Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Rhodium(I)-catalysed Decarbonylative Direct C-H Vinylation and Dienylation of Arenes

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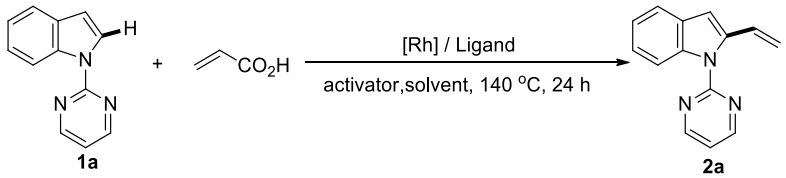
1. General information:

Unless otherwise noted, all experiments were carried out under nitrogen atmosphere, and all commercially available chemicals were used as received from Aldrich, Acros or Strem without further purification. All organic solvents were dried using standard, published methods and were distilled before use. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Model Avance DMX 400 Spectrometer (^{1}H 400 MHz and ^{13}C 100.6 MHz, respectively). Chemical shifts (δ) are given in ppm and are referenced to residual solvent peaks. *N*-(2-pyrimidyl)-indoles (**1a**-**n**),[1] 2-arylpyridines (**3a**-**p**),[2] 2-arylpyrimidine (**3s** and **3t**),[3] 3-phenylbenzo[*d*]isothiazole 1,1-dioxide (**3u**)[4], 6-arylpurine derivatives (**5a**-**e**)[5], [2-^{2}H]-1-(pyrimidin-2-yl)-1*H*-indole,[6] [Rh(CO)(DPPP)Cl]$_2$[7] and [Rh(DPPP)Cl][8] were prepared according to the previous reports.

2. Screening of reaction conditions

Table S1. Screening conditions for direct vinylation of indole **1a** with acrylic acid[a]

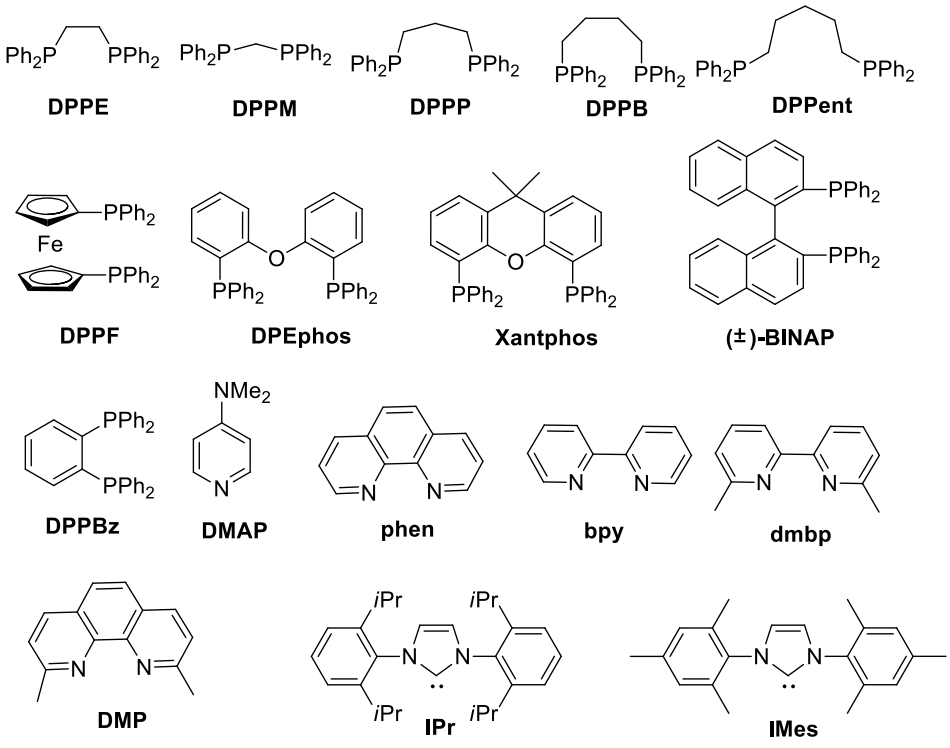


Entry	[Rh]	Ligand	Solvent	Activator	Yield(%)[b]
1	$[Rh(CO)_2Cl]_2$	none	toluene	(*t*BuCO)$_2$O	NR
2	$[Rh(COD)Cl]_2$	none	toluene	(*t*BuCO)$_2$O	NR
3	$[Rh(COD)_2]OTf$	none	toluene	(*t*BuCO)$_2$O	NR
4	$[Rh(COD)_2]BF_4$	none	toluene	(*t*BuCO)$_2$O	NR
5	$[Rh(NBD)Cl]_2$	none	toluene	(*t*BuCO)$_2$O	NR
6	$[Rh(NBD)_2]BF_4$	none	toluene	(*t*BuCO)$_2$O	NR
7	$[Rh(PPh_3)_3Cl]$	none	toluene	(*t*BuCO)$_2$O	NR
8	$[Rh(1,5\text{-}HD)Cl]_2$	none	toluene	(*t*BuCO)$_2$O	NR
9	$[Rh(C_2H_4)_2Cl]_2$	none	toluene	(*t*BuCO)$_2$O	NR
10	$[Rh(acac)(CO)_2]$	none	toluene	(*t*BuCO)$_2$O	NR
11	$[Rh(acac)(C_2H_4)_2]$	none	toluene	(*t*BuCO)$_2$O	NR
12	$[Rh(CO)_2Cl]_2$	DPPE	toluene	(*t*BuCO)$_2$O	20
13	$[Rh(CO)_2Cl]_2$	DPPM	toluene	(*t*BuCO)$_2$O	26
14	**$[Rh(CO)_2Cl]_2$**	**DPPP**	**toluene**	**(*t*BuCO)$_2$O**	**95**
15	$[Rh(CO)_2Cl]_2$	DPPB	toluene	(*t*BuCO)$_2$O	35
16	$[Rh(CO)_2Cl]_2$	DPPF	toluene	(*t*BuCO)$_2$O	68
17	$[Rh(CO)_2Cl]_2$	DPPent	toluene	(*t*BuCO)$_2$O	30
18	$[Rh(CO)_2Cl]_2$	DPEPhos	toluene	(*t*BuCO)$_2$O	43
19	$[Rh(CO)_2Cl]_2$	Xantphos	toluene	(*t*BuCO)$_2$O	52
20	$[Rh(CO)_2Cl]_2$	(±)-BINAP	toluene	(*t*BuCO)$_2$O	21
21	$[Rh(CO)_2Cl]_2$	DPPBz	toluene	(*t*BuCO)$_2$O	16

22	$[Rh(CO)_2Cl]_2$	PPh_3	toluene	$(tBuCO)_2O$	NR
23	$[Rh(CO)_2Cl]_2$	$P(2\text{-furyl})_3$	toluene	$(tBuCO)_2O$	NR
24	$[Rh(CO)_2Cl]_2$	$P(o\text{-tolyl})_3$	toluene	$(tBuCO)_2O$	NR
25	$[Rh(CO)_2Cl]_2$	$P(p\text{-tolyl})_3$	toluene	$(tBuCO)_2O$	NR
26	$[Rh(CO)_2Cl]_2$	$P(o\text{-MeOPh})_3$	toluene	$(tBuCO)_2O$	NR
27	$[Rh(CO)_2Cl]_2$	$P(p\text{-MeOPh})_3$	toluene	$(tBuCO)_2O$	NR
28	$[Rh(CO)_2Cl]_2$	$P(p\text{-}CF_3Ph)_3$	toluene	$(tBuCO)_2O$	NR
29	$[Rh(CO)_2Cl]_2$	$P(2\text{-furyl})_3$	toluene	$(tBuCO)_2O$	NR
30	$[Rh(CO)_2Cl]_2$	$P(C_6F_5)_3$	toluene	$(tBuCO)_2O$	NR
31	$[Rh(CO)_2Cl]_2$	PCy_3	toluene	$(tBuCO)_2O$	8
32	$[Rh(CO)_2Cl]_2$	$AsPh_3$	toluene	$(tBuCO)_2O$	NR
33	$[Rh(CO)_2Cl]_2$	pyridine	toluene	$(tBuCO)_2O$	NR
34	$[Rh(CO)_2Cl]_2$	DMAP	toluene	$(tBuCO)_2O$	NR
35	$[Rh(CO)_2Cl]_2$	phen	toluene	$(tBuCO)_2O$	16
36	$[Rh(CO)_2Cl]_2$	bpy	toluene	$(tBuCO)_2O$	21
37	$[Rh(CO)_2Cl]_2$	dmbp	toluene	$(tBuCO)_2O$	NR
38	$[Rh(CO)_2Cl]_2$	DMP	toluene	$(tBuCO)_2O$	NR
39	$[Rh(CO)_2Cl]_2$	IPr	toluene	$(tBuCO)_2O$	35
40	$[Rh(CO)_2Cl]_2$	IMes	toluene	$(tBuCO)_2O$	48
41	$[Rh(COD)Cl]_2$	DPPP	toluene	$(tBuCO)_2O$	39
42	$[Rh(COD)_2]OTf$	DPPP	toluene	$(tBuCO)_2O$	NR
43	$[Rh(COD)_2]BF_4$	DPPP	toluene	$(tBuCO)_2O$	NR
44	$[Rh(NBD)Cl]_2$	DPPP	toluene	$(tBuCO)_2O$	NR
45	$[Rh(NBD)_2]BF_4$	DPPP	toluene	$(tBuCO)_2O$	NR
46	$[Rh(PPh_3)_3Cl]$	DPPP	toluene	$(tBuCO)_2O$	NR
47	$[Rh(1,5\text{-HD})Cl]_2$	DPPP	toluene	$(tBuCO)_2O$	10
48	$[Rh(C_2H_4)_2Cl]_2$	DPPP	toluene	$(tBuCO)_2O$	NR
49	$[Rh(acac)(CO)_2]$	DPPP	toluene	$(tBuCO)_2O$	23
50	$[Rh(acac)(C_2H_4)_2]$	DPPP	toluene	$(tBuCO)_2O$	NR
51	$RhCl_3.3H_2O$	DPPP	toluene	$(tBuCO)_2O$	NR
52	$[Cp^*RhCl]_2$	DPPP	toluene	$(tBuCO)_2O$	11
53	$[(p\text{-cymene})_2RuCl_2]_2$	DPPP	toluene	$(tBuCO)_2O$	NR
54	$[RuCl_2(PPh_3)_3]$	DPPP	toluene	$(tBuCO)_2O$	NR
55	$[Cp^*IrCl_2]_2$	DPPP	toluene	$(tBuCO)_2O$	NR
56	$[IrCl(COD)]_2$	DPPP	toluene	$(tBuCO)_2O$	NR
57	$Pd(OAc)_2$	DPPP	toluene	$(tBuCO)_2O$	NR
58	$[Rh(CO)_2Cl]_2$	DPPP	DMF	$(tBuCO)_2O$	38
59	$[Rh(CO)_2Cl]_2$	DPPP	DMSO	$(tBuCO)_2O$	44
60	$[Rh(CO)_2Cl]_2$	DPPP	PhCl	$(tBuCO)_2O$	NR
61	$[Rh(CO)_2Cl]_2$	DPPP	THF	$(tBuCO)_2O$	65
62	$[Rh(CO)_2Cl]_2$	DPPP	1,4-Dioxane	$(tBuCO)_2O$	73
63	$[Rh(CO)_2Cl]_2$	DPPP	CH_3CN	$(tBuCO)_2O$	55
64	$[Rh(CO)_2Cl]_2$	DPPP	DCE	$(tBuCO)_2O$	NR
65	$[Rh(CO)_2Cl]_2$	DPPP	CH_2Cl_2	$(tBuCO)_2O$	NR

66	$[Rh(CO)_2Cl]_2$	DPPP	*p*-xylene	$(t\text{BuCO})_2O$	66
67	$[Rh(CO)_2Cl]_2$	DPPP	toluene	Ac_2O	38
68	$[Rh(CO)_2Cl]_2$	DPPP	toluene	Boc_2O	25
69	$[Rh(CO)_2Cl]_2$	DPPP	toluene	$(CF_3CO)_2O$	NR
70	$[Rh(CO)_2Cl]_2$	DPPP	toluene	$(MeOCO)_2O$	NR
71	$[Rh(CO)_2Cl]_2$	DPPP	ttoluene	*t*BuCOCl	24
72[c]	$[Rh(CO)_2Cl]_2$	DPPP	toluene	$(t\text{BuCO})_2O$	77
73[d]	$[Rh(CO)_2Cl]_2$	DPPP	toluene	$(t\text{BuCO})_2O$	51
74[e]	$[Rh(CO)_2Cl]_2$	DPPP	toluene	$(t\text{BuCO})_2O$	93
75	$[Rh(CO)_2Cl]_2$	DPPP	toluene	none	NR
76	none	DPPP	toluene	$(t\text{BuCO})_2O$	NR

[a] Reaction Conditions: **1a** (0.5 mmol.), acrylic acid (0.6 mmol), [Rh] (4.0 mol%), ligand (6.0 mol%), activator (0.6 mmol), solvent (3.0 mL), 140 °C, 24 h, NR: no reaction. [b] Isolated yield. [c] Reaction temperature 120 °C. [d] $[Rh(CO)_2Cl]_2$ (1.0 mol%) and DPPP (1.5 mol%) were used. [e] acrylic acid (1.5 mmol) and $(t\text{BuCO})_2O$ (1.8 mmol) were used, but no double (C2 and C7) vinylation was observed.



3. The general procedure for the direct olefination of arenes

(a) Direct vinylation of arenes with acrylic acid

To an oven-dried pressure tube were sequentially added indole **1** (0.5 mmol), $[Rh(CO)_2Cl]_2$ (7.8 mg, 4.0 mol%), DPPP (12.4 mg, 6.0 mol%), acrylic acid (43.3 mg, 0.6 mmol), $(t\text{BuCO})_2O$ (111.8 mg, 0.6 mmol) and anhydrous toluene (3.0 mL). After being degassed three times, the tube was heated and stirred vigorously at 140 °C for 24 h in the oil bath under nitrogen atmosphere. Then the tube was removed from the oil bath and cooled to room temperature. The solvent was removed by vacuum evaporation, and the residue was purified by column chromatography on silica gel

using a mixture of ethyl acetate and hexane to give the pure product.

To an oven-dried pressure tube were sequentially added indole **1a** (1.17 g, 6.0 mmol), $[Rh(CO)_2Cl]_2$ (93.3 mg, 4.0 mol%), DPPP (148.5 mg, 6.0 mol%), acrylic acid (518.8 mg, 7.2 mmol), $(t\text{BuCO})_2O$ (1.34 g, 7.2 mmol) and anhydrous toluene (30.0 mL). After being degassed three times, the tube was heated and stirred vigorously at 140 °C for 24 h in the oil bath under nitrogen atmosphere. Then the tube was removed from the oil bath and cooled to room temperature. The solvent was removed by vacuum evaporation, and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure product **2a** (1.18 g, 89% yield).

1-(Pyrimidin-2-yl)-2-vinyl-1*H*-indole (2a), white solid, mp: 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.28 (dd, *J* = 11.0, 1.5 Hz, 1H), 5.79 (dd, *J* = 17.4, 1.5 Hz, 1H), 6.80 (s, 1H), 6.96 (d, *J* = 10.5 Hz, 1H), 7.17-7.19 (m, 1H), 7.20-7.22 (m, 1H), 7.22-7.24 (m, 1H), 7.55 (d, *J* = 6.04 Hz, 1H), 8.23 (d, *J* = 5.4 Hz, 1H), 8.82 (d, *J* = 3.2 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 108.0, 116.0, 117.0, 117.7, 118.0, 123.1, 127.3, 127.5, 130.2, 134.6, 139.4, 158.1, 158.2; HRMS (ESI) calcd. for $C_{14}H_{12}N_3$ $[M+H]^+$: 222.1026, found: 222.1036.

5-Methoxy-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2b), white solid, mp: 118-119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.89 (s, 3H), 5.30 (dd, *J* = 11.1, 1.5 Hz, 1H), 5.80 (dd, *J* = 17.4, 1.5 Hz, 1H), 6.86 (s, 1H), 6.90 (d, *J* = 2.6 Hz, 1H), 7.06 (d, *J* = 2.5 Hz, 1H), 7.16-7.18 (m, 1H), 7.24-7.27 (m, 1H), 8.26 (d, *J* = 9.1 Hz, 1H), 8.82 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 55.7, 107.1, 115.9, 116.9, 117.7, 118.1, 123.1, 127.4, 130.2, 134.6, 139.4, 158.1, 158.2; HRMS (ESI) calcd. for $C_{15}H_{14}N_3O$ $[M+H]^+$: 252.1131, found: 252.1144.

5-Methyl-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2c), white solid, mp: 106-107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.58 (s, 3H), 5.40 (dd, *J* = 11.1, 1.5 Hz, 1H), 5.91 (dd, *J* = 17.5, 1.5 Hz, 1H), 7.00 (s, 1H), 7.31-7.36 (m, 3H), 7.60 (d, *J* = 7.9 Hz, 1H), 8.2 (s, 1H), 8.97 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 21.5, 108.0, 115.9, 116.9, 117.7, 118.2, 123.2, 127.4, 130.2, 134.6, 139.5, 158.1, 158.2; HRMS (ESI) calcd. For $C_{15}H_{14}N_3$ $[M+H]^+$: 236.1182, found: 236.1171.

5-Fluoro-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2d), yellow solid, mp: 110-111 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.35 (dd, *J* = 11.0, 1.4 Hz, 1H), 5.87 (dd, *J* = 17.4, 1.4 Hz, 1H), 6.64 (d, *J* = 3.2 Hz, 1H), 7.03-7.05 (m, 2H), 7.25-7.27 (m, 2H), 8.30 (d, *J* = 3.3 Hz, 1H), 8.67 (d, *J* = 4.6 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 107.9, 115.4, 116.8, 117.5, 121.3, 122.5, 125.4, 125.5, 130.7, 135.0, 139.0, 158.1, 158.4; HRMS (ESI) calcd. for $C_{14}H_{11}FN_3$ $[M+H]^+$: 240.0932, found: 240.0944.

5-Chloro-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2e), yellow solid, mp: 122-123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.30 (d, *J* = 10.9 Hz, 1H), 5.83 (d, *J* = 17.4 Hz, 1H), 6.63-6.64 (m, 1H), 7.05-7.08 (m, 1H), 7.26-7.29 (m, 2H), 7.57 (d, *J* = 2.1 Hz, 1H), 8.29 (d, *J* = 3.4 Hz, 1H), 8.69 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 107.9, 115.8, 116.9, 117.9, 118.3, 123.0, 127.2, 127.4, 130.1, 134.5, 139.3, 158.0, 158.1; HRMS (ESI) calcd. for $C_{14}H_{11}ClN_3$ $[M+H]^+$: 256.0636, found: 256.0628.

5-Bromo-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2f), white solid, mp: 128-129 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.35 (dd, *J* = 11.1, 1.4 Hz, 1H), 5.84 (dd, *J* = 17.4, 1.4 Hz, 1H), 6.90 (s, 1H), 7.21-7.24 (m, 2H), 7.56-7.57 (m, 2H), 8.25 (d, *J* = 8.9 Hz, 1H), 8.84 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 108.0, 115.9, 117.0, 117.7, 118.0, 123.1, 127.3, 127.5, 130.2, 134.6, 139.4, 158.1, 158.2; HRMS (ESI) calcd. for $C_{14}H_{11}BrN_3$ $[M+H]^+$: 300.0131, found: 300.0122.

Methyl 1-(pyrimidin-2-yl)-2-vinyl-1H-indole-5-carboxylate (2g), white solid, mp: 98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.97 (s, 3H), 5.36 (dd, *J* = 11.1, 1.5 Hz, 1H), 5.87 (dd, *J* = 17.4, 1.4 Hz, 1H), 6.98 (s, 1H), 7.25-7.27 (m, 3H), 7.97 (dd, J = 8.8, 1.7 Hz, 1H), 8.29 (d, *J* = 8.8 Hz, 1H), 8.88 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 51.1, 107.9, 115.8, 116.9, 117.8, 118.3, 123.0, 127.2, 127.4, 130.1, 134.5, 141.3, 158.1, 158.3, 167.3; HRMS (ESI) calcd. for $C_{16}H_{14}N_3O_2$ $[M+H]^+$: 280.1081, found: 280.1092.

5-Nitro-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2h), 49% yield, 133-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.40 (dd, *J* = 11.1, 1.5 Hz, 1H), 5.92 (dd, *J* = 17.4, 1.5 Hz, 1H), 7.00 (s, 1H), 7.31-7.36 (m, 3H), 7.60 (d, *J* = 7.9 Hz, 1H), 8.22 (s, 1H), 8.97 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 107.7, 115.4, 116.7, 117.5, 121.3, 122.5, 125.4, 125.5, 130.7, 135.1, 139.1, 158.1, 158.4; HRMS (ESI) calcd. for $C_{14}H_{11}N_4O_2$ $[M+H]^+$: 267.0877, found: 267.0863.

6-Methyl-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2i), white solid, mp: 88-89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.51 (s, 3H), 5.28 (dd, *J* = 11.04, 1.48 Hz, 1H), 5.80 (dd, *J* = 17.44, 1.48 Hz, 1H), 6.88 (s, 1H), 7.06-7.08 (m, 1H), 7.19-7.24 (m, 2H), 7.49 (d, *J* = 7.96 Hz, 1H), 8.10 (s, 1H), 8.85 (d, *J* = 4.80 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 21.2, 111.9, 115.0, 115.8, 116.9, 117.9, 118.2, 123.0, 127.3, 130.3, 134.5, 140.8, 158.1, 158.2; HRMS (ESI) calcd. For $C_{15}H_{14}N_3$ $[M+H]^+$: 236.1182, found: 236.1169.

7-Methyl-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2j), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.50 (s, 3H), 5.28 (dd, *J* = 11.04, 1.48 Hz, 1H), 5.80 (dd, *J* = 17.4, 1.48 Hz, 1H), 6.88 (s, 1H), 7.06-7.08 (m, 1H), 7.19-7.24 (m, 2H), 7.49 (d, *J* = 7.9 Hz, 1H), 8.10 (s, 1H), 8.85 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 19.9, 113.7, 115.5, 116.8, 118.8, 121.8, 123.9, 128.8, 130.7, 133.9, 136.2, 144.1, 158.1, 158.2; HRMS (ESI) calcd. for $C_{15}H_{14}N_3$ $[M+H]^+$: 236.1182, found: 236.1188.

4-Methyl-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2k), white solid, mp: 98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 5.25 (dd, *J* = 11.1, 1.5 Hz, 1H), 5.77 (dd, *J* = 17.4, 1.5Hz, 1H), 6.86 (s, 1H), 7.05 (d, *J* = 8.8 Hz, 1H), 7.16-7.21 (m, 2H), 7.45-7.48 (m, 1H), 8.08 (s, 1H), 8.82 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 20.0, 111.9, 115.9, 116.3, 118.0, 118.4, 123.0, 127.2, 127.9, 130.7, 134.5, 140.3, 158.2, 158.3; HRMS (ESI) calcd. for $C_{15}H_{14}N_3$ $[M+H]^+$: 236.1182, found: 236.1196.

3-Methyl-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2l), yellow solid, mp: 132-133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 5.42-5.49 (m, 2H), 7.05 (dd, *J* = 17.67, 11.5 Hz, 1H), 7.12 (t, *J* = 4.7 Hz, 1H), 7.21-7.30 (m, 2H), 7.57-7.59 (m, 1H), 8.27 (d, *J* = 7.8 Hz, 1H), 8.78 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 10.3, 113.7, 115.5, 116.7, 118.8, 123.9, 128.9, 130.7, 133.9, 136.2, 158.1, 158.2; HRMS (ESI) calcd. for $C_{15}H_{14}N_3$ $[M+H]^+$: 236.1182, found: 236.1171.

3-Phenyl-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2m), colorless oil; ^{1}H NMR (400

MHz, $CDCl_3$) δ 5.09 (dd, *J* = 17.8, 1.4 Hz, 1H), 5.23 (dd, *J* = 11.6, 1.3 Hz, 1H), 7.05 (dd, *J* = 17.8, 11.6 Hz, 1H), 7.22-7.26 (m, 2H), 7.30-7.42 (m, 2H), 7.48-7.58 (m, 5H), 8.15 (d, *J* = 8.4 Hz, 1H), 8.88 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 116.8, 118.9, 119.7, 121.6, 122.4, 124.3, 126.4, 127.0, 127.6, 128.7, 129.8, 130.6, 133.2, 133.7, 134.8, 137.3, 137.6, 158.1, 158.2; HRMS (ESI) calcd. for $C_{20}H_{16}N_3$ $[M+H]^+$: 298.1339, found: 298.1348.

3-Bromo-1-(pyrimidin-2-yl)-2-vinyl-1H-indole (2n), colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 5.08 (dd, *J* = 17.8, 1.4 Hz, 1H), 5.23 (dd, *J* = 11.6, 1.3 Hz, 1H), 7.05 (dd, *J* = 17.8, 11.6 Hz, 1H), 7.10-7.34 (m, 1H), 7.39-7.42 (m, 1H), 7.48-7.51 (m, 2H), 8.15 (d, *J* = 8.4 Hz, 1H), 8.89 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 113.5, 115.3, 116.7, 118.7, 121.7 123.8, 128.7, 130.6, 133.8, 136.1, 138.1, 158.0, 158.1; HRMS (ESI) calcd. for $C_{14}H_{11}BrN_3$ $[M+H]^+$: 300.0131, found: 300.0142.

2-(2-Vinylphenyl)pyridine (4a)[9], colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 5.24 (d, *J* = 11.0 Hz, 1H), 5.62 (d, *J* = 17.4 Hz, 1H), 6.82 (dd, *J* = 17.4, 11.0 Hz, 1H), 7.29-7.31 (m, 1H), 7.36-7.41 (m, 2H), 7.44 (d, *J* = 7.2 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.66 (d, *J* = 7.4 Hz, 1H), 8.72-8.75 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 115.4, 118.7, 121.8, 124.8, 125.0, 126.2, 127.8, 128.6, 130.0, 135.6, 136.1, 139.3, 149.2; HRMS (ESI) calcd. for $C_{13}H_{12}N$ $[M+H]^+$: 182.0964, found: 182.0972.

2-(2-Methoxy-6-vinylphenyl)pyridine (4b), yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 3.75 (s, 3H), 5.13 (dd, *J* = 11.0, 0.9 Hz, 1H), 5.66 (dd, *J* = 17.5, 0.9 Hz, 1H), 6.38 (dd, *J* = 17.4, 11.0 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 7.32 (s, 1H), 7.34-7.35 (m, 1H), 7.39-7.40 (m, 1H), 7.70-7.73 (m, 1H), 7.76-7.77 (m, 1H), 8.77 (d, J = 4.9 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 55.6, 111.4, 115.5, 118.3, 121.0, 121.7, 125.1, 126.2, 129.1, 129.9, 131.2, 135.6, 139.0, 149.4; HRMS (ESI) calcd. for $C_{14}H_{14}NO$ $[M+H]^+$: 212.1070, found: 212.1056.

2-(5-Methoxy-2-vinylphenyl)pyridine (4c), colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 3H), 5.14 (dd, *J* = 11.0, 1.2 Hz, 1H), 5.63 (d, *J* = 17.4, 1.2 Hz, 1H), 6.76 (dd, *J* = 17.4, 11.0 Hz, 1H), 6.96-6.99 (m, 1H), 7.05 (d, *J* = 2.7 Hz, 1H), 7.27-7.29 (m, 1H), 7.43-7.45 (m, 1H), 7.61 (d, *J* = 8.6 Hz, 1H), 7.74 (d, *J* = 1.4 Hz, 1H), 8.73-8.75 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 55.4, 108.2, 113.3, 114.3, 115.1, 121.9, 125.0, 127.4, 129.1, 130.6, 135.0, 135.9, 139.9, 149.6; HRMS (ESI) calcd. for $C_{14}H_{14}NO$ $[M+H]^+$: 212.1070, found: 212.1062.

2-(5-Methyl-2-vinylphenyl)pyridine (4d)[10], colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 2.42 (s, 3H), 5.21 (dd, *J* = 11.0, 1.1 Hz, 1H), 5.71 (dd, J = 17.5, 1.1 Hz, 1H), 6.82 (dd, *J* = 17.4, 11.0 Hz, 1H), 7.22-7.28 (m, 2H), 7.36 (s, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.71-7.76 (m, 1H), 8.74 (dd, *J* = 4.8, 0.7 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 21.1, 114.4, 121.7, 125.0, 126.1, 129.4, 130.5, 133.2, 135.4, 135.8, 137.6, 139.2, 149.4, 158.9; HRMS (ESI) calcd. for $C_{14}H_{14}N$ $[M+H]^+$: 196.1121, found:196.1112.

2-(4-Methoxy-2-vinylphenyl)pyridine (4e), colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 3.91 (s, 3H), 5.28 (d, *J* = 10.9 Hz, 1H), 5.75 (d, *J* = 17.5 Hz, 1H), 6.87 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.95 (dd, *J* = 8.5, 2.6 Hz, 1H), 7.18 (d, *J* = 2.6 Hz, 1H), 7.23-7.26 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.71-7.75 (m,

1H), 8.71 (d, *J* = 4.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 55.3, 111.1, 113.7, 114.1, 115.4, 119.8, 121.4, 124.9, 128.2, 131.4, 135.8, 136.6, 149.5; HRMS (ESI) calcd. for $C_{14}H_{14}NO$ $[M+H]^+$: 212.1070, found: 212.1058.

2-(4-methyl-2-vinylphenyl)pyridine (4f), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.42 (s, 3H), 5.27 (d, *J* = 11.0 Hz, 1H), 5.74 (d, *J* = 17.4 Hz, 1H), 6.87 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.95 (dd, *J* = 8.4, 2.5 Hz, 1H), 7.16-7.21 (m, 3H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.49 (d, *J* = 8.5 Hz, 1H), 8.71 (d, *J* = 4.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 20.4, 111.1, 113.6, 114.1, 115.3, 119.7, 121.3, 124.8, 128.1, 131.4, 135.8, 136.6, 149.5; HRMS (ESI) calcd. for $C_{14}H_{14}N$ $[M+H]^+$: 196.1121, found: 196.1134

2-(3-Vinyl-[1,1'-biphenyl]-4-yl)pyridine (4g), yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.32 (d, *J* = 1.1 Hz, 1H), 5.35 (d, *J* = 1.1 Hz, 1H), 6.96 (dd, *J* = 17.5, 11.0 Hz, 1H), 7.25-7.30 (m, 2H), 7.64 (d, *J* = 1.0 Hz, 2H), 7.69~7.72 (m, 4H), 7.76~7.78 (m, 2H), 7.92 (s, 1H), 8.72~8.76 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 115.6, 120.5, 121.8, 122.1, 123.8, 125.0, 125.1, 126.7, 127.1, 127.2, 128.9, 130.6, 135.8, 136.0, 136.8, 138.3, 149.5; HRMS (ESI) calcd. for $C_{19}H_{16}N$ $[M+H]^+$: 258.1277, found: 258.1286.

2-(4-Fluoro-2-vinylphenyl)pyridine (4h), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.32 (d, *J* = 11.0 Hz, 1H), 5.75 (d, *J* = 17.6 Hz, 1H), 6.81 (dd, *J* = 17.6, 9.6 Hz, 1H), 7.06-7.11 (m, 1H), 7.34-7.37 (m, 1H), 7.41-7.43 (m, 1H), 7.50-7.52 (m, 1H), 7.79 (d, *J* = 1.8 Hz, 2H), 8.7 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 115.3, 120.6, 122.1, 123.3, 124.9, 126.5, 126.9, 128.5, 128.8, 130.0, 134.0, 136.7, 149.7; HRMS (ESI) calcd. for $C_{13}H_{11}FN$ $[M+H]^+$: 200.0870, found: 200.0883

2-(4-Chloro-2-vinylphenyl)pyridine (4i), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.29 (d, *J* = 11.0 Hz, 1H), 5.73 (d, *J* = 17.6 Hz, 1H), 6.80 (dd, *J* = 17.6, 9.6 Hz, 1H), 7.03-7.08 (m, 1H), 7.32-7.40 (m, 2H), 7.46-7.49 (m, 1H), 7.76 (d, *J* = 1.7 Hz, 2H), 8.7 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 115.0, 121.8, 123.1, 124.7, 126.3, 126.7, 128.3, 128.5, 128.7, 129.7, 133.7, 136.5, 149.4; HRMS (ESI) calcd. for $C_{13}H_{11}ClN$ $[M+H]^+$: 216.0575, found: 216.0560.

(*E*)-2-(4-Bromo-2-vinylphenyl)pyridine (4j), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.29 (d, *J* = 11.0 Hz, 1H), 5.73 (d, *J* = 17.6 Hz, 1H), 6.80 (dd, *J* = 17.6, 9.6 Hz, 1H), 7.03-7.09 (m, 1H), 7.32-7.35 (m, 2H), 7.39 (d, J = 7.7 Hz, 1H), 7.46-7.50 (m, 1H), 7.77 (d, *J* = 1.7 Hz, 1H), 8.67 (d, *J* = 4.7 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 115.0, 121.9, 123.1, 124.7, 126.3, 126.7, 128.3, 128.5, 128.7, 129.7, 133.6, 136.5, 149.5; HRMS (ESI) calcd. for $C_{13}H_{11}BrN$ $[M+H]^+$: 260.0069, found: 260.0081.

Methyl-4-(pyridin-2-yl)-3-vinylbenzoate (4k), yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.92 (s, 3H), 5.29 (d, *J* = 11.0 Hz, 1H), 5.73 (d, *J* = 17.6 Hz, 1H), 6.80 (dd, *J* = 17.1, 9.4 Hz, 1H), 7.04-7.09 (m, 1H), 7.32-7.40 (m, 2H), 7.40-7.50 (m, 1H), 7.77 (d, *J* = 1.7 Hz, 2H), 8.70 (d, *J* = 6.1 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 53.2, 112.6, 115.4, 120.7, 121.8, 124.8, 126.2, 127.8, 128.6, 130.0, 135.6, 136.4, 139.6, 149.2, 167.1; HRMS (ESI) calcd. for $C_{15}H_{14}NO_2$ $[M+H]^+$: 240.1019, found: 240.1027.

4-(Pyridin-2-yl)-3-vinylbenzonitrile (4l), brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.28 (d, *J* = 11.6 Hz, 1H), 5.74 (d, *J* = 17.4 Hz, 1H), 6.87 (dd, *J* = 17.4, 11.0 Hz, 1H), 6.94 (dd, *J* = 8.4, 2.6 Hz, 1H), 7.14 -7.26 (m, 2H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.49 (d, *J*

= 8.5 Hz, 1H), 7.71-7.75 (m, 1H), 8.71 (d, *J* = 4.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 110.1, 113.7, 114.0, 115.3, 120.7, 121.2, 124.9, 128.2, 131.5, 135.8, 136.6, 140.5, 149.2, 152.1; HRMS (ESI) calcd. for $C_{14}H_{11}N_2$ $[M+H]^+$: 207.0917, found: 207.0922.

2-(4-Acetyl-2-vinylphenyl)pyridine (4m), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.60 (s, 3H), 5.25 (m, 1H), 5.76 (d, *J* = 17.4 Hz, 1H), 6.77 (dd, *J* = 17.4, 11.0 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.70-7.73 (m, 2H), 7.86 (dd, *J* = 8.0, 1.8 Hz, 1H), 8.16 (d, *J* = 1.6 Hz, 1H), 8.67 (d, *J* = 4.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 53.2, 112.6, 115.4, 120.7, 121.8, 124.8, 126.2, 127.8, 128.6, 130.0, 135.6, 136.4, 139.6, 149.2, 167.1; HRMS (ESI) calcd. for $C_{15}H_{14}NO$ $[M+H]^+$: 224.1070, found: 224.1058.

4-(Pyridin-2-yl)-3-vinylbenzaldehyde (4n), yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.27 (d, *J* = 11.4 Hz, 1H), 5.73 (d, *J* = 17.6 Hz, 1H), 6.88 (dd, *J* = 17.4, 10.8 Hz, 1H), 6.95 (dd, *J* = 8.5, 2.6 Hz, 1H), 7.16-7.21 (m, 3H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 8.5 Hz,1H), 8.70 (d, *J* = 4.8 Hz, 1H), 9.99 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 111.0, 113.7, 114.1, 115.9, 120.2, 121.8, 124.6, 128.3, 131.4, 135.7, 136.6, 140.1, 150.1, 198.8; HRMS (ESI) calcd. for $C_{14}H_{14}NO$ $[M+H]^+$: 212.1070, found: 212.1062.

2-(3-Vinylnaphthalen-2-yl)pyridine (4o), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.30 (d, *J* = 12.0 Hz, 1H), 5.83 (d, *J* = 17.4 Hz, 1H), 6.94 (dd, *J* = 10.9, 6.5 Hz, 1H), 7.28-7.31 (m, 1H), 7.45-7.55 (m, 3H), 7.76-7.80 (m, 2 H), 7.87 (t, *J* = 8.9 Hz, 1H), 7.98 (s, 1H), 8.09 (s, 1H), 8.76 (d, *J* = 4.80 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 114.9, 120.5, 123.3, 125.3, 127.6, 128.2, 128.3, 128.4, 128.9, 132.4, 133.6, 134.5, 134.6, 135.6, 137.6, 147.9; HRMS (ESI) calcd. for $C_{17}H_{14}N$ $[M+H]^+$: 232.1121, found: 232.1115.

5-Methyl-2-(2-vinylphenyl)pyridine (4p), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 5.24 (d, *J* = 11.0 Hz, 1H), 5.82 (d, *J* = 17.4 Hz, 1H), 6.42 (dd, *J* = 17.4, 11.0 Hz, 1H), 7.30-7.37 (m, 2H), 7.41-7.54 (m, 3H), 7.86 (d, *J* = 7.4 Hz, 1H), 8.72 (d, *J* = 4.9 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 18.2, 115.4, 119.9, 127.3, 128.5, 128.6, 131.6, 133.9, 137.4, 139.1, 141.6, 149.8, 154.6; HRMS (ESI) calcd. for $C_{14}H_{14}N$ $[M+H]^+$: 196.1121, found: 196.1130.

Pyridin-2-yl(2-vinylphenyl)methanone (4q), red oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.15 (dd, *J* = 11.0, 1.0 Hz, 1H), 5.59 (dd, *J* = 17.4, 1.0 Hz, 1H), 6.78 (dd, *J* = 17.4, 11.0 Hz, 1H), 7.28-7.30 (m, 1H), 7.40-7.41 (m, 1H), 7.42-7.43 (m, 2H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.84 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.97-7.99 (m, 1H), 8.03 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 114.2, 123.5, 125.9, 127.0, 127.1, 127.9, 128.2, 128.5, 131.5, 132.1, 134.2, 136.8, 160.9, 167.5; HRMS (ESI) calcd. for $C_{14}H_{12}NO$ $[M+H]^+$: 210.0913, found: 210.0922.

10-Vinylbenzo[h]quinoline (4r)[11], white soild, mp: 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.29 (d, *J* = 11.0 Hz, 1H), 5.73 (d, *J* = 17.4 Hz, 1H), 7.04 (d, *J* = 9.3 Hz, 1H), 7.24 (d, *J* = 7.9 Hz, 1H), 7.62 (d, *J* = 6.5 Hz, 1H), 7.89-7.91 (m, 2H), 8.00 (dd, *J* = 9.2, 1.0 Hz, 1H), 8.11 (d, *J* = 9.3 Hz, 1H), 8.20-8.23 (m, 1H), 8.74 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 115.9, 120.2, 121.5, 122.1, 124.5, 126.4, 127.5, 128.2, 128.9, 129.2, 130.9, 135.6, 138.3, 147.9; HRMS (ESI) calcd. for $C_{15}H_{12}N$

$[M+H]^+$: 206.0964, found: 206.0976.

2-(2-Vinylphenyl)pyrimidine (4s), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.29 (d, *J* = 8.0 Hz, 1H), 5.72 (d, *J* = 16.6 Hz, 1H), 6.48-6.49 (m, 1H), 7.12-7.15 (m, 2H), 7.25-7.28 (m, 2H), 7.76 (d, *J* = 3.0 Hz, 1H), 8.57 (s, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 116.4, 124.1, 125.1, 127.9, 128.5, 130.0, 132.4, 133.9, 136.0, 139.3, 158.3; HRMS (ESI) calcd. for $C_{12}H_{11}N_2$ $[M+H]^+$: 183.0917, found: 183.0930.

2-(3-Vinylthiophen-2-yl)pyrimidine (4t), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.16 (dd, *J* = 10.9, 0.8 Hz, 1H), 5.64 (dd, *J* = 17.4, 0.8 Hz, 1H), 6.35 (dd, *J* = 17.4, 11.0 Hz, 1H), 7.33 (t, *J* = 4.96 Hz, 1H), 7.41-7.44 (m, 1H), 7.60 (d, *J* = 7.76 Hz, 1H), 8.91 (d, *J* = 4.96 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 116.0, 119.0, 121.7, 125.1, 128.9, 134.6, 136.4, 136.7, 157.0, 167.4; HRMS (ESI) calcd. for $C_{10}H_9N_2S$ $[M+H]^+$: 189.0481, found: 189.0466.

3-(2-Vinylphenyl)benzo[d]isothiazole 1,1-dioxide (4u)[11], white solid, mp : 86-87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.28 (d, *J* = 11.0 Hz, 1H), 5.71 (d, *J* = 17.6 Hz, 1H), 6.18 (m, 1H), 7.45-7.48 (m, 2H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.78 (t, *J* = 7.6 Hz, 2H), 7.99 (d, *J* = 7.5 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 118.5, 122.7, 126.6, 126.7, 127.9, 128.5, 129.3, 131.4, 131.8, 133.5, 133.7, 133.8, 137.4, 140.2, 172.8; HRMS (ESI) calcd. for $C_{15}H_{12}NO_2S$ $[M + H]^+$: 270.0583, found: 270.0596.

9-Isopropyl-6-(2-vinylphenyl)-9H-purine (6a), colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.69 (d, *J* = 6.8 Hz, 6H), 4.97-5.01 (m, 1H), 5.23 (d, *J* = 19.4 Hz, 1H), 5.79 (d, *J* = 11.4 Hz, 1H), 6.95-7.02 (m, 1H), 7.43-7.52 (m, 2H), 7.78-7.80 (m, 2H), 8.12 (s, 1H), 9.08 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 22.6, 47.4, 115.4, 126.3, 127.6, 129.9, 131.2, 132.4, 133.9, 135.4, 136.7, 144.8, 152.1, 152.2, 158.1; HRMS (ESI) calcd. for $C_{16}H_{17}N_4$ $[M+H]^+$: 265.1448, found: 265.1454.

9-Isopropyl-6-(4-methoxy-2-vinylphenyl)-9H-purine (6b), colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.69 (d, *J* = 6.8 Hz, 6H), 3.90 (s, 3H), 4.96-5.00 (m, 1H), 5.24 (d, *J* = 11.7 Hz, 1H), 5.76 (d, *J* = 16.7 Hz, 1H), 6.98-7.00 (m, 1H), 7.04-7.08 (m, 1H), 7.27 (d, *J* = 2.6 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 8.13 (s, 1H), 9.02 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 22.6, 47.4, 55.4, 111.6, 113.5, 115.3, 126.8, 132.7, 133.1, 135.6, 138.8, 142.0, 151.5, 151.8, 157.7, 160.9; HRMS (ESI) calcd. for $C_{17}H_{19}N_4O$ $[M+H]^+$: 295.1553, found: 295.1570.

6-(4-Chloro-2-vinylphenyl)-9-isopropyl-9H-purine (6c), colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.69 (d, *J* = 6.8 Hz, 6H), 4.97-5.01 (m, 1H), 5.27 (d, *J* = 11.0 Hz, 1H), 5.78 (d, *J* = 17.5 Hz, 1H), 6.93-6.98 (m, 1H), 7.40 (dd, *J* = 10.4, 2.1 Hz, 1H), 7.74-7.76 (m, 2H), 8.15 (s, 1H), 9.04 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 22.5, 47.6, 116.5, 126.3, 127.7, 132.3, 132.6, 132.7, 134.3, 136.1, 138.7, 142.6, 151.7, 151.9, 156.7; HRMS (ESI) calcd. for $C_{16}H_{16}ClN_4$ $[M+H]^+$: 299.1058, found: 299.1076.

9-Butyl-6-(2-vinylphenyl)-9H-purine (6d), brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (t, *J* = 7.4 Hz, 3H), 1.40-1.49 (m, 2H), 1.94-2.01 (m, 2H), 4.34 (t, *J* = 7.3 Hz, 2H), 5.24 (d, *J* = 11.0 Hz, 1H), 5.78 (d, *J* = 17.4 Hz, 1H), 6.95-7.02 (m, 1H), 7.43-7.52 (m, 2H), 7.80 (t, *J* = 6.2 Hz, 2H), 8.10 (s, 1H), 9.09 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 13.5, 20.0, 32.0, 43.8, 115.3, 126.2, 127.6, 129.9, 131.2,

132.4, 133.9, 135.2, 136.8, 144.7, 152.0, 152.1, 157.9; HRMS (ESI) calcd. for $C_{17}H_{19}N_4$ $[M+H]^+$: 279.1604, found: 279.1594.

9-Benzyl-6-(2-vinylphenyl)-9H-purine (6e), brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.24 (d, *J* = 11.0 Hz, 1H), 5.52 (s, 2H), 5.79 (d, *J* = 17.4 Hz, 1H), 6.96-7.03 (m, 1H), 7.36-7.53 (m, 7H), 7.80 (t, *J* = 6.0 Hz, 2H), 8.10 (s, 1H), 9.13 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 47.4, 115.3, 126.3, 127.6, 128.0, 128.7, 129.2, 129.9, 131.2, 133.8, 135.1, 135.2, 136.9, 144.5, 152.0, 152.4, 158.1; HRMS (ESI) calcd. for $C_{20}H_{17}N_4$ $[M+H]^+$: 313.1448, found: 313.1454.

(b) Direct dienylation of arenes with (*E*)-penta-2,4-dienoic acid

To an oven-dried pressure tube were sequentially added indole **1a** (97.5 mg, 0.5 mmol), $[Rh(CO)_2Cl]_2$ (7.8 mg, 4.0 mol%), BINAP (18.7 mg, 6.0 mol%), (*E*)-penta-2,4-dienoic acid (58.9 mg, 0.6 mmol), (*t*BuCO)$_2$O (111.8 mg, 0.6 mmol) and anhydrous toluene (3.0 mL). After being degassed three times, the tube was heated and stirred vigorously at 140 °C for 24 h in the oil bath under nitrogen atmosphere. Then the tube was removed from the oil bath and cooled to room temperature. The solvent was removed by vacuum evaporation, and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure product.

(*E*)-2-(Buta-1,3-dien-1-yl)-1-(pyrimidin-2-yl)-1H-indole (7a), white solid, mp: 166-167 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.18 (d, *J* = 9.9 Hz, 1H), 5.35 (d, *J* = 16.6 Hz, 1H), 5.94-6.04 (m, 1H), 6.30-6.36 (m, 1H), 6.93 (s, 1H), 7.20-7.27 (m, 4H), 7.61 (d, *J* = 7.3 Hz, 1H), 8.31 (d, *J* = 8.2 Hz, 1H), 8.85 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 105.0, 115.8, 117.0, 117.7, 118.0, 123.1, 127.3, 127.5, 130.2, 131.5, 134.6, 137.4, 139.4, 158.1, 158.2; HRMS (ESI) calcd. for $C_{16}H_{14}N_3$ $[M+H]^+$: 248.1182, found: 248.1175.

(*E*)-2-(buta-1,3-dien-1-yl)-5-methyl-1-(pyrimidin-2-yl)-1H-indole (7b), white solid, mp: 145-146 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.60 (s, 3H), 5.18 (d, *J* = 9.9 Hz, 1H), 5.34 (d, *J* = 16.6 Hz, 1H), 5.94-6.04 (m, 1H), 6.30-6.36 (m, 1H), 6.93 (s, 1H), 7.19-7.23 (m, 2H), 7.24-7.27 (m, 1H), 7.61 (d, *J* = 7.3 Hz, 1H), 8.32 (d, *J* = 8.2 Hz,1H), 8.86 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 21.5, 115.0, 116.2, 116.5, 117.5, 121.1, 122.0, 125.4, 125.7, 130.4, 135.5, 137.0, 139.3, 158.4, 158.8; HRMS (ESI) calcd. for $C_{17}H_{16}N_3$ $[M+H]^+$: 262.1339, found: 262.1346.

(*E*)-2-(Buta-1,3-dien-1-yl)-5-fluoro-1-(pyrimidin-2-yl)-1H-indole (7c), yellow solid, mp: 156-157 °C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.07 (dd, *J* = 9.6, 1.0 Hz, 1H), 5.23 (dd, *J* = 15.8, 1.8 Hz, 1H), 5.95-6.04 (m, 1H), 6.30-6.36 (m, 1H), 7.12 (d, *J* = 1.4 Hz, 1H), 7.22-7.24 (m, 1H), 7.25-7.38 (m, 2H), 7.48 (d, *J* = 15.5 Hz, 1H), 7.88 (d, *J* = 1.5 Hz, 1H), 8.76 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 105.8, 115.4, 116.1, 116.7, 117.5, 121.3, 122.5, 125.4, 125.5, 131.0, 135.0, 137.2, 139.0, 158.0, 158.4; HRMS (ESI) calcd. for $C_{16}H_{13}FN_3$ $[M+H]^+$: 266.1088, found: 266.1079.

(*E*)-2-(Buta-1,3-dien-1-yl)-5-chloro-1-(pyrimidin-2-yl)-1H-indole (7d), yellow solid, mp: 163-164 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.08 (d, *J* = 10.0 Hz, 1H), 5.26

(d, *J* = 16.0 Hz, 1H), 5.92-6.01 (m, 1H), 6.27-6.34 (m, 1H), 7.09 (d, *J* = 1.3 Hz, 1H), 7.19-7.22 (m, 1H), 7.26-7.37 (m, 2H), 7.45 (d, *J* = 15.5 Hz, 1H), 7.85 (d, *J* = 1.5 Hz, 1H), 8.73 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 106.0, 115.5, 116.0, 116.6, 117.6, 121.4, 122.5, 125.4, 125.5, 130.7, 135.0, 137.2, 139.0, 158.1, 158.4; HRMS (ESI) calcd. for $C_{16}H_{13}ClN_3$ $[M+H]^+$: 282.0793, found: 282.0779.

(*E*)-2-(Buta-1,3-dien-1-yl)-4-methyl-1-(pyrimidin-2-yl)-1H-indole (7e), yellow solid, mp: 122-123 °C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.3 (s, 3H), 5.16 (d, *J* = 9.9 Hz, 1H), 5.35 (d, *J* = 16.6 Hz, 1H), 5.95-6.04 (m, 1H), 6.30-6.36 (m, 1H), 6.92 (s, 1H), 7.19-7.27 (m, 3H), 7.61 (d, *J* = 7.3 Hz, 1H), 8.32 (d, *J* = 8.2 Hz, 1H), 8.86 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 18.8, 113.7, 115.5, 116.8, 118.8, 121.8, 123.9, 128.9, 130.7, 133.2, 133.9, 136.2, 137.2, 139.4, 158.1, 158.2; HRMS (ESI) calcd. for $C_{17}H_{16}N_3$ $[M+H]^+$: 262.1339, found: 262.1346.

(*E*)-2-(Buta-1,3-dien-1-yl)-3-methyl-1-(pyrimidin-2-yl)-1H-indole (7f), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.40 (s, 3H), 5.42-5.49 (m, 2H), 5.99-6.29 (m, 1H), 6.30-6.34 (m, 1H), 7.01-7.09 (dd, *J* = 17.4, 11.6 Hz, 1H), 7.10-7.13 (m, 1H), 7.22 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.25-7.30 (m, 2H), 7.57-7.59 (m, 1H), 8.77 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 10.7, 109.7, 116.9, 118.9, 120.9, 122.0, 124.1, 126.5, 127.5, 128.7, 130.9, 134.0, 136.6, 137.9, 158.2, 158.4; HRMS (ESI) calcd. for $C_{17}H_{16}N_3$ $[M+H]^+$: 262.1339, found: 262.1328.

(*E*)-2-(2-(Buta-1,3-dien-1-yl)phenyl)pyridine (7g), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.12-5.14 (m, 1H), 5.29-5.33 (m, 1H), 6.39-6.65 (m, 1H), 6.69-6.76 (m, 1H), 7.27 (d, *J* = 1.2 Hz, 1H), 7.28-7.39 (m, 2H), 7.40-7.48 (m, 2H), 7.49 (d, *J* = 1.4 Hz, 1H), 7.66-7.69 (m, 1H), 7.72-7.77 (m, 1H), 8.72-8.74 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 114.2, 117.4, 121.8, 124.8, 125.0, 126.2, 128.6, 130.0, 131.2, 135.6, 136.1, 138.1, 149.4; HRMS (ESI) calcd. for $C_{15}H_{14}N$ $[M+H]^+$: 208.1121, found: 208.1112.

(*E*)-2-(2-(Buta-1,3-dien-1-yl)-4-methylphenyl)pyridine (7h), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.32 (s, 3H), 5.13-5.14 (m, 1H), 6.35-6.42 (m, 1H), 6.44-6.74 (m, 1H), 7.26-7.28 (m, 1H), 7.33-7.35 (m, 3H), 7.37-7.41 (m, 1H), 7.42-7.49 (m, 2H), 7.68 (d, *J* = 7.6 Hz, 1H), 8.73-8.78 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 21.3, 112.5, 113.3, 114.1, 115.5, 119.8, 121.1, 124.3, 128.3, 131.6, 132.3, 135.8, 136.5, 137.2, 149.4; HRMS (ESI) calcd. for $C_{16}H_{16}N$ $[M+H]^+$: 222.1277, found: 222.1260.

(*E*)-2-(2-(Buta-1,3-dien-1-yl)-4-fluorophenyl)pyridine (7i), yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.11-5.14 (m, 1H), 5.28-5.32 (m, 1H), 6.35-6.44 (m, 1H), 6.64-6.74 (m, 1H), 7.26-7.28 (m, 1H), 7.33-7.40 (m, 3H), 7.41-7.42 (m, 1H), 7.48 (d, *J* = 1.4 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 8.68 (d, *J* = 4.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 115.0, 120.3, 121.9, 123.1, 124.7, 126.3, 126.7, 128.3, 128.5, 128.7, 129.7, 133.6, 136.5, 137.5, 149.4; HRMS (ESI) calcd. for $C_{15}H_{13}FN$ $[M+H]^+$: 226.1027, found: 226.1036

(*E*)-2-(2-(Buta-1,3-dien-1-yl)-4-chlorophenyl)pyridine (7j), brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.20 (d, *J* = 10.0 Hz, 1H), 5.38 (d, *J* = 16.0 Hz, 1H), 6.43-6.52 (m, 1H), 6.73-6.82 (m, 1H), 7.39-7.44 (m, 3H), 7.46-7.48 (m, 1H), 7.54 (d, *J* = 1.7 Hz, 1H), 7.56 (d, *J* = 1.4 Hz, 1H), 7.73-7.75 (m, 1H), 8.72 (d, *J* = 4.7 Hz, 1H); ^{13}C NMR

(100.6 MHz, $CDCl_3$) δ 115.0, 120.3, 121.9, 123.2, 124.6, 126.3, 126.7, 128.3, 128.5, 128.7, 129.7, 130.9, 133.6, 137.4, 149.4; HRMS (ESI) calcd. for $C_{15}H_{13}ClN$ $[M+H]^+$: 242.0731, found: 242.0722.

(*E*)-2-(2-(Buta-1,3-dien-1-yl)-4-(trifluoromethyl)phenyl)pyridine (7k), yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 5.11-5.14 (m, 1H), 5.28-5.32 (m, 1H), 6.35-6.44 (m, 1H), 6.64-6.74 (m, 1H), 7.26-7.33 (m, 1H), 7.35-7.39 (m, 3H), 7.40-7.42 (m, 1H), 7.48 (d, *J* = 1.4 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 8.76 (d, *J* = 4.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 113.6, 120.1, 121.9, 123.1, 124.6, 126.3, 126.7, 128.3, 128.5, 128.8, 129.8, 131.8, 133.7, 137.3, 138.1, 150.3; HRMS (ESI) calcd. for $C_{16}H_{13}F_3N$ $[M+H]^+$: 276.0995, found: 276.0982.

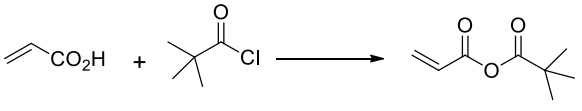
(*E*)-2-(3-(Buta-1,3-dien-1-yl)naphthalen-2-yl)pyridine (7l), yellow solid, mp: 154-155 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 5.34 (d, *J* = 10.8 Hz, 1H), 5.84 (d, *J* = 17.4 Hz, 1H), 6.35-6.44 (m, 1H), 6.64-6.74 (m, 1H), 7.29-7.32 (m, 1H), 7.47-7.55 (m, 3H), 7.76-7.88 (m, 1H), 7.80-7.90 (m, 2H), 7.99 (s, 1H), 8.10 (s, 2H), 8.76 (d, *J* = 4.7 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 116.2, 120.7, 121.2, 122.8, 123.3, 124.1, 126.9, 127.2, 128.2, 128.5, 129.5, 130.9, 131.5, 135.3, 137.9, 138.4, 147.6; HRMS (ESI) calcd. For $C_{19}H_{16}N$ $[M+H]^+$: 258.1277, found: 258.1284.

(*E*)-10-(Buta-1,3-dien-1-yl)benzo[h]quinoline (7m), brown solid, mp: 178-179 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 5.28 (d, *J* = 11.0 Hz, 1H), 5.50 (d, *J* = 17.8 Hz, 1H), 6.25-6.42 (m, 1H), 6.44-6.74 (m, 1H), 7.04 (d, *J* = 9.3 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 6.5 Hz, 1H), 7.89-7.91 (m, 2H), 8.00 (dd, *J* = 8.0, 1.1Hz, 1H), 8.11 (d, *J* = 9.3 Hz, 1H), 8.20-8.23 (m, 1H), 8.74 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 112.4, 120.9, 123.4, 123.6, 125.5, 127.6, 128.8, 128.9, 129.2, 129.6, 131.6, 133.3, 134.4, 135.5, 137.3, 138.3, 148.2; HRMS (ESI) calcd. for $C_{17}H_{14}N$ $[M+H]^+$: 232.1121, found: 232.1176.

(*E*)-6-(2-(Buta-1,3-dien-1-yl)phenyl)-9-isopropyl-9H-purine (7n), yellow solid, mp: 143-144 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 1.69 (d, *J* = 4.5 Hz, 6H), 4.99-5.01 (m, 1H), 5.01 (d, *J* = 4.6 Hz, 1H), 5.24 (d, *J* = 19.3 Hz, 1H), 5.83-5.97 (m, 1H), 6.76 (dd, *J* = 13.8, 7.3 Hz, 1H), 6.95-7.02 (m, 1H), 7.42~7.52 (m, 2H), 7.78~7.85 (m, 2H), 8.12 (s, 1H), 9.15 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 23.4, 46.4, 115.9, 126.7, 127.2, 129.4, 131.7, 132.4, 133.4, 135.1, 136.4, 139.3, 144.1, 152.8, 152.9, 158.6; HRMS (ESI) calcd. For $C_{18}H_{19}N_4$ $[M+H]^+$: 291.1604, found: 2901.1596.

4. The mechanistic study

a) **Preparation of acrylic pivalic anhydride**



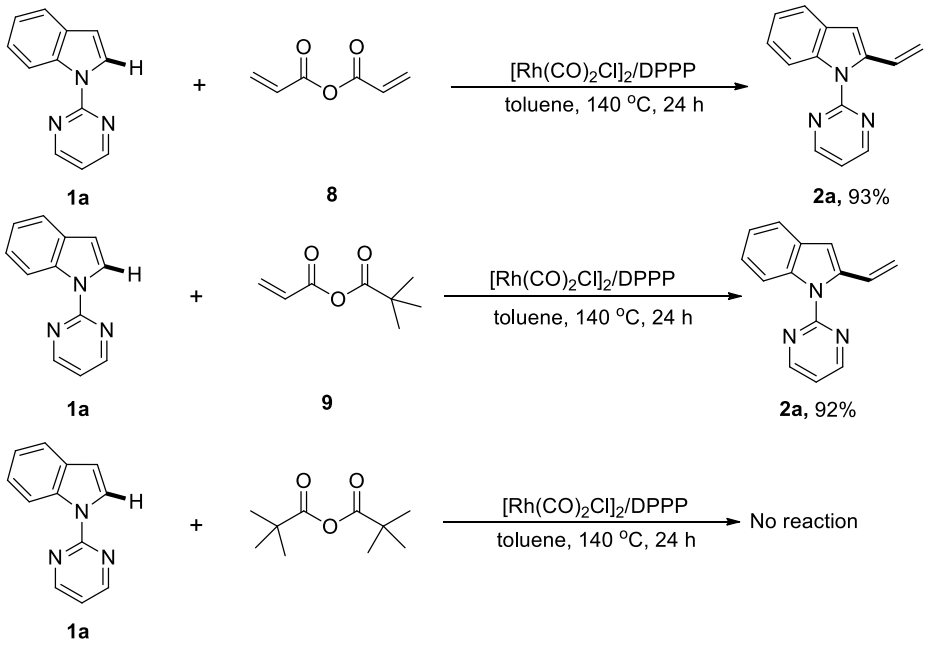
acrylic pivalic anhydride (**9**)

Preparation of acrylic pivalic anhydride (**9**): distilled NEt_3 (1.01 g, 10.0 mmol) in 20.0 mL of dry THF was added dropwise to a solution of acrylic acid (0.72 g, 10 mmol) at -15 °C, and then trimethyacetyl chloride (1.20 g, 10.0 mmol) in 10.0 mL dry THF at -15 °C was introduced. The reaction mixture was stirred vigorously at -15 °C, and

was monitored by TLC. When the acid disappeared, the reaction was poured into ice-cold saturated $NaHCO_3$ aqueous solution (20.0 mL). The organic layer was separated and the aqueous solution was extracted with CH_2Cl_2 (20.0 mL × 3). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated under vacuum to give acrylic pivalic anhydride (1.28 g, 82%).

Acrylic pivalic anhydride (9), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20-1.22 (m, 9H), 5.97-6.00 (m, 1H), 6.04-6.12 (m, 1H), 6.40-6.45 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 25.4, 39.0, 126.8, 133.1, 160.7, 172.7; HRMS (ESI) calcd. for $C_8H_{13}O_3$ $[M+H]^+$: 157.0859, found: 157.0846.

b) The coupling reaction of anhydrides with 1a:



General procedure for the reaction of anhydrides with 1a: To an oven-dried pressure tube were sequentially added **1a** (97.5 mg, 0.5 mmol), $[Rh(CO)_2Cl]_2$ (7.8 mg, 4 mol%), DPPP (12.4 mg, 6 mol%), anhydride (0.5 mmol) and anhydrous toluene (3.0 mL). The reaction mixture was degassed three times with nitrogen, and then heated and stirred vigorously at 140 °C in an oil bath. After 24 h, the tube was removed from the oil bath, and cooled to room temperature. The solvent was removed and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure product **2a**.

c) The in situ generation of anhydrides

A mixture of equimolar amounts of acrylic acid and $(t\text{BuCO})_2O$ in toluene was stirred at 140 °C for 1 h, and subsequent analysis by ^{1}H NMR revealed the formation of acrylic anhydride (**8**) and acrylic pivalic anhydride (**9**) in a ratio of 1:3.8. After 24 h stirring, the ratio became 1:6.3.

d) Procedure for the analysis of the gaseous products by GC-TCD:

To an oven-dried pressure tube were sequentially added indole **1a** (97.5 mg, 0.5 mmol), $[Rh(CO)_2Cl]_2$ (7.8 mg, 4.0 mol%), DPPP (12.4 mg, 6.0 mol%), acrylic acid (43.3 mg, 0.6 mmol), $(t\text{BuCO})_2O$ (111.8 mg, 0.6 mmol) and anhydrous toluene (3.0 mL). After being degassed three times, the tube was heated and stirred vigorously at 140 °C for 24 h in an oil bath under argon atmosphere. After cooling, the reaction gas was analyzed by GC-TDC with argon as the carrier gas.

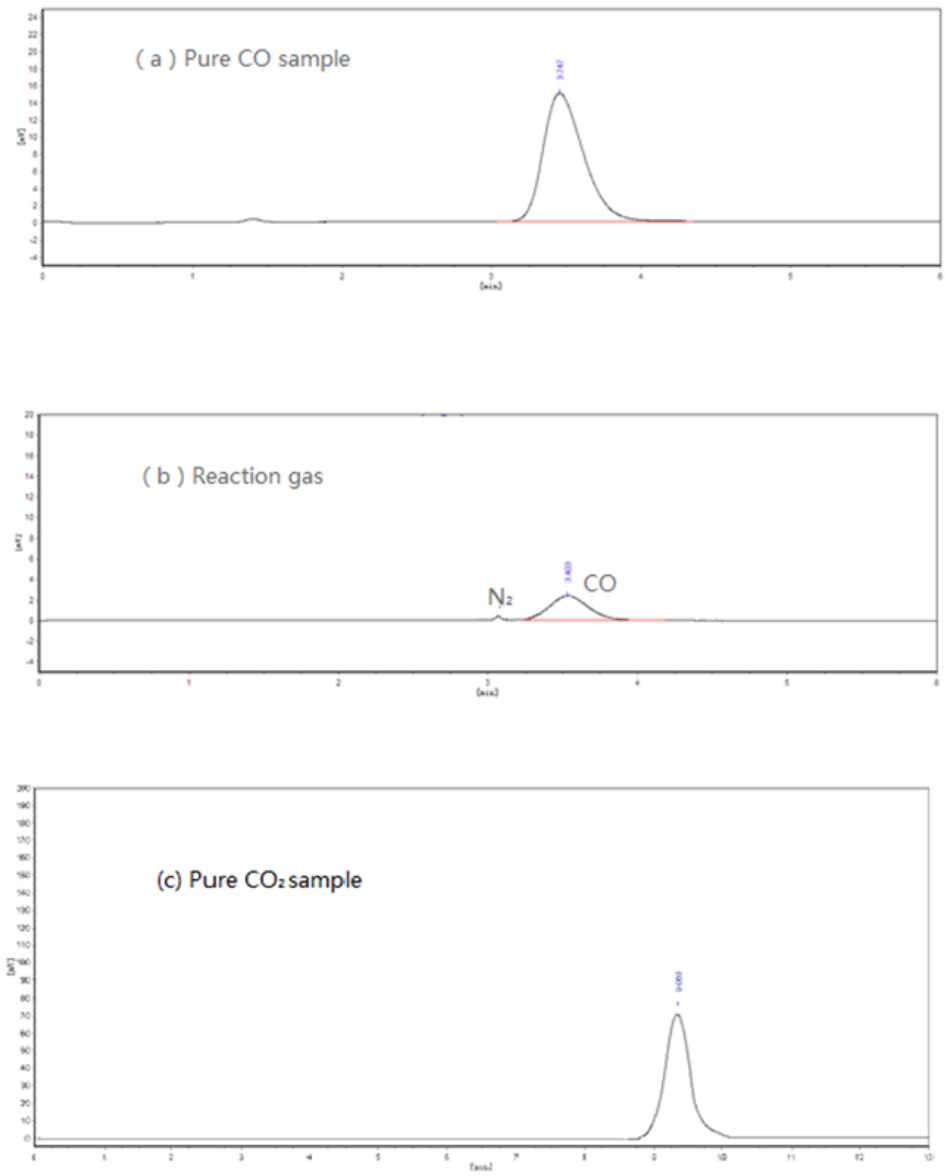
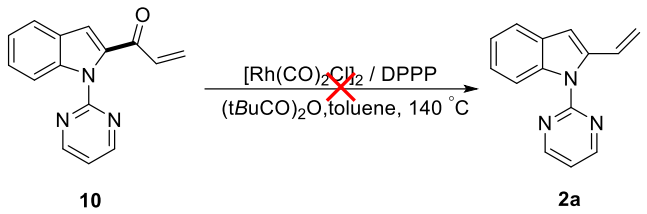


Figure S1. GC analysis indicated the existenc CO, and no CO_2 was produced.

d) Decarbonylation of 1-(1-(pyrimidin-2-yl)-1*H*-indol-2-yl)prop-2-en-1-one

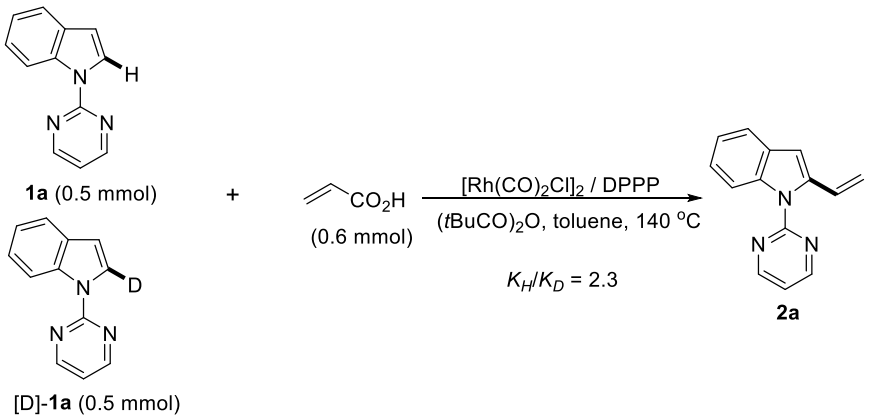


10 **2a**

Preparation of 1-(1-(Pyrimidin-2-yl)-1*H*-indol-2-yl)prop-2-en-1-one (10): A solution of 1-(pyrimidin-2-yl)-1*H*-indole (**1a**) (390.0 mg, 2.0 mmol) in dry THF (10.0 mL) was cooled to -78 °C and *n*-BuLi (1.6 M, 1.3 mL, 2.0 mmol) was added dropwise under N_2. The mixture was stirred for 5 min at -78 °C and for 30 min at room temperature. Then the reaction was cooled to -78 °C for 20 min, acrylic acid (72.0 mg, 1.0 mmol) in 2.0 mL THF was added to the mixture. The mixture was allowed to warm to room temperature over 30 min, and stirred for 2 h. Then the reaction mixture was slowly quenched with a saturated aqueous solution of sodium bicarbonate. The aqueous layer was extracted with ethyl acetate (20.0 mL × 3). The organic layers were combined and dried with Na_2SO_4. The solvent was removed by vacuum evaporation, and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure product (144.0 mg, 58% yield).

1-(1-(Pyrimidin-2-yl)-1*H*-indol-2-yl)prop-2-en-1-one (10), white solid, mp: 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.42 (d, *J* = 11.1 Hz, 1H), 5.93 (d, *J* = 17.4 Hz, 1H), 6.38 (dd, *J* = 17.4, 11.0 Hz, 1H), 7.29-7.35 (m, 4H), 7.71 (d, *J* = 7.4 Hz, 1H), 8.41 (d, *J* = 8.2 Hz, 1H), 8.95 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 109.1, 115.2, 115.8, 116.9, 117.7, 118.0, 123.1, 127.3, 127.5, 130.2, 133.2, 138.2, 158.1, 158.2, 182.5; HRMS (ESI) calcd. for $C_{15}H_{12}N_3O$ $[M+H]^+$: 250.0975, found: 250.0984.

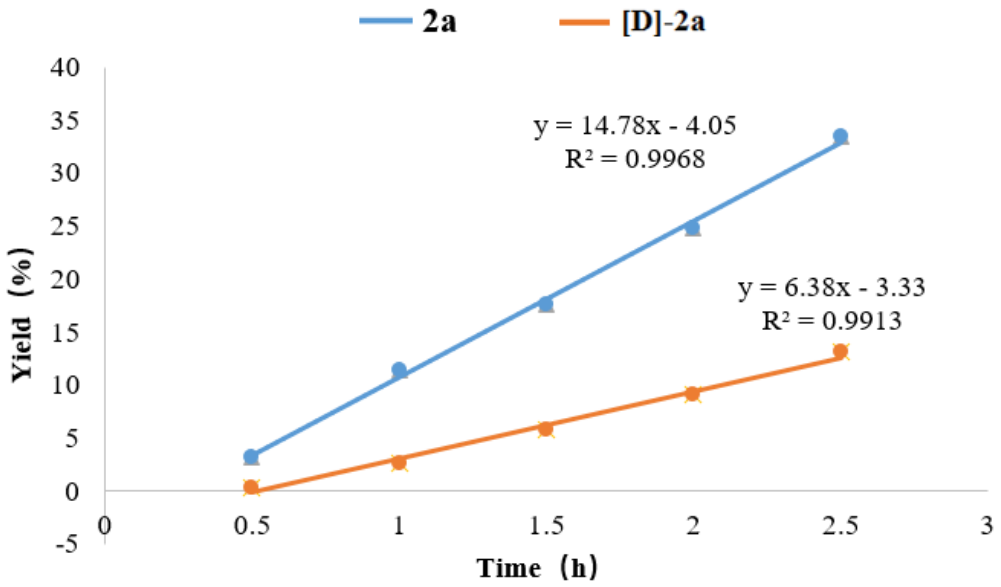
e) Kinetic isotope effect



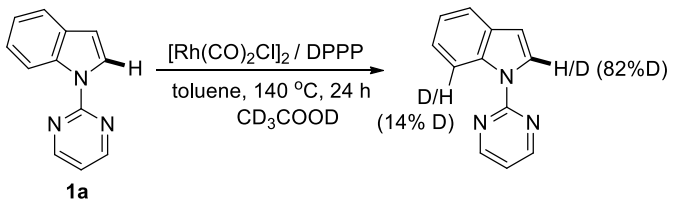
Following the general procedure, to an oven-dried pressure tube were sequentially added indole **1a** (97.5 mg, 0.5 mmol), $[Rh(CO)_2Cl]_2$ (7.8 mg, 4.0 mol%), DPPP (12.4 mg, 6.0 mol%), acrylic acid (43.3 mg, 0.6 mmol), $(t$BuCO$)_2$O (111.8 mg, 0.6 mmol)

and anhydrous toluene (3.0 mL). In another reaction vessel, **[D]-1a** (([2-^{2}H]-1-(pyrimidin-2-yl)-1*H*-indole))(0.5 mmol) was used instead of **1a**. After being degassed three times, the two reactions was heated and stirred vigorously at 130 °C in the oil bath under nitrogen atmosphere. An aliquot of each reaction mixture was taken at the time of 30 min, 1 h, 2 h, 3 h and 4 h. The yields were determined by ^{1}H NMR analysis of the crude reaction mixture. A kinetic isotope effect value K_H/K_D = 2.3 was obtained.

Time (h)		0.5	1	1.5	2	2.5
NMR Yield (%)	**2a**	3.2	11.5	17.6	24.8	33.5
	[D]-2a	0.4	2.7	5.8	9.2	13.1

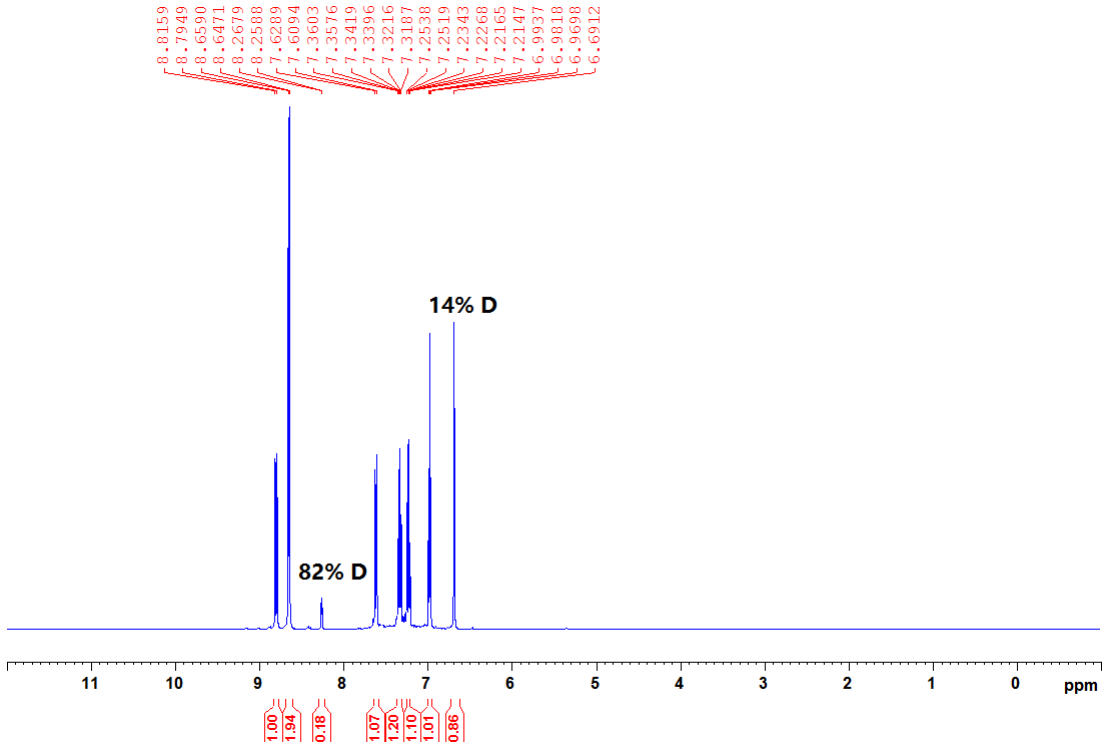


f) H/D exchange experiment

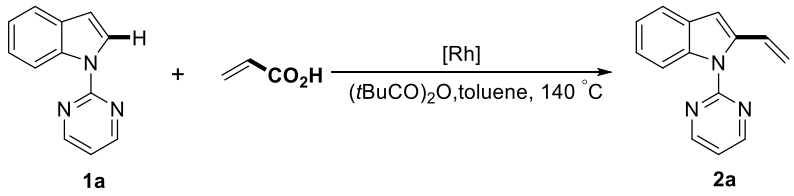


To an oven-dried pressure tube were sequentially added indole **1a** (97.5 mg, 0.5 mmol), $[Rh(CO)_2Cl]_2$ (7.8 mg, 4.0 mol%), DPPP (12.4 mg, 6.0 mol%), CD_3CO_2D (20.0 eq) and anhydrous toluene (3.0 mL). After being degassed three times, the tube was heated and stirred vigorously at 140 °C for 24 h in the oil bath under nitrogen atmosphere. Then the tube was removed from the oil bath and cooled to room temperature. The solvent was removed by vacuum evaporation, and ^{1}H NMR analysis

indicated that 82% deuterium incorporation was detected at the C2-position, and only 14% D was observed at the C7-postion.



g) The working mode of catalyst and ^{31}P NMR studies



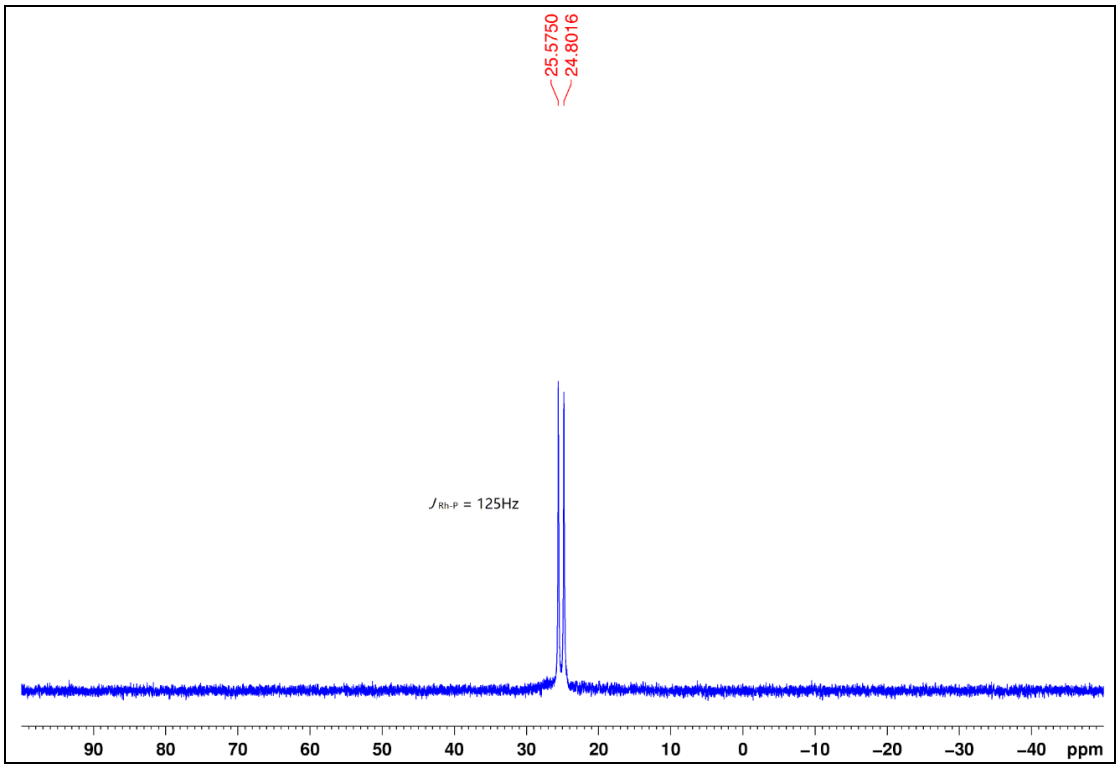
1a **2a**

[Rh(DPPP)Cl]: 58%

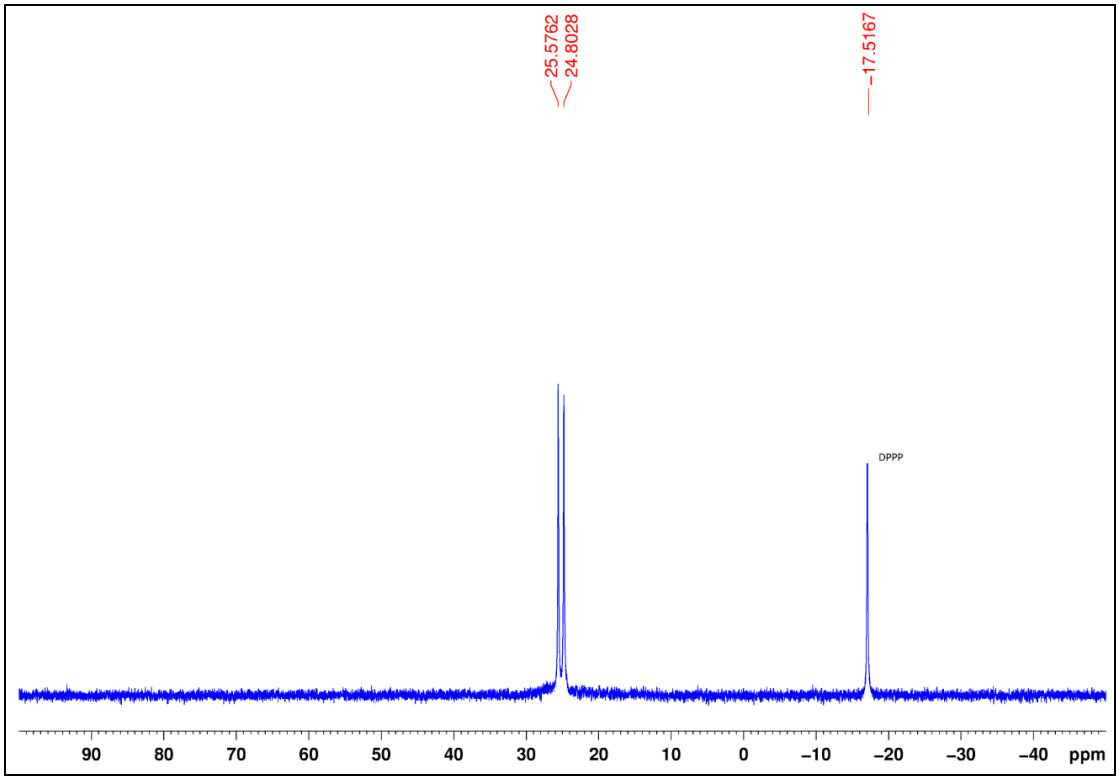
[Rh(DPPP)(CO)Cl]$_2$: 92%

These results clearly indicated that [Rh(DPPP)(CO)Cl]$_2$ is the reactive intermediate in the catalytic cycle.

^{31}P-NMR spectrum of the [Rh(CO)Cl(DPPP)]$_2$

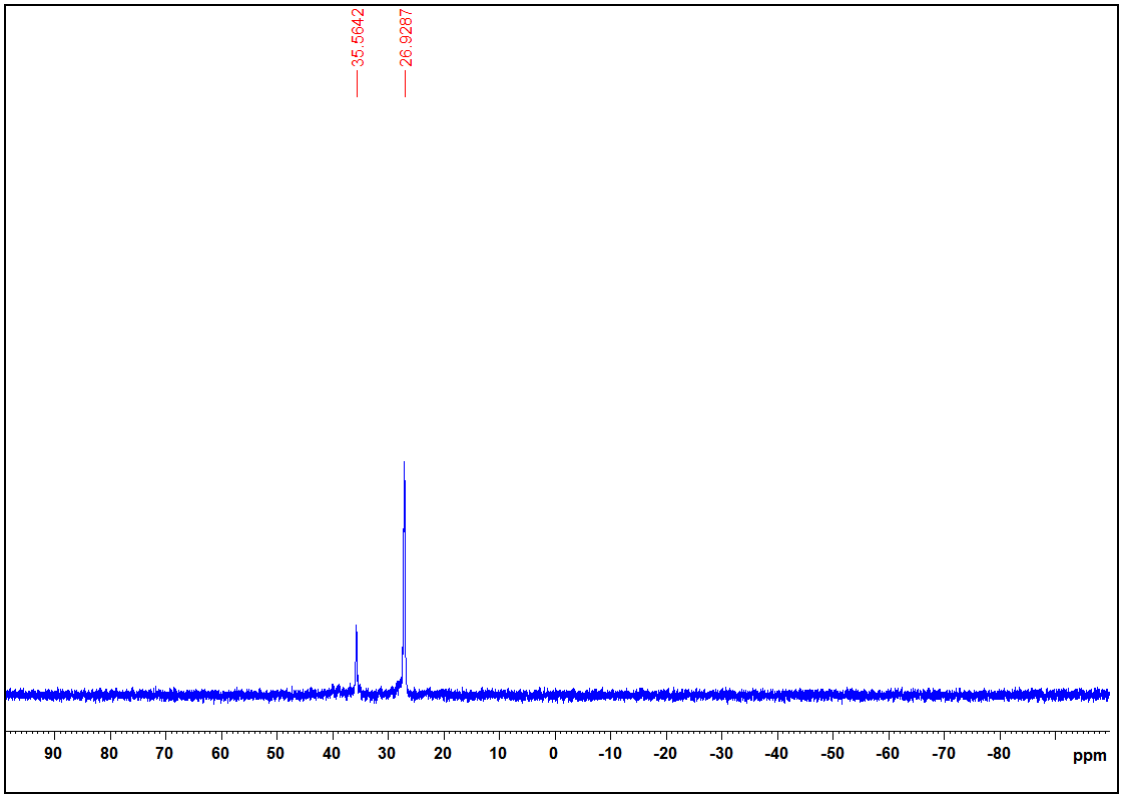


^{31}P-NMR spectrum of the mixture [Rh(CO)$_2$Cl]$_2$, DPPP and indole 1a



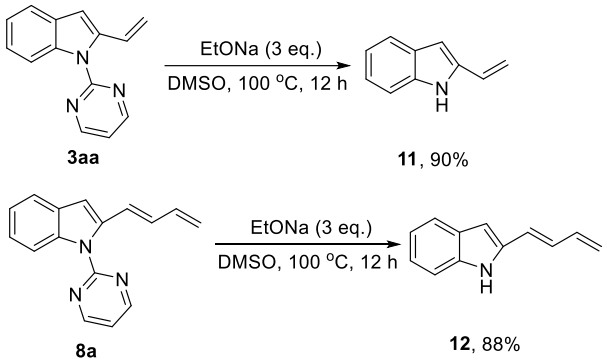
^{31}P-NMR spectrum of the mixture of [Rh(CO)$_2$Cl]$_2$(7.8 mg, 0.02 mmol), DPPP (9.9 mg, 1.2 eq.) and indole **1a** (156.0 mg, 40.0 eq.) after 60 min at room temperature.

^{31}P-NMR spectrum of the mixture $[Rh(CO)_2Cl]_2$, DPPP, acrylic acid and $(tBuCO)_2O$



^{31}P-NMR spectrum of the mixture of $[Rh(CO)_2Cl]_2$(7.8 mg, 0.02 mmol), DPPP (9.9 mg, 1.2 eq.), acrylic acid (57.6 mg, 40.0 eq.) and $(tBuCO)_2O$ (148.8 mg, 40.0 eq.) after 60 min at room temperature.

5. The general procedure for the deprotection of indole products



To an oven-dried pressure tube was added the olefinated indole (0.5 mmol), freshly prepared EtONa (1.5 mmol) and dry DMSO (3.0 mL). After being degassed by nitrogen for three times, the tube was heated and stirred vigorously at 100 °C for 12 h in an oil bath. Then the tube was removed from the oil bath and cooled to room temperature. The mixture was poured into 25 mL water and extracted with CH_2Cl_2

(20 mL × 3). The organic phase was dried by Na_2SO_4 and filtered. The filtrate was concentrated and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the unprotected indoles.

2-Vinyl-1H-indole (11), colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.98 (dd, *J* = 11.1, 1.2 Hz, 1H), 5.49 (dd, *J* = 17.4, 1.2 Hz, 1H), 6.60 (s, 1H), 6.85-6.88 (m, 2H), 6.90-6.92 (m, 2H), 7.28 (d, *J* = 7.4 Hz, 1H), 11.3 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 108.4, 115.0, 115.7, 117.0, 117.8, 118.1, 125.7, 134.7, 138.2; HRMS (ESI) calcd. for $C_{10}H_{10}N$ $[M+H]^+$: 144.0808, found: 144.0816.

(*E*)-2-(buta-1,3-dien-1-yl)-1H-indole (12), white solid, mp: 143-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.18 (d, *J* = 9.9 Hz, 1H), 5.35 (d, *J* = 16.6 Hz, 1H), 5.94-6.04 (m, 1H), 6.30-6.36 (m, 1H), 6.93 (s, 1H), 7.20-7.27 (m, 4H), 7.61 (d, *J* = 7.3 Hz, 1H), 11.34 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 105.8, 115.4, 116.1, 116.7, 117.5, 121.3, 122.5, 125.4, 125.5, 130.7, 135.0, 137.2; HRMS (ESI) calcd. for $C_{12}H_{12}N$ $[M+H]^+$: 170.0964, found: 170.0952.

6. References:

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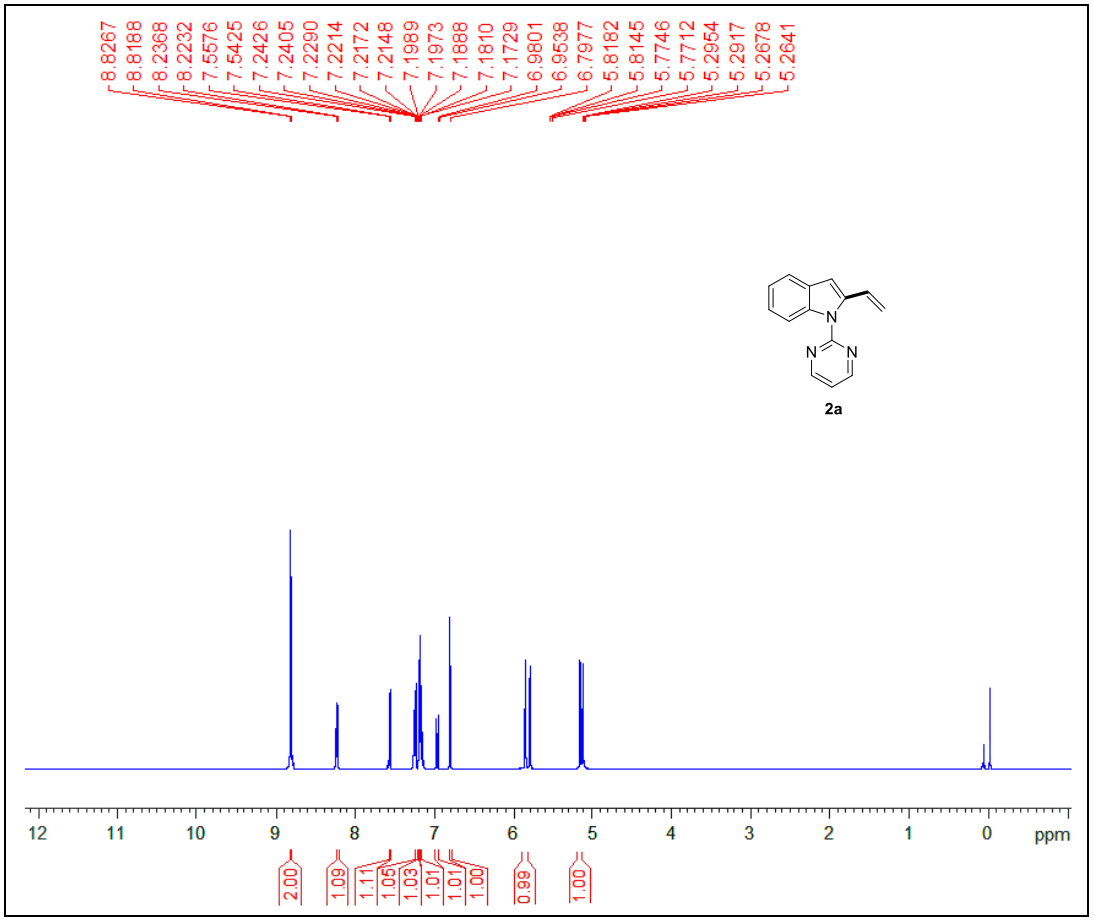
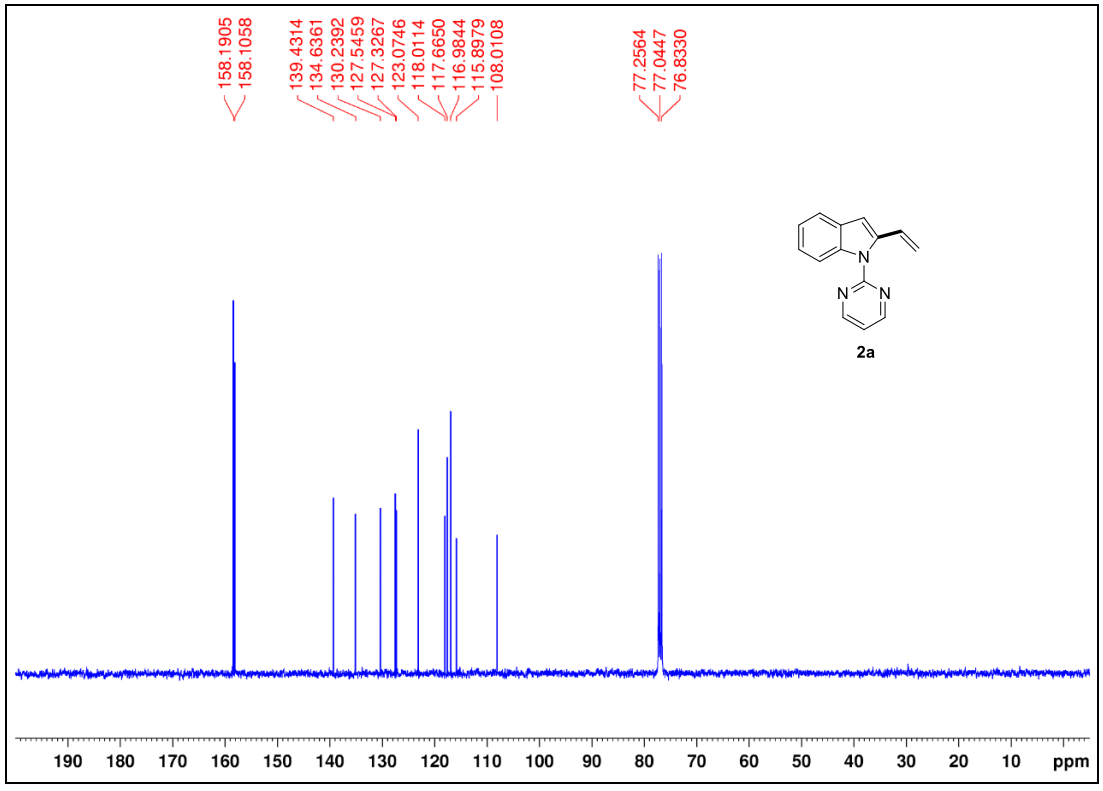
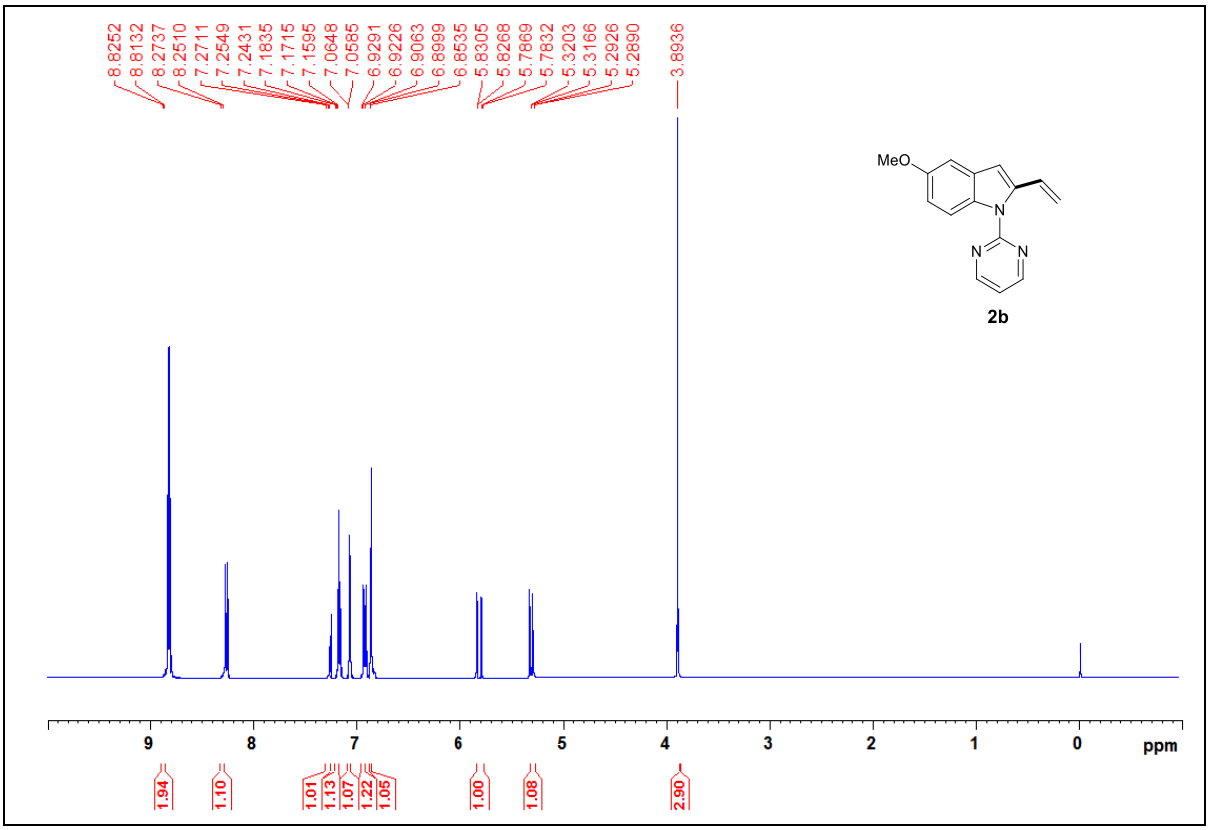
7. ^{1}H and ^{13}C NMR spectra of the products



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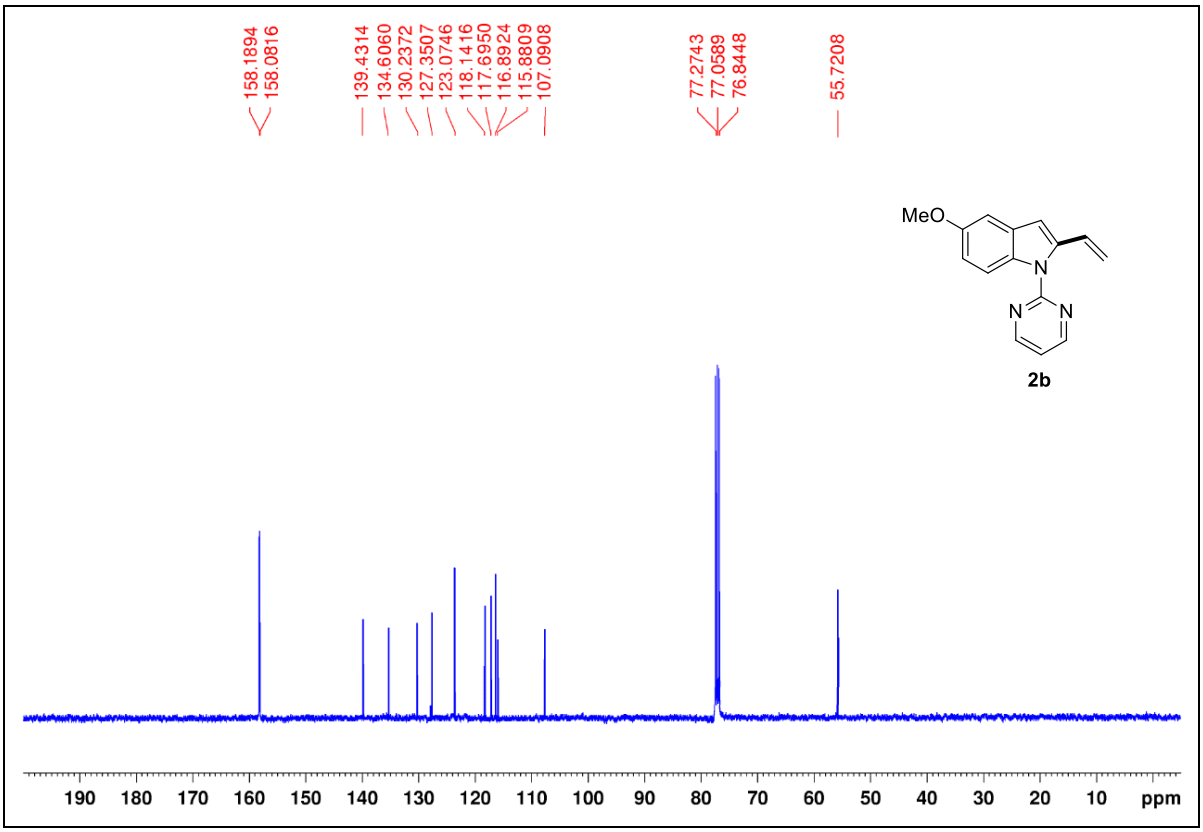
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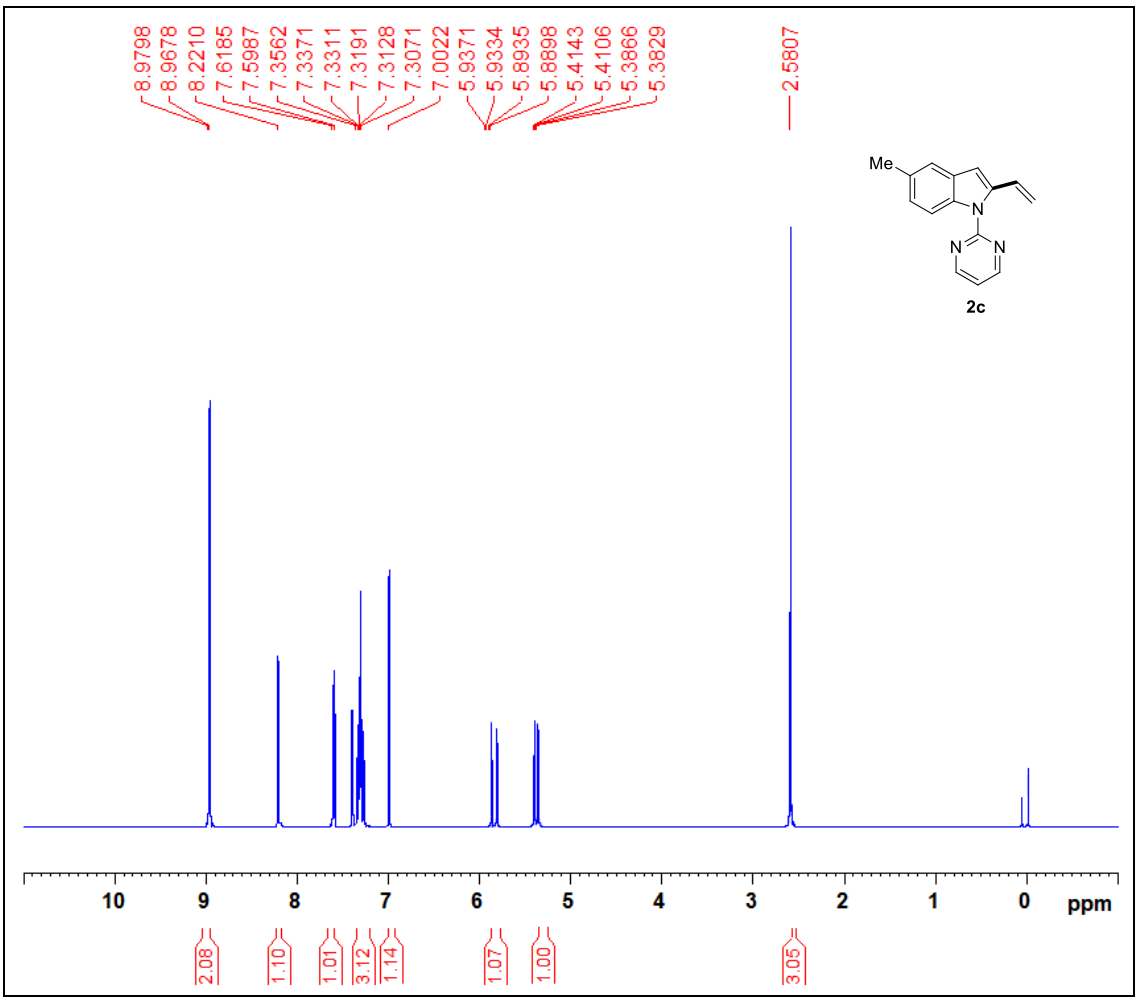
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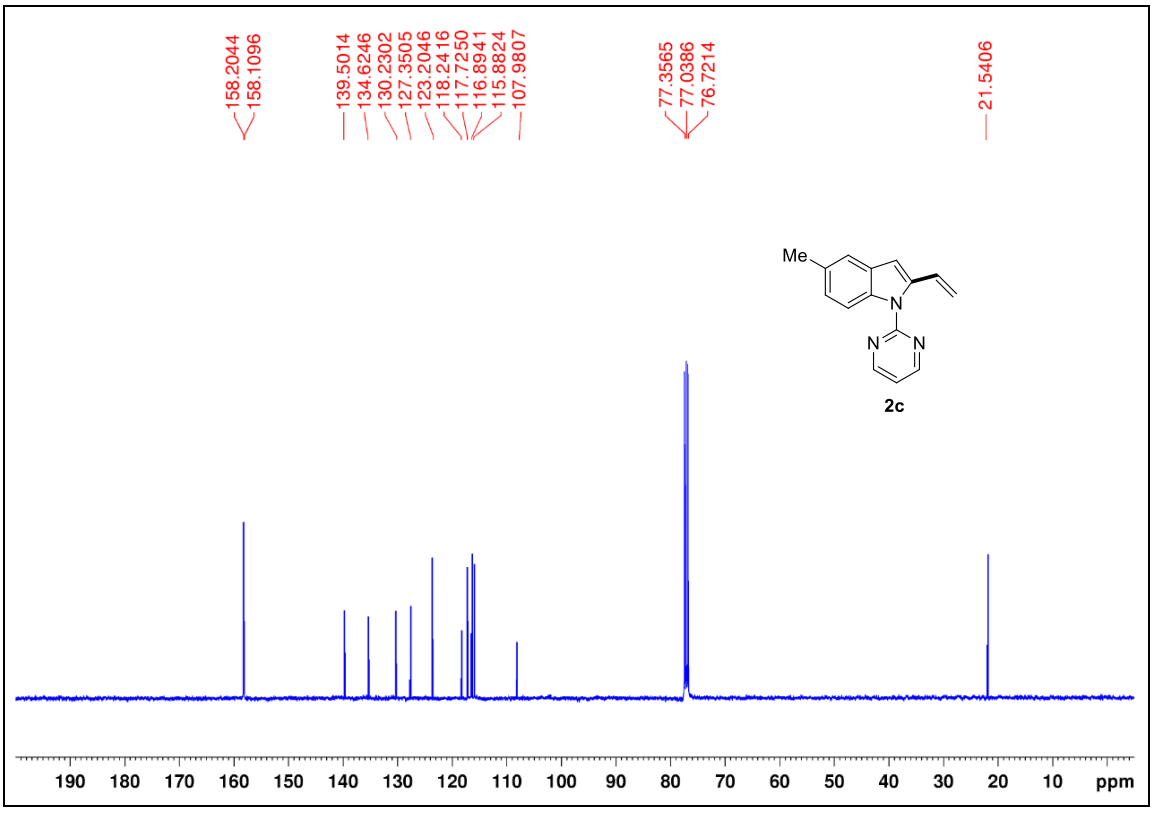
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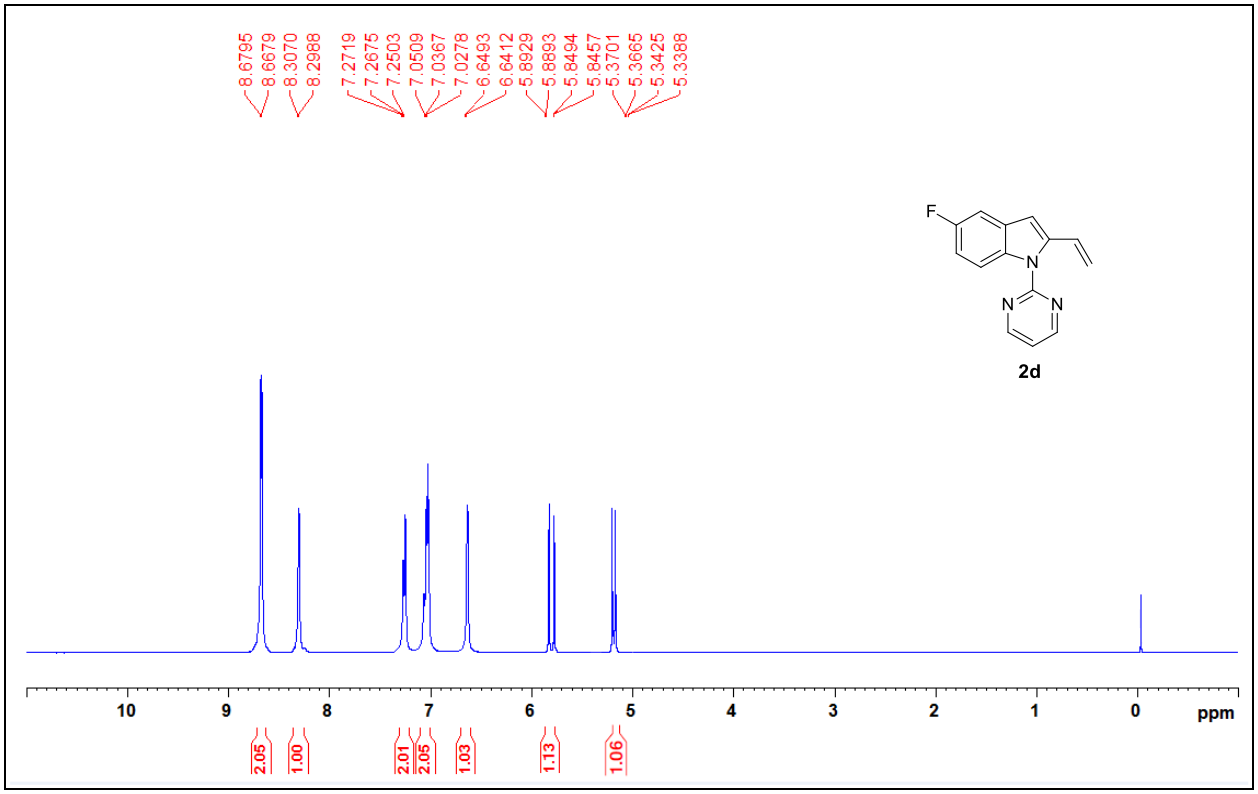
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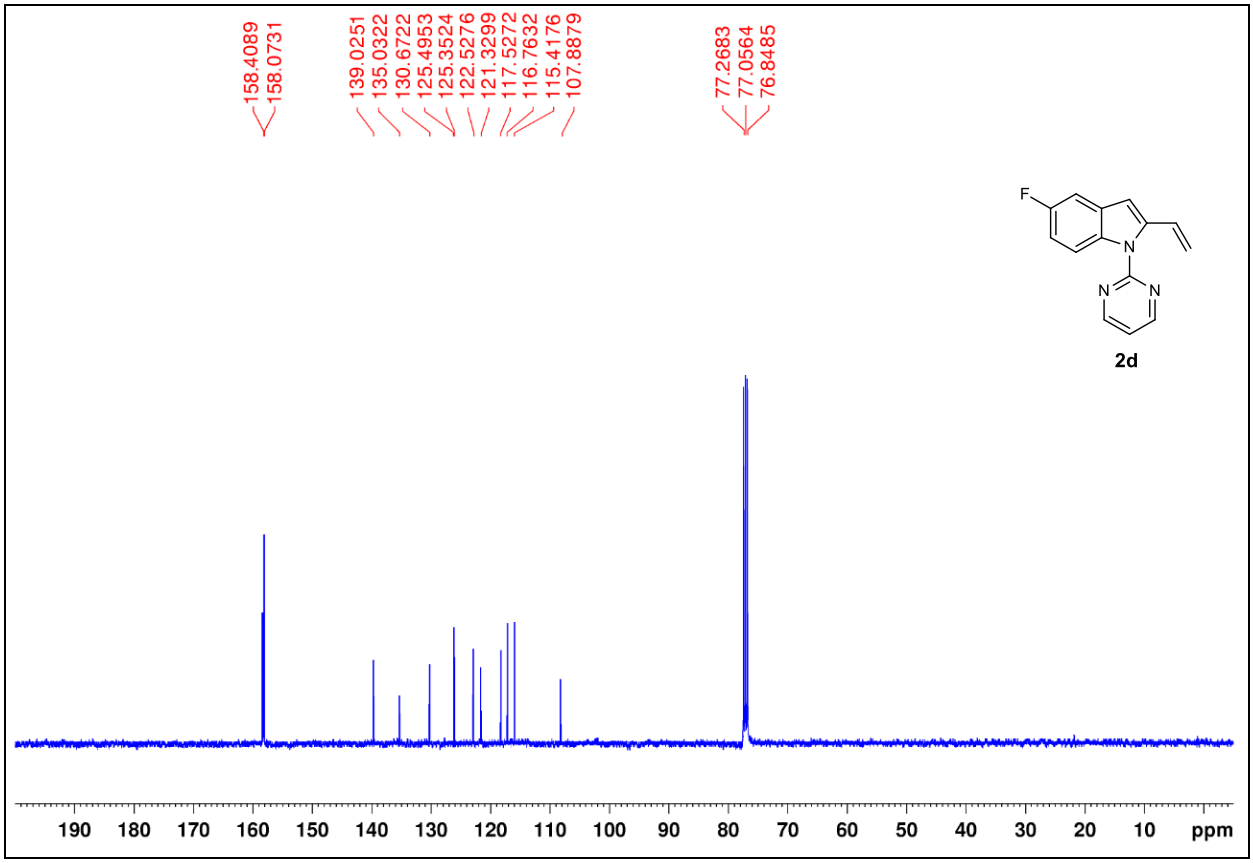
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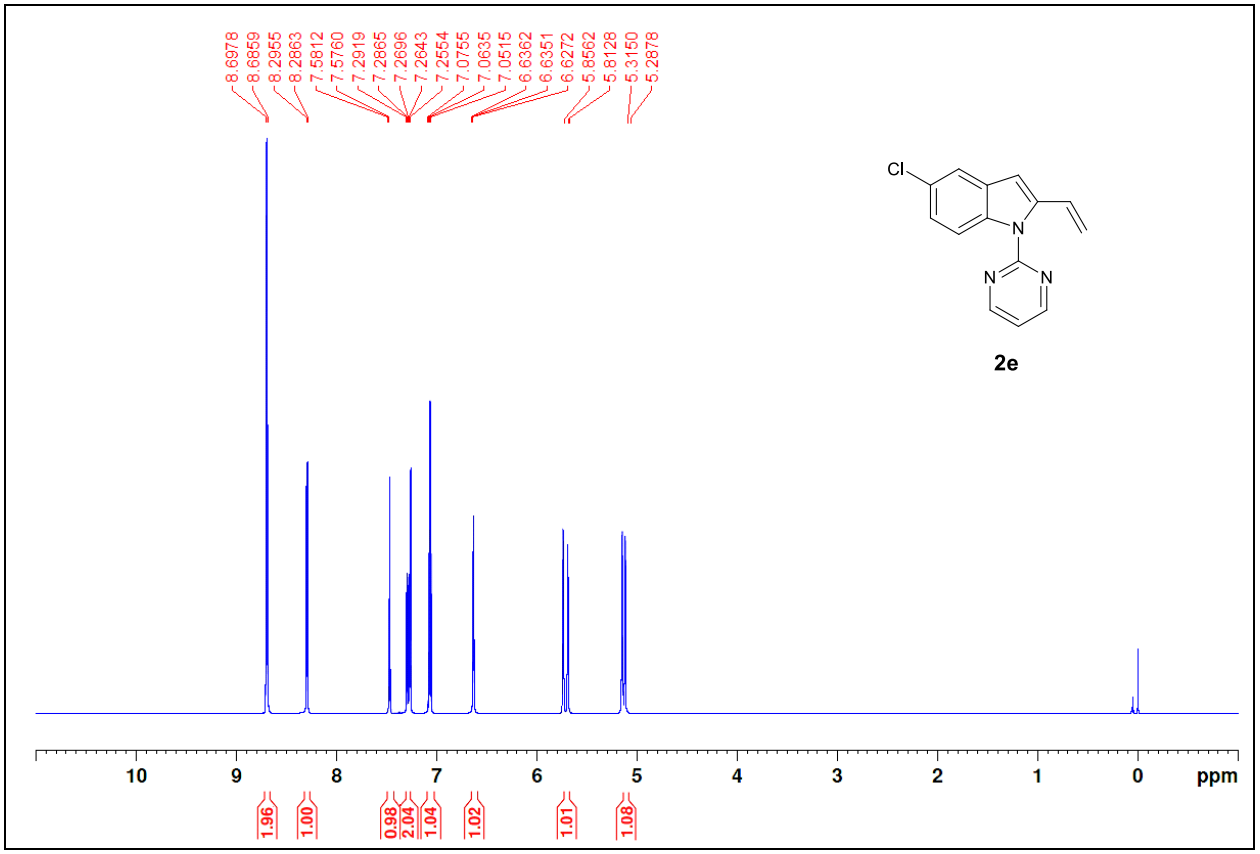
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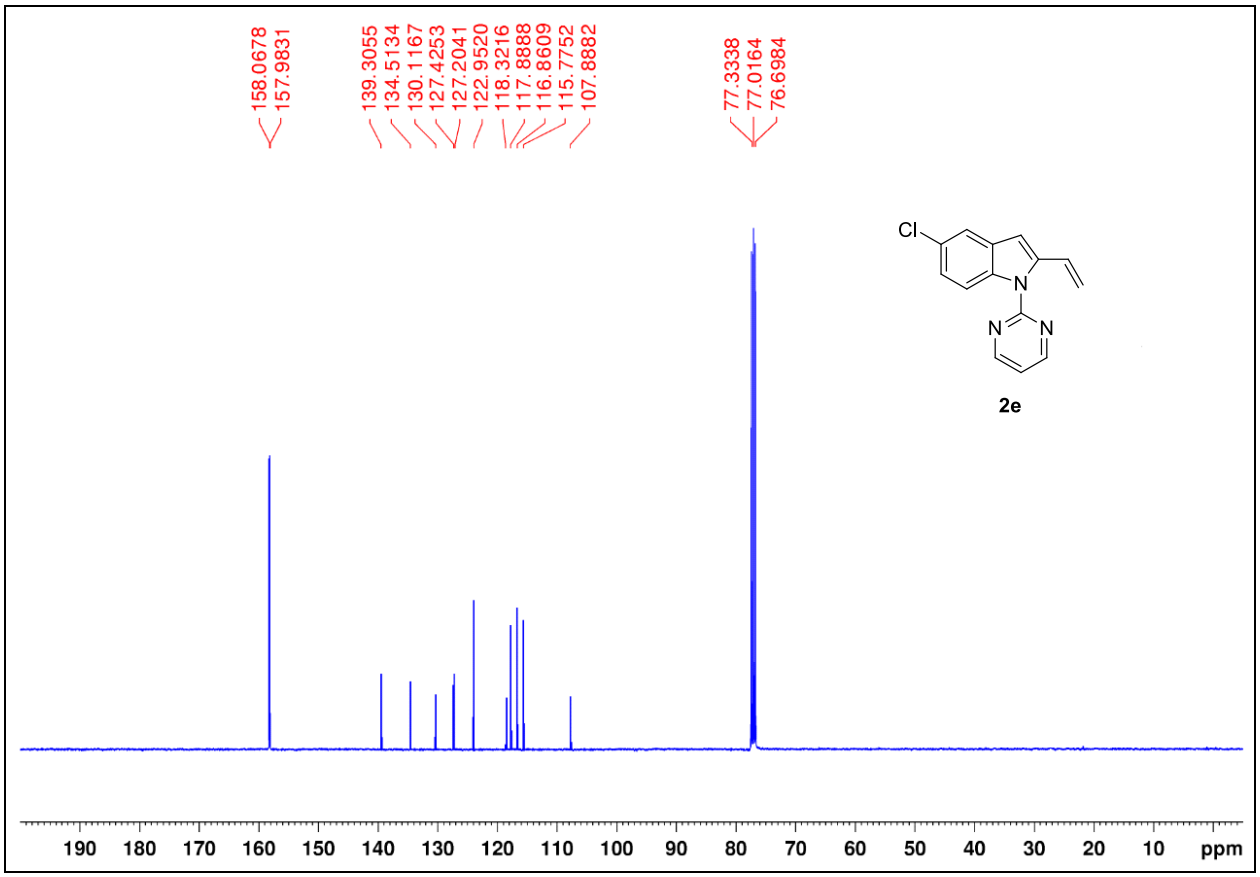
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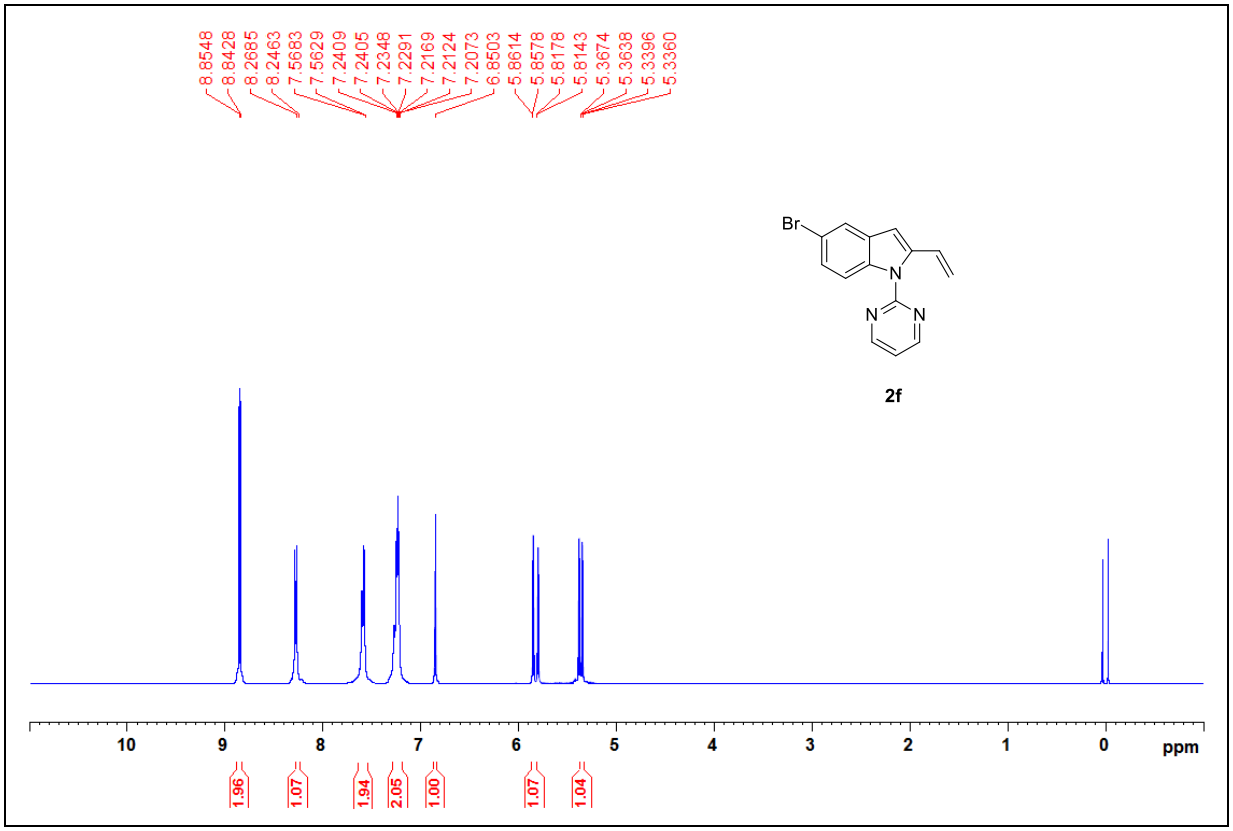
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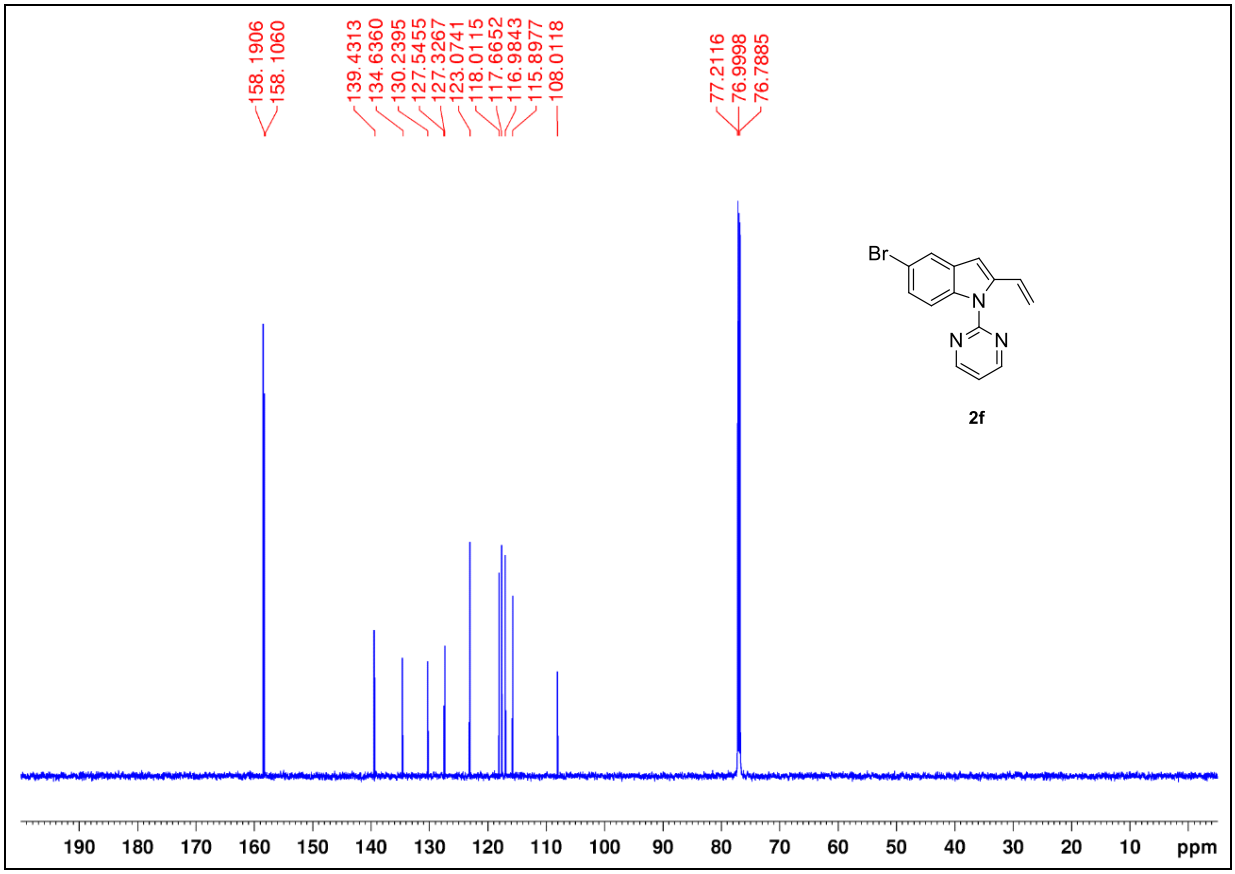
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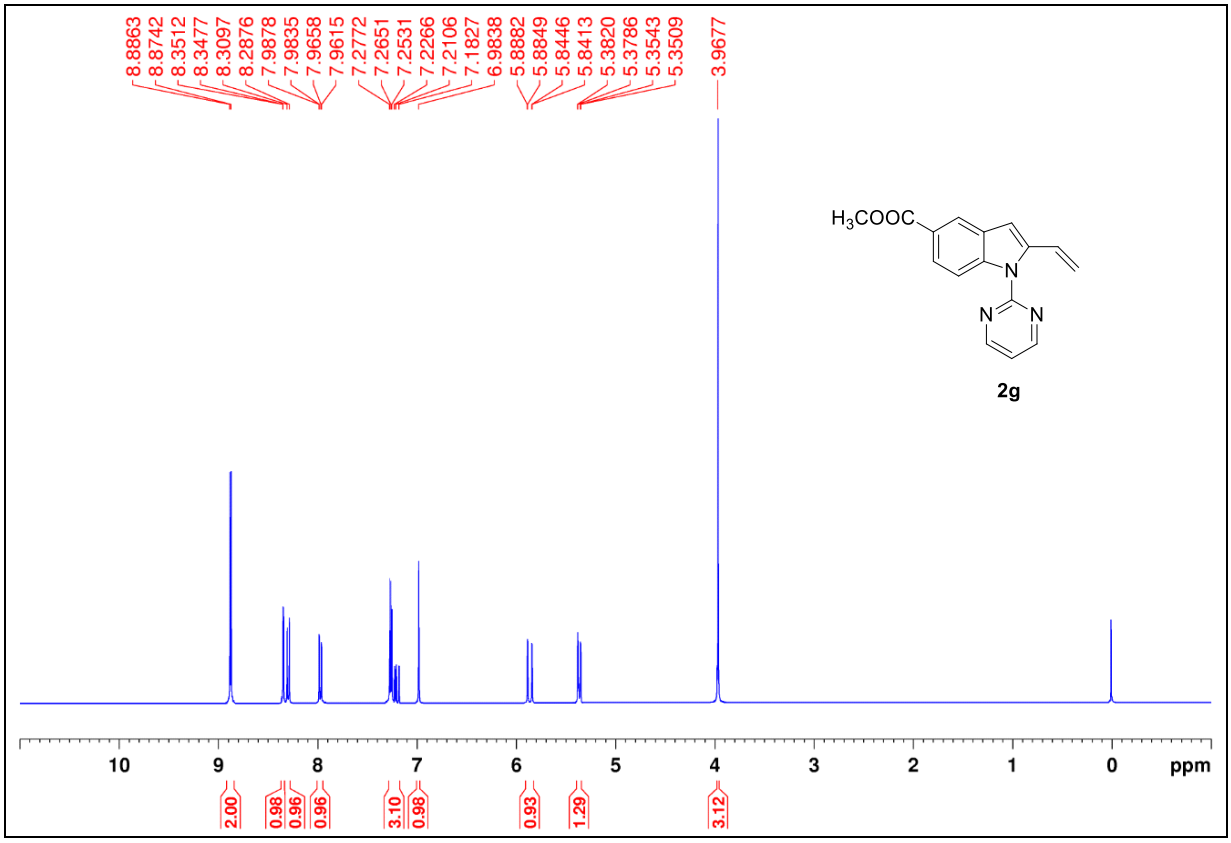
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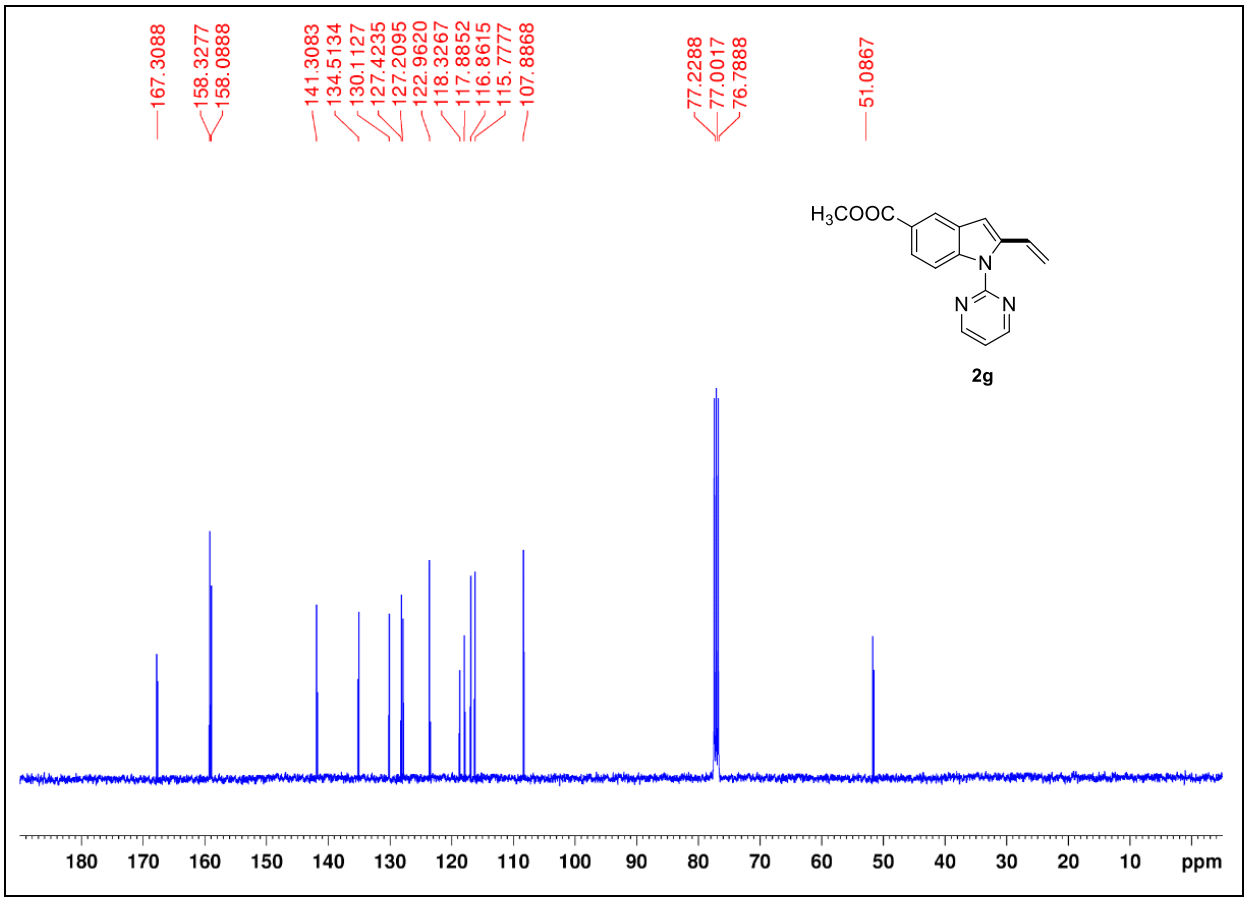
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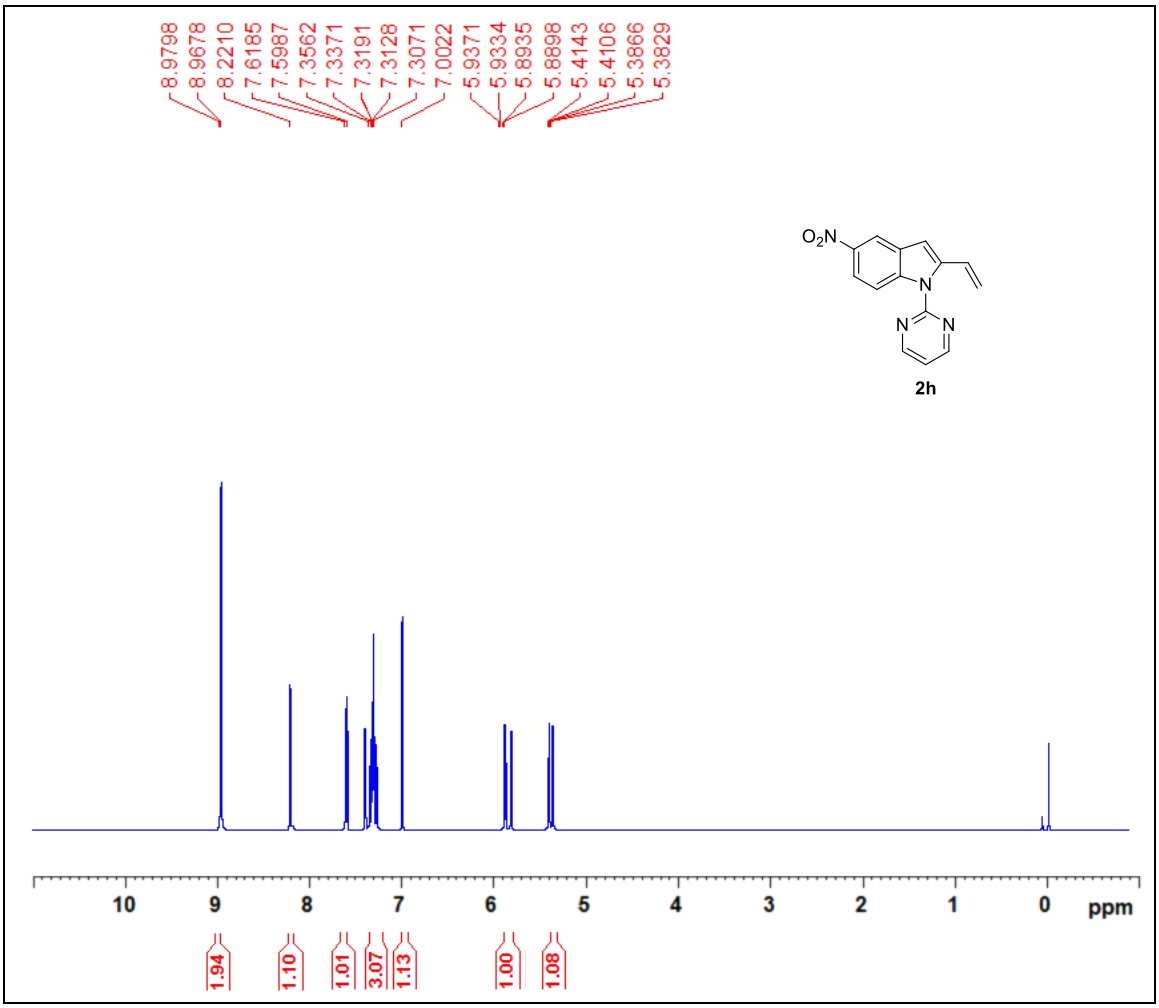
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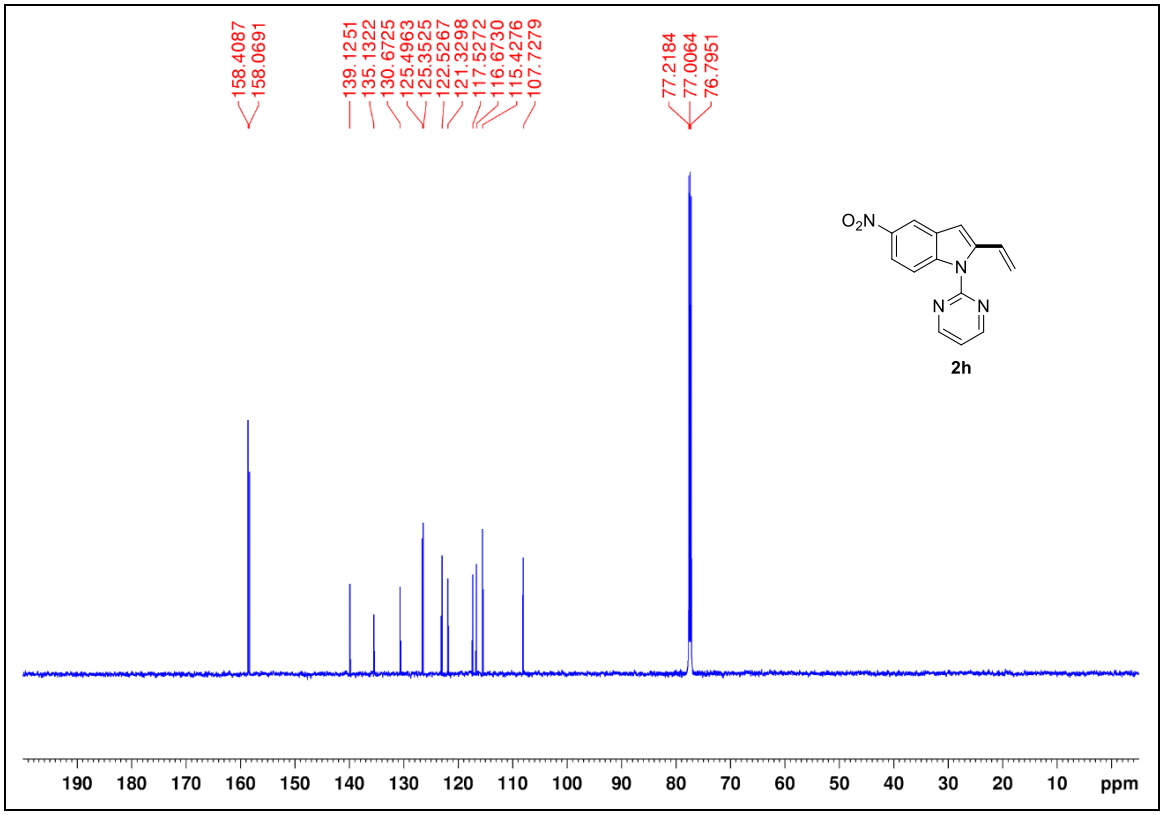
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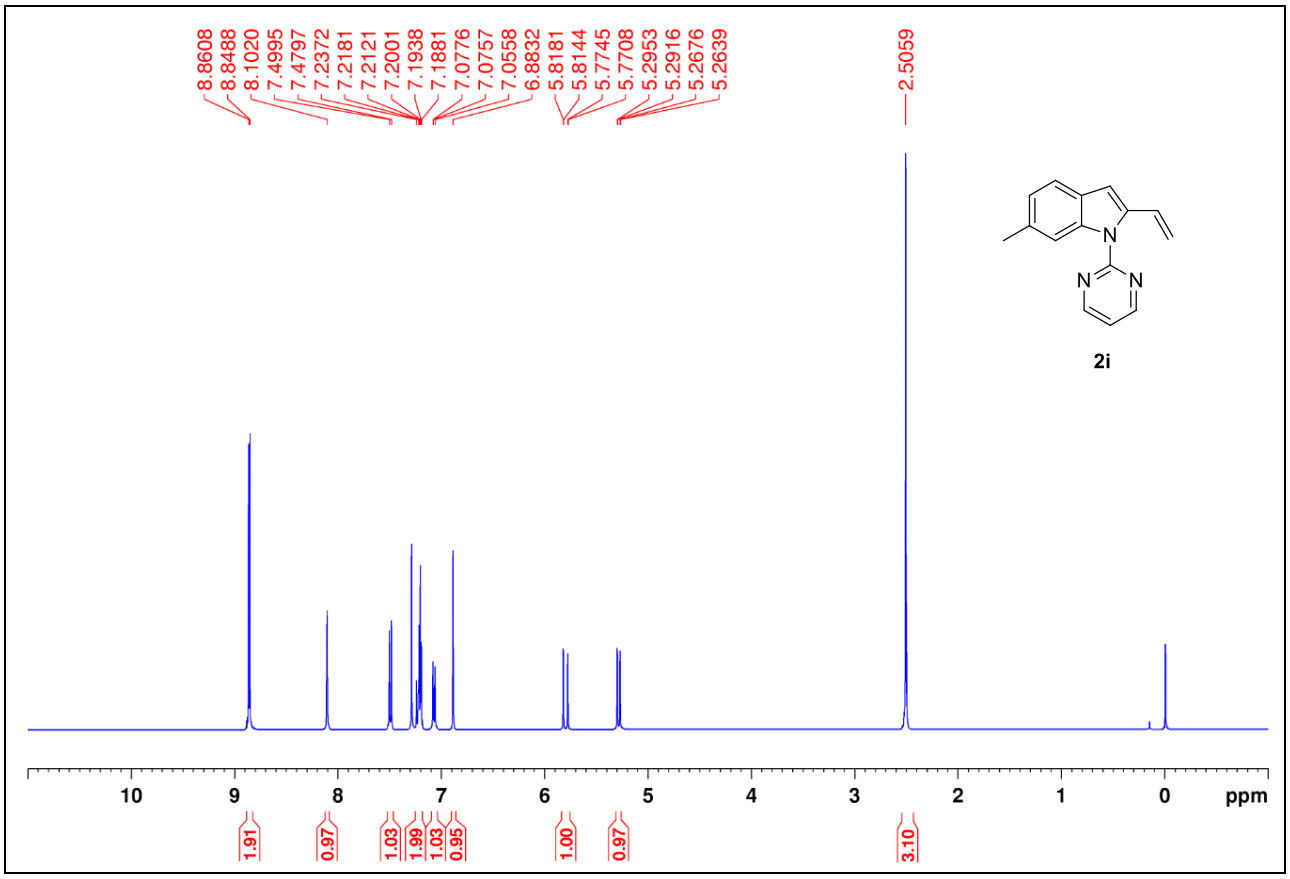
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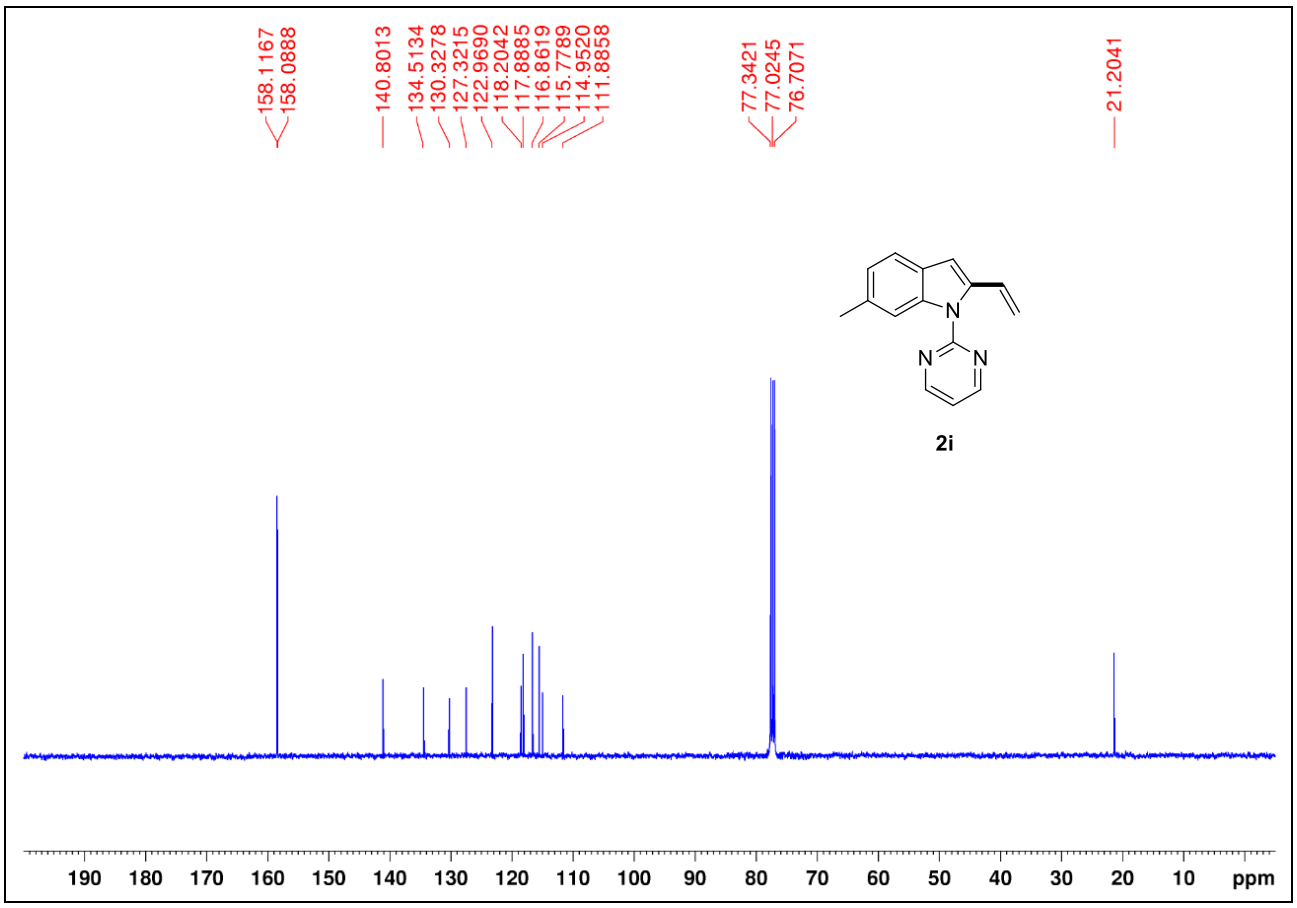
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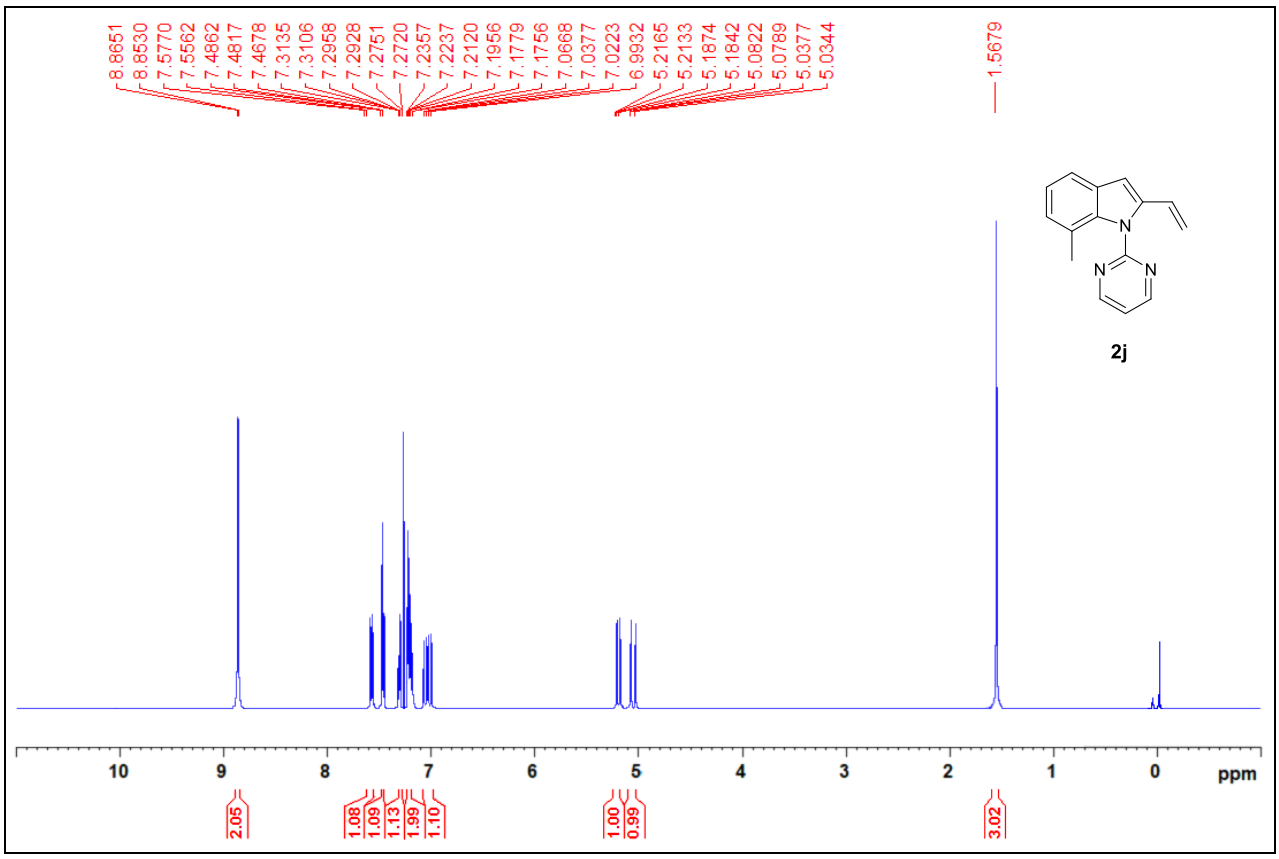
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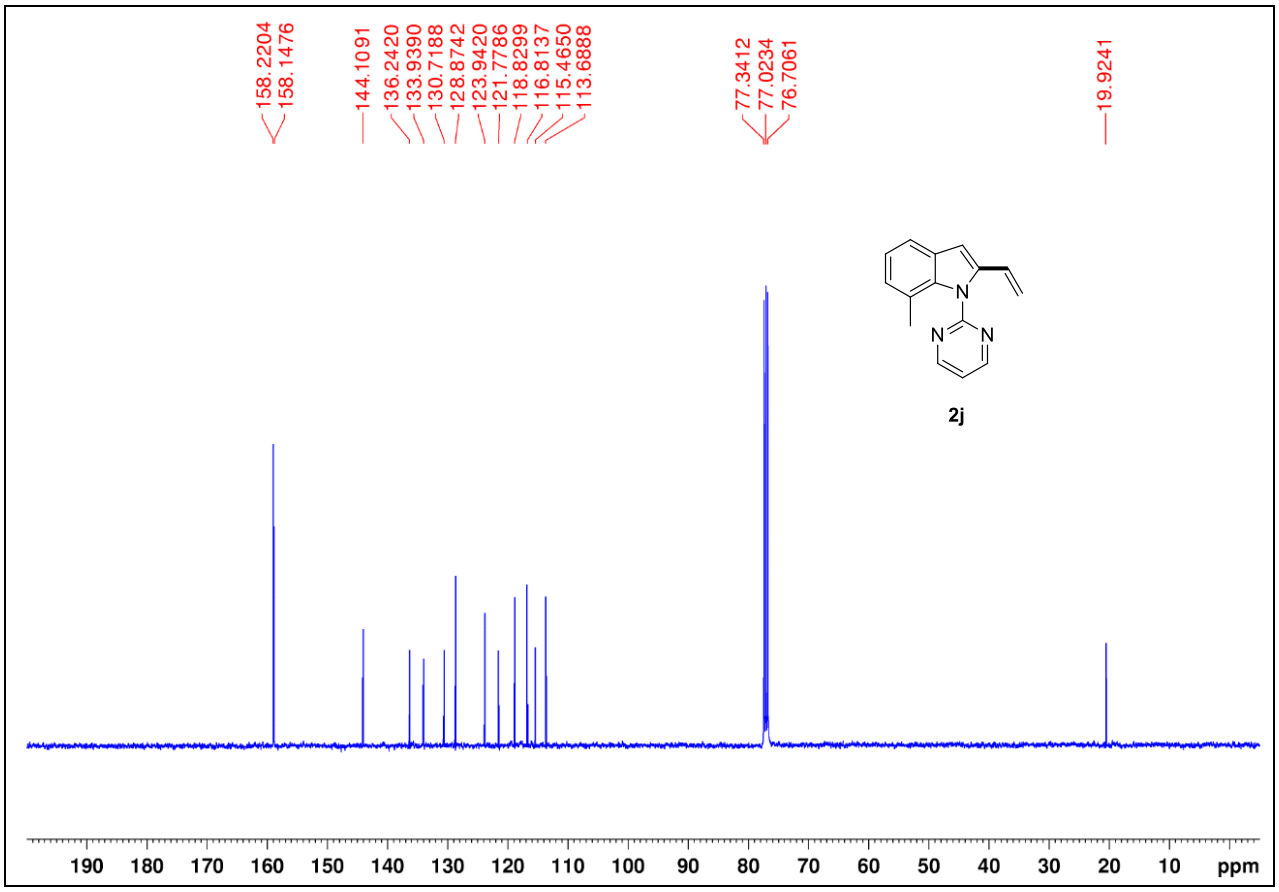
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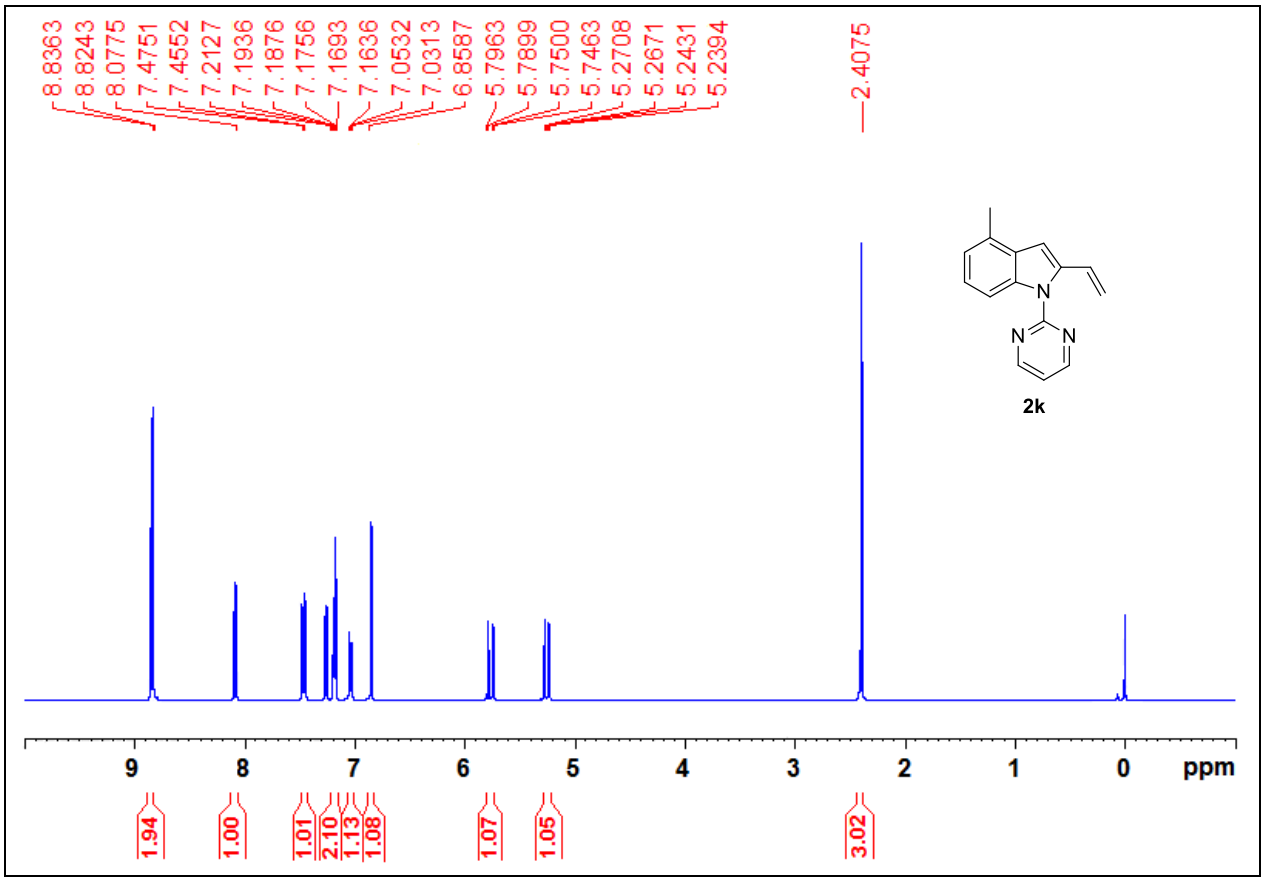
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6.8587
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5.2671
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8
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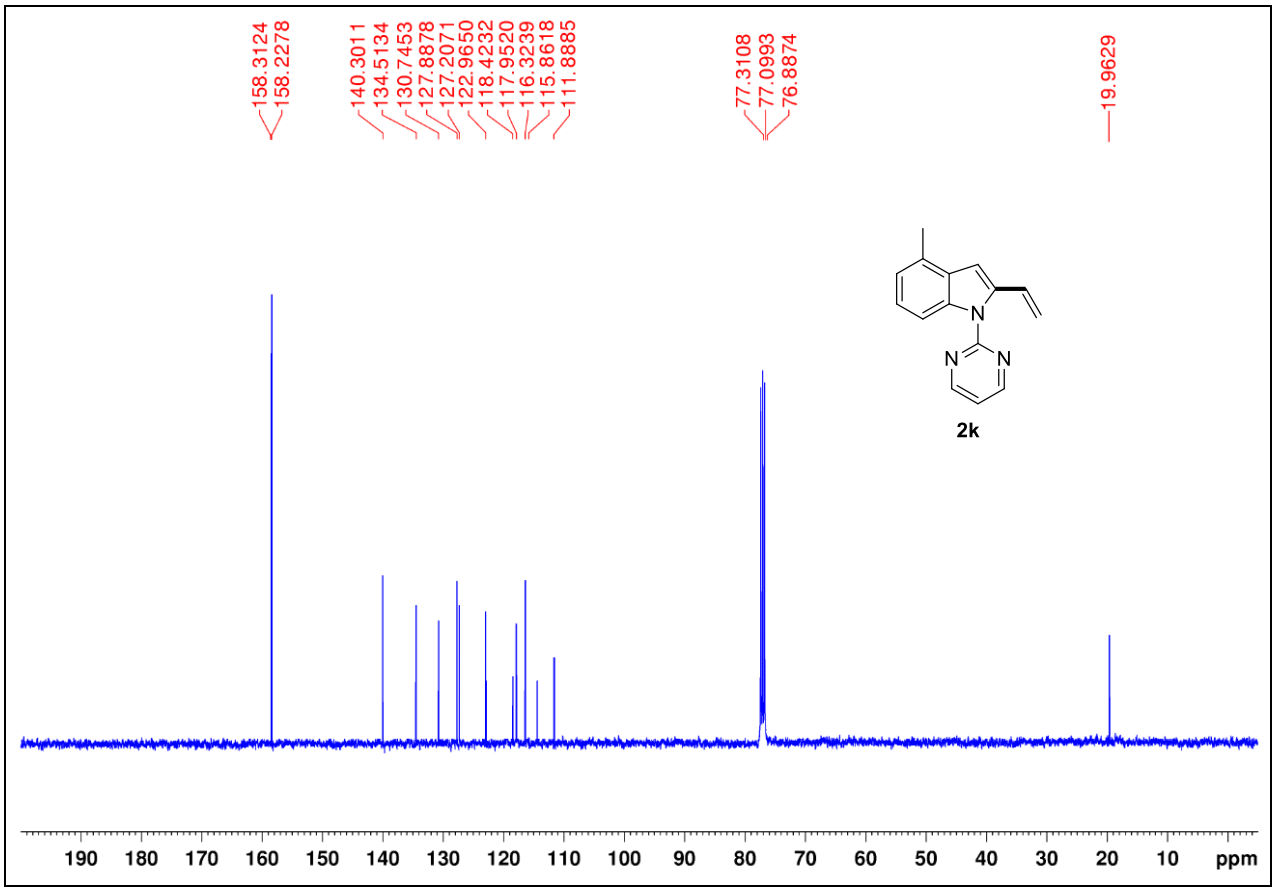
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N
N
2k
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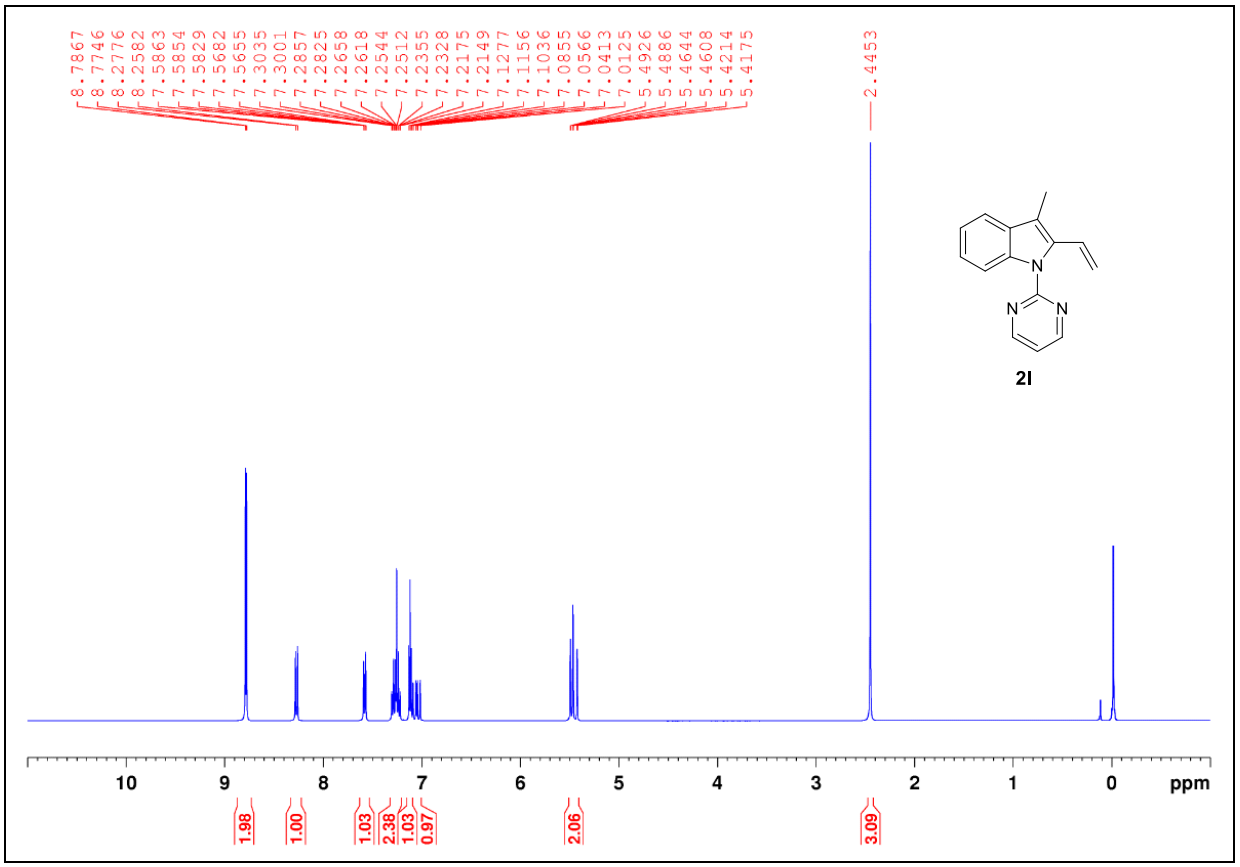
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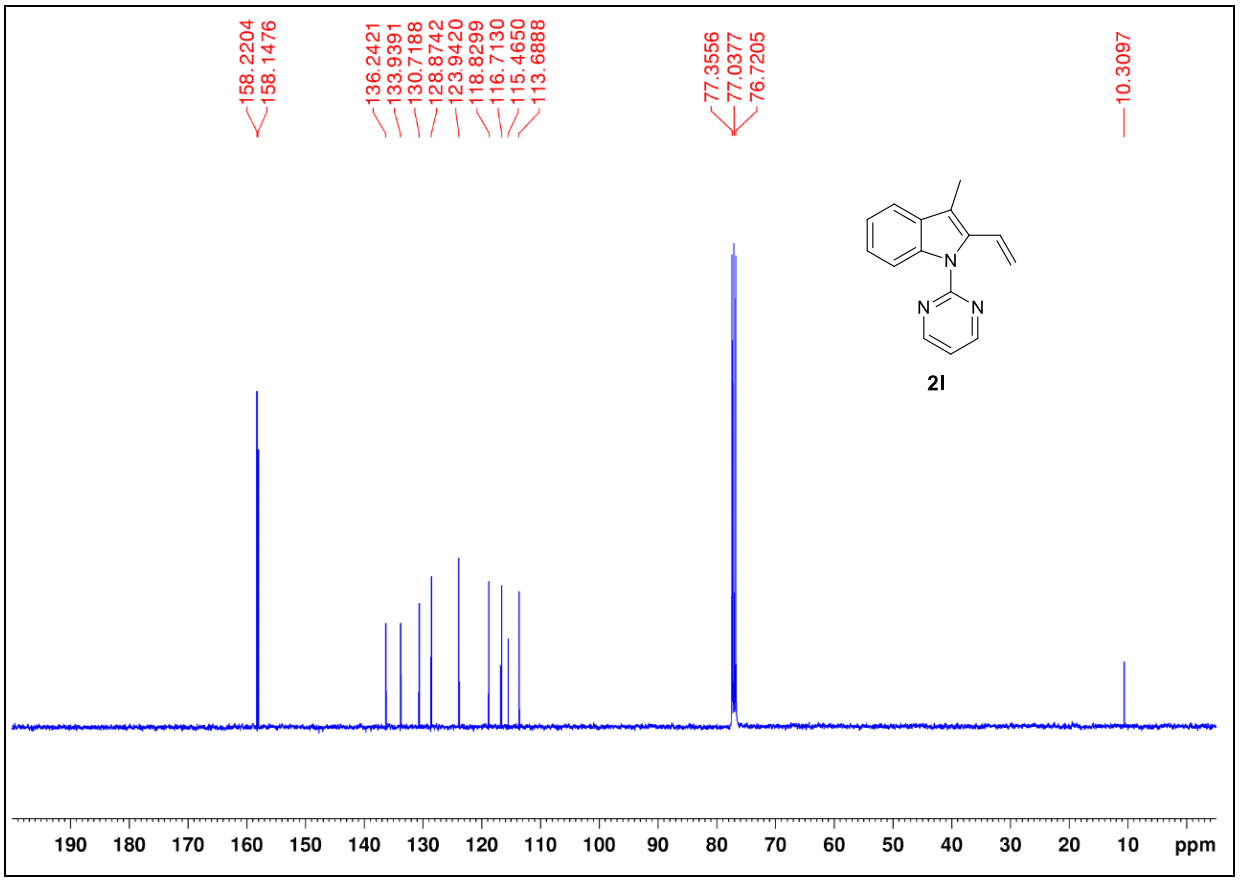
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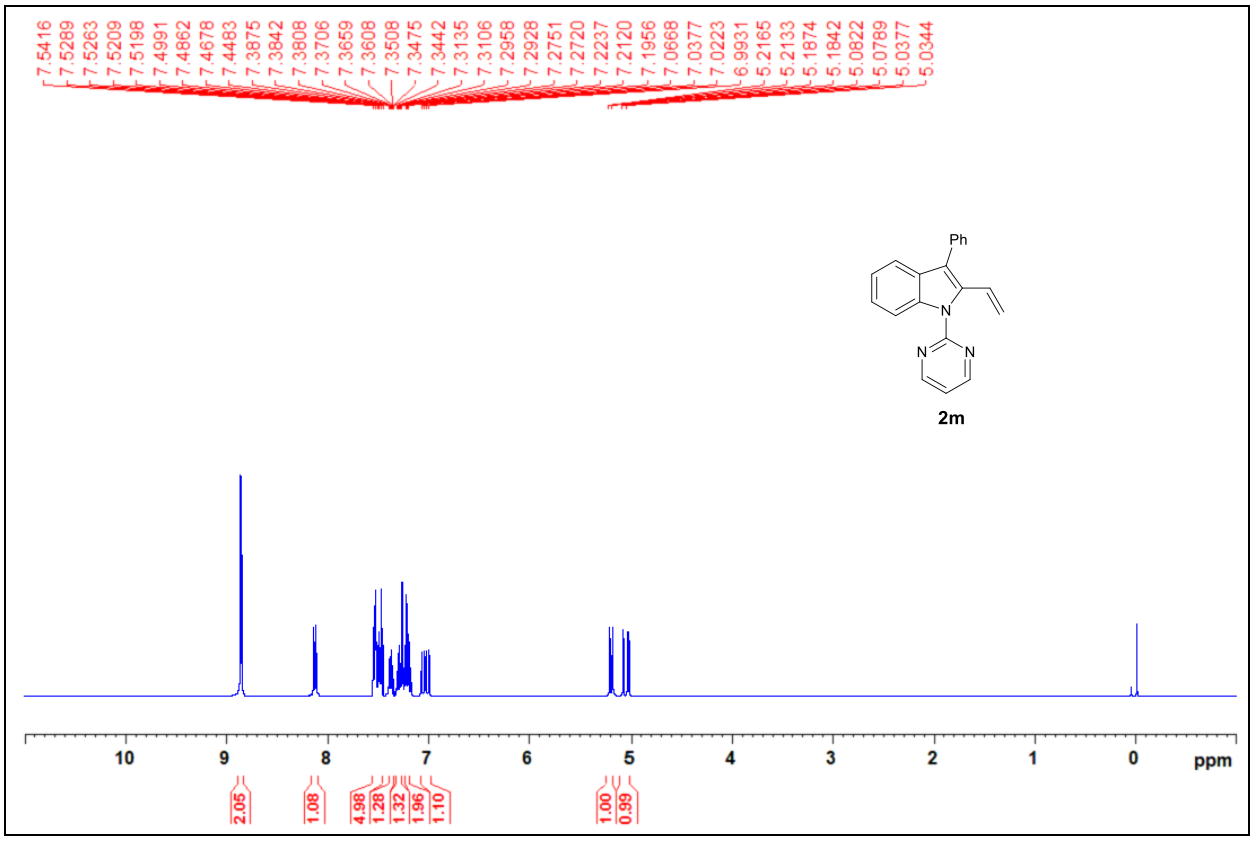
ppm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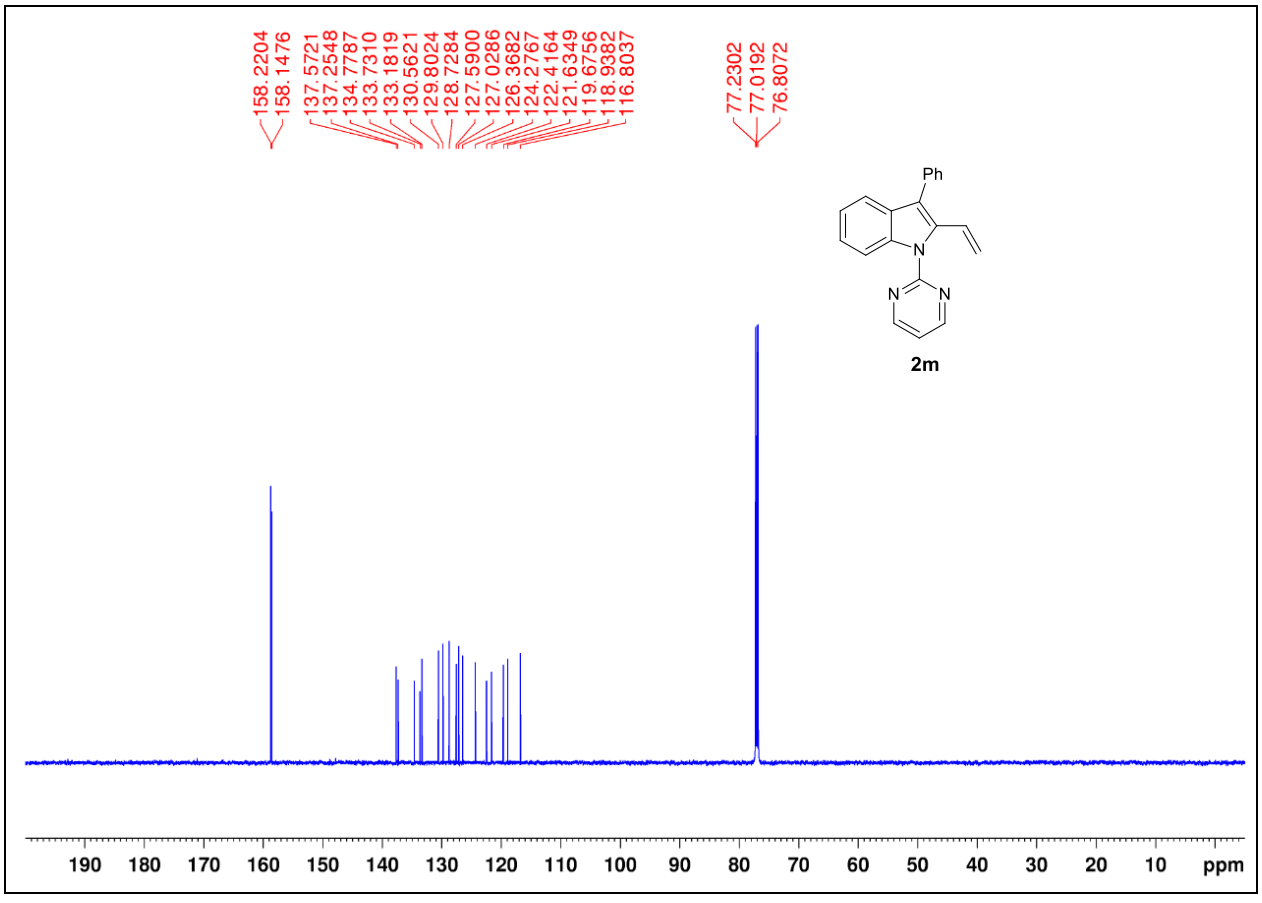
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N
N
2m
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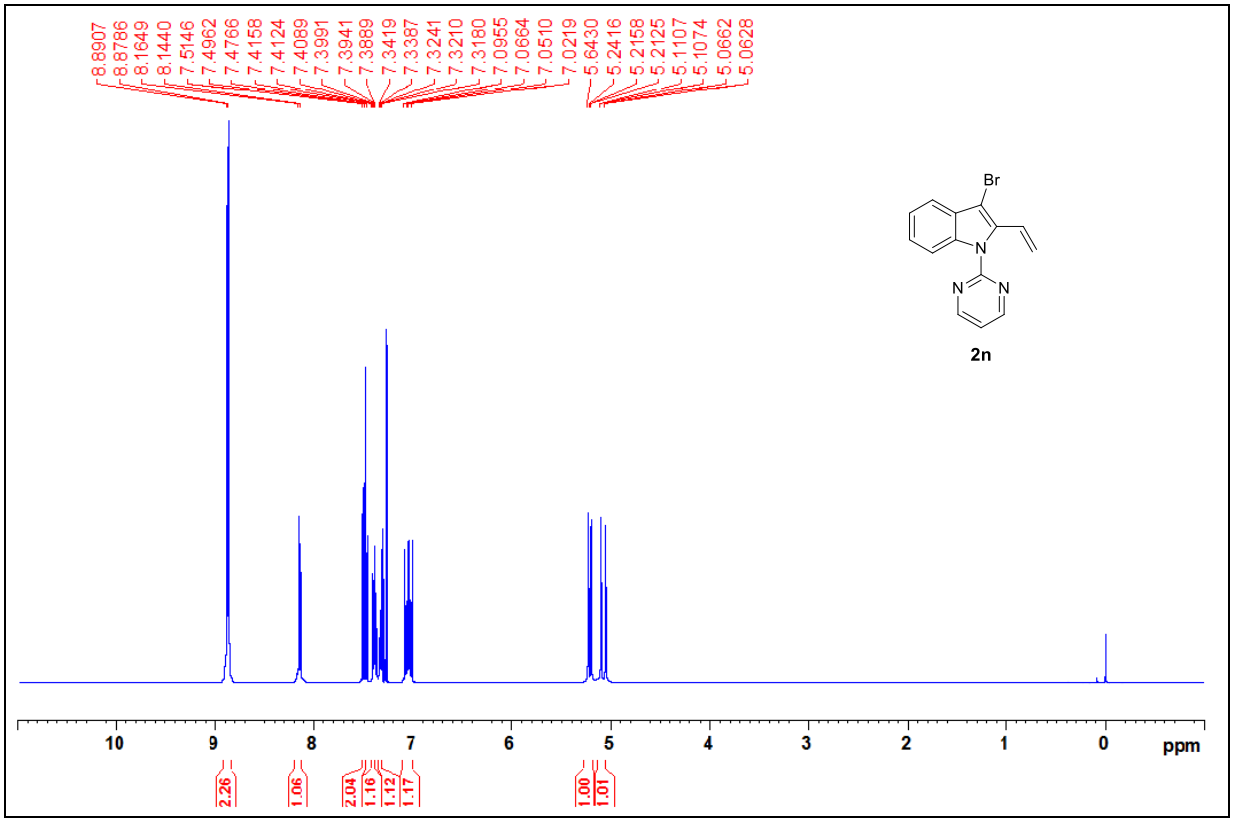
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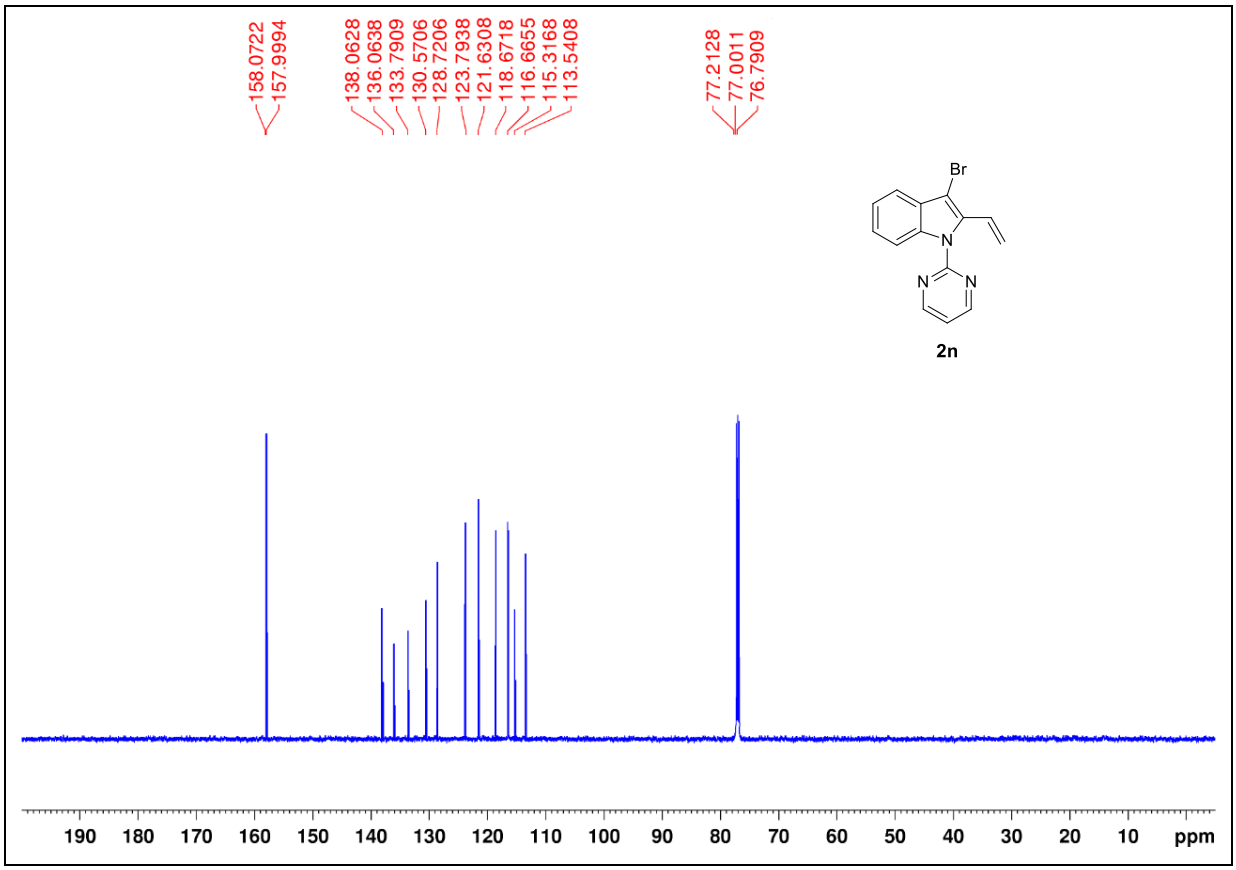
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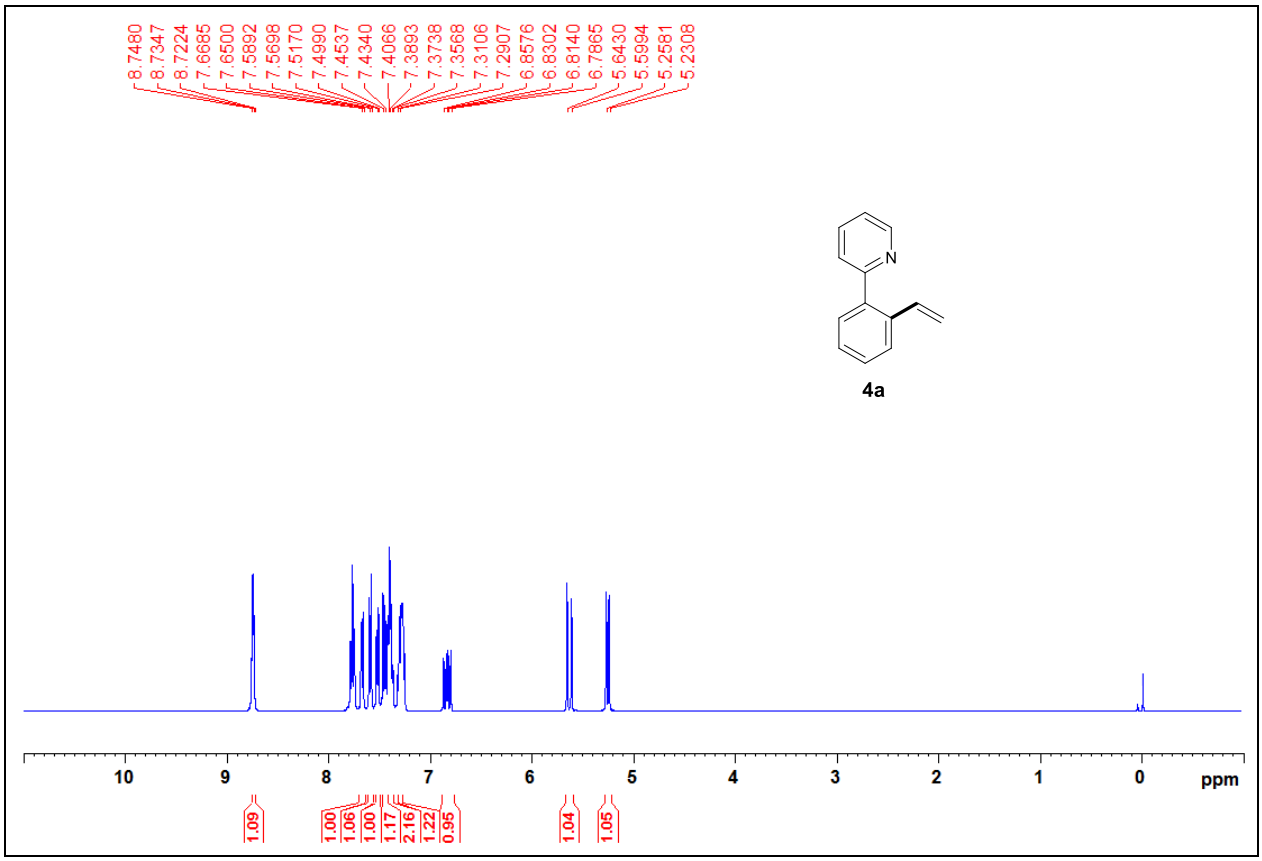
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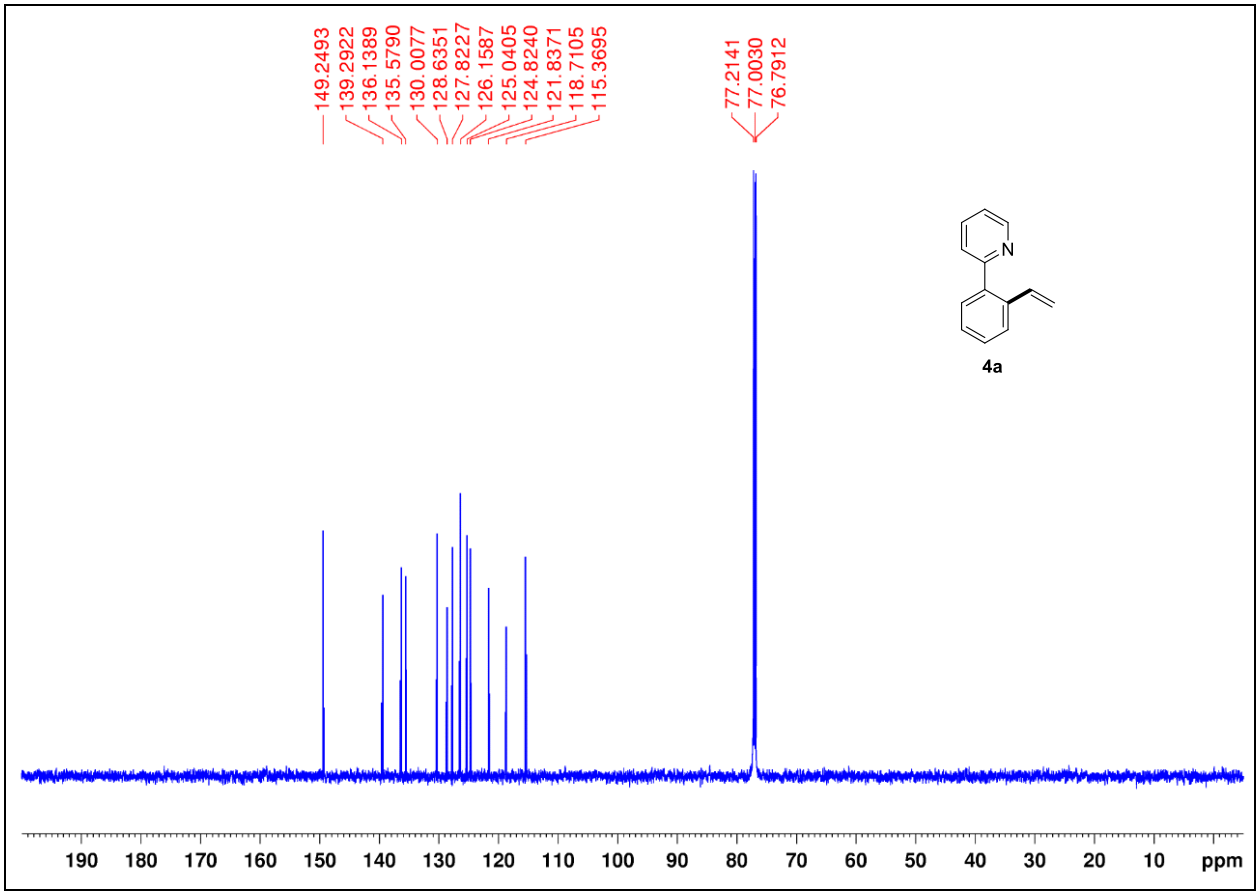
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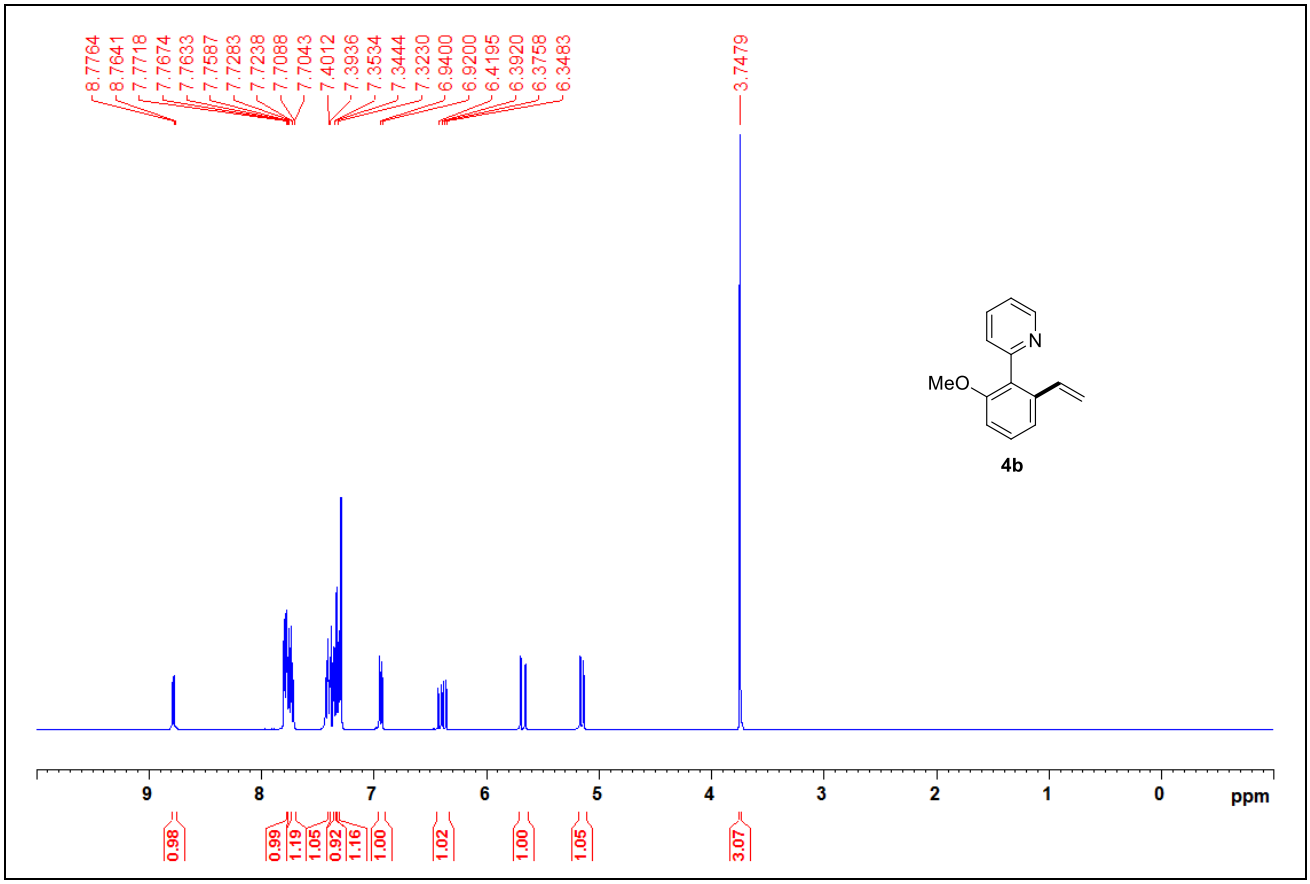
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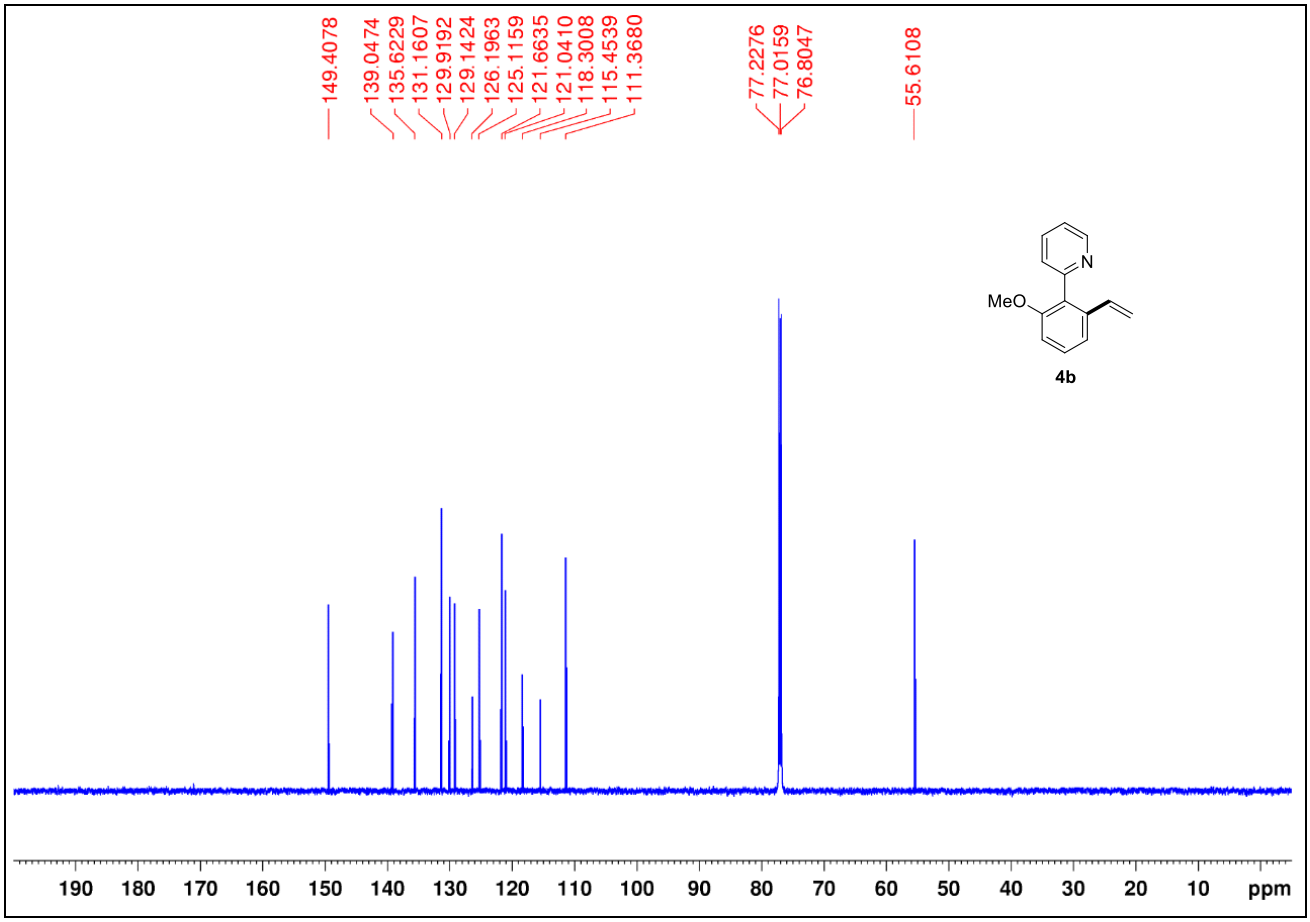
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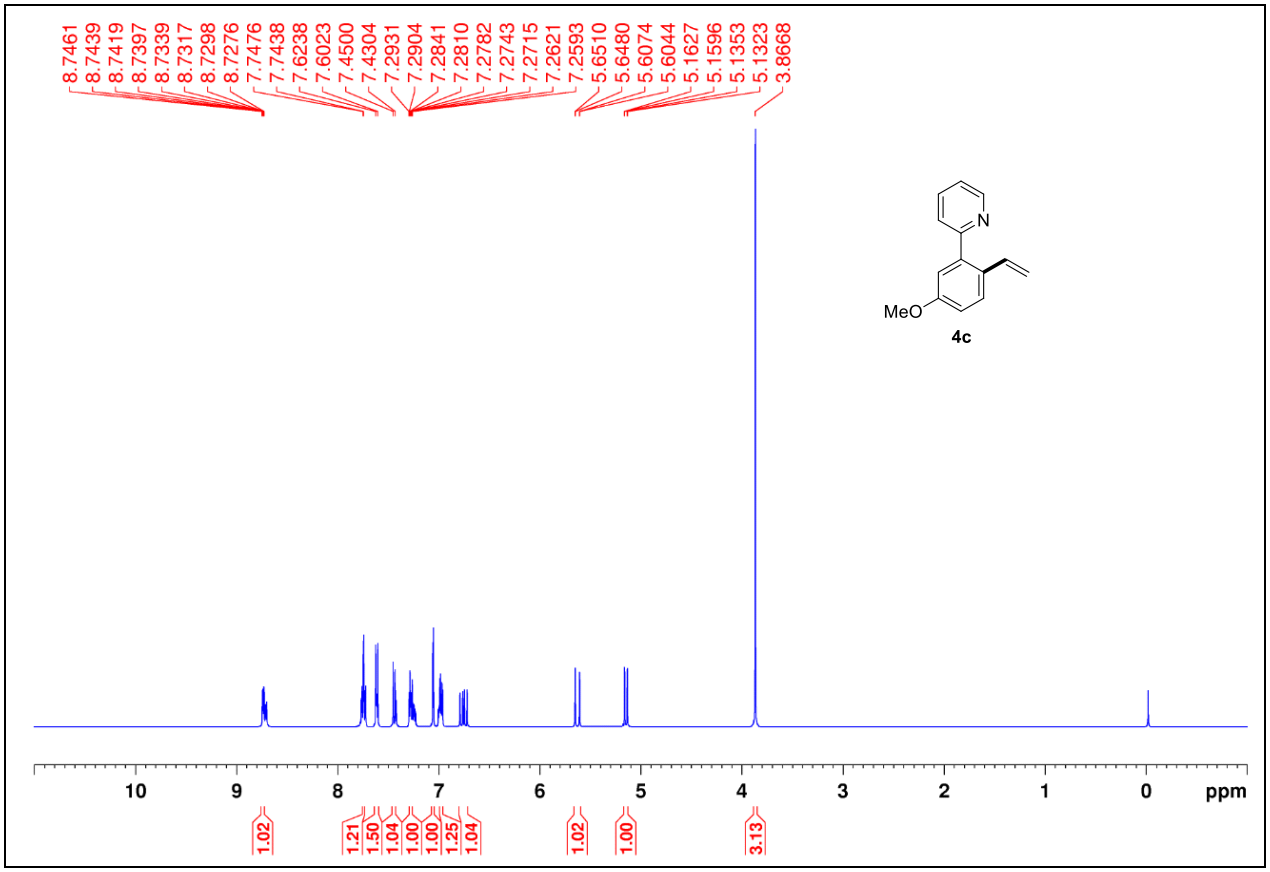
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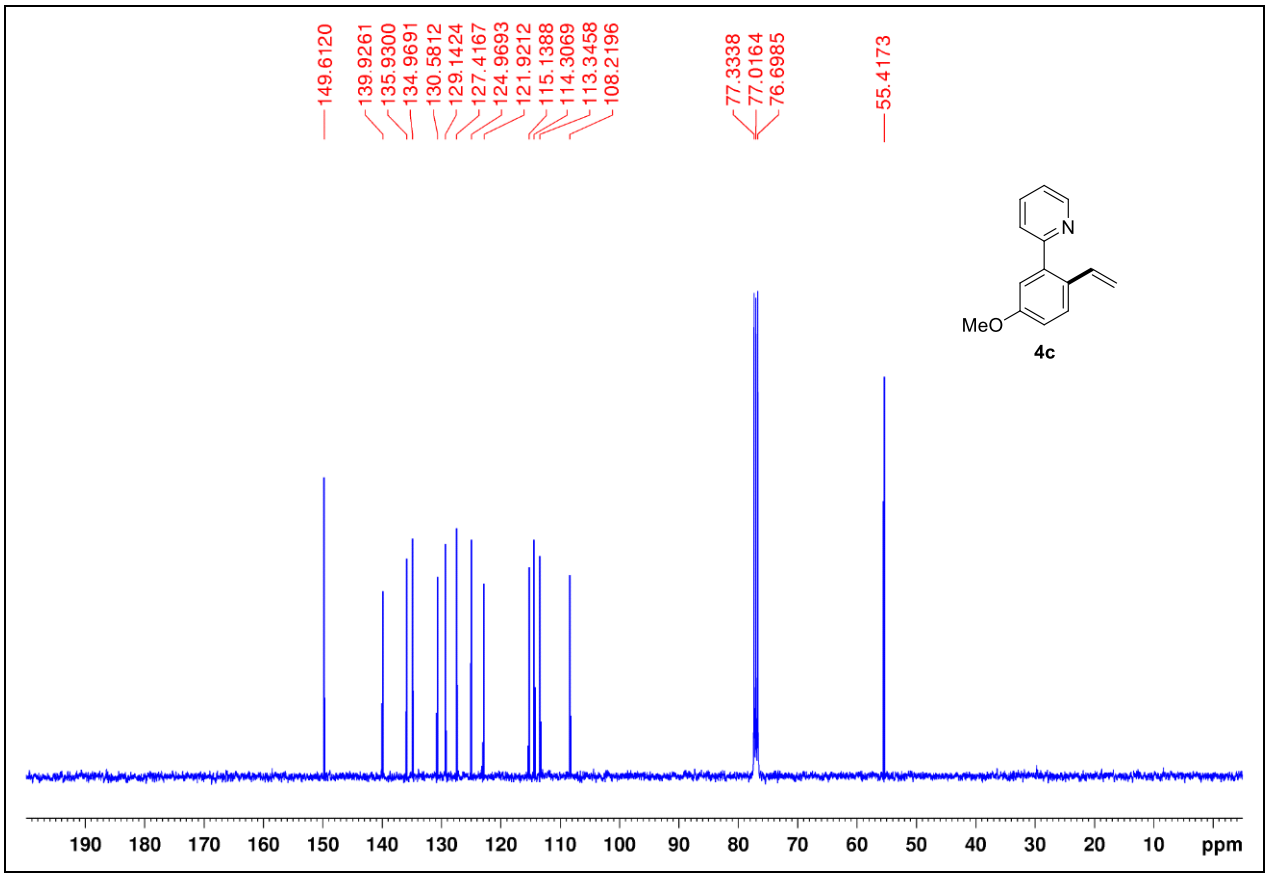
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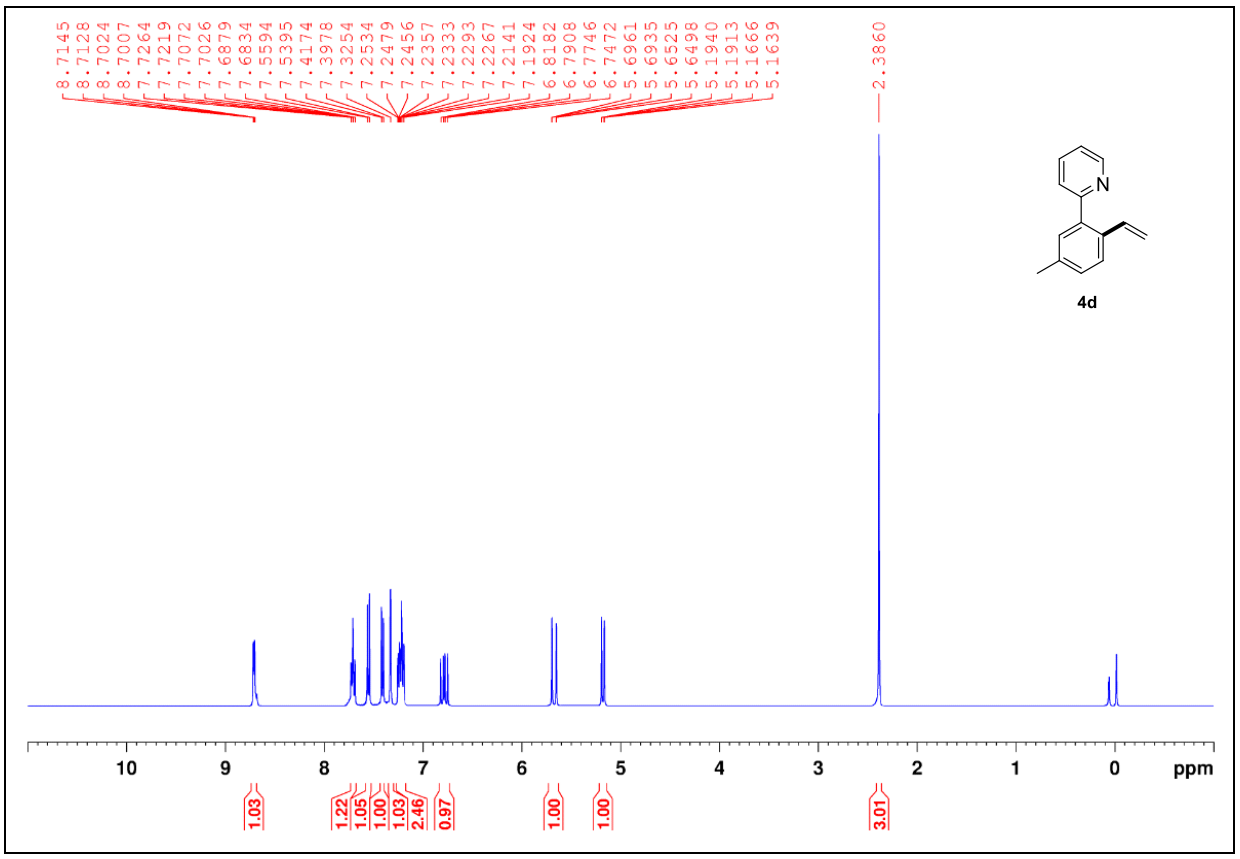
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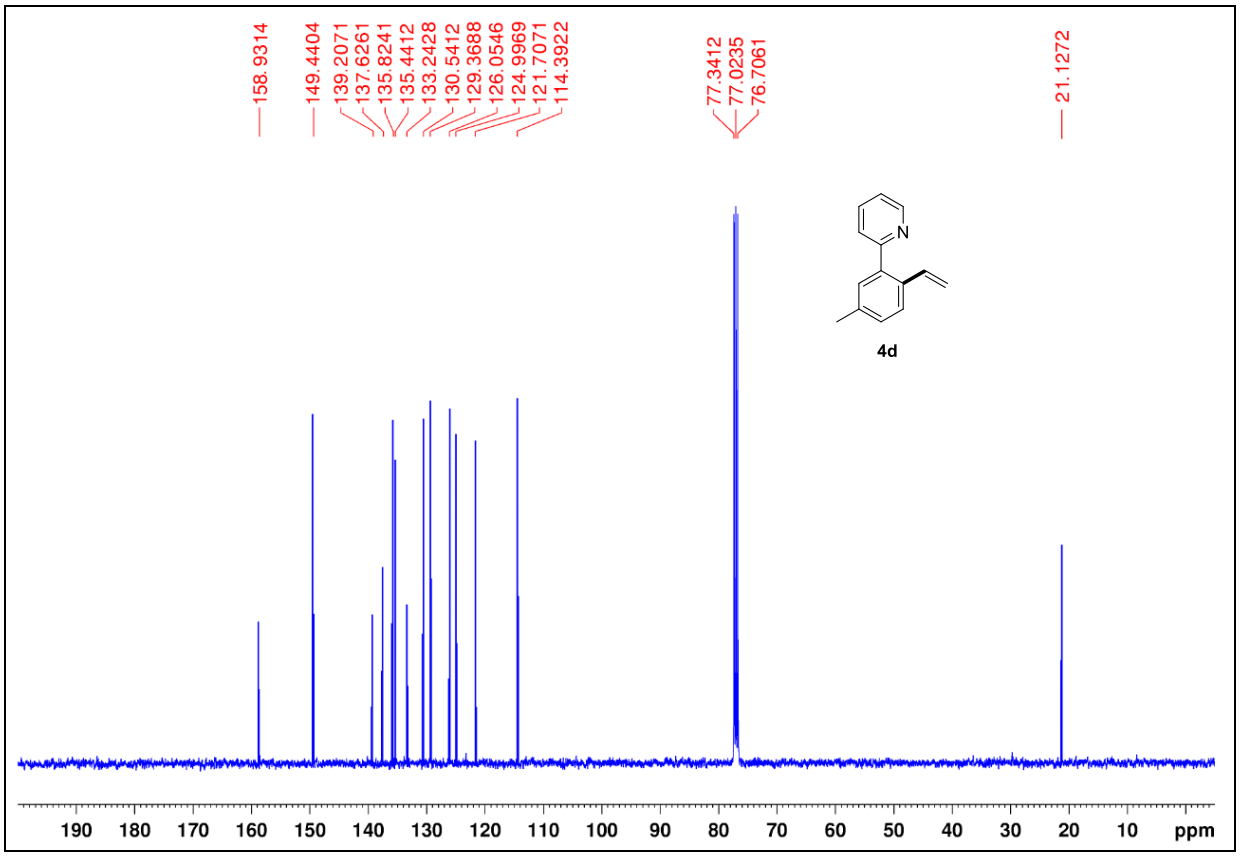
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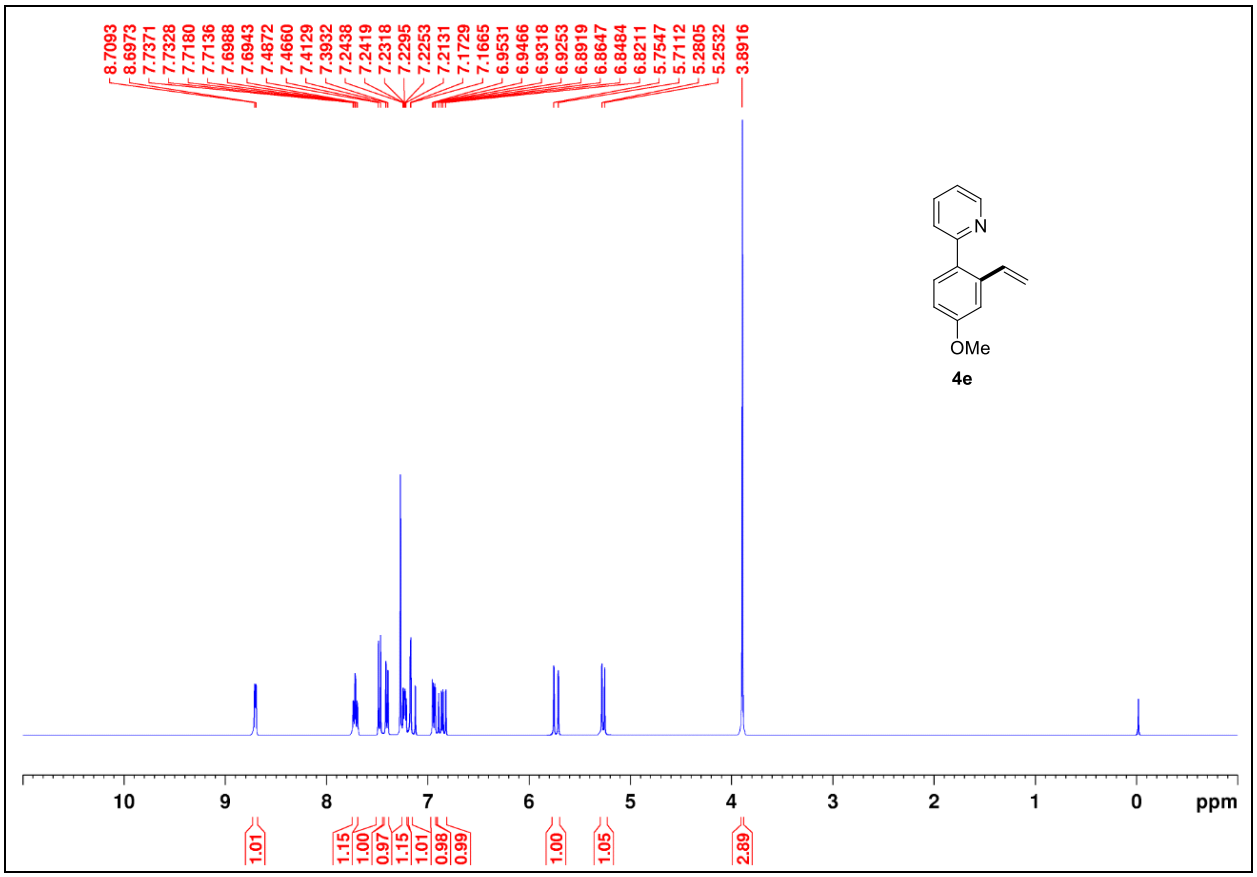
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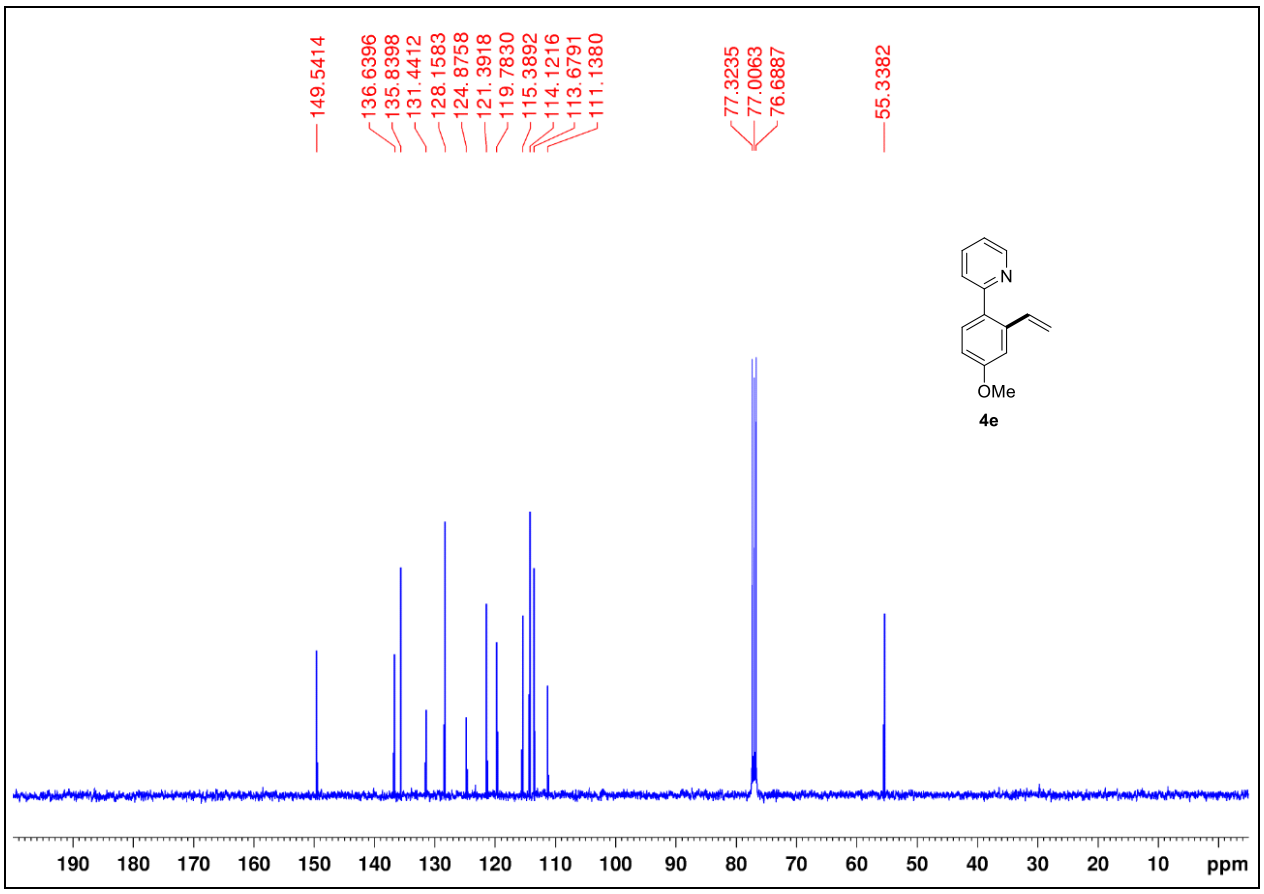
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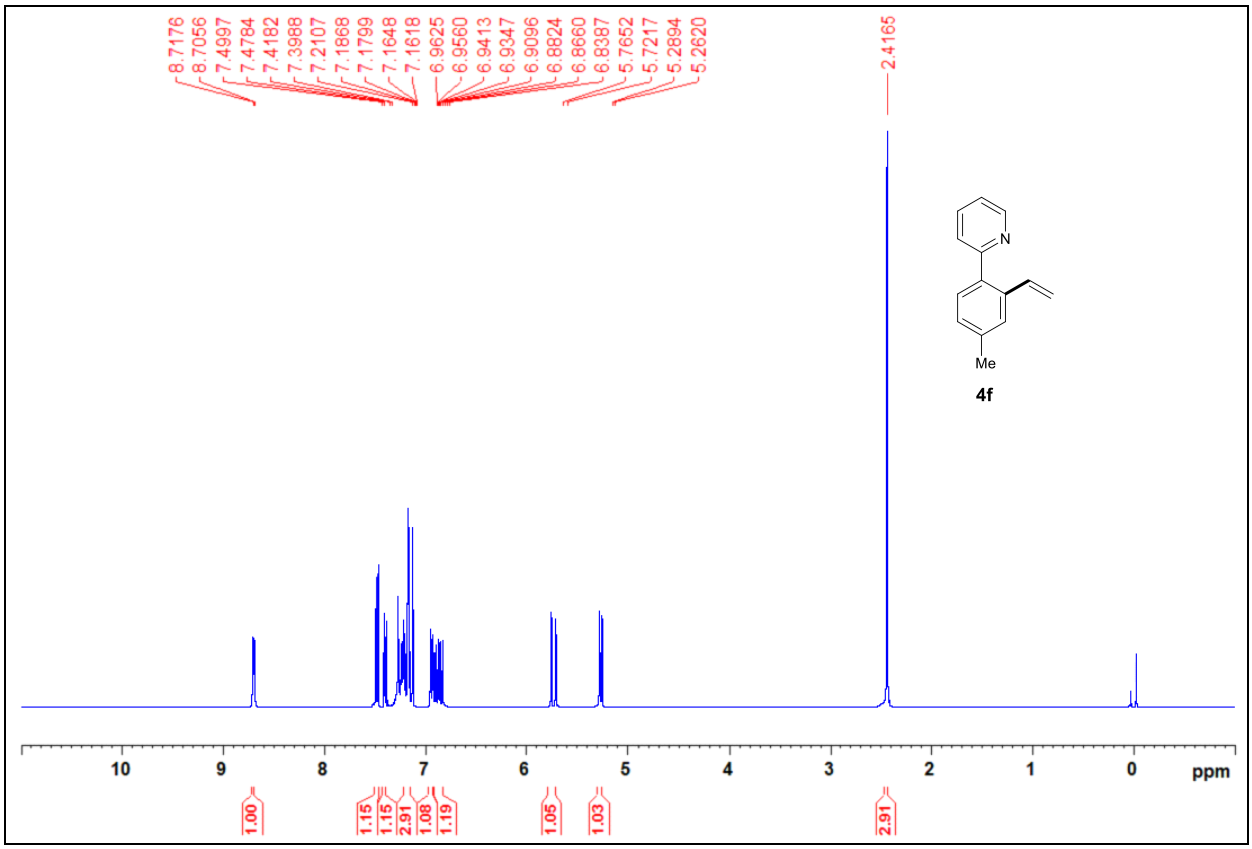
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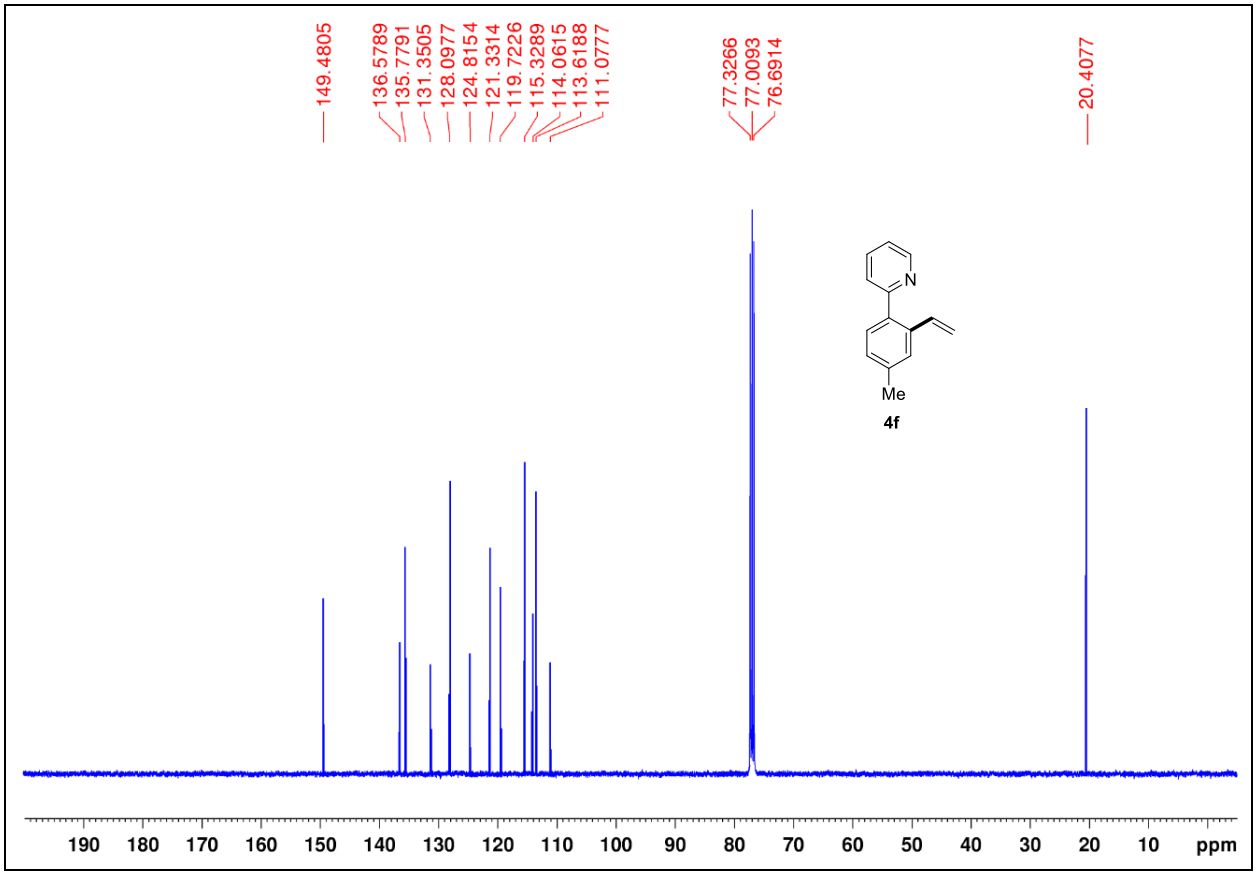
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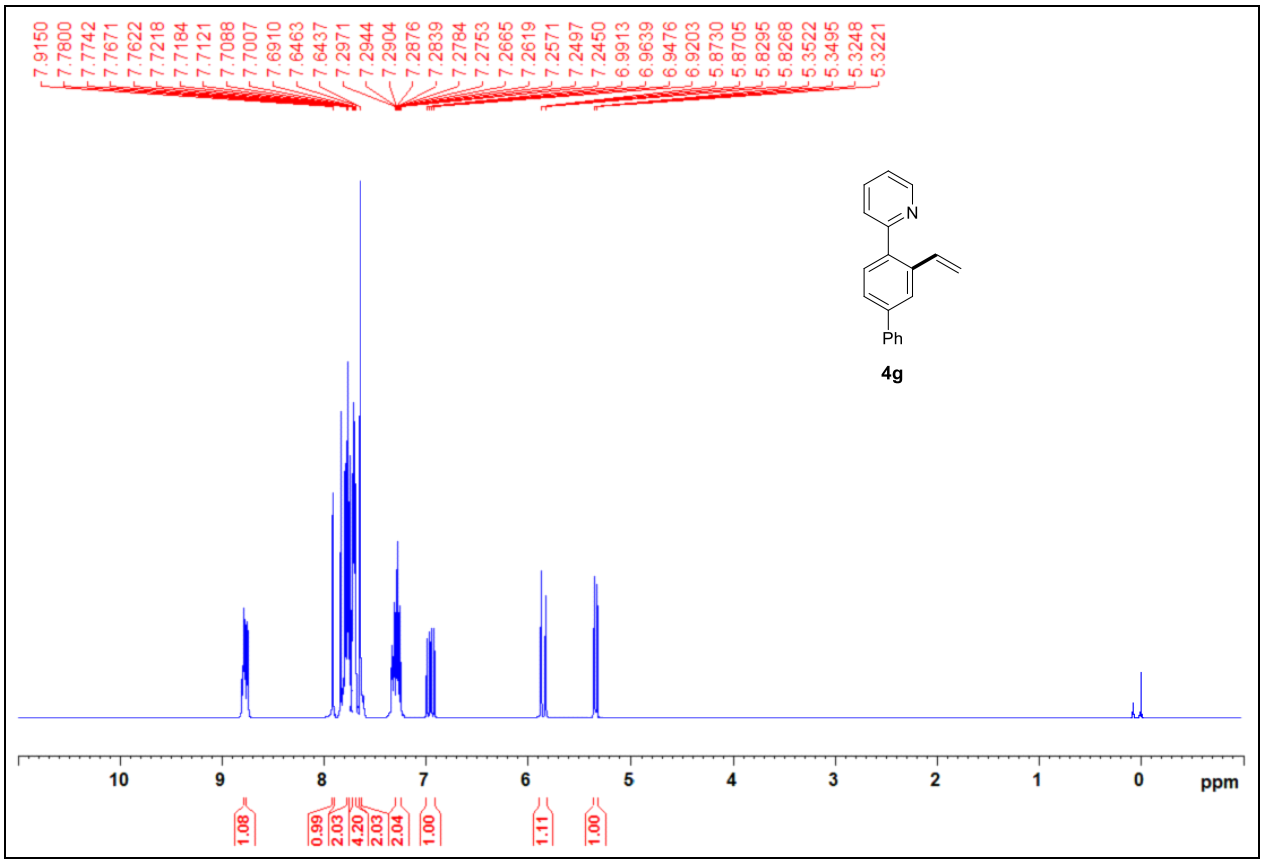
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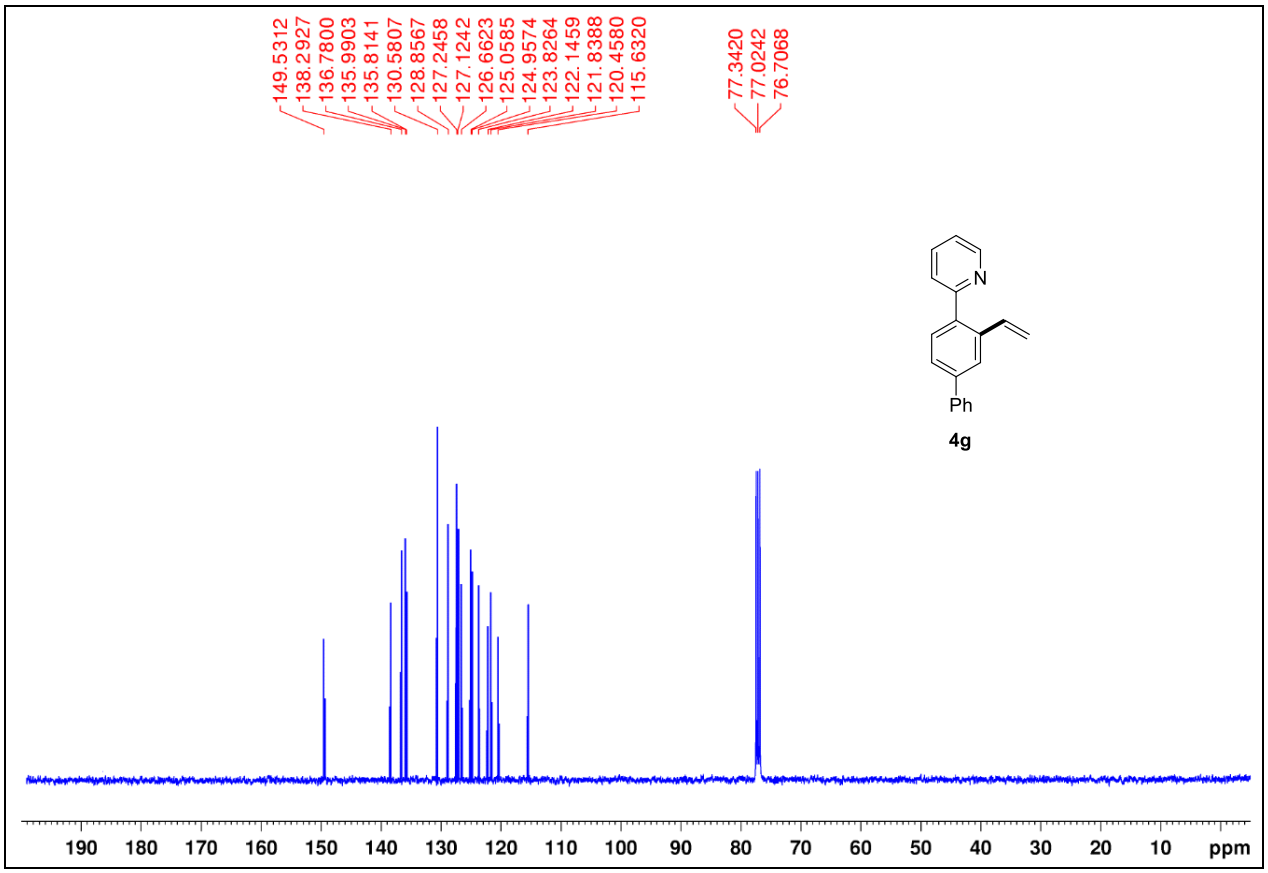
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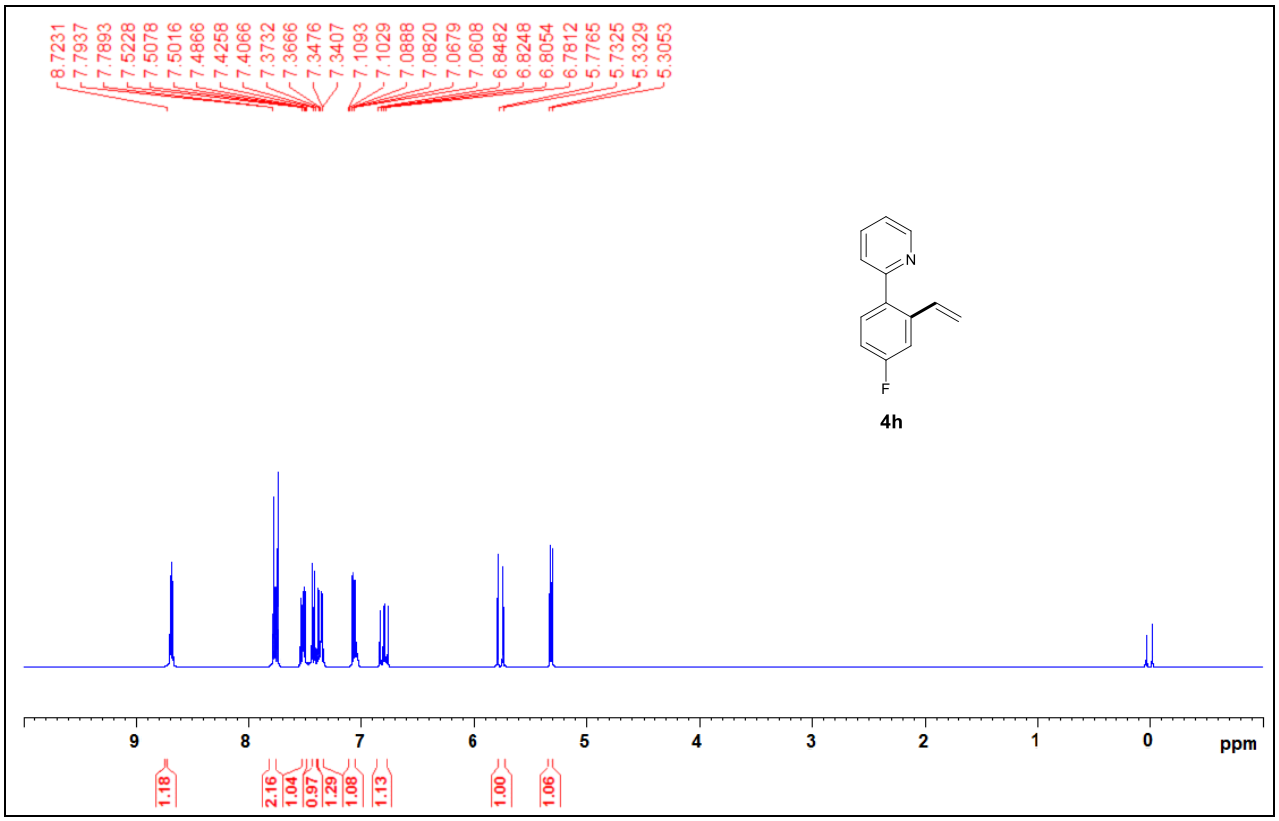
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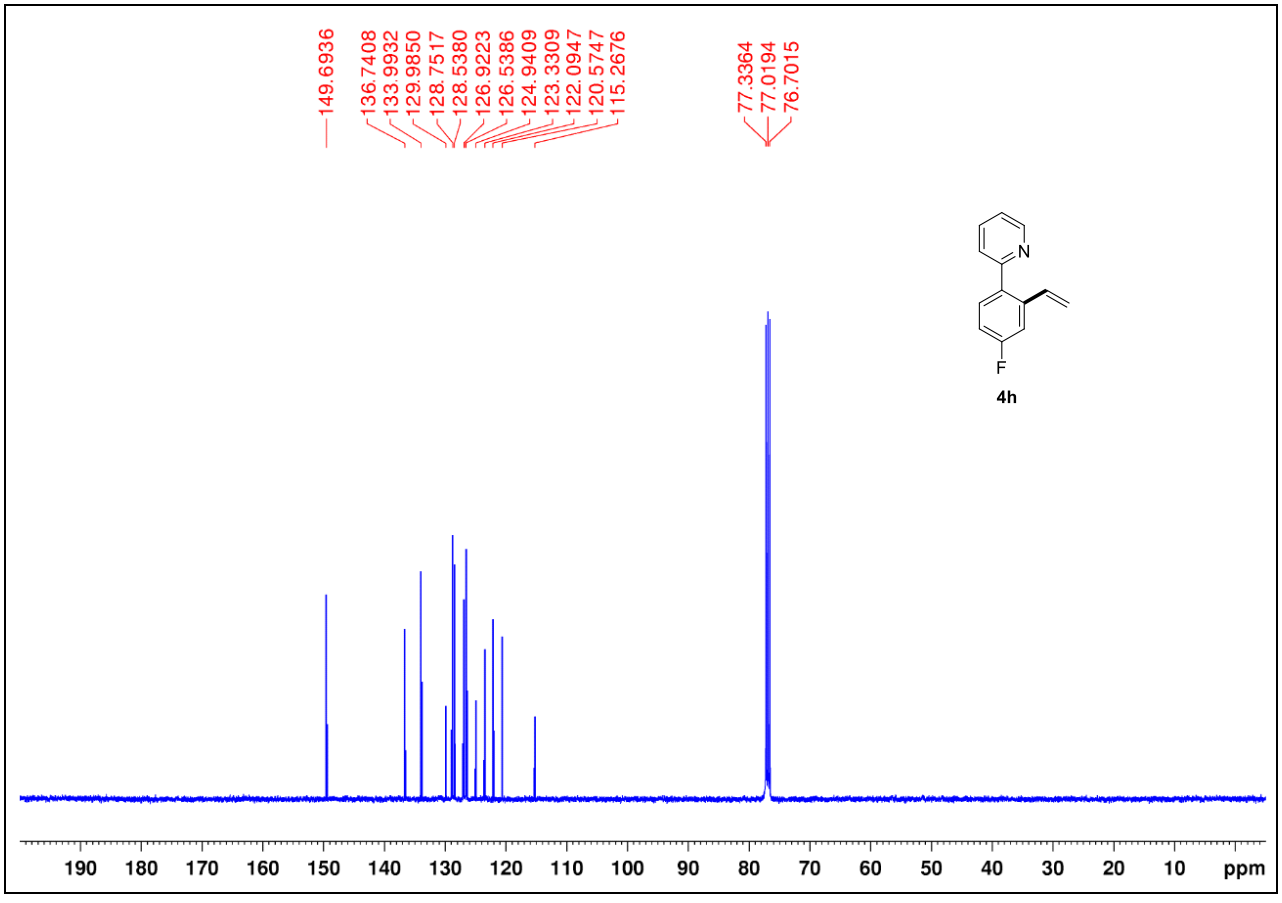
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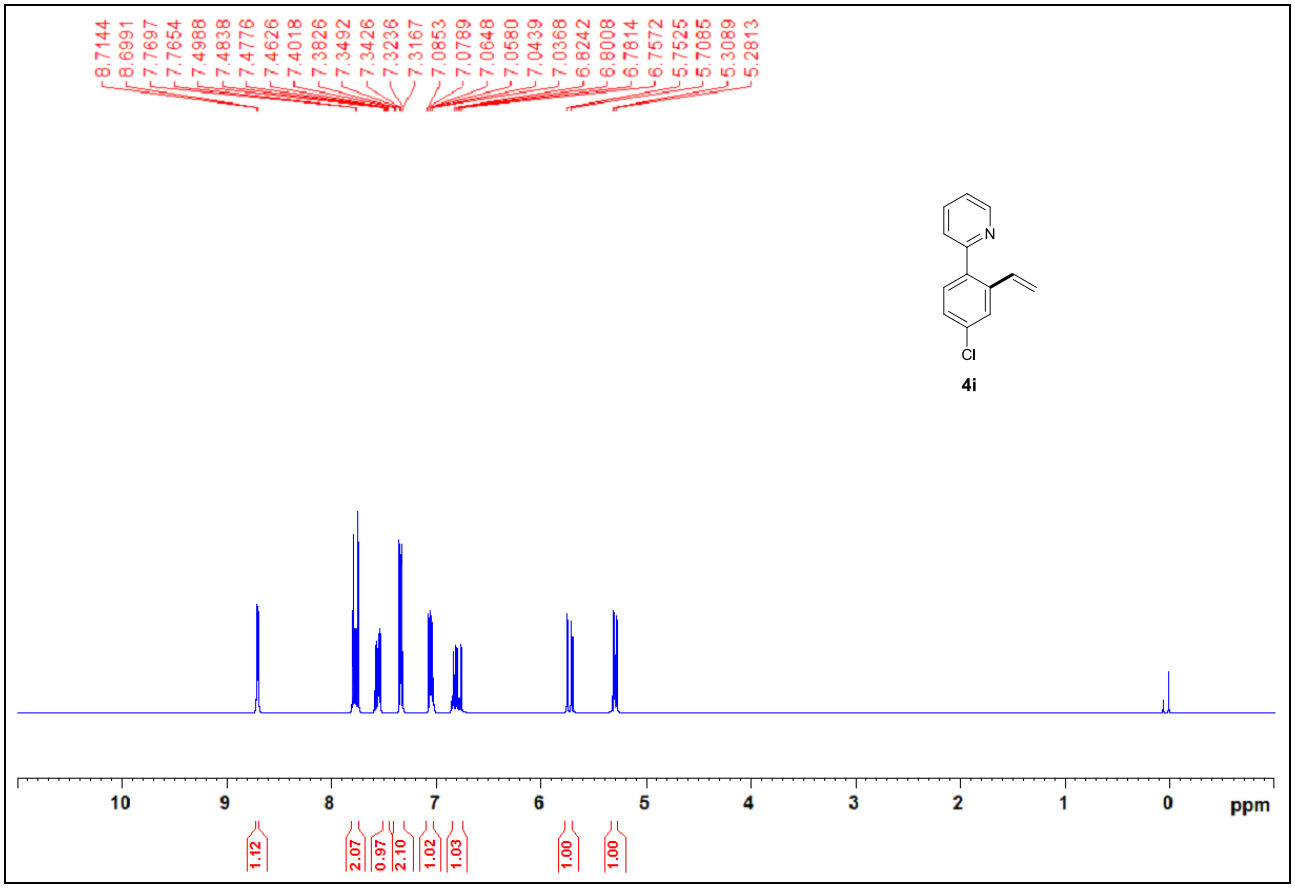
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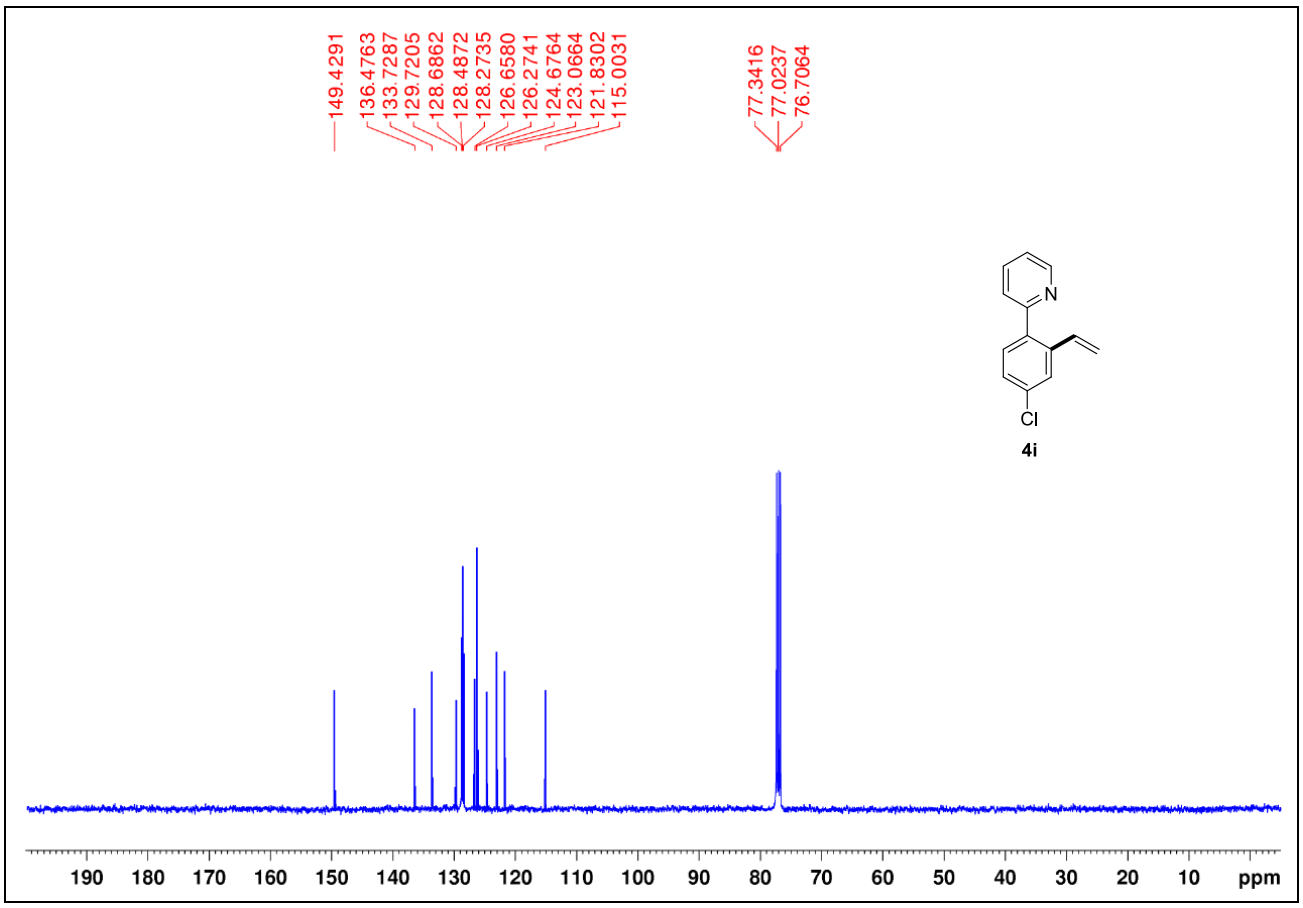
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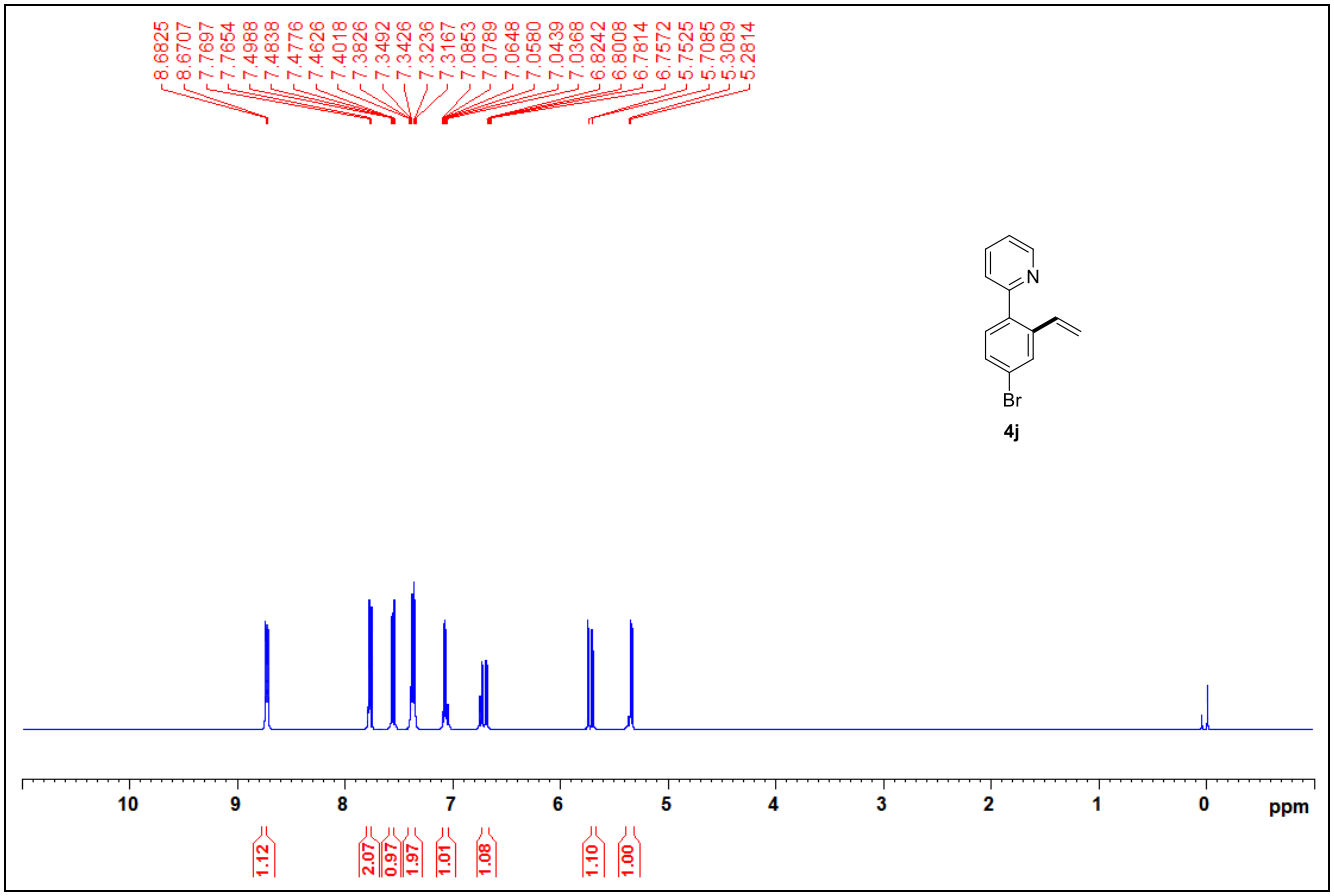
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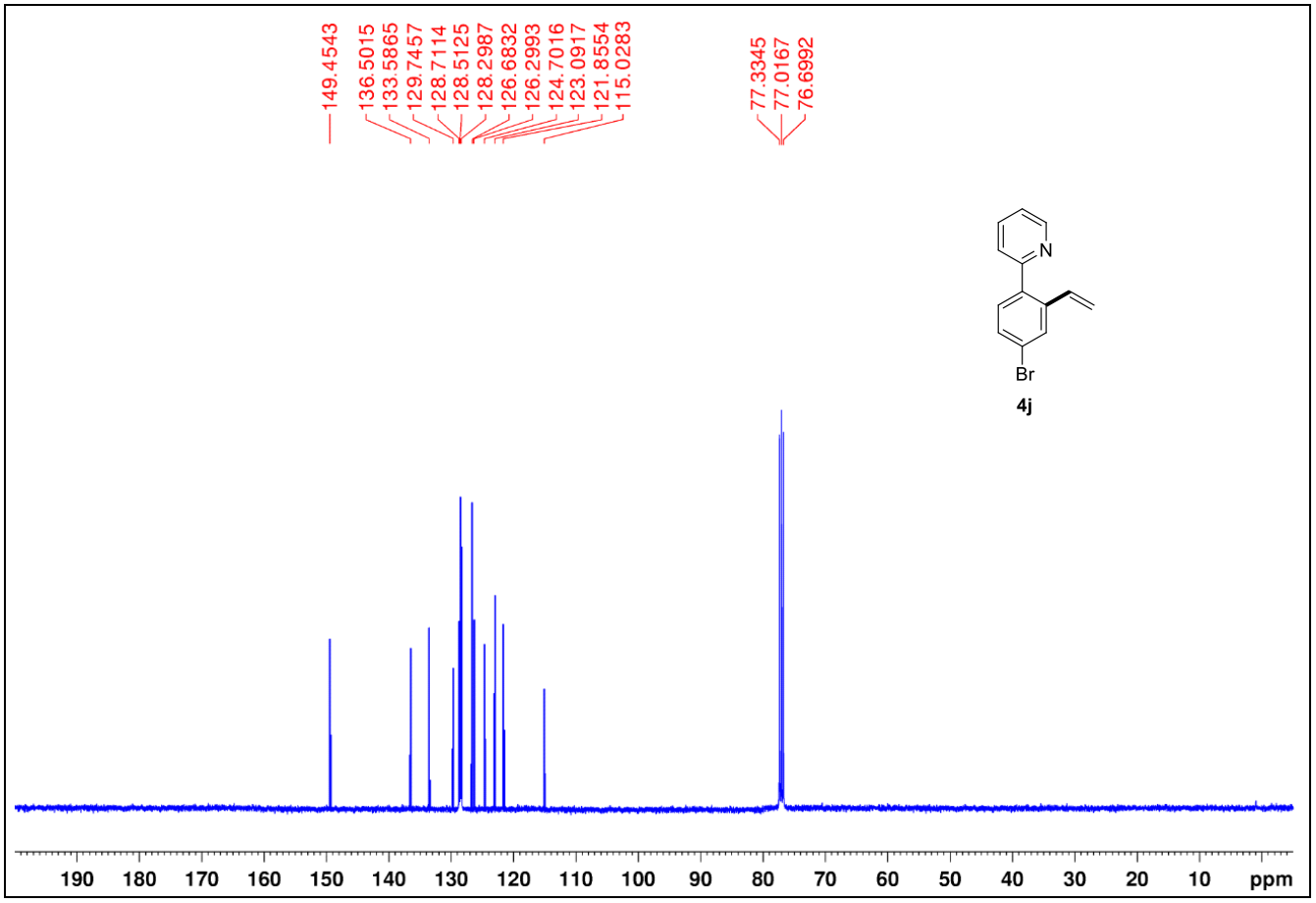
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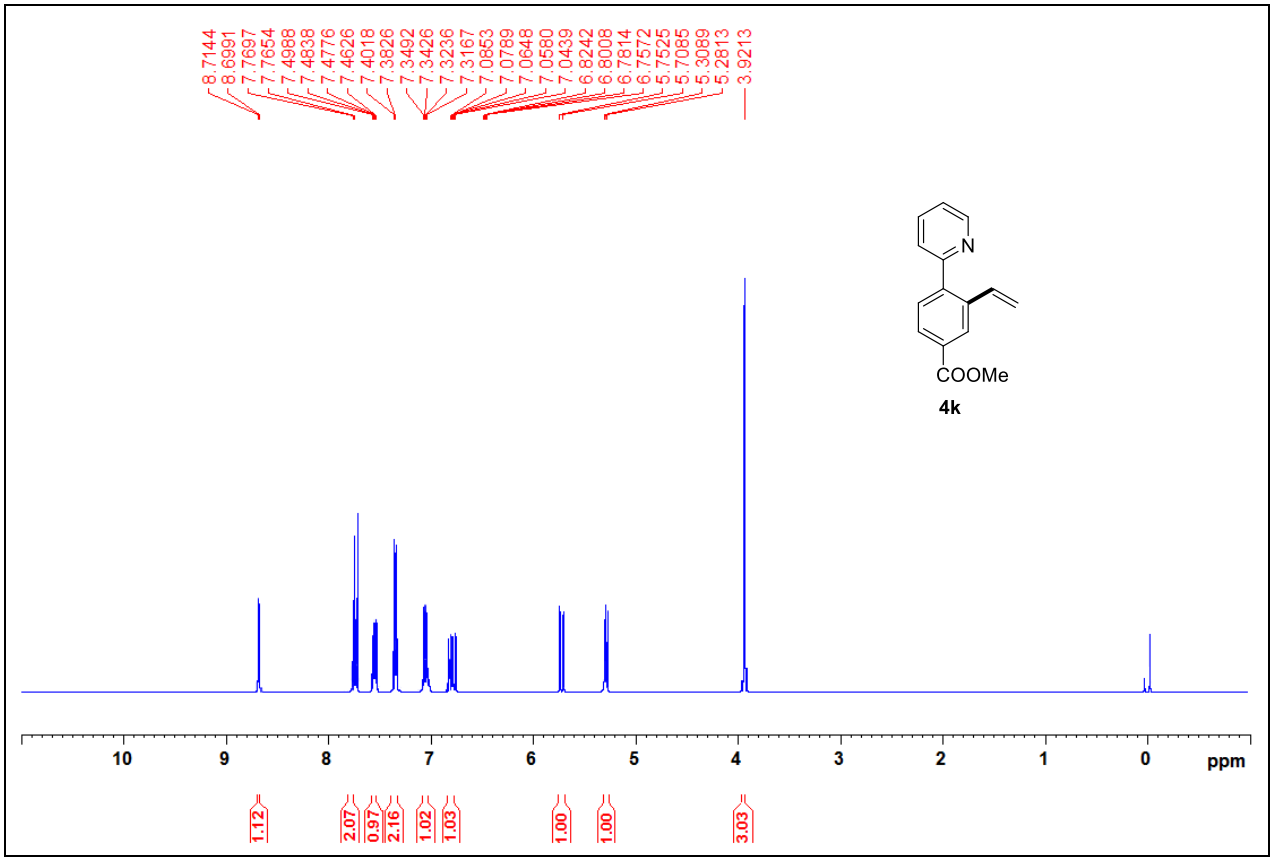
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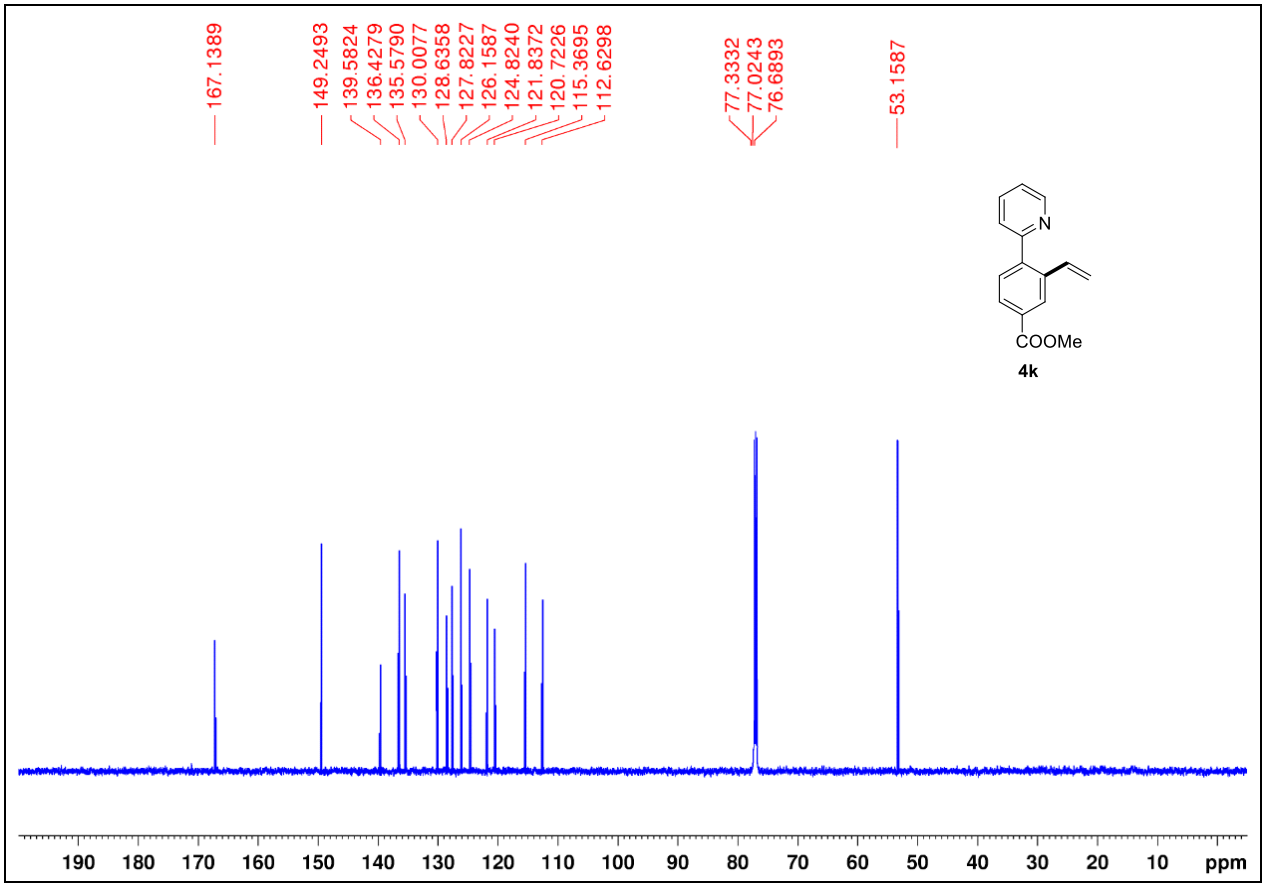
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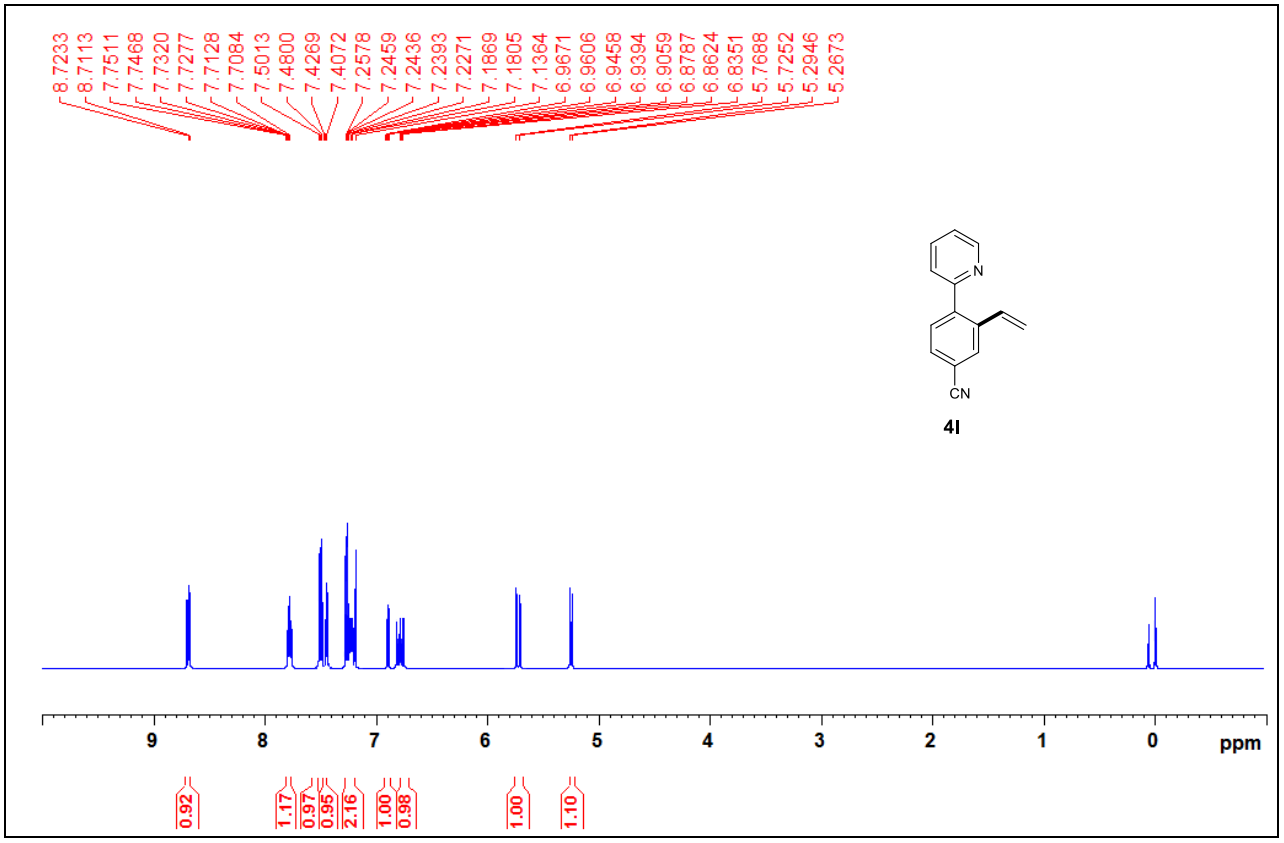
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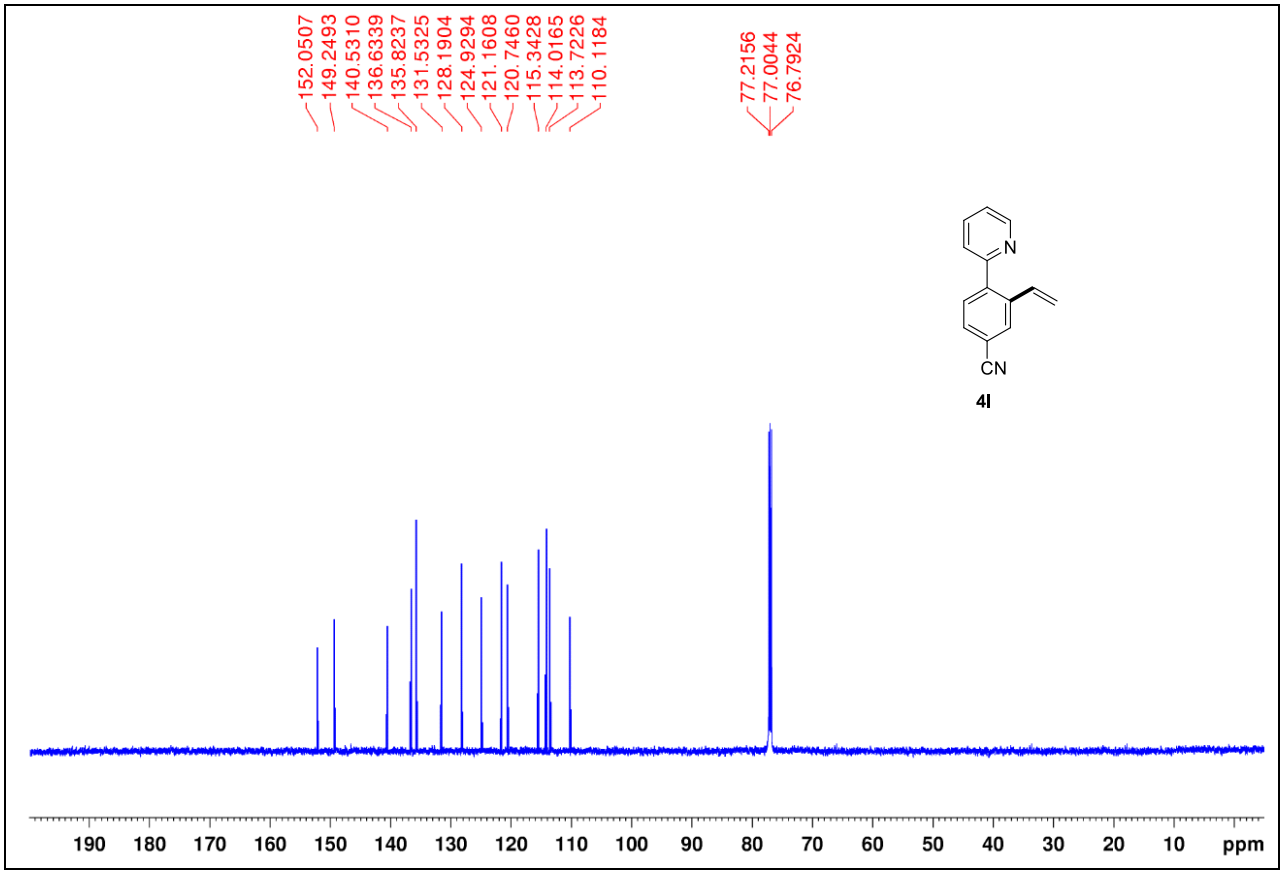
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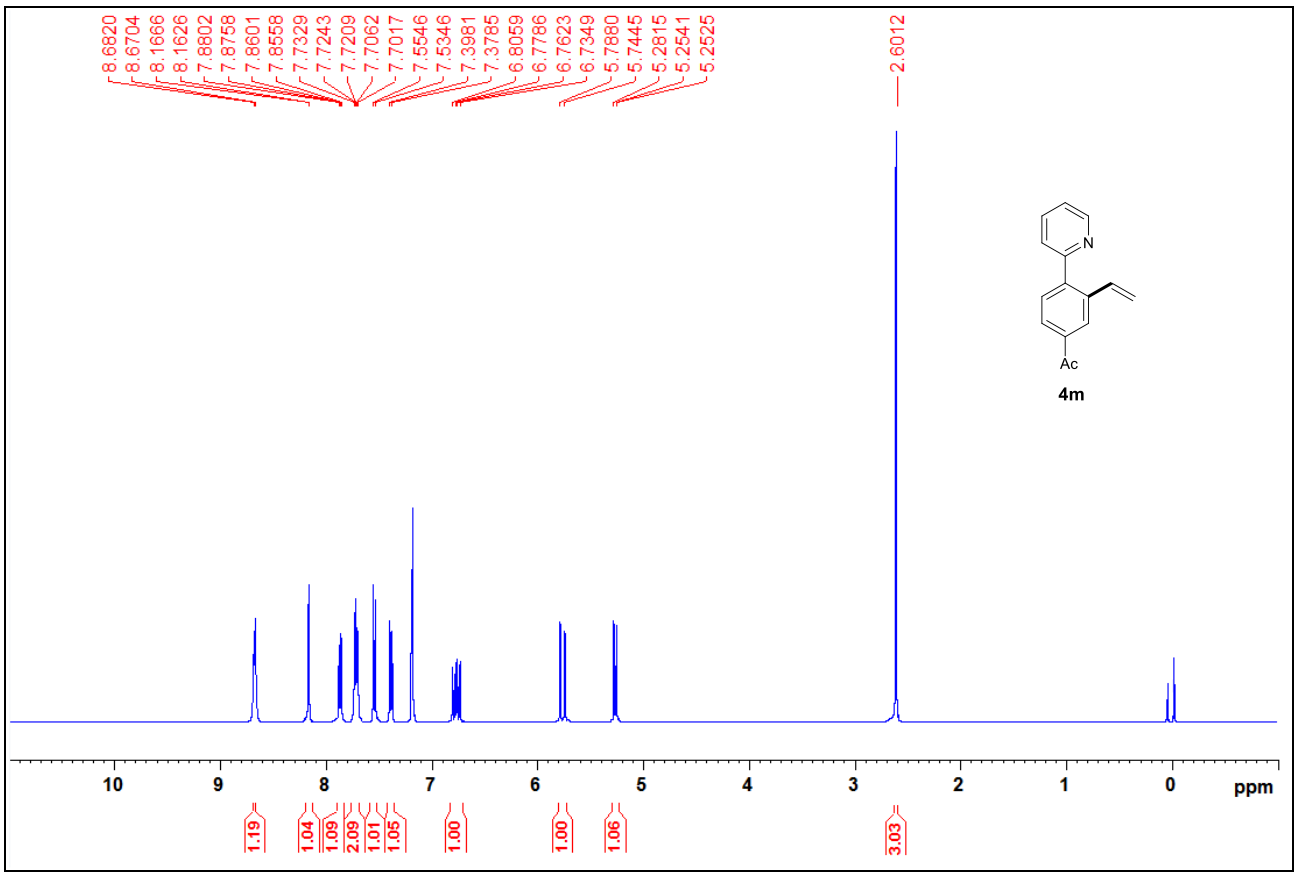
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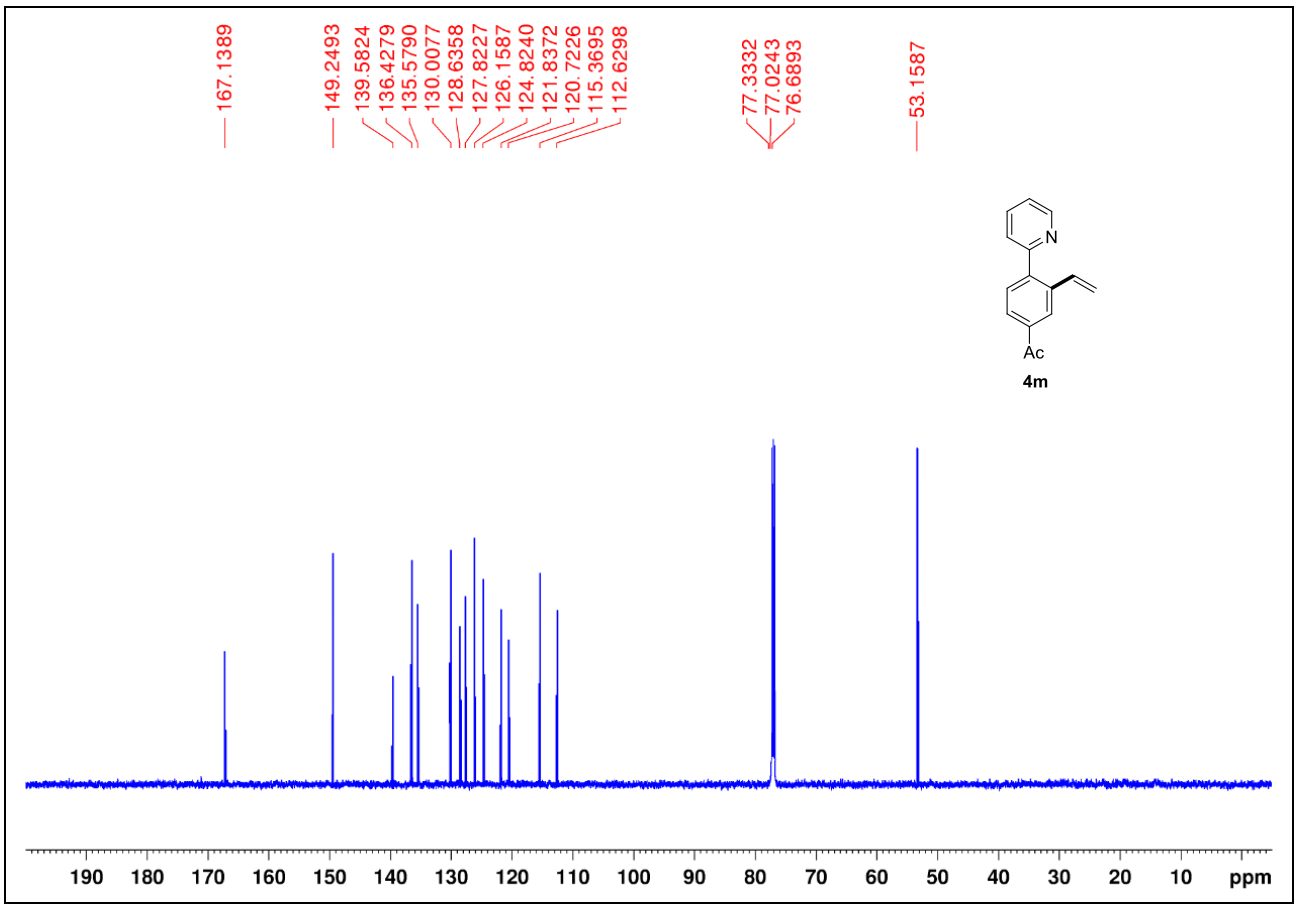
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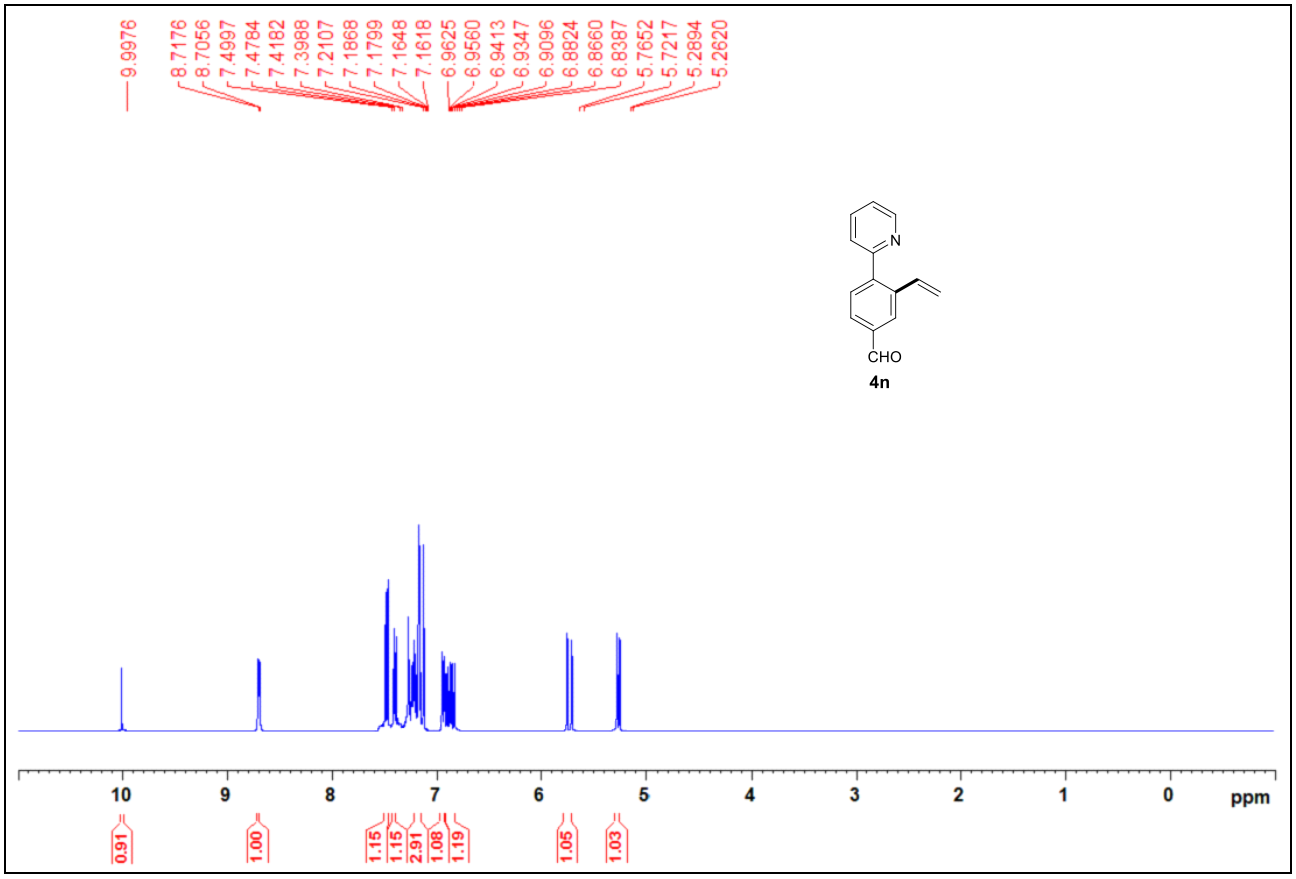
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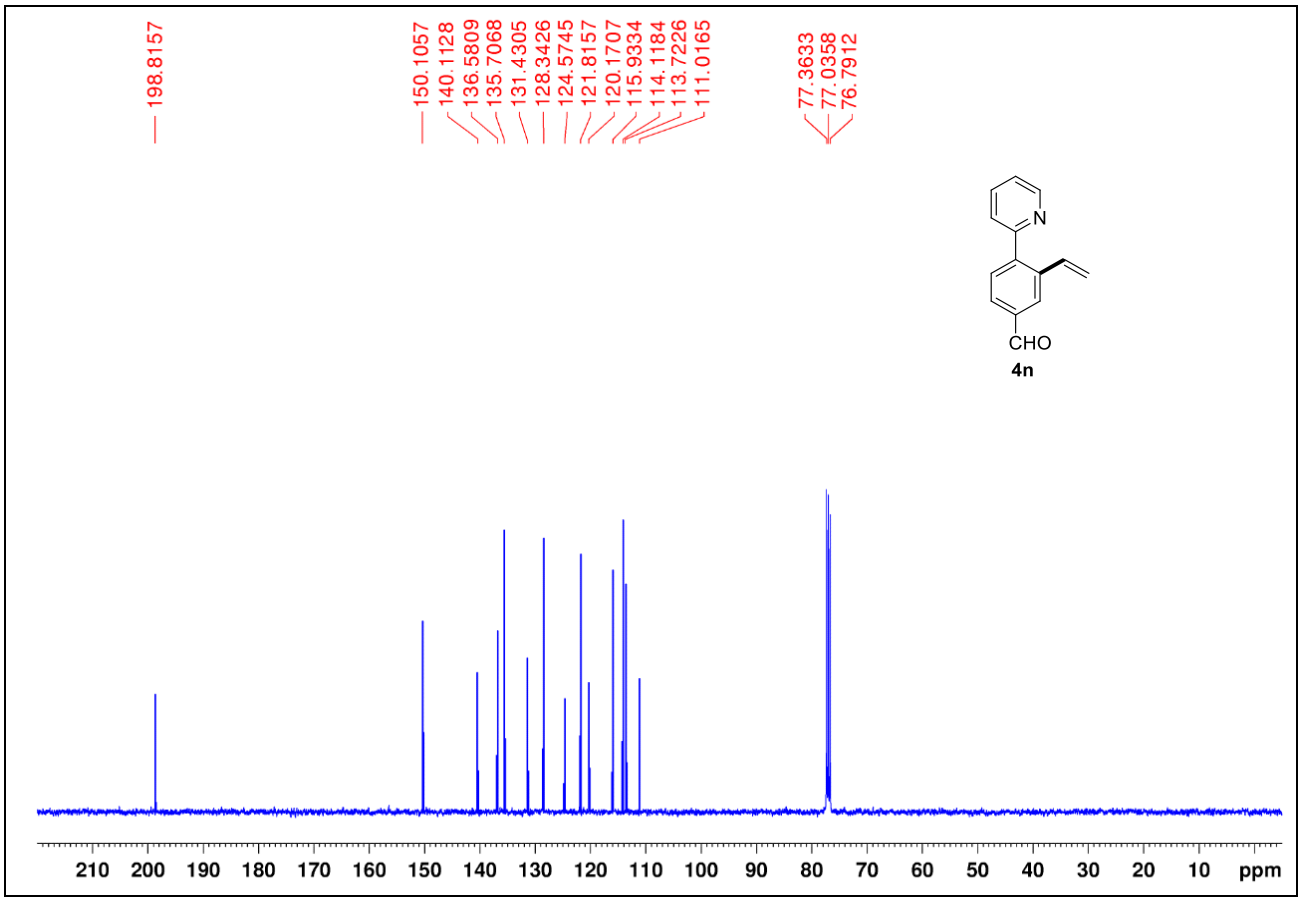
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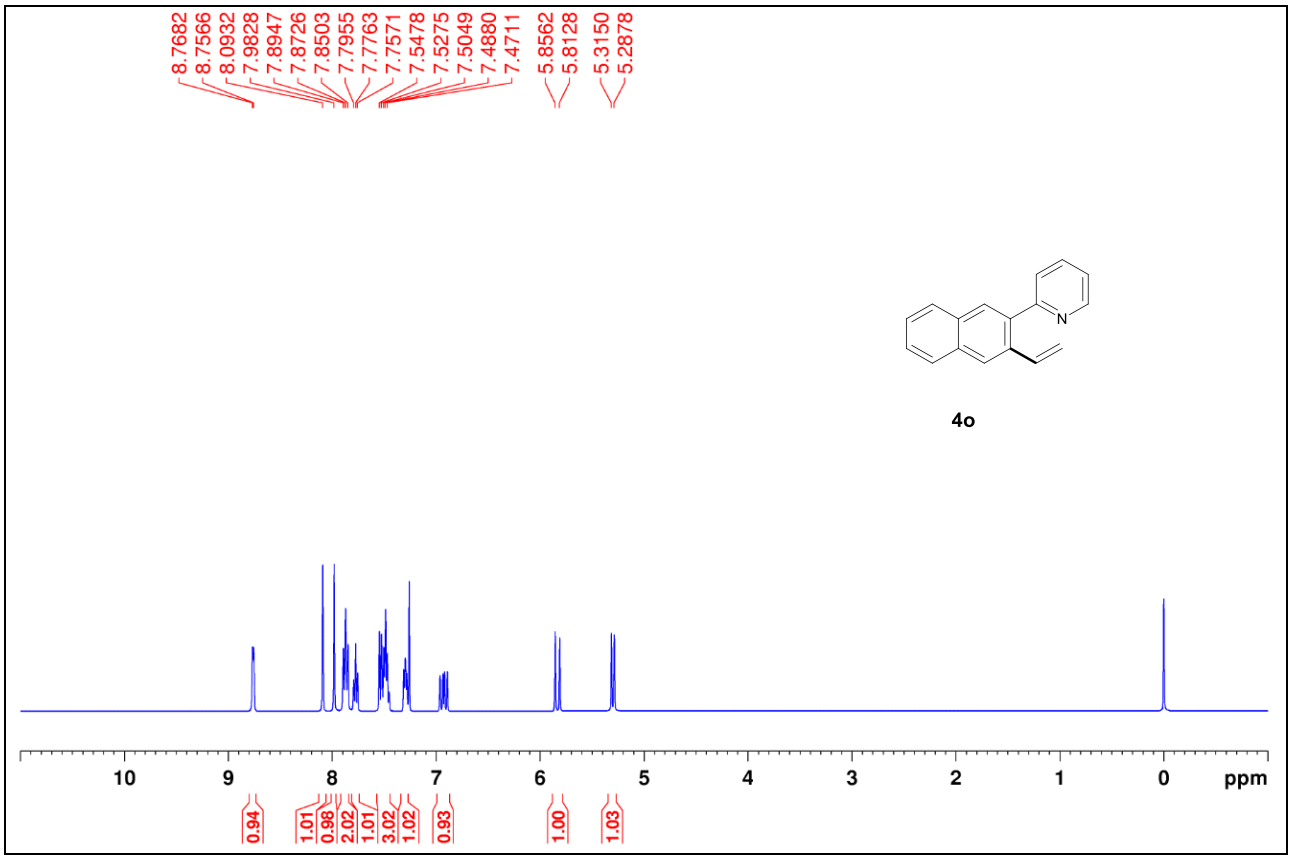
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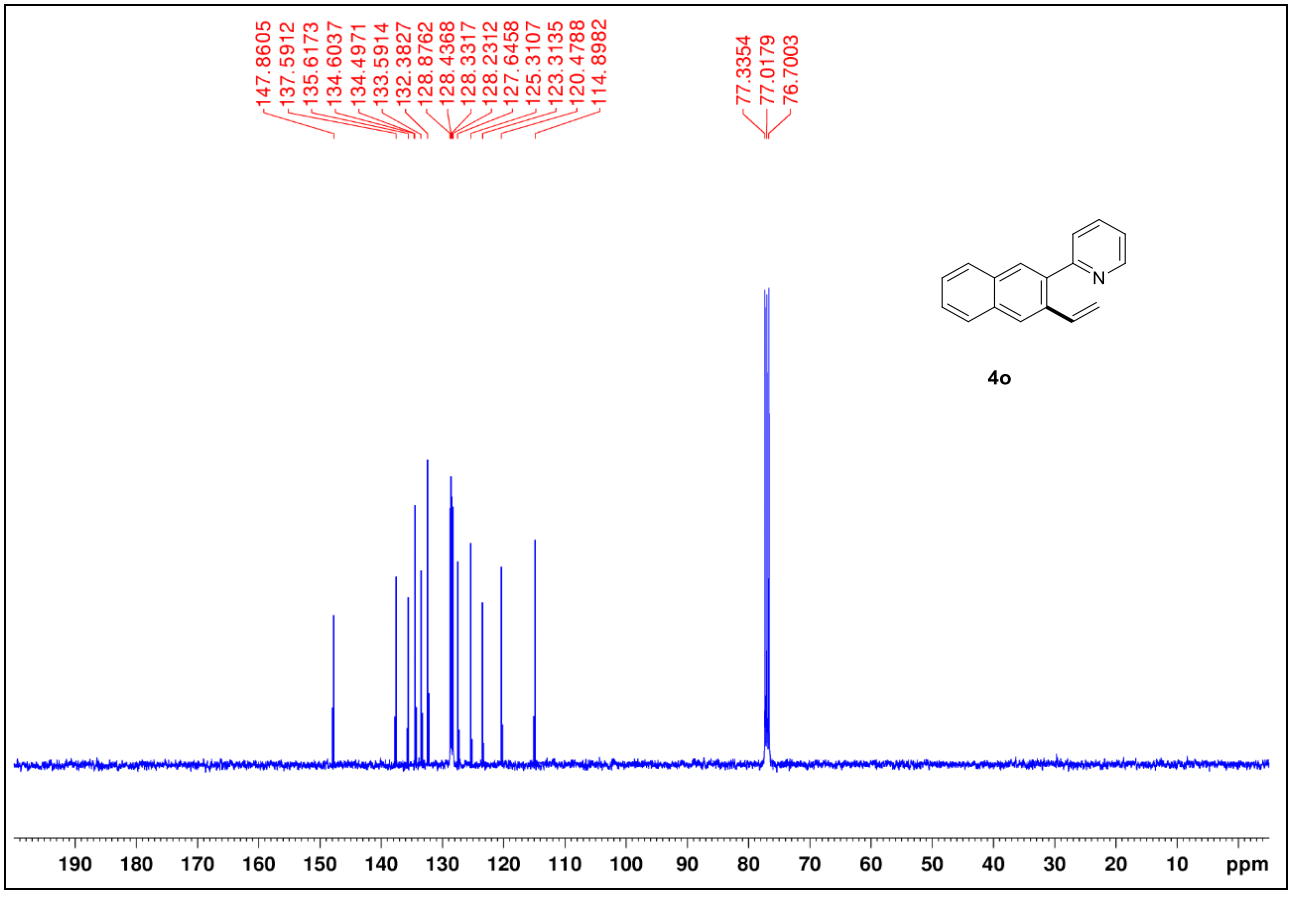
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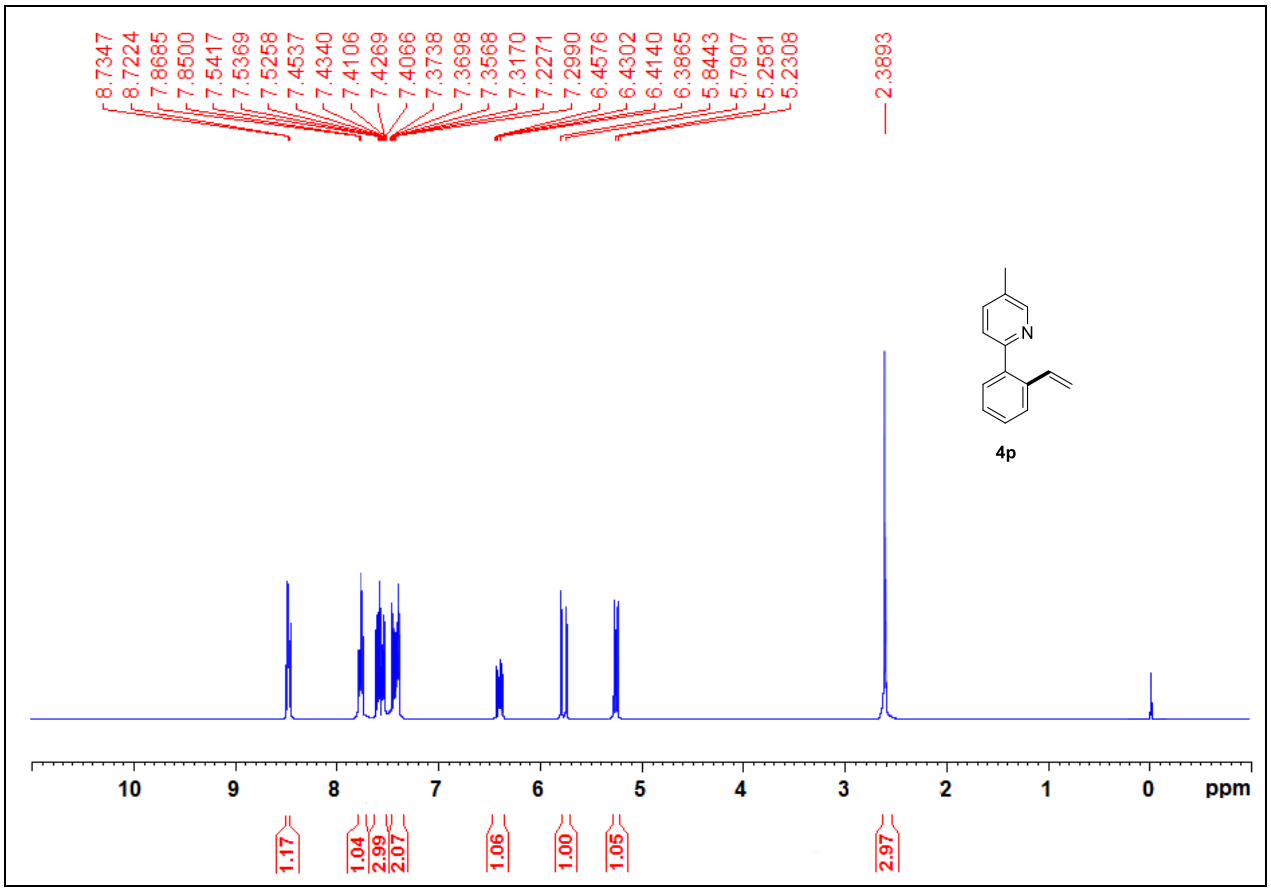
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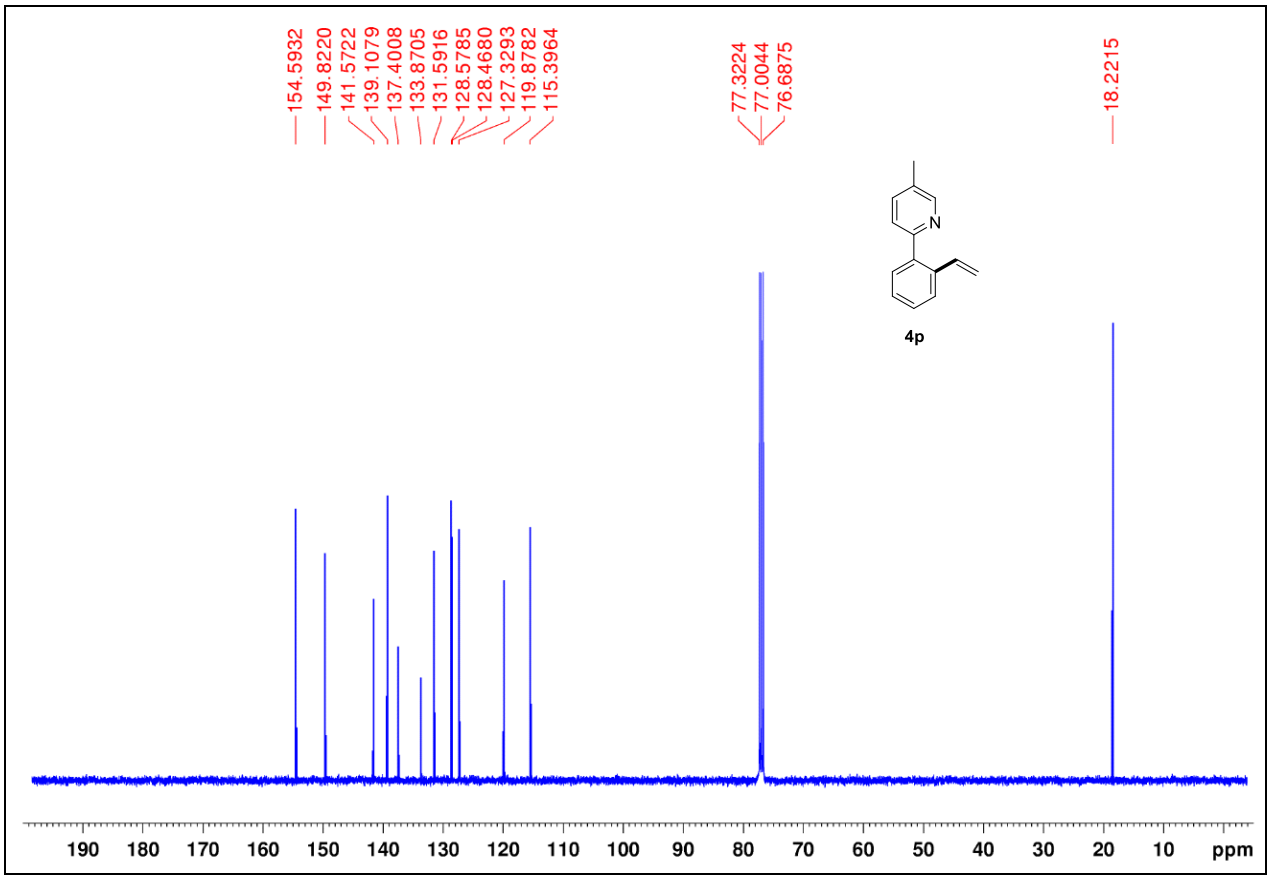
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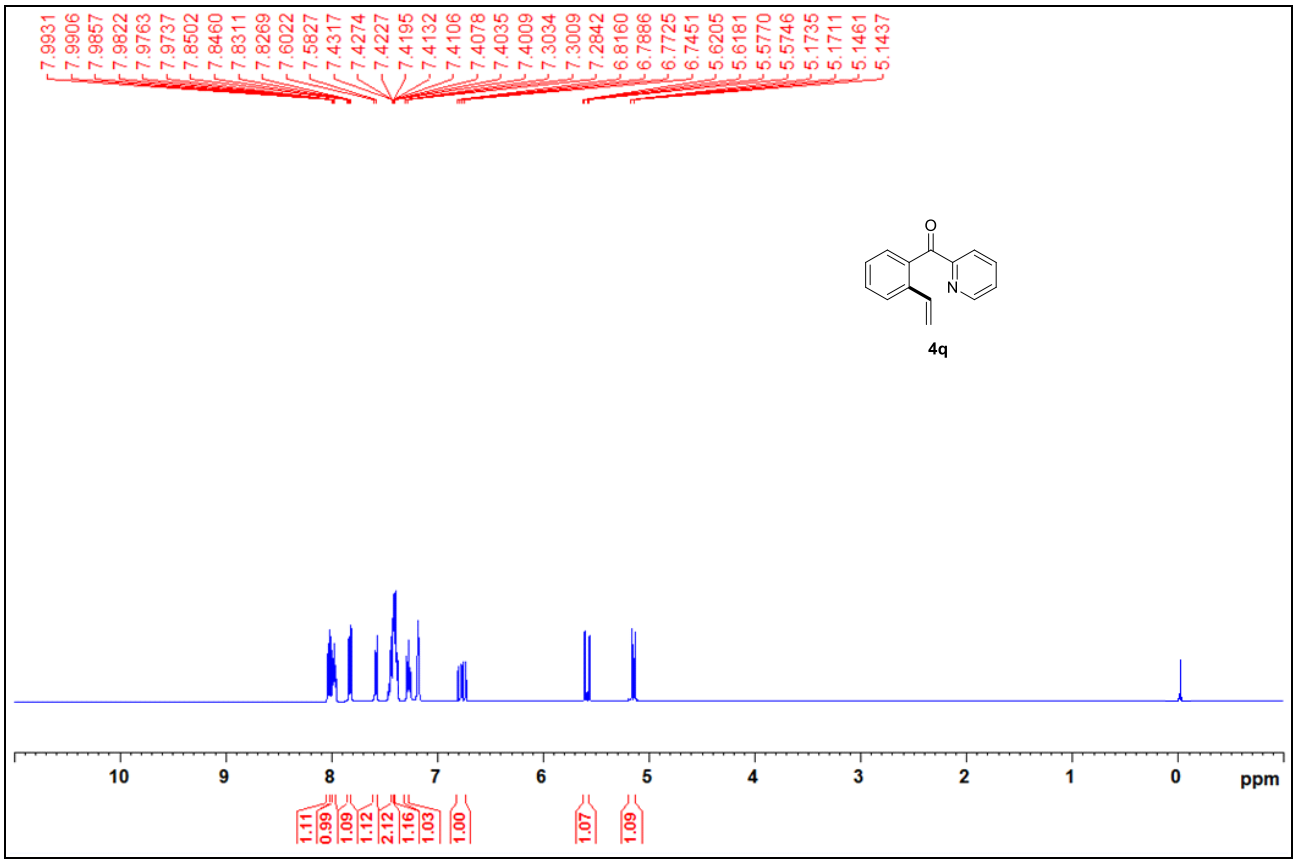
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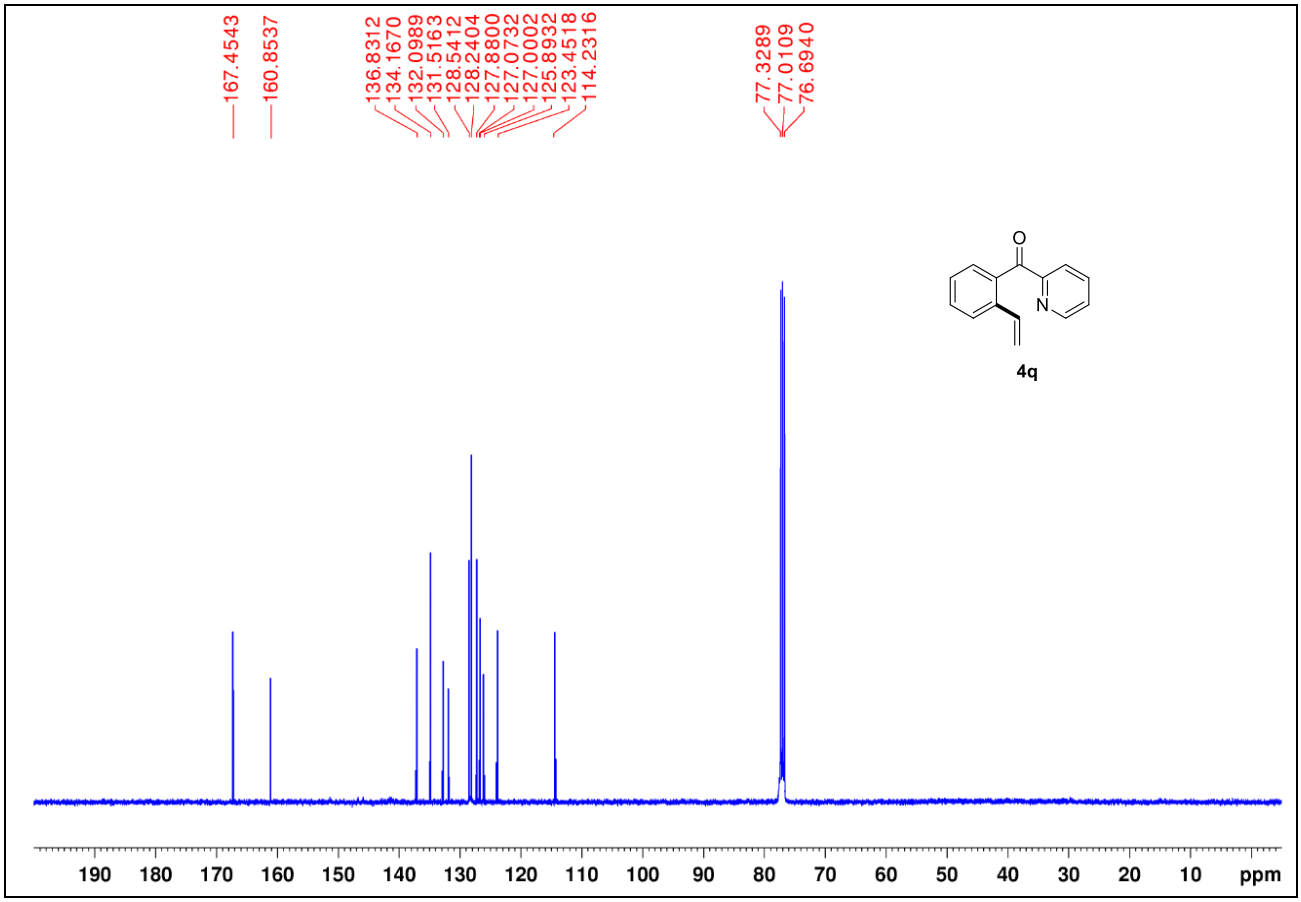
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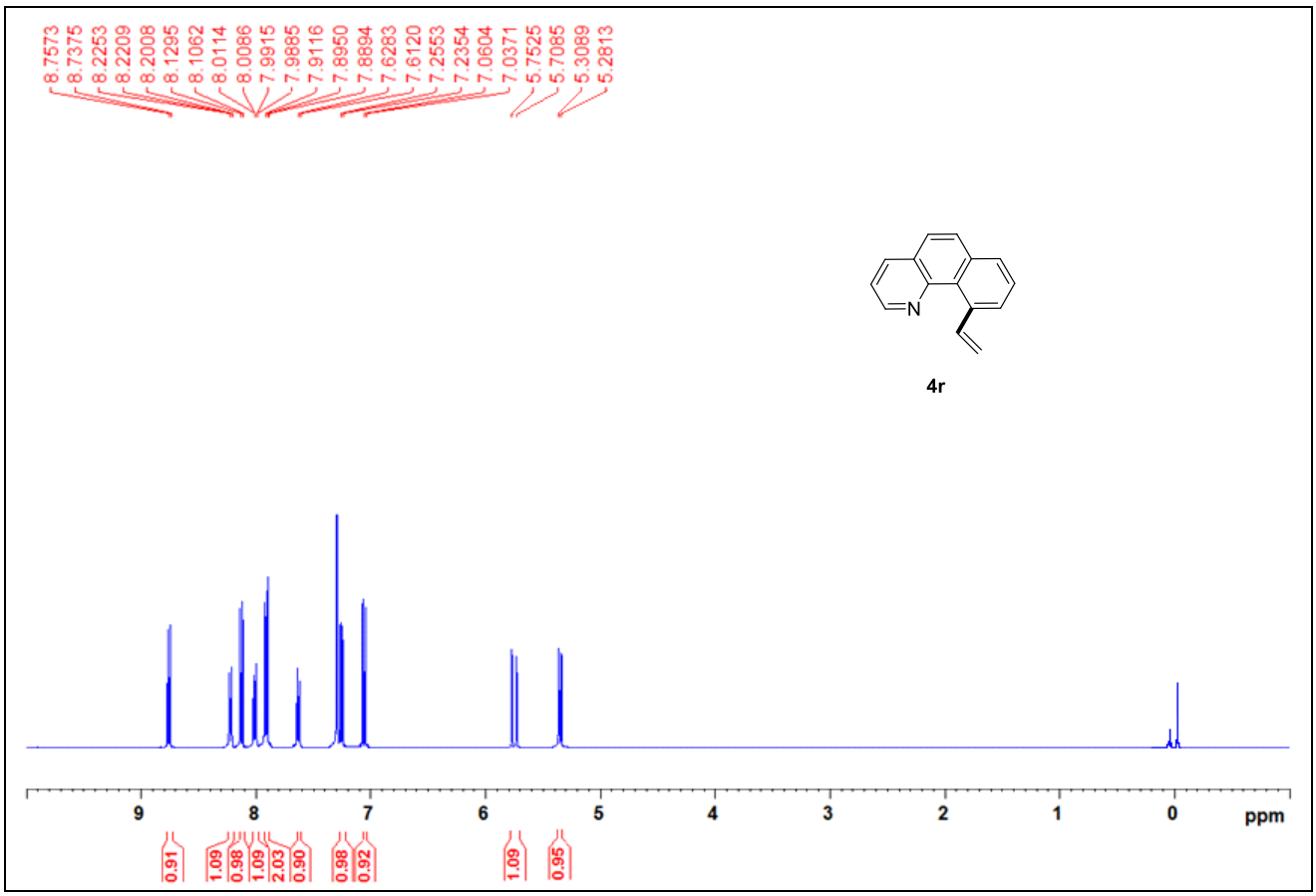
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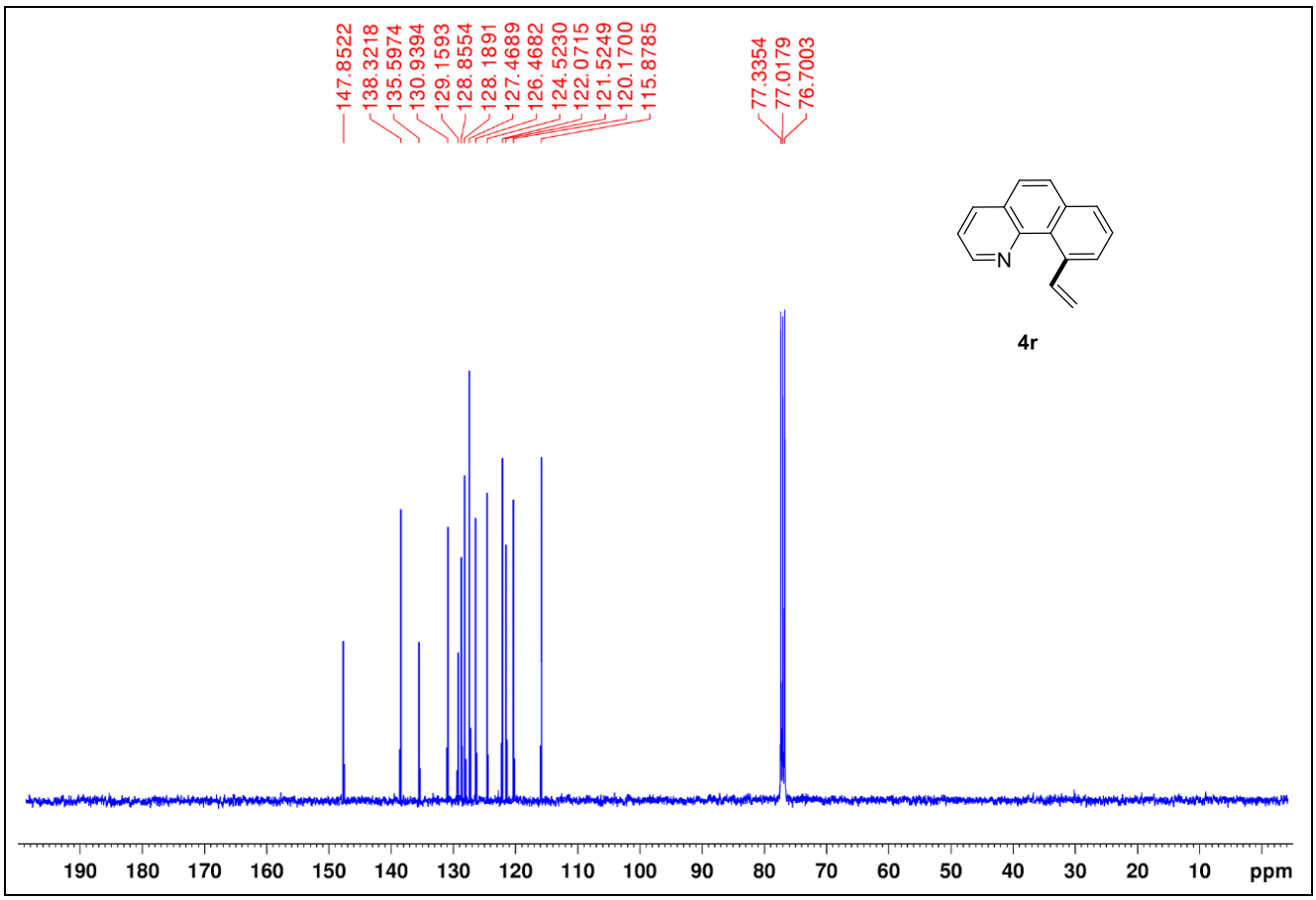
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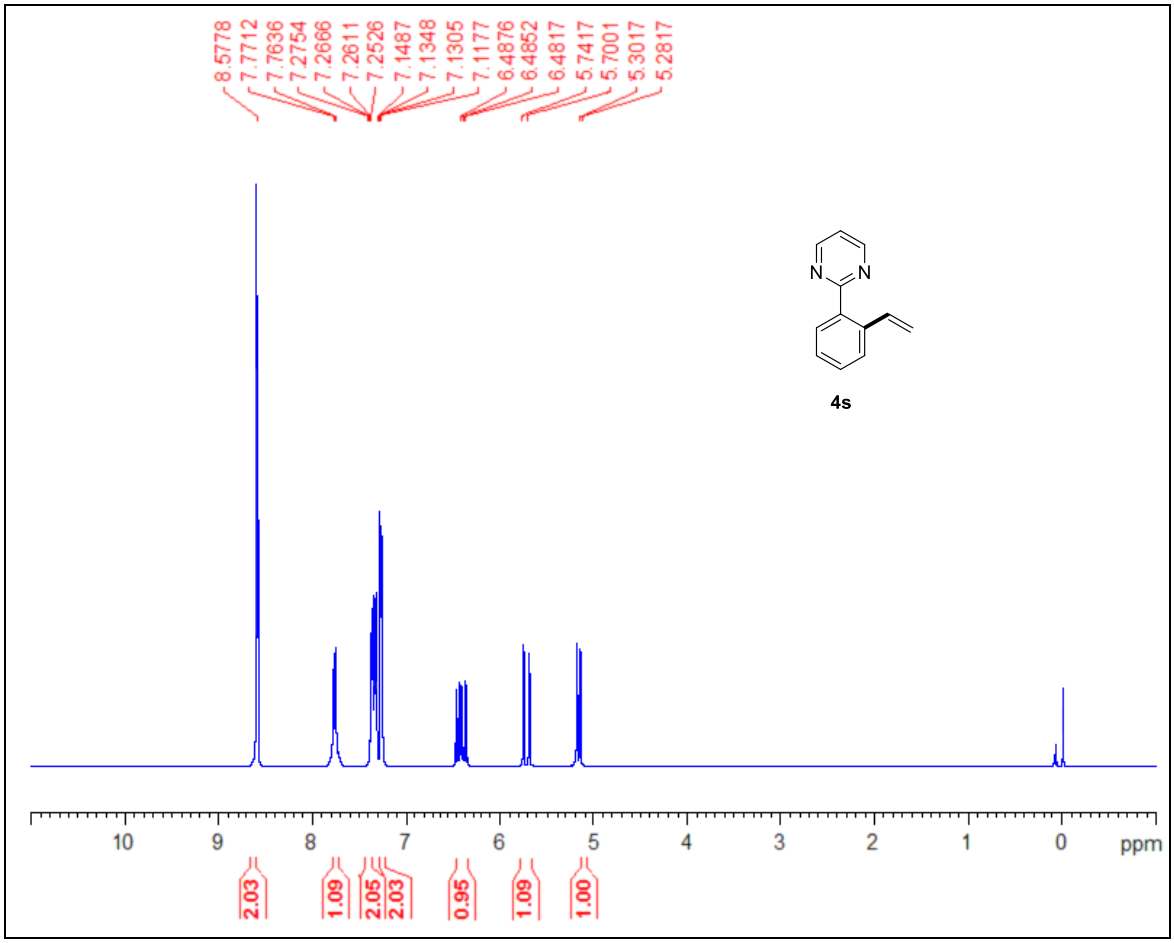
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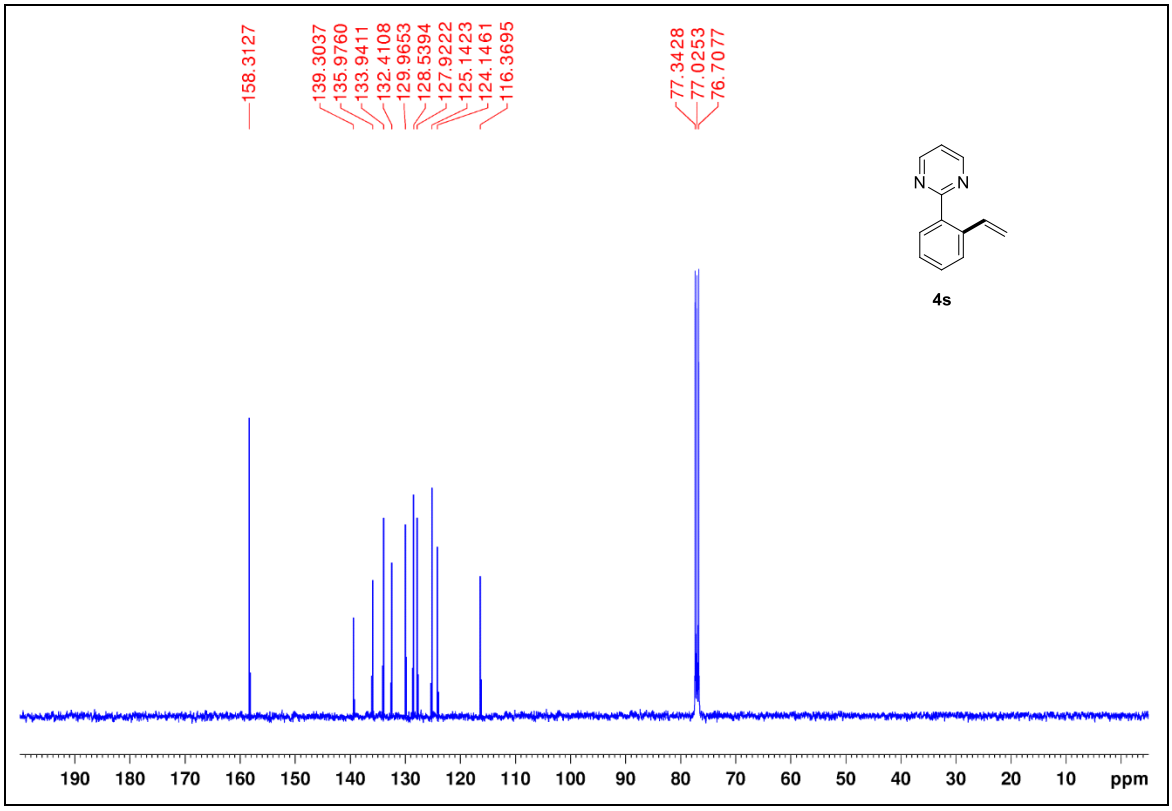
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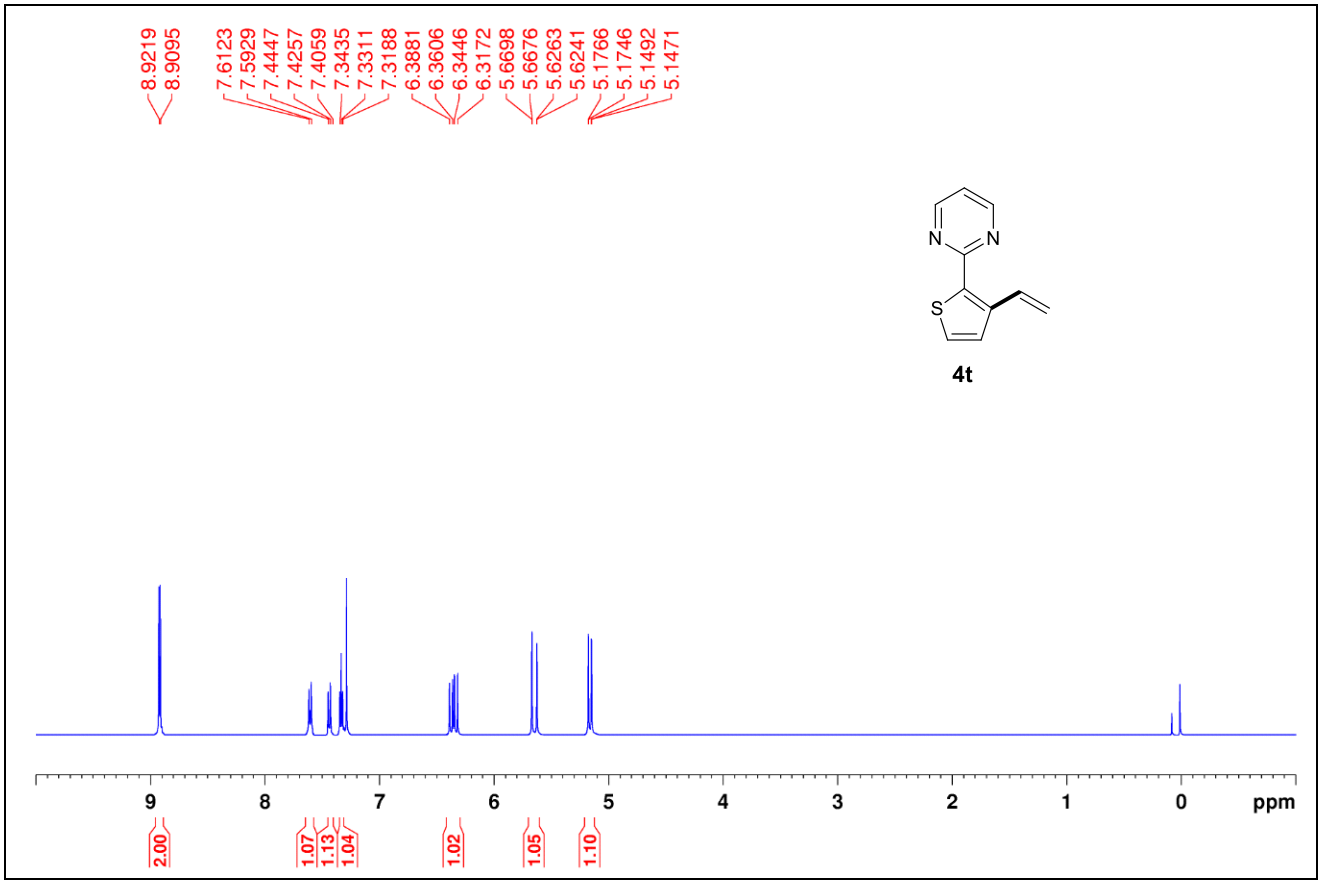
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S
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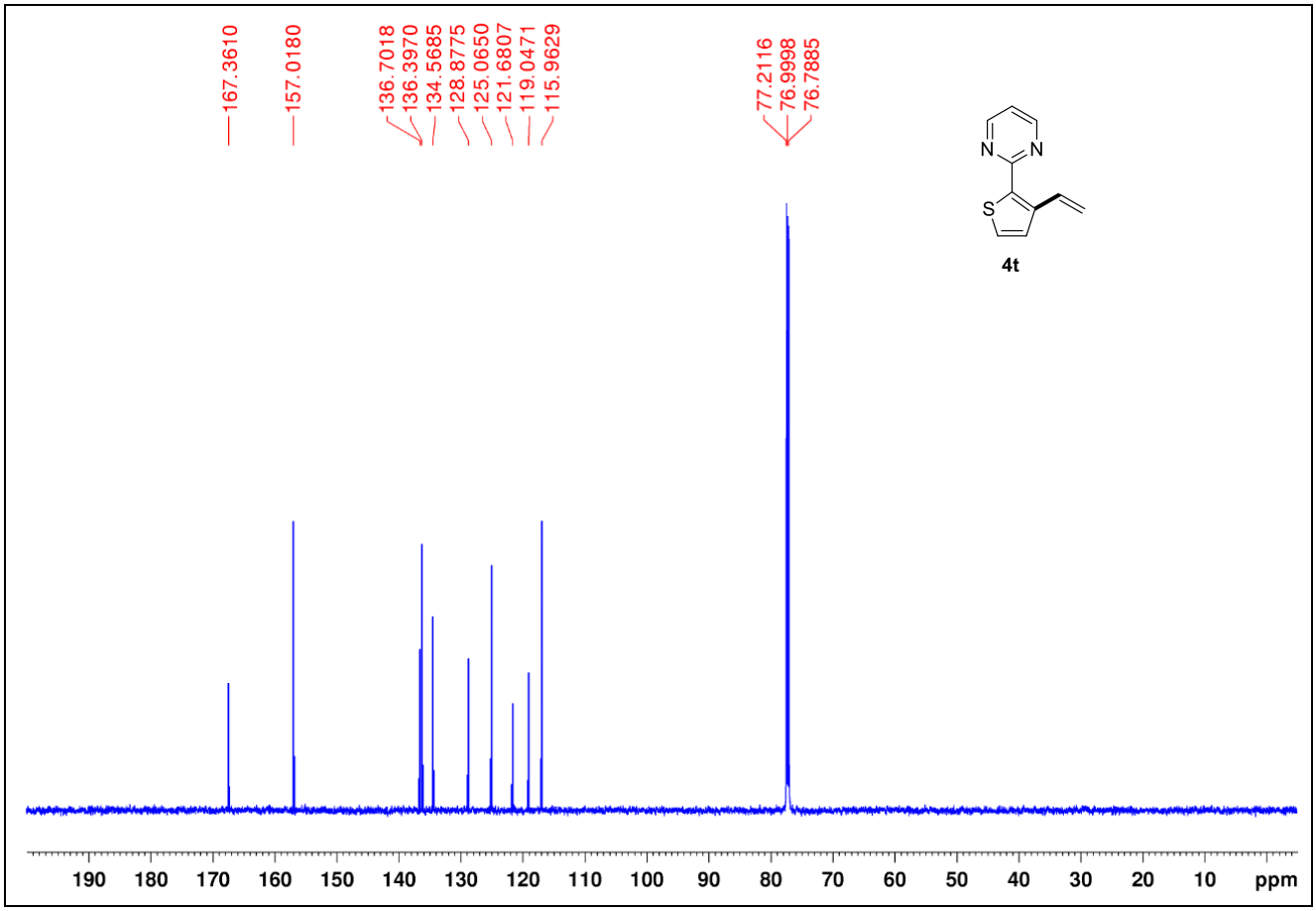
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N
S
4t
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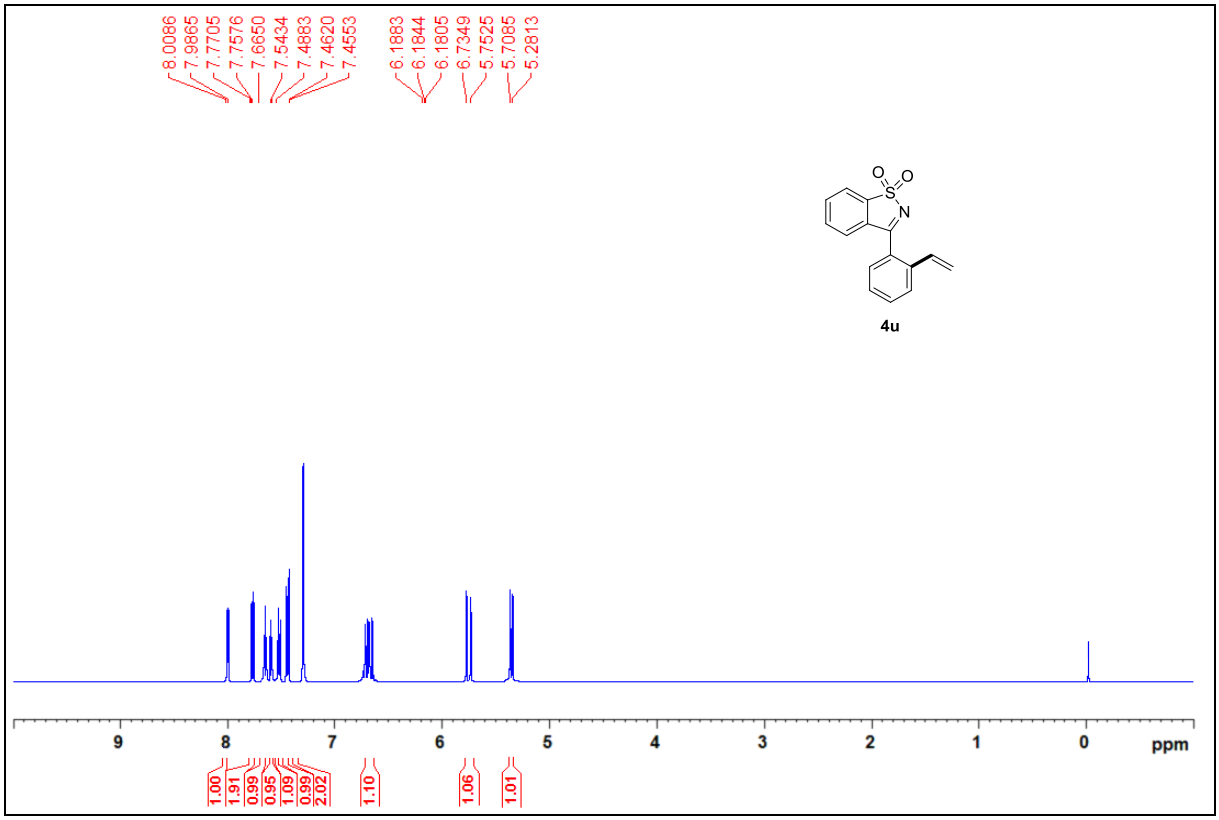
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5.7525
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8
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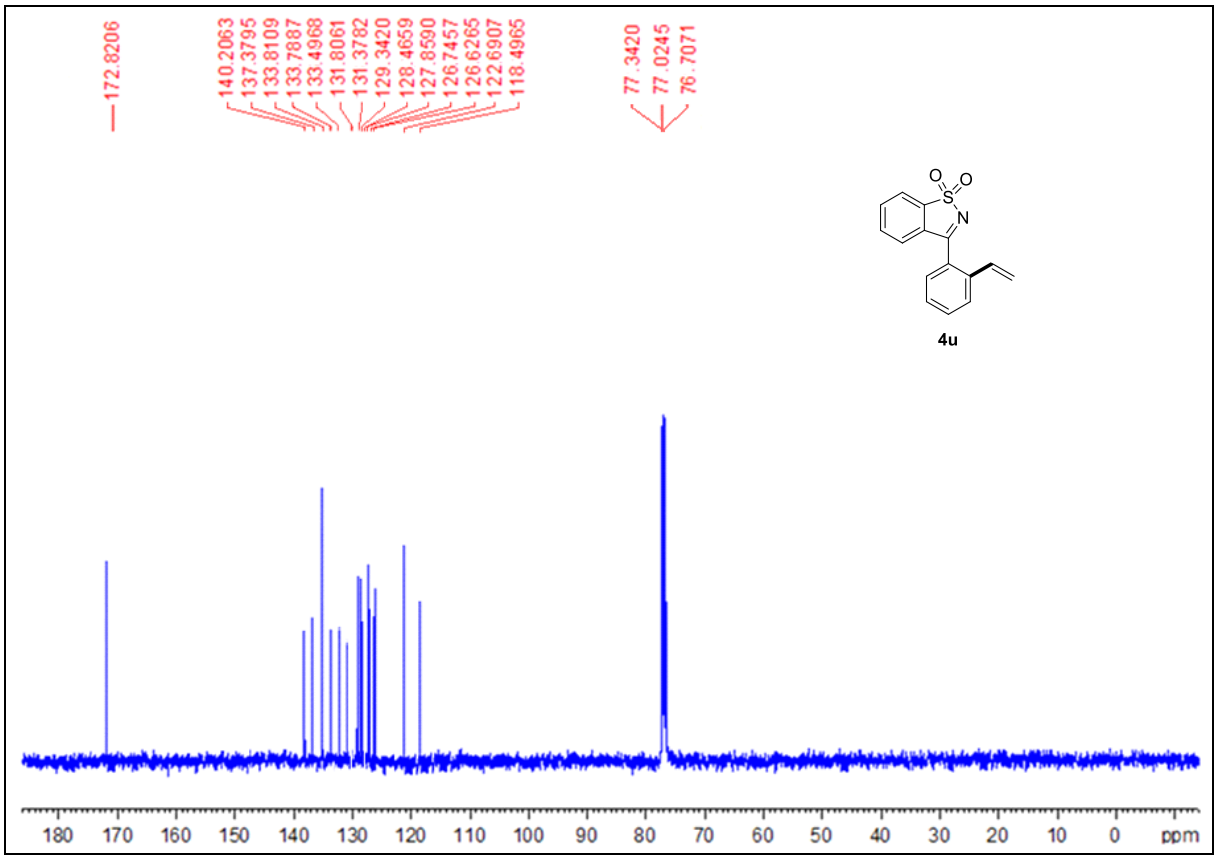
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4u
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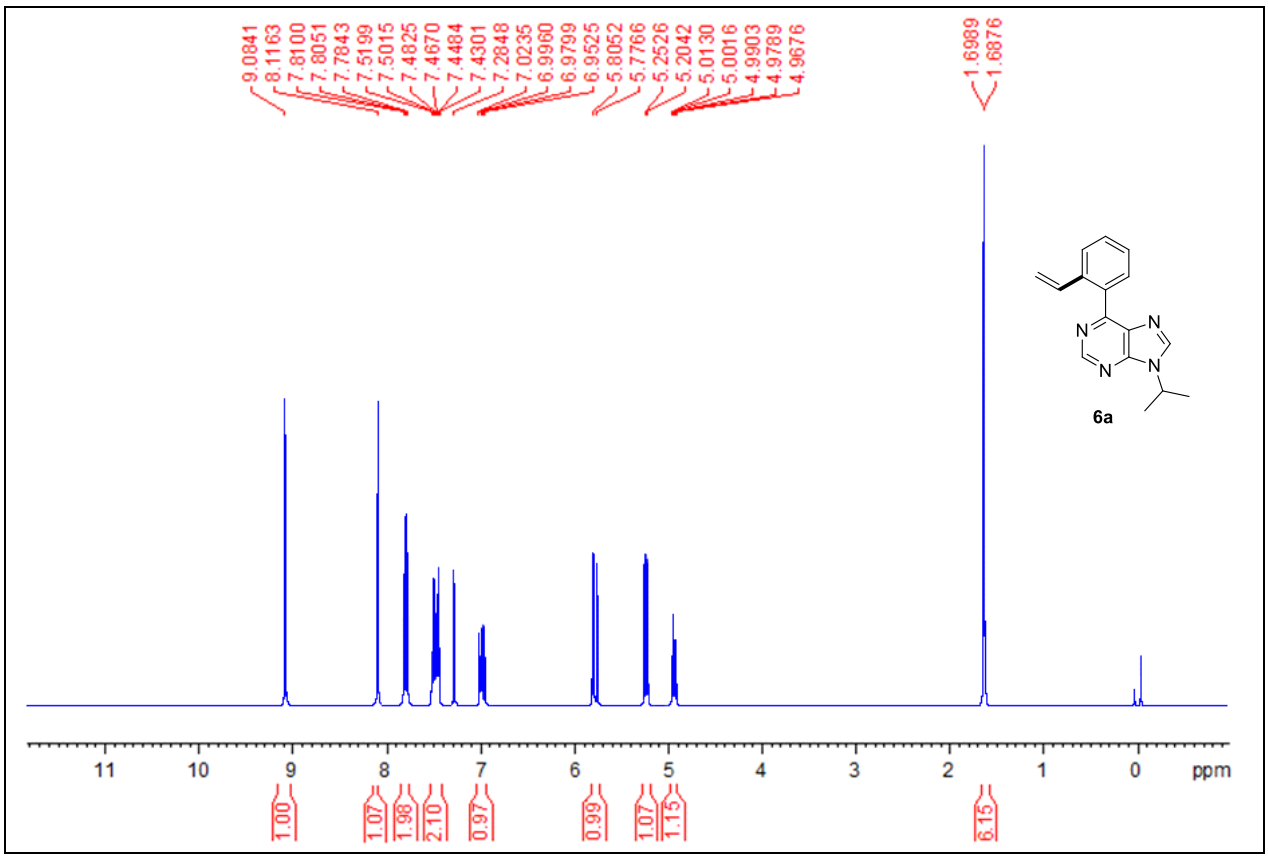
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6.9799
6.9525
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5.2042
5.0130
5.0016
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8
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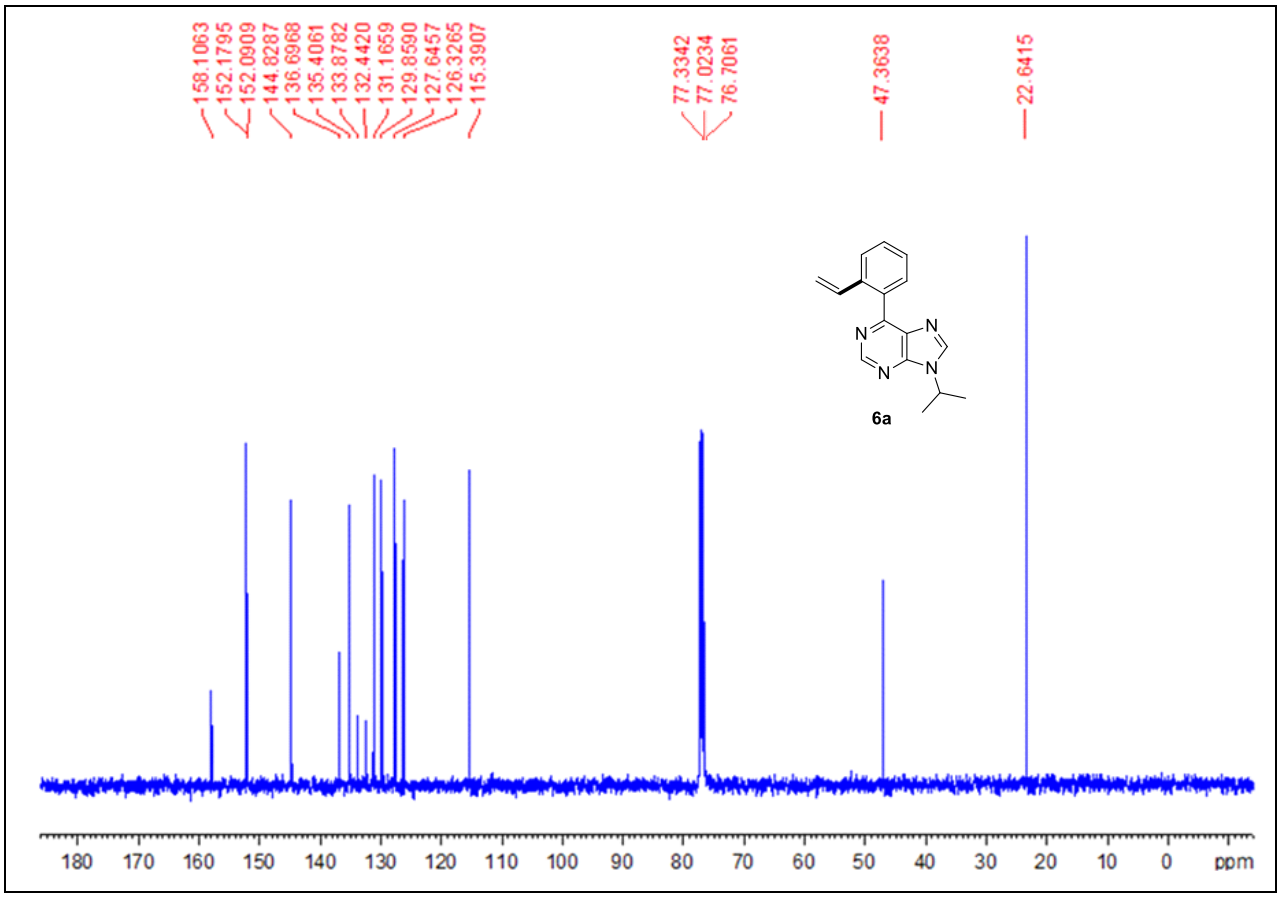
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ppm
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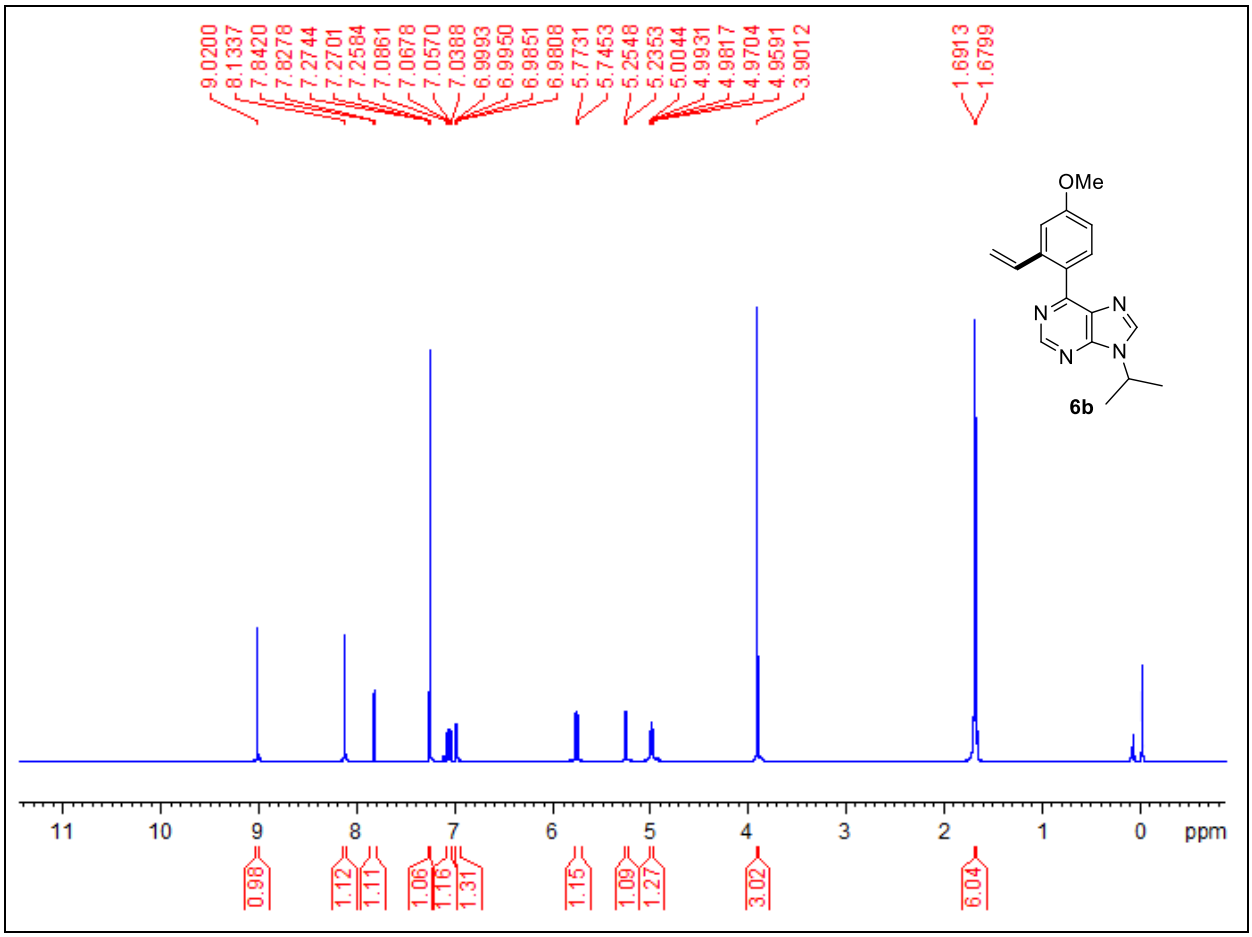
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5.2353
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3.9012
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1.6799
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10
9
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7
6
5
4
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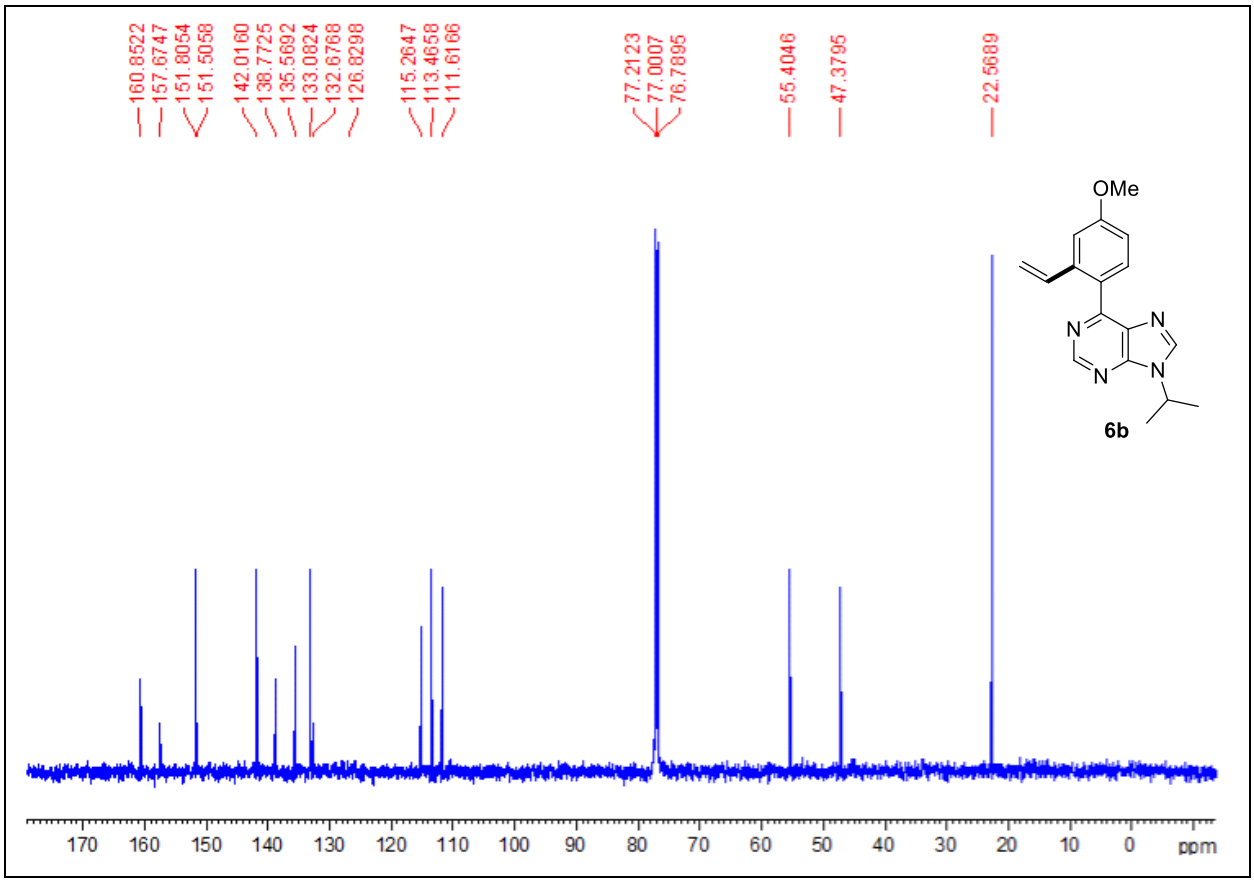
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22.5689
OMe
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N
N
N
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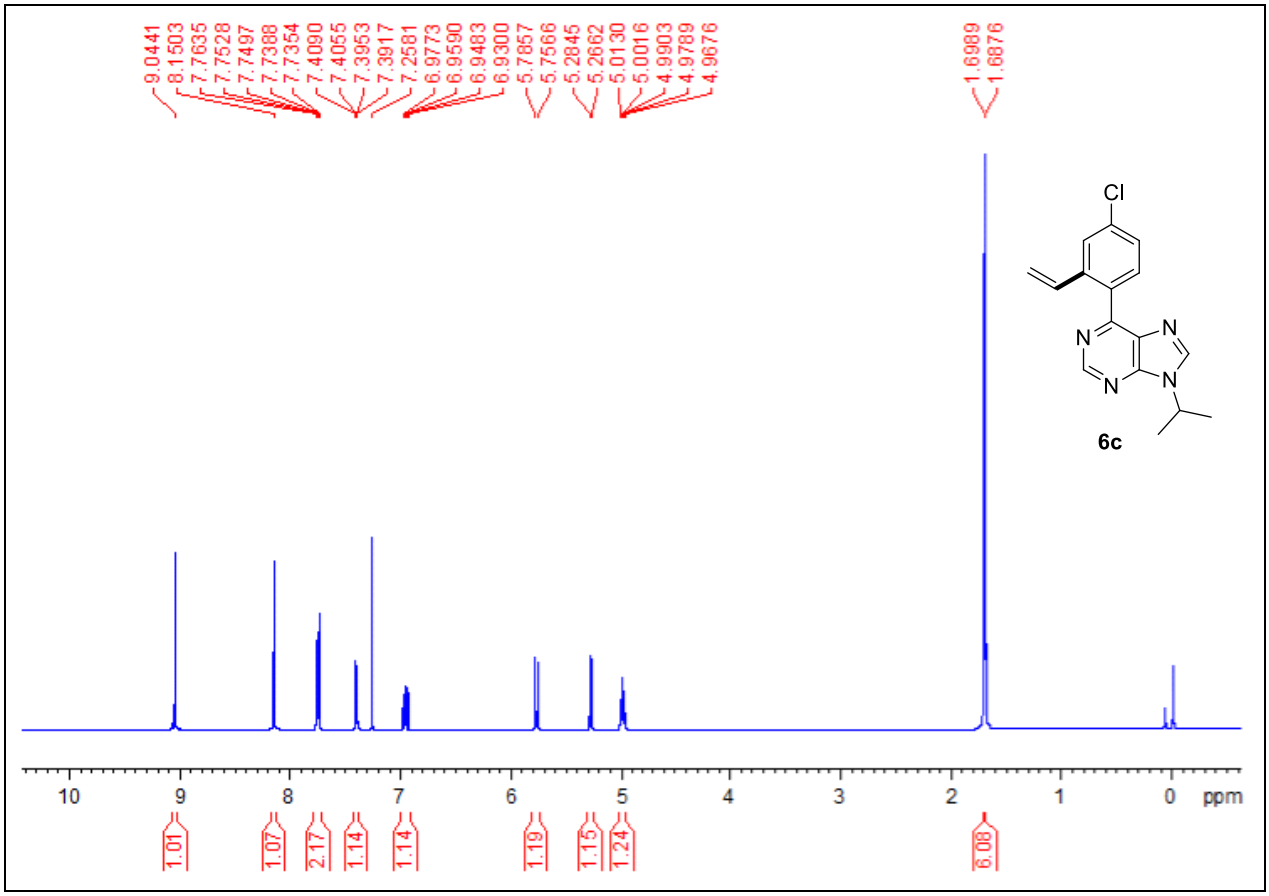
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1.6876
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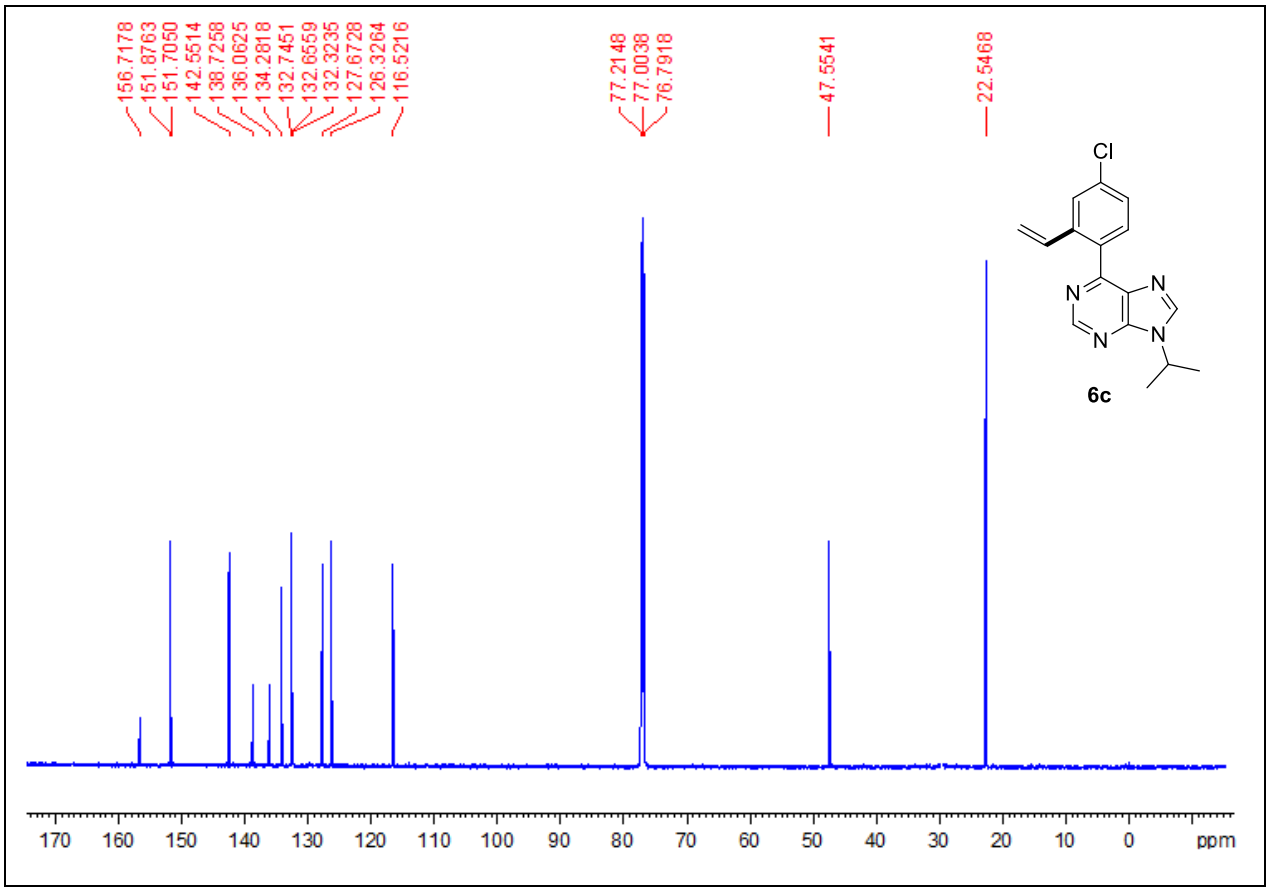
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N
N
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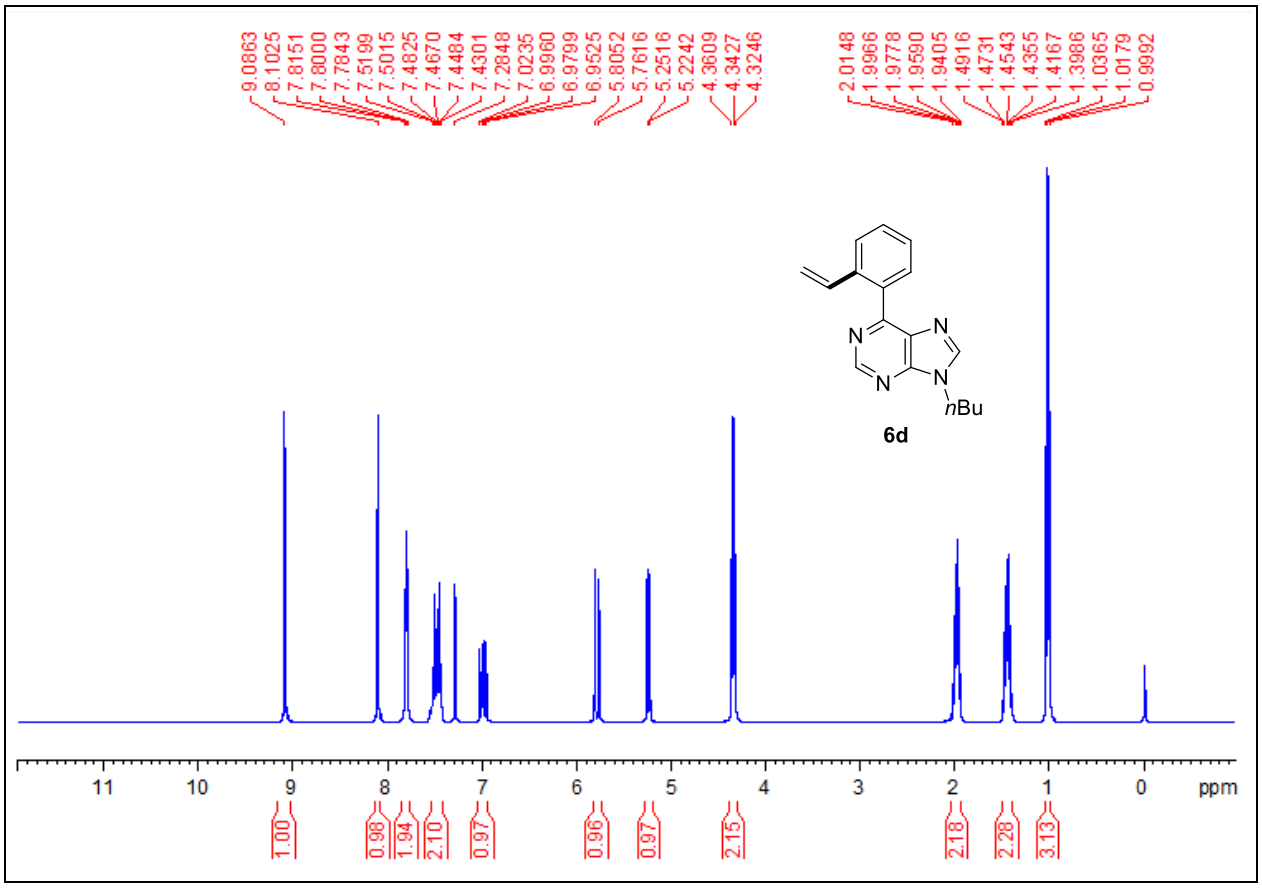
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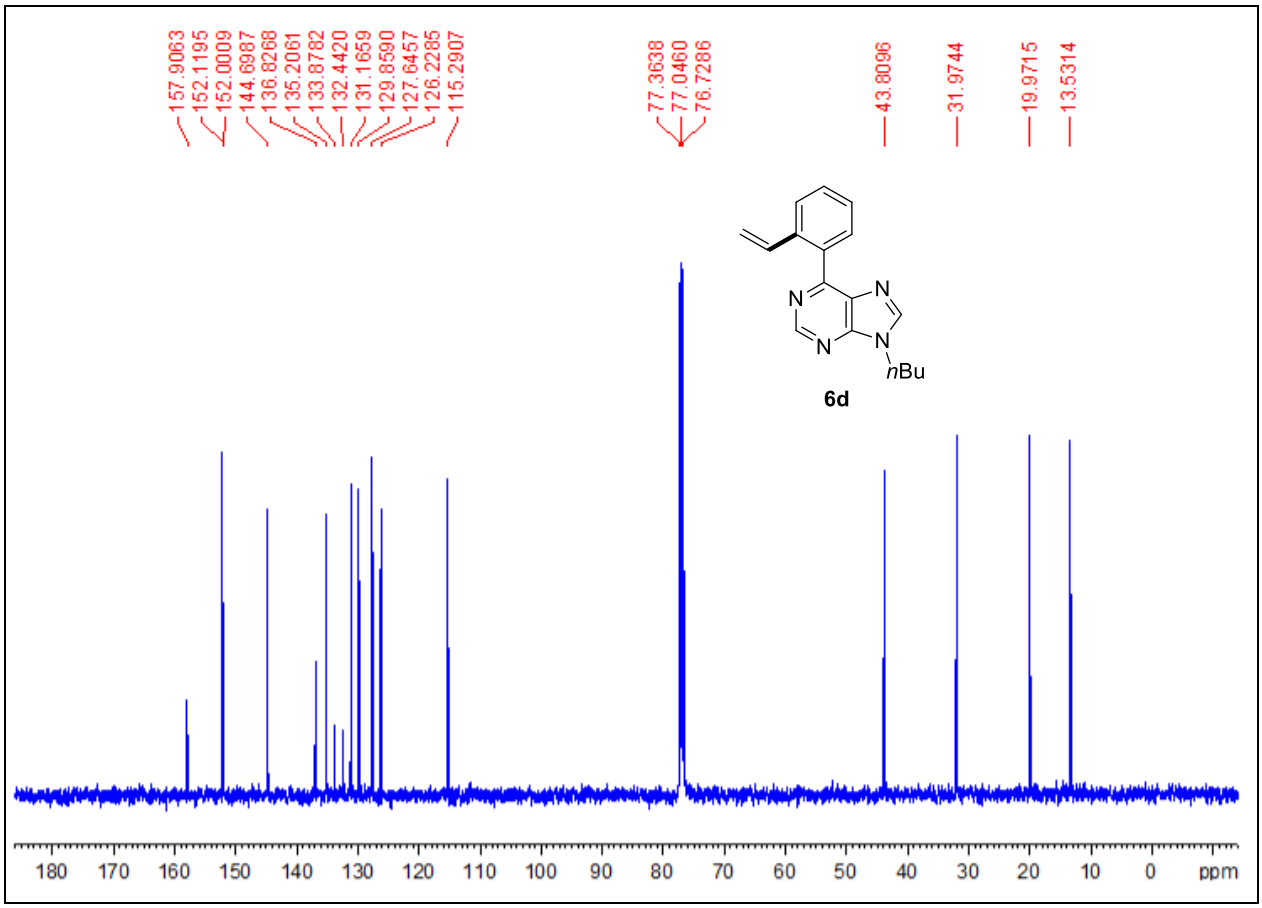
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N
N
N
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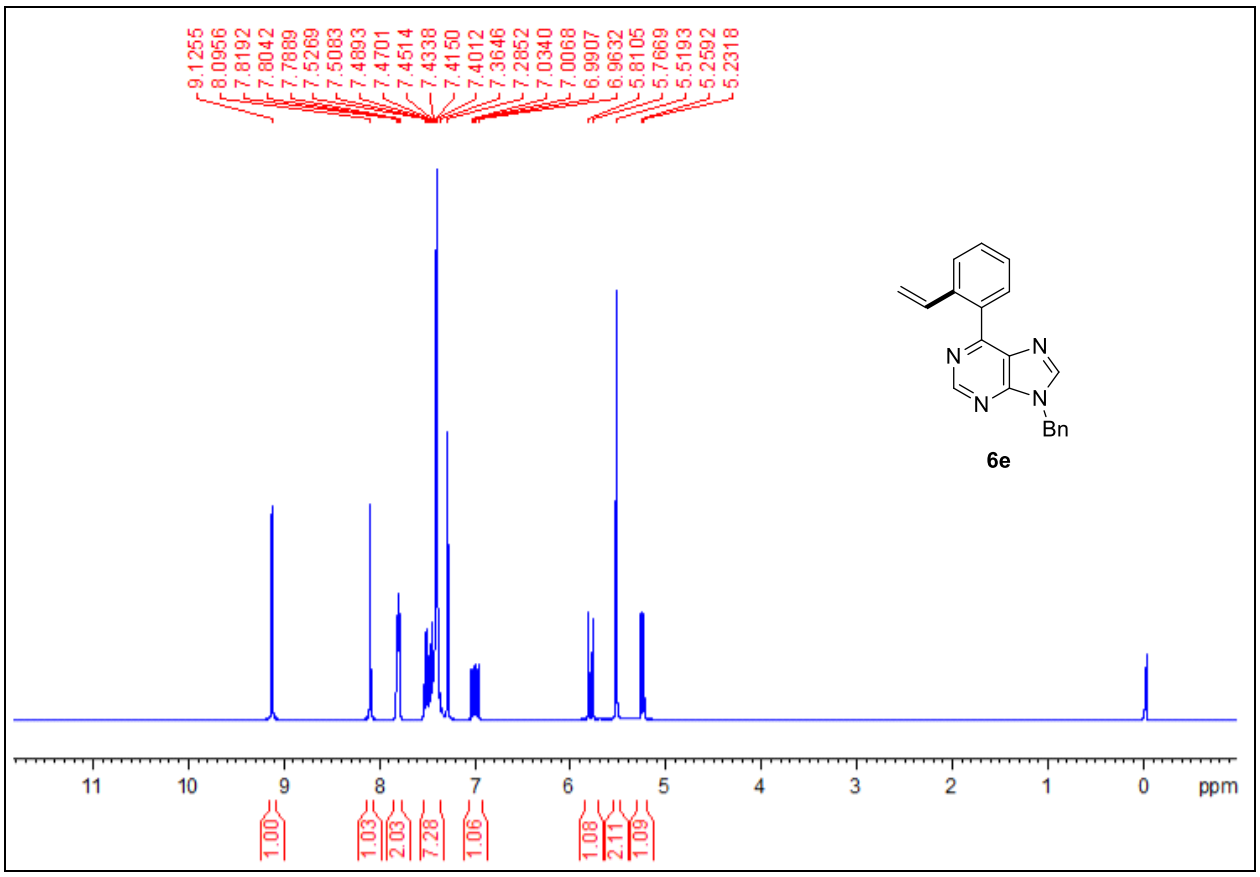
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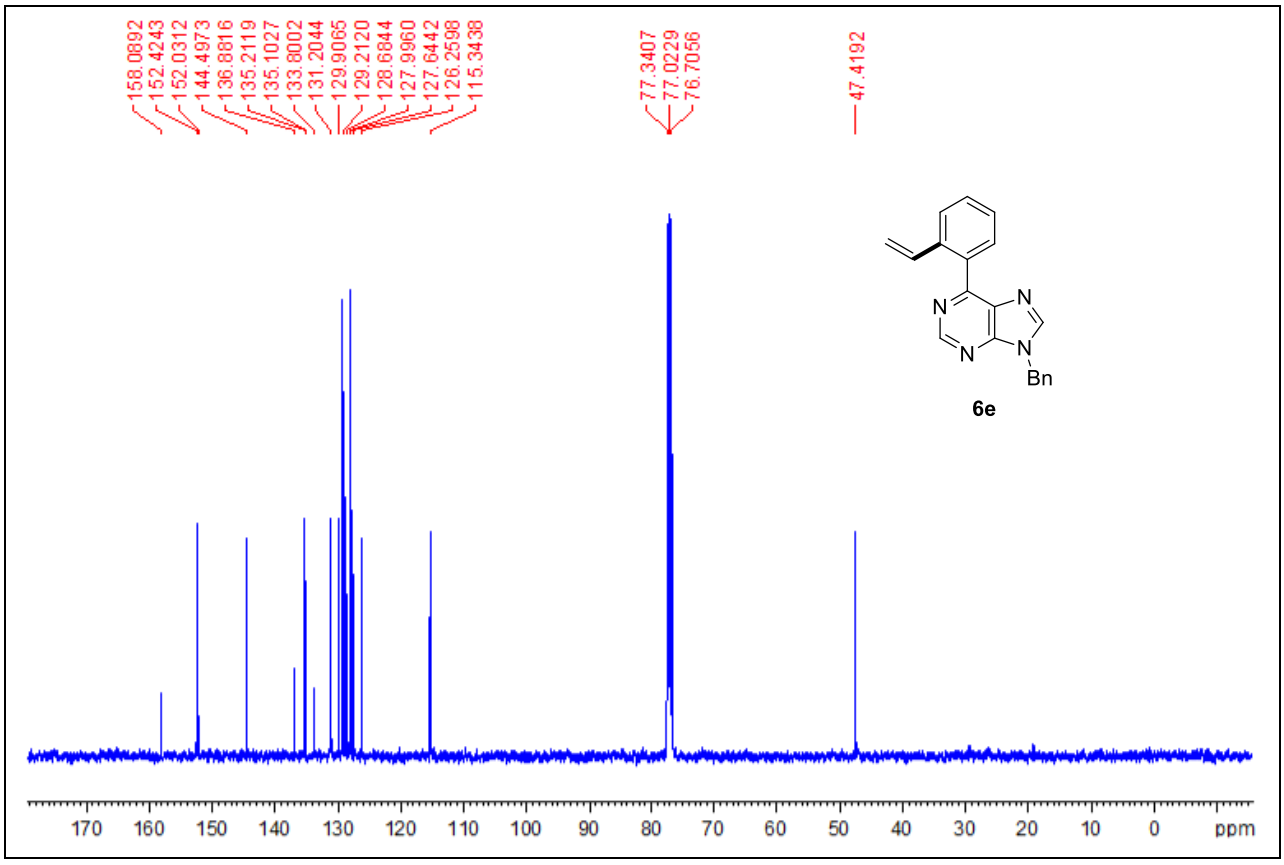
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N
Bn
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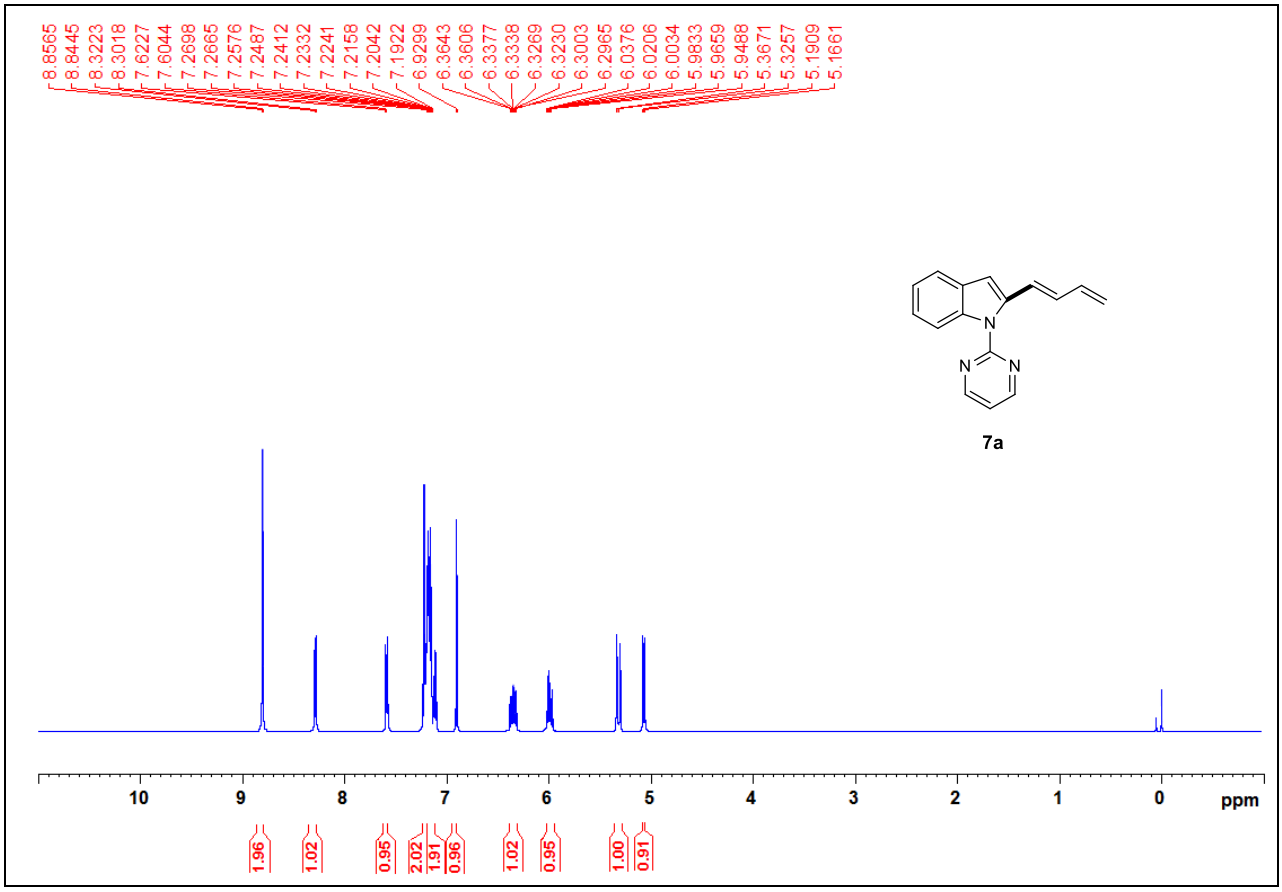
6e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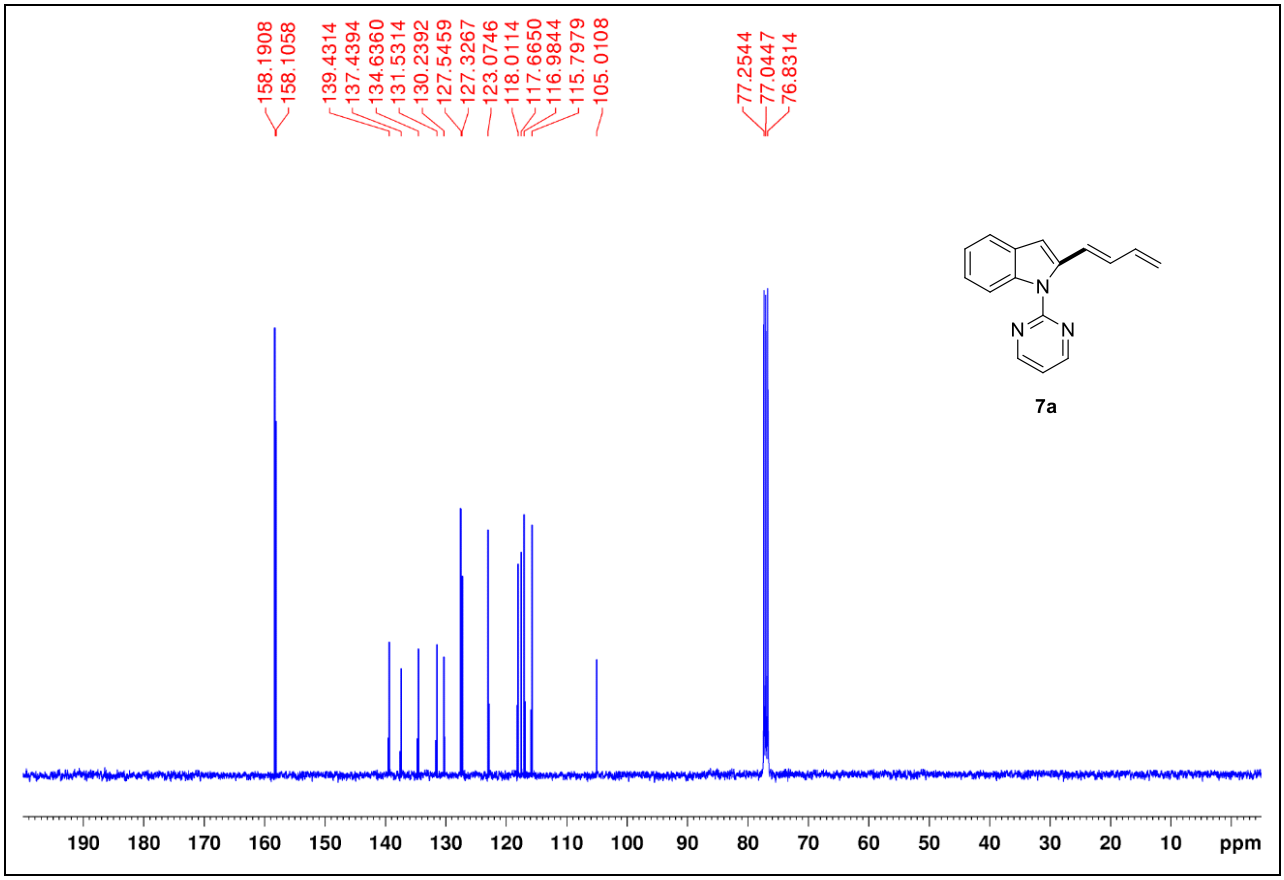
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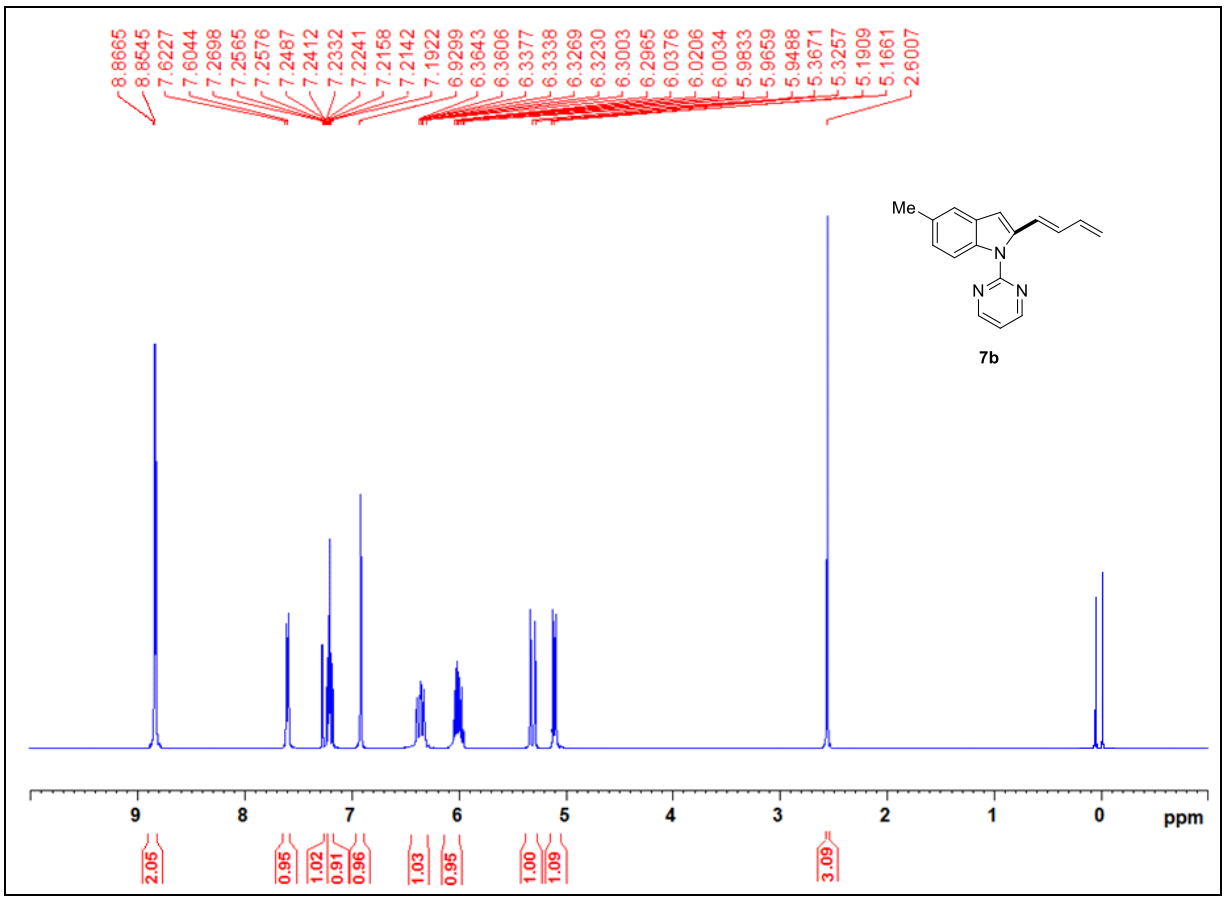
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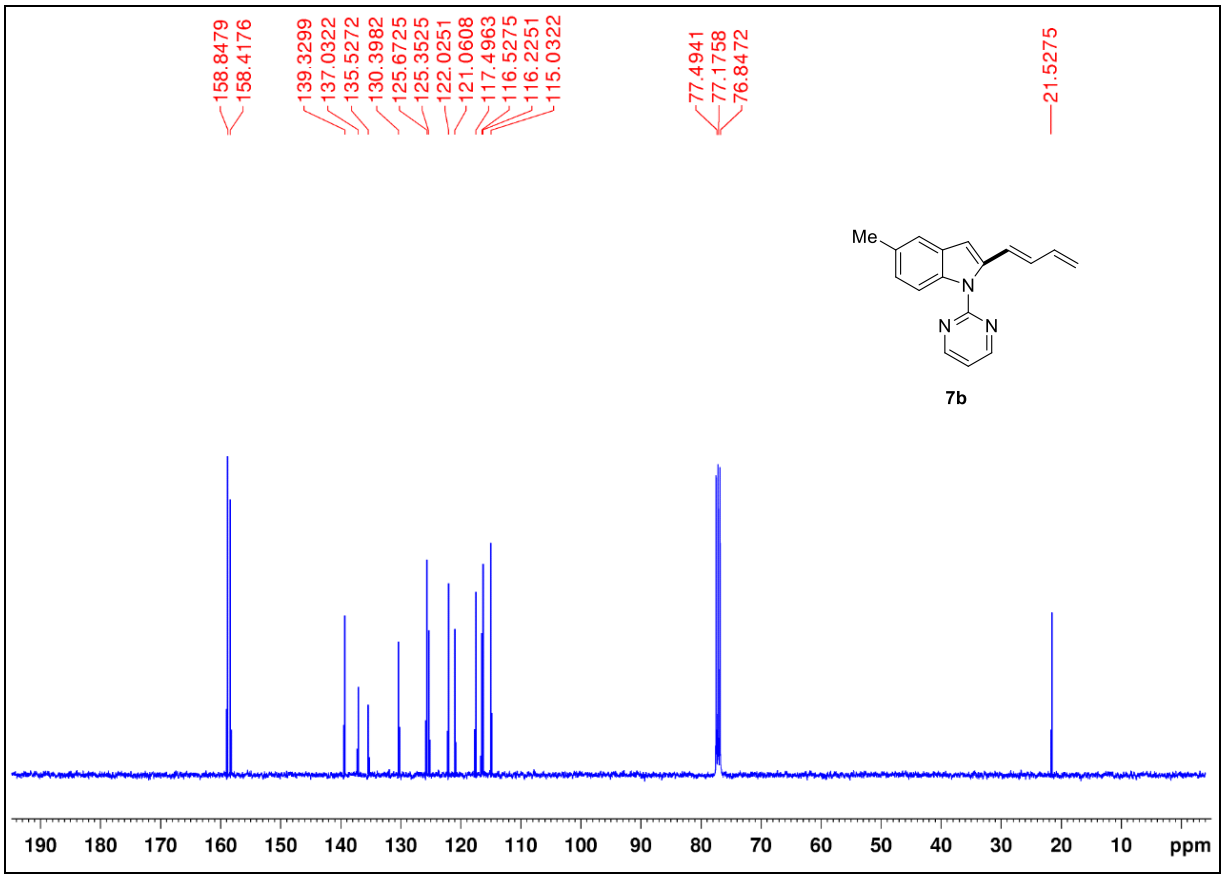
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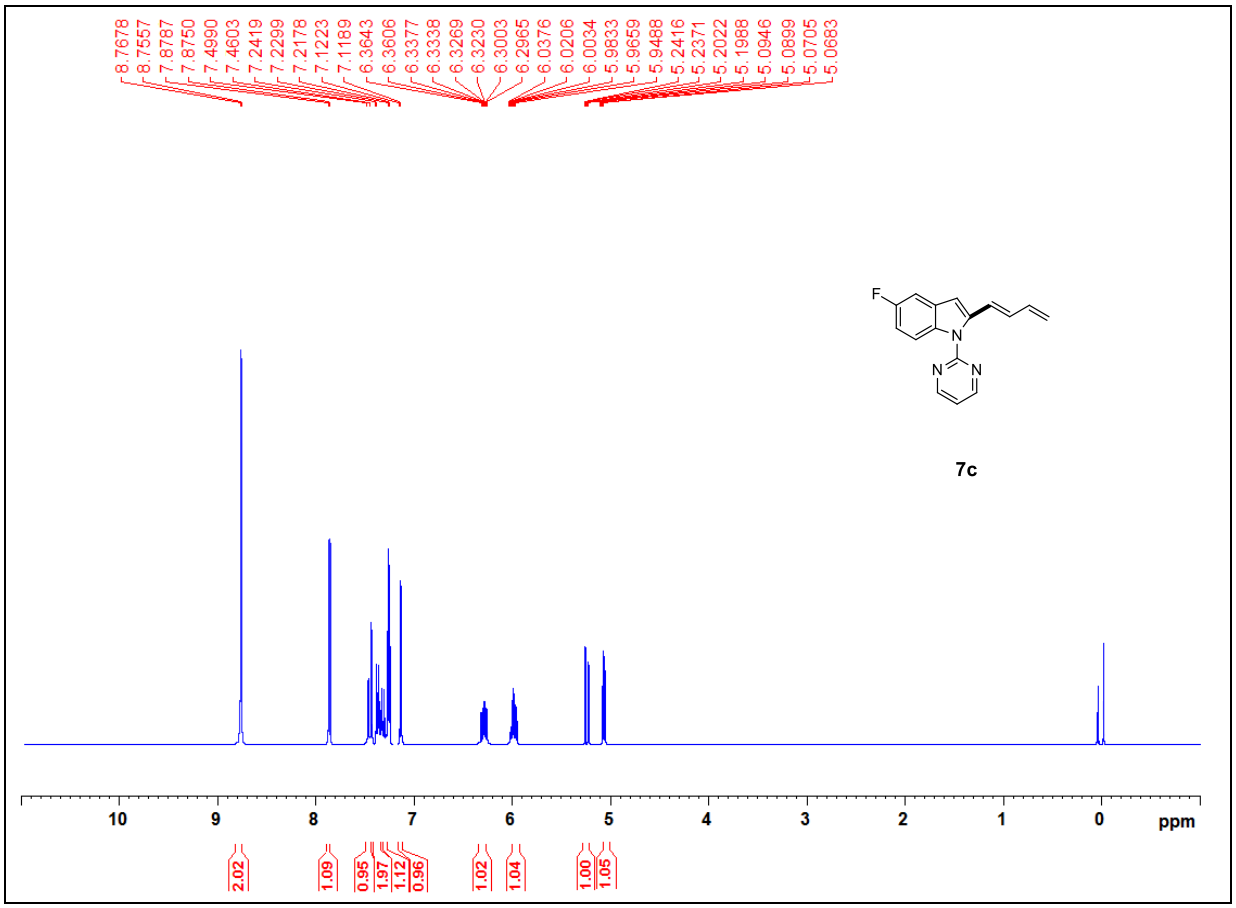
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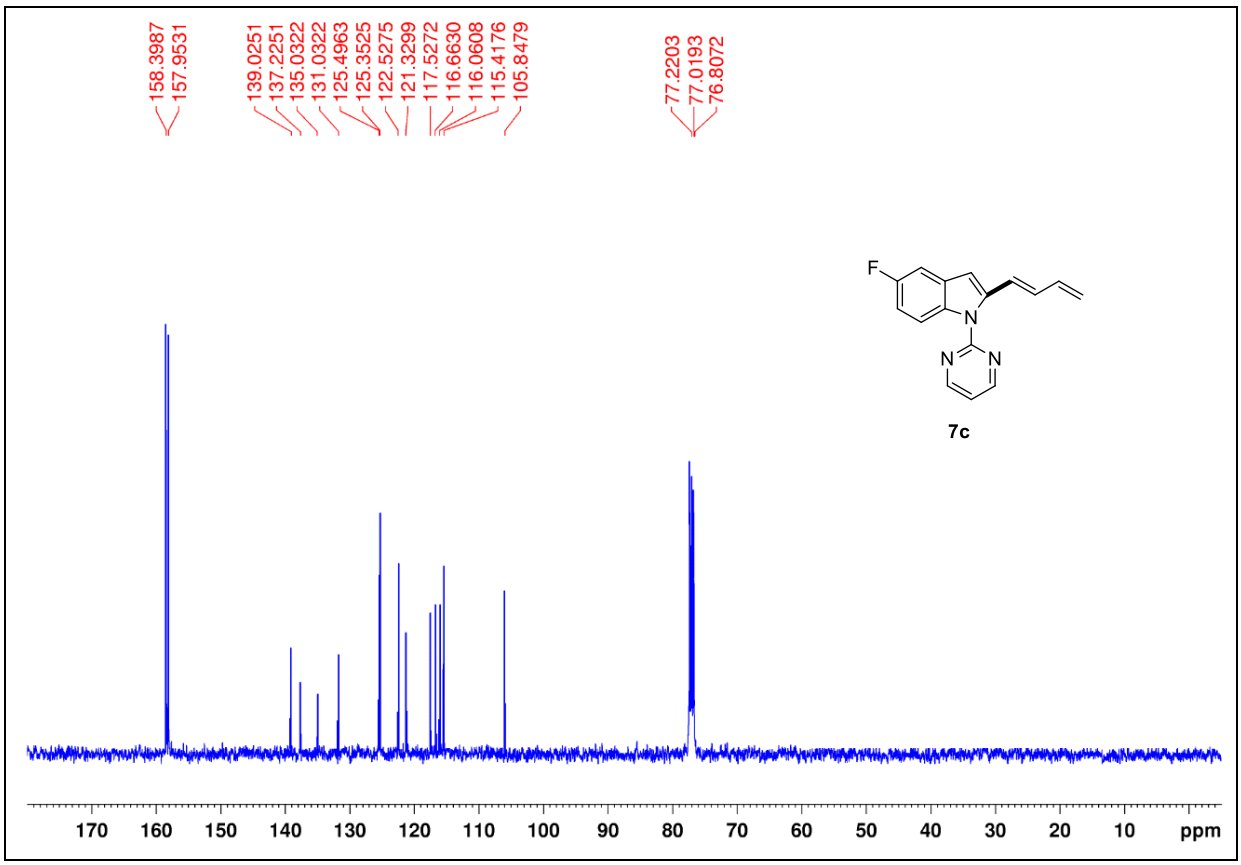
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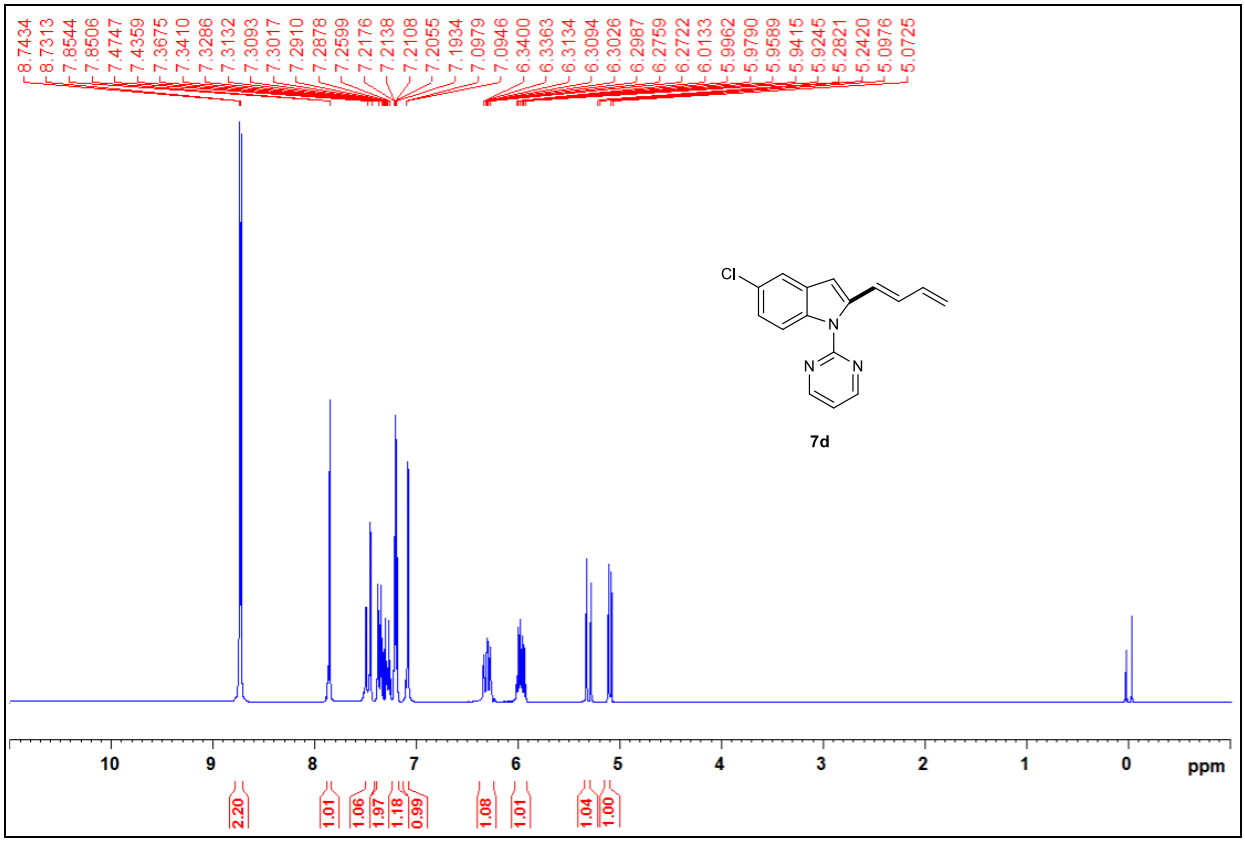
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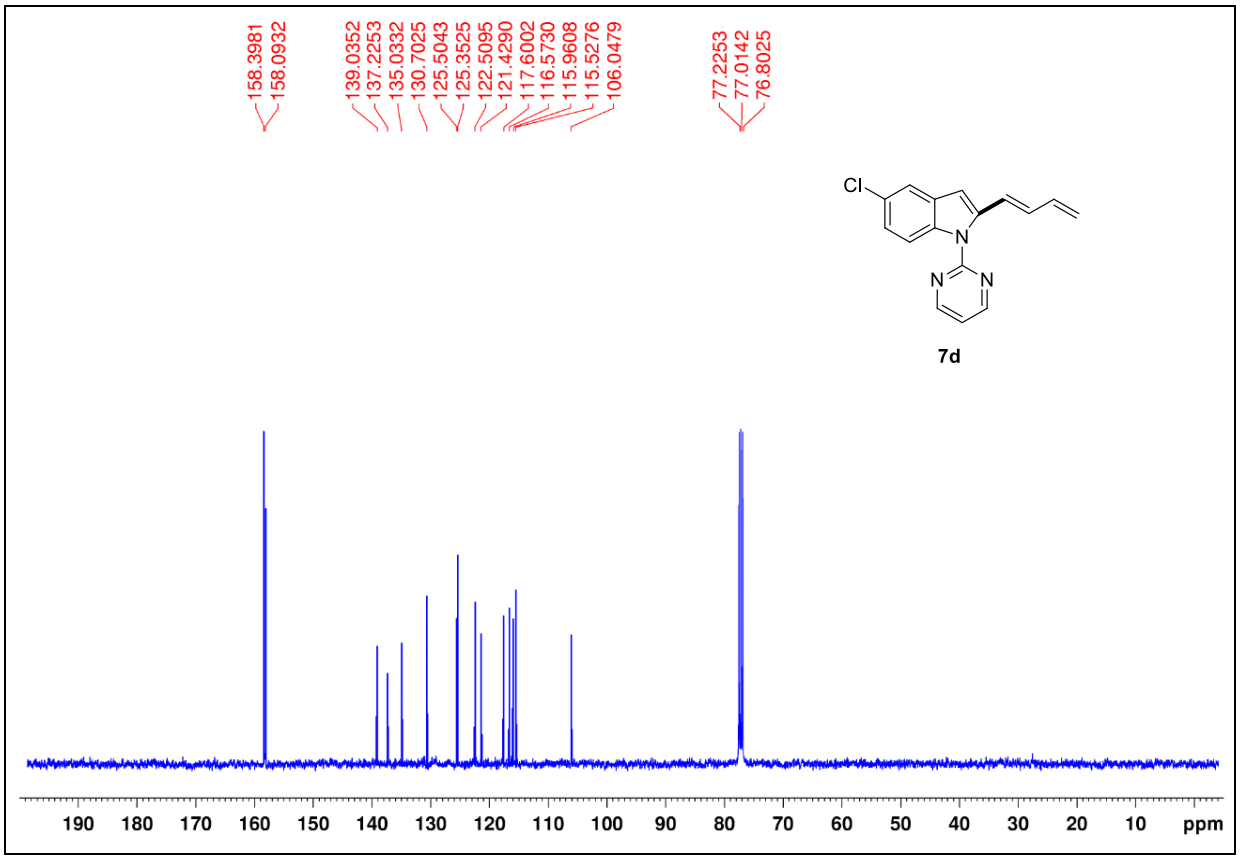
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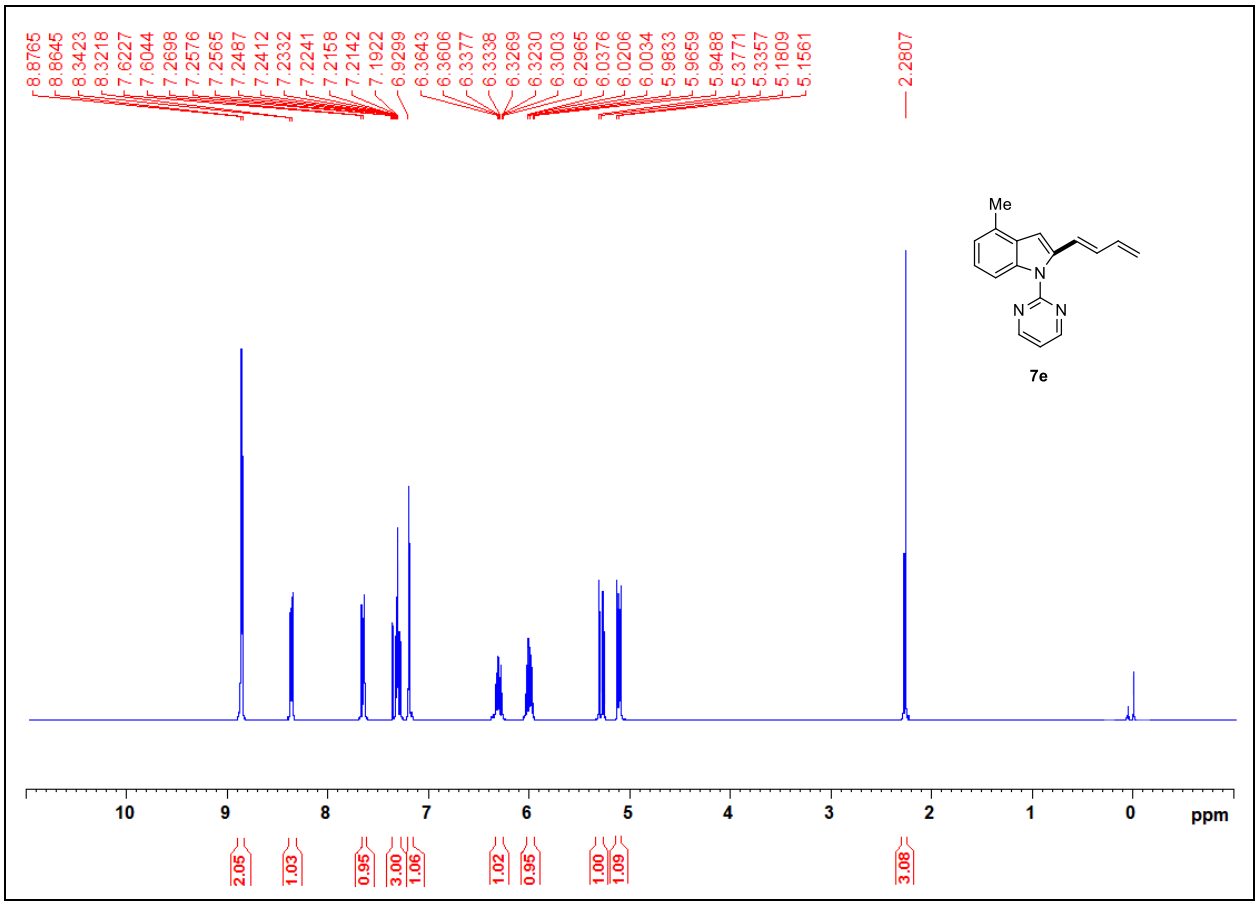
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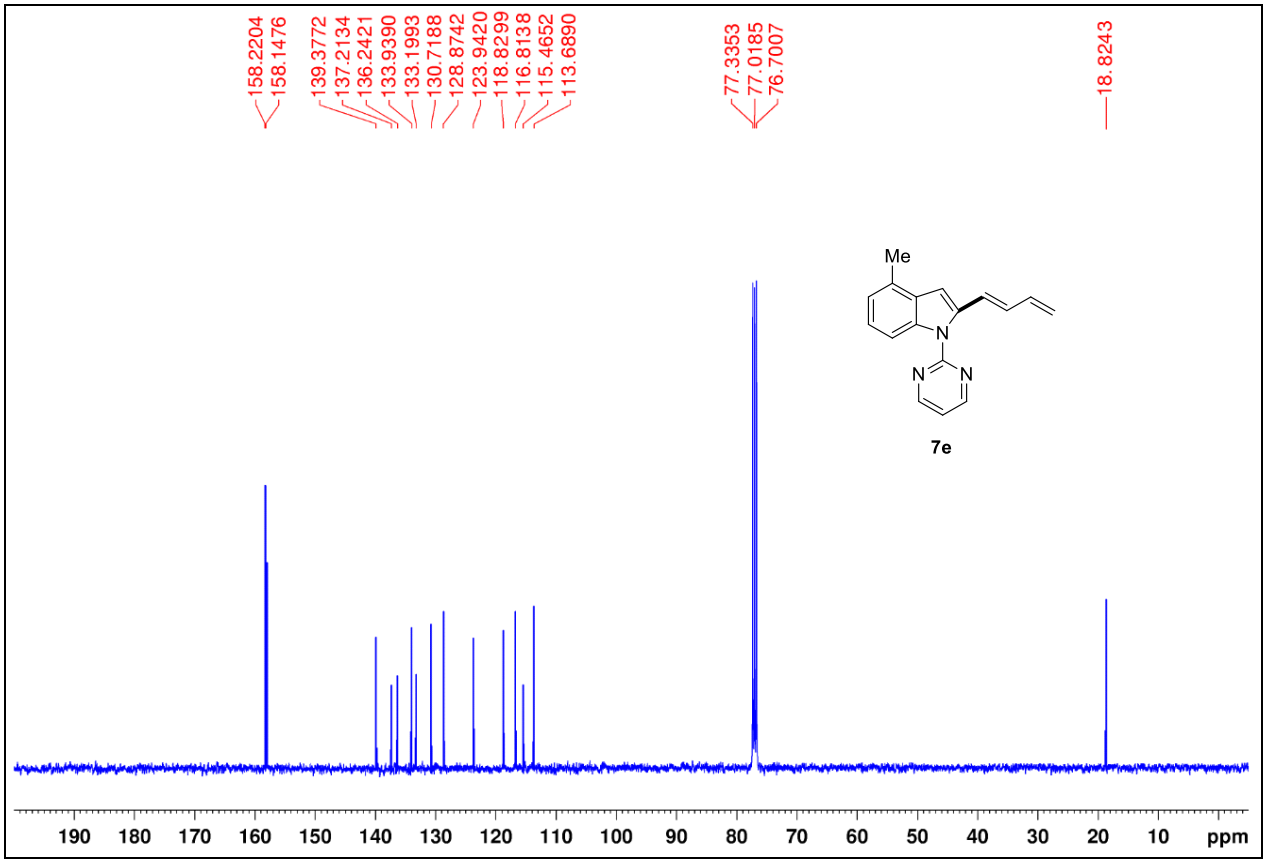
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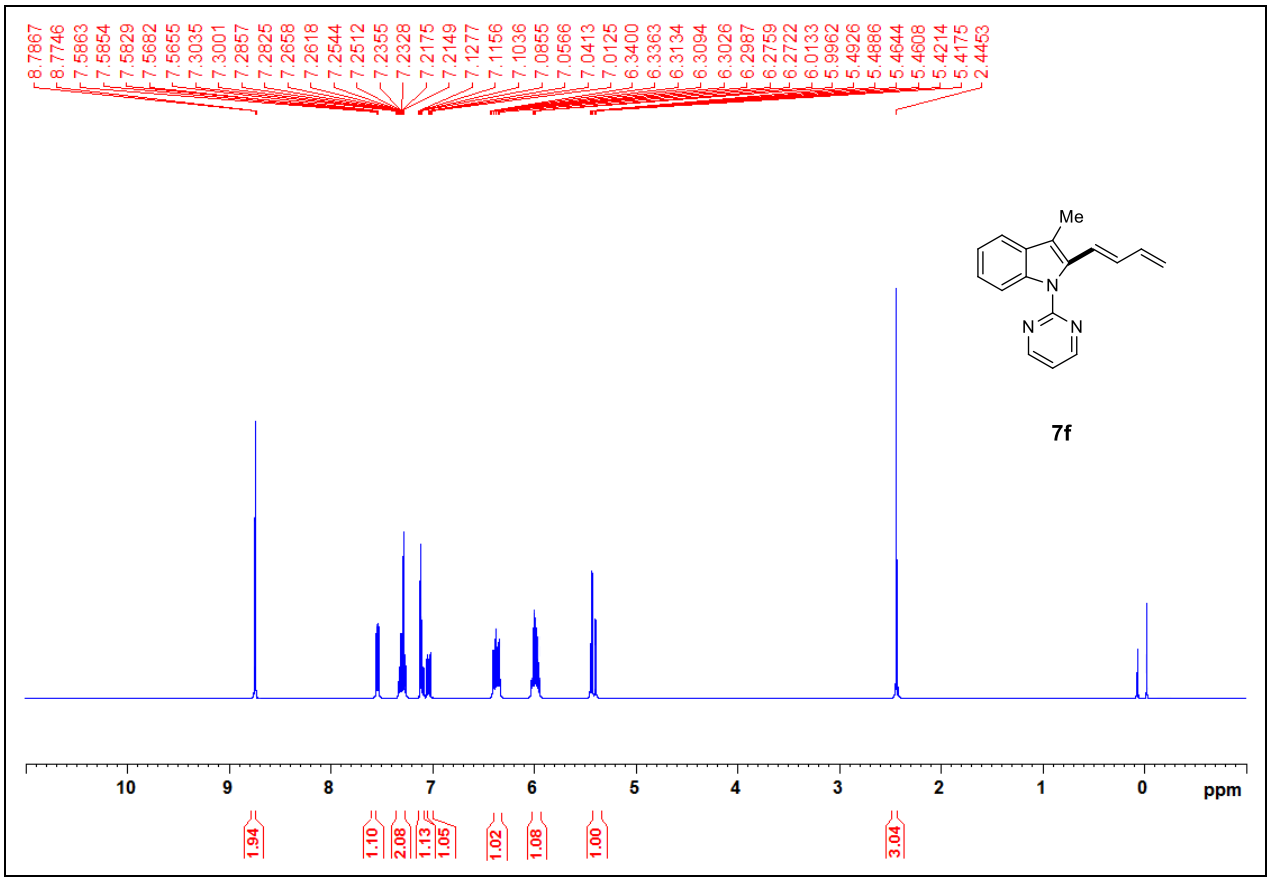
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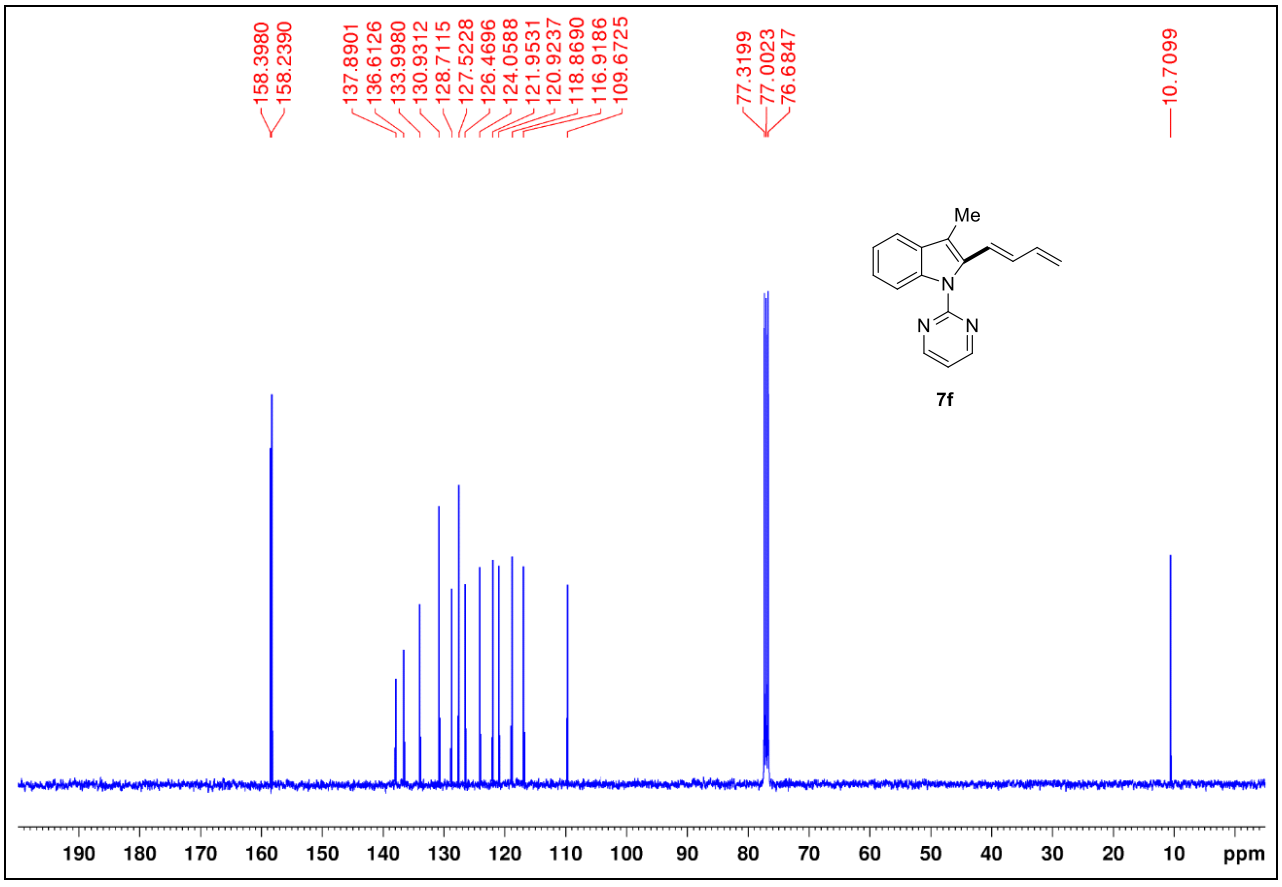
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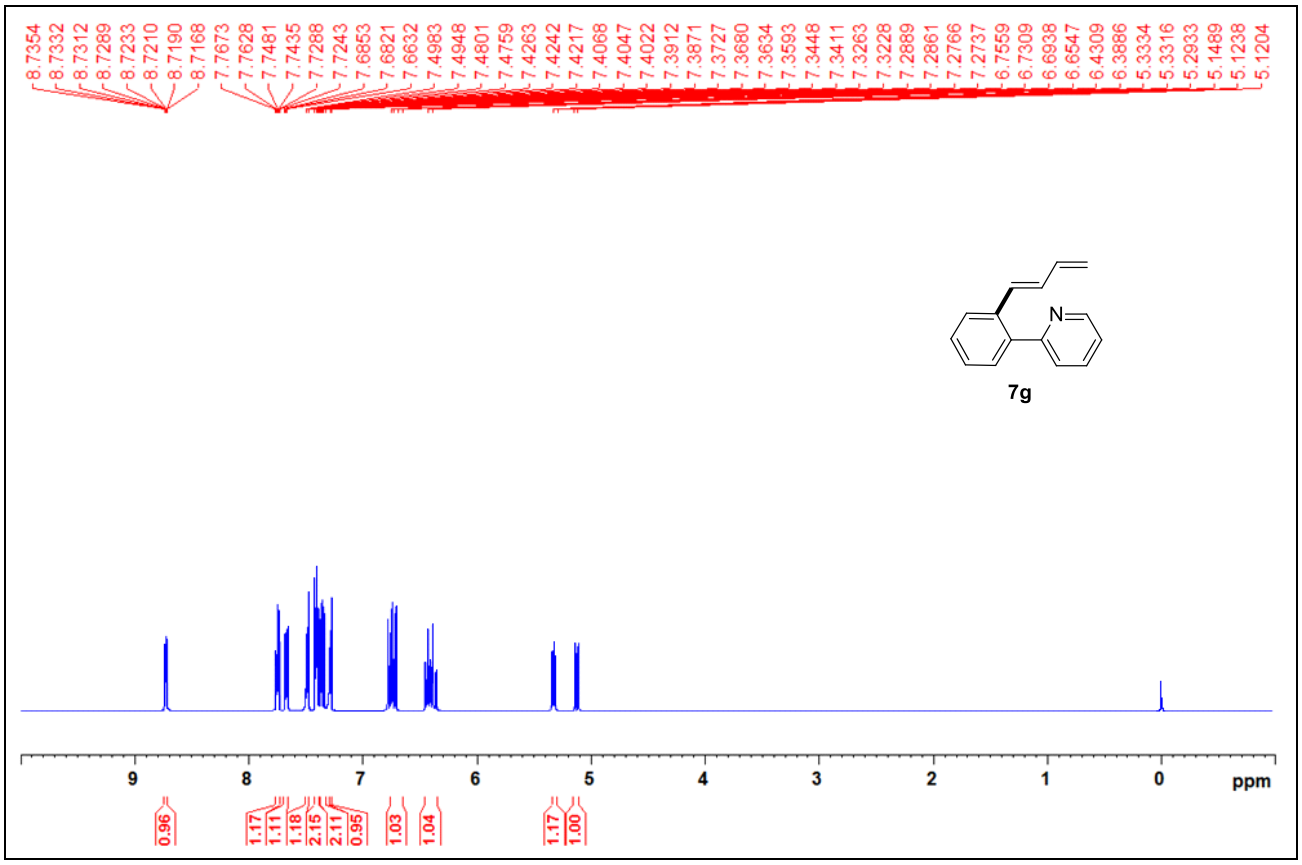
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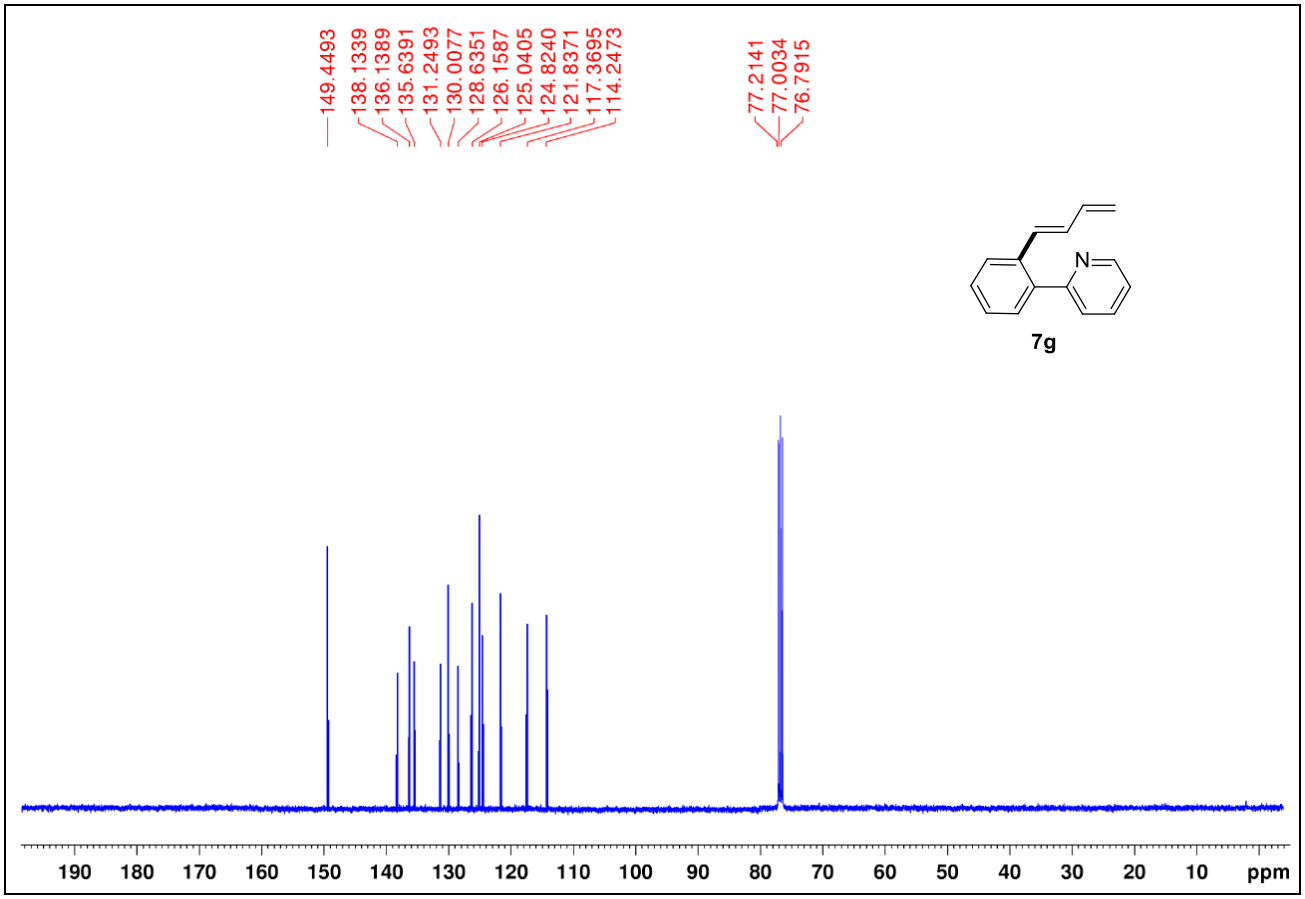
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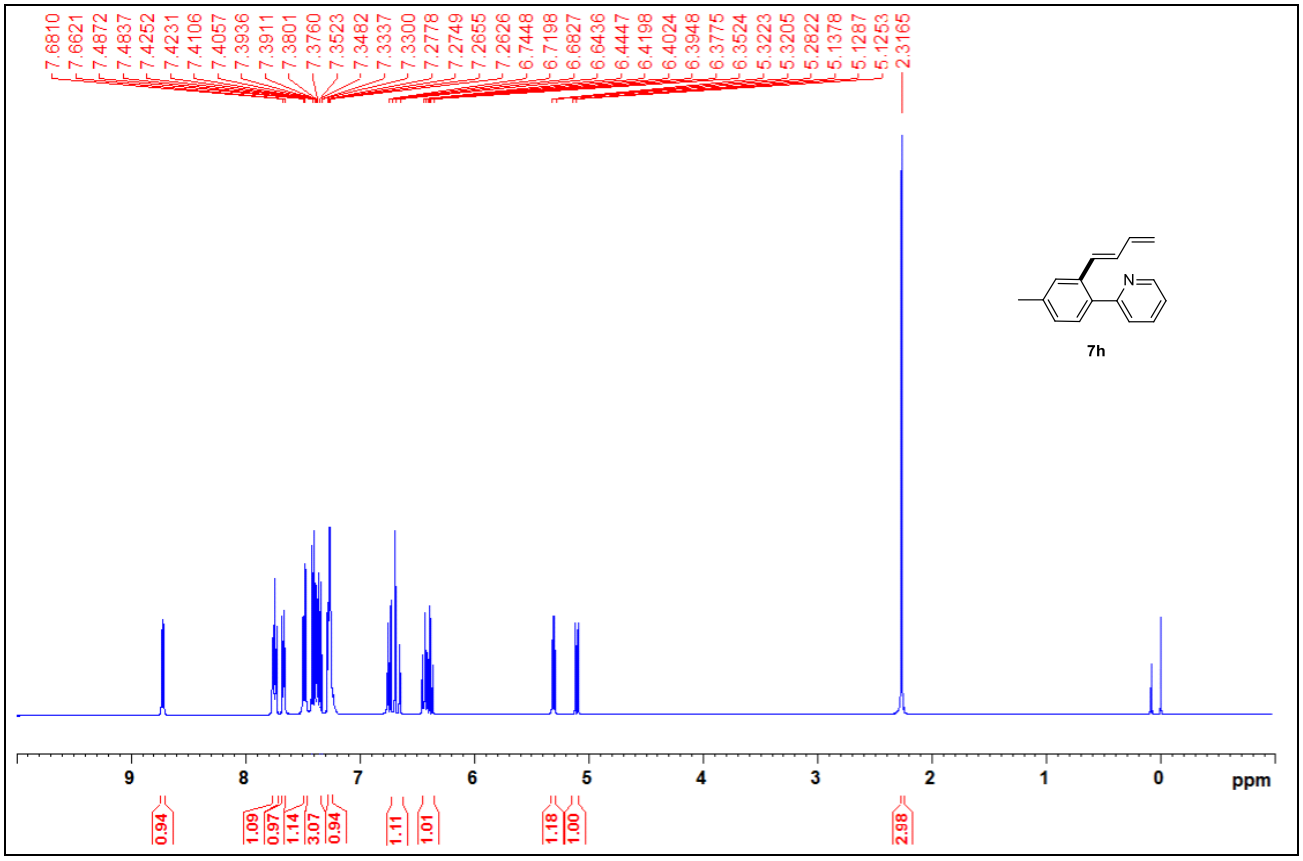
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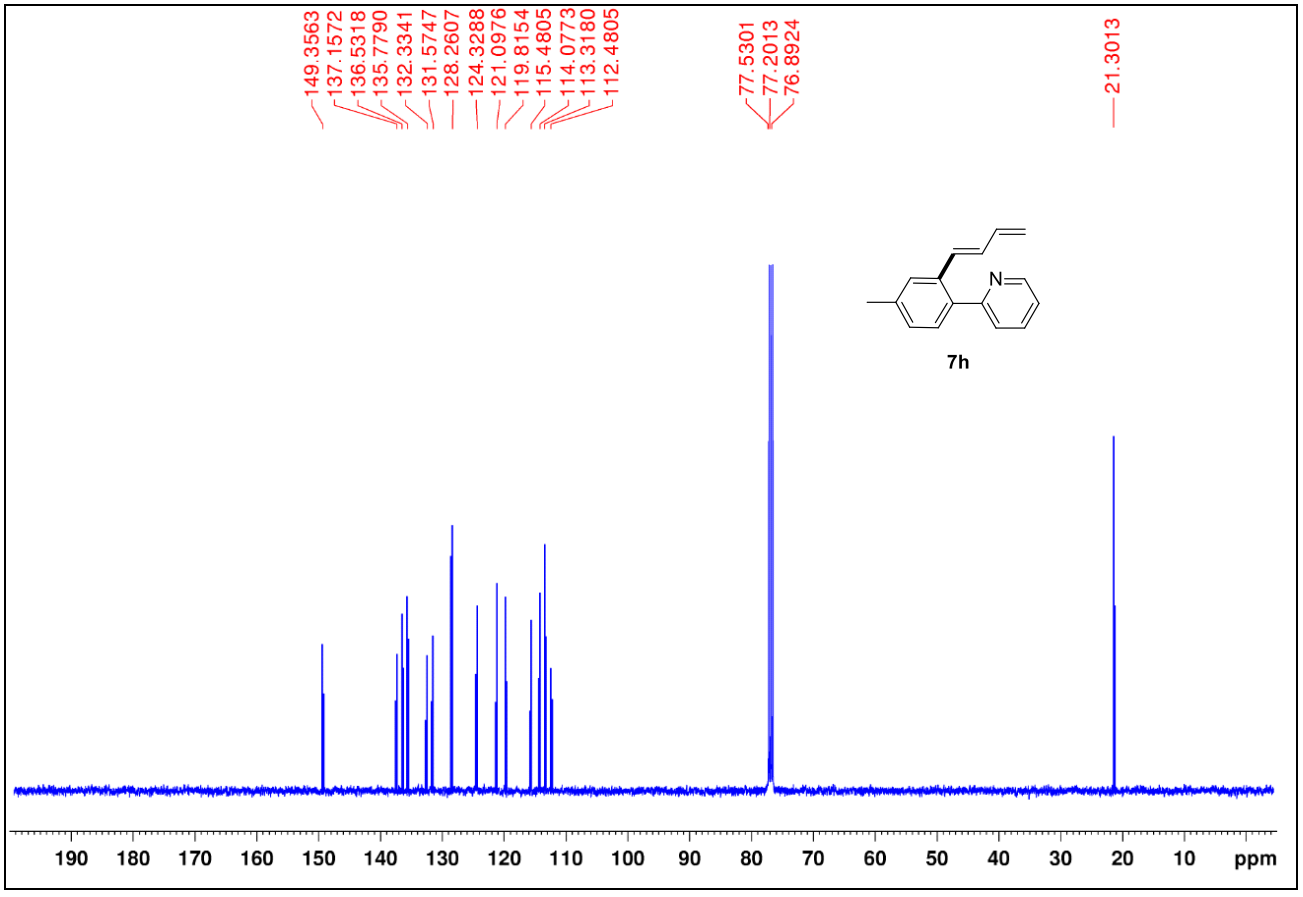
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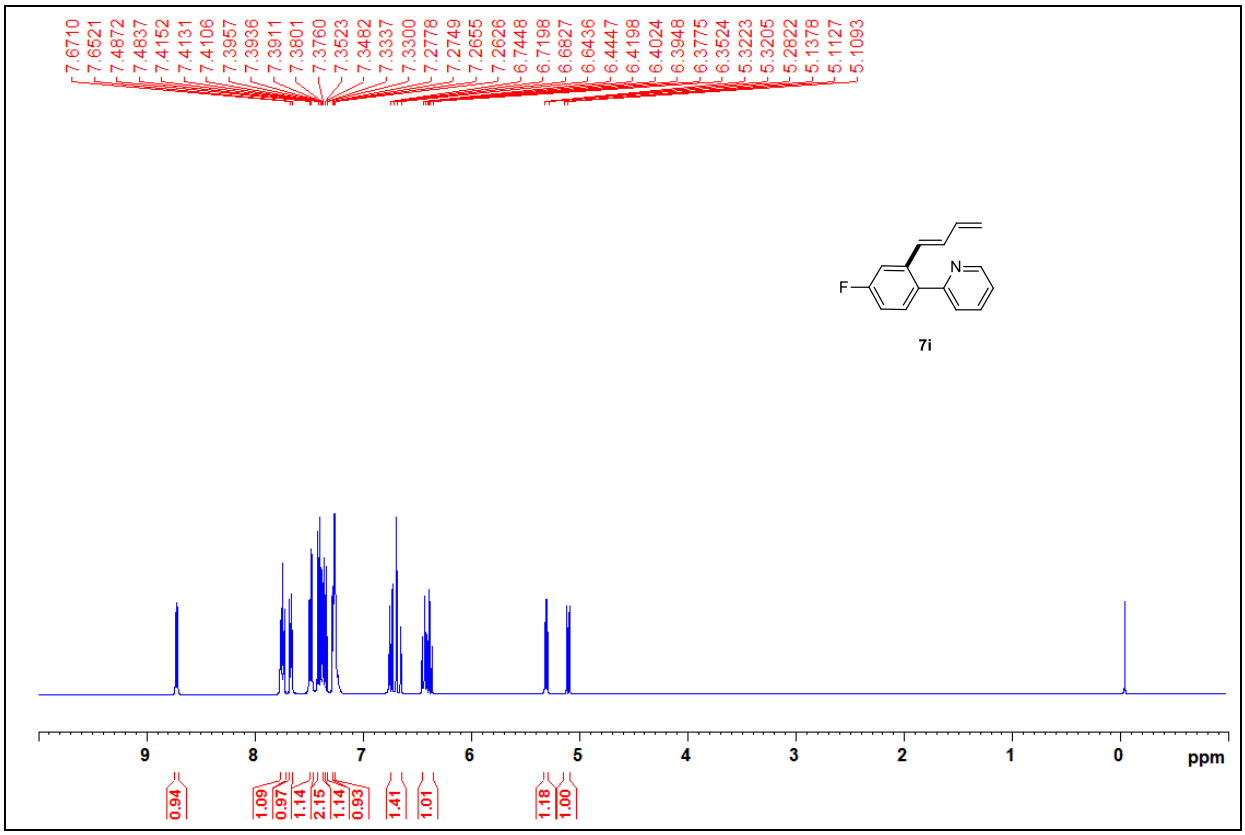
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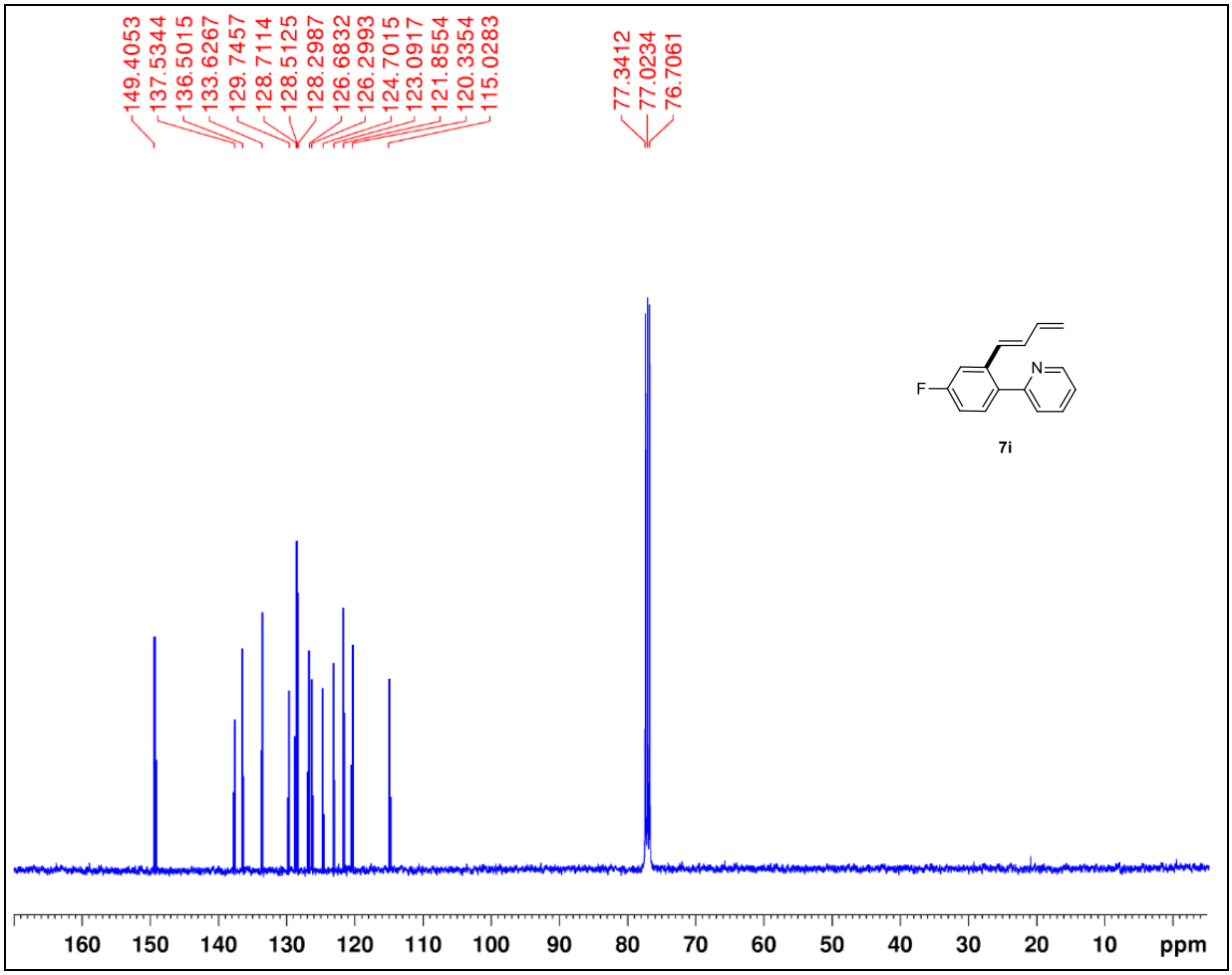
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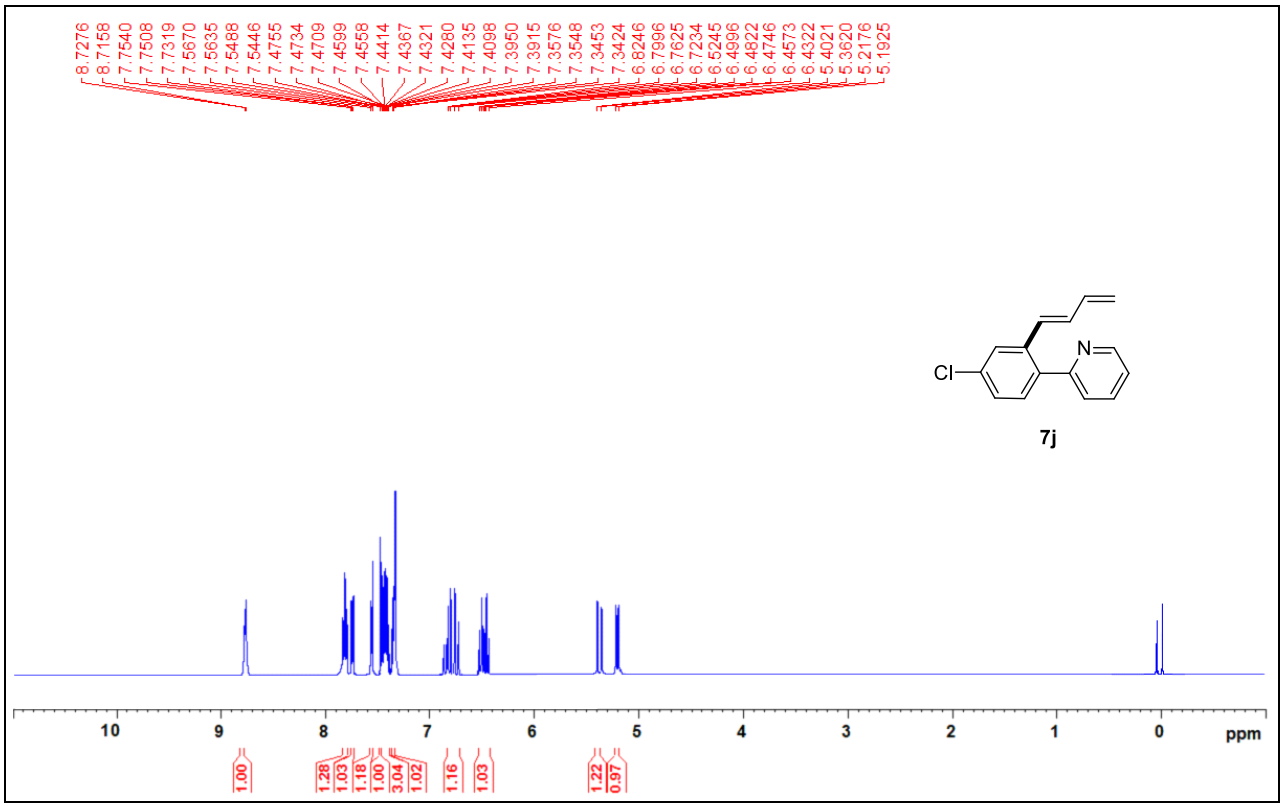
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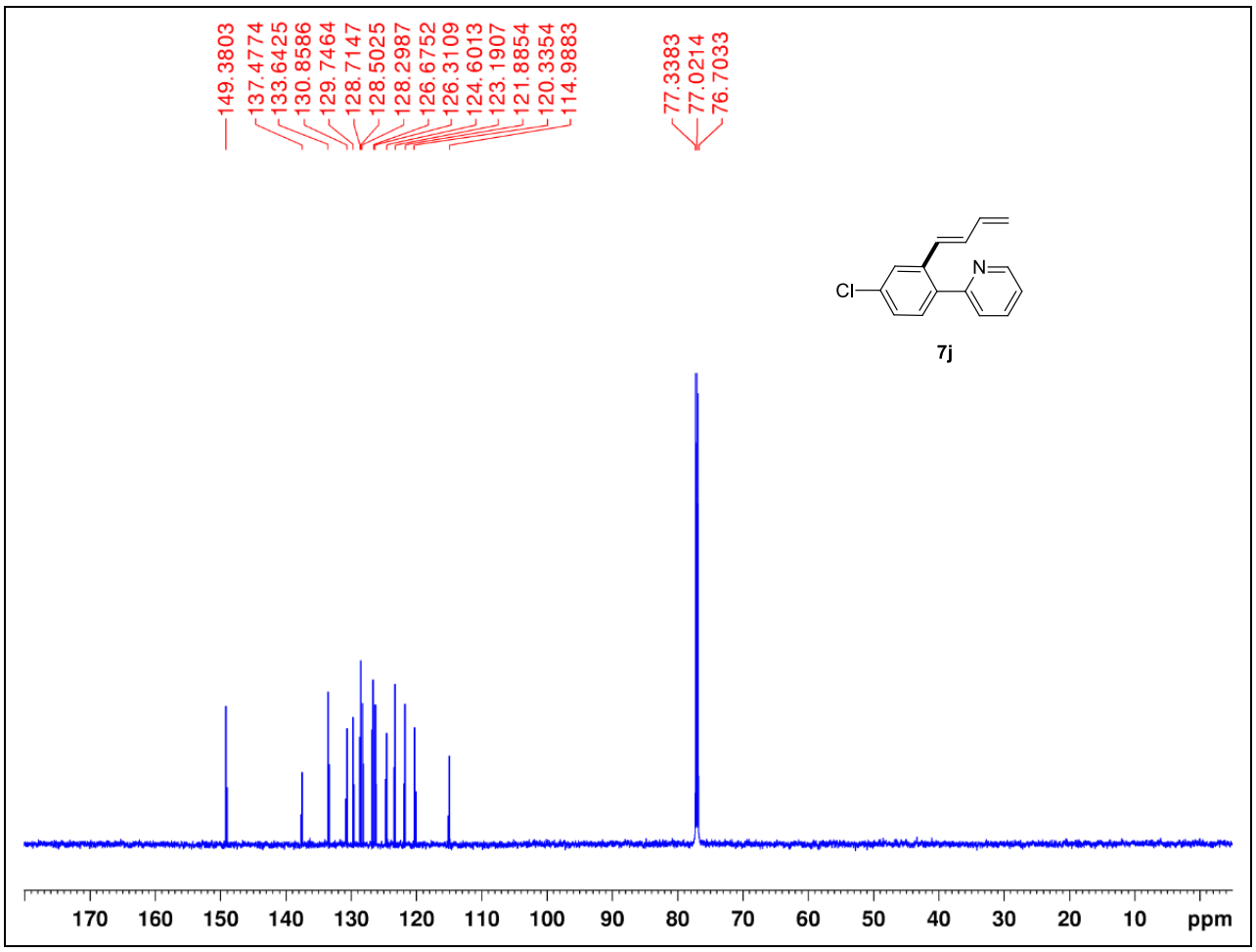
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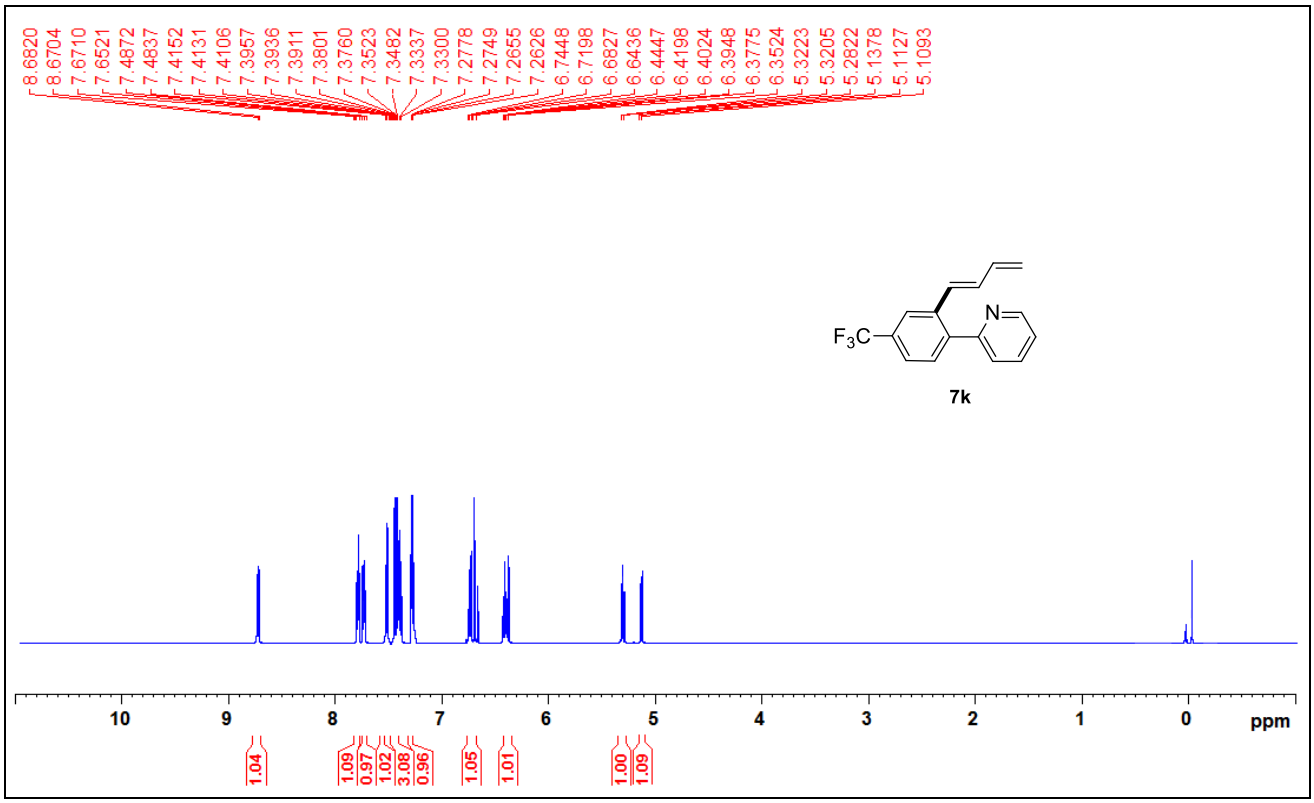
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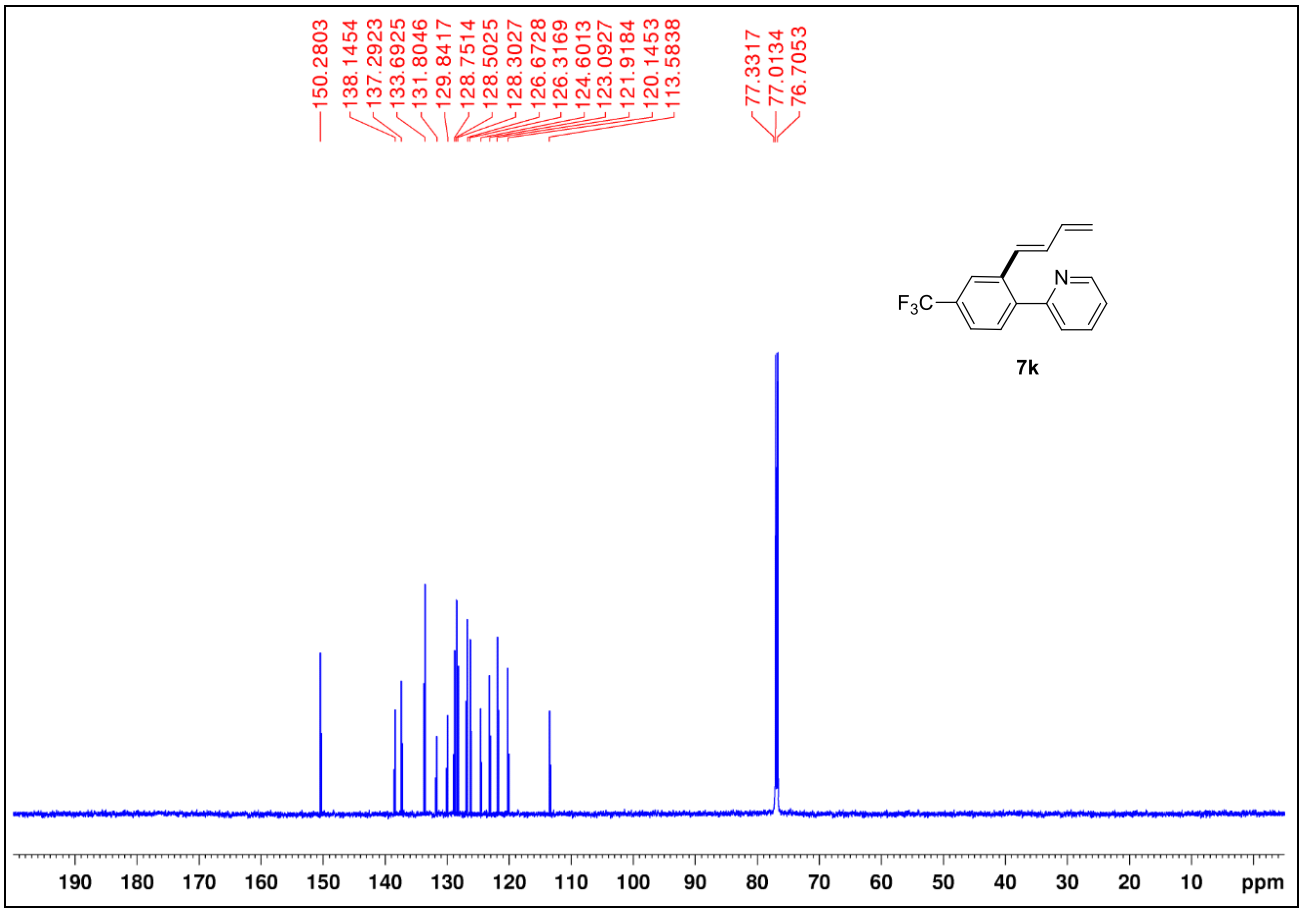
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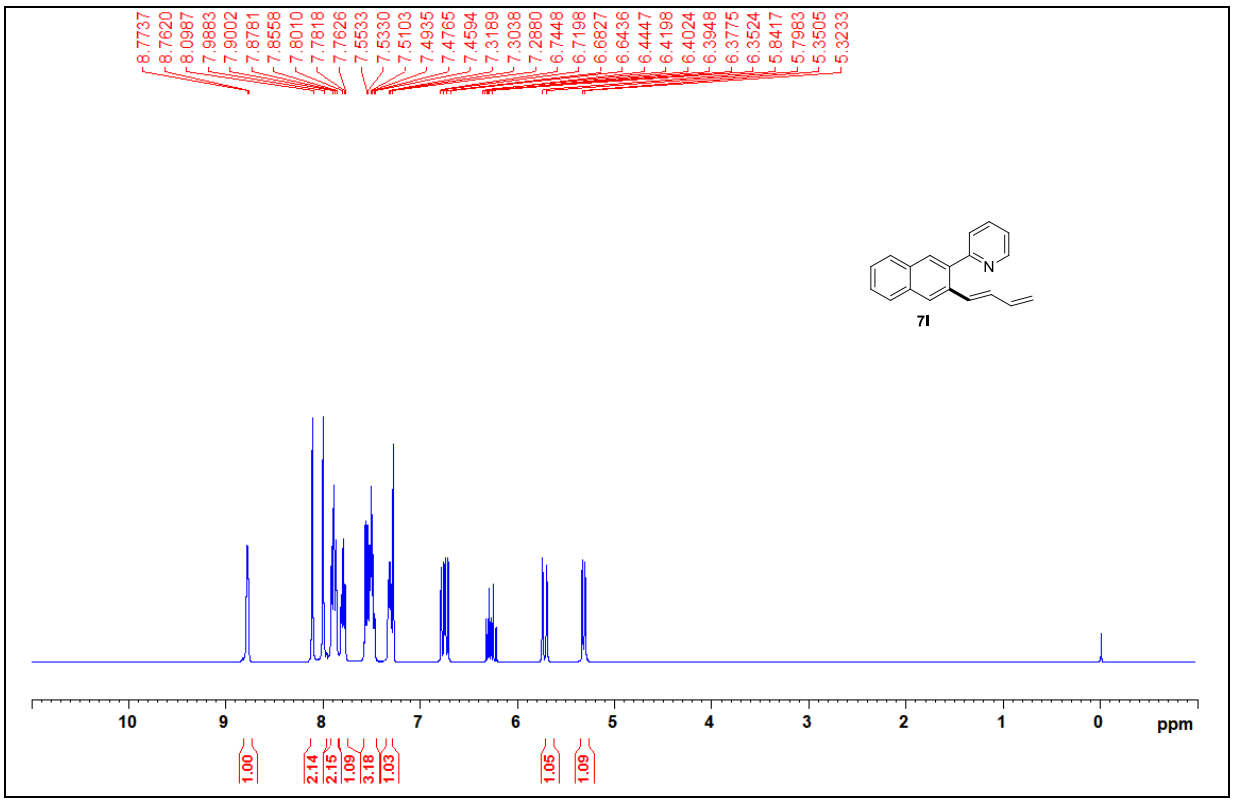
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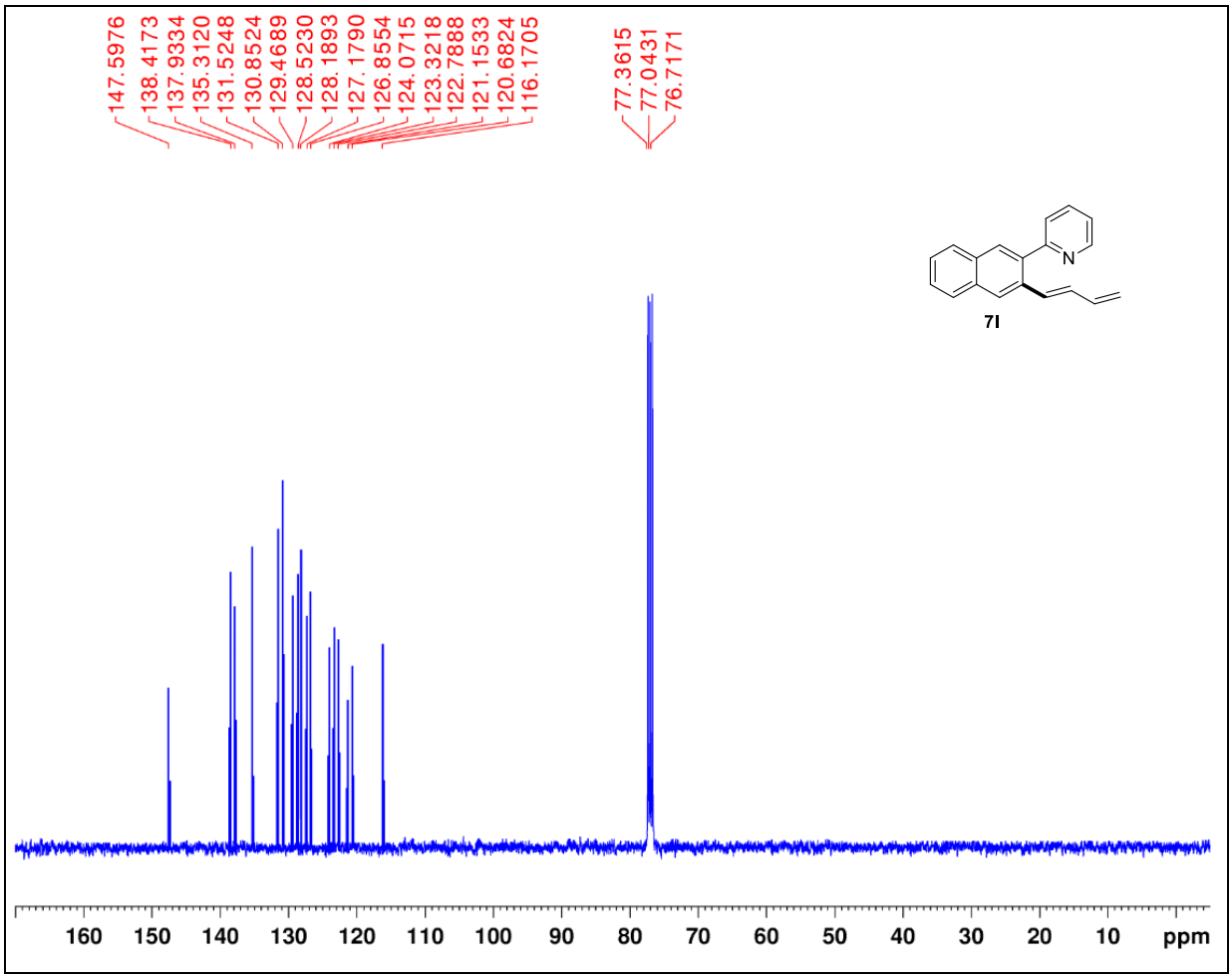
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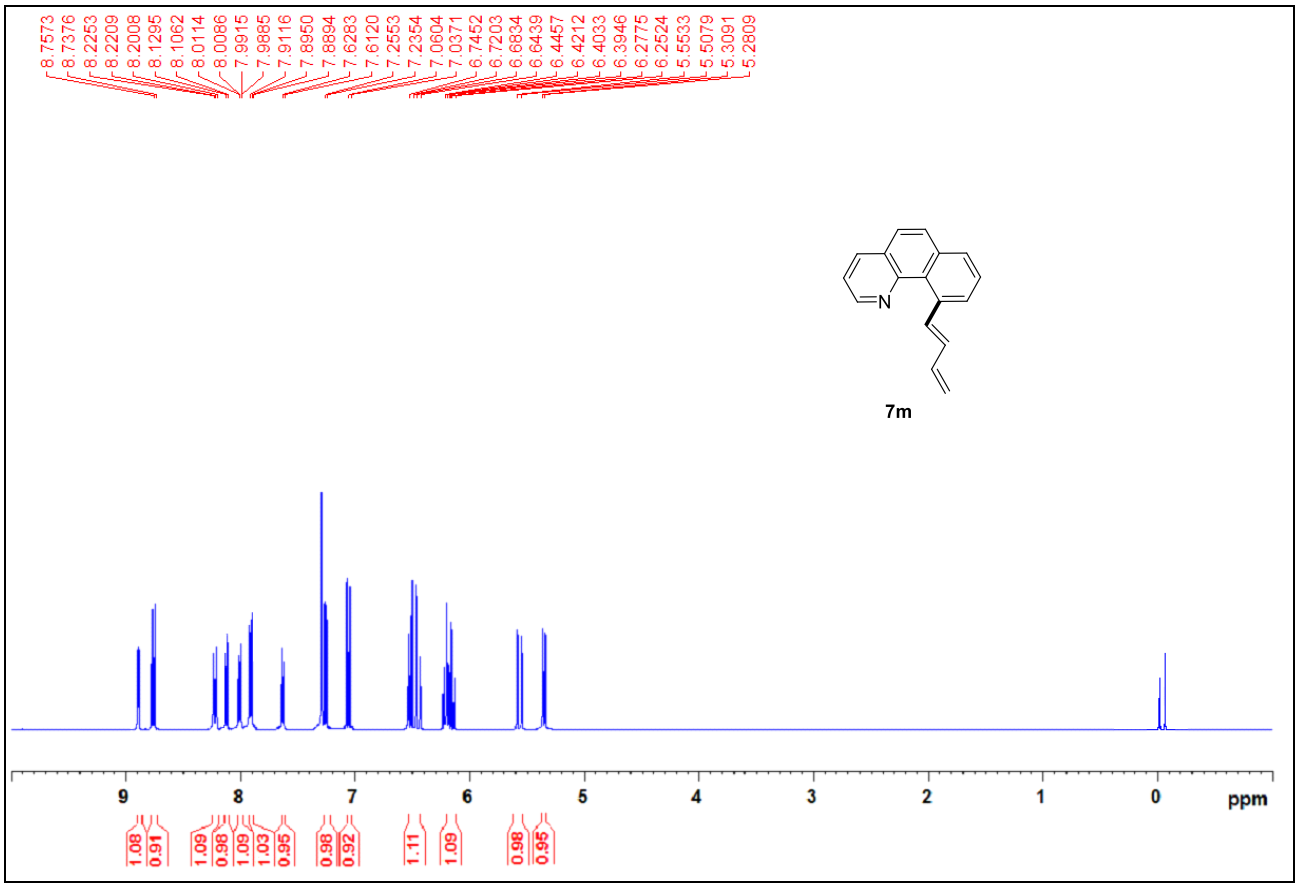
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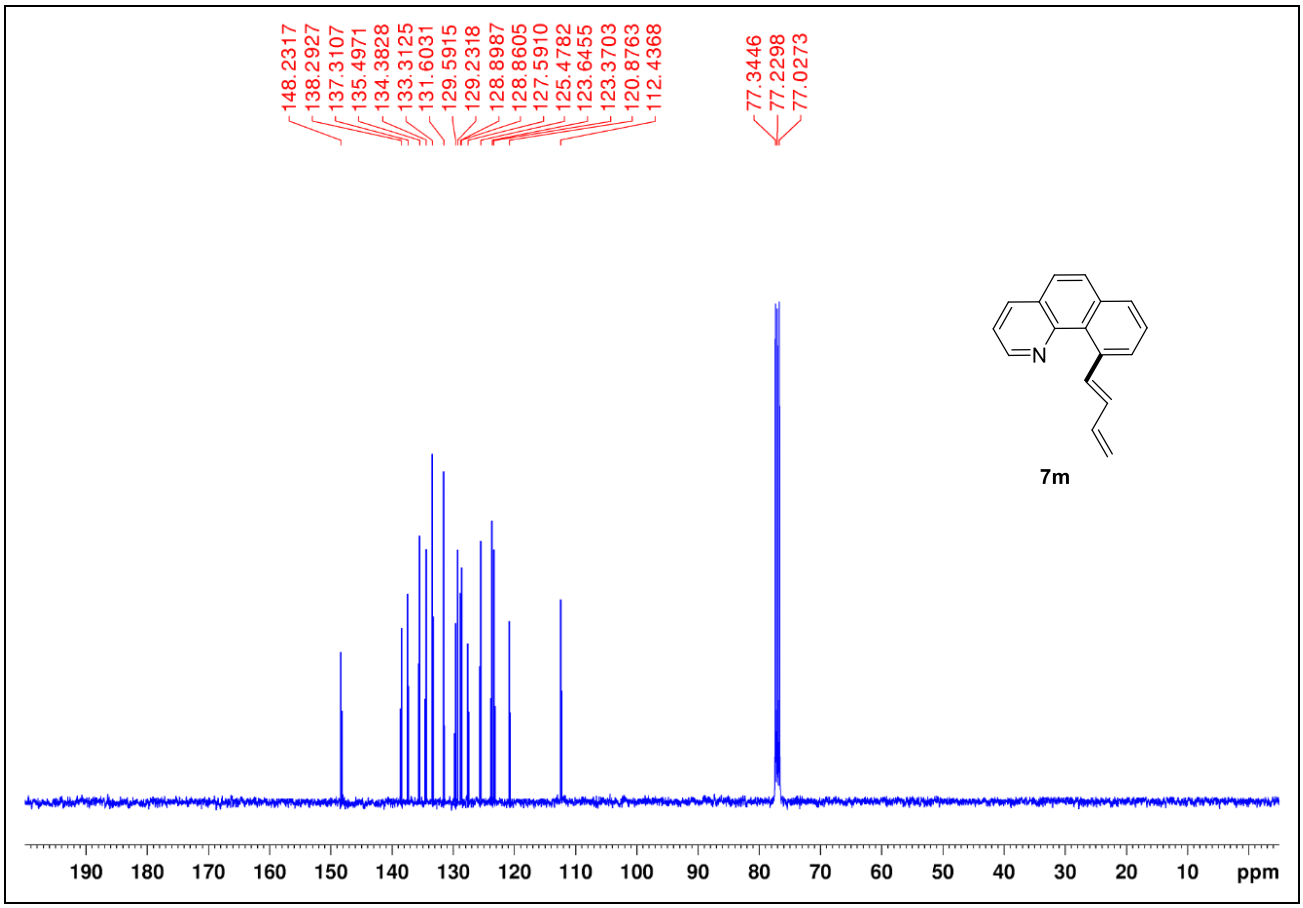
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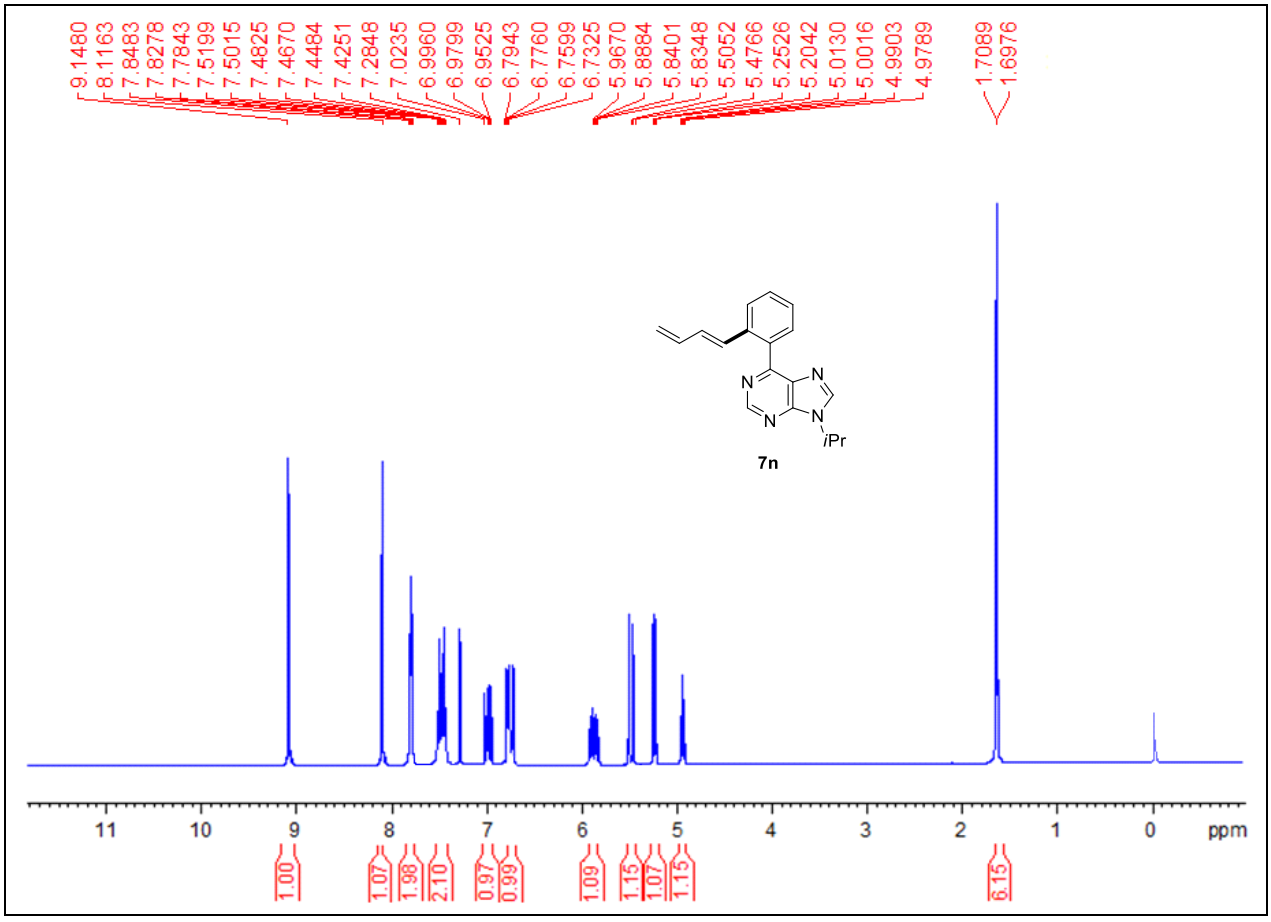
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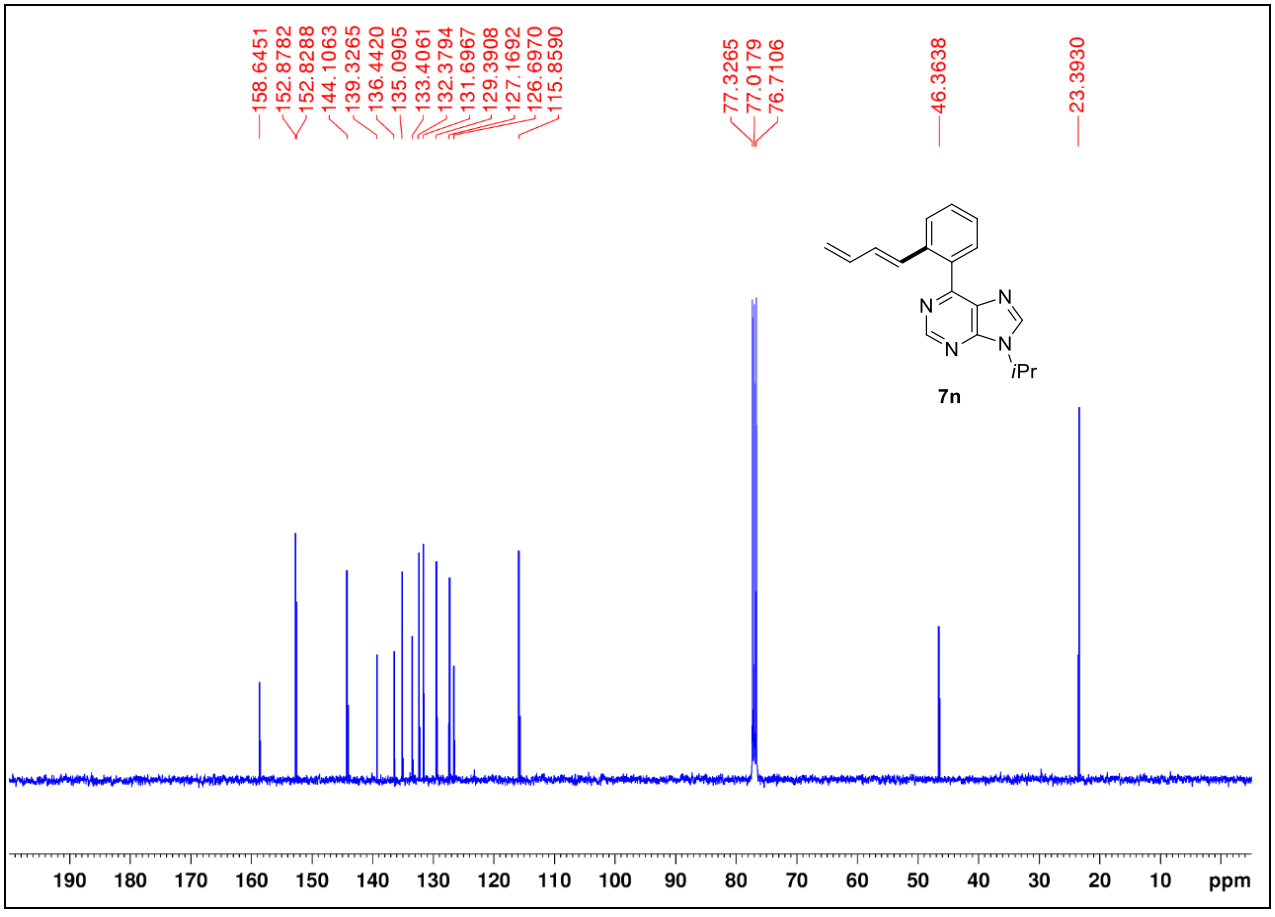
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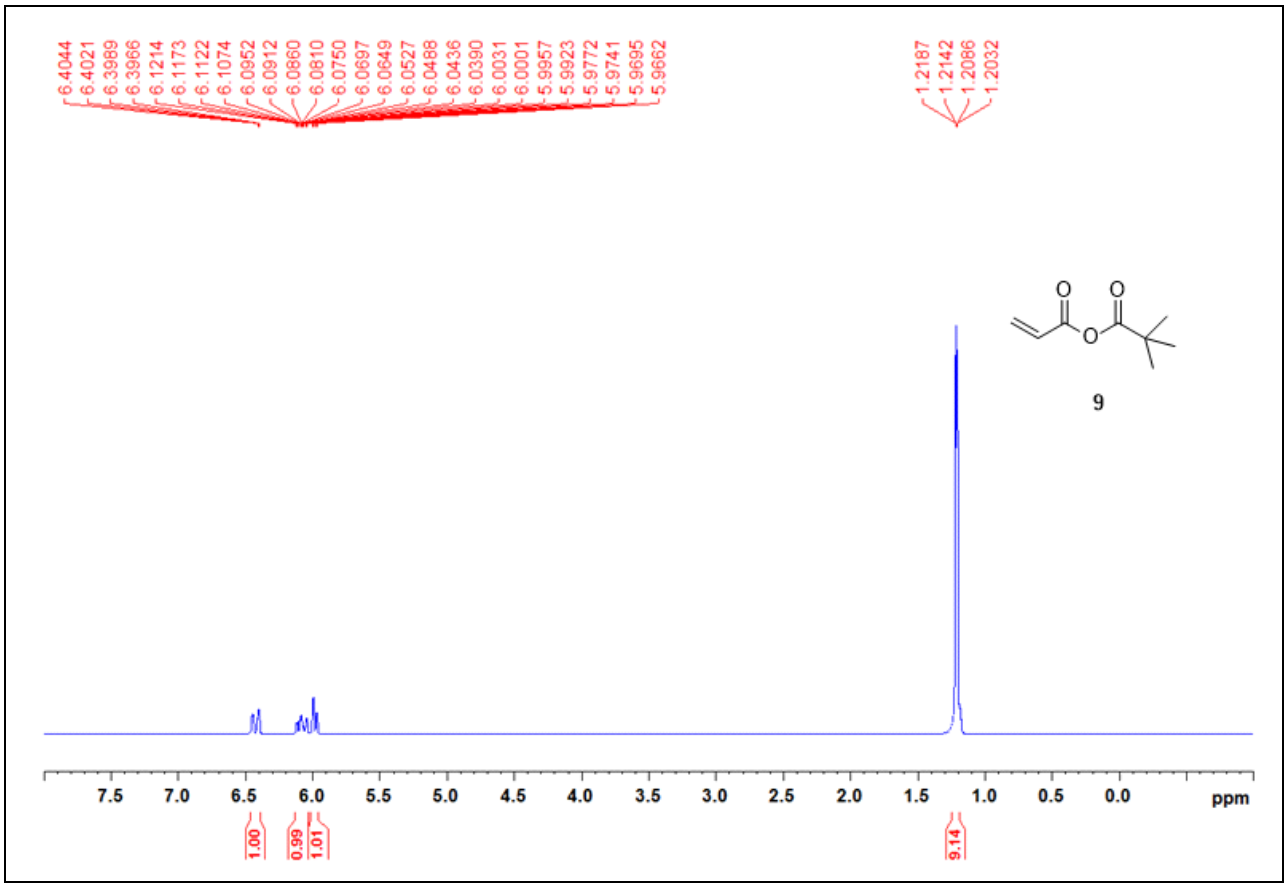
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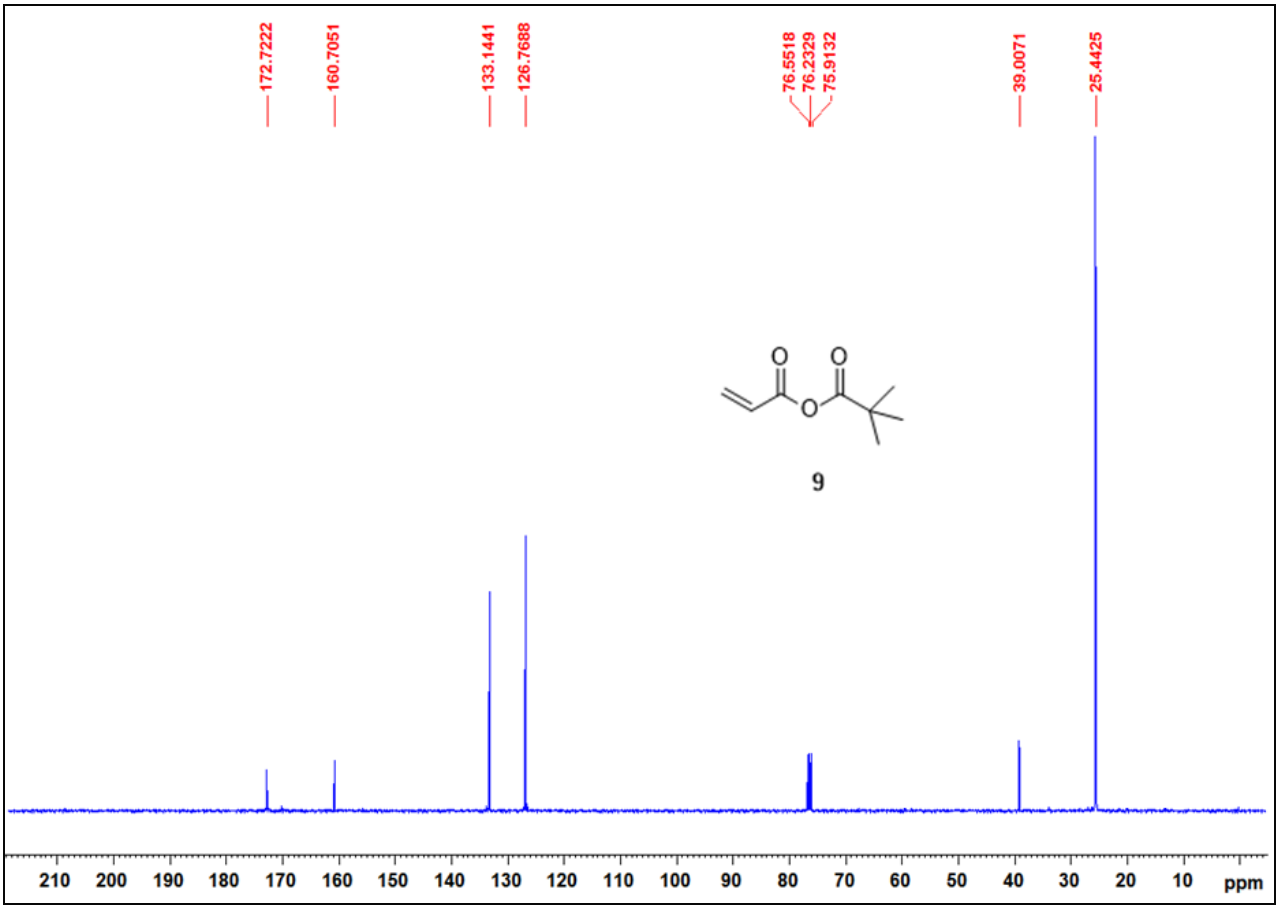
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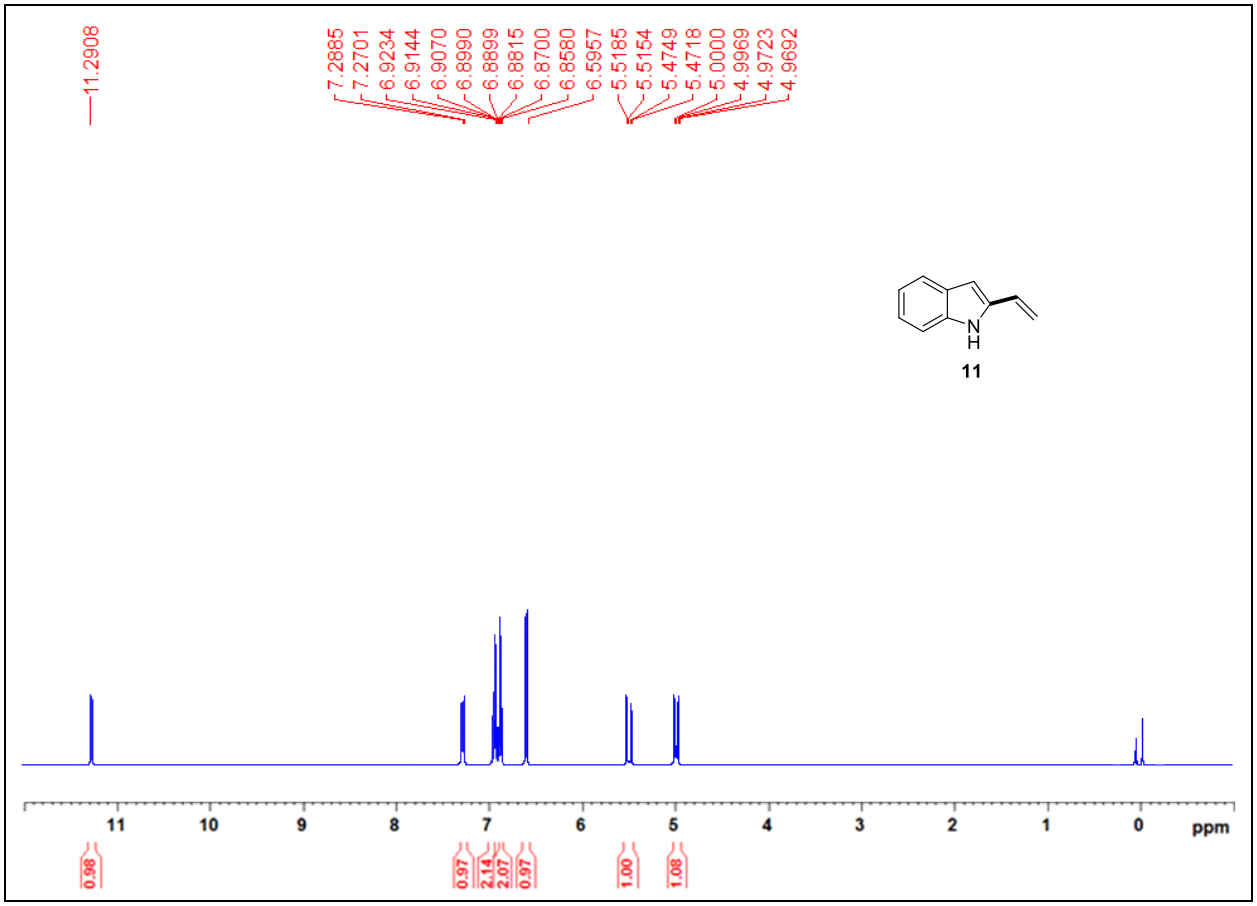
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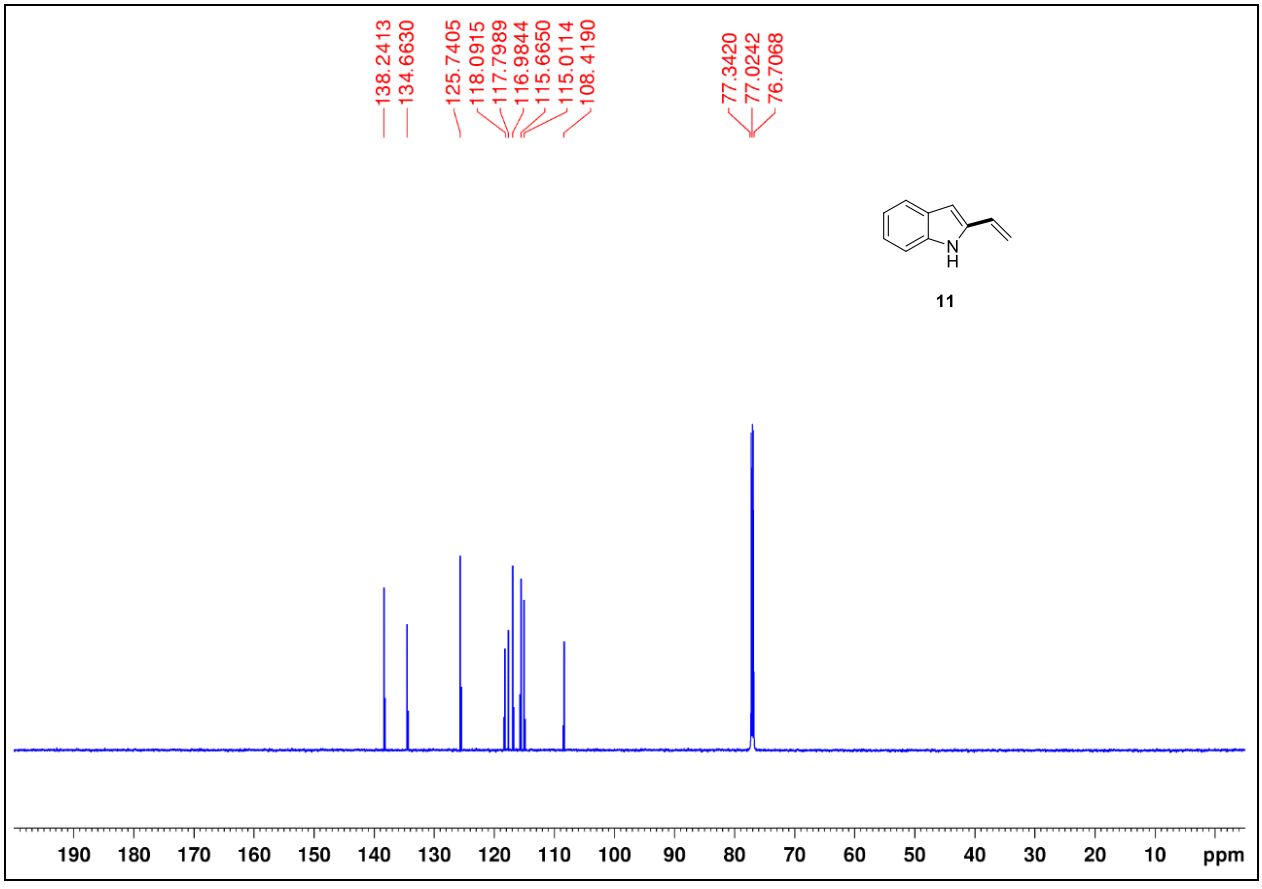
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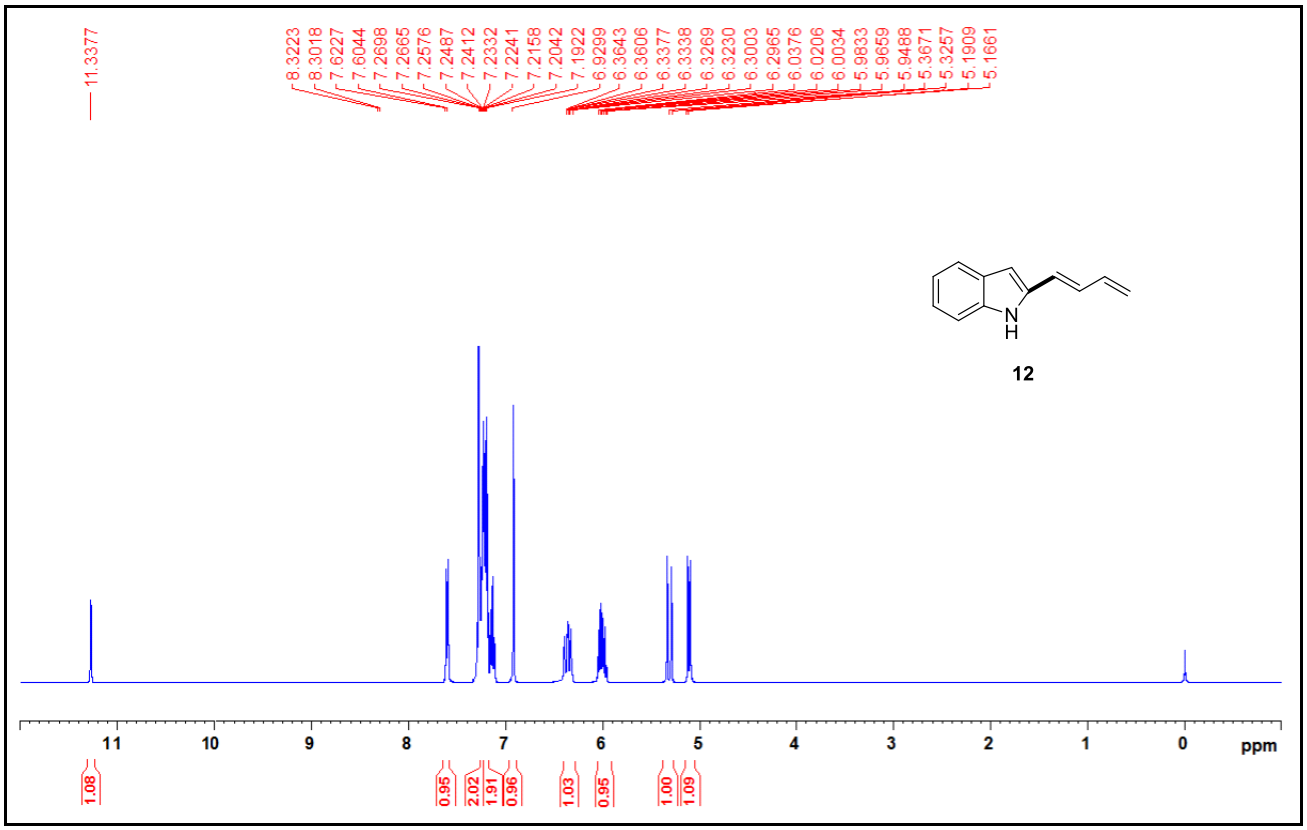
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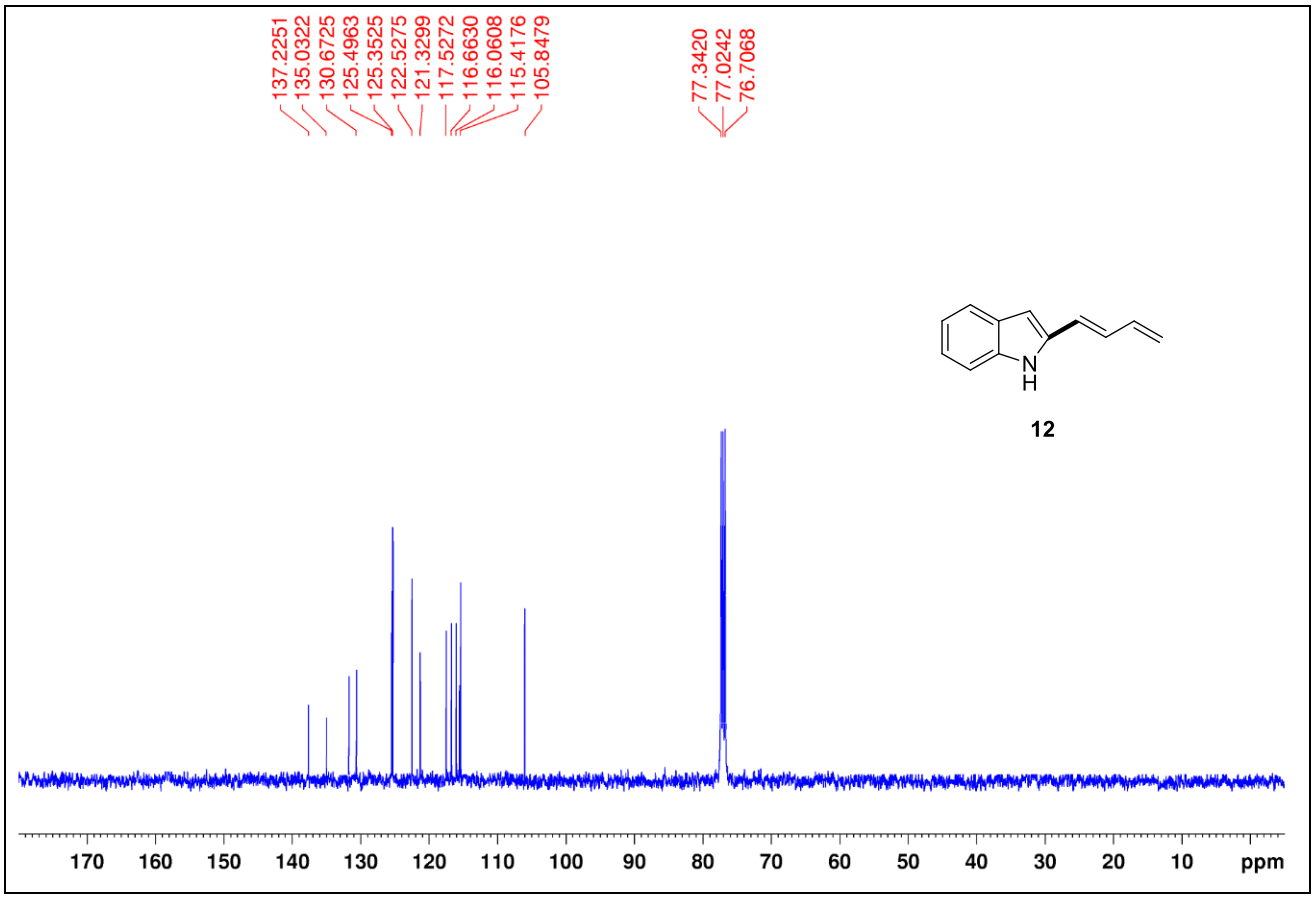
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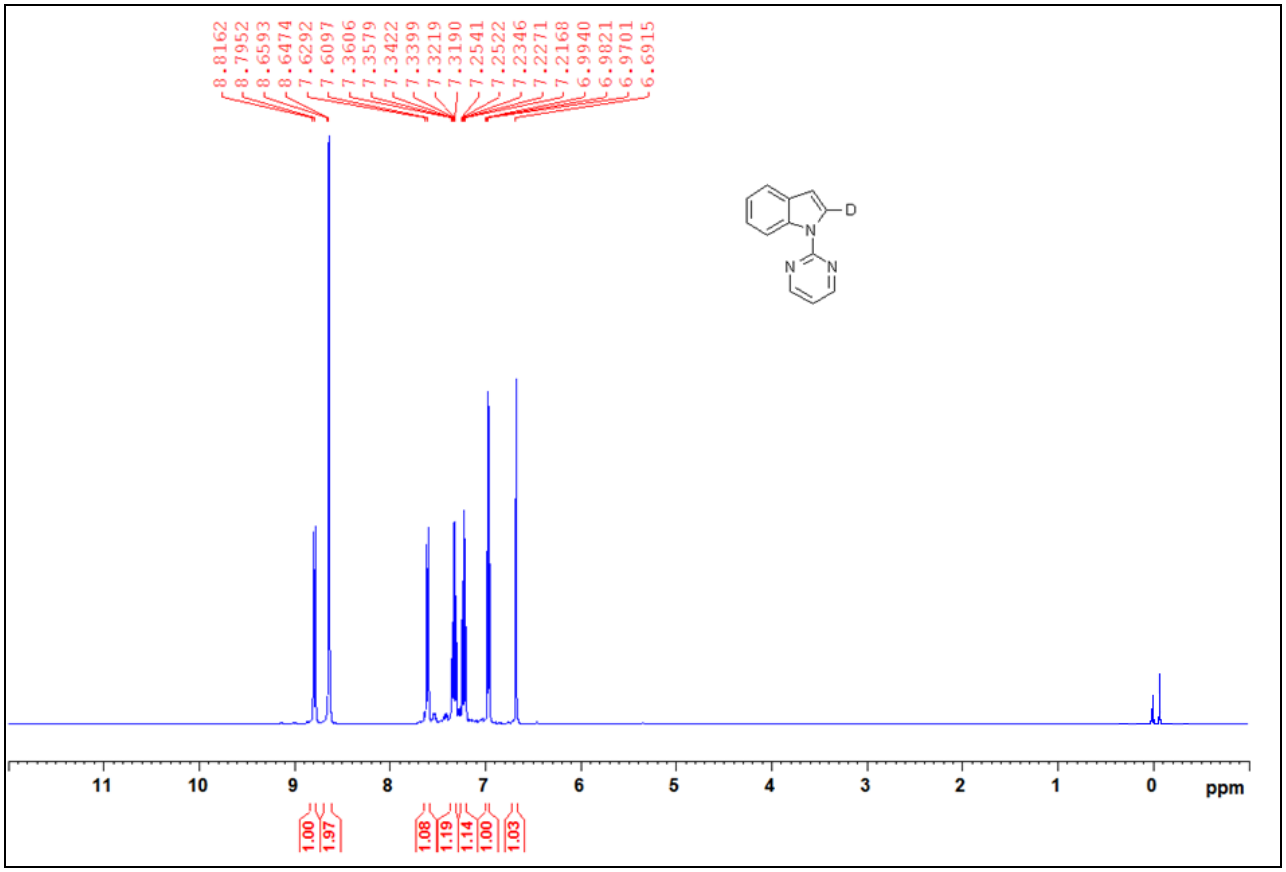
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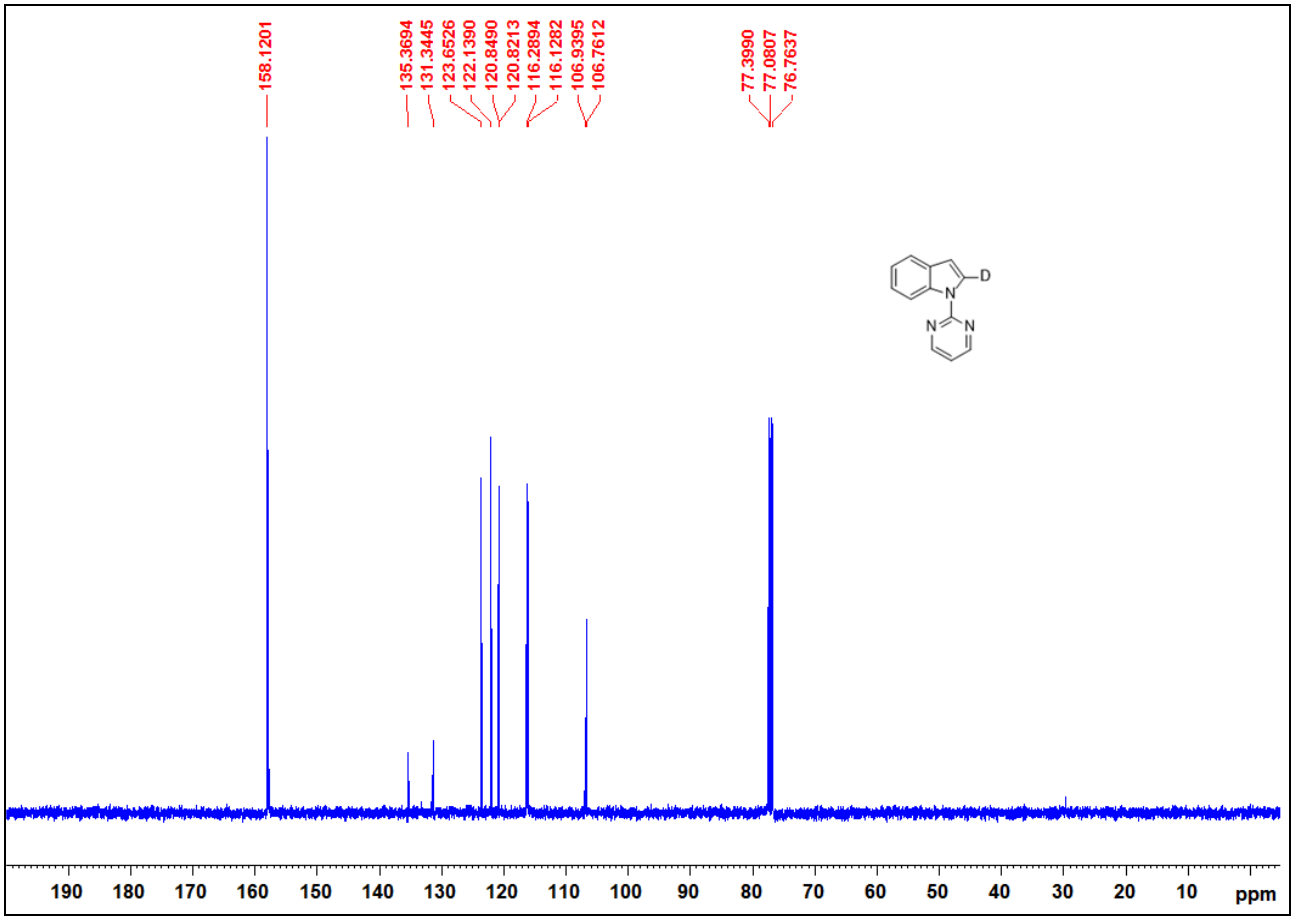
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ppm