Supporting Information for

Synthesis of Fused N-Heterocycles via Tandem C-H Activation

Ge Meng, Hong-Ying Niu, Gui-Rong Qu, John S. Fossey, Jian-Ping Li,* and Hai-Ming Guo*

College of Chemistry and Environmental Science, Key Laboratory of Green Chemical Media and Reactions of Ministry of Education, Henan Normal University, Xinxiang 453007, Henan, China.
Fax: +86 373 3329276
E-mail: jplig@163.com; guohm518@hotmail.com

General information:

NMR spectra were recorded with a 400 MHz spectrometer for ^{1}H NMR, 100 MHz for ^{13}C NMR. Chemical shifts δ are given in ppm relative to the residual signals of tetramethylsilane in $CDCl_3$ or deuterated solvent $CDCl_3$ for ^{1}H and ^{13}C NMR. Multiplicities are reported as follows: singlet (s), doublet (d), triplet (t), multiplet (m). High resolution mass spectra were taken with a 3000 mass spectrometer, using Waters Q-TofMS/MS system. For column chromatography silica gel (200-300 mesh) was used as the stationary phase. All reactions were monitored by thin layer chromatography (TLC). All reagents were purchased from commercial sources and purified commonly before used. All Starting materials were synthesized by Suzuki cross-coupling reactions according to references 1 and 2.

General procedure for the intramolecular cyclization of 2, 6-substituted-9-benzyl purine.

A 25 mL Schlenk tube, containing a Teflon stirbar, was charged with **2**, 6-substituted-9-benzyl purine (0.3 mmol), $Pd(OAc)_2$ (0.03 mmol, 6.9 mg) and AgOAc (0.6 mmol, 100.2 mg), then AcOH (1.5 mL) was added and the reaction mixture was heated at 110 ^{o}C for indicated hours. The resulting mixture was cooled down to room temperature, filtered through a pad of celite, and the celite was rinsed with copious EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc) affording the corresponding intramolecular cyclization product.

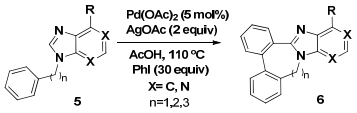
General procedure for the intramolecular cyclization of 1-benzyl benzimidazole.

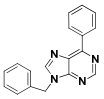
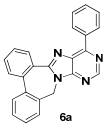
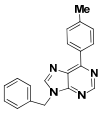
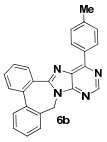
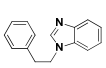
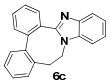
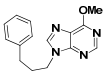
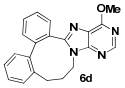
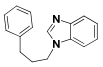
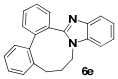
A 25 mL Schlenk tube, containing a Teflon stirbar, was charged with 1-benzyl benzimidazole (0.3 mmol), $Pd(OAc)_2$ (0.03 mmol, 6.9 mg) and AgOAc (0.6 mmol, 100.2 mg), then AcOH (1.5 mL) was added and the reaction mixture was heated at 110 ^{o}C for indicated hours. The resulting mixture was cooled down to room temperature, filtered through a pad of celite, and the celite was rinsed with copious EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc) affording the corresponding intramolecular cyclization product.

General procedure for the intramolecular cyclization of purines and benzimidazoles with iodobenzene

A 25 mL Schlenk tube, containing a Teflon stirbar, was charged with substrate (0.3 mmol), $Pd(OAc)_2$ (0.03 mmol, 6.9 mg), AgOAc (0.6 mmol, 100.2 mg) and PhI (9 mmol, 1.836 g), then AcOH (1.5 mL) was added and the reaction mixture was heated at 110 ^{o}C～120 ^{o}C for indicated hours. The resulting mixture was cooled down to room temperature, filtered through a pad of celite, and the celite was rinsed with copious EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc) affording the corresponding intramolecular cyclization product.

Table for Intramolecular cyclisation of purines and benzimidazoles with iodobenzene[a]

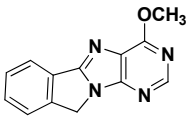


entry	substrate	product	yield/%[b]
1[c]			45
2			63
3			69
4			49
5			79

[a] Unless otherwise mentioned, all of the reactions were carried out with **1a** (0.3 mmol), catalyst (5 mol %), AgOAc (2 equiv), AcOH (1.8 mL) in a Schlenk tube at 110 °C for 36 h. [b] Isolated yield. [c] 120 °C for 48 h.

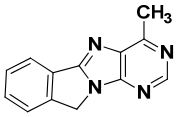
Characterization of compounds

4-methoxy-10*H*-isoindolo[2,1-*e*]purine (2a):



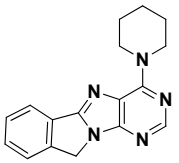
White solid. mp 183-185 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.10 (t, *J* = 4.4 Hz, 1H), 7.63 (t, *J* = 4.0 Hz, 1H), 7.58-7.53 (m, 2H), 5.18 (s, 2H), 4.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 157.6, 151.4, 150.7, 143.5, 130.4, 129.0, 128.3, 125.9, 124.1, 122.3, 54.1, 47.1; HRMS: calcd for $C_{13}H_{11}N_4O$ $[M+H]^+$ 239.0933, found 239.0929.

4-methyl-10*H*-isoindolo[2,1-*e*]purine (2b):



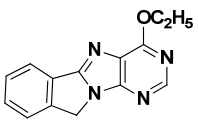
Light yellow solid. mp 175-177 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.11 (t, *J* = 4.0 Hz, 1H), 7.61 (d, *J* = 4.8 Hz, 1H), 7.57-7.54 (m, 2H), 5.15 (s, 2H), 2.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 158.4, 151.5, 149.4, 143.9, 137.9, 131.0, 129.1, 127.9, 124.3, 122.7, 46.9, 19.7; HRMS: calcd for $C_{13}H_{11}N_4$ $[M+H]^+$ 223.0984, found 223.0986.

4-(piperidin-1-yl)-10*H*-isoindolo[2,1-*e*]purine (2c):



Light yellow solid. mp 180-182 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.01 (d, *J* = 7.2 Hz, 1H), 7.58 (d, *J* = 6.8 Hz, 1H), 7.51-7.48 (m, 2H), 5.08 (s, 2H), 4.30 (s, 4H), 1.75 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 153.4, 151.9, 149.5, 143.2, 129.5, 128.9, 128.6, 124.1, 121.7, 46.7, 46.4, 29.7, 26.2, 24.9; HRMS: calcd for $C_{17}H_{18}N_5$ $[M+H]^+$ 292.1562, found 292.1563.

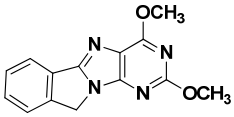
4-ethoxy-10*H*-isoindolo[2,1-*e*]purine (2d):



White solid. mp 188-190 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.06 (t, *J* = 4.2 Hz, 1H), 7.57 (t, *J* = 3.8 Hz, 1H), 7.51-7.49 (m, 2H), 5.12 (s, 2H), 4.68-4.63 (m, 2H), 1.53 (t, *J* =7.2 Hz,

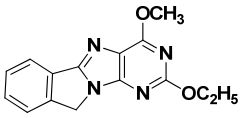
3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 157.4, 151.4, 150.7, 143.5, 130.3, 129.0, 128.3, 125.8, 124.1, 122.3, 63.1, 47.0, 14.6; HRMS: calcd for $C_{14}H_{13}N_4O$ $[M+H]^+$ 253.1089, found 253.1091.

2,4-dimethoxy-10*H*-isoindolo[2,1-*e*]purine (2e):



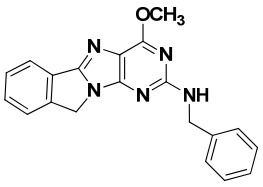
Light yellow solid. mp 200-202 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.92 (m, 1H), 7.50-7.49 (m, 1H), 7.46-7.42 (m, 2H), 4.99 (s, 2H), 4.13 (s, 3H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6, 161.2, 156.0, 152.0, 143.1, 129.8, 128.8, 128.4, 124.0, 121.8, 121.3, 55.0, 54.1, 46.8; HRMS: calcd for $C_{14}H_{13}N_4O_2$ $[M+H]^+$ 269.1039, found 269.1034.

2-ethoxy-4-methoxy-10*H*-isoindolo[2,1-*e*]purine (2f):



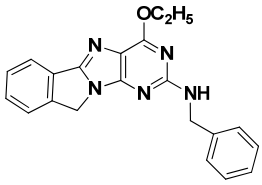
White solid. mp 190-192 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 6.4 Hz, 1H), 7.54 (d, J = 7.6 Hz, 1H), 7.48-7.45 (m, 2H), 5.03 (s, 2H), 4.66-4.60 (m, 2H), 4.02 (s, 3H), 1.51 (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 161.2, 156.0, 152.1, 143.2, 129.8, 128.8, 128.5, 124.0, 121.9, 121.4, 63.1, 55.1, 46.8, 14.6; HRMS: calcd for $C_{15}H_{15}N_4O_2$ $[M+H]^+$ 283.1195, found 283.1199.

N-benzyl-4-methoxy-10*H*-isoindolo[2,1-*e*]purin-2-amine (2g):



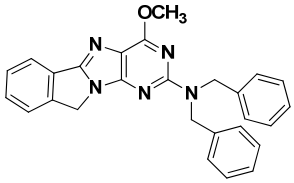
Light yellow solid. mp 216-218 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 7.2 Hz, 1H), 7.54-7.26 (m, 8H), 5.39 (s, 1H), 4.98 (s, 2H), 4.70 (d, J = 5.6 Hz, 2H), 4.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2, 158.6, 154.4, 152.3, 143.0, 139.6, 129.3, 129.0, 128.8, 128.5, 127.6, 127.1, 124.0, 121.6, 119.5, 53.6, 46.5, 46.1; HRMS: calcd for $C_{20}H_{18}N_5O$ $[M+H]^+$ 344.1511, found 344.1510.

N-benzyl-4-ethoxy-10*H*-isoindolo[2,1-*e*]purin-2-amine (2h):



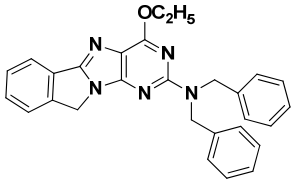
Light yellow solid. mp 165-167 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.2 Hz, 1H), 7.55-7.32 (m, 8H), 5.37-5.34 (m, 1H), 4.99 (s, 2H), 4.69 (d, *J* = 5.6 Hz, 2H), 4.59-4.52 (m, 2H), 1.46 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 158.5, 154.3, 152.2, 143.0, 139.6, 129.3, 129.0, 128.7, 128.5, 127.5, 127.1, 124.0, 121.6, 119.4, 62.5, 46.5, 46.1, 14.6; HRMS: calcd for $C_{21}H_{20}N_5O$ $[M+H]^+$ 358.1668, found 358.1666.

N,N-dibenzyl-4-methoxy-10*H*-isoindolo[2,1-*e*]purin-2-amine (2i):



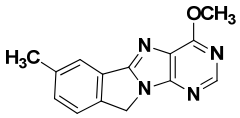
Light yellow solid. mp 140-142 °C. ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 7.86-7.85 (m, 1H), 7.64 (d, *J* = 6.0 Hz, 1H), 7.51-7.50 (m, 2H), 7.31-7.30 (m, 8H), 7.24-7.23 (m, 2H), 5.11 (s, 2H), 4.87 (s, 3H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 158.7, 154.4, 152.8, 143.1, 138.9, 129.2, 129.0, 128.7, 128.4, 127.7, 126.9, 123.9, 121.6, 118.7, 53.5, 49.8, 46.5; HRMS: calcd for $C_{27}H_{24}N_5O$ $[M+H]^+$ 434.1981, found 434.1978.

N,N-dibenzyl-4-ethoxy-10*H*-isoindolo[2,1-*e*]purin-2-amine (2j):



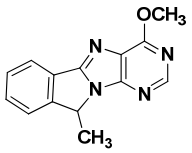
Light yellow solid. mp 145-147 °C. ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.02 (d, *J* = 7.2 Hz, 1H), 7.51-7.42 (m, 3H), 7.35-7.24 (m, 10H), 4.96 (s, 2H), 4.93 (s, 4H), 4.53-4.47 (m, 2H), 1.41 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 158.7, 154.3, 152.8, 143.1, 139.0, 129.1, 128.7, 128.4, 127.7, 126.9, 123.9, 121.5, 118.7, 62.3, 49.7, 46.5, 14.5; HRMS: calcd for $C_{28}H_{26}N_5O$ $[M+H]^+$ 448.2137, found 448.2133.

4-methoxy-7-methyl-10*H*-isoindolo[2,1-*e*]purine (2k):



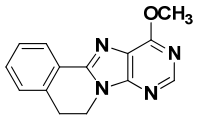
White solid. mp 220-222 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.88 (s, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 5.11 (s, 2H), 4.22 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 157.7, 151.3, 150.7, 140.7, 139.1, 131.4, 128.3, 125.8, 123.8, 122.7, 54.1, 46.9, 21.5; HRMS: calcd for $C_{14}H_{13}N_4O$ $[M+H]^+$ 253.1089, found 253.1085.

4-methoxy-10-methyl-10*H*-isoindolo[2,1-*e*]purine (2l):



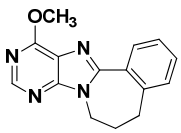
Light yellow solid. mp 165-167 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.08-8.06 (m, 1H), 7.55-7.53 (m, 3H), 5.47-5.42 (m, 1H), 4.22 (s, 3H), 1.89 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 156.6, 151.3, 150.7, 149.5, 130.5, 129.0, 127.6, 126.1, 123.1, 122.3, 55.9, 54.1, 18.9; HRMS: calcd for $C_{14}H_{13}N_4O$ $[M+H]^+$ 253.1089, found 253.1090.

11-methoxy-5,6-dihydropurino[8,9-*a*]isoquinoline (2m):



White solid. mp 100-102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.37 (d, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 4.0 Hz, 2H), 7.36 (d, *J* = 6.4 Hz, 1H), 4.48 (t, *J* = 6.8 Hz, 2H), 4.25 (s, 3H), 3.31 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 151.5, 142.0, 138.4, 134.8, 132.2, 131.0, 129.7, 128.2, 127.8, 125.8, 54.2, 47.3, 21.1; HRMS: calcd for $C_{14}H_{13}N_4O$ $[M+H]^+$ 253.1089, found 253.1085.

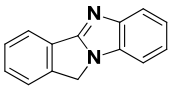
12-methoxy-6,7-dihydro-5*H*-benzo[3,4]azepino[1,2-*e*]purine (2n):



White solid. mp 90-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.00-7.98 (m, 1H),

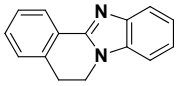
7.45-7.41 (m, 2H), 7.33 (d, *J* = 6.8 Hz, 1H), 4.26-4.22 (m, 5H), 2.79 (t, *J* = 7.0 Hz, 2H), 2.42 (t, *J* = 7.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 154.0, 153.0, 151.4, 139.0, 130.8, 129.9, 129.7, 129.6, 127.3, 121.5, 54.2, 40.2, 30.8, 30.1; HRMS: calcd for $C_{15}H_{15}N_4O$ $[M+H]^+$ 267.1246, found 267.1245.

11*H*-benzo[4,5]imidazo[2,1-*a*]isoindole (4a):



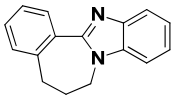
Light yellow solid. mp 180-182 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 6.8 Hz, 1H), 7.85-7.82 (m, 1H), 7.57 (t, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.47-7.44 (m, 1H), 7.31-7.28 (m, 2H), 5.06 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 148.2, 143.5, 132.6, 129.5, 129.2, 128.6, 123.8, 122.6, 122.1, 121.9, 120.4, 109.3, 47.1; HRMS: calcd for $C_{14}H_{11}N_2$ $[M+H]^+$ 207.0922, found 207.0923.

5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline (4b):



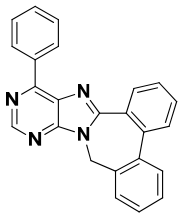
White solid. mp 115-117 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (t, *J* = 4.2 Hz, 1H), 7.84-7.81 (m, 1H), 7.42-7.37 (m, 2H), 7.36-7.31 (m, 1H), 7.28 (t, *J* = 4.8 Hz, 2H), 4.28 (t, *J* = 7.0 Hz, 2H), 3.24 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 143.8, 134.6, 134.3, 130.2, 128.1, 127.7, 126.6, 125.6, 122.7, 122.4, 119.7, 109.1, 40.4, 28.2; HRMS: calcd for $C_{15}H_{13}N_2$ $[M+H]^+$ 221.1079, found 221.1080.

6,7-dihydro-5*H*-benzo[*c*]benzo[4,5]imidazo[1,2-*a*]azepine (4c):



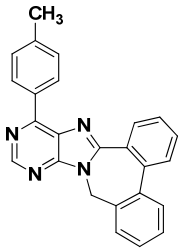
White pasty. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.97 (m, 1H), 7.89-7.86 (m, 1H), 7.44-7.37 (m, 3H), 7.32-7.27 (m, 3H), 4.10 (t, *J* = 6.8 Hz, 2H), 2.77 (t, *J* = 7.0 Hz, 2H), 2.43-2.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 143.1, 138.8, 135.4, 130.8, 130.3, 129.5, 129.4, 127.3, 122.5, 122.1, 119.9, 108.9, 41.3, 30.9, 30.6; HRMS: calcd for $C_{16}H_{15}N_2$ $[M+H]^+$ 235.1235, found 235.1237.

14-phenyl-9*H*-dibenzo[3,4:5,6]azepino[1,2-*e*]purine (6a):



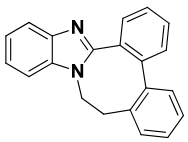
Light yellow solid. mp 173-175 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.07 (t, *J* = 4.2 Hz, 1H), 7.87 (d, *J* = 7.2 Hz, 1H), 7.62 (d, *J* = 6.4 Hz, 1H), 7.58-7.51 (m, 6H), 7.22-7.20 (m, 2H), 7.15-7.09 (m, 3H), 5.17 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 158.3, 151.3, 150.5, 144.0, 142.0, 141.4, 137.5, 134.6, 131.1, 131.0, 130.9, 129.7, 129.3, 129.0, 128.0, 127.7, 127.3, 126.5, 124.2, 123.0, 46.9; HRMS: calcd for $C_{24}H_{17}N_4$ $[M+H]^+$ 361.1453, found 361.1450.

14-(*p*-tolyl)-9*H*-dibenzo[3,4:5,6]azepino[1,2-*e*]purine (6b):



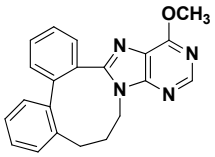
Light yellow pasty. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H), 8.08-8.06 (m, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 6.0 Hz, 1H), 7.57-7.54 (m, 2H), 7.36 (t, *J* = 8.2 Hz, 1H), 7.21-7.18 (m, 2H), 7.14-7.08 (m, 3H), 5.16 (s, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 158.4, 151.3, 150.5, 144.0, 141.8, 141.5, 139.7, 137.5, 131.8, 131.7, 131.1, 130.9, 129.2, 128.1, 127.7, 126.4, 124.2, 123.0, 46.9, 21.4; HRMS: calcd for $C_{25}H_{19}N_4$ $[M+H]^+$ 375.1610, found 375.1605.

9,10-dihydrodibenzo[*c*,*e*]benzo[4,5]imidazo[1,2-*a*]azocine (6c):



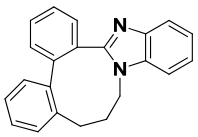
Light yellow solid. mp 136-138 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.39 (s, 5H), 7.34-7.32 (m, 3H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.18-7.14 (m, 1H), 4.37 (t, *J* = 6.6 Hz, 2H), 3.26 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 143.4, 141.9, 141.7, 136.6, 133.7, 131.2, 129.5, 129.3, 127.7, 127.2, 126.9, 124.8, 122.5, 121.8, 120.4, 108.6, 40.1, 30.0; HRMS: calcd for $C_{21}H_{17}N_2$ $[M+H]^+$ 297.1392, found 297.1390.

10-methoxy-16,17-dihydro-15*H*-dibenzo[3,4:5,6]azonino[1,2-*e*]purine (6d):



White solid. mp 190-192 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 6.8 Hz, 1H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.24-7.22 (m, 3H), 7.14-7.11 (m, 2H), 4.38 (s, 2H), 4.06 (s, 3H), 2.62 (t, *J* = 6.8 Hz, 2H), 2.37-2.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 152.0, 151.9, 151.3, 147.6, 143.3, 140.5, 139.8, 130.4, 129.6, 129.1, 128.1, 127.9, 127.0, 121.3, 54.3, 39.2, 30.6, 30.1; HRMS: calcd for $C_{21}H_{19}N_4O$ $[M+H]^+$ 343.1559, found 343.1557.

16,17-dihydro-15*H*-dibenzo[*c*,*e*]benzo[4,5]imidazo[1,2-*a*]azonine (6e):



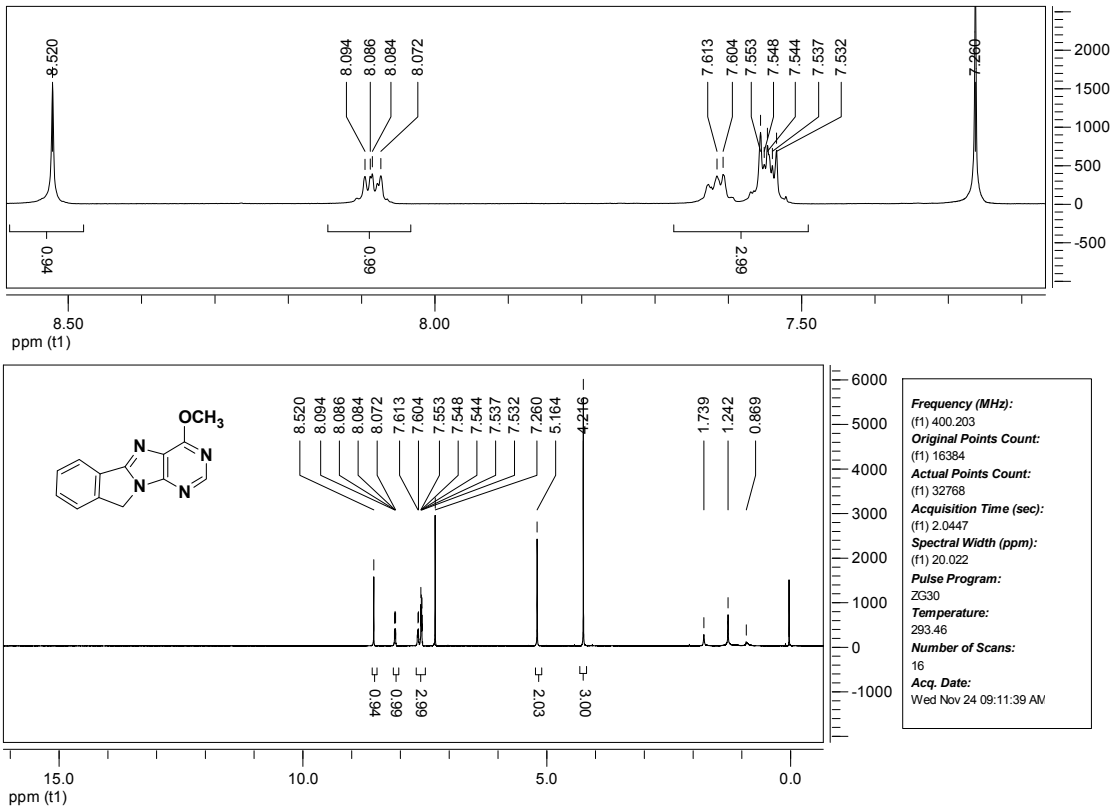
Light yellow solid. mp 120-122 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.51-7.45 (m, 2H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 6.4 Hz, 2H), 7.23-7.15 (m, 6H), 4.30 (s, 2H), 2.60 (t, *J* = 6.4 Hz, 2H), 2.33 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 143.3, 142.9, 140.8, 139.7, 133.8, 130.0, 129.5, 129.1, 128.8, 128.1, 128.0, 127.9, 126.9, 122.2, 121.6, 108.5, 40.2, 30.7, 30.5; HRMS: calcd for $C_{22}H_{19}N_2$ $[M+H]^+$ 311.1548, found 311.1552.

References:

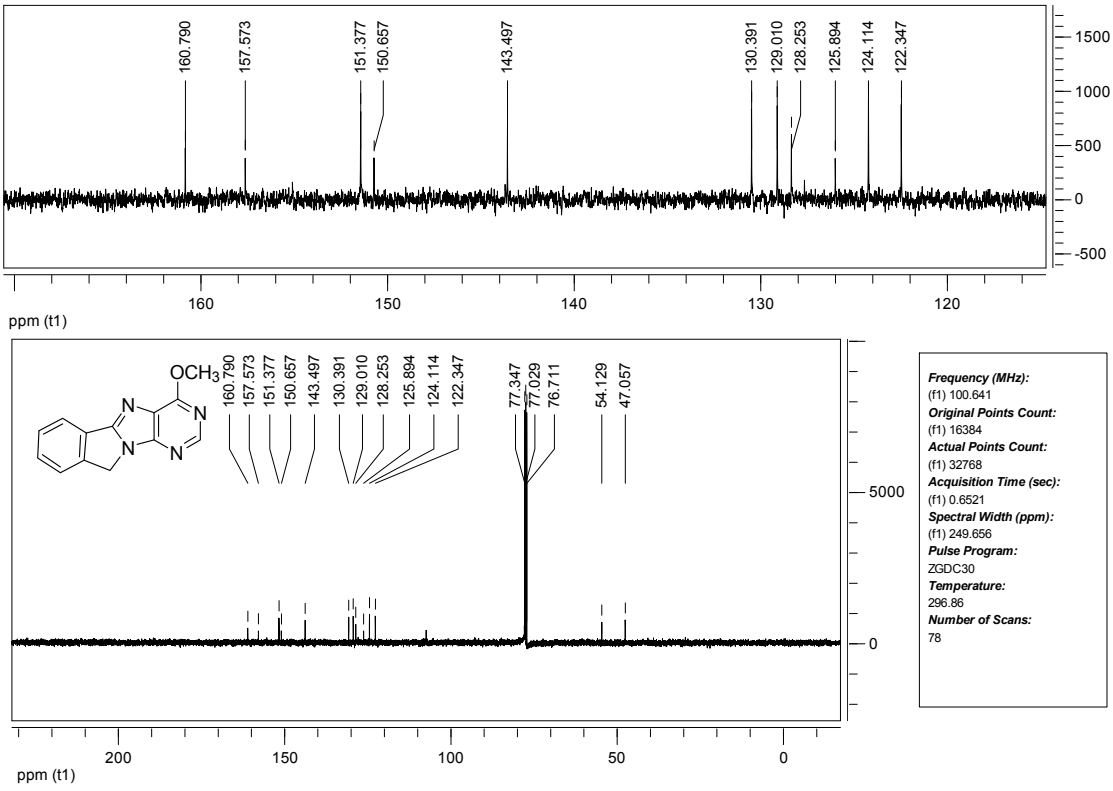
1. Černă, I.; Pohl, R.; Klepetářová, B.; Hocek, M. *J. Org. Chem*. **2008**, *73*, 9048-9054.
2. Lakshman, M.K.; Hilmer, J.H.; Martin, J.Q.; Keeler, J.C.; Dinh, Y.Q.V.; Ngassa, F.N.; Russon, L.M. *J. Am. Chem. Soc*. **2001**, *123*, 779-7787.

Copies of ^{1}H and ^{13}C NMR Spectrum

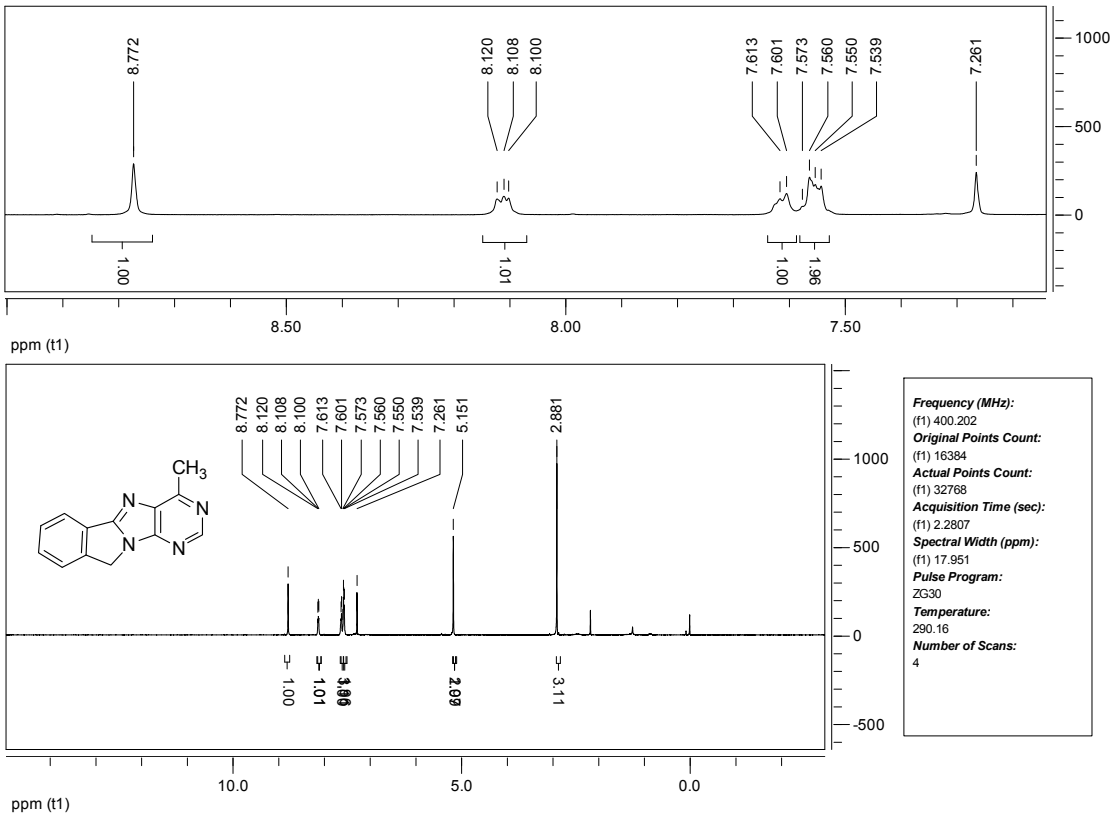
^{1}H NMR Spectrum for 2a



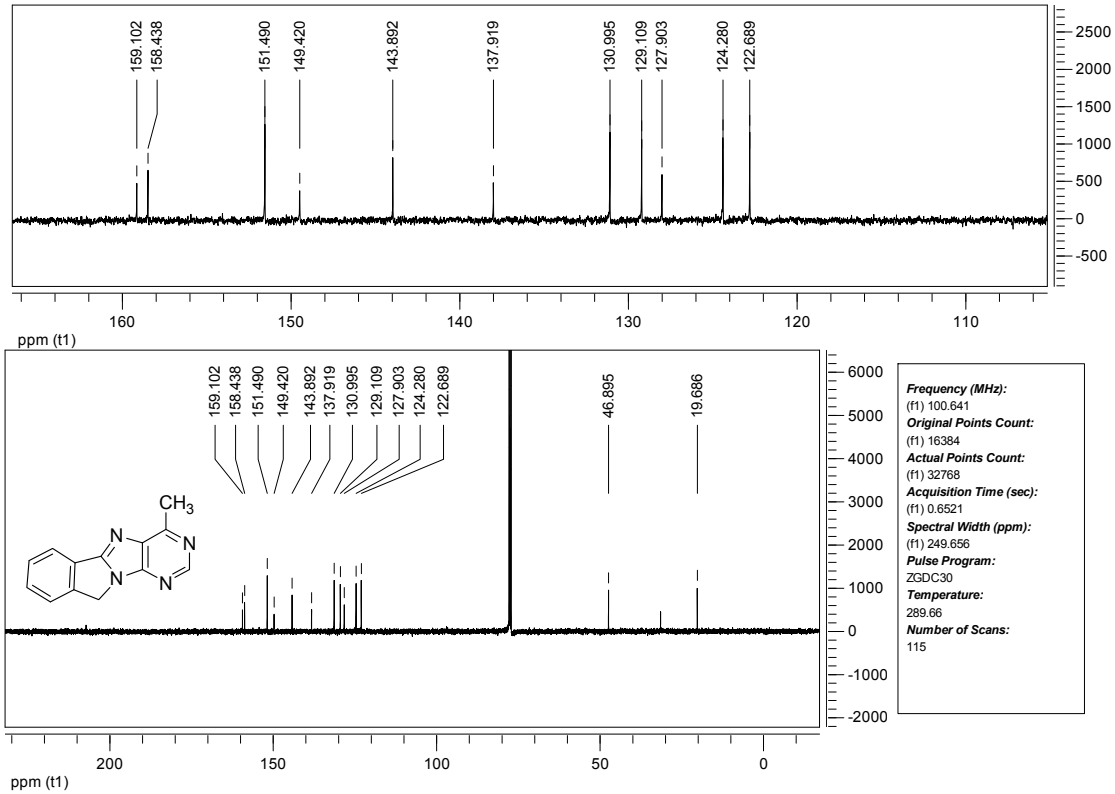
^{13}C NMR Spectrum for 2a



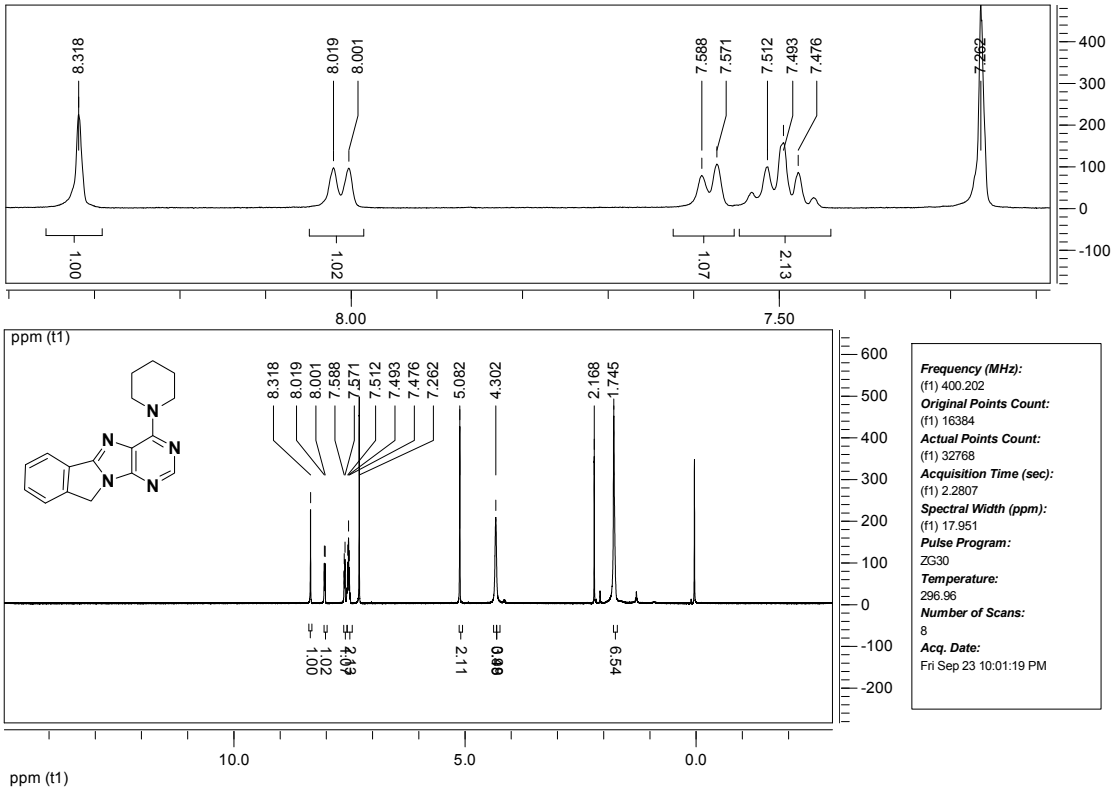
^{1}H NMR Spectrum for 2b



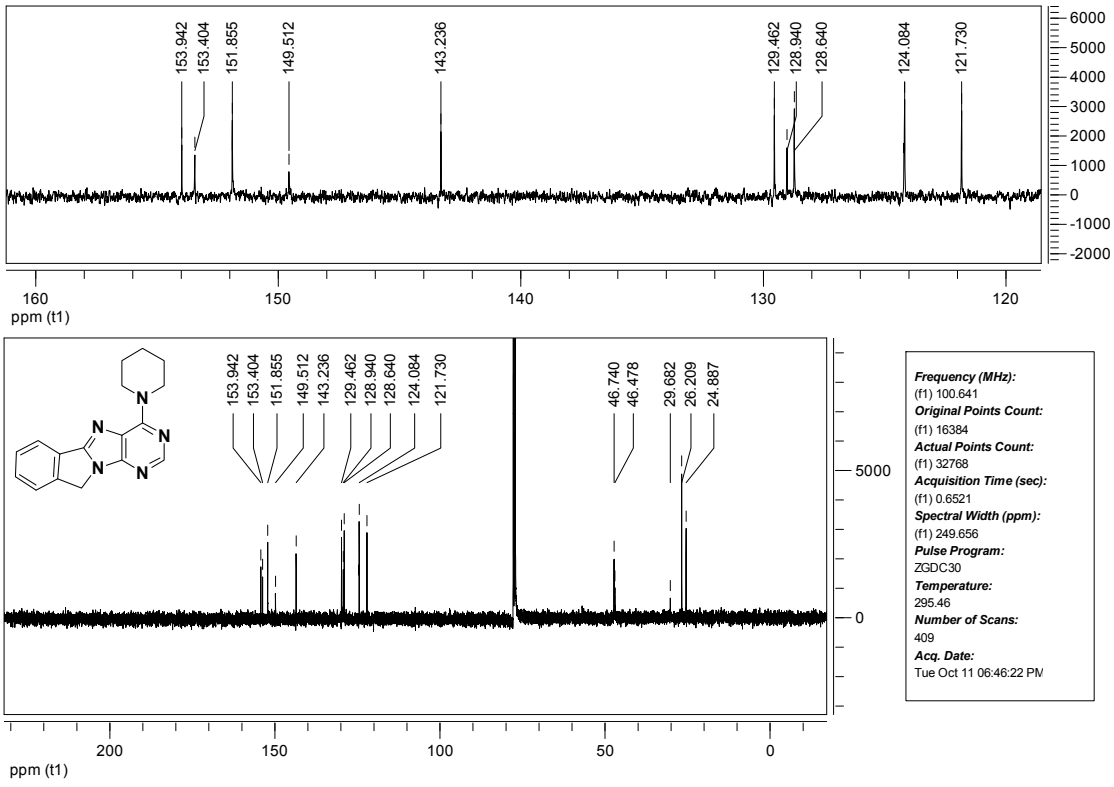
^{13}C NMR Spectrum for 2b



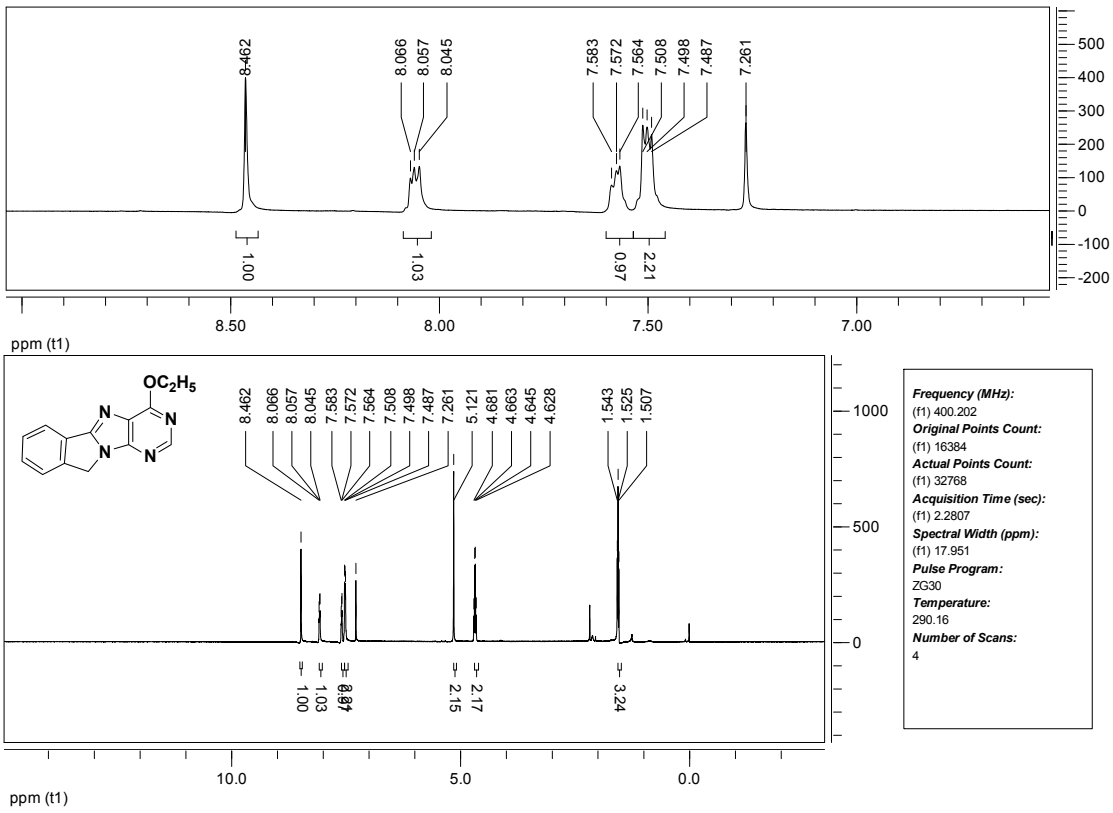
^{1}H NMR Spectrum for 2c



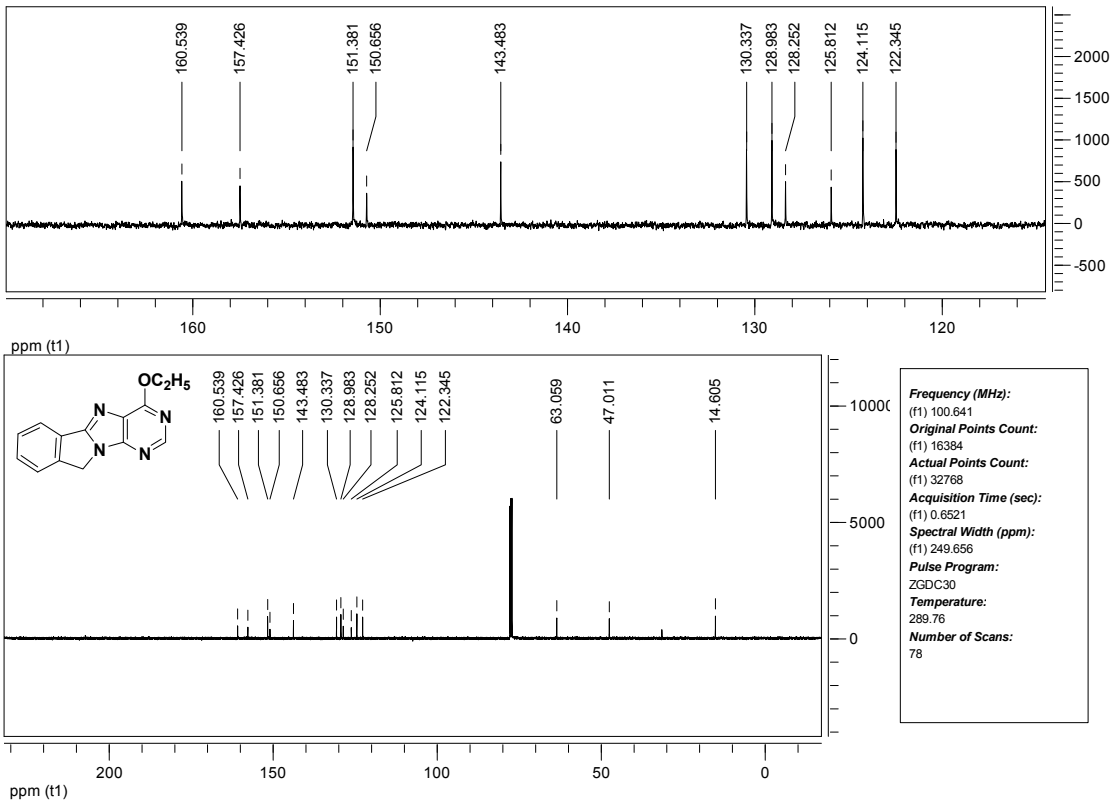
^{13}C NMR Spectrum for 2c



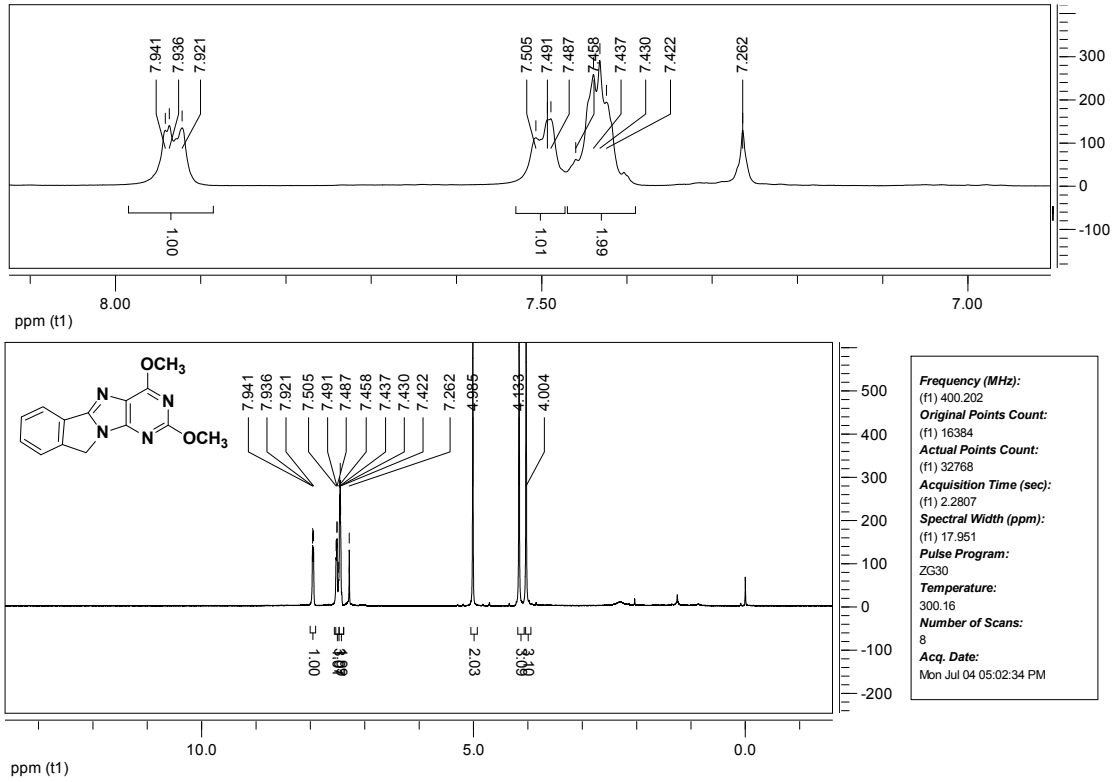
^{1}H NMR Spectrum for 2d



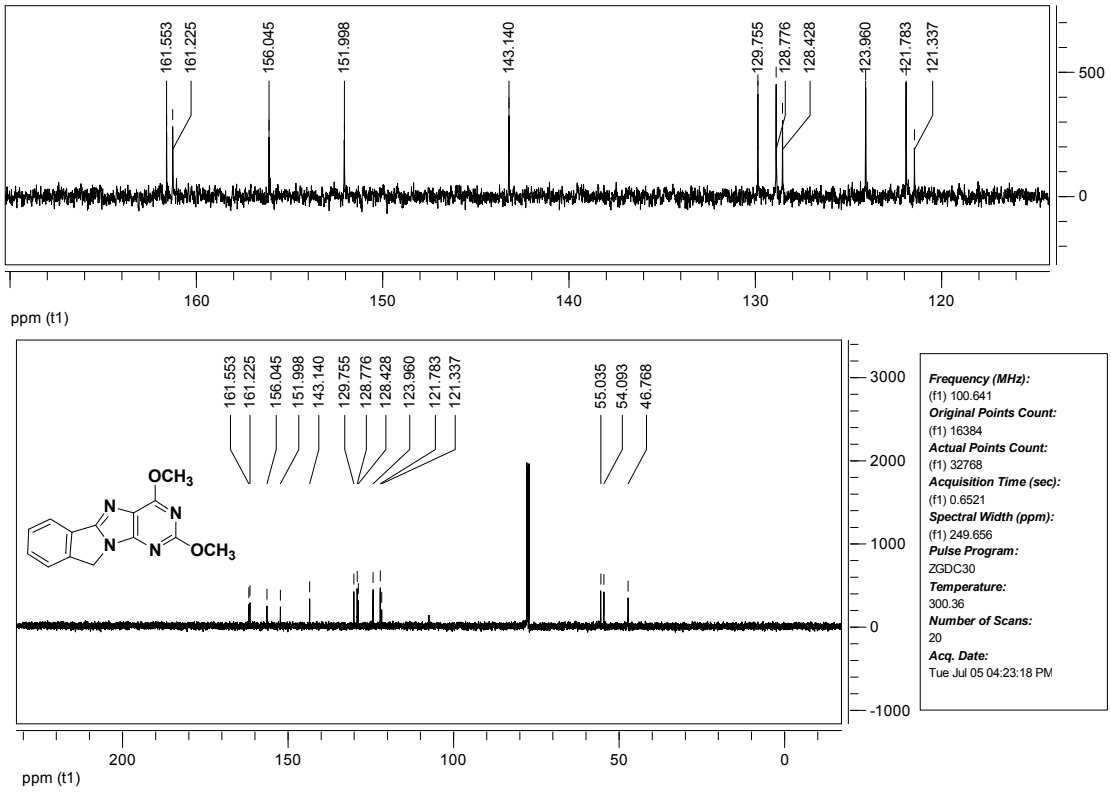
^{13}C NMR Spectrum for 2d



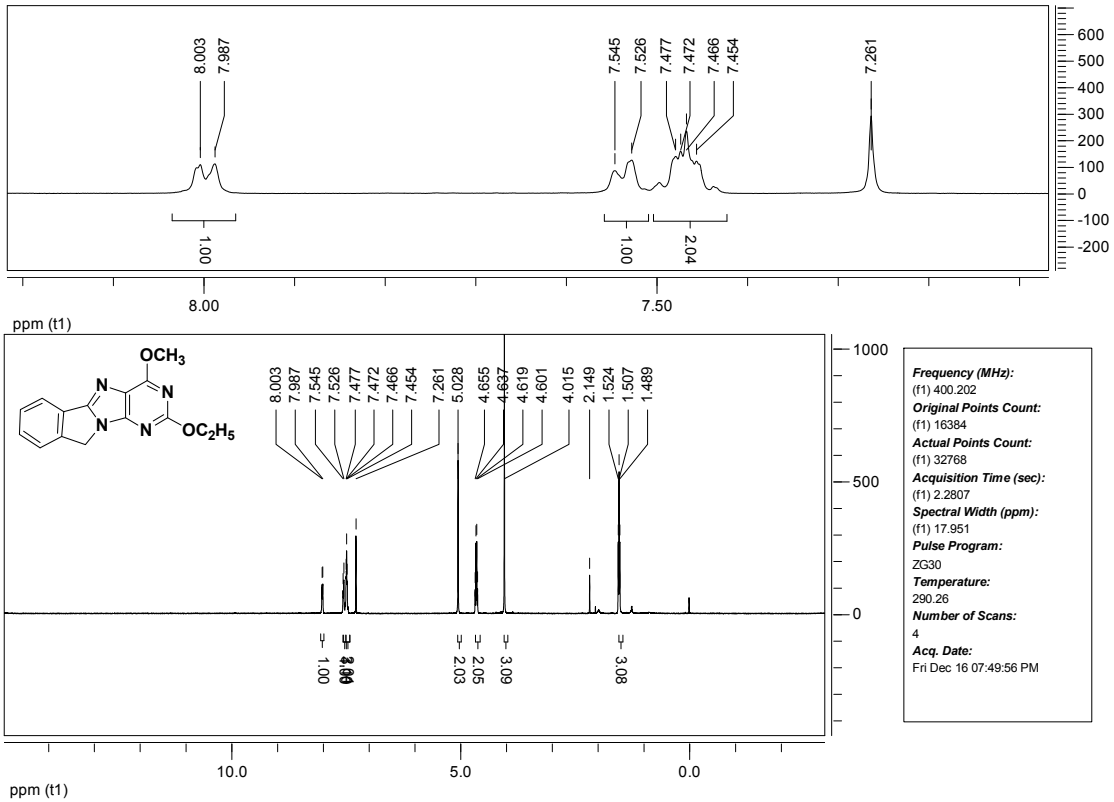
^{1}H NMR Spectrum for 2e



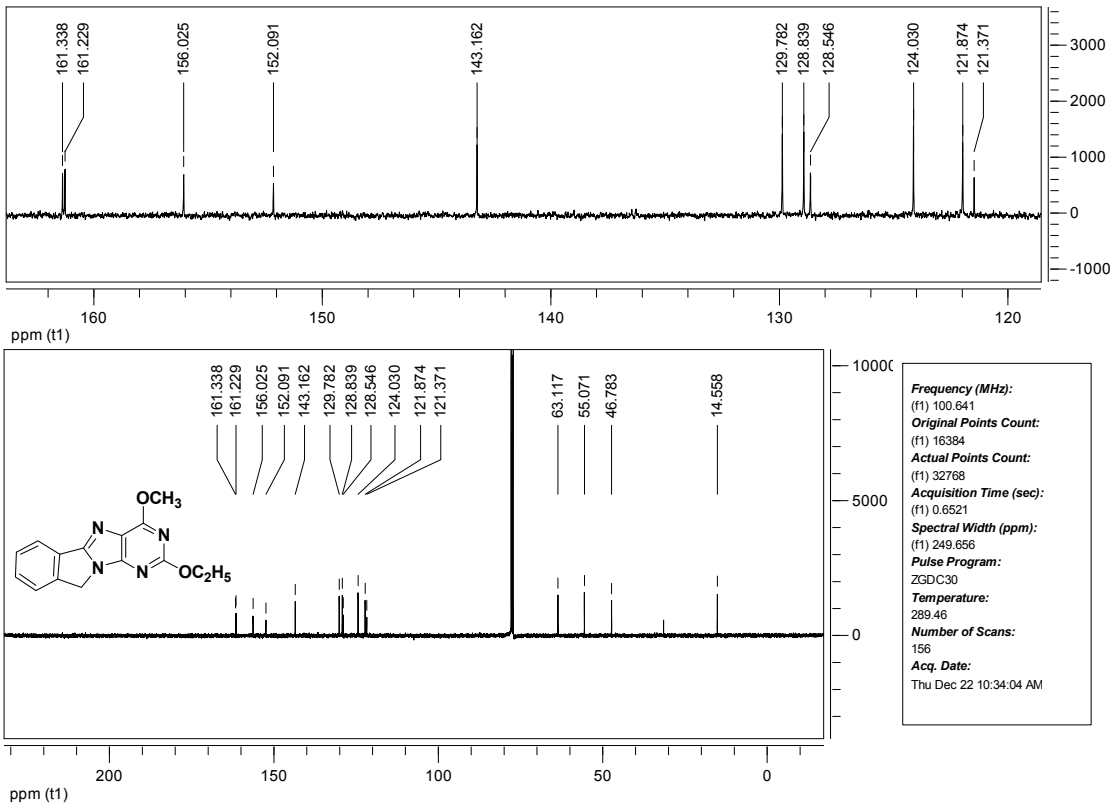
^{13}C NMR Spectrum for 2e



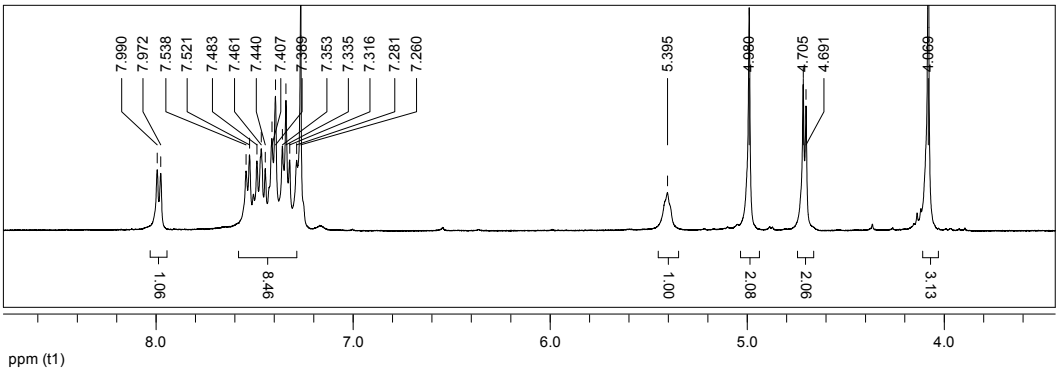
^{1}H NMR Spectrum for 2f

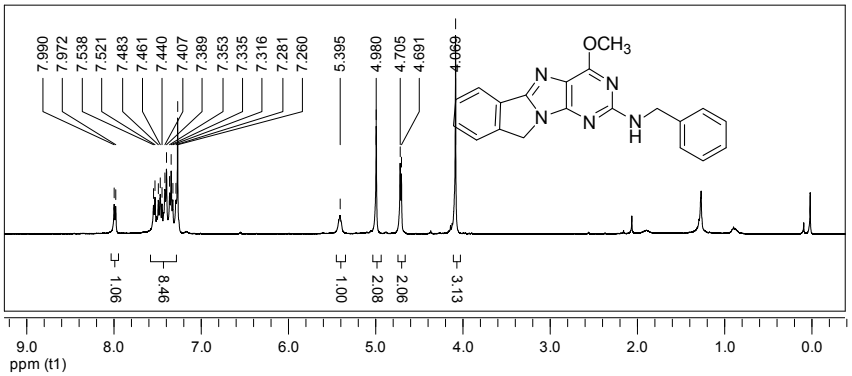


^{13}C NMR Spectrum for 2f



^{1}H NMR Spectrum for 2g





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Actual Points Count:
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Acquisition Time (sec):
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Spectral Width (ppm):
(f1) 15.089
Pulse Program:
ZG30
Temperature:
290.26
Number of Scans:
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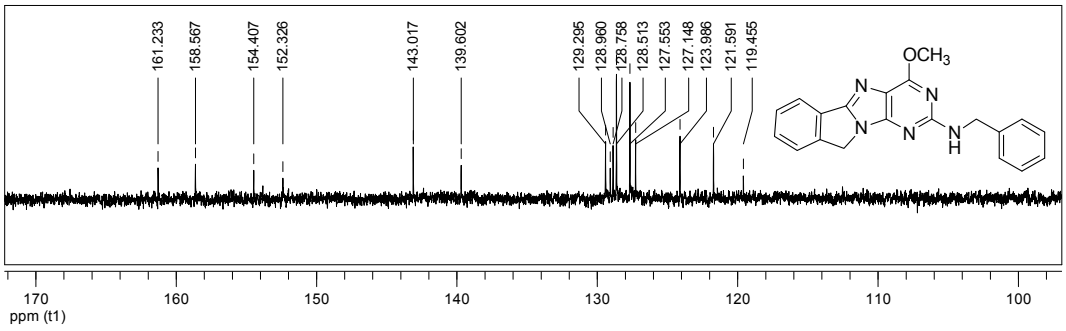
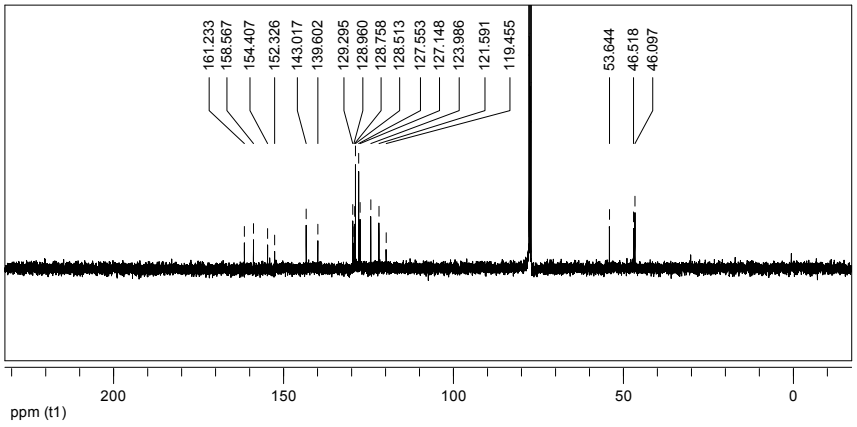
^{13}C NMR Spectrum for 2g





Frequency (MHz):
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Temperature:
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Number of Scans:
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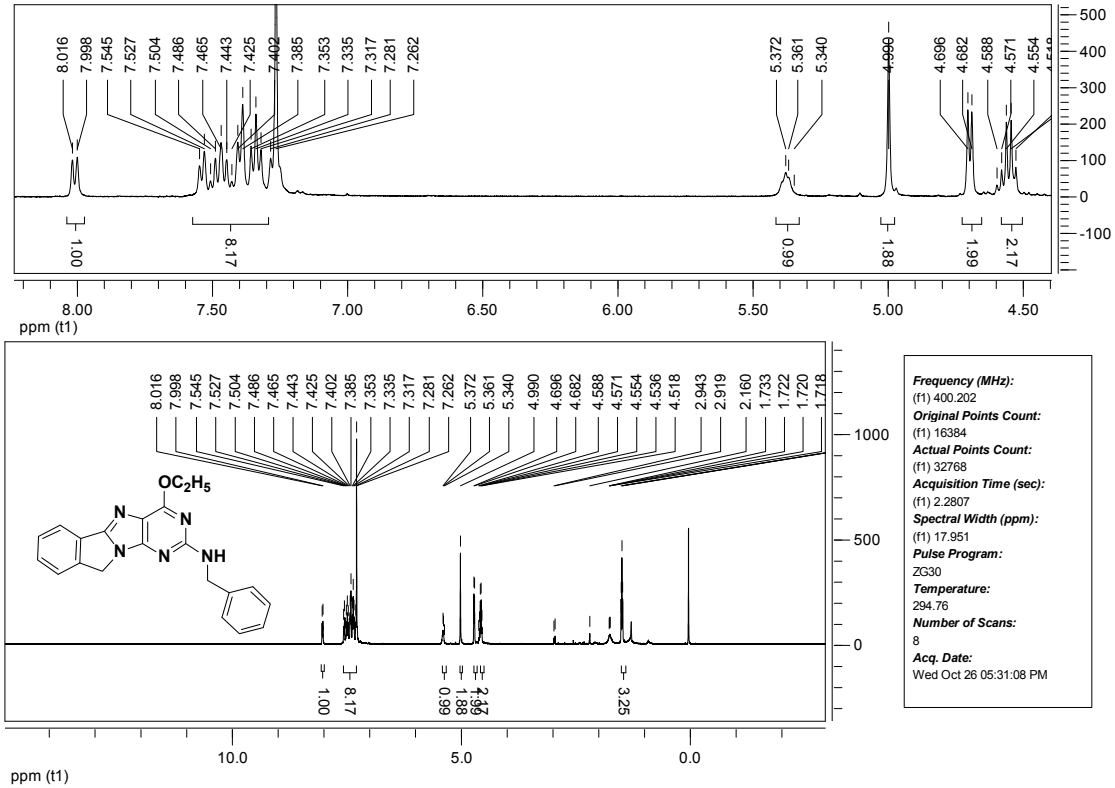
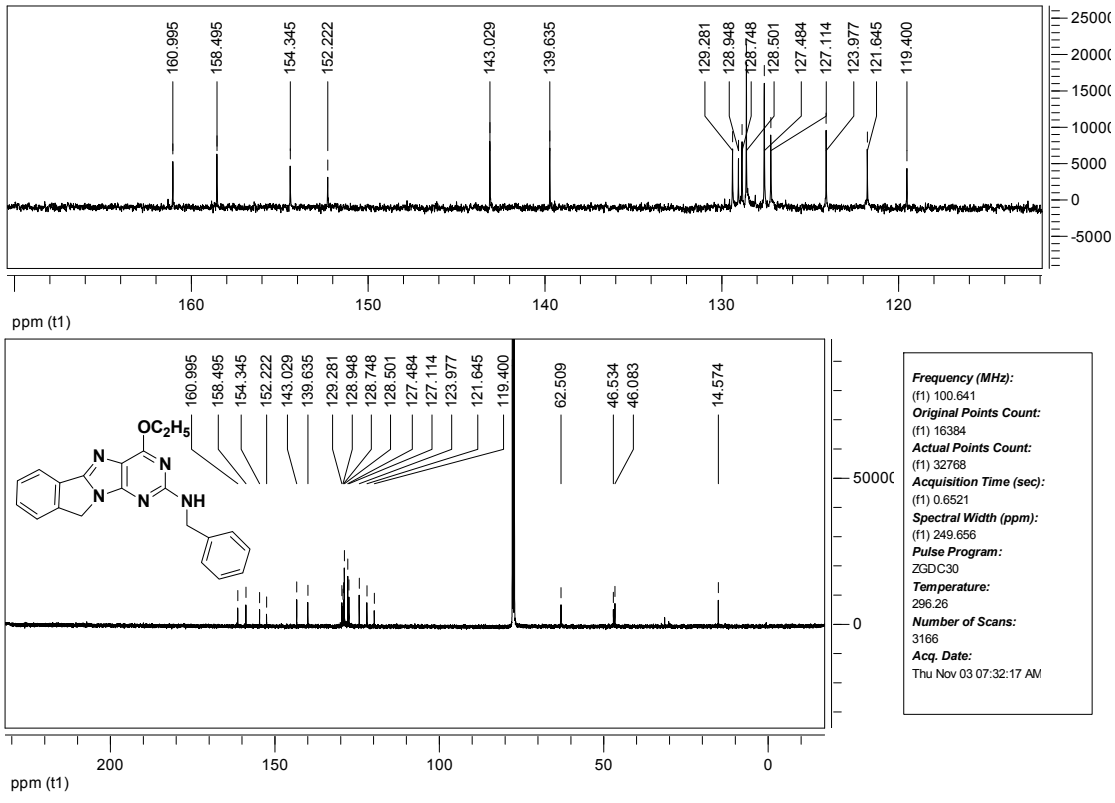
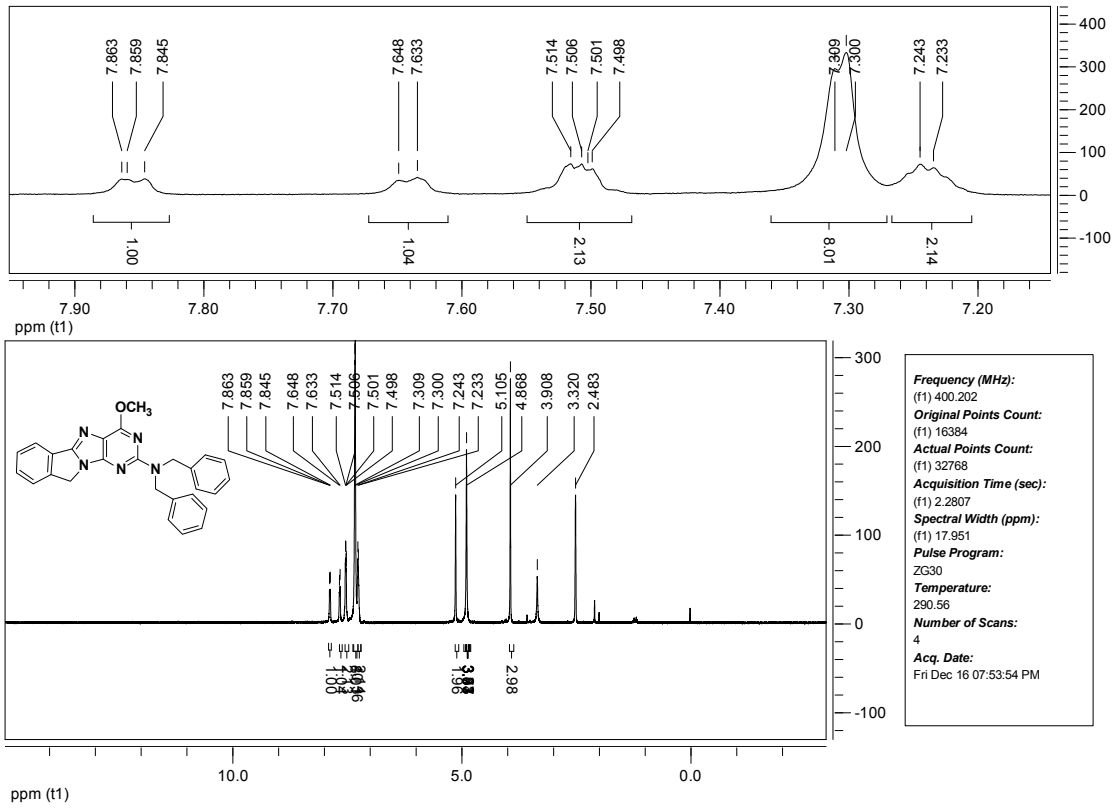
^{1}H NMR Spectrum for 2h



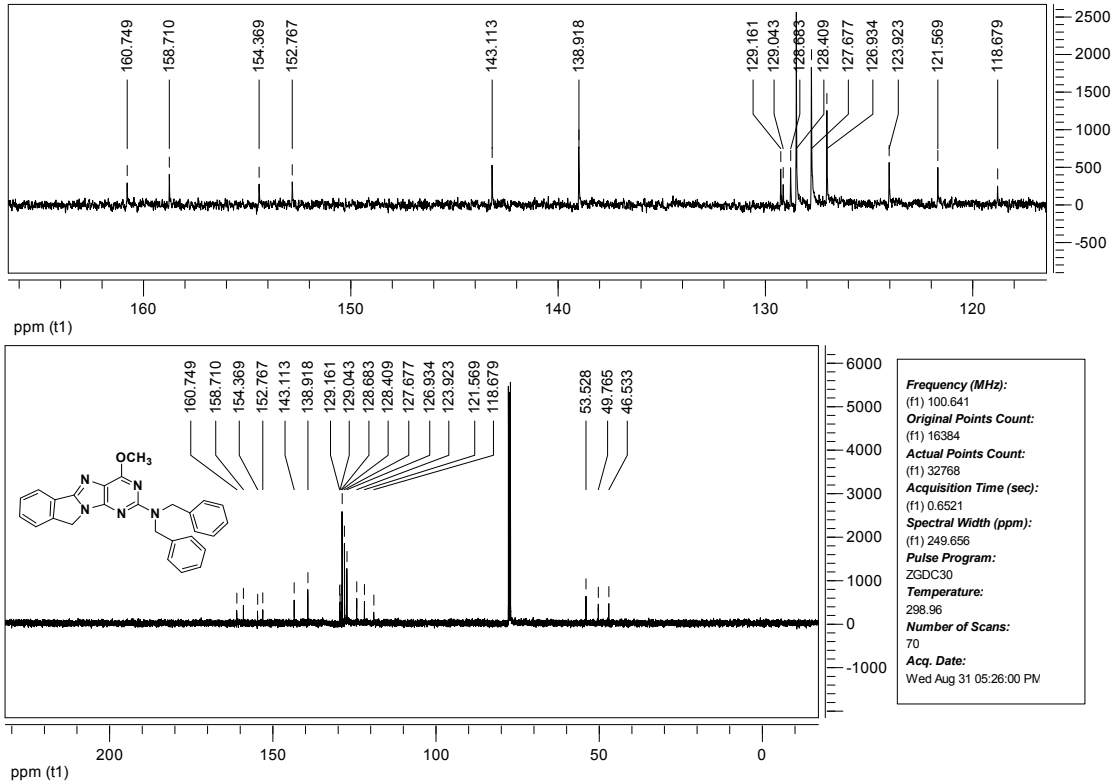
^{13}C NMR Spectrum for 2h



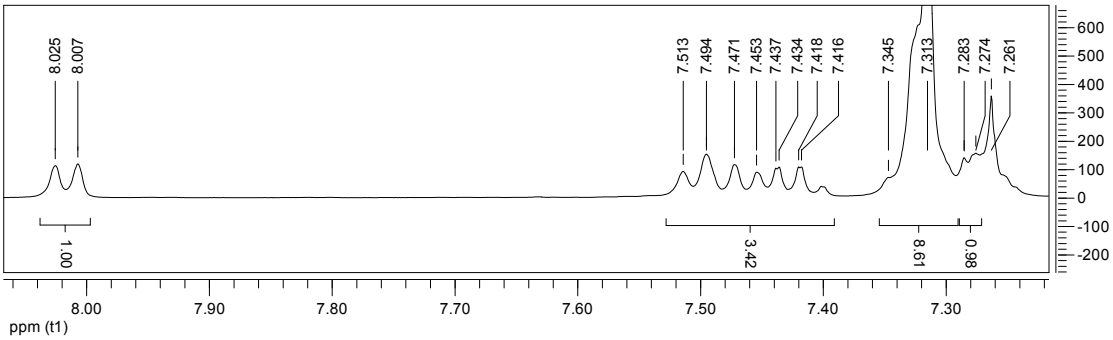
^{1}H NMR Spectrum for 2i

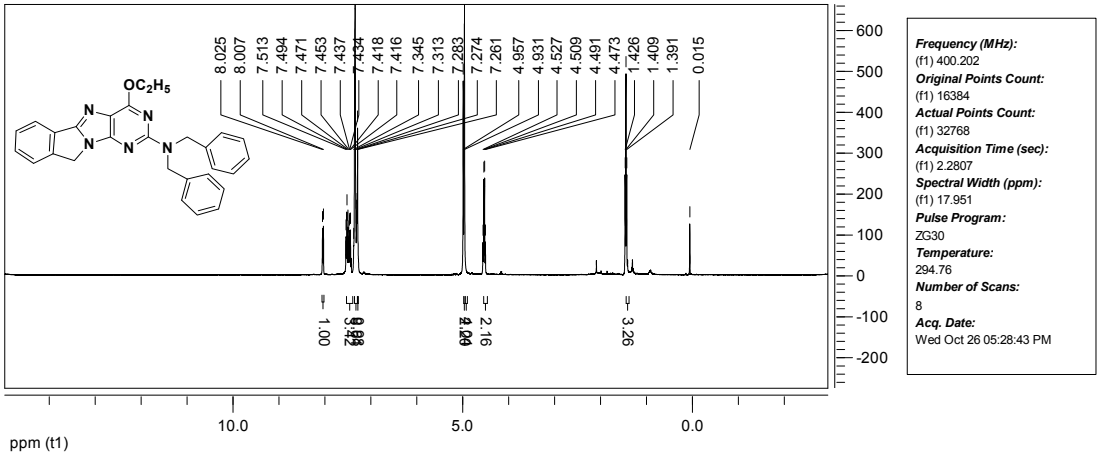


^{13}C NMR Spectrum for 2i

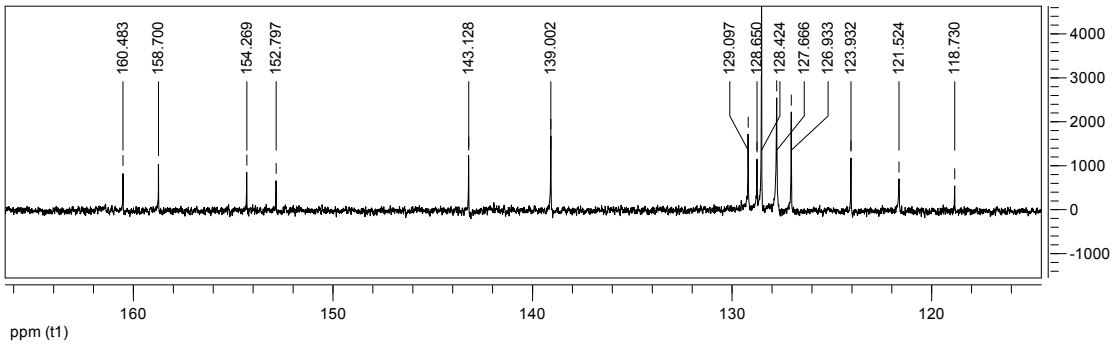


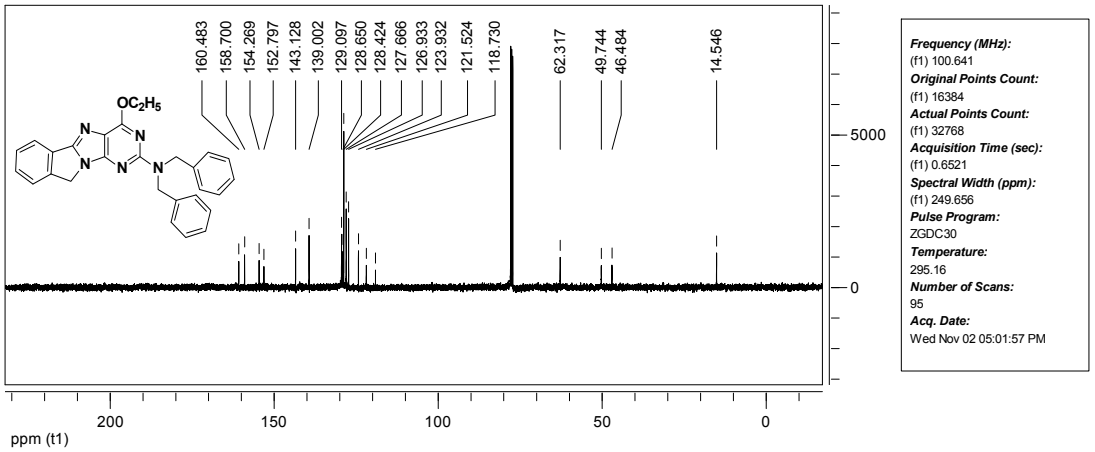
^{1}H NMR Spectrum for 2j



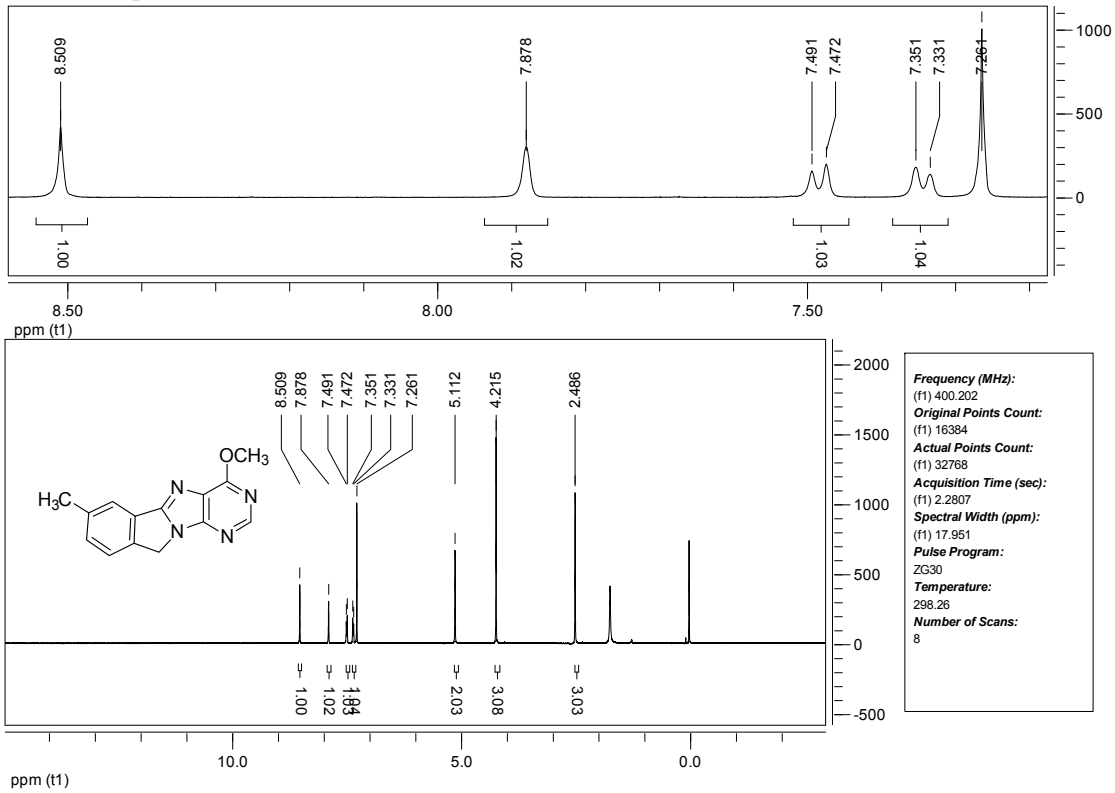


^{13}C NMR Spectrum for 2j

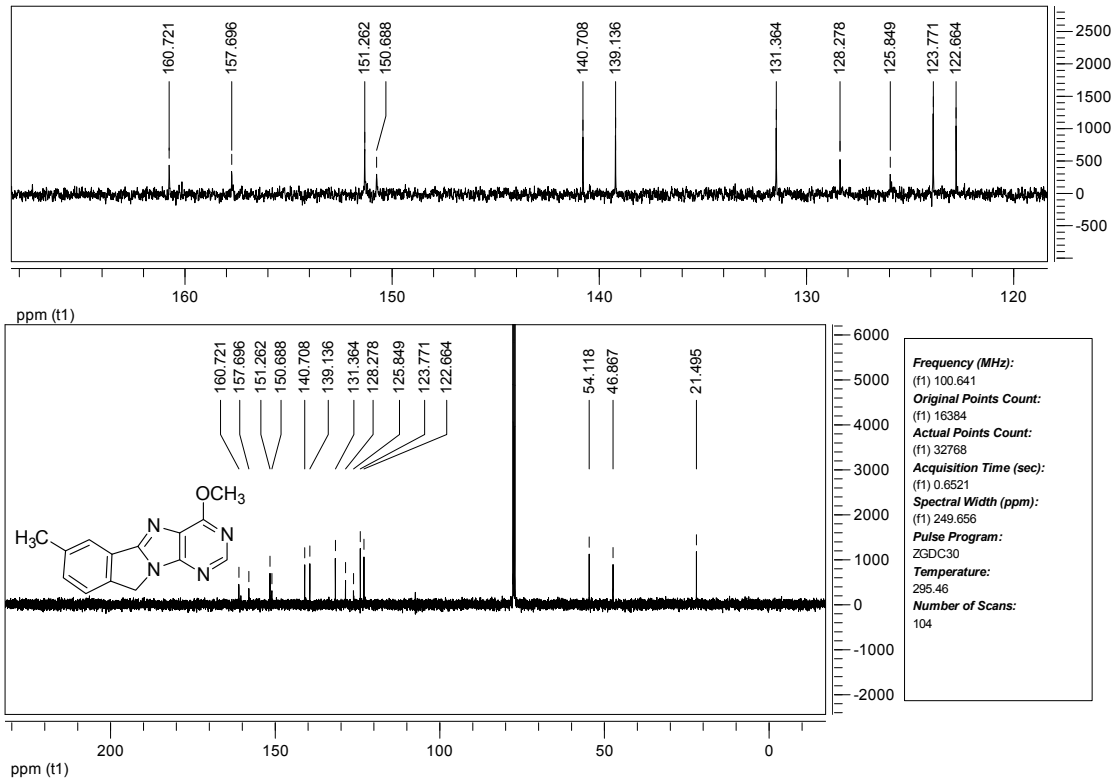




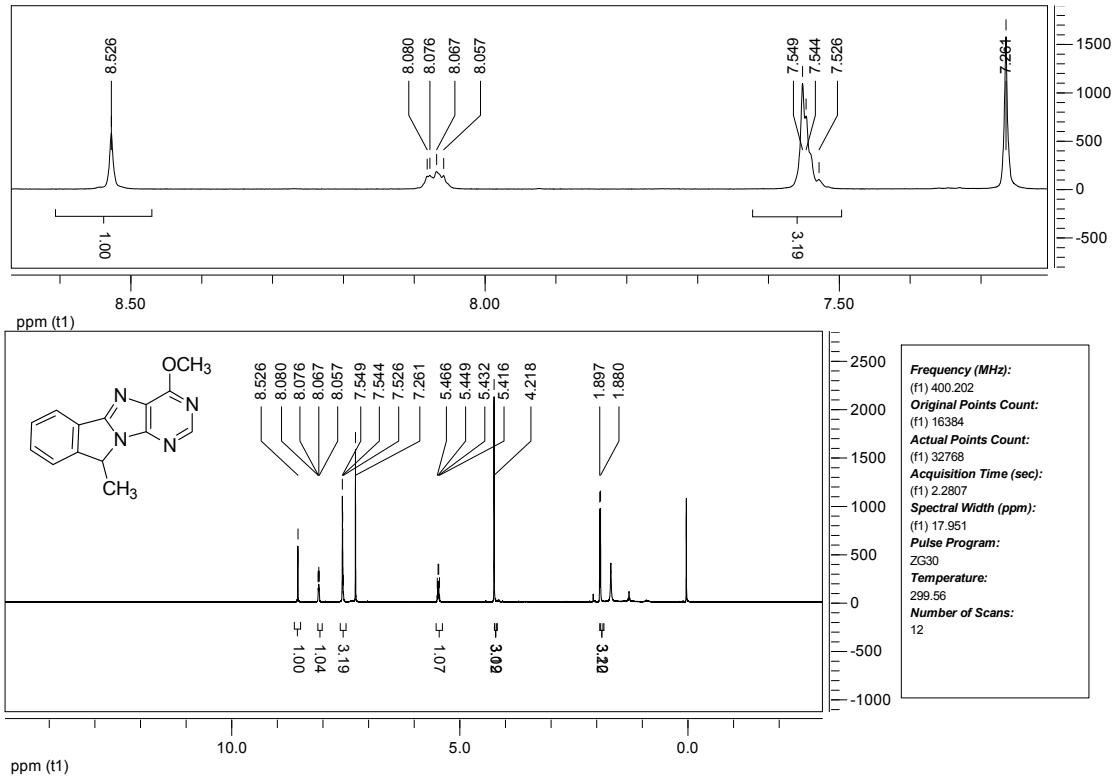
^{1}H NMR Spectrum for 2k



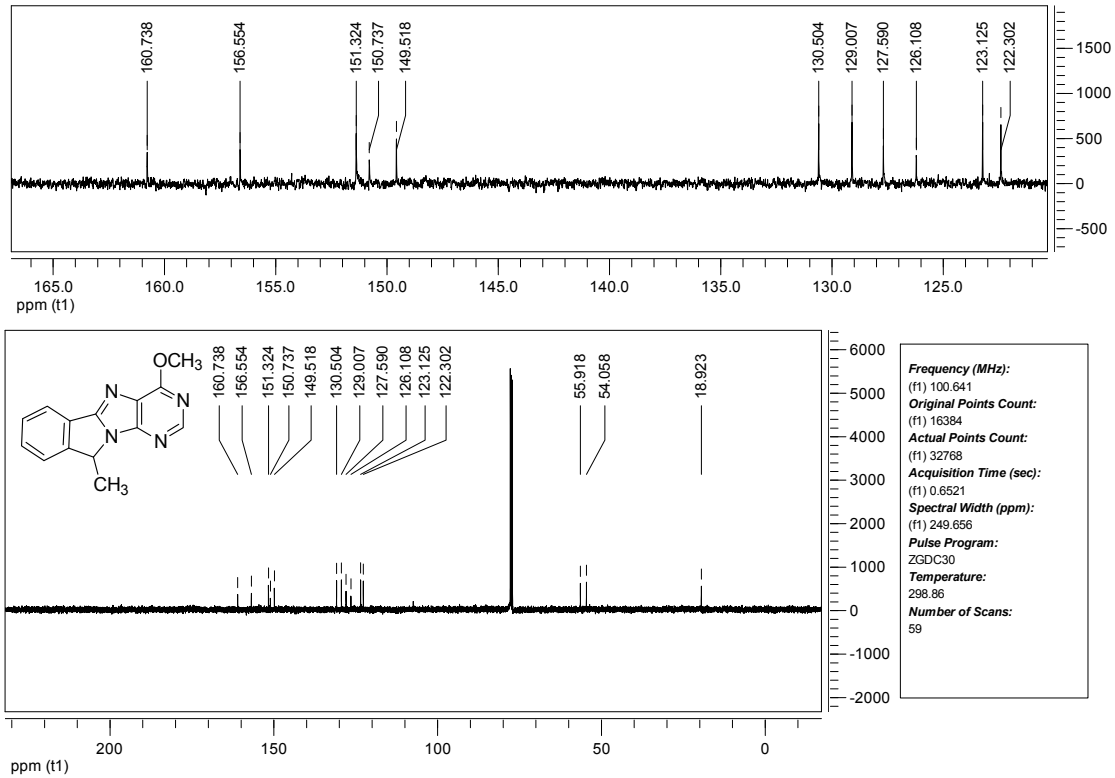
^{13}C NMR Spectrum for 2k



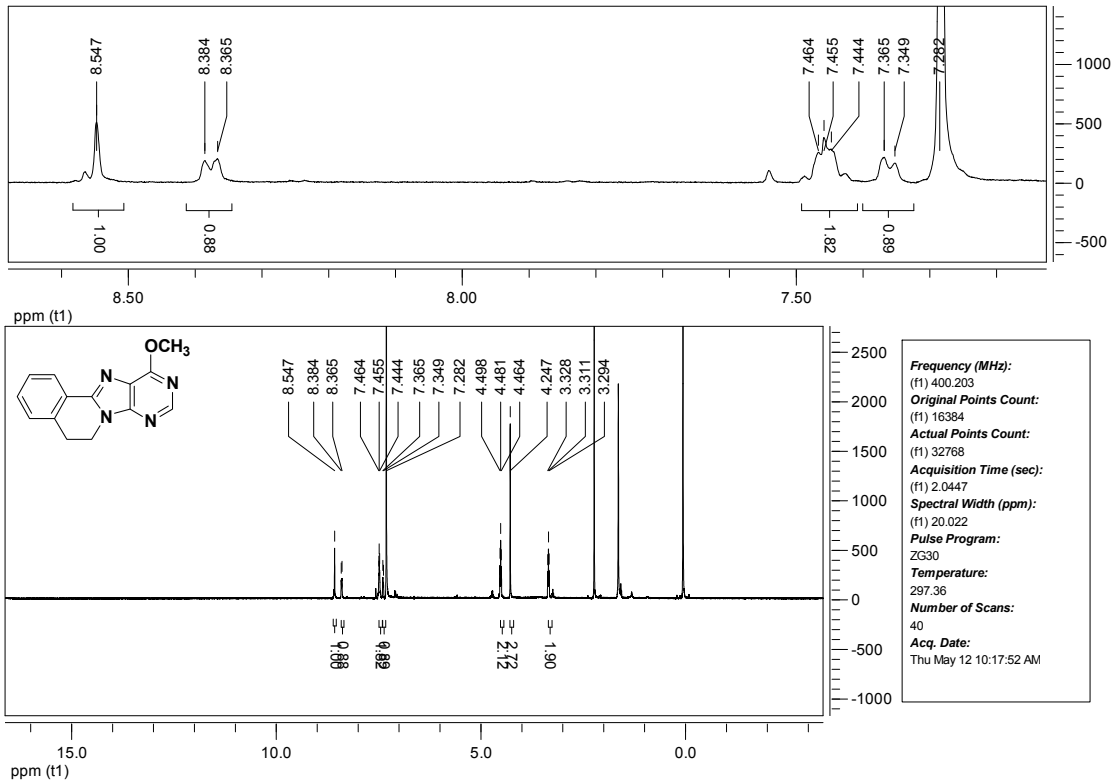
^{1}H NMR Spectrum for 2l



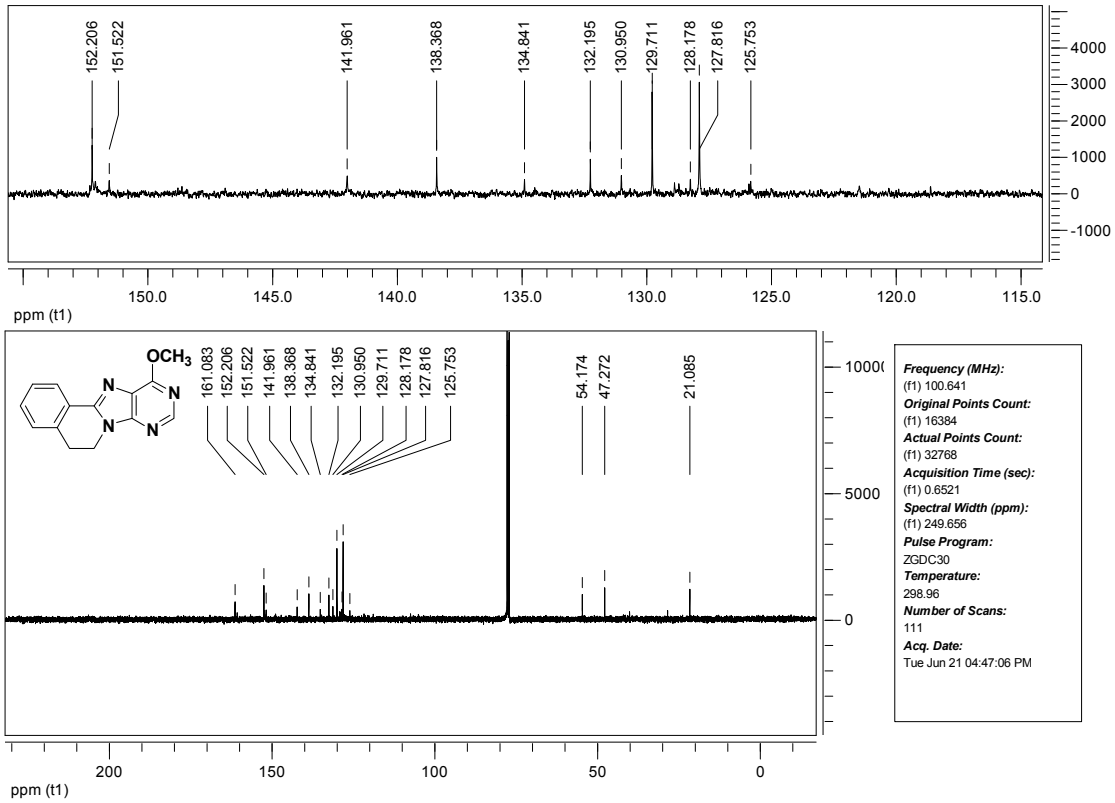
^{13}C NMR Spectrum for 2l



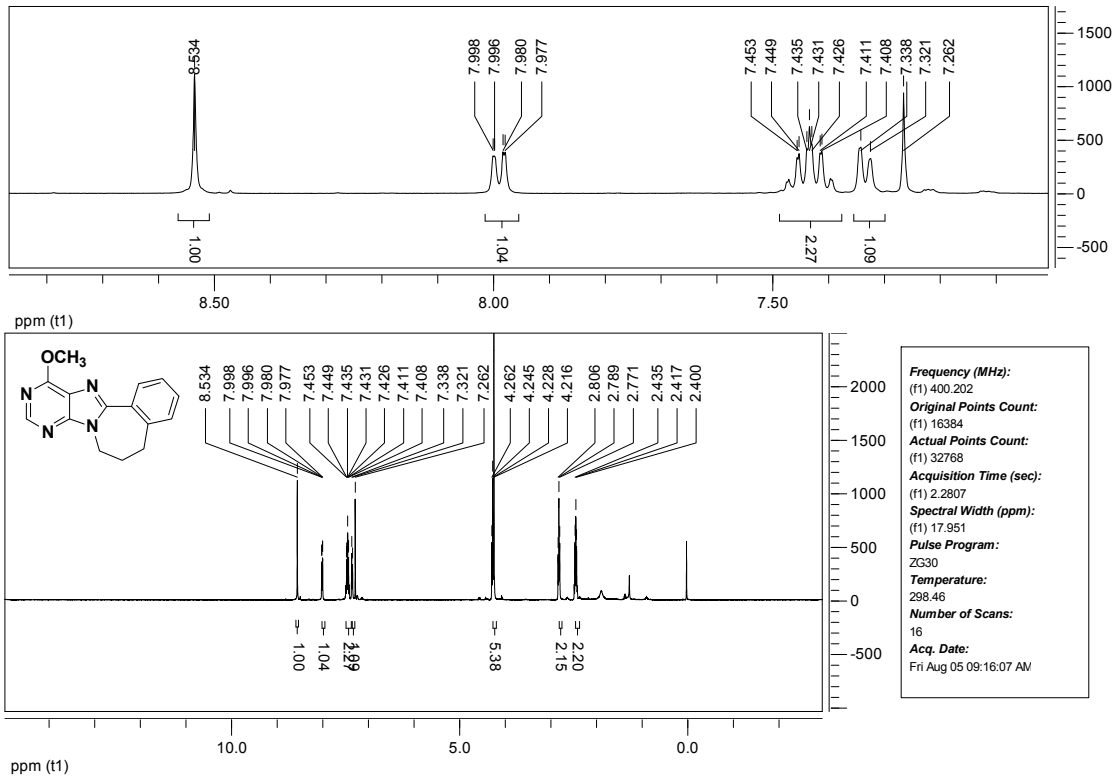
^{1}H NMR Spectrum for 2m



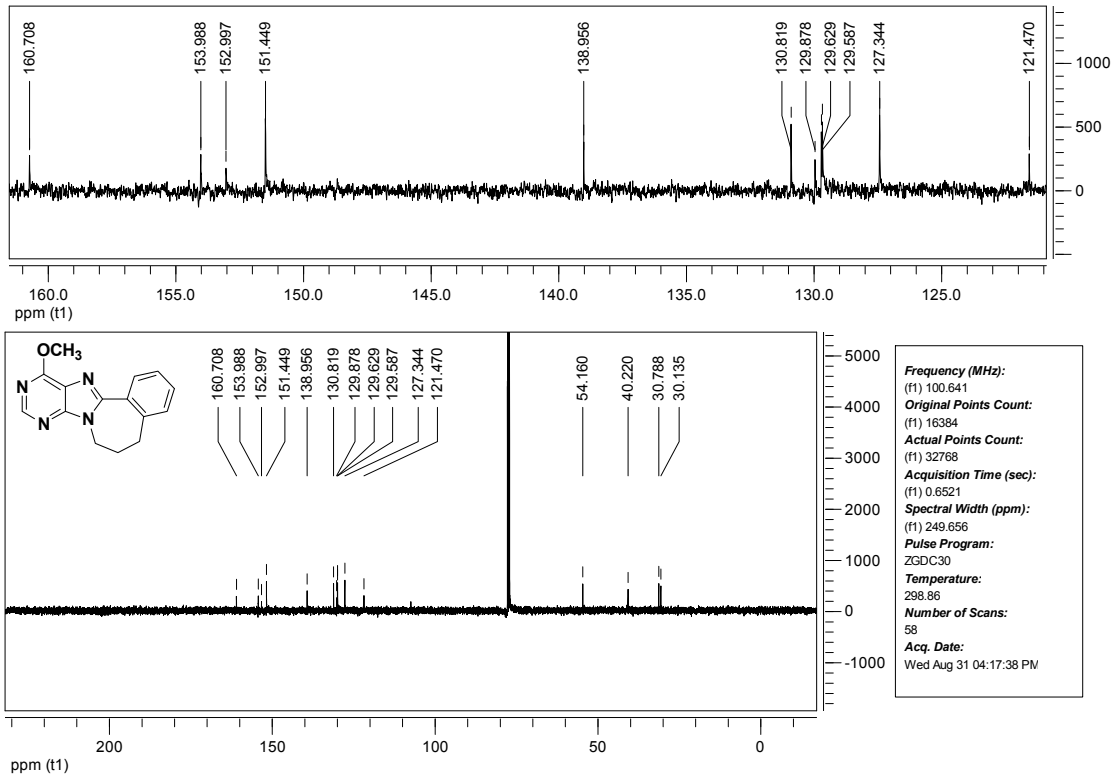
^{13}C NMR Spectrum for 2m



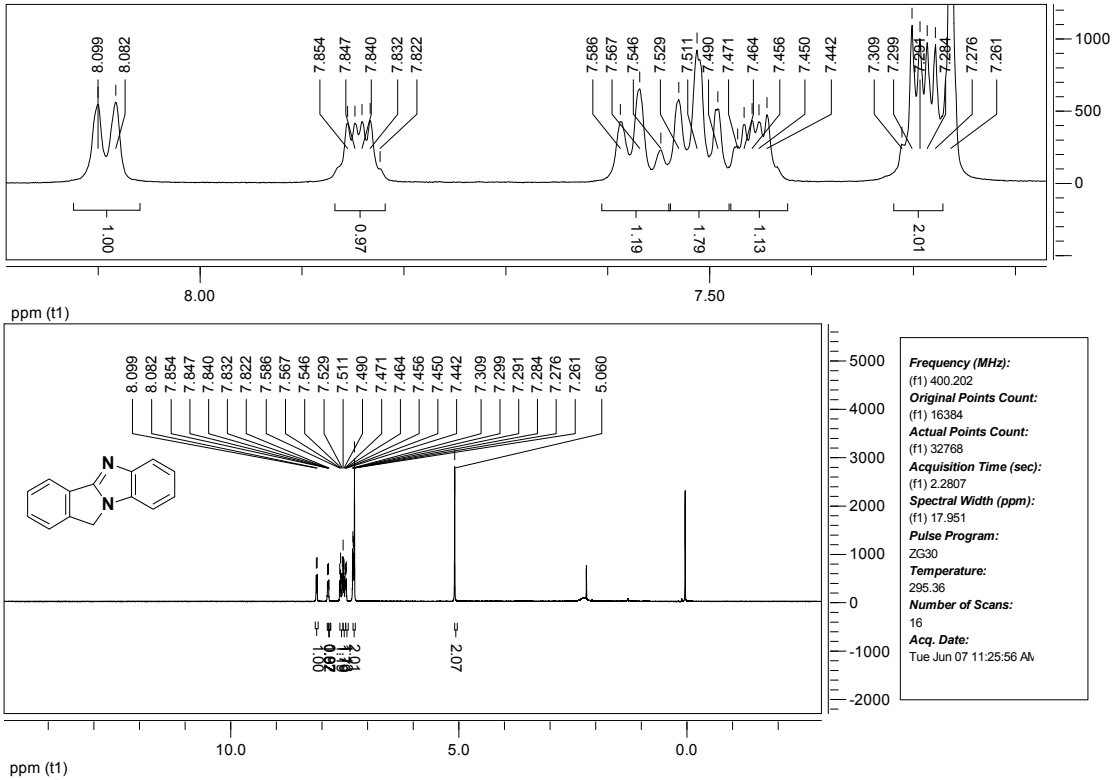
^{1}H NMR Spectrum for 2n



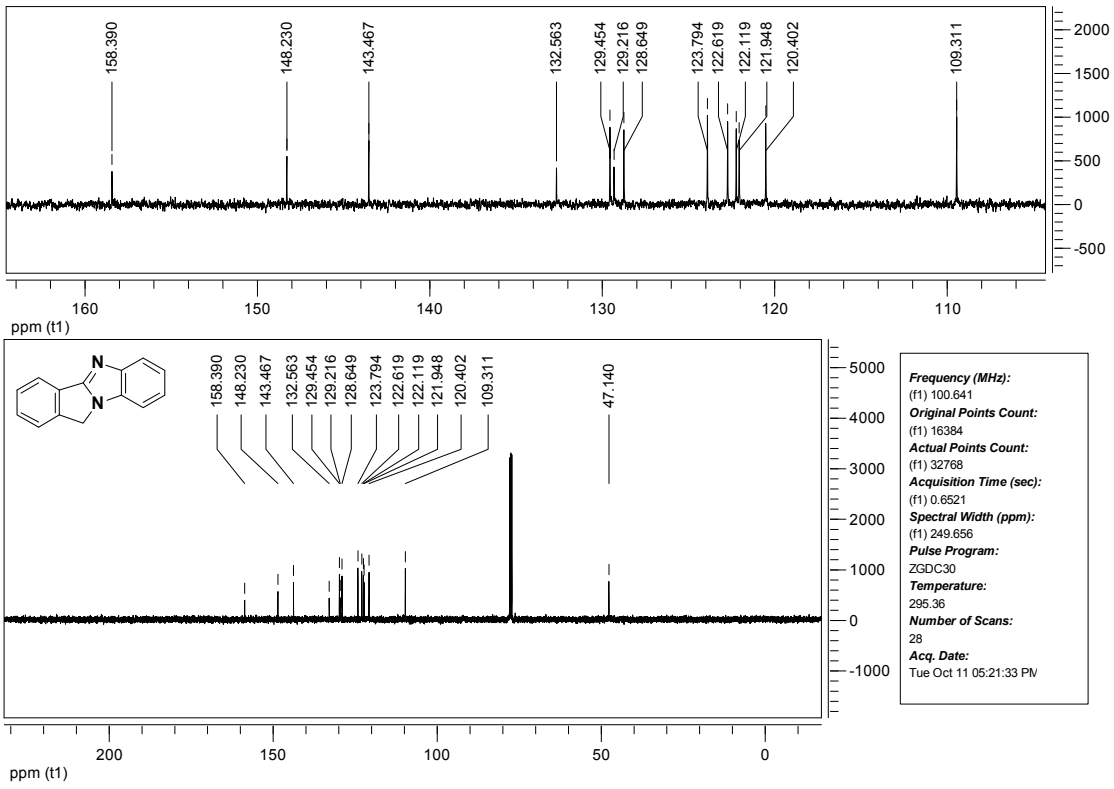
^{13}C NMR Spectrum for 2n



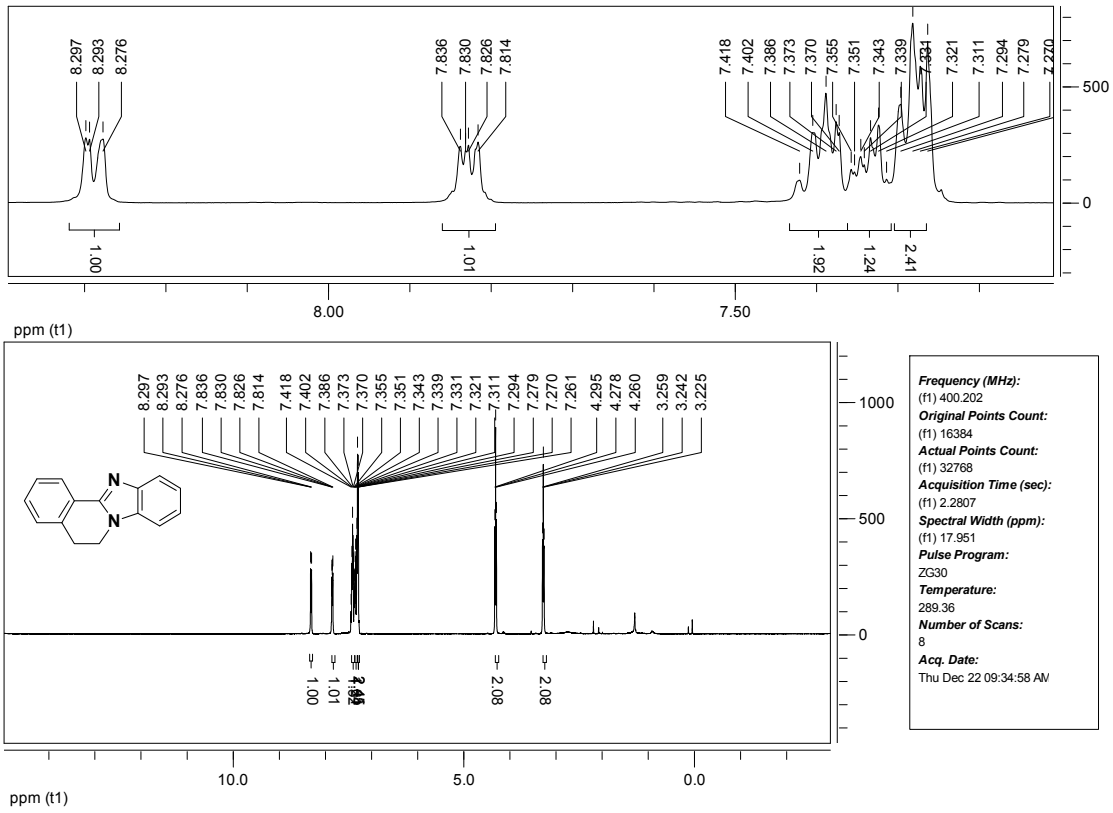
^{1}H NMR Spectrum for 4a



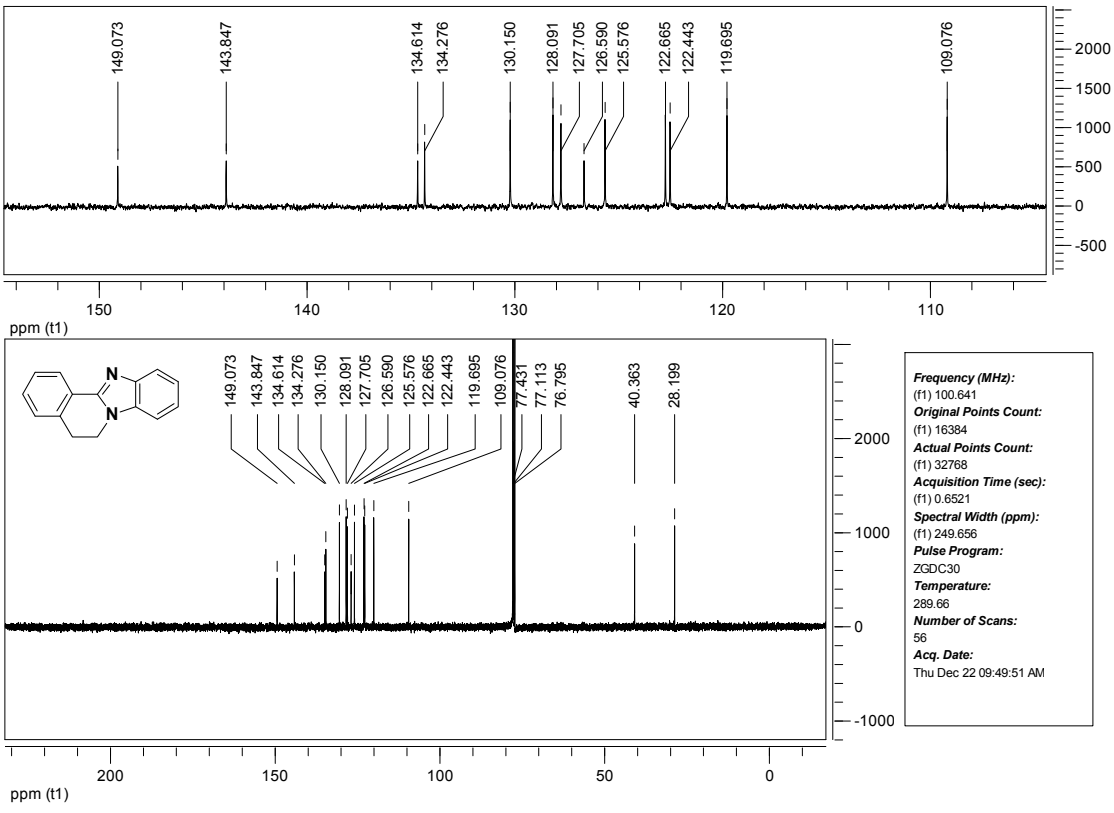
^{13}C NMR Spectrum for 4a



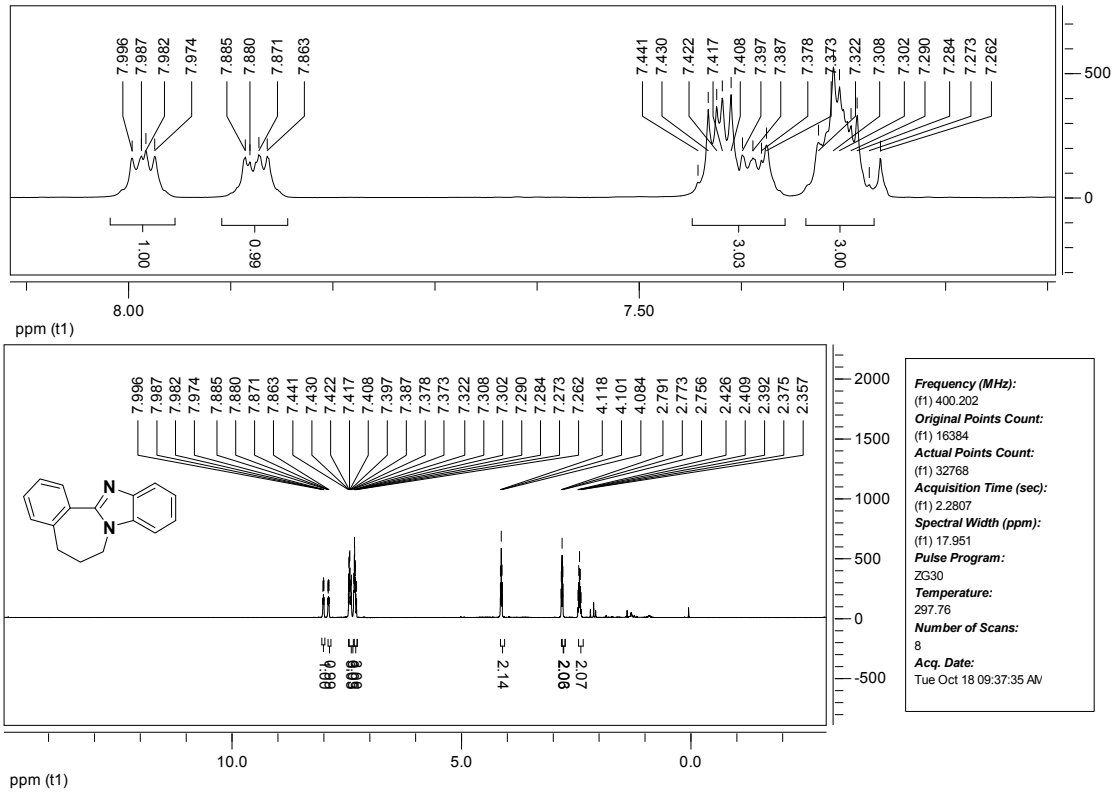
^{1}H NMR Spectrum for 4b



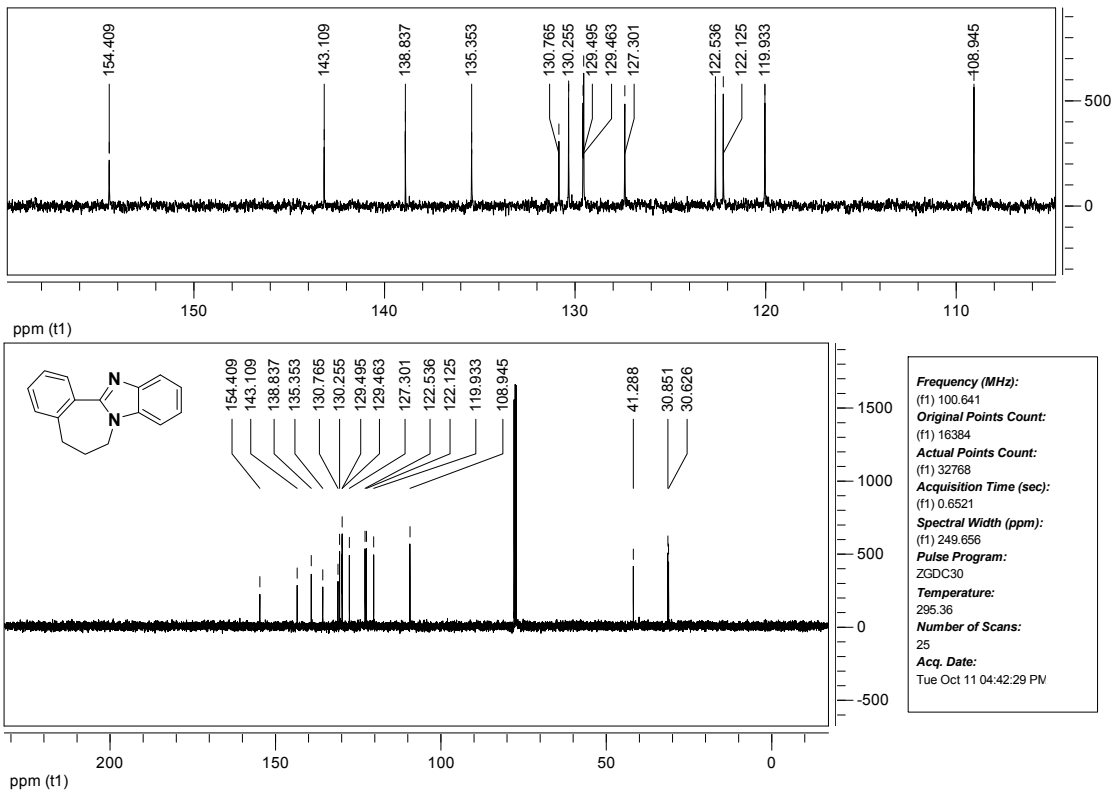
^{13}C NMR Spectrum for 4b



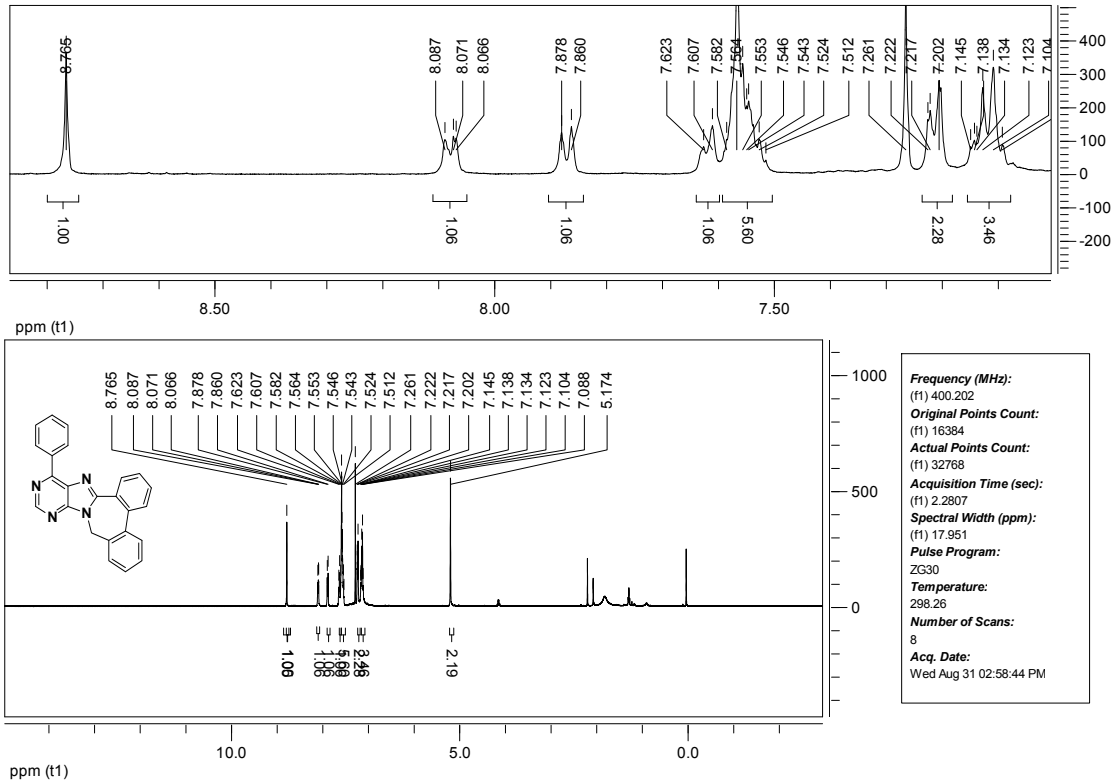
^{1}H NMR Spectrum for 4c



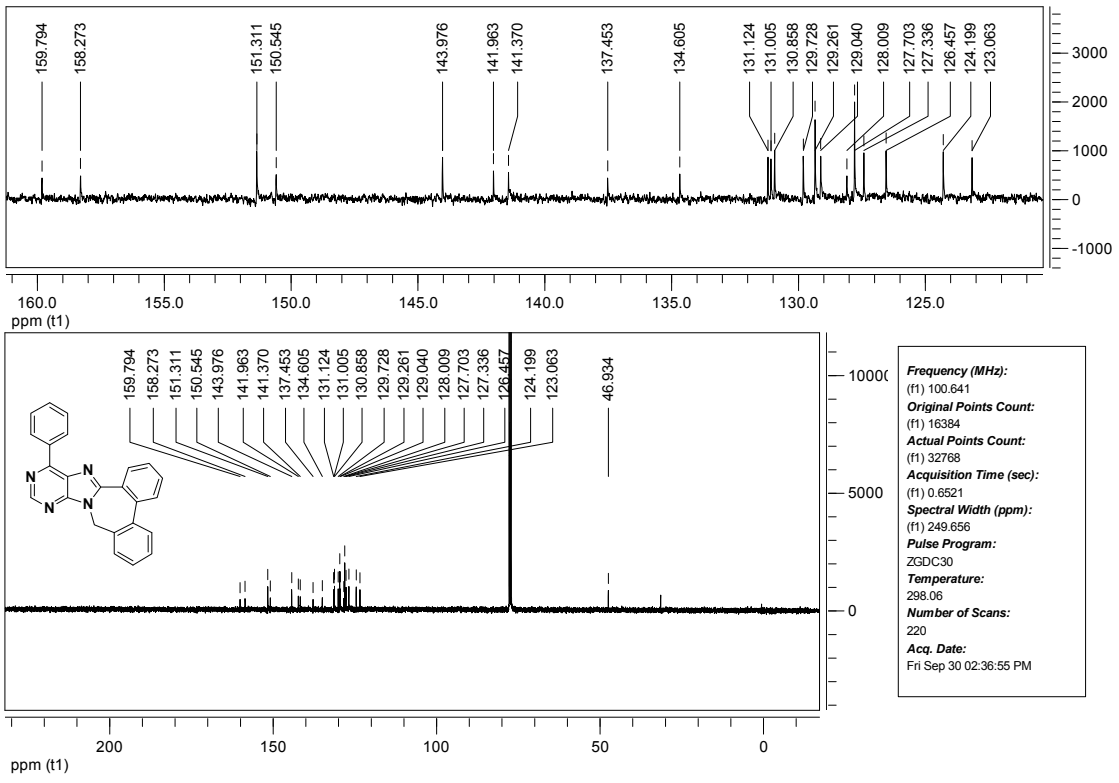
^{13}C NMR Spectrum for 4c



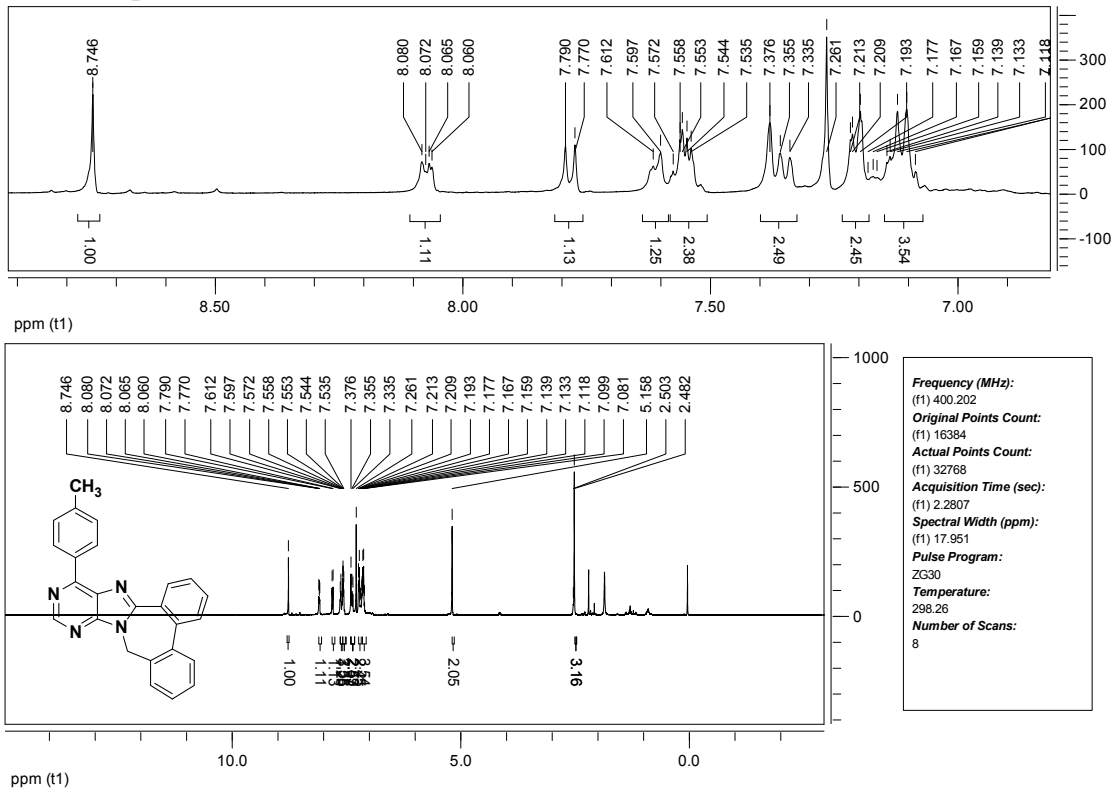
^{1}H NMR Spectrum for 6a



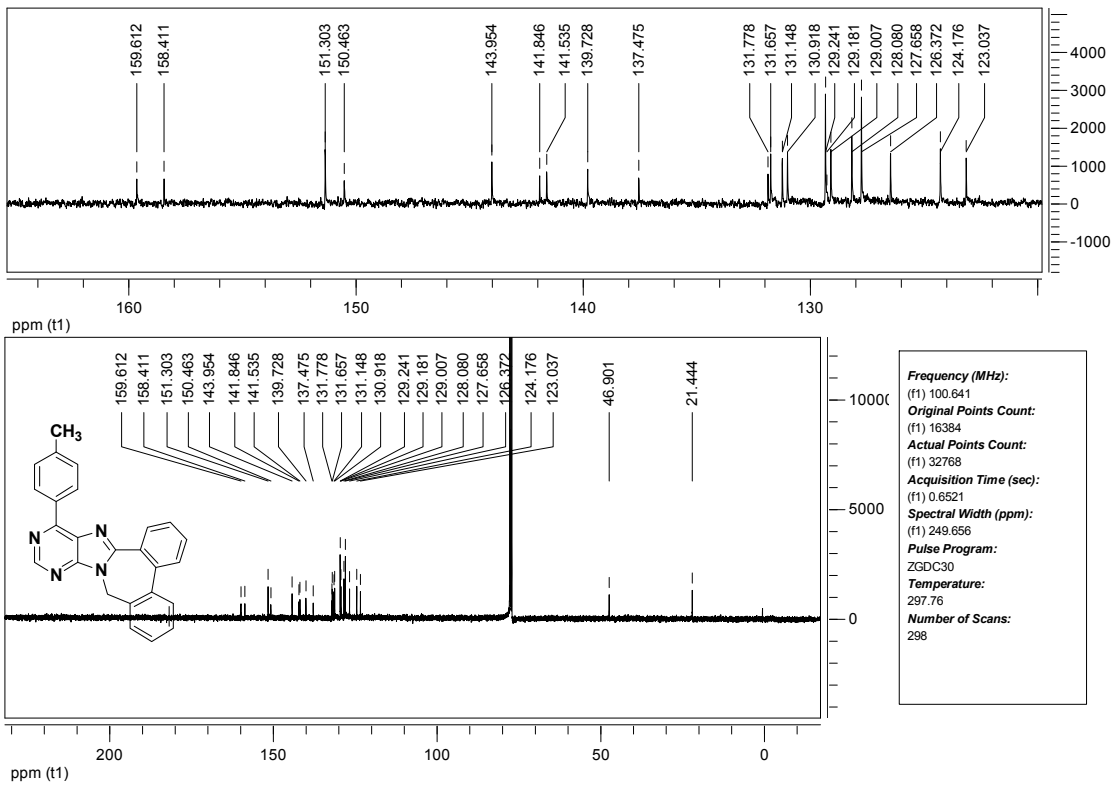
^{13}C NMR Spectrum for 6a



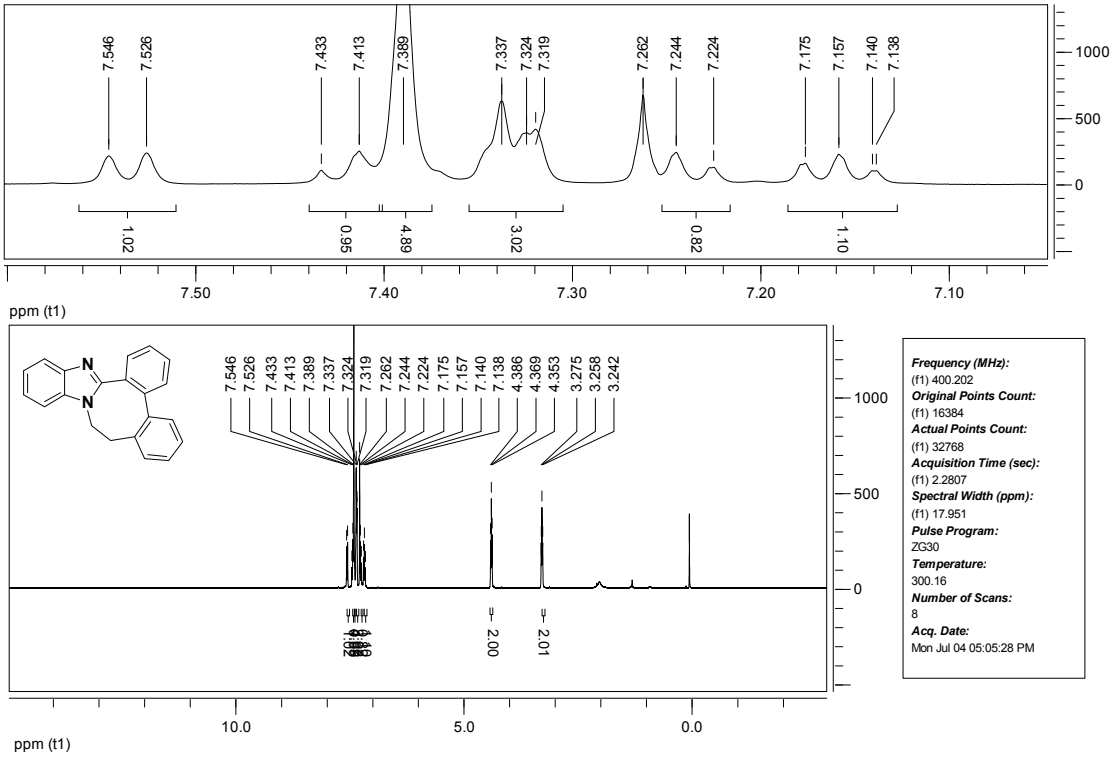
^{1}H NMR Spectrum for 6b



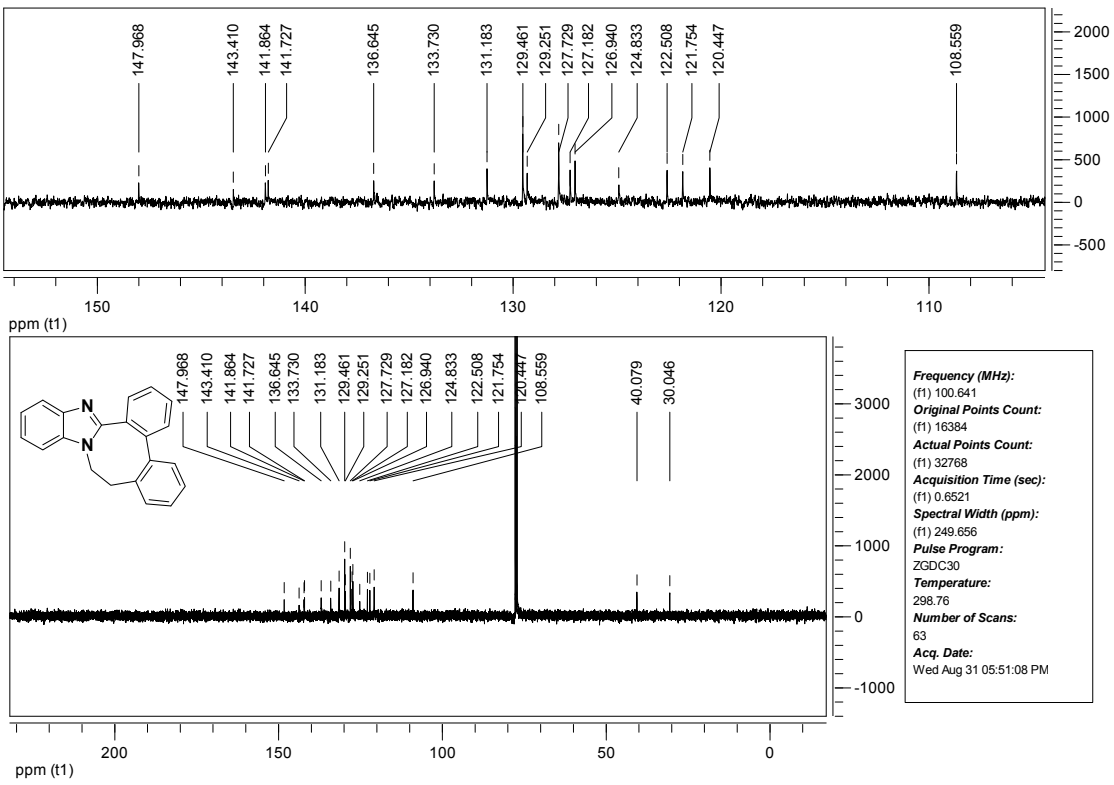
^{13}C NMR Spectrum for 6b



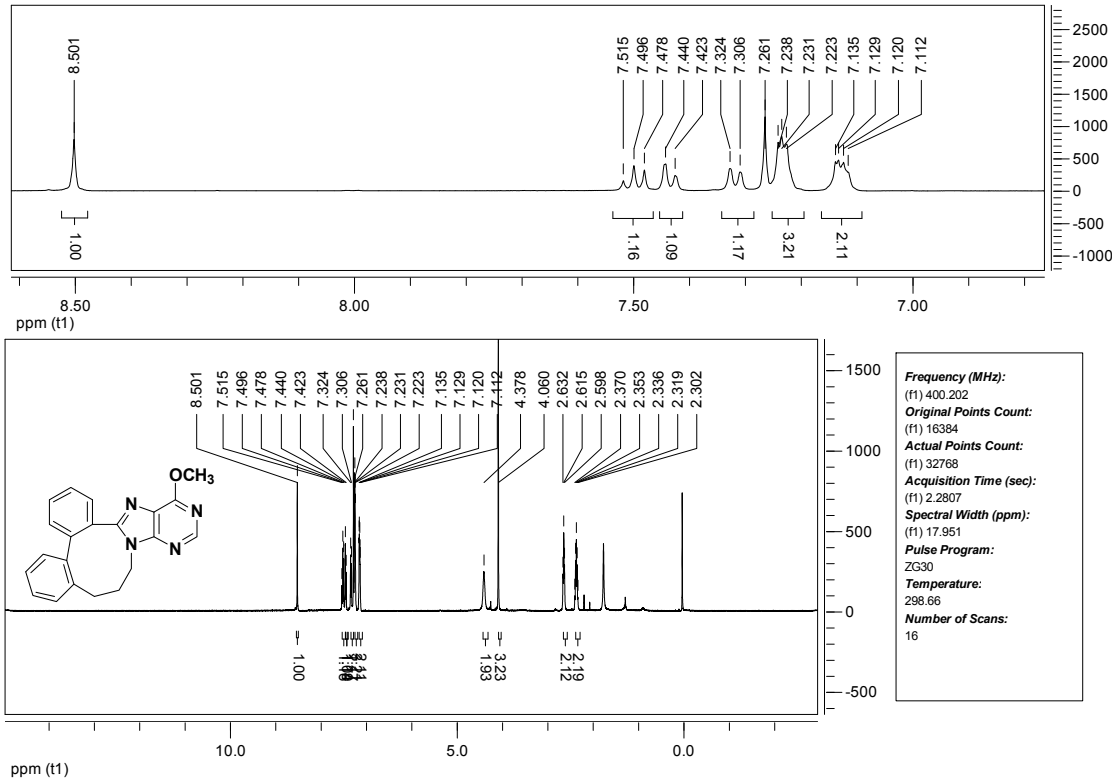
^{1}H NMR Spectrum for 6c



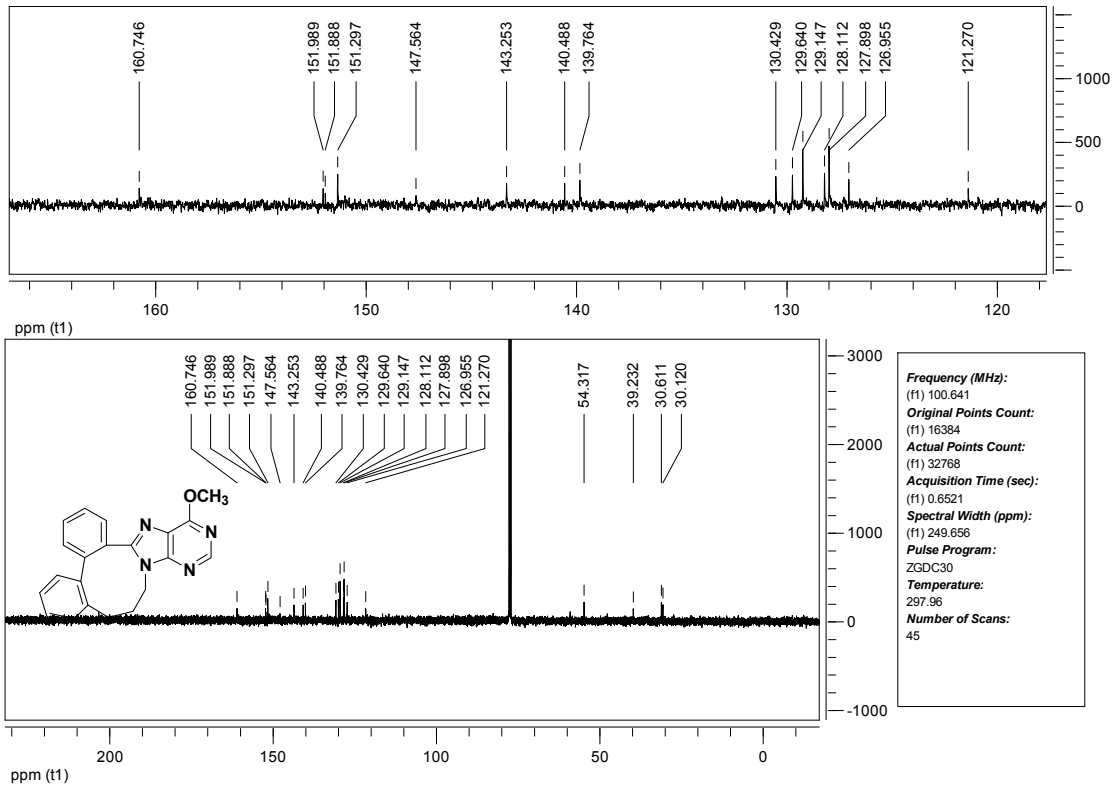
^{13}C NMR Spectrum for 6c



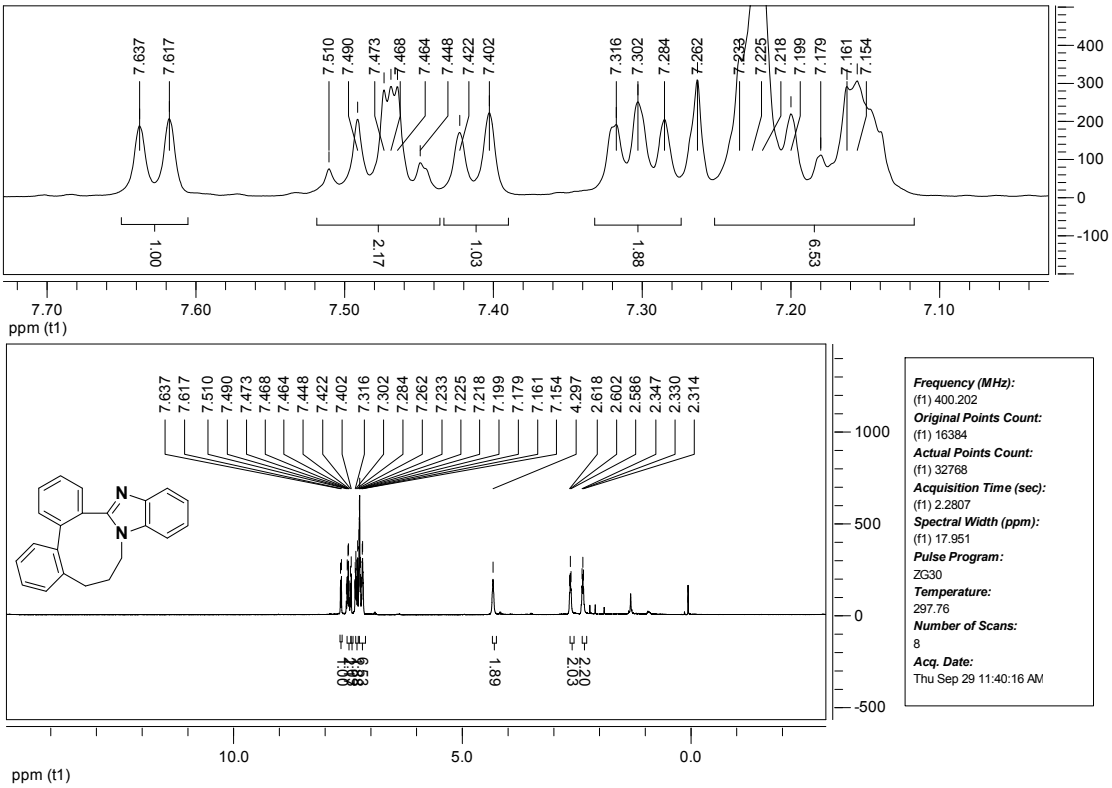
^{1}H NMR Spectrum for 6d



^{13}C NMR Spectrum for 6d



^{1}H NMR Spectrum for 6e



^{13}C NMR Spectrum for 6e