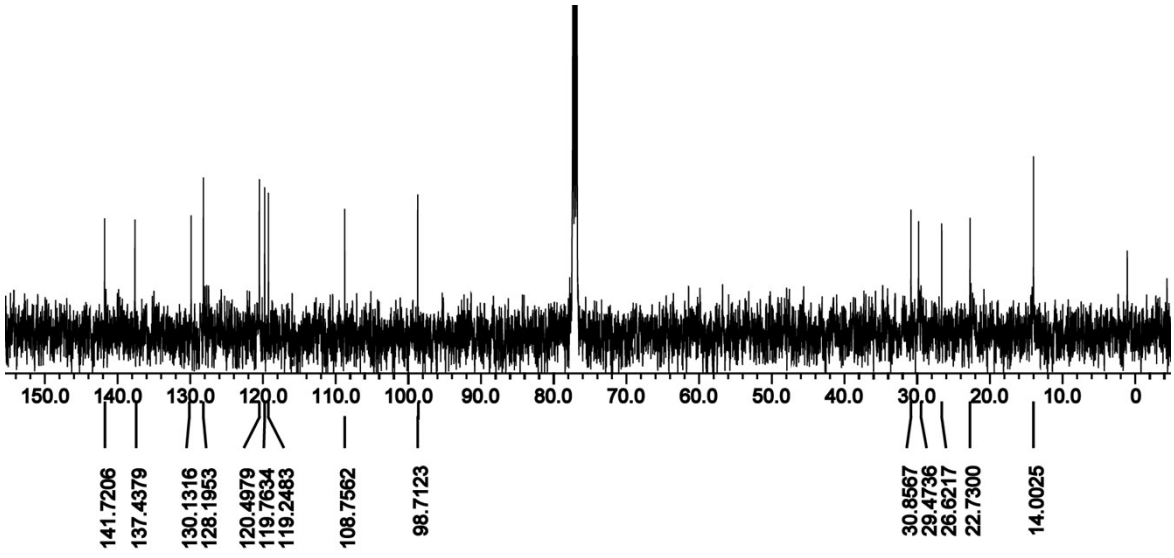
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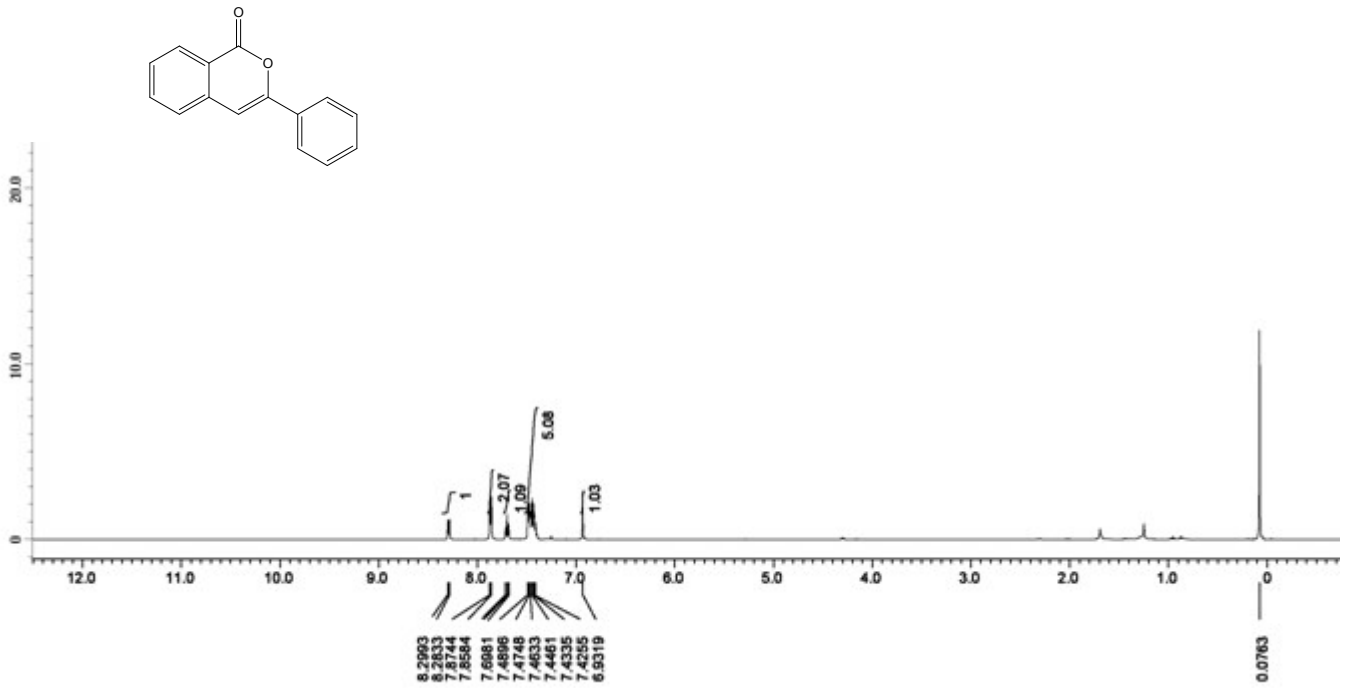
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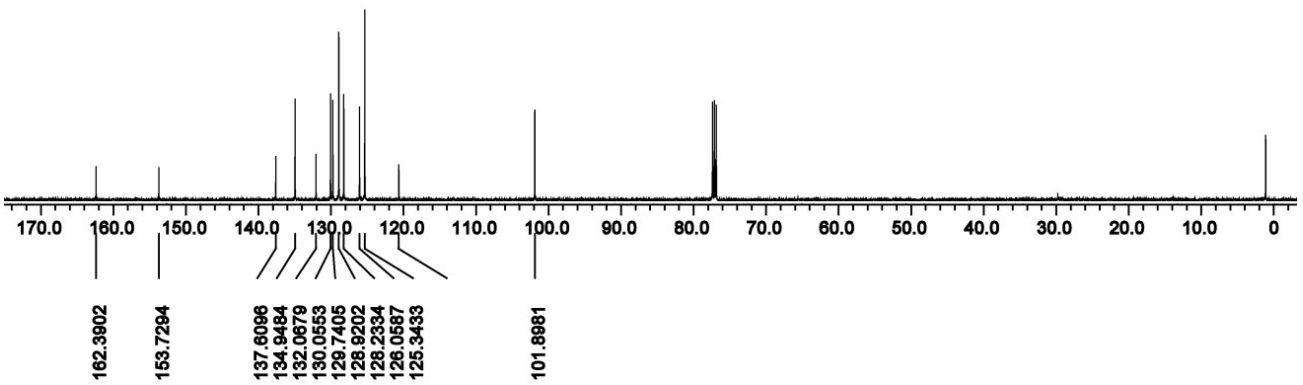
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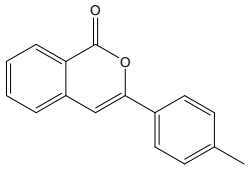

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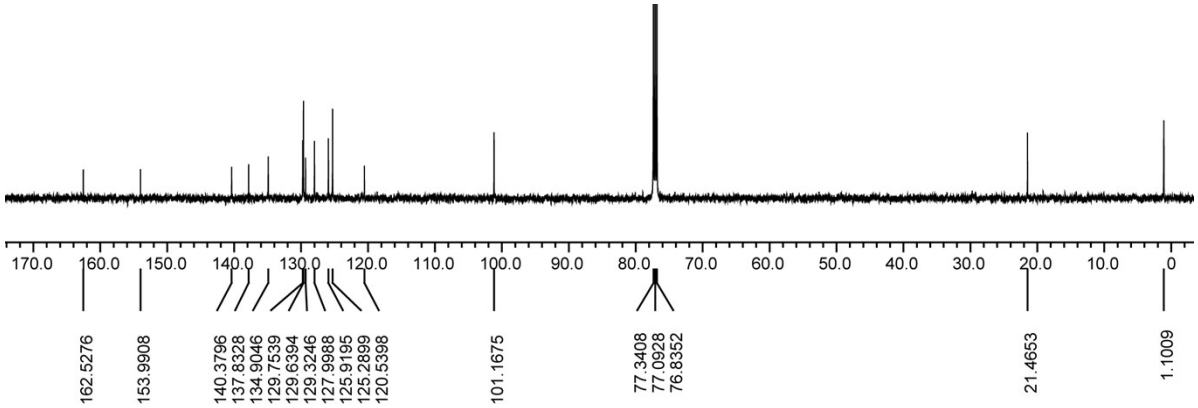
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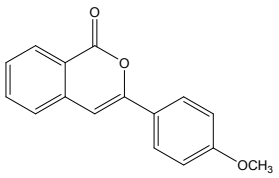
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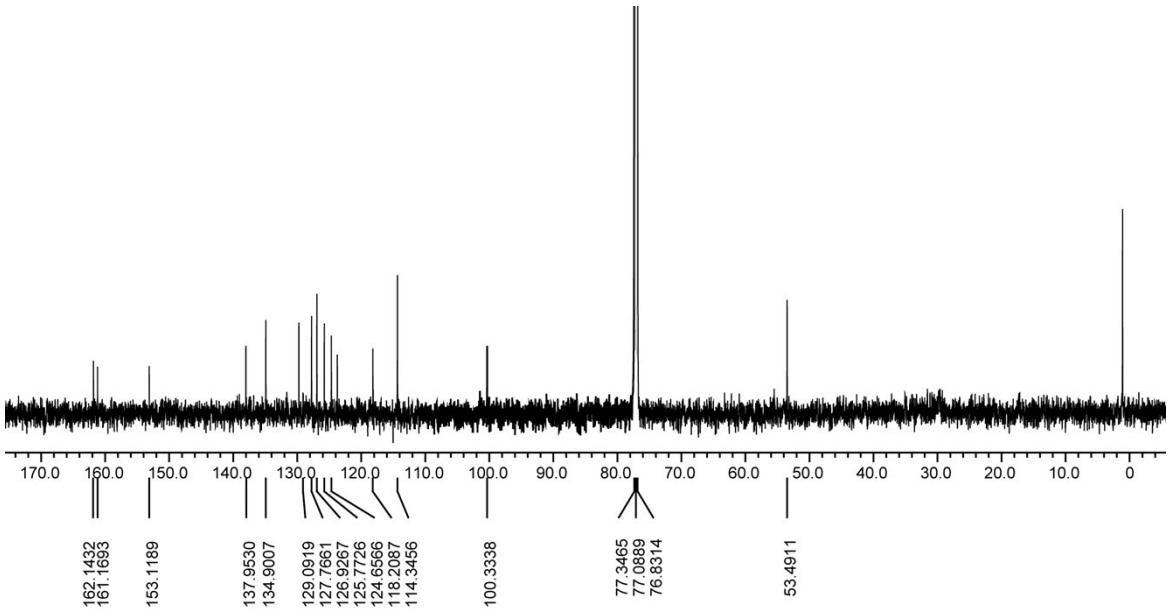
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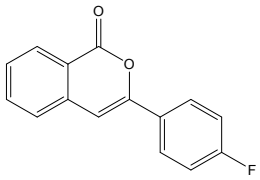
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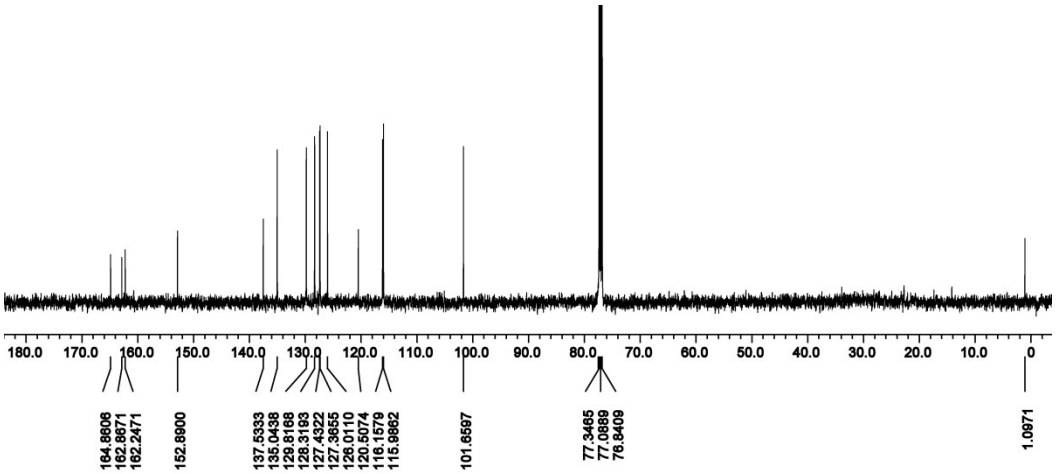
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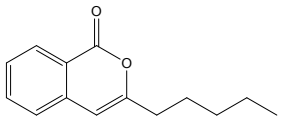

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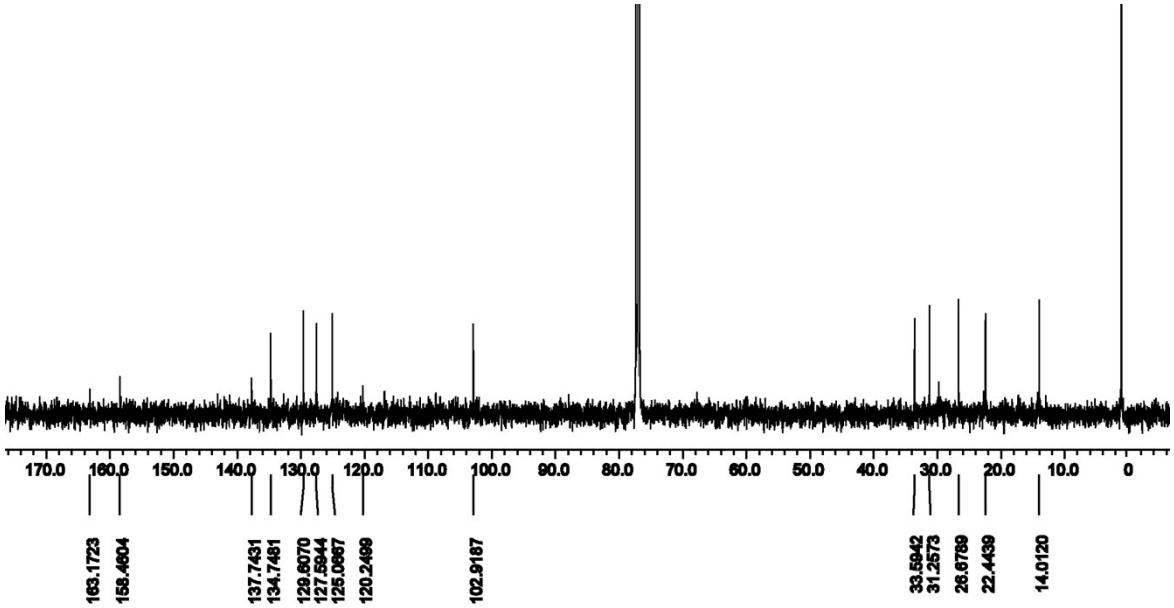
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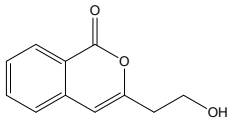
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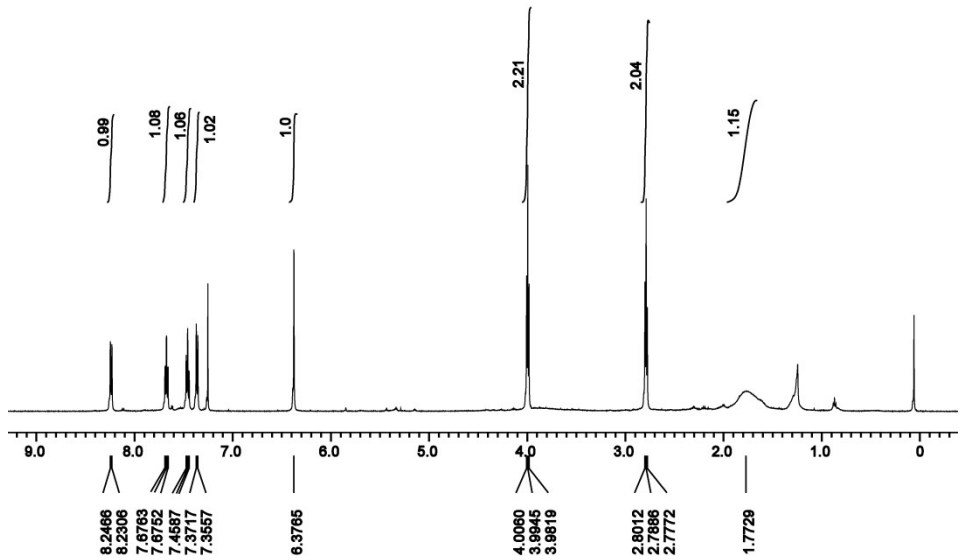
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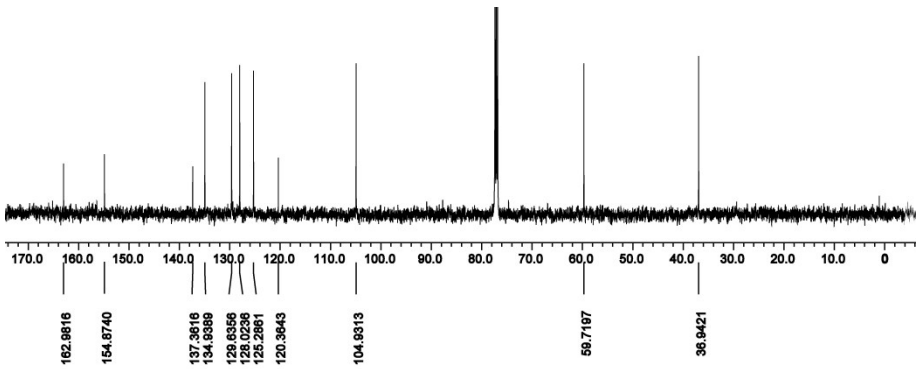
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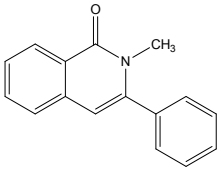
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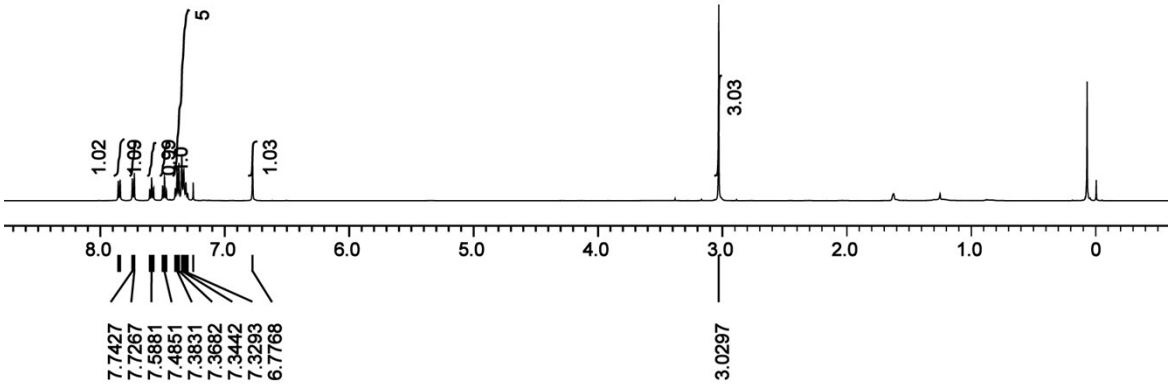
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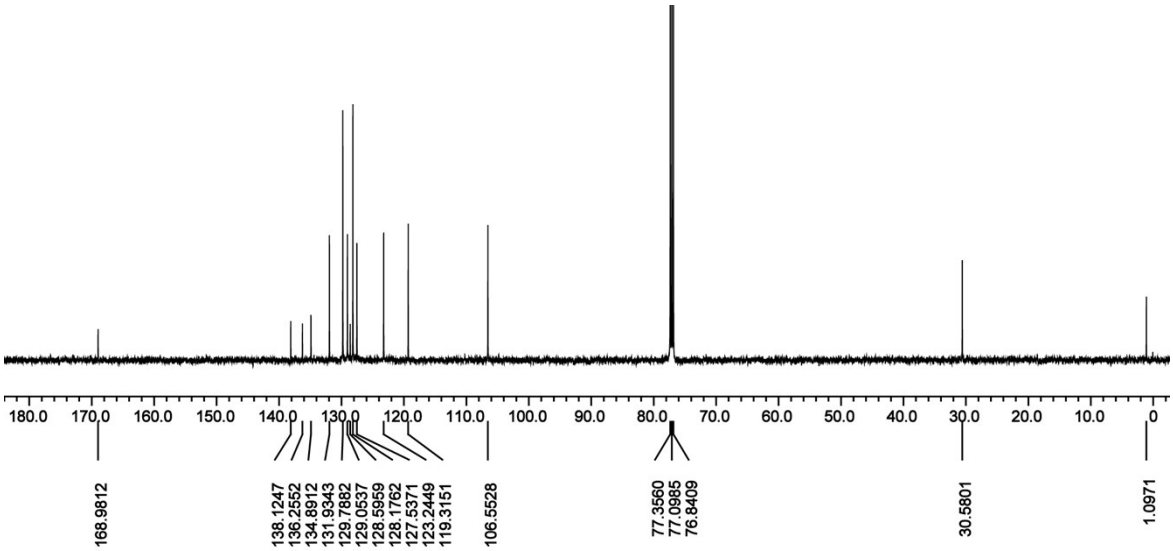
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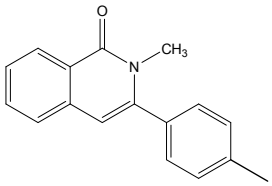
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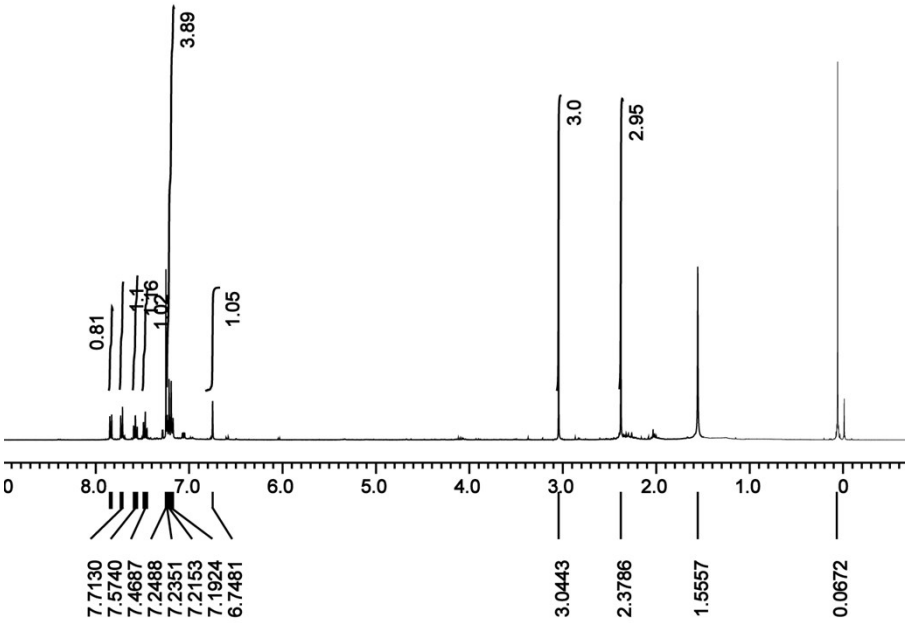
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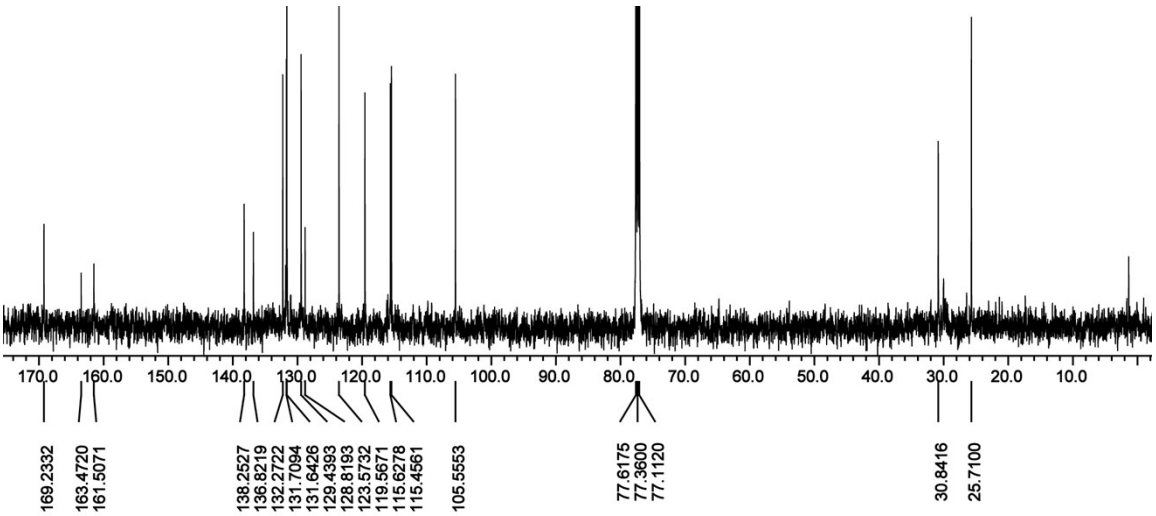
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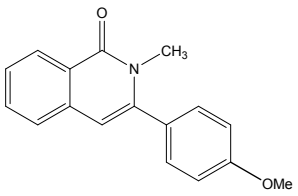
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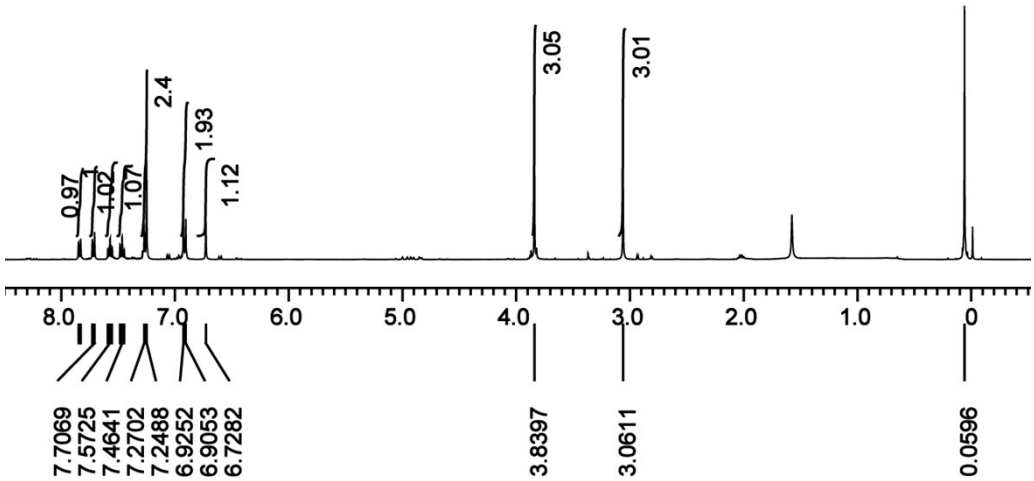
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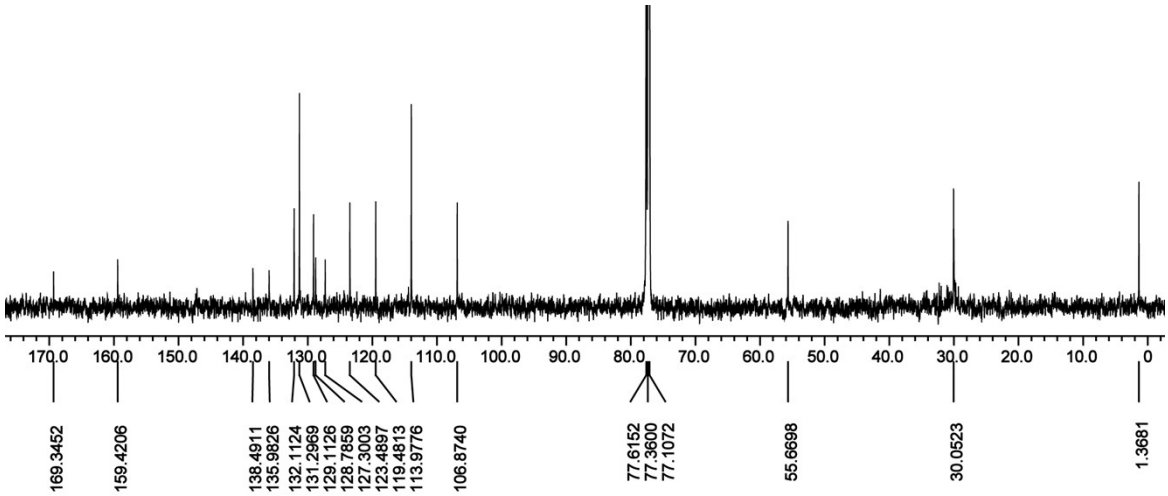
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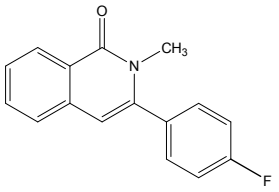
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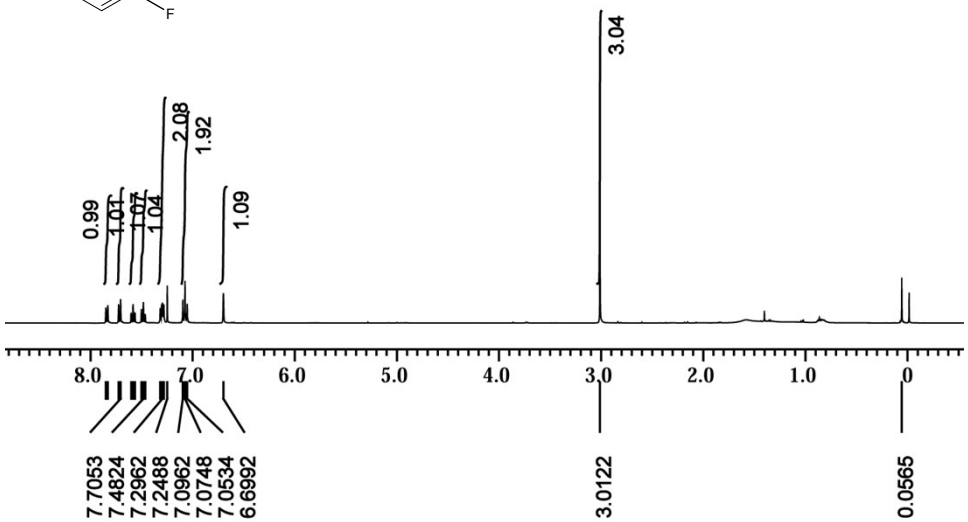
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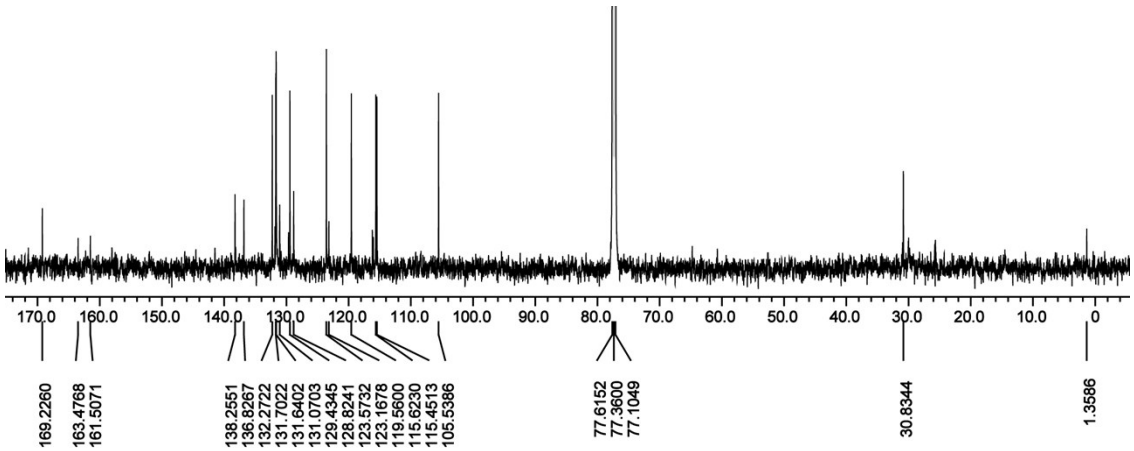
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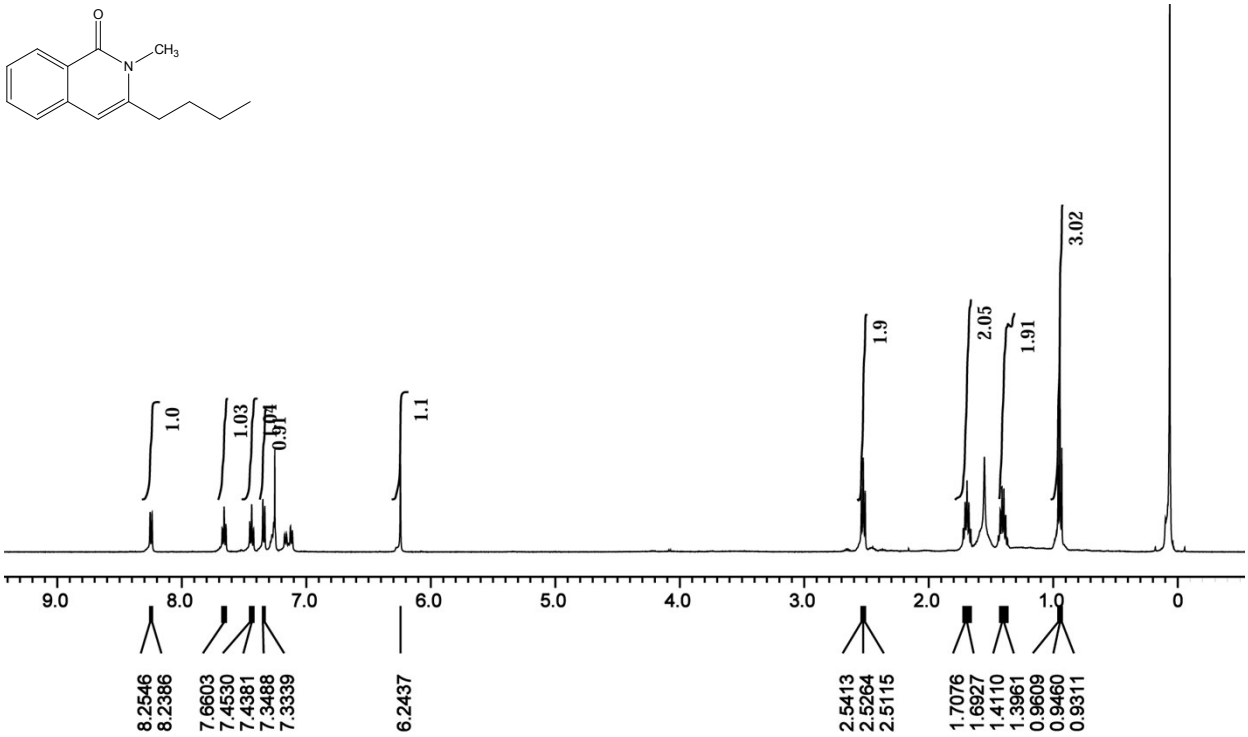
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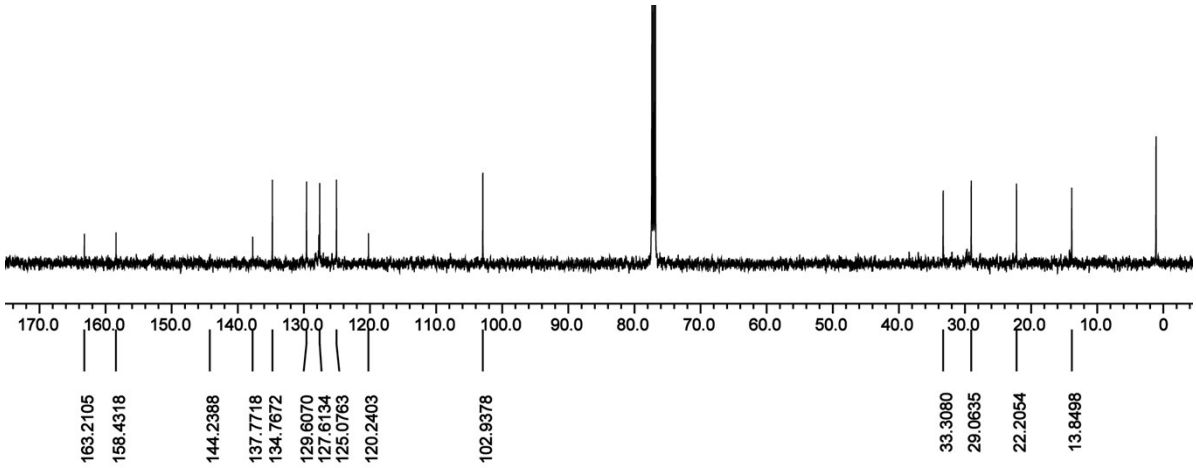
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