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Tetramethylguanidiniumchlorosulfonate ionic liquid (TMG IL): An efficient reusable catalyst for the synthesis of tetrahydro-1*H*-benzo[*a*]chromeno[2,3-*c*]phenazin-1-ones under solvent-free conditions and evaluation for their *in vitro* bioassay

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Supporting Information

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Synthesis of 16-(4-ethoxyphenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4a).

A mixture of benzo[a]phenazin-5-ol (1, 1mmol), 4-ethoxybenzaldehyde (2a, 1mmol), and 5,5-dimethylcyclohexane-1,3-dione (3a, 1mmol), was taken in TMG IL (5% mol) and stirred at 60 °C for 45 min. After completion of the reaction (monitored by thin layer chromatography (TLC)), the product was extracted with 20 mL of ethyl acetate (EA). The solvent was evaporated under reduced pressure, and the obtained solid was washed with hexane and recrystallized from ethanol to afford the product. The insoluble IL was separated by simple filtration, washed twice with EA, and then dried under vacuum before reuse.

16-(4-ethoxyphenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4a). Yield 95%; yellow powder; mp 223-225 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.26 (dd, *J* = 2.0, 8.1 Hz, 1H), 8.29 (dd, *J* = 2.1, 8.0 Hz, 1H), 8.21-8.17 (m, 2H), 7.79-7.70 (m, 4H), 7.48 (d, *J* = 8.0 Hz, 2H), 6.67 (d, *J* = 8.0 Hz, 2H), 6.04 (s, 1H), 3.87-3.82 (q, 2H), 2.78 and 2.73 (AB System, *J* = 16.4 Hz, 2H), 2.39 and 2.32 (AB System, *J* = 16.4 Hz, 2H), 1.25 (t, *J* = 6.9 Hz, 3H), 1.19 (s, 3H), 1.14 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.0, 163.4, 157.4, 147.0, 142.7, 142.1, 140.5, 140.4, 137.2, 130.5, 130.2, 130.0, 129.8, 129.5, 129.1, 128.5, 126.8, 125.7, 122.1, 116.6, 115.4, 113.9, 63.2, 51.1, 41.4, 32.8, 32.6, 29.6, 27.5, 14.9 ppm. HRMS (ESI, m/z): calcd for $C_{33}H_{28}N_2O_3$ ($M+H^+$) 500.210; found: 500.202.

16-(2,5-dimethylphenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4b). Yield 90%; yellow powder; mp 286-288 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.21 (d, *J* = 8.0 Hz, 1H), 8.29 (d, *J* = 8.0 Hz, 1H), 8.14-8.11 (m, 2H), 7.80-7.69 (m, 4H), 6.695 (d, *J* = 6.9 Hz, 1H), 6.78 (s, 1H), 6.68 (d, *J* = 6.9 Hz, 1H), 5.88 (s, 1H), 3.24 (s, 3H), 2.74 (s, 2H), 2.38 and 2.28 (AB System, *J* = 16.4 Hz, 2H), 1.99 (s, 3H), 1.20 (s, 3H), 1.06 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.1, 163.1, 147.0, 144.0, 142.7, 142.1, 141.1, 140.7, 134.8, 134.6, 130.8, 130.0, 129.9, 129.8, 129.5, 129.3, 128.3, 127.1, 126.7, 125.5, 122.0, 117.8, 116.4, 51.2, 41.5, 32.6, 30.2, 29.6, 27.3, 21.3, 20.3 ppm. HRMS (ESI, m/z): calcd for $C_{33}H_{28}N_2O_2$ ($M+H^+$) 484.215; found: 484.211.

16-(benzo[d][1,3]dioxol-5-yl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4c). Yield 88%; yellow powder; mp 230-232 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.34-9.32 (m, 1H), 8.36-8.34 (m, 1H), 8.26-8.23 (m, 2H), 7.83-7.73 (m, 4H), 7.14 (d, *J* = 6.9 Hz, 1H), 7.04-7.02 (m, 1H), 6.69 (d, *J* = 6.9 Hz, 1H), 6.05 (s, 1H), 5.78 (dd, *J* = 1.4, 10.6 Hz, 2H), 2.82 and 2.74 (AB System, *J* = 16.4 Hz, 2H), 2.40 and 2.34 (AB System, *J* = 16.4 Hz, 2H), 1.20 (s, 3H), 1.14 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.1, 163.6, 147.2, 146.9, 145.9, 142.7, 142.0, 141.0, 140.9, 139.2, 131.0, 130.0, 129.6, 129.5, 128.5, 126.5, 125.6, 122.2, 122.0, 116.4, 115.3, 110.0, 107.8, 100.8, 51.1, 41.4, 33.3, 32.6, 29.6, 27.7 ppm. HRMS (ESI, m/z): calcd for $C_{32}H_{24}N_2O_4$ ($M+H^+$) 500.174; found: 500.170.

3,3-dimethyl-16-(o-tolyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4d). Yield 90%; yellow powder; mp 248-250 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.30 (dd, *J* = 2.0, 8.0 Hz, 1H), 8.35 (dd, *J* = 2.2, 7.6 Hz, 1H), 8.24-8.20 (m, 2H), 7.83-7.73 (m, 4H), 7.43 (s, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.03 (t, *J* = 6.9 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.09 (s, 1H), 2.82 and 2.75 (AB System, *J* = 16.4 Hz, 2H), 2.39 and 2.33 (AB System, *J* = 16.4 Hz, 2H), 2.22 (s, 3H), 1.19 (s, 3H), 1.13 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.1, 163.1, 147.0, 144.3, 142.6, 142.0, 141.0, 137.6, 130.8, 130.1, 129.9, 129.8, 129.5, 129.4, 128.5, 128.3, 126.6, 126.2, 125.6, 122.0, 117.8, 116.3, 51.1, 41.4, 32.5, 30.1, 29.6, 27.3, 20.7 ppm. HRMS (ESI, m/z): calcd for $C_{32}H_{26}N_2O_2$ ($M+H^+$) 470.199; found: 470.192.

16-(3-bromophenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4e). Yield 90%; yellow powder; mp 239-241 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.32-9.30 (m, 1H), 8.39-8.33 (m, 2H), 8.24-8.21 (m, 1H), 7.83-7.76 (m, 4H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.30 (s, 1H), 7.06-7.01 (m, 1H), 6.86-6.82 (m, 1H), 6.22 (s, 1H), 2.77 (s, 2H), 2.40 and 2.34 (AB System, *J* = 16.4 Hz, 2H), 1.20 (s, 3H), 1.10 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.0, 163.4, 148.0, 142.9, 142.1, 140.5, 140.3, 133.3, 130.2, 130.0, 129.9, 129.7,

129.1, 128.7, 127.7, 126.9, 126.6, 125.7, 122.2, 115.8, 51.1, 41.6, 35.1, 32.4, 29.5, 27.6 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{23}BrN_2O_2$ ($M+H^+$) 535.431; found: 535.425.

16-(2-bromophenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4f). Yield 91%; yellow powder; mp 247-249 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.31 (dd, *J* = 1.8, 7.2 Hz, 1H), 8.38-8.33 (m, 1H), 8.25-8.19 (m, 2H), 7.83-7.77 (m, 4H), 7.72-7.71 (m, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.15-7.13 (m, 1H), 7.05-6.99 (m, 1H), 6.05 (s, 1H), 2.83 and 2.76 (AB System, *J* = 16.4 Hz, 2H), 2.40 and 2.34 (AB System, *J* = 16.4 Hz, 2H), 1.20 (s, 3H), 1.14 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 196.8, 163.9, 147.3, 147.0, 142.6, 141.7, 141.0, 140.9, 132.3, 131.3, 131.1, 130.1, 130.4, 129.7, 129.5, 128.6, 128.1, 126.4, 125.6, 122.1, 115.6, 114.6, 51.0, 41.4, 33.7, 32.6, 29.6, 27.6 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{23}BrN_2O_2$ ($M+H^+$) 534.094; found: 534.098.

16-(3-hydroxyphenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4g). Yield 89%; yellow powder; mp 209-211 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.24 (dd, *J* = 2.1, 8.1 Hz, 1H), 8.30 (dd, *J* = 2.0, 8.6 Hz, 1H), 8.17-8.14 (m, 2H), 7.84-7.69 (m, 4H), 7.07-7.02 (m, 2H), 6.88-6.83 (m, 2H), 5.97 (s, 1H), 2.75 (s, 2H), 2.38 and 2.28 (AB System, *J* = 16.2 Hz, 2H), 1.19 (s, 3H), 1.05 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.1, 164.1, 152.7, 146.9, 142.5, 142.0, 141.5, 140.4, 130.9, 130.1, 129.7, 129.6, 129.1, 128.5, 126.6, 125.6, 122.0, 116.4, 114.9, 106.5, 51.0, 41.4, 33.7, 32.5, 29.9, 27.3 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{24}N_2O_3$ ($M+H^+$) 472.179; found: 472.172.

16-(3-methoxyphenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4h). Yield 91%; yellow powder; mp 222-224 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.33 (dd, *J* = 2.1, 8.1 Hz, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 8.22-8.18 (m, 2H), 7.89-7.71 (m, 5H), 7.04-7.00 (m, 1H), 6.91-6.85 (m, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 6.19 (s, 1H), 3.69 (s, 3H), 2.77 and 2.72 (AB System, *J* = 16.4 Hz, 2H), 2.37 and 2.28 (AB System, *J* = 16.2 Hz, 2H), 1.19 (s, 3H), 1.08 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 196.7, 163.8, 159.3, 146.6, 140.8, 130.0, 129.7, 129.5, 128.8, 128.5, 126.6, 125.8, 122.1, 121.5, 115.3, 111.8, 52.2, 51.1, 41.4, 33.7, 32.6, 29.6, 27.6 ppm. HRMS (ESI, m/z): calcd for $C_{32}H_{26}N_2O_3$ ($M+H^+$) 486.194; found: 486.190.

4-(3,3-dimethyl-1-oxo-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-16-yl)benzonitrile (4i). Yield 89%; yellow powder; mp 236-238 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.31 (d, *J* = 5.8 Hz, 1H), 8.34-8.14 (m, 3H), 7.82-7.79 (m, 4H), 7.79 (d, *J* = 6.9 Hz, 2H), 7.44 (d, *J* = 6.9 Hz, 2H), 6.08 (s, 1H), 2.83 (s, 2H), 2.41 and 2.32 (AB System, *J* = 16.4 Hz, 2H), 1.21 (s, 3H), 1.09 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.0, 164.0, 150.6, 147.2, 141.5, 140.9, 131.8, 130.3, 130.2, 130.0, 129.5, 129.2, 128.8, 125.6, 122.1, 114.8, 114.0, 110.1, 50.9, 41.3, 34.3, 32.6, 29.6, 27.4 ppm. HRMS (ESI, m/z): calcd for $C_{32}H_{23}N_3O_2$ ($M+H^+$) 481.179; found: 481.173.

16-(4-fluorophenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4j). Yield 92%; yellow powder; mp 232-234 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.41 (dd, *J* = 2.0, 8.1 Hz, 1H), 8.40-8.36 (m, 2H), 8.27-8.23 (m, 1H), 7.90-7.82 (m, 4H), 7.56-7.52 (m, 2H), 6.85-6.81 (m, 2H), 6.10 (s, 1H), 2.82 and 2.77 (AB System, *J* = 16.4 Hz, 2H), 2.43 and 2.37 (AB System, *J* = 16.4 Hz, 2H), 1.21 (s, 3H), 1.12 (s, 3H) ppm. ^{13}C-

NMR (100 MHz, $CDCl_3$): 197.0, 163.6, 162.4 (d, *J* = 241.2 Hz), 147.3, 142.7, 142.0, 139.7, 130.6, 130.5, 129.4, 128.9, 128.7, 126.8, 126.4, 126.0, 122.3, 116.0, 114.9, 114.7, 51.0, 41.4, 33.1, 32.6, 29.6, 27.5 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{23}FN_2O_2$ ($M+H^+$) 474.174; found: 474.168.

16-(2-methoxyphenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4k). Yield 93%; yellow powder; mp 280-282 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.37 (d, *J* = 7.3 Hz, 1H), 8.36 (d, *J* = 8.0 Hz, 1H), 8.27 (t, *J* = 7.2 Hz, 2H), 7.85-7.81 (m, 5H), 7.16 (d, *J* = 6.9 Hz, 1H), 7.06 (t, *J* = 6.9 Hz, 1H), 6.56 (d, *J* = 7.3 Hz, 1H), 6.14 (s, 1H), 3.73 (s, 3H), 2.83 and 2.76 (AB System, *J* = 16.4 Hz, 2H), 2.37 (d, *J* = 16.2 Hz, 2H), 1.20 (s, 3H), 1.15 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.1, 164.2, 158.1, 147.5, 142.7, 142.6, 140.8, 133.2, 131.6, 130.9, 129.8, 129.7, 129.5, 129.4, 129.2, 128.1, 127.8, 126.7, 125.5, 121.9, 120.1, 114.7, 113.0, 110.9, 55.4, 51.1, 41.5, 32.5, 31.7, 29.8, 27.0 ppm. HRMS (ESI, m/z): calcd for $C_{32}H_{26}N_2O_3$ ($M+H^+$) 486.194; found: 486.188.

16-(1H-indol-3-yl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4l). Yield 89%; yellow powder; mp 240-242 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.32 (d, *J* = 8.0 Hz, 1H), 8.35 (d, *J* = 8.0 Hz, 1H), 8.25-8.22 (m, 1H), 8.16-8.13 (m, 1H), 7.87-7.78 (m, 3H), 7.74-7.71 (m, 3H), 7.41 (d, *J* = 6.9 Hz, 2H), 7.09 (d, *J* = 6.9 Hz, 2H), 6.09 (s, 1H), 2.84 and 2.78 (AB System, *J* = 16.4 Hz, 2H), 2.41 and 2.32 (AB System, *J* = 16.4 Hz, 2H), 1.22 (s, 3H), 1.12 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.1, 164.3, 147.7, 147.2, 142.5, 142.2, 140.7, 140.2, 131.3, 130.2, 129.8, 129.6, 129.2, 128.9, 126.0, 122.2, 120.9, 115.1, 114.2, 51.0, 41.4, 33.7, 32.6, 29.5, 27.8 ppm. HRMS (ESI, m/z): calcd for $C_{33}H_{25}N_3O_2$ ($M+H^+$) 495.195; found: 495.191.

3,3-dimethyl-16-(3,4,5-trimethoxyphenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4m). Yield 90%; yellow powder; mp 239-241 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.39 (d, *J* = 7.7 Hz, 1H), 8.39-8.34 (m, 2H), 8.28-8.25 (m, 1H), 7.86-7.80 (m, 4H), 6.89 (s, 2H), 6.12 (s, 1H), 3.78 (s, 6H), 3.67 (s, 3H), 2.83 (s, 2H), 2.42 and 2.38 (AB System, *J* = 16.4 Hz, 2H), 1.23 (s, 3H), 1.21 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.0, 164.0, 152.7, 142.3, 141.9, 140.3, 130.3, 130.2, 130.0, 129.2, 129.0, 128.6, 126.6, 125.7, 122.1, 116.2, 114.8, 106.5, 60.7, 56.2, 51.0, 41.3, 33.6, 32.5, 29.9, 27.3 ppm. HRMS (ESI, m/z): calcd for $C_{34}H_{30}N_2O_5$ ($M+H^+$) 546.215; found: 546.208.

3,3-dimethyl-16-(thiophen-2-yl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4n). Yield 90%; yellow powder; mp 259-261 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.31 (dd, *J* = 2.0, 8.0 Hz, 1H), 8.32-8.29 (m, 2H), 8.26-8.23 (m, 1H), 7.82-7.77 (m, 4H), 7.10 (d, *J* = 6.9 Hz, 1H), 6.97-6.95 (q, 1H), 6.75-6.73 (m, 1H), 6.50 (s, 1H), 2.83 and 2.72 (AB System, *J* = 16.4 Hz, 2H), 2.44 (s, 2H), 1.23 (s, 3H), 1.22 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 196.8, 164.4, 148.7, 147.1, 142.6, 141.7, 141.1, 140.9, 130.9, 130.1, 130.0, 129.6, 128.5, 126.5, 125.5, 123.7, 122.1, 115.8, 114.7, 51.1, 41.4, 32.5, 29.7, 28.2, 27.7 ppm. HRMS (ESI, m/z): calcd for $C_{29}H_{22}N_2O_2S$ ($M+H^+$) 462.140; found: 462.130.

3,3-dimethyl-16-(3-nitrophenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4o). Yield 91%; yellow powder; mp 280-282 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.31-9.26 (m, 1H), 8.68 (d, *J* = 8.6 Hz, 1H), 8.56-8.54 (m, 1H), 8.30-8.25 (m, 2H), 8.21 (d, *J* = 8.0

Hz, 2H), 8.02-799 (m, 3H), 7.34-729 (m, 2H), 6.15 (s, 1H), 2.87 and 2.80 (AB System, J = 16.2 Hz, 2H), 2.42 and 2.32 (AB System, J = 16.2 Hz, 2H), 1.22 (s, 3H), 1.13 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 196.6, 164.6, 148.3, 147.2, 142.6, 141.5, 140.4, 135.6, 131.3, 129.9, 129.6, 129.3, 128.9, 126.4, 125.6, 124.4, 122.3, 121.6, 114.9, 51.1, 41.5, 34.1, 32.7, 29.5, 27.6 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{23}N_3O_4$ ($M+H^+$) 501.169; found: 501.162.

16-(3-fluorophenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4p). Yield 90%; yellow powder; mp 313-315°C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.27 (dd, J = 2.2, 8.9 Hz, 1H), 8.30 (dd, J = 2.2, 9.8 Hz, 1H), 8.19 (dd, J = 2.0, 10.1 Hz, 2H), 7.81-7.72 (m, 4H), 7.36 (d, J = 8.0 Hz, 1H), 7.32-7.28 (m, 1H), 7.12-7.07 (m, 1H),, 6.72-6.67 (m, 1H), 6.08 (s, 1H), 2.80 and 2.74 (AB System, J = 17.6 Hz, 2H), 2.40 and 2.33 (AB System, J = 16.4 Hz, 2H), 1.20 (s, 3H), 1.12 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 196.9, 163.9, 147.1, 142.6, 141.7, 141.0, 140.8, 131.0, 129.7, 129.5, 129.2, 128.6, 126.4, 125.6, 124.8, 122.0, 116.3, 116.1, 115.7, 114.8, 113.4, 51.1, 41.4, 33.6, 32.6, 29.6, 27.5 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{23}FN_2O_2$ ($M+H^+$) 474.174; found: 474.170.

3,3-dimethyl-16-(4-nitrophenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4q). Yield 90%; yellow powder; mp 296-298 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.32-9.30 (m, 1H), 8.38-8.33 (m, 1H), 8.30-8.27 (m, 1H), 8.25-8.20 (m, 1H), 8.17-8.13 (m, 1H), 8.06-7.98 (m, 2H), 7.82-7.77 (m, 6H), 6.13 (s, 1H), 2.80 (s, 2H), 2.41 and 2.31 (AB System, J = 16.4 Hz, 2H), 1.22 (s, 3H), 1.10 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 196.8, 164.2, 152.6, 147.2, 146.4, 142.5, 141.5, 141.1, 130.3, 130.1, 129.9, 129.6, 129.2, 128.9, 125.6, 123.3, 122.2, 114.8, 114.1, 50.9, 41.4, 34.3, 32.6, 29.6, 27.4 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{23}N_3O_4$ ($M+H^+$) 501.169; found: 501.162.

16-(4-(dimethylamino)phenyl)-3,3-dimethyl-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4r). Yield 93%; yellow powder; mp 248-250 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.36 (d, J = 5.6 Hz, 1H), 8.39 (d, J = 8.0 Hz, 1H), 8.30-8.27 (m, 1H), 8.20-8.17 (m, 1H), 7.76-7.72 (m, 4H), 7.41 (d, J = 6.9 Hz, 2H), 7.11 (d, J = 6.9 Hz, 2H), 6.12 (s, 1H), 3.08 (s, 6H), 2.85 and 2.78 (AB System, J = 16.4 Hz, 2H), 2.44 and 2.37 (AB System, J = 16.4 Hz, 2H), 1.22 (s, 3H), 1.12 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.2, 164.4, 147.7, 141.9, 140.7, 140.3, 131.3, 130.3, 129.5, 129.3, 128.9, 126.1, 125.7, 122.3, 120.1, 115.1, 114.2, 51.0, 47.1, 41.3, 33.7, 32.6, 29.4, 27.7 ppm. HRMS (ESI, m/z): calcd for $C_{33}H_{29}N_3O_2$ ($M+H^+$) 499.226; found: 499.219.

16-(4-ethoxyphenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4s). Yield 90%; yellow powder; mp 224-226 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.35 (d, J = 7.6 Hz, 1H), 8.37 (d, J = 6.9 Hz, 1H), 8.27-8.23 (m, 2H), 7.84-7.76 (m, 4H), 7.48 (d, J = 8.0 Hz, 2H), 6.67 (d, J = 8.0 Hz, 2H), 6.11 (s, 1H), 3.88-3.83 (q, 2H), 3.02-2.95 (m, 1H), 2.89-2.81 (m, 1H), 2.57-2.42 (m, 2H), 2.21-2.12 (m, 2H), 1.27 (t, J = 6.9 Hz, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.2, 165.2, 157.4, 147.0, 142.7, 142.1, 140.7, 137.4, 130.0, 129.9, 129.3, 128.4, 125.6, 122.0, 113.9, 63.2, 37.3, 32.7, 27.7, 20.7, 14.9 ppm. HRMS (ESI, m/z): calcd for $C_{31}H_{24}N_2O_3$ ($M+H^+$) 472.179; found: 472.172.

16-(4-isopropylphenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4t). Yield 95%; yellow powder; mp 250-252 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.31 (dd, J =

1.8, 8.2 Hz, 1H), 8.36-8.33 (m, 1H), 8.26-8.22 (m, 2H), 7.83-7.745 (m, 4H), 7.49 (d, *J* = 8.0 Hz, 2H), 6.69 (d, *J* = 8.0 Hz, 2H), 6.15 (s, 1H), 3.01-2.95 (m, 1H), 2.89-2.82 (m, 1H), 2.75-2.68 (m, 1H), 2.55-2.48 (m, 2H), 2.21-2.10 (m, 2H), 1.08 (dd, *J* = 2.2, 6.6 Hz, 6H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.2, 165.2, 147.0, 146.6, 142.6, 142.4, 142.0, 140.7, 130.7, 130.0, 129.9, 129.6, 129.3, 128.8, 128.3, 126.7, 126.1, 125.6, 122.0, 116.7, 37.3, 33.6, 33.0, 27.7, 24.0, 20.7 ppm. HRMS (ESI, m/z): calcd for $C_{32}H_{26}N_2O_2$ ($M+H^+$) 470.199; found: 470.192.

16-(2-chlorophenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4u). Yield 90%; yellow powder; mp 230-232 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.29-9.26 (m, 1H), 8.32-8.30 (m, 1H), 8.21-8.18 (m, 2H), 7.80-7.75 (m, 4H),7.53-7.47 (m, 2H), 7.10-6.97 (m, 2H), 6.07 (s, 1H), 3.00-2.96 (m, 1H), 2.87-2.80 (m, 1H), 2.52-2.48 (m, 2H), 2.21-2.14 (m, 2H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.0, 165.6, 147.2, 142.6, 141.9, 141.1, 133.7, 130.1, 129.7, 129.4, 129.2, 129.1, 128.6, 127.7, 126.6, 126.4, 125.6, 122.1, 115.9, 37.2, 33.6, 27.7, 20.6 ppm. HRMS (ESI, m/z): calcd for $C_{29}H_{19}ClN_2O_2$ ($M+H^+$) 462.114; found: 462.110.

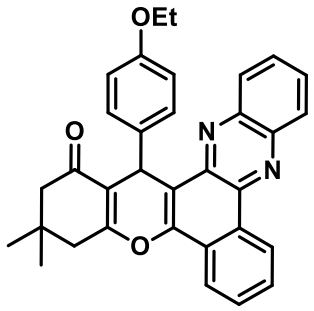
16-(2-methoxyphenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4v). Yield 91%; yellow powder; mp 302-304 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.28 (dd, *J* = 2.2, 7.9 Hz, 1H), 8.32-8.30 (m, 1H), 8.24-8.20 (m, 2H), 7.80-7.74 (m, 4H), 7.21-7.19 (m, 1H), 7.15 (d, *J* = 6.9 Hz, 1H), 7.06 (t, *J* = 6.9 Hz, 1H), 6.12 (s, 1H), 3.72 (s, 3H), 3.00-2.93 (m, 1H), 2.88-2.80 (m, 1H), 2.57-2.46 (m, 2H), 2.20-2.10 (m, 2H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.1, 165.3, 159.2, 146.9, 146.7, 142.5, 141.9, 140.6, 130.6, 130.0, 129.6, 129.4, 129.3, 128.8, 128.4, 126.5, 125.5, 121.9, 121.5, 116.3, 116.1, 115.4, 111.4, 55.2, 37.2, 33.5, 27.6, 20.6 ppm. HRMS (ESI, m/z): calcd for $C_{30}H_{22}N_2O_3$ ($M+H^+$) 458.163; found: 458.155.

16-(3-methoxyphenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4w). Yield 95%; yellow powder; mp 241-243 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.28 (d, *J* = 7.9 Hz, 1H), 8.36-8.32 (m, 1H), 8.21-8.16 (m, 2H), 7.81-7.73 (m, 4H), 7.08-7.03 (m, 2H), 6.88-6.84 (m, 2H), 6.03 (s, 1H), 3.76 (s, 3H), 3.00-2.94 (m, 1H), 2.87-2.81 (m, 1H), 2.57-2.46 (m, 2H), 2.20-2.11 (m, 2H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.2, 164.8, 147.1, 144.6, 142.7, 142.0, 140.6, 137.6, 130.0, 129.6, 129.5, 128.7, 128.4, 126.2, 125.8, 122.5, 121.5, 116.2, 115.4, 111.4, 56.2, 37.3, 30.2, 27.8, 20.6 ppm. HRMS (ESI, m/z): calcd for $C_{30}H_{22}N_2O_3$ ($M+H^+$) 458.163; found: 458.155.

16-(3-chlorophenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4x). Yield 90%; yellow powder; mp 289-291 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.29-9.27 (m, 1H), 8.33-8.31 (m, 1H), 8.21-8.17 (m, 2H), 7.82-7.75 (m, 5H),7.37 (d, *J* = 8.0 Hz, 1H), 67.29-7.24 (m, 1H), 7.12-7.01 (m, 1H), 6.73-6.68 (m, 1H), 6.11 (s, 1H), 3.00-2.94 (m, 1H), 2.89-2.82 (m, 1H), 2.58-2.44 (m, 2H), 2.22-2.10 (m, 2H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.0, 165.5, 147.2, 147.0, 142.5, 141.7, 140.8, 140.6, 133.8, 131.1, 130.8, 130.5, 130.1, 129.7, 129.4, 129.2, 129.1, 128.6, 127.8, 127.7, 126.6, 126.4, 125.5, 125.1, 122.0, 115.9, 115.5, 37.2, 33.6, 27.7, 20.6 ppm. HRMS (ESI, m/z): calcd for $C_{29}H_{19}ClN_2O_2$ ($M+H^+$) 462.114; found: 462.118.

16-(3-fluorophenyl)-2,3,4,16-tetrahydro-1H-benzo[a]chromeno[2,3-c]phenazin-1-one (4y). Yield 92%; yellow powder; mp 285-287 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.33 (dd, *J* = 1.9, 7.6 Hz, 1H), 8.38-8.25 (m, 3H), 8.16-8.14 (m, 1H), 7.86-7.67 (m, 3H),7.44 (d, *J* = 8.0 Hz, 2H), 6.68 (d, *J* = 8.0 Hz, 2H), 6.11 (s, 1H), 3.1-2.95 (m, 1H), 2.91-2.85 (m, 1H), 2.52-2.48 (m, 2H),

2.22-2.10 (m, 2H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): 197.0, 165.5, 162.5 (d, J = 240.2 Hz), 147.7, 147.0, 142.5, 141.7, 141.0, 140.8, 130.9, 130.0, 129.6, 129.5, 129.2, 128.5, 126.4, 125.5, 124.8, 122.0, 116.2, 116.0, 115.7, 113.3, 37.2, 33.5, 27.7, 20.6 ppm. HRMS (ESI, m/z): calcd for $C_{29}H_{19}FN_2O_2$ ($M+H^+$) 446.143; found: 446.135.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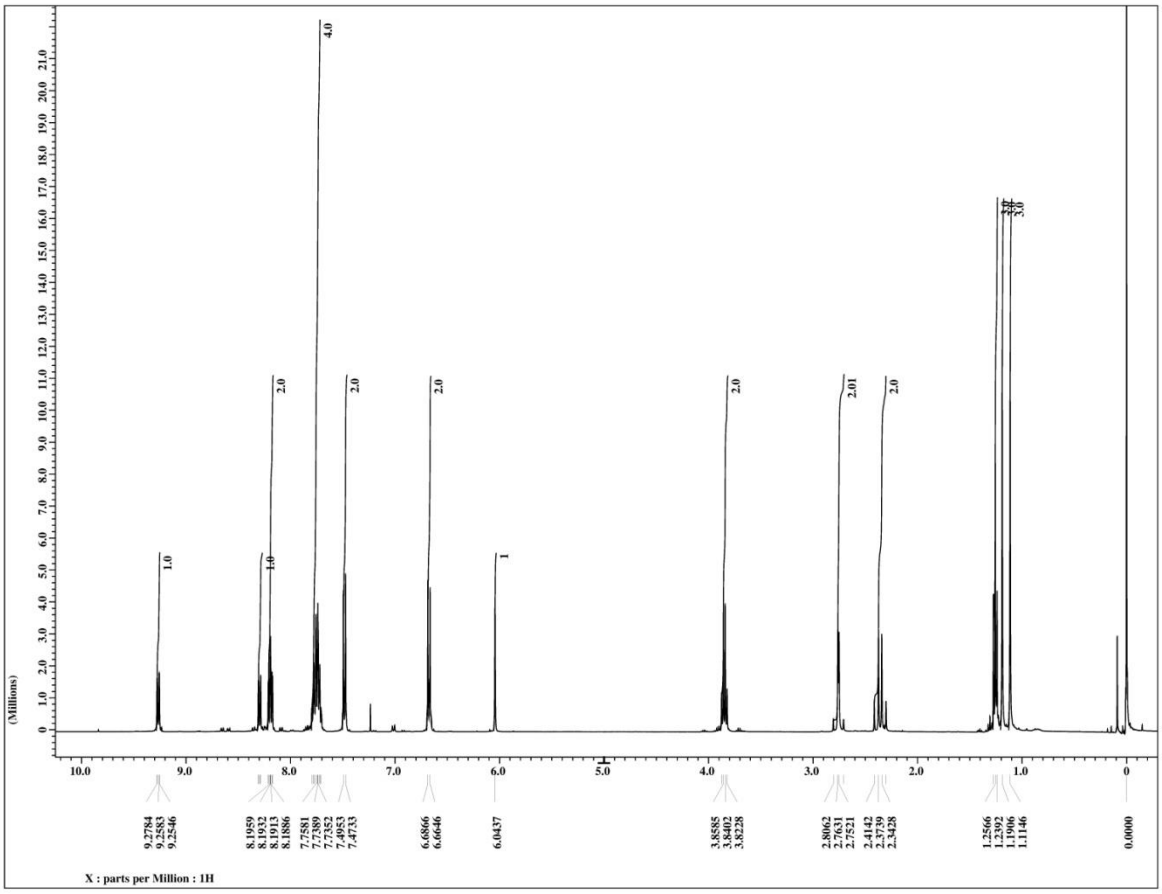
O

4a-^{1}H-NMR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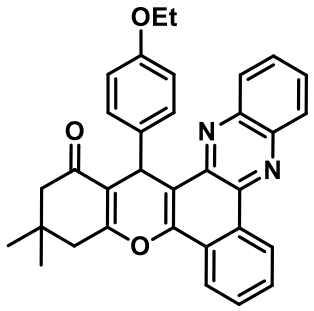
OEt
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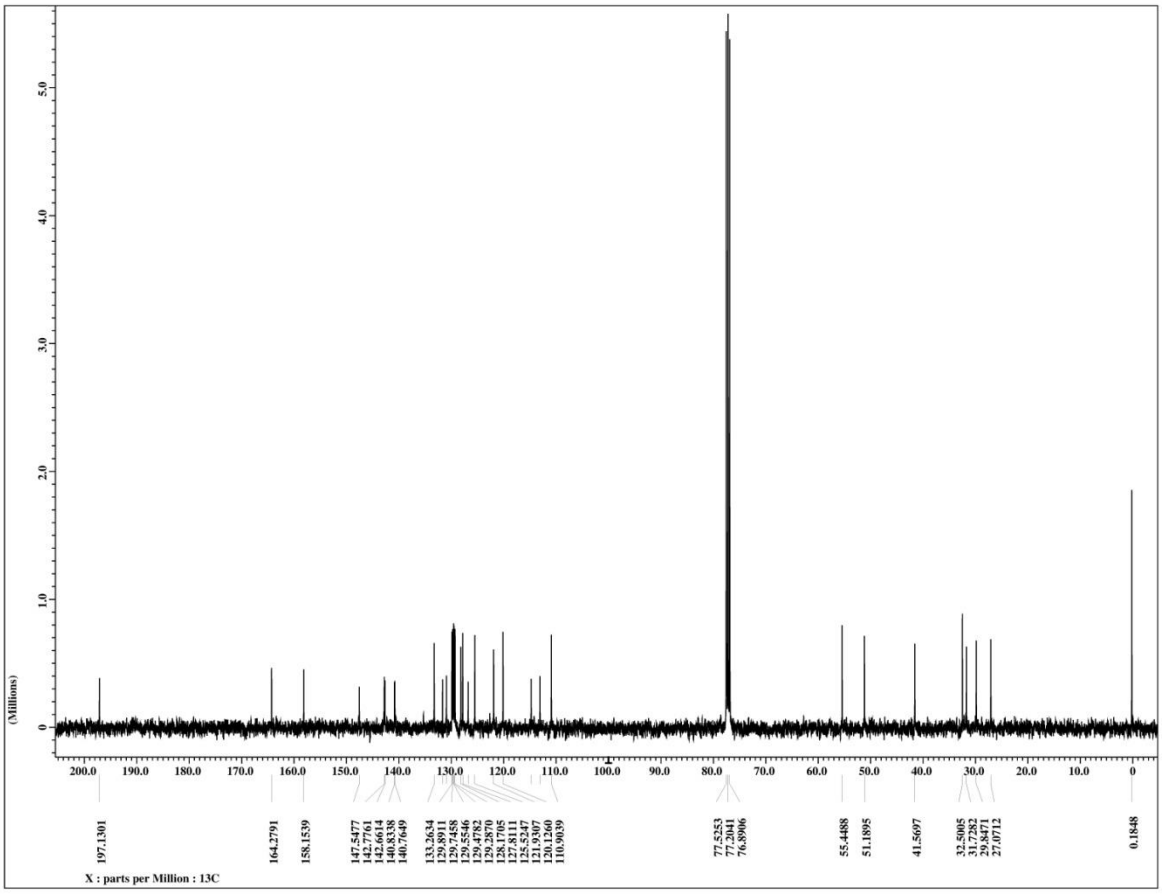
N
O

4a-^{13}C-NMR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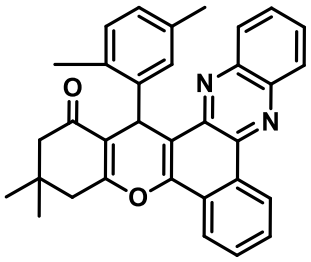
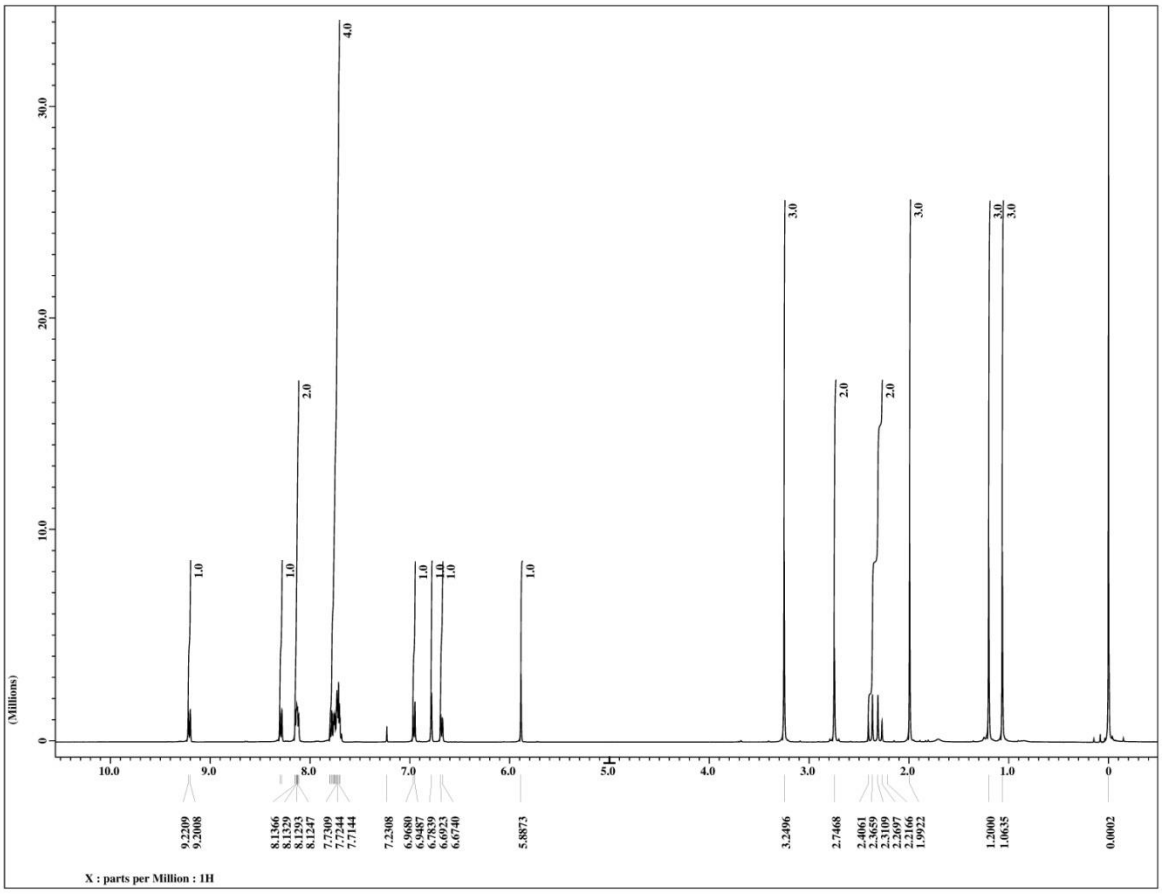

O
N
N
O

4b-^{1}H-NMR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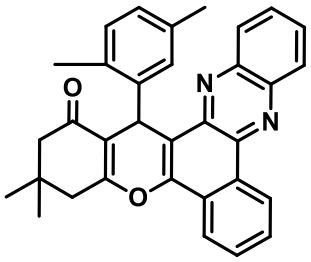
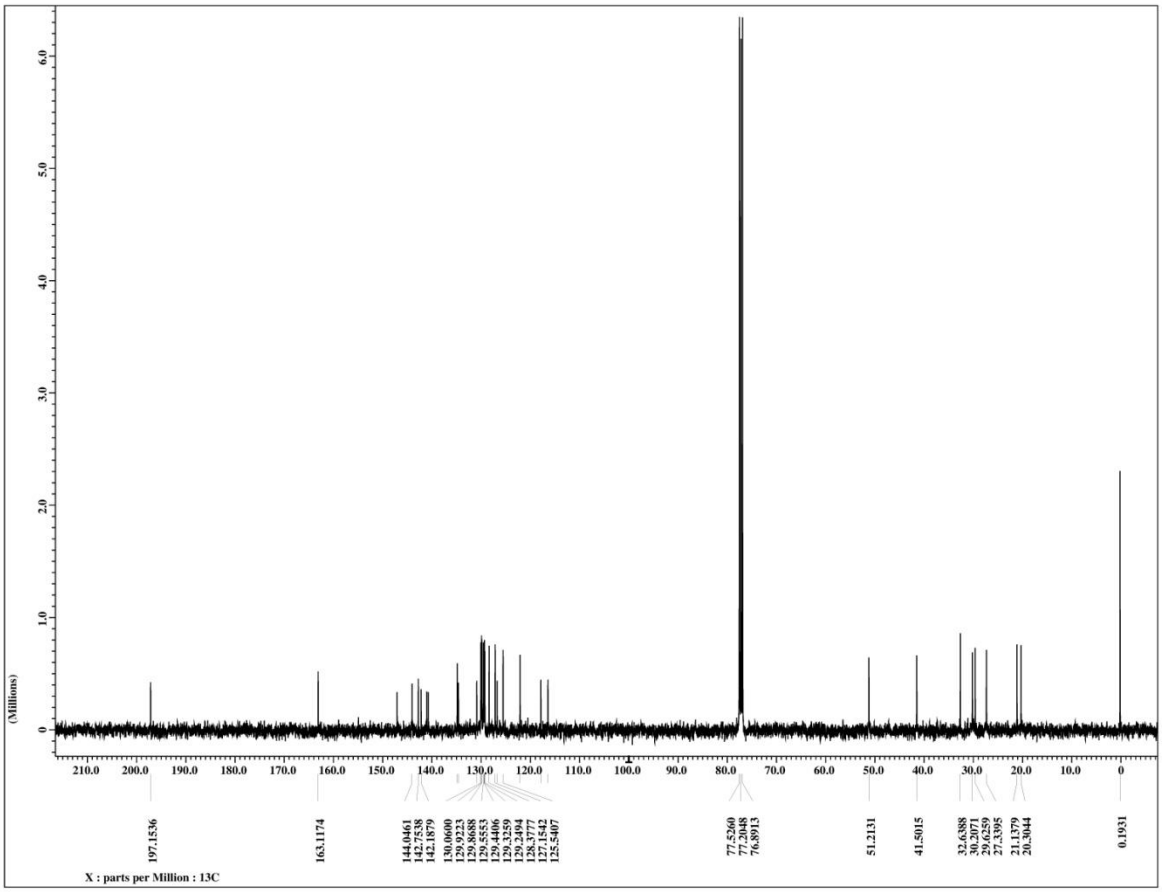

O
N
N
O

4b-^{13}C-NMR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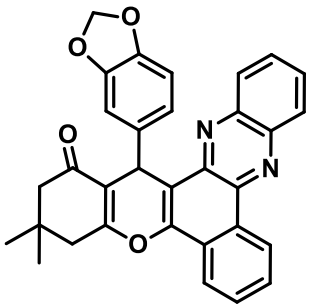
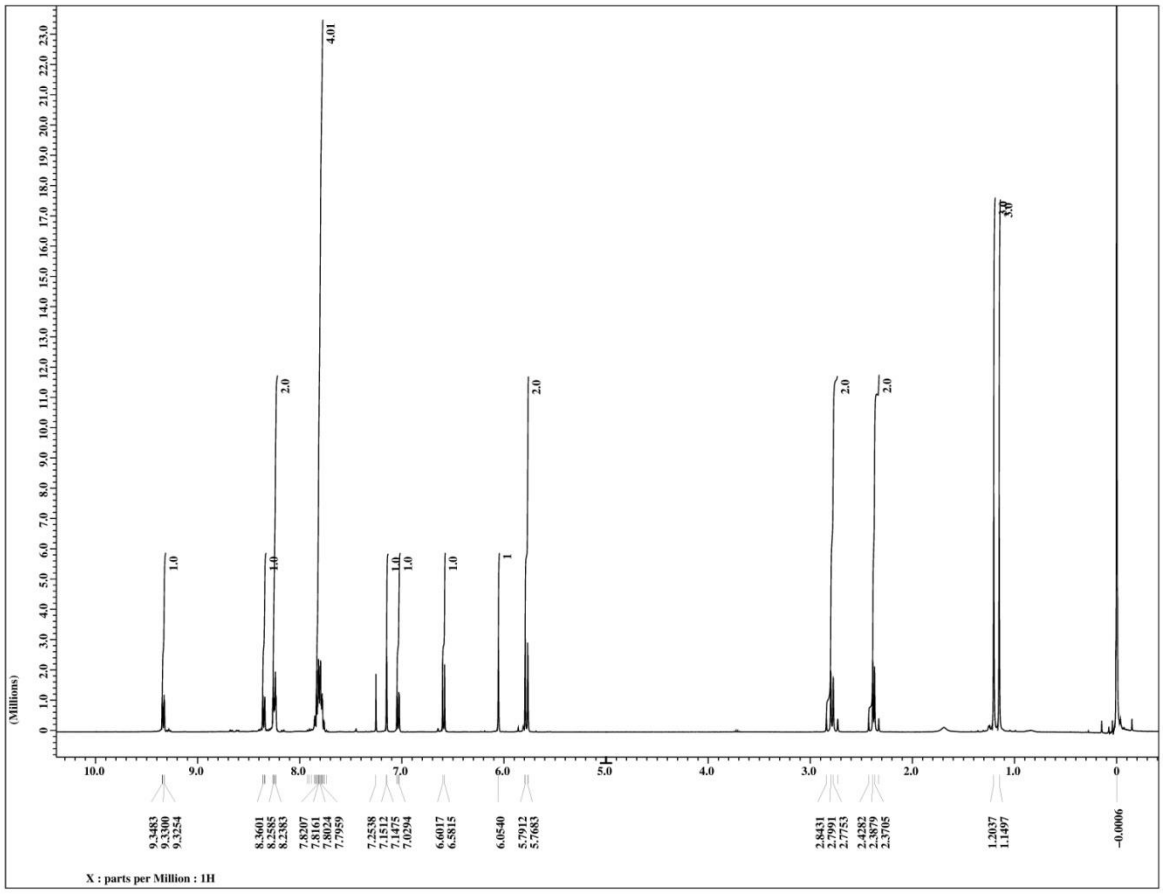


4c-^{1}H-NMR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7.0
6.0
5.0
4.0
3.0
2.0
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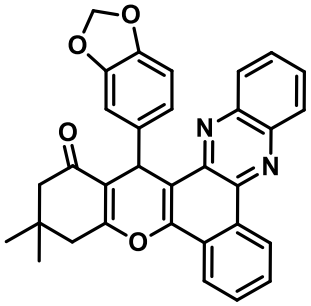
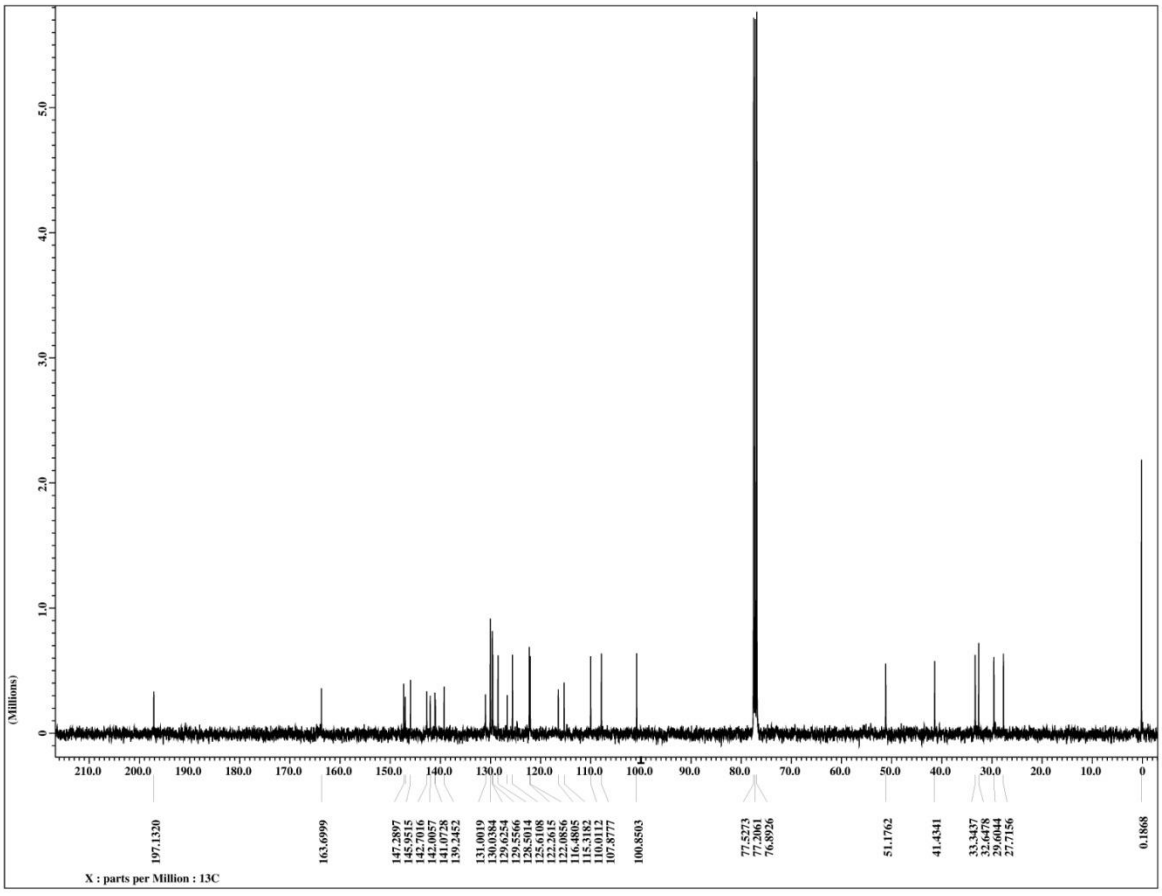


4c-^{13}C-NMR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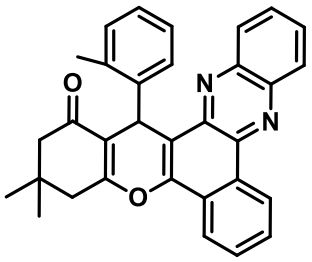
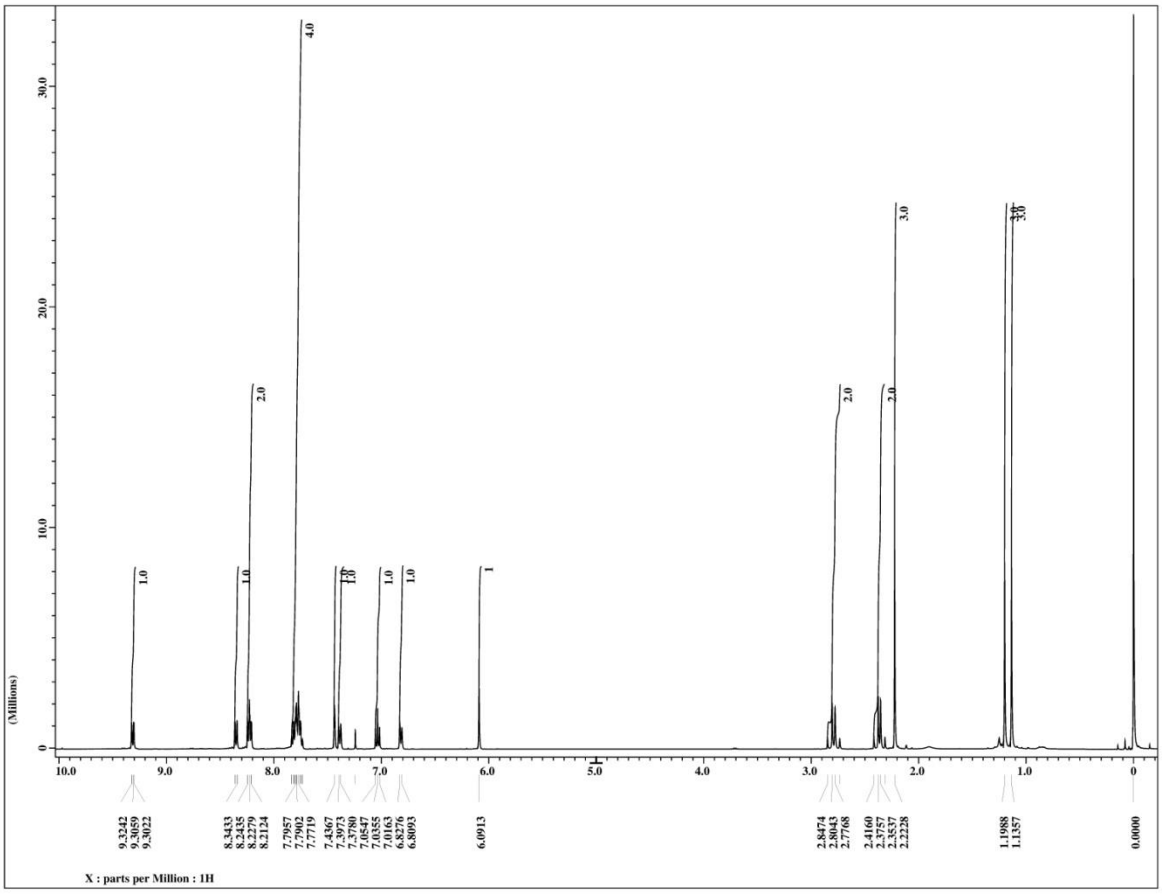

O
N
N
O

4d-^{1}H-NMR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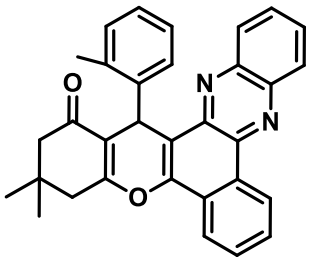
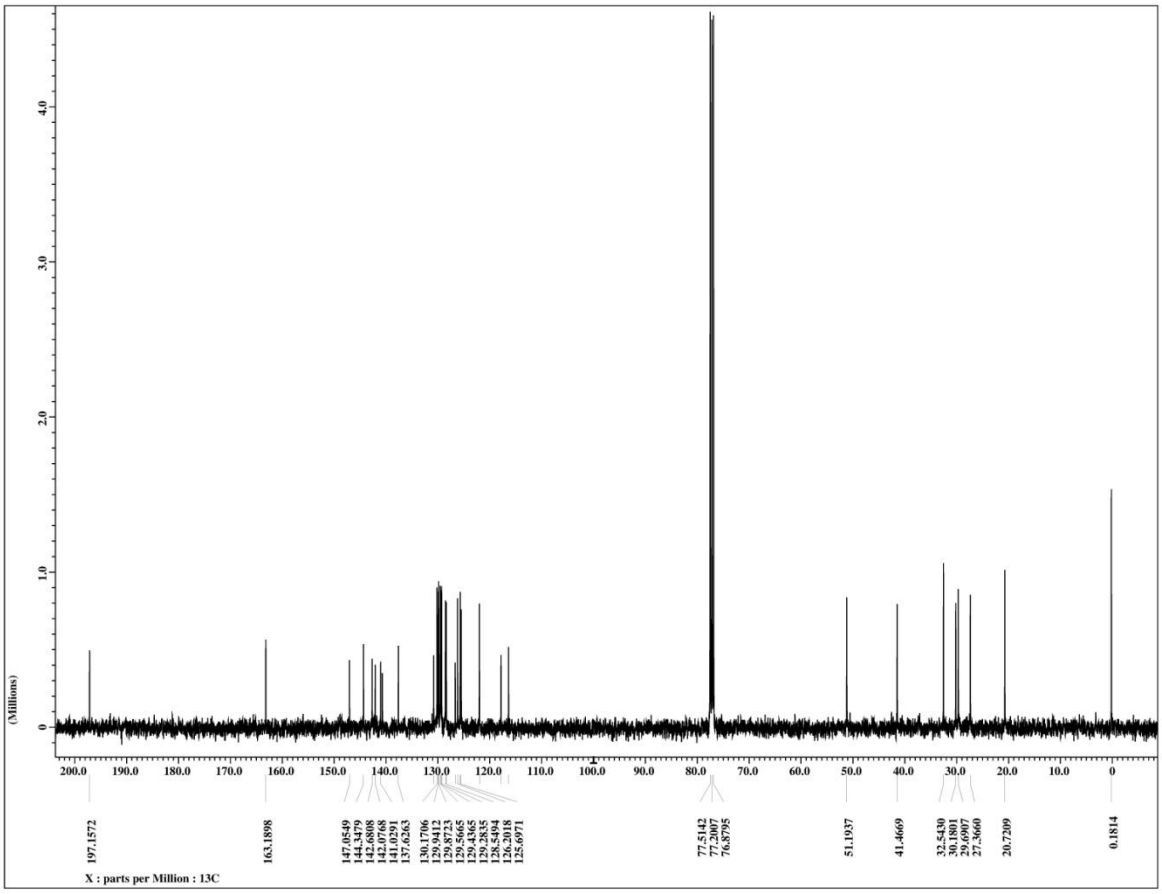
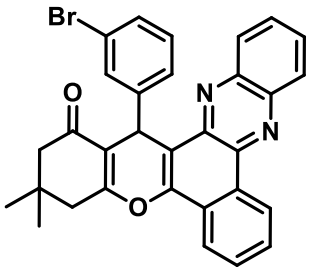
0.0000
X : parts per Million : 1H

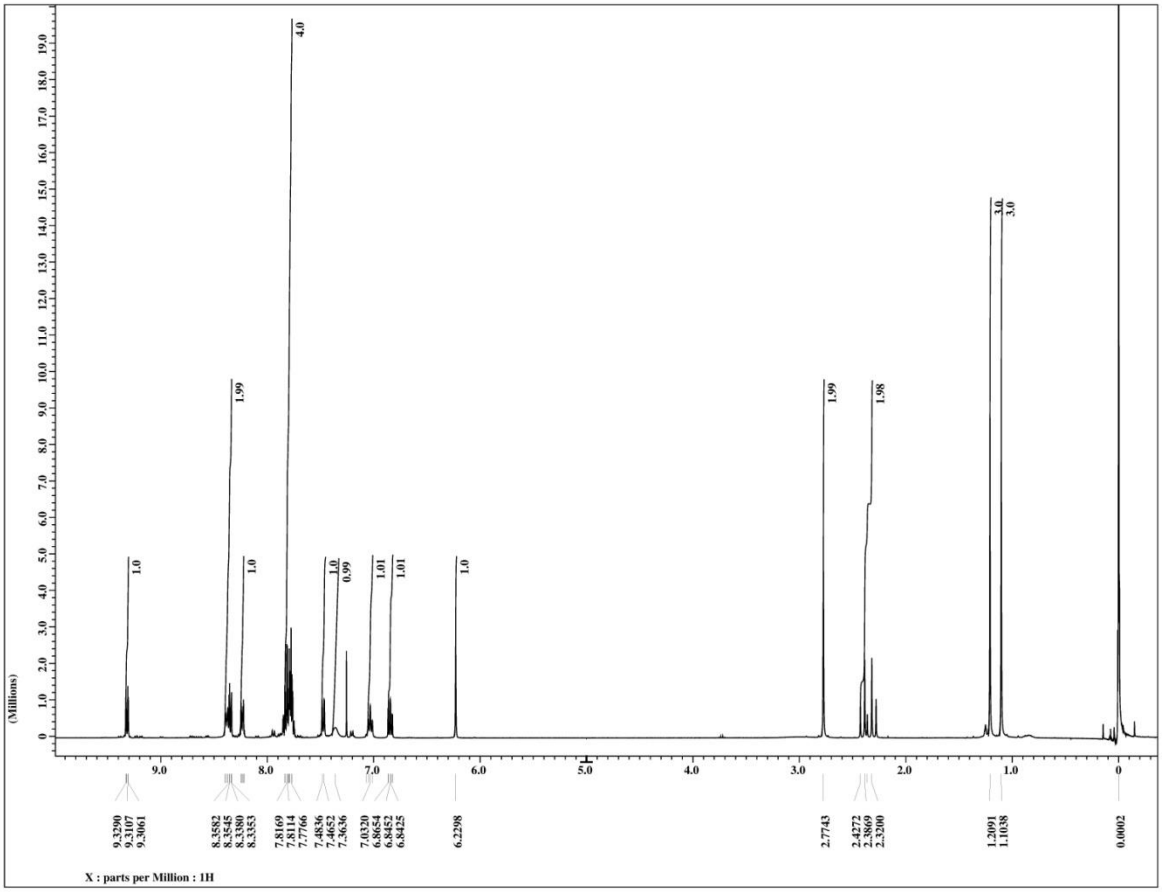

O
N
N
O

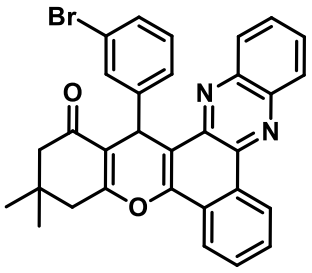
4d-^{13}C-NMR


(Millions)
4.0
3.0
2.0
1.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.1572
163.1898
147.0549
144.3479
142.6808
141.0764
141.0291
137.6263
130.1706
129.9412
129.8723
129.5665
129.4365
129.2835
128.5494
126.7018
125.6971
77.5142
77.2007
76.8795
51.1937
41.4669
32.5430
30.1801
29.6907
27.3660
20.7209
0.1814
X : parts per Million : 13C

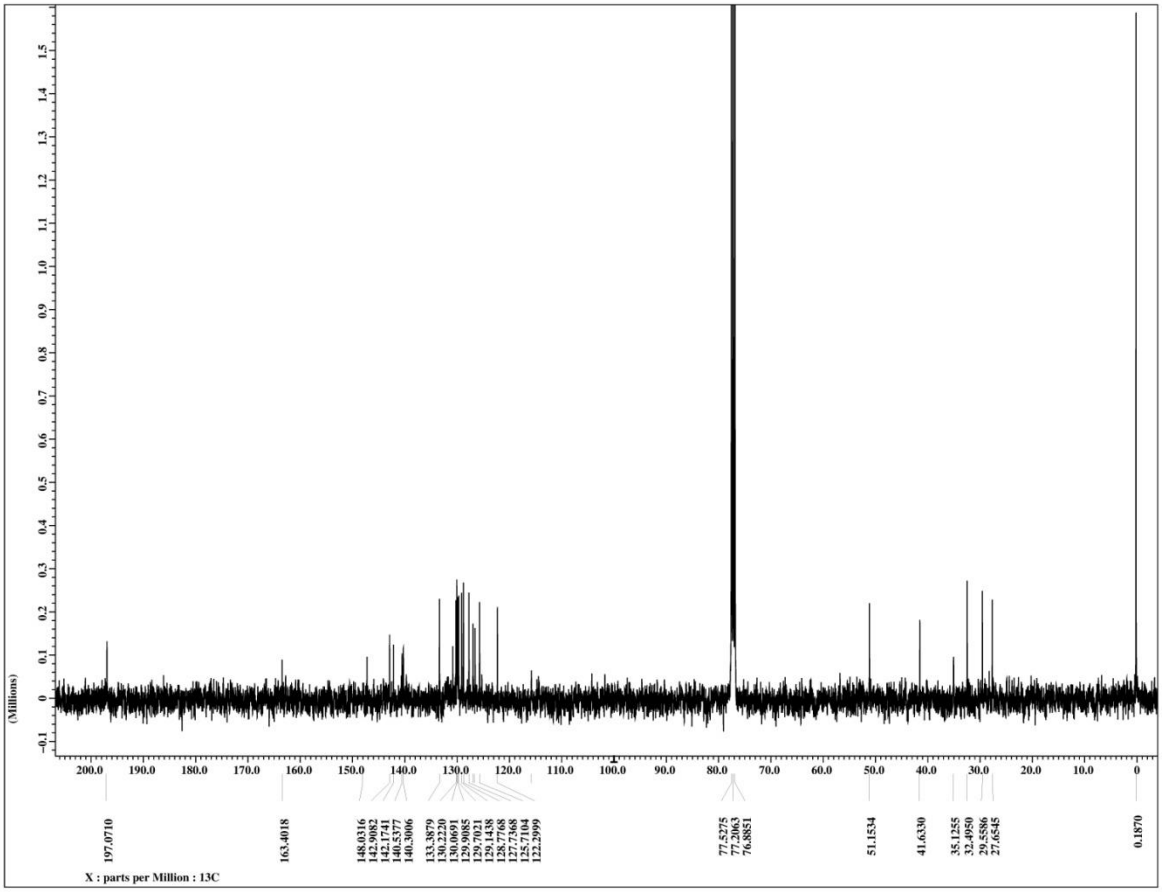


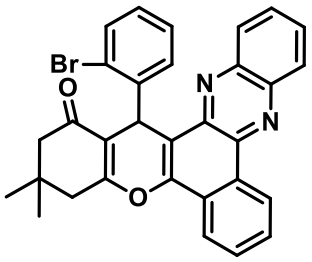
4e-^{1}H-NMR



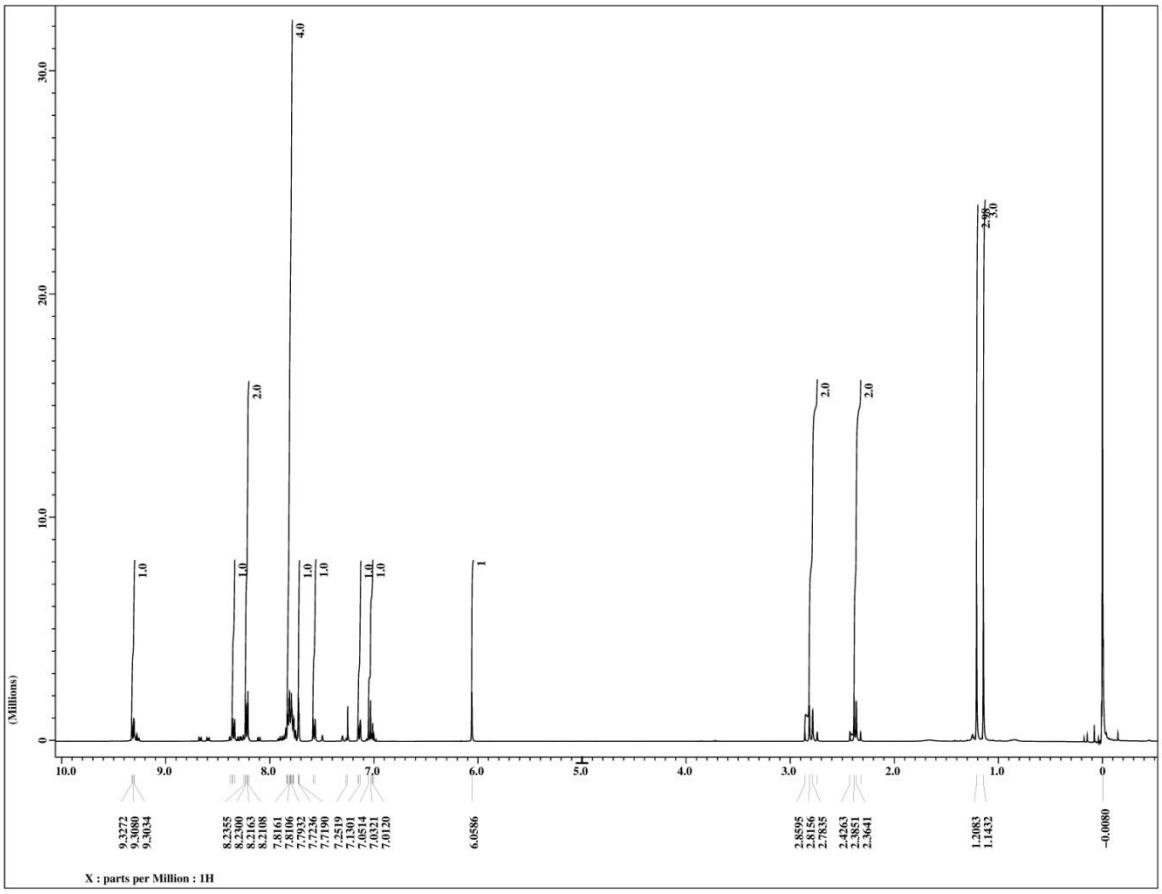

Br
O
N
N
O

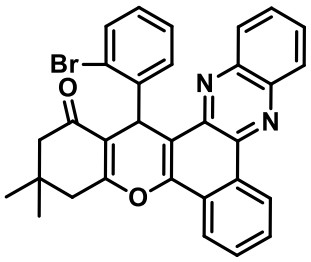
4e-^{13}C-NMR


(Millions)
X : parts per Million : 13C
197.0710
163.4018
148.0316
142.9082
142.1741
140.5377
140.3006
133.3879
130.2220
130.0691
129.9055
129.7021
129.1438
128.7768
127.7368
125.7104
122.2999
77.5275
77.2063
76.8851
51.1534
41.6330
35.1255
32.4950
29.5586
27.6545
0.1870

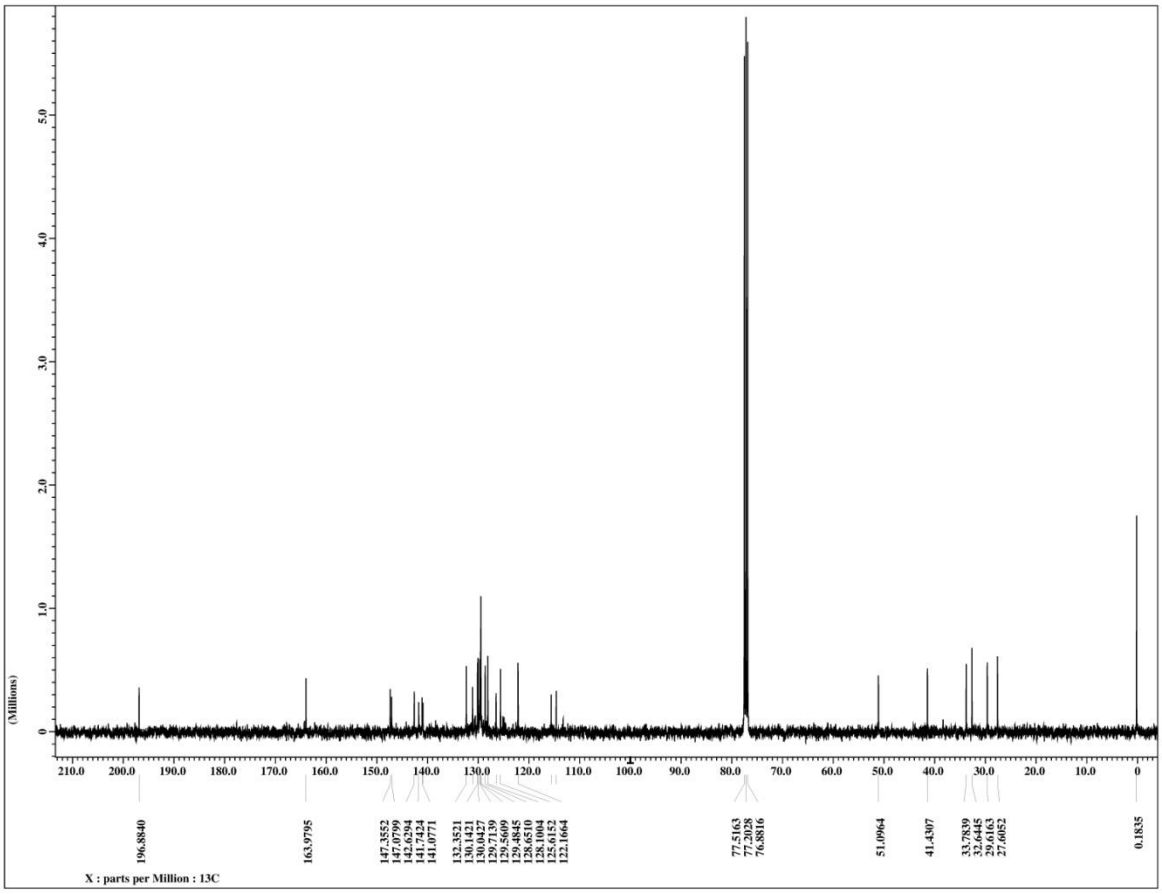

Br
O
N
N
O

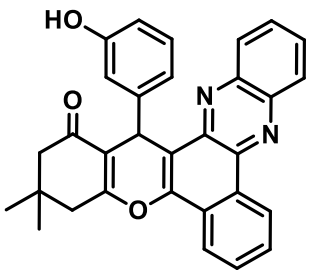
4f-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.3272
9.3080
9.3034
8.2355
8.2300
8.2163
8.2108
7.8161
7.8106
7.7932
7.7736
7.7190
7.2519
7.1301
7.0514
7.0321
7.0120
6.0586
2.8595
2.8156
2.7835
2.4263
2.3851
2.3641
1.2083
1.1432
-0.0080

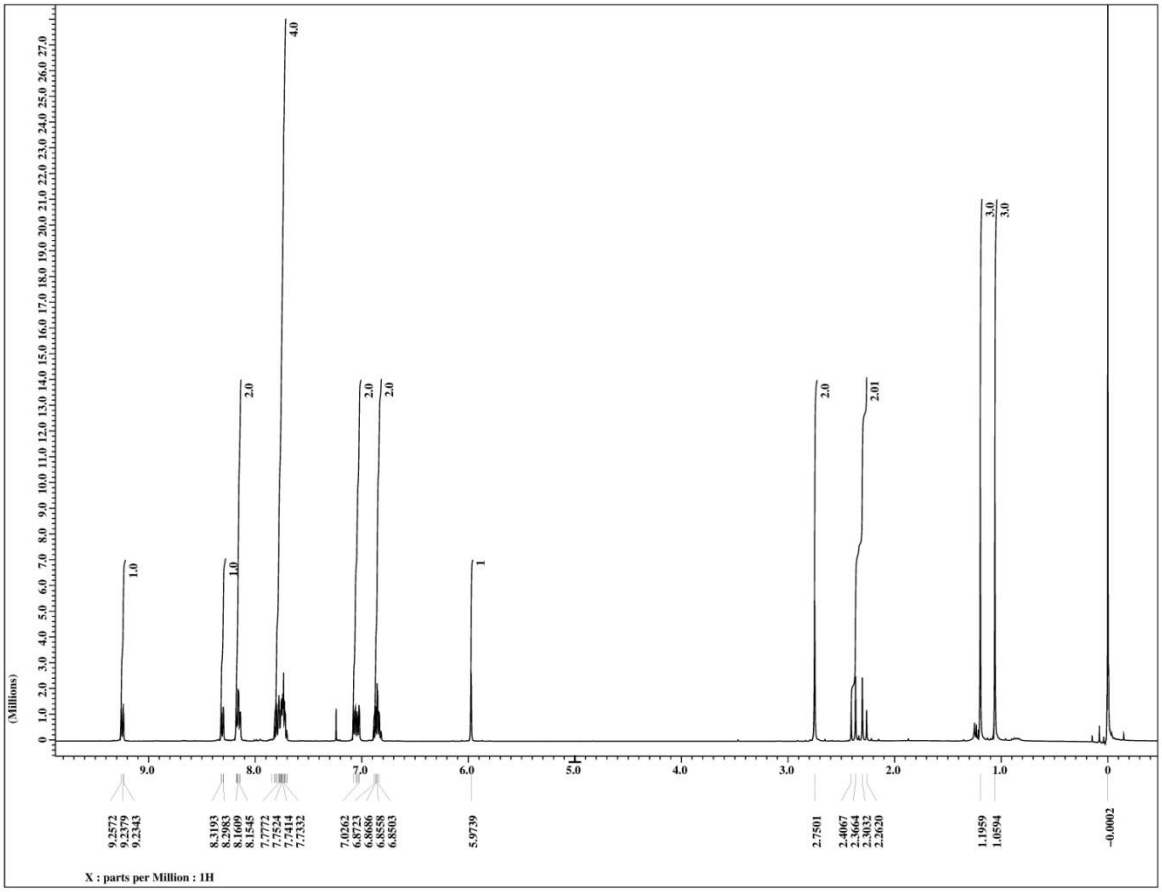

Br
O
N
N
O

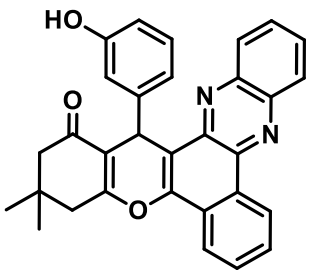
4f-^{13}C-NMR


(Millions)
0
1.0
2.0
3.0
4.0
5.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.8840
163.9795
147.3552
147.0799
142.4294
141.7424
141.0771
132.3521
130.1421
130.0137
129.7139
129.5609
129.4845
128.6510
128.1004
125.0152
122.1664
77.5163
77.2028
76.8816
51.0964
41.4307
33.7839
32.6445
29.6163
27.6052
0.1835
X : parts per Million : 13C

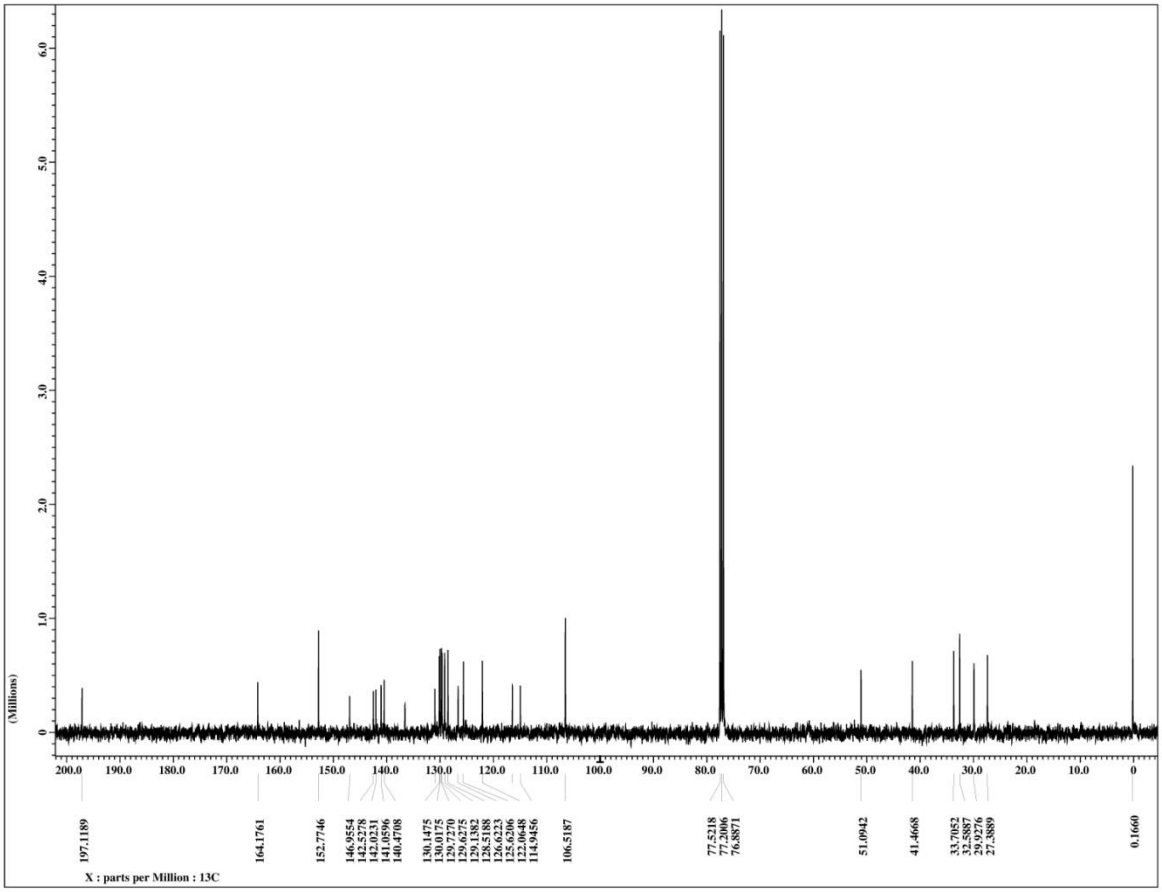

HO
O
N
N
O

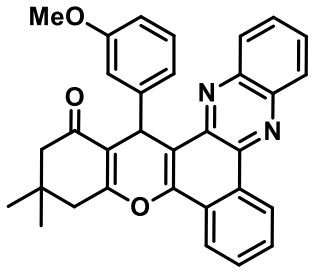
4g-^{1}H-NMR


(Millions)
4.0
2.0
2.0
2.0
1.0
1.0
1
2.0
2.01
3.0
3.0
9.2572
9.2379
9.2343
8.3193
8.2983
8.1609
8.1545
7.7772
7.7524
7.7414
7.7332
7.0262
6.8723
6.8686
6.8558
6.8503
5.9739
2.7501
2.4067
2.3664
2.3032
2.2620
1.1959
1.0594
-0.0002
X : parts per Million : 1H

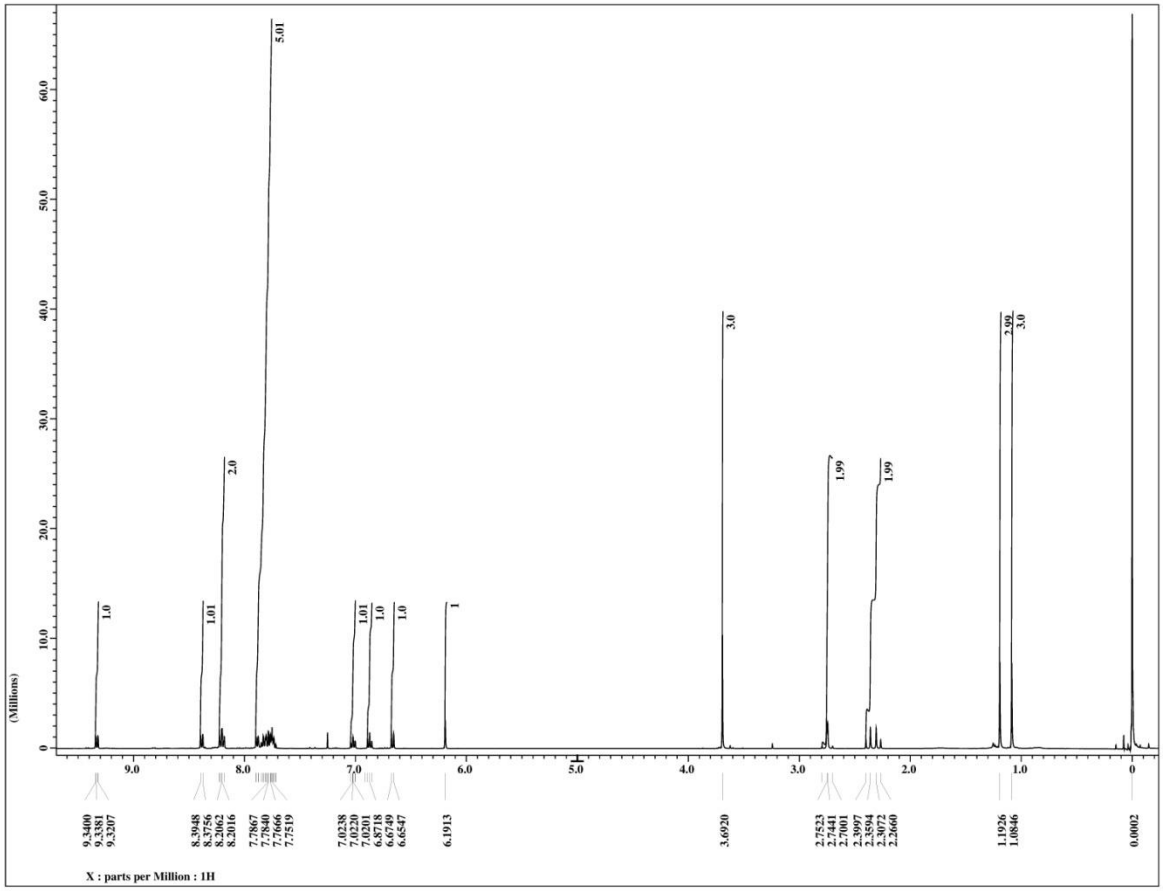

HO
O
N
N
O

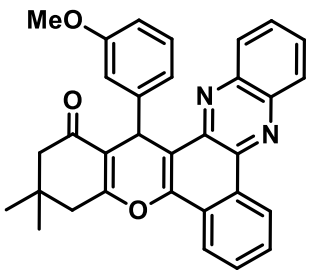
4g-^{13}C-NMR


(Millions)
6.0
5.0
4.0
3.0
2.0
1.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.1189
164.1761
152.7746
146.9554
142.5278
142.0231
141.0596
140.4708
130.1475
130.0175
129.7770
129.6275
129.1382
128.5188
126.6223
125.6206
123.1648
114.9456
106.5187
77.5218
77.2006
76.8871
51.0942
41.4668
33.7052
32.5887
29.9276
27.3889
0.1660
X : parts per Million : 13C

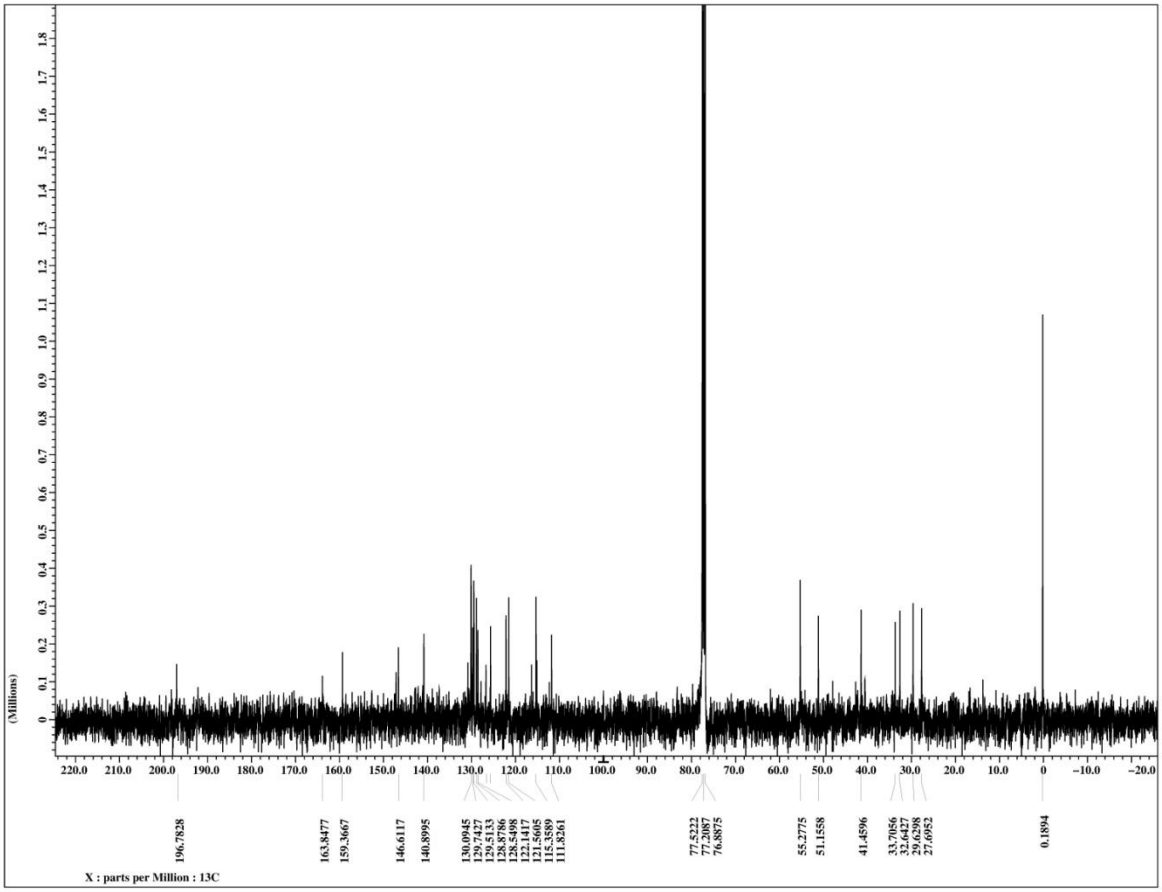


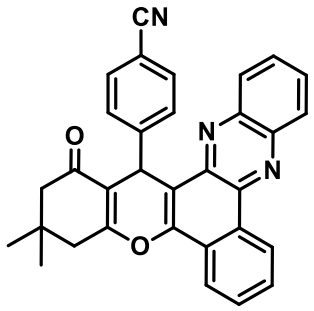
4h-^{1}H-NMR



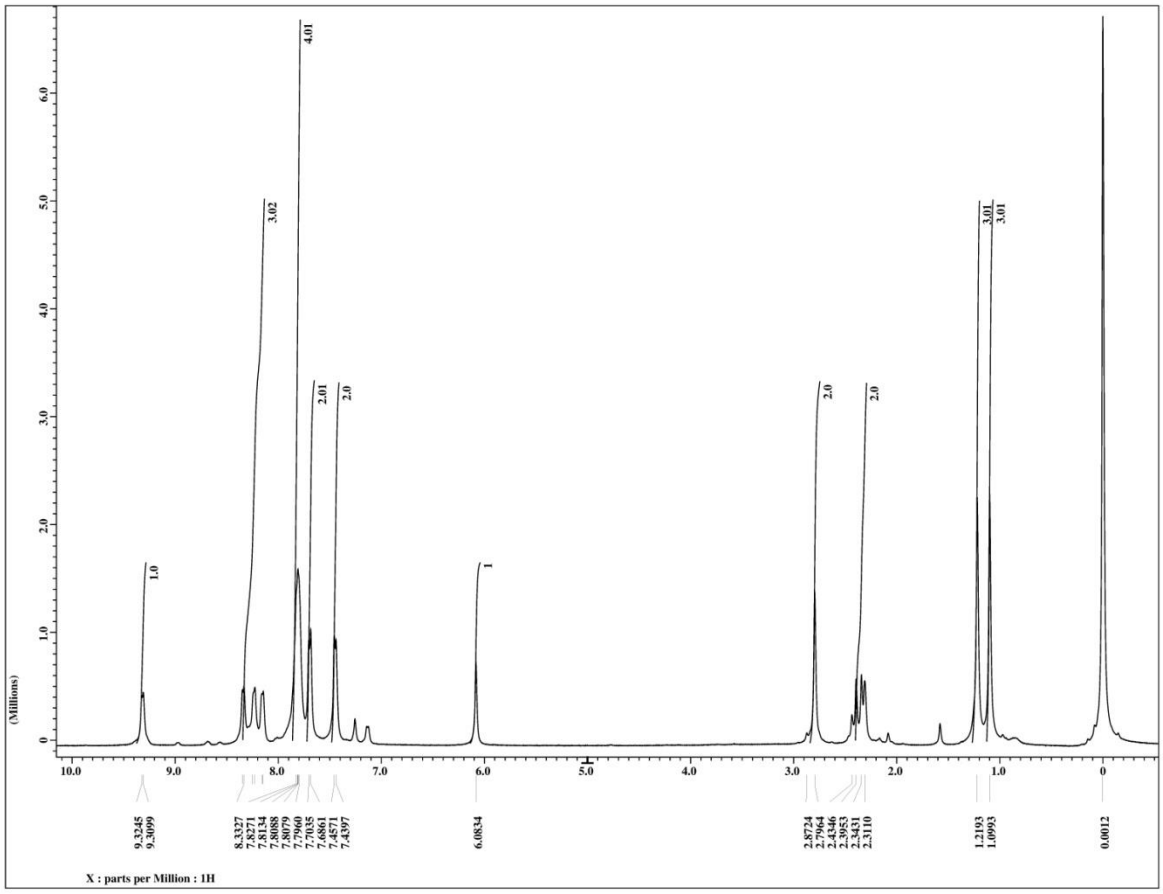

MeO
O
N
N
O

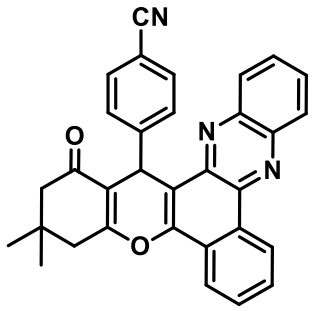
4h-^{13}C-NMR


(Millions)
X : parts per Million : 13C
196.7828
163.8477
159.3667
146.6117
140.8995
130.0945
129.7427
129.5133
128.8786
128.5498
122.1417
121.5468
115.1589
111.8361
77.5222
77.2087
76.8875
55.2775
51.1558
41.4596
33.7056
32.6427
29.6298
27.6952
0.1894

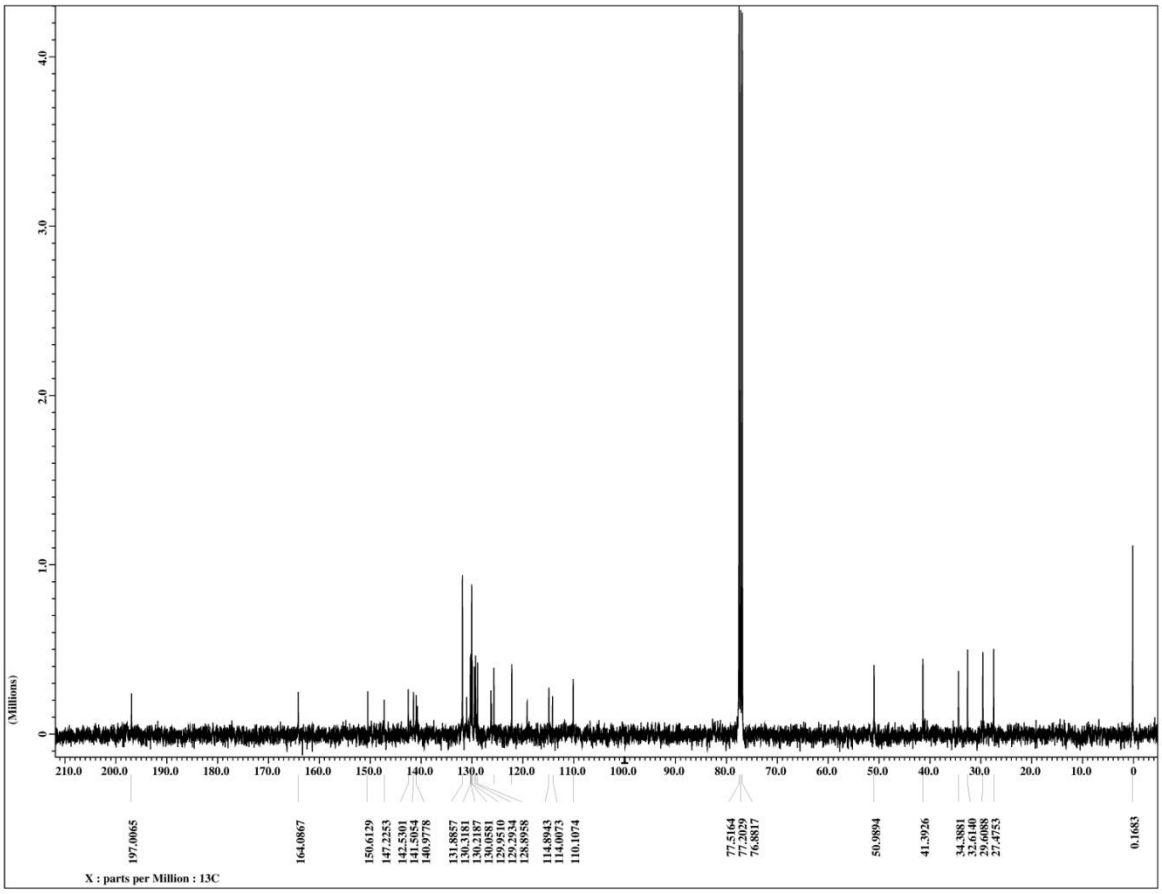

CN
O
N
N
O

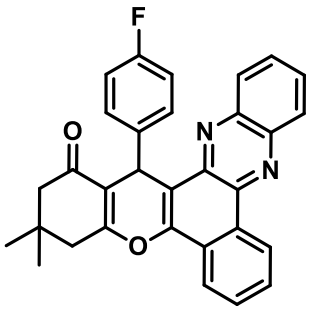
4i-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.3245
9.3099
8.3327
7.8271
7.8134
7.8088
7.8079
7.7960
7.7035
7.6861
7.4571
7.4397
6.0834
2.8724
2.7964
2.3446
2.3355
2.3431
2.3110
1.2193
1.0993
0.0012

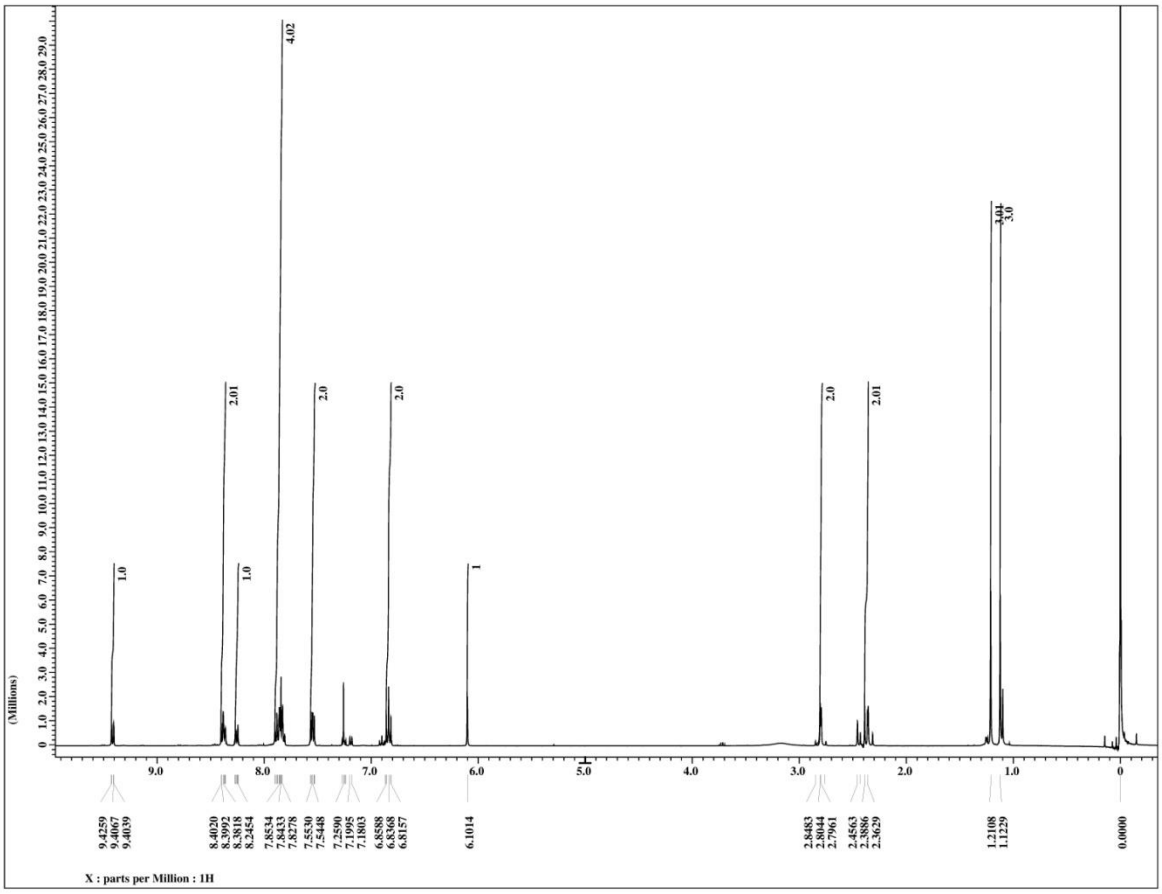

CN
O
N
N
O

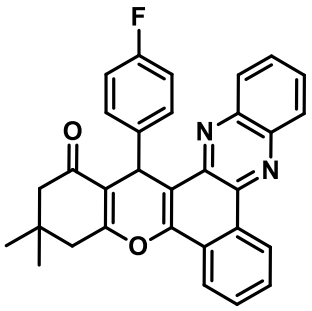
4i-^{13}C-NMR


(Millions)
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.0065
164.0867
150.6129
147.2253
142.5301
141.5054
140.9778
131.8857
130.3181
130.2187
130.0581
129.9510
129.2934
128.8958
114.8943
114.0073
110.1074
77.5164
77.2029
76.8817
50.9894
41.3926
34.3881
32.6140
29.6698
27.4783
0.1683
X : parts per Million : 13C

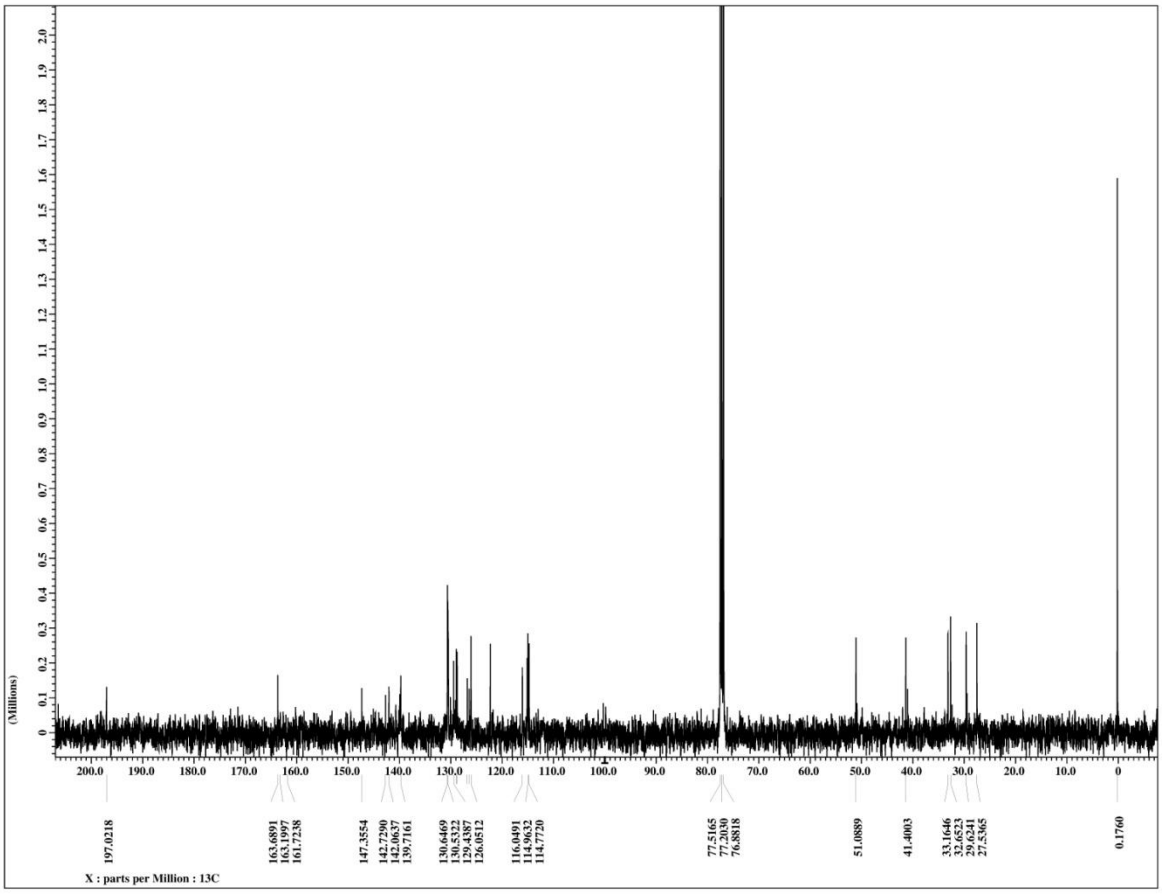

F
O
N
N
O

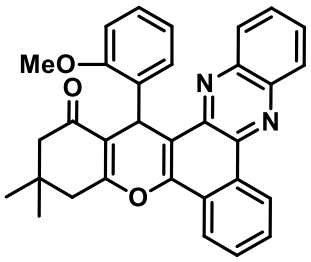
4j-^{1}H-NMR


(Millions)
4.02
2.01
2.0
2.0
1.0
1.0
1
2.0
2.01
3.01
3.0
9.4259
9.4067
9.4039
8.4020
8.3992
8.3818
8.2454
7.8534
7.8433
7.8278
7.5530
7.5448
7.2590
7.1995
7.1803
6.8588
6.8368
6.8157
6.1014
2.8483
2.8044
2.7961
2.4563
2.3886
2.3629
1.2108
1.1229
0.0000
X : parts per Million : 1H

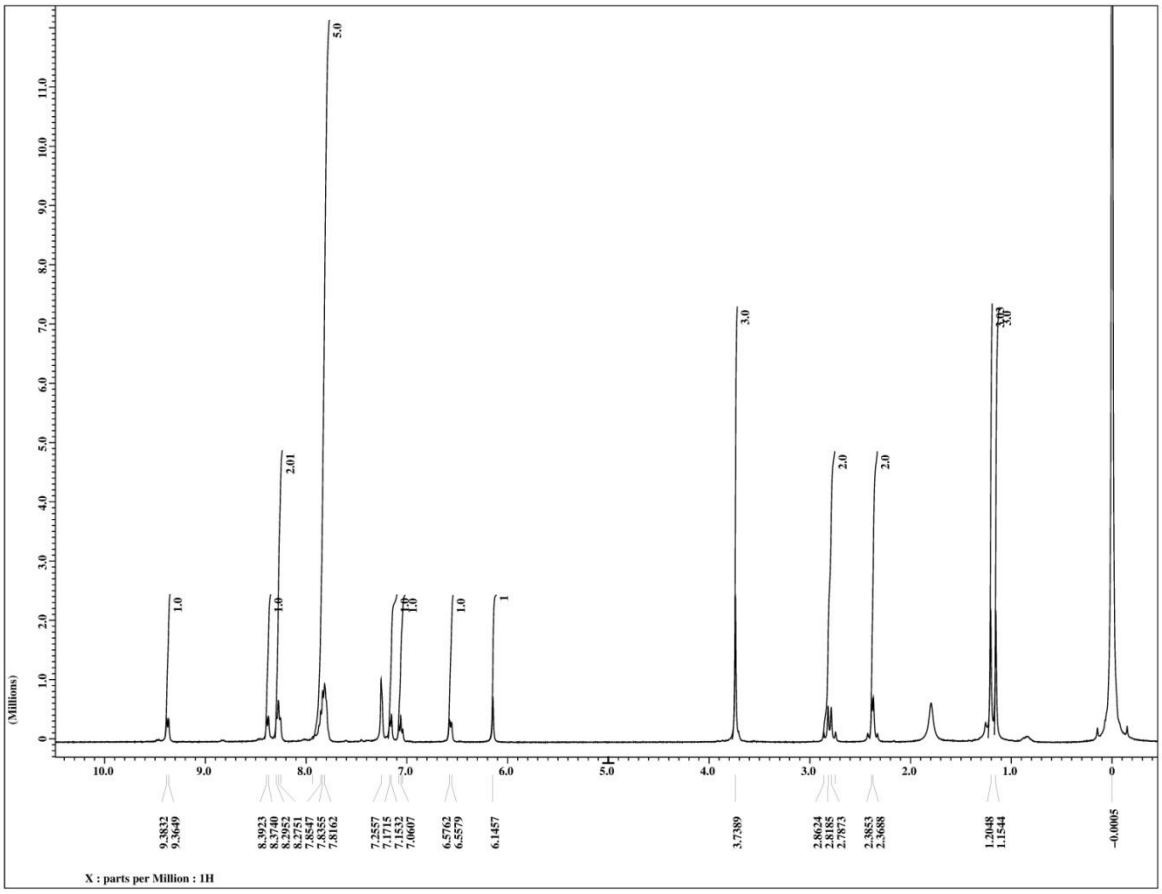

F
O
N
N
O

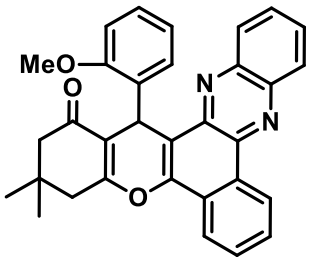
4j-^{13}C-NMR


(Millions)
X : parts per Million : 13C
197.0218
163.6891
163.1597
161.7238
147.3554
142.7390
142.0637
139.7161
130.6469
130.5322
129.4387
126.0512
116.0491
114.9632
114.7720
77.5165
77.2030
76.8818
51.0889
41.4003
33.1646
32.6523
29.6141
27.2565
0.1760

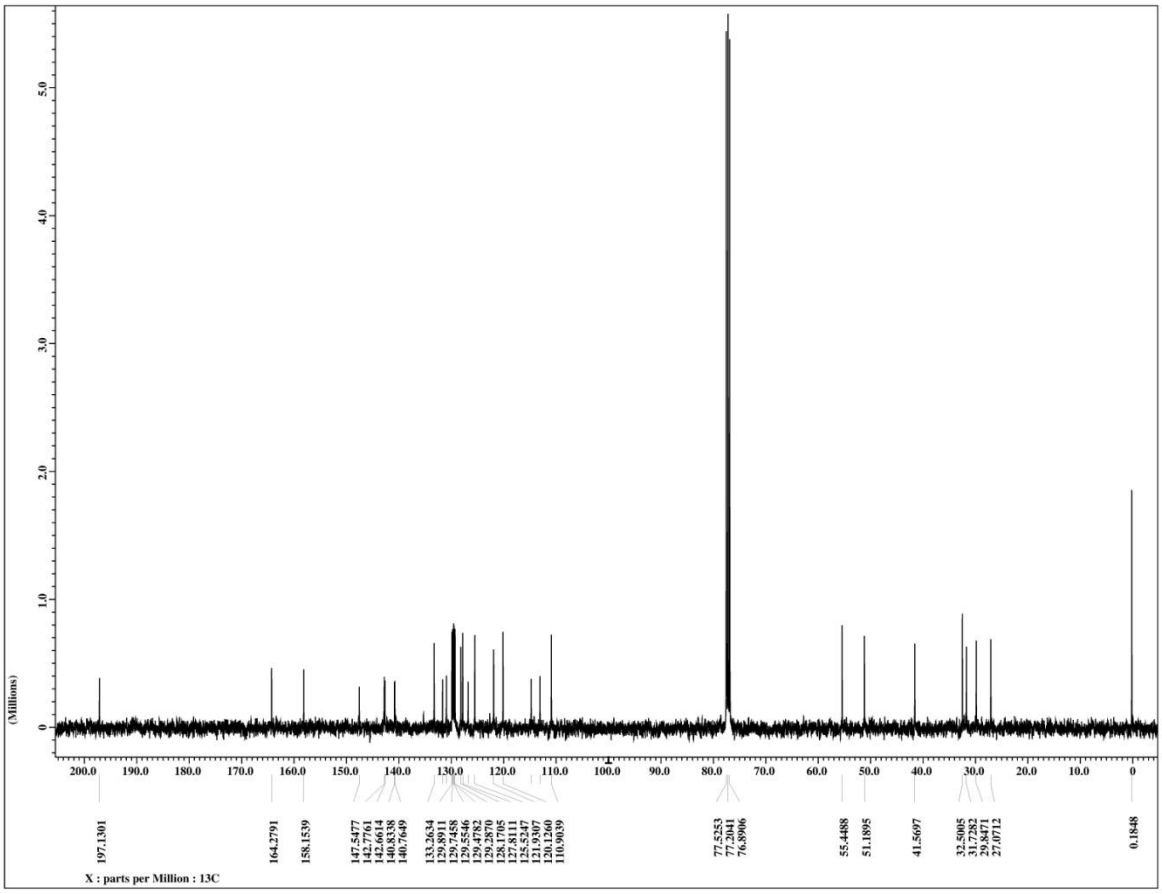

MeO
O
N
N
O

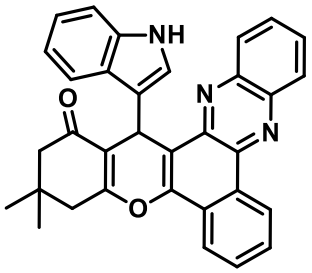
4k-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.3832
9.3649
8.3923
8.3740
8.2952
8.2753
7.8547
7.8355
7.8162
7.2557
7.1715
7.1532
7.0607
6.5762
6.5579
6.1457
3.7389
2.8624
2.8435
2.7873
2.3853
2.3688
1.2048
1.1544
-0.0005

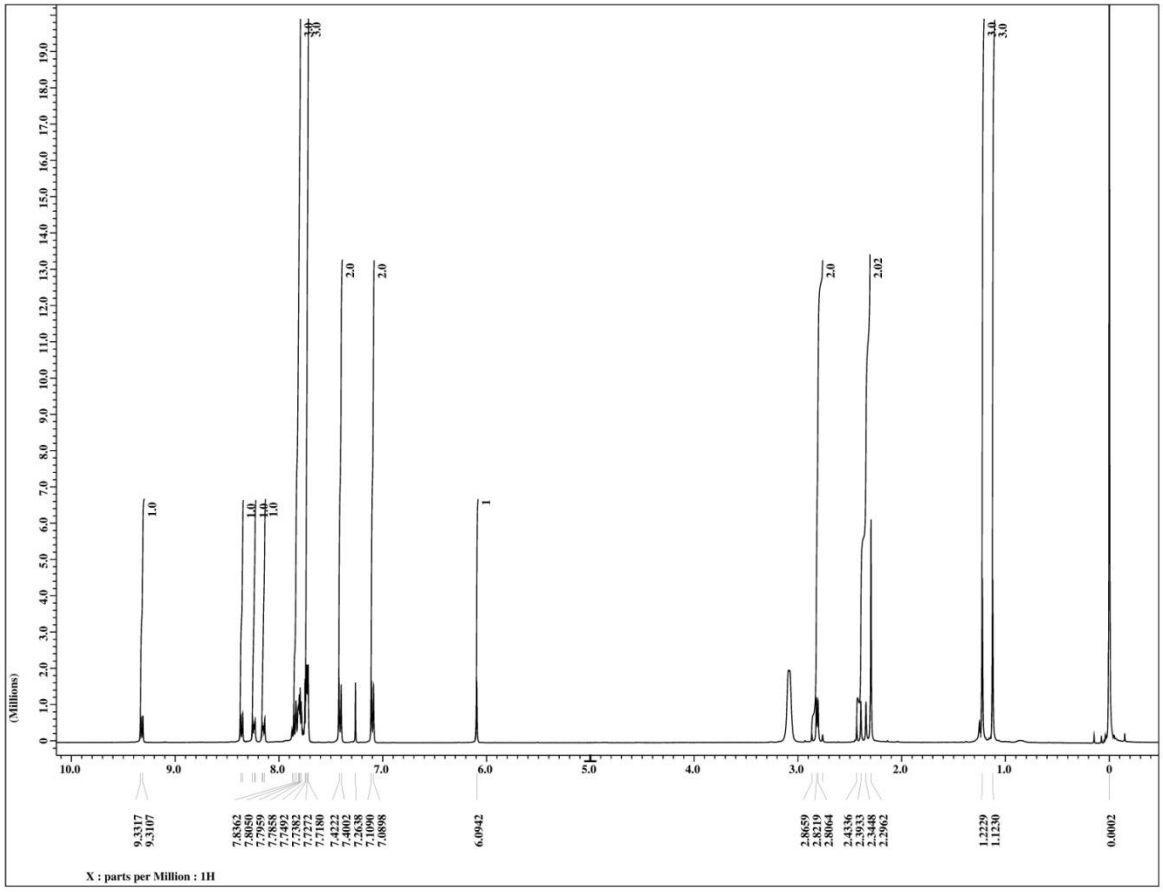

MeO
O
N
N
O

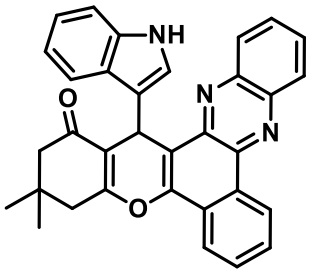
4k-^{13}C-NMR


(Millions)
X : parts per Million : 13C
197.1301
164.2791
158.1539
147.5477
142.6614
140.8338
140.7649
133.2634
129.8911
129.7458
129.4782
129.2870
128.1705
127.8111
125.5347
121.1007
120.1260
110.9039
77.5353
77.2041
76.8906
55.4488
51.1895
41.5697
32.5005
31.7282
29.9471
27.0712
0.1848

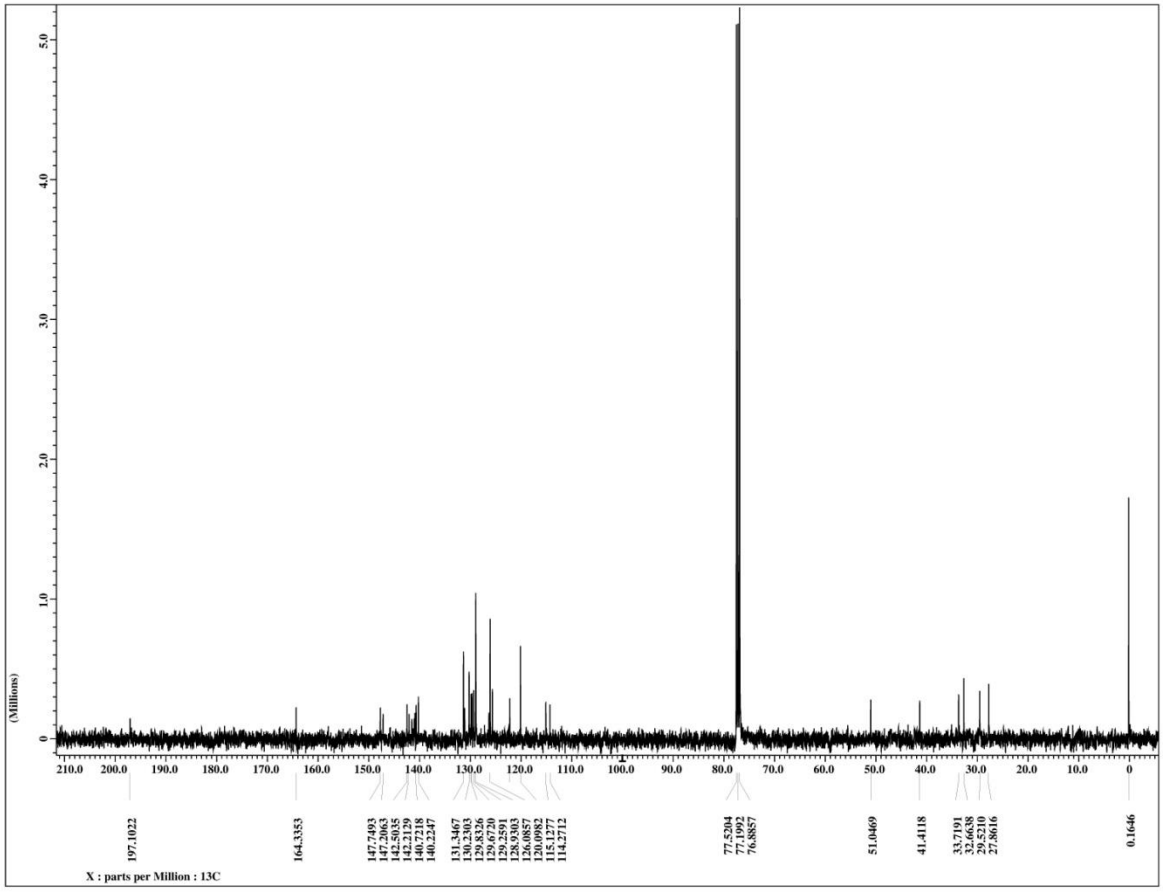

NH
O
N
N
O

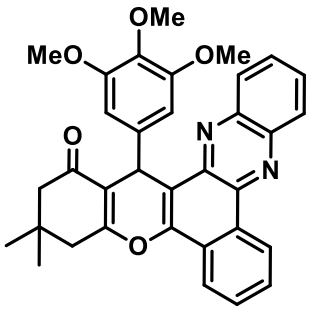
4l-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.3317
9.3107
7.8362
7.8050
7.7959
7.7858
7.7692
7.7382
7.7272
7.7180
7.4222
7.4002
7.2638
7.1090
7.0898
6.0942
2.8659
2.8319
2.8064
2.4336
2.3933
2.3648
2.2962
1.2229
1.1230
0.0002

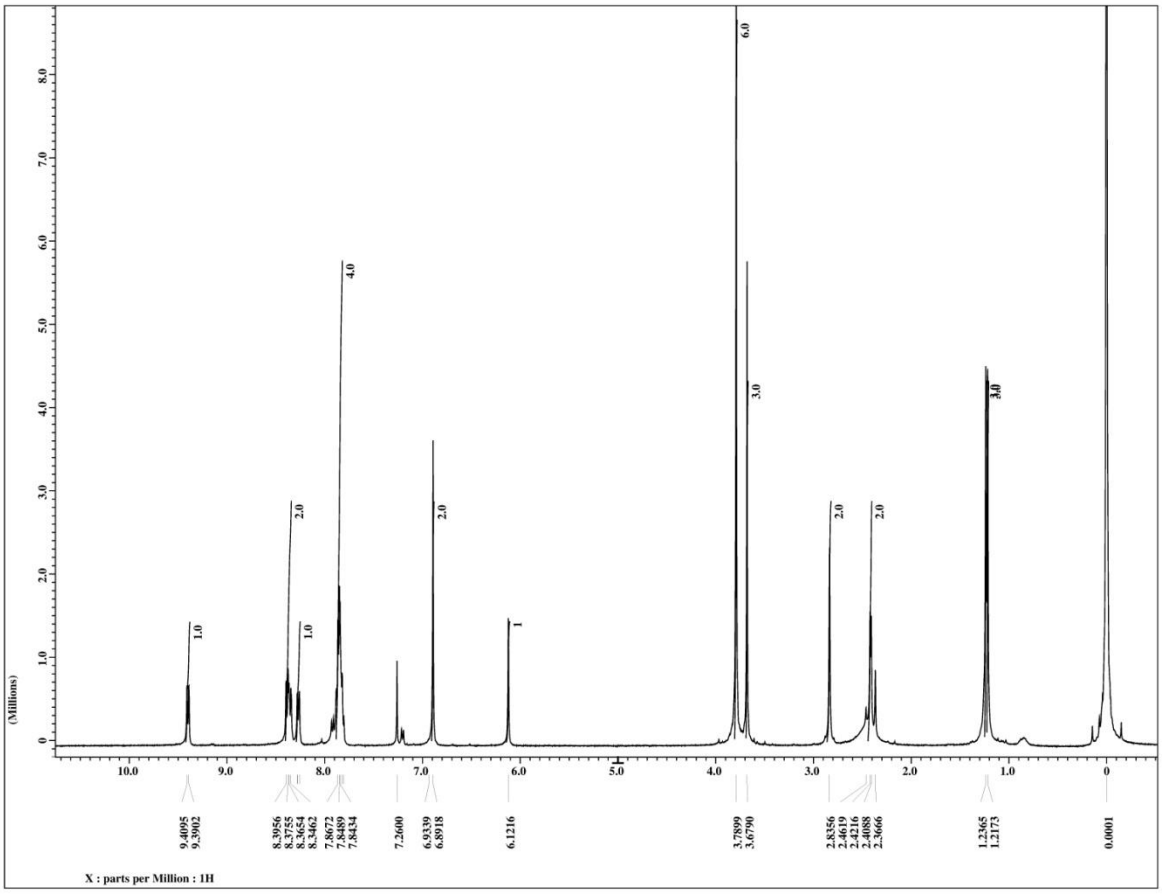

NH
O
N
N
O

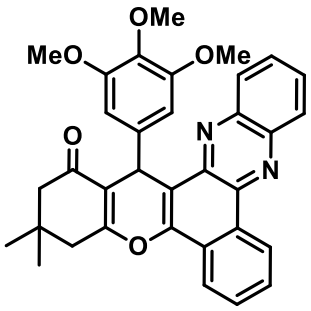
4l-^{13}C-NMR


(Millions)
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.1022
164.3353
147.7493
147.2063
142.5035
142.2129
140.7218
140.2247
131.3467
130.3303
129.8326
129.6720
129.2591
128.9303
126.0857
120.0992
115.1277
114.2712
77.5204
77.1992
76.8857
51.0469
41.4118
33.7191
32.6638
29.5210
27.8616
0.1646
X : parts per Million : 13C

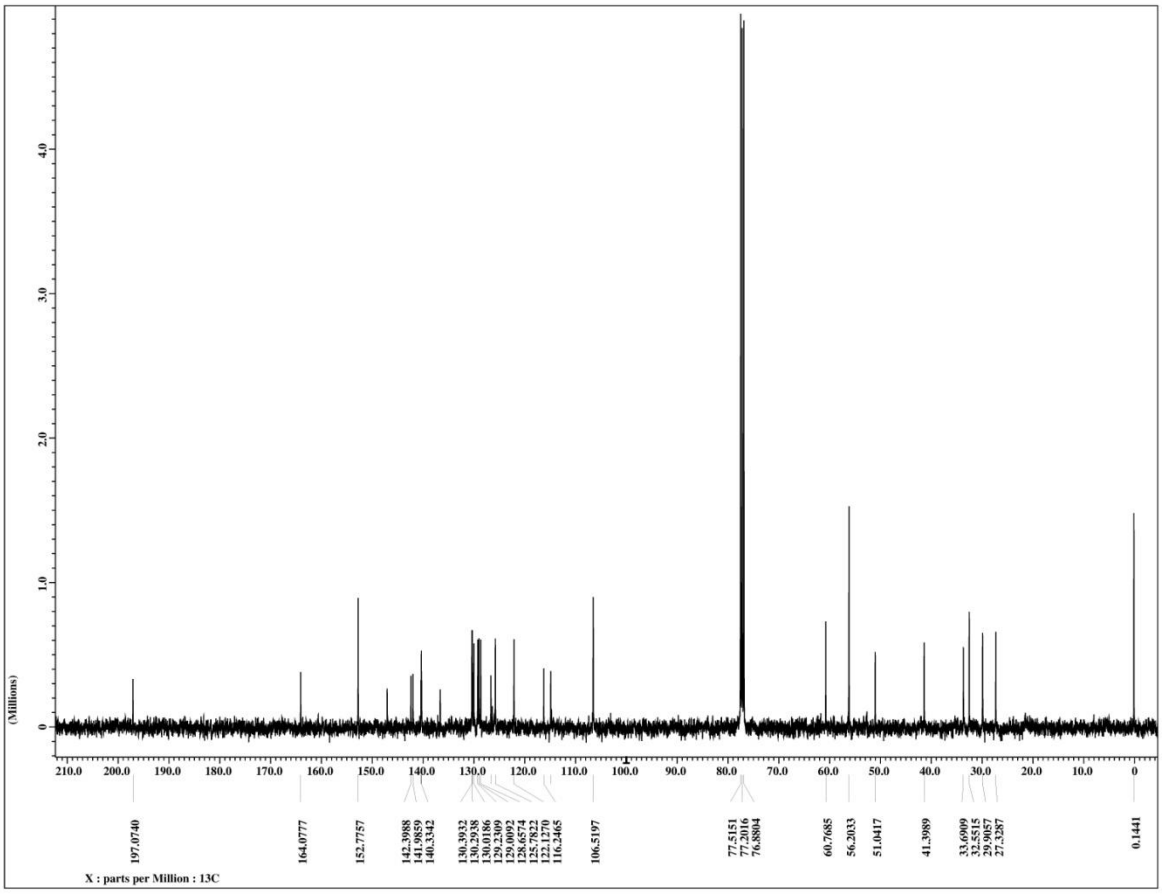

OMe
MeO
OMe
O
N
N
O

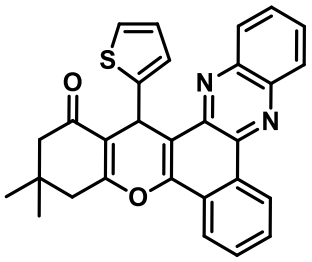
4m-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.4095
9.3902
8.3956
8.3755
8.3654
8.3462
7.8672
7.8489
7.8434
7.2600
6.9339
6.8918
6.1216
3.7899
3.6790
2.8356
2.4619
2.4216
2.4088
2.3666
1.2365
1.2173
0.0001

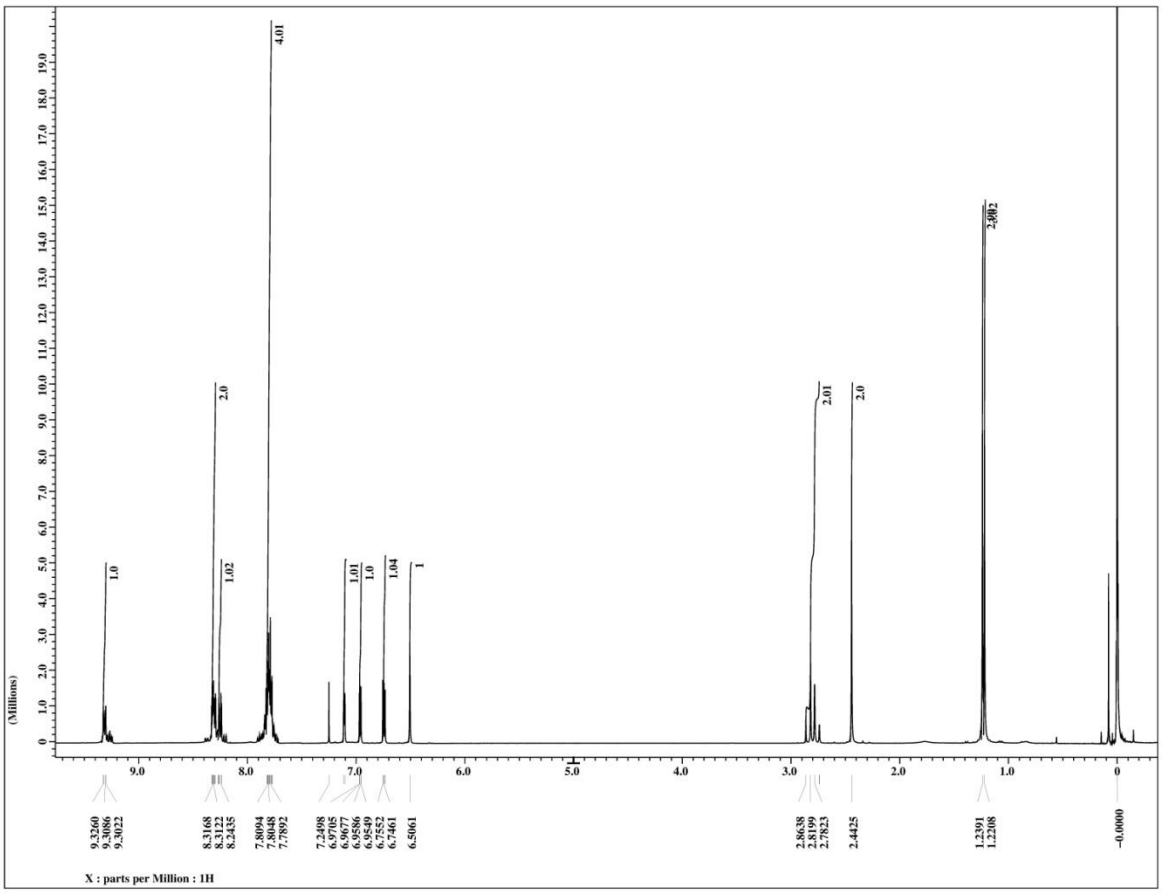

OMe
MeO
OMe
O
N
N
O

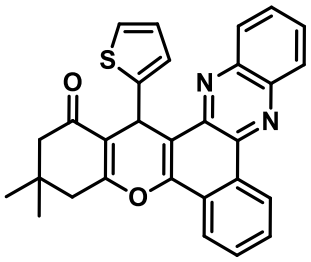
4m-^{13}C-NMR


(Millions)
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.0740
164.0777
152.7757
142.3988
141.9859
140.3342
130.3932
130.2938
130.0186
129.2309
129.0092
126.6574
125.7823
122.1270
116.2465
106.5197
77.5151
77.2016
76.8804
60.7685
56.2033
51.0417
41.3989
33.6909
32.5515
29.9087
27.3287
0.1441
X : parts per Million : 13C

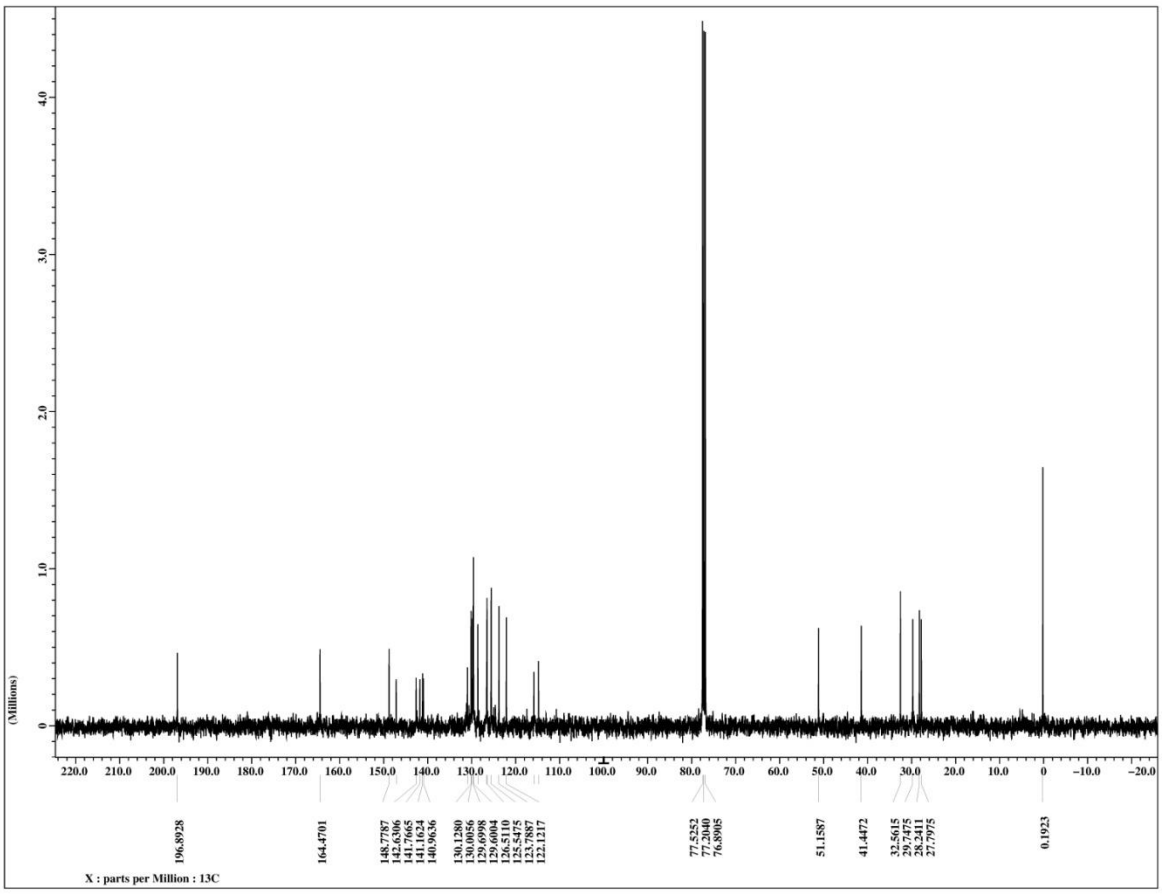

S
O
N
N
O

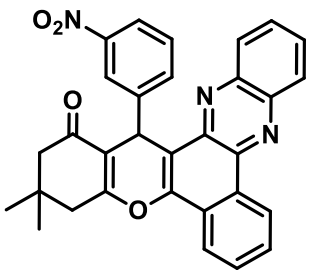
4n-^{1}H-NMR


(Millions)
4.01
2.0
1.02
1.0
1.01
1.0
1.04
1
2.01
2.0
2.982
9.3260
9.3086
9.3022
8.3168
8.3122
8.2435
7.8094
7.8048
7.7892
7.2498
6.9705
6.9677
6.9586
6.7552
6.7461
6.5061
2.8638
2.8199
2.7823
2.4425
1.2391
1.2208
-0.0000
X : parts per Million : 1H

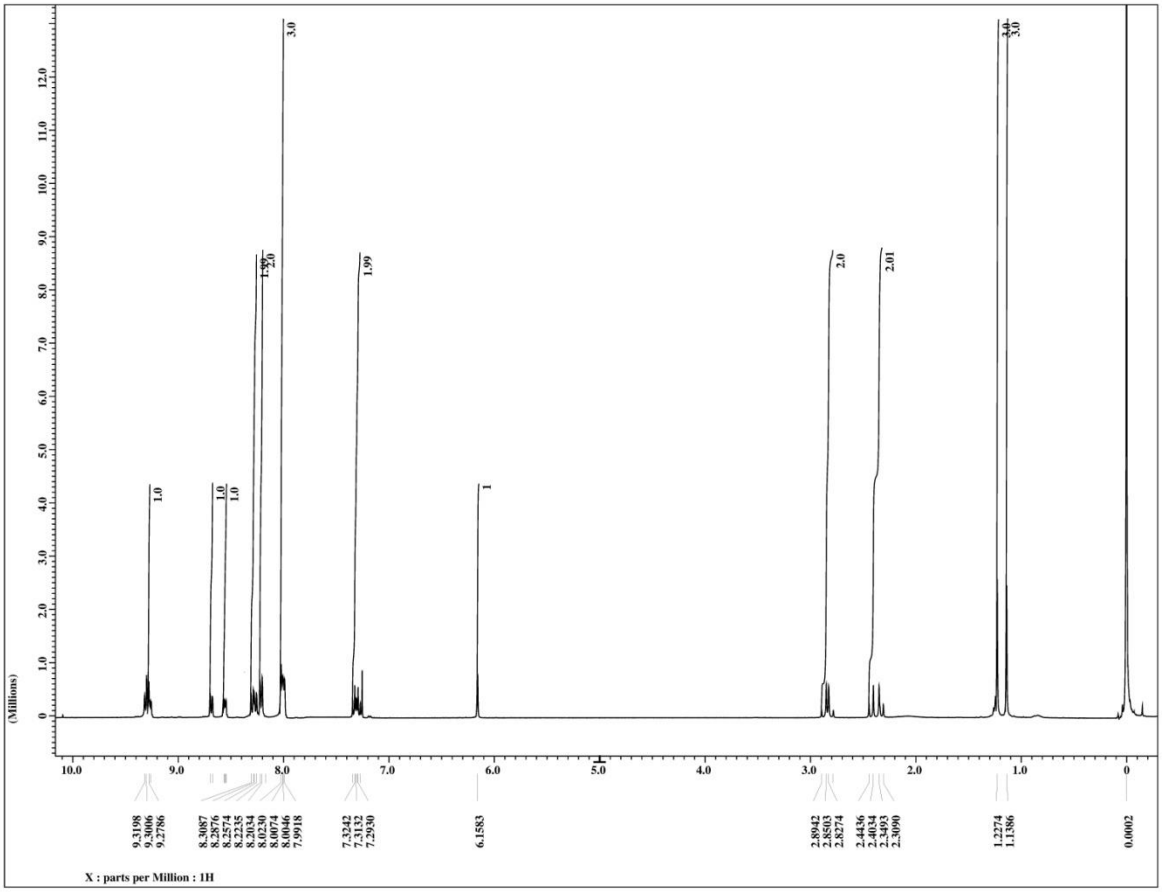

S
O
N
N
O

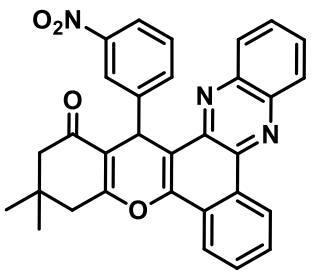
4n-^{13}C-NMR


(Millions)
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0 −20.0
196.8928
164.4701
148.7787
142.7566
141.1665
141.1624
140.9636
130.1280
130.0056
129.6998
129.6014
126.5110
125.5475
123.7887
122.1217
77.5252
77.2040
76.8905
51.1587
41.4472
32.5615
29.7475
28.2411
27.7975
0.1923
X : parts per Million : 13C

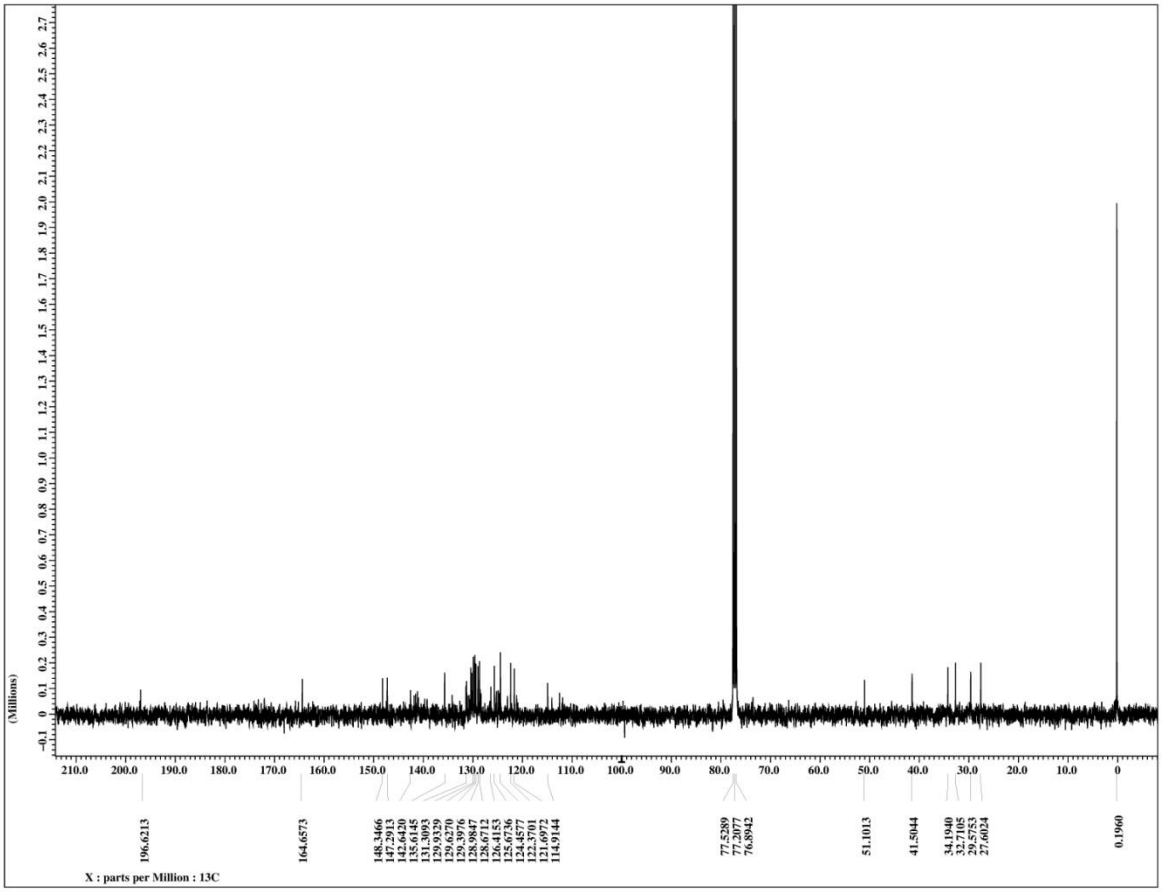


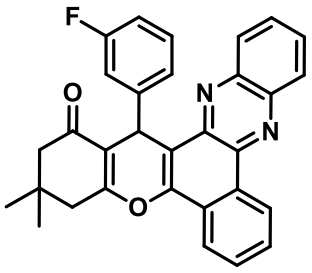
4o-^{1}H-NMR



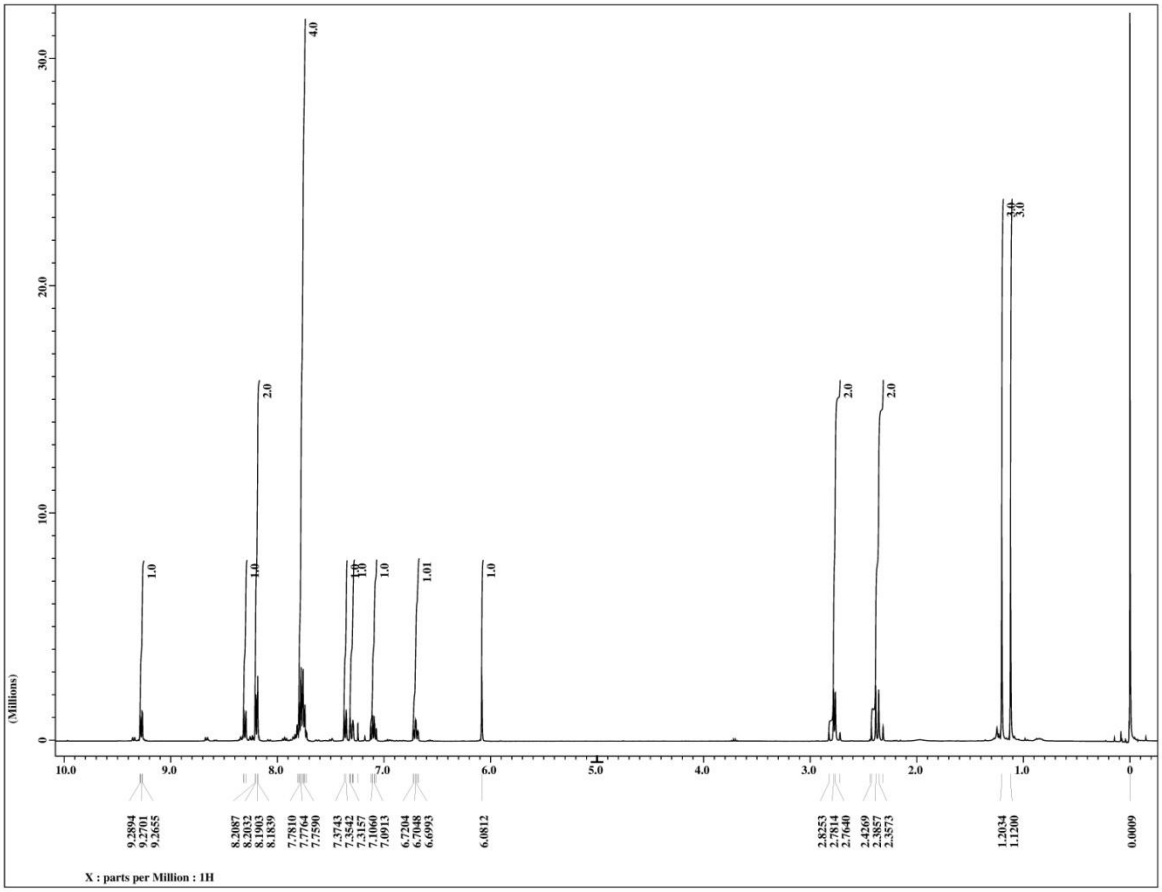

O2N
O
N
N
O

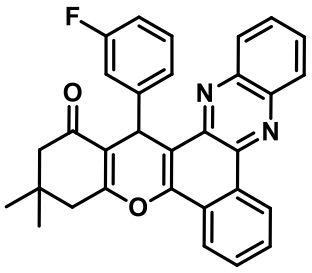
4o-^{13}C-NMR


(Millions)
X : parts per Million : 13C
196.6213
164.6573
148.3466
147.2913
142.6420
135.6145
131.3093
130.1939
129.6270
129.3976
128.9847
128.6712
126.4153
125.4756
124.4577
122.3701
121.6972
114.9144
77.5289
77.2077
76.8942
51.1013
41.5044
34.1940
32.7105
29.5753
27.6024
0.1960

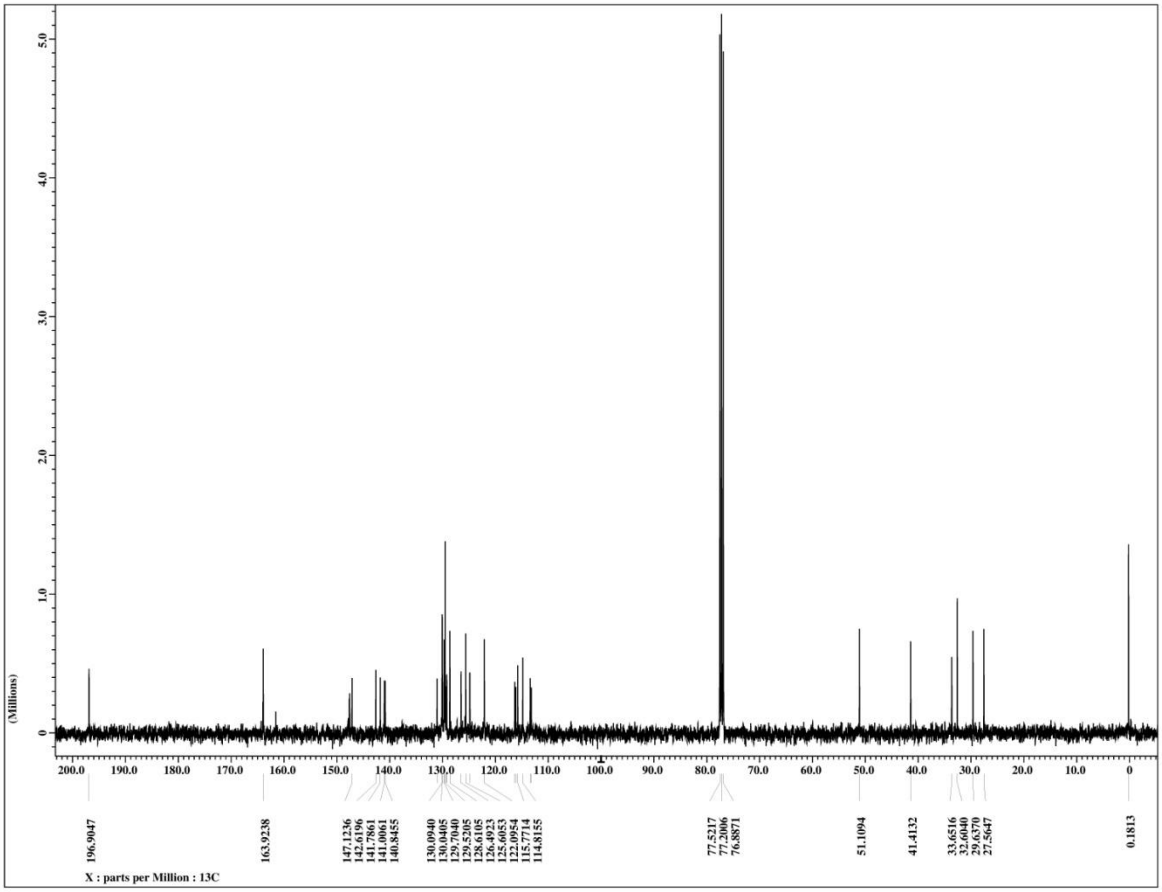

F
O
N
N
O

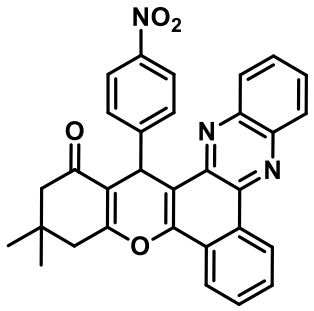
4p-^{1}H-NMR


(Millions)
30.0
20.0
10.0
0
4.0
2.0
1.0
1.0
1.0
1.0
1.01
1.0
2.0
2.0
1.0
3.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.2894
9.2701
9.2655
8.2087
8.2032
8.1903
8.1839
7.7810
7.7764
7.7590
7.3743
7.3542
7.3157
7.1060
7.0913
6.7204
6.7048
6.6993
6.0812
2.8253
2.7814
2.7640
2.4269
2.3857
2.3573
1.2034
1.1200
0.0009
X : parts per Million : 1H

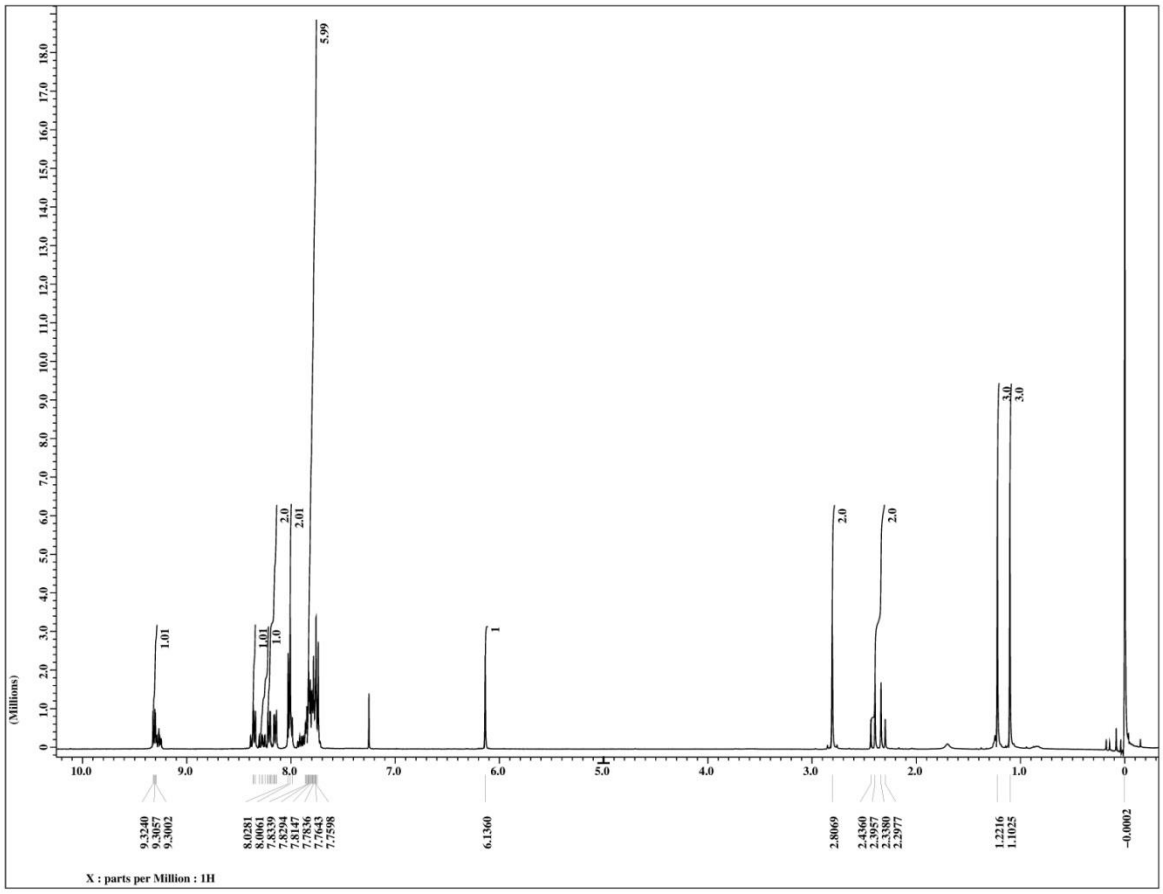

F
O
N
N
O

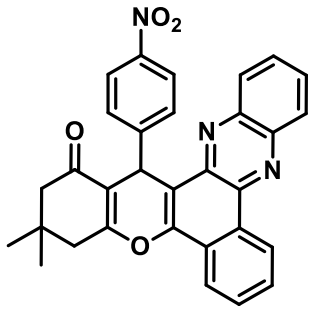
4p-^{13}C-NMR


(Millions)
5.0
4.0
3.0
2.0
1.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
196.9047
163.9238
147.1236
142.6196
141.7861
141.0061
140.8455
130.0940
130.0405
129.7040
129.5508
126.4923
125.6053
122.0954
115.7714
114.8155
77.5217
77.2006
76.8871
51.1094
41.4132
33.6516
32.6040
29.6370
27.5647
0.1813
X : parts per Million : 13C

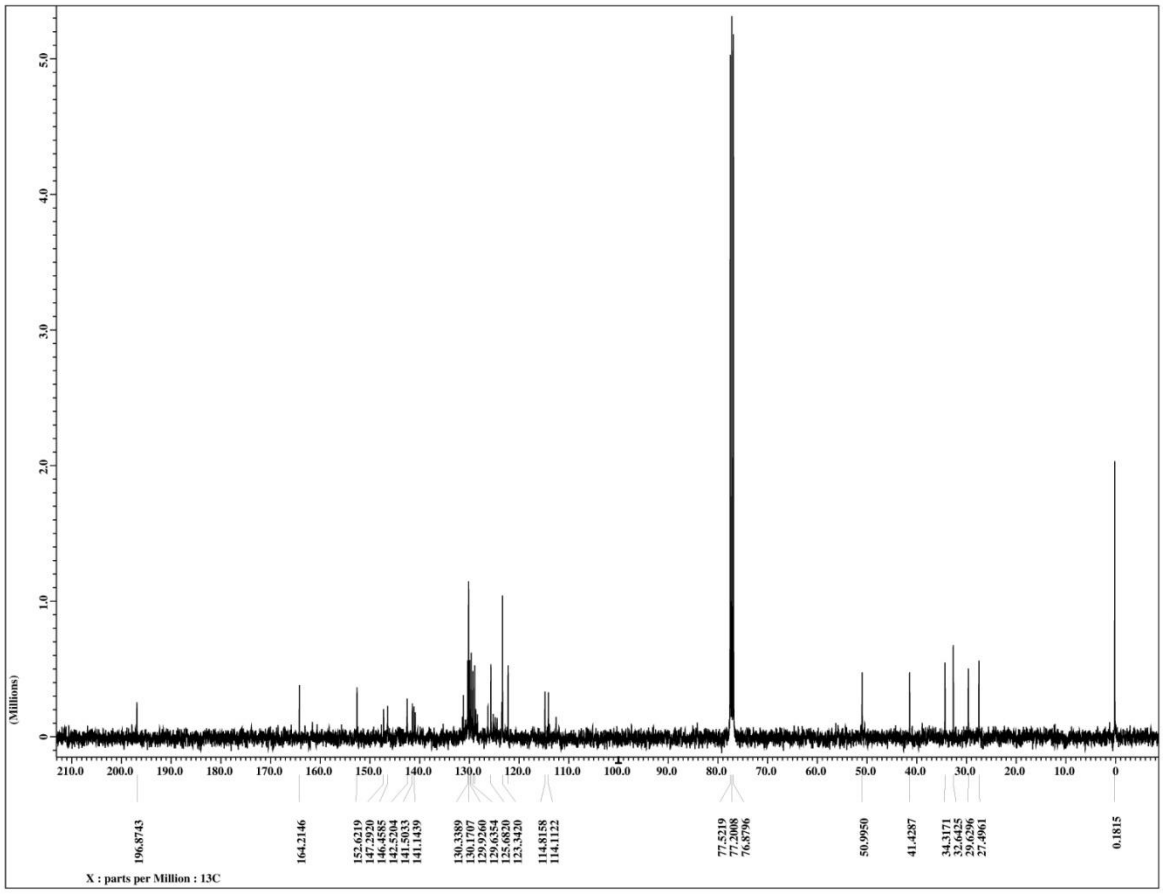

NO2
O
N
N
O

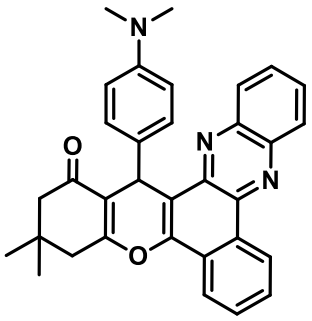
4q-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.3240
9.3057
9.3002
8.0281
8.0061
7.8339
7.8294
7.8147
7.7836
7.7643
7.7598
6.1360
2.8069
2.4360
2.3987
2.3980
2.2977
1.2216
1.1025
-0.0002

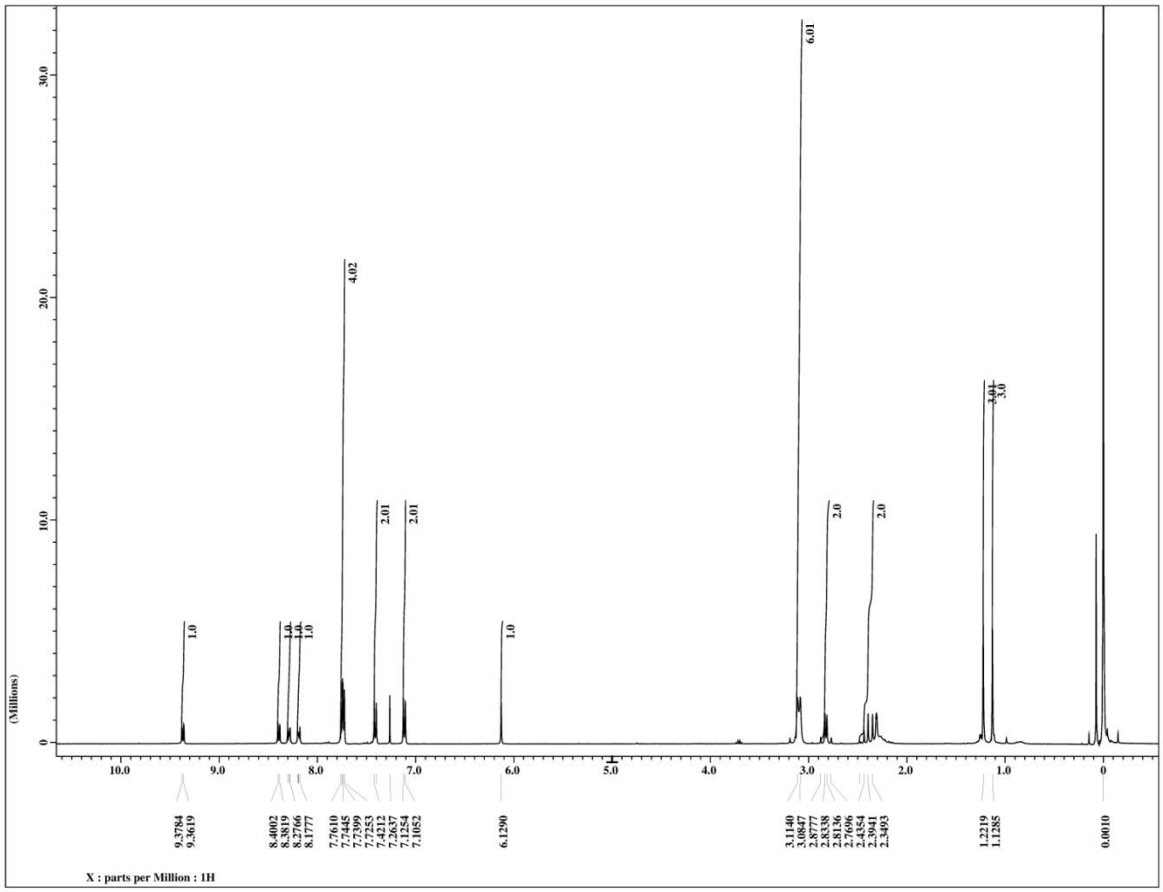

NO2
O
N
N
O

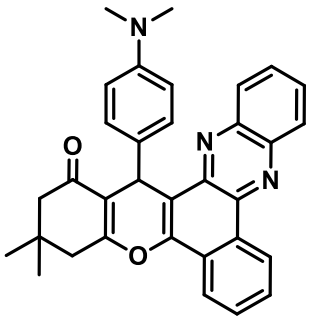
4q-^{13}C-NMR


(Millions)
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
196.8743
164.2146
152.6219
147.2920
146.4455
142.5204
141.5033
141.1439
130.3389
130.1707
129.9260
129.6154
125.6820
123.3420
114.8158
114.1122
77.5219
77.2008
76.8796
50.9950
41.4287
34.3171
33.6425
29.4936
27.4961
0.1815
X : parts per Million : 13C

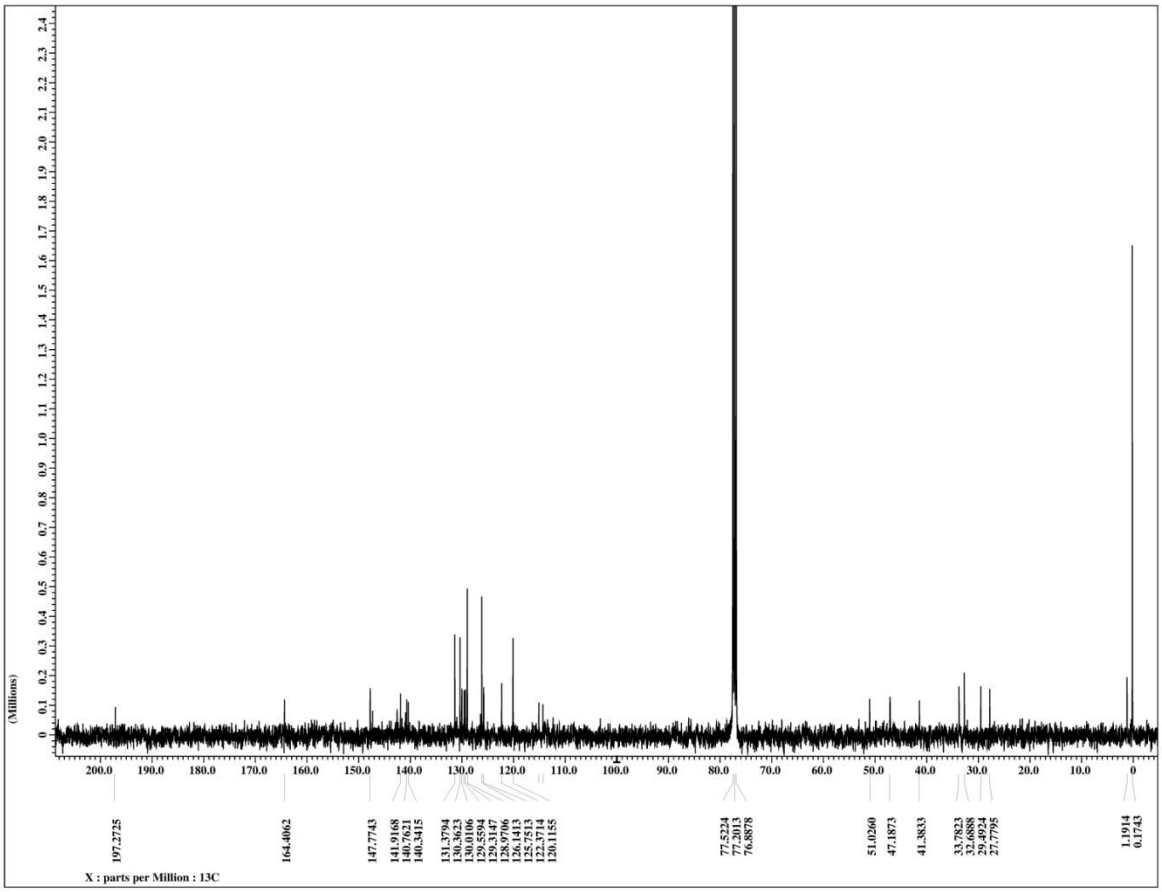


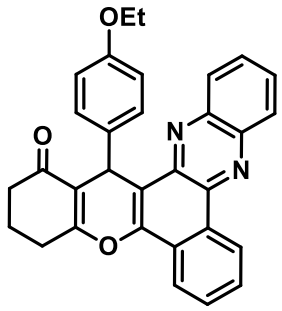
4r-^{1}H-NMR


(Millions)
30.0
20.0
10.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
6.01
4.02
2.01
2.01
2.0
2.0
3.01
3.0
1.0
1.0
1.0
1.0
1.0
9.3784
9.3619
8.4002
8.3819
8.2766
8.1777
7.7610
7.7448
7.7399
7.7253
7.4231
7.2637
7.1254
7.1052
6.1290
3.1140
3.0847
2.8777
2.8338
2.8136
2.7696
2.4354
2.3041
2.3493
1.2219
1.1285
0.0010
X : parts per Million : 1H

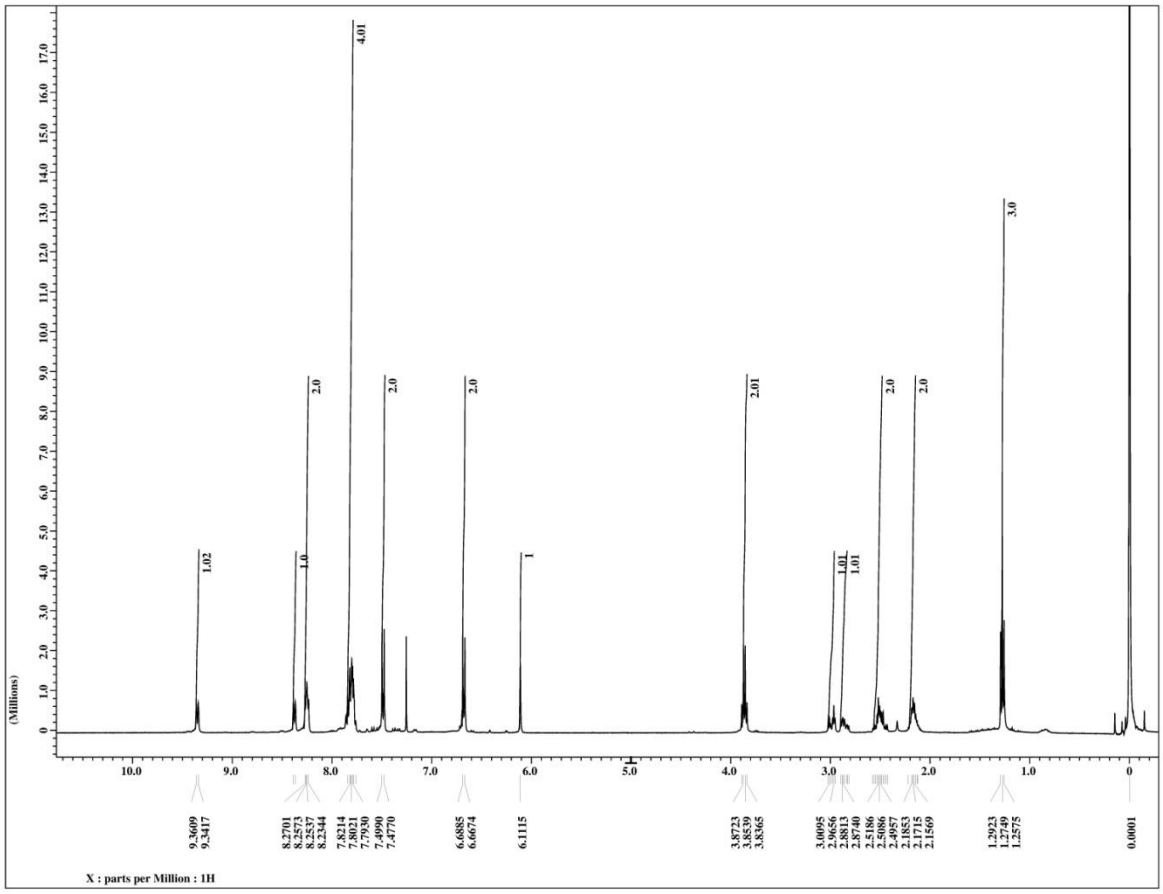


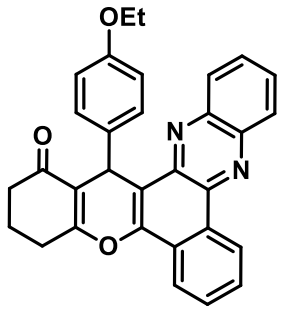
4r-^{13}C-NMR


(Millions)
X : parts per Million : 13C
197.2725
164.4062
147.7743
141.9168
140.7621
140.3415
131.3794
130.3623
130.0106
129.5594
129.3147
128.9706
126.1413
125.7513
122.3714
120.1155
77.5234
77.2013
76.8878
51.0260
47.1873
41.3833
33.7823
32.4698
29.4914
27.7795
1.1914
0.1743

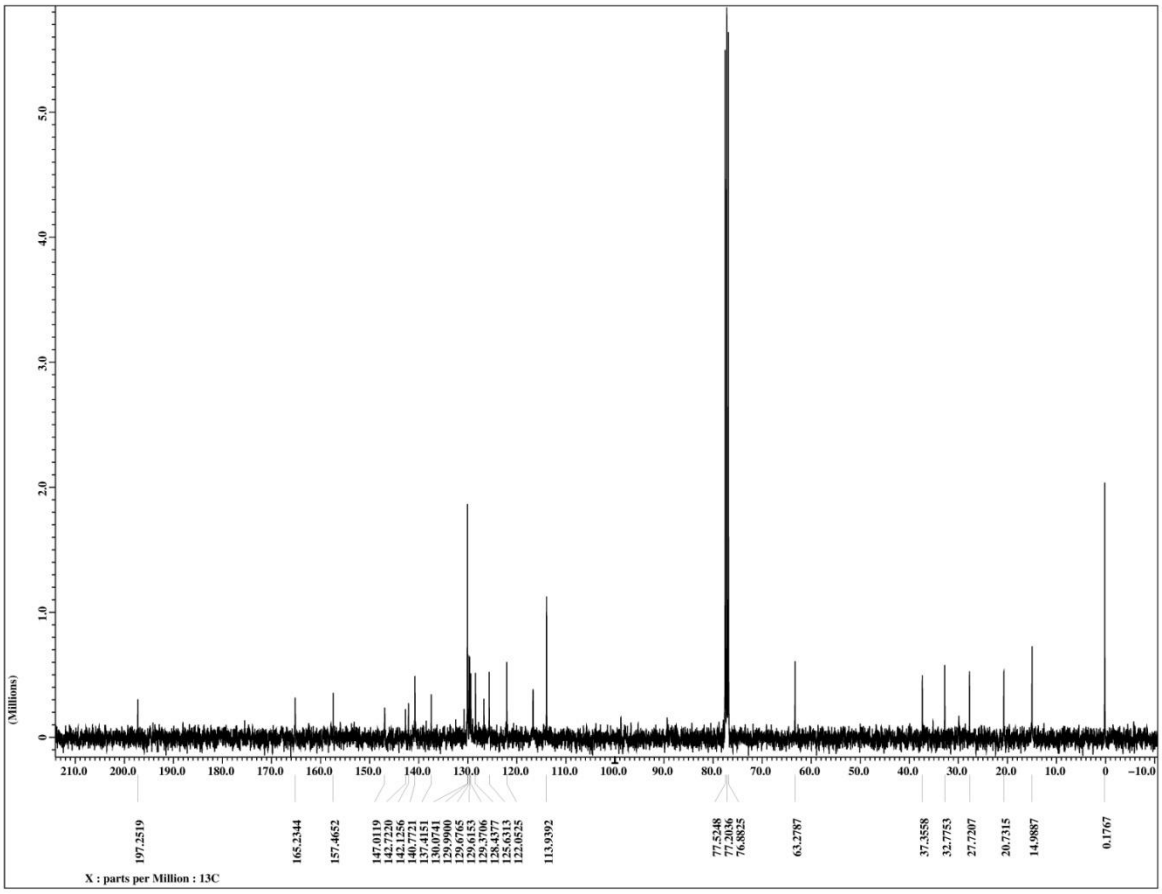

OEt
O
N
N
O

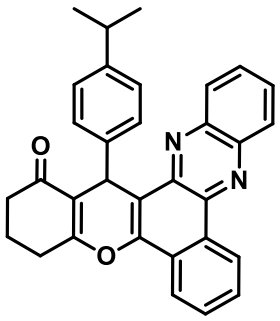
4s-^{1}H-NMR


(Millions)
X : parts per Million : 1H
1.02
1.0
2.0
4.01
2.0
2.0
1
2.01
1.01
1.01
2.0
2.0
3.0
9.3609
9.3417
8.2701
8.2573
8.2537
8.2344
7.8214
7.8021
7.7930
7.4990
7.4770
6.6885
6.6674
6.1115
3.8723
3.8539
3.8365
3.0095
2.8656
2.8513
2.8740
2.5186
2.5086
2.4957
2.1853
2.1715
2.1569
1.2923
1.2749
1.2575
0.0001

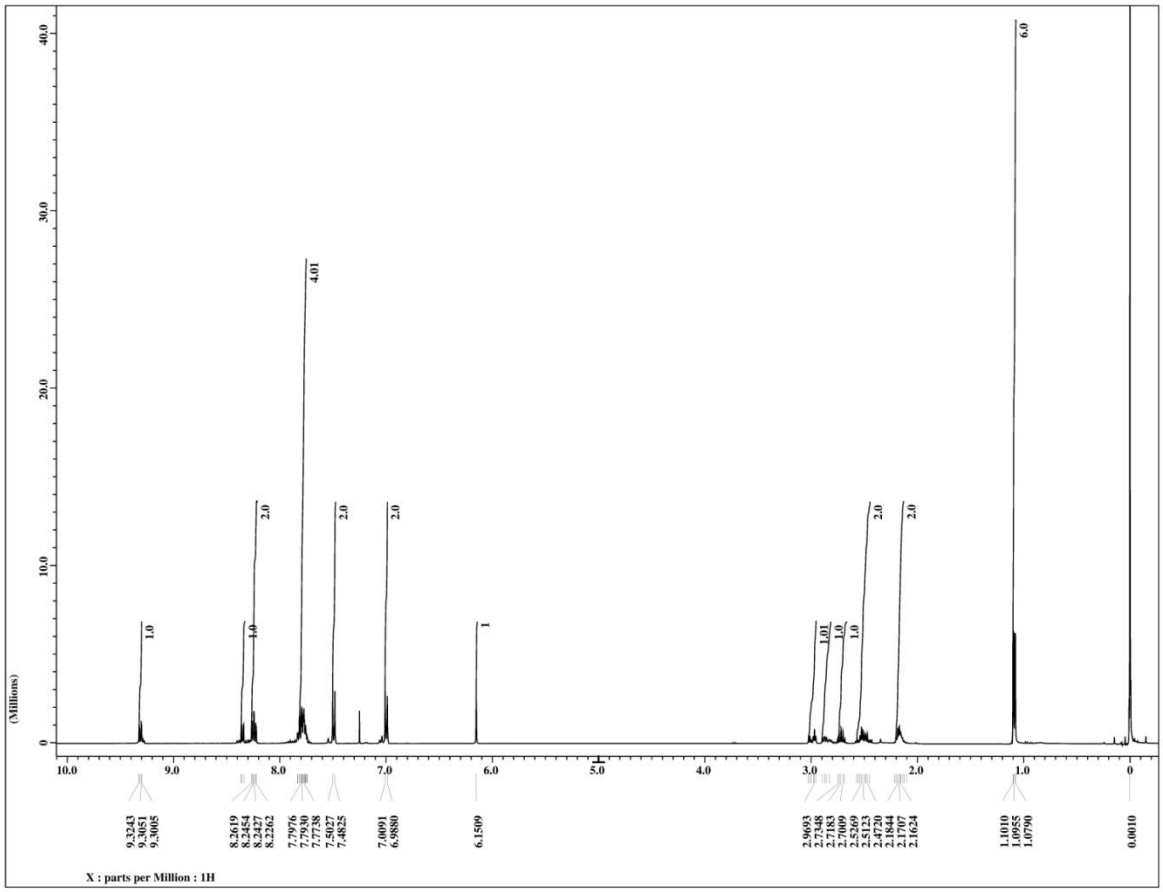

OEt
O
N
N
O

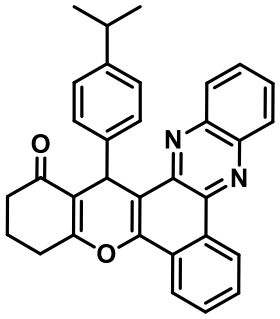
4s-^{13}C-NMR


(Millions)
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0
197.2519
165.2344
157.4652
147.0119
142.7220
142.1256
140.7721
137.1451
130.0741
129.9900
129.6765
129.6153
129.3706
128.4377
125.6111
122.0525
113.9392
77.5248
77.2036
76.8825
63.2787
37.3558
32.7753
27.7207
20.7315
14.9887
0.1767
X : parts per Million : 13C

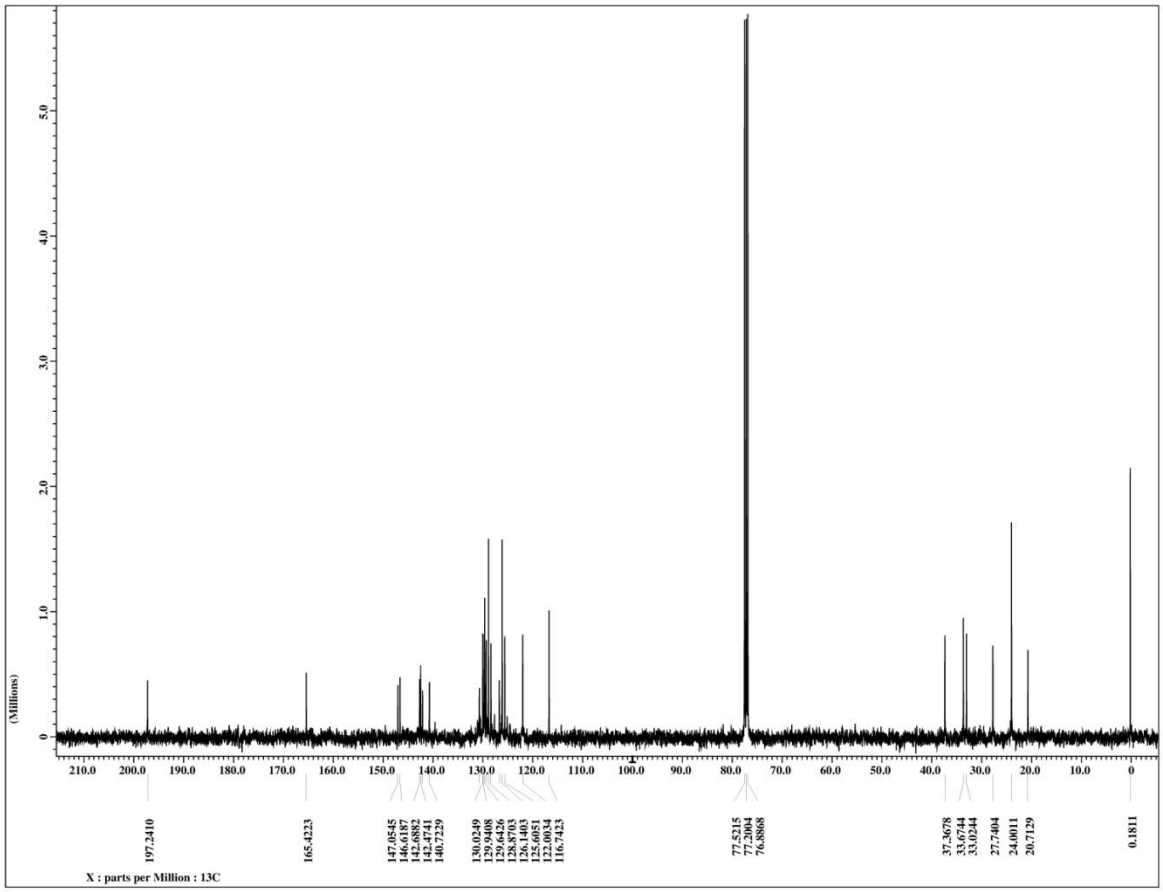

O
N
N
O

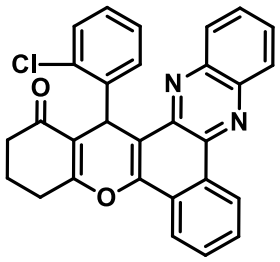
4t-^{1}H-NMR


(Millions)
40.0
30.0
20.0
10.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.0
2.0
1.0
4.01
2.0
2.0
1
1.01
1.0
1.0
2.0
2.0
6.0
9.3343
9.3051
9.3005
8.2619
8.2454
8.2427
8.2262
7.7976
7.7930
7.7738
7.5027
7.4825
7.0091
6.9880
6.1509
2.9693
2.7548
2.7334
2.7009
2.5269
2.5123
2.4720
2.1844
2.1707
2.1624
1.1010
1.0955
1.0790
0.0010
X : parts per Million : 1H

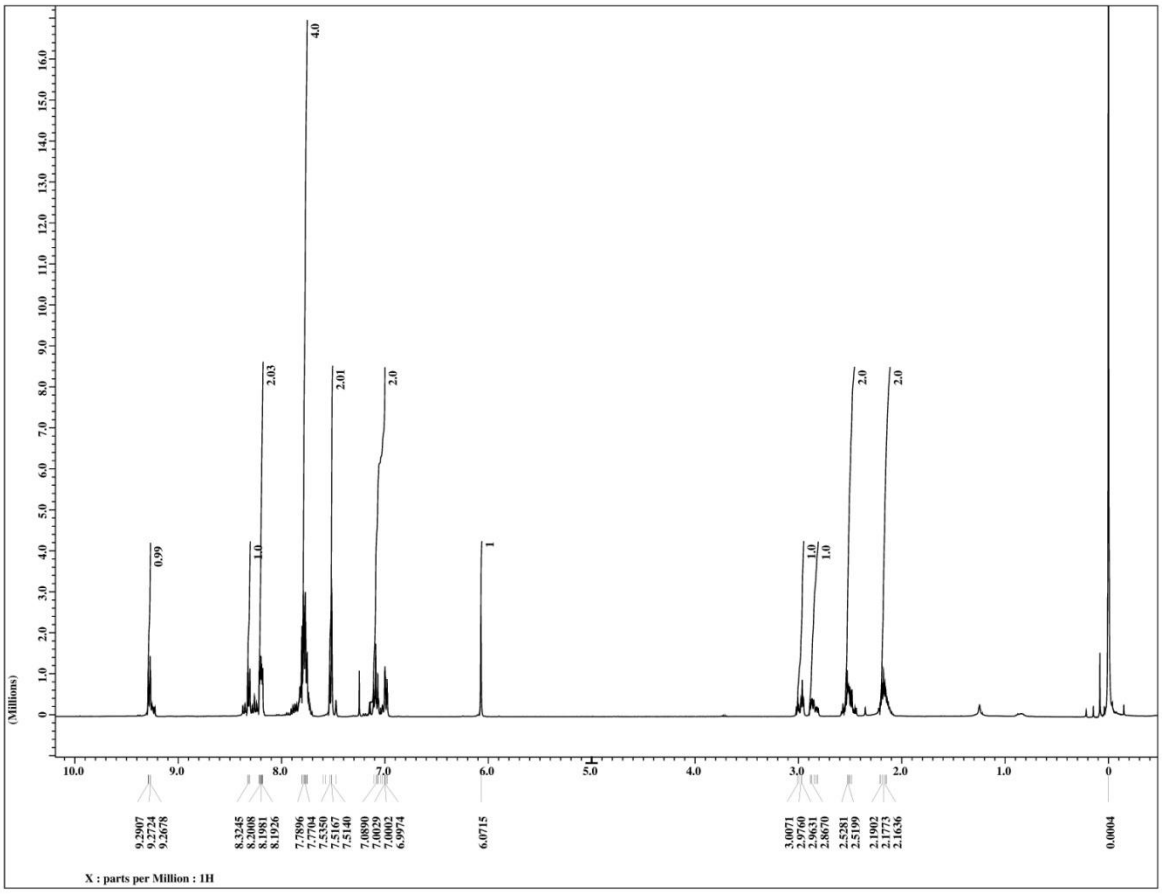

O
N
N
O

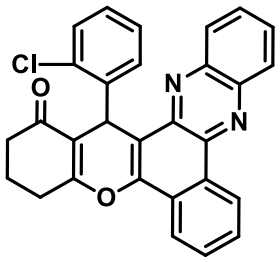
4t-^{13}C-NMR


(Millions)
0
1.0
2.0
3.0
4.0
5.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.2410
165.4223
147.0545
146.6187
142.6882
142.3741
140.7229
130.0249
129.9408
129.6426
128.8703
126.1403
125.6051
122.0034
116.7423
77.5215
77.2004
76.8868
37.3678
33.6744
33.0244
27.7404
24.9011
20.7129
0.1811
X : parts per Million : 13C

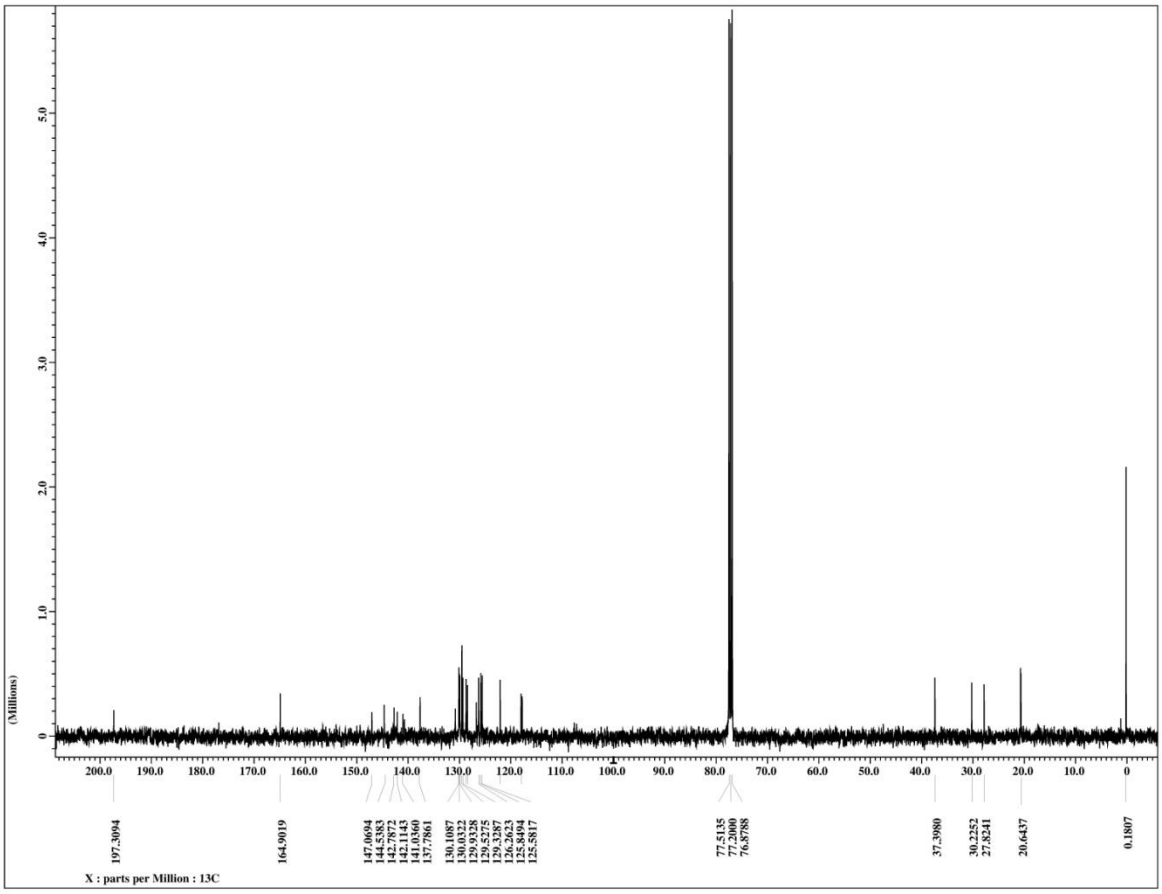

Cl
O
N
N
O

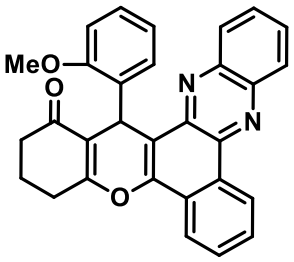
4u-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.2907
9.2724
9.2678
8.3345
8.2008
8.1981
8.1926
7.7896
7.7704
7.5350
7.5167
7.5140
7.0890
7.0029
7.0002
6.9974
6.0715
3.0071
2.9760
2.9631
2.8670
2.5381
2.5199
2.1902
2.1773
2.1636
0.0004

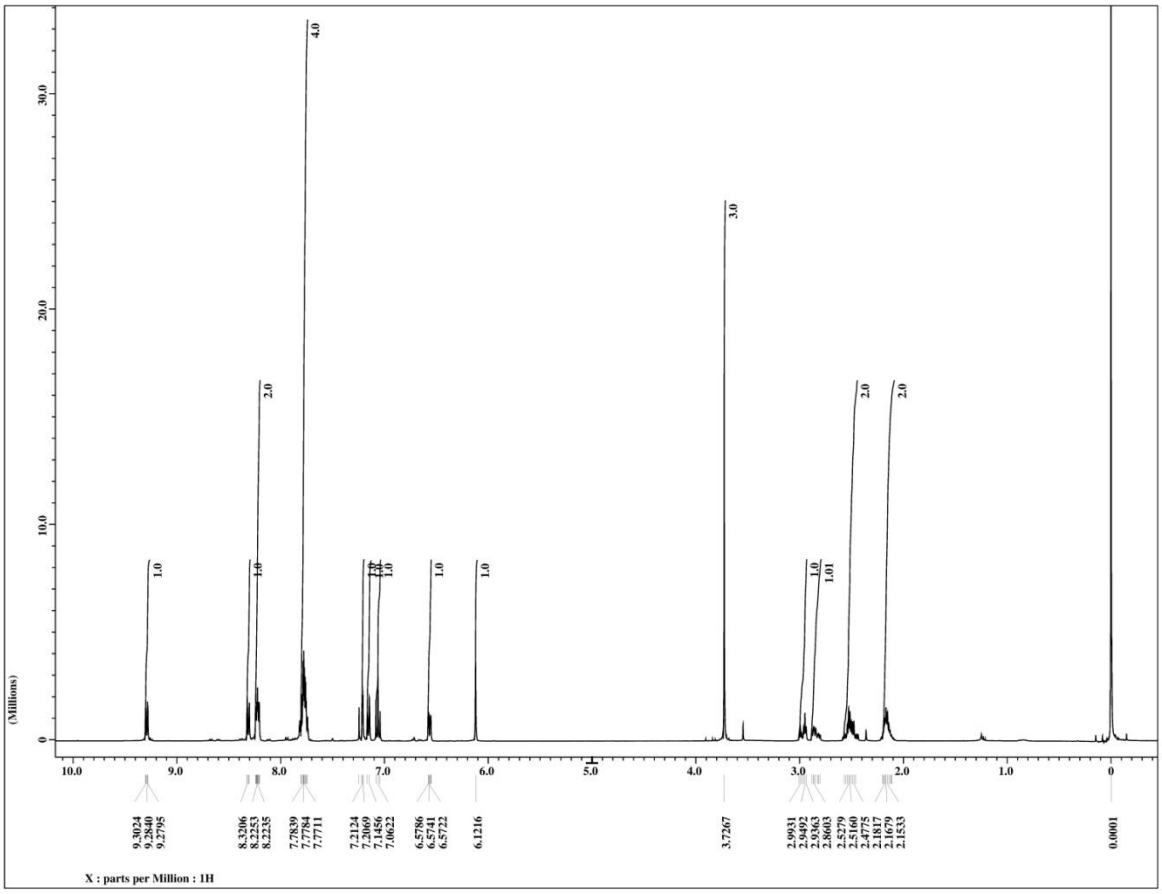

Cl
O
N
N
O

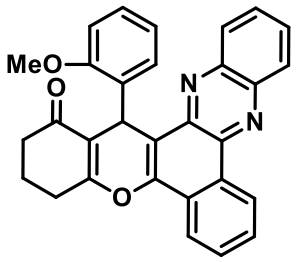
4u-^{13}C-NMR


(Millions)
0
1.0
2.0
3.0
4.0
5.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
197.3094
164.9019
147.0694
144.5383
142.7872
142.1143
141.0360
137.7861
130.1087
130.0322
129.9328
129.5275
129.3287
126.5023
125.8404
125.5817
77.5135
77.3000
76.8788
37.3980
30.2252
27.8241
20.6437
0.1807
X : parts per Million : 13C

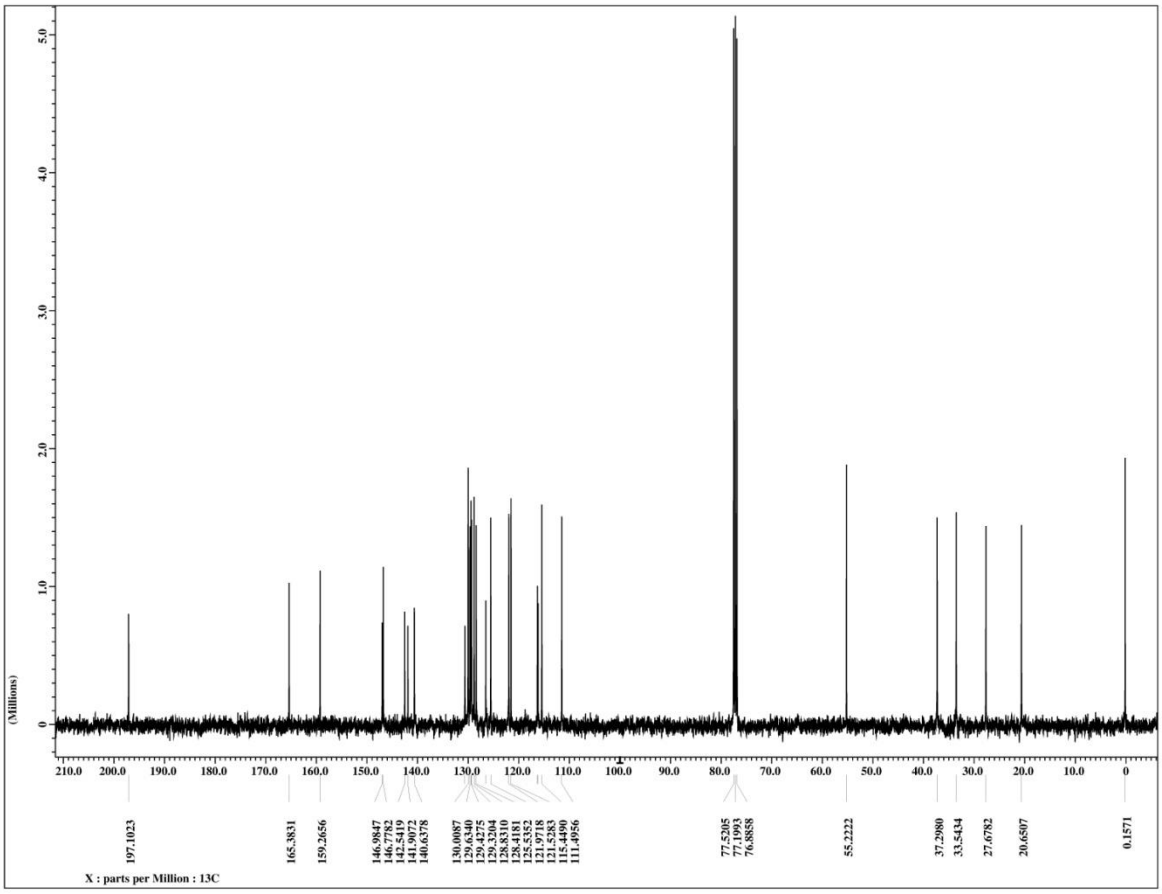

MeO
O
N
N
O

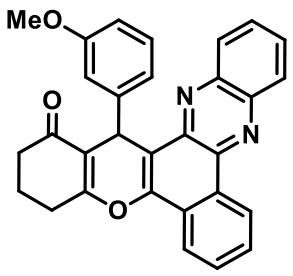
4v-^{1}H-NMR


(Millions)
30.0
20.0
10.0
0
4.0
3.0
2.0
2.0
2.0
1.0
1.0
1.0
1.0
1.0
1.0
1.0
1.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.3024
9.2840
9.2795
8.3306
8.2253
8.2235
7.7839
7.7784
7.7711
7.2124
7.2069
7.1456
7.0622
6.5786
6.5741
6.5722
6.1216
3.7267
2.9931
2.9492
2.8663
2.8603
2.5279
2.5160
2.4775
2.1817
2.1679
2.1533
0.0001
X : parts per Million : 1H

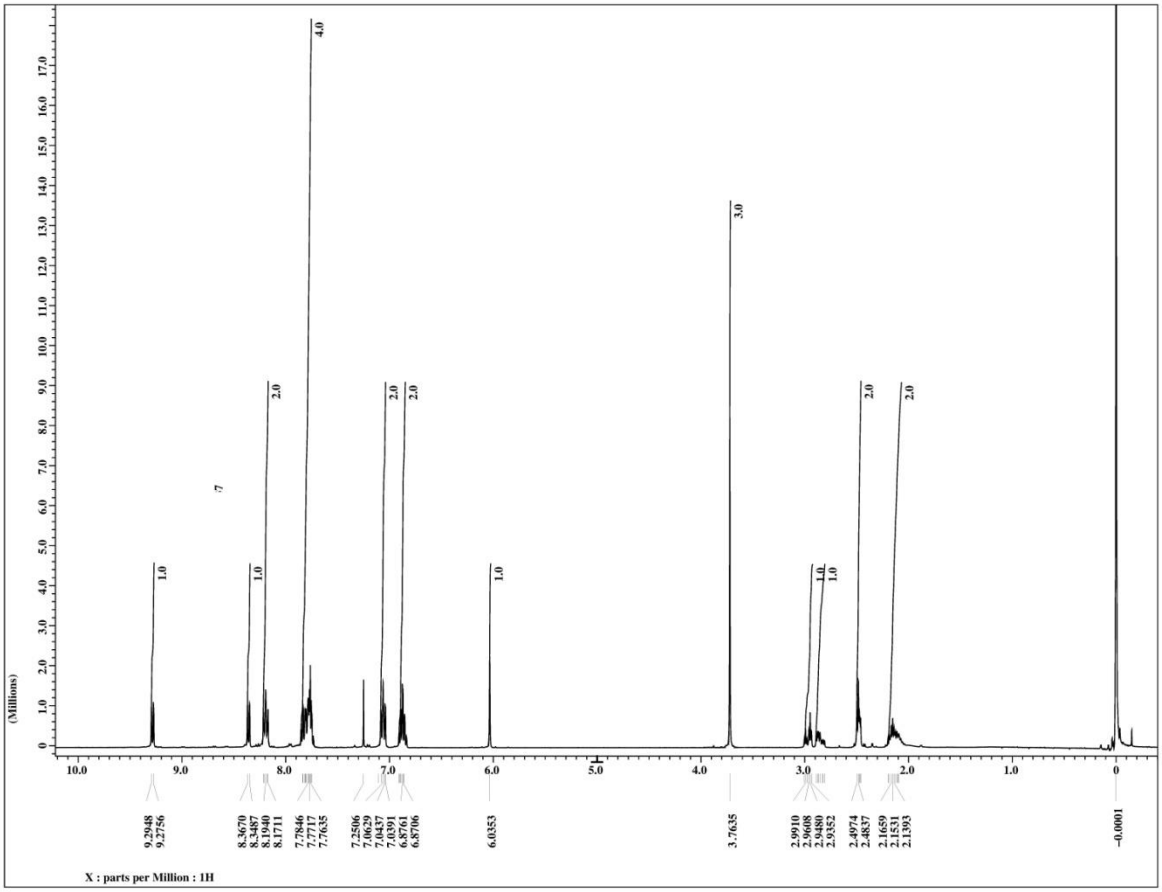

MeO
O
N
N
O

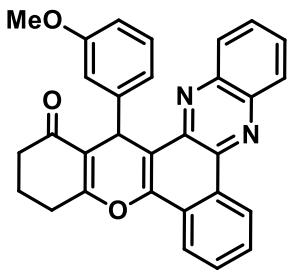
4v-^{13}C-NMR


(Millions)
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.1023
165.3831
159.2656
146.9847
146.7782
142.5419
141.9072
140.6378
130.0087
129.6340
129.3275
129.2034
128.8310
128.4181
125.5352
121.9718
121.5283
115.4460
111.4956
77.5205
77.1993
76.8858
55.2222
37.2980
33.5434
27.6782
20.6507
0.1571
X : parts per Million : 13C

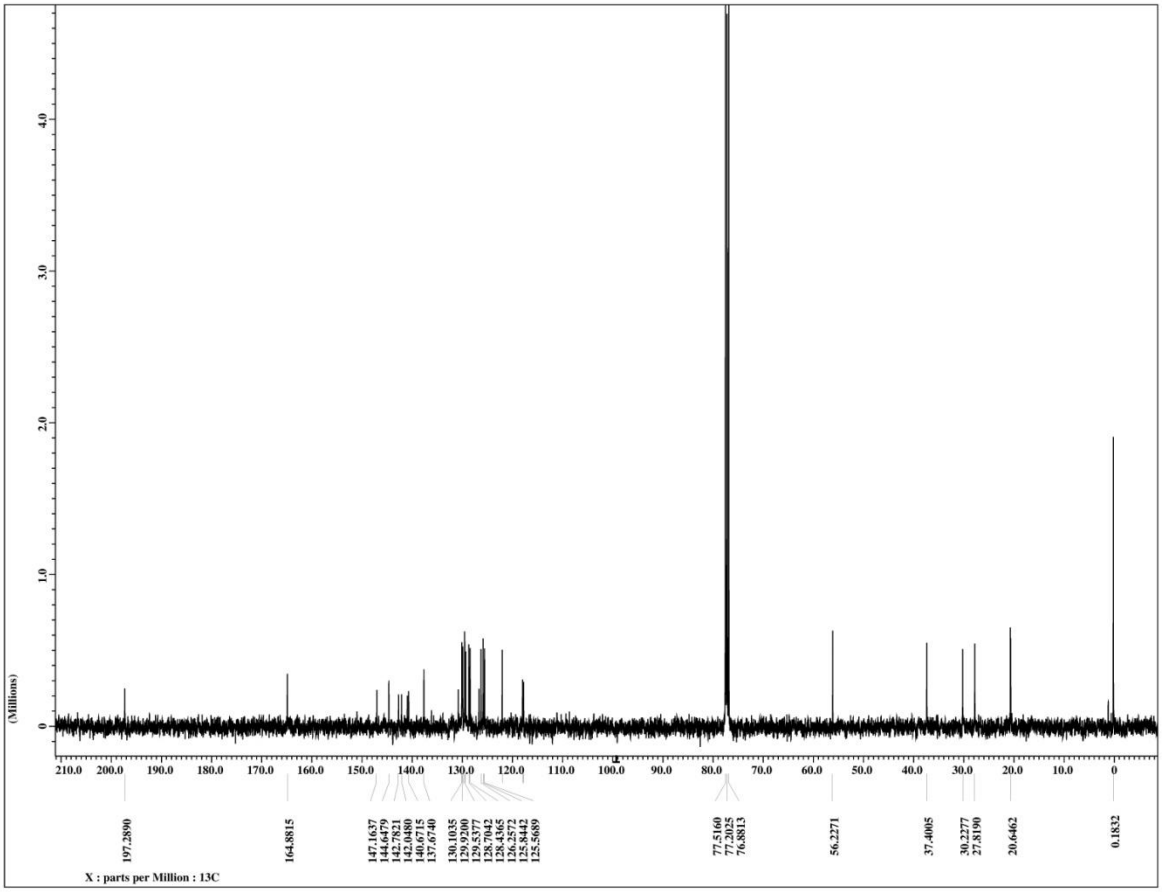

MeO
O
N
N
O

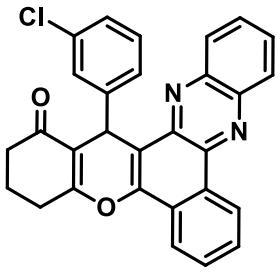
4w-^{1}H-NMR


(Millions)
X : parts per Million : 1H
9.2948
9.2756
8.3670
8.3487
8.1940
8.1711
7.7846
7.7777
7.7635
7.2506
7.0437
7.0391
6.8761
6.8706
6.0353
3.7635
2.9910
2.9608
2.9480
2.9352
2.4974
2.4837
2.1659
2.1531
2.1393
-0.0001

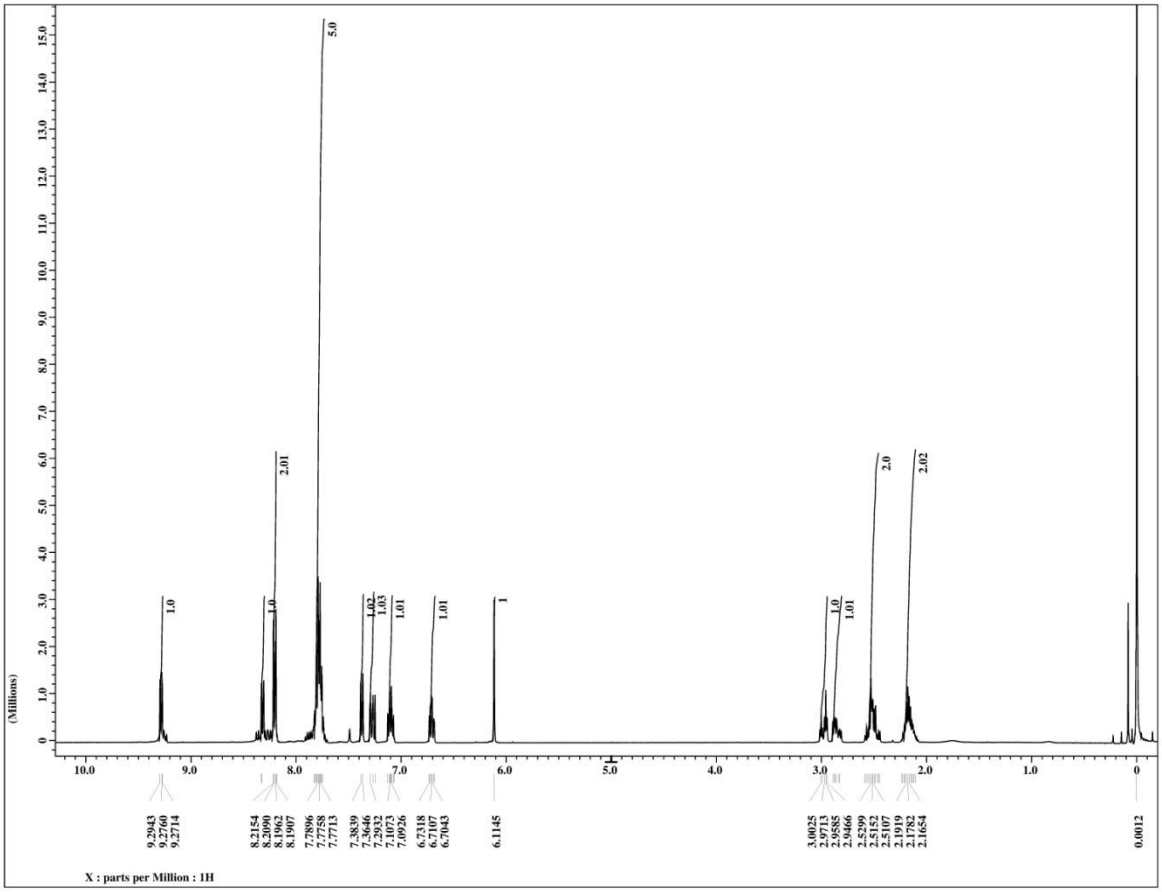

MeO
O
N
N
O

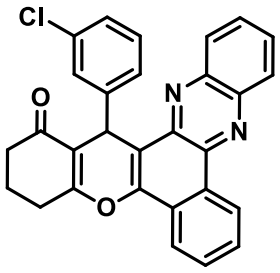
4w-^{13}C-NMR


(Millions)
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.2890
164.8815
147.1637
144.6479
143.7971
142.0480
140.6715
137.6740
130.1035
129.9200
129.5377
128.7042
128.4365
126.2572
125.8442
125.5689
77.5160
77.2025
76.8813
56.2271
37.4005
30.2277
27.8190
20.6462
0.1832
X : parts per Million : 13C

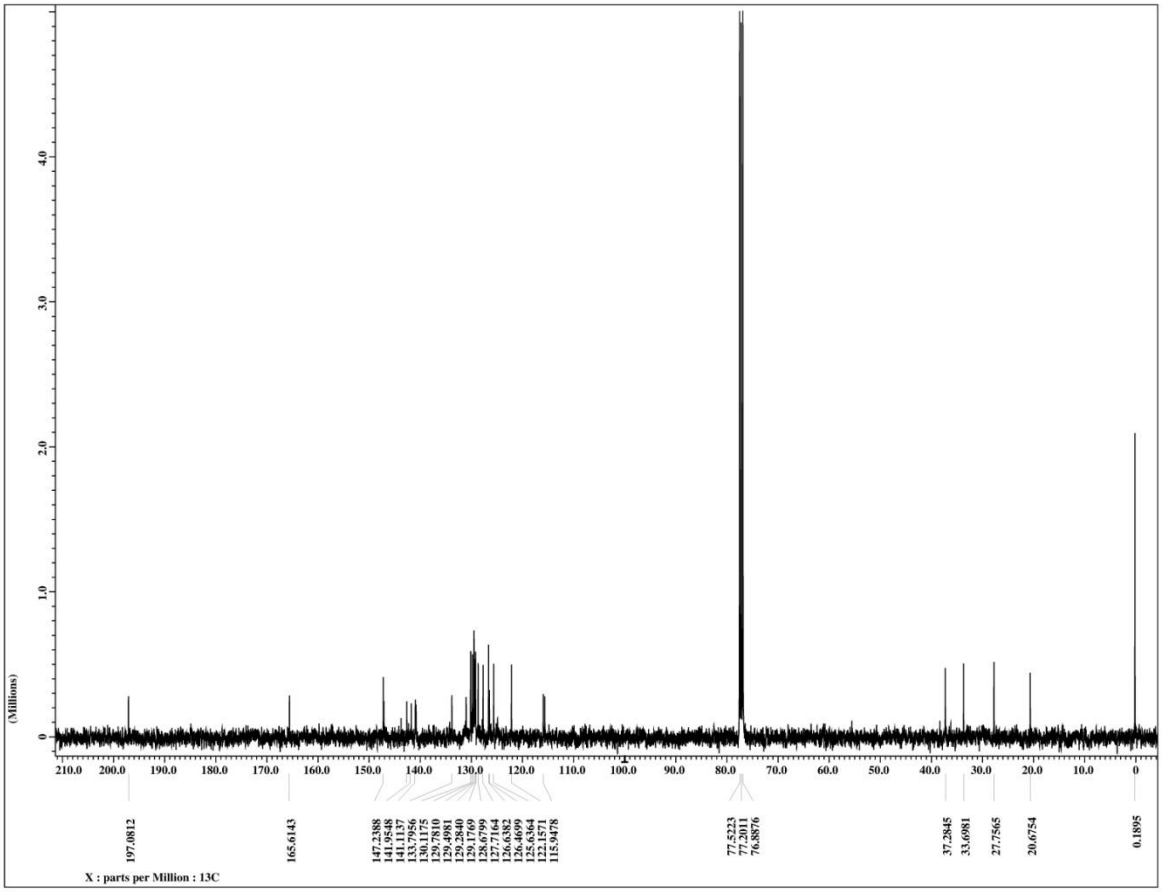


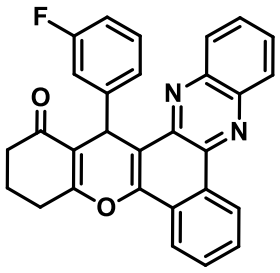
4x-^{1}H-NMR



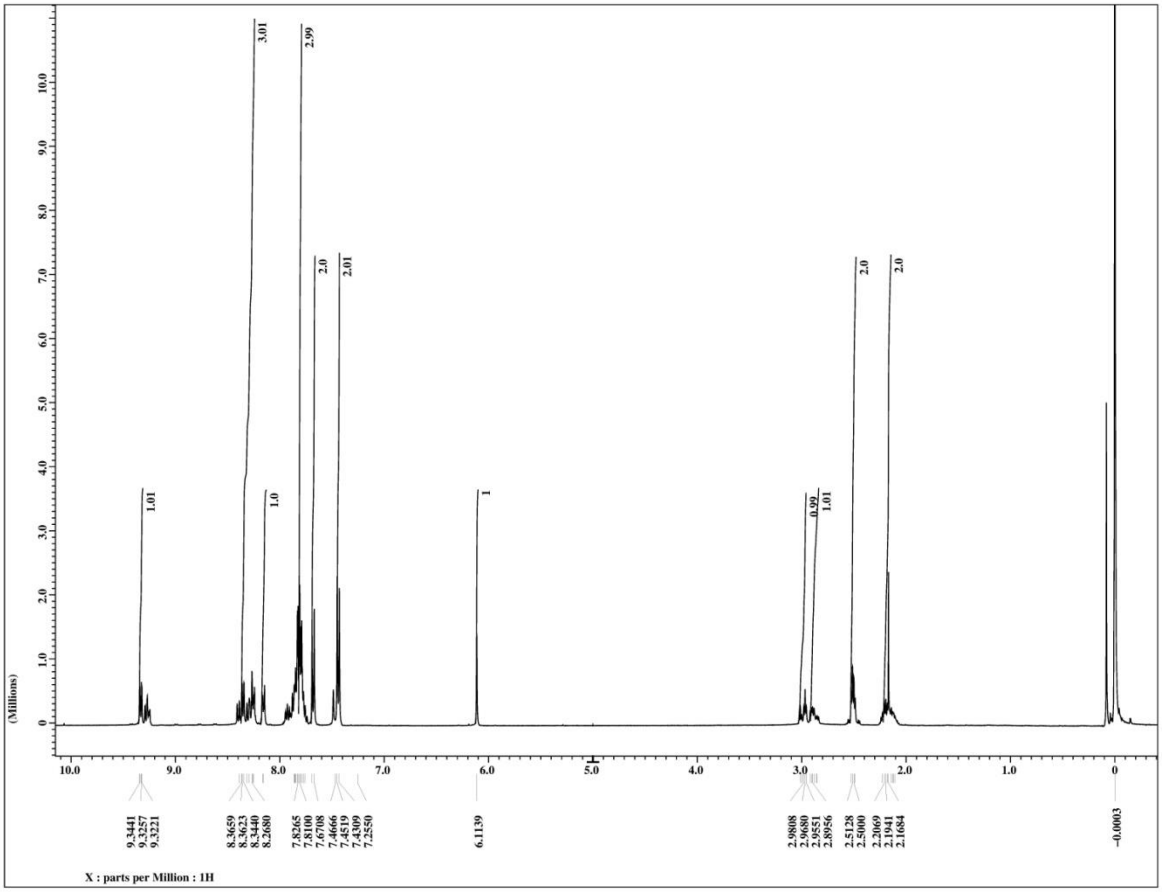

Cl
O
N
N
O

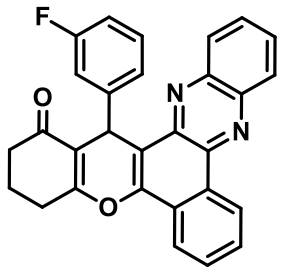
4x-^{13}C-NMR


(Millions)
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.0812
165.6143
147.2388
141.9548
141.1137
133.7956
131.1135
129.7810
129.4981
129.2840
129.1769
128.6799
127.7164
126.6452
126.4699
125.6364
122.1571
115.9478
77.5223
77.2011
76.8876
37.2845
33.6981
27.7565
20.6754
0.1895
X : parts per Million : 13C

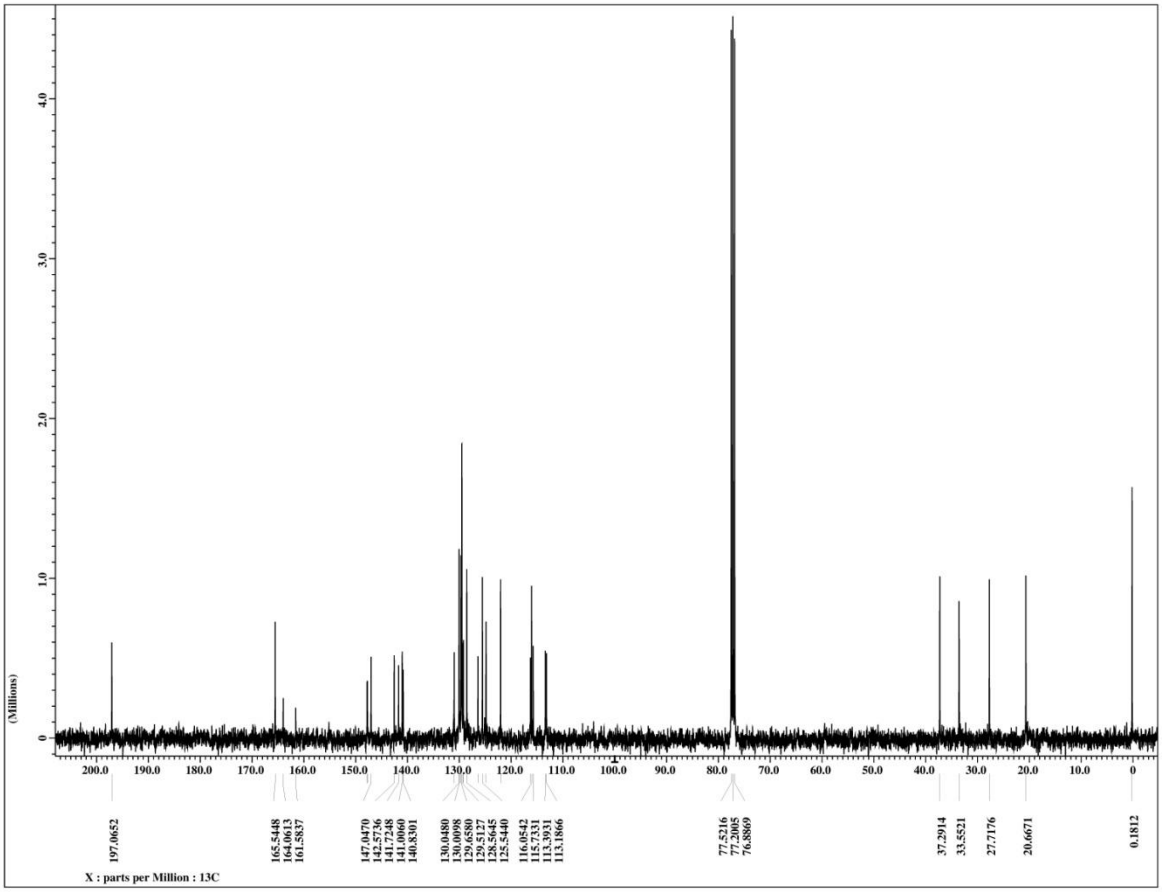

F
O
N
N
O

4y-^{1}H-NMR


(Millions)
3.01
2.99
2.0
2.01
1.01
1.0
1
0.99
1.01
2.0
2.0
9.3441
9.3257
9.3221
8.3659
8.3423
8.3401
8.2680
7.8265
7.8100
7.6708
7.4666
7.4519
7.4309
7.2550
6.1139
2.9808
2.9680
2.9551
2.8956
2.5128
2.5000
2.2069
2.1941
2.1684
-0.0003
X : parts per Million : 1H


F
O
N
N
O

4y-^{13}C-NMR


(Millions)
4.0
3.0
2.0
1.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.0652
165.5448
164.0613
161.5837
147.0470
142.5736
141.7248
141.0060
140.8301
130.0480
130.0098
129.6580
129.5147
128.5645
125.5440
116.0542
115.7731
113.3931
113.1866
77.5216
77.2005
76.8869
37.2914
33.5521
27.7176
20.6671
0.1812
X : parts per Million : 13C