Supporting Information

Tandem Isomerization and C-H Activation: Regioselective Hydroheteroarylation of Allylarenes

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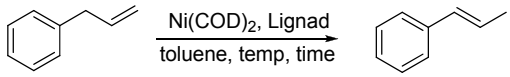
General. All air-sensitive manipulations were performed under an atmosphere of nitrogen using Schlenk technique or in a glovebox. ^{1}H and ^{13}C NMR spectra were run a Bruker 300 MHz, or 400 MHz spectrometer using the residual proton of the deuterated solvent for reference ($CDCl_3$, ^{1}H NMR: 7.24 ppm. ^{13}C NMR: 77.2 ppm). Chemical shifts are reported in ppm (δ); coupling constants, *J*, are reported in Hz. Standard abbreviations are used: s = singlet, d = doublet, t = triplet, q = quartet, qn = quintet, m = multiplet. Column chromatography was performed using silica gel (spherical, 40-63 m). Visualization was performed with UV light (254 nm). GC analyses were performed on an Agilent Technologies 7890 GC instrument. High resolution mass spectra were obtained with a JEOL, JMS-700 (EI or FAB+) spectrometer. High resolution MALDI-mass spectra were conducted on an Applied Biosystems 4800 Proteomics Analyzer (Applied Biosystem, Foster City).

Chemicals. All reagents were purchased from Acros, Aldrich, and Alfa Aesar without further purification in advance before use. Solvents for chromatography were reagent grade. Toluene was dried over sodium with benzophenone-ketyl intermediate as an indicator. Deuterated benzene and chloroform were dried by vacuum transfer from activated molecular sieve. $AlMe_3$ (2.0 M in toluene) was purchased from Aldrich and diluted with dried toluene to 0.5 M. IMes and IPr were synthesized according to the literature.[1] Amino-NHC was prepared in accord to our previous work.[2] All allylbenzene derivatives were purchased from Acros, Aldrich, and Alfa Aesar and used without further purification. Starting materials of benzoxazole,[3] oxazole,[4] and benzimidazole[5] derivatives were prepared according to the literature procedures.

General procedure A for Nickel-catalyzed hydroheteroarylation of allylarenes (Branch): To the toluene solution of $Ni(COD)_2$ (14 mg, 0.05 mmol), IMes (14 mg, 0.05 mmol), and 1-methylbenzimidazole (0.5 mmol) was added allylbenzene (1.0 mmol) into the vial. After the vial was screw-capped, the reaction solution was taken outside the glovebox and heated at 130 ^{o}C for 16 h. The resulting mixture was filtered through *Celite* and washed with dichloromethane. The filtrate solution was concentrated in *vacuo* to afford crude product. The crude was further purified by flash chromatography using hexane/ethyl acetate (3:1) as eluent.

General procedure B for Nickel/$AlMe_3$ mediated hydroheteroarylation of allylarenes (Linear): To the toluene solution of $Ni(COD)_2$ (14 mg, 0.05 mmol), IPr (19 mg, 0.05 mmol), and 1-methylbenzimidazole (0.5 mmol) was added allylbenzene (1.0 mmol) and $AlMe_3$ in toluene (0.05 mmol, 0.1 mL) into the vial. After the vial was screw-capped, the reaction solution was taken outside the glovebox and heated at 130 ^{o}C for 16 h. The resulting mixture was filtered through *Celite* and washed with dichloromethane. The filtrate solution was concentrated in *vacuo* to afford crude product. The crude was further purified by flash chromatography using hexane/ethyl acetate (1:3) as eluent.

Table S1. Isomerization of Allylbenzene



entry	Ligand	cat. mol%	Temp(^{o}C)	Time(h)	GC Yield (%)
1	PCy_3	10	130	18	40
2	PPh_3	10	130	18	0
3	Cy_2P ⌒ PCy_2	10	130	18	95
4	bipyridine	10	130	18	0
5	1,10-phenanthroline	10	130	18	0
6	IMes	10	130	18	99
7	IMes	3	130	18	99
8	IMes	3	130	1	99
9	IMes	3	60	1	4
10	IMes	1	130	1	99
11	IMes	0.1	130	1	0
12	IMes	0.5	130	1	99
13	IMes	0.2	130	1	21

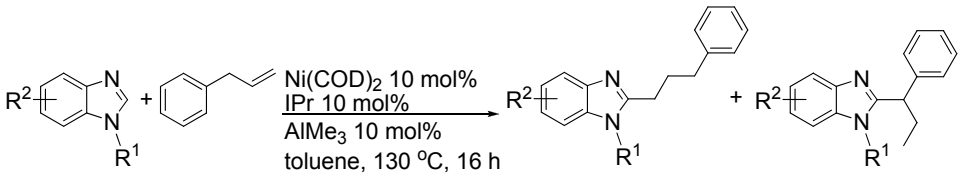
[a] Conditons: Allylbenzene (0.5 mmol), $Ni(COD)_2$ (0.05 mmol), ligand (IMes: 0.05 mmol; PCy_3: 0.1 mmol; dcpe, bipyridine, 1,10-Phen: 0.05 mmol), toluene (1 mL).

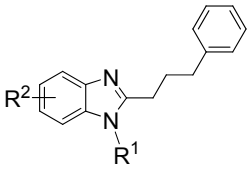
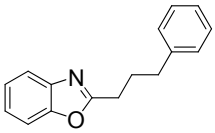
Table S2. Optimization.

Entry	Ligand (eq)	Additive (eq)	Yield (%)[b]	**3a**:**4a**
1	bipyridine (0.1)	-	NR	-
2	1,10-Phen (0.1)	-	NR	-
3	PCy_3 (0.2)	-	27	15:85
4	IMes (0.1)	-	97	6:94
5	IPr (0.1)	-	80	36:64
6	Amino NHC (0.1)	-	88	9:91
7	PCy_3 (0.2)	$AlMe_3$ (0.1)	69	81:19
8	IMes (0.1)	$AlMe_3$ (0.1)	80	80:20
9	IPr (0.1)	$AlMe_3$ (0.1)	94	93:7
10	Amino NHC (0.1)	$AlMe_3$ (0.1)	53	79:21

[a] Reaction Conditions: **1a** (0.5 mmol), **2a** (1.0 mmol), $Ni(COD)_2$ (0.05 mmol), and ligand in toluene (1 mL) at 130 ˚C for 16 hours. [b] Isolated yield.
1,10-Phen = 1,10-phenanthroline, PCy_3 = tricyclohexyl-phosphine,
IMes =1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene,
IPr =1,3-bis(2,6-diisopropyl-phenyl)imidazol-2-ylidene,
Amino NHC = N-(2-(3-mesityl-2,3-dihydro-1H-imidazol-1-yl)ethyl)-2-methylpropan-2-amine.

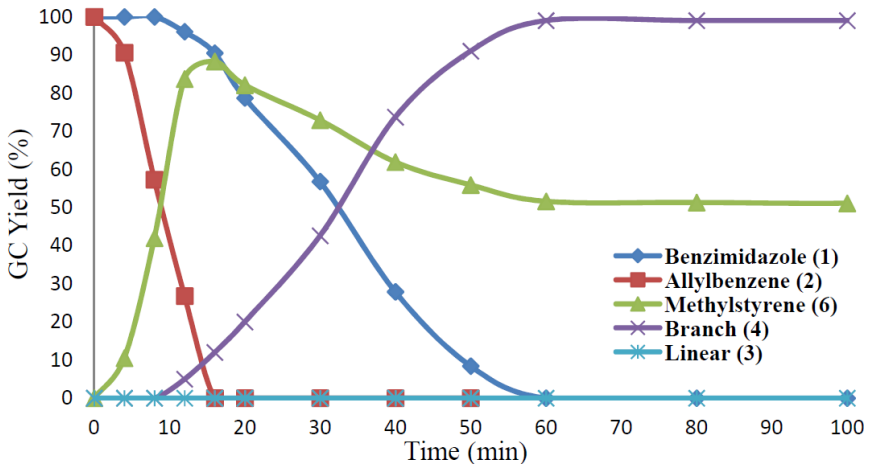
Table S3. Scope with various heteroarenes (Linear Selectivity).[a]

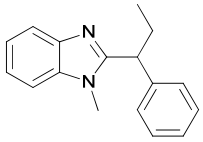


entry		1	major product	yield (%)	3:4
1	**1a**	R^1 = Me, R^2 = H		92	92:8
2	**1l**	R^1 = $(CH_2)_7CH_3$, R^2 = H		73	>99:1
3	**1m**	R^1 = CH_2-*o*-py, R^2 = H		65	95:5
4	**1n**	R^1 = CH_2Ph, R^2 = H		67	>99:1
5	**1o**	R^1 = *p*-C_6H_4Me, R^2 = H		80	91:9
6	**1p**	R^1 = *o*-C_6H_4Me, R^2 = H		65	>99:1
7	**1q**	R^1 = *p*-C_6H_4OMe, R^2 = H		76	91:9
8	**1r**	R^1 = *p*-$C_6H_4CF_3$, R^2 = H		81	>99:1
9	**1s**	R^1 = Me, R^2 = 5-Me		87	>99:1
10	**1t**	R^1 = Me, R^2 = 5,6-Me_2		85	98:2
11	**1u**	R^1 = Me, R^2 = 5-OMe		88	>99:1
12	**1x**			81	91:9

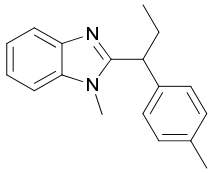
[a] Conditions: benzimidazole (0.5 mmol), allylbenzene derivative (1.0 mmol), $Ni(COD)_2$ (0.05 mmol), IPr (0.05 mmol), and $AlMe_3$ (0.05 mmol) in toluene (1 mL) at 130 °C for 16 hours unless otherwise noted.

Figure S1. GC yield of each components plot vs reaction time for tandem olefin isomerization/CH activation process of **1a** with **2a**.

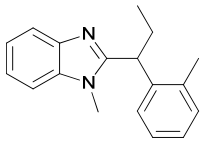




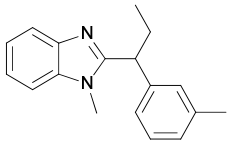
1-methyl-2-(1-phenylpropyl)-1*H*-benzo[*d*]imidazole (4a): The reaction was performed according to the above general procedure A. Yield: 91%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84-7.81 (m, 1H, Ar), 7.28-7.16 (m, 8H), 3.99 (t, 1H, $^{3}J_{HH}$ = 7.5 Hz), 3.50 (s, 3H, N-CH_3), 2.56-2.46 (m, 1H), 2.22-2.11 (m, 1H), 0.99 (t, 3H, $^{3}J_{HH}$ = 7.5 Hz). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 156.5 (s, Ar), 142.7 (s, Ar), 141.4 (s, Ar), 136.1 (s, Ar), 128.9 (s, Ar), 128.3 (s, Ar), 127.1 (s, Ar), 122.3 (s, Ar), 121.9 (s, Ar), 119.8 (s, Ar), 109.1 (s, Ar), 46.6 (s, CH), 29.9 (s, N-CH_3), 29.0 (s, CH_2), 12.8 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{17}H_{18}N_2$ ([M+H]$^{+}$) 251.1548, found 251.1554.



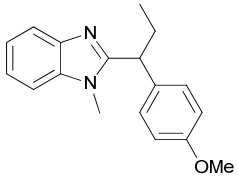
1-methyl-2-(1-(p-tolyl)propyl)-1*H*-benzo[*d*]imidazole (4b): The reaction was performed according to the above general procedure A. Yield: 87%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83-7.80 (m, 1H), 7.24-7.21 (m, 3H), 7.12 and 7.06 (AB quartet, $^{3}J_{HH}$ = 6.0 Hz, 4H), 3.95 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H), 3.50 (s, 3H), 2.53-2.41 (m, 1H), 2.27 (s, 3H), 2.21-2.07 (m, 1H), 0.98 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 156.7 (s, Ar), 142.7 (s, Ar), 138.3 (s, Ar), 136.7 (s, Ar), 136.1 (s, Ar), 129.6 (s, Ar), 128.1 (s, Ar), 122.3 (s, Ar), 121.9 (s, Ar), 119.8 (s, Ar), 109.0 (s, Ar), 46.2 (s, CH), 29.9 (s, N-CH_3), 28.9 (s, CH_2), 21.2 (s, CH_3), 12.8 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ([M+H]$^{+}$) 265.1705, found 265.1711.



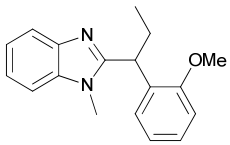
1-methyl-2-(1-(o-tolyl)propyl)-1*H*-benzo[*d*]imidazole (4c): The reaction was performed according to the above general procedure A. Yield: 83%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84-7.82 (m, 1H), 7.26-6.97 (m, 8H), 4.24 (t, $^{3}J_{HH}$ = 6.0 Hz, 1H), 3.40 (s, 3H), 2.59-2.46 (m, 1H), 2.49 (s, 3H), 2.11-1.97 (m, 1H), 1.05 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 156.7 (s, Ar), 142.7 (s, Ar), 139.9 (s, Ar), 136.2 (s, Ar), 135.1 (s, Ar), 130.7 (s, Ar), 128.0 (s, Ar), 126.9 (s, Ar), 122.3 (s, Ar), 121.9 (s, Ar), 119.8 (s, Ar), 109.0 (s, Ar), 42.2 (s, CH), 29.5 (s, N-CH_3), 28.6 (s, CH_2), 19.8 (s, CH_3), 13.0 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ([M+H]$^{+}$) 265.1705, found 265.1718.



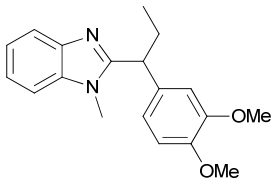
1-methyl-2-(1-(m-tolyl)propyl)-1*H*-benzo[*d*]imidazole (4d): The reaction was performed according to the above general procedure A. Yield: 90%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84-7.81 (m, 1H), 7.24-6.99 (m, 8H), 3.94 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H), 3.51 (s, 3H), 2.54-2.45 (m, 1H), 2.26 (s, 3H), 2.19-2.10 (m, 1H), 0.98 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 156.5 (s, Ar), 141.2 (s, Ar), 138.7 (s, Ar), 136.1 (s, Ar), 128.8 (s, Ar), 128.7 (s, Ar), 127.9 (s, Ar), 125.4 (s, Ar), 122.3 (s, Ar), 121.9 (s, Ar), 119.8 (s, Ar), 109.1 (s, Ar), 46.5 (s, CH), 29.9 (s, N-CH_3), 28.9 (s, CH_2), 21.6 (s, CH_3), 12.9 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ([M+H]$^{+}$) 265.1705, found 265.1718.



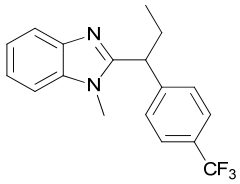
2-(1-(3-methoxyphenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (4e): The reaction was performed according to the above general procedure A. Yield: 55%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.87-7.84 (m, 1H), 7.29-7.18 (m, 3H), 7.19 (d, 2H, $^{3}J_{HH}$ = 6.0 Hz), 6.84 (d, 2H, $^{3}J_{HH}$ = 6.0 Hz), 3.97 (t, 1H, $^{3}J_{HH}$ = 7.5 Hz), 3.78 (s, 3H), 3.54 (s, 3H), 2.58-2.44 (m, 1H), 2.22-2.13 (m, 1H), 1.01 (t, 1H, $^{3}J_{HH}$ = 7.5 Hz). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 158.7 (s, Ar), 156.8 (s, Ar), 142.7 (s, Ar), 136.6 (s, Ar), 136.1 (s, Ar), 133.4 (s, Ar), 129.2 (s, Ar), 122.3 (s, Ar), 121.9 (s, Ar), 119.8 (s, Ar), 114.3 (s, Ar), 109.0 (s, Ar), 55.4 (s, O-CH_3), 45.7 (s, CH), 29.8 (s, N-CH_3), 29.0 (s, CH_2), 12.8 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2O$ ([M+H]$^{+}$) 281.1654, found 281.1665.



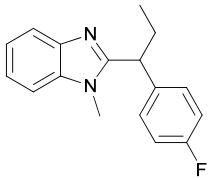
2-(1-(2-methoxyphenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (4f): The reaction was performed according to the above general procedure A. Yield: 66%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83-7.79 (m, 1H), 7.24-7.09 (m, 5H), 6.90-6.79 (m, 2H), 4.63 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H), 3.90 (s, 3H), 3.50 (s, 3H), 2.52-2.38 (m, 1H), 2.16-2.02 (m, 1H), 0.97 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 157.4 (s, Ar), 156.4 (s, Ar), 142.8 (s, Ar), 136.1 (s, Ar), 129.9 (s, Ar), 128.9 (s, Ar), 128.0 (s, Ar), 122.1 (s, Ar), 121.7 (s, Ar), 121.4 (s, Ar), 119.6 (s, Ar), 110.5 (s, Ar), 109.0 (s, Ar), 55.8 (s, O-CH_3), 37.2 (s, CH), 29.5 (s, N-CH_3), 28.3 (s, CH_2), 12.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2O$ ([M+H]$^{+}$) 281.1654, found 281.1663.



2-(1-(3,4-dimethoxyphenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (4g): The reaction was performed according to the above general procedure A. Yield: 46%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.81-7.78 (m, 1H), 7.21-7.20 (m, 3H), 6.77-6.71 (m, 3H), 3.90 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H), 3.79 (s, 3H, OCH_3), 3.75 (s, 3H, OCH_3), 2.25-2.38 (m, 1H), 2.21-2.06 (m, 1H), 0.96 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 156.5 (s, Ar), 149.4 (s, Ar), 148.1 (s, Ar), 142.5 (s, Ar), 136.0 (s, Ar), 133.8 (s, Ar), 122.2 (s, Ar), 121.8 (s, Ar), 120.4 (s, Ar), 119.5 (s, Ar), 111.2 (s, Ar), 111.0 (s, Ar), 109.0 (s, Ar), 56.0 (s, O-CH_3), 56.0 (s, O-CH_3), 46.0 (s, CH), 29.8(s, N-CH_3), 28.8 (s, CH_2), 12.7 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{19}H_{23}N_2O_2$ ([M+H]$^{+}$) 311.1759, found 311.1771.

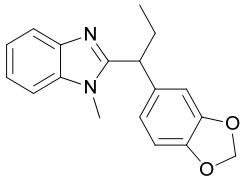


1-methyl-2-(1-(4-(trifluoromethyl)phenyl)propyl)-1*H*-benzo[*d*]imidazole (4h): The reaction was performed according to the above general procedure A. Yield: 79%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84-7.80 (m, 1H), 7.53 and 7.39 (AB quartet, $^{3}J_{HH}$ = 9.0 Hz, 4H), 7.27-7.24 (m, 3H), 4.07 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H), 3.52 (s, 3H), 2.59-2.45 (m, 1H), 2.24-2.10 (m, 1H), 0.99 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 155.4 (s, Ar), 145.4 (s, Ar), 142.6 (s, Ar), 136.0 (s, Ar), 129.5 (q, $^{2}J_{CF}$ = 30.0 Hz, *C*-CF_3), 128.6 (s, Ar), 125.9 (s, Ar), 124.3 (q, $^{1}J_{CF}$ = 270.0 Hz, *C*F_3), 122.6 (s, Ar), 122.1 (s, Ar), 119.8 (s, Ar), 109.2 (s, Ar), 46.2 (s, CH), 29.8(s, N-CH_3), 29.0 (s, CH_2), 12.7 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{18}N_2F_3$ ([M+H]$^{+}$) 319.1422, found 319.1435.

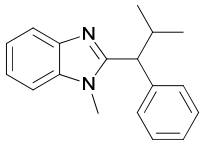


2-(1-(4-fluorophenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (4i): The reaction was performed according to the above general procedure A. Yield: 61%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83-7.80 (m, 1H), 7.24-7.18 (m, 5H), 6.94 (t, $^{3}J_{HH}$ = 9.0 Hz, 2H), 3.97 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H), 3.50 (s, 3H), 2.55-2.40 (m, 1H), 2.20-2.06 (m, 1H), 0.97 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 162.0 (d, $^{1}J_{CF}$ = 247.5 Hz, *C*-F), 156.2 (s, Ar), 142.6 (s, Ar), 136.5 (d, $^{2}J_{CF}$ = 75.0 Hz, *C*-C-F), 129.7 (s, Ar), 129.6 (s, Ar), 122.4 (s, Ar), 122.0 (s, Ar), 119.7 (s, Ar), 115.9 (s, Ar), 115.6 (s, Ar), 109.1 (s, Ar), 45.7 (s, CH), 29.8(s, N-CH_3), 29.0 (s, CH_2), 12.7 (s, CH_3).

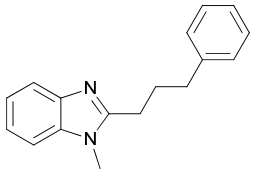
HR-MS (MALDI): *m/z* calcd. for $C_{17}H_{18}N_2F$ ($[M+H]^+$) 269.1454, found 269.1466. HR-MS (MALDI): *m/z* calcd. for $C_{17}H_{18}N_2F$ ($[M+H]^+$) 269.1454, found 269.1462.



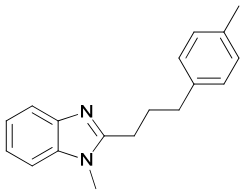
2-(1-(benzo[d][1,3]dioxol-5-yl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (4j): The reaction was performed according to the above general procedure A. Yield: 62%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83-7.79 (m, 1H), 7.23-7.22 (m, 3H), 6.73 (s, 1H), 6.70 (s, 2H), 5.87 (d, $^3J_{HH}$ = 6.0 Hz, 2H), 3.90 (t, $^3J_{HH}$ = 7.5 Hz, 1H), 3.52 (s, 3H), 2.52-2.38 (m, 1H), 2.19-2.05 (m, 1H), 0.97 (t, $^3J_{HH}$ = 7.5 Hz, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 156.4 (s, Ar), 148.2 (s, Ar), 146.7 (s, Ar), 142.6 (s, Ar), 136.1 (s, Ar), 135.2 (s, Ar), 122.3 (s, Ar), 121.9 (s, Ar), 121.4 (s, Ar), 119.7 (s, Ar), 109.1 (s, Ar), 108.5 (s, Ar), 108.4 (s, Ar), 101.2 (s, Ar), 46.1 (s, CH), 29.8(s, N-CH_3), 29.0 (s, CH_2), 12.7 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{19}N_2O_2$ ($[M+H]^+$) 295.1446, found 295.1453.



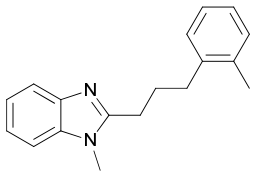
1-methyl-2-(2-methyl-1-phenylpropyl)-1*H*-benzo[*d*]imidazole (4k): The reaction was performed according to the above general procedure A. Yield: 31%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84-7.81 (m, 1H), 7.37-7.17 (m, 8H), 3.67 (d, $^3J_{HH}$ = 9.0 Hz, 1H), 3.59 (s, 3H), 2.94-2.81 (m, 1H), 1.08 (d, $^3J_{HH}$ = 6.0 Hz, 3H), 0.84 (d, $^3J_{HH}$ = 9.0 Hz, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 156.5 (s, Ar), 142.9 (s, Ar), 140.3 (s, Ar), 135.7 (s, Ar), 128.9 (s, Ar), 128.7 (s, Ar), 127.1 (s, Ar), 122.1 (s, Ar), 121.9 (s, Ar), 119.7 (s, Ar), 109.1 (s, Ar), 52.5 (s, CH), 32.9 (s, CH), 29.8 (s, N-CH_3), 22.6 (s, CH_3), 21.2 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ($[M+H]^+$) 265.1705, found 265.1715.



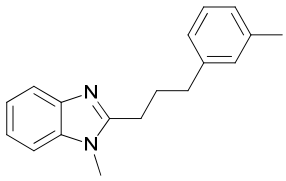
1-methyl-2-(3-phenylpropyl)-1*H*-benzo[*d*]imidazole (3a): The reaction was performed according to the above general procedure B. Yield: 85%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.71-7.67 (m, 1H), 7.27-7.12 (m, 8H), 3.55 (s, 3H), 2.80 (t, $^3J_{HH}$ = 6.0 Hz, 2H), 2.74 (t, $^3J_{HH}$ = 6.0 Hz, 2H), 2.17 (qn, $^3J_{HH}$ = 8.0 Hz, 2H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 155.0 (s, Ar), 142.7 (s, Ar), 141.5 (s, Ar), 135.8 (s, Ar), 128.6 (s, Ar), 128.5 (s, Ar), 126.1 (s, Ar), 122.1 (s, Ar), 121.8 (s, Ar), 119.2 (s, Ar), 109.0 (s, Ar), 35.4 (s, N-CH_3), 29.7 (s, CH_2), 29.0 (s, CH_2), 26.8 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{17}H_{19}N_2$ ($[M+H]^+$) 251.1548, found 251.1554.



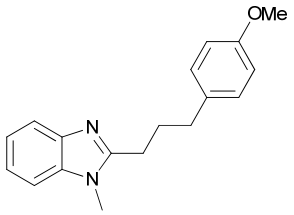
1-methyl-2-(3-(p-tolyl)propyl)-1*H*-benzo[*d*]imidazole (3b): The reaction was performed according to the above general procedure B. Yield: 85%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74-7.71 (m, 1H), 7.25-7.20 (m, 3H), 7.09 (s, 4H), 3.62 (s, 3H), 2.85 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H). 2.75 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 2.31 (s, 3H), 2.19 (qn, $^{3}J_{HH}$ = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 155.0 (s, Ar), 142.6 (s, Ar), 138.3 (s, Ar), 135.7 (s, Ar), 135.4 (s, Ar), 129.1 (s, Ar), 128.4 (s, Ar), 121.9 (s, Ar), 121.7 (s, Ar), 119.1 (s, Ar), 108.9 (s, Ar), 34.9 (s, N-CH_3), 29.5 (s, CH_2), 28.9 (s, CH_2), 26.6 (s, CH_2), 21.0 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ([M+H]$^{+}$) 265.1705, found 265.1716.



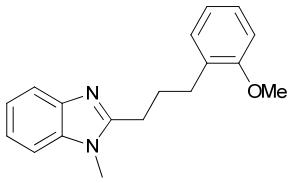
1-methyl-2-(3-(*o*-tolyl)propyl)-1*H*-benzo[*d*]imidazole (3c): The reaction was performed according to the above general procedure B. Yield: 90%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74-7.69 (m, 1H), 7.29-7.19 (m, 3H), 7.16-7.08 (m, 4H), 3.55 (s, 3H), 2.91 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H). 2.78 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 2.29 (s, 3H), 2.17 (qn, $^{3}J_{HH}$ = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 154.9 (s, Ar), 142.6 (s, Ar), 139.6 (s, Ar), 136.0 (s, Ar), 135.8 (s, Ar), 130.3 (s, Ar), 128.9 (s, Ar), 126.1 (s, Ar), 126.0 (s, Ar), 122.0 (s, Ar), 121.7 (s, Ar), 119.1 (s, Ar), 108.9 (s, Ar), 32.7 (s, N-CH_3), 29.54 (s, CH_2), 27.6 (s, CH_2), 27.0 (s, CH_2), 19.3 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ([M+H]$^{+}$) 265.1705, found 265.1716.



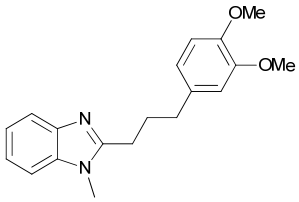
1-methyl-2-(3-(m-tolyl)propyl)-1*H*-benzo[*d*]imidazole (3d): The reaction was performed according to the above general procedure B. Yield: 88%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74-7.71 (m, 1H), 7.24-7.15 (m, 4H), 7.01 (s, 1H), 7.00 (d, $^{3}J_{HH}$ = 6.0 Hz, 2H), 3.61 (s, 3H), 2.86 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H). 2.75 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 2.31 (s, 3H), 2.21 (qn, $^{3}J_{HH}$ = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 155.0 (s, Ar), 142.6 (s, Ar), 141.3 (s, Ar), 137.9 (s, Ar), 135.8 (s, Ar), 129.3 (s, Ar), 128.3 (s, Ar), 126.7 (s, Ar), 125.5 (s, Ar), 121.9 (s, Ar), 121.7 (s, Ar), 119.1 (s, Ar), 108.9 (s, Ar), 35.3 (s, N-CH_3), 29.5 (s, CH_2), 28.9 (s, CH_2), 26.7 (s, CH_2), 21.4 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ([M+H]$^{+}$) 265.1705, found 265.1710.



2-(3-(3-methoxyphenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (3e): The reaction was performed according to the above general procedure B. Yield: 81%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73-7.68 (m, 1H), 7.26-7.20 (m, 3H), 7.12 (d, $^{3}J_{HH}$ = 9.0 Hz, 2H), 6.82 (d, $^{3}J_{HH}$ = 9.0 Hz, 2H), 3.77 (s, 3H), 3.61 (s, 3H), 2.84 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H). 2.72 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 2.17 (qn, $^{3}J_{HH}$ = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 157.9 (s, Ar), 155.0 (s, Ar), 142.6 (s, Ar), 135.7 (s, Ar), 133.4 (s, Ar), 129.4 (s, Ar), 121.9 (s, Ar), 121.7 (s, Ar), 119.0 (s, Ar), 113.8 (s, Ar), 108.9 (s, Ar), 55.2 (s, O-CH_3), 34.4 (s, CH_2), 29.5 (s, N-CH_3), 29.1 (s, CH_2), 26.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2O$ ([M+H]$^{+}$) 281.1654, found 281.1663.

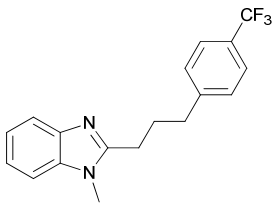


2-(3-(2-methoxyphenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (3f): The reaction was performed according to the above general procedure B. Yield: 87%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73-7.69 (m, 1H), 7.26-7.20 (m, 3H), 7.17-7.13 (m, 2H), 6.89-6.82 (m, 2H), 3.78 (s, 3H), 3.63 (s, 3H), 2.88 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H). 2.78 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 2.17 (qn, $^{3}J_{HH}$ = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 157.5 (s, Ar), 155.3 (s, Ar), 142.6 (s, Ar), 135.8 (s, Ar), 130.0 (s, Ar), 129.8 (s, Ar), 127.3 (s, Ar), 121.9 (s, Ar), 121.7 (s, Ar), 120.4 (s, Ar), 119.1 (s, Ar), 110.2 (s, Ar), 108.8 (s, Ar), 55.2 (s, O-CH_3), 29.9 (s, N-CH_3), 29.5 (s, CH_2), 27.5 (s, CH_2), 27.1 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2O$ ([M+H]$^{+}$) 281.1654, found 281.1667.

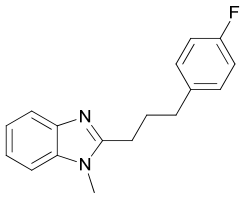


2-(3-(3,4-dimethoxyphenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (3g): The reaction was performed according to the above general procedure B. Yield: 79%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.72-7.67 (m, 1H), 7.24-7.19 (m, 3H), 6.78-6.70 (m, 3H), 3.82 (s, 6H), 3.60 (s, 3H), 2.84 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H). 2.71 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 2.18 (qn, $^{3}J_{HH}$ = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 154.9 (s, Ar), 148.8 (s, Ar), 147.2 (s, Ar), 142.5 (s, Ar), 135.7 (s, Ar), 134.0 (s, Ar), 121.9 (s, Ar), 121.7 (s, Ar), 120.3 (s, Ar), 119.0 (s, Ar), 111.8 (s, Ar), 111.2 (s, Ar), 108.8 (s,

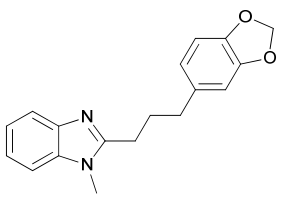
Ar), 55.9 (s, O-CH_3), 55.8 (s, O-CH_3), 34.9 (s, CH_2), 29.5 (s, N-CH_3), 29.0 (s, CH_2), 26.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{19}H_{23}N_2O_2$ ($[M+H]^+$) 311.1759, found 311.1768.



1-methyl-2-(3-(4-(trifluoromethyl)phenyl)propyl)-1*H*-benzo[*d*]imidazole (3h): The reaction was performed according to the above general procedure B. Yield: 33%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73-7.68 (m, 1H), 7.52 (d, $^3J_{HH}$ = 7.5 Hz, 2H), 7.31 (d, $^3J_{HH}$ = 7.5 Hz, 2H), 7.26-7.21 (m, 3H), 3.65 (s, 3H), 2.87 (t, $^3J_{HH}$ = 7.5 Hz, 2H). 2.84 (t, $^3J_{HH}$ = 7.5 Hz, 2H), 2.24 (qn, $^3J_{HH}$ = 7.5 Hz, 2H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 154.6 (s, Ar), 145.7 (s, Ar), 142.7 (s, Ar), 135.9 (s, Ar), 129.0 ((s, Ar), 128.6 (q, $^2J_{CF}$ = 32.0 Hz, *C*-CF_3), 125.5 (s, Ar), 124.5 (q, $^1J_{CF}$ = 270.0 Hz, -*C*F_3), 122.3 (s, Ar), 122.1 (s, Ar), 119.4 (s, Ar), 109.1 (s, Ar), 35.3 (s, CH_2), 29.8 (s, N-CH_3), 28.7 (s, CH_2), 26.8 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{18}N_2F_3$ ($[M+H]^+$) 319.1422, found 319.1435.

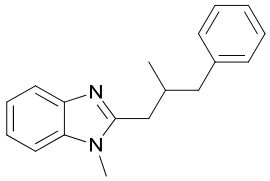


2-(3-(4-fluorophenyl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (3i): The reaction was performed according to the above general procedure B. Yield: 77%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73-7.68 (m, 1H), 7.26-7.20 (m, 3H), 7.16-7.12 (m, 2H), 6.95 (t, $^3J_{HH}$ = 7.5 Hz, 2H), 3.62 (s, 3H), 2.84 (t, $^3J_{HH}$ = 7.5 Hz, 2H). 2.74 (t, $^3J_{HH}$ = 7.5 Hz, 2H), 2.18 (qn, $^3J_{HH}$ = 7.5 Hz, 2H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 161.4 (d, $^1J_{CF}$ = 240.0 Hz, *C*-F), 154.8 (s, Ar), 142.6 (s, Ar), 136.5 (d, $^2J_{CF}$ = 97.5 Hz, *C*-C-F), 129.9 (s, Ar), 129.8 (s, Ar), 122.1 (s, Ar), 121.8 (s, Ar), 119.2 (s, Ar), 115.3 (s, Ar), 115.0 (s, Ar), 109.0 (s, Ar), 34.5 (s, CH_2), 29.6 (s, N-CH_3), 29.0 (s, CH_2), 26.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{17}H_{18}N_2F$ ($[M+H]^+$) 269.1454, found 269.1462.

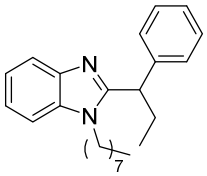


2-(3-(benzo[d][1,3]dioxol-5-yl)propyl)-1-methyl-1*H*-benzo[*d*]imidazole (3j): The reaction was performed according to the above general procedure B. Yield: 83%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.72-7.67 (m, 1H), 7.26-7.20 (m, 3H), 6.72-6.61 (m, 3H), 5.89 (s, 2H), 3.63 (s, 3H), 2.83 (t,

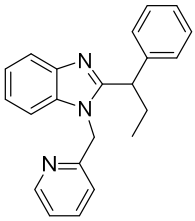
$^3J_{HH}$ = 7.5 Hz, 2H). 2.69 (t, $^3J_{HH}$ = 7.5 Hz, 2H), 2.15 (qn, $^3J_{HH}$ = 7.5 Hz, 2H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 154.8 (s, Ar), 147.6 (s, Ar), 145.7 (s, Ar), 142.5 (s, Ar), 135.7 (s, Ar), 135.2 (s, Ar), 121.9 (s, Ar), 121.7 (s, Ar), 121.2 (s, Ar), 119.0 (s, Ar), 108.9 (s, Ar), 108.1 (s, Ar), 100.7 (s, Ar), 35.0 (s, CH_2), 29.5 (s, N-CH_3), 29.0 (s, CH_2), 26.5 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{19}N_2O_2$ ($[M+H]^+$)295.1446, found 295.1459.



1-methyl-2-(2-methyl-3-phenylpropyl)-1*H*-benzo[*d*]imidazole (3k): The reaction was performed according to the above general procedure B. Yield: 67%. ^1H NMR (300 MHz, $CDCl_3$): δ 7.73-7.68 (m, 1H), 7.29-7.16 (m, 8H), 3.58 (s, 3H), 2.93-2.86 (m, 1H), 2.75-2.59 (m, 3H), 2.46-2.34 (m, 1H), 0.99 (d, $^3J_{HH}$ = 9.0 Hz, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 154.4 (s, Ar), 142.6 (s, Ar), 140.4 (s, Ar), 135.7 (s, Ar), 129.3 (s, Ar), 128.3 (s, Ar), 126.1 (s, Ar), 122.0 (s, Ar), 121.8 (s, Ar), 119.1 (s, Ar), 109.0 (s, Ar), 43.5 (s, CH_3), 34.9 (s, CH), 34.0 (s, CH_2), 29.7 (s, N-CH_3), 19.8 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ($[M+H]^+$) 265.1705, found 265.1717.

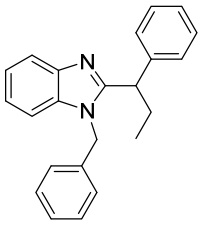


1-octyl-2-(1-phenylpropyl)-1*H*-benzo[*d*]imidazole (4l): The reaction was performed according to the above general procedure A. Yield: 79%. ^1H NMR (300 MHz, $CDCl_3$): δ 7.84-7.81 (m, 1H), 7.26-7.17 (m, 8H), 3.97 (t, 1H, $^3J_{HH}$ = 9.0 Hz), 3.92 (d, 2H, $^3J_{HH}$ = 6.0 Hz), 2.53-2.46 (m, 1H), 2.20-2.10 (m, 1H), 1.24-1.17 (m, 12H), 0.98 (t, 3H, $^3J_{HH}$ = 7.5 Hz), 0.86 (t, 3H, $^3J_{HH}$ = 7.5 Hz). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 155.8 (s, Ar), 142.7 (s, Ar), 141.7 (s, Ar), 135.2 (s, Ar), 128.7 (s, Ar), 128.0 (s, Ar), 126.9 (s, Ar), 122.0 (s, Ar), 121.6 (s, Ar), 119.6 (s, Ar), 109.3 (s, Ar), 46.4 (s, CH), 43.6 (s, CH_2), 31.7 (s, CH_2), 29.4 (s, CH_2), 29.2 (s, CH_2), 29.1 (s, CH_2), 29.0 (s, CH_2), 26.9 (s, CH_2), 22.6 (s, CH_2), 14.0 (s, CH_3), 12.7 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{24}H_{32}N_2$ ($[M+H]^+$) 349.2644, found 349.2650.

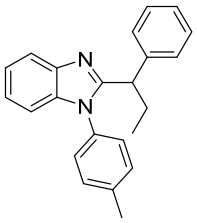


2-(1-phenylpropyl)-1-(pyridin-2-ylmethyl)-1H- benzo[d]imidazole (4m): The reaction was

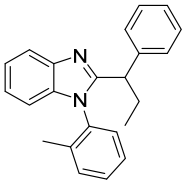
performed according to the above general procedure A. Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.54 (d, 1H, $^{3}J_{HH}$ =4.0 Hz), 7.87 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.34-7.07 (m, 10H), 6.27 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 5.32 (AB quartet, 2H, $^{2}J_{HH}$ = 13.3 Hz), 3.97 (t, 1H, $^{3}J_{HH}$ = 6.0 Hz), 2.52-2.47 (m, 1H), 2.18-2.11 (m, 1H), 0.91 (t, 3H, $^{3}J_{HH}$ = 8.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.4 (s, Ar), 155.9 (s, Ar), 149.4 (s, Ar), 142.7 (s, Ar), 141.0 (s, Ar), 136.8 (s, Ar), 135.4 (s, Ar), 128.6 (s, Ar), 128.0 (s, Ar), 126.8 (s, Ar), 122.5 (s, Ar), 122.4 (s, Ar), 122.1 (s, Ar), 120.2 (s, Ar), 119.7 (s, Ar), 109.3 (s, Ar), 48.6 (s, CH), 46.2 (s, N-CH_2), 29.0 (s, CH_2), 12.5 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{22}H_{21}N_3$ ([M+H]$^{+}$) 328.1814, found 328.1823.



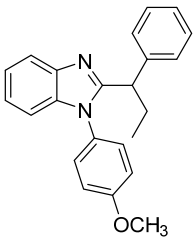
1-benzyl-2-(1-phenylpropyl)-1H-benzo[d]imidazole (4n): The reaction was performed according to the above general procedure A. Yield: 81%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.26-7.12 (m, 11H), 6.89-6.86 (m, 2H), 5.15 (AB quartet, 2H, $^{2}J_{HH}$ = 22.4 Hz), 3.88 (t, 1H, $^{3}J_{HH}$ = 8.0 Hz), 2.50-2.47 (m, 1H), 2.14-2.08 (m, 1H), 0.89 (t, 3H, , $^{3}J_{HH}$ = 8.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.3 (s, Ar), 142.7 (s, Ar), 141.3 (s, Ar), 136.1 (s, Ar), 135.6 (s, Ar), 128.8 (s, Ar), 128.7 (s, Ar), 128.0 (s, Ar), 127.7 (s, Ar), 126.9 (s, Ar), 126.1 (s, Ar), 122.4 (s, Ar), 121.9 (s, Ar), 119.7 (s, Ar), 109.5 (s, Ar), 46.7 (s, CH), 46.3 (s, N-CH_2), 29.0 (s, CH_2), 12.5 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2$ ([M+H]$^{+}$) 327.1861, found 327.1866.



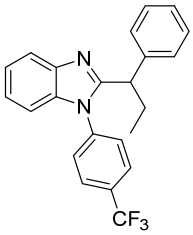
2-(1-phenylpropyl)-1-(p-tolyl)-1H-benzo[d]imidazole (4o): The reaction was performed according to the above general procedure A. Yield: 94%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.28-7.11 (m, 11H), 6.99 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 3.84 (t, 1H, $^{3}J_{HH}$ = 8.0 Hz), 2.53-2.42 (m, 1H), 2.45 (s, 3H), 2.17-2.06 (m, 1H), 0.90 (t, 3H, $^{3}J_{HH}$ = 8.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.5 (s, Ar), 142.6 (s, Ar), 141.7 (s, Ar), 138.9 (s, Ar), 136.8 (s, Ar), 133.0 (s, Ar), 130.1 (s, Ar), 128.3 (s, Ar), 128.0 (s, Ar), 126.5 (s, Ar), 122.4 (s, Ar), 122.1 (s, Ar), 119.4 (s, Ar), 110.0 (s, Ar), 45.9 (s, CH), 29.2 (s, CH_2), 21.2 (s, CH_3), 12.5 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2$ ([M+H]$^{+}$) 327.1861, found 327.1875.



2-(1-phenylpropyl)-1-(o-tolyl)-1H-benzo[d]imidazole (4p): The reaction was performed according to the above general procedure A. Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.41-7.02 (m, 10H), 6.82 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 6.54 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 3.53 (t, 1H, $^{3}J_{HH}$ = 8.0 Hz), 2.51-2.42 (m, 1H), 2.15-2.04 (m, 1H), 1.96 (s, 3H), 0.91 (t, 3H, $^{3}J_{HH}$ = 8.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.3 (s, Ar), 142.8 (s, Ar), 141.7 (s, Ar), 136.3 (s, Ar), 136.1 (s, Ar), 134.4 (s, Ar), 131.1 (s, Ar), 129.6 (s, Ar), 129.5 (s, Ar), 128.3 (s, Ar), 128.1(s, Ar), 126.8(s, Ar), 126.6(s, Ar), 122.6 (s, Ar), 122.1 (s, Ar), 119.6 (s, Ar), 109.9 (s, Ar), 46.6 (s, CH), 29.2 (s, CH_2), 17.3 (s, CH_3), 12.8 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2$ ([M+H]$^{+}$) 327.1861, found 327.1870.

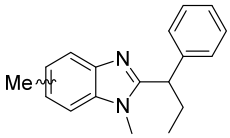


1-(4-methoxyphenyl)-2-(1-phenylpropyl)-1H-benzo[d]imidazole (4q): The reaction was performed according to the above general procedure A. Yield: 79%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.27-7.08 (m, 11H), 6.97 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 3.87 (s, 3H), 3.80 (t, 1H, $^{3}J_{HH}$ = 8.0 Hz), 2.50-2.39 (m, 1H), 2.14-2.04 (m, 1H), 0.89 (t, 3H, $^{3}J_{HH}$ = 6.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 159.8 (s, Ar), 156.8 (s, Ar), 142.5 (s, Ar), 141.7 (s, Ar), 137.0 (s, Ar), 128.3 (s, Ar), 128.1 (s, Ar), 126.6 (s, Ar), 122.5 (s, Ar), 122.1 (s, Ar), 119.4 (s, Ar), 114.7 (s, Ar), 110.0 (s, Ar), 55.6 (s, OCH_3), 46.0 (s, CH), 29.1 (s, CH_2), 12.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2O$ ([M+H]$^{+}$) 343.1810, found 343.1822.

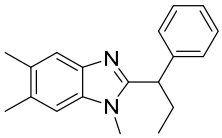


2-(1-phenylpropyl)-1-(4-(trifluoromethyl)phenyl)-1H-benzo[d]imidazole (4r): The reaction was performed according to the above general procedure A. Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.71 (br s, 2H), 7.31-7.13 (m, 7H), 7.04-6.97 (m, 3H), 3.78 (t, 1H, $^{3}J_{HH}$ = 8.0 Hz), 2.53-2.42 (m, 1H), 2.16-2.06 (m, 1H), 0.90 (t, 3H, $^{3}J_{HH}$ = 6.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.1 (s, Ar), 142.7 (s, Ar), 141.3 (s, Ar), 139.1 (s, Ar), 136.4 (s, Ar), 131.1 (q, $^{2}J_{CF}$ = 33.3 Hz, *C*-CF_3), 128.5 (s, Ar), 128.0 (s, Ar), 127.3-119.6(q, $^{1}J_{CF}$ =

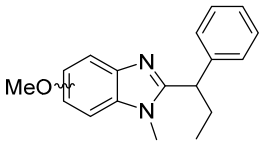
256 Hz, CF_3), 126.8 (s, Ar), 123.1 (s, Ar), 122.7 (s, Ar), 119.8 (s, Ar), 109.7 (s, Ar), 46.3 (s, CH), 29.2 (s, CH_2), 12.5 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{19}F_3N_2$ ($[M+H]^+$) 381.1578, found 381.1588.



1,5/6-dimethyl-2-(1-phenylpropyl)-1H-benzo[d]imidazole (4s): The reaction was performed according to the above general procedure A. Yield: 92%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.69 (d, 0.5H, $^3J_{HH}$ = 6.0 Hz), 7.61 (s, 0.5H), 7.28-7.01 (m, 7H), 3.96 (t, 1H, $^3J_{HH}$ = 7.5 Hz), 3.47 (s, 1.5H), 3.45 (s, 1.5H), 2.56-2.42 (m, 1H), 2.46 (s, 3H), 2.22-2.07 (m, 1H), 0.98 (t, 3H, $^3J_{HH}$ = 7.5 Hz). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 156.1 (s, Ar), 155.7 (s, Ar), 142.7 (s, Ar), 141.3 (s, Ar), 140.5 (s, Ar), 136.1 (s, Ar), 134.0 (s, Ar), 132.0 (s, Ar), 131.3 (s, Ar), 128.7 (s, Ar), 128.0 (s, Ar), 126.8 (s, Ar), 123.5 (s, Ar), 123.2 (s, Ar), 119.4 (s, Ar), 119.0 (s, Ar), 108.9 (s, Ar), 108.4 (s, Ar), 46.3(s, CH), 29.5 (s, N-CH_3), 28.7 (s, CH_2), 21.8 (s, Ar-CH_3), 21.5 (s, Ar-CH_3), 12.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{20}N_2$ ($[M+H]^+$) 265.1705, found 265.1712.

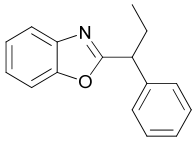


1,5,6-trimethyl-2-(1-phenylpropyl)-1H-benzo[d]imidazole (4t): The reaction was performed according to the above general procedure A. Yield: 91%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (s, 1H), 7.26-7.17 (m, 5H), 6.99 (s, 1H), 3.95 (t, 1H, $^3J_{HH}$ = 8.0 Hz), 3.44 (s, 3H), 2.52-2.40 (m, 1H), 2.36 (s, 3H), 2.35 (s, 3H), 2.19-2.08 (m, 1H), 0.97 (t, 3H, $^3J_{HH}$ = 6.0 Hz). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 155.4 (s, Ar), 141.4 (s, Ar), 141.0 (s, Ar), 134.5 (s, Ar), 131.1 (s, Ar), 130.3 (q, CF_3), 128.6 (s, Ar), 128.0 (s, Ar), 126.8 (s, Ar), 119.7 (s, Ar), 109.2 (s, Ar), 46.3 (s, CH), 29.6 (s, N-CH_3), 28.7 (s, CH_2), 20.4 (s, Ar-CH_3), 20.2 (s, Ar-CH_3), 12.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{19}H_{22}N_2$ ($[M+H]^+$) 279.1861, found 279.1870.

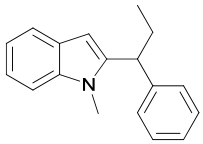


5/6-methoxy-1-methyl-2-(1-phenylpropyl)-1H-benzo[d]imidazole (4u): The reaction was performed according to the above general procedure A. Yield: 77%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73 (d, 0.5H, $^3J_{HH}$ = 9.0 Hz), 7.38 (d, 0.5H, $^3J_{HH}$ = 3.0 Hz), 7.30-7.22 (m, 5H), 7.14 (d, 0.5H, $^3J_{HH}$ = 9.0 Hz), 6.91 (dd, 1H, $^3J_{HH}$ = 9.0 Hz, , $^3J_{HH}$ = 2.4 Hz), 6.73 (d, 0.5H, $^3J_{HH}$ = 3.0 Hz), 3.99 (t, 1H, $^3J_{HH}$ = 7.5 Hz), 3.89 (s, 1.5H), 3.87 (s, 1.5H), 3.52 (s, 1.5H), 3.48 (s, 1.5H), 2.57-2.47 (m, 1H), 2.24-2.13 (m, 1H), 1.02 (t, 3H, $^3J_{HH}$ = 7.5 Hz). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 156.4 (s, Ar), 156.3 (s, Ar), 155.9 (s, Ar), 155.5 (s, Ar), 143.1 (s, Ar), 141.3 (s, Ar), 141.2 (s, Ar), 136.9 (s,

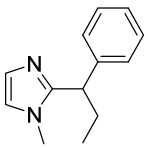
Ar), 136.5 (s, Ar), 130.5 (s, Ar), 128.7 (s, Ar), 128.0 (s, Ar), 126.8 (s, Ar), 120.0 (s, Ar), 112.0 (s, Ar), 110.5 (s, Ar), 109.2 (s, Ar), 102.0 (s, Ar), 93.0 (s, Ar), 55.9 (s, Ar-O*C*H_3), 55.8 (s, Ar-O*C*H_3), 46.4(s, CH), 29.6 (s, N-CH_3), 28.7 (s, CH_2), 12.6 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{20}N_2O$ ($[M+H]^+$) 281.1654, found 281.1667.



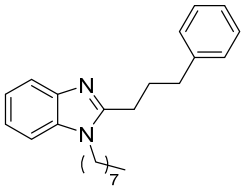
2-(1-phenylpropyl)benzo[*d*]oxazole (4v): The reaction was performed according to the above general procedure A. Yield: 62%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73-7.70 (m, 1H), 7.45-7.24 (m, 8H), 4.13 (t, 1H, $^3J_{HH}$ = 7.5 Hz), 2.49-2.35 (m, 1H), 2.22-2.08 (m, 1H), 0.99 (t, 3H, $^3J_{HH}$ = 7.5 Hz, CH_3). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 168.3 (s, Ar), 150.9 (s, Ar), 141.4 (s, Ar), 140.0 (s, Ar), 128.9 (s, Ar), 128.1 (s, Ar), 127.4 (s, Ar), 124.7 (s, Ar), 124.2 (s, Ar), 120.0 (s, Ar), 110.6 (s, Ar), 48.0 (s, CH), 27.8 (s, CH_2), 12.5 (s, CH_3). HR-MS (EI): *m/z* calculated for $C_{16}H_{15}ON$ ($[M^+]$) 237.1160, found 237.1154.



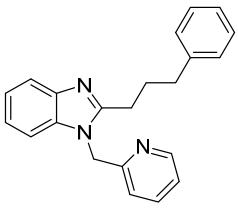
1-methyl-2-(1-phenylpropyl)-1*H*-indole (4w): The reaction was performed according to the above general procedure A. Yield: 58%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.65-7.62 (m, 1H, Ar), 7.30-7.08 (m, 8H, Ar), 6.54 (s, 1H), 3.93 (t, $^3J_{HH}$ = 7.5 Hz, 1H, CH), 3.44 (s, 3H, N-CH_3), 2.33-2.19 (m, 1H), 2.09-1.94 (m, 1H), 1.03 (t, $^3J_{HH}$ = 7.5 Hz, 3H, CH_3). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 143.4 (s, Ar), 143.4 (s, Ar), 137.7 (s, Ar), 128.7 (s, Ar), 128.3 (s, Ar), 127.9 (s, Ar), 126.6 (s, Ar), 121.0 (s, Ar), 120.3 (s, Ar), 119.4 (s, Ar), 109.0 (s, Ar), 99.2 (s, Ar), 46.1 (s, CH), 29.9 (s, N-CH_3), 29.5 (s, CH_2), 13.0 (s, CH_3). HR-MS (EI): *m/z* calculated for $C_{18}H_{19}N$ ($[M^+]$) 249.1517, found 249.1514.



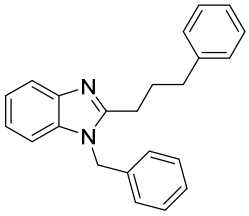
1-methyl-2-(1-phenylpropyl)-1H-imidazole (4x): The reaction was performed according to the above general procedure A. Yield: 45%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.24 (m, 2H), 7.19-7.15 (m, 3H), 6.99 (s, 1H), 6.73 (s, 1H), 3.76 (t, 1H, $^3J_{HH}$ = 8.0 Hz), 3.34 (s, 3H), 2.37-2.30 (m, 1H), 2.06-1.97 (m, 1H), 0.92 (t, 3H, $^3J_{HH}$ = 6.0 Hz). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 149.6 (s, Ar), 142.0 (s, Ar), 128.6 (s, Ar), 127.9 (s, Ar), 127.0 (s, Ar), 126.5 (s, Ar), 120.6 (s, Ar), 45.6 (s, CH), 32.5 (s, N-CH_3), 28.8 (s, CH_2), 12.6 (s, CH_3). HR-MS (FAB): *m/z* calculated for $C_{13}H_{17}N_2$ ($[M+H]^+$) 201.1392, found 201.1394.



1-octyl-2-(3-phenylpropyl)-1H-benzo[d]imidazole (3l): The reaction was performed according to the above general procedure B. Yield: 73%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72-7.70 (m, 1H), 7.29-7.16 (m, 8H), 3.97 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.83 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.79 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.24 (qn, 2H, $^{3}J_{HH}$ = 8.0 Hz), 1.72-1.68 (m, 2H), 1.27-1.24 (m, 10H,), 0.87 (t, 3H, $^{3}J_{HH}$ = 8.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 154.3 (s, Ar), 142.6 (s, Ar), 141.2 (s, Ar), 134.8 (s, Ar), 128.3 (s, Ar), 128.2 (s, Ar), 125.8 (s, Ar), 121.6 (s, Ar), 121.4 (s, Ar), 118.9 (s, Ar), 109.0 (s, Ar), 43.3 (s, CH_2), 35.1 (s, CH_2), 31.5 (s, CH_2), 29.6 (s, CH_2), 28.9 (s, CH_2), 28.9 (s, CH_2), 26.7 (s, CH_2), 26.3 (s, CH_2), 22.4 (s, CH_2), 13.9 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{24}H_{32}N_2$ ([M+H]$^{+}$) 349.2644, found 349.2657.

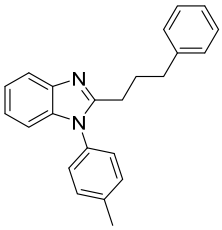


2-(3-phenylpropyl)-1-(pyridin-2-ylmethyl)-1H-benzo[d]imidazole (3m): The reaction was performed according to the above general procedure B. Yield: 62%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, 1H, $^{3}J_{HH}$ =4.0 Hz), 7.75 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.53-7.49 (td, 1H, $^{3}J_{HH}$ =8.0 Hz, $^{3}J_{HH}$ =1.6 Hz), 7.24-7.11 (m, 9H), 6.65 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 5.37 (s, 2H), 2.87 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.72 (t, 2H, $^{3}J_{HH}$ = 6.0 Hz), 2.18 (qn, 2H, $^{3}J_{HH}$ = 8.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 155.9 (s, Ar), 155.1 (s, Ar), 149.7 (s, Ar), 142.8 (s, Ar), 141.3 (s, Ar), 137.2 (s, Ar), 135.2 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 125.9 (s, Ar), 122.8 (s, Ar), 122.4 (s, Ar), 122.1 (s, Ar), 120.3 (s, Ar), 119.4 (s, Ar), 109.3 (s, Ar), 48.8 (s, CH_2), 35.3 (s, CH_2), 28.9 (s, CH_2), 26.8 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{22}H_{21}N_3$ ([M+H]$^{+}$) 328.1814, found 328.1821.

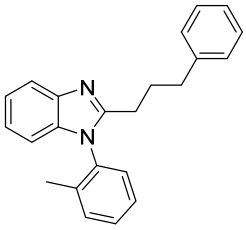


1-benzyl-2-(3-phenylpropyl)-1H-benzo[d]imidazole (3n): The reaction was performed according to the above general procedure B. Yield: 67%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.25-7.10 (m, 11H), 6.97-6.95 (m, 2H), 5.23 (s, 2H), 2.81 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.71 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.15 (qn, 2H, $^{3}J_{HH}$ = 7.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$):

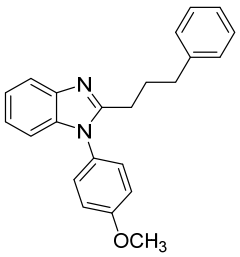
δ 154.9 (s, Ar), 142.6 (s, Ar), 141.3 (s, Ar), 135.9 (s, Ar), 135.4 (s, Ar), 128.8 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 127.7 (s, Ar), 126.1 (s, Ar), 125.8 (s, Ar), 122.2 (s, Ar), 121.9 (s, Ar), 119.2 (s, Ar), 109.3 (s, Ar), 46.7 (s, CH_2), 35.2 (s, CH_2), 28.8 (s, CH_2), 26.7 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2$ ($[M+H]^+$) 327.1861, found 327.1870.



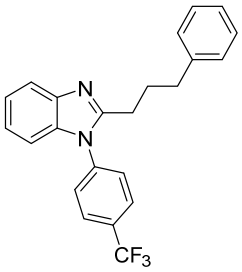
2-(3-phenylpropyl)-1-(p-tolyl)-1H-benzo[d]imidazole (3o): The reaction was performed according to the above general procedure B. Yield: 73%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, 1H, $^3J_{HH}$ = 8.0 Hz), 7.33-7.08 (m, 12H), 2.80 (t, 2H, $^3J_{HH}$ = 8.0 Hz), 2.66 (t, 2H, $^3J_{HH}$ = 8.0 Hz), 2.47 (s, 3H), 2.11 (qn, 2H, $^3J_{HH}$ = 9.0 Hz). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 154.9 (s, Ar), 142.6 (s, Ar), 141.3 (s, Ar), 138.8 (s, Ar), 136.6 (s, Ar), 133.2 (s, Ar), 130.4 (s, Ar), 128.3 (s, Ar), 128.2 (s, Ar), 127.0 (s, Ar), 125.7 (s, Ar), 122.4 (s, Ar), 122.1 (s, Ar), 119.0 (s, Ar), 109.9 (s, Ar), 35.2 (s, CH_2), 29.1 (s, CH_2), 27.0 (s, CH_2), 21.1 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2$ ($[M+H]^+$) 327.1861, found 327.1876.



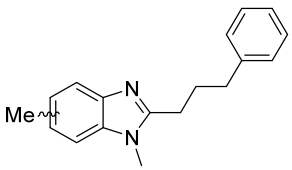
2-(3-phenylpropyl)-1-(o-tolyl)-1H-benzo[d]imidazole (3p): The reaction was performed according to the above general procedure B. Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, 1H, $^3J_{HH}$ = 8.0 Hz), 7.46-7.07 (m, 11H), 6.89 (d, 1H, $^3J_{HH}$ = 8.0 Hz), 2.74-2.61 (m, 4H), 2.16-2.04 (m, 2H), 1.93 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 154.9 (s, Ar), 142.7 (s, Ar), 141.3 (s, Ar), 136.3 (s, Ar), 136.1 (s, Ar), 134.6 (s, Ar), 131.4 (s, Ar), 129.5 (s, Ar), 128.5 (s, Ar), 128.3 (s, Ar), 128.2 (s, Ar), 127.2 (s, Ar), 125.8 (s, Ar), 122.4 (s, Ar), 122.1 (s, Ar), 119.1 (s, Ar), 109.9 (s, Ar), 35.2 (s, CH_2), 28.9 (s, CH_2), 27.0 (s, CH_2), 17.2 (s, CH_3). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2$ ($[M+H]^+$) 327.1861, found 327.1874.



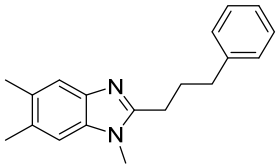
1-(4-methoxyphenyl)-2-(3-phenylpropyl)-1H-benzo[d]imidazole (3q): The reaction was performed according to the above general procedure B. Yield: 69%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.27-7.00 (m, 12H), 3.88 (s, 3H), 2.78 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.66 (t, 2H, $^{3}J_{HH}$ = 6.0 Hz), 2.11 (qn, 2H, $^{3}J_{HH}$ = 8.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 159.6 (s, Ar), 155.1 (s, Ar), 142.5 (s, Ar), 141.3 (s, Ar), 136.8 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 128.2 (s, Ar), 125.7 (s, Ar), 122.3 (s, Ar), 122.1 (s, Ar), 119.0 (s, Ar), 114.9 (s, Ar), 109.8 (s, Ar), 55.5 (s, CH_3), 35.1 (s, CH_2), 29.1 (s, CH_2), 27.0 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{22}N_2O$ ([M+H]$^{+}$) 343.1810, found 343.1822.



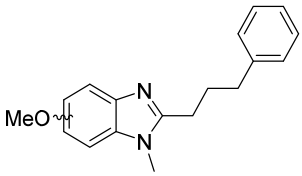
2-(3-phenylpropyl)-1-(4-(trifluoromethyl)phenyl)-1H-benzo[d]imidazole (3r): The reaction was performed according to the above general procedure B. Yield: 81%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, 2H, $^{3}J_{HH}$ = 8.0 Hz), 7.79 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.41 (d, 2H, $^{3}J_{HH}$ = 8.0 Hz), 7.31-7.05 (m, 8H), 2.79 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.67 (t, 2H, $^{3}J_{HH}$ = 6.0 Hz), 2.12 (qn, 2H, $^{3}J_{HH}$ = 7.0 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 154.4 (s, Ar), 142.7 (s, Ar), 141.1 (s, Ar), 139.2 (s, Ar), 136.0 (s, Ar), 130.9 (q, $^{2}J_{CF}$ = 33.3 Hz, *C*-CF_3), 128.3 (s, Ar), 128.3 (s, Ar), 127.5 (s, Ar), 127.1 (s, Ar), 127.1 (s, Ar), 125.9 (s, Ar), 123.3 (q, $^{1}J_{CF}$ = 270 Hz, *C*F_3), 123.0 (s, Ar), 122.8 (s, Ar), 119.4 (s, Ar), 109.6 (s, Ar), 35.1 (s, CH_2), 29.1 (s, CH_2), 26.9 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{23}H_{19}F_3N_2$ ([M+H]$^{+}$) 381.1578, found 381.1588.



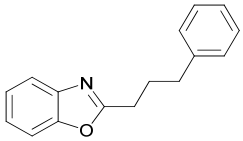
1,5/6-dimethyl-2-(3-phenylpropyl)-1H-benzo[d]imidazole (3s): The reaction was performed according to the above general procedure B. Yield: 87%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, 0.5H, $^{3}J_{HH}$ = 8.0 Hz), 7.52 (s, 0.5H), 7.29-7.16 (m, 5H), 7.10-7.02 (m, 2H), 3.51 (s, 3H), 2.81-2.74 (m, 4H), 2.48 (s, 1.5H), 2.47 (s, 1.5H), 2.19 (qnd, 2H, $^{3}J_{HH}$ = 8.0 Hz, $^{2}J_{HH}$ = 2.4 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 154.6 (s, Ar), 154.2 (s, Ar), 142.7 (s, Ar), 141.2 (s, Ar), 140.5 (s, Ar), 135.8 (s, Ar), 133.7 (s, Ar), 131.6 (s, Ar), 131.0 (s, Ar), 128.3 (s, Ar), 128.2 (s, Ar), 125.8 (s, Ar), 123.1 (s, Ar), 123.0 (s, Ar), 118.8 (s, Ar), 118.4 (s, Ar), 108.7 (s, Ar), 108.2 (s, Ar), 35.1 (s, CH_2), 29.3 (s, N-CH_3), 29.2 (s, N-CH_3), 28.7 (s, *C*H_2), 28.7 (s, *C*H_2), 26.5 (s, CH_2), 21.6 (s, Ar-*C*H_3), 21.3 (s, Ar-*C*H_3). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{20}N_2$ ([M+H]$^{+}$) 265.1705, found 265.1713.



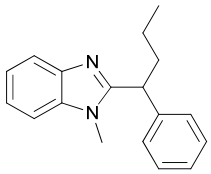
1,5,6-trimethyl-2-(3-phenylpropyl)-1H-benzo[d]imidazole (3t): The reaction was performed according to the above general procedure B. Yield: 83%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (s, 1H), 7.29-7.16 (m, 5H), 7.01 (s, 1H), 3.55 (s, 3H), 2.82 (t, 2H, $^{3}J_{HH}$ = 6.0 Hz), 2.76 (t, 2H, $^{3}J_{HH}$ = 8.0 Hz), 2.38 (s, 3H), 2.36 (s, 3H), 2.19 (qn, 2H, $^{3}J_{HH}$ = 7.0 Hz). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 153.9 (s, Ar), 141.4 (s, Ar), 141.1 (s, Ar), 134.2 (s, Ar), 130.7 (s, Ar), 130.2 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 125.8 (s, Ar), 119.2 (s, Ar), 109.1 (s, Ar), 35.2 (s, CH_2), 29.4 (s, N-CH_3), 28.9 (s, CH_2), 26.6 (s, CH_2), 20.4 (s, Ar-*C*H_3), 20.1 (s, Ar-*C*H_3). HR-MS (MALDI): *m/z* calcd. for $C_{19}H_{22}N_2$ ($[M+H]^+$) 279.1861, found 279.1872.



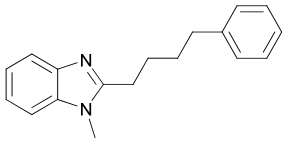
5/6-methoxy-1-methyl-2-(3-phenylpropyl)-1H-benzo[d]imidazole (3u): The reaction was performed according to the above general procedure B. Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.28-7.15 (m, 5H), 6.86 (d, 0.5H, $^{3}J_{HH}$ = 4.0 Hz), 6.84 (d, 0.5H, $^{3}J_{HH}$ = 4.0 Hz), 6.71 (d, 1H, $^{3}J_{HH}$ = 2.4 Hz), 3.84 (s, 3H), 3.55 (s, 3H), 2.83-2.74 (m, 4H), 2.18 (qn, 2H, $^{3}J_{HH}$ = 7.0 Hz). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 156.1 (s, Ar), 154.0 (s, Ar), 141.4 (s, Ar), 137.0 (s, Ar), 136.3 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 125.9 (s, Ar), 119.4 (s, Ar), 110.4 (s, Ar), 93.1 (s, Ar), 55.9 (s, O-*C*H_3), 35.2 (s, CH_2), 29.5 (s, N-CH_3), 28.8 (s, *C*H_2), 26.7 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{20}N_2O$ ($[M+H]^+$) 281.1654, found 281.1660.



2-(3-phenylpropyl)benzo[*d*]oxazole (3x): The reaction was performed according to the above general procedure B. Yield: 74%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.68-7.65 (m, 1H, Ar), 7.48-7.43 (m, 1H, Ar), 7.30-7.16 (m, 7H, Ar), 2.94 (t, 2H, $^{3}J_{HH}$ = 7.5 Hz, CH_2), 2.75 (t, 2H, $^{3}J_{HH}$ = 7.5 Hz, CH_2), 2.22 (qn, $^{3}J_{HH}$ = 7.5 Hz, 2H, CH_2). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$): δ 167.1 (s, Ar), 151.0 (s, Ar), 141.6 (s, Ar), 141.3 (s, Ar), 128.7 (s, Ar), 128.7 (s, Ar), 126.3 (s, Ar), 124.7 (s, Ar), 124.3 (s, Ar), 119.8 (s, Ar), 110.5 (s, Ar), 35.3 (s, CH_2), 28.5 (s, CH_2), 28.2 (s, CH_2). HR-MS (FAB): *m/z* calculated for $C_{16}H_{16}ON$ ($[M+H]^+$) 238.1232, found 238.1236.



1-methyl-2-(1-phenylbutyl)-1*H*-benzo[*d*]imidazole (11-B): The reaction was performed according to the above general procedure A. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.87-7.82 (m, 1H), 7.26-7.15 (m, 8H), 4.10 (t, $^{3}J_{HH}$ = 7.5 Hz, 1H), 3.49 (s, 3H), 2.52-2.40 (m, 1H), 2.22-2.10 (m, 1H), 1.47-1.24 (m, 2H), 0.96 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 156.5 (s, Ar), 142.5 (s, Ar), 141.4 (s, Ar), 136.0 (s, Ar), 128.9 (s, Ar), 128.2 (s, Ar), 127.0 (s, Ar), 122.3 (s, Ar), 121.8 (s, Ar), 119.7 (s, Ar), 109.0 (s, Ar), 44.4 (s, CH), 37.7 (s, N-CH_3), 29.8 (s, CH_2), 21.1 (s, CH_2), 14.1 (s, CH_3). HR-MS (EI): *m/z* calculated for $C_{18}H_{20}N_2$ ([M^+]) 264.1626, found 264.1623.

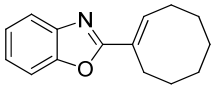


1-methyl-2-(4-phenylbutyl)-1*H*-benzo[*d*]imidazole (11-L): The reaction was performed according to the above general procedure B. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74-7.69 (m, 1H), 7.29-7.14 (m, 8H), 3.65 (s, 3H), 2.88 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 2.69 (t, $^{3}J_{HH}$ = 7.5 Hz, 2H), 1.97-1.87 (m, 2H), 1.83-1.73 (m, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 155.1 (s, Ar), 142.5 (s, Ar), 142.1 (s, Ar), 135.7 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 125.8 (s, Ar), 121.9 (s, Ar), 121.7 (s, Ar), 119.0 (s, Ar), 108.9 (s, Ar), 35.6 (s, CH_2), 31.1 (s, N-CH_3), 29.6 (s, CH_2), 27.3 (s, CH_2), 27.1 (s, CH_2). HR-MS (MALDI): *m/z* calcd. for $C_{18}H_{21}N_2$ ([M+H]$^+$) 265.1705, found 265.1711.

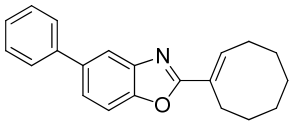
General procedure for Nickel-mediated alkenylation of benzoxazoles (12-13), and oxazoles (14): The product **12a** is a representative reaction. To a vial (5 mL) containing $Ni(COD)_2$ (14 mg, 0.050 mmol) and IMes (15 mg, 0.050 mmol) was added 1,5-cyclooctadiene (1.0 mL) as solvent in a glove box atmosphere. After the substances were completely dissolved in 1,5-cyclooctadiene, the solution was transferred into a screw-capped vial (5 mL) containing benzoxazole (60 mg, 0.50 mmol). The vial was closed and heated at 130 ^{o}C for 2 hours. The resulting mixture was filtered through *Celite* and washed with dichloromethane. The filtrate solution was concentrated *in vacuo* to afford the crude product, which was further purified by column chromatography using hexane/ethyl acetate (19:1 v/v) as eluent to furnish (E)-2-(cyclooctenyl)-benzoxazole (109 mg, 0.480 mmol) in 96% yield.

General procedure for Nickel-mediated alkenylation of 1-methylbenzimidazole (15) and caffeine (16): The product **15a** is a representative reaction. To a screw-capped vial (5 mL) containing $Ni(COD)_2$ (14 mg, 0.050 mmol), IMes (15 mg, 0.050 mmol), 1-methylbenzimidazole (66 mg, 0.50 mmol), and potassium *tert*-butoxide (5.6 mg, 0.050 mmol) was added toluene (1.0 mL) followed by the addition of 1,5-cyclooctadiene (43 mg, 0.040 mmol) in a glove box

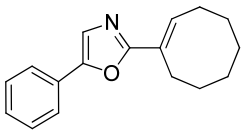
atmosphere. The reaction vial was closed and heated at 80 ^{o}C for 2 hours outside of the glove box. The resulting mixture was filtered through *Celite* and washed with dichloromethane. The filtrate solution was concentrated *in vacuo* to afford the crude product, which was further purified by column chromatography using hexane/ethyl acetate (4:1 v/v) as eluent to furnish (E)-2-(cyclooctenyl)-1-methyl-benzimidazole **15a** (117 mg, 0.49 mmol) in 97% yield.



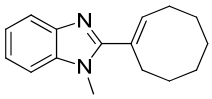
(E)-2-(cyclooct-1-en-1-yl)benzo[d]oxazole (12a): The reaction was performed according to the above general procedure. Yield: 96%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70-7.66 (m, 1H), 7.47-7.42 (m, 1H), 7.28-7.24 (m, 2H), 7.08 (t, *J* = 8.6 Hz, 1H), 2.81 (t, *J* = 6.4 Hz, 2H), 2.42-2.37 (m, 2H), 1.76-1.72 (m, 2H), 1.65-1.64 (m, 2H), 1.55-1.51 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.3, 150.5, 142.1, 138.1, 129.4, 124.6, 124.1, 119.7, 110.1, 29.5, 29.0, 27.2, 26.5, 26.0, 25.6. HR-MS (EI): calculated for: $[C_{15}H_{17}NO]^{+}$: 227.1310. Found: 227.1308.



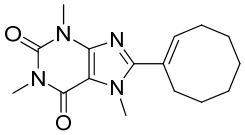
(E)-2-(cyclooct-1-en-1-yl)-5-phenylbenzo[d]oxazole (13a): The reaction was performed according to the above general procedure. Yield: 66%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (s, 1H), 7.60-7.58 (m, 2H), 7.50 (m, 2H), 7.44 (t, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.11 (t, *J* = 8.6 Hz, 1H), 2.82 (t, *J* = 6.2 Hz, 2H), 2.44-2.39 (m, 2H), 1.75 (m, 2H), 1.66-1.65 (m, 2H) 1.53-1.52 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.9, 150.0, 142.7, 141.2, 138.3, 137.9, 129.4, 128.8, 127.3, 127.1, 124.2, 118.2, 110.1, 29.5, 29.0, 27.2, 26.5, 26.0, 25.6. HR-MS (FAB): calculated for: $[C_{21}H_{21}ON]^{+}$: 303.1623. Found: 303.1629.



(E)-2-(cyclooct-1-en-1-yl)-5-phenyloxazole (14a): The reaction was performed according to the above general procedure. Yield: 92%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 7.2, 2H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.29-7.24 (m, 2H), 6.84 (t, *J* = 8.6 Hz, 1H), 2.72 (t, *J* = 6.2 Hz, 2H), 2.37-2.31 (m, 2H), 1.70 (m, 2H), 1.62-1.61 (m, 2H), 1.51-1.50 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.5, 150.3, 134.0, 129.1, 128.7, 128.0, 128.2,123.9, 122.8, 29.5, 28.9, 26.9, 26.5, 26.0, 25.4. HR-MS (EI): calculated for: $[C_{17}H_{19}NO]^{+}$: 253.1467. Found: 253.1460.



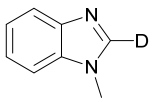
(*E*)-2-(cyclooct-1-en-1-yl)-1-methyl-1*H*-benzo[*d*]imidazole (15a): The reaction was performed according to the above general procedure. Yield: 97%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.75-7.71 (m, 1H), 7.25-7.19 (m, 3H), 6.06 (t, J = 8.1 Hz, 1H), 3.72 (s, 3H), 2.75-2.71 (m, 2H), 2.36 (dd, J = 8.1 Hz, 11.4, 2H), 1.66-1.59 (m, 8H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 155.6, 142.4, 136.1, 135.8, 131.6, 122.1, 121.8, 119.3, 109.2, 31.6, 29.3, 29.0, 28.9, 26.9, 26.4, 26.1. HR-MS (EI): calculated for: $[C_{16}H_{20}N_2]^+$: 240.1626. Found: 240.1620.



(*E*)-8-(cyclooct-1-en-1-yl)-1,3,7-trimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (16a): The reaction was performed according to the above general procedure. Yield: 93%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.07 (t, J = 8.0 Hz, 1H), 3.96 (s, 3H), 3.54 (s, 3H), 3.38 (s, 3H), 2.65-2.62 (m, 2H), 2.38-2.33 (m, 2H), 1.66-1.56 (m, 8H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 155.4, 154.2, 151.7, 147.9, 136.8, 130.5, 107.7, 33.9, 29.6, 29.4, 29.1, 28.8, 27.8, 27.1, 26.6, 26.2. HR-MS (EI): calculated for: $[C_{16}H_{22}N_4O_2]^+$: 302.1743. Found: 302.1735.

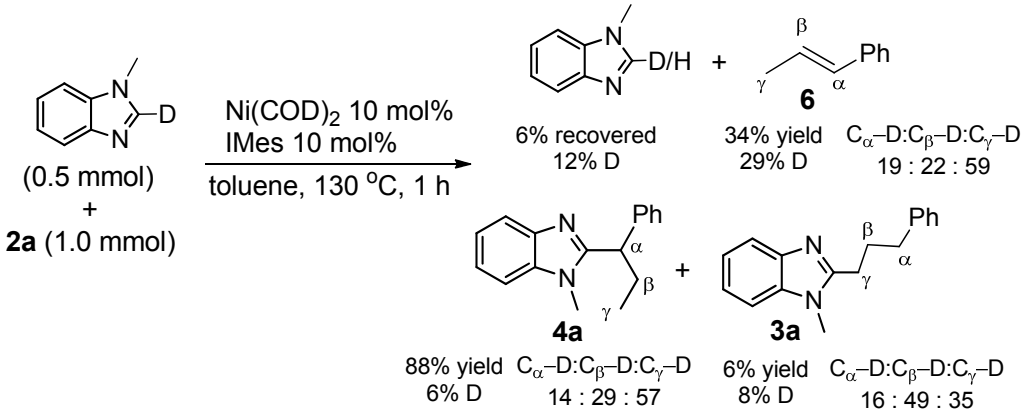
Mechanism study

(a) Synthesis of 1-methylbenzimidazole-d



A 50 mL Schlenk flask equipped with a stir-bar was charged with 1-methylbenzimidazole (1.32 g, 10 mmol) in diethyl ether (40 mL) under nitrogen. The solution was cooled to -78 ^{o}C and *n*-butyllithium (4.8 mL of 2.5 M in hexane solution, 12 mmol) was added dropwise followed by removing the slush bath. After 20 minutes the temperature was lowered to -78 ^{o}C again, followed by slow addition of D_2O (2 mL). The solution was then slowly warmed to room temperature. Solvent was removed under reduced pressure. The residue was purified by flash chromatography using ethyl acetate as eluent to give amber oil (1.02 g, 77%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, $^{3}J_{HH}$ = 8.0 Hz, 1H, Ar), 7.36-7.24 (m, 3H, Ar), 3.78 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): 143.8 (s, Ar), 143.4 (1:1:1 triplet, $^{1}J_{CD}$ = 40 Hz, C-D), 134.6 (s, Ar), 123.0 (s, Ar), 122.2 (s, Ar), 120.4 (s, Ar), 109.5 (s, Ar), 31.1 (s, CH_3).

(b) Isotopic labeling Experiments



To the toluene solution of $Ni(COD)_2$ (14 mg, 0.05 mmol), IMes (14 mg, 0.05 mmol), and 1-methylbenzimidazole-d (0.5 mmol) was added allylbenzene (1.0 mmol) into the vial. After the vial was screw-capped, the reaction solution was taken outside the glovebox and heated at 130 ^{o}C for 1 h. The resulting mixture was filtered through *Celite* and washed with dichloromethane. The filtrate solution was concentrated in *vacuo* to afford crude product. The crude was further purified by flash chromatography using hexane/ethyl acetate (3:1) as eluent.

Deuterium-labeling experiments were performed. Reaction of C2-deuterated **1a** with **2a** shows deuteration at α, β and γ positions of **4a**, the isomerized **6**, as well as the loss of deuteration and H/D scrambling in [D_1]-**1a**, revealing that the C-H bond cleavage and migratory insertion steps are reversible. These results may suggest that the final reductive elimination step could be the rate-determining step, which has been discussed for the nickel-catalyzed hydroheteroarylation[6] and hydroalkynylation[7] of vinylarenes.

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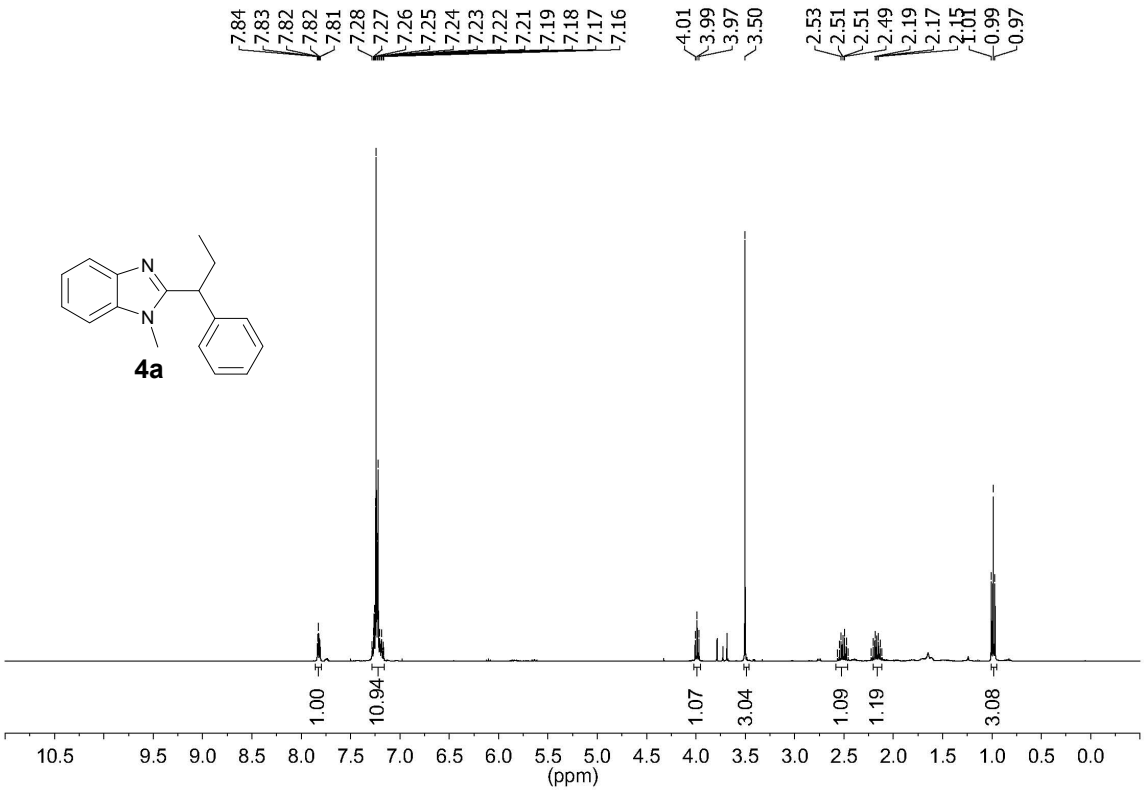
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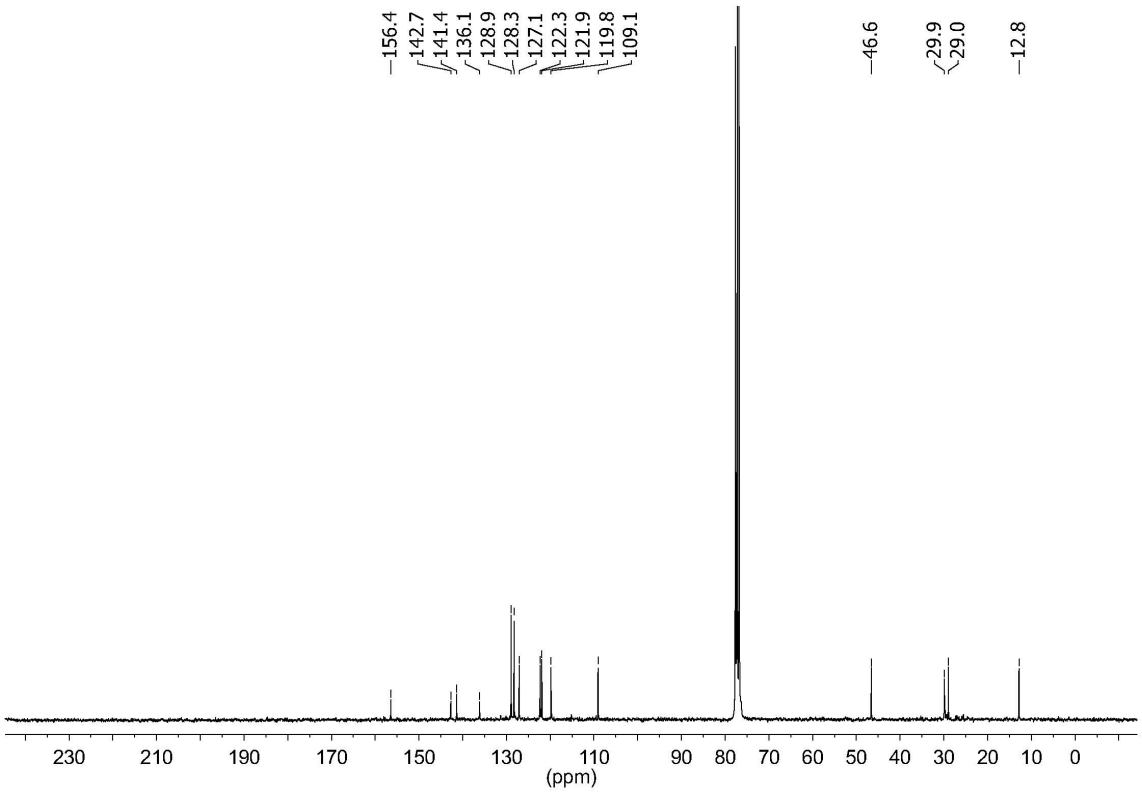
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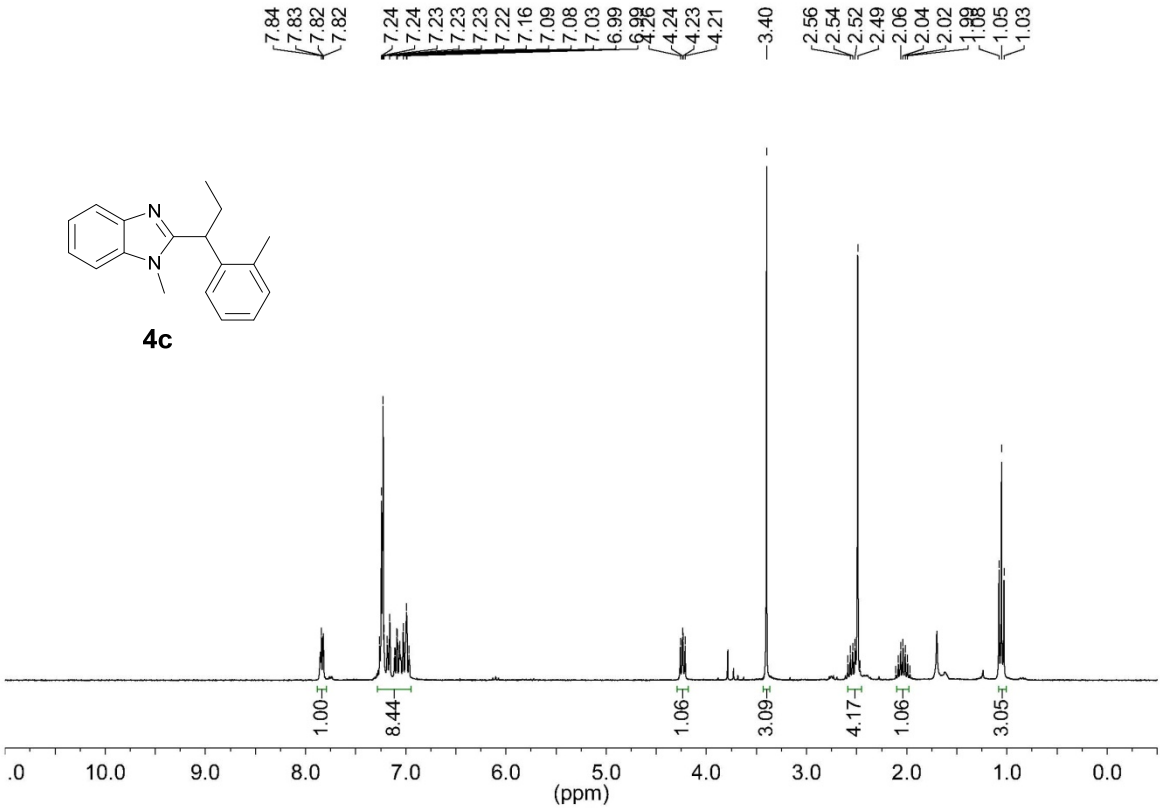
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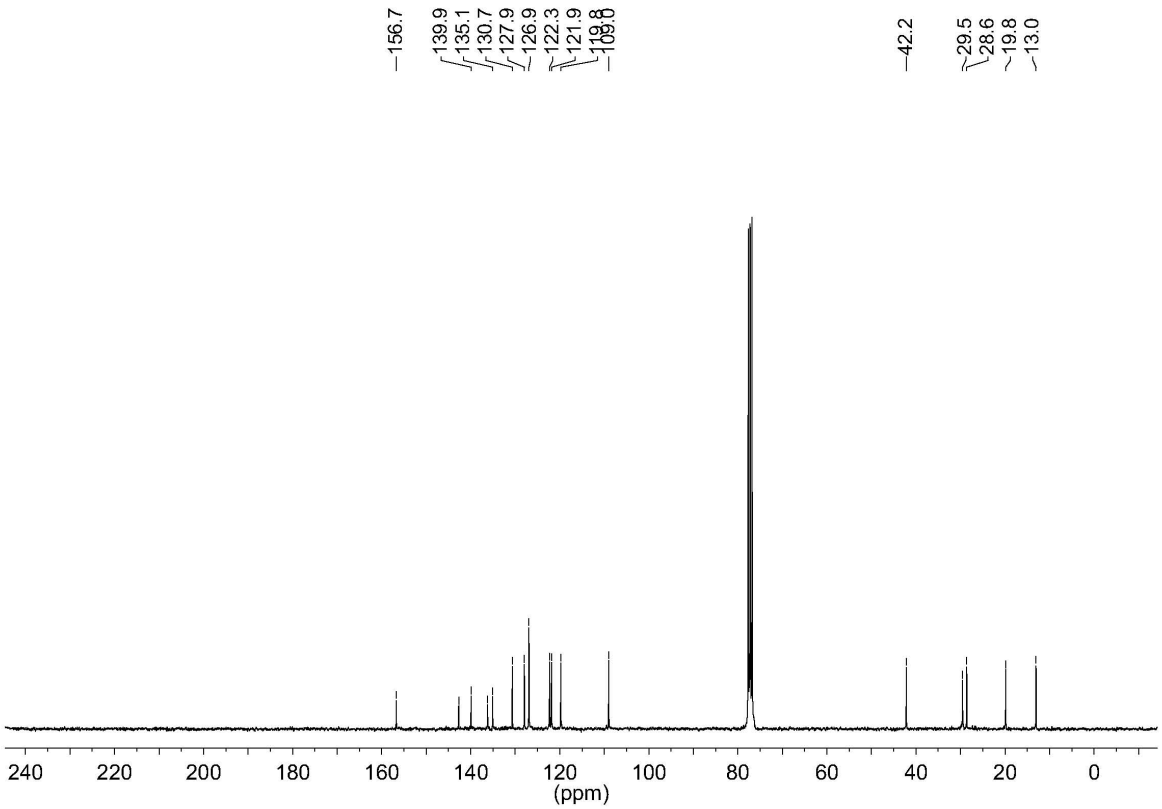
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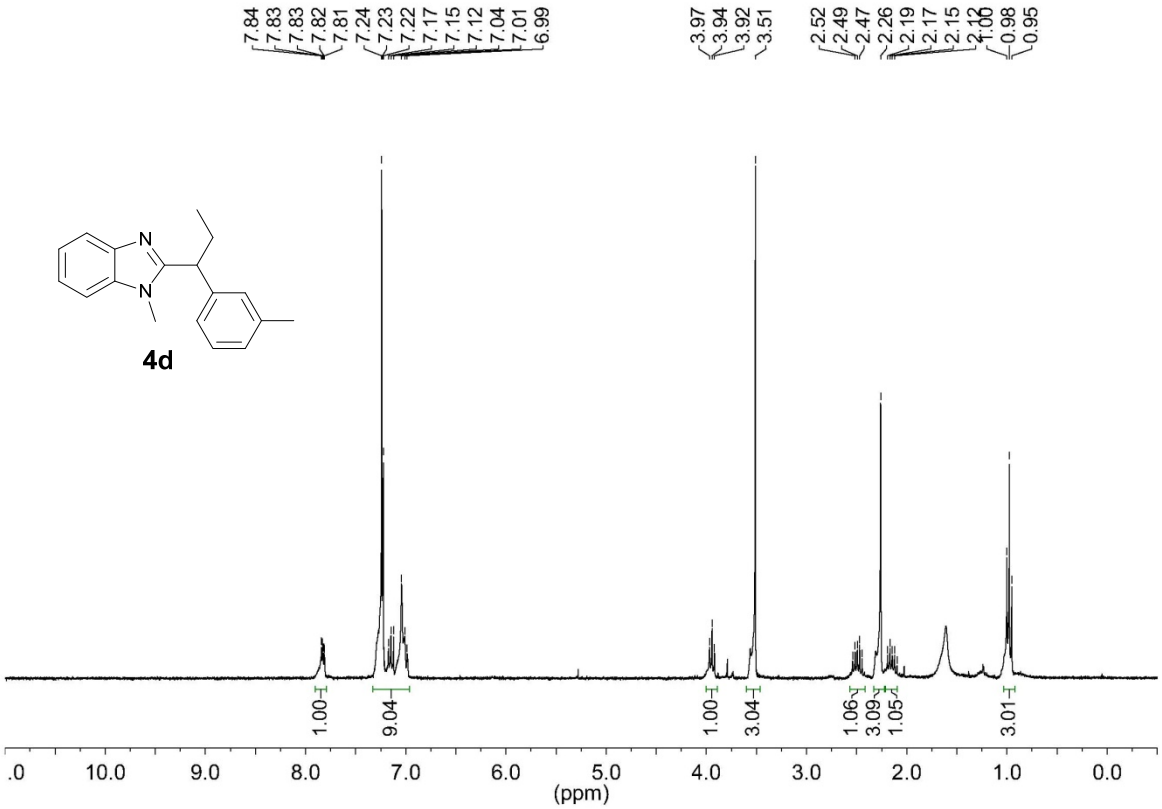
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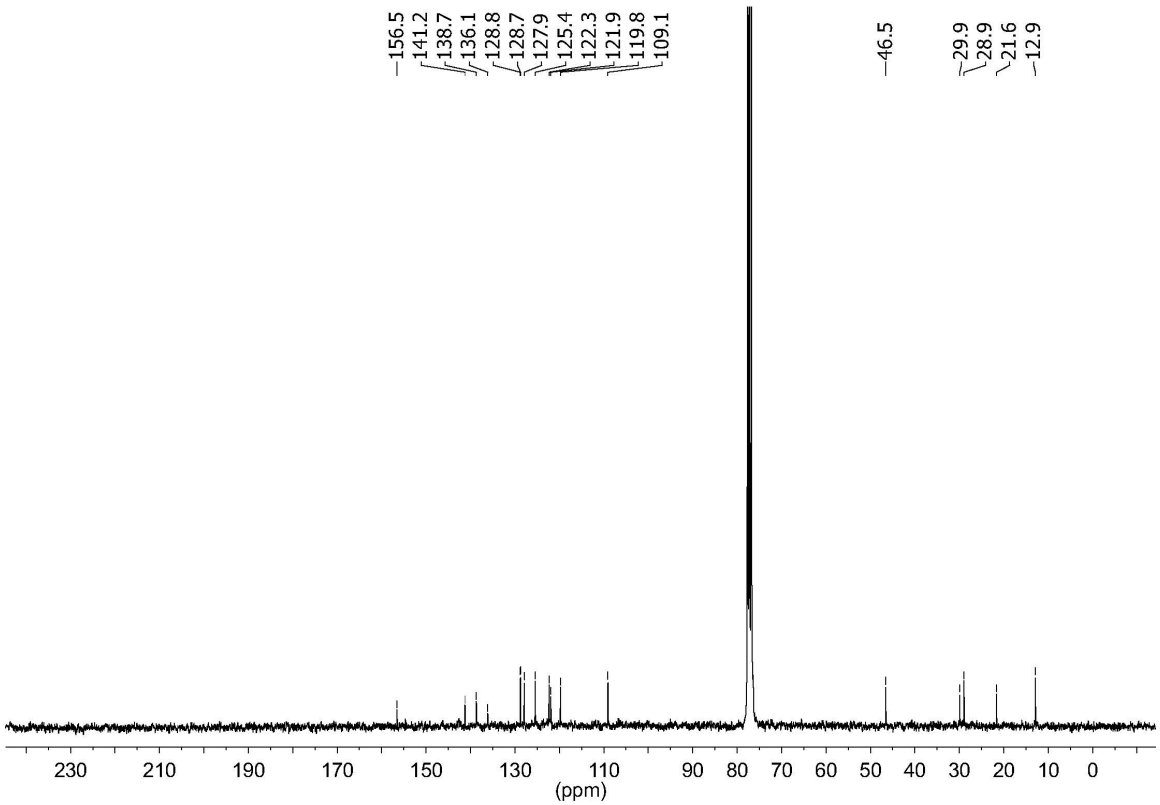
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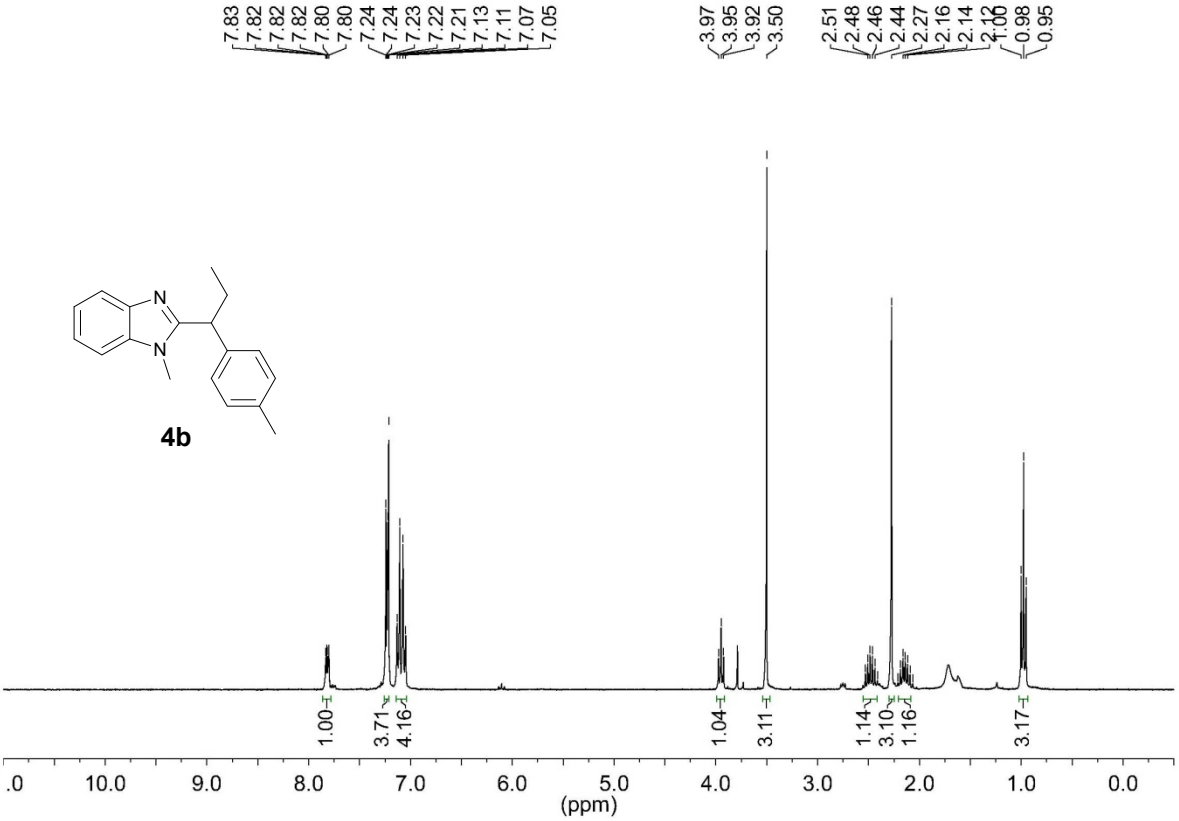
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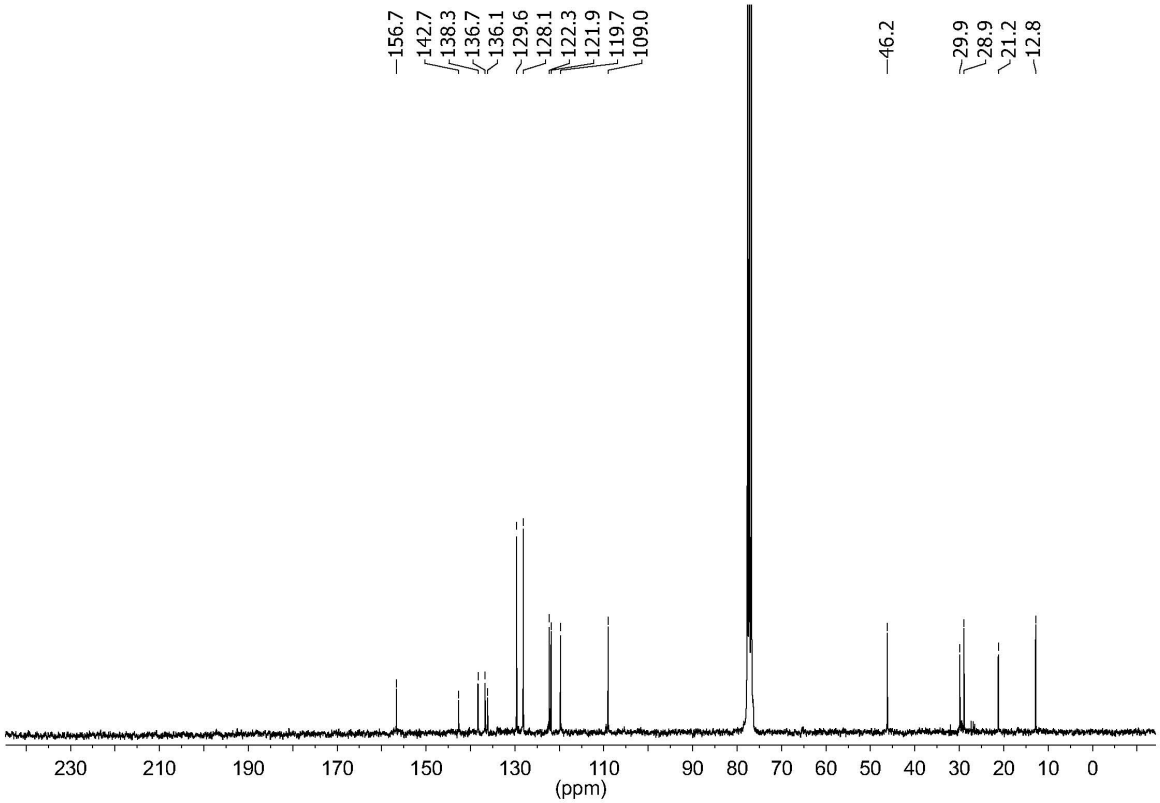
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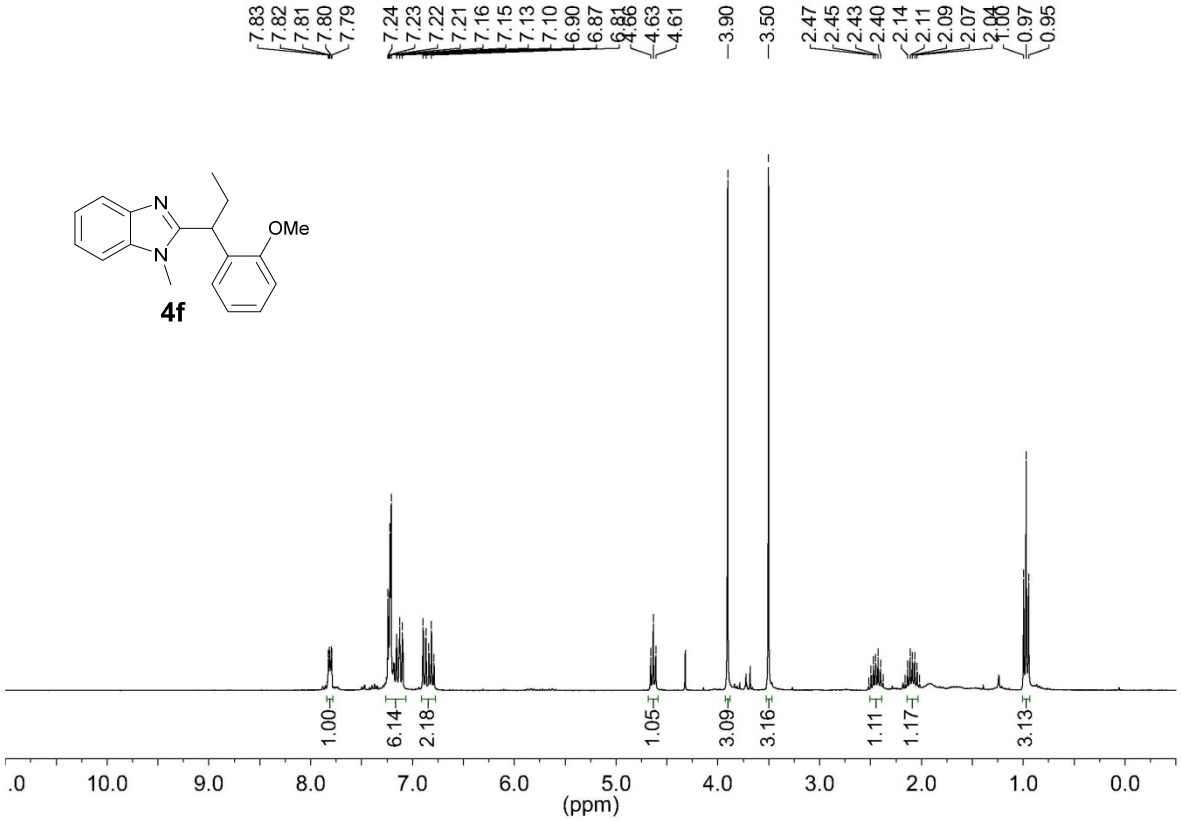
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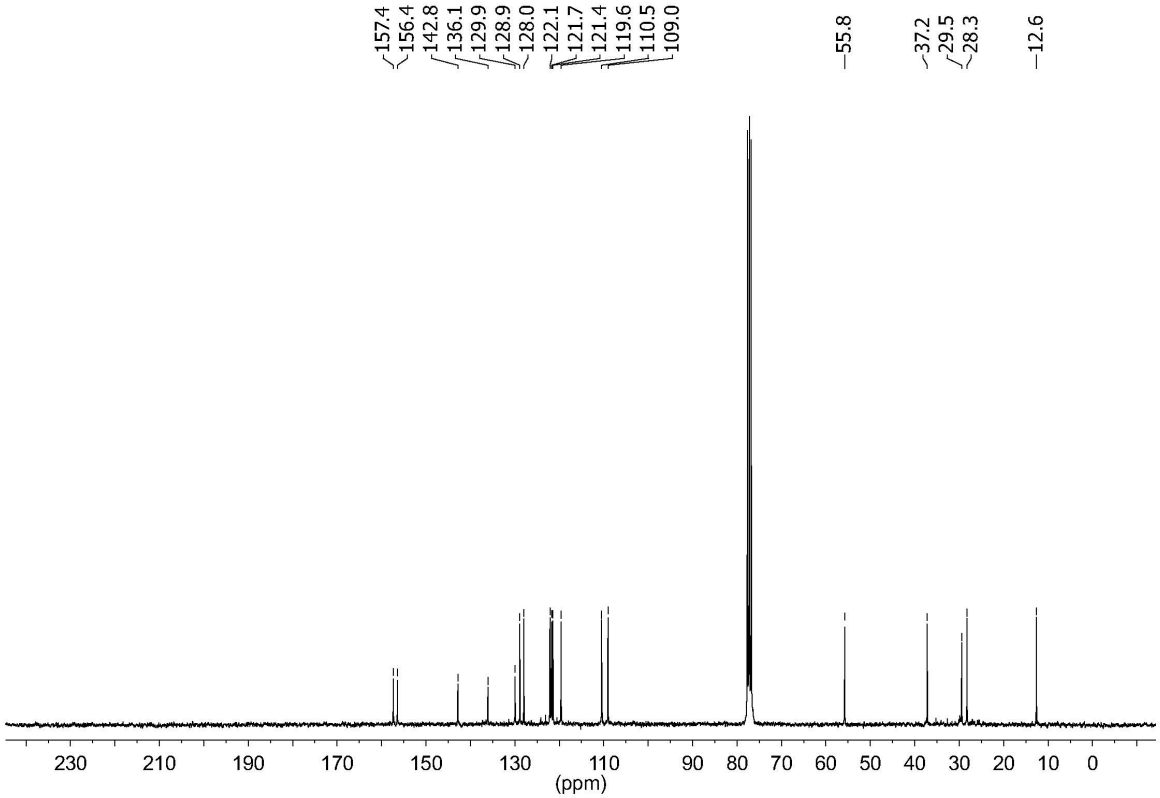
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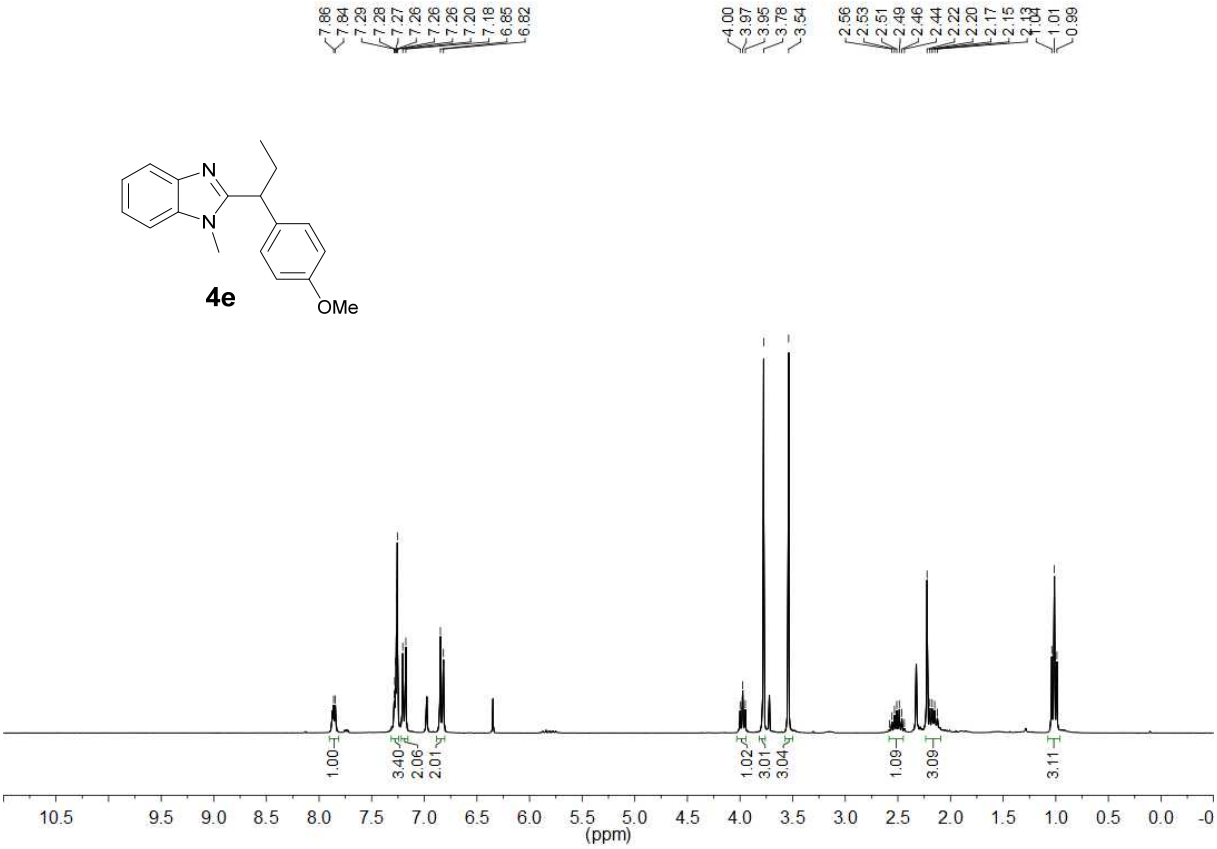
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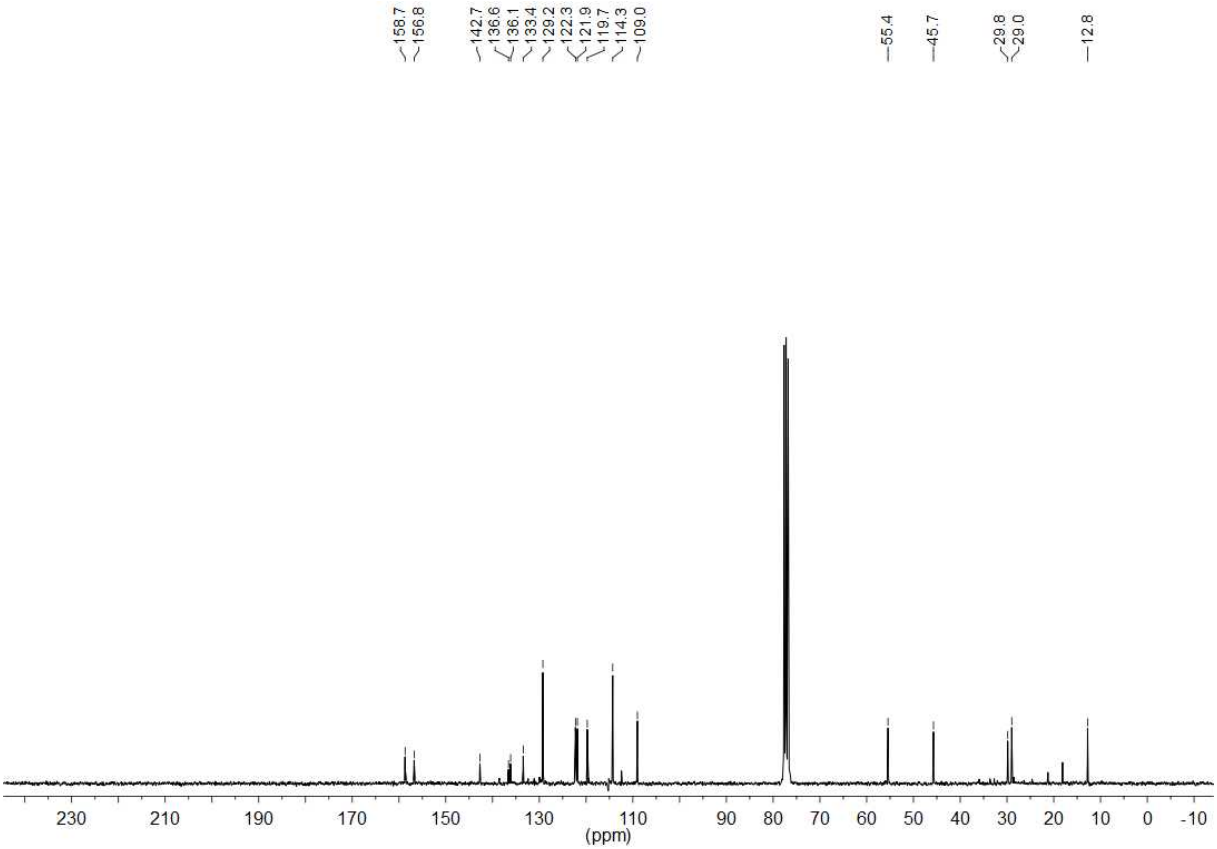
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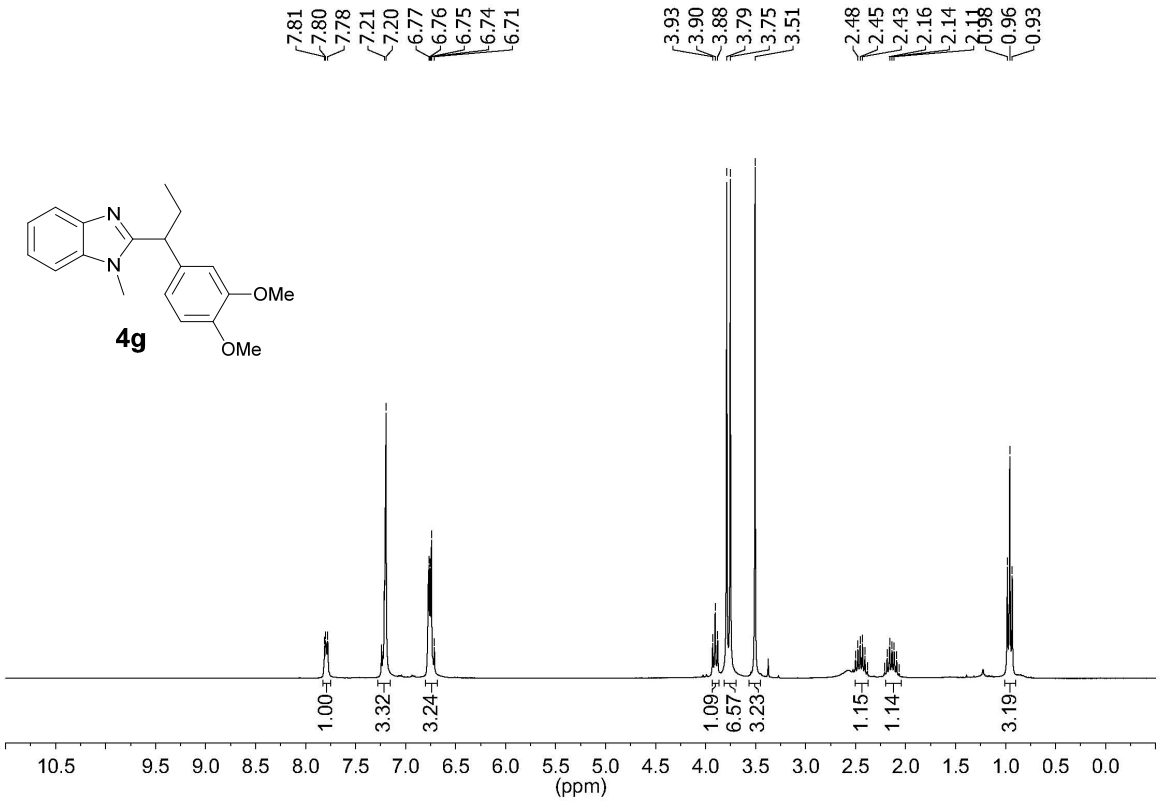
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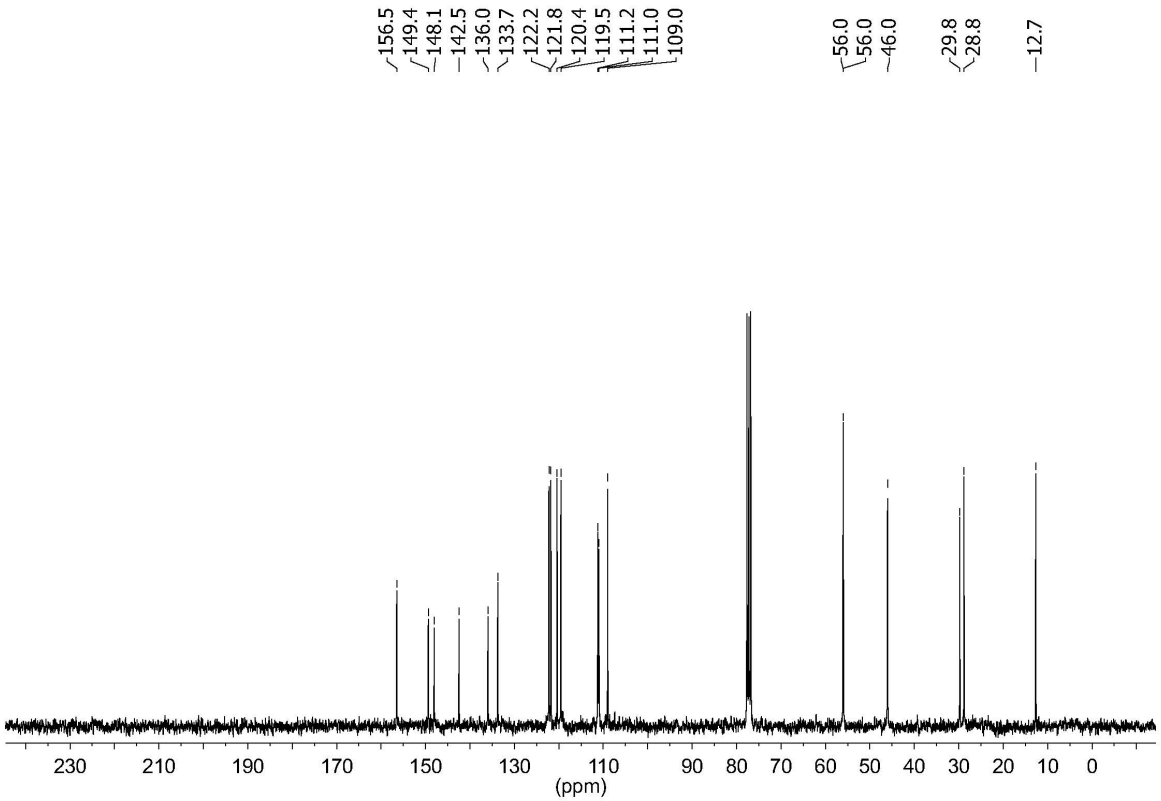
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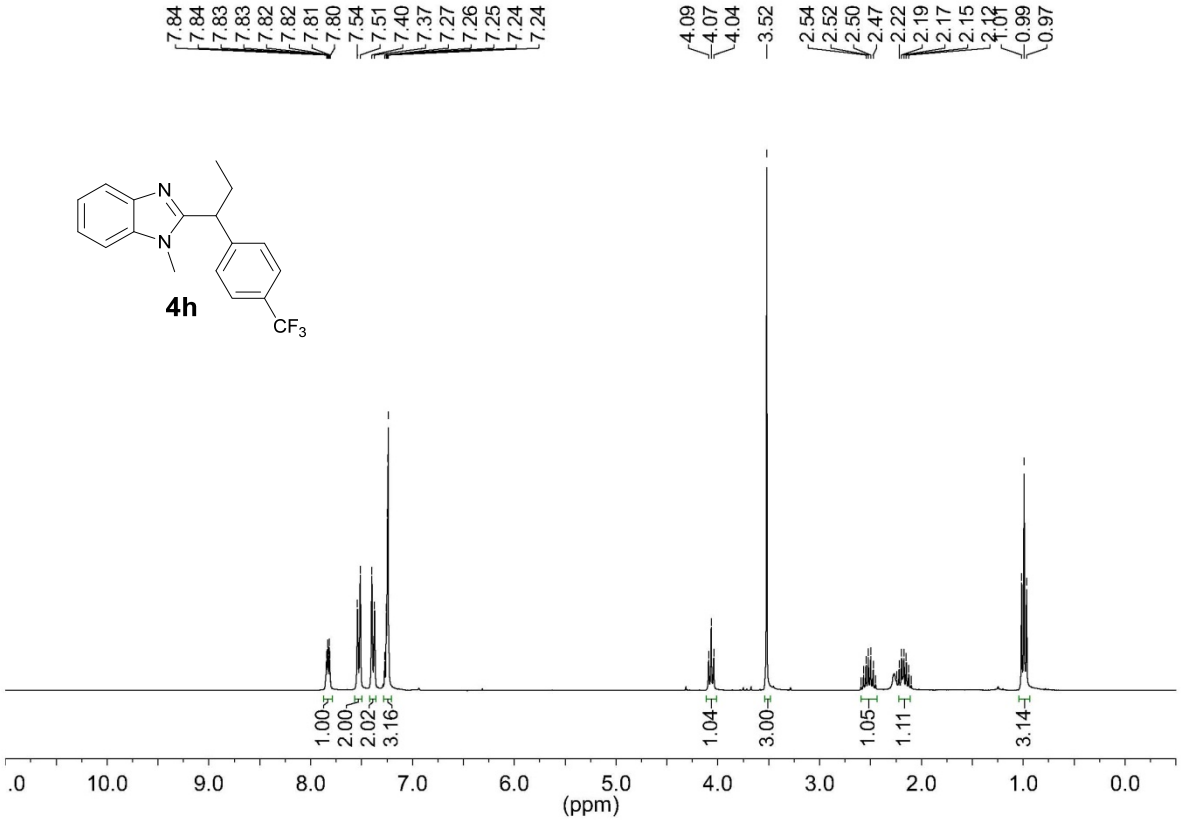
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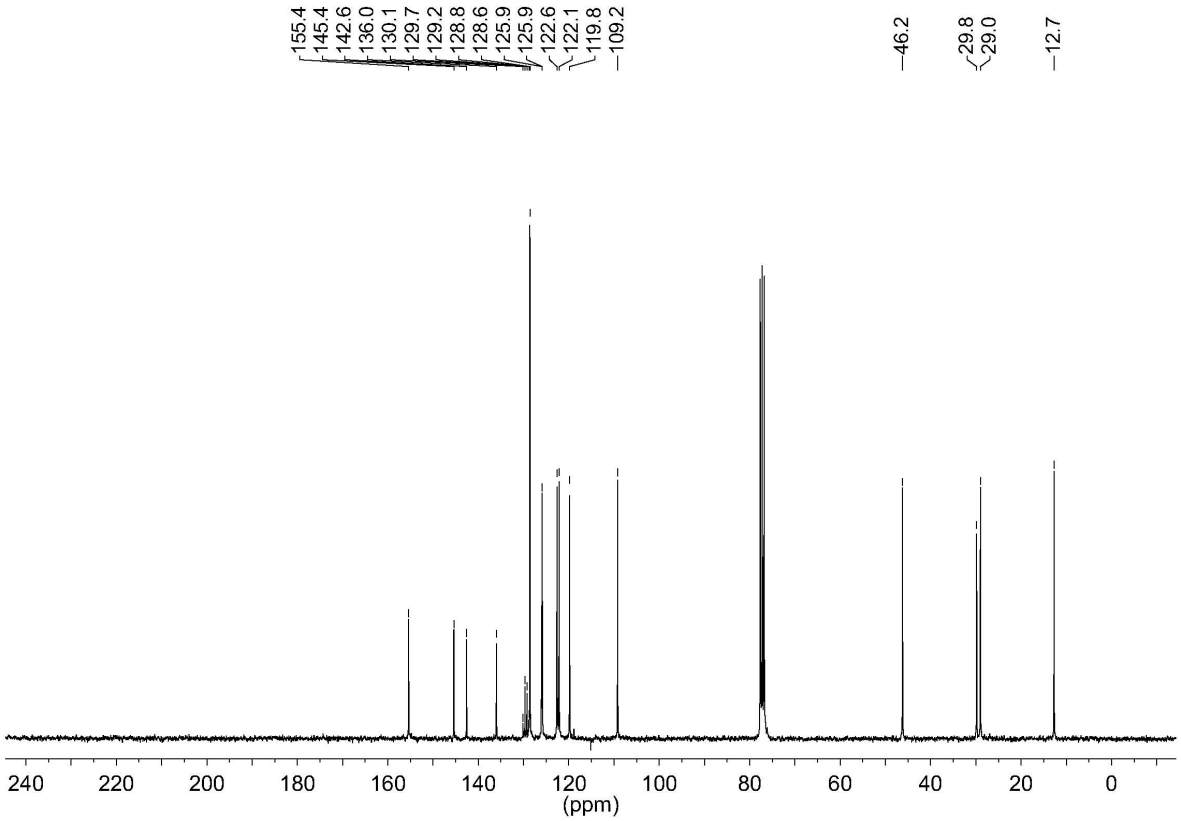
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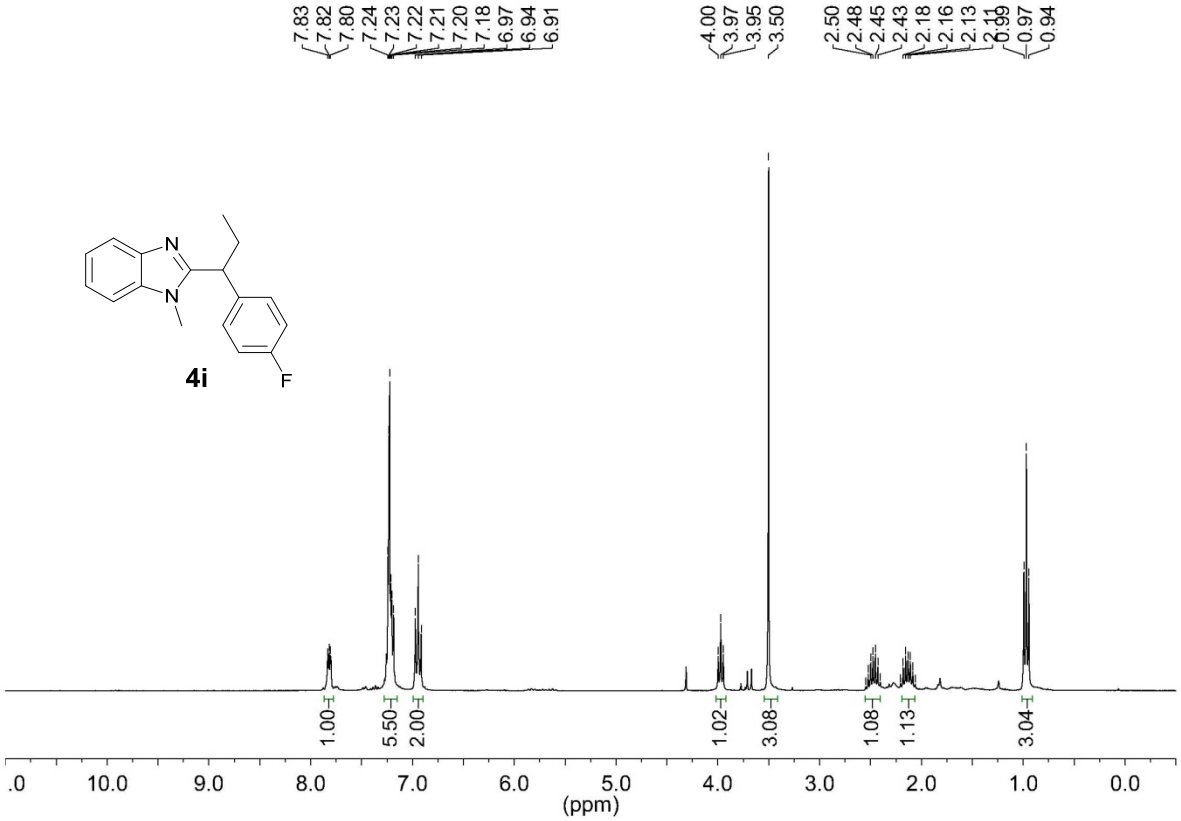
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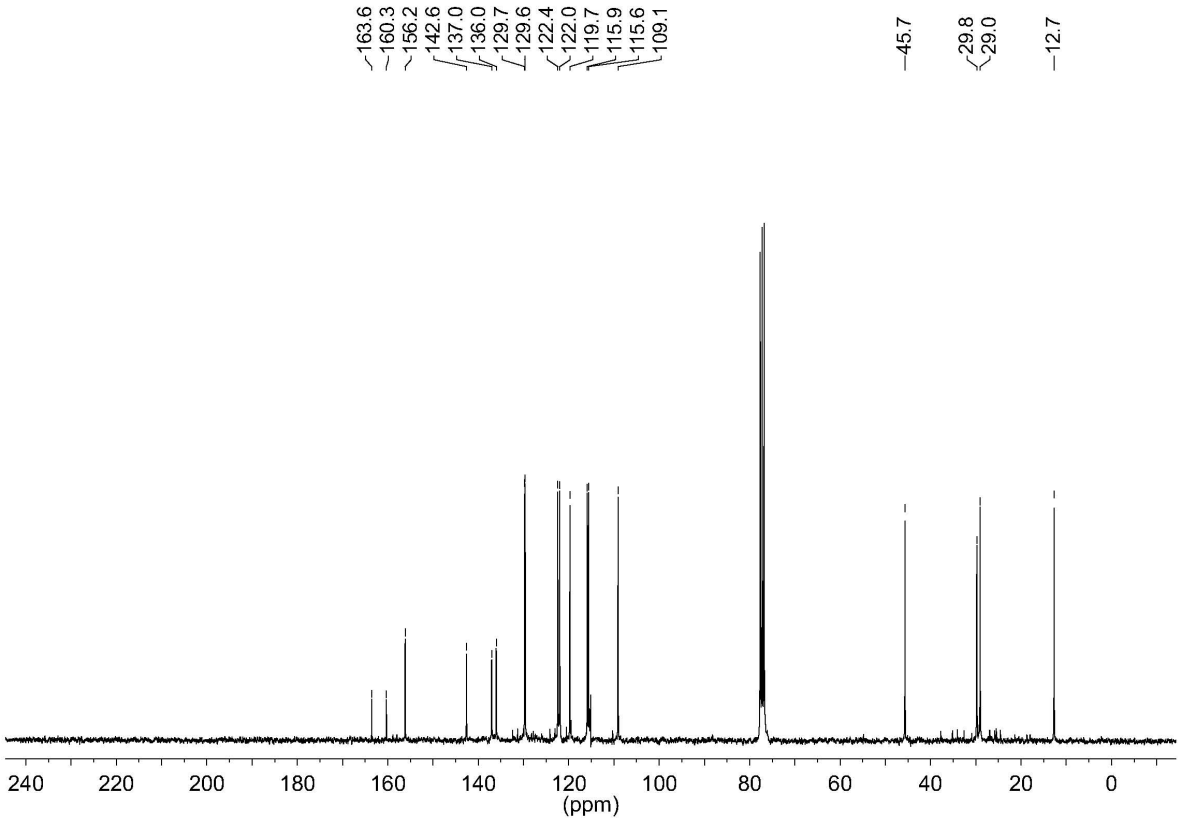
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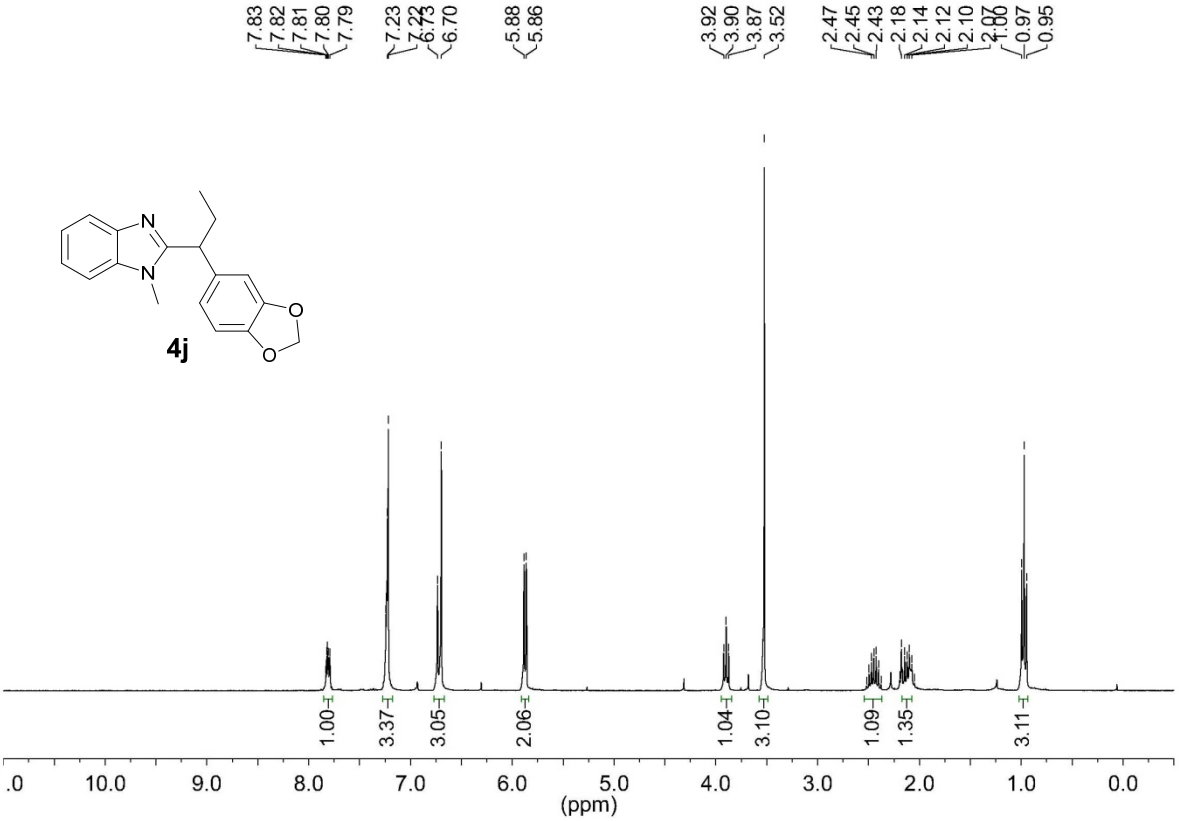
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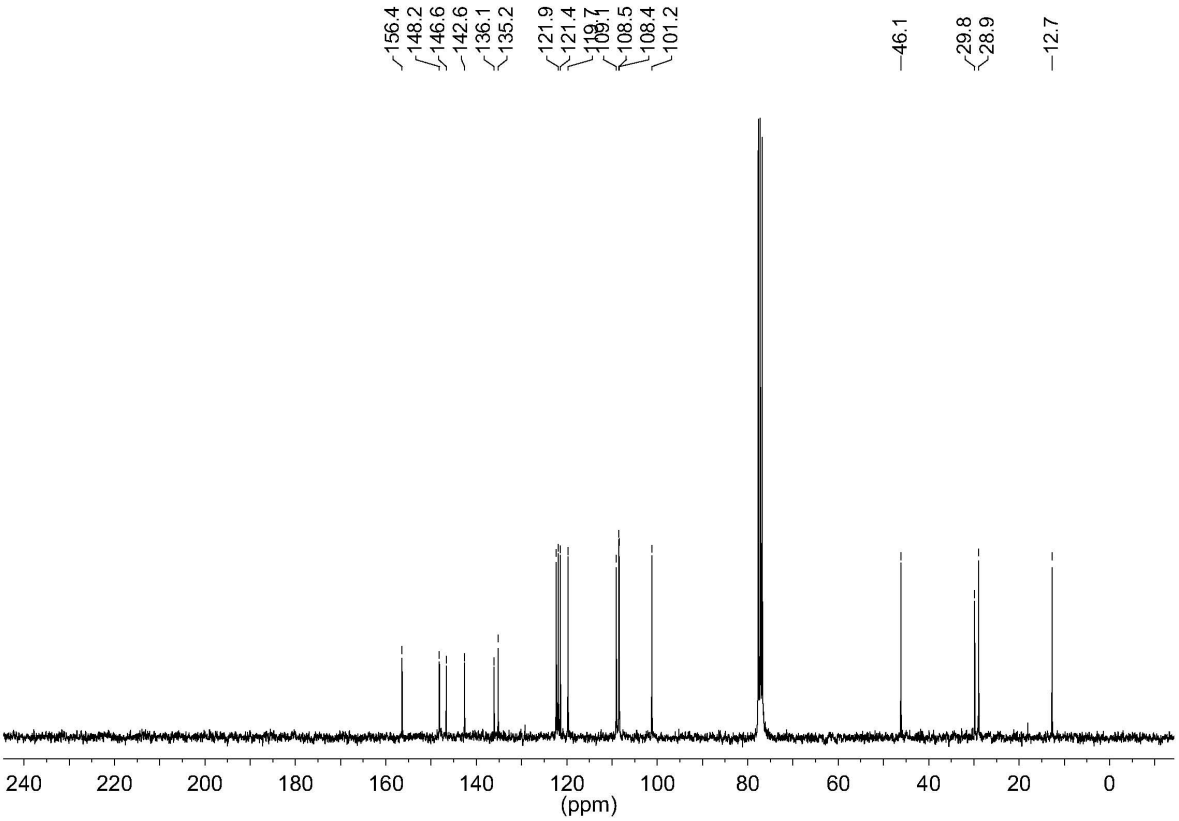
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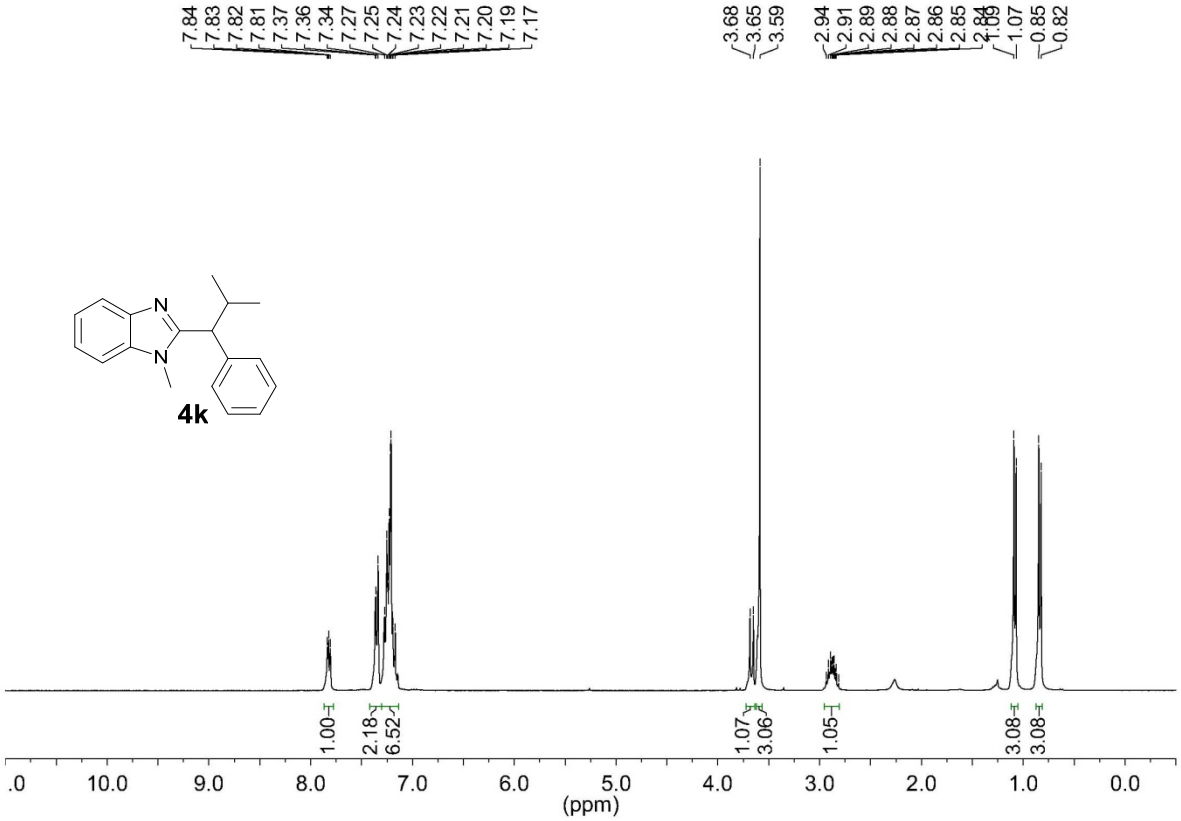
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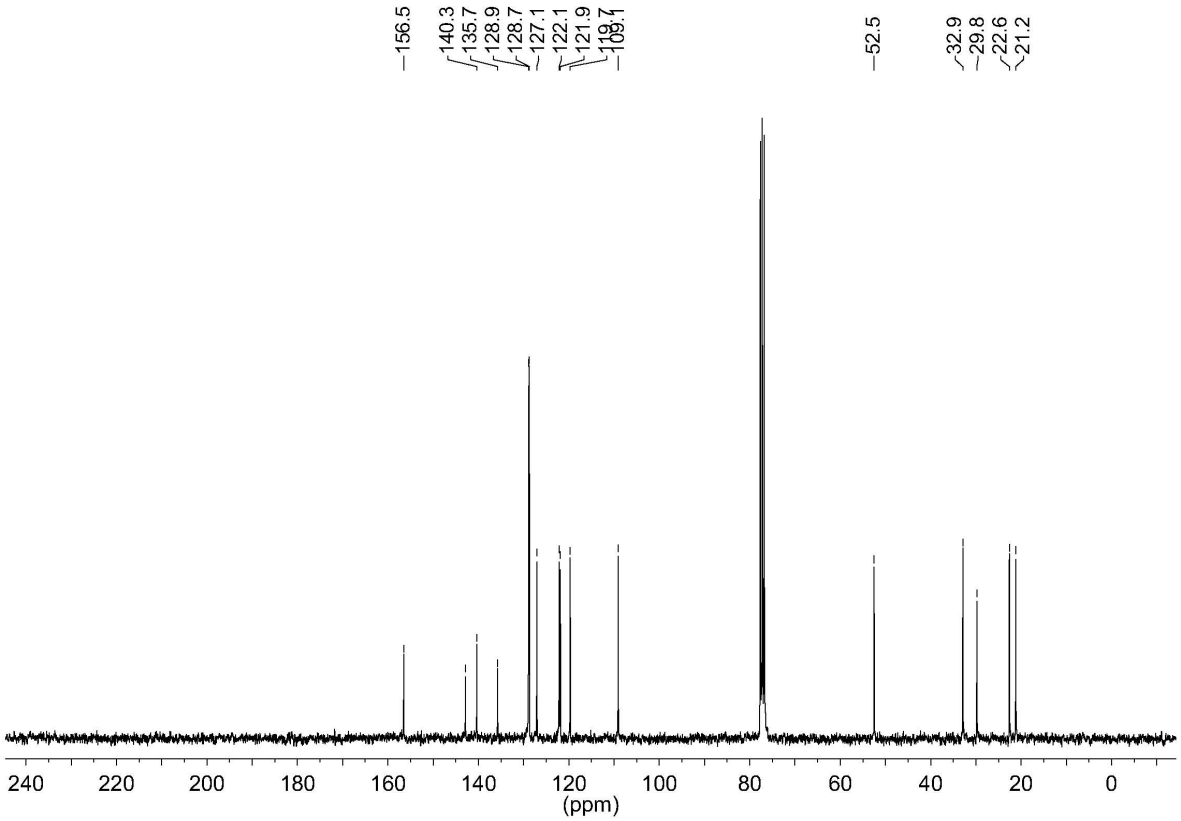
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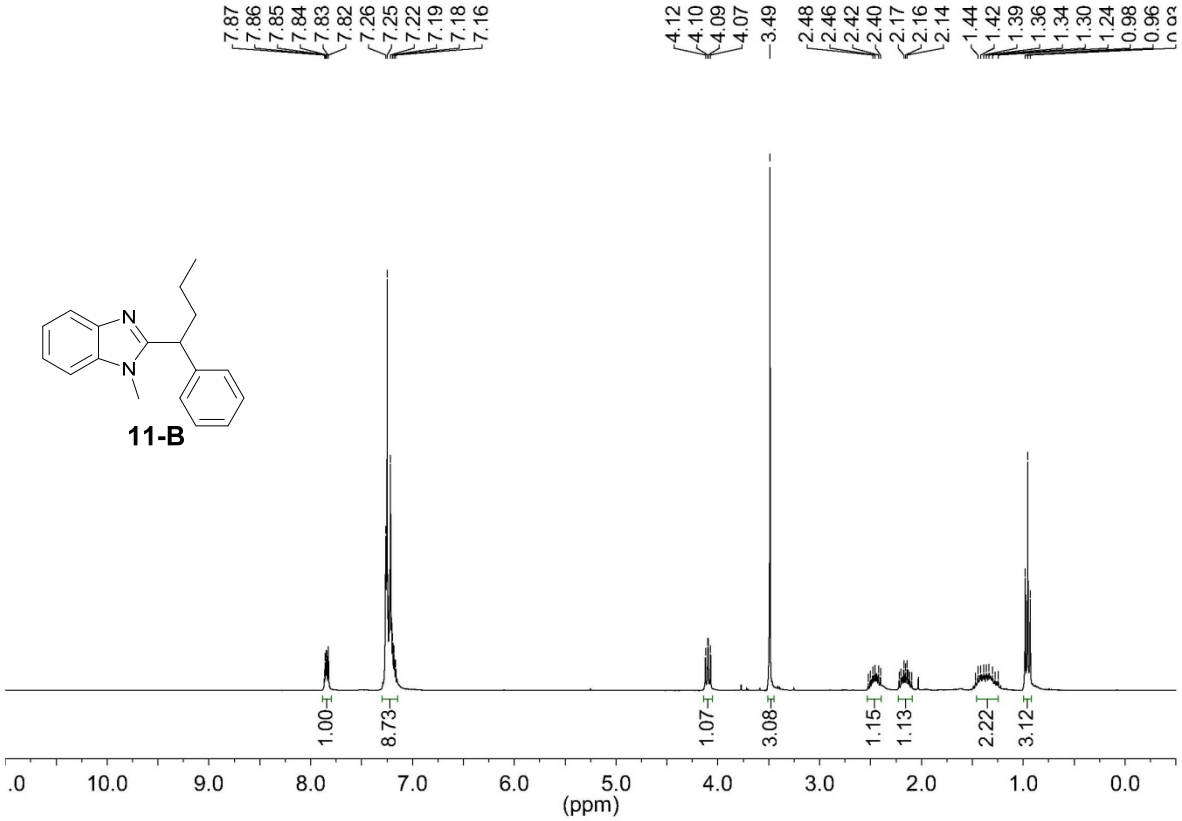
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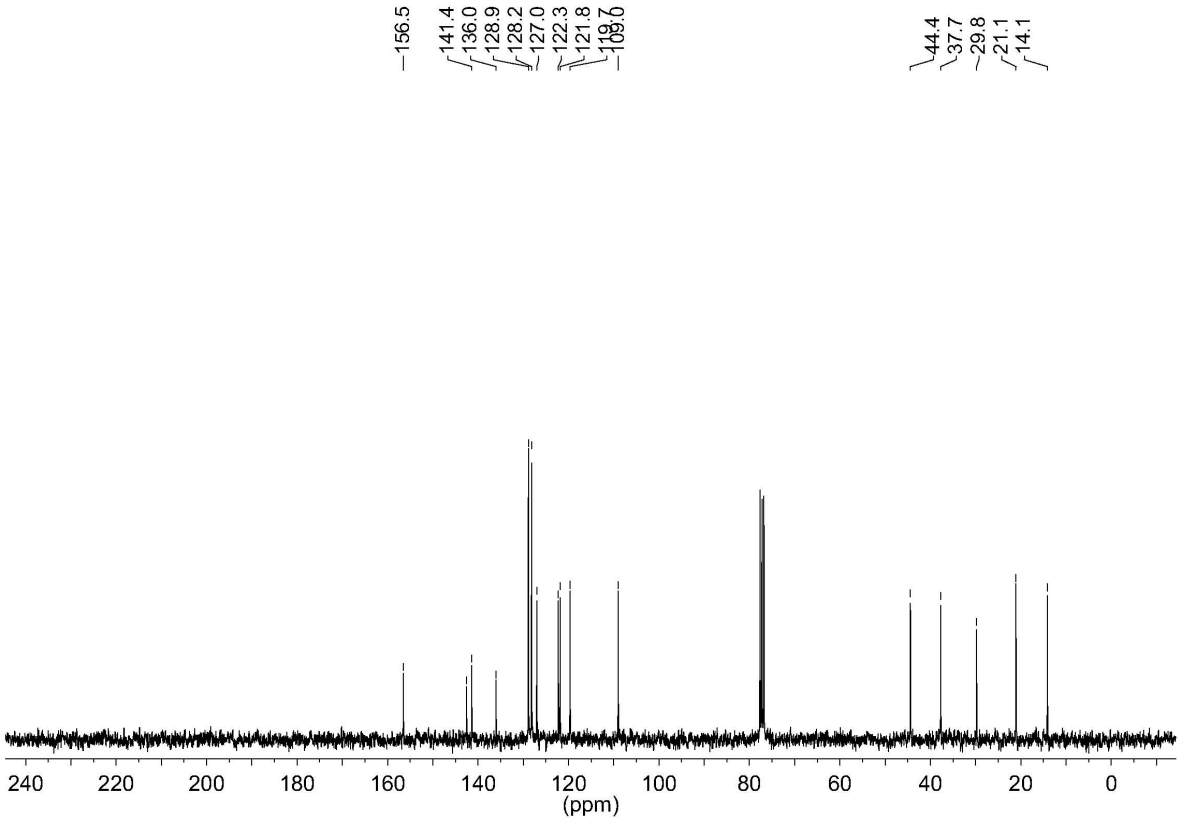
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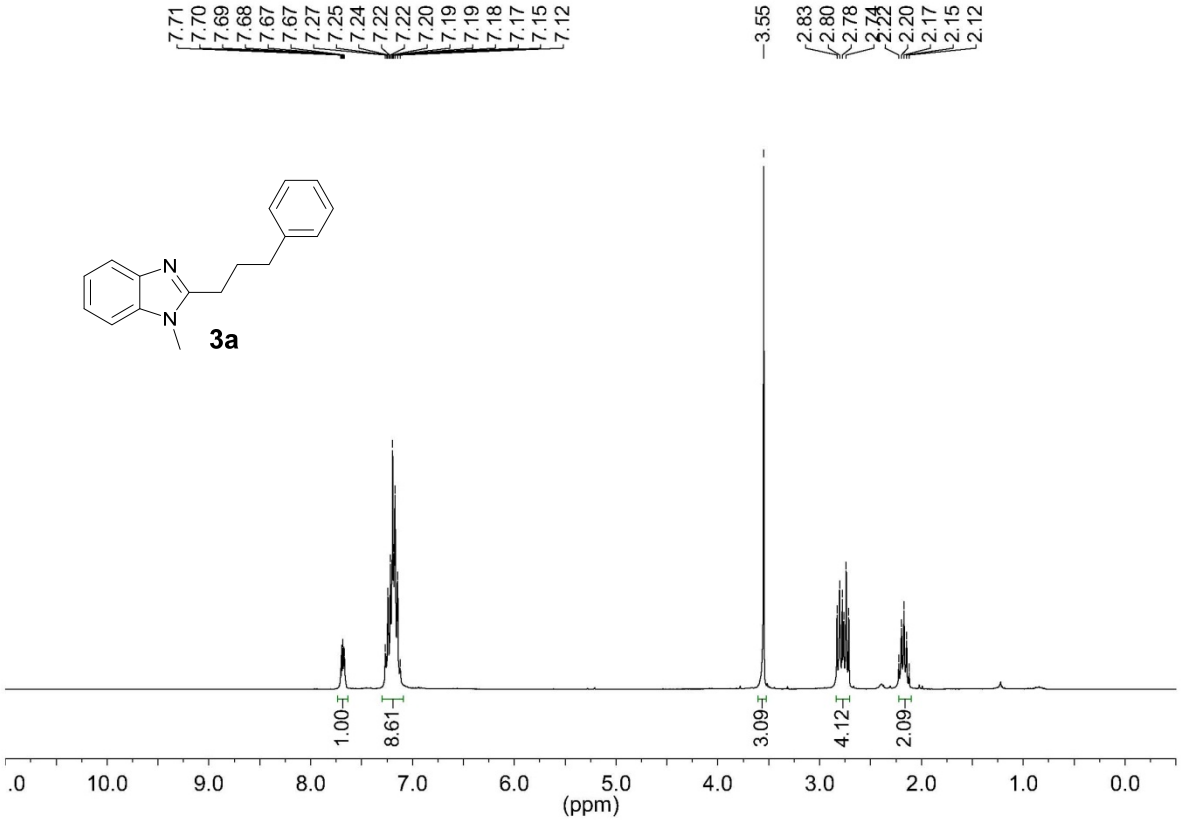
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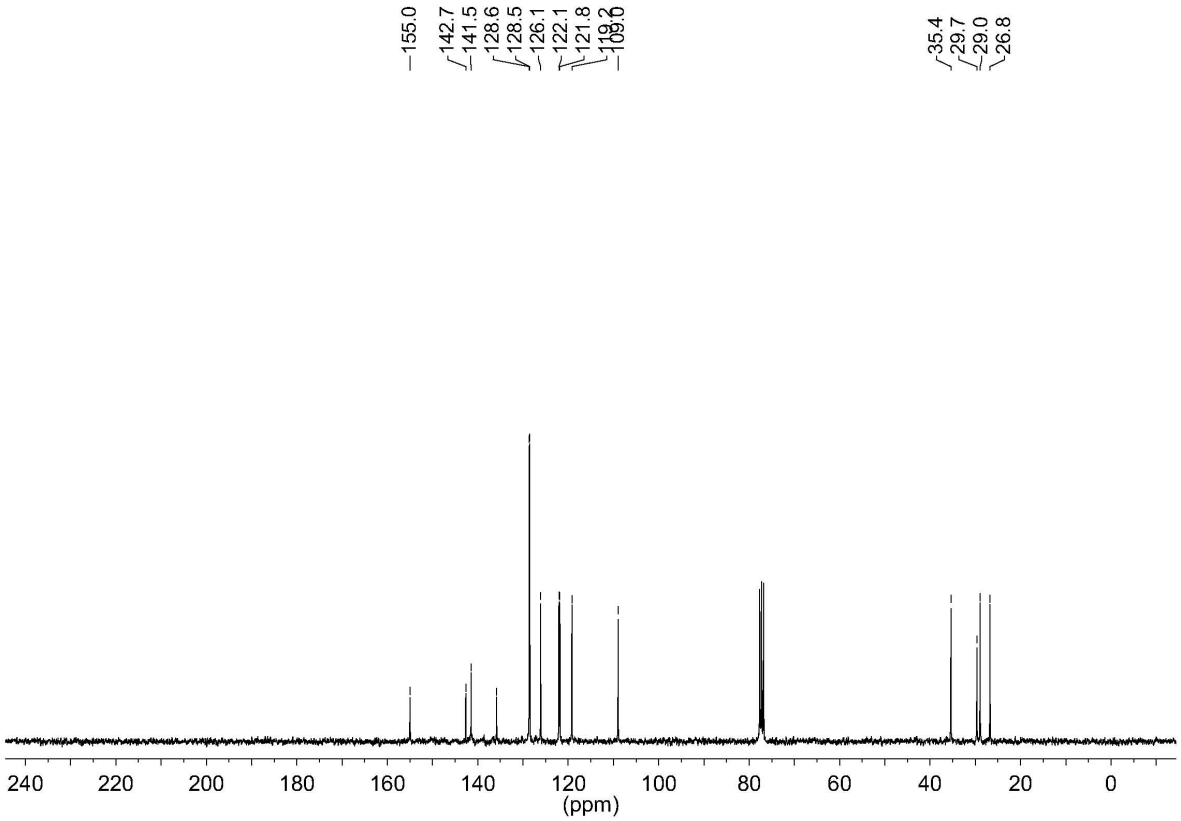
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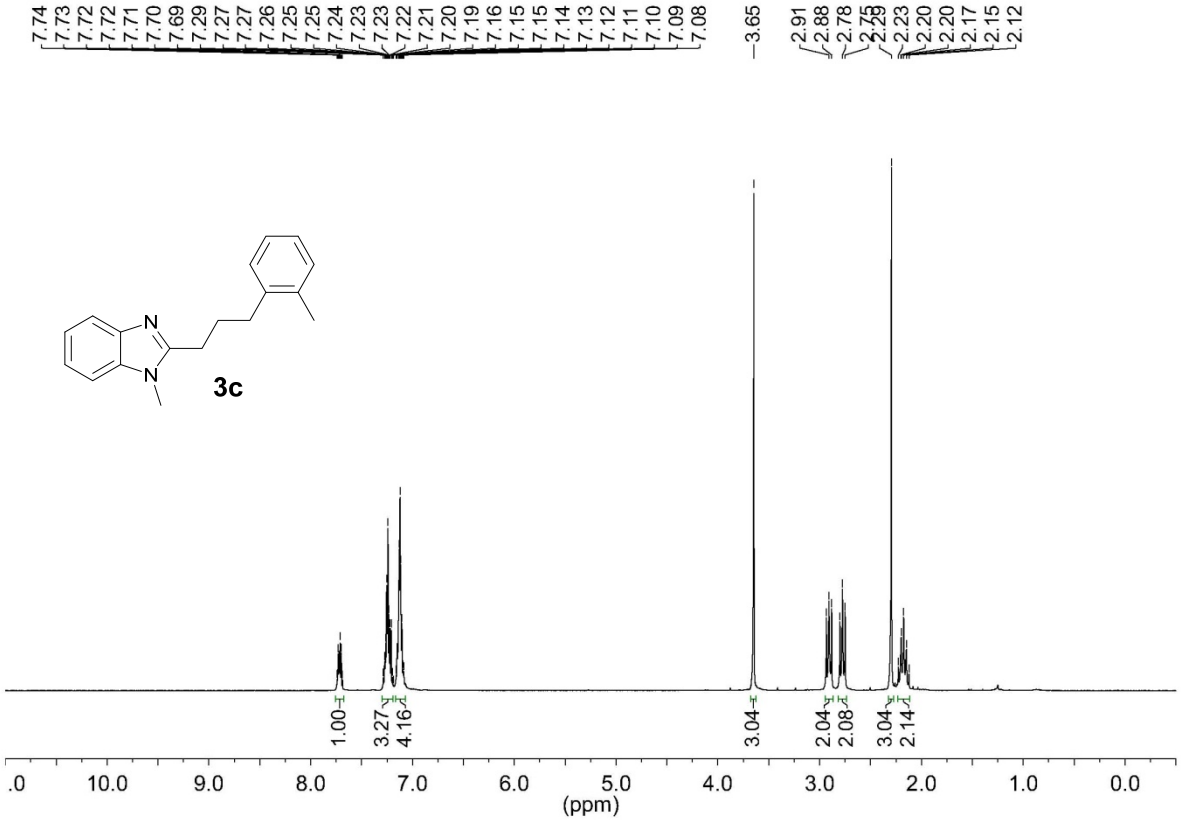
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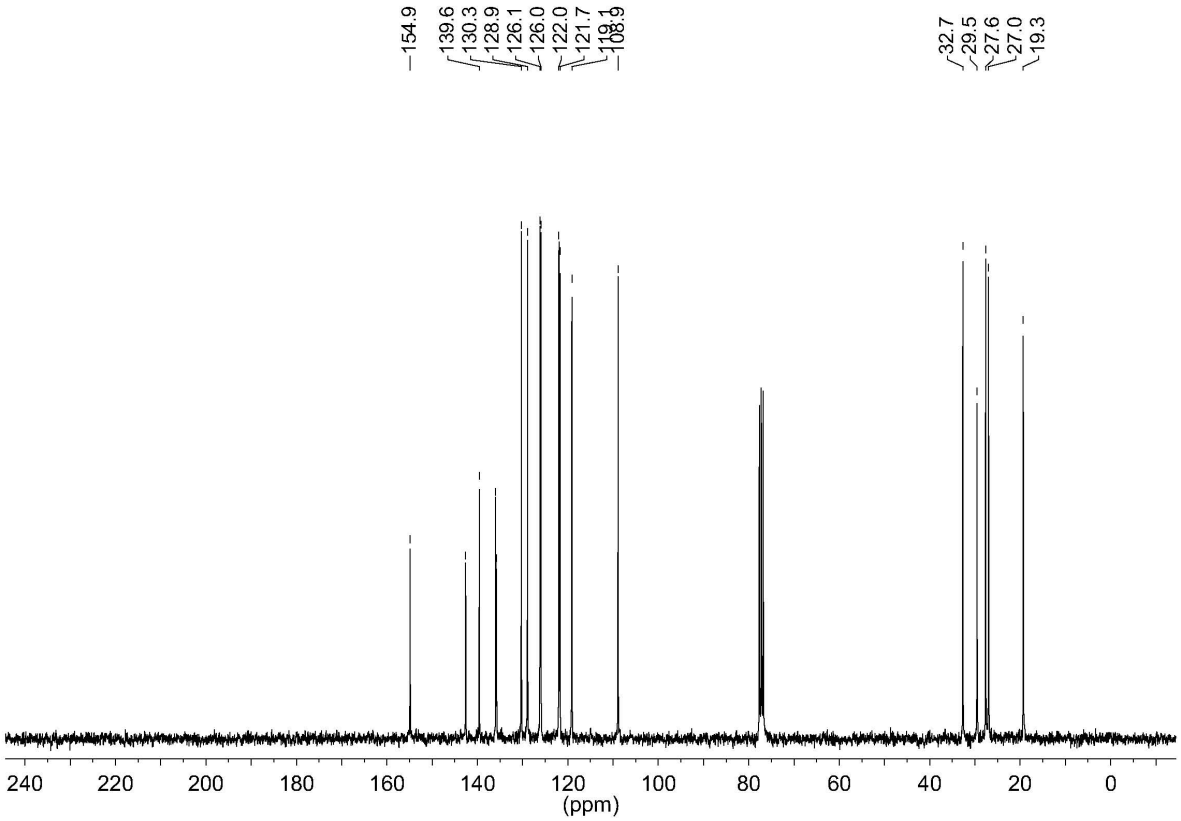
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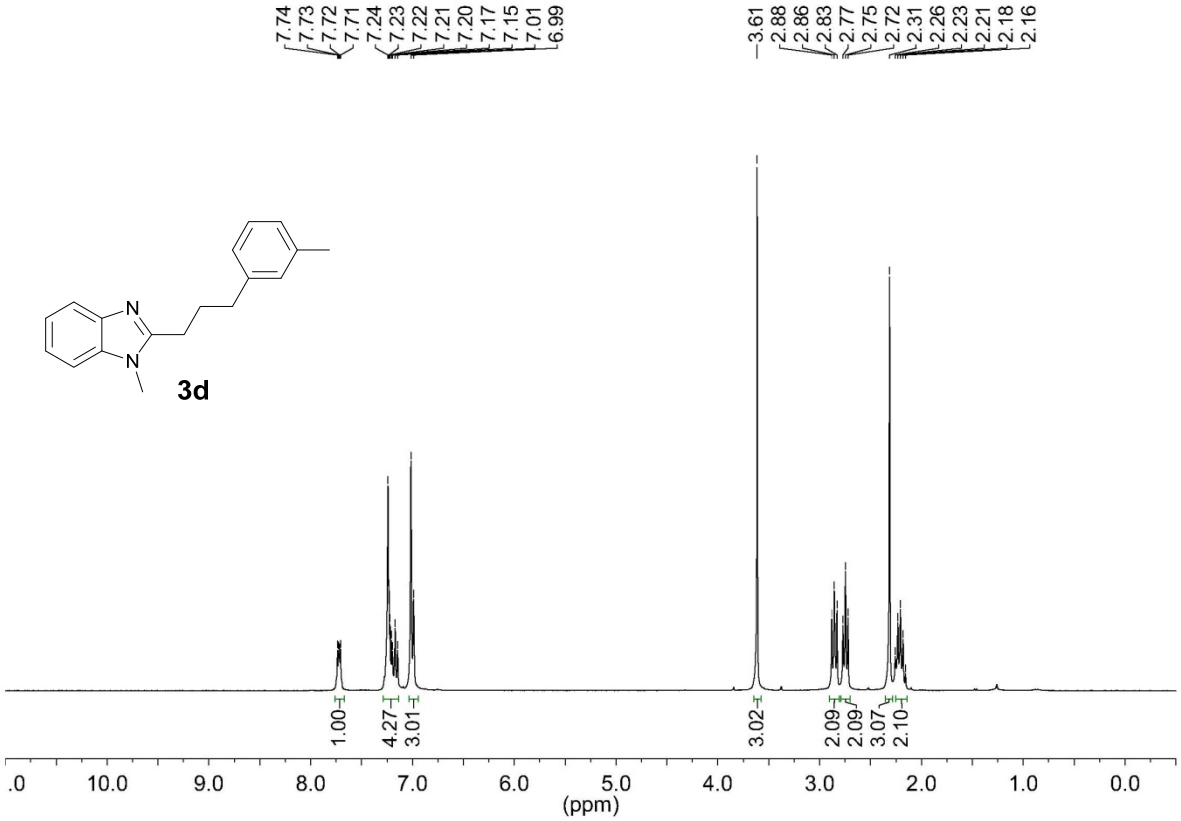
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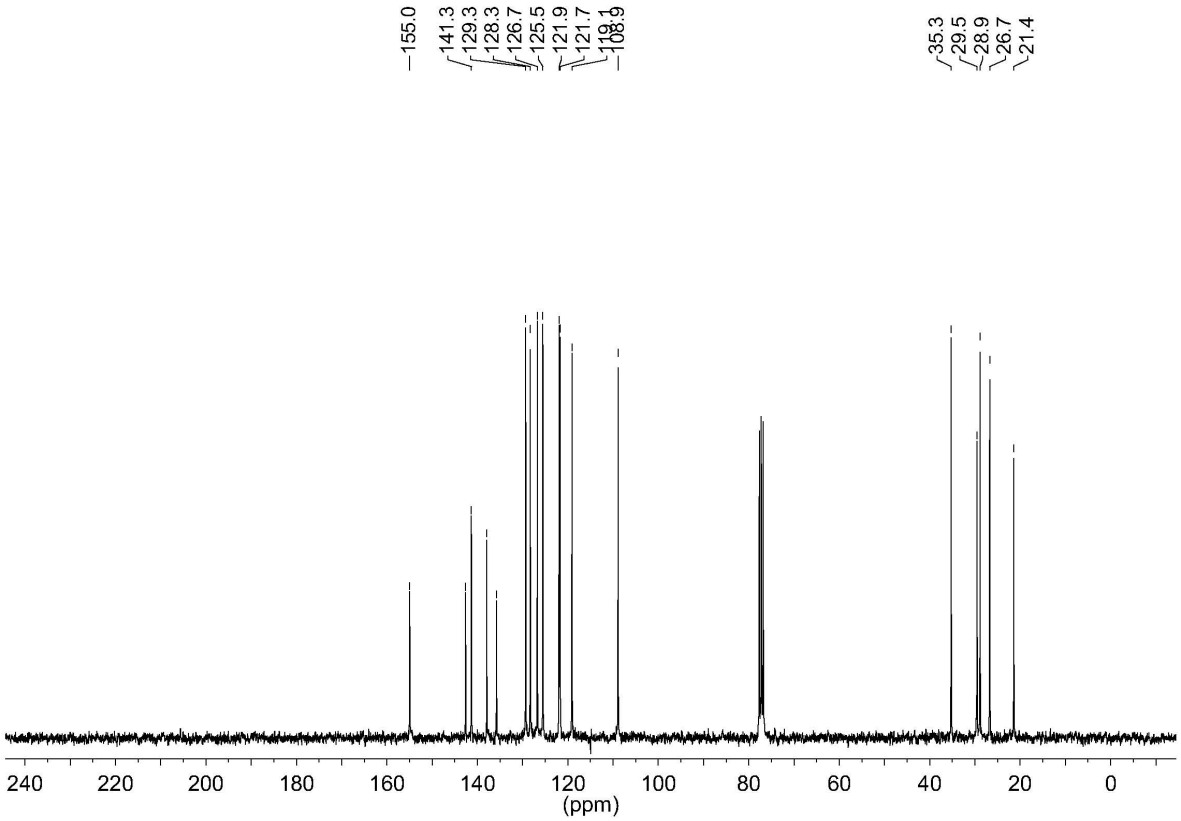
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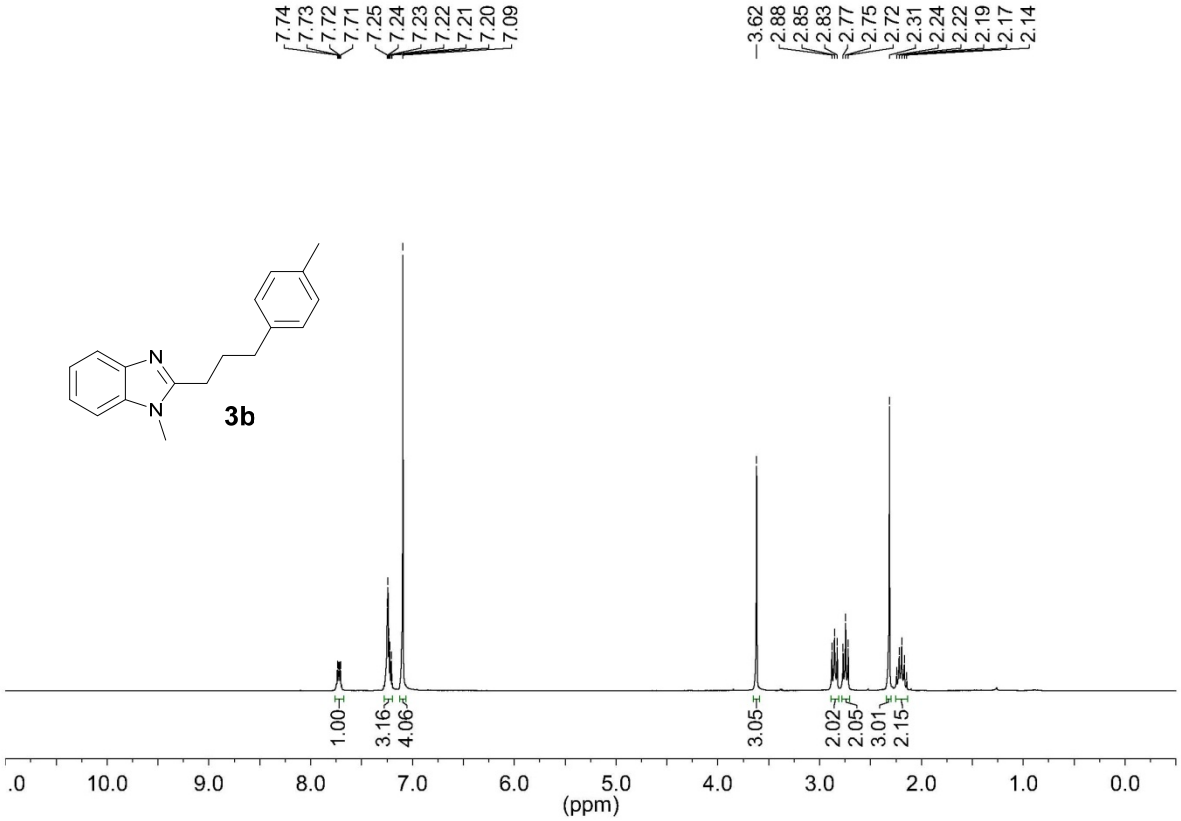
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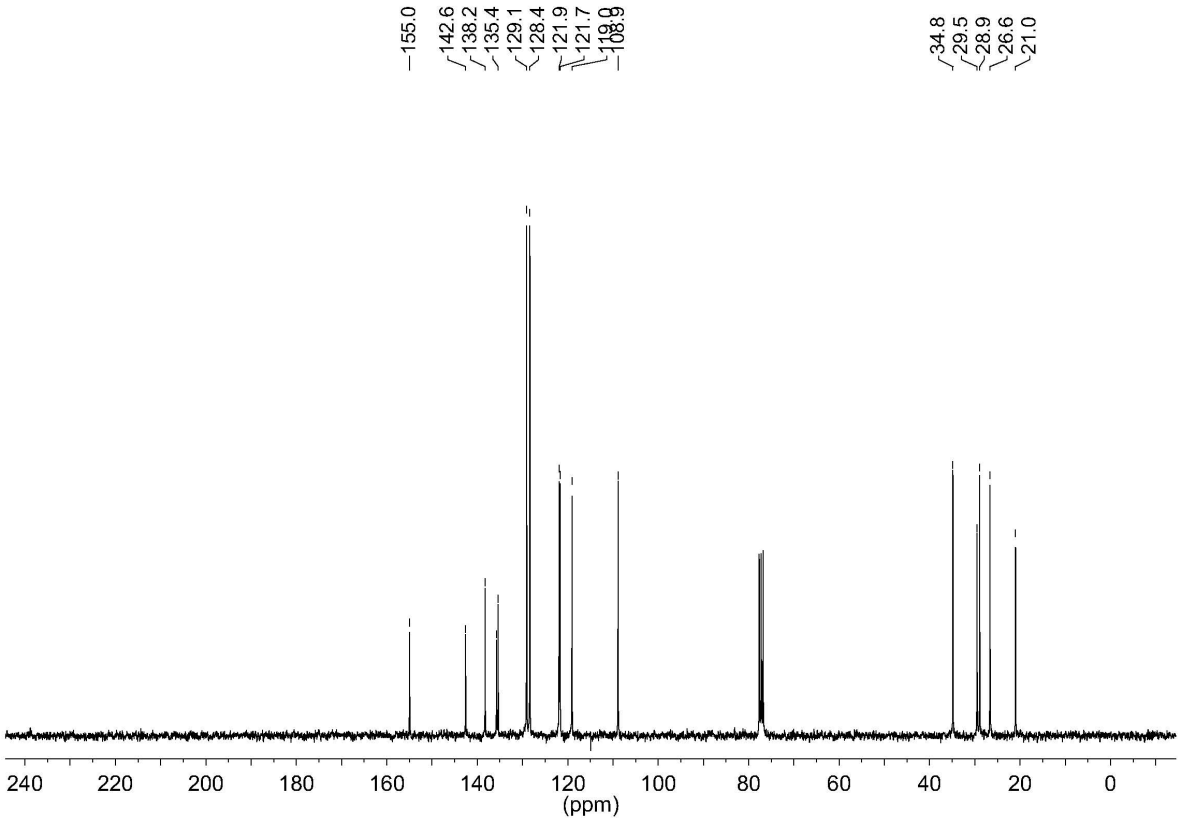
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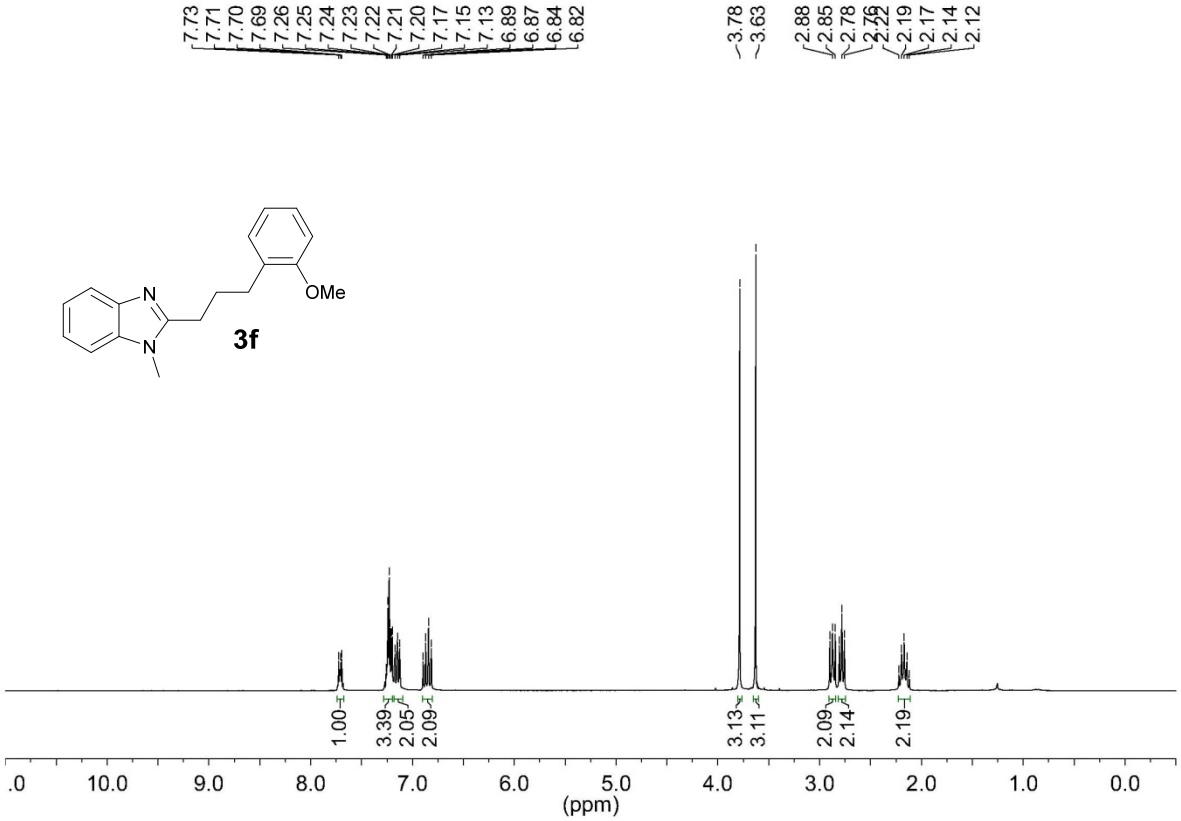
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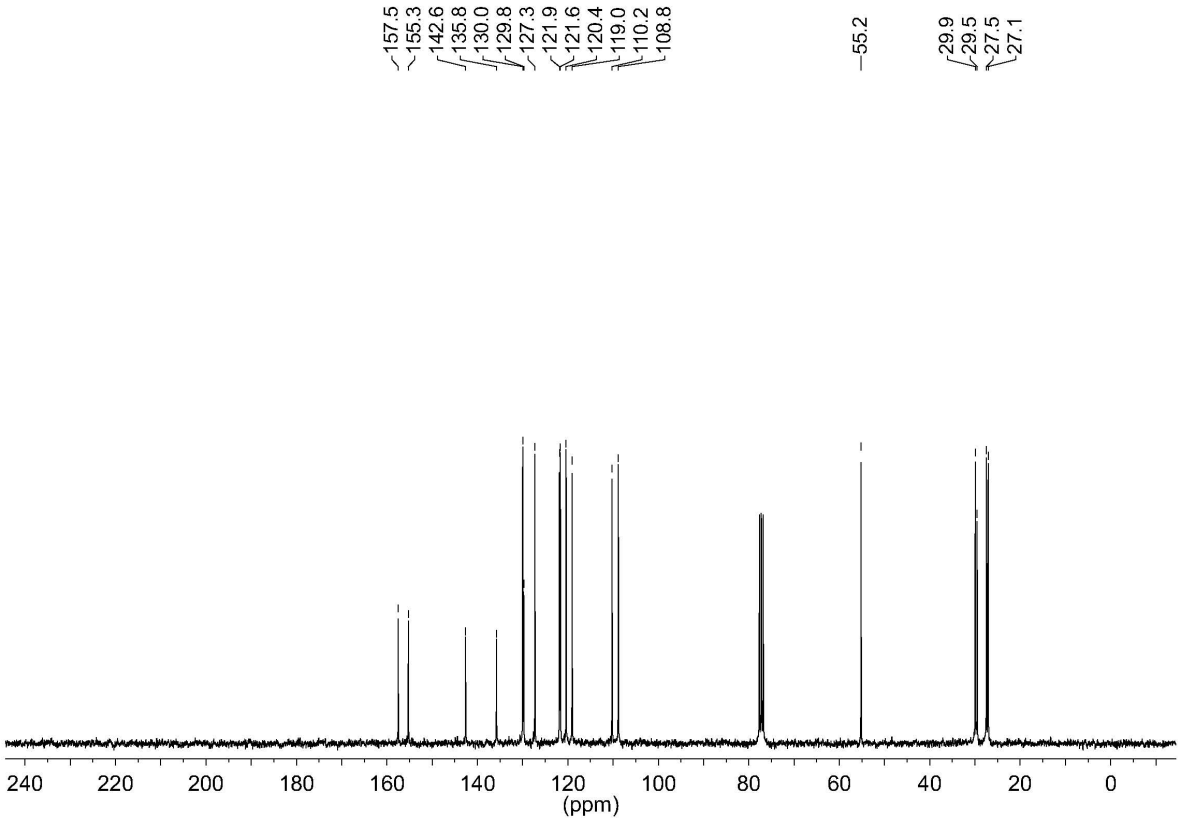
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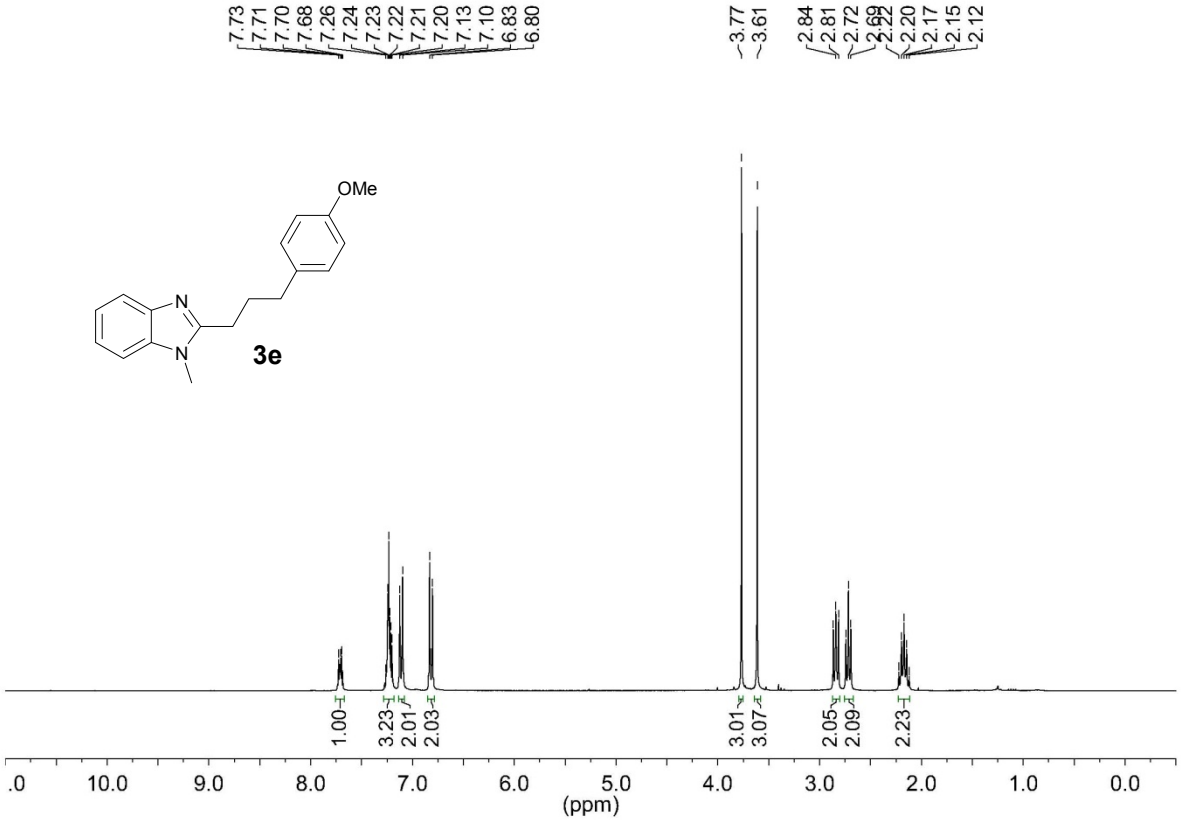
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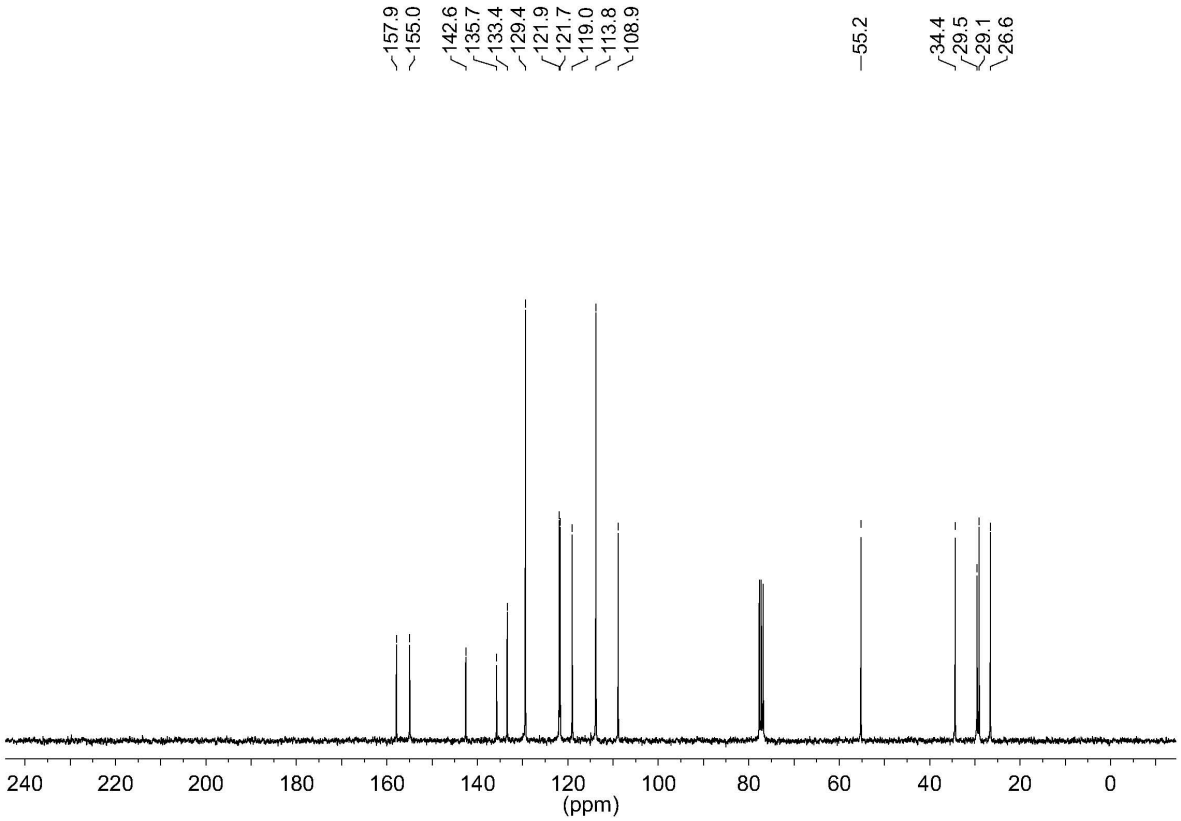
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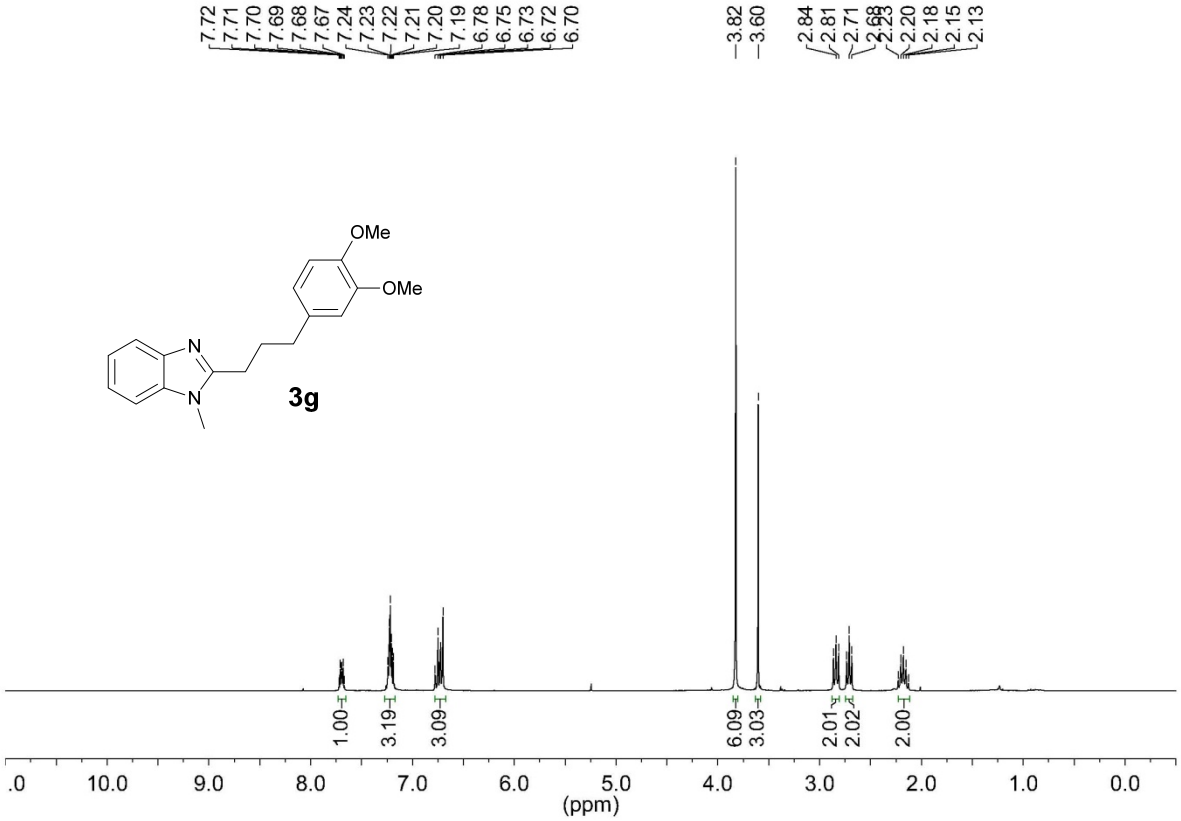
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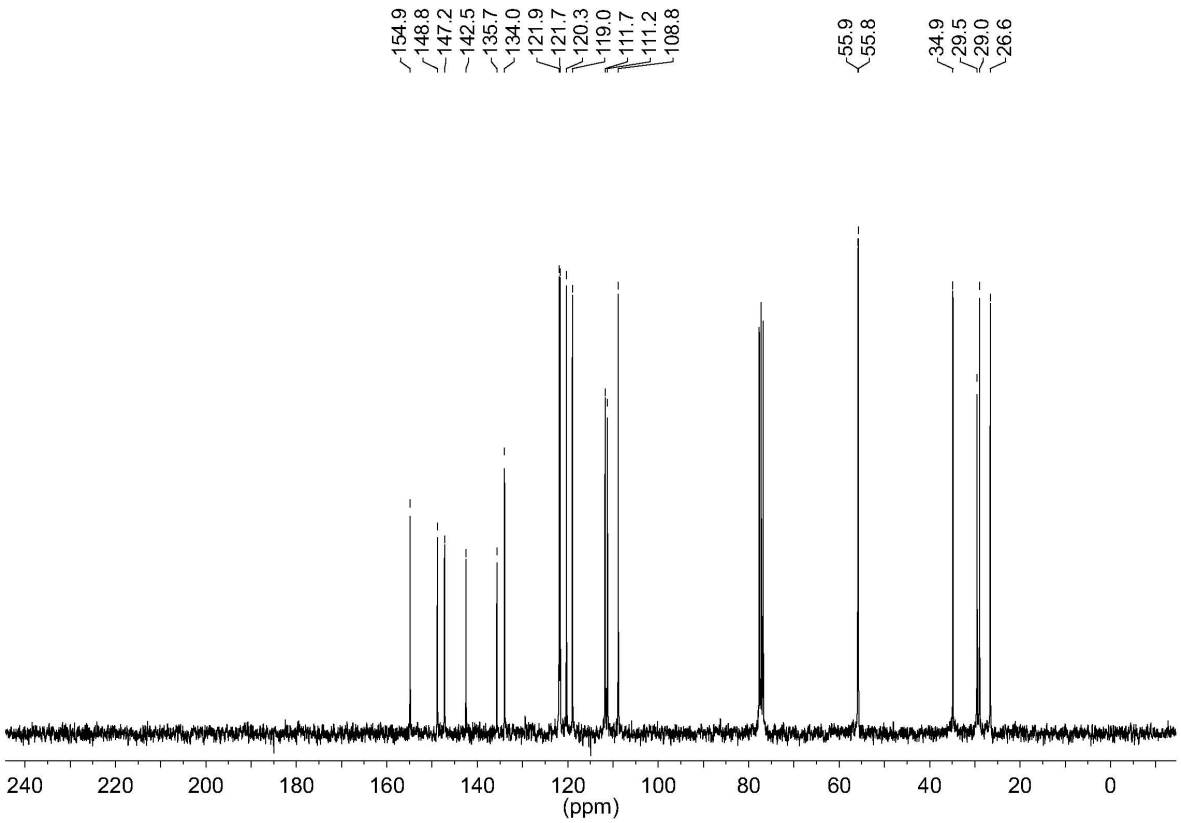
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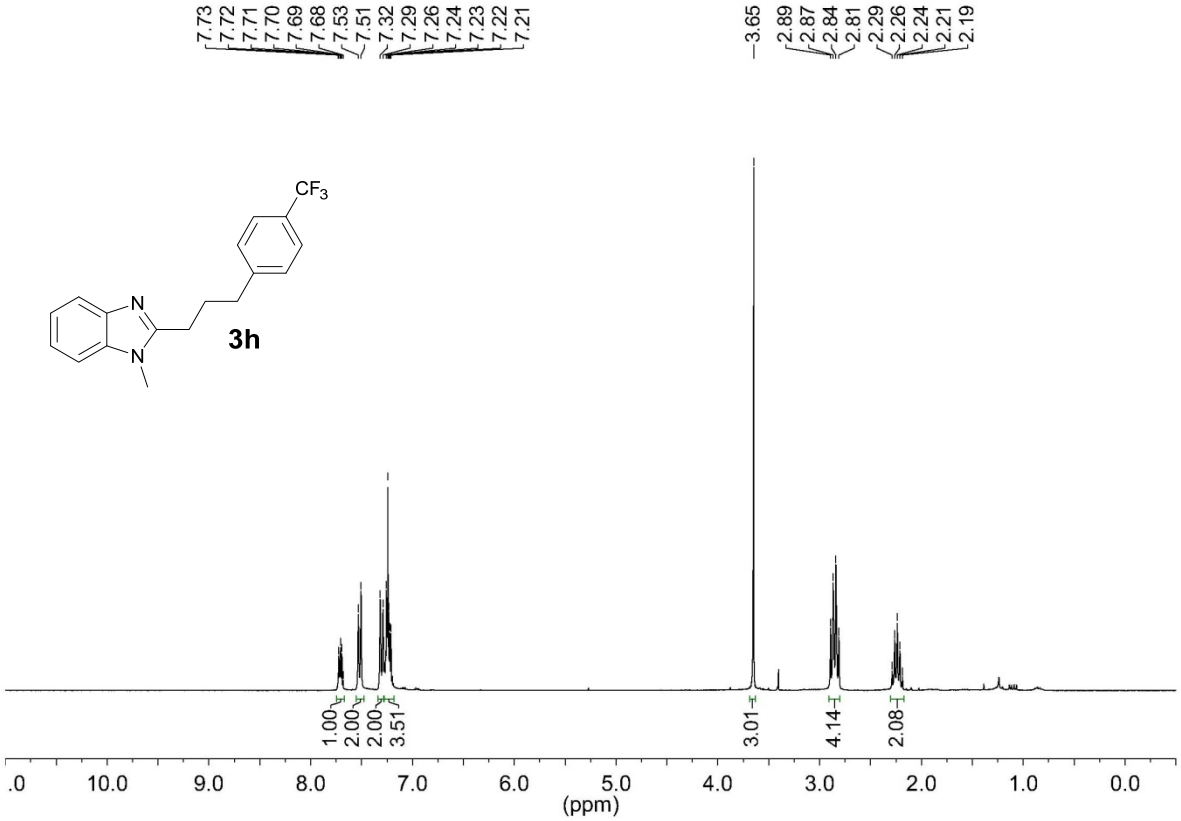
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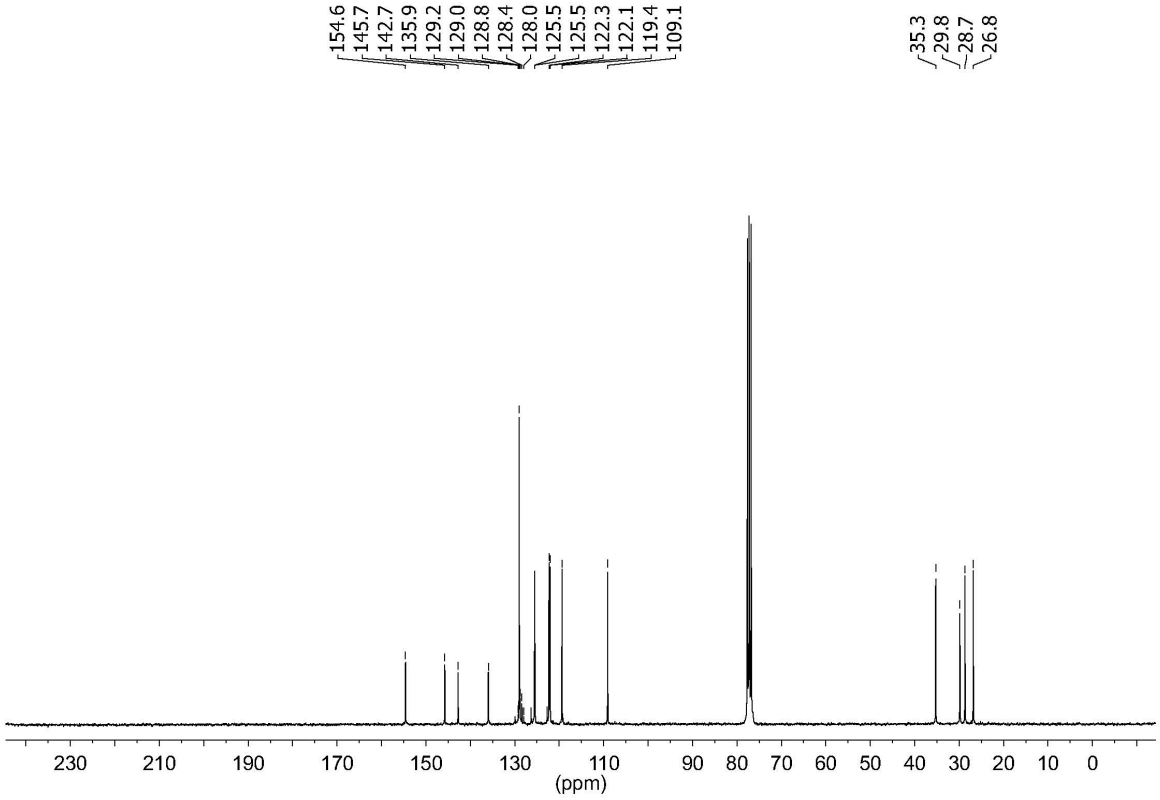
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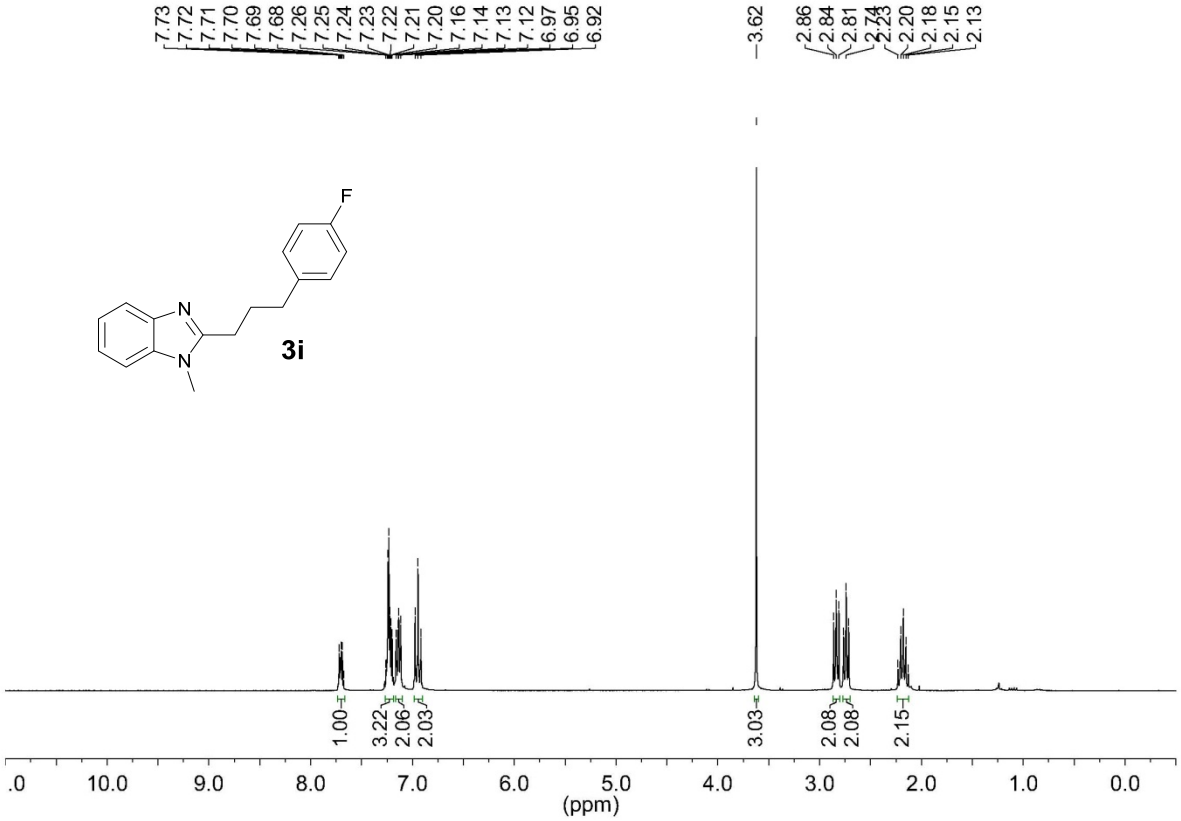
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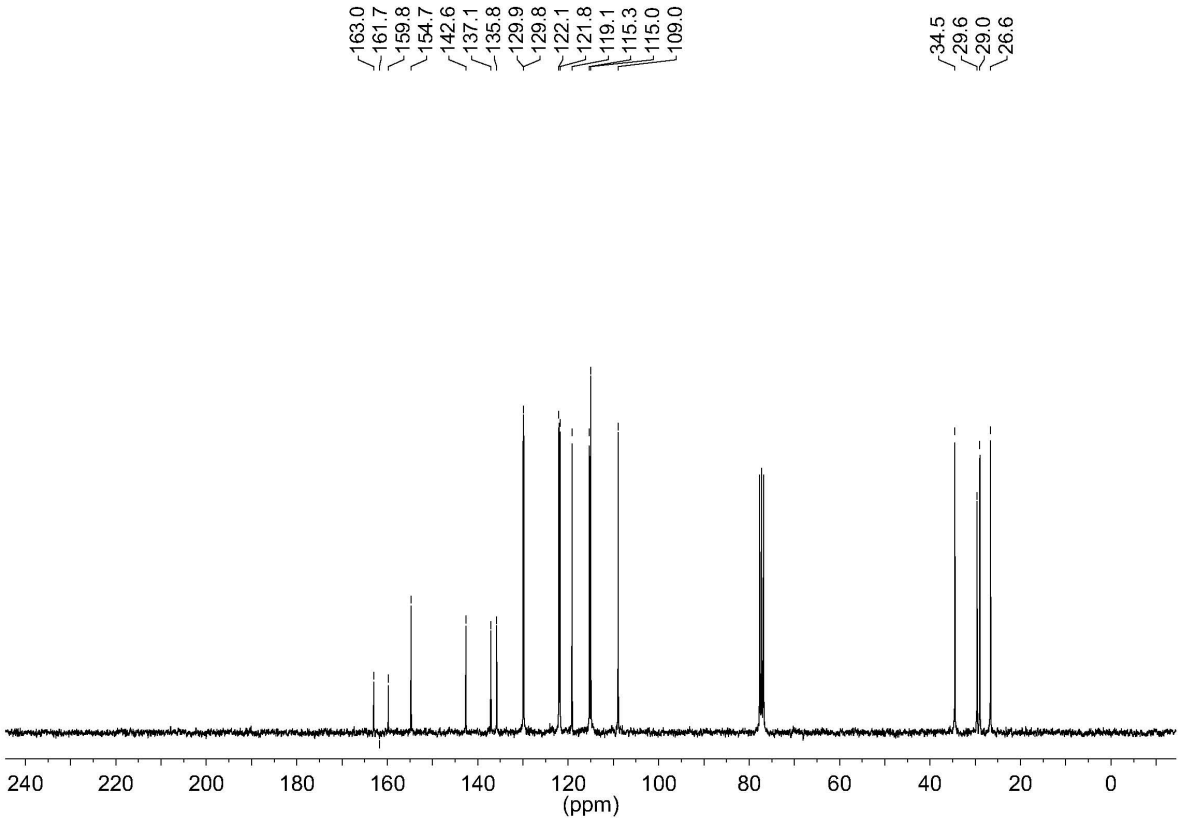
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121.8
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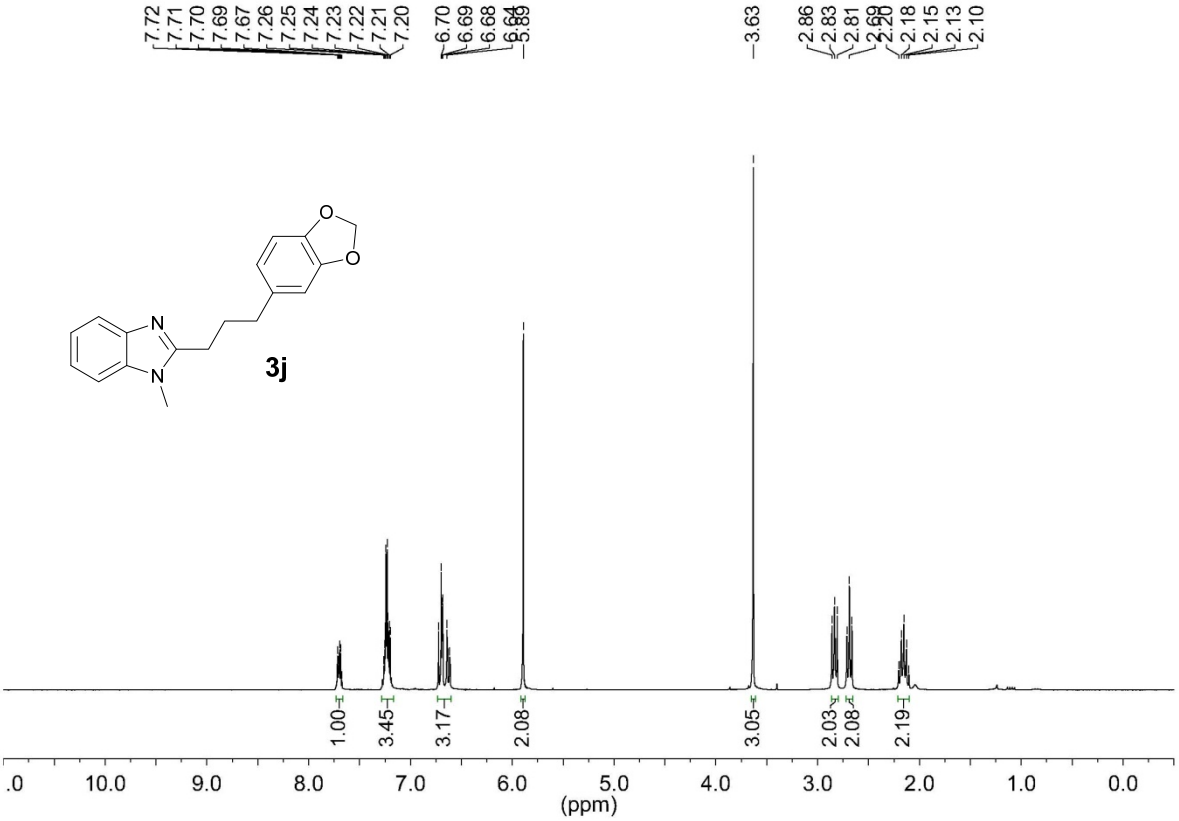
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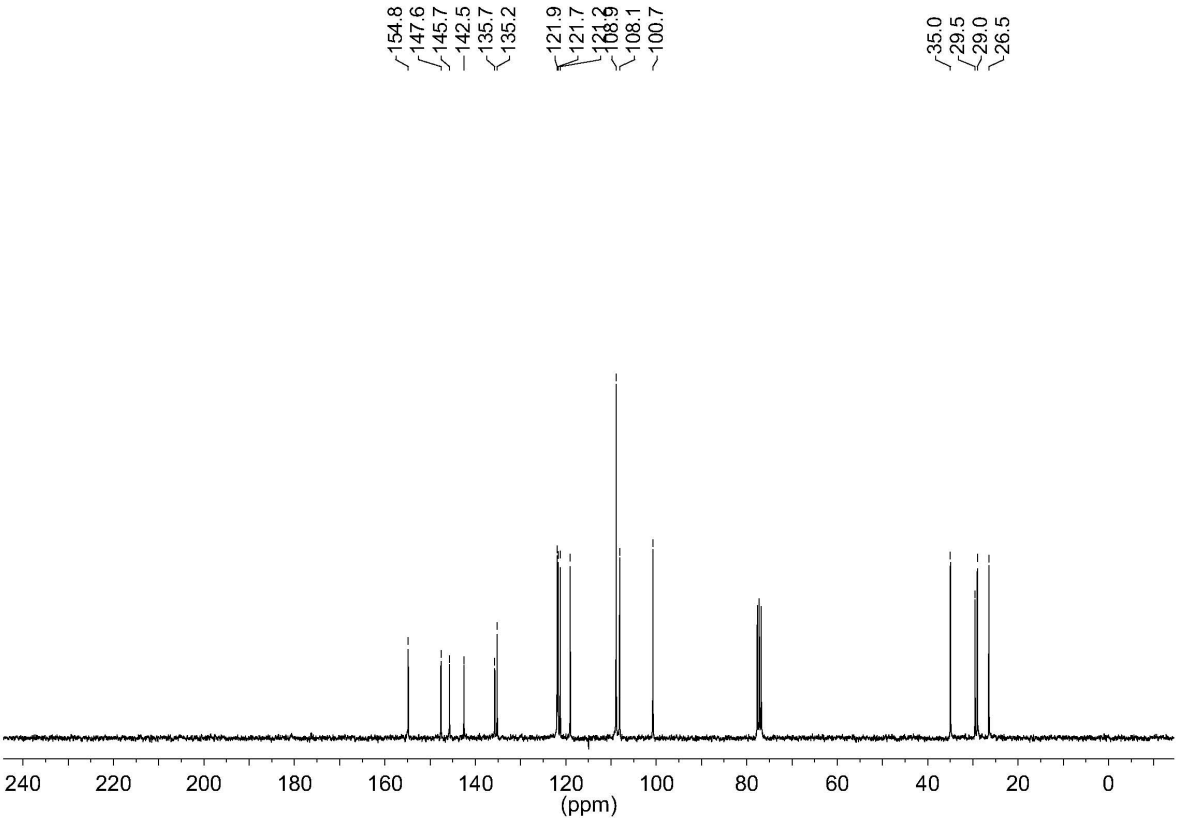
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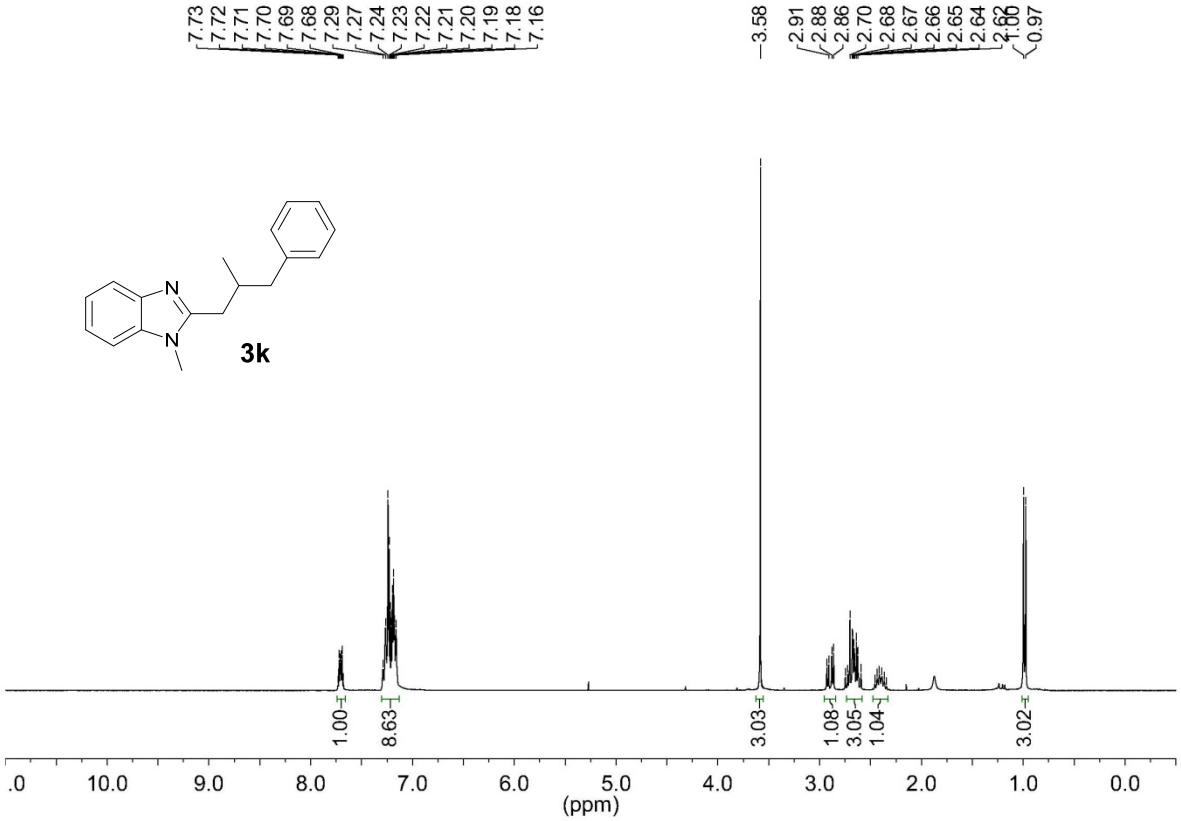
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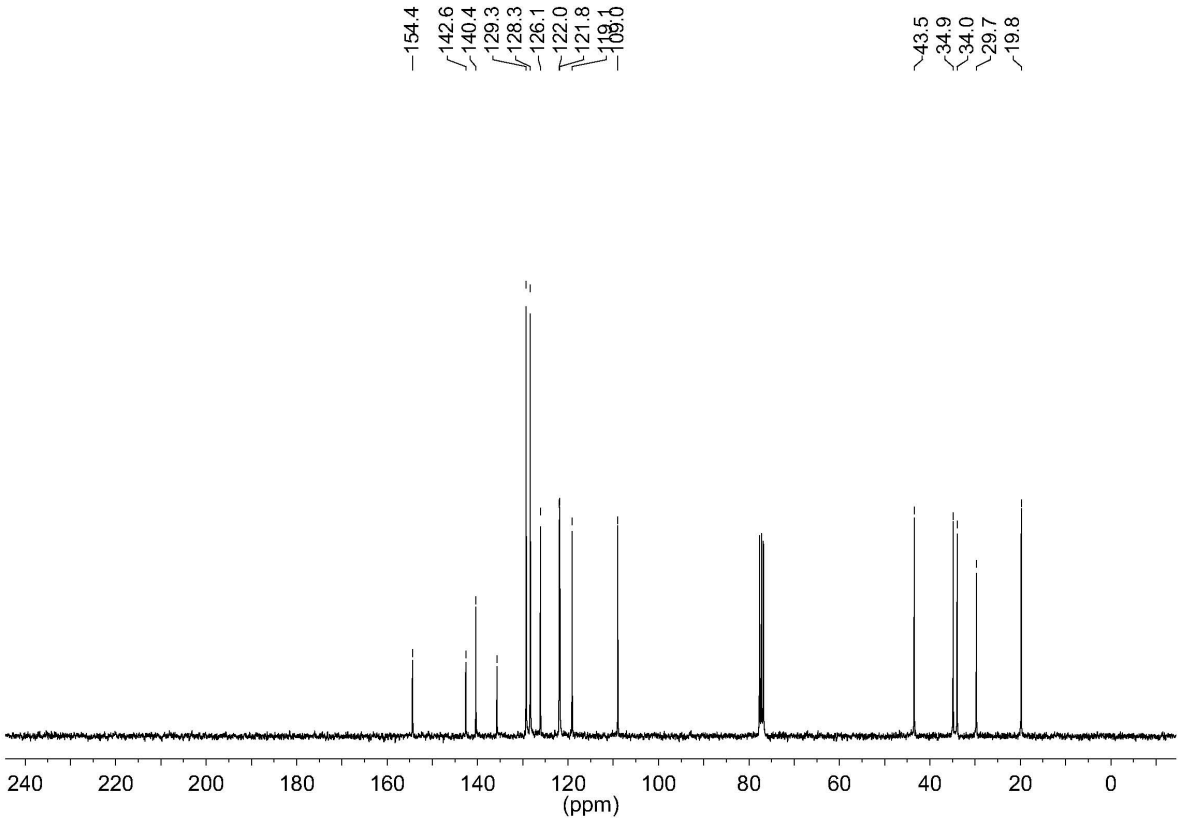
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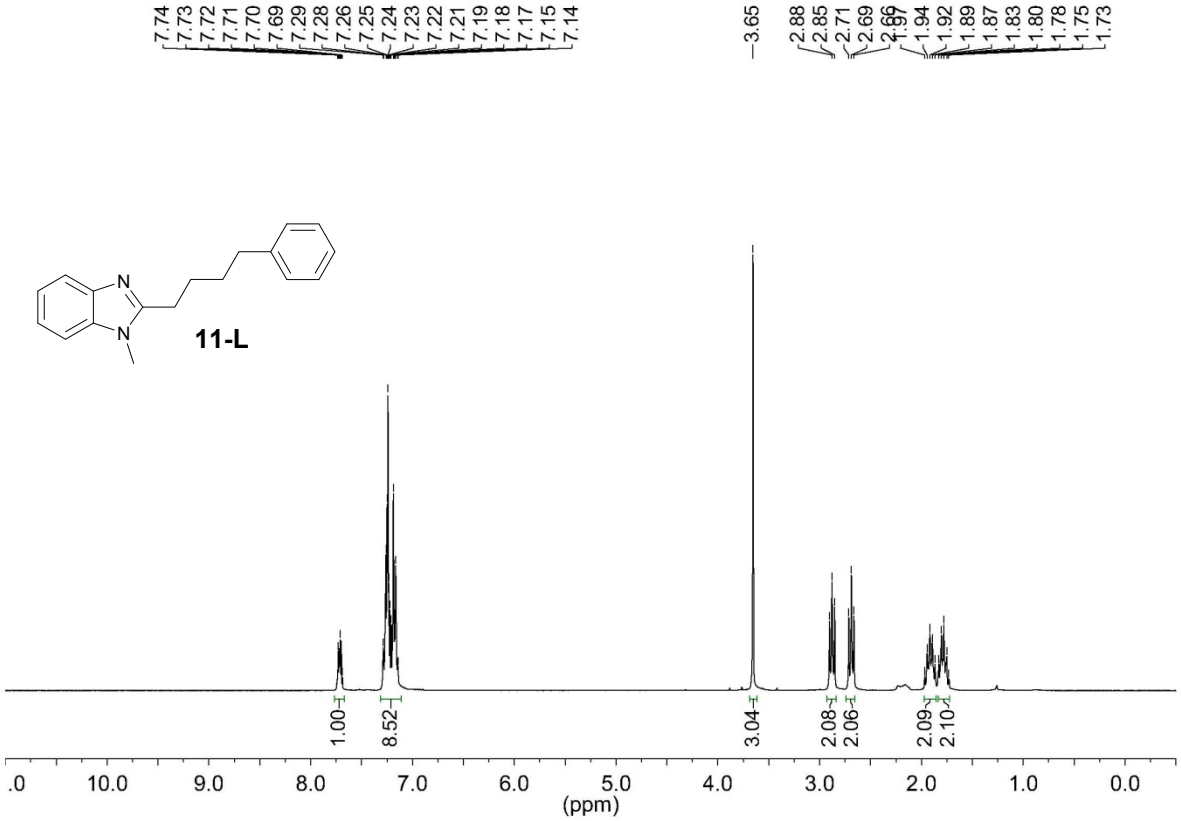
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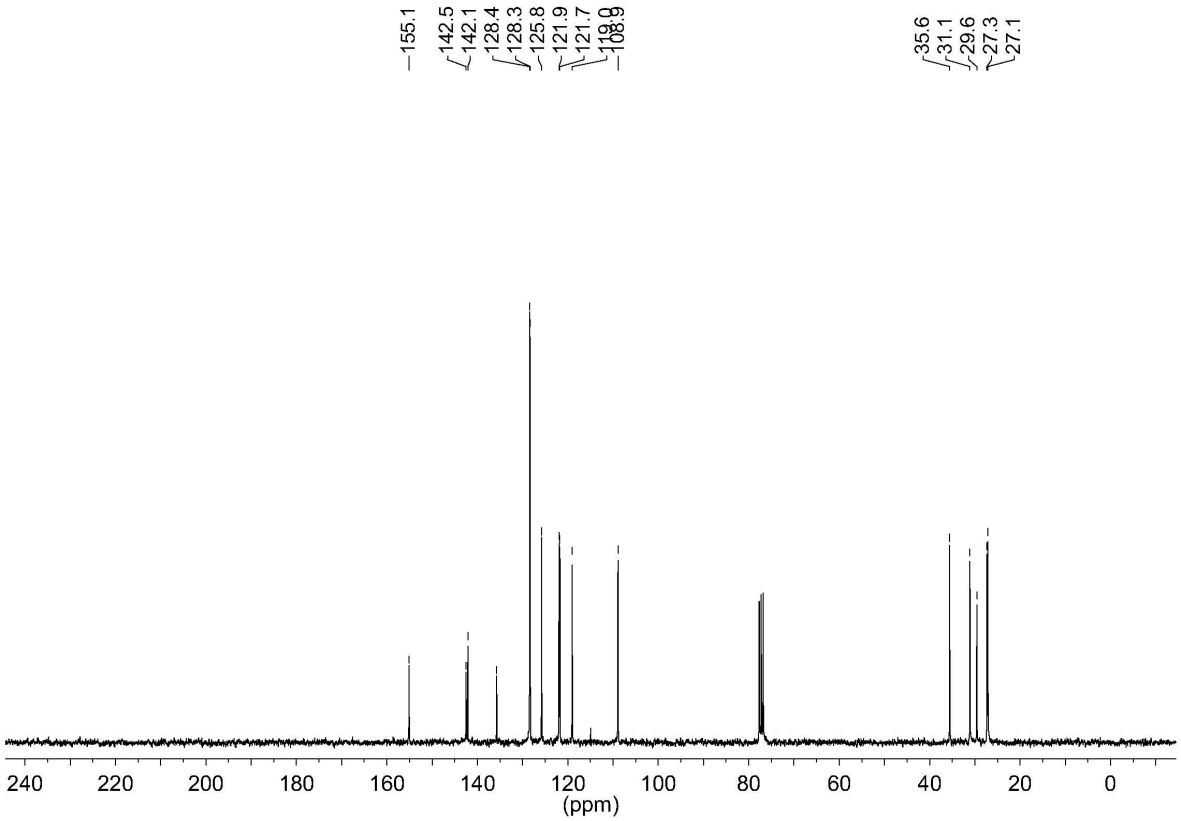
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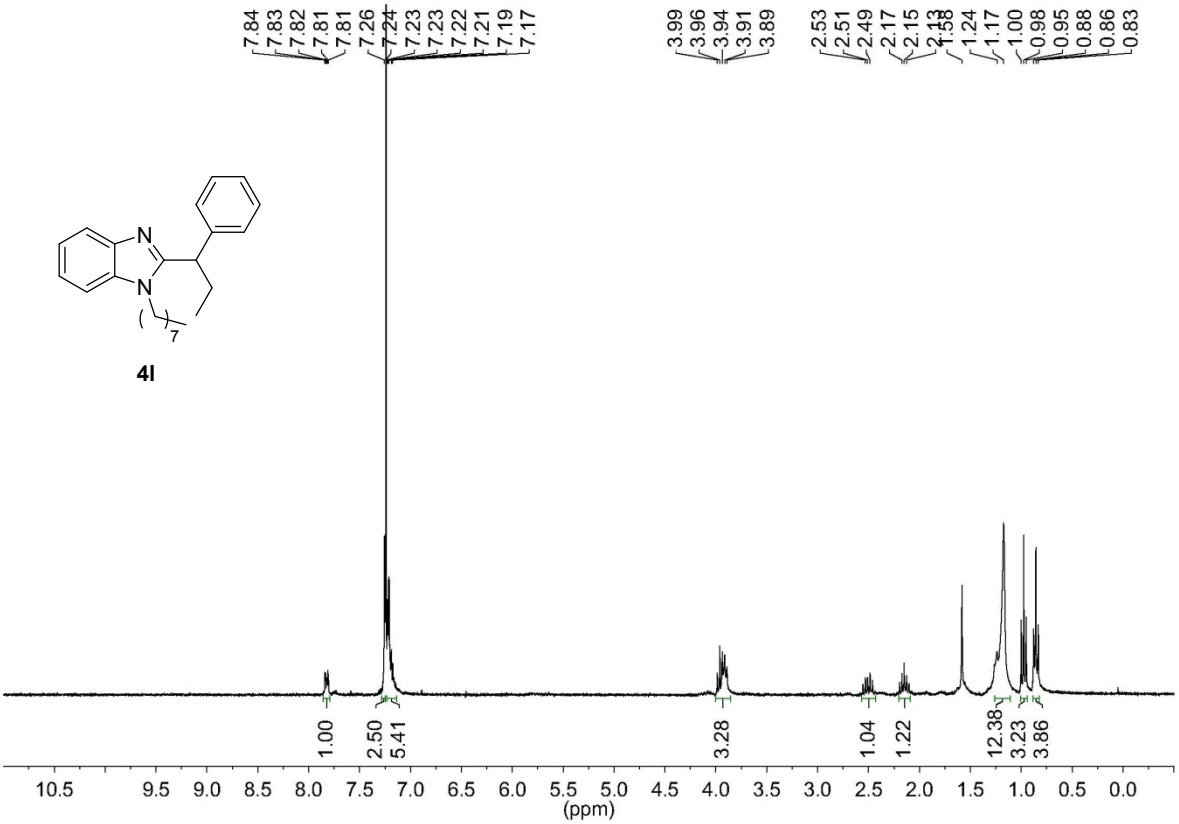
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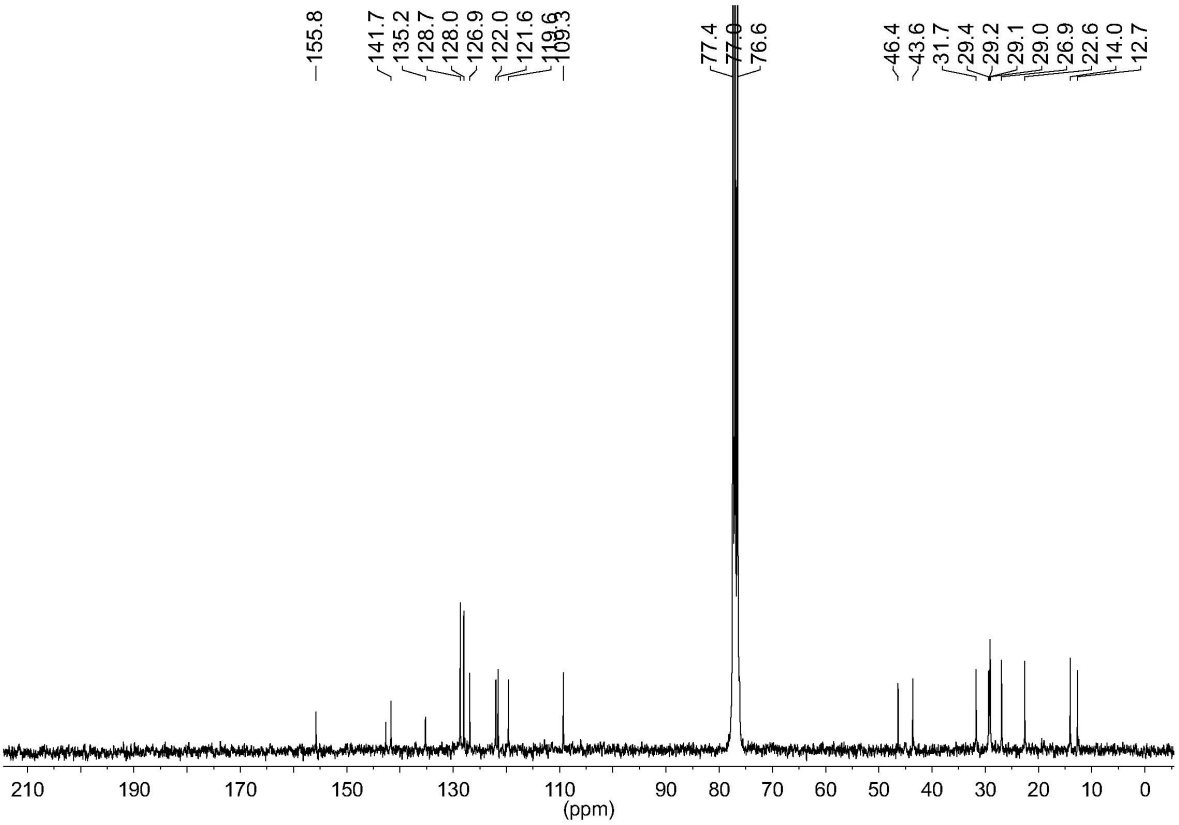
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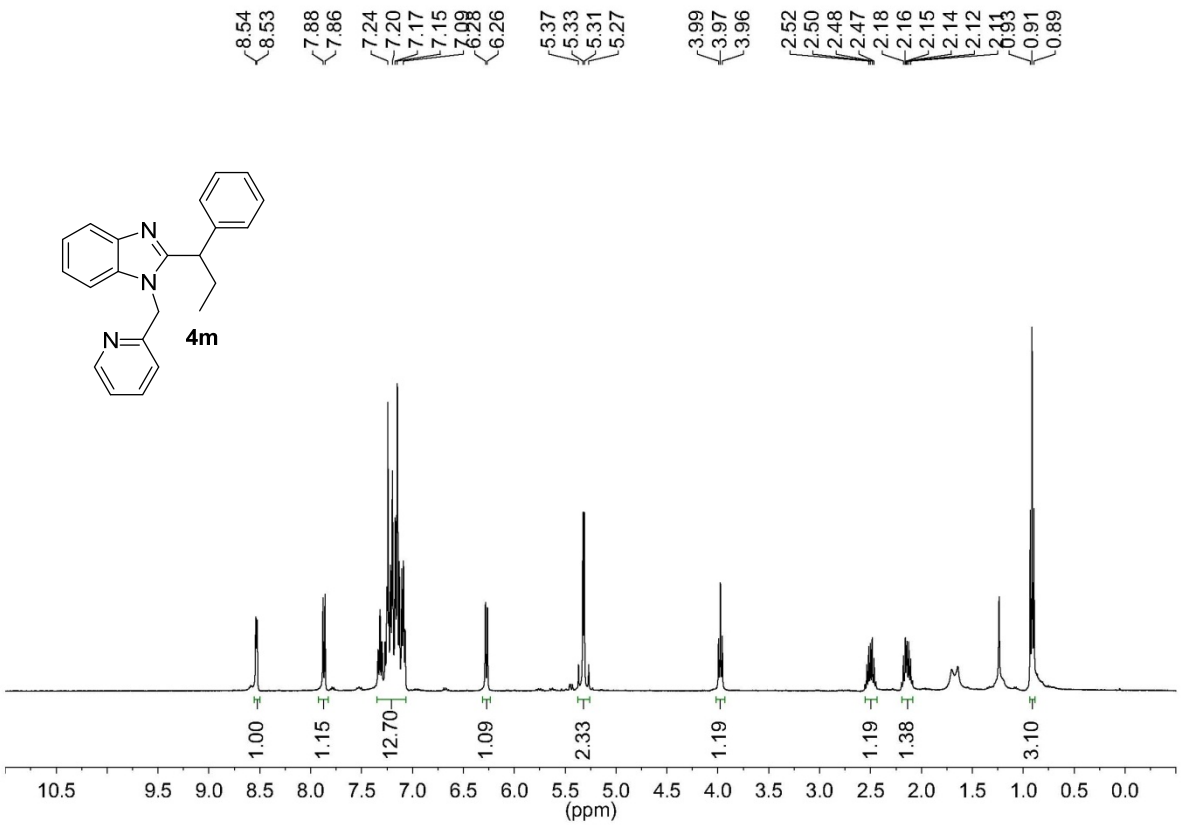
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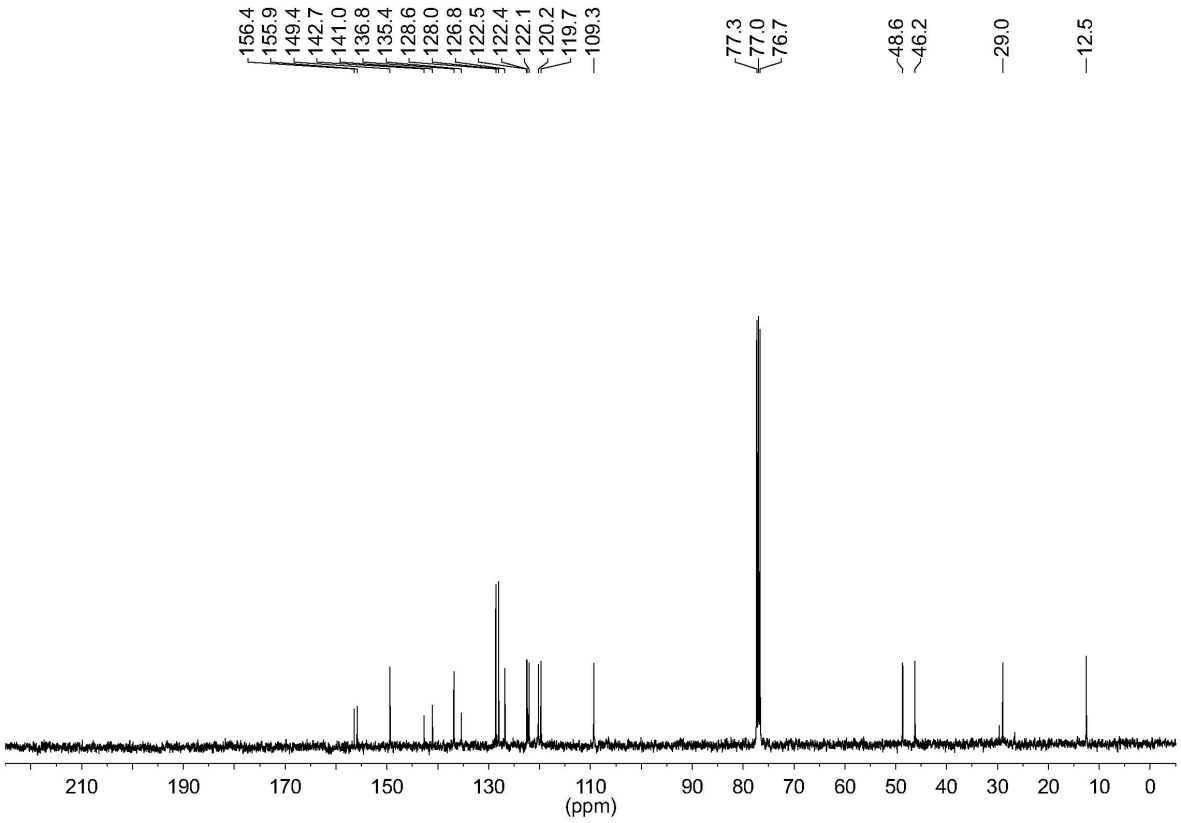
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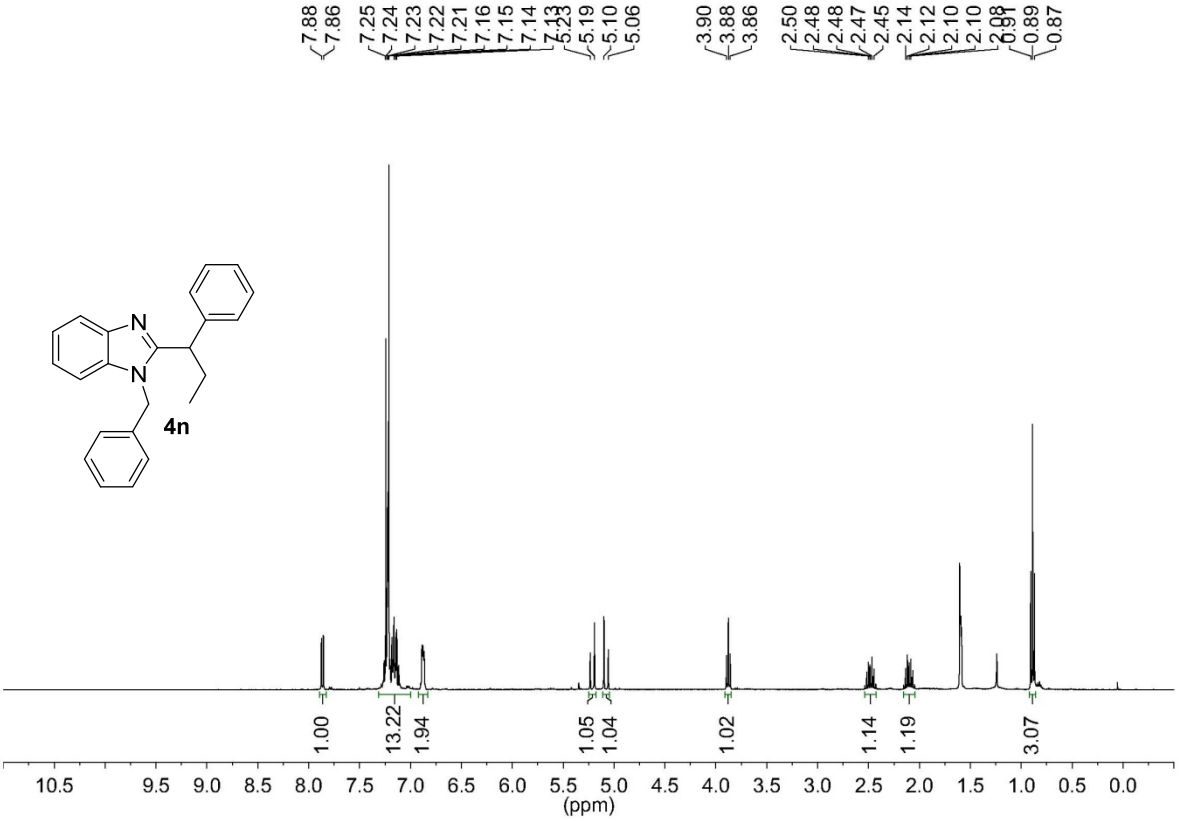
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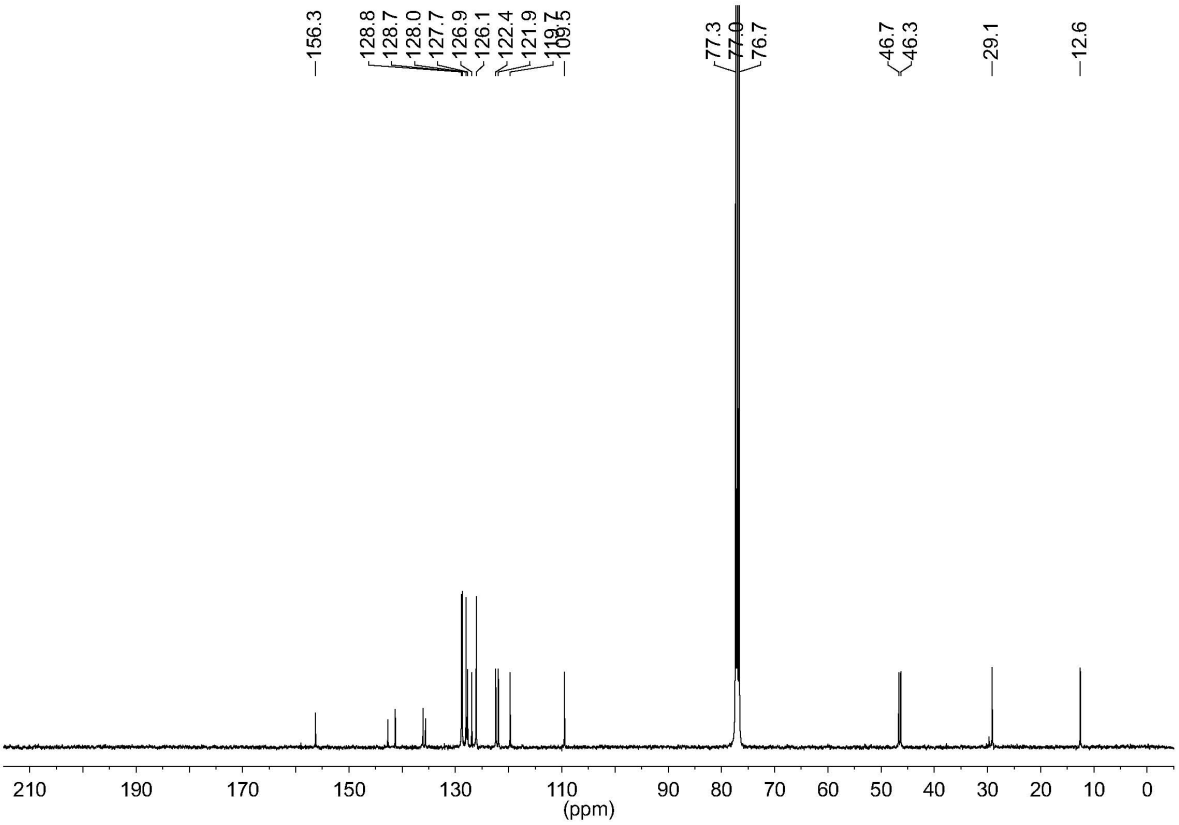
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46.3
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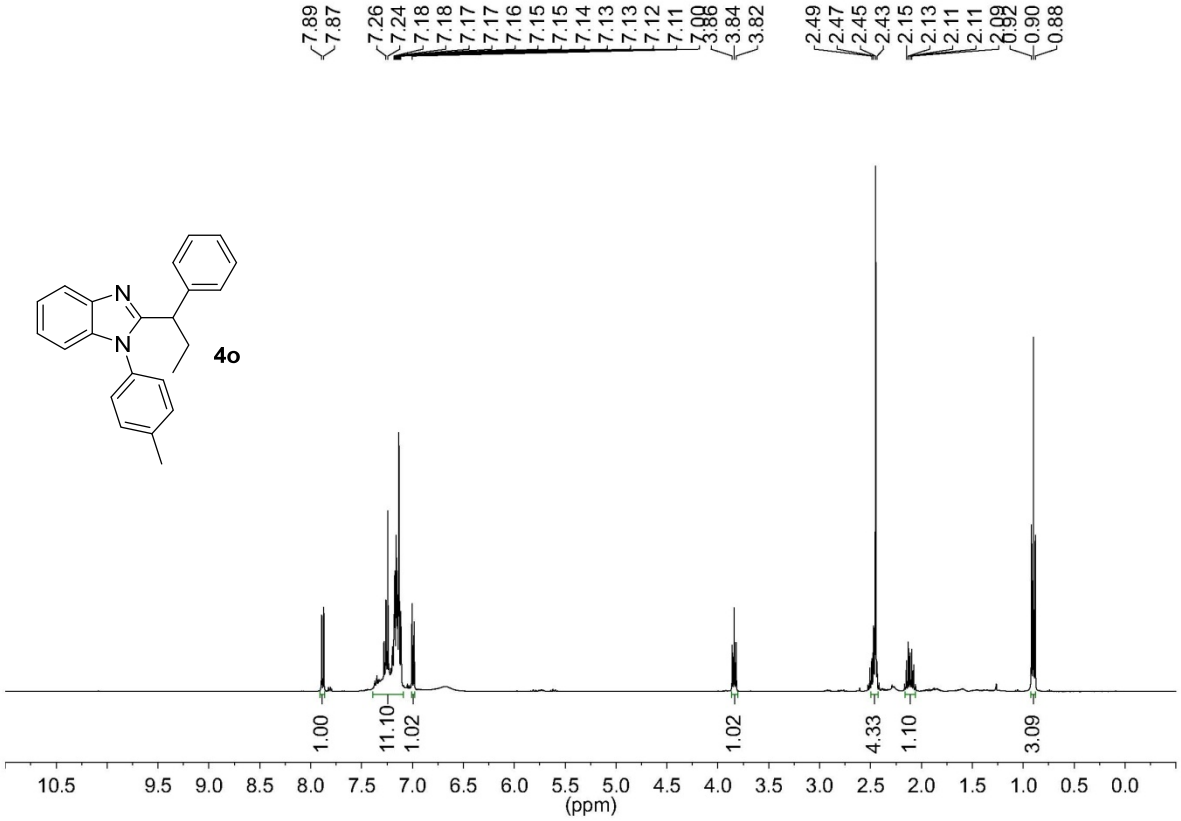
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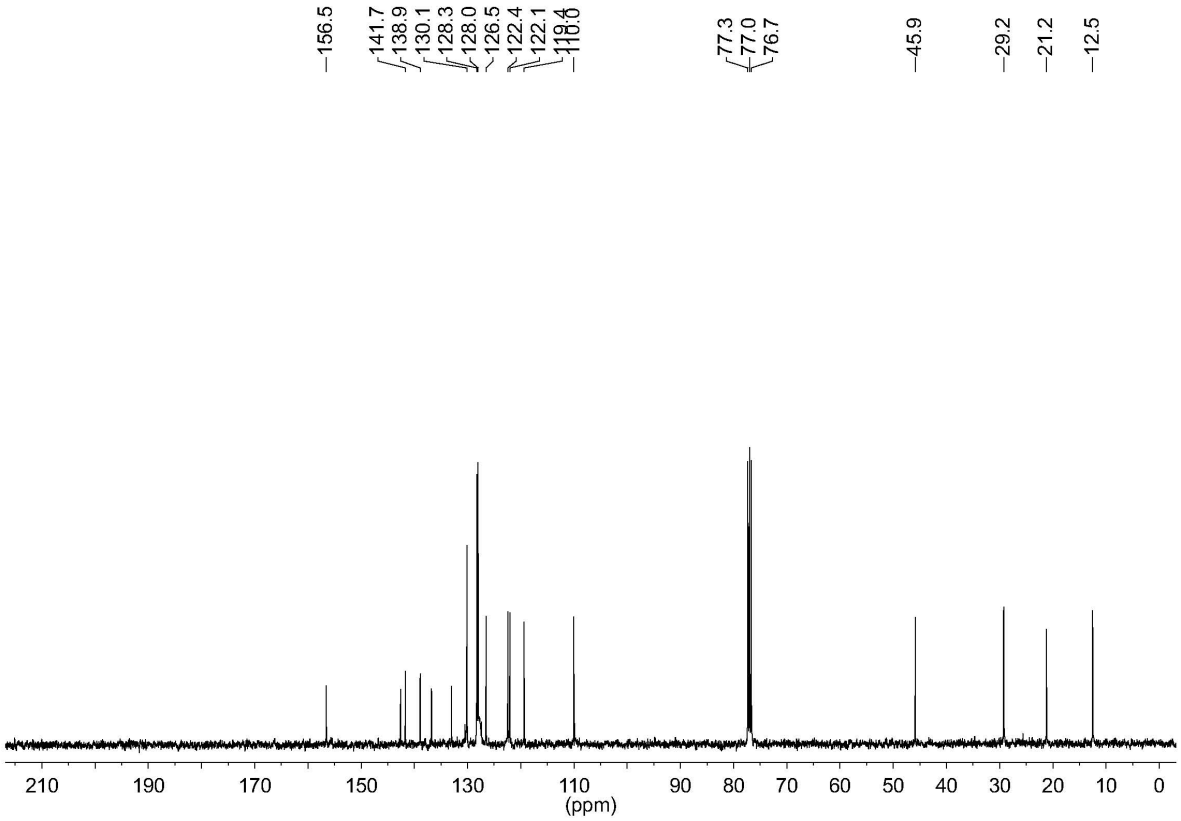
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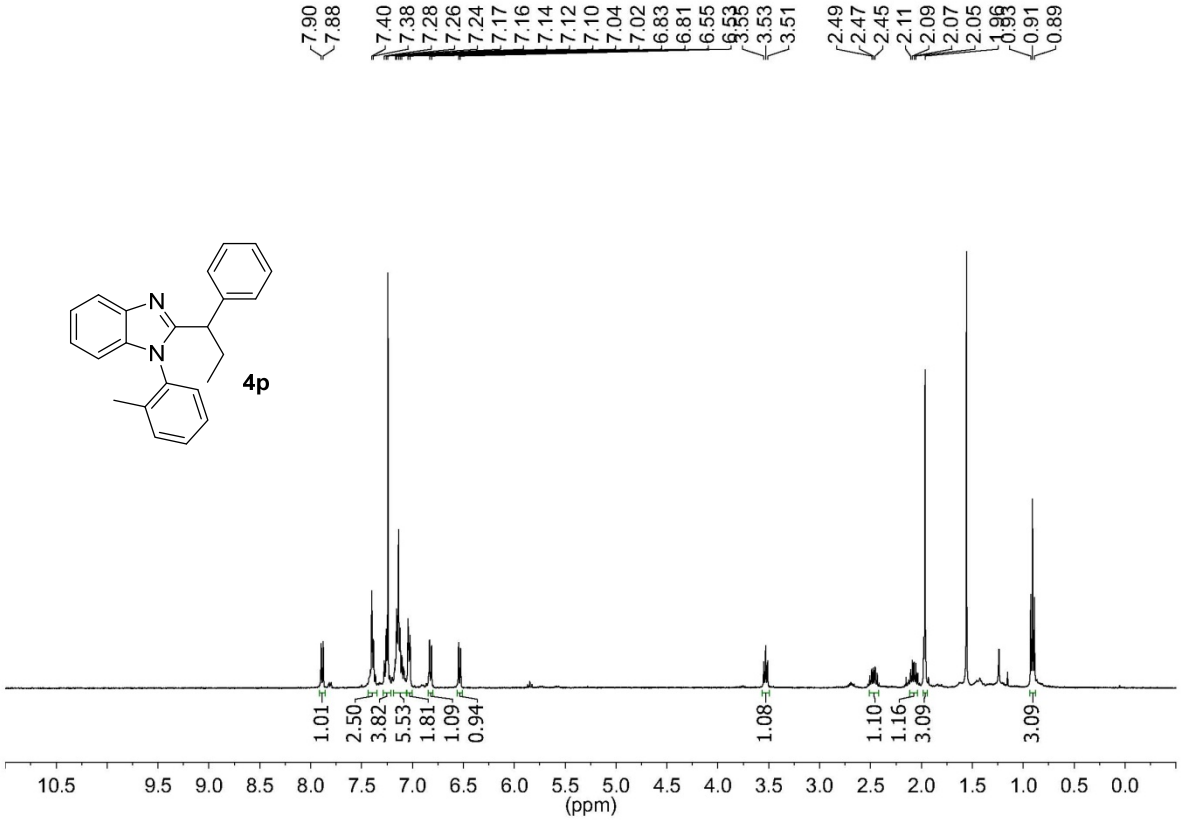
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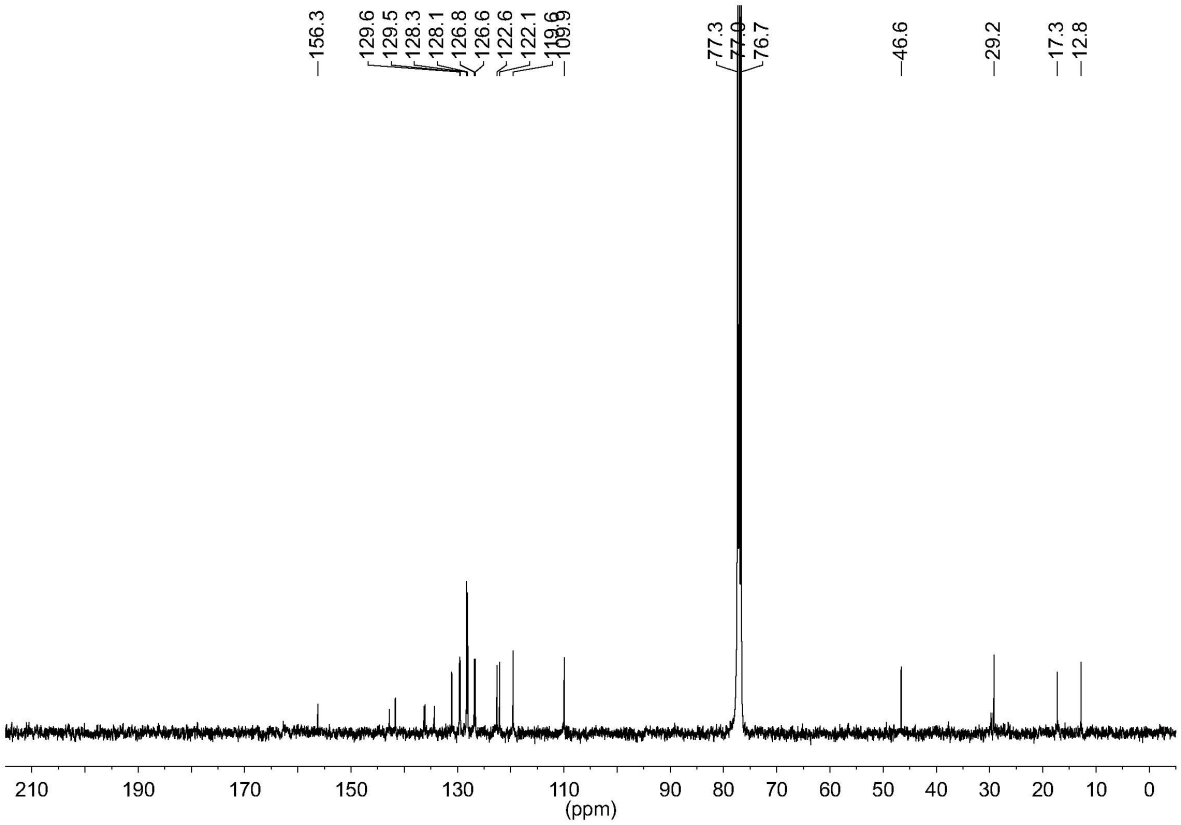
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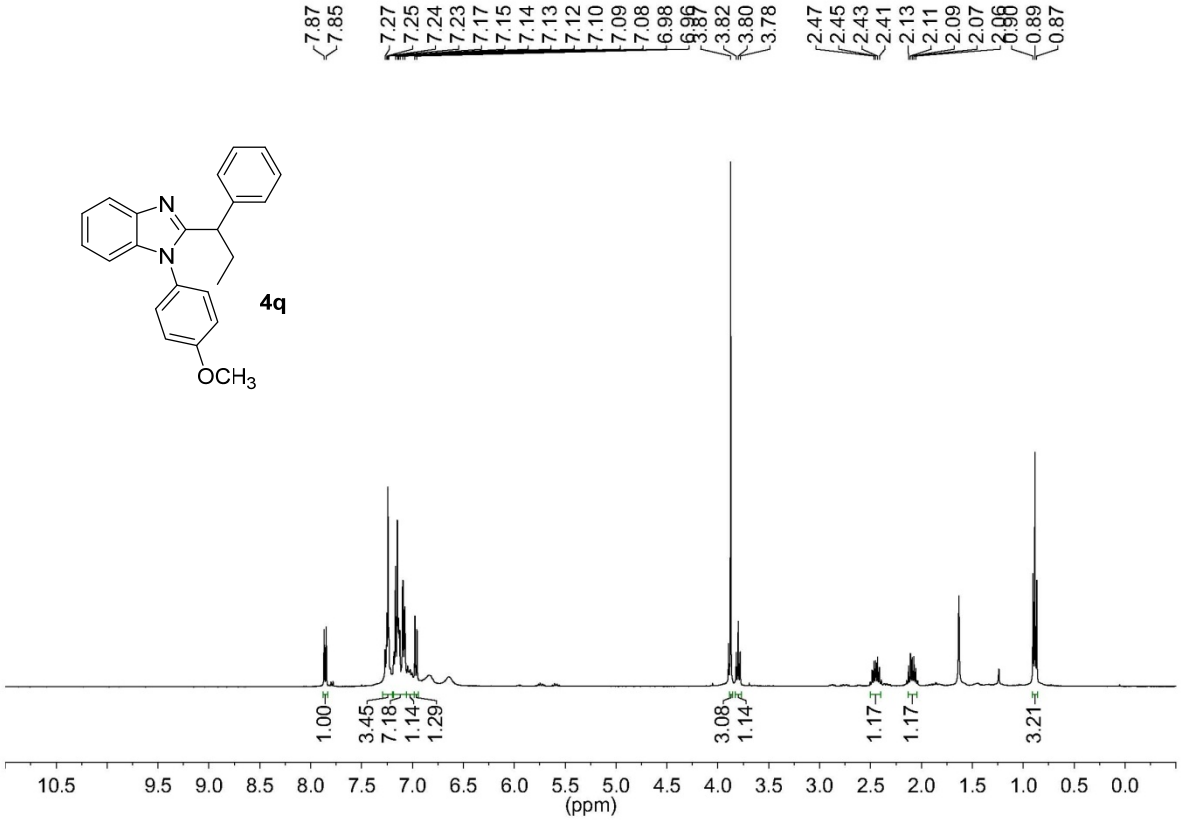
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1.17
1.17
3.21
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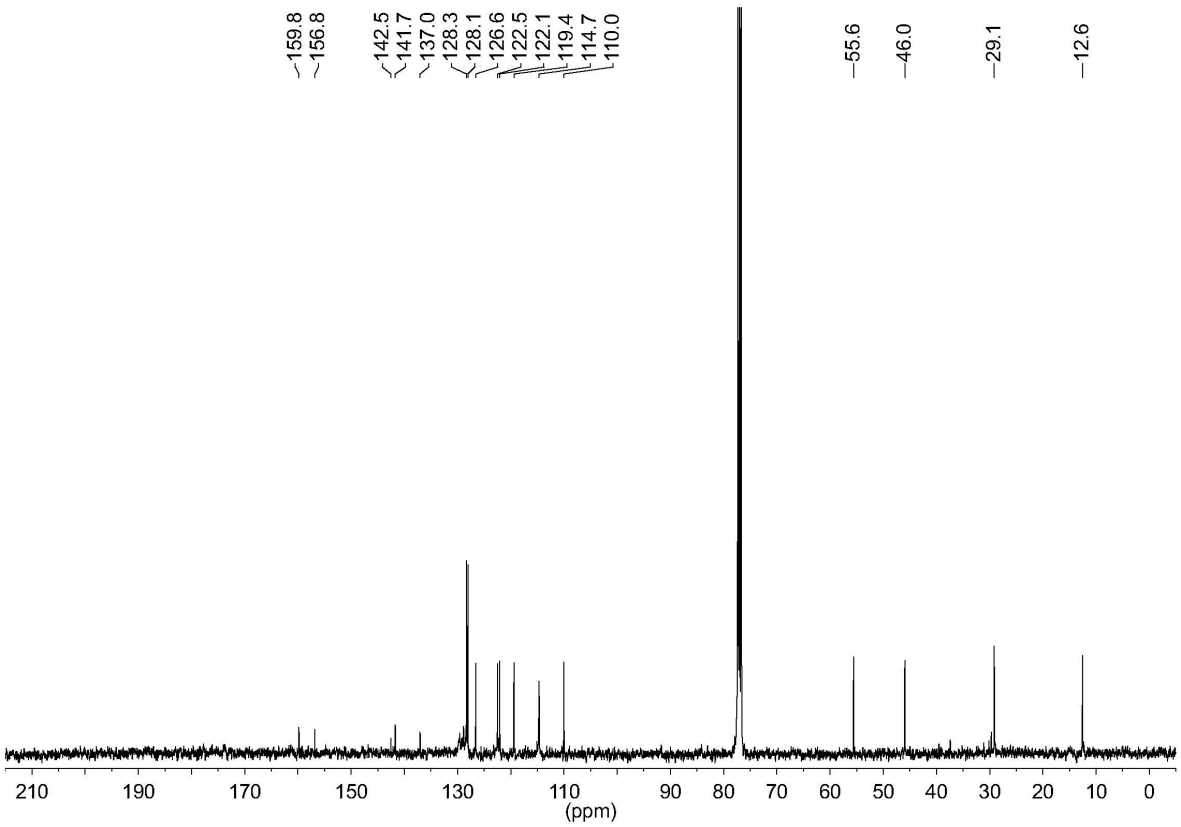
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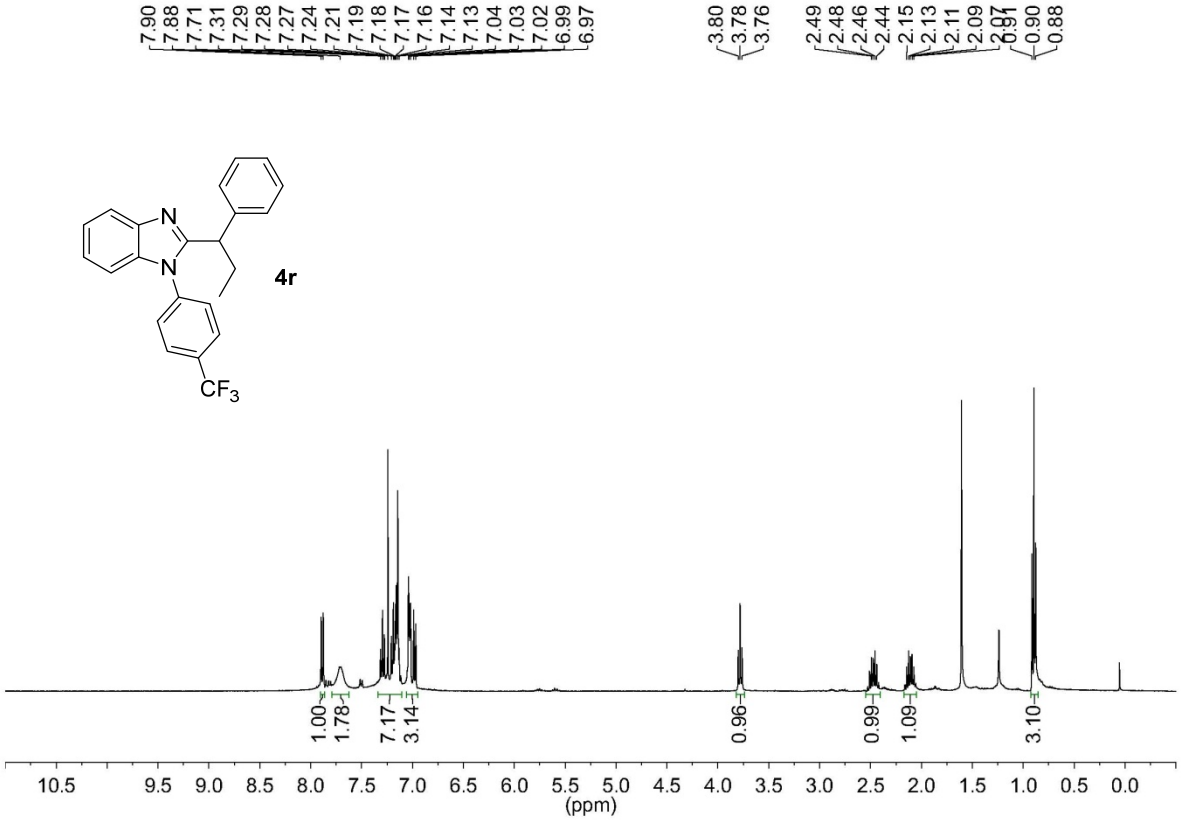
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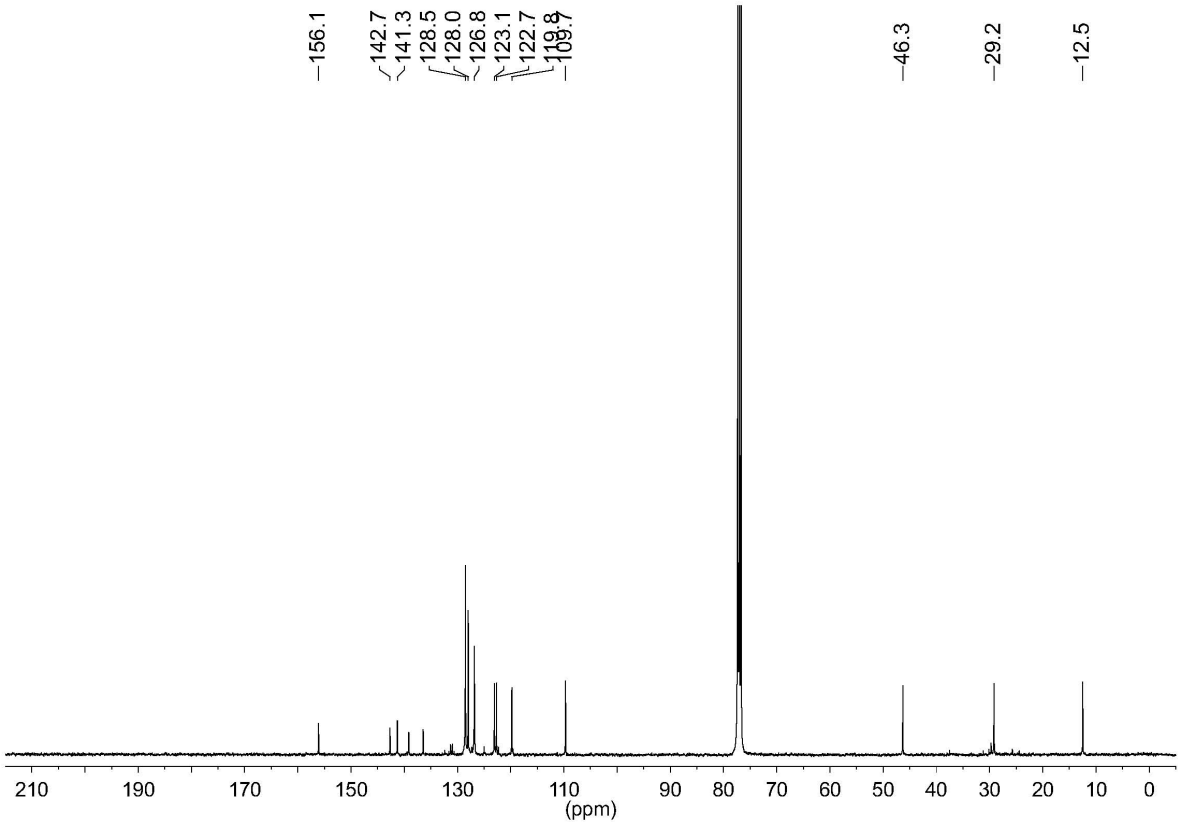
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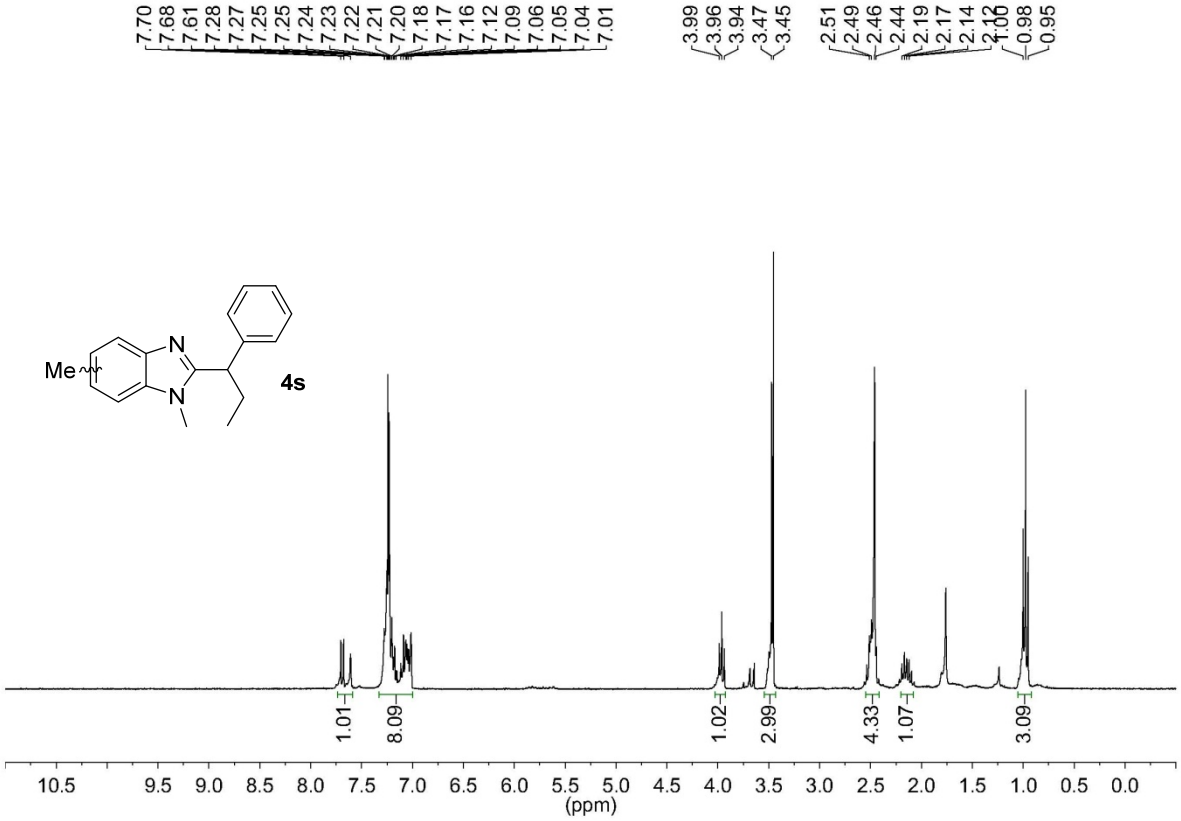
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7.12
7.09
7.06
7.05
7.04
7.01
3.99
3.96
3.94
3.47
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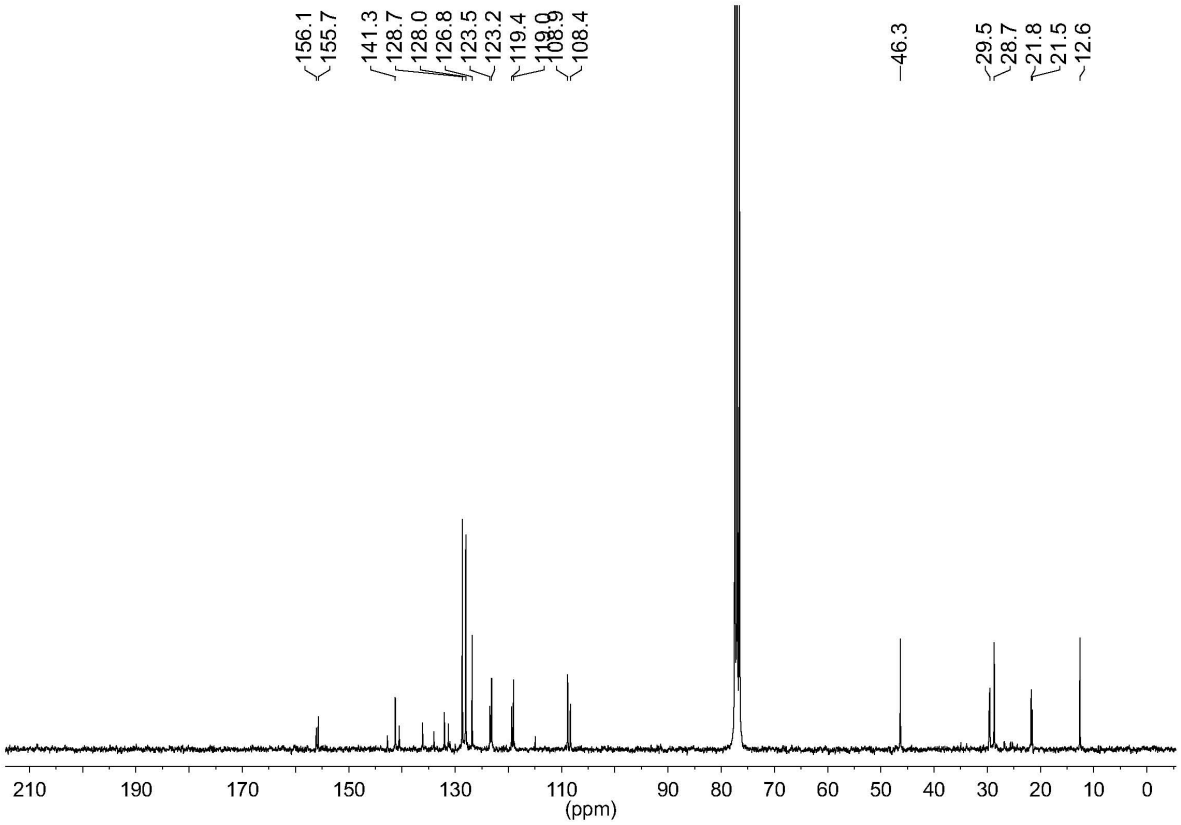
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21.8
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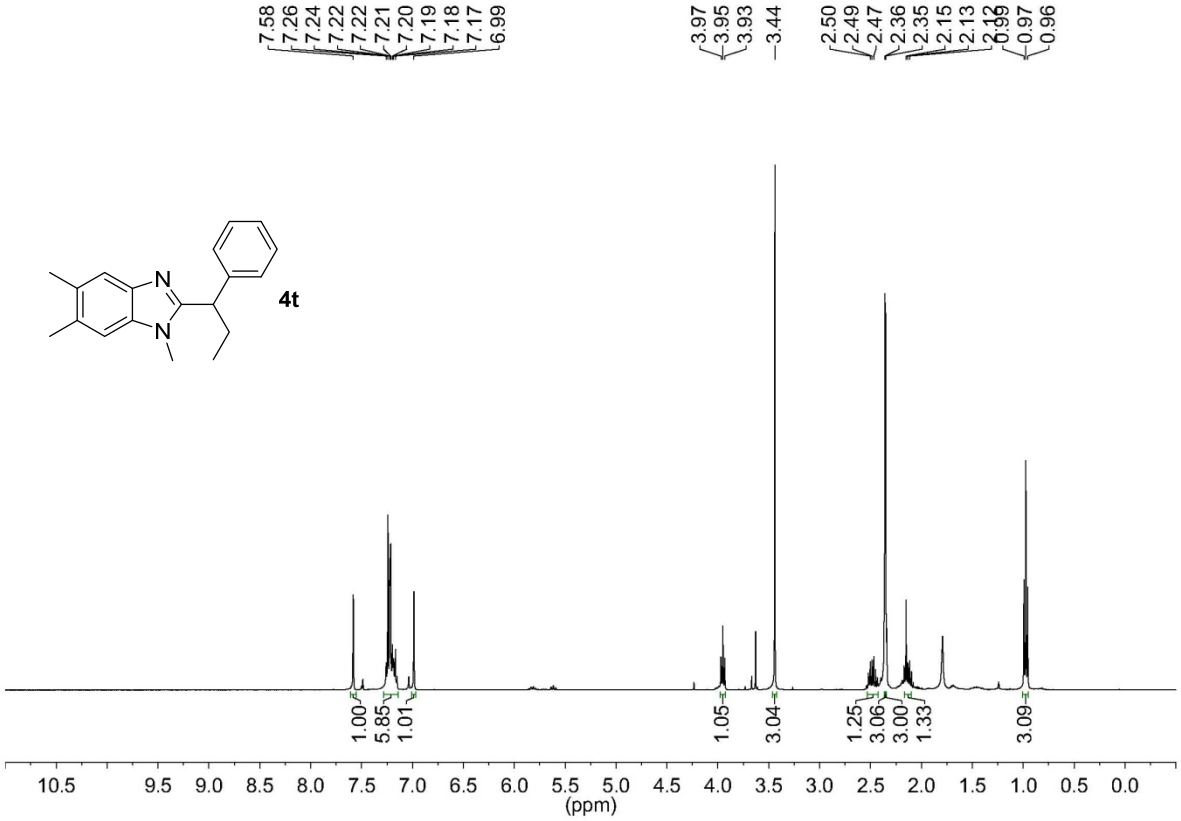
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1.01
1.05
3.04
1.25
3.06
3.00
1.33
3.09
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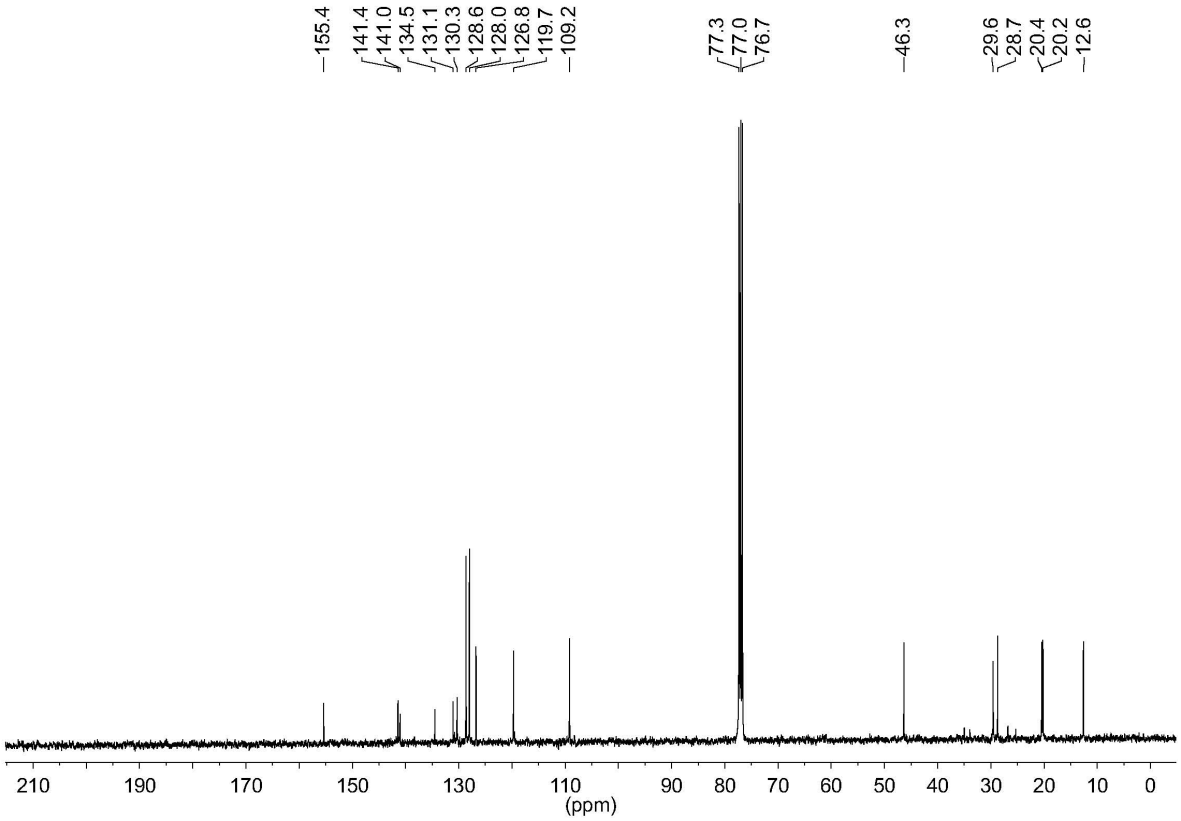
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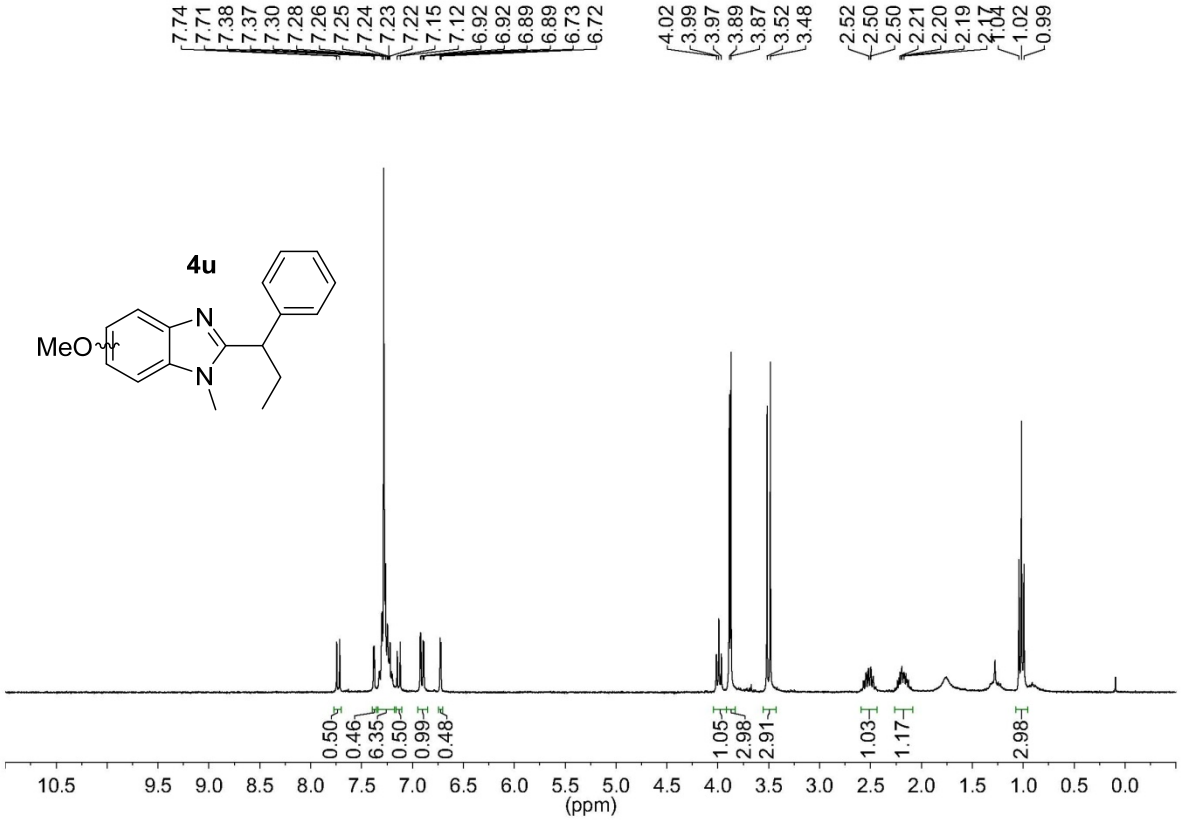
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7.15
7.12
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6.92
6.89
6.89
6.73
6.72
4.02
3.99
3.97
3.89
3.87
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2.50
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2.19
2.17
2.04
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0.99
0.48
1.05
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2.91
1.03
1.17
2.98
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9.5
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8.5
8.0
7.5
7.0
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6.0
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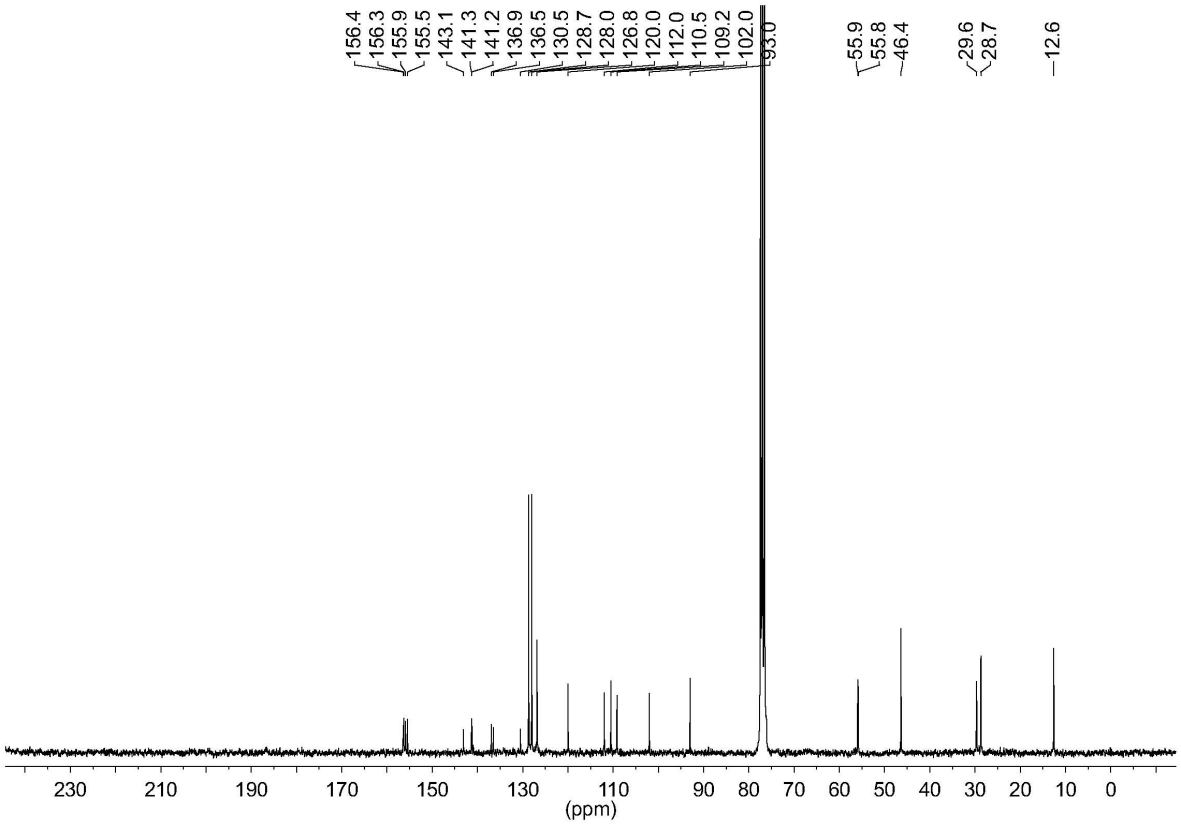
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112.0
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102.0
93.0
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55.8
46.4
29.6
28.7
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190
170
150
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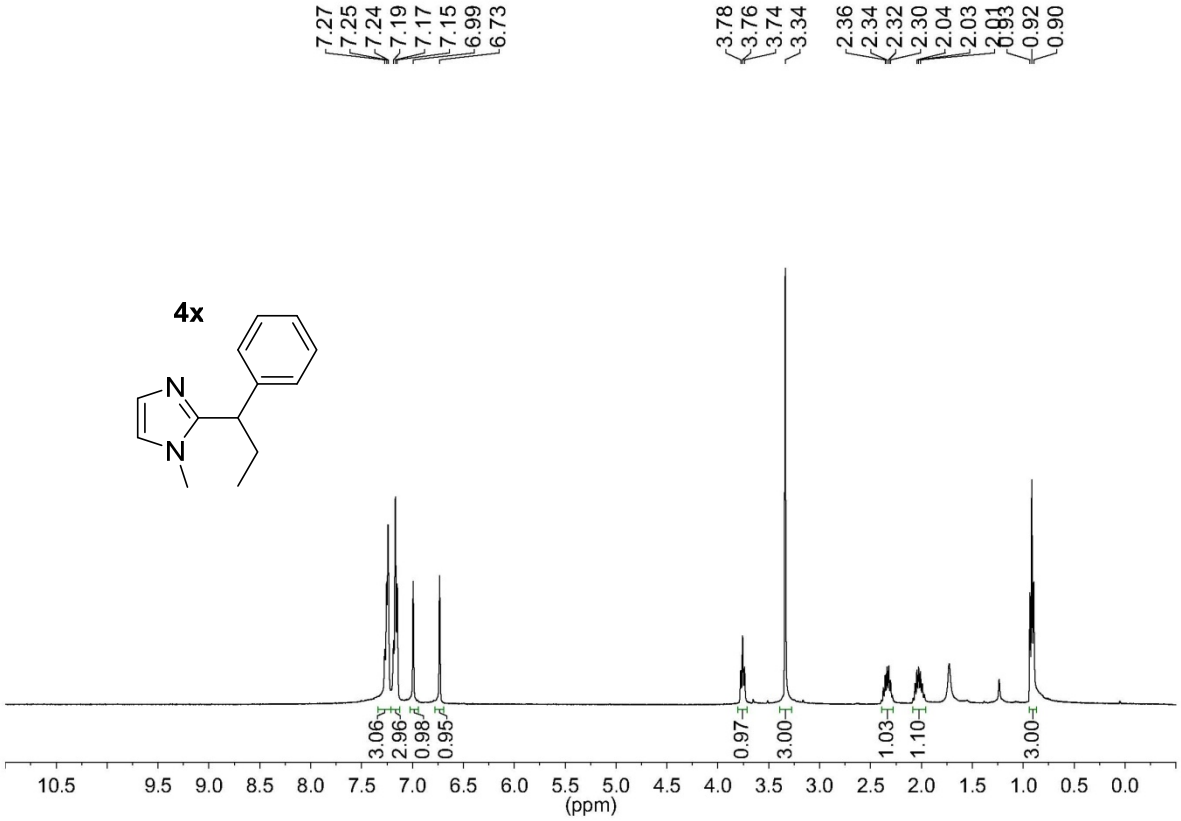
(ppm)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2.34
2.32
2.30
2.04
2.03
2.01
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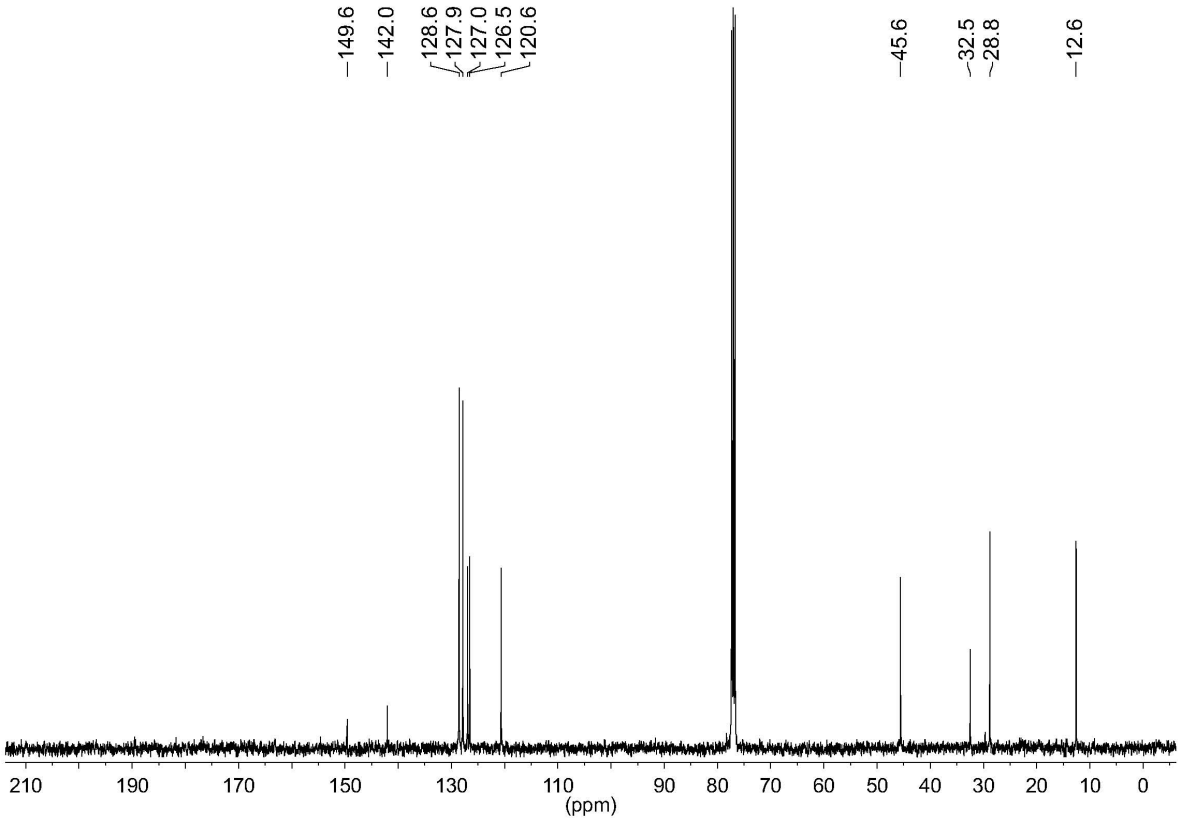
0.92
0.90
4x
N
N
3.06
2.96
0.98
0.95
0.97
3.00
1.03
1.10
3.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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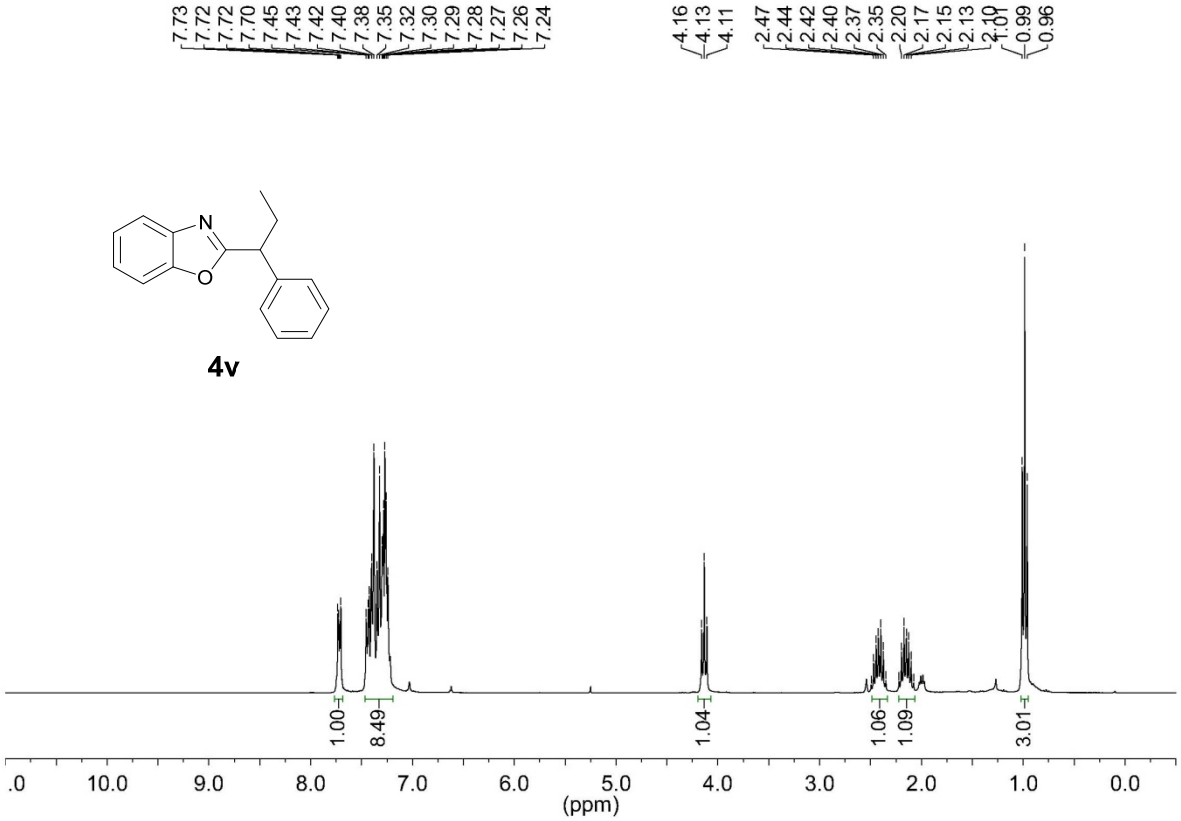
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7.72
7.72
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7.40
7.38
7.35
7.32
7.30
7.29
7.28
7.27
7.26
7.24
4.16
4.13
4.11
2.47
2.44
2.42
2.40
2.37
2.35
2.20
2.17
2.15
2.13
2.10
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0.96
N
O
4v
1.00
8.49
1.04
1.06
1.09
3.01
.0
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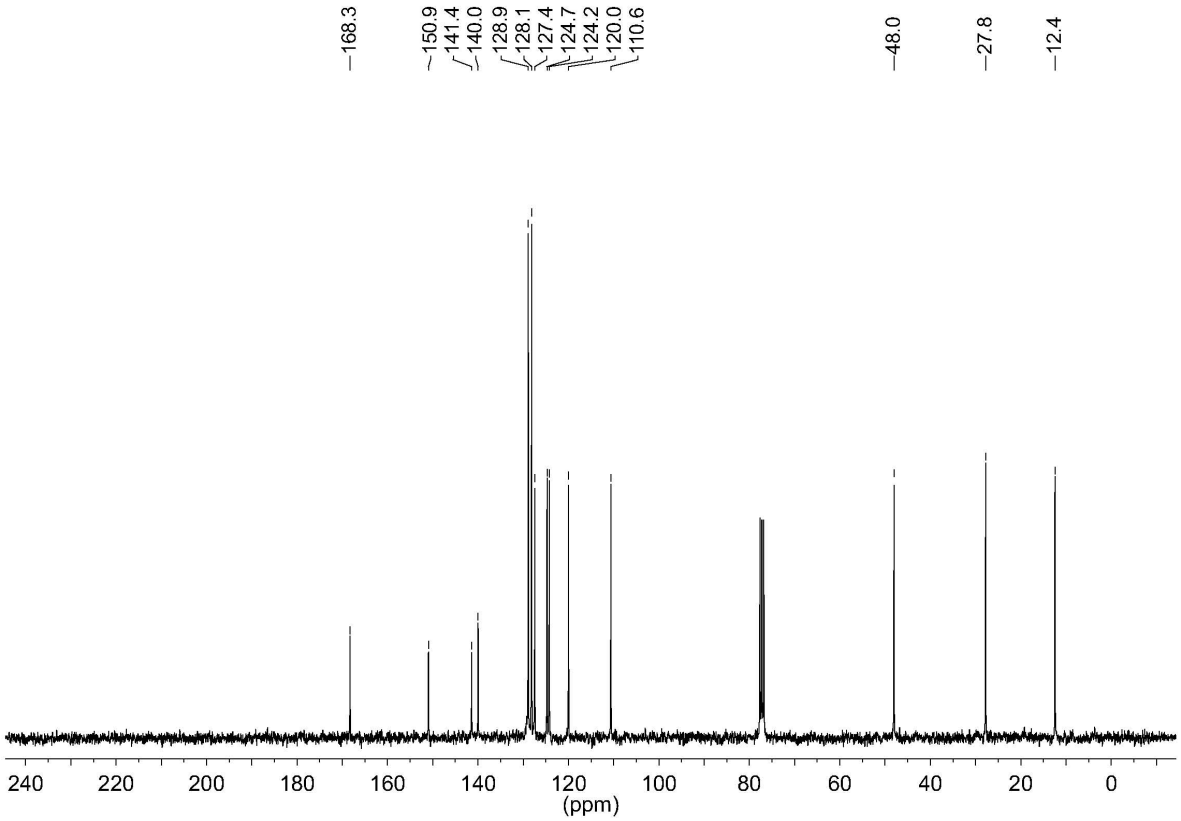
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110.6
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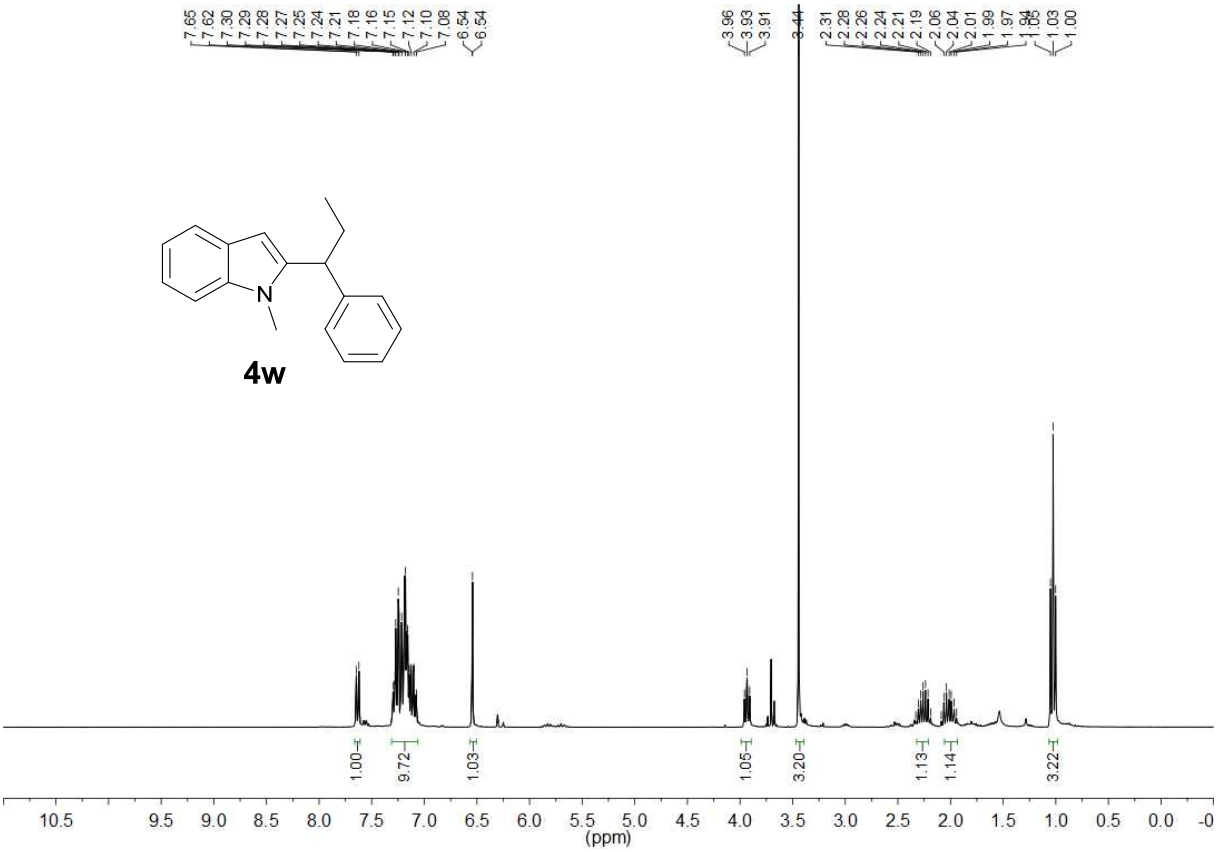
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7.12
7.10
7.08
6.54
6.54
3.96
3.93
3.91
3.44
2.31
2.28
2.26
2.24
2.21
2.19
2.06
2.04
2.01
1.99
1.97
1.03
1.00
N
4w
1.00
9.72
1.03
1.05
3.20
1.13
1.14
3.22
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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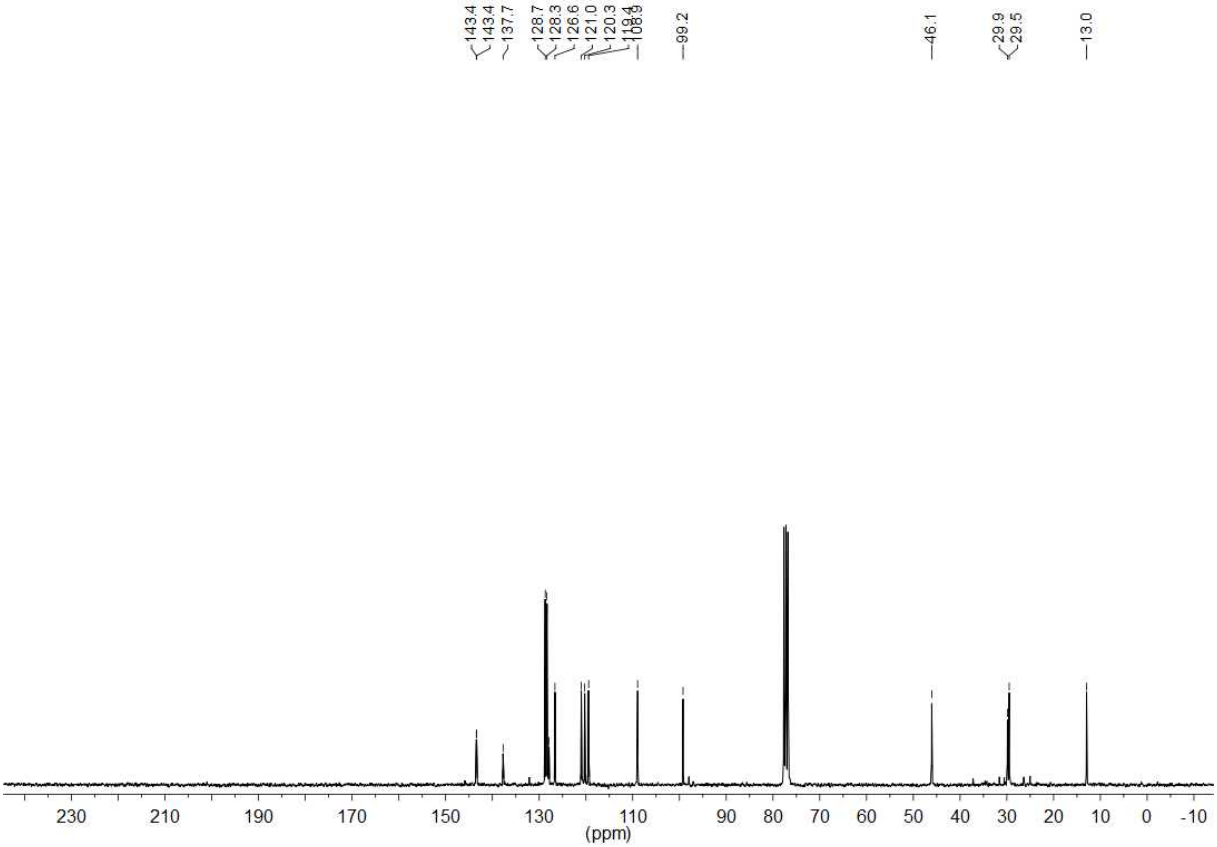
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143.4
137.7
128.7
128.3
126.6
121.0
120.3
99.2
46.1
29.9
29.5
13.0
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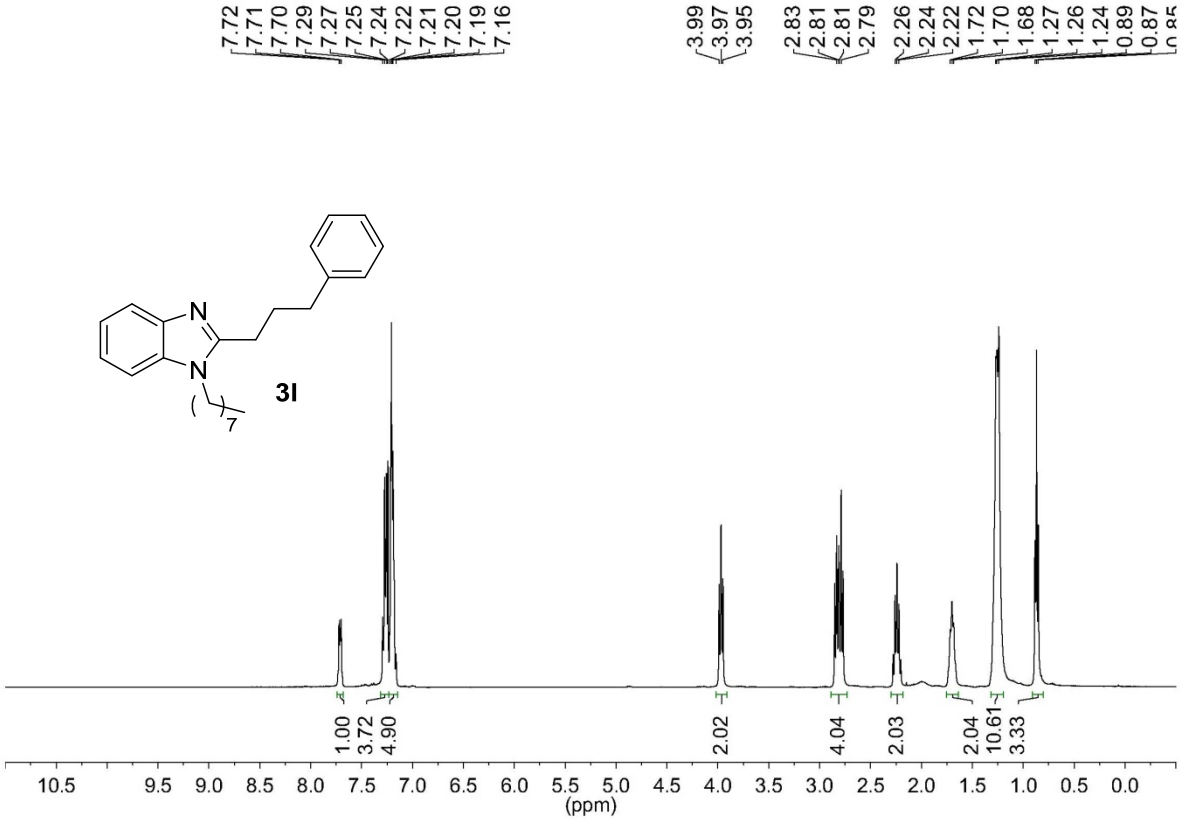
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
(ppm)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7.16
3.99
3.97
3.95
2.83
2.81
2.81
2.79
2.26
2.24
2.22
1.72
1.70
1.68
1.27
1.26
1.24
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0.87
0.85
N
N
7
3l
1.00
3.72
4.90
2.02
4.04
2.03
2.04
10.61
3.33
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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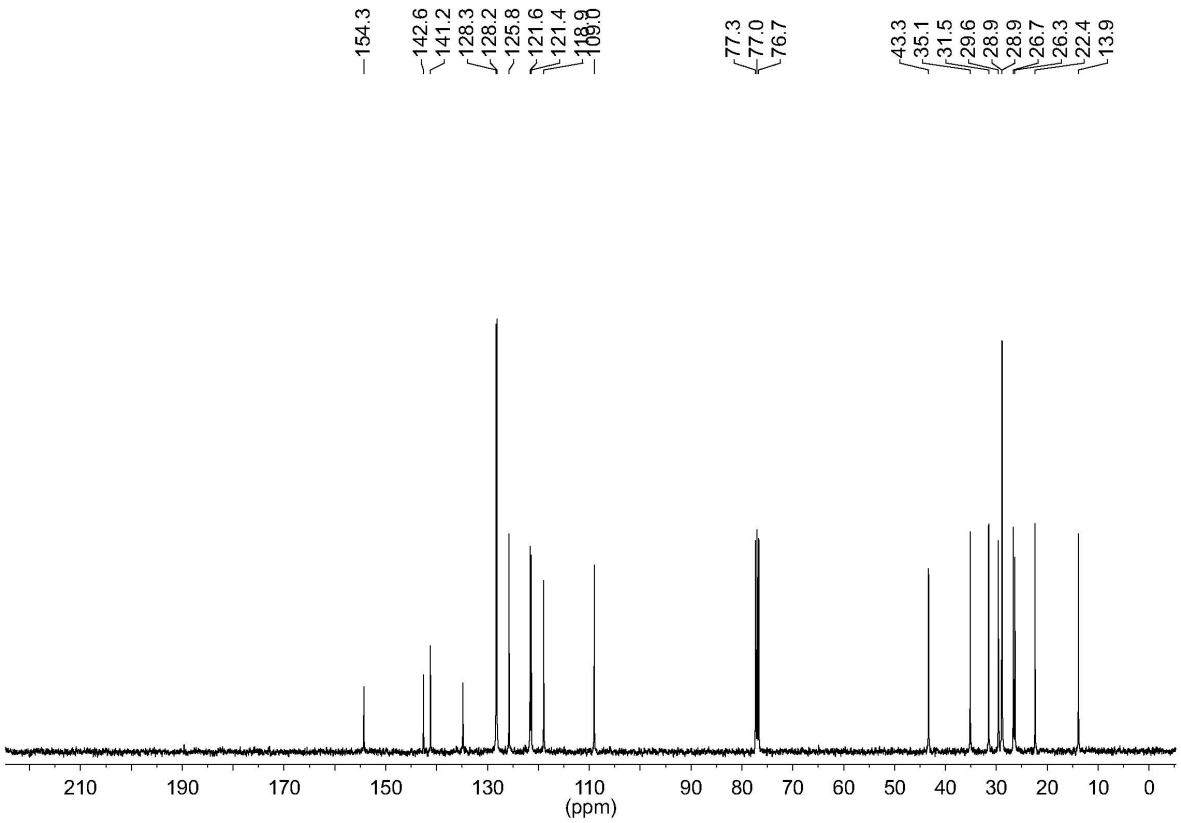
(ppm)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77.0
76.7
43.3
35.1
31.5
29.6
28.9
28.9
26.7
26.3
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150
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110
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80
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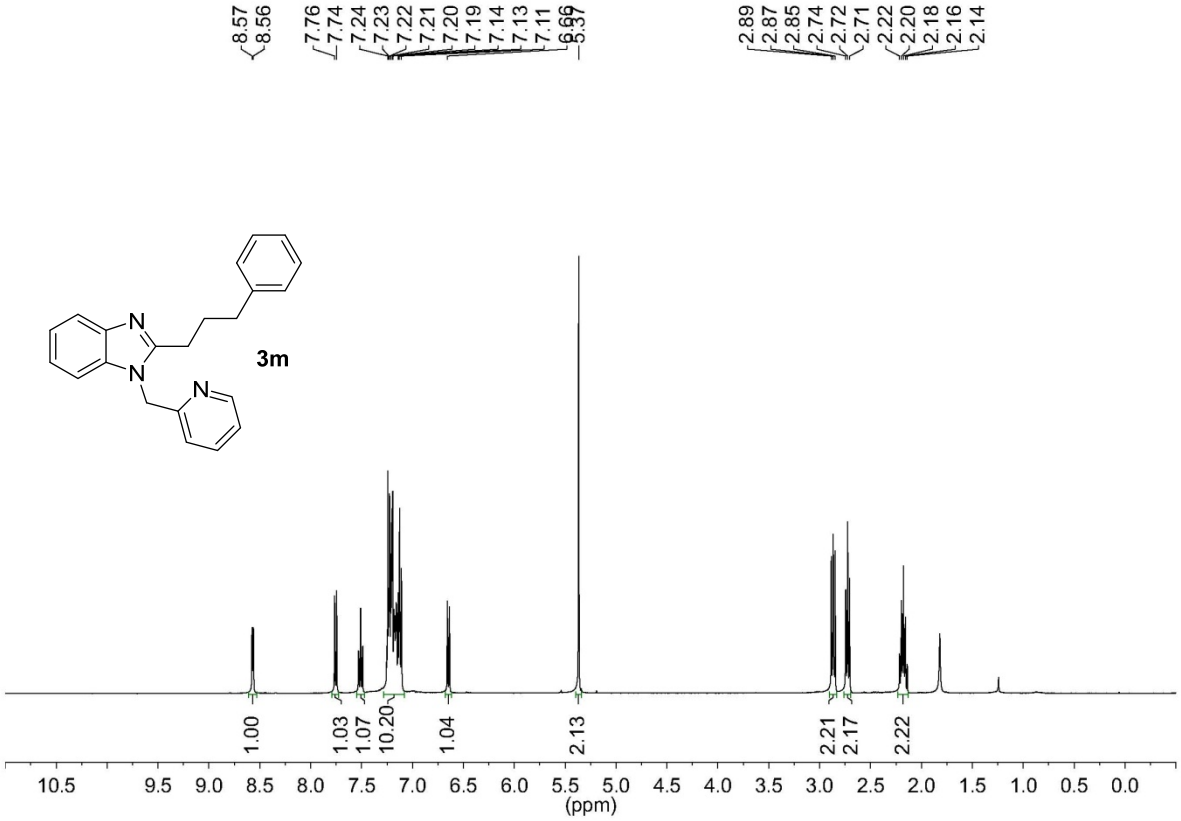
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5.37
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2.87
2.85
2.74
2.72
2.71
2.22
2.20
2.18
2.16
2.14
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N
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1.03
1.07
10.20
1.04
2.13
2.21
2.17
2.22
10.5
9.5
9.0
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7.5
7.0
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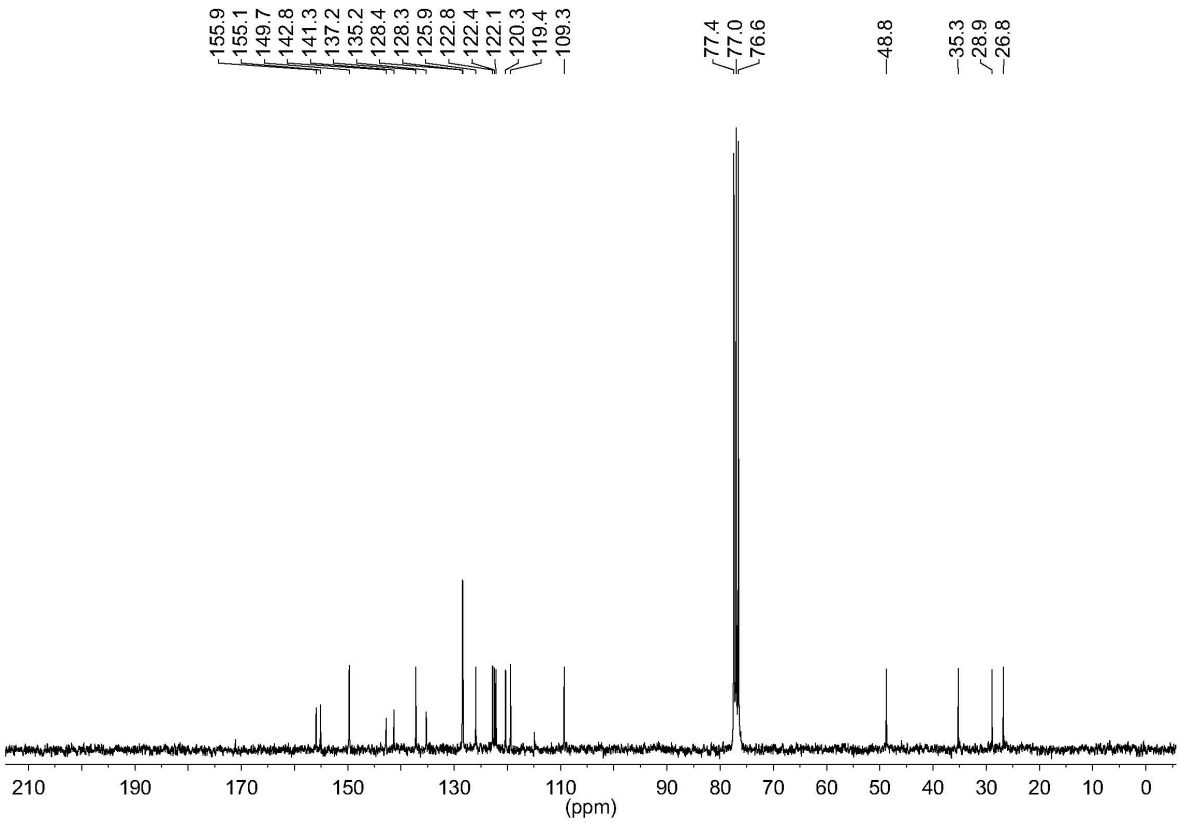
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122.1
120.3
119.4
109.3
77.4
77.0
76.6
48.8
35.3
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150
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110
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80
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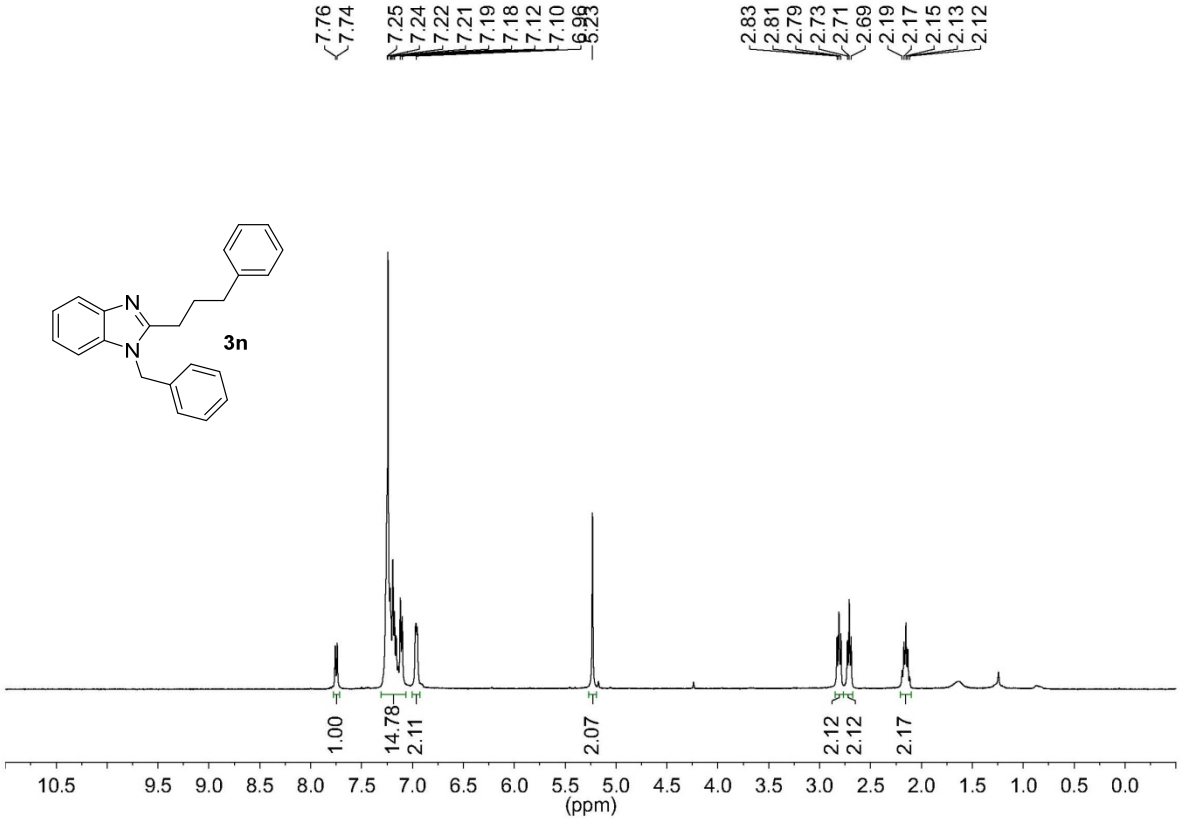
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2.73
2.71
2.69
2.19
2.17
2.15
2.13
2.12
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N
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14.78
2.11
2.07
2.12
2.12
2.17
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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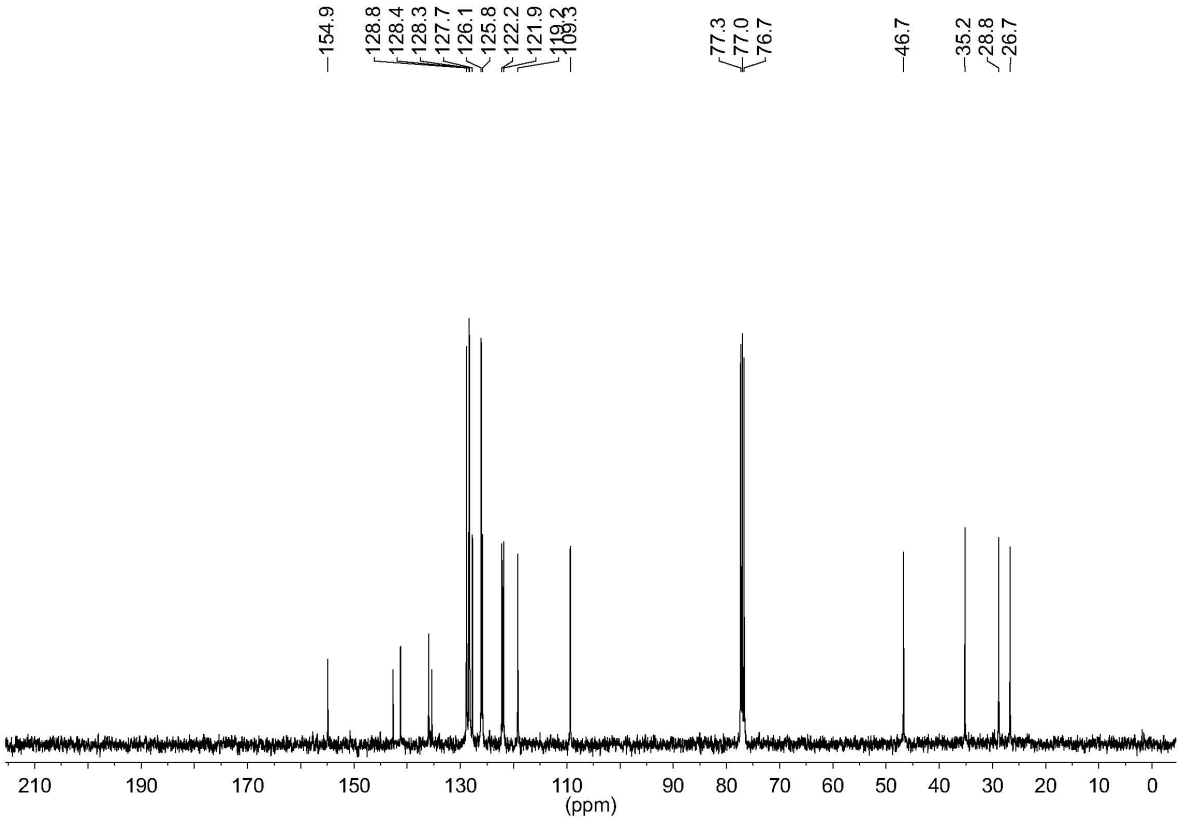
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26.7
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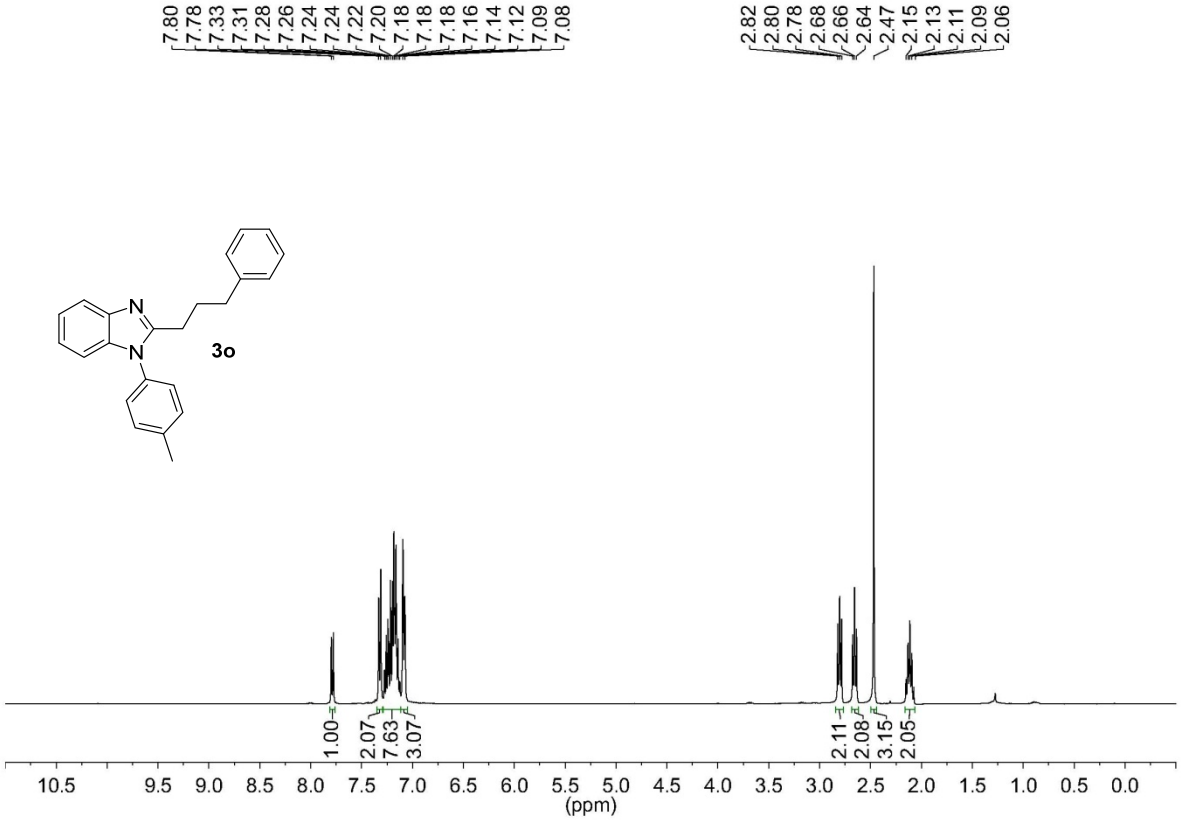
(ppm)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7.18
7.16
7.14
7.12
7.09
7.08
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2.80
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2.64
2.47
2.15
2.13
2.11
2.09
2.06
N
N
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2.07
7.63
3.07
2.11
2.08
3.15
2.05
10.5
9.5
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8.0
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7.0
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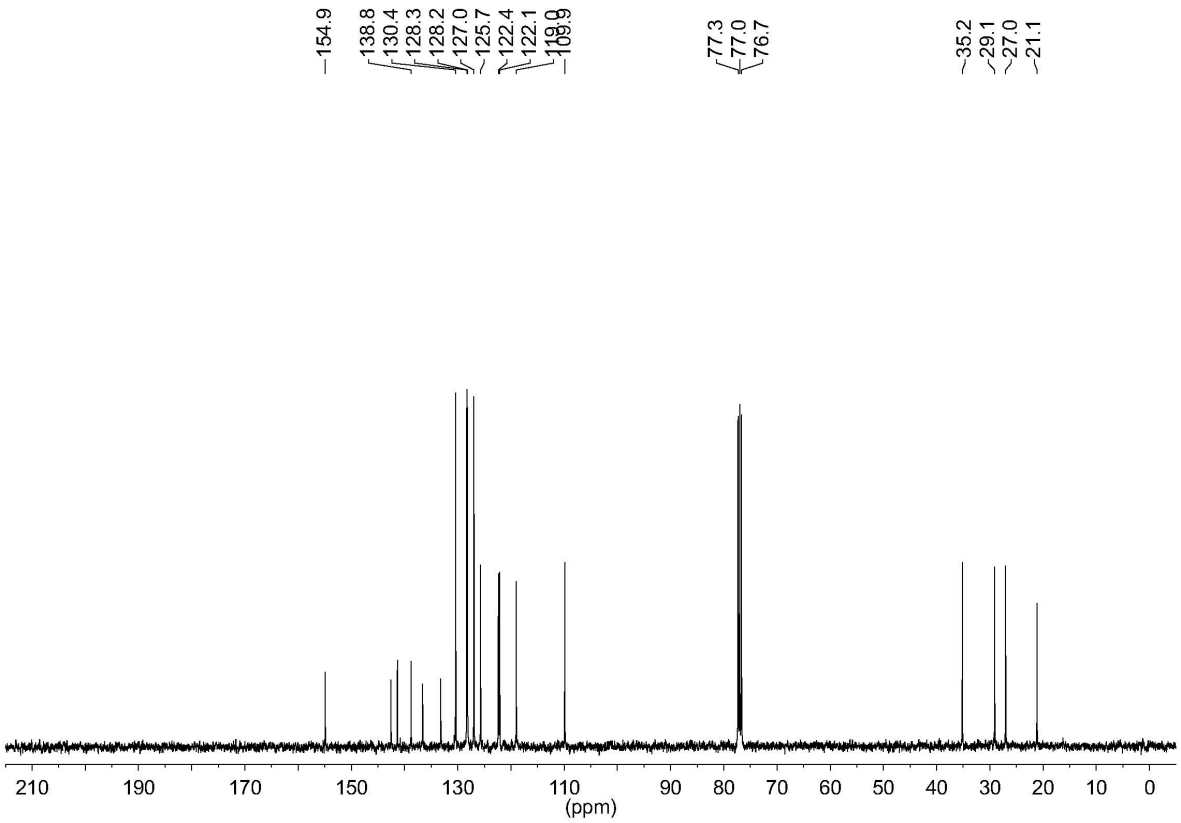
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128.2
127.0
125.7
122.4
122.1
77.3
77.0
76.7
35.2
29.1
27.0
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170
150
130
110
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80
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50
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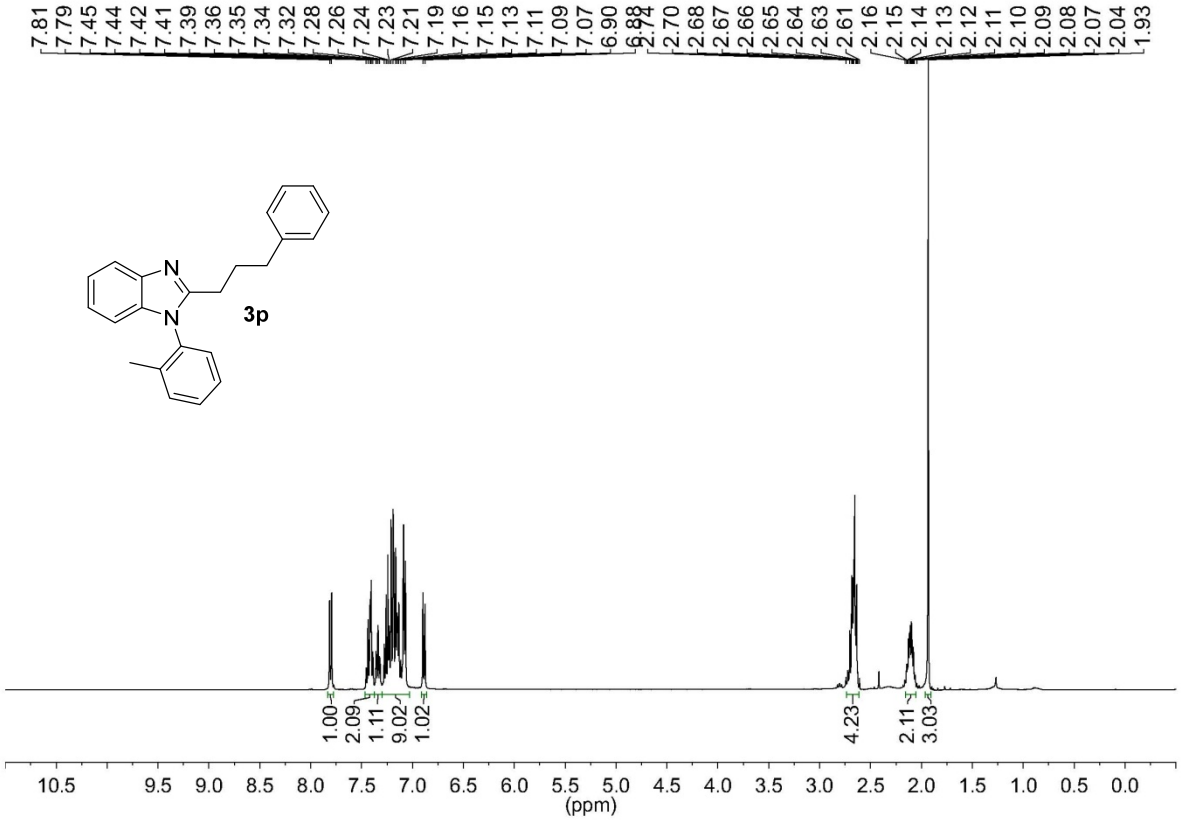
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7.13
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7.07
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2.10
2.09
2.08
2.07
2.04
1.93
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N
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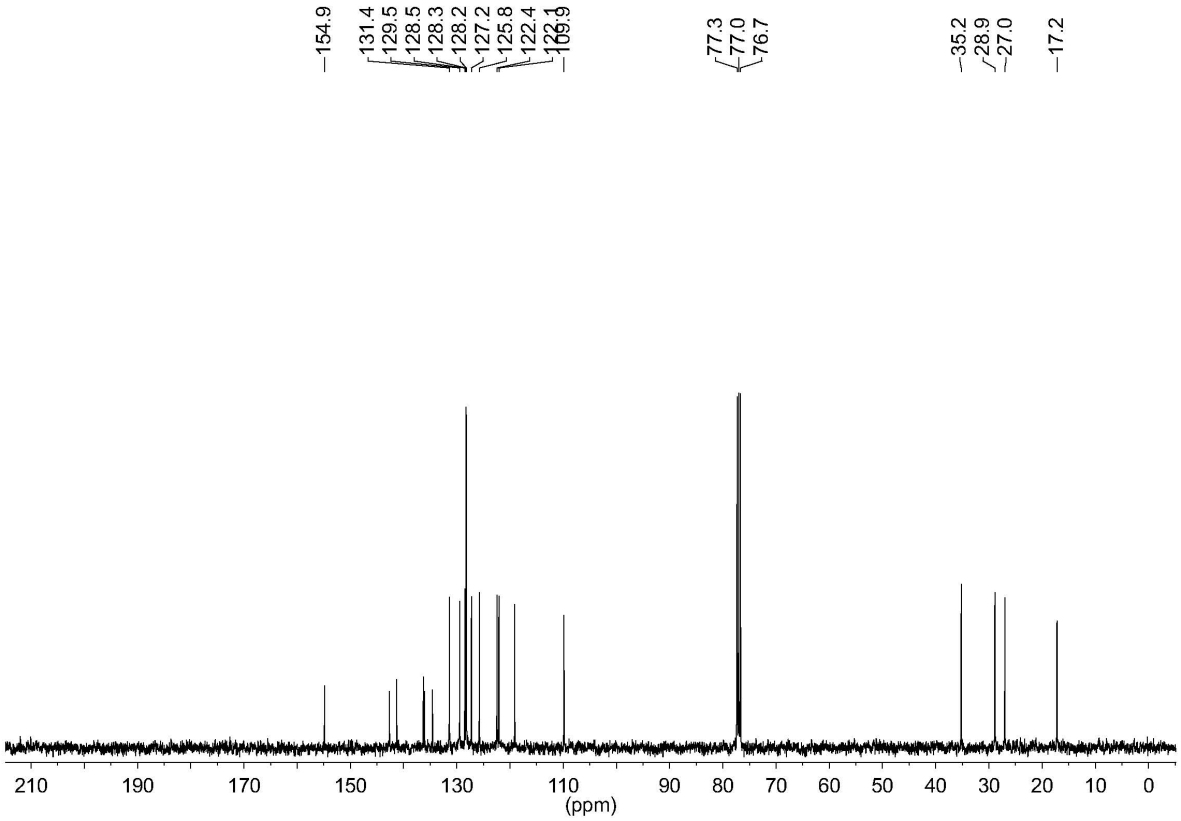
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122.4
77.3
77.0
76.7
35.2
28.9
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170
150
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110
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80
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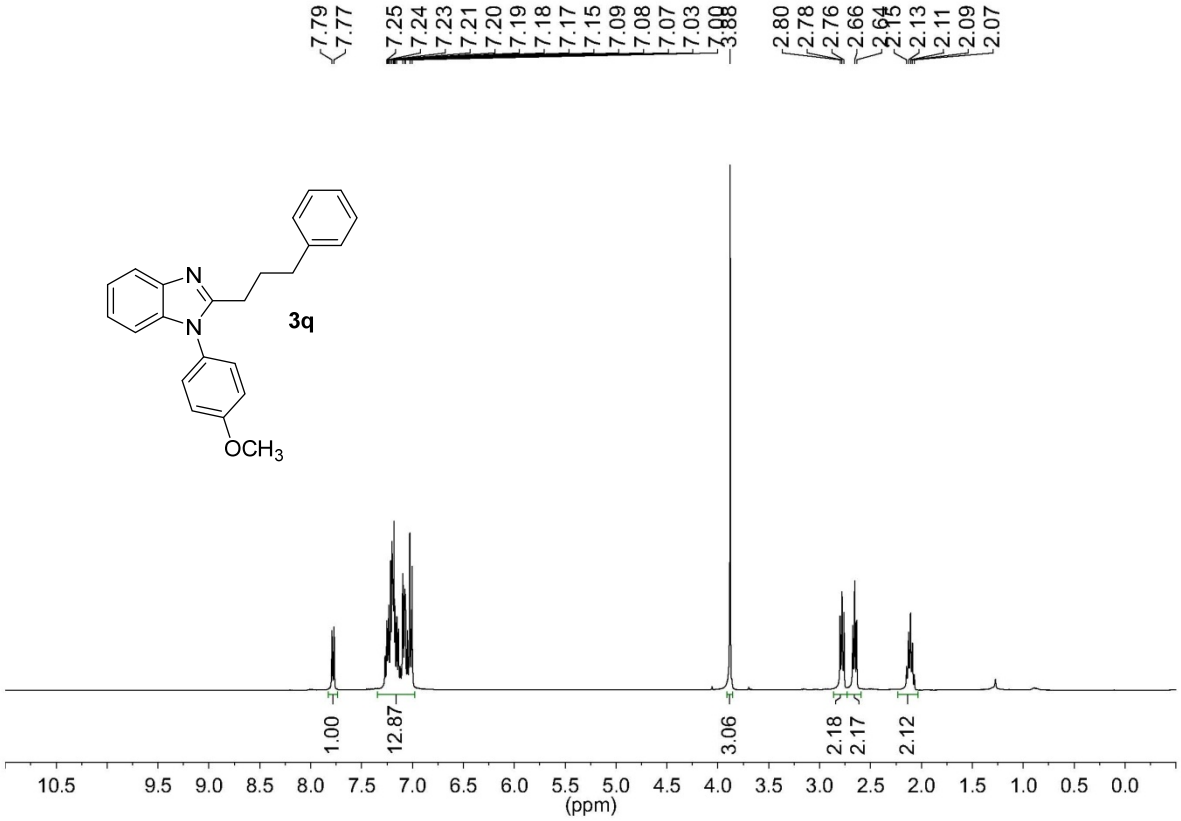
(ppm)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7.09
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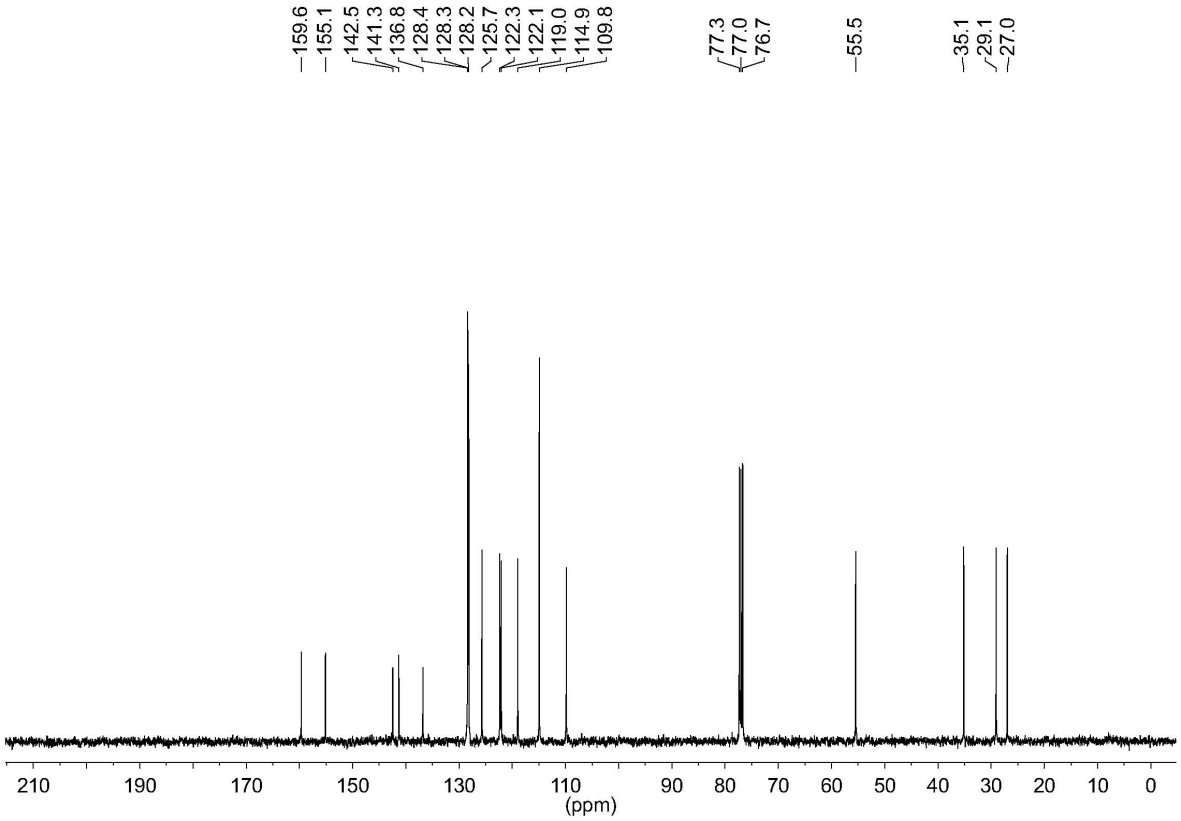
(ppm)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109.8
77.3
77.0
76.7
55.5
35.1
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150
130
110
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80
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50
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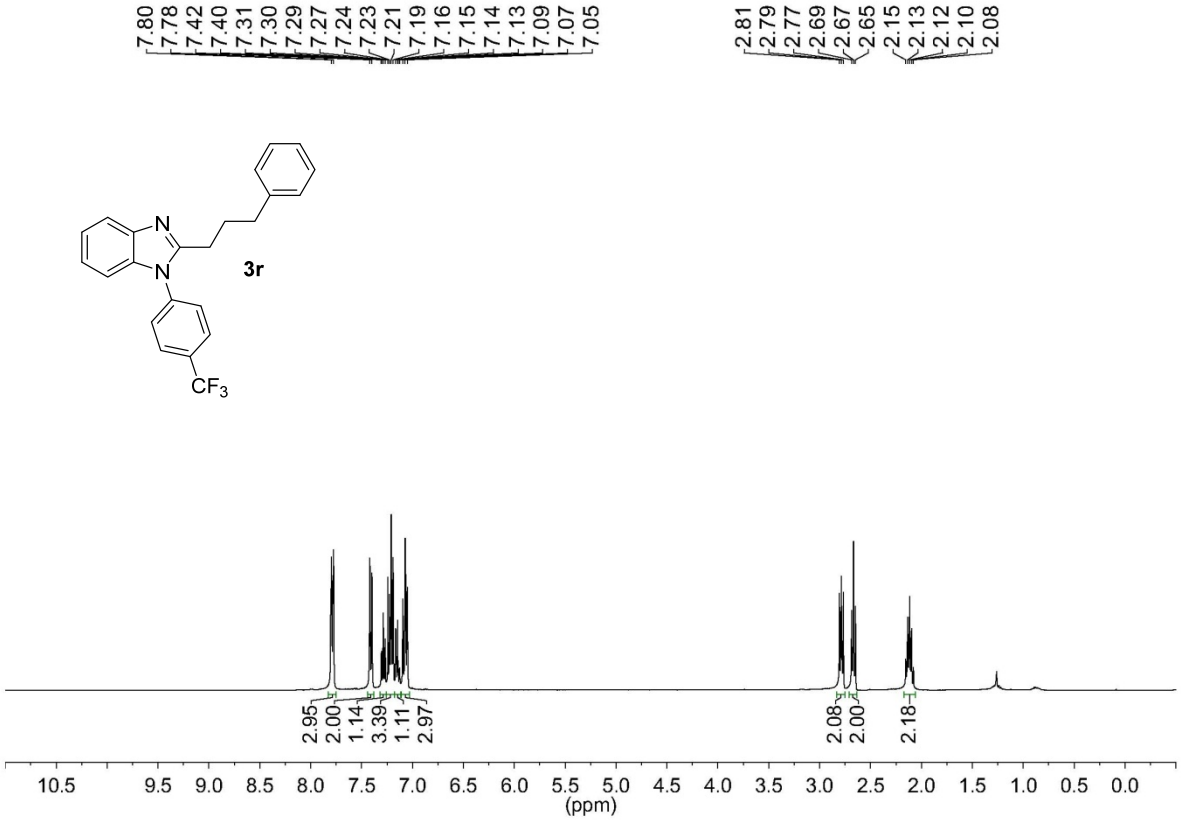
(ppm)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7.14
7.13
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7.07
7.05
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2.67
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2.13
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2.10
2.08
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6.0
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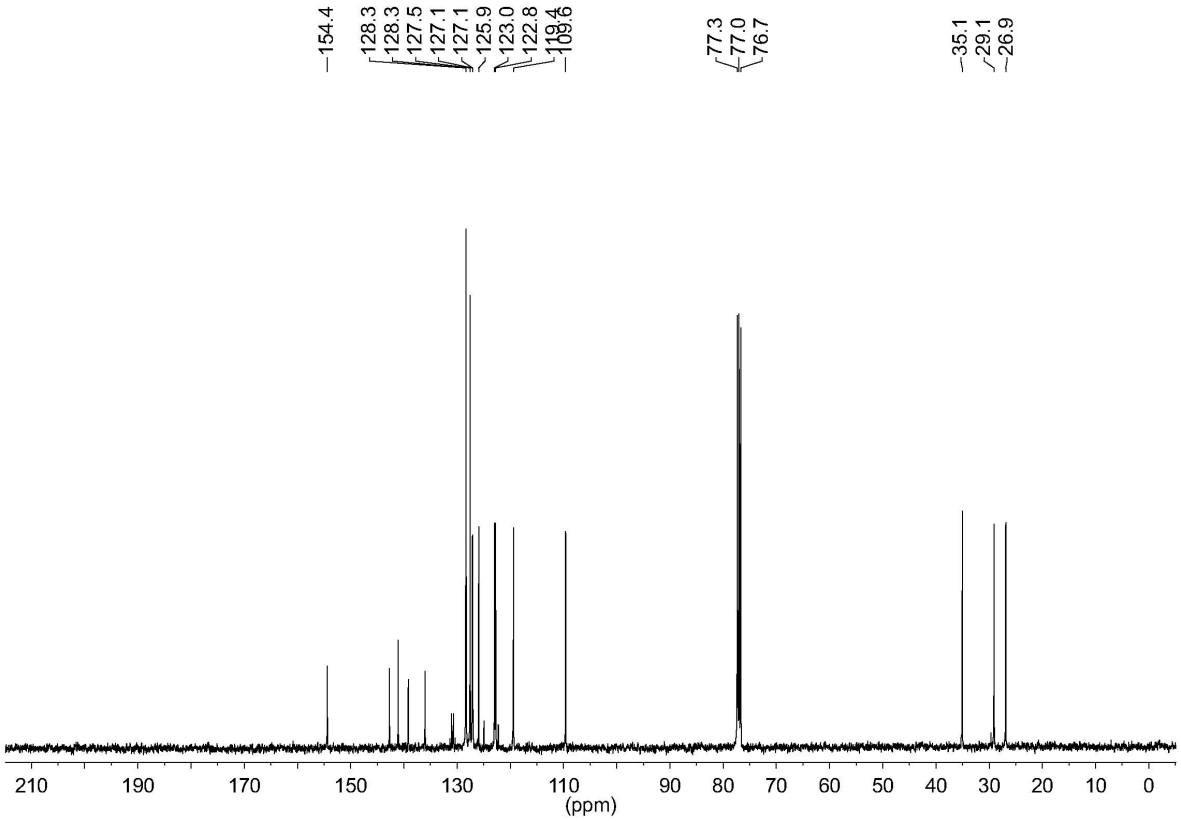
(ppm)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127.1
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119.4
109.6
77.3
77.0
76.7
35.1
29.1
26.9
210
190
170
150
130
110
90
80
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60
50
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30
20
10
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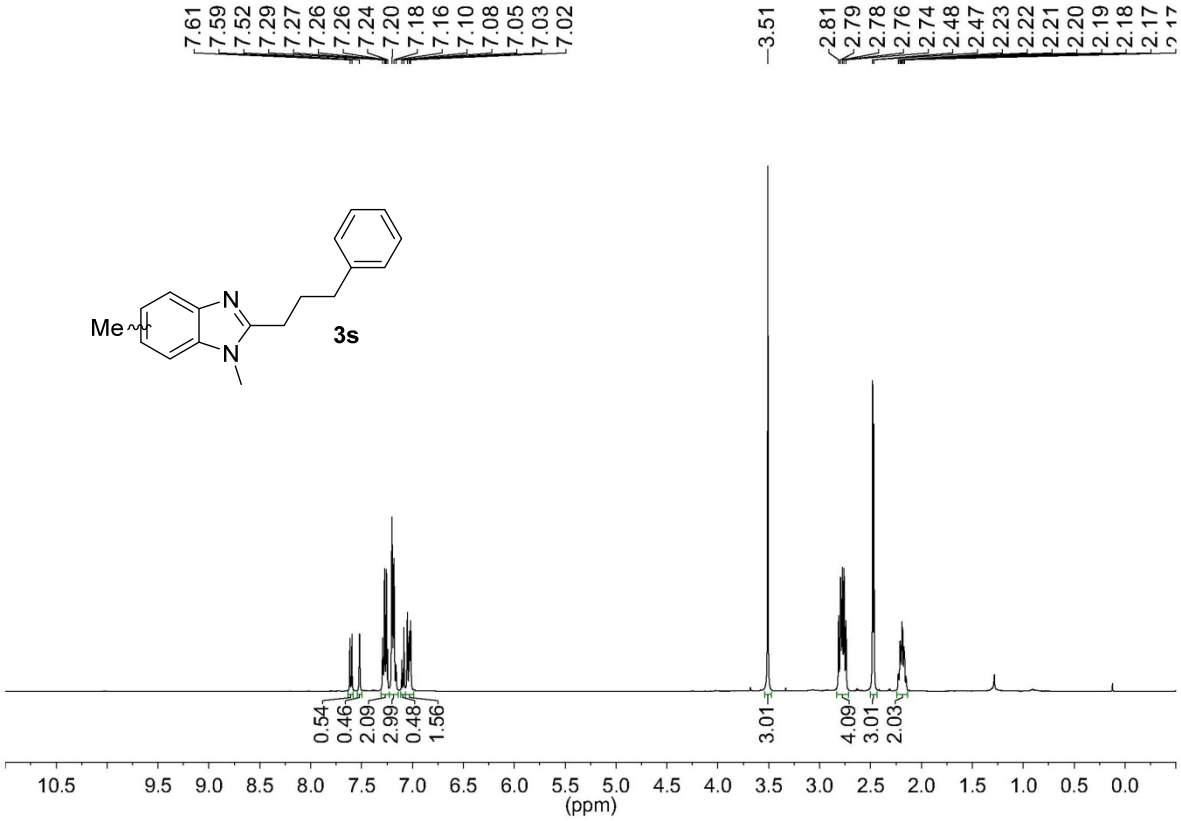
(ppm)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7.02
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2.20
2.19
2.18
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Me
N
N
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3.01
2.03
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5.5
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4.5
4.0
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3.0
2.5
2.0
1.5
1.0
0.5
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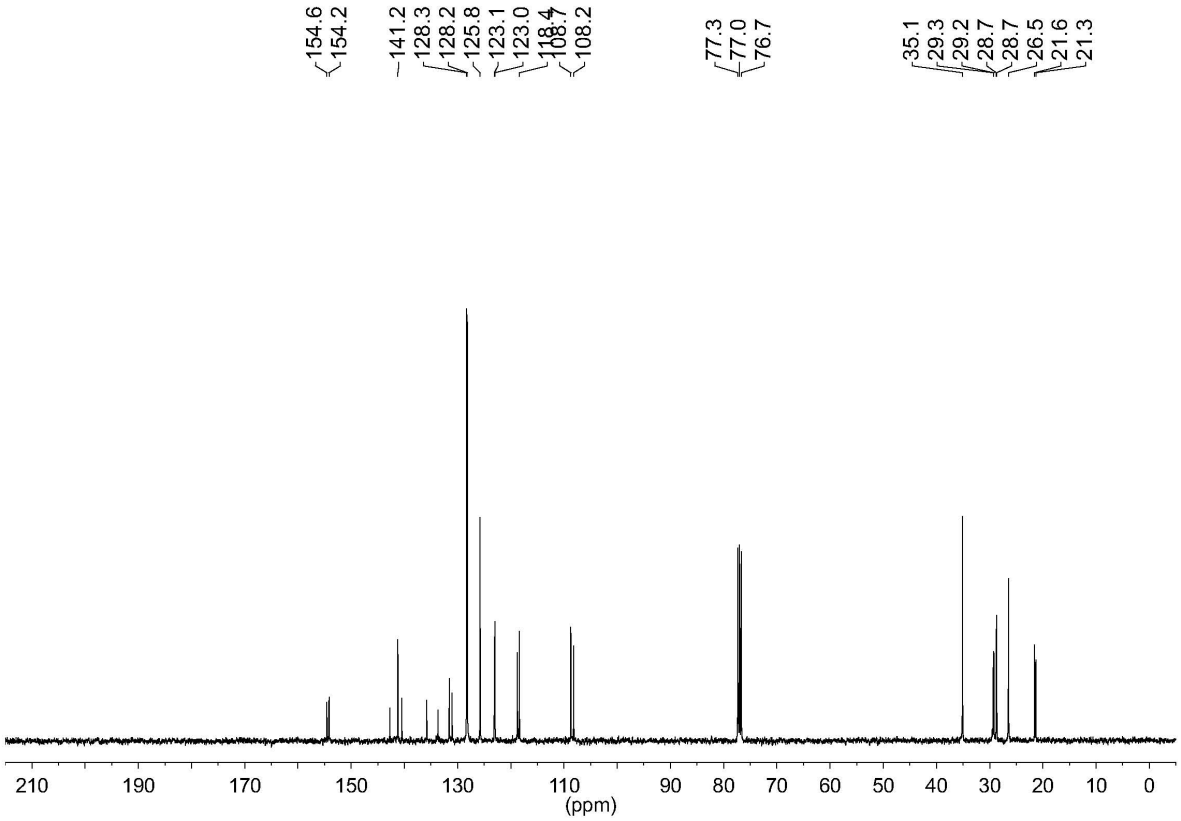
(ppm)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154.2
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128.2
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123.0
118.4
108.7
108.2
77.3
77.0
76.7
35.1
29.3
29.2
28.7
28.7
26.5
21.6
21.3
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190
170
150
130
110
90
80
70
60
50
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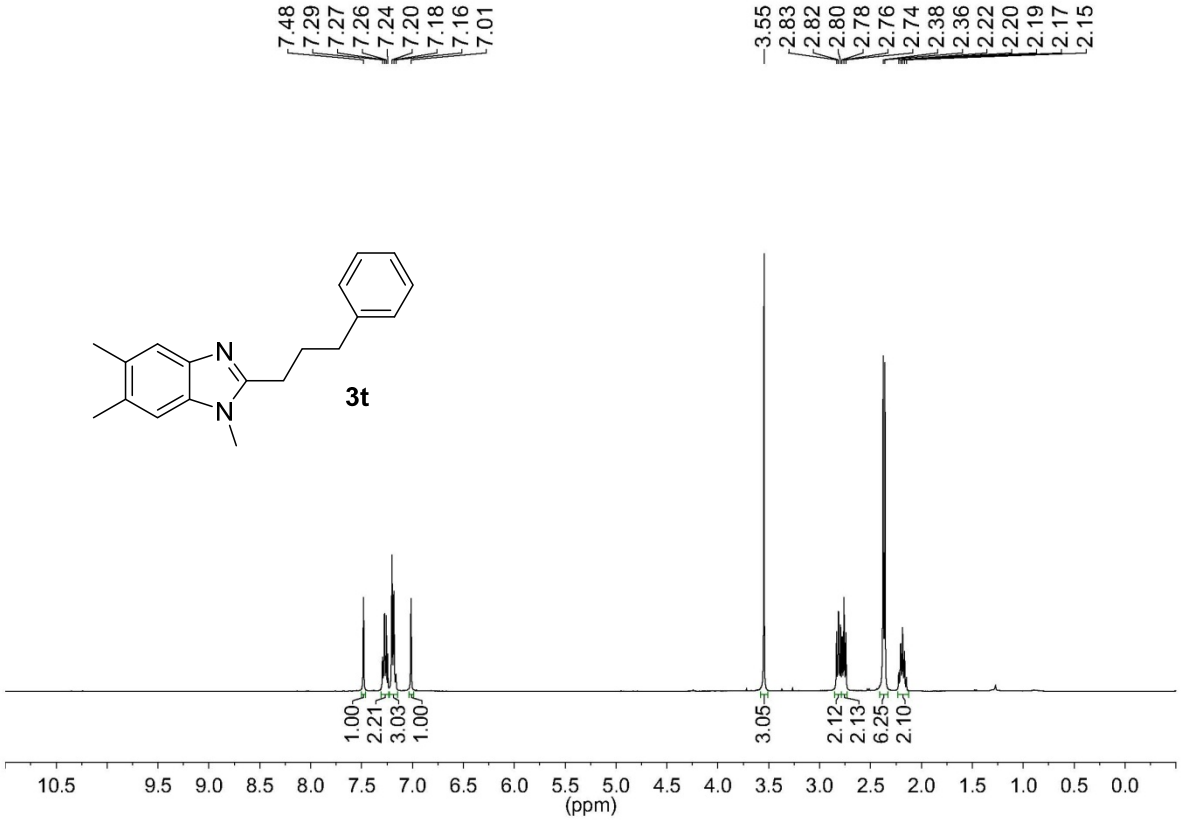
(ppm)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7.01
3.55
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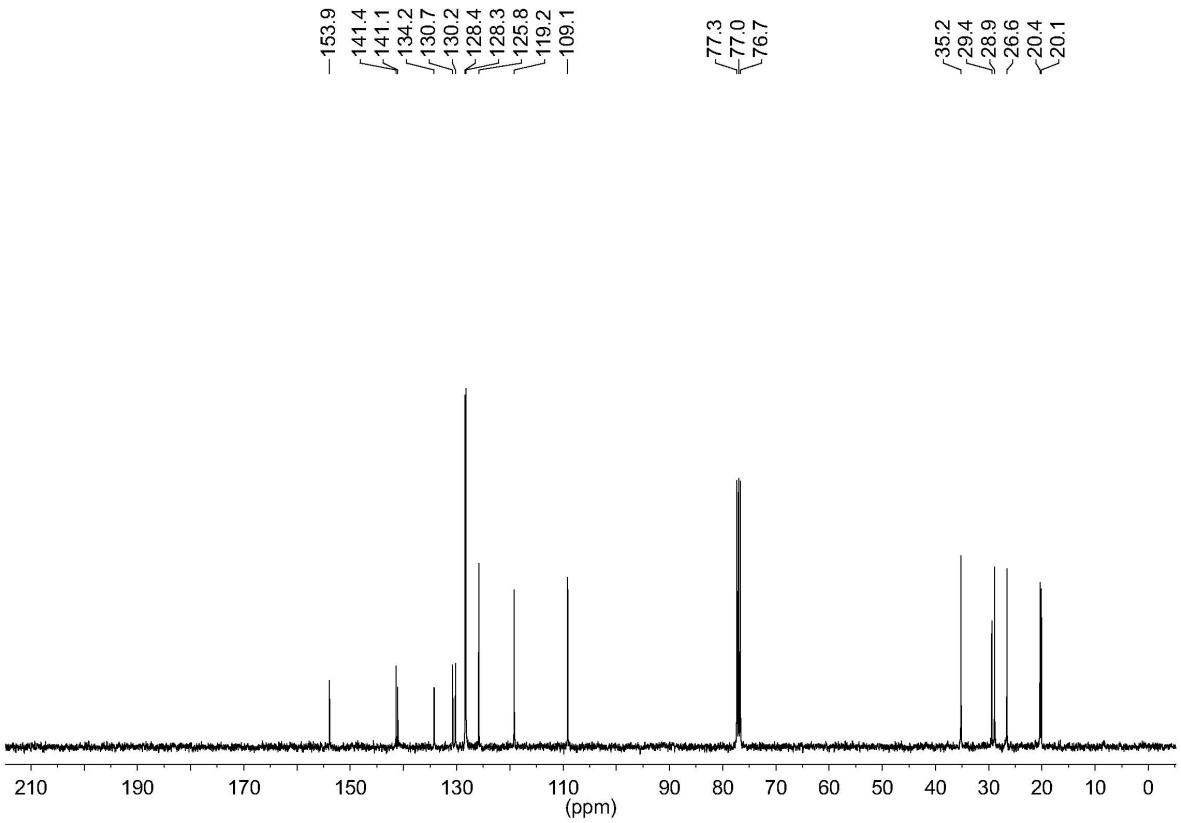
2.82
2.80
2.78
2.76
2.74
2.38
2.36
2.22
2.20
2.19
2.17
2.15
N
N
3t
1.00
2.21
3.03
1.00
3.05
2.12
2.13
6.25
2.10
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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130.2
128.4
128.3
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119.2
109.1
77.3
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29.4
28.9
26.6
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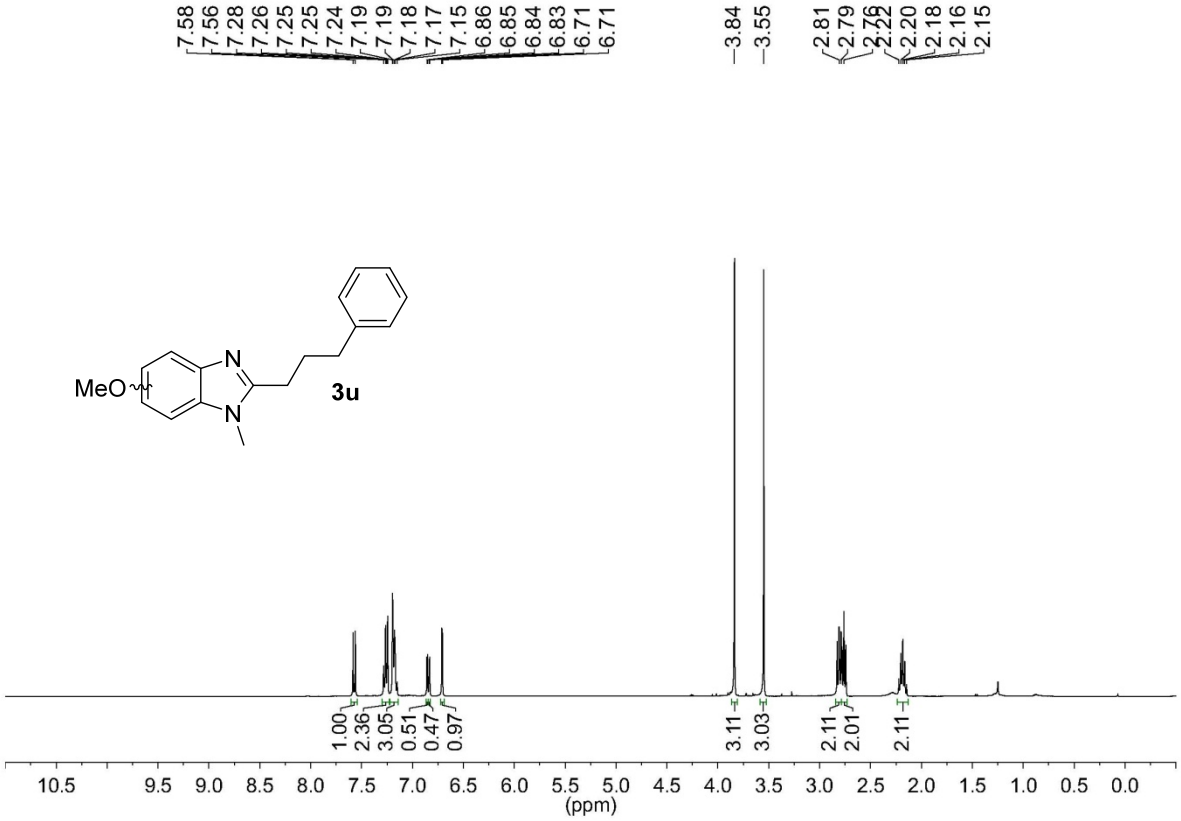
20.1
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
(ppm)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7.17
7.15
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6.85
6.84
6.83
6.71
6.71
3.84
3.55
2.81
2.79
2.76
2.22
2.20
2.18
2.16
2.15
MeO
N
N
3u
1.00
2.36
3.05
0.51
0.47
0.97
3.11
3.03
2.11
2.01
2.11
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
1.5
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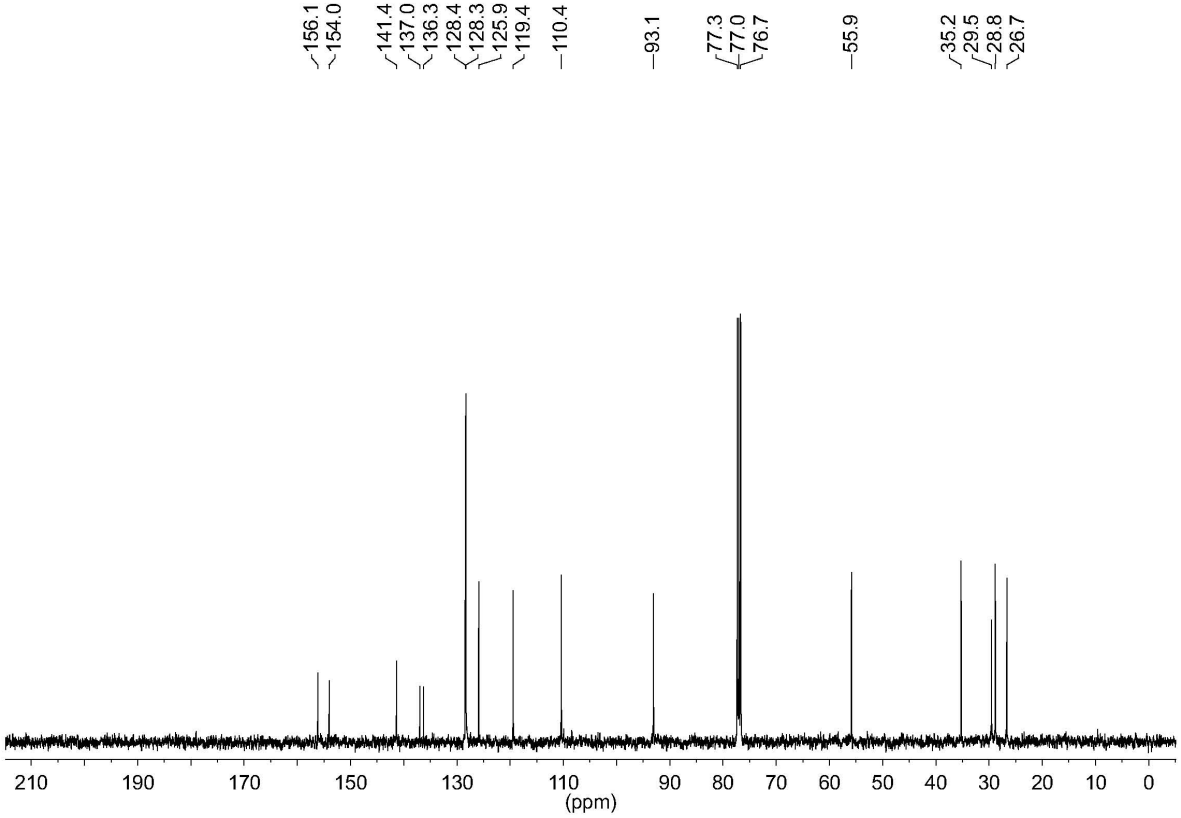
0.0
(ppm)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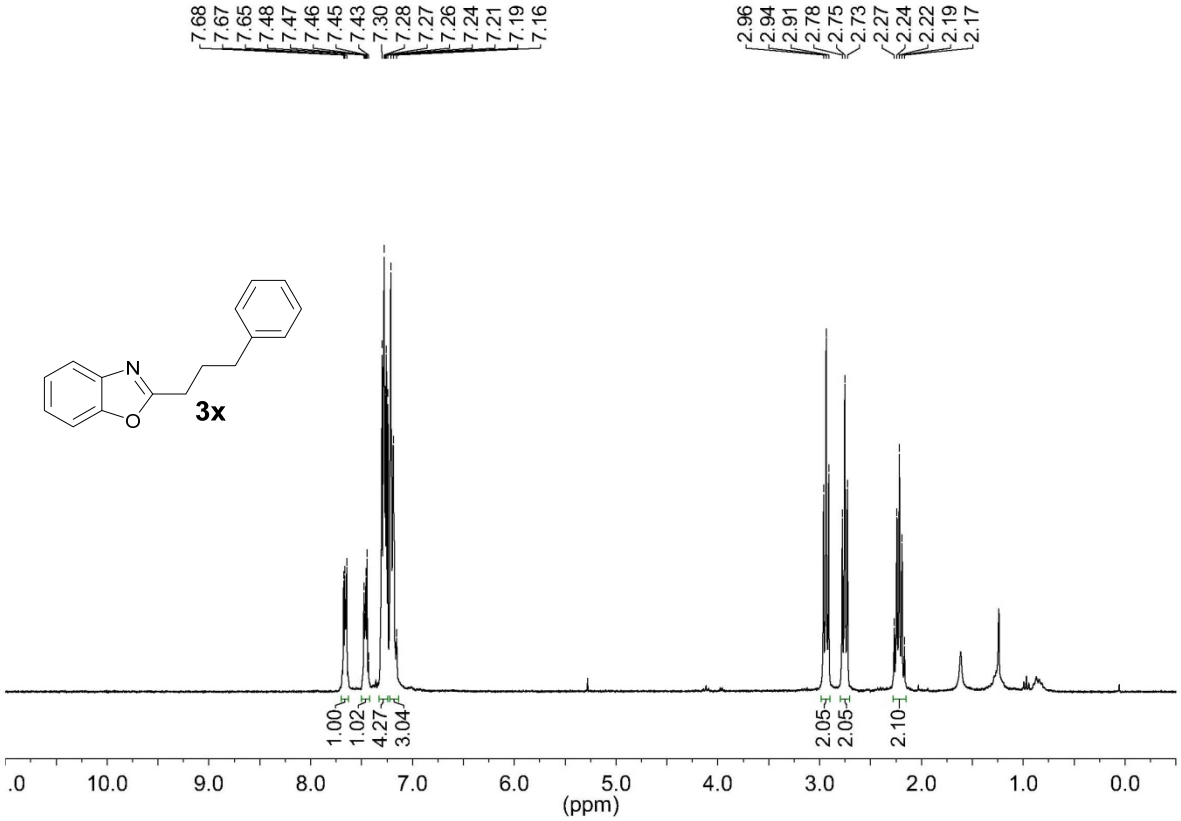
154.0
141.4
137.0
136.3
128.4
128.3
125.9
119.4
110.4
93.1
77.3
77.0
76.7
55.9
35.2
29.5
28.8
26.7
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
(ppm)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7.43
7.30
7.28
7.27
7.26
7.24
7.21
7.19
7.16
2.96
2.94
2.91
2.78
2.75
2.73
2.27
2.24
2.22
2.19
2.17
N
O
3x
1.00
1.02
4.27
3.04
2.05
2.05
2.10
.0
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8.0
7.0
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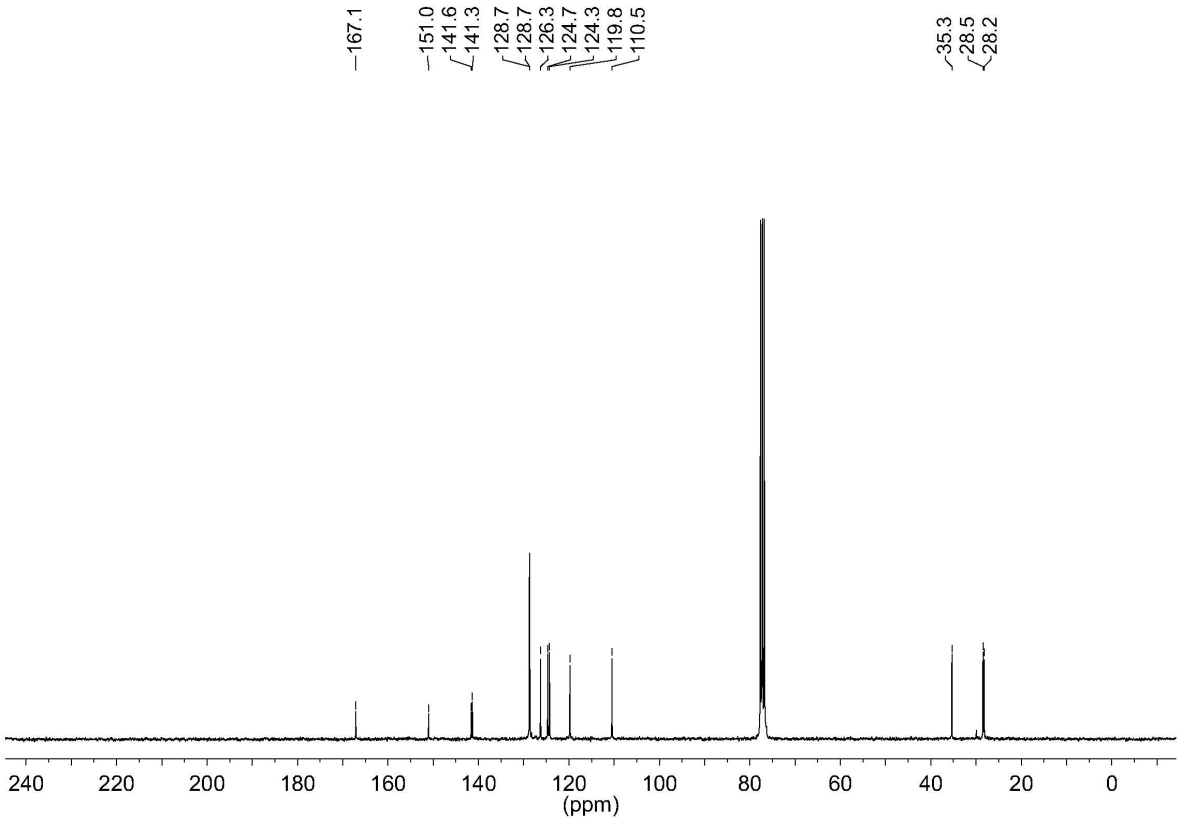
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)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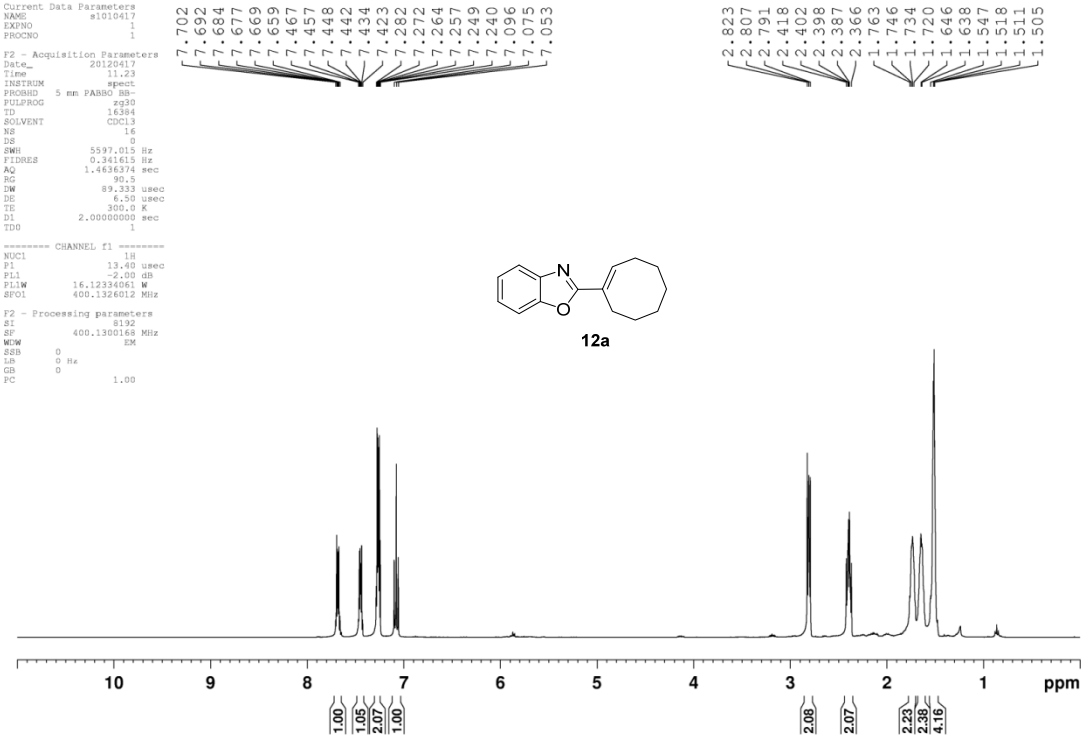
141.6
141.3
128.7
128.7
126.3
124.7
124.3
119.8
110.5
35.3
28.5
28.2
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)


Current Data Parameters
NAME s1010417
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120417
Time 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636374 sec
RG 90.5
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.40 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1326012 MHz
F2 - Processing parameters
SI 8192
SF 400.1300168 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
7.702
7.692
7.684
7.677
7.669
7.659
7.467
7.457
7.448
7.442
7.434
7.423
7.282
7.272
7.264
7.257
7.249
7.240
7.096
7.075
7.053
2.823
2.807
2.791
2.418
2.402
2.398
2.387
2.366
1.763
1.746
1.734
1.720
1.646
1.638
1.547
1.518
1.511
1.505
N
O
12a
10
9
8
7
6
5
4
3
2
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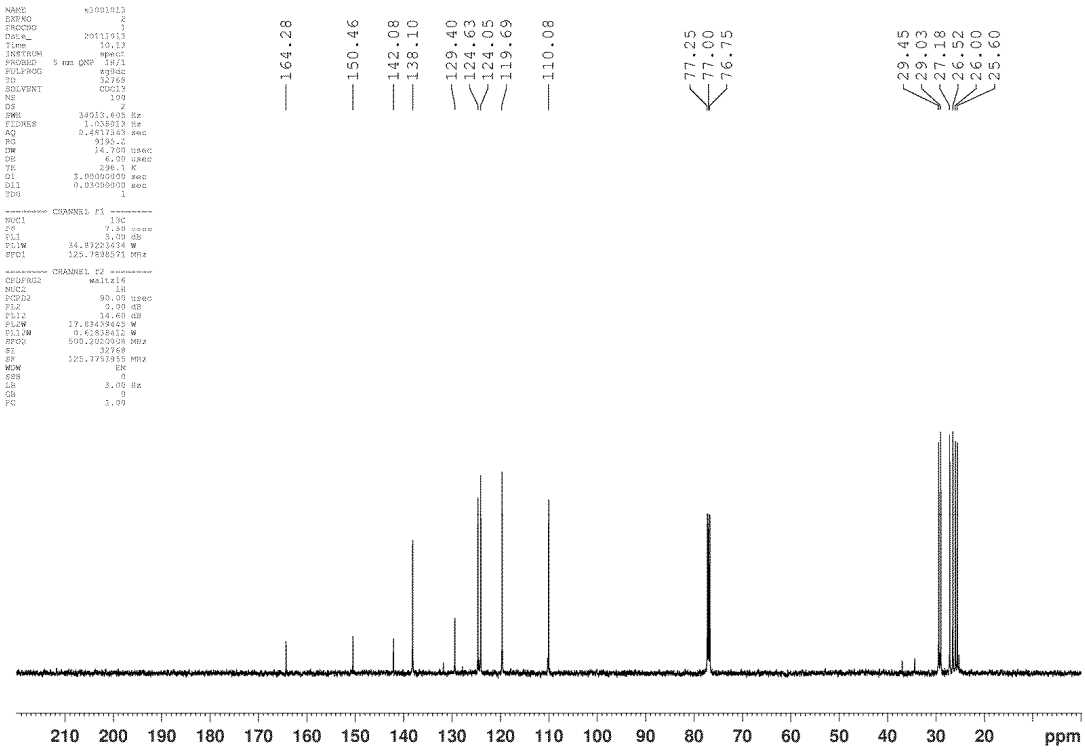
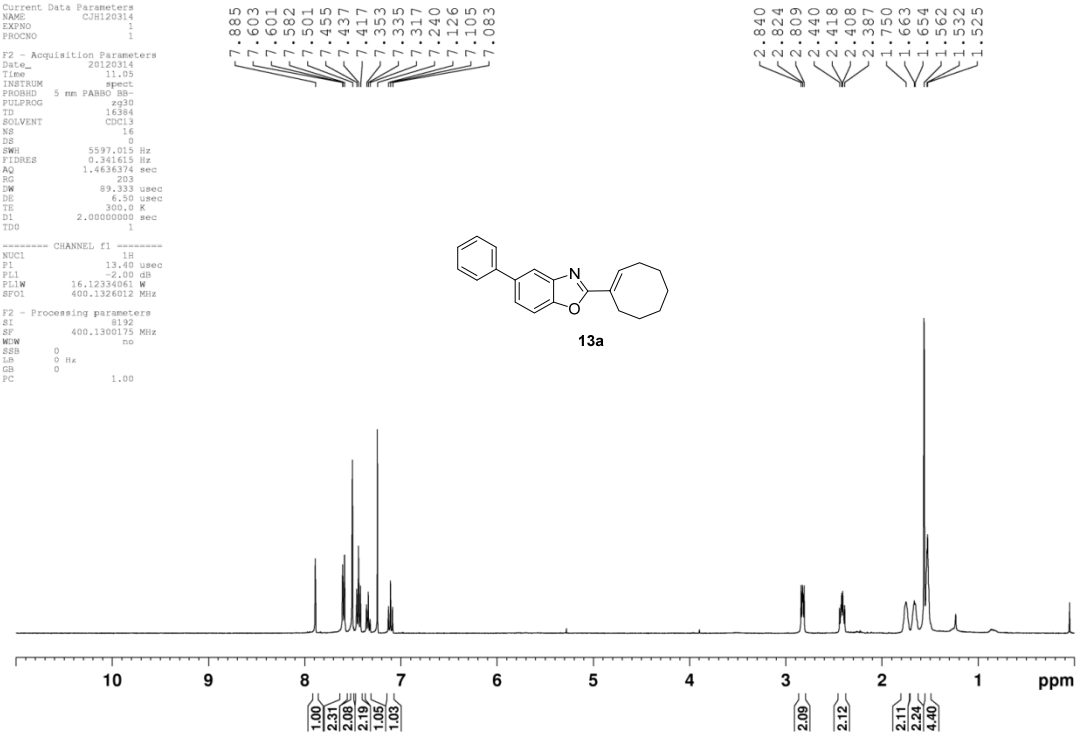
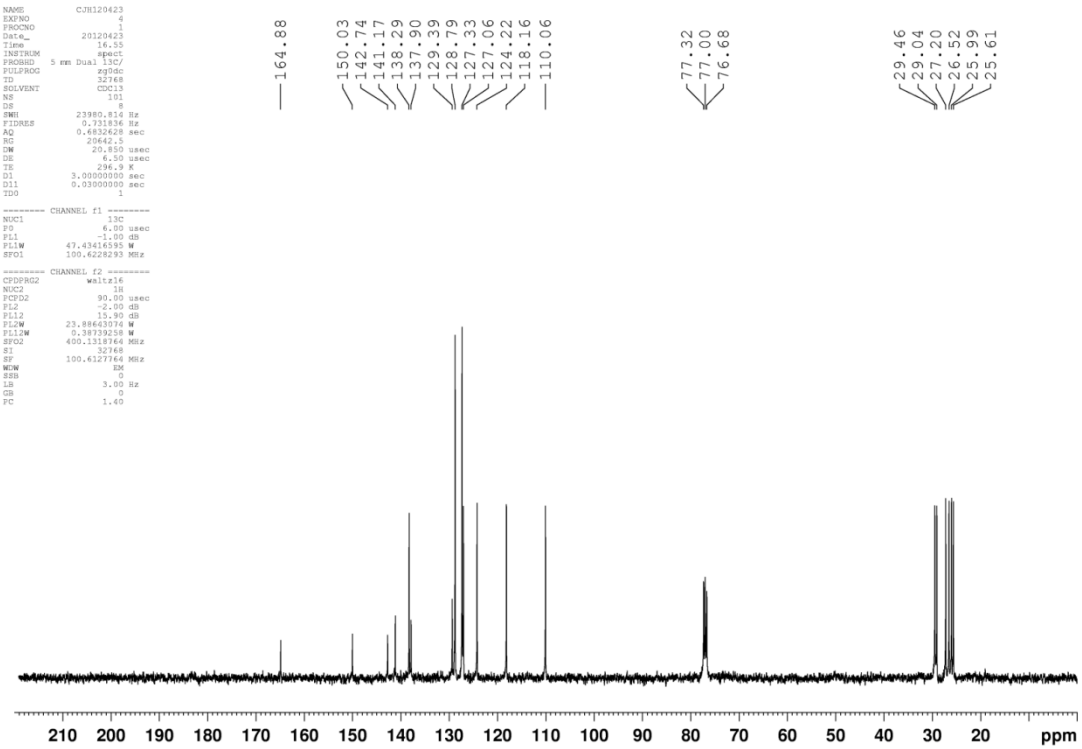
ppm
1.00
1.05
2.07
1.00
2.08
2.07
2.23
2.38
4.16

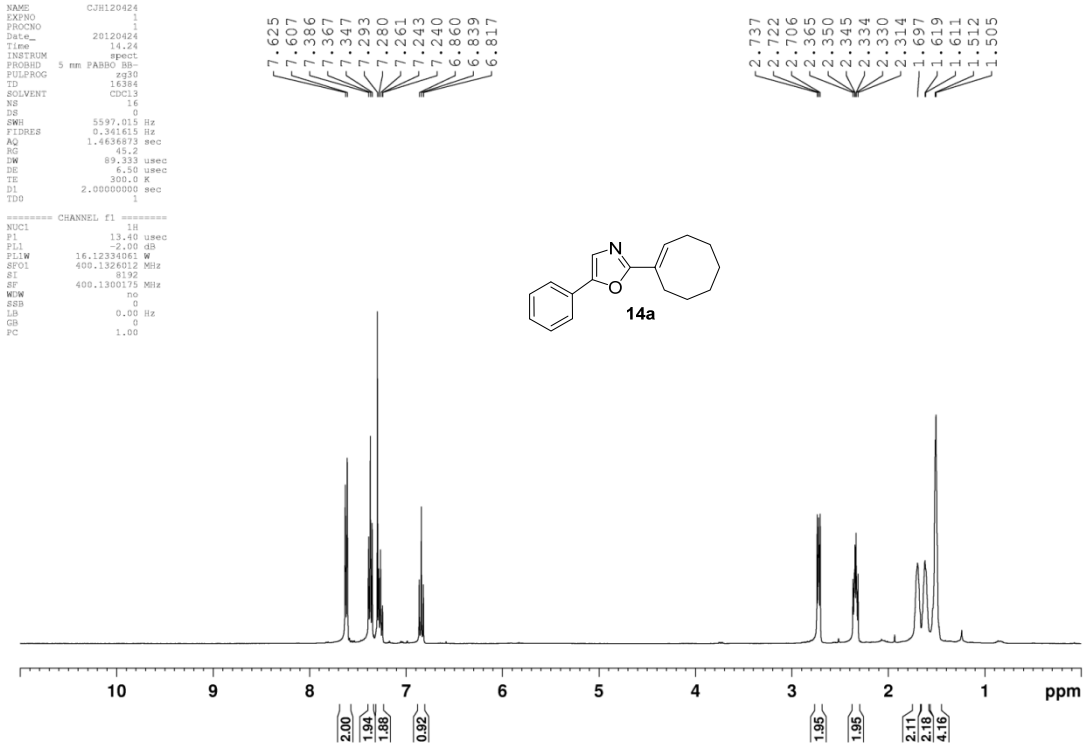

NAME s1001013
EXPNO 2
PROCNO 1
Date_ 20111913
Time 10.13
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgdec
TD 32768
SOLVENT CDCl3
NS 109
DS 2
SWH 34013.605 Hz
FIDRES 1.038513 Hz
AQ 0.4817543 sec
RG 9193.2
DW 14.700 usec
DE 6.00 usec
TE 296.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P0 7.80 usec
PL1 3.00 dB
PL1W 34.87223434 W
SFO1 125.7898571 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 14.60 dB
PL2W 17.83439443 W
PL12W 0.62838412 W
SFO2 500.2020004 MHz
SI 32768
SF 125.7753955 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
164.28
150.46
142.08
138.10
129.40
124.63
124.05
119.69
110.08
77.25
77.00
76.75
29.45
29.03
27.18
26.52
26.00
25.60
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

```
Current Data Parameters
NAME          CJH120314
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20120314
Time               11.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5597.015 Hz
FIDRES         0.341615 Hz
AQ            1.4636374 sec
RG                  203
DW               89.333 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                13.40 usec
PL1               -2.00 dB
PL1W        16.12334061 W
SFO1       400.1326012 MHz

F2 - Processing parameters
SI                 8192
SF          400.1300175 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```




```
NAME          CJH120423
EXPNO                 4
PROCNO                1
Date_           20120423
Time               16.55
INSTRUM            spect
PROBHD   5 mm Dual 13C/
PULPROG           zgdc
TD                32768
SOLVENT           CDCl3
NS                  101
DS                    8
SWH            23980.814 Hz
FIDRES         0.731836 Hz
AQ            0.6832628 sec
RG              20642.5
DW               20.850 usec
DE                6.50 usec
TE               296.9 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P0                 6.00 usec
PL1               -1.00 dB
PL1W        47.43416595 W
SFO1       100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -2.00 dB
PL12              15.90 dB
PL2W        23.88643074 W
PL12W        0.38739258 W
SFO2       400.1318764 MHz
SI                32768
SF         100.6127764 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.40
```




NAME CJH120424
EXPNO 1
PROCNO 1
Date_ 20120424
Time 14.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 45.2
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.40 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1326012 MHz
SI 8192
SF 400.1300175 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.625
7.607
7.386
7.367
7.347
7.293
7.280
7.261
7.243
7.240
6.860
6.839
6.817
2.737
2.722
2.706
2.365
2.350
2.345
2.334
2.330
2.314
1.697
1.619
1.611
1.512
1.505
N
O
14a
10
9
8
7
6
5
4
3
2
1
ppm
2.00
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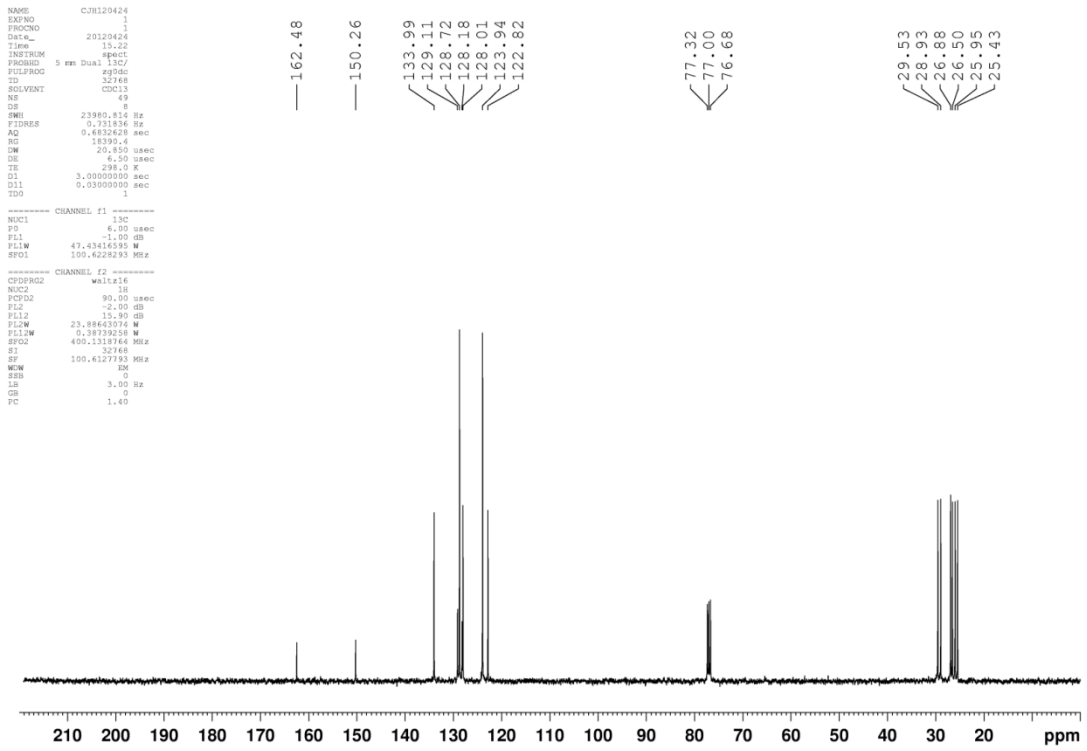
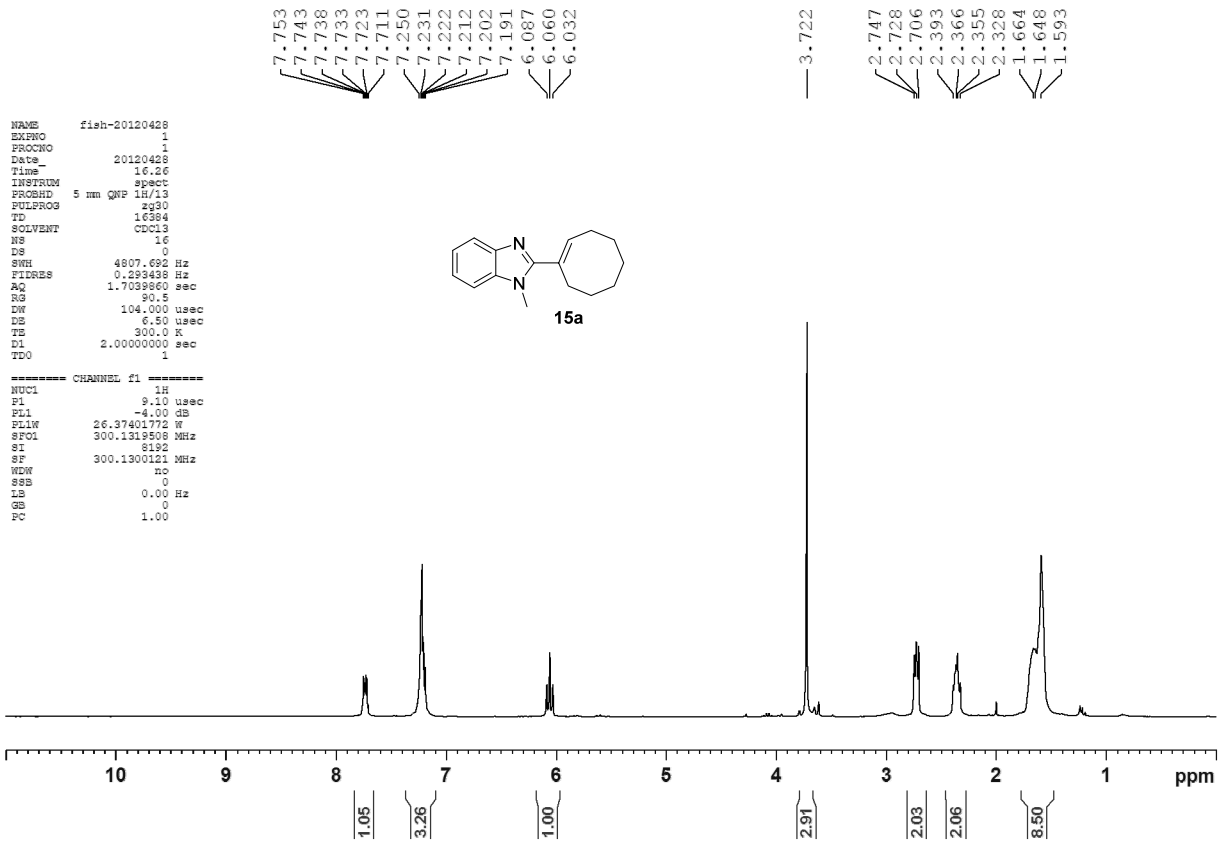
1.88
0.92
1.95
1.95
2.11
2.18
4.16


NAME CJH120424
EXPNO 1
PROCNO 1
Date_ 20120424
Time 15.22
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpdc
TD 32768
SOLVENT CDCl3
NS 49
DS 8
SWH 23980.814 Hz
FIDRES 0.731836 Hz
AQ 0.6832628 sec
RG 18390.4
DW 20.850 usec
DE 6.50 usec
TE 298.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P0 6.00 usec
PL1 -1.00 dB
PL1W 47.43416595 W
SFO1 100.6228293 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.90 dB
PL2W 23.88643074 W
PL12W 0.38739258 W
SFO2 400.1318764 MHz
SI 32768
SF 100.6127793 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
162.48
150.26
133.99
129.11
128.72
128.18
128.01
123.94
122.82
77.32
77.00
76.68
29.53
28.93
26.88
26.50
25.95
25.43
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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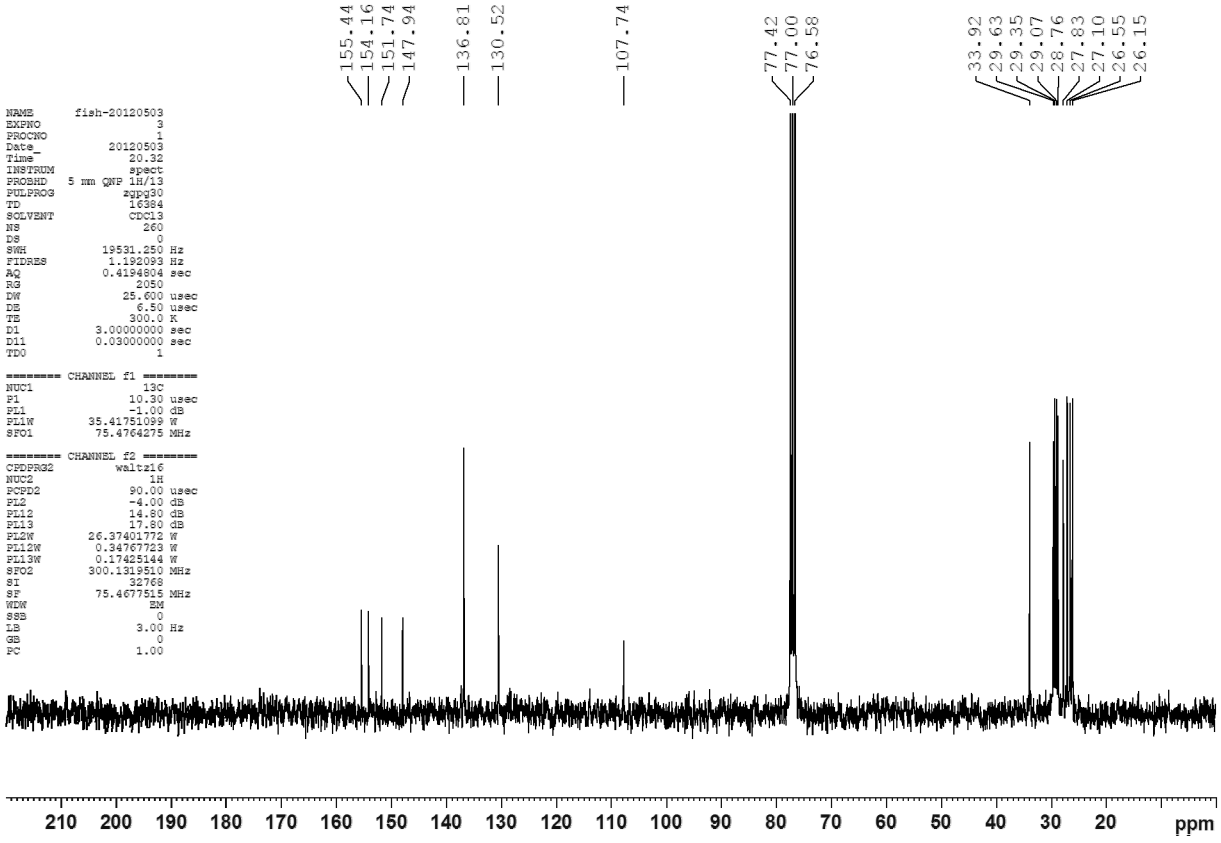
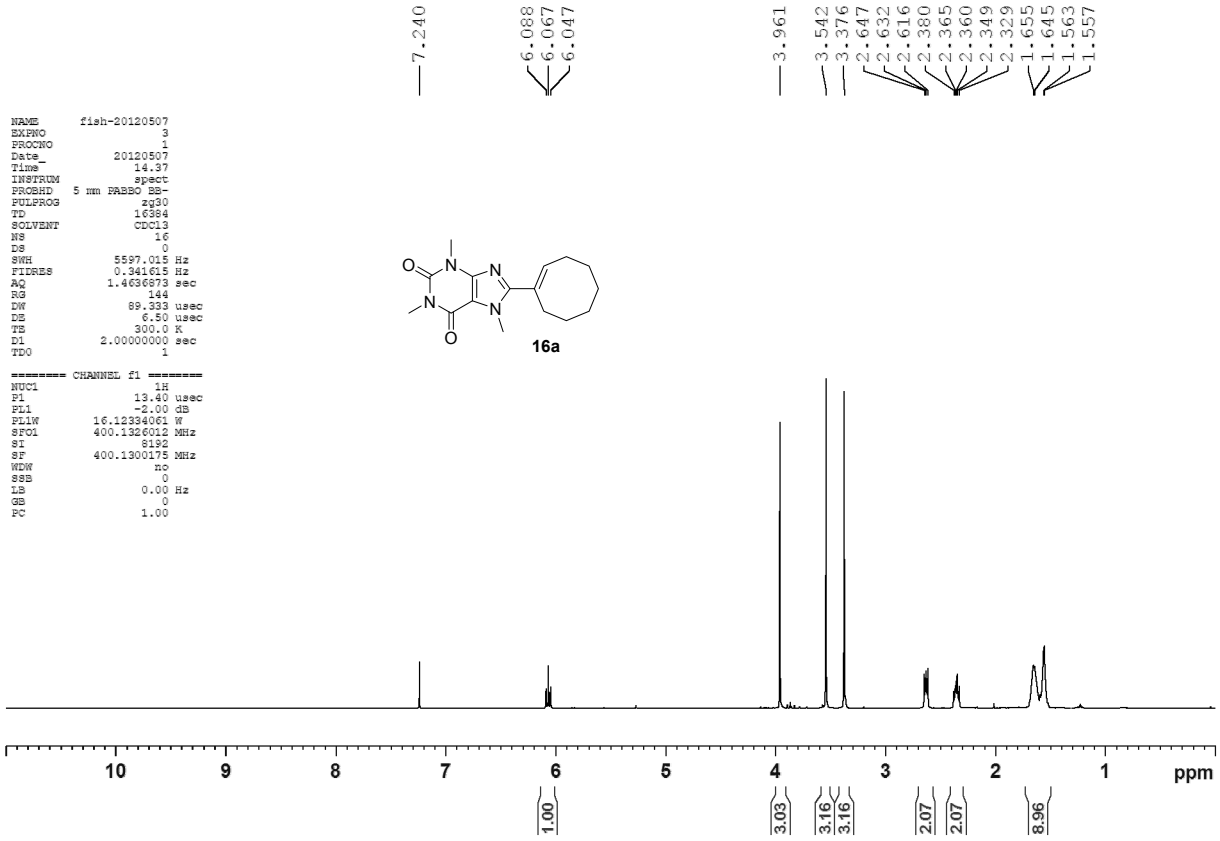
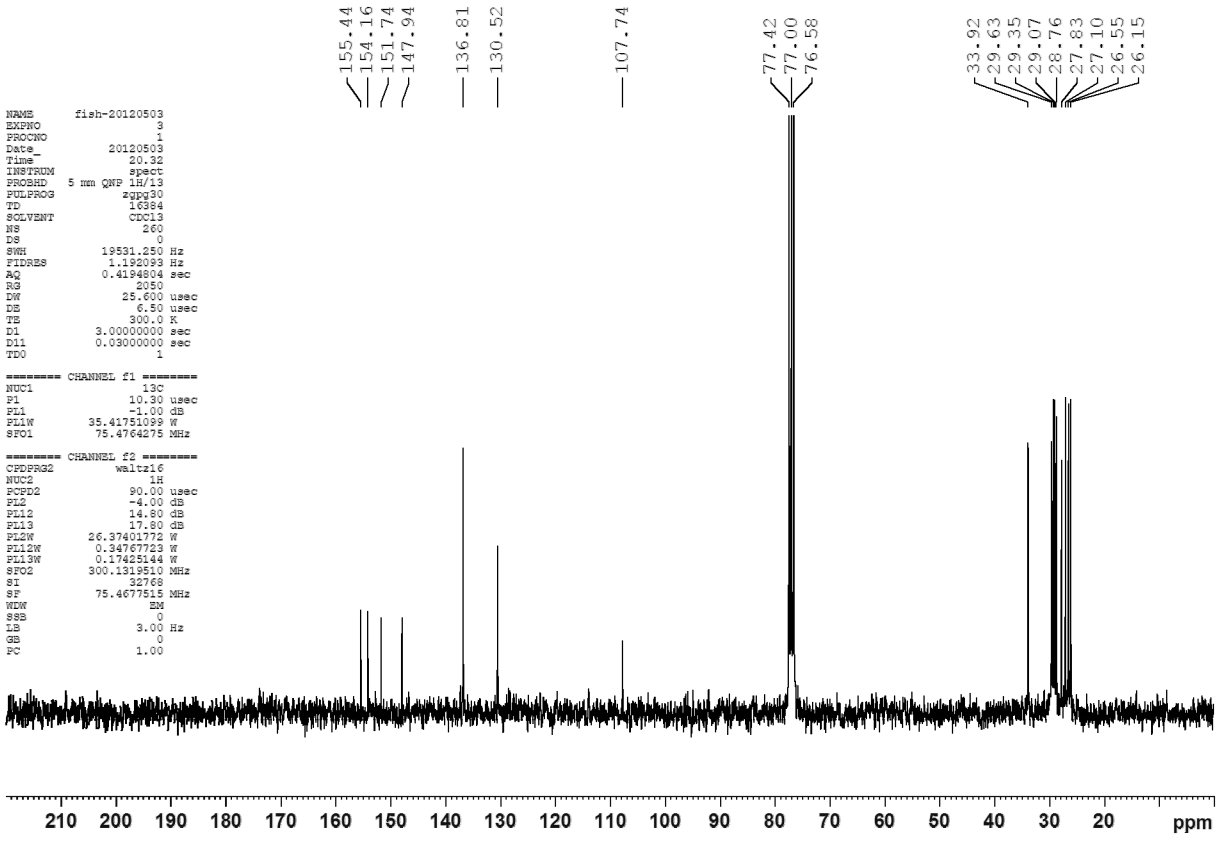
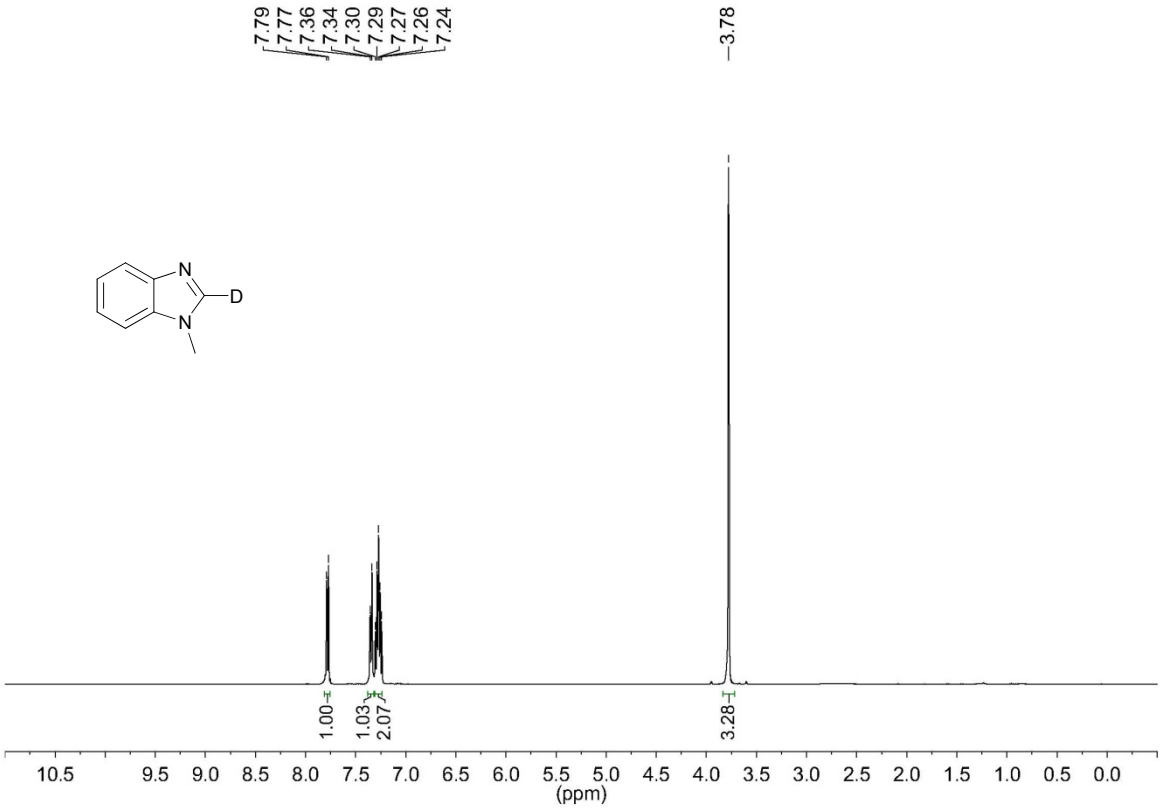
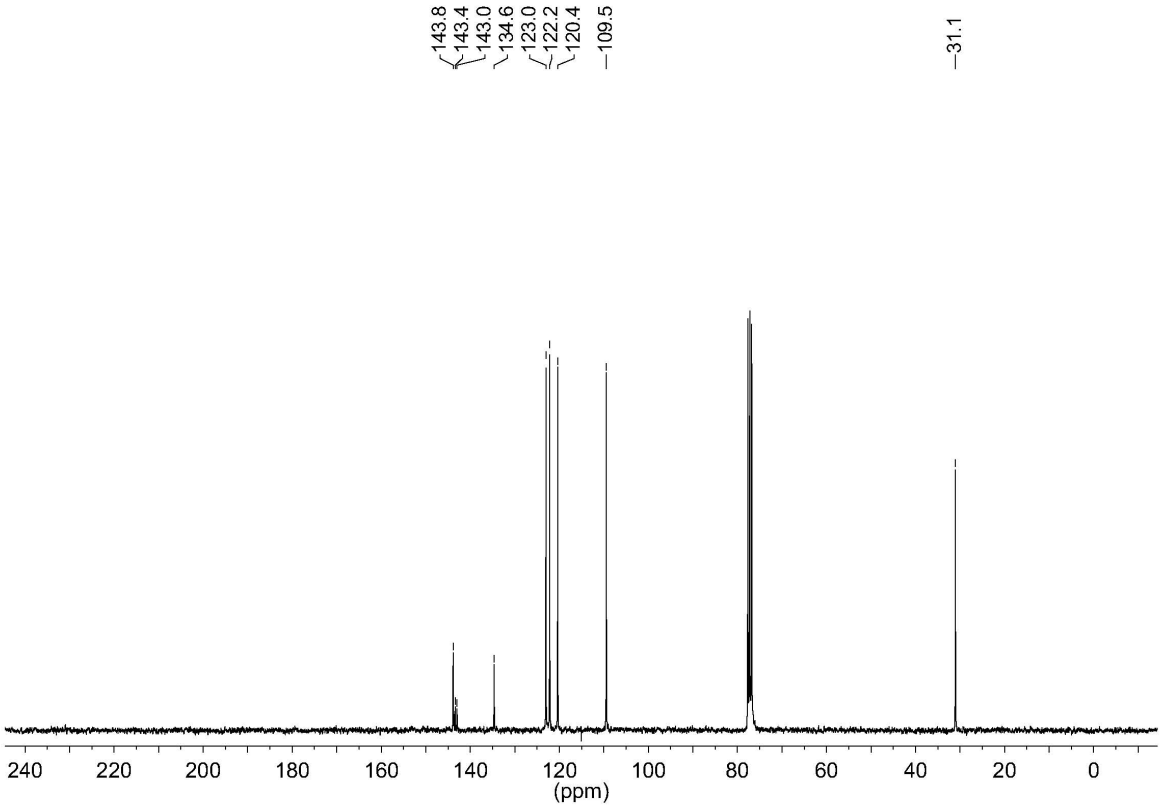
7.733
7.723
7.711
7.250
7.231
7.222
7.212
7.202
7.191
6.087
6.060
6.032
3.722
2.747
2.728
2.706
2.393
2.366
2.355
2.328
1.664
1.648
1.593
NAME fish-20120428
EXPNO 1
PROCNO 1
Date_ 20120428
Time 16.26
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 4807.692 Hz
FIDRES 0.293438 Hz
AQ 1.7039860 sec
RG 90.5
DW 104.000 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.10 usec
PL1 -4.00 dB
PL1W 26.37401772 W
SFO1 300.1319508 MHz
SI 8192
SF 300.1300121 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
N
15a
10
9
8
7
6
5
4
3
2
1
ppm
1.05
3.26
1.00
2.91
2.03
2.06
8.50


155.44
154.16
151.74
147.94
136.81
130.52
107.74
77.42
77.00
76.58
33.92
29.63
29.35
29.07
28.76
27.83
27.10
26.55
26.15
NAME fish-20120503
EXPNO 3
PROCNO 1
Date_ 20120503
Time 20.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 260
DS 0
SWH 19531.250 Hz
FIDRES 1.192093 Hz
AQ 0.4194804 sec
RG 2050
DW 25.600 usec
DE 6.50 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.30 usec
PL1 -1.00 dB
PL1W 35.41751099 W
SFO1 75.4764275 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 14.80 dB
PL13 17.80 dB
PL2W 26.37401772 W
PL12W 0.34767723 W
PL13W 0.17425144 W
SFO2 300.1319510 MHz
SI 32768
SF 75.4677515 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.240
6.088
6.067
6.047
3.961
3.542
3.376
2.647
2.632
2.616
2.380
2.365
2.360
2.349
2.329
1.655
1.645
1.563
1.557
NAME fish-20120507
EXPNO 3
PROCNO 1
Date_ 20120507
Time 14.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5597.015 Hz
FIDRES 0.341615 Hz
AQ 1.4636873 sec
RG 144
DW 89.333 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.40 usec
PL1 -2.00 dB
PL1W 16.12334061 W
SFO1 400.1326012 MHz
SI 8192
SF 400.1300175 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
16a
10
9
8
7
6
5
4
3
2
1
ppm
1.00
3.03
3.16
3.16
2.07
2.07
8.96


155.44
154.16
151.74
147.94
136.81
130.52
107.74
77.42
77.00
76.58
33.92
29.63
29.35
29.07
28.76
27.83
27.10
26.55
26.15
NAME fish-20120503
EXPNO 3
PROCNO 1
Date_ 20120503
Time 20.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 260
DS 0
SWH 19531.250 Hz
FIDRES 1.192093 Hz
AQ 0.4194304 sec
RG 2050
DW 25.600 usec
DE 6.50 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.30 usec
PL1 -1.00 dB
PL1W 35.41751099 W
SFO1 75.4764275 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 14.80 dB
PL13 17.80 dB
PL2W 26.37401772 W
PL12W 0.34767723 W
PL13W 0.17425144 W
SFO2 300.1319510 MHz
SI 32768
SF 75.4677515 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.79
7.77
7.36
7.34
7.30
7.29
7.27
7.26
7.24
3.78
N
D
N
1.00
1.03
2.07
3.28
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)


143.8
143.4
143.0
134.6
123.0
122.2
120.4
109.5
31.1
240 220 200 180 160 140 120 100 80 60 40 20 0
(ppm)