Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Three Component Photoredox 1,2-Alkylamination of Styrenes with Alkanes and Nitrogen Nucleophiles via C(sp^3)-H bond Cleavage

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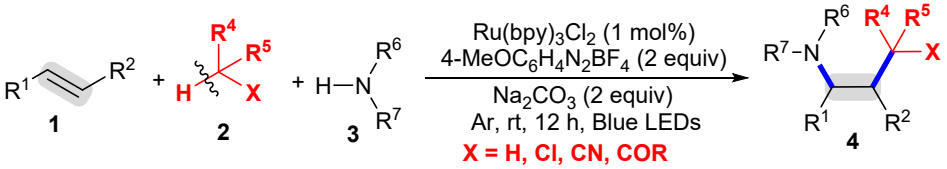
(A) Typical experimental procedure

(a) General

The ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ solvent on a NMR spectrometer using TMS as internal standard. HRMS was measured on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry. Melting points are uncorrected.

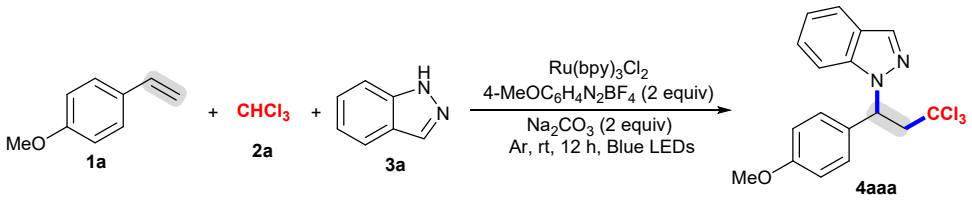
(b) General procedure for the synthesis of 4.



To a Schlenk tube were added $Ru(bpy)_3Cl_2$ (0.002 mmol, 1 mol%), Na_2CO_3 (0.4 mmol, 2 equiv), Nitrogen Nucleophiles **3** (0.4 mmol), alkanes **2** (1 mL). Finally, to this Schlenk tube was successively added 4-$MeOC_6H_4N_2BF_4$ (0.4 mmol, 2 equiv), alkene **1** (0.2 mmol), and alkanes **2** (3 mL), the tube was then charged with argon. The mixture was stirred under 18 W blue LEDs at room temperature until complete consumption of starting material as monitored by TLC and/or GC-MS analysis (about 12 h). After the reaction was finished, the combined organic phases concentrated, and the resulting residue was purified by silica gel column chromatography (petroleum/ethyl acetate) to afford the desired product **4**.

(c) Screening of optimal reaction conditions

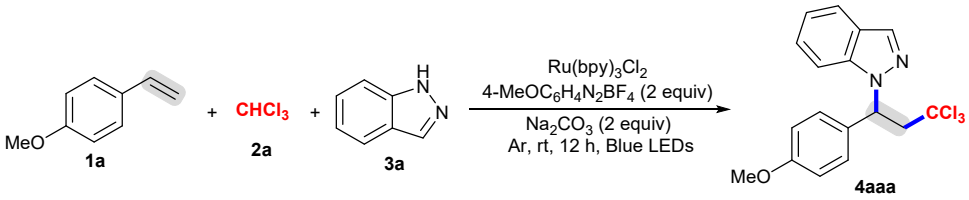
Table S1. Screening of optimal reaction conditions[a]



Entry	Additive/10 mol%	Ligand/20 mol%	Solvent	Yield (%)
1	CuTc	Phen	$CHCl_3$	71
2	$Cu(MeCN)_4BF_4$	Phen	$CHCl_3$	47
3	$Cu(MeCN)_4PF_6$	Phen	$CHCl_3$	46
4	\	Phen	$CHCl_3$	60
5	CuTc	\	$CHCl_3$	70
6	$FeCl_2$	\	$CHCl_3$	67
7	$B(C_6F_5)_3$	\	$CHCl_3$	44
8	$Yb(OTf)_3$	\	$CHCl_3$	38
9	$In(OTf)_3$	\	$CHCl_3$	40
10	$FeCl_3$	\	$CHCl_3$	61
11[b]	\	\	PhCl	20
12[b]	\	\	$PhCF_3$	28
13[b]	\	\	DMSO	trace
14[b]	\	\	DMA	trace
15[b]	\	\	DMF	trace
16[b]	\	\	toluene	12
17[c]	\	\	$CHCl_3$	22
18[d]	\	\	$CHCl_3$	60
19[e]	\	\	$CHCl_3$	80

[a] Reaction conditions: **1a** (0.2 mmol), $CHCl_3$ **2a** (4 mL), **3a** (2 equiv), $Ru(bpy)_3Cl_2$ (1 mol%), Na_2CO_3 (2 equiv), 4-$MeOC_6H_4N_2BF_4$ (2 equiv), room temperature, 18 W blue LEDs, argon, and 12 h. [b] $CHCl_3$ (2 mmol), solvents (4 mL). [c] 18 W White LEDs. [d] 4-$MeOC_6H_4N_2BF_4$ (1 equiv). [e] 4-$MeOC_6H_4N_2BF_4$ (3 equiv).

Table S2. Screening of optimal reaction conditions for base [a]

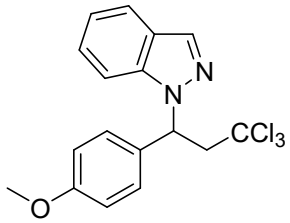


Entry	base	Yield (%)
1	Cs_2CO_3 instead of Na_2CO_3	14
2	K_3PO_4 instead of Na_2CO_3	20
3	Et_3N instead of Na_2CO_3	42
4	2,6-Lutidine instead of Na_2CO_3	41
5	$NaHCO_3$ instead of Na_2CO_3	44
6	*t*-BuONa instead of Na_2CO_3	NR
7	NaOH instead of Na_2CO_3	8
8	K_2CO_3 instead of Na_2CO_3	56
9	KOAc instead of Na_2CO_3	46
10	DBU instead of Na_2CO_3	24
11	Without Na_2CO_3	34
12	Na_2CO_3 (1 equiv)	70
13	Na_2CO_3 (3 equiv)	77

[a] Reaction conditions: **1a** (0.2 mmol), $CHCl_3$ **2a** (4 mL), **3a** (2 equiv), $Ru(bpy)_3Cl_2$ (1 mol%), Na_2CO_3 (2 equiv), 4-$MeOC_6H_4N_2BF_4$ (2 equiv), room temperature, 18 W blue LEDs, argon, and 12 h.

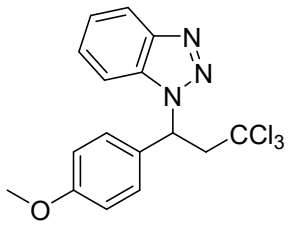
(B) Analytical data

1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-indazole (4aaa)



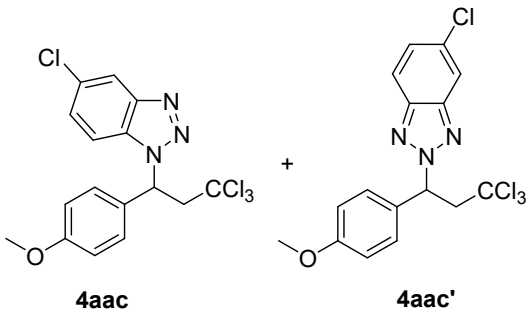
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.76-7.74 (m, 1H), 7.61-7.59 (m, 1H), 7.36 (d, *J* = 9.0 Hz, 2H), 7.27-7.24 (m, 1H), 7.07-7.05 (m, 1H), 6.85 (d, *J* = 9.0 Hz,, 2H), 6.00-5.98 (m, 1H), 4.54-4.49 (m, 1H), 3.75 (s, 3H), 3.57-3.54 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 148.8, 131.4, 128.2, 126.0, 123.2, 121.9, 121.7, 120.2, 117.8, 114.2, 97.1, 64.4, 58.7, 55.3; LRMS (EI, 70eV) *m/z* (%): 370 (M^+ + 2, 12), 368 (M^+, 212), 244 (25), 217 (100), 155 (48); HRMS *m/z* (ESI) calcd for $C_{17}H_{16}ON_2{}^{35}Cl_3$ ($[M+H]^+$) 369.0323, found 369.0321.

1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*][1,2,3]triazole (4aab)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87-7.85 (m, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.38-7.36 (m, 2H), 6.87 (d, *J* = 8.5 Hz, 2H), 6.48-6.46 (m, 1H), 4.60-4.57 (m, 1H), 3.77 (s, 3H), 3.63-3.59 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.9, 144.3, 130.3, 128.4, 126.5, 118.3, 114.4, 96.6, 67.5, 58.8, 55.3; LRMS (EI, 70eV) *m/z* (%): 371 (M^+ + 2, 16), 369 (M^+, 16), 251 (48), 155 (100), 134 (10); HRMS *m/z* (ESI) calcd for $C_{16}H_{15}ON_3{}^{35}Cl_3$ ($[M+H]^+$) 370.0275, found 370.0274.

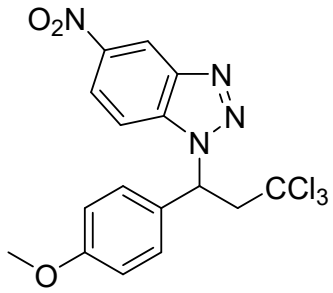
5-Chloro-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*][1,2,3]triazole (4aac) and 5-chloro-2-(3,3,3-trichloro-1-(4-methoxyphenyl)propyl)-2*H*-benzo[*d*][1,2,3]triazole (4aac')



4aac **4aac'**

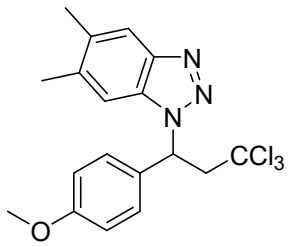
4aac:**4aac'** = 1:1; Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (s, 0.53H), 7.99 (m, 0.48H), 7.54-7.44 (m, 2H), 7.37-7.27 (m, 2H), 6.92-6.82 (m, 2H), 6.20-6.16 (m, 1H), 4.61 (s, 1H), 3.77 (s, 3H), 3.67-3.65 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 146.7, 134.2, 129.9 128.6, 128.1, 125.5, 121.1, 119.5, 114.6, 110.2, 109.1, 96.6, 60.2 (2C), 58.4, 55.3; LRMS (EI, 70eV) *m/z* (%): 405 (M^+ + 2, 16), 403 (M^+, 12), 251 (53), 201 (27), 155 (100); HRMS *m/z* (ESI) calcd for $C_{16}H_{14}ON_3{}^{35}Cl_4$ ($[M+H]^+$) 403.9885, found 403.9886.

5-Nitro-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*][1,2,3]triazole (4aad)



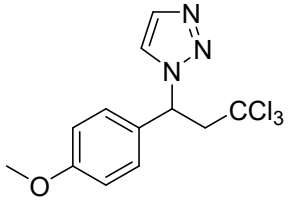
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (s, 1H), 8.33 (s, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 9.5 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.05-6.03 (m, 1H), 4.52-4.47 (m, 1H), 3.79 (s, 3H), 3.58-3.54 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 149.7, 143.2, 130.3, 128.4, 127.4, 120.4, 120.0, 119.5, 118.8, 114.5, 96.7, 65.2, 58.4, 55.3.

5,6-Dimethyl-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*][1,2,3]triazole (4aae)



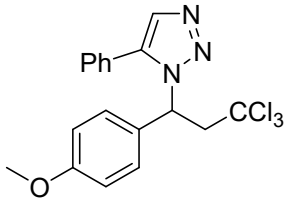
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (s, 2H), 7.43 (d, *J* = 8.5 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 6.44-6.40 (m, 1H), 4.58-4.53 (m, 1H), 3.75 (s, 3H), 3.58-3.54 (m, 1H), 2.37 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 143.7, 137.0, 130.5, 128.2, 116.7, 114.3, 96.7, 67.1, 58.8, 55.3, 20.8; LRMS (EI, 70eV) *m/z* (%): 399 (M^+ + 2, 15), 397 (M^+, 15), 238 (26), 215 (18), 155 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{19}ON_3{}^{35}Cl_3$ ($[M+H]^+$) 398.0588, found 398.0586.

1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1H-1,2,3-triazole (4aaf)



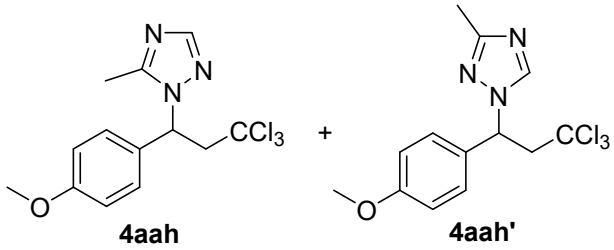
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.59 (s, 1H), 7.33 (d, *J* = 8.5 Hz, 2H), 6.89 (d, *J* = 8.5 Hz, 2H), 6.01-5.99 (m, 1H), 4.39-4.34 (m, 1H), 3.79 (s, 3H), 3.56-3.53 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 134.0, 130.2, 128.2, 123.8, 114.5, 96.5, 62.1, 58.6, 55.3; LRMS (EI, 70eV) *m/z* (%): 321 (M^+ + 2, 15), 319 (M^+, 15), 174 (61), 155 (77), 133 (100); HRMS *m/z* (ESI) calcd for $C_{12}H_{13}ON_3{}^{35}Cl_3$ ($[M+H]^+$) 320.0119, found 320.0115.

5-Phenyl-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-1,2,3-triazole (4aag)



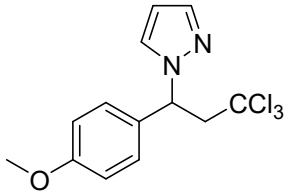
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.79 (d, *J* = 7.5 Hz, 2H), 7.42-9.39 (m, 4H), 7.35-7.32 (m, 1H), 6.87 (d, *J* = 9.0 Hz, 2H), 6.23-6.20 (m, 1H), 4.41-4.36 (m, 1H), 3.76 (s, 3H), 3.49-3.45 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.7 147.9, 131.2, 130.7, 130.2, 128.8, 128.5, 128.1, 126.0, 114.3, 96.7, 65.8, 58.8, 55.2; LRMS (EI, 70eV) *m/z* (%): 397 (M^+ + 2, 14), 395 (M^+, 14), 264 (38), 251 (36), 155 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{17}ON_3{}^{35}Cl_3$ ($[M+H]^+$) 396.0432, found 396.0435.

5-Methyl-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-1,2,4-triazole (4aah) and 3-Methyl-1-(3,3,3-trichloro-1-(4-methoxyphenyl)propyl)-1*H*-1,2,4-triazole (4aah')



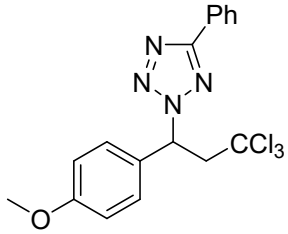
(**4aah**:**4aah'** = 4:1)Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (s, 0.8H), 7.86 (s, 0.2H), 7.35 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 9.0 Hz, 2H), 5.73-5.71 (m, 1H), 4.29-4.24 (m, 0.2H), 4.15-4.10 (m, 0.8H), 3.80 (s, 3H), 3.41-3.37 (m, 1H), 2.52 (s, 0.6H), 2.42 (s, 2.4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 150.4, 143.5, 130.3, 128.4, 128.0, 114.4, 96.7, 60.7, 58.3, 55.3, 14.1; LRMS (EI, 70eV) *m/z* (%): 335 (M^+ + 2, 17), 333 (M^+, 17), 202 (100), 155 (55), 134 (51); HRMS *m/z* (ESI) calcd for $C_{13}H_{15}ON_3{}^{35}Cl_3$ ([M+H]$^+$) 334.0275, found 334.0279.

1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-pyrazole (4aai)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59-7.58 (m, 1H), 7.46-7.45 (m, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.24-6.23 (m, 1H), 5.74-5.72 (m, 1H), 4.30-4.25 (m, 1H), 3.77 (s, 3H), 3.43-3.40 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 139.7, 132.0, 129.6, 128.0, 114.2, 105.8, 97.2, 62.7, 58.6, 55.3; LRMS (EI, 70eV) *m/z* (%): 320 (M^+ + 2, 11), 318 (M^+, 11), 215 (18), 187 (100), 155 (48); HRMS *m/z* (ESI) calcd for $C_{13}H_{14}N_2O^{35}Cl_3$ ([M+H]$^+$) 319.0166, found 319.0169.

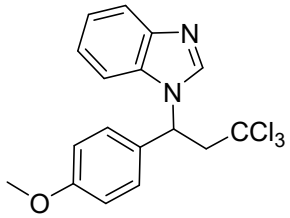
5-Phenyl-2-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-2*H*-tetrazole (4aaj)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.0 Hz,

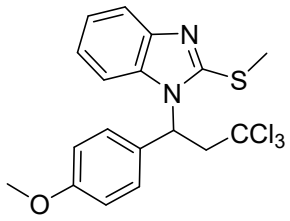
2H), 7.48-7.46 (m, 5H), 6.91 (d, *J* = 7.5 Hz, 2H), 6.48 (d, *J* = 8.5 Hz, 1H), 4.39-4.34 (m, 1H), 3.79 (s, 3H), 3.56 (d, *J* = 15.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.2, 160.2, 130.4, 128.9, 128.8, 128.42 (s), 127.2, 126.9, 114.6, 96.0, 64.7, 58.5, 55.3; HRMS *m/z* (ESI) calcd for $C_{17}H_{16}ON_4{}^{35}Cl_3$ ($[M+H]^+$) 397.0384, found 397.0384.

1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*]imidazole (4aak)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.82 (t, *J* = 8.5 Hz, 1H), 7.38 (t, *J* = 8.5 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.5 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 2H), 6.05-6.01 (m, 1H), 3.88-3.83 (m, 1H), 3.78 (s, 3H), 3.75-3.71 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 144.0, 141.9, 129.4, 127.8, 123.2, 122.5, 120.6, 114.5, 110.5, 96.6, 57.1, 56.7, 55.2; LRMS (EI, 70eV) m/z (%): 370 (M^+ + 2, 12), 368 (M^+, 12), 251 (34), 157 (32), 155 (100), 91 (12); HRMS m/z (ESI) calcd for $C_{17}H_{16}ON_2{}^{35}Cl_3$ ([M+H]+) 369.0323, found 369.0319.

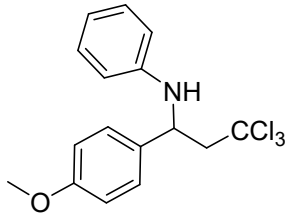
2-(Methylthio)-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*]imidazole (4aal)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.23-7.19 (m, 4H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.179-6.16 (m, 1H), 4.12-4.07 (m, 1H), 3.77 (s, 3H), 3.75-3.71 (m, 1H), 2.81 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.4, 144.0, 129.2, 127.8, 122.0, 121.9, 118.7, 114.3, 110.6, 97.0, 55.8, 55.3, 55.3, 15.5; LRMS (EI, 70eV) m/z (%): 414 (M^+ + 2, 11), 414 (M^+, 11), 251 (32), 155 (100), 134 (13), 119

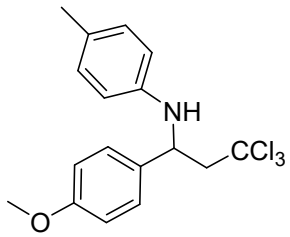
(11); HRMS m/z (ESI) calcd for $C_{18}H_{18}N_2OS^{35}Cl_3$ ([M+H]+) 415.0200, found 415.0201.

_N_-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)aniline (4aam)



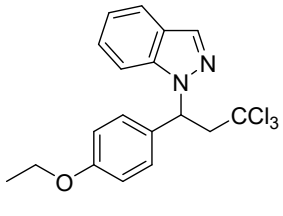
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, J = 8.0 Hz, 2H), 7.26 (s, 1H), 7.13 (t, J = 8.0 Hz, 2H), 6.89 (d, J = 8.0 Hz, 2H), 6.70 (t, J = 7.5 Hz, 1H), 6.57 (d, J = 8.0 Hz, 2H), 4.85 (t, J = 4.5Hz, 1H), 4.31 (br, 1H), 3.80 (s, 3H), 3.21 (d, J = 7.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.1, 146.5, 134.4, 129.2, 127.5, 118.0, 114.4, 113.6, 97.4, 61.7, 56.4, 55.3; LRMS (EI, 70eV) m/z (%): 345 (M^+ + 2, 12), 343 (M^+, 12), 251 (19), 212 (90), 155 (100), 104 (22); HRMS m/z (ESI) calcd for $C_{16}H_{17}NO^{35}Cl_3$ ([M+H]$^+$) 344.0370, found 344.0373.

4-methyl-_N_-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)aniline (4aan)



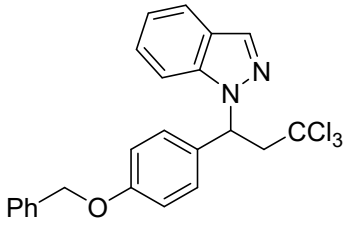
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, J = 8.0 Hz, 2H), 7.26 (s, 1H), 6.93 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 8.0 Hz, 2H), 6.49 (d, J = 8.0 Hz, 2H), 4.82-4.80 (m, 1H), 4.22 (br, 1H), 3.79 (s, 3H), 3.19 (d, J = 7.0Hz, 2H), 2.20 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.0, 144.2, 134.6, 129.7, 127.5, 114.3, 113.7, 100.0, 97.8, 61.7, 56.7, 55.3, 20.4; LRMS (EI, 70eV) m/z (%): 359 (M^+ + 2, 3), 357 (M+, 3), 269 (100), 254 (20), 226 (38), 191 (45); HRMS m/z (ESI) calcd for $C_{17}H_{19}ON^{35}Cl_3$ ([M+H]+) 358.0527, found 358.0526.

1-(3,3,3-Trichloro-1-(4-ethoxyphenyl)propyl)-1_H_-indazole (4baa)



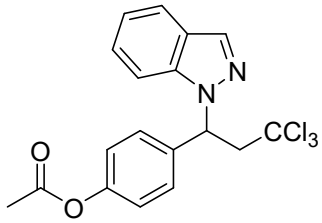
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.29-7.27 (m, 1H), 7.07-7.04 (m, 1H), 6.85 (d, *J* = 9.0 Hz, 2H), 6.00-5.98 (m, 1H), 4.53-4.49 (m, 1H), 4.01-3.96 (m, 2H), 3.58-3.54 (m, 1H), 1.38 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.0, 148.8, 131.2, 128.2, 126.0, 123.2, 121.9, 121.7, 120.2, 117.8, 114.8, 97.1, 64.5, 63.5, 58.7, 14.7; LRMS (EI, 70eV) m/z (%): 384 (M^+ + 2, 10), 382 (M^+, 10), 265 (18), 217 (24), 155 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{18}ON_2{}^{35}Cl_3$ ($[M+H]^+$) 383.0479, found 383.0483.

1-(1-(4-(Benzyloxy)phenyl)-3,3,3-Trichloropropyl)-1*H*-indazole (4caa)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.39-7.34 (m, 5H), 7.30 (d, *J* = 7.0 Hz, 1H), 7.28-7.23 (m, 2H), 7.07-7.04 (m, 1H), 6.92 (d, *J* = 9.0 Hz, 2H), 6.00-5.97 (m, 1H), 5.01 (s, 2H), 4.53-4.49 (m, 1H), 3.56-3.53 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 148.8, 136.6, 131.7, 128.6, 128.2, 128.0, 127.4, 126.0, 123.2, 121.9, 121.9, 120.2, 117.8, 115.2, 97.1, 70.0, 64.4, 58.7; HRMS *m/z* (ESI) calcd for $C_{23}H_{20}ON_2{}^{35}Cl_3$ ($[M+H]^+$) 445.0636, found 445.0640.

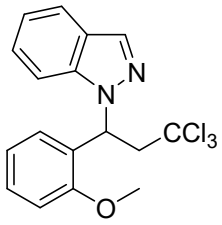
4-(3,3,3-Trichloro-1-(1*H*-indazol-1-yl)propyl)phenyl acetate (4daa)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.44 (d, *J* = 9.0 Hz, 2H), 7.31-7.28 (m, 1H), 7.09 (s, 1H), 7.06 (d, *J* = 8.5 Hz, 2H), 6.05-6.03 (m, 1H), 4.61-4.56 (m, 1H), 3.55-3.52 (m, 1H), 2.27 (s, 3H); ^{13}C

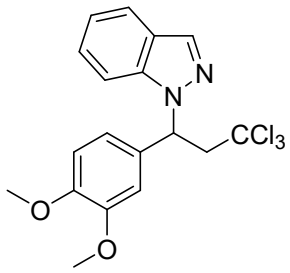
NMR (125 MHz, $CDCl_3$) δ 169.2, 150.6, 148.9, 136.9, 128.0, 126.2, 123.5, 122.1, 122.0, 121.8, 120.2, 117.9, 100.0, 97.0, 64.3, 58.7, 21.1; LRMS (EI, 70eV) *m/z* (%): 398 (M^+ + 2, 5), 396 (M^+, 5), 265 (7), 237 (8), 118 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{16}O_2N_2{}^{35}Cl_3$ ($[M+H]^+$) 397.0272, found 397.0270.

1-(3,3,3-Trichloro-1-(2-methoxyphenyl)propyl)-1*H*-indazole (4eaa)



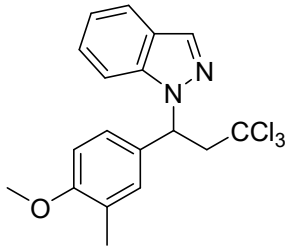
Yellow oil; ^1H NMR (500 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.26-7.24 (m, 2H), 7.06-7.03 (m, 1H), 6.91-6.88 (m, 2H), 6.57-6.54 (m, 1H), 4.50-4.45 (m, 1H), 3.91 (s, 3H), 3.52-3.49 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 148.6, 129.7, 128.0, 127.5, 125.9, 123.9, 121.7, 121.6, 121.0, 120.2, 117.8, 110.6, 97.4, 58.4, 57.1, 55.5; LRMS (EI, 70eV) *m/z* (%): 370 (M^+ + 2, 23), 368 (M^+, 23), 337 (50), 155 (100), 118 (81); HRMS *m/z* (ESI) calcd for $C_{17}H_{16}ON_2{}^{35}Cl_3$ ($[M+H]^+$) 369.0323, found 369.0319.

1-(3,3,3-Trichloro-1-(3,4-dimethoxyphenyl)propyl)-1*H*-indazole (4faa)



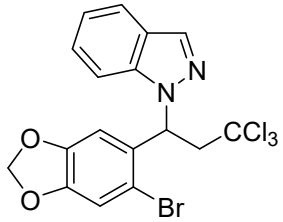
Yellow oil; ^1H NMR (500 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.27-7.25 (m, 1H), 7.15-7.14 (m, 1H), 7.05-7.02 (m, 2H), 6.87-6.85 (m, 1H), 6.60-6.57 (m, 1H), 4.54-4.49 (m, 1H), 3.95 (s, 3H), 3.85 (s, 3H), 3.55-3.52 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.5, 148.7, 145.7, 132.7, 125.9, 124.4, 123.7, 121.7 (2C), 120.2, 119.6, 117.8, 112.6, 97.3, 61.0, 58.1, 57.5, 55.8; LRMS (EI, 70eV) *m/z* (%): 400 (M^+ + 2, 3), 398 (M^+, 3), 367 (100), 185 (38), 91 (45); HRMS *m/z* (ESI) calcd for $C_{18}H_{18}O_2N_2{}^{35}Cl_3$ ($[M+H]^+$) 399.0428, found 399.0431.

1-(3,3,3-Trichloro-1-(4-methoxy-3-methylphenyl)propyl)-1*H*-indazole (4gaa)



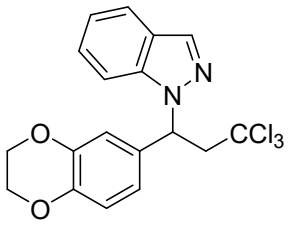
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.29-7.26 (m, 1H), 7.24-7.22 (m, 2H), 7.07-7.04 (m, 1H), 6.76 (d, *J* = 9.0 Hz, 1H), 5.97-5.95 (m, 1H), 4.53-4.49 (m, 1H), 3.79 (s, 3H), 3.58-3.54 (m, 1H), 2.19 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.9, 148.8, 130.9, 129.2, 127.3, 126.0, 125.5, 123.1, 121. 8 (2C), 120.2, 117.8, 110.0, 97.2, 64.5, 58.6, 55.3, 16.3; LRMS (EI, 70eV) *m/z* (%): 384 (M^+ + 2, 7), 382 (M^+, 7), 265 (23), 251 (17), 169 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{18}ON_2{}^{35}Cl_3$ ($[M+H]^+$) 383.0479, found 383.0483.

1-(1-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)-3,3,3-Trichloropropyl)-1*H*-indazole (4haa)



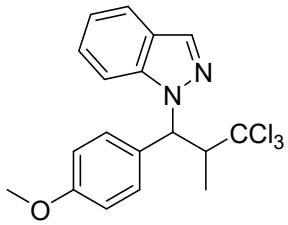
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.42 (s, 1H), 7.28-7.25 (m, 1H), 7.07-7.04 (m, 1H), 6.98 (s, 1H), 6.59-6.57 (m, 1H), 5.96 (s, 1H), 5.89 (s, 1H), 4.46-4.43 (m, 1H), 3.49-3.45 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.8, 148.6, 148.0, 131.3, 126.2, 123.7, 121.9, 121.6, 120.3, 117.8, 113.6, 112.4, 109.0, 102.1, 96.7, 62.8, 57.9; LRMS (EI, 70eV) *m/z* (%): 464 (M^+ + 4, 2), 462 (M^+ + 2, 3), 460 (M^+, 2), 381 (50), 345 (28), 249 (100); HRMS *m/z* (ESI) calcd for $C_{17}H_{13}O_2N_2{}^{35}Cl_3{}^{80}Br$ ($[M+H]^+$) 460.9220, found 460.9221.

1-(3,3,3-Trichloro-1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)propyl)-1H-indazole (4iaa)



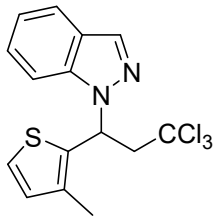
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.28-7.25 (m, 1H), 7.07-7.04 (m, 1H), 6.96 (s, 1H), 6.90-6.88 (m, 1H), 6.81 (d, *J* = 8.5 Hz, 1H), 5.94-5.91 (m, 1H), 4.53-4.48 (m, 1H), 4.20 (s, 4H), 3.55-3.51 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.8, 143.7, 143.6, 132.6, 126.0, 123.2, 121.9, 121.8, 120.2, 119.9, 117.9, 117.69, 116.0, 97.2, 64.4, 64.3, 58.6; LRMS (EI, 70eV) *m/z* (%): 398 (M^+ + 2, 10), 396 (M^+, 10), 265 (20), 243 (14), 183 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{16}O_2N_2{}^{35}Cl_3$ ($[M+H]^+$) 397.0272, found 397.0269.

1-(3,3,3-Trichloro-1-(4-methoxyphenyl)-2-methylpropyl)-1*H*-indazole (4jaa)



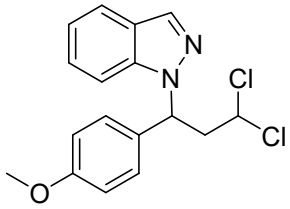
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.49 (d, *J* = 8.5 Hz, 2H), 7.28-7.26 (m, 1H), 7.07-7.04 (m, 1H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.08 (d, *J* = 6.0 Hz, 1H), 3.77 (s, 3H), 3.735-3.73 (m, 1H), 1.41 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 149.0, 130.7, 129.3, 125.9, 124.3, 121.8, 121.1, 120.2, 118.0, 114.0, 103.4, 67.9, 58.4, 55.2, 14.0; LRMS (EI, 70eV) *m/z* (%): 384 (M^+ + 2, 8), 382 (M^+, 8), 265 (35), 251 (23), 169 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{19}ON_2{}^{35}Cl_3$ ($[M+H]^+$) 383.0479, found 383.0484.

1-(3,3,3-Trichloro-1-(3-methylthiophen-2-yl)propyl)-1*H*-indazole (4kaa)



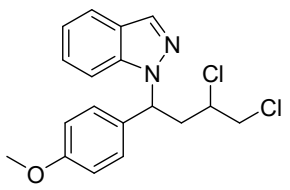
Yellow oil; 1H NMR (500 MHz, CDCl3) δ 8.02 (s, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.28-7.26 (m, 1H), 7.21 (d, *J* = 5.0 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.79 (d, *J* = 5.0 Hz, 1H), 6.40-6.38 (m, 1H), 4.39 (dd, *J* = 15.0, 7.0 Hz, 1H), 3.57 (dd, *J* = 15.0, 4.0 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.9, 135.2, 135.0, 129.8, 126.2, 125.2, 122.7, 122.0, 121.7, 120.2, 117.9, 96.5, 59.5, 58.7, 14.0; LRMS (EI, 70eV) *m/z* (%): 360 (M^+ + 2, 8), 358 (M^+, 8), 242 (22), 145 (100), 118 (46); HRMS *m/z* (ESI) calcd for $C_{15}H_{14}N_2S^{35}Cl_3$ ($[M+H]^+$) 358.9938, found 358. 9940.

1-(3,3-dichloro-1-(4-methoxyphenyl)propyl)-1H-indazole (4aba)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.30-7.25 (m, 1H), 7.09-7.06 (m, 1H), 6.87 (d, *J* = 8.5 Hz, 2H), 5.80-5.77 (m, 1H), 5.48-5.46 (m, 1H), 3.78 (s, 3H), 3.66-3.60 (m, 1H), 3.07-3.01 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 149.0, 130.3, 128.2, 126.1, 123.0, 122.0, 121.6, 120.2, 117.8, 114.4, 70.3, 64.0, 55.3, 48.8; LRMS (EI, 70eV) *m/z* (%): 336 (M^+ + 2, 12), 334 (M^+, 18), 217 (98), 181 (47), 155 (100); HRMS *m/z* (ESI) calcd for $C_{17}H_{17}ON_2^{35}Cl_2$ ($[M+H]^+$) 335.0712, found 335.0711.

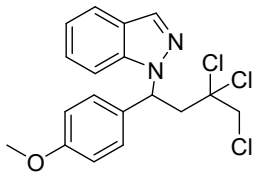
1-(3,4-dichloro-1-(4-methoxyphenyl)butyl)-1H-indazole (4aca)



dr = 3:2; Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (s, 0.6H), 7.87 (s, 0.4H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.64-7.57 (m, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 1H), 7.28-7.25 (m, 1H), 7.09-7.06 (m, 1H), 6.91 (d, *J* = 8.5 Hz, 0.8H), 6.85 (d, *J* = 8.5 Hz, 1.2H),

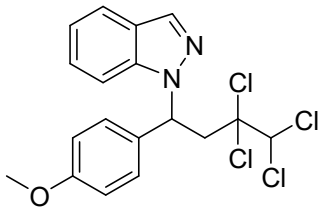
5.90-5.88 (m, 0.6H), 5.85-5.82 (m, 0.4H), 3.80 (s, 2H), 3.77 (s, 3H), 3.73-3.67 (m, 1H), 3.42-3.41 (m, 0.6H), 3.25-3.22 (m, 0.4H), 2.86-2.81 (m, 0,4H), 2.45-2.40 (m, 0.6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 159.5, 149.0, 148.7, 131.6, 129.5, 128.9, 128.0, 126.0, 123.4, 122.1, 121.9, 121.8, 121.5, 120.3, 120.1, 117.9, 117.6, 114.5, 114.1, 64.2, 63.7, 58.0, 57.7, 55.3, 48.7, 48.1, 41.3, 40.9; LRMS (EI, 70eV) *m/z* (%): 350 (M^+ + 2, 7), 348 (M^+, 12), 237 (45), 155(100); HRMS *m/z* (ESI) calcd for $C_{18}H_{19}ON_2{}^{35}Cl_2$ ($[M+H]^+$) 349.0869, found 349.0868.

1-(3,4,4-Trichloro-1-(4-methoxyphenyl)butyl)-1*H*-indazole (4ada)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.37 (d, *J* = 9.0 Hz, 2H), 7.29-7.25 (m, 1H), 7.07-7.04 (m, 1H), 6.86 (d, *J* = 9.0 Hz, 2H), 6.03-6.01 (m, 1H), 3.95-3.91 (m, 1H), 3.85-3.79 (m, 2H), 3.76 (s, 3H), 3.29-3.25 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.7, 148.7, 131.5, 128.3, 126.0, 122.8, 121.9, 121.8, 120.2, 117.8, 114.2, 88.8, 63.9, 55.3, 54.4, 48.9; LRMS (EI, 70eV) *m/z* (%): 384 (M^+ + 2, 11), 382 (M^+, 11), 265 (43), 237 (55), 155 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{18}ON_2{}^{35}Cl_3$ ($[M+H]^+$) 383.0479, found 383.0480.

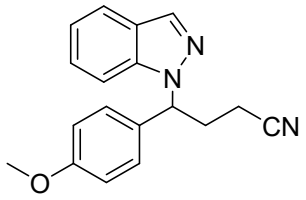
1-(3,3,4,4-Tetrachloro-1-(4-methoxyphenyl)butyl)-1*H*-indazole (4aea)



Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.37 (d, *J* = 9.0 Hz, 2H), 7.28-7.23 (m, 1H), 7.07-7.04 (m, 1H), 6.85 (d, *J* = 9.0 Hz, 2H), 6.10-6.08 (m, 1H), 5.87 (s, 1H), 4.09-4.04 (m, 1H), 3.75 (s, 3H), 3.34-3.31 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 148.7, 131.5, 128.3, 126.0, 122.8, 121.8

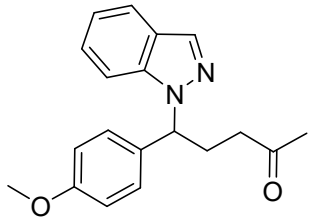
(2C), 120.2, 117.8, 114.2, 92.1, 78.1, 63.8, 55.2, 47.3; LRMS (EI, 70eV) *m/z* (%): 418 (M^+ + 2, 12), 416 (M^+, 9), 301 (51), 237 (68), 155 (100); HRMS *m/z* (ESI) calcd for $C_{18}H_{17}ON_2Cl_4$ ($[M+H]^+$) 417.0090, found 417.0089.

4-(1*H*-indazol-1-yl)-4-(4-methoxyphenyl)butanenitrile (4afa)



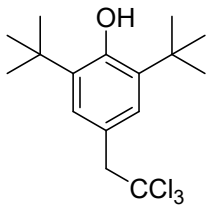
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.70-7.27 (m, 1H), 7.10-7.06 (m, 1H), 6.88 (d, *J* = 8.5 Hz, 2H), 5.66-5.63 (m, 1H), 3.78 (s, 3H), 3.06-3.02 (m, 1H), 2.60-2.53 (m, 1H), 2.41-2.35 (m, 2H), 2.33-2.26 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 149.0, 130.5, 128.2, 126.2, 123.0, 122.0, 121.6, 120.3, 118.7, 117.7, 114.4, 65.1, 55.3, 31.1, 14.7; LRMS (EI, 70eV) *m/z* (%): 291 (24), 237 (23), 174 (100), 134 (53); HRMS *m/z* (ESI) calcd for $C_{18}H_{18}ON_3$ ($[M+H]^+$) 292.1444, found 292.1447.

5-(1*H*-indazol-1-yl)-5-(4-methoxyphenyl)pentan-2-one (4aga)



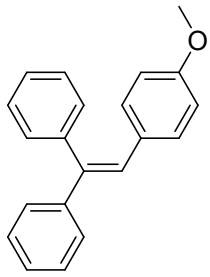
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.34-7.28 (m, 3H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 7.5 Hz, 2H), 5.60 (t, *J* = 6.5Hz, 1H), 3.78 (s, 3H), 2.81-2.75 (m, 1H), 2.58 (dd, J = 14.1, 7.0 Hz, 1H), 2.42 (d, *J* = 7.0 Hz, 2H), 2.07 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 207.7, 159.5, 131.7, 128.2, 125.8, 121.9, 121.7, 120.2, 117.7, 114.1, 65.9, 55.3, 40.0, 30.1, 29.3; LRMS (EI, 70eV) m/z (%): 308 (M^+ + 25), 237 (46), 191 (100), 173 (36), 147 (28); HRMS m/z (ESI) calcd for $C_{19}H_{21}O_2N_2$ ($[M+H]^+$) 309.1598, found 309.1597.

2,6-Di-tert-butyl-4-(2,2,2-trichloroethyl)phenol (5a)



Light yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (s, 2H), 5.26 (s, 1H), 3.83 (s, 1H), 1.45 (s, 18H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.9, 135.4, 128.4, 124.14, 99.9, 59.9, 34.3, 30.3; LRMS (EI, 70eV) m/z (%): 336(M^++2, 5), 336(M^+, 6), 321 (18.87), 220 (17), 219 (100), 203 (7).

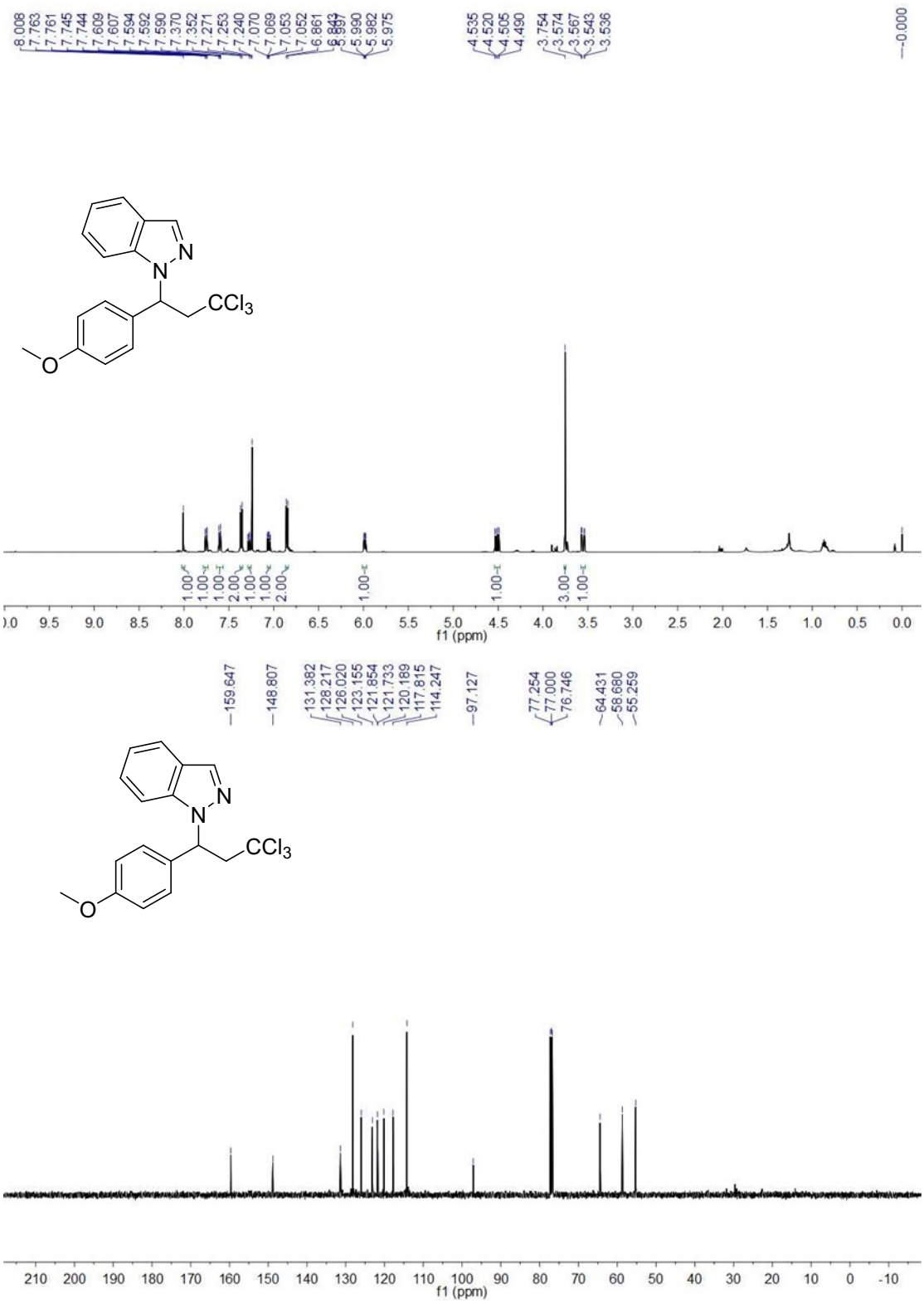
(2-(4-Methoxyphenyl)ethene-1,1-diyl)dibenzene (5b)



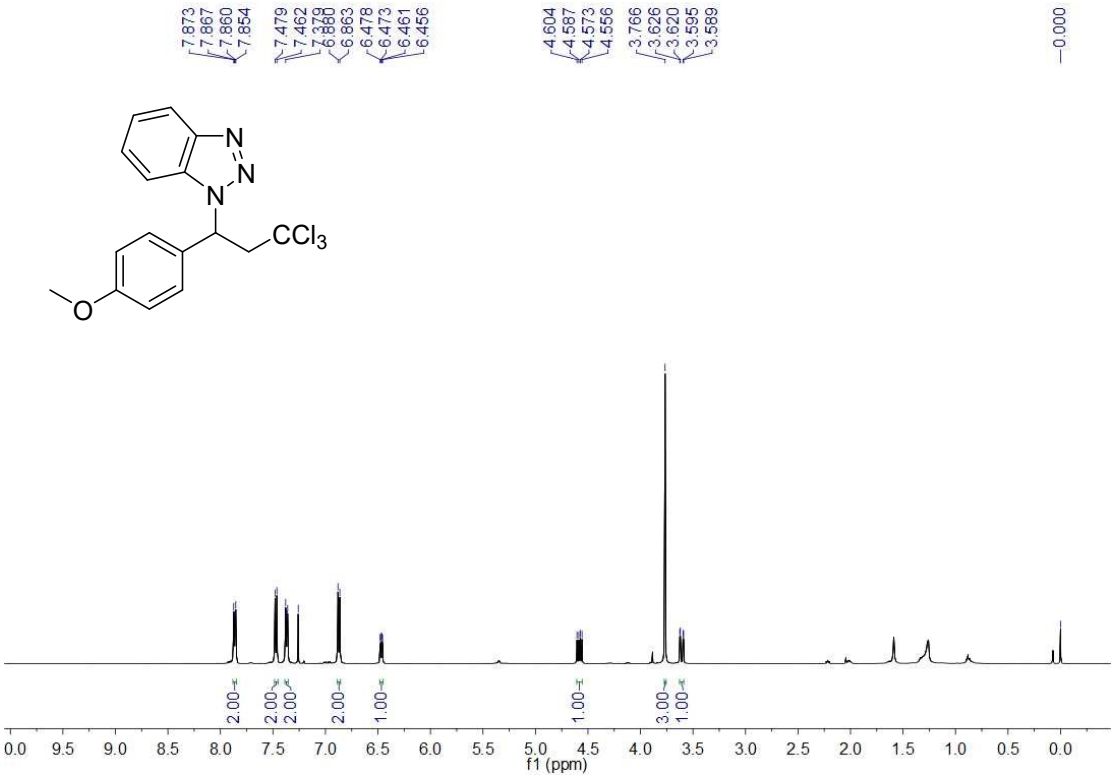
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.28 (m, 8H), 7.22 (d, J = 7.0 Hz, 2H), 6.95 (d, J = 8.5 Hz, 2H), 6.92 (s, 1H), 6.67 (d, J = 8.0 Hz, 2H), 3.75 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.3, 143.6, 140.6, 140.6, 130.8, 130.4, 130.0, 128.7, 128.1, 127.6, 127.4, 113.4, 55.1; 286 (M^+, 100), 253 (8), 243 (9), 228 (9), 165 (31).

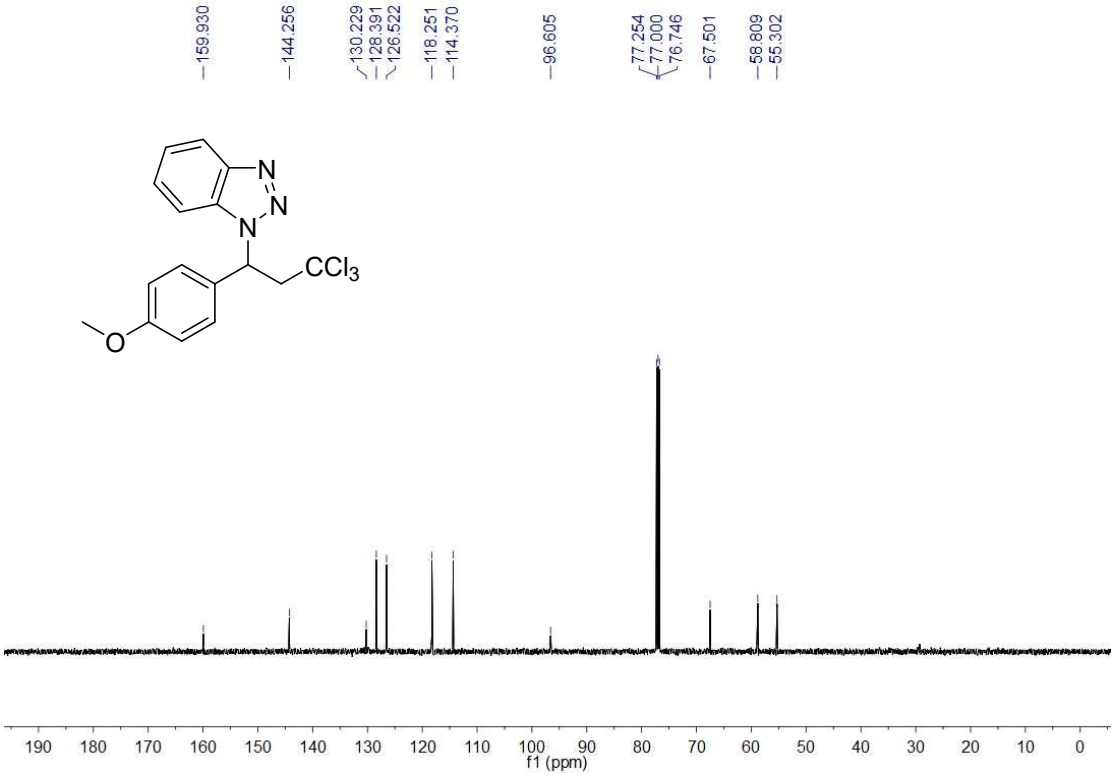
(C) Spectra

1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-indazole (4aaa)

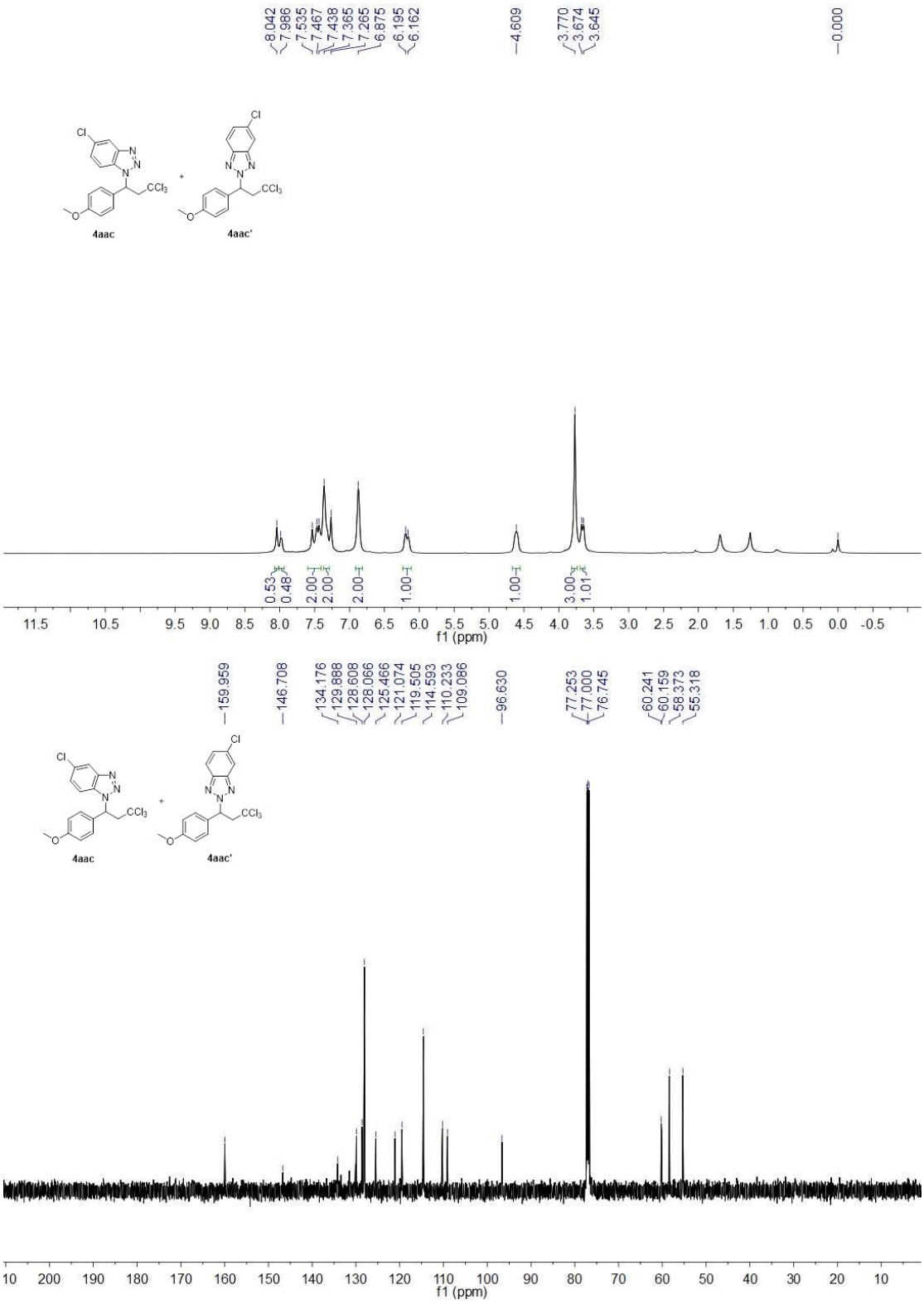


1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*][1,2,3]triazole (4aab)

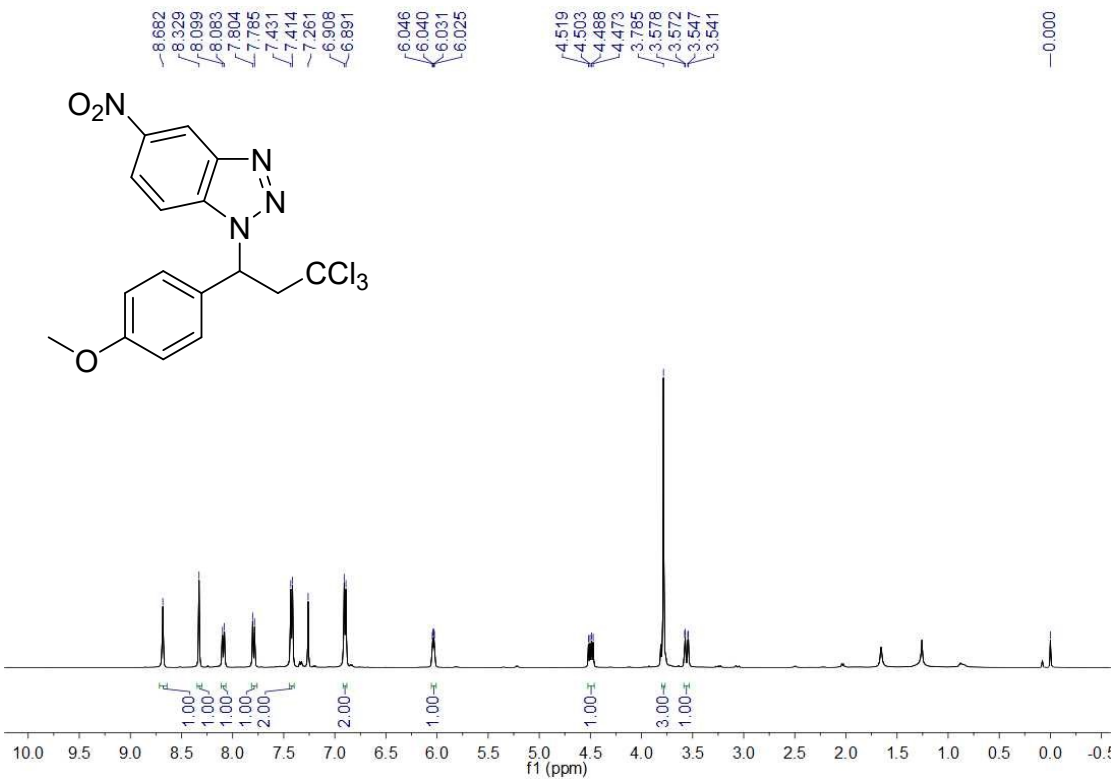

7.873
7.867
7.860
7.854
7.479
7.462
7.379
6.880
6.863
6.478
6.473
6.461
6.456
4.604
4.587
4.573
4.556
3.766
3.626
3.620
3.595
3.589
0.000
N
N
N
CCl3
O
2.00
2.00
2.00
2.00
1.00
1.00
3.00
1.00
f1 (ppm)

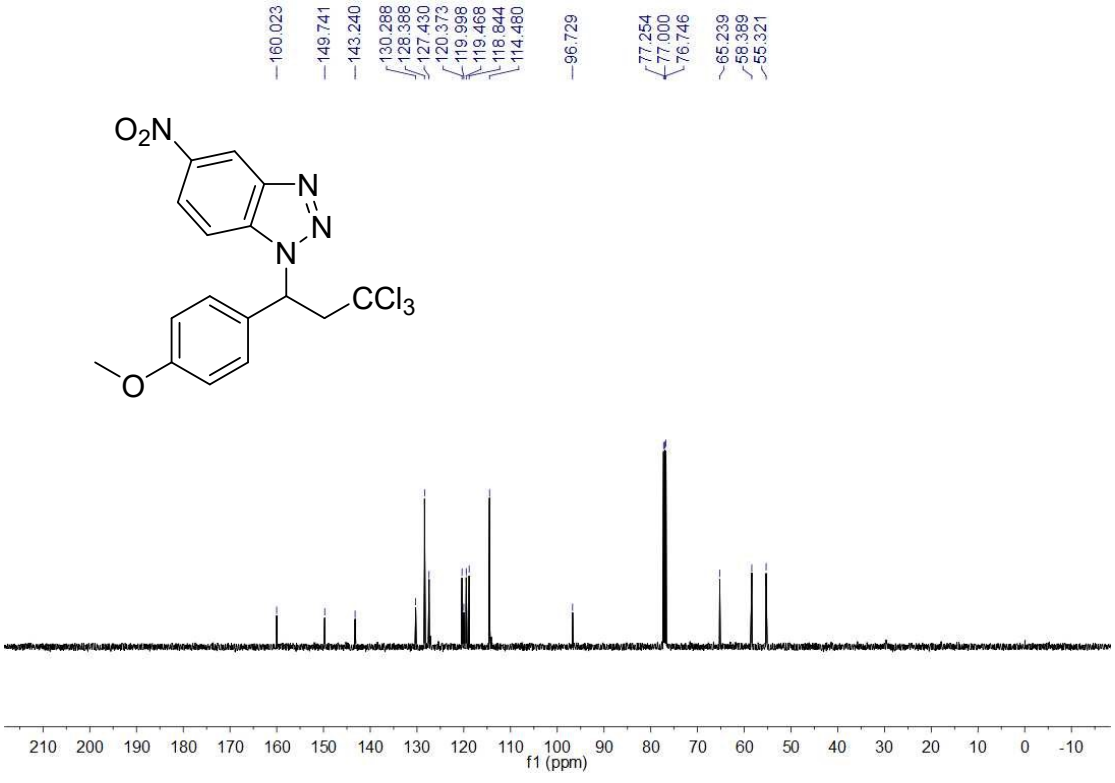

159.930
144.256
130.229
128.391
126.522
118.251
114.370
96.605
77.254
77.000
76.746
67.501
58.809
55.302
N
N
N
CCl3
O
f1 (ppm)

5-Chloro-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*][1,2,3]triazole (4aac) and 5-Chloro-2-(3,3,3-trichloro-1-(4-methoxyphenyl)propyl)-2H-benzo[*d*][1,2,3]triazole (4aac')

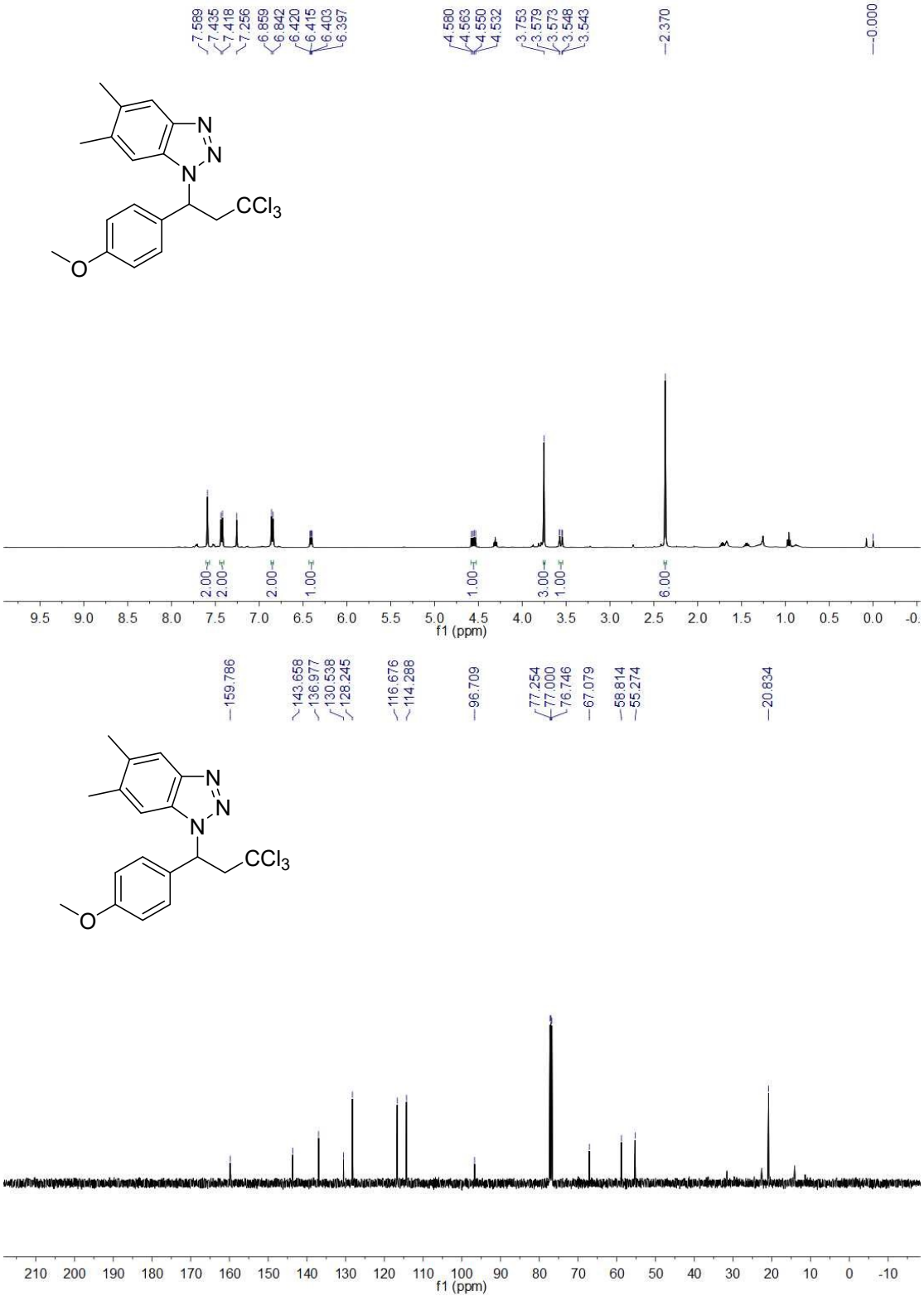


5-Nitro-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*][1,2,3]triazole (4aad)

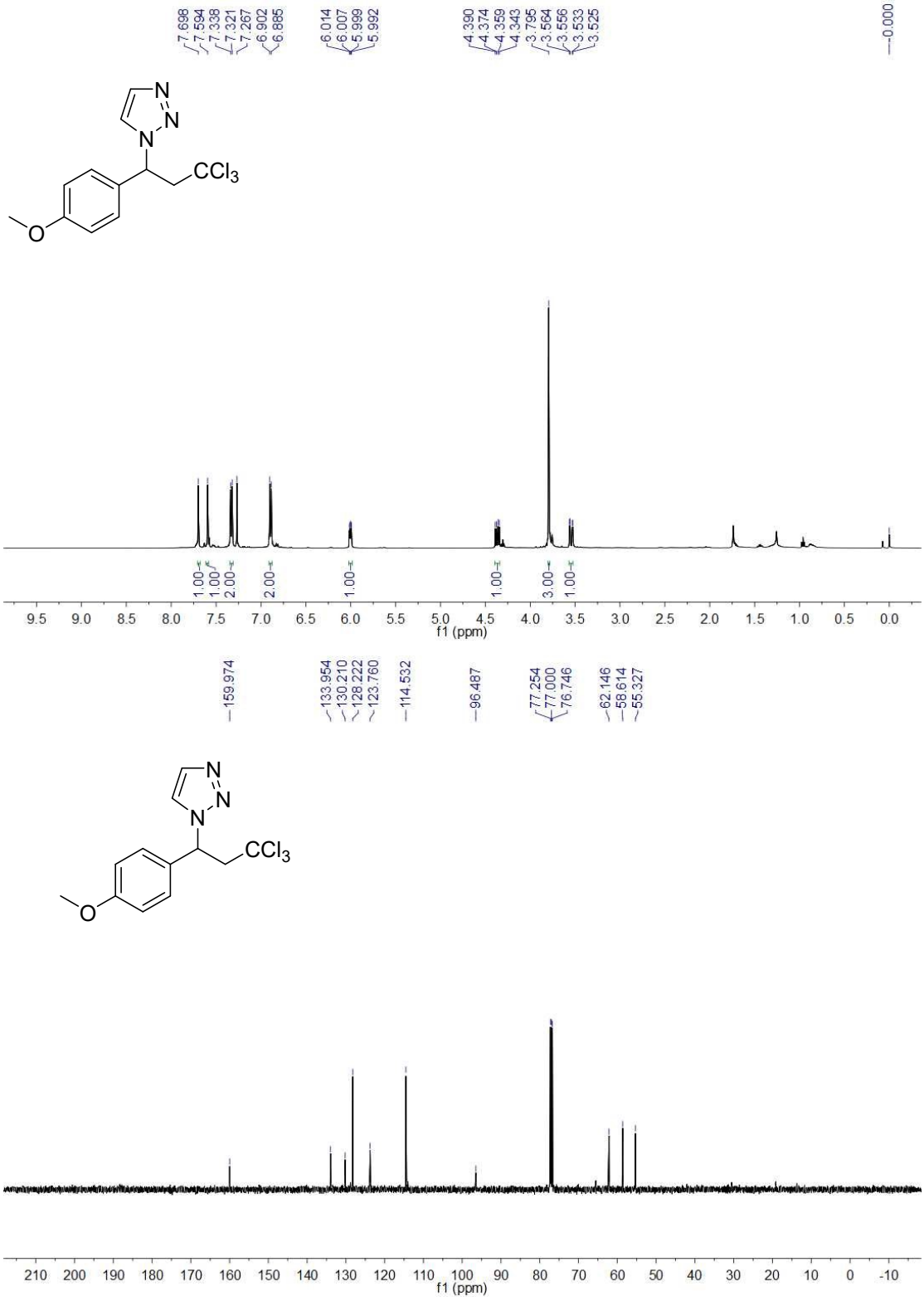




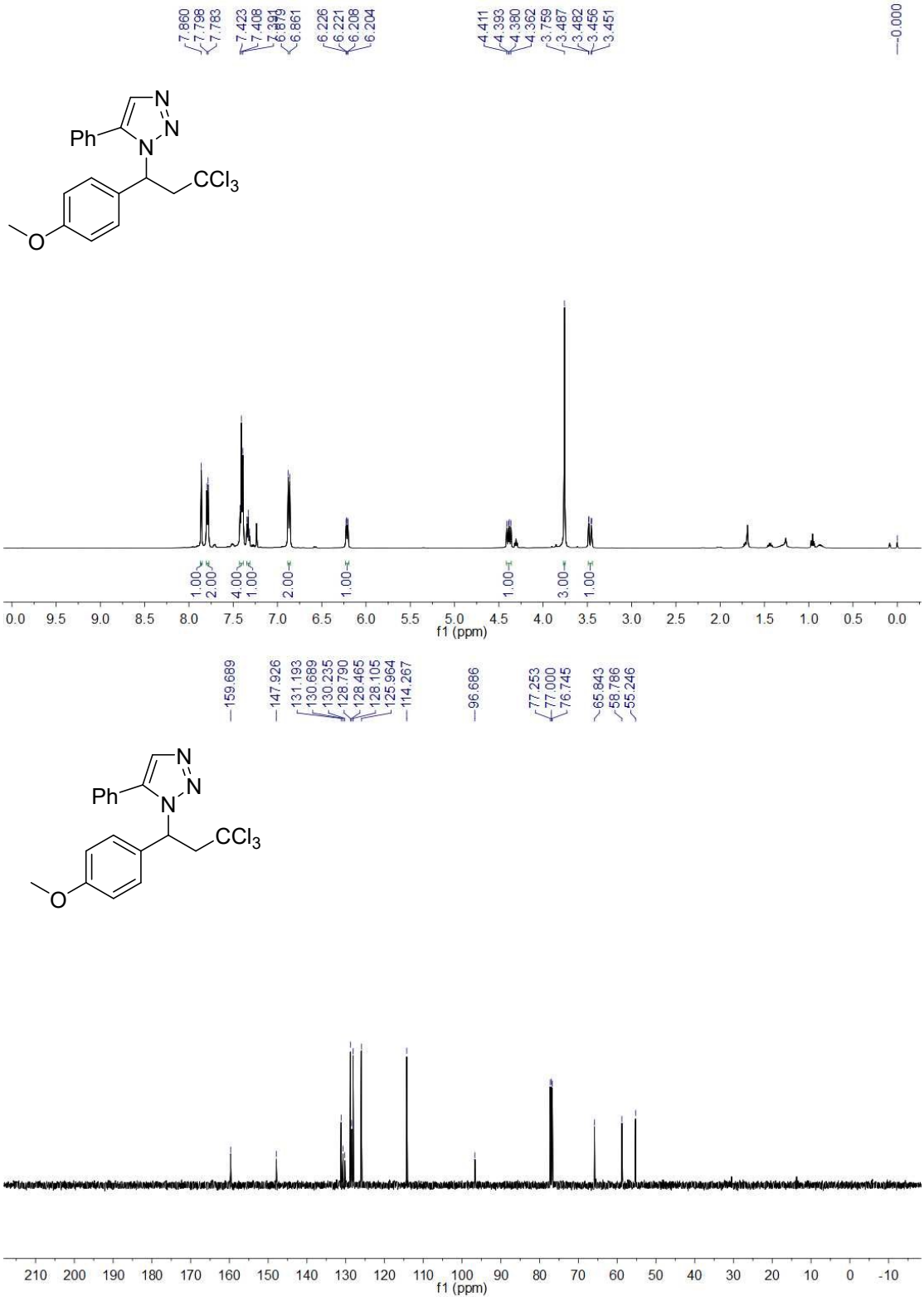
5,6-Dimethyl-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1H-benzo[d][1,2,3]triazole (4aae)



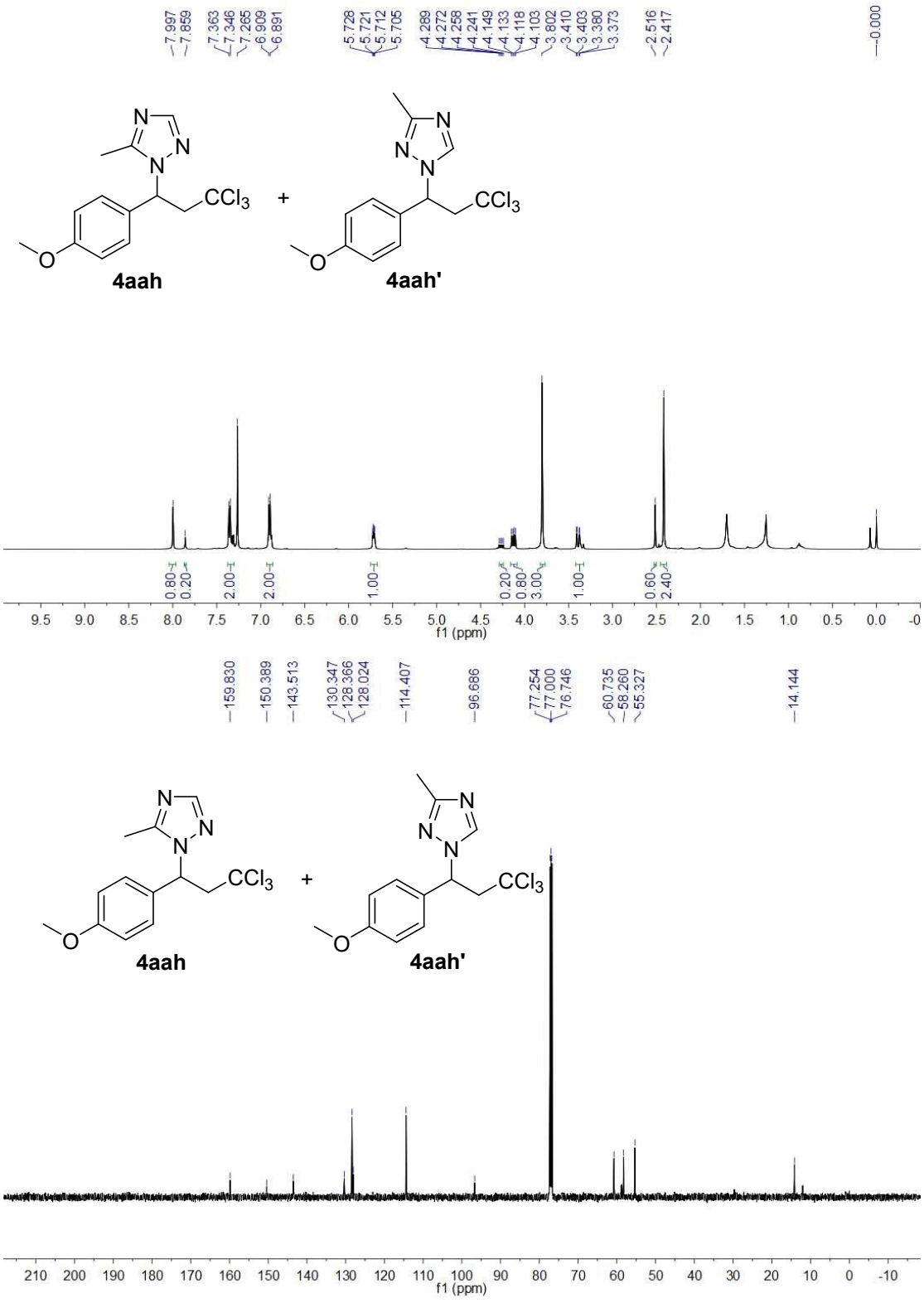
1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-1,2,3-triazole (4aaf)



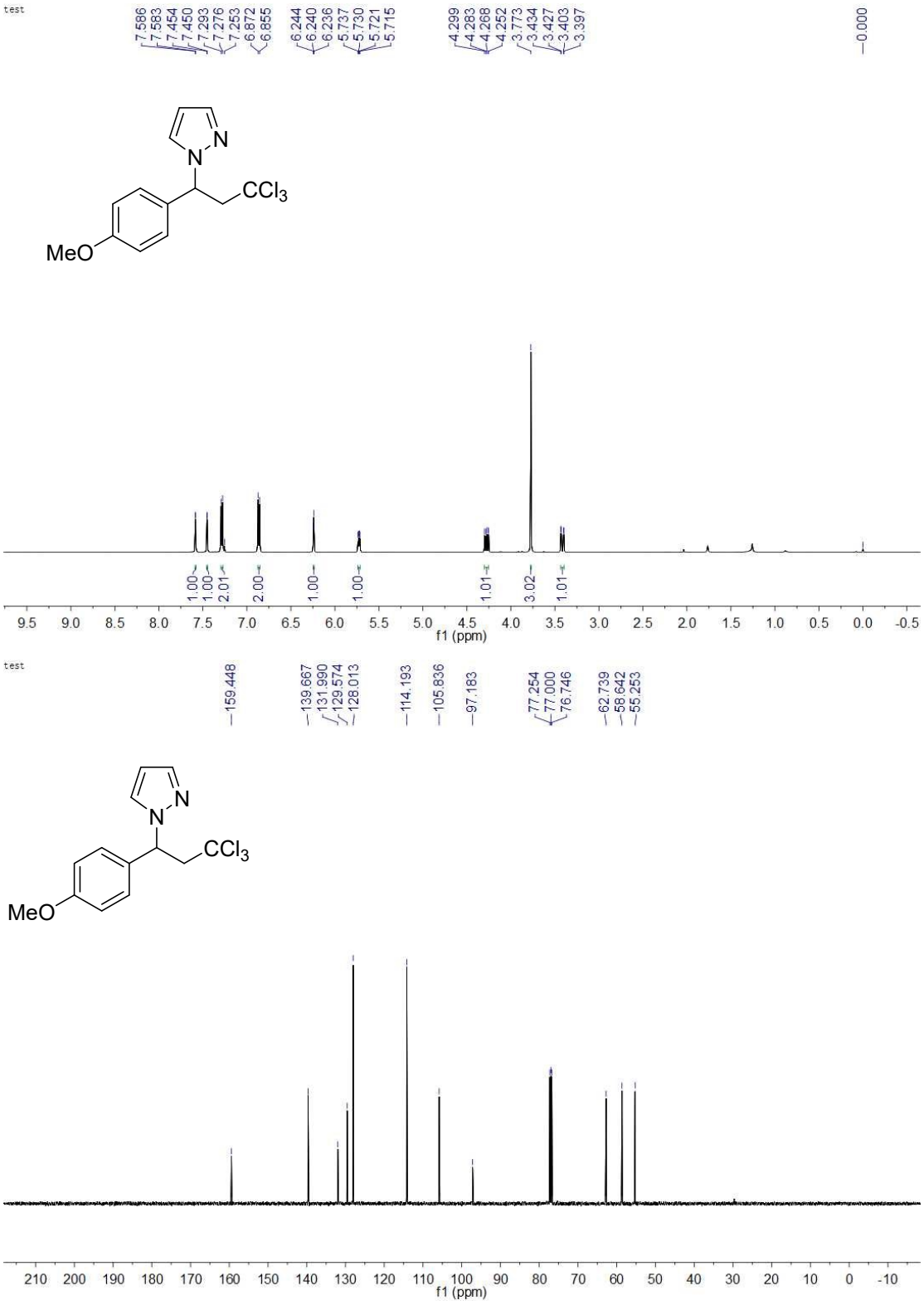
5-Phenyl-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-1,2,3-triazole (4aag)



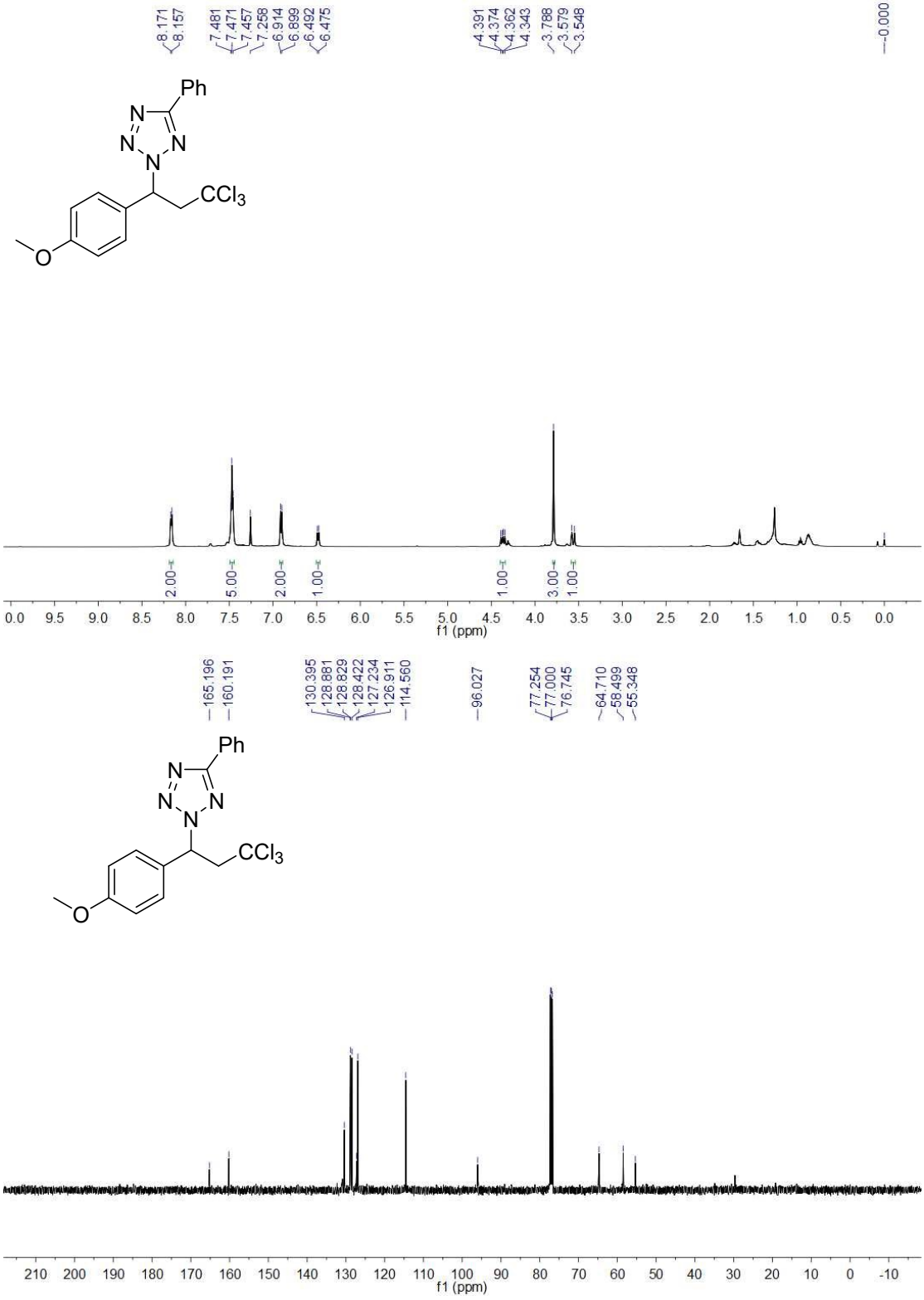
5-Methyl-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-1,2,4-triazole (4aah) and 3-Methyl-1-(3,3,3-trichloro-1-(4-methoxyphenyl)propyl)-1*H*-1,2,4-triazole (4aah')



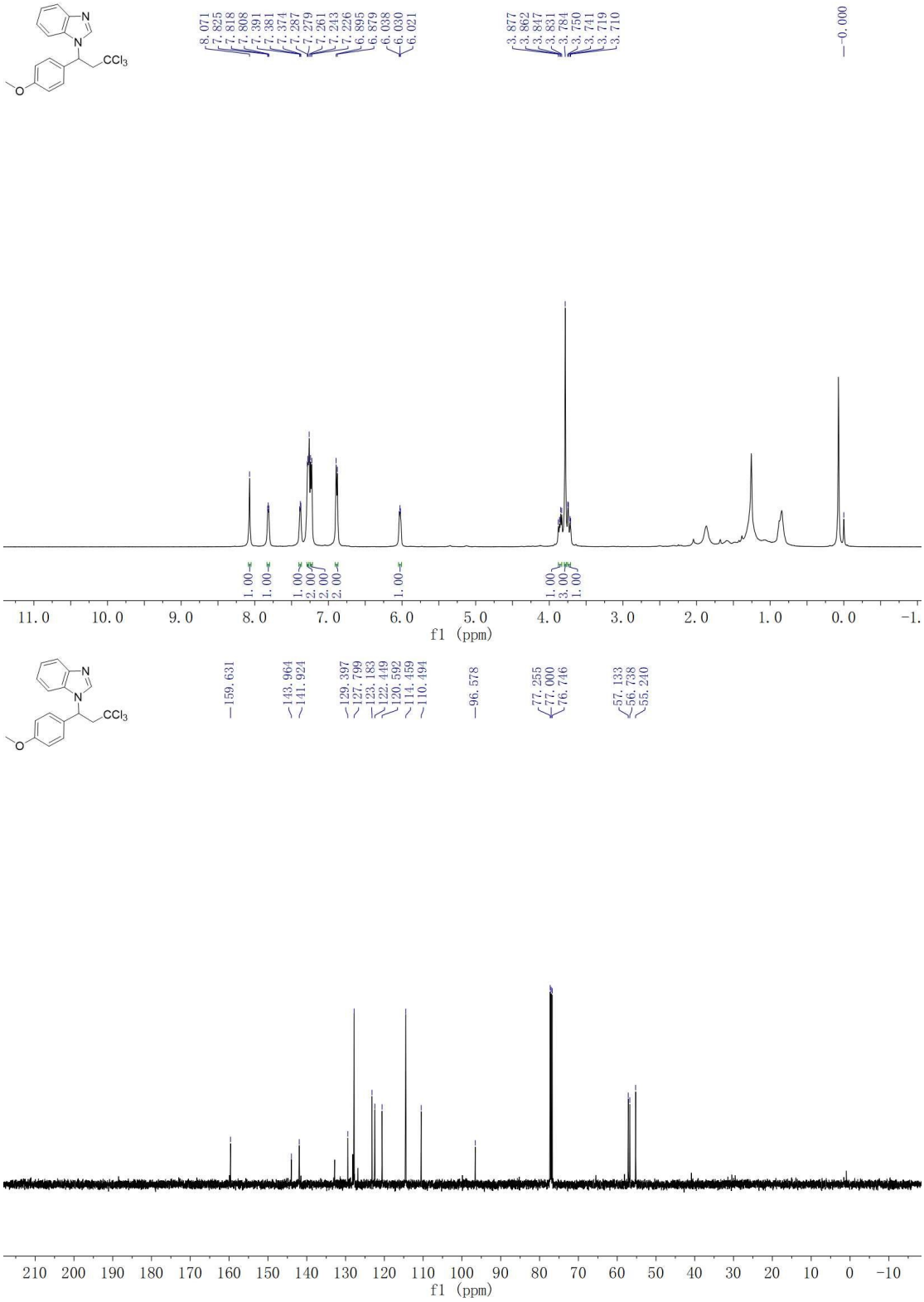
1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1H-pyrazole (4aai)



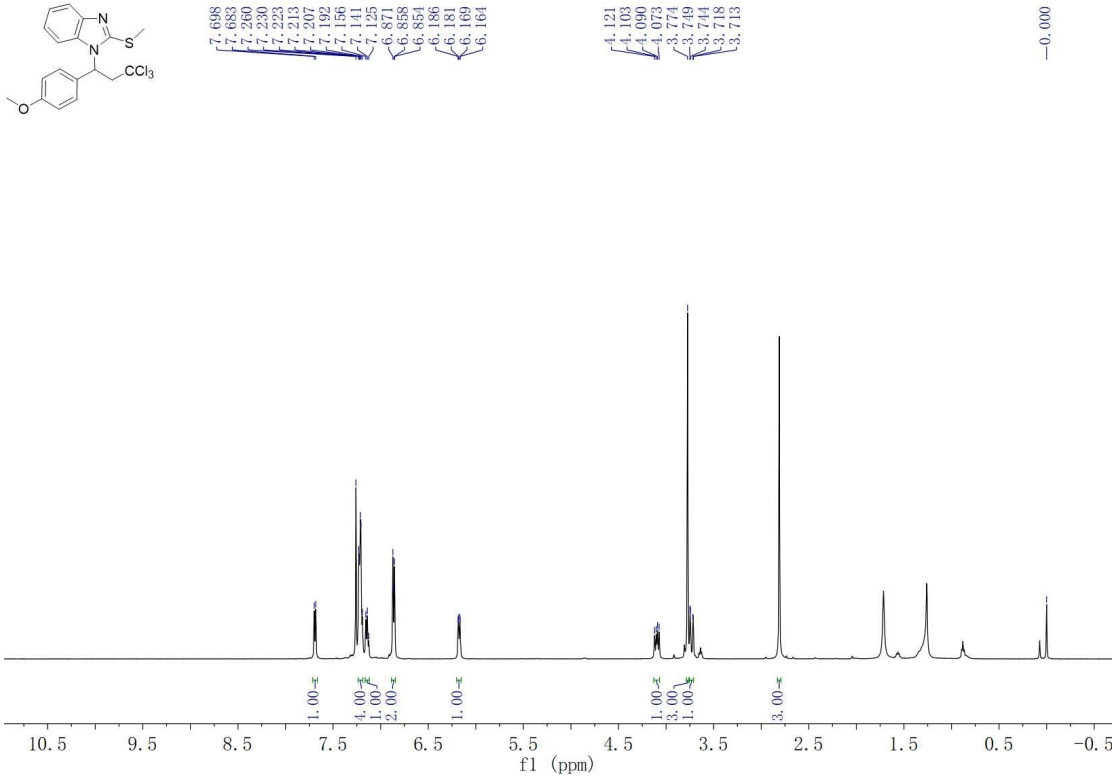
5-phenyl-2-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-2H-tetrazole (4aaj)

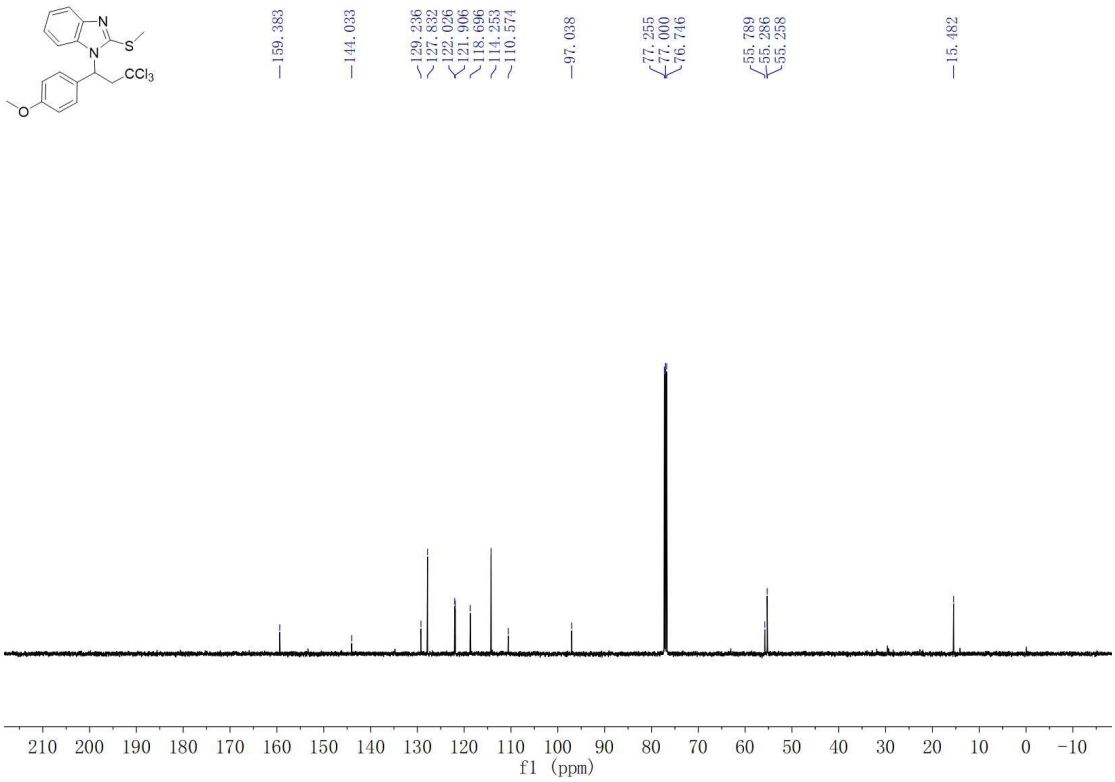


1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*]imidazole (4aak)

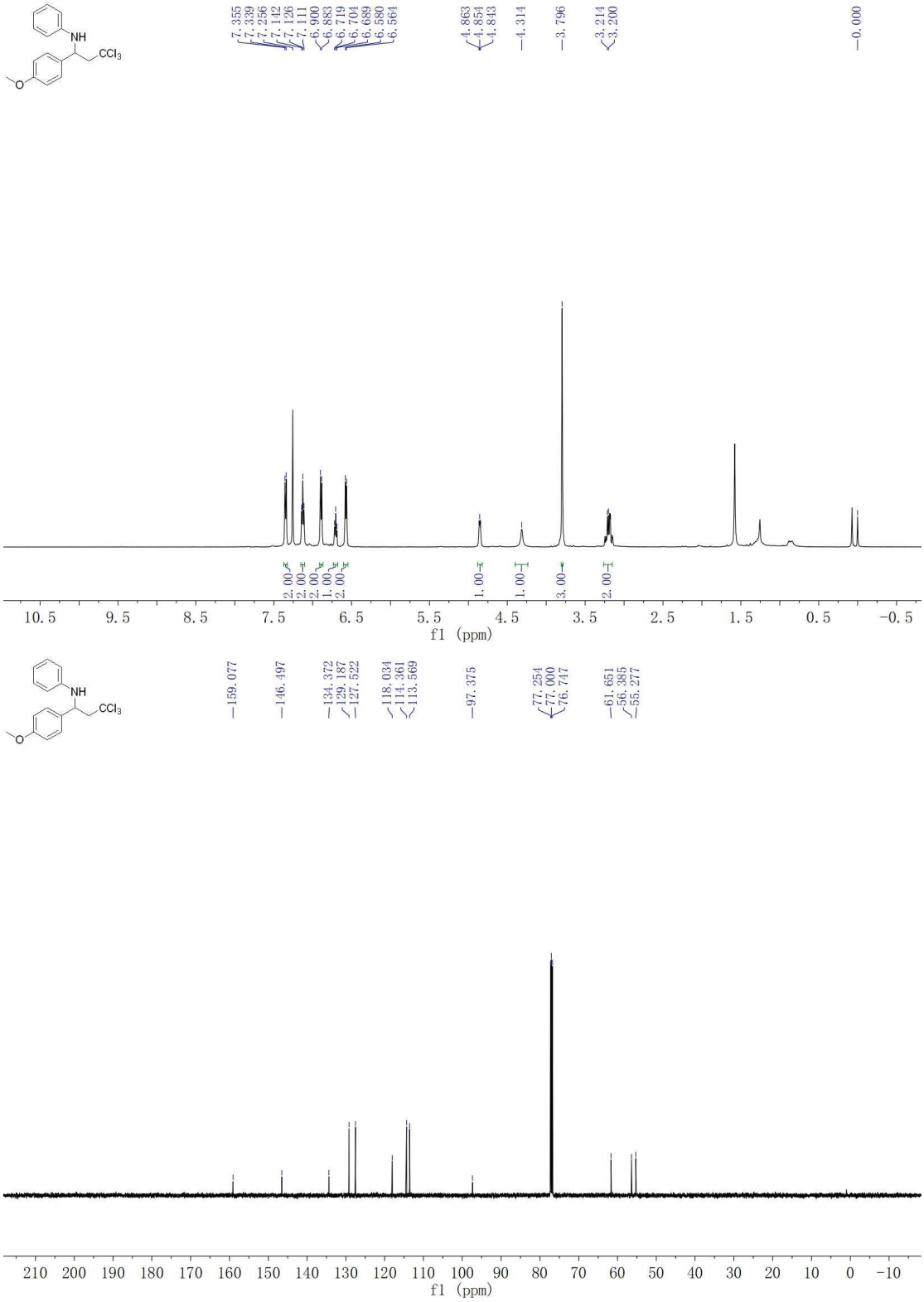


2-(methylthio)-1-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)-1*H*-benzo[*d*]imidazole (4aal)

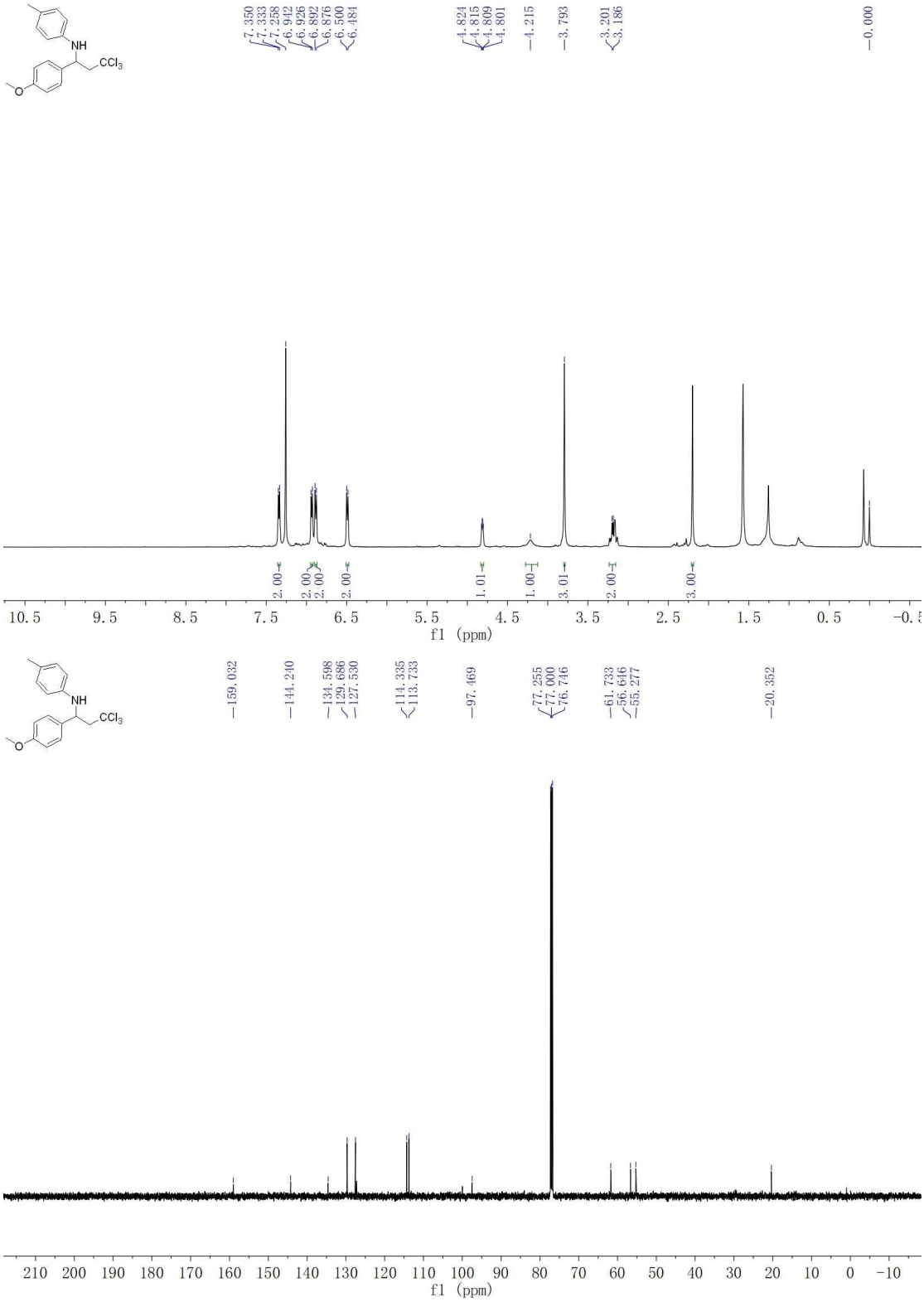




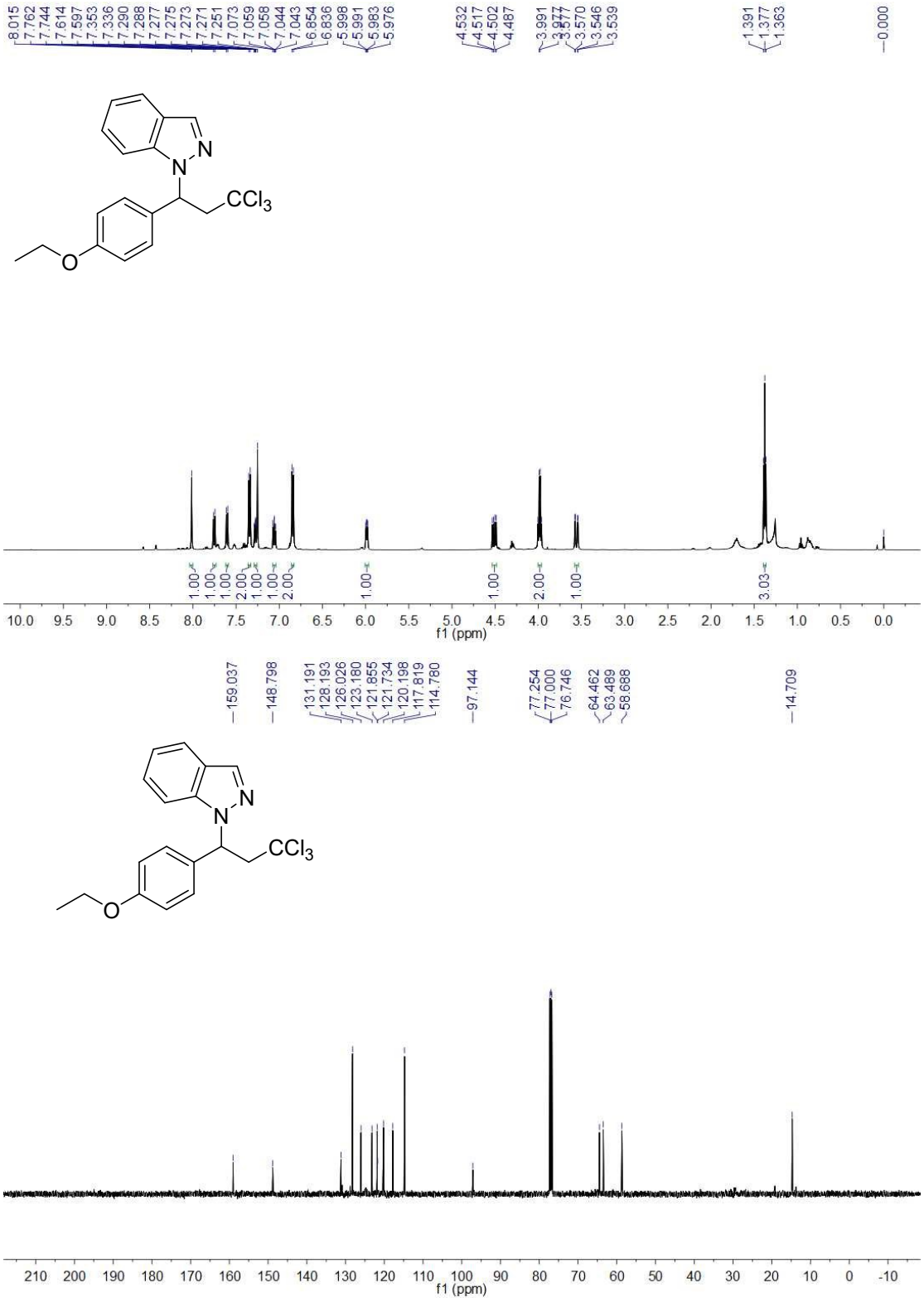
N-(3,3,3-Trichloro-1-(4-methoxyphenyl)propyl)aniline (4aam)



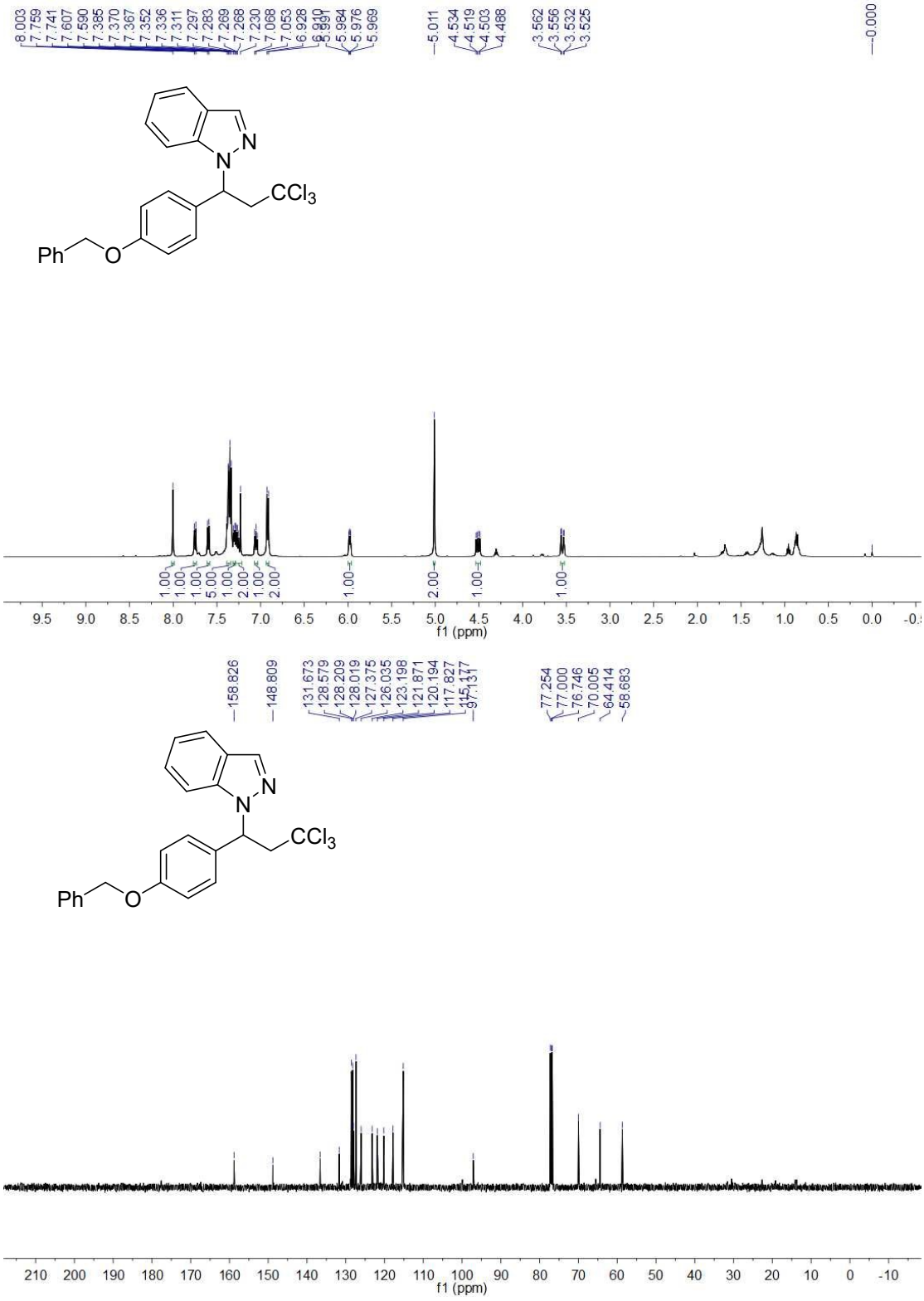
4-Methyl-*N*-(3,3,3-trichloro-1-(4-methoxyphenyl)propyl)aniline (4aan)



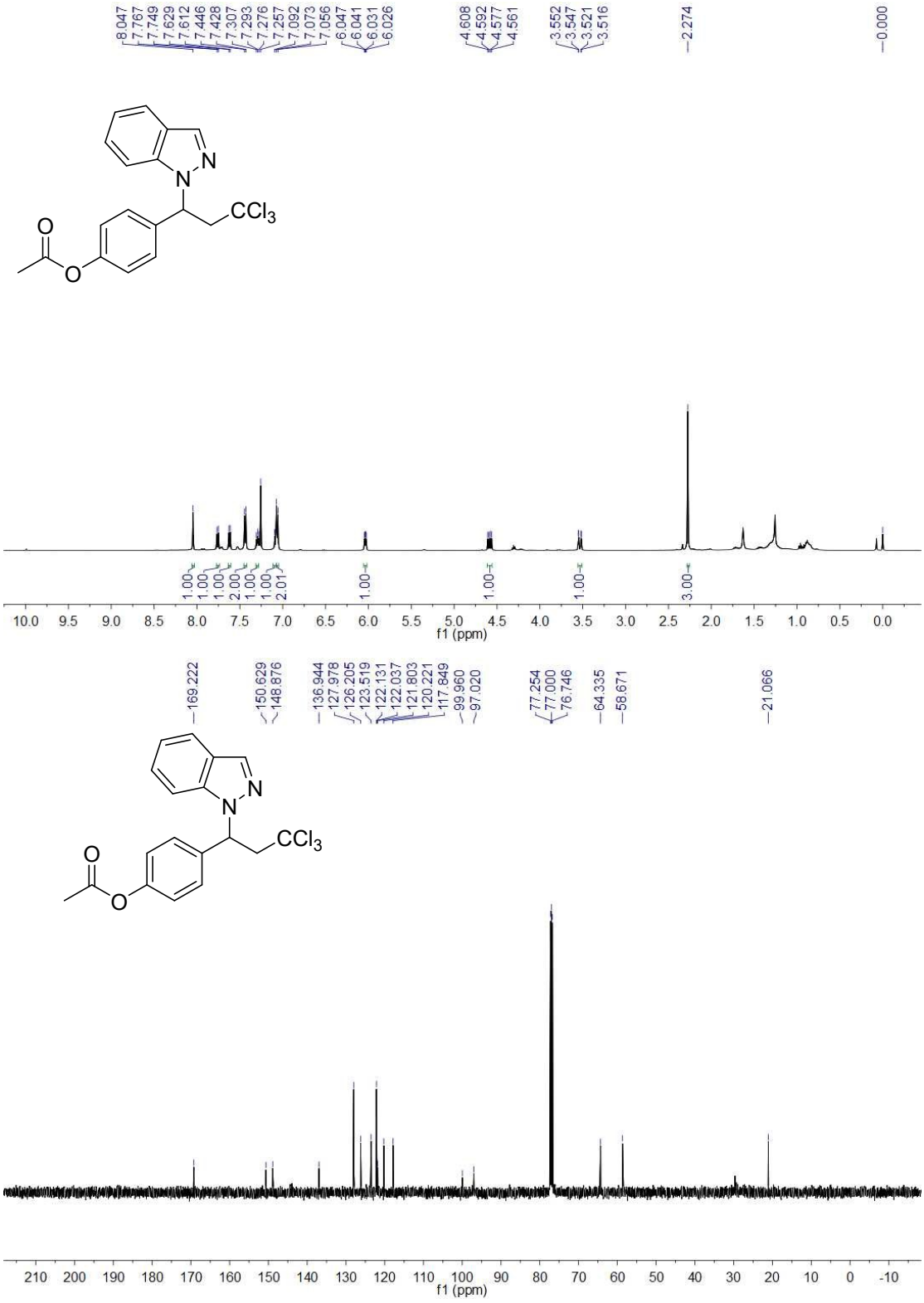
1-(3,3,3-Trichloro-1-(4-ethoxyphenyl)propyl)-1H-indazole (4baa)



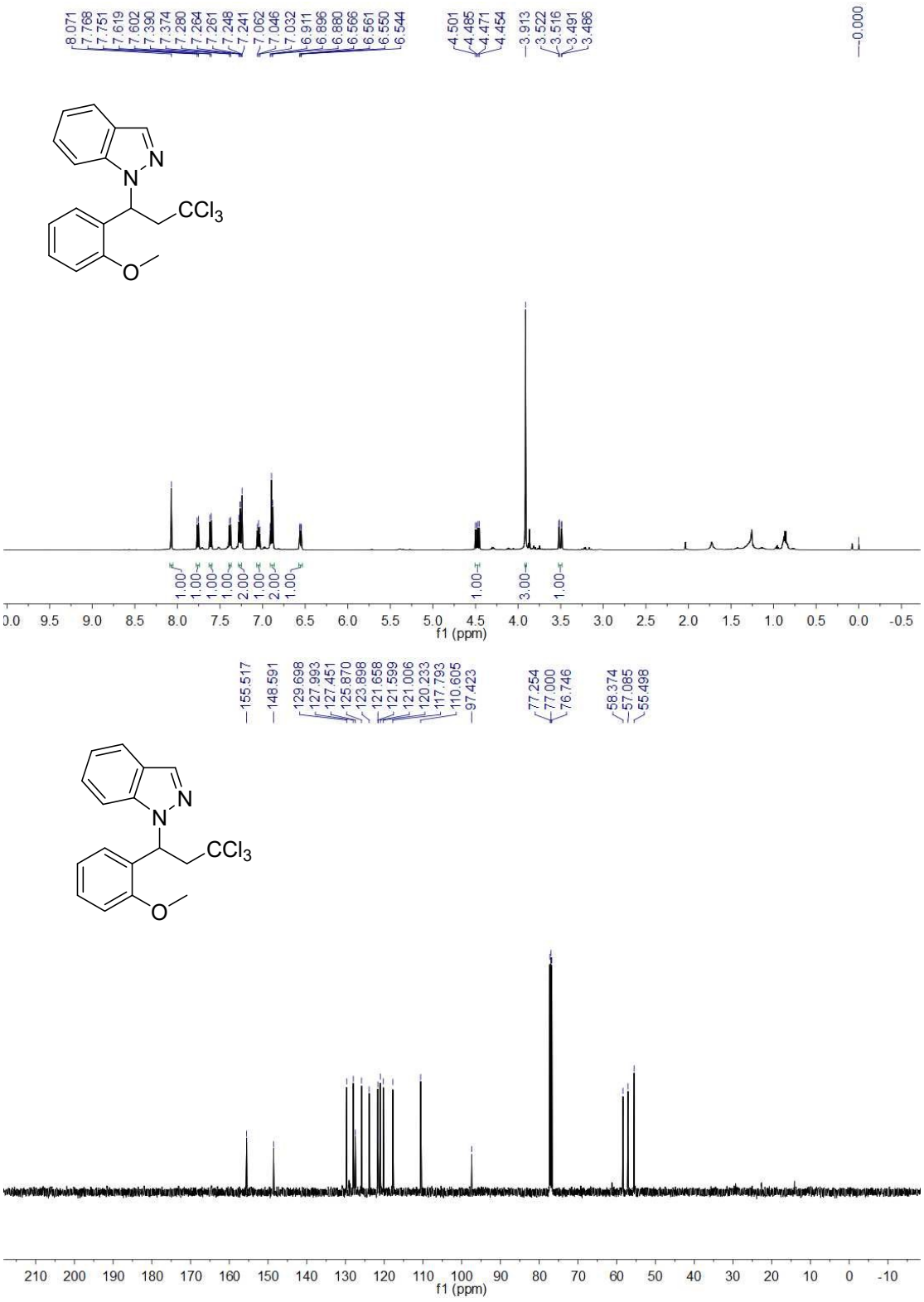
1-(1-(4-(benzyloxy)phenyl)-3,3,3-Trichloropropyl)-1H-indazole (4caa)



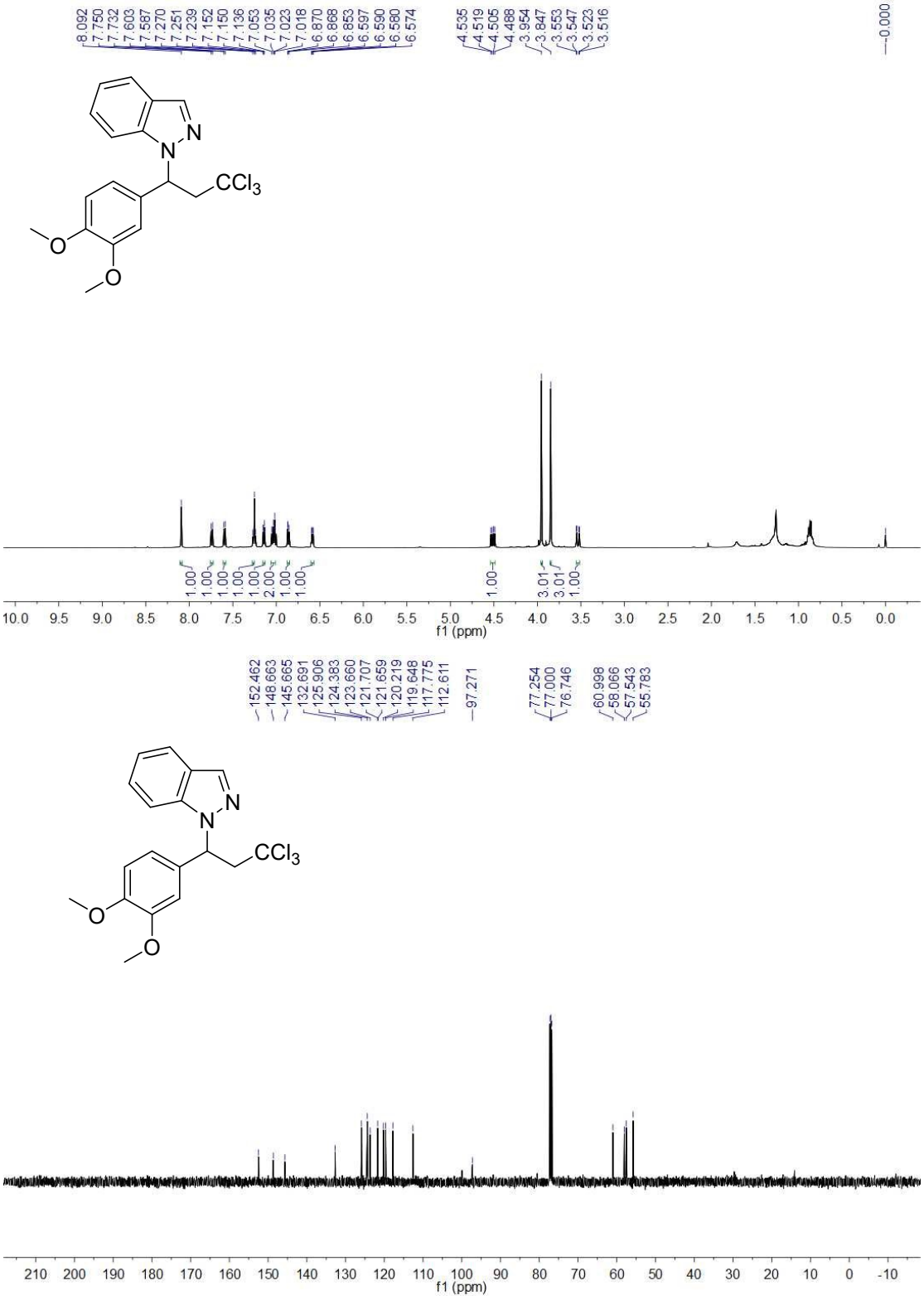
4-(3,3,3-Trichloro-1-(1H-indazol-1-yl)propyl)phenyl acetate (4daa)



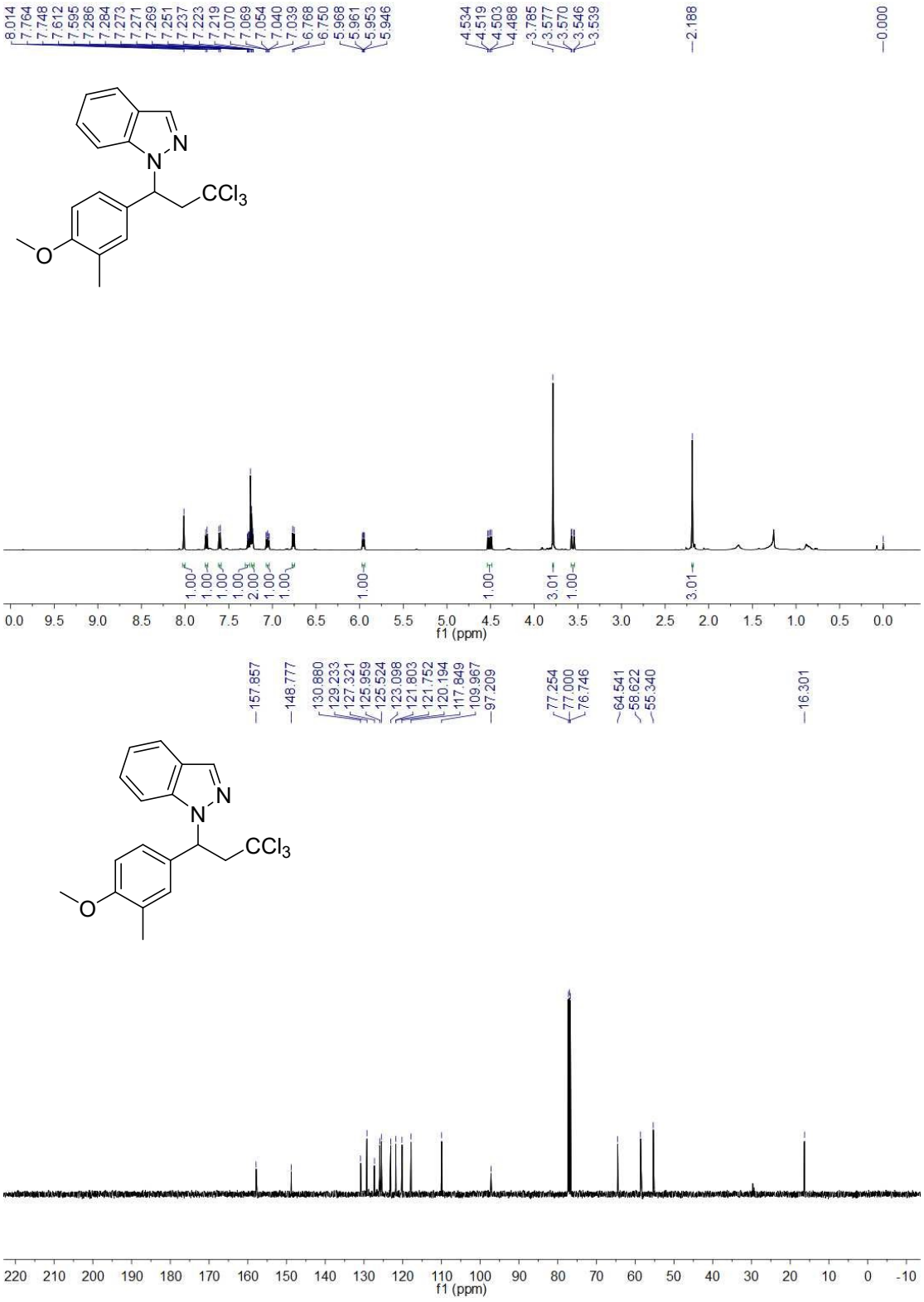
1-(3,3,3-Trichloro-1-(2-methoxyphenyl)propyl)-1H-indazole (4eaa)



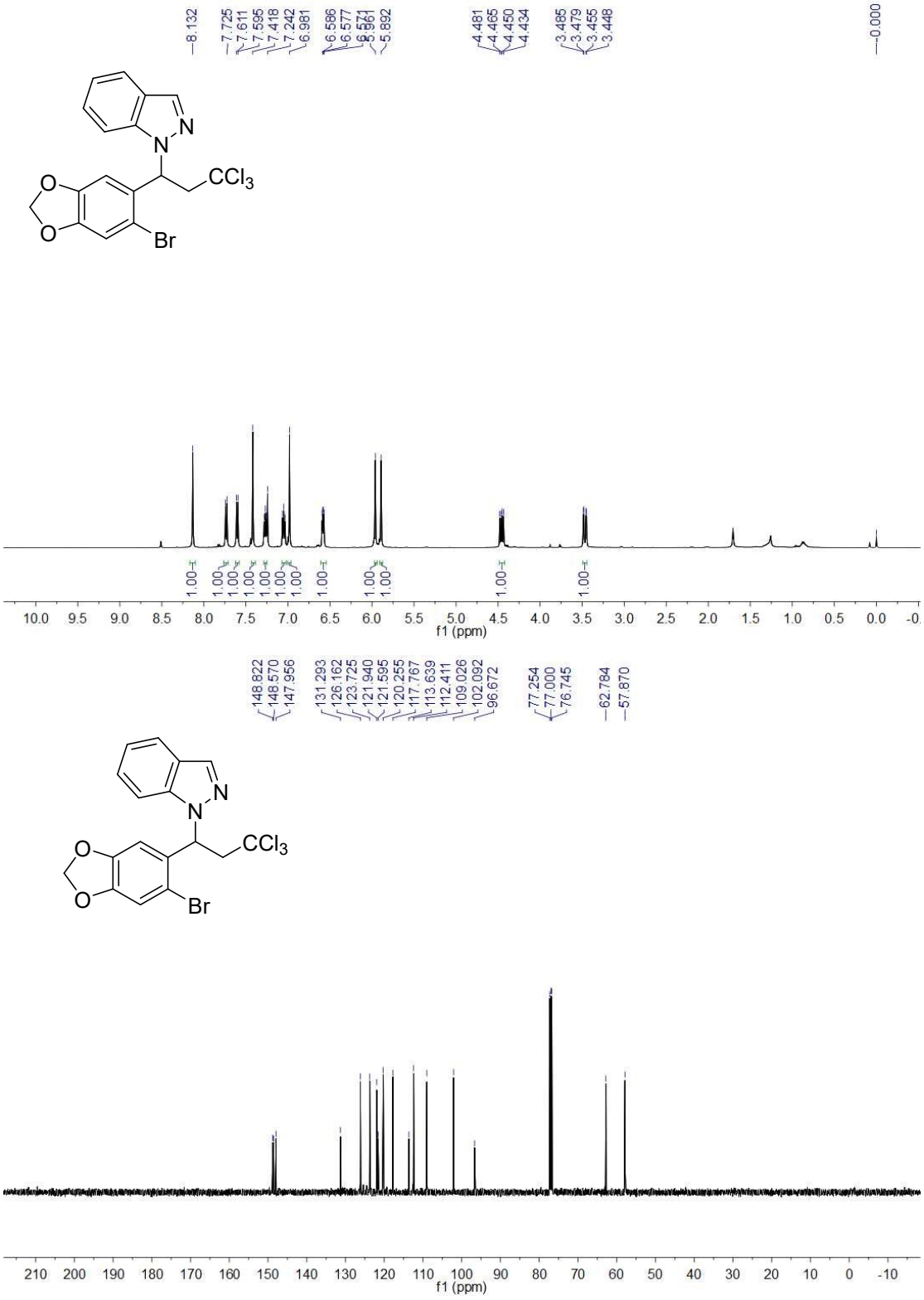
1-(3,3,3-Trichloro-1-(3,4-dimethoxyphenyl)propyl)-1H-indazole (4faa)



1-(3,3,3-Trichloro-1-(4-methoxy-3-methylphenyl)propyl)-1H-indazole (4gaa)

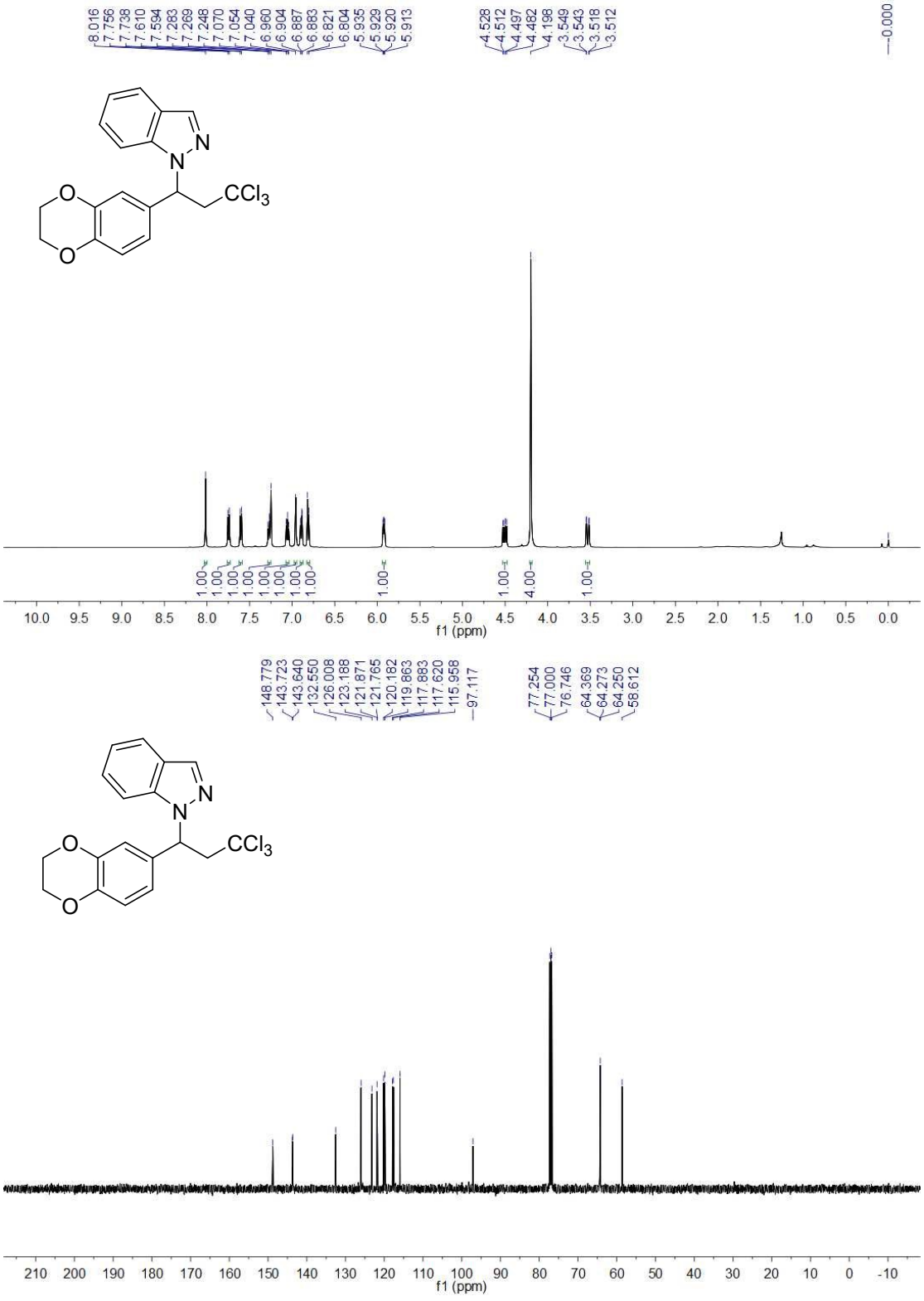


1-(1-(6-bromobenzo[d][1,3]dioxol-5-yl)-3,3,3-Trichloropropyl)-1H-indazole (4haa)

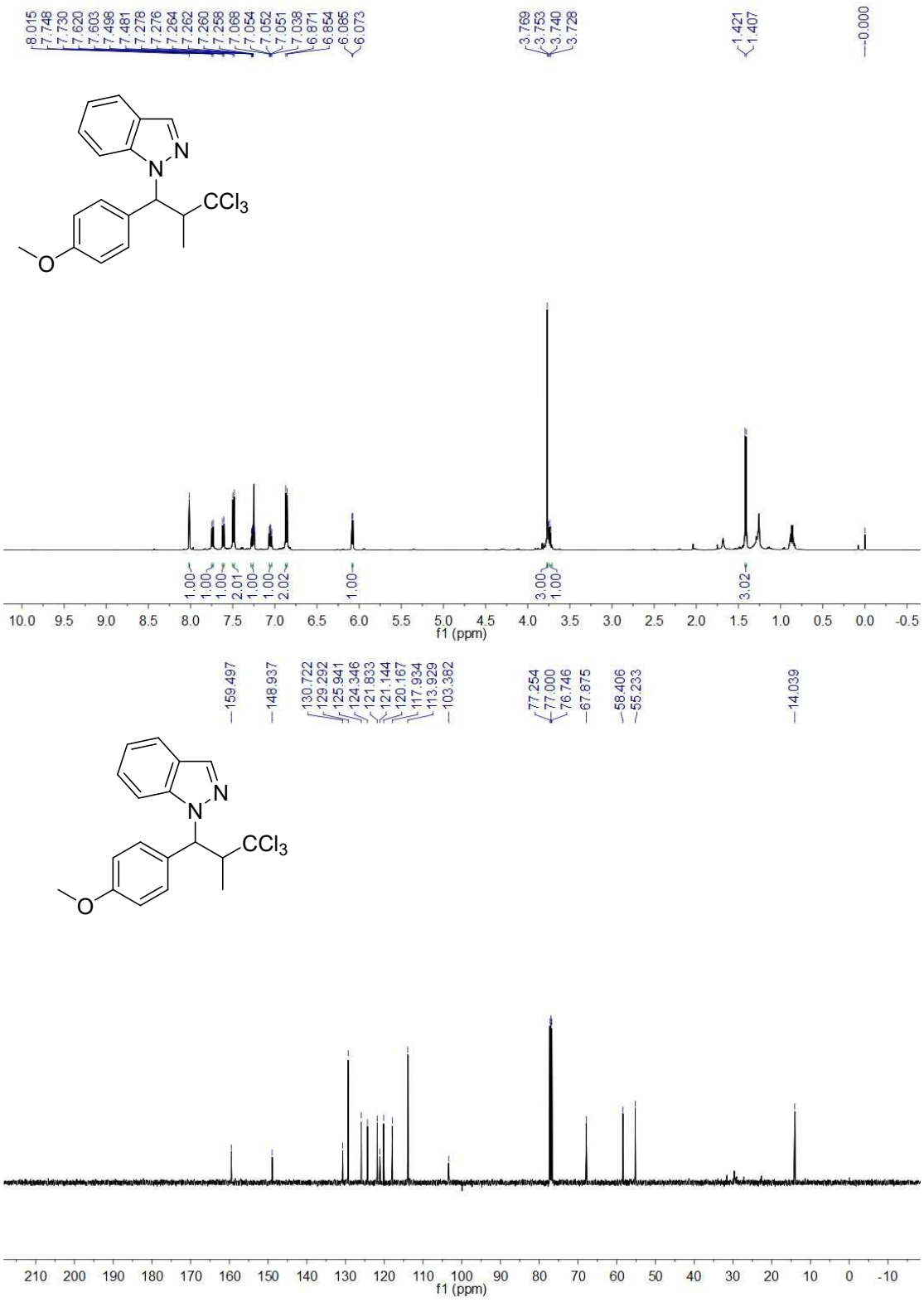


1-(3,3,3-Trichloro-1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)propyl)-1H-indazole

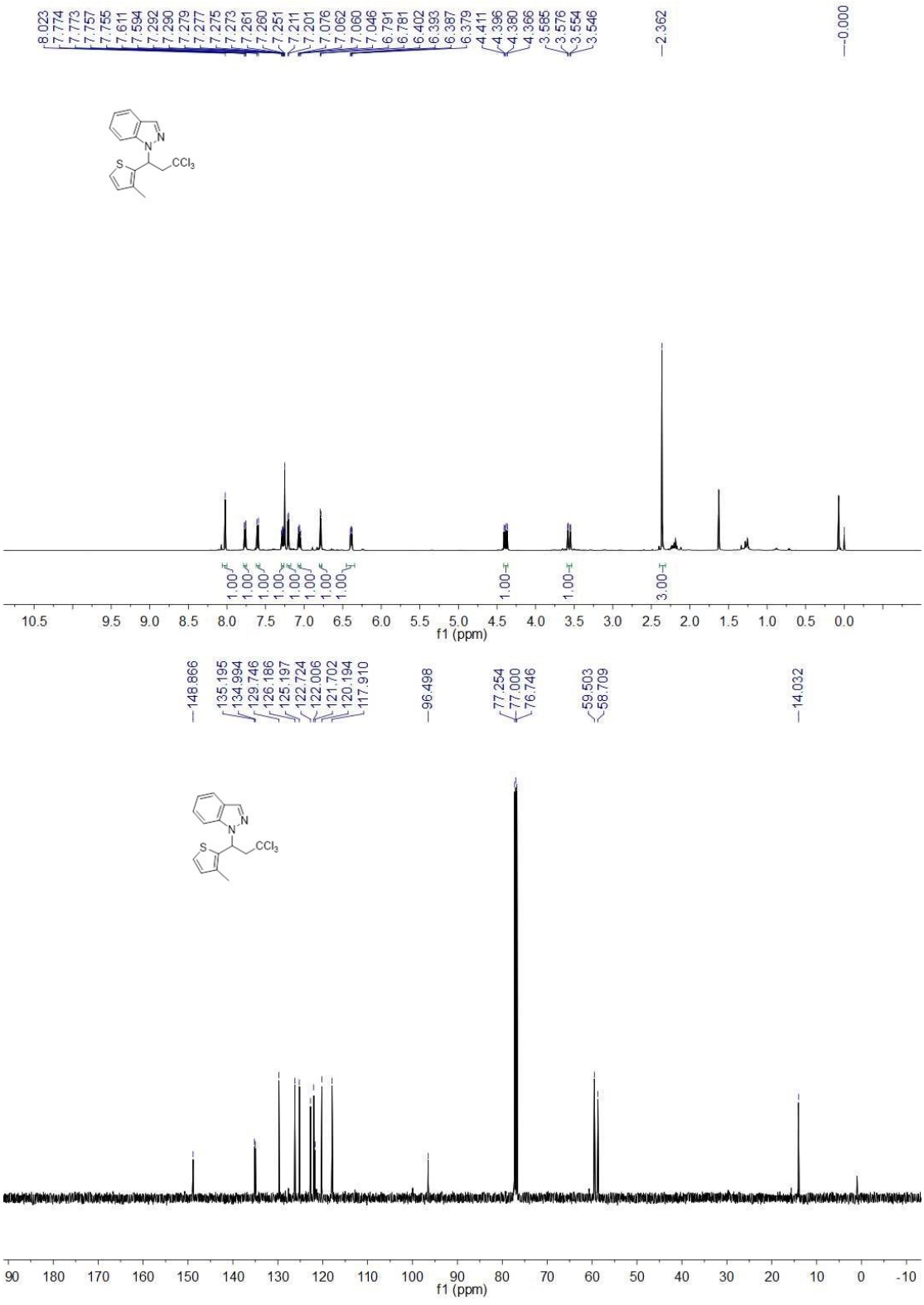
(4iaa)



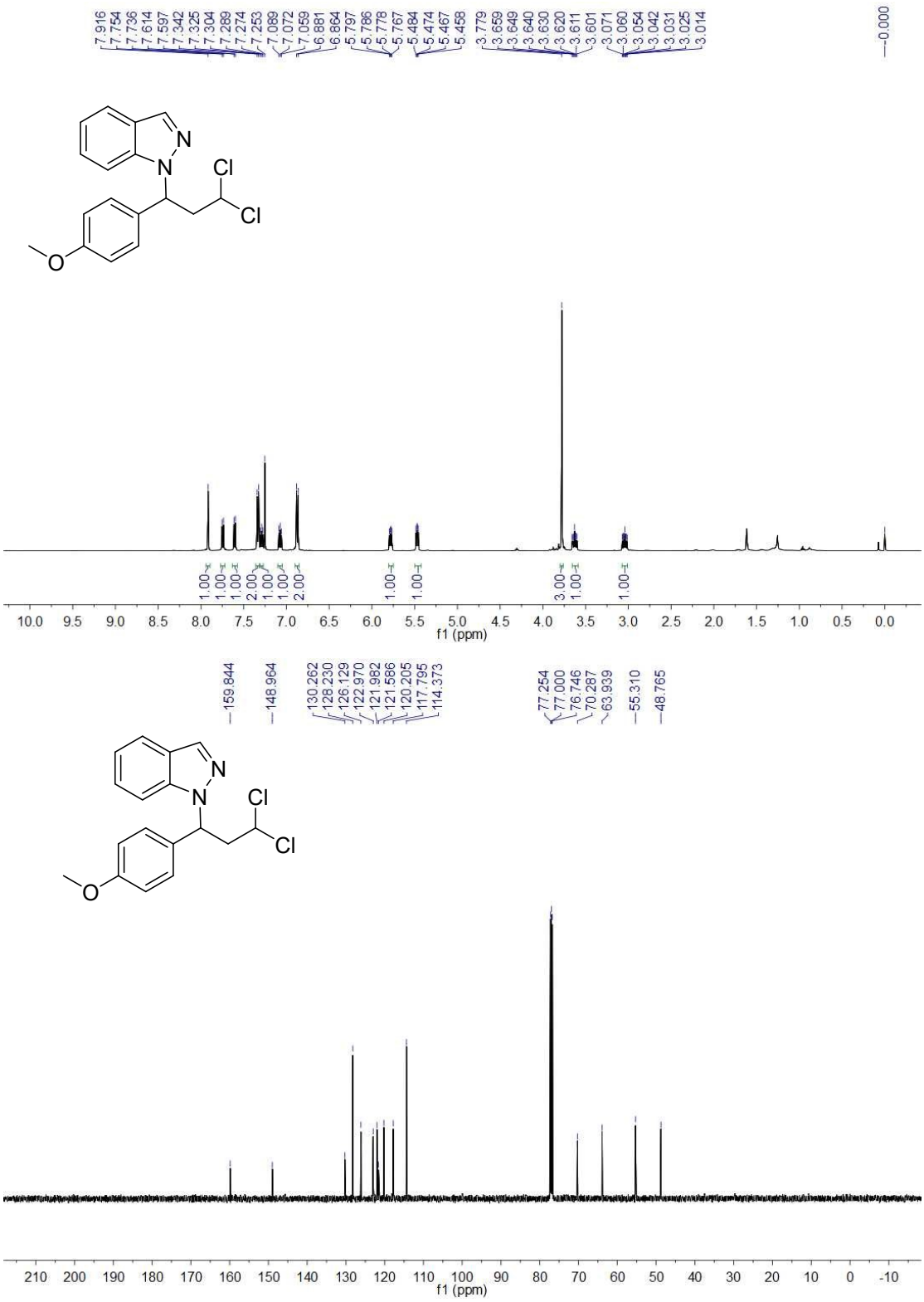
1-(3,3,3-Trichloro-1-(4-methoxyphenyl)-2-methylpropyl)-1*H*-indazole (4jaa)



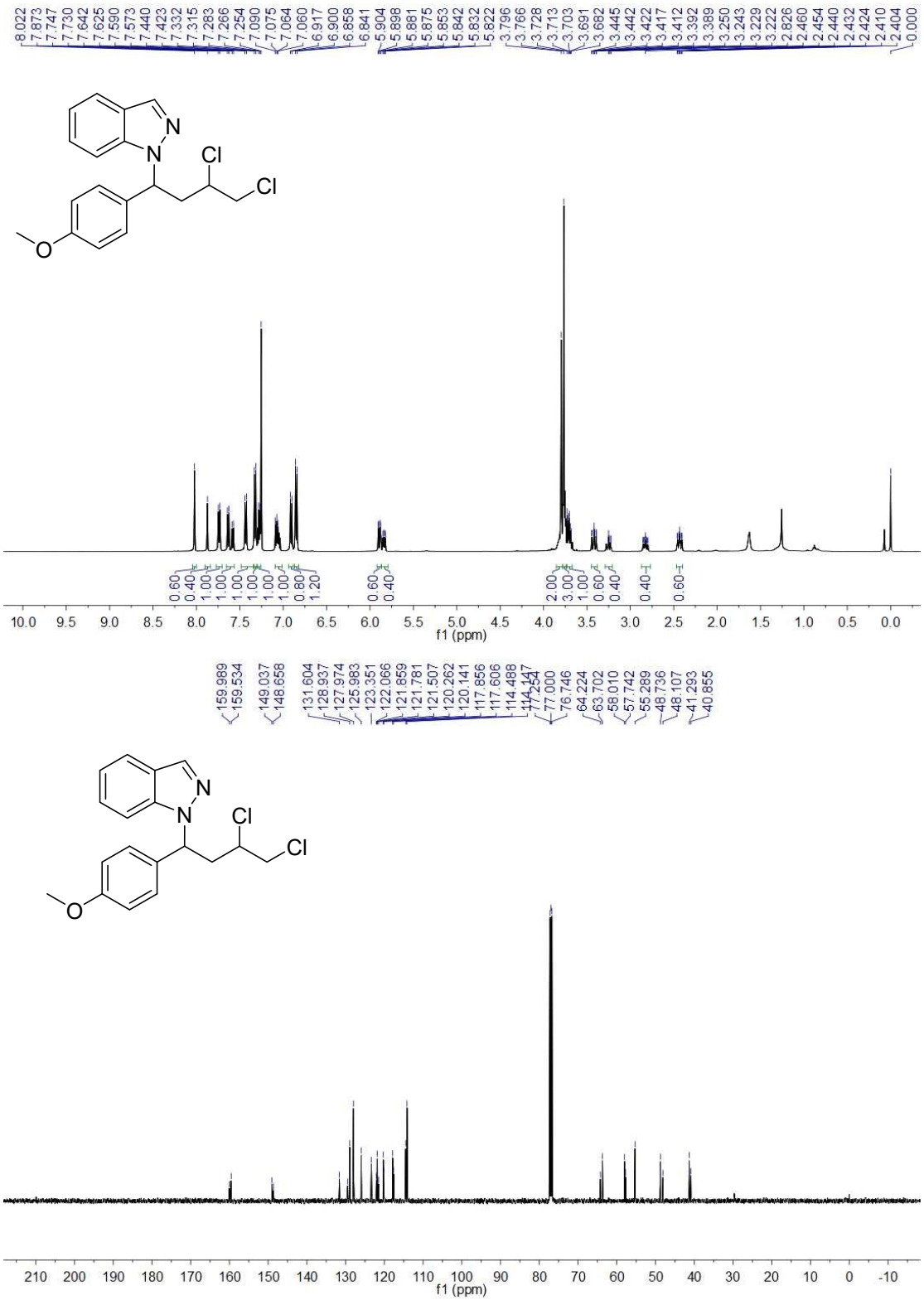
1-(3,3,3-Trichloro-1-(3-methylthiophen-2-yl)propyl)-1*H*-indazole (4kaa)



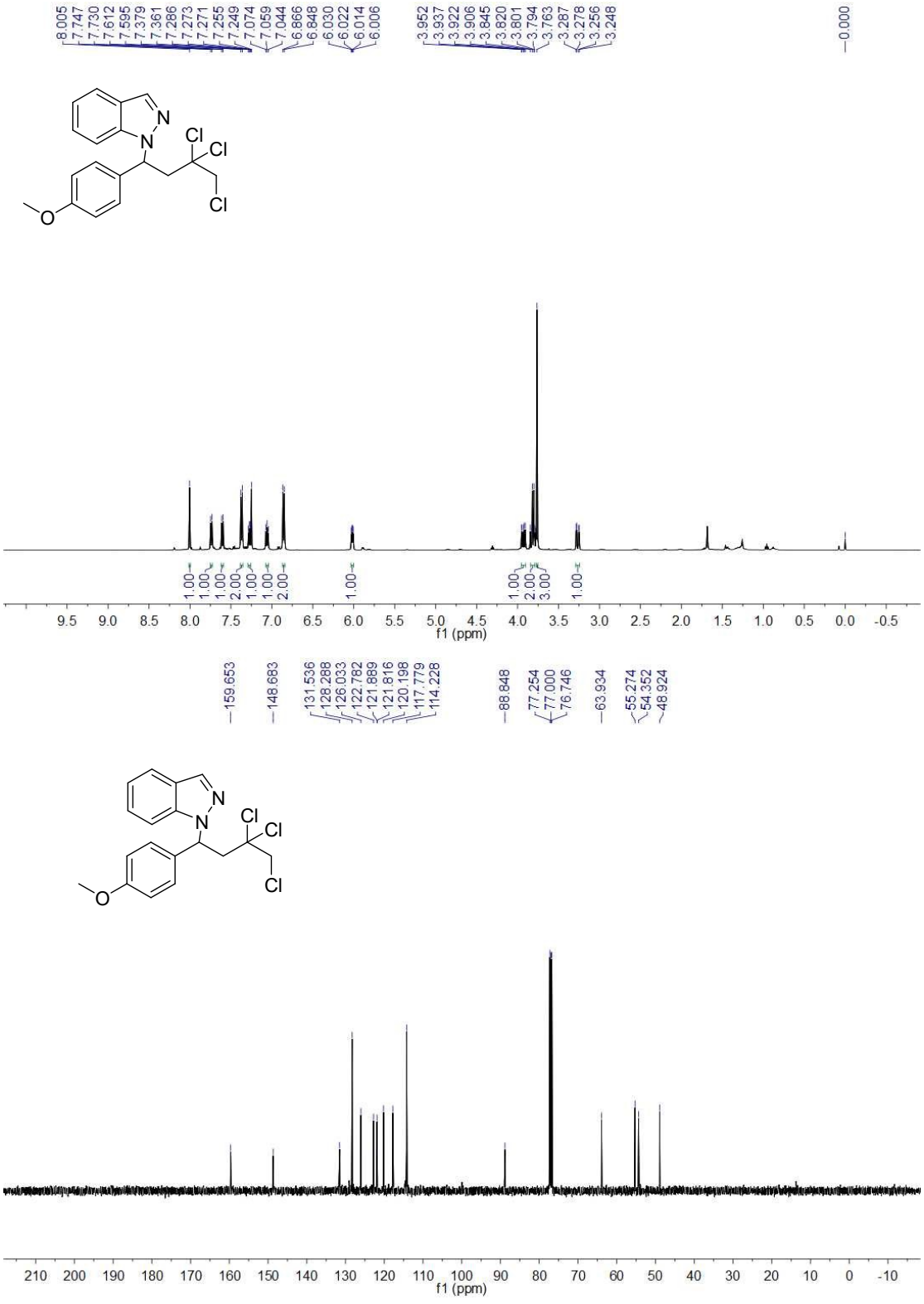
1-(3,3-dichloro-1-(4-methoxyphenyl)propyl)-1*H*-indazole (4aba)



1-(3,4-dichloro-1-(4-methoxyphenyl)butyl)-1H-indazole (4aca)



1-(3,4,4-Trichloro-1-(4-methoxyphenyl)butyl)-1H-indazole (4ada)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7.271
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7.044
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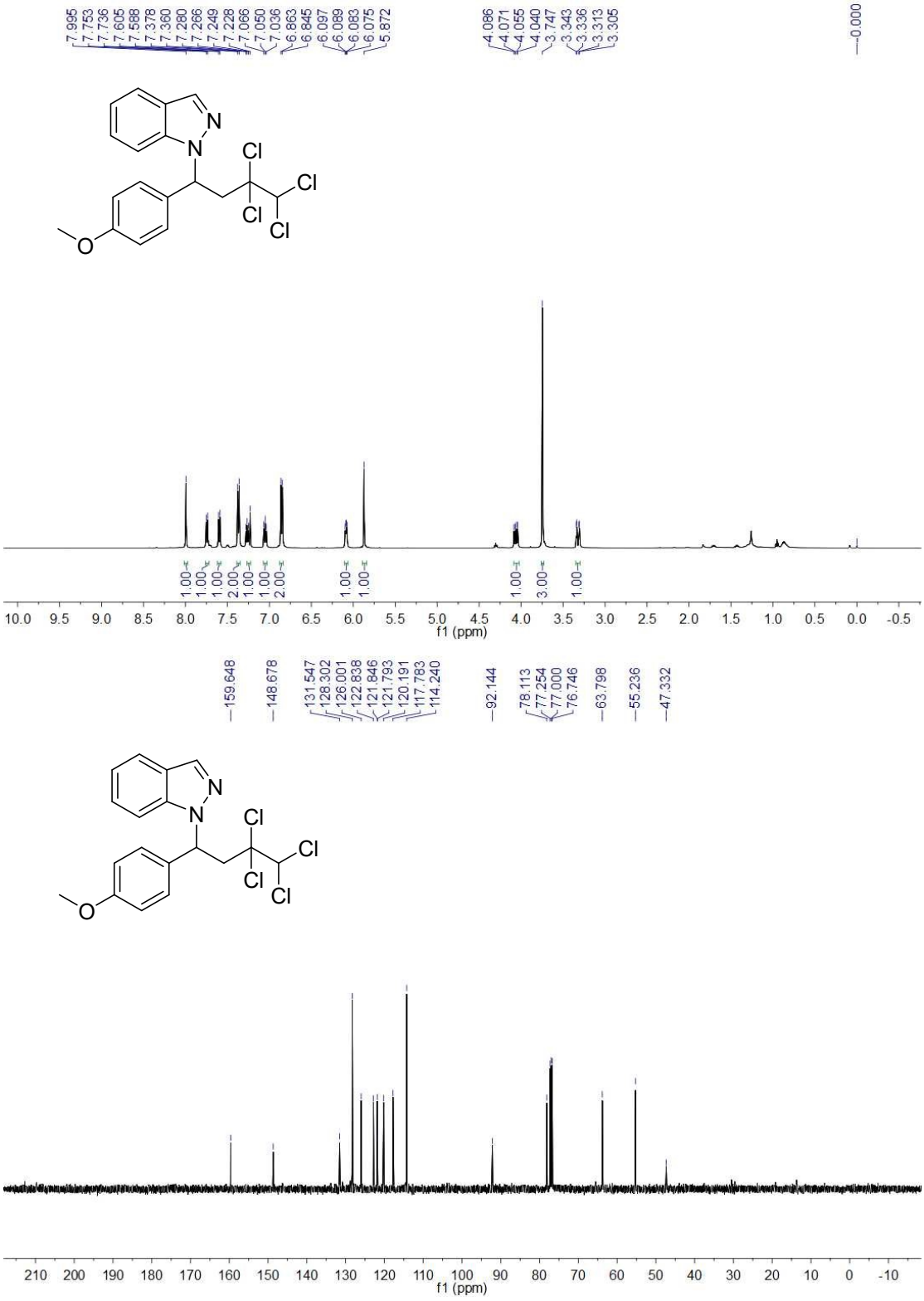
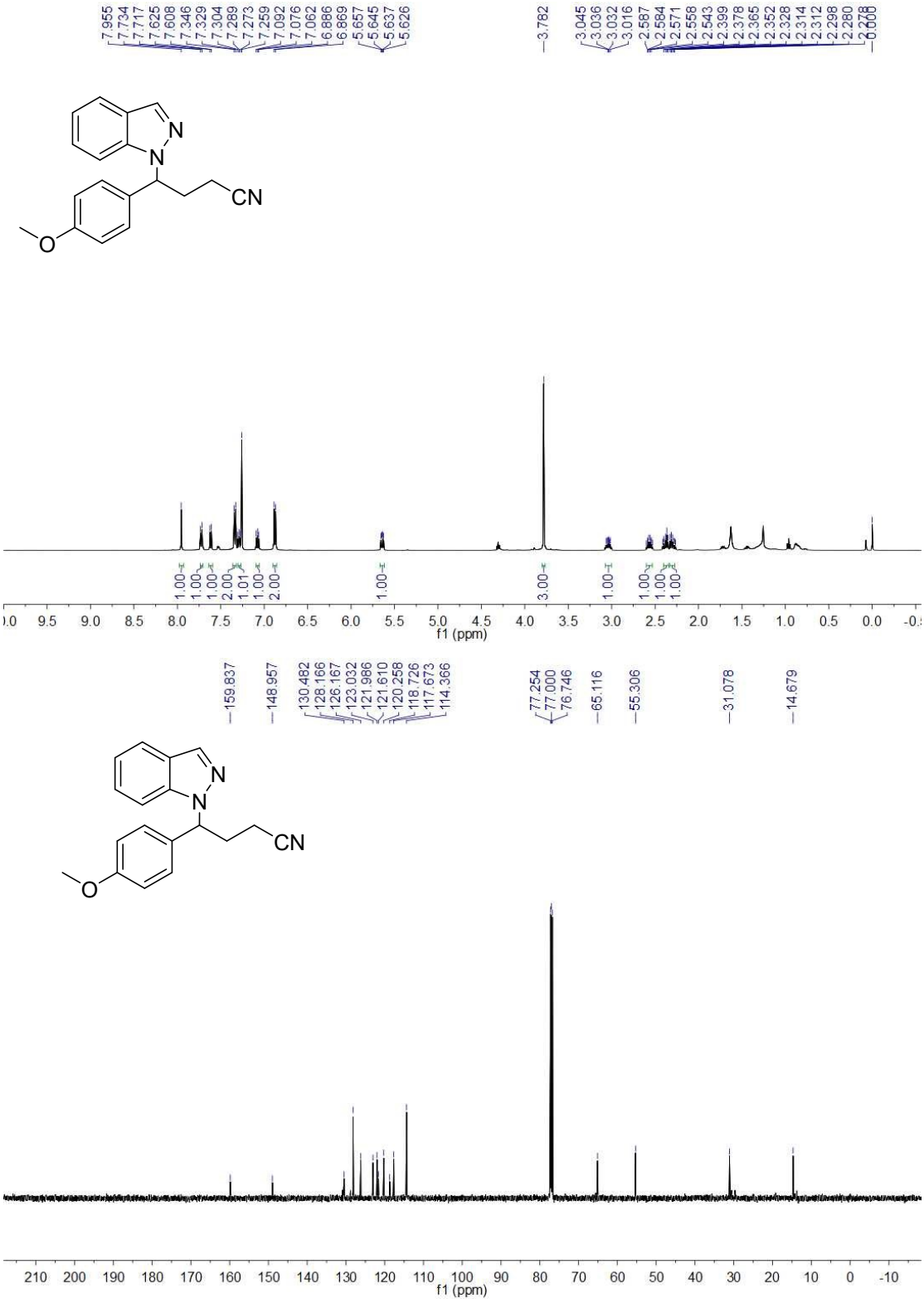
6.848
6.030
6.022
6.014
6.006
3.952
3.937
3.922
3.906
3.845
3.820
3.801
3.794
3.763
3.287
3.278
3.256
3.248
0.000
N
N
Cl
Cl
Cl
O
1.00
1.00
1.00
2.00
1.00
1.00
2.00
1.00
1.00
2.00
3.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
159.653
148.683
131.536
128.288
126.033
122.782
121.889
121.816
120.198
117.779
114.228
88.848
77.254
77.000
76.746
63.934
55.274
54.352
48.924
N
N
Cl
Cl
Cl
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

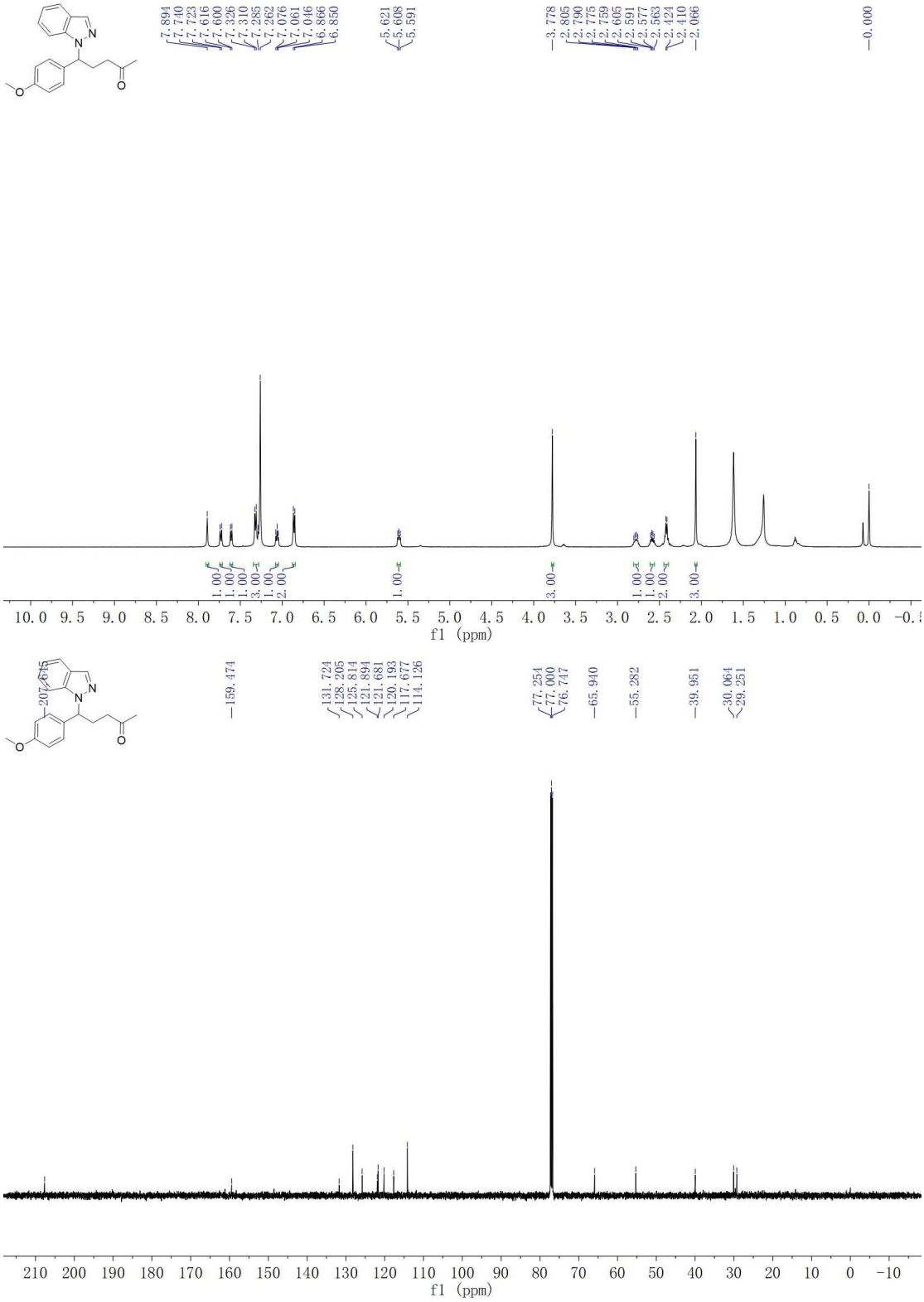
1-(3,3,4,4-tetrachloro- a1-(4-methoxyphenyl)butyl)-1*H*-indazole (4aea)



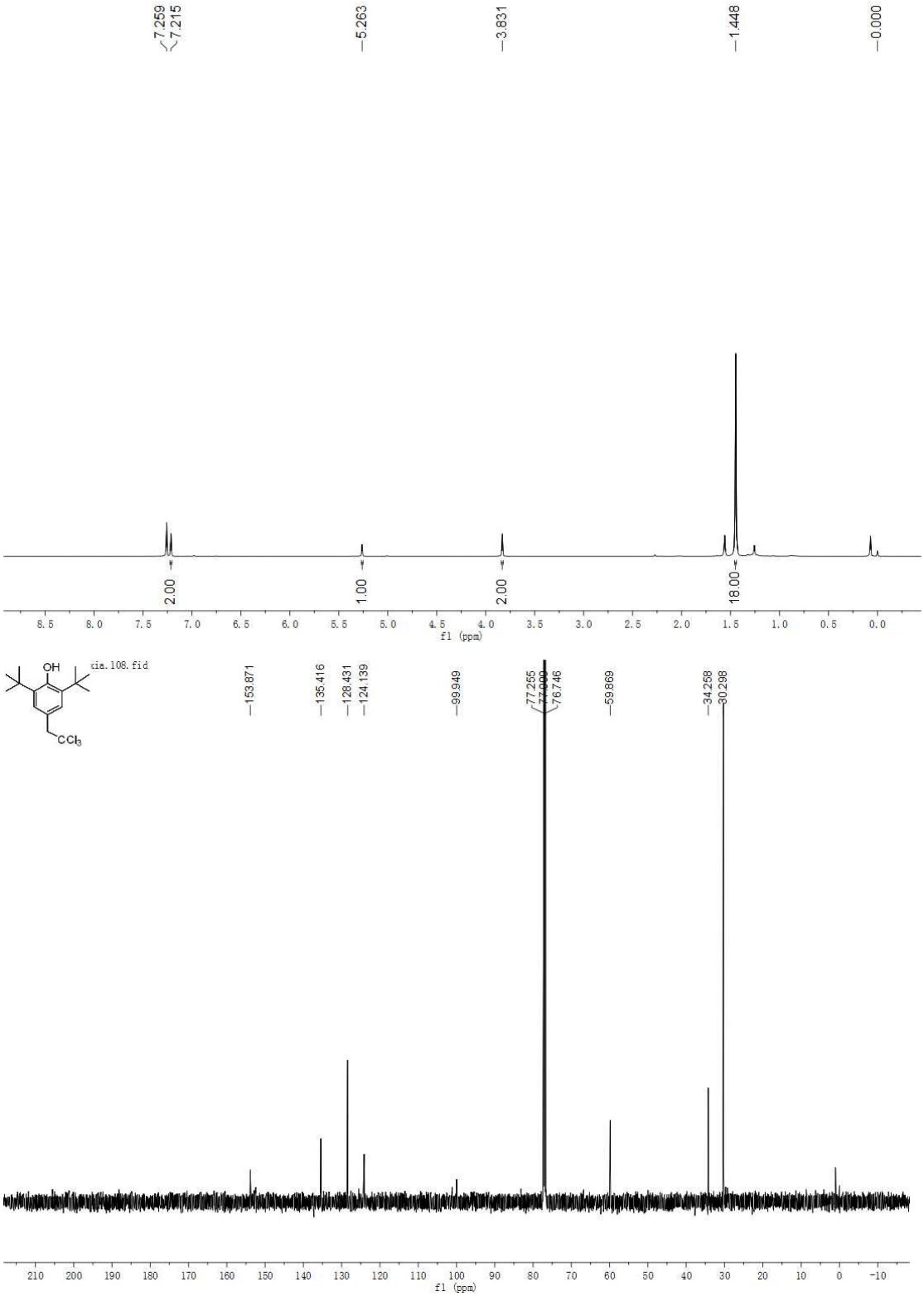
4-(1H-indazol-1-yl)-4-(4-methoxyphenyl)butanenitrile (4afa)



5-(1*H*-indazol-1-yl)-5-(4-methoxyphenyl)pentan-2-one (4aga)



2,6-Di-tert-butyl-4-(2,2,2-trichloroethyl)phenol (5a)



(2-(4-Methoxyphenyl)ethene-1,1-diyl)dibenzene (5b)