Regiochemistry of the Microwave-Assisted Reaction between Aromatic Amines and α-Bromoketones to Yield Substituted 1H-Indoles

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Supporting Information

List of Contents:

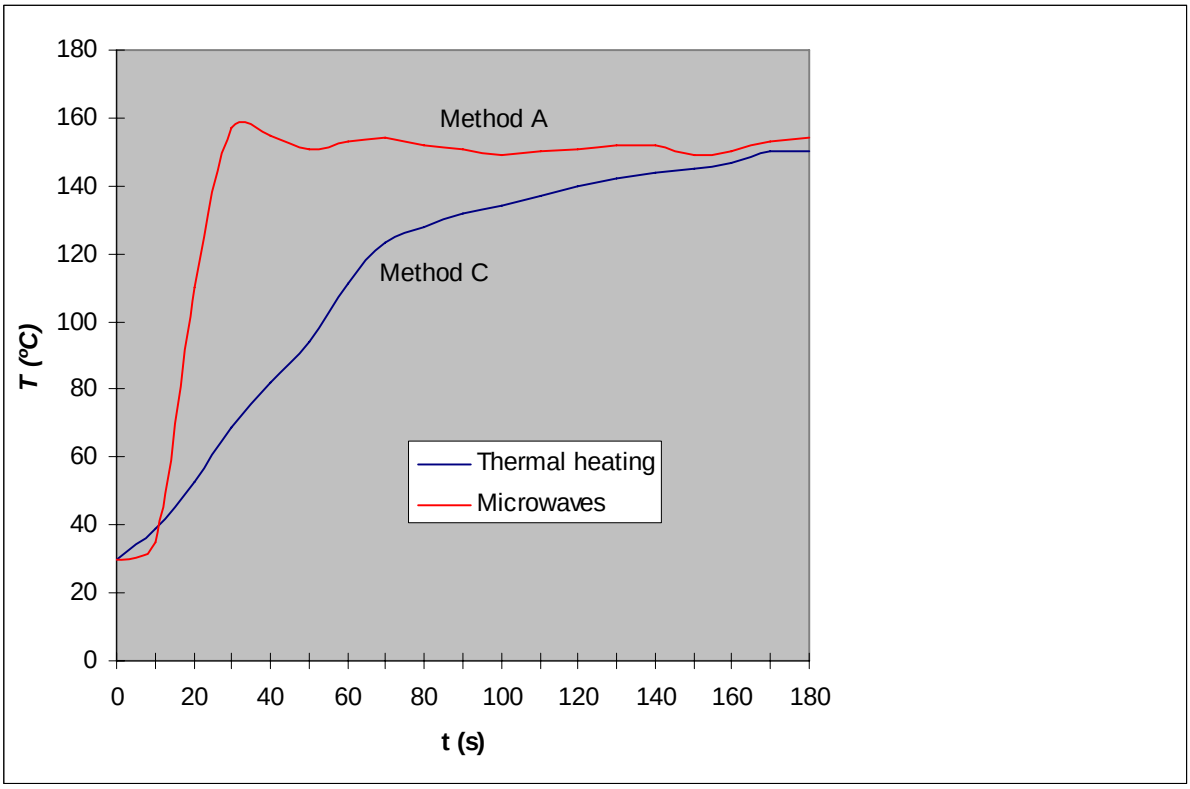


Figure S1. Temperature profiles for the reaction between **1d** and **2c** under microwave irradiation (100 W, 20 psi, Method A) and under thermal heating (Solvent-free conditions, Method C).

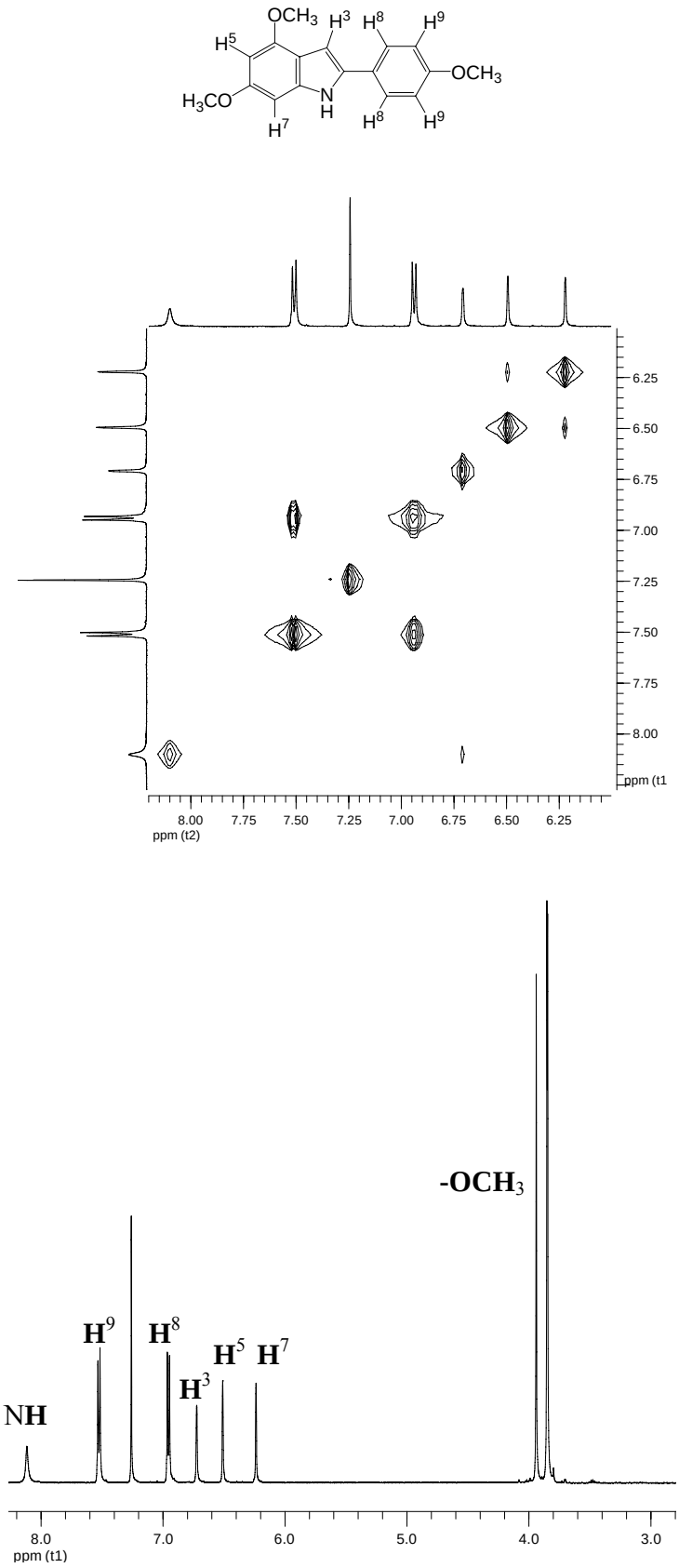


Figure S2. COSY spectrum and assignation of compound **3c**.

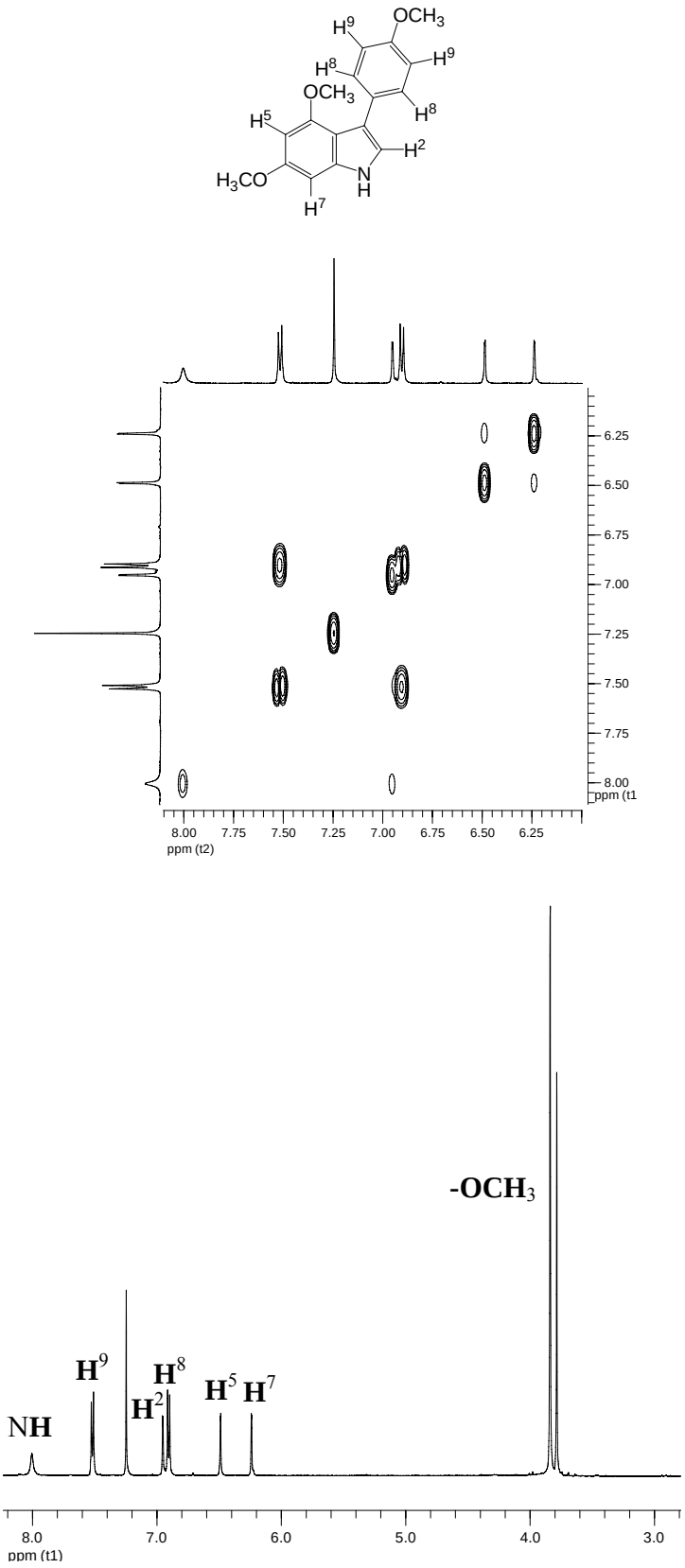


Figure S3. COSY spectrum and assignation of compound **4c**.

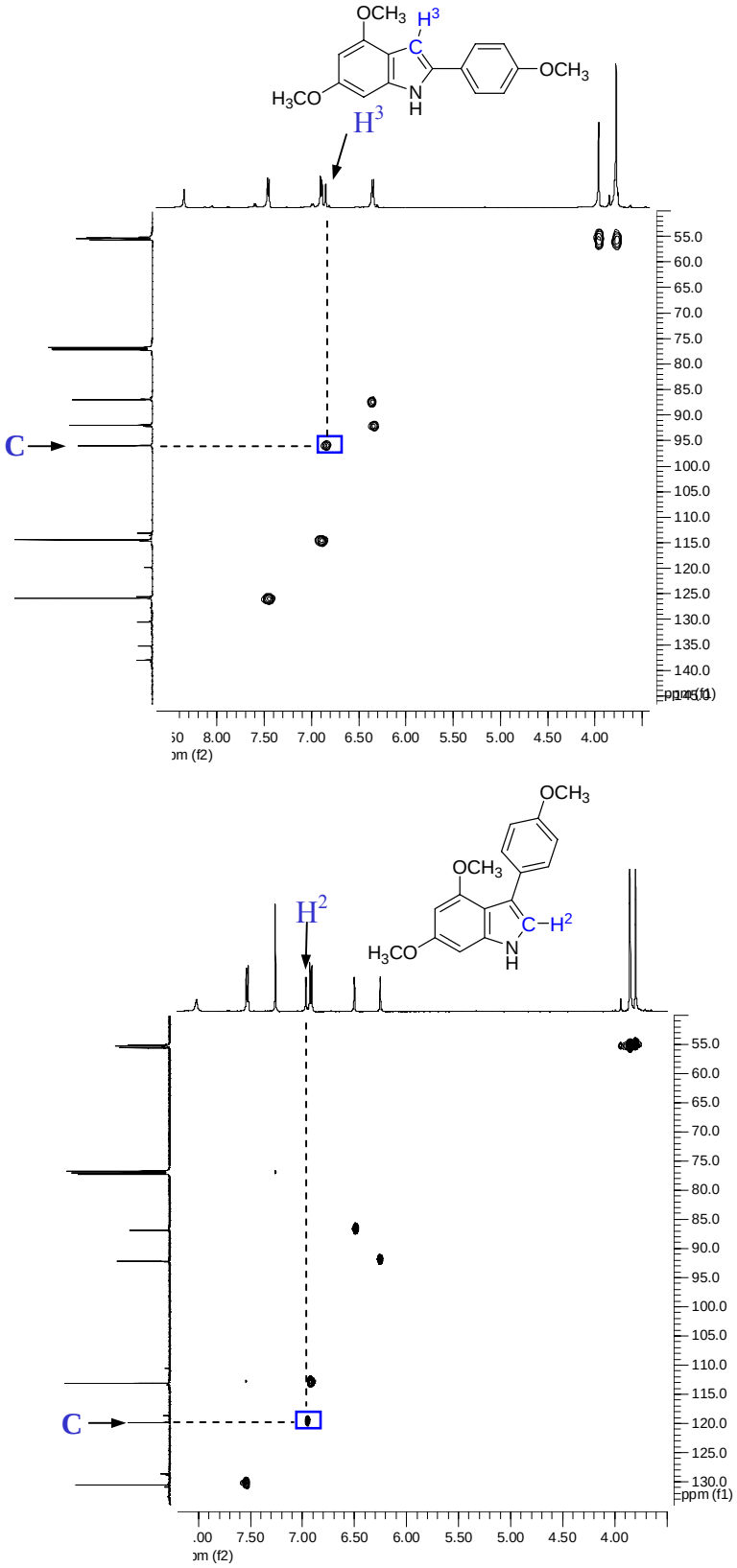


Figure S4. HSQC spectra of compounds **3c** (up) and **4c** (down).

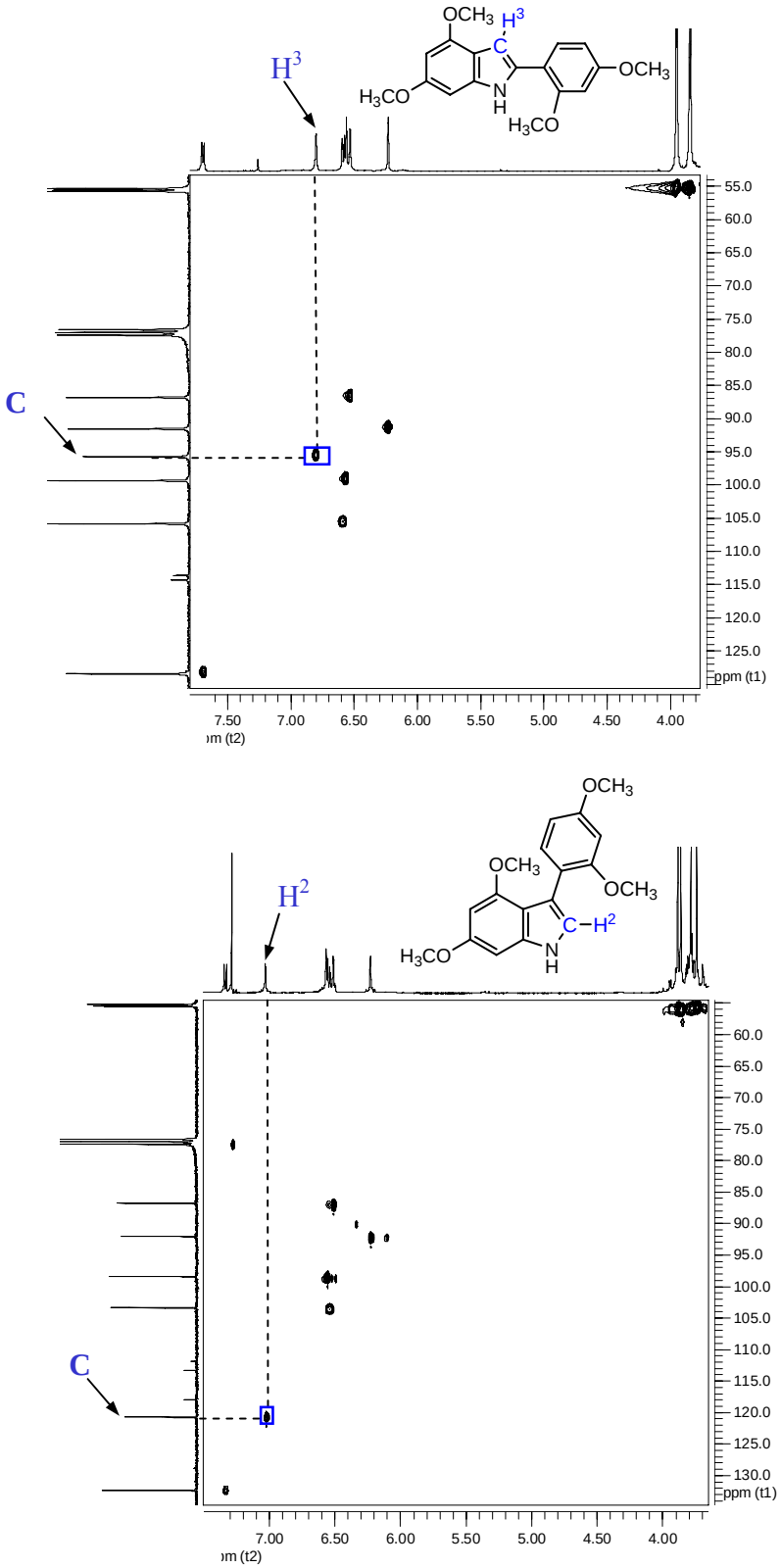


Figure S5. HSQC spectra of compounds **3e** (up) and **4e** (down).

Experimental Procedures and Characterization of Compounds 1i,l,m, 2c, 3,4a-r, 15a,b and 16a-c.

***N*-*tert*-Butylaniline**[1] (**1i**). Colourless oil, 69% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.14 (2 H, t), 6.74 (3H, m), 3.34 (1 H, br s), 1.33 (9 H, s).

***N*-*tert*-Butyl-*N*-methylaniline** (**1m**)[2]. Colourless oil, 72% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.35-7.04 (5 H, m), 2.80 (3 H, s), 1.16 (9 H, s).

***N*-Isopropyl-*N*-methylaniline**[3] (**1l**). Colourless oil, 45 % yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.30-7.16 (1 H,m), 6.86-6.62 (3H, m), 4.10 (1 H, m), 2.73 (3 H, s), 1.17 (6 H, d, J = 6.6 Hz).

2-Bromo-1-(3,5-dimethoxyphenyl)ethanone[4] (2c). White solid, 82% yield. ^{1}H NMR (δ ppm, 500 MHz, CDCl3), 7.10 (2H, d, J = 2.2 Hz), 6.69 (1H, t, J = 2.2 Hz), 4.43 (2H, s), 3.85 (6H, s).

5,7-Dimethoxy-2-(4-methoxyphenyl)-1*H*-indole (3b): White solid, 30% yield; mp 164ºC (Et_2O-hexanes); ν_{max}/cm^{-1} (KBr) 3376, 1592, 1498, 1141; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.30 (1H, s), 7.59 (2H, d, J = 8.7 Hz), 6.98 (2H, d, J = 8.7 Hz), 6.67 (1H, d, J = 1.7 Hz), 6.62 (1H, d, J = 2.2 Hz), 6.34 (1H, d, J = 1.9 Hz), 3.96 (3H, s), 3.86 (6H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 159.2, 155.2, 146.2, 137.9, 130.0, 126.4, 122.3, 114.4, 99.0, 94.1, 93.6, 55.8, 55.4. Anal. Calcd. For $C_{17}H_{17}NO_3$: C, 72.1; H, 6.0; N, 4.9. Found: C, 72.0; H, 5.9; N, 5.0.

4,6-Dimethoxy-2-(4-methoxyphenyl)-1*H*-indole (3c): White solid, 52% yield; mp 131ºC (Et_2O-hexanes); ν_{max}/cm^{-1} (KBr) 3457, 1587, 1497, 1121; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.10 (1H, s), 7.51 (2H, d, J = 8.5 Hz), 6.94 (2H, d, J = 8.6 Hz), 6.71 (1H, s), 6.50 (1H, s), 6.22 (1H, s), 3.92 (3H, s),

3.84 (3H, s), 3.83 (3H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 158.9, 157.6, 153.5, 138.0, 135.3, 130.5, 125.9, 125.6, 119.8, 114.5, 113.1, 96.0, 92.0, 87.0, 55.7, 55.4, 55.3 Anal. Calcd. For $C_{17}H_{17}NO_3$: C, 72.1; H, 6.0; N, 4.9. Found: C, 71.8; H, 5.7; N, 5.1.

5-Methoxy-2-(3,5-dimethoxyphenyl)-1*H*-indole (3d): White solid, 48% yield; mp 105-107ºC (Et_2O-hexanes); ν_{max}/cm^{-1} (KBr) 3377, 1597, 1206, 1156; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.17 (1H, s), 7.27 (1H, d, J = 8.8 Hz), 7.07 (1H, d, J = 1.8 Hz), 6.85 (1H, dd, J = 8.7, 2.2 Hz), 6.77 (2H, d, J = 1.8 Hz), 6.73 (1H, s), 6.43 (1H, s), 3.85 (9H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 161.4**,** 154.7, 138.7, 134.6, 132.1, 129.8, 112.9, 111.8, 103.7, 102.5, 100.4, 99.8, 55.6**.** Anal. Calcd. For $C_{17}H_{17}NO_3$: C, 72.1; H, 6.0; N, 4.9. Found: C, 71.8; H, 6.3; N, 4.8.

4,6-Dimethoxy-2-(2,4-dimethoxyphenyl)-1*H*-indole (3e): White solid, 43% yield; mp 171-172ºC (Et_2O-hexanes); ν_{max}/cm^{-1} (KBr) 3427, 1587, 1472, 1301, 1216, 1126; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 9.38 (1H, s), 7.68 (1H, d, J = 8.4 Hz), 6.77 (1H, s), 6.57 (1H, d, J = 8.7 Hz), 6.55 (1H, s), 6.51 (1H, s), 6.20 (1H, s), 3.95 (3H, s), 3.93 (3H, s), 3.84 (3H, s), 3.83 (3H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 159.9, 157.4, 156.7, 153.4, 137.2, 133.5, 128.6, 114.5, 113.8, 106.0, 99.5, 95.5, 91.7, 87.0, 56.0, 55.8, 55.6, 55.5. Anal. Calcd. For $C_{18}H_{19}NO_4$: C, 69.0; H, 6.1; N, 4.5. Found: C, 68.8; H, 6.1; N, 4.6.

4,6-Dimethoxy-2-(2,5-dimethoxyphenyl)-1*H*-indole (3f): White solid, 61% yield; mp 148-150ºC (Et_2O-hexanes); ν_{max}/cm^{-1} (KBr) 3407, 1542, 1487, 1211, 1141; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 9.62 (1H, s), 7.32 (1H, d, J = 3.0 Hz), 6.92 (1H, d, J = 8.9 Hz), 6.90 (1H, d, J = 1.3 Hz), 6.76 (1H, dd, J = 8.9, 3.0 Hz), 6.52 (1H, s), 6.21 (1H, d, J = 1.4 Hz), 3.94 (6H, s), 3.84 (3H, s), 3.81 (3H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 157.7, 154.3, 153.5, 149.9, 137.4, 133.1, 121.7, 113.5, 113.4, 112.3, 97.2, 91.7, 86.8, 56.6, 55.8, 55.7, 55.4. Anal. Calcd. For $C_{18}H_{19}NO_4$: C, 69.0; H, 6.1; N, 4.5. Found: C, 68.7; H, 6.4; N, 4.4.

5,7-Dimethoxy-2-(3,5-dimethoxyphenyl)-1*H*-indole (3g): Oil, 16% yield; ν_{max}/cm^{-1} (KBr) 3477, 1597, 1206, 1150; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.42 (1H, s), 6.76 (2H, d, J = 2.1 Hz), 6.68 (1H, s), 6.63 (1H, d, J = 1.5 Hz), 6.39 (1H, t, J = 2.1 Hz), 6.32 (1H, d, J = 1.7 Hz), 3.90 (3H, s), 3.82 (3H, s), 3.81 (6H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 161.3, 155.3, 146.4, 137.9, 134.5, 129.7, 122.7, 103.5, 100.6, 99.7, 94.7, 93.7, 55.9, 55.5. Anal. Calcd. For $C_{18}H_{19}NO_4$: C, 69.0; H, 6.1; N, 4.5. Found: C, 68.9; H, 6.2; N, 4.6.

4,6-Dimethoxy-2-(3,5-dimethoxyphenyl)-1*H*-indole (3h): White solid, 80% yield; mp 126-128ºC (Et_2O-hexanes); ν_{max}/cm^{-1} (KBr) 3407, 1608, 1206, 1160; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.18 (1H, s), 6.82 (1H, s), 6.73 (2H, d, J = 1.8 Hz), 6.49 (1H, s), 6.38 (1H, s), 6.22 (1H, s), 3.92 (3H, s), 3.83 (9H, s); ^{13}C ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 161.4, 158.2, 153.9, 138.3, 135.3, 134.7, 114.6, 103.1, 99.4, 97.8, 92.2, 87.1, 55.8, 55.6. Anal. Calcd. For $C_{18}H_{19}NO_4$: C, 69.0; H, 6.1; N, 4.5. Found: C, 68.9; H, 5.8; N, 4.5.

6-Methoxy-2-(4-methoxyphenyl)-1*H*-indole (**3i**): White solid, 75% yield**;** mp 220-222ºC (Et_2O-hexanes); ν_{max}/cm^{-1} (KBr) 3441, 3383, 1685, 1656, 1485, 1247, 1177; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$ + DMSO) 9.88 (1H, s), 7.63 (2H, d, J = 8.7), 7.41 (1H, d, J = 8.5), 6.94 (2H, d, J = 8.7), 6.91 (1H, d, J = 1.4), 6.71 (1H, dd, J = 8.5, 2.1 Hz)**,** 6.59 (1H, s)**,** 3.83 (6H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$ + DMSO) 157.8, 154.9, 137.0, 136.2, 125.2, 124.8, 122.6, 119.4, 113.3, 108.5, 96.5, 93.9, 54.7, 54.4 Anal. Calcd. For $C_{16}H_{15}NO_2$: C, 75.9; H, 6.0; N, 5.5. Found: C, 75.8; H, 5.8; N, 5.6.

4,6-Dimethoxy-3-methyl-2-phenyl-1*H*-indole (3j): Oil, 28% yield; ν_{max}/cm^{-1} (KBr) 3447, 1608, 1121; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.84 (1H, s), 7.46 (2H, d, J = 7.5 Hz), 7.40 (2H, t, J = 7.8 Hz, 7.5 Hz), 7.26 (1H, t, J = 7.5 Hz, 6.9 Hz), 6.37 (1H, s), 6.16 (1H, d, J = 1.5 Hz), 3.85 (3H, s), 3.78 (3H, s), 2.55 (3H, s) ; ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 157.6, 155.7, 137.5, 133.5, 131.3, 128.6, 127.5,

126.6, 114.3, 109.1, 98.9, 97.0, 91.6, 86.6, 55.5, 55.2, 11.7. Anal. Calcd. For $C_{17}H_{17}NO_2$: C, 76.4; H, 6.4; N, 5.2. Found: C, 76.2; H, 6.5; N, 5.0.

4,6-Dimethoxy-3-(4-methoxyphenyl)-1*H*-indole (4c): Oil, 24% yield; ν_{max}/cm^{-1} (KBr) 3407, 1628, 1502, 1246, 1166; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.00 (1H, s), 7.52 (2H, d, J = 8.6 Hz), 6.95 (1H, d, J = 2.2 Hz), 6.90 (2H, d, J = 8.6 Hz), 6.49 (1H, d, J = 1.6 Hz), 6.24 (1H, d, J = 1.5 Hz), 3.84 (6H, s), 3.78 (3H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 158.1, 157.7, 155.1, 138.4, 130.6, 128.7, 119.9, 118.7, 113.2, 110.7, 92.3, 87.0, 55.7, 55.4, 55.2.

4,6-Dimethoxy-3-(2,4-dimethoxyphenyl)-1*H*-indole (4e): Oil, 23% yield; ν_{max}/cm^{-1} (KBr) 3407, 1552, 1211, 1161; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.02 (1H, s), 7.32 (1H, d, J = 8.2 Hz), 7.01 (1H, d, J = 2.0 Hz), 6.57-6.51 (2H, m), 6.49 (1H, d, J = 1.3 Hz), 6.21 (1H, d, J = 1.3 Hz), 3.87 (3H, s), 3.85 (3H, s), 3.77 (3H, s), 3.73 (3H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 159.6, 158.7, 157.5, 155.2, 137.8, 132.5, 120.9, 118.1, 113.4, 112.0, 103.5, 98.6, 92.2, 86.9, 55.7, 55.6, 55.5, 55.4.

4,6-Dimethoxy-3-(2,5-dimethoxyphenyl)-1*H*-indole (4f): Oil, 13% yield; ν_{max}/cm^{-1} (KBr) 3397, 1502, 1216, 1141; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.08 (1H, s), 7.06 (1H, s), 7.04 (1H, d, J = 2.9 Hz), 6.84 (1H, d, J = 8.8 Hz), 6.78 (1H, dd, J = 8.9, 3.0 Hz), 6.44 (1H, s), 6.20 (1H, s), 3.80 (3H, s), 3.78 (3H, s), 3.72 (3H, s), 3.71 (3H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 157.6, 155.0, 153.1, 152.0, 137.9, 126.3, 121.7, 118.3, 113.4, 112.4, 111.8, 92.4, 87.1, 56.3, 55.9, 55.8, 55.3.

4,6-Dimethoxy-3-(3,5-dimethoxyphenyl)-1*H*-indole (4h): Oil, 13% yield; ν_{max}/cm^{-1} (KBr) 3407, 1608, 1542, 1341, 1216, 1161; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.05 (1H, s), 7.05 (1H, d, J = 2.2 Hz), 6.82 (2H, d, J = 2.1 Hz), 6.50 (1H, d, J = 1.7 Hz), 6.40 (1H, t, J = 1.9, 2.2 Hz), 6.27 (1H, d, J = 1.6 Hz), 3.84 (3H, s), 3.82 (9H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 160.0, 157.6, 154.7, 138.4, 137.9,

120.7, 118.9, 110.2, 107.6, 98.5, 92.4, 86.9, 55.6, 55.3, 55.1. Anal. Calcd. For $C_{18}H_{19}NO_4$: C, 69.0; H, 6.1; N, 4.5. Found: C, 68.8; H, 5.9; N, 4.4.

4,6-Dimethoxy-2-methyl-3-phenyl-1*H*-indole (4j): Oil, 42% yield; ν_{max}/cm^{-1} (KBr) 3477, 1597, 1206, 1156; ^1H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.72 (1H, s), 7.39 (2H, d, J = 7.2 Hz), 7.32 (2H, t, J = 7.8, 7.5 Hz), 7.22 (1H, d, J = 7.4, 7.3 Hz), 6.32 (1H, d, J = 1.8 Hz), 6.18 (1H, d, J = 1.8 Hz), 3.75 (3H, s), 3.64 (3H, s), 2.24 (3H, s); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 156.8, 154.2, 136.7, 136.1, 130.9, 129.0, 114.1, 111.8, 92.0, 86.7, 55.6, 55.1, 12.1. Anal. Calcd. For $C_{17}H_{17}NO_2$: C, 76.4; H, 6.4; N, 5.2. Found: C, 76.4; H, 6.3; N, 5.3.

General procedure for the synthesis of 1*H*-indoles from *N*-alkyl anilines 1f-i. A mixture of *N*-alkyl aniline (1.0 mmol) and **2a** (1.0 mmol) was irradiated at 150 ºC, 150 W, 20 psi for 10 minutes in a microwave vessel. The resulting mixture was dissolved in EtOAc and washed with HCl 2N. After drying (Na_2SO_4), the solution was evaporated and purified by flash chromatography (Ethyl acetate/hexanes) to yield the corresponding indol**.**

2-Phenyl-1*H*-indole[5] (**3a**)**:** 100% yield. ^1H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.32 (1H, s), 7.67 (3H, t, J = 7.5 Hz), 7.45 (2H, t, J = 7.5 Hz), 7.40 (1H, d, J = 7.5 Hz), 7.34 (1H, t, J = 7.5 Hz), 7.22 (1H, t, J = 7.5 Hz), 7.15 (1H, t, J = 7.5 Hz), 6.85 (1H, s).

1-Methyl-3-phenyl-1*H*-indole[6] (**4k**): 53% yield. ^1H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.03 (1H, d, J = 8.0 Hz), 7.73 (2H, d, J = 8.2 Hz), 7.51 (2H, t, J = 7.6 Hz), 7.42 (1H, d, J = 8.2 Hz), 7.36 (2H, m), 7.27 (2H, m), 3.86 (3H, s).

1-Ethyl-3-phenyl-1*H*-indole[7] (**4l**): 57% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.99 (1H, d, J = 8.3 Hz), 7.71 (2H, d, J = 7.8 Hz), 7.57-7.38 (3H, m), 7.34 (1H, s), 7.31-7.15 (3H, m), 4.27 (2H, q, J = 7.3 Hz), 1.55 (3H, t, J = 7.3 Hz).

1-Isopropyl-3-phenyl-1*H*-indole (**4m**): Oil, 34% yield**.** ν_{max}/cm^{-1} (KBr) 3053, 2983, 2920, 1600, 1205; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.06 (1H, d, J = 8.0 Hz), 7.77 (2H, d, J = 8.1 Hz), 7.52 (3H, m), 7.48 (1H, s), 7.35 (2H, m), 7.28 (1H, m), 4.80 (1H, m), 1.65 (6H, d, J = 6.7 Hz); ^{13}C NMR (δ ppm, 500 MHz, $CDCl_3$) 136.4, 135.9, 128.7, 127.3, 126.3, 125.6, 121.7, 121.4, 120.0, 119.8, 116.9, 109.7, 47.0, 22.8. Anal. Calcd. For $C_{17}H_{17}N$**:** C, 86.8; H, 7.3; N, 6.0. Found: C, 86.7; H, 7.3; N, 6.0.

General procedure for the synthesis of 1*H*-indoles from *N,N*-dialkyl anilines 1j-m. A mixture of *N,N*-dialkyl aniline (1.0 mmol) and the corresponding α-bromoketone **2** (1.0 mmol) was irradiated at 150ºC, 150 W, 20 psi for 10 minutes in a microwave vessel. The resulting mixture was dissolved in EtOAc and washed with HCl 2N. After drying (Na_2SO_4), the solution is evaporated and purified by flash chromatography (Ethyl acetate/hexanes) to yield the corresponding indole**.**

Ethyl 1*H*-indole-2-carboxylate[8] **(3o):** 31% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 9.00 (1H, s), 7.72 (1H, d, J = 7.9 Hz), 7.45 (1H, d, J = 7.9 Hz), 7.36, (1H, t, J = 7.2 Hz), 7.26 (1H, s), 7.19 (1H, t, J = 7.2 Hz), 4.45 (2H, q, J = 7.1 Hz), 1.45 (3H, t, J = 7.1 Hz).

Ethyl 1-methyl-1*H*-indole-3-carboxylate[9] (**4p**): 34% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.22-8.14 (1H, m), 7.81 (1H, s), 7.40-7.27 (3H, m), 4.40 (2H, q, J = 7.1 Hz), 3.82 (3H, s), 1.43 (3H, t, J = 7.1 Hz).

3-(4-Metoxyphenyl)-1-methyl-1*H*-indole[5] (**4q**): 60% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.93 (2H, d, J = 8.0 Hz), 7.66 (2H, d, J = 8.7 Hz), 7.38 (2H, d, J = 8.2 Hz), 7.30 (1H, m), 7.21 (1H, m), 7.17 (1H, s), 7.02 (2H, d, J = 8.7 Hz), 3.88 (3H, s), 3.84 (3H, s).

1,2-Dimethyl-3-phenyl-1H-indole[10] (**4r**): 51% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 7.72 (1H, d, J = 7.9 Hz), 7.60-7.50 (4H, m), 7.38-7.33 (2H, m), 7.26 (1H, m), 7.17 (1H, m), 3.79 (3H, s), 2.54 (3H, s).

2-(4-methoxyphenyl)quinoxaline (20a). A mixture of phenylendiamine (0.227 g, 2.1 mmol), 2-bromo-1-(4methoxyphenyl)ethanone (0.229 g, 1.0 mmol), and N,N-dimethylaniline (0.42 ml, 3.3 mmol) was heated at 150ºC, 150 W in a microwave vessel for 10 minutes. The resulting mixture was dissolved in EtOAc and washed with HCl 2N. After drying (Na_2SO_4), the solution is evaporated and purified by flash chromatography (Ethyl acetate/hexanes) to yield the title product[11] in 61 % yield. m.p.100-101 ºC; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 9.30 (1H, s), 8.20 (2H, d, J = 8.8 Hz), 8.10 (2H, m), 7.73 (2H, m), 7.10 (2H, d, J = 8.8 Hz), 3.90 (3H, s).

2-(4-Nitrophenyl)quinoxaline[11] **(20b)**. 37 % yield. m.p.190 ºC; ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 9.40 (1H, s), 8.43 (4H, m), 8.20 (2H, m), 7.85 (2H, m).

2-(4-Methoxyphenyl)imidazo[1,2-a]pyridine (21a). A mixture of pyridin-2-amine (1 mmol), 2-bromo-1-(4methoxyphenyl)ethanone (1.0 mmol), and neutral Al_2O_3 (1 g.) was irradiated at 150ºC, 150 W and 20 psi in a microwave vessel for 10 minutes. After completion of the reaction, the contents were diluted with chloroform (5 ml) and filtered through a celite pad, washed with 2 ml of chloroform, and evaporated. The residue was purified by chromatography on silica gel using hexane-ethyl acetate as eluent to give the title product[12] in 70% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.11 (1H, dt, J = 6.8,

1.2 Hz)**,** 7.89 (2H, d, J = 8.9 Hz), 7.79 (1H, s), 7.61 (1H, dd, J = 9.1, 0.8 Hz), 7.15 (1H, m), 6.98 (2H, d, J = 8.9 Hz), 6.76 (1H, t, J = 6.8, 1.2 Hz), 3.86 (3H, s).

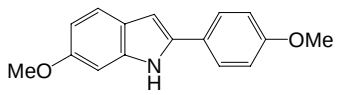
2-(4-Nitrophenyl)imidazo[1,2-a]pyridine[11] **(21b)**. 61 % yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.30 (2H, d, J = 8.9 Hz), 8.16 (1H, dt, J = 6.8, 1.0 Hz), 8.12 (2H, d, J = 8.9 Hz), 8.0 (1H, s), 7.66 (1H, dd, J = 8.9, 0.7 Hz), 7.24 (1H, m), 6.85 (1H, t, J = 6.8, 1.0 Hz).

2-(4-Methoxyphenyl)imidazo[1,2-a]pyrimidine[13] **(21c)**. 75% yield. ^{1}H NMR (δ ppm, 500 MHz, $CDCl_3$) 8.51-8.50 (1H, m), 8.42-8.39 (1H, m), 7.99-7.95 (2H, m), 7.74 (1H, m), 7.00-6.97 (2H, m), 6.85-6.82 (1H, m), 3.86 (3H, s).

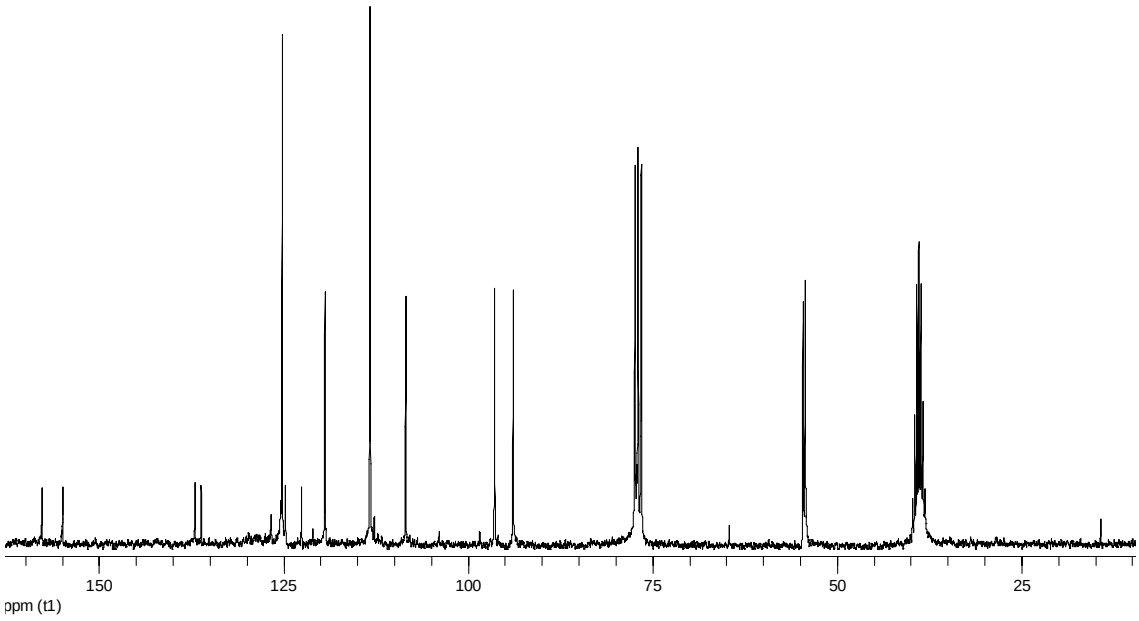
^{1}H and ^{13}C NMR Spectra for Compounds 3b-j and 4c,e,f,h,j,m

^{1}H-NMR ($CDCl_3$ + DMSO)

Compound 3i

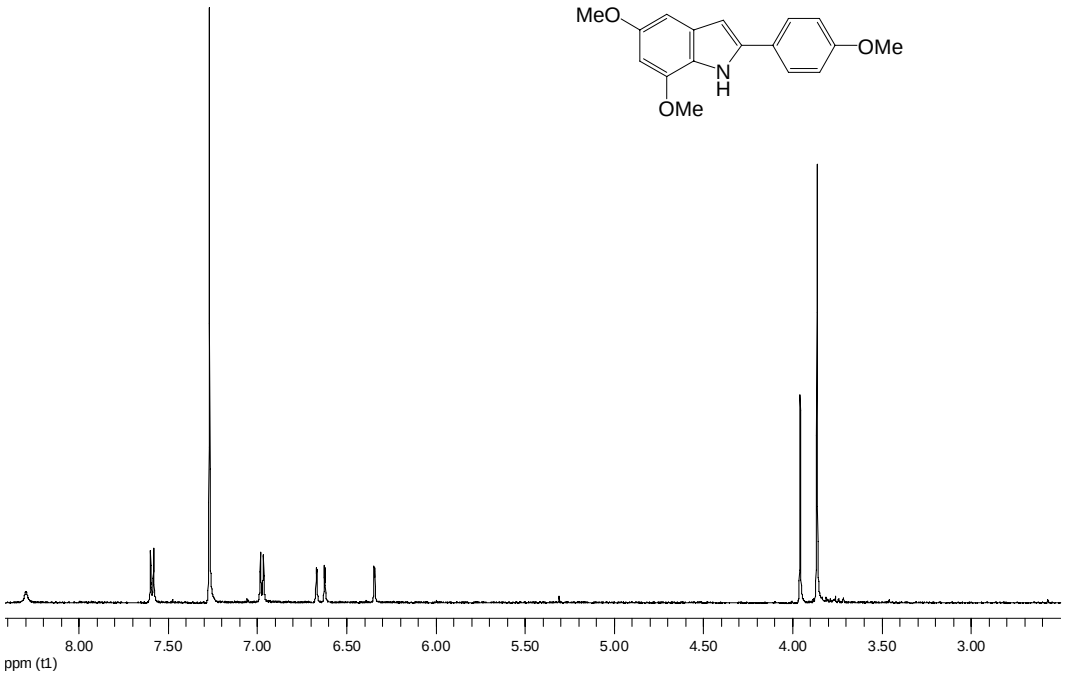


^{13}C-NMR ($CDCl_3$ + DMSO)

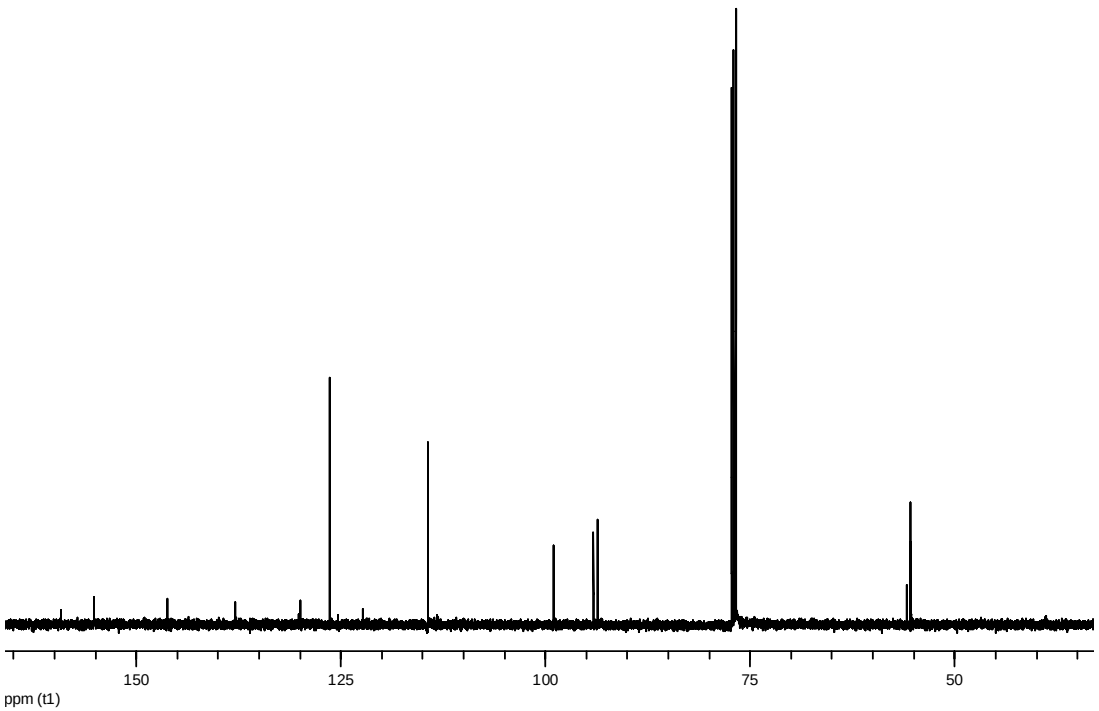


^{1}H-NMR ($CDCl_3$)

Compound 3b

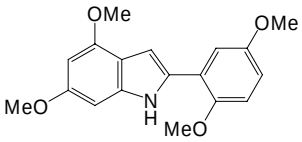


^{13}C-NMR ($CDCl_3$)

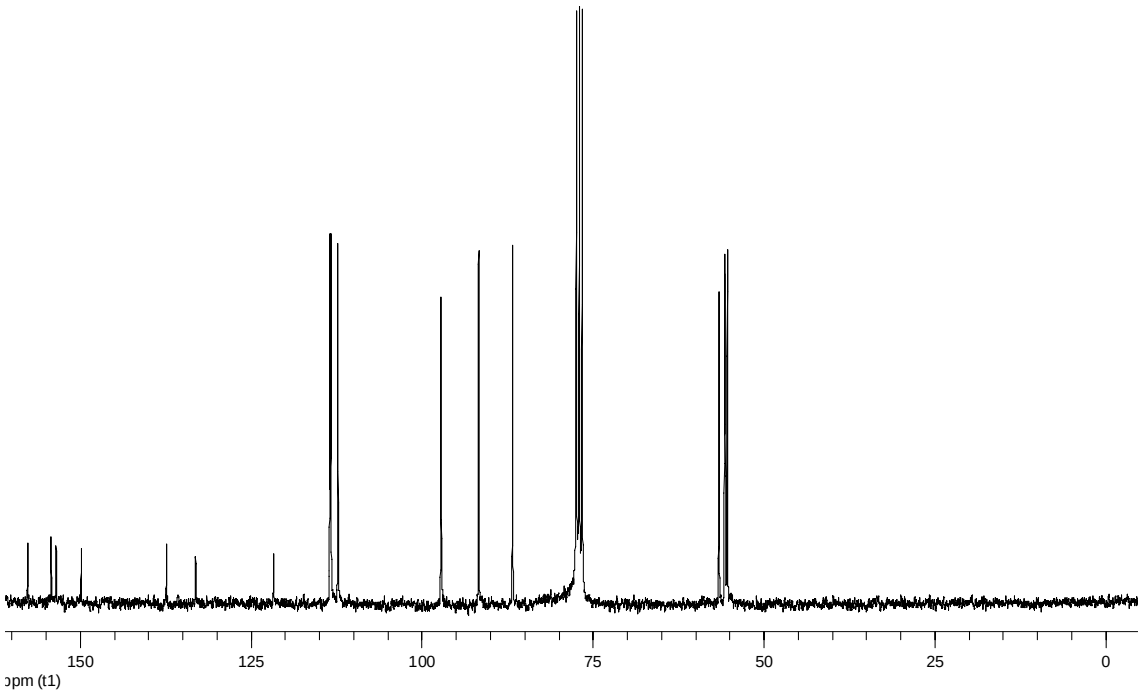


^{1}H-NMR ($CDCl_3$)

Compound 3f

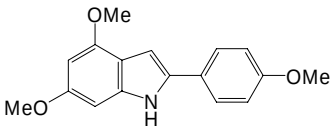


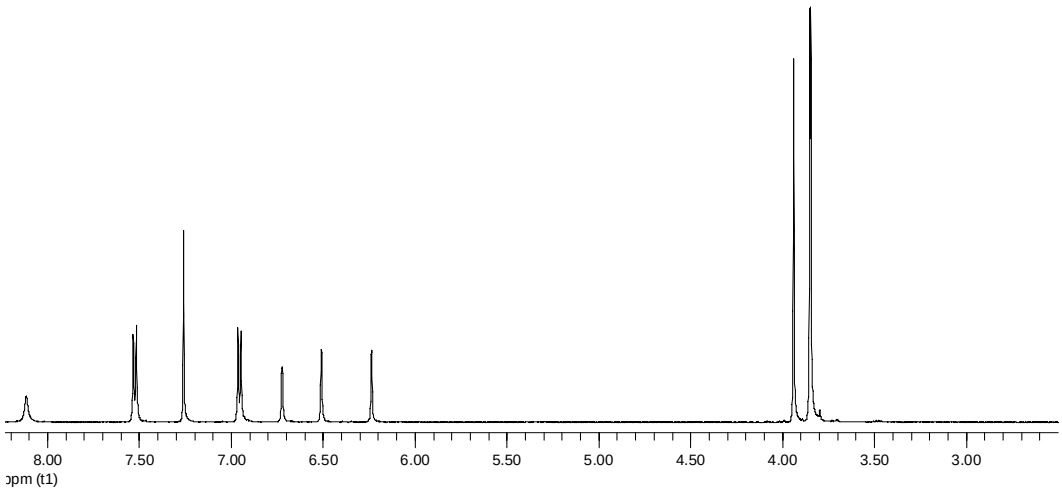
^{13}C-NMR ($CDCl_3$)



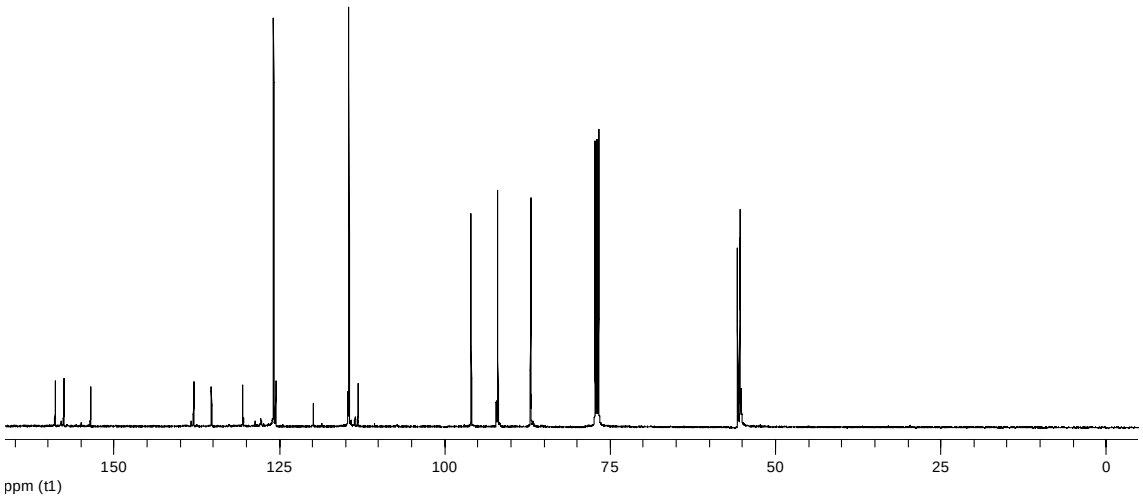
^{1}H-NMR ($CDCl_3$)

Compound 3c



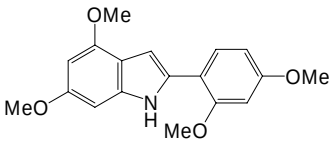


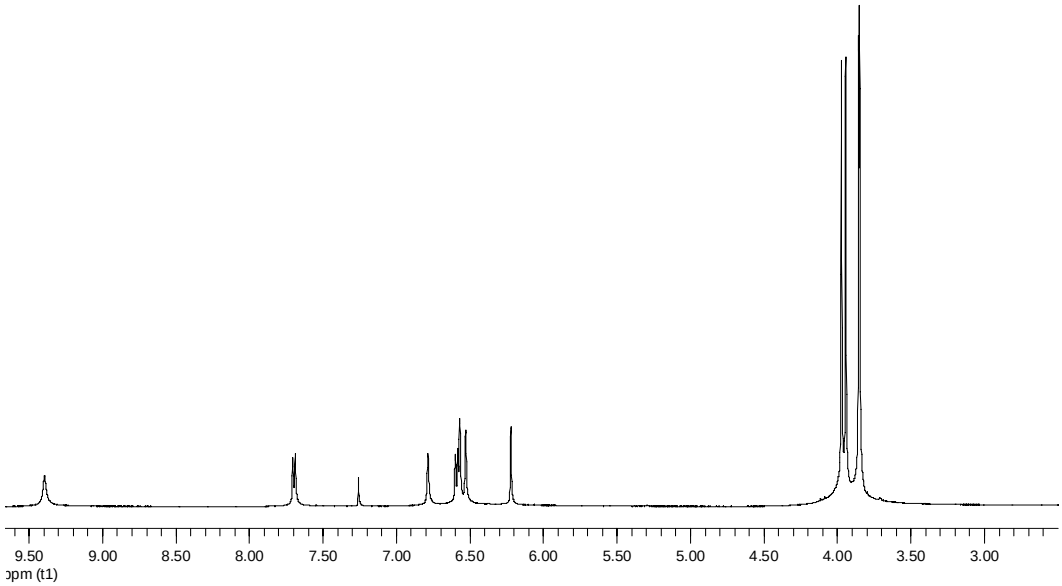
^{13}C-NMR ($CDCl_3$)



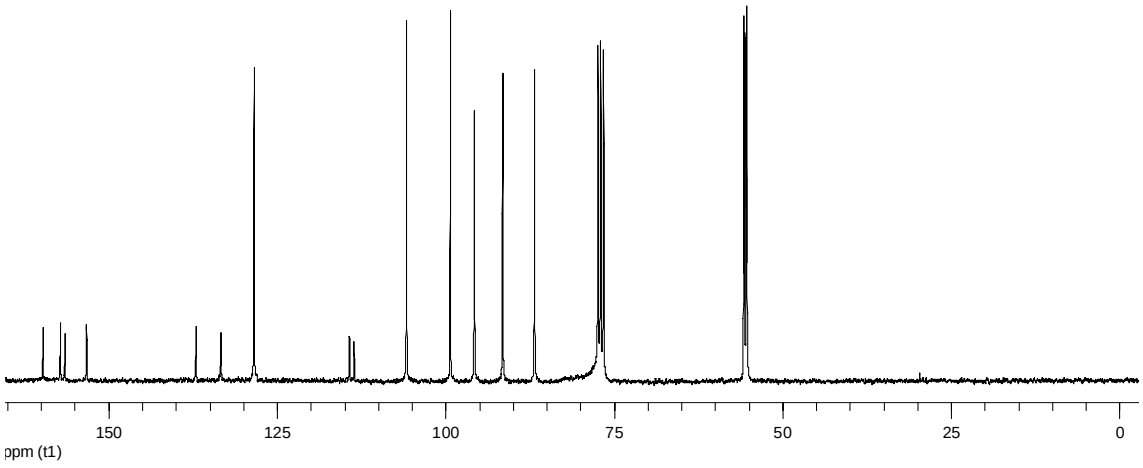
^{1}H-NMR ($CDCl_3$)

Compound 3e



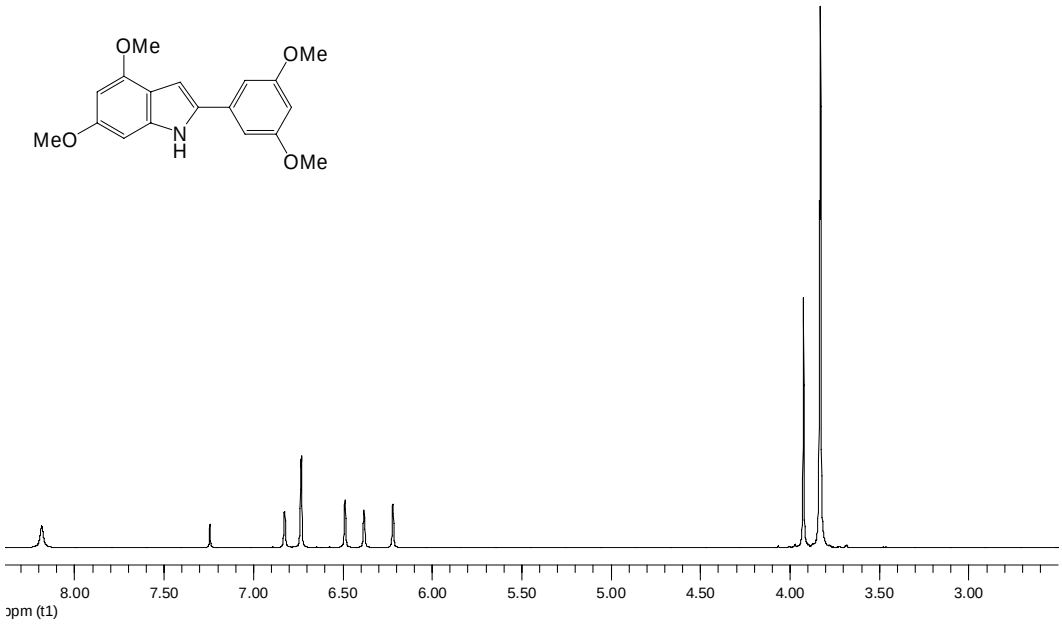


^{13}C-NMR ($CDCl_3$)

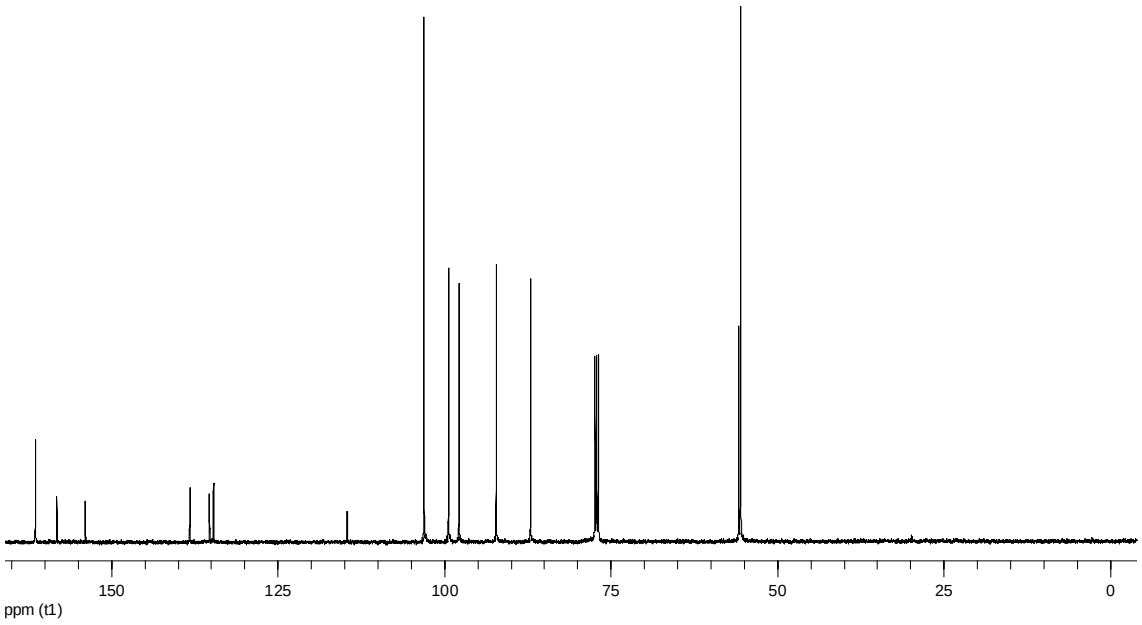


^{1}H-NMR ($CDCl_3$)

Compound 3h

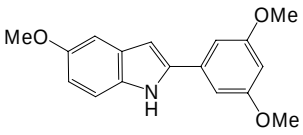


^{13}C-NMR ($CDCl_3$)

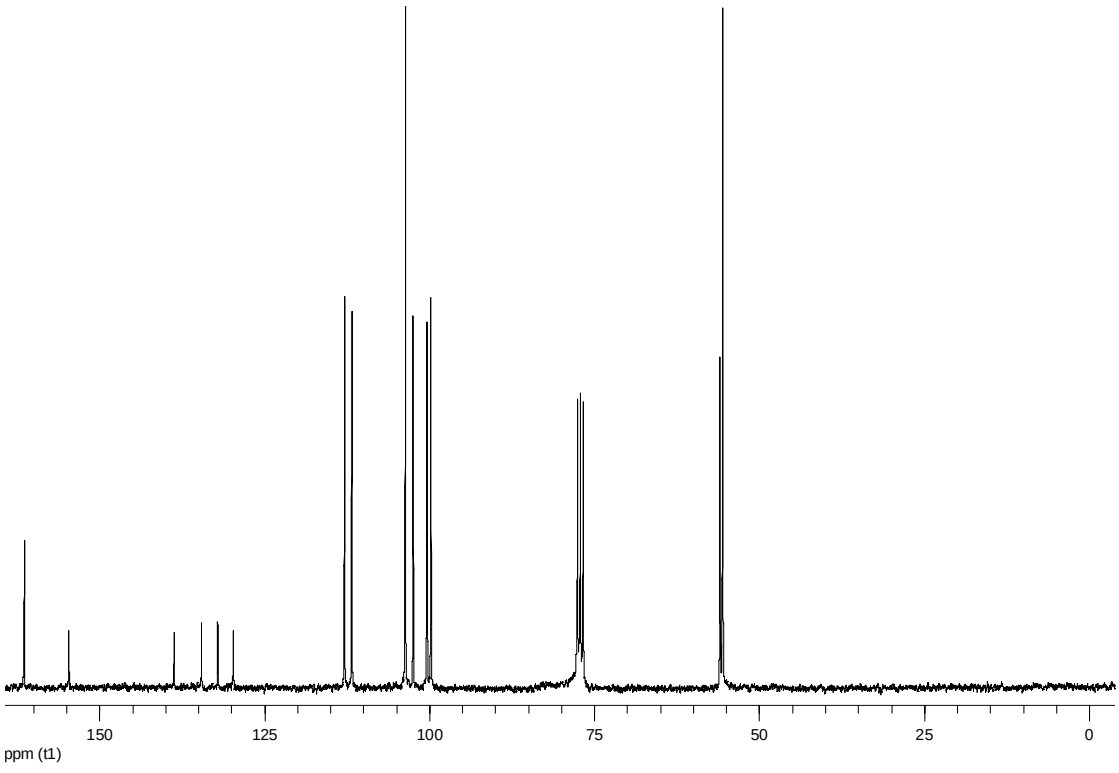


^{1}H-NMR ($CDCl_3$)

Compound 3d

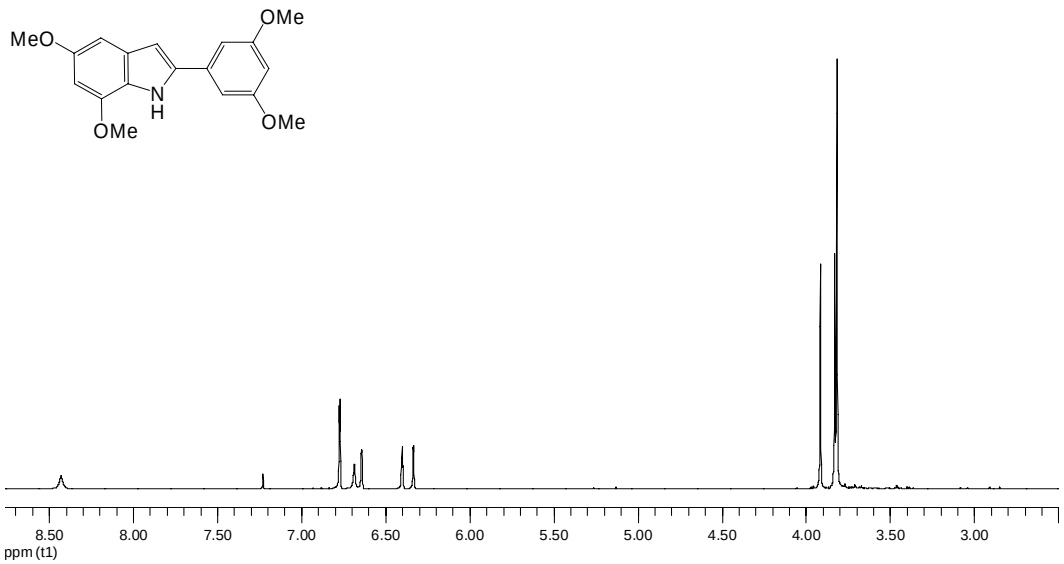


^{13}C-NMR ($CDCl_3$)

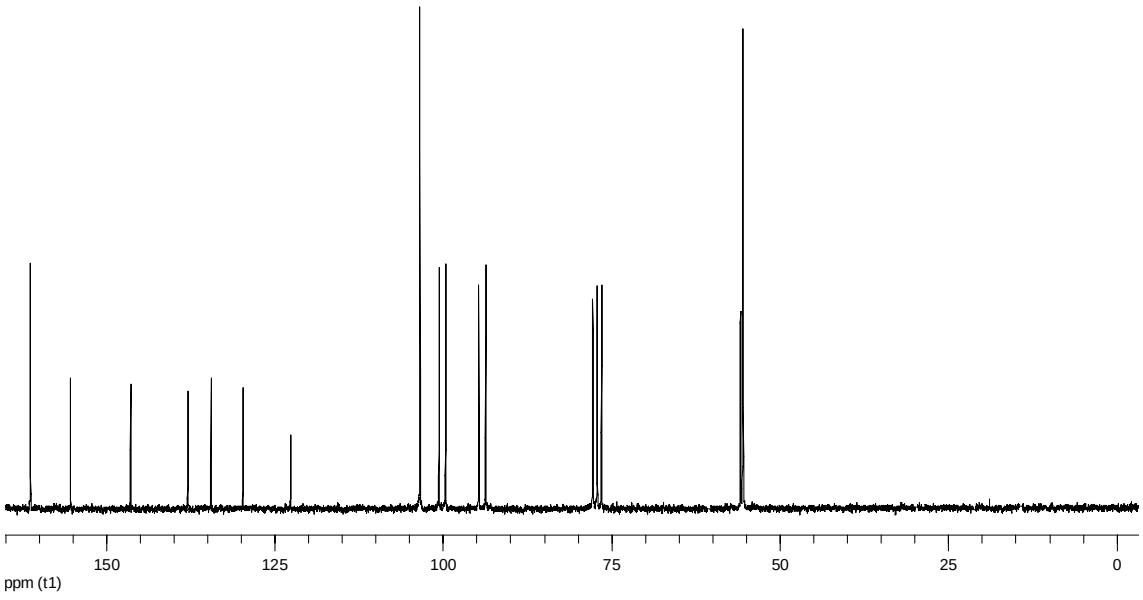


^{1}H-NMR ($CDCl_3$)

Compound 3g

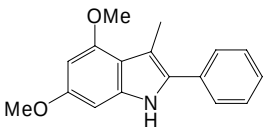


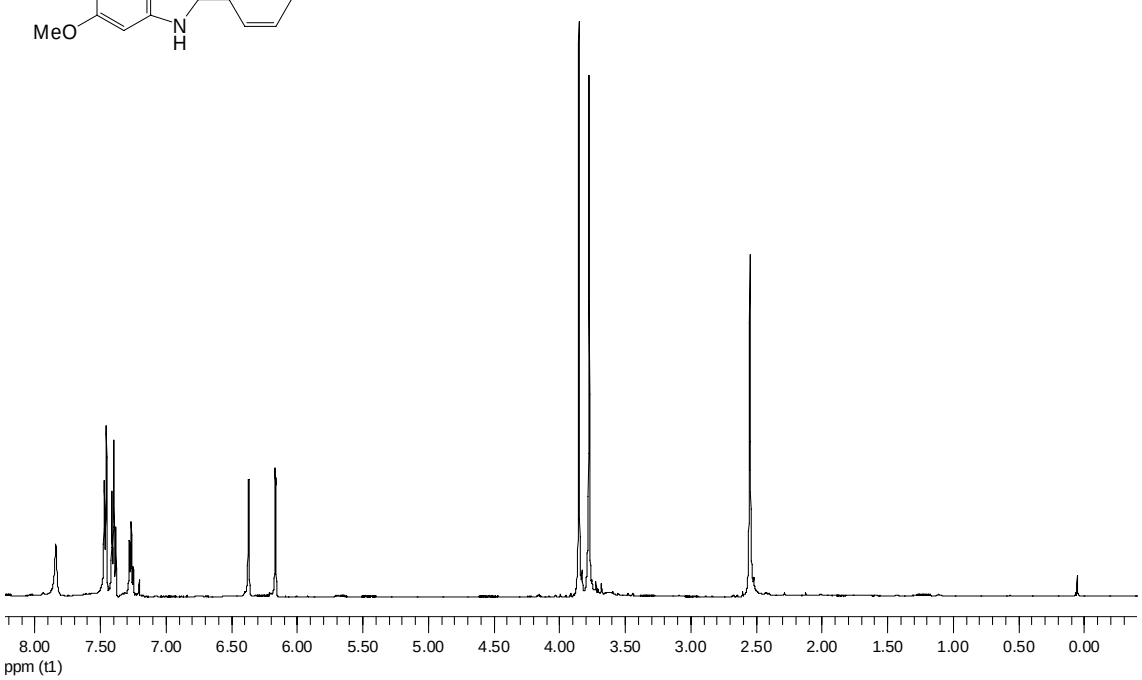
^{13}C-NMR ($CDCl_3$)



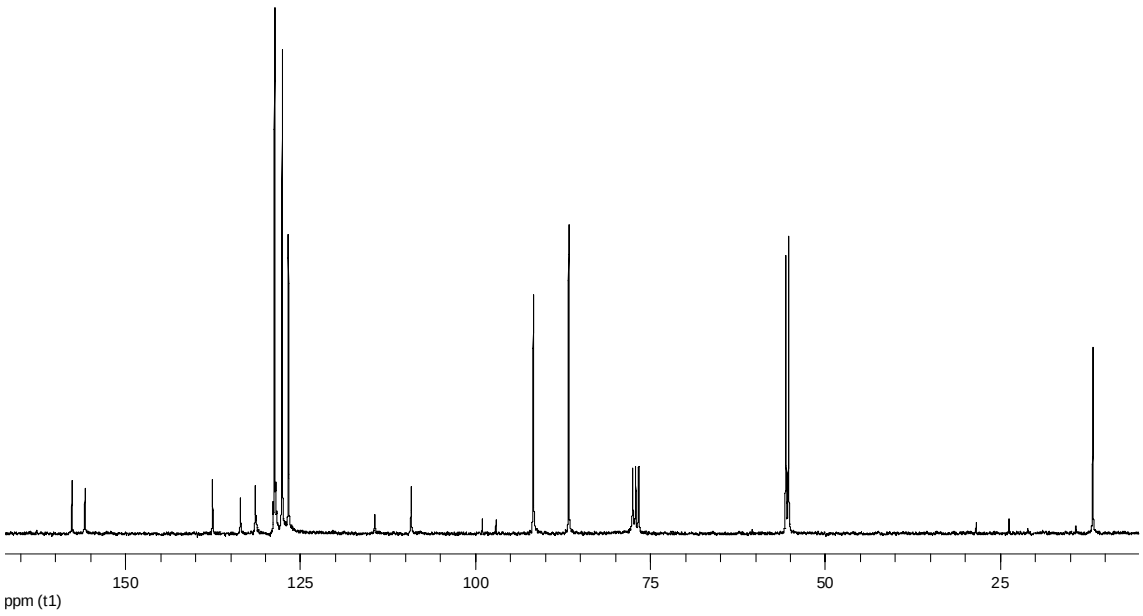
^{1}H-NMR ($CDCl_3$)

Compound 3j



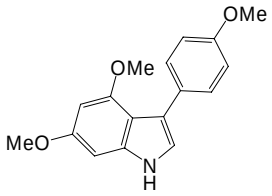


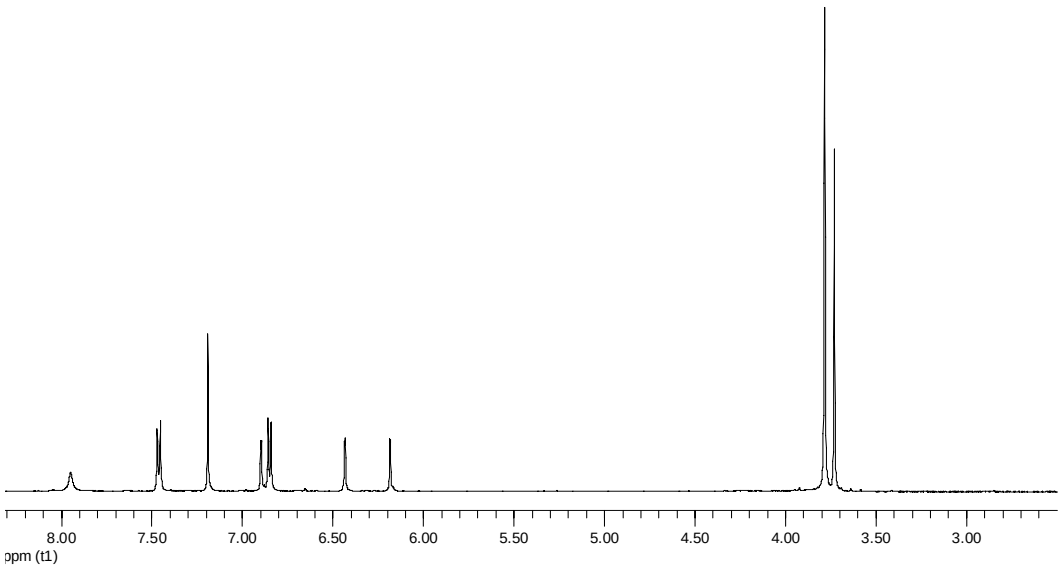
^{13}C-NMR ($CDCl_3$)



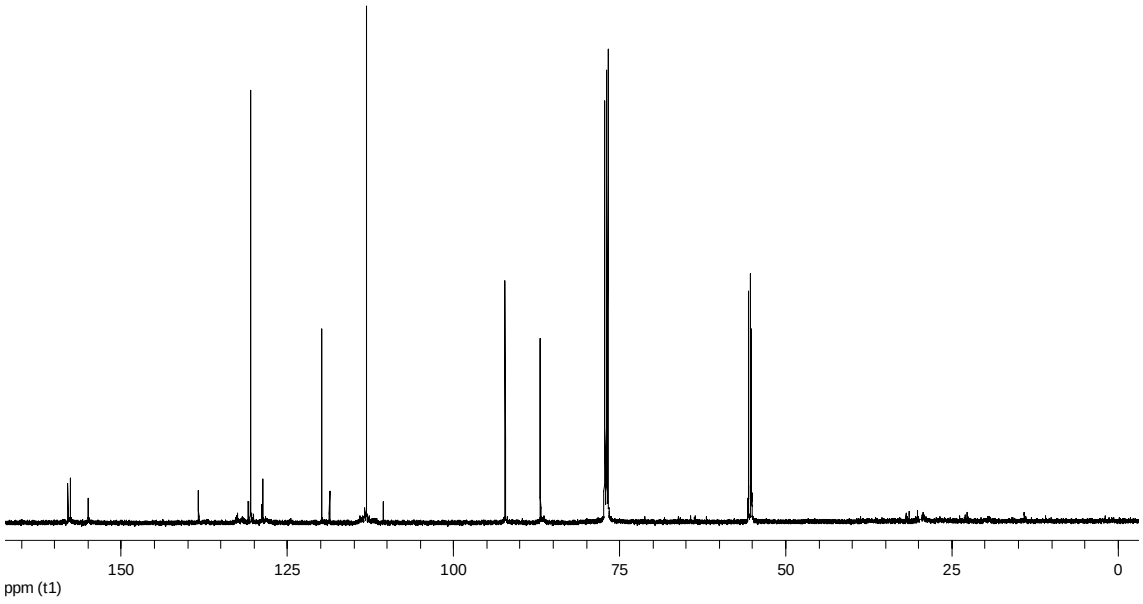
^{1}H-NMR ($CDCl_3$)

Compound 4c



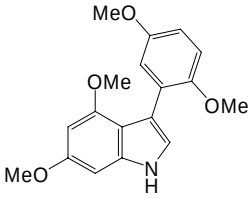


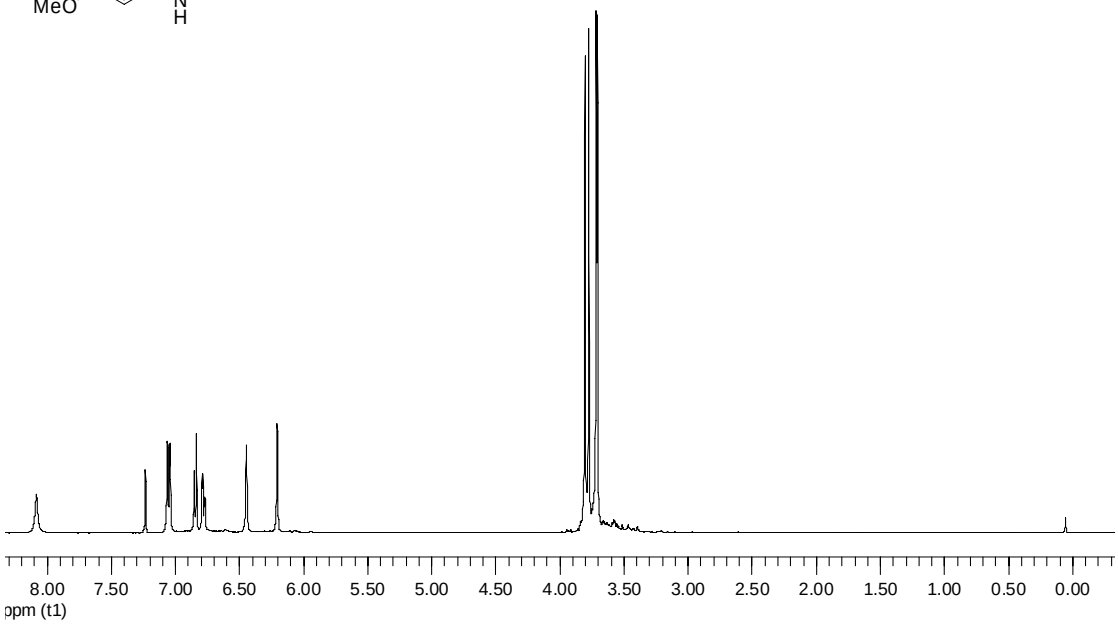
^{13}C-NMR ($CDCl_3$)



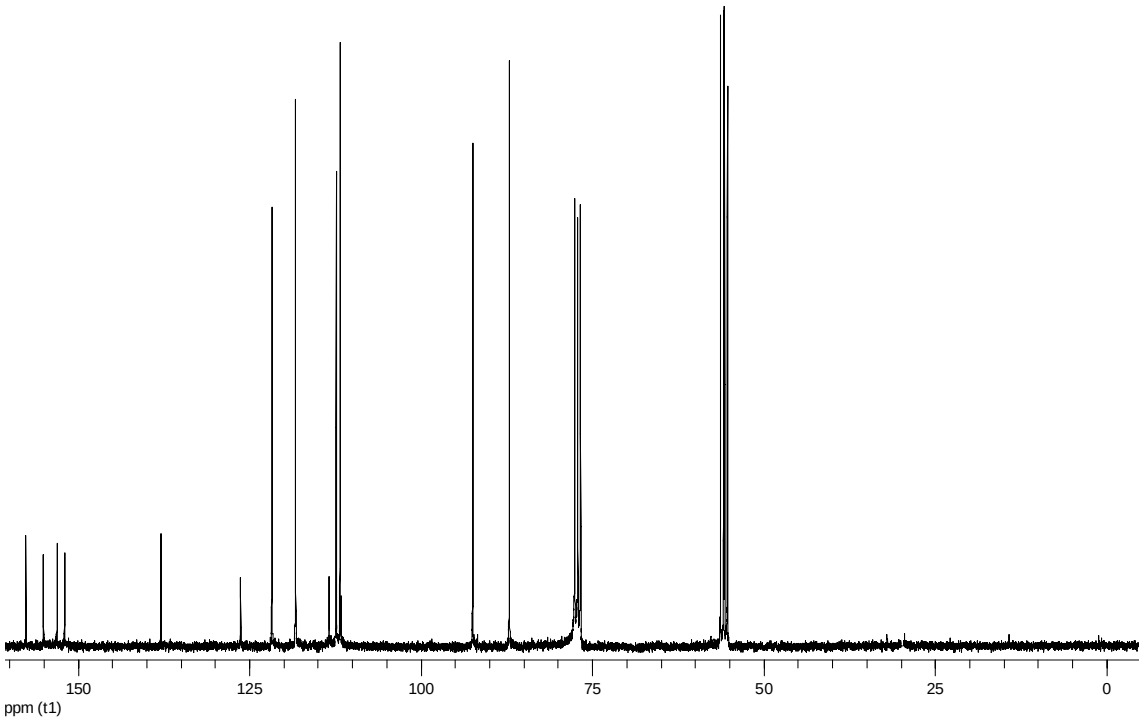
^{1}H-NMR ($CDCl_3$)

Compound 4f



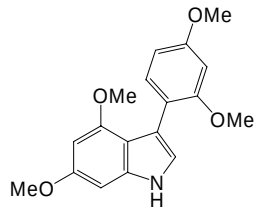


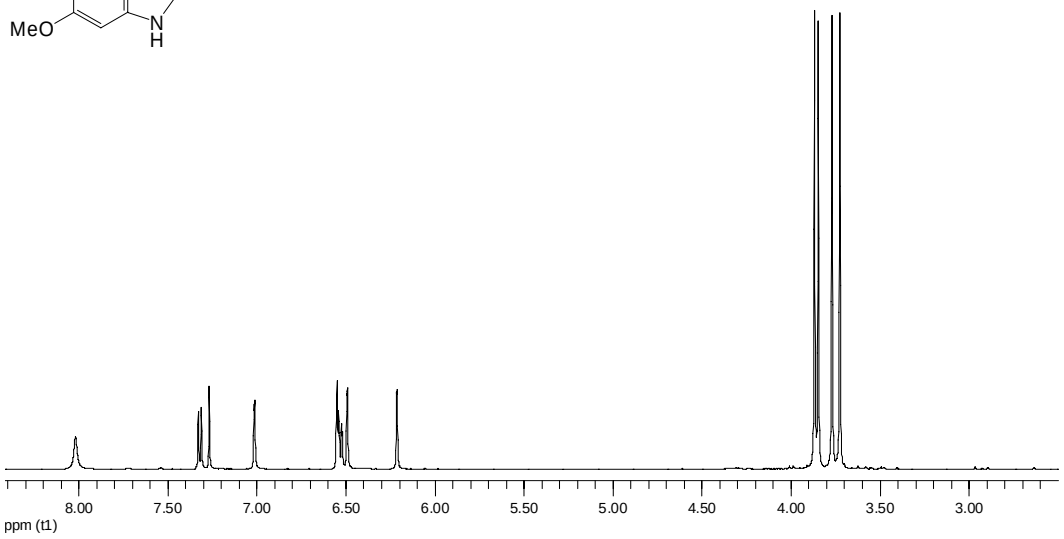
^{13}C-NMR (CDCl3)



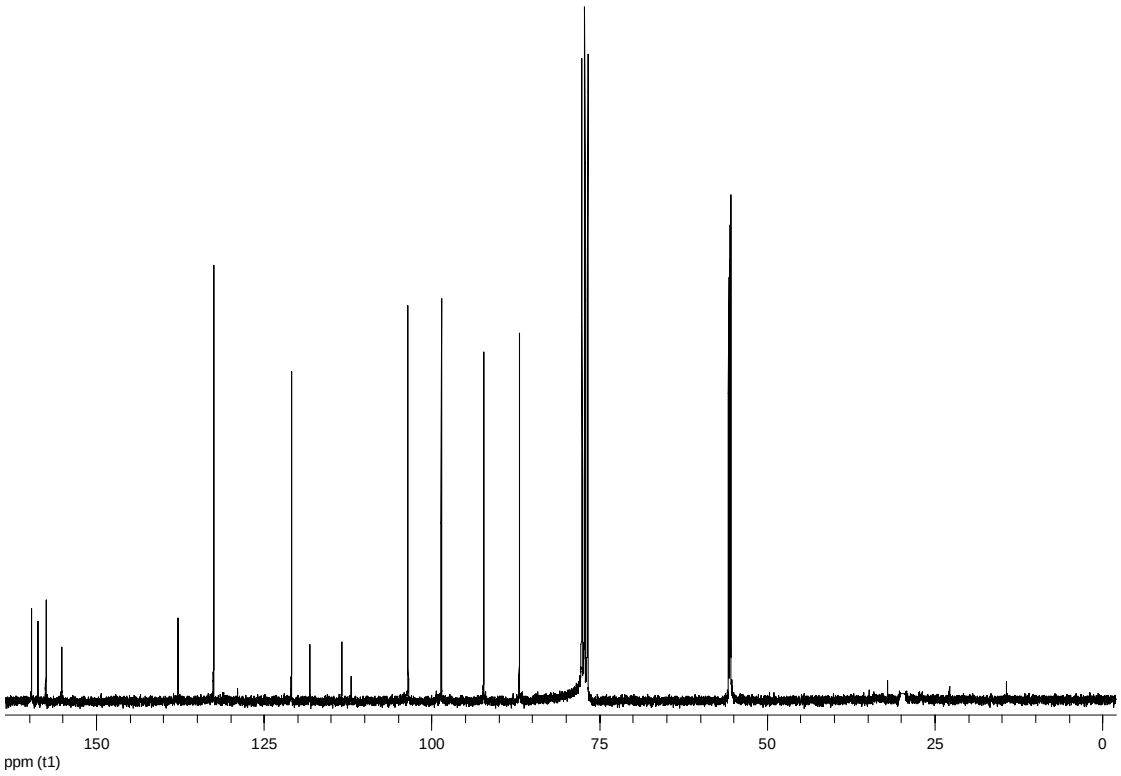
^{1}H-NMR ($CDCl_3$)

Compound 4e



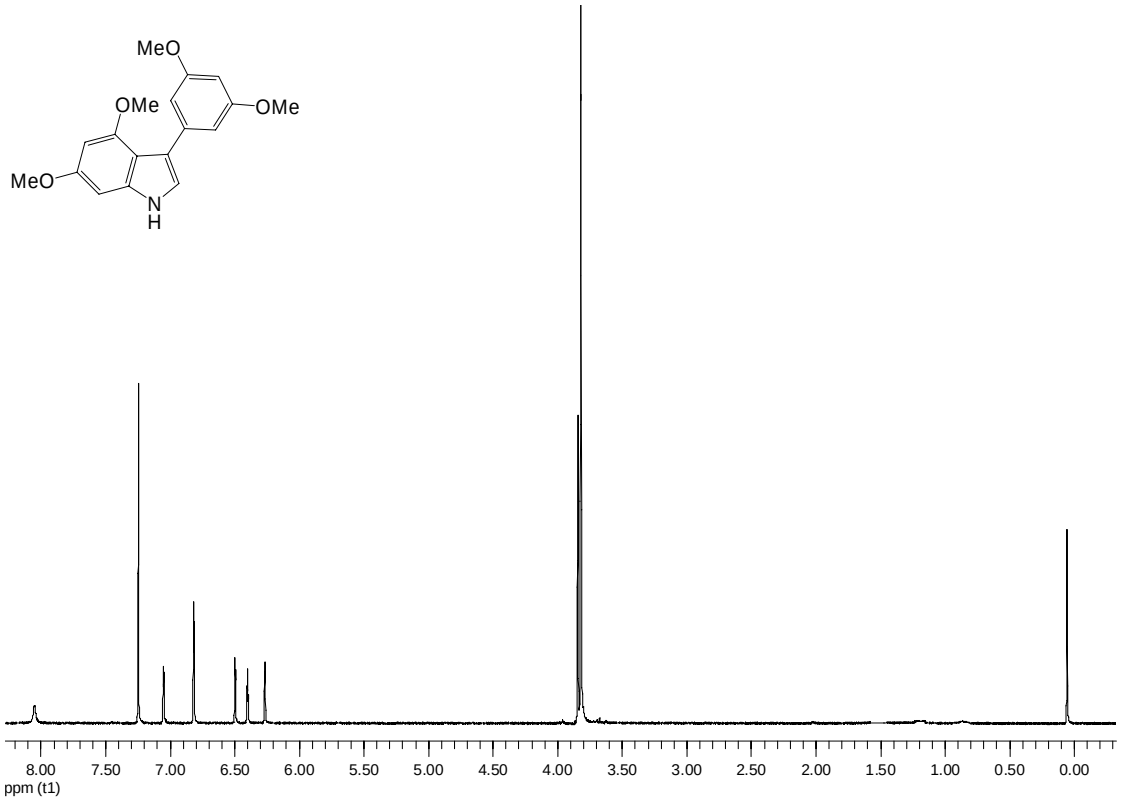


^{13}C-NMR ($CDCl_3$)

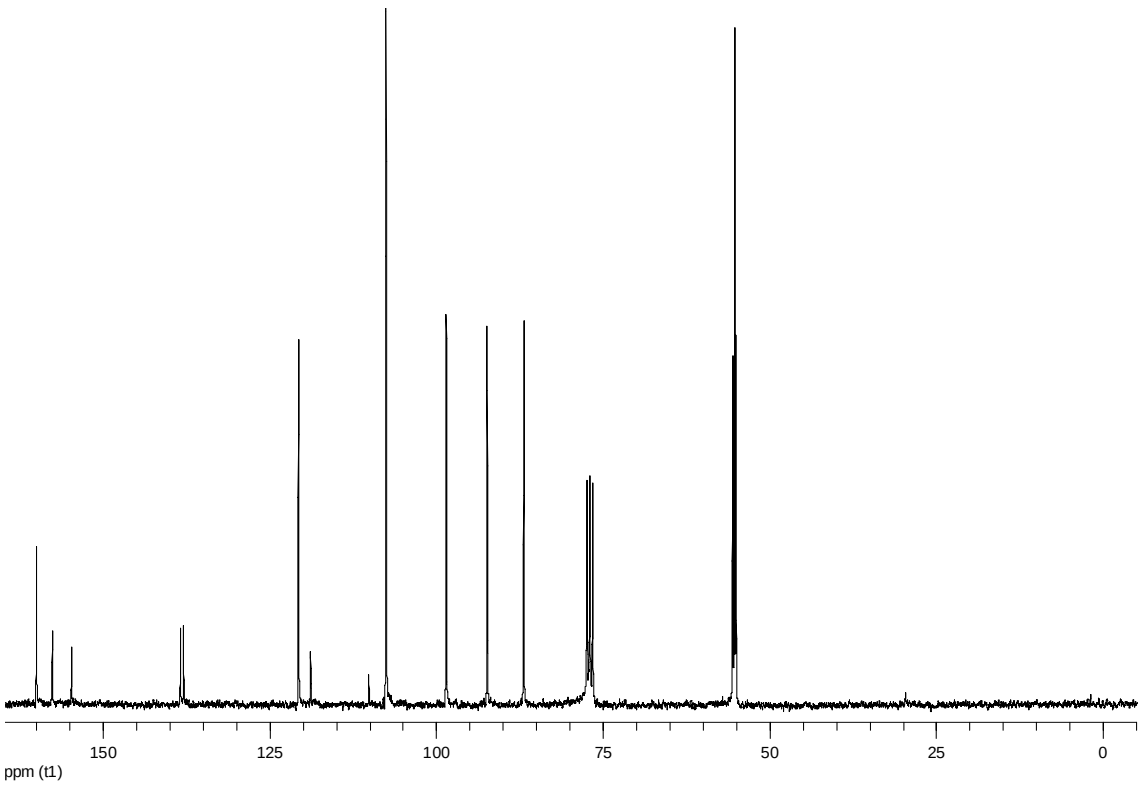


^{1}H-NMR (CDCl3)

Compound 4h

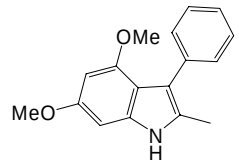


^{13}C-NMR ($CDCl_3$)

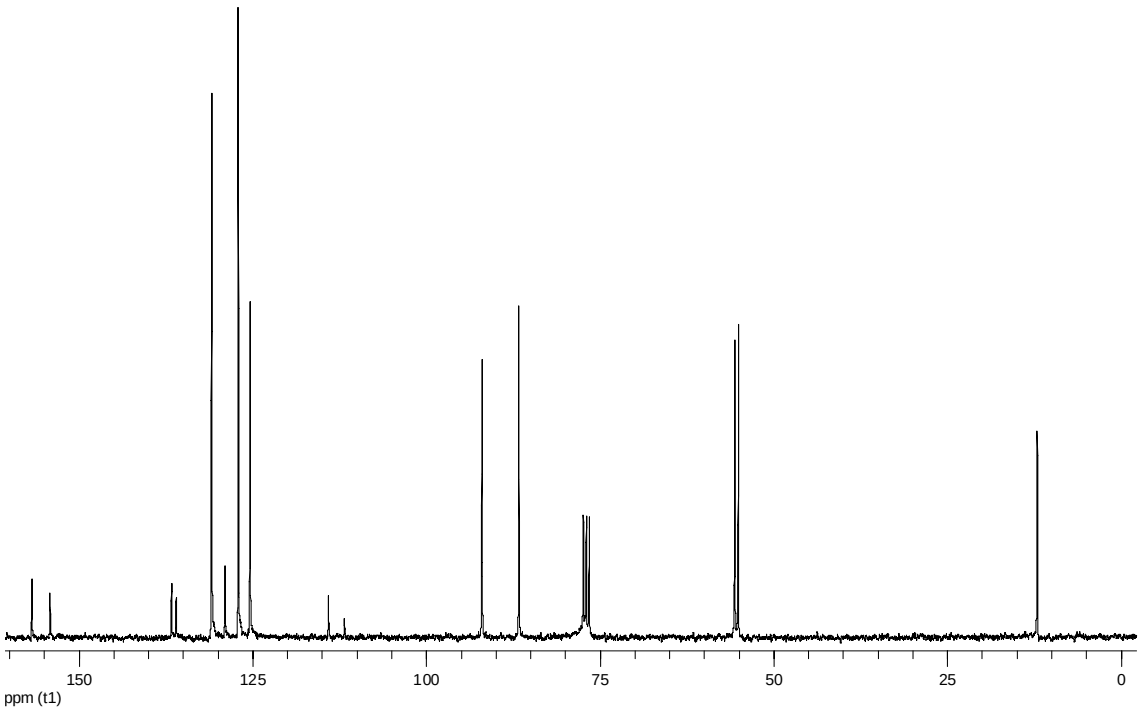


^{1}H-NMR ($CDCl_3$)

Compound 4j

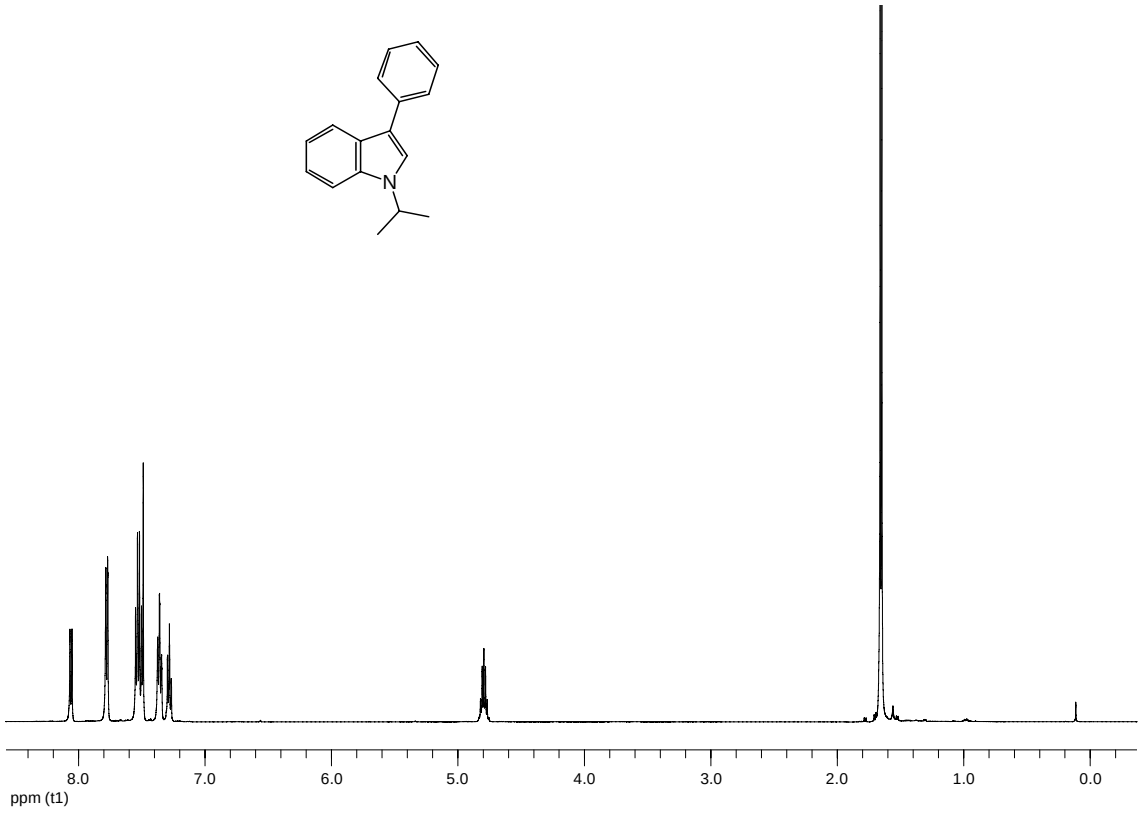


^{13}C-NMR ($CDCl_3$)



^{1}H-NMR ($CDCl_3$)

Compound 4m



^{13}C-NMR ($CDCl_3$)

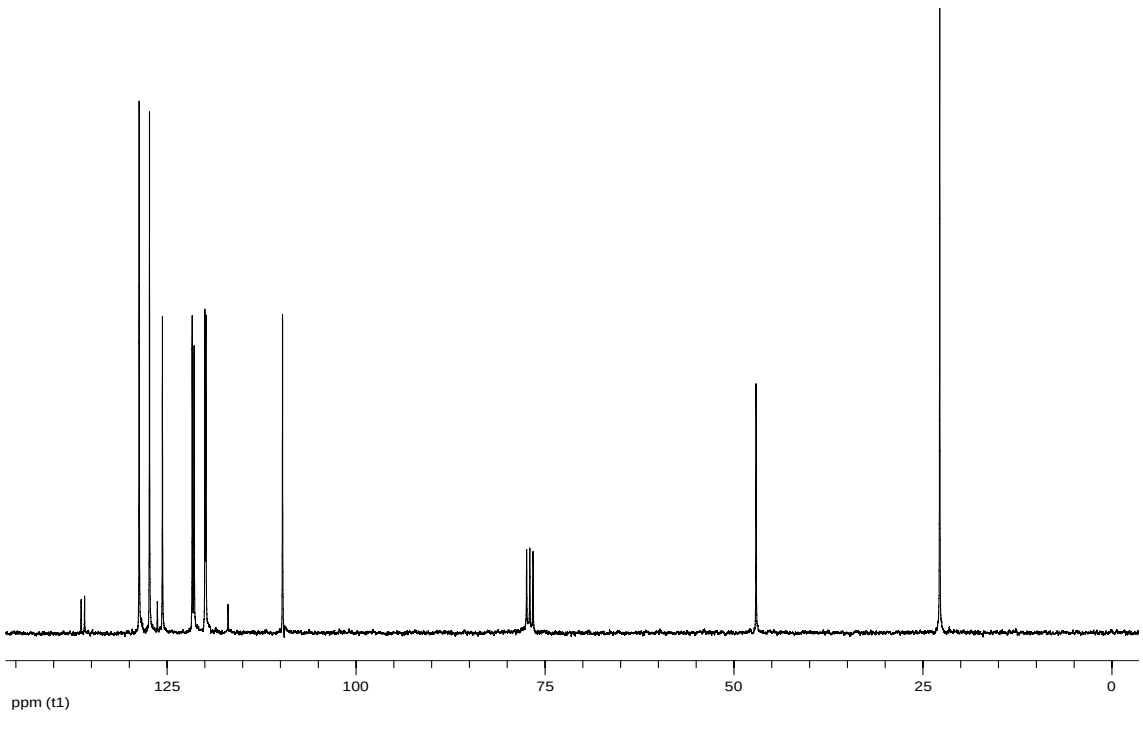


Table 1. Total electronic energies[a] (E, in a.u.), zero-point correction of energies (ΔZPE, in a.u.), thermal corrections to Gibbs free energies (TCGE, in a.u.) and number of imaginary frequencies[b] (NIMAG) of all the stationary points discussed in the main text.

Structure	E	ΔZPE	TCGE	NIMAG(ν)
5a	-651.772599	0.264013	0.221837	0
5b	-3167.169216	0.222768	0.180024	0
6a	-595.205314	0.222389	0.184599	0
TS1	-651.7253617	0.258389	0.216581	1 (-357.4288)
TS2	-3167.092174	0.220691	0.178256	1 (-476.8558)
5c	-728.227698	0.287900	0.240116	0
6b	-728.211840	0.288381	0.243884	0
5d	-728.220518	0.288531	0.242578	0
6c	-744.302689	0.277982	0.231928	0
TS3	-728.199462	0.287048	0.242926	1 (-304.2720)
TS4	-728.197246	0.285956	0.241270	1 (-207.0281)
8	-959.265516	0.372640	0.321831	0
10	-671.651291	0.250270	0.207869	0
1a	-287.601761	0.117390	0.088240	0
TS5	-959.207607	0.368334	0.316507	1 (-534.9066)
14.HBr	-3454.782222	0.342706	0.290079	0
16.HBr	-3454.780277	0.340409	0.286492	0
TS6.HBr	-3454.752885	0.343005	0.291579	1 (-259.6462)

[a]Computed at the B3LYP/6-31G* level of theory. [b]The imaginary frequency ν (in parentheses) is given in cm^{-1}

Cartesian coordinates (optimized at the B3LYP/6-31G* level) of all the stationary points discussed in the main text.

5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.742560	-1.596243	-1.522765
2	6	0	-4.103972	-1.052367	-0.833094
3	6	0	-2.460003	0.332225	0.942995
4	6	0	-2.724982	-1.237454	-0.888893
5	6	0	-4.670221	-0.192544	0.113464
6	6	0	-3.845843	0.487237	1.009884
7	6	0	-1.889046	-0.523083	-0.016562
8	1	0	-2.280975	-1.922123	-1.604468
9	1	0	-5.747610	-0.070678	0.164059
10	1	0	-4.278820	1.130423	1.770668
11	7	0	-0.501532	-0.758180	-0.058090
12	1	0	-1.821820	0.805833	1.688551
13	6	0	0.376471	0.144986	-0.283604
14	6	0	0.010839	1.572921	-0.691754
15	6	0	1.823182	-0.163661	-0.142198
16	1	0	0.484391	1.864991	-1.631222
17	7	0	0.522887	2.551583	0.363095
18	1	0	-1.067149	1.711478	-0.761345
19	1	0	1.522161	2.362392	0.541531
20	1	0	0.016622	2.423420	1.247989
21	1	0	0.417969	3.532633	0.076471
22	6	0	4.542885	-0.778258	0.220068
23	6	0	2.209332	-1.285748	0.614097
24	6	0	2.827222	0.643193	-0.716683
25	6	0	4.176847	0.335371	-0.536144
26	6	0	3.555155	-1.589750	0.788390

27	1	0	1.437167	-1.907408	1.054377
28	1	0	2.576148	1.476245	-1.371291
29	1	0	4.937735	0.955077	-1.000770
30	1	0	3.837619	-2.460441	1.372346
31	1	0	5.592445	-1.017824	0.361029

5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.693207	-2.797998	0.769107
2	6	0	4.099939	-1.964827	0.401484
3	6	0	2.563709	0.167368	-0.549119
4	6	0	2.713003	-2.068051	0.376044
5	6	0	4.730556	-0.806632	-0.063722
6	6	0	3.956655	0.248979	-0.546802
7	6	0	1.923662	-0.992644	-0.073581
8	1	0	2.213433	-2.973083	0.708488
9	1	0	5.814536	-0.734439	-0.060318
10	1	0	4.436494	1.147598	-0.925785
11	7	0	0.538196	-1.195962	-0.122430
12	1	0	1.970528	0.990772	-0.933842
13	6	0	-0.364240	-0.373999	0.280350
14	6	0	-0.060089	0.908316	1.022859
15	6	0	-1.792597	-0.762244	0.101960
16	1	0	-0.745017	1.065805	1.854613
17	1	0	0.971258	0.938319	1.365578
18	35	0	-0.272642	2.529048	-0.120960
19	6	0	-4.470061	-1.567232	-0.214902
20	6	0	-2.106694	-2.071285	-0.305840
21	6	0	-2.845213	0.137328	0.339208
22	6	0	-4.172005	-0.263791	0.180647

23	6	0	-3.429974	-2.469397	-0.459633
24	1	0	-1.291955	-2.762340	-0.490891
25	1	0	-2.637731	1.166336	0.611374
26	1	0	-4.971912	0.448777	0.362421
27	1	0	-3.653492	-3.487017	-0.768746
28	1	0	-5.504163	-1.879013	-0.335111

6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.053413	0.927707	-0.254286
2	6	0	2.829884	1.527786	-0.035538
3	6	0	1.724830	0.683780	0.178250
4	6	0	1.910841	-0.777546	0.458444
5	6	0	3.224834	-1.342275	0.041198
6	6	0	4.247436	-0.501058	-0.253626
7	7	0	0.433915	1.045918	0.085194
8	6	0	-0.305193	-0.068152	0.035046
9	6	0	0.534423	-1.338465	0.015996
10	6	0	-1.736798	-0.021433	-0.004693
11	6	0	-2.398695	1.231509	0.069711
12	6	0	-3.782637	1.288212	0.032424
13	6	0	-4.527744	0.106724	-0.081382
14	6	0	-3.888690	-1.138343	-0.160211
15	6	0	-2.504579	-1.206290	-0.122704
16	1	0	4.909640	1.555987	-0.486210
17	1	0	2.688934	2.598217	-0.138084
18	1	0	1.936427	-0.856736	1.566185
19	1	0	3.374180	-2.417448	0.090508
20	1	0	5.233293	-0.889742	-0.487092
21	1	0	0.138991	-2.125259	0.662098

22	1	0	0.589062	-1.736242	-1.004901
23	1	0	-1.803701	2.133820	0.153815
24	1	0	-4.288897	2.246377	0.090303
25	1	0	-5.612391	0.155528	-0.111294
26	1	0	-4.475880	-2.046238	-0.252243
27	1	0	-2.015020	-2.172632	-0.191221

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.833825	-0.774847	0.071550
2	6	0	3.386250	0.607584	-1.265112
3	7	0	0.538196	-1.024499	0.410307
4	6	0	-0.239927	-0.006342	0.108004
5	6	0	-1.688978	-0.188527	-0.044825
6	6	0	4.420483	0.174676	-0.459439
7	1	0	3.580051	1.260130	-2.110937
8	6	0	4.186298	-0.777043	0.568358
9	1	0	5.434048	0.517624	-0.642182
10	6	0	2.920556	-1.270833	0.823781
11	1	0	5.022505	-1.113589	1.174242
12	1	0	2.729443	-1.966554	1.633713
13	6	0	2.073346	0.125310	-1.033504
14	6	0	0.436931	1.290881	-0.071563
15	1	0	1.380993	0.106741	-1.871728
16	1	0	1.200302	1.591407	0.626655
17	1	0	0.106953	2.046668	-0.773313
18	7	0	-0.853146	2.544698	1.512965
19	1	0	-0.578441	2.258578	2.452553
20	1	0	-1.856232	2.386462	1.432631
21	1	0	-0.689535	3.549062	1.442108

22	6	0	-4.437003	-0.640959	-0.384017
23	6	0	-2.516409	0.810591	-0.595682
24	6	0	-2.261640	-1.422801	0.324275
25	6	0	-3.625609	-1.638481	0.165776
26	6	0	-3.878008	0.579546	-0.771769
27	1	0	-2.100632	1.761587	-0.913429
28	1	0	-1.624393	-2.197233	0.736234
29	1	0	-4.057519	-2.589201	0.462676
30	1	0	-4.502876	1.350310	-1.212471
31	1	0	-5.500699	-0.815915	-0.514657

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.034077	-1.293676	-0.221231
2	6	0	-3.440230	-0.014156	1.364406
3	7	0	-0.748234	-1.570669	-0.588345
4	6	0	0.067633	-0.708320	-0.016520
5	6	0	1.502527	-0.991284	0.051817
6	6	0	-4.489053	-0.126636	0.479355
7	1	0	-3.574823	0.480984	2.321783
8	6	0	-4.344501	-0.870331	-0.720155
9	1	0	-5.452464	0.315151	0.715501
10	6	0	-3.140769	-1.465109	-1.066927
11	1	0	-5.193821	-0.955803	-1.392211
12	1	0	-3.010793	-1.982188	-2.011805
13	6	0	-2.171763	-0.601275	1.047411
14	6	0	-0.613475	0.480703	0.596884
15	1	0	-1.623390	-1.019862	1.891475
16	1	0	-1.122890	1.162187	-0.072081
17	1	0	-0.248207	0.941251	1.506132

18	35	0	0.759572	2.708542	-0.388006
19	6	0	4.217252	-1.667212	0.235150
20	6	0	1.967567	-2.234226	-0.431681
21	6	0	2.420429	-0.094123	0.629566
22	6	0	3.767792	-0.438140	0.718728
23	6	0	3.312698	-2.564492	-0.345164
24	1	0	1.254784	-2.922253	-0.872604
25	1	0	2.091783	0.889033	0.945822
26	1	0	4.469423	0.264763	1.158268
27	1	0	3.660430	-3.520861	-0.725541
28	1	0	5.270414	-1.927004	0.304053

5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.231251	-0.854882	-1.734764
2	6	0	4.513920	-0.439647	-1.032630
3	6	0	2.653406	0.596670	0.769246
4	6	0	3.283633	-1.067467	-0.867222
5	6	0	4.829857	0.708351	-0.301575
6	6	0	3.893188	1.216755	0.595845
7	6	0	2.338562	-0.560035	0.041030
8	1	0	3.050309	-1.962791	-1.440244
9	1	0	5.790866	1.195991	-0.429960
10	1	0	4.121038	2.107050	1.175167
11	7	0	1.091803	-1.219961	0.135204
12	1	0	1.951159	1.025975	1.477434
13	1	0	1.103901	-2.145820	-0.274680
14	6	0	0.209337	-1.129239	1.283822
15	1	0	0.456985	-0.255946	1.886958
16	1	0	0.245714	-2.017023	1.928762

17	6	0	-1.198975	-1.005818	0.713345
18	8	0	-1.864474	-2.056436	0.602889
19	6	0	-1.746963	0.298007	0.287272
20	1	0	-3.018795	-2.219461	-0.325428
21	7	0	-3.828082	-2.457322	-1.053206
22	1	0	-4.613507	-2.908172	-0.574123
23	1	0	-3.476536	-3.091997	-1.776558
24	1	0	-4.155946	-1.593150	-1.494873
25	6	0	-2.872304	2.752307	-0.462899
26	6	0	-3.133764	0.519290	0.416821
27	6	0	-0.929152	1.330165	-0.207958
28	6	0	-1.496841	2.542918	-0.592421
29	6	0	-3.690128	1.742485	0.053905
30	1	0	-3.755821	-0.242489	0.880597
31	1	0	0.137299	1.172947	-0.325037
32	1	0	-0.862642	3.328464	-0.991514
33	1	0	-4.752857	1.919366	0.191443
34	1	0	-3.305333	3.705944	-0.749756

6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.536362	1.006854	-0.478362
2	6	0	3.305348	0.242360	0.640147
3	6	0	2.125430	-0.537027	0.646455
4	6	0	1.310060	-0.740107	-0.582995
5	6	0	1.574034	0.225382	-1.679944
6	6	0	2.661358	1.030674	-1.626522
7	7	0	1.535927	-1.131517	1.666536
8	6	0	0.238440	-1.732522	1.313990
9	6	0	-0.150721	-1.023233	-0.037235

10	8	0	-0.741149	-1.903498	-0.935922
11	6	0	-0.958716	0.266064	0.154897
12	6	0	-0.933356	1.016131	1.338806
13	6	0	-1.668913	2.197860	1.451076
14	6	0	-2.440012	2.649476	0.380390
15	6	0	-2.471534	1.911284	-0.804620
16	6	0	-1.737514	0.730959	-0.916183
17	7	0	-3.407244	-2.402202	-0.475921
18	1	0	4.408175	1.656007	-0.489786
19	1	0	3.949395	0.300886	1.511692
20	1	0	1.606322	-1.731202	-0.984172
21	1	0	0.924947	0.194938	-2.549226
22	1	0	2.902039	1.699593	-2.445988
23	1	0	1.933755	-1.168754	2.599337
24	1	0	-0.477516	-1.592121	2.126243
25	1	0	0.358987	-2.802107	1.110209
26	1	0	-1.715466	-2.048167	-0.712701
27	1	0	-0.342757	0.691910	2.190848
28	1	0	-1.640937	2.760932	2.379462
29	1	0	-3.013879	3.567088	0.469190
30	1	0	-3.070478	2.253453	-1.643891
31	1	0	-1.773838	0.152356	-1.833732
32	1	0	-3.636696	-3.058604	0.269960
33	1	0	-3.959852	-1.562265	-0.306360
34	1	0	-3.765385	-2.814860	-1.337425

5d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.642443	0.500113	0.740687
2	6	0	3.292831	0.804257	0.907151

3	6	0	2.313232	0.047210	0.249655
4	6	0	2.702691	-1.013945	-0.579729
5	6	0	4.056727	-1.297777	-0.753186
6	6	0	5.032708	-0.546703	-0.096001
7	7	0	0.943633	0.331103	0.487438
8	6	0	-0.066138	0.276745	-0.566047
9	6	0	-0.299779	1.740982	-0.906170
10	6	0	-1.345530	-0.459938	-0.204870
11	8	0	-1.289213	2.396461	-0.586322
12	6	0	-1.658238	-0.791262	1.117649
13	6	0	-2.883621	-1.392614	1.426084
14	6	0	-3.806451	-1.672153	0.411006
15	6	0	-3.487569	-1.364304	-0.918949
16	6	0	-2.266209	-0.759441	-1.221012
17	1	0	5.389913	1.093541	1.259082
18	1	0	2.997386	1.633320	1.547386
19	1	0	1.958225	-1.638561	-1.066000
20	1	0	4.346598	-2.123219	-1.396871
21	1	0	6.084730	-0.776304	-0.232514
22	1	0	0.799385	1.064576	1.172644
23	1	0	0.394845	-0.190062	-1.441743
24	1	0	0.557379	2.254810	-1.371423
25	1	0	-0.930075	-0.602407	1.900156
26	1	0	-3.109356	-1.659861	2.454739
27	1	0	-4.749124	-2.157609	0.647814
28	1	0	-4.182896	-1.609656	-1.716885
29	1	0	-2.025198	-0.526827	-2.256430
30	7	0	-3.747254	1.756963	0.378249
31	1	0	-2.756807	1.911257	0.006920
32	1	0	-3.877905	2.272531	1.253619
33	1	0	-3.892895	0.746632	0.542548
34	1	0	-4.427742	2.092679	-0.309882

6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.857932	0.193000	0.007134
2	6	0	1.839991	-1.155862	-0.151542
3	7	0	0.578387	-1.574948	-0.396675
4	6	0	-0.297399	-0.436549	-0.748846
5	6	0	0.445881	0.761396	-0.087060
6	6	0	2.985628	0.896766	0.253512
7	6	0	4.185063	0.233998	0.371469
8	6	0	4.198719	-1.170871	0.228187
9	6	0	3.039171	-1.879220	-0.035272
10	6	0	-1.731455	-0.596140	-0.304240
11	6	0	-2.758882	-0.145007	-1.140818
12	6	0	-4.090570	-0.237509	-0.733500
13	6	0	-4.404087	-0.787908	0.510098
14	6	0	-3.382684	-1.243398	1.347608
15	6	0	-2.051098	-1.145587	0.945149
16	8	0	0.418547	1.906952	-0.815843
17	7	0	-0.645753	3.967755	0.573456
18	1	0	5.138522	-1.707423	0.315113
19	1	0	3.039956	-2.955709	-0.162191
20	1	0	2.862669	1.971215	0.320747
21	1	0	5.096017	0.788531	0.560227
22	1	0	0.401757	-2.499090	-0.769273
23	1	0	-0.258181	-0.262354	-1.832944
24	1	0	0.107161	0.898090	0.949632
25	1	0	0.051831	2.673132	-0.259025
26	1	0	-1.261435	-1.511845	1.596422
27	1	0	-3.623439	-1.679365	2.312808
28	1	0	-5.440664	-0.868974	0.823721
29	1	0	-4.881133	0.110208	-1.391908

30	1	0	-2.517479	0.276001	-2.113860
31	1	0	-0.619512	4.766383	-0.061438
32	1	0	-0.217198	4.280351	1.444460
33	1	0	-1.630883	3.799920	0.778374

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.090655	3.311640	-0.461377
2	6	0	0.306633	2.810705	0.762845
3	6	0	0.925271	1.546018	0.791076
4	6	0	1.263334	0.849232	-0.431843
5	6	0	0.829373	1.433560	-1.674011
6	6	0	0.135435	2.613895	-1.683698
7	7	0	1.074700	0.776484	1.888920
8	6	0	1.275644	-0.630929	1.601203
9	6	0	0.604188	-0.918946	0.216960
10	1	0	-0.615462	4.262530	-0.491276
11	1	0	0.080712	3.338271	1.684722
12	1	0	2.261111	0.413087	-0.464430
13	1	0	1.093896	0.937094	-2.603186
14	1	0	-0.204737	3.052645	-2.615665
15	1	0	0.772577	1.089438	2.801740
16	1	0	0.849359	-1.253010	2.394612
17	1	0	2.340236	-0.880711	1.509115
18	6	0	-0.882960	-0.933114	0.120205
19	8	0	1.158942	-1.878635	-0.509779
20	1	0	2.173703	-1.971854	-0.415945
21	7	0	3.802419	-2.422770	-0.498098
22	1	0	4.539023	-1.716942	-0.508215
23	1	0	3.884363	-2.931350	-1.379868

24	1	0	4.051908	-3.088951	0.233858
25	6	0	-3.675567	-1.044811	-0.135604
26	6	0	-1.712577	-0.592772	1.201240
27	6	0	-1.474246	-1.336150	-1.090541
28	6	0	-2.858008	-1.387903	-1.216745
29	6	0	-3.099594	-0.651840	1.072750
30	1	0	-1.289585	-0.301460	2.156553
31	1	0	-0.839985	-1.614267	-1.925188
32	1	0	-3.301433	-1.702104	-2.156759
33	1	0	-3.728596	-0.399844	1.921181
34	1	0	-4.756075	-1.091009	-0.233530

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.081688	-1.472666	0.060656
2	6	0	2.854441	-1.770208	-0.505113
3	6	0	1.910592	-0.736779	-0.664480
4	6	0	2.257268	0.612758	-0.332942
5	6	0	3.527278	0.868735	0.257728
6	6	0	4.415091	-0.160748	0.478737
7	7	0	0.593961	-0.948081	-0.951429
8	6	0	-0.312569	0.106537	-0.536033
9	6	0	0.344775	0.715081	0.732272
10	6	0	-1.709992	-0.396501	-0.226293
11	8	0	0.041050	1.876803	1.180603
12	6	0	-1.910386	-1.435770	0.695232
13	6	0	-3.200905	-1.880695	0.981139
14	6	0	-4.300120	-1.291097	0.353435
15	6	0	-4.107476	-0.257103	-0.565525
16	6	0	-2.817799	0.189246	-0.851977

17	1	0	4.799525	-2.274393	0.209252
18	1	0	2.597866	-2.790734	-0.774820
19	1	0	1.799336	1.424846	-0.890335
20	1	0	3.800445	1.893054	0.493262
21	1	0	5.382532	0.029460	0.931104
22	1	0	0.231500	-1.878567	-1.110021
23	1	0	-0.380605	0.901952	-1.294378
24	1	0	0.637967	0.004976	1.507209
25	1	0	-0.410238	2.575937	0.505903
26	1	0	-1.062381	-1.902103	1.191077
27	1	0	-3.347626	-2.685997	1.694480
28	1	0	-5.304023	-1.639799	0.575991
29	1	0	-4.959581	0.192941	-1.066118
30	1	0	-2.668535	0.976884	-1.587589
31	7	0	-1.123155	3.733762	-0.201345
32	1	0	-1.071479	4.542249	0.421138
33	1	0	-2.115008	3.537597	-0.341776
34	1	0	-0.745051	4.032782	-1.100791

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.561107	-0.150361	0.172565
2	6	0	2.902500	-1.502932	0.313639
3	6	0	4.138977	-1.981059	-0.127115
4	6	0	5.063081	-1.111375	-0.703813
5	6	0	4.747775	0.242665	-0.827865
6	6	0	3.510697	0.717718	-0.393790
7	6	0	1.237564	0.431411	0.696366
8	6	0	0.170336	-0.639253	1.040917
9	7	0	-0.301796	-1.263104	-0.252623

10	6	0	-1.620926	-1.931503	-0.219717
11	6	0	-1.676941	-3.302276	0.013233
12	6	0	-2.928421	-3.918442	0.059259
13	6	0	-4.088332	-3.162897	-0.123679
14	6	0	-4.005826	-1.787963	-0.355968
15	6	0	-2.762625	-1.156193	-0.406154
16	7	0	0.655225	1.262474	-0.357098
17	6	0	-0.453251	2.160583	-0.197087
18	6	0	-1.009880	2.680327	-1.378282
19	6	0	-2.100231	3.545024	-1.325519
20	6	0	-2.671736	3.884603	-0.096483
21	6	0	-2.125888	3.363042	1.074562
22	6	0	-1.015516	2.513464	1.037904
23	8	0	1.435763	1.064527	1.951147
24	1	0	2.231174	-2.204456	0.802484
25	1	0	4.380210	-3.032958	-0.006902
26	1	0	6.025051	-1.482313	-1.043578
27	1	0	5.465597	0.933517	-1.259610
28	1	0	3.302749	1.781810	-0.486200
29	1	0	-0.695600	-0.155091	1.490299
30	1	0	0.534131	-1.414426	1.712408
31	1	0	0.419968	-1.908568	-0.594376
32	1	0	-0.287503	-0.453795	-0.910236
33	1	0	-0.770427	-3.886259	0.153471
34	1	0	-2.992715	-4.987297	0.235579
35	1	0	-5.058939	-3.647480	-0.088425
36	1	0	-4.907973	-1.203046	-0.503330
37	1	0	-2.689145	-0.086774	-0.588226
38	1	0	1.321926	1.580559	-1.048789
39	1	0	-0.579418	2.407288	-2.339754
40	1	0	-2.507170	3.947303	-2.248747
41	1	0	-3.525612	4.553543	-0.054801
42	1	0	-2.549002	3.631379	2.038427
43	1	0	-0.570780	2.167345	1.961814

44	1	0	2.258600	1.580405	1.919542

10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.486945	0.164015	0.285105
2	6	0	0.008605	1.410806	1.025579
3	8	0	-0.099920	2.477343	0.100386
4	6	0	1.903349	-0.102732	0.111365
5	7	0	-0.412299	-0.639425	-0.236846
6	6	0	-1.854318	-0.487276	-0.167673
7	6	0	-2.581791	-1.245634	0.750128
8	6	0	-3.971095	-1.113215	0.778551
9	6	0	-4.613841	-0.242330	-0.104442
10	6	0	-3.872534	0.500537	-1.026037
11	6	0	-2.482075	0.380820	-1.065748
12	6	0	2.813729	0.977306	0.144046
13	6	0	4.169313	0.750222	-0.065432
14	6	0	4.637613	-0.549347	-0.276738
15	6	0	3.747528	-1.630842	-0.289881
16	6	0	2.389565	-1.412855	-0.106803
17	1	0	0.752469	1.688306	1.773465
18	1	0	-0.931764	1.194533	1.541724
19	1	0	-1.014678	2.520666	-0.221890
20	1	0	-0.071657	-1.415361	-0.803049
21	1	0	-2.073135	-1.921635	1.430939
22	1	0	-4.548803	-1.692790	1.491595
23	1	0	-5.694831	-0.147236	-0.078472
24	1	0	-4.373381	1.167276	-1.720969
25	1	0	-1.895767	0.923304	-1.802475

26	1	0	2.451871	1.991113	0.277212
27	1	0	4.861354	1.586043	-0.061629
28	1	0	5.699239	-0.724416	-0.422893
29	1	0	4.118834	-2.640807	-0.430498
30	1	0	1.719756	-2.268614	-0.070343

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.938686	-0.000006	-0.010109
2	6	0	0.221276	-1.208222	-0.005170
3	7	0	2.337277	-0.000039	-0.078907
4	6	0	-1.171791	-1.202614	0.003362
5	6	0	-1.881644	0.000005	0.008311
6	6	0	-1.171779	1.202619	0.003367
7	6	0	0.221278	1.208219	-0.005122
8	1	0	0.763395	-2.151716	-0.013087
9	1	0	2.777518	0.835099	0.287984
10	1	0	2.777595	-0.834843	0.288680
11	1	0	-1.705693	-2.149783	0.008705
12	1	0	-2.967642	0.000003	0.016573
13	1	0	-1.705675	2.149795	0.008766
14	1	0	0.763403	2.151707	-0.013100

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.090099	2.152419	0.089297

2	6	0	1.303618	2.221802	-0.024268
3	6	0	1.930039	3.453076	-0.221262
4	6	0	1.173064	4.622171	-0.295116
5	6	0	-0.216387	4.561310	-0.162605
6	6	0	-0.845439	3.334307	0.030413
7	6	0	-0.795748	0.846928	0.282977
8	6	0	-0.100452	-0.297259	0.872910
9	7	0	1.042709	-1.204842	-0.777866
10	6	0	2.375735	-1.589123	-0.397628
11	6	0	3.477068	-0.843196	-0.829056
12	6	0	4.759091	-1.193365	-0.402018
13	6	0	4.945817	-2.284018	0.447851
14	6	0	3.842256	-3.028421	0.870971
15	6	0	2.556711	-2.682441	0.456365
16	7	0	-1.851306	0.624121	-0.576914
17	6	0	-2.781701	-0.467436	-0.414899
18	6	0	-3.864184	-0.343812	0.467818
19	6	0	-4.765580	-1.400678	0.615454
20	6	0	-4.589874	-2.576610	-0.116054
21	6	0	-3.521060	-2.692201	-1.007915
22	6	0	-2.619326	-1.637787	-1.162592
23	8	0	-1.149623	0.742812	1.905133
24	1	0	1.911436	1.325248	0.040885
25	1	0	3.011172	3.496597	-0.311051
26	1	0	1.663171	5.579476	-0.444096
27	1	0	-0.808946	5.470234	-0.197522
28	1	0	-1.922814	3.308028	0.174095
29	1	0	-0.610287	-1.245794	0.948277
30	1	0	0.832516	-0.165697	1.397917
31	1	0	1.045093	-0.550481	-1.559142
32	1	0	0.482778	-2.011101	-1.051960
33	1	0	3.338661	-0.007521	-1.511615
34	1	0	5.612295	-0.616731	-0.746289
35	1	0	5.944481	-2.556857	0.773743

36	1	0	3.979875	-3.883247	1.526169
37	1	0	1.700767	-3.266463	0.787373
38	1	0	-2.241771	1.470765	-0.975654
39	1	0	-4.020622	0.587915	1.007809
40	1	0	-5.606548	-1.299613	1.294632
41	1	0	-5.292470	-3.396356	-0.002405
42	1	0	-3.397589	-3.597392	-1.594825
43	1	0	-1.811459	-1.700717	-1.886084
44	1	0	-1.993867	0.248266	1.968283

14.HBr

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.482671	2.943045	-1.343436
2	6	0	-1.016751	2.231840	-0.229268
3	6	0	-0.441305	2.922037	0.847483
4	6	0	-0.360512	4.313315	0.815402
5	6	0	-0.842466	5.023263	-0.287751
6	6	0	-1.401668	4.336658	-1.366415
7	6	0	-1.075808	0.705120	-0.167661
8	6	0	0.151659	0.198503	-0.888222
9	7	0	1.230130	-0.118103	-0.263126
10	6	0	2.467513	-0.558920	-0.805837
11	6	0	3.333489	-1.210690	0.081119
12	6	0	4.559436	-1.676026	-0.389706
13	6	0	4.920171	-1.485649	-1.724947
14	6	0	4.053977	-0.817797	-2.596012
15	6	0	2.824806	-0.346784	-2.142348
16	7	0	-2.248660	0.173628	-0.840657
17	6	0	-2.661718	-1.161254	-0.602993
18	6	0	-3.804491	-1.619919	-1.281837
19	6	0	-4.250305	-2.926563	-1.115704

20	6	0	-3.557308	-3.810211	-0.282735
21	6	0	-2.425451	-3.356891	0.391196
22	6	0	-1.973749	-2.041482	0.247369
23	35	0	0.798946	-0.331274	2.748936
24	1	0	-4.331972	-0.941447	-1.948965
25	1	0	-1.124877	-1.717060	0.843488
26	1	0	-1.885667	-4.022694	1.059301
27	1	0	-3.901118	-4.832912	-0.157808
28	1	0	-5.138895	-3.258493	-1.646717
29	1	0	-3.019641	0.831567	-0.844111
30	1	0	-1.000188	0.410646	0.889164
31	1	0	0.101346	0.122444	-1.974287
32	1	0	1.164557	-0.132732	0.841540
33	1	0	3.028225	-1.337768	1.116891
34	1	0	5.233569	-2.185780	0.291979
35	1	0	5.878577	-1.846607	-2.086714
36	1	0	4.340835	-0.653303	-3.630473
37	1	0	2.169645	0.197234	-2.815823
38	1	0	-0.057751	2.357414	1.695806
39	1	0	0.076093	4.843682	1.657057
40	1	0	-0.780357	6.107960	-0.306950
41	1	0	-1.773146	4.883679	-2.228788
42	1	0	-1.913706	2.410491	-2.187045

16.HBr

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.701800	-1.498183	-0.340807
2	6	0	-2.785434	-0.919793	0.545985
3	6	0	-3.247569	0.008318	1.488958
4	6	0	-4.597912	0.354727	1.541881
5	6	0	-5.506600	-0.229139	0.656852

6	6	0	-5.054104	-1.156878	-0.283049
7	6	0	-1.305908	-1.232477	0.475697
8	6	0	-0.480065	-0.227784	-0.407113
9	7	0	0.005407	0.901781	0.378846
10	6	0	0.130894	2.187239	-0.182615
11	6	0	1.300181	2.935519	0.044163
12	6	0	1.417107	4.233951	-0.448209
13	6	0	0.384570	4.808902	-1.191242
14	6	0	-0.776064	4.067112	-1.422847
15	6	0	-0.912650	2.775063	-0.919093
16	7	0	-0.996609	-2.546629	-0.118890
17	6	0	0.243874	-2.468319	-0.755825
18	6	0	1.081851	-3.511204	-1.160209
19	6	0	2.275821	-3.186046	-1.810230
20	6	0	2.627607	-1.855005	-2.064511
21	6	0	1.771460	-0.816351	-1.661940
22	6	0	0.594172	-1.130729	-0.993868
23	35	0	3.360314	-0.296426	1.663133
24	1	0	0.819710	-4.548094	-0.966489
25	1	0	3.204235	-0.860146	0.337063
26	1	0	2.031626	0.221489	-1.856341
27	1	0	3.552887	-1.626702	-2.585543
28	1	0	2.941974	-3.985623	-2.123501
29	1	0	-1.156659	-3.349084	0.479874
30	1	0	-0.882479	-1.166079	1.491106
31	1	0	-1.123634	0.163297	-1.201262
32	1	0	0.830647	0.644764	0.913955
33	1	0	2.121150	2.480516	0.594380
34	1	0	2.330369	4.792946	-0.259469
35	1	0	0.480783	5.818191	-1.580892
36	1	0	-1.595027	4.502766	-1.989915
37	1	0	-1.840568	2.231258	-1.070242
38	1	0	-2.541170	0.465418	2.177106
39	1	0	-4.940670	1.076688	2.278529

40	1	0	-6.560024	0.034412	0.702160
41	1	0	-5.755417	-1.618372	-0.973723
42	1	0	-3.346884	-2.222339	-1.068018

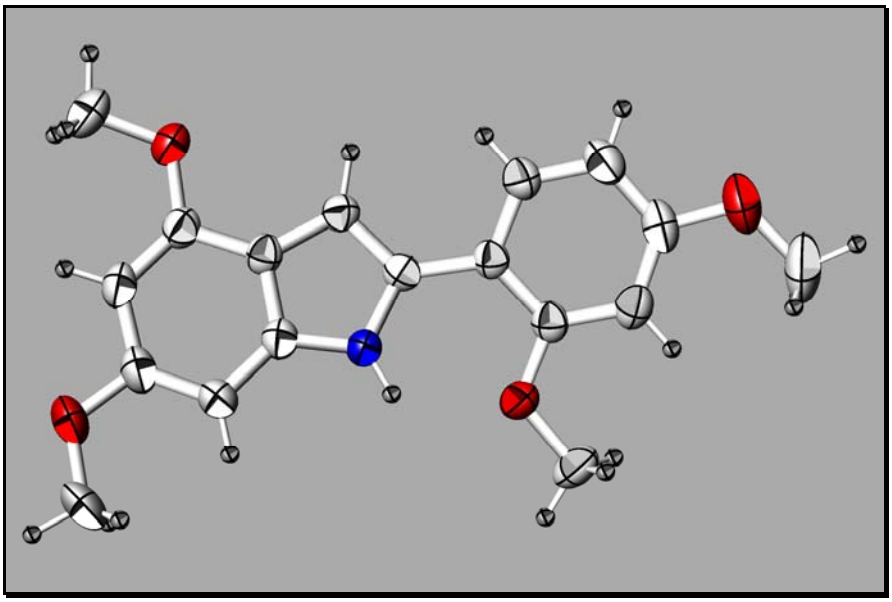
TS6.HBr

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.605994	4.221155	-1.667009
2	6	0	0.601163	3.794856	-1.140184
3	6	0	0.617998	2.615368	-0.370190
4	6	0	-0.606008	1.933594	-0.020656
5	6	0	-1.816770	2.411362	-0.619977
6	6	0	-1.814275	3.513422	-1.445128
7	7	0	1.724100	1.904924	-0.050392
8	6	0	1.460270	0.507645	0.306318
9	6	0	0.135183	0.180436	-0.444000
10	7	0	-0.586705	-0.852642	0.034112
11	35	0	-0.904408	0.097311	3.019227
12	1	0	1.526099	4.319344	-1.364887
13	1	0	-0.720424	1.577800	1.025881
14	1	0	-2.747177	1.915266	-0.358086
15	1	0	-2.736262	3.877498	-1.887647
16	1	0	-0.621706	5.112801	-2.288665
17	1	0	2.653658	2.201411	-0.311266
18	6	0	2.597629	-0.419847	-0.060701
19	1	0	1.237888	0.415714	1.377158
20	1	0	0.200185	0.240551	-1.530299
21	6	0	-1.645095	-1.492601	-0.643589
22	1	0	-0.674439	-0.839972	1.079517
23	6	0	-2.748447	-1.905059	0.121213
24	6	0	-3.808725	-2.561499	-0.497621
25	6	0	-3.786039	-2.807686	-1.873154

26	6	0	-2.685751	-2.396637	-2.628515
27	6	0	-1.612485	-1.745702	-2.021906
28	1	0	-2.760160	-1.677366	1.184382
29	1	0	-4.660923	-2.875269	0.098897
30	1	0	-4.615996	-3.319587	-2.351712
31	1	0	-2.653774	-2.594745	-3.696545
32	1	0	-0.745086	-1.464641	-2.612229
33	6	0	2.994651	-1.403893	0.853245
34	6	0	4.025862	-2.286776	0.533703
35	6	0	4.672847	-2.193009	-0.700424
36	6	0	4.280524	-1.216598	-1.618121
37	6	0	3.244090	-0.337695	-1.301884
38	1	0	2.486625	-1.473464	1.811909
39	1	0	4.326798	-3.045235	1.250933
40	1	0	5.478752	-2.878826	-0.946911
41	1	0	4.777863	-1.141898	-2.581456
42	1	0	2.936857	0.413734	-2.026487

Crystallographic data for Compound 3e:

A)



B)

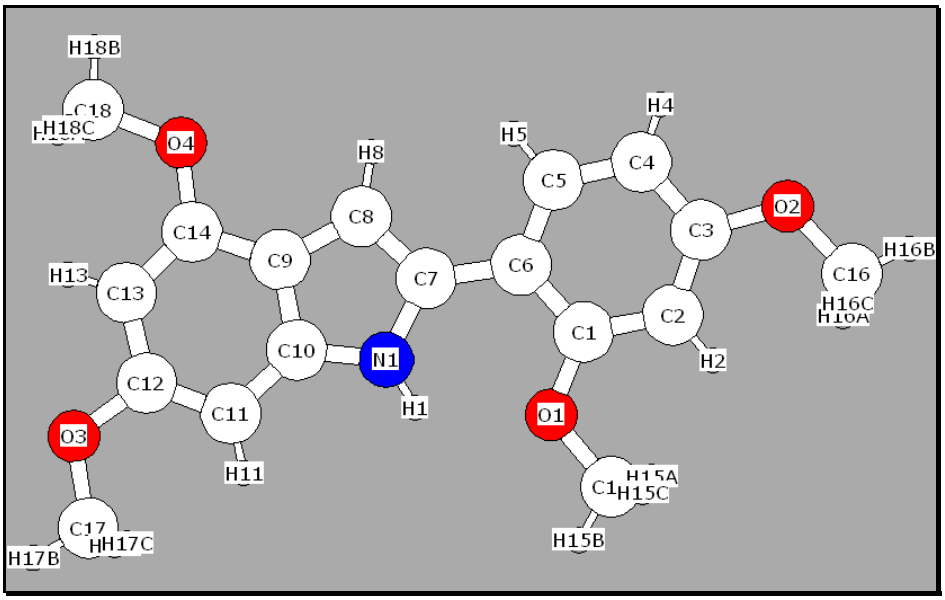


Figure 1. (A)ORTEP diagram of compound **3e** (Identification code: FC9abs).(B)Atom numbering for compound **3e**.

Table 1. Crystal data and structure refinement for fc9abs.

Identification code	fc9abs
Empirical formula	C72 H76 N4 O16
Formula weight	1253.37
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 14.5050(10) A alpha = 90 deg. b = 10.7366(7) A beta = 100.855(7) deg. c = 10.6755(10) A gamma = 90 deg.
Volume	1632.8(2) A^3
Z, Calculated density	1, 1.275 Mg/m^3
Absorption coefficient	0.090 mm^-1
F(000)	664
Crystal size	0.21 x 0.11 x 0.03 mm
Theta range for data collection	3.43 to 26.37 deg.
Limiting indices	-17<=h<=18, -13<=k<=13, -13<=l<=7
Reflections collected / unique	11596 / 3308 [R(int) = 0.0449]
Completeness to theta = 26.37	99.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3308 / 0 / 220
Goodness-of-fit on F^2	1.134
Final R indices [I>2sigma(I)]	R1 = 0.0584, wR2 = 0.1164
R indices (all data)	R1 = 0.1049, wR2 = 0.1363
Largest diff. peak and hole	0.162 and -0.159 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic

displacement parameters (A^2 x 10^3) for fc9abs.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4619(1)	4114(2)	6164(2)	43(1)
C(2)	3688(2)	4448(2)	6106(2)	54(1)
C(3)	2993(2)	3785(2)	5335(2)	61(1)
C(4)	3214(2)	2796(2)	4622(2)	60(1)
C(5)	4137(1)	2483(2)	4689(2)	51(1)
C(6)	4872(1)	3115(2)	5457(2)	39(1)
C(7)	5834(1)	2694(2)	5501(2)	40(1)
C(8)	6151(1)	1819(2)	4749(2)	42(1)
C(9)	7117(1)	1649(2)	5201(2)	42(1)
C(10)	7387(1)	2452(2)	6239(2)	47(1)
C(11)	8301(1)	2525(2)	6932(2)	60(1)
C(12)	8945(2)	1761(2)	6547(2)	65(1)
C(13)	8710(1)	934(2)	5513(2)	57(1)
C(14)	7808(1)	883(2)	4841(2)	46(1)
C(15)	5139(2)	5748(2)	7675(2)	61(1)
C(16)	1779(2)	5045(3)	5935(3)	108(1)
C(17)	10180(2)	2550(4)	8142(3)	131(2)
C(18)	8145(2)	-744(2)	3464(3)	78(1)
N(1)	6594(1)	3076(2)	6401(2)	46(1)
O(1)	5344(1)	4728(1)	6917(1)	52(1)
O(2)	2051(1)	4035(2)	5218(2)	90(1)
O(3)	9875(1)	1699(2)	7139(2)	100(1)
O(4)	7500(1)	140(1)	3810(1)	60(1)

Table 3. Bond lengths [A] and angles [deg] for fc9abs.

C(1)-O(1)	1.367(2)
C(1)-C(2)	1.387(3)
C(1)-C(6)	1.399(3)
C(2)-C(3)	1.374(3)
C(3)-O(2)	1.375(3)
C(3)-C(4)	1.379(3)
C(4)-C(5)	1.370(3)
C(5)-C(6)	1.393(3)
C(6)-C(7)	1.459(3)
C(7)-C(8)	1.370(3)
C(7)-N(1)	1.381(2)
C(8)-C(9)	1.406(3)
C(9)-C(10)	1.400(3)
C(9)-C(14)	1.405(3)
C(10)-N(1)	1.370(2)
C(10)-C(11)	1.393(3)
C(11)-C(12)	1.363(3)
C(12)-O(3)	1.380(3)
C(12)-C(13)	1.408(3)
C(13)-C(14)	1.369(3)
C(14)-O(4)	1.365(2)
C(15)-O(1)	1.425(2)
C(16)-O(2)	1.425(3)
C(17)-O(3)	1.413(3)
C(18)-O(4)	1.429(3)

O(1)-C(1)-C(2)	122.41(18)
O(1)-C(1)-C(6)	115.89(16)
C(2)-C(1)-C(6)	121.69(19)
C(3)-C(2)-C(1)	119.5(2)
C(2)-C(3)-O(2)	124.0(2)
C(2)-C(3)-C(4)	120.55(19)
O(2)-C(3)-C(4)	115.5(2)
C(5)-C(4)-C(3)	119.1(2)
C(4)-C(5)-C(6)	122.9(2)
C(5)-C(6)-C(1)	116.23(17)
C(5)-C(6)-C(7)	119.24(17)
C(1)-C(6)-C(7)	124.51(17)

C(8)-C(7)-N(1)	107.40(17)
C(8)-C(7)-C(6)	128.23(17)
N(1)-C(7)-C(6)	124.25(16)
C(7)-C(8)-C(9)	108.14(17)
C(10)-C(9)-C(14)	118.03(17)
C(10)-C(9)-C(8)	107.63(16)
C(14)-C(9)-C(8)	134.34(18)
N(1)-C(10)-C(11)	130.02(18)
N(1)-C(10)-C(9)	106.58(17)
C(11)-C(10)-C(9)	123.39(18)
C(12)-C(11)-C(10)	116.36(19)
C(11)-C(12)-O(3)	123.9(2)
C(11)-C(12)-C(13)	122.49(19)
O(3)-C(12)-C(13)	113.57(19)
C(14)-C(13)-C(12)	120.14(19)
O(4)-C(14)-C(13)	125.55(18)
O(4)-C(14)-C(9)	114.87(17)
C(13)-C(14)-C(9)	119.58(18)
C(10)-N(1)-C(7)	110.24(16)
C(1)-O(1)-C(15)	119.04(16)
C(3)-O(2)-C(16)	118.0(2)
C(12)-O(3)-C(17)	117.06(18)
C(14)-O(4)-C(18)	117.72(17)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for fc9abs.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	42(1)	45(1)	41(1)	6(1)	7(1)	6(1)
C(2)	54(1)	55(1)	55(1)	2(1)	14(1)	13(1)
C(3)	40(1)	69(2)	74(2)	9(1)	8(1)	12(1)
C(4)	43(1)	67(1)	68(1)	2(1)	1(1)	0(1)
C(5)	45(1)	52(1)	53(1)	-1(1)	4(1)	5(1)
C(6)	39(1)	42(1)	36(1)	5(1)	6(1)	4(1)
C(7)	41(1)	41(1)	37(1)	4(1)	5(1)	1(1)
C(8)	43(1)	43(1)	39(1)	-2(1)	6(1)	2(1)
C(9)	43(1)	44(1)	40(1)	2(1)	11(1)	4(1)
C(10)	41(1)	53(1)	48(1)	-3(1)	10(1)	5(1)
C(11)	42(1)	76(2)	58(1)	-19(1)	0(1)	5(1)
C(12)	39(1)	88(2)	66(1)	-12(1)	5(1)	13(1)
C(13)	45(1)	67(1)	60(1)	-8(1)	15(1)	15(1)
C(14)	47(1)	50(1)	43(1)	-3(1)	12(1)	6(1)
C(15)	78(2)	49(1)	54(1)	-10(1)	12(1)	14(1)
C(16)	61(2)	123(2)	146(3)	-8(2)	34(2)	36(2)
C(17)	43(2)	200(4)	136(3)	-84(3)	-24(2)	15(2)
C(18)	79(2)	74(2)	85(2)	-25(1)	21(1)	22(1)
N(1)	39(1)	53(1)	46(1)	-12(1)	4(1)	7(1)
O(1)	52(1)	50(1)	51(1)	-12(1)	3(1)	10(1)
O(2)	43(1)	106(1)	118(2)	-7(1)	10(1)	18(1)
O(3)	39(1)	142(2)	109(1)	-49(1)	-10(1)	24(1)
O(4)	55(1)	64(1)	61(1)	-17(1)	12(1)	14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for fc9abs.

	x	y	z	U(eq)
H(2)	3536	5114	6585	65
H(4)	2742	2347	4103	72
H(5)	4280	1818	4200	61
H(11)	8462	3065	7619	72
H(13)	9168	421	5286	68
H(15A)	4790	6367	7135	91
H(15B)	5715	6104	8122	91
H(15C)	4774	5458	8280	91
H(16A)	1993	4892	6829	162
H(16B)	1108	5120	5762	162
H(16C)	2054	5803	5699	162
H(17A)	10108	3385	7818	197
H(17B)	10828	2398	8498	197
H(17C)	9810	2444	8792	197
H(18A)	8668	-312	3232	118
H(18B)	7836	-1231	2754	118
H(18C)	8366	-1283	4175	118
H(1)	6556(15)	3680(20)	6920(20)	63(7)
H(8)	5751(14)	1384(17)	4017(18)	55(6)

Table 6. Hydrogen bonds for fc9abs [A and deg.].

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.862	2.089	123.89	2.668	O1
N1-H1	0.862	2.550	142.69	3.277	O4 [x, -y+1/2, z+1/2]

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