# Temperature-Dependence of Radical-Trapping Activity of Phenoxazine, Phenothiazine and their Aza-Analogs Clarifies the Way Forward for New Antioxidant Design

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Supporting Information

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## Synthesis

**General.** Reagents were purchased from commercial suppliers and used without further purification. 2-Amino-3-(2-bromophenoxy)-pyridine,[1] *N*-acetyl-2-aminothiophenol,[2] 4-(2'-bromophenylthio)-3-nitropyridine,[3] 3-*tert*-butyl-6-aminophenol,[4] phenothiazine-3-one[5] and phenoxazine-N-oxyl[6] were synthesized according to literature procedures. Column chromatography was carried out using flash silica gel (40−63 μm, 230−400 mesh). $^{1}$H and $^{13}$C NMR were recorded on a Bruker AVANCE spectrometer at 600 and 151 MHz, respectively, unless specified otherwise. High-resolution mass spectra were obtained on a Kratos Concept Tandem mass spectrometer. Reported melting points are uncorrected.

***1-Azaphenoxazine.***[7] To 2-aminophenol (1.09 g, 10.0 mmol) in anhydrous DMSO (40 mL) were added 3-bromo-2-chloropyridine (1.93 g, 10.0 mmol) and cesium carbonate (3.25 g, 10 mmol) under an inert atmosphere. After stirring at 120 °C overnight, the solvent was removed under reduced pressure and the residue was dry-loaded onto a silica gel column. The crude material was purified by column chromatography using EtOAC/hexanes (4:6 to 10:0) as eluent to afford the title compound as a solid (350 mg, 19%). $^{1}$H-NMR (500 MHz; DMSO-$d_6$): δ 9.00 (s, 1H), 7.52 (dd, *J* = 5.0, 1.4 Hz, 1H), 6.89-6.87 (m, 1H), 6.75 (ddd, *J* = 7.7, 6.9, 2.0 Hz, 1H), 6.66-6.60 (m, 2H), 6.58-6.54 (m, 2H). $^{13}$C NMR (126 MHz; DMSO-$d_6$): δ 146.0, 142.3, 142.7, 139.0, 131.3, 124.2, 121.3, 120.6, 116.5, 115.0, 114.1 HRMS (EI): Calc'd for $C_{11}H_8N_2O$: 184.0636, Found: 184.0651, Mp 209 – 211 °C.

***2-Azaphenoxazine.*** To a Schlenk tube was added 2-amino-3-(2-bromophenoxy)-pyridine (395 mg, 1.5 mmol), $Pd_2dba_3$ (54 mg, 0.06 mmol), Bippy Phos (122 mg, 0.24 mmol), KOH (126 mg, 2.25 mmol) and degassed tert-amyl alcohol (1 mL) under an inert atmosphere. After stirring at 120 °C for 3 days, EtOAc (50 mL) was added. The reaction mixture was filtered through celite and concentrated under reduced pressure. The residue was purified by column chromatography using EtOAc as eluent to afford the title compound as a solid (150 mg, 54%). $^{1}$H-NMR (600 MHz; DMSO-$d_6$): δ 8.36 (s, 1H), 7.74 (d, *J* = 5.2 Hz, 1H), 7.64 (s, 1H), 6.76 (td, *J* = 7.6, 1.5 Hz, 1H), 6.66-6.56 (m, 3H), 6.47 (dd, *J* = 7.8, 1.5 Hz, 1H). $^{13}$C NMR (151 MHz; DMSO-$d_6$): δ 149.1, 143.3, 141.8, 134.6, 131.9, 129.6, 124.8, 120.8, 115.5, 114.0, 110.2 HRMS (EI): Calc'd for $C_{11}H_8N_2O$: 184.0636, Found: 184.0615. Mp 207 – 210 °C.

***3-Azaphenoxazine.*** To 2-aminophenol (560 mg, 5.2 mmol) in DMSO (21 mL) were added 3-bromo-4-chloropyridine (1.0 g, 5.2 mmol) and cesium carbonate (3.4 g, 10.4 mmol) under an inert atmosphere. After stirring at 120 °C overnight, acetone and silica gel were added. The solvent was removed under reduced pressure and the residue was dry-loaded onto a silica gel column. The crude material was purified by column chromatography using EtOAC/MeOH (100:0 to 95:5) as eluent to afford the title compound as a pinkish solid (180 mg, 19%). $^{1}$H-NMR (400 MHz; DMSO-$d_6$): δ 8.80 (s, 1H), 7.78 (d, J = 5.1 Hz, 1H), 7.69 (s, 1H), 6.79-6.75 (m, 1H), 6.66-6.64 (m, 2H), 6.50 (dt, *J* = 7.4, 0.7 Hz, 1H), 6.39 (d, *J* = 5.1 Hz, 1H). $^{13}$C NMR (151 MHz; DMSO-$d_6$): δ 146.1, 143.0, 140.2, 139.0, 135.3, 130.4, 124.3, 121.9, 115.5, 114.1, 107.8 HRMS (EI): Calc'd for $C_{11}H_8N_2O$: 184.0636, Found: 184.0646. Mp 243 – 244 °C.

***4-Azaphenoxazine.***[7] 10-Acetyl-4-azaphenoxazine (160 mg, 0.72 mmol), was added to 5 ml of a freshly prepared solution of sodium methoxide in MeOH (0.6 M). The reaction was stirred for 15 minutes under an inert atmosphere. The precipitate was filtered, washed with water, and dried under vacuum. The solid was recrystallized from benzene to afford the title compound as a solid (54 mg, 40%). $^{1}$H-NMR (500 MHz; DMSO-$d_6$): δ 8.47 (s, 1H), 7.36 (dd, *J* = 4.8, 1.8 Hz, 1H), 6.78-6.72 (m, 3H), 6.68 (dd, *J* = 7.9, 1.4 Hz, 1H), 6.61 (td, *J* = 7.7, 1.4 Hz, 1H), 6.47 (dd, *J* = 7.7, 1.4 Hz, 1H). $^{13}$C NMR (126 MHz; DMSO-$d_6$): δ 150.4, 142.8, 137.2, 131.2, 128.2, 124.5, 120.9, 120.7, 119.4, 115.6, 113.3. HRMS (EI): Calc'd for $C_{11}H_8N_2O$: 184.06366, Found: 184.06365 Mp (dec.) 217 – 220 °C.

***1-Azaphenothiazine.*** To *N*-acetyl-2-Aminothiophenol (167 mg, 1.0 mmol) in DMF (6.6 mL) were added 2,3-dibromopyridine (355 mg, 1.5 mmol), $Fe(II)SO_4 \cdot 7H_2O$ (56 mg, 0.2 mmol), 1,10-phenanthroline monohydrate (40mg, 0.2 mmol) and potassium tert-butoxide (448 mg, 0.4 mmol) under an inert atmosphere. After stirring at 135 °C overnight, $H_2O$ (70 mL) was added and the reaction mixture was extracted with EtOAc (3 x 70 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by column chromatography using $Et_2O$/Petroleum ether (4:6) as eluent and recrystallized in hexane to afford the title compound as a solid (51 mg, 25%). $^{1}$H-NMR (300 MHz; $C_6D_6$): δ 9.19 (s, 1H), 7.81 (dd, *J* = 4.9, 1.6 Hz, 1H), 7.27 (ddd, *J* = 7.5, 1.6, 0.5 Hz, 1H), 7.00 (ddd, *J* = 8.0, 7.2, 1.5 Hz, 1H), 6.92 (dd, *J* = 7.7, 1.5 Hz, 1H), 6.84-6.73 (m, 3H). $^{13}$C NMR

(76 MHz; DMSO-$d_6$): δ 153.2, 145.6, 140.8, 133.8, 127.7, 125.9, 122.5, 117.9, 115.3, 115.2, 112.2 HRMS (EI): Calc'd for $C_{11}H_8N_2S$: 200.0408, Found: 200.0400. Mp 116 °C.

***N-Acetyl-3-amino-4-(2'-bromophenylthio)pyridine.*** To 4-(2'-bromophenylthio)-3-nitropyridine (3.0 g, 9.6 mmol) in EtOH (32 mL) were added iron powder (4.3 g, 77 mmol) and acetic acid (8.7 mL, 153 mmol). After stirring at r.t. for 2 h, the reaction mixture was neutralized with saturated $NaHCO_3$ solution and extracted with EtOAc (2 × 300 mL). The organic phase was washed with brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure. To the crude material in THF were added acetic anhydride (1.8 mL, 19.2 mmol) and DMAP (122 mg, 1 mmol) and the reaction was allowed to stir at r.t overnight prior to addition of a second portion of acetic anhydride (0.9 mL, 9.6 mmol). After stirring at r.t. for another 12 h, the reaction was quenched with saturated $NaHCO_3$ solution and extracted with EtOAc (3 x 100 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by column chromatography using EtOAc/Hexane (1:1) as eluent to afford the title compound as white needles (1.43g 46%). $^1$H-NMR (400 MHz; $CDCl_6$): δ 9.39 (s, 1H), 8.30 (d, *J* = 4.8 Hz, 1H), 7.66 (s, *J* = 9.2 Hz, 2H), 7.29 – 7.11 (m, 6H), 2.15 (s, 1H). $^{13}$C-NMR (100 MHz; $CDCl_6$): δ 168.3, 145.6, 144.2, 134.2, 133.7, 133.5, 133.1, 132.3, 129.7, 128.6, 126.5, 125.6, 24.4. HRMS (EI): Calc'd for $C_{13}H_{11}BrN_2OS$: 321.9776, Found: 321.9797. Mp 144 – 146 °C.

***10-Acetyl-2-azaphenothiazine.*** To *N*-acetyl-3-amino-4-(2'-bromophenylthio)pyridine (1.1 g, 3.4 mmol) in DMF (17 mL) were added were added copper(I) iodide (130 mg, 0.68 mmol), DMEDA (73 μL, 0.68 mmol) and potassium *tert*-butoxide (540 mg, 4.8 mmol) under an inert atmosphere. After stirring at 110 °C overnight, $H_2O$ (170 mL) was added and the reaction mixture was extracted with EtOAc (3 × 170 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. Recrystallization in EtOAc/Hexane afforded the title compound as a brown needels(400 mg, 49%). $^1$H-NMR (600 MHz; DMSO-$d_6$): δ 8.73 (s, 1H), 8.40 (d, *J* = 5.4 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.65 (dd, *J* = 5.4, 1.2 Hz, 1H), 7.59 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.45 (td, *J* = 7.2, 1.2 Hz, 1H), 7.36 (td, J = 7.2, 1.2 Hz, 1H), 2.17 (s, 3H). $^{13}$C NMR (151 MHz; DMSO-$d_6$): δ 169.0, 151.5, 146.6, 135.7, 134.0, 133.3,132.9, 132.6, 130.2, 128.4, 128.0, 121.6, 23.1. HRMS (EI): Calc'd for $C_{13}H_{10}N_2OS$: 242.0514, Found: 242.0531. Mp 127 – 129 °C.

***2-Azaphenothiazine.*** To 10-Acetyl-2-azaphenothiazine (350 mg, 1.45 mmol) in MeOH (10 mL) was added HCL (1 mL, 11.8 mmol) under an inert atmosphere. After stirring at 60 °C for 90 min, the reaction mixture was neutralized with 1M NaOH solution and extracted with EtOAc (3 × 50 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. Recrystallisation from benzene/hexadecane afford the title compound as a solid (247 mg, 84%). $^1$H-NMR (600 MHz; DMSO-$d_6$): δ 8.72 (s, 1H), 7.83 (d, *J* = 4.8 Hz, 1H), 7.80 (s, 1H), 7.00 (t, *J* = 8.4 Hz, 1H), 6.92 (d, *J* = 4.8, 1H) 6.89 (d, *J* = 7.8 Hz, 1H), 6.76 (t, *J* = 7.8 Hz, 1H), 6.66 (d, *J* = 7.8 Hz, 1H). $^{13}$C NMR (151 MHz; DMSO-$d_6$): δ 142.6, 141.1, 138.0, 134.7, 128.3, 126.9, 126.5, 122.3, 120.6, 115.0, 114.3 HRMS (EI): Calc'd for $C_{11}H_8N_2S$: 200.0408, Found: 200.0388. Mp 169 °C.

***3-Azaphenothiazine.*** To 2-aminothiophenol (0.66 mL, 6.2 mmol) in DMF (21 mL) were added 3-bromo-4-chloropyridine (1.0 g, 5.2 mmol) and caesium carbonate (3.4 g, 10.4 mmol) under an inert atmosphere. After stirring at 120 °C overnight, acetone and silica gel were added. The solvent was removed under reduced pressure and the residue was dry-loaded onto a silica gel column. The crude material was purified by column chromatography using EtOAC/MeOH (100:0 to 95:5) as eluent to afford the title compound as a solid (734 mg, 71%). $^1$H-NMR (400 MHz; DMSO-$d_6$): δ 9.09 (s, 1H), 7.98 (d, *J* = 5.4 Hz, 1H), 7.88 (s, 1H), 7.02 (td, *J* = 7.6, 1.3 Hz, 1H), 6.94 (dd, *J* = 7.7, 1.2 Hz, 1H), 6.81 (td, *J* = 7.5, 1.2 Hz, 1H), 6.68 (dd, *J* = 7.9, 1.1 Hz, 1H), 6.54 (d, *J* = 5.4 Hz, 1H). $^{13}$C NMR (151 MHz; DMSO-$d_6$): δ 148.7, 148.0, 145.6, 139.7, 127.9, 126.7, 123.1, 115.7, 115.1, 113.2, 108.7. HRMS (EI): Calc'd for $C_{11}H_8N_2S$: 200.0408, Found: 200.0414. Mp 247 – 248 °C.

***2'-((2-Bromophenyl)thio)-3-nitropyridine.*** To 2-chloro-3-nitropyridine (1.58 g, 10 mmol) in DMF (25 mL) was added $K_2CO_3$ (1.38 g, 10 mmol) and 2-bromothiophenol (1.2 mL, 10 mmol). After stirring at r.t. overnight, the reaction mixture was poured into $H_2O$ (400 mL) and stirred at 0 °C for 1 h. The precipitate was filtrated and washed with $H_2O$ to afford the title compound as yellow needles (2.9 g, 93%). $^1$H-NMR (600 MHz; DMSO-$d_6$): δ 8.66 (dd, *J* = 8.4, 1.8 Hz, 1H), 8.61 (dd, *J* = 4.8, 1.8 Hz, 1H), 7.51 – 7.44 (m, 3H). $^{13}$C NMR (151 MHz; DMSO-$d_6$): δ 154.9, 154.0, 141.4, 138.2, 134.5, 133.5, 132.0, 130.6, 130.5, 128.7, 121.1. HRMS (EI): Calc'd for $C_{11}H_7BrN_2O_2S$: 309.9412, Found: 309.9429. Mp 115 – 118 °C.

***N-Acetyl-3-amino-2-(2'-bromophenylthio)pyridine.*** To 2'-(2-bromophenylthio)-3-nitropyridine (2.8 g, 9 mmol) in EtOH (36 mL) were added tin (II) chloride (5.5 g, 29 mmol and HCl (4.9 mL, 58 mmol). After stirring at 70 °C for 1 h, the reaction mixture was concentrated under reduced pressure followed by addition of $H_2O$ (100 mL) and extraction with EtOAc (3 × 100 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. To the crude material in $Et_2O$ (45 mL) was added acetic anhydride (1.2 mL, 12.6 mmol) and the reaction was allowed to stir at r.t. overnight prior to addition of a second portion of acetic anhydride (1.2 mL, 12.6 mmol). After stirring at r.t. for another 12 h, the reaction was quenched with $H_2O$ (100 mL) and extracted with EtOAc (3 x 100 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by column chromatography using 70 % $Et_2O$/petroleum ether to 100% EtOAc as eluent to afford the title compound as a light yellow needles (1.1 g, 39%). $^1$H-NMR (600 MHz; DMSO-$d_6$): δ 9.80 (s, 1H), 8.19 (dd, *J* = 4.2, 1.2 Hz, 1H), 7.78 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.73 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.31 (td, *J* = 7.2, 1.8 Hz, 1H), 7.25 (dd, *J* = 9.0, 4.2 Hz, 1H), 2.09 (s, 3H). $^{13}$C NMR (151 MHz; DMSO-$d_6$): δ 169.0, 151.5, 146.6, 135.7, 134.0, 133.3, 132.9, 132.6, 130.2, 128.4, 128.0, 121.6, 23.1. HRMS (EI): Calc'd for $C_{13}H_{11}BrN_2OS$: 321.9776, Found: 321.9778. Mp 145 – 148 °C.

***4-Azaphenothiazine.*** To *N*-acetyl-3-amino-2-(2'-bromophenylthio)pyridine (900 mg, 2.8 mmol) in DMF (14 mL) were added copper(I) iodide (530 mg, 2.8 mmol), DMEDA (300 µL, 2.8 mmol) and caesium carbonate (390 mg, 3.4 mmol) under an inert atmosphere. After stirring at 90 °C overnight, $H_2O$ (140 mL) was added and the reaction mixture was extracted with EtOAc (3 × 140 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. Recrystallization in hexane afforded the title compound as a solid (300 mg, 44%). $^1$H-NMR (400 MHz; DMSO-$d_6$): δ 8.61 (s, 1H), 7.75 (dd, *J* = 4.7, 1.5 Hz, 1H), 6.99-6.91 (m, 2H), 6.88 (dd, *J* = 7.7, 1.4 Hz, 1H), 6.83 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.74 (td, *J* = 7.5, 1.3 Hz, 1H), 6.62 (dd, *J* = 7.9, 1.1 Hz, 1H). $^{13}$C NMR (76 MHz; DMSO-$d_6$): δ 141.6, 140.3, 139.9, 137.6, 127.8, 126.4, 122.6, 121.9, 119.5, 116.3, 114.5 HRMS (EI): Calc'd for $C_{11}H_8N_2S$: 200.0408, Found: 200.0383. Mp 248 – 250 °C.

***2-((5-Bromo-2-(diethylamino)pyrimidin-4-yl)amino)-5-(tert-butyl)phenol.*** 3-*tert*-Butyl-6-aminophenol (2.58g, 15.6 mmol) was dissolved in EtOH (110 mL) followed by addition of NaOH (625 mg, 15.6 mmol) at r.t. under $N_2$. The reaction mixture was allowed to stir for 10 min before addition of 5-bromo-2,4-dichloropyrimidine (3.56 g, 15.6 mmol) in EtOH (10 mL) under $N_2$. After reflux overnight, the reaction mixture was neutralized with 1M HCl and extracted with EtOAc (3 × 100 mL). The organic solution was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was washed with hexane and the obtained yellow powder (4.3 g, 12 mmol) was dissolved in THF (80 mL) followed by addition of diethylamine (7.3 mL, 72 mmol) under $N_2$. After reflux for 37 hours, the reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography using hexane/EtOAc (7:3 to 6:4) as eluent to afford the title compound as a light beige solid (2.7g, 44% over two steps). $^1$H-NMR (400 MHz; DMSO-$d_6$): δ 10.05 (s, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.08 (s, 1H), 6.94 (d, *J* = 2.4 Hz, 1H), 6.83 (dd, J = 8.4, 2.4 Hz, 1H), 3.53 (q, *J* = 6.8 Hz, 4H), 1.24 (s, 9H), 1.12 (t, *J* = 6.8 Hz, 6H). $^{13}$C NMR (76 MHz; DMSO-$d_6$): δ 159.1, 156.5, 154.9, 145.9, 145.4, 124.8, 118.6, 115.6, 111.5, 91.1, 41.8, 33.9, 31.2, 13.0. Calc'd for $C_{18}H_{25}BrN_4O$: 392.1212, Found: 392.1191. Mp 148 – 151 °C.

***7-tert-Butyl-2-diethylamino-1,3-diazaphenoxazine.*** To 2-((5-Bromo-2-(diethylamino)pyrimidin-4-yl)amino)-5-(*tert*-butyl)phenol (1.18 g, 3 mmol) in anhydrous DMF (15 mL) were added copper(I) iodide (83 mg, 0.6 mmol), DMEDA (60 µL, 0.6 mmol) and cesium carbonate (1.17 g, 3.6 mmol) under an inert atmosphere. After stirring at 110 °C overnight, $H_2O$ (150 mL) was added and the reaction mixture was extracted with EtOAc (3 × 100 mL). The organic phase was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by column chromatography using hexane/EtOAc (7:3) as eluent to afford the title compound as a white powder (300 mg, 32%). $^1$H-NMR (400 MHz; DMSO-$d_6$): δ 9.31 (s, 1H), 7.43 (s, 1H), 6.76 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.68 (d, *J* = 2.0 Hz, 1H), 6.58 (d, J = 8.4 Hz, 1H), 3.44 (q, *J* = 6.8 Hz, 4H), 1.18 (s, 9H), 1.06 (t, *J* = 6.8 Hz, 6H). $^{13}$C NMR (76 MHz; DMSO-$d_6$): δ 156.8, 151.1, 145.3, 142.7, 138.9, 129.3, 126.7, 119.6, 114.3, 112.3, 41.1, 33.8, 30.9, 13.3. Calc'd for $C_{18}H_{24}N_4O$: 312.1950, Found: 312.1949. Mp 226 – 229 °C.

***3H-phenoxazin-3-one.*** The synthesis of 3*H*-phenoxazin-3-one was based on the method described by Barret and Daudon.[8] A flame dried 100 mL round bottom flask was charged with 60 mL of benzene, 1.10 g of phenoxazine (6 mmol), 2.83 g of iodoxybenzene (12 mmol) and 320 mg vanadyl acetylacetonate (1.2 mmol). With stirring, the

reaction mixture was brought to reflux for 3 hours. The benzene was removed under reduced pressure, and the residue was purified using column chromatography (8:2 hexane/EtOAc). The fractions containing the product were consolidated into a single round bottom flask and the solvent was removed under reduced pressure. The partially purified product was dissolved in a minimum of ethyl acetate, after which hexanes were added to precipitate 3*H*-phenoxazin-3-one as an orange solid. The obtained solid was filtered and rinsed with hexanes to afford the title compound (0.23 g, 18%). $^{1}$H-NMR (400 MHz; DMSO-$d_6$): δ 7.85 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.66 (ddd, *J* = 7.4, 7.3, 1.6 Hz, 1H), 7.57 (d, *J* = 9.8 Hz, 1H), 7.50 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.45 (ddd, *J* = 7.9, 7.4, 1.3 Hz, 1H), 6.84 (dd, *J* = 9.8, 2.1 Hz, 1H), 6.30 (d, *J* = 2.1 Hz, 1H). $^{13}$C NMR (101 MHz; DMSO-$d_6$): δ 185.7, 149.7, 148.6, 143.5, 135.0, 134.8, 133.1, 133.0, 130.0, 125.6, 116.2, 105.8. Mp 216 – 218 °C (lit. 214 °C)[8]

***Phenothiazine-5-oxide.*** In 10 mL round bottom flask was dissolved 0.40 g of phenothiazine (2 mmol) into 4 mL of ethyl acetate with stirring. *m*-CPBA (4 mmol) were dissolved in 2 mL of diethyl ether. The ether layer (commercial m-CPBA contains a large amount of $H_2O$) was dropped into the flask containing the phenothiazine solution while stirring which resulted in immediate and quantitative precipitation of phenothiazine-5-oxide. After filtration, the light-yellow product was rinsed with ethyl acetate, diethyl ether and hexanes to afford the title compound (0.41g, 95%). This product was recrystallized out of absolute ethanol. The $^{1}$H-NMR was consistent with the previously reported characterization of phenothiazine-5-oxide.[9] $^{1}$H-NMR (400 MHz; DMSO-$d_6$): δ 10.98 (s, 1H), 7.89 (d, *J* = 7.0 Hz, 2H), 7.61 (ddd, *J* = 8.3, 8.3, 1.3 Hz, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.18 (dd, *J* = 7.4, 7.4 Hz, 2H).

# UPLC Product Analysis and Quantification

## I. Key products arising in PNX- and PTZ-inhibited autoxidations

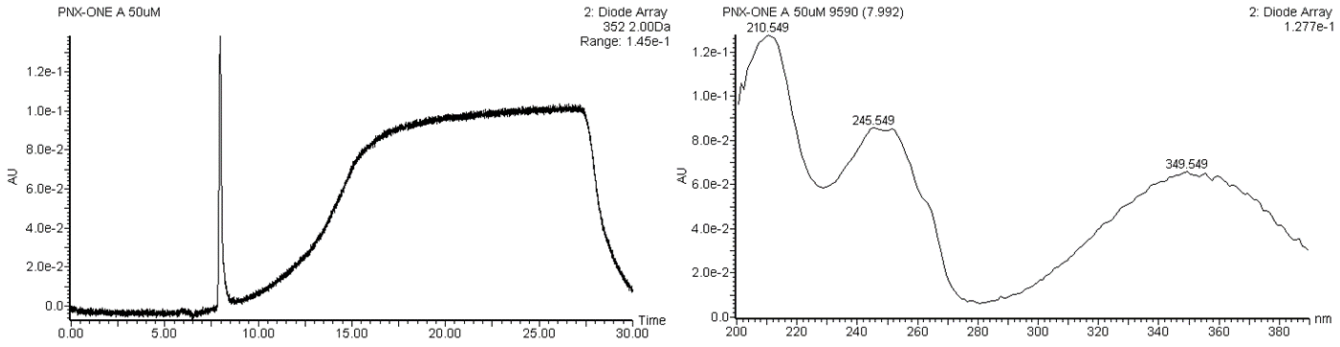



**Figure S1**. *(Left)* Representative chromatogram of PNX-ONE standard (50 μM) monitored at 352 nm; *(Right)* UV-Vis spectrum of PNX-ONE standard.

| Concentration (µM) | Integral (at 352nm) | Error (±) |
|---|---|---|
| 5 | 2746 | 194 |
| 10 | 5330 | 709 |
| 25 | 12578 | 1256 |
| 50 | 25392 | 1233 |
| 100 | 52536 | 678 |

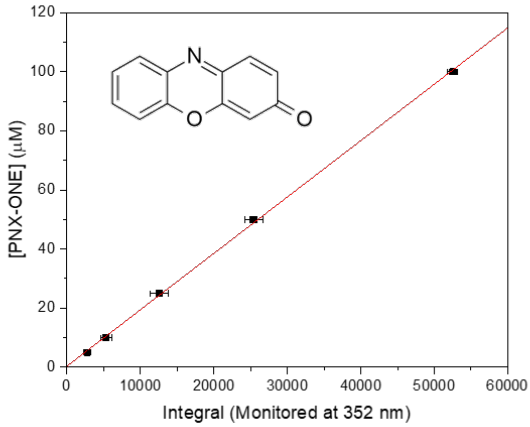



**Figure S2**. *(Left)* Table of integrals of PNX-ONE standard monitored at 352 nm; *(Right)* Calibration curve for PNX-ONE at 352 nm ($R^2$ = 0.9995, y = 0.00191x + 0.3768).

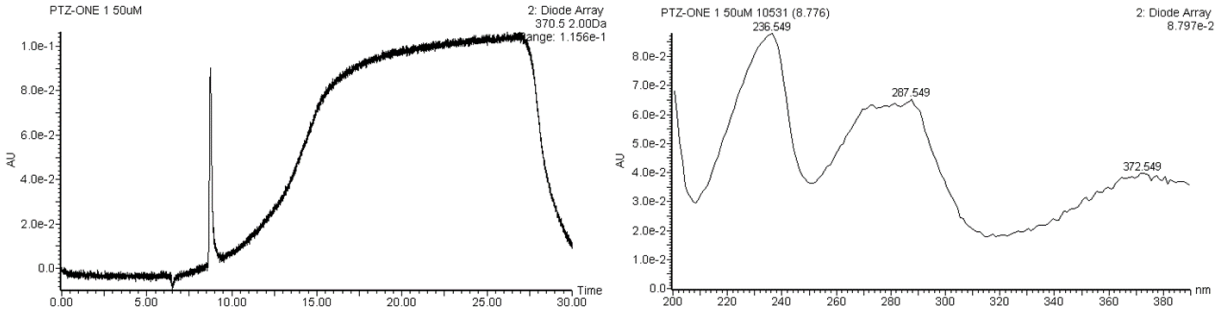



**Figure S3**. *(Left)* Representative chromatogram of PTZ-ONE standard (50 µM) monitored at 370.5 nm; *(Right)* UV-Vis spectrum of PTZ-ONE standard.

| Concentration (µM) | Integral (at 370.5nm) | Error (±) |
|---|---|---|
| 5 | 1587 | 154 |
| 25 | 10271 | 157 |
| 50 | 20166 | 575 |
| 100 | 38469 | 892 |
| 250 | 95120 | 1617 |

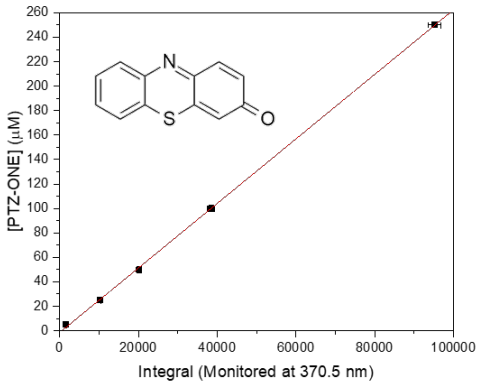



**Figure S4**. *(Left)* Table of integrals of PTZ-ONE standard monitored at 370.5 nm; *(Right)* Calibration curve for PTZ-ONE at 370.5 nm ($R^2$ = 0.9998, y = 0.00264x – 1.3676).

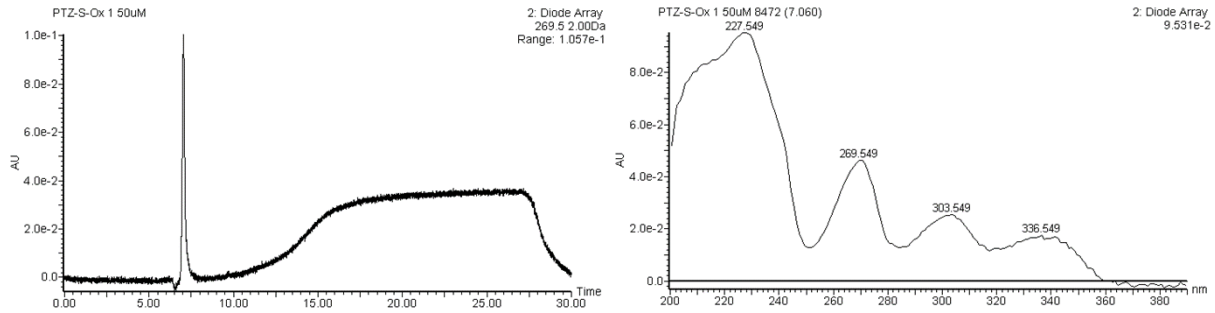



**Figure S5**. *(Left)* Representative chromatogram of PTZ-SO standard (50 μM) monitored at 269.5 nm; *(Right)* UV-Vis spectrum of PTZ-SO standard.

| Concentration (μM) | Integral (at 269.5nm) | Error (±) |
|---|---|---|
| 5 | 2282 | 127 |
| 25 | 15732 | 1778 |
| 50 | 28549 | 1161 |
| 100 | 56115 | 1153 |
| 250 | 140131 | 4974 |

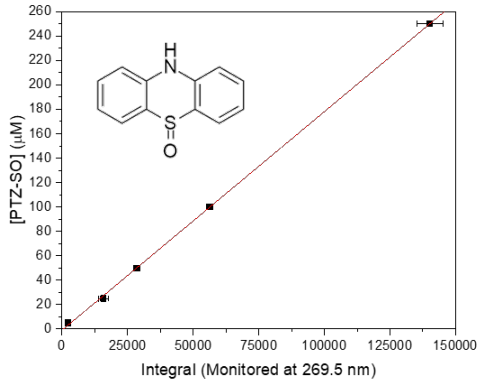



**Figure S6**. *(Left)* Table of integrals of PTZ-SO standard monitored at 269.5 nm; *(Right)* Calibration curve for PTZ-SO at 269.5 nm ($R^2 = 0.9998$, $y = 0.00179x - 0.9414$).

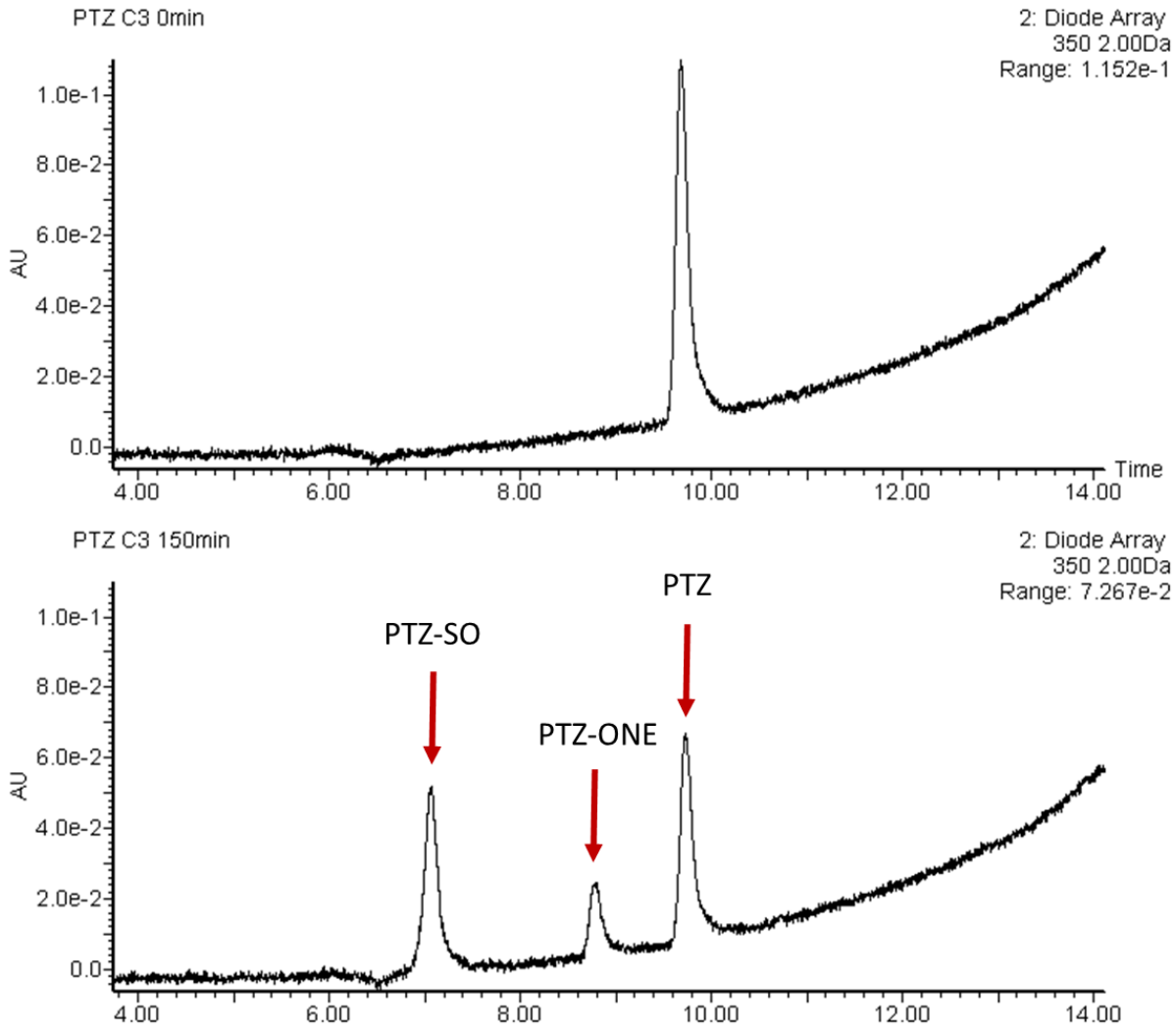



**Figure S7**. *(Top)* Representative UPLC-PDA trace of unoxidized PTZ extracted from hexadecane (monitored at 350nm); *(Bottom)* Representative UPLC-PDA trace of PTZ derived products extracted from hexadecane from an intermediate state of autoxidation (monitored at 350nm).

Interestingly, in the PNX inhibited autoxidation PNX-NO is the most abundant oxidation product, accumulating to well over half of the original [PNX]. While formation of PNX-NO is not unexpected, the rapid oxidation/consumption of PNX compared to PTZ implies significant pro-oxidant activity on the part of PNX. What is not entirely clear is why PNX-NO actually increases between during the 15 minutes spanning 7200s and 8100s (observed by both EPR spin counting and UPLC) despite that fact that no trace of PNX can be detected by 7200s. One would expect if the only source of PNX-NO originates from the oxidation of PNX that PNX-NO should only decrease once PNX is depleted. Of the species that can be observed by UPLC upon sample extraction, there are two products in addition to PNX-NO and PNX-ONE for which we do not have authentic standards (Figure S1A). Of particular interest is 'Unknown 1' which has m/z values consistent with [M + H]+ and [M – HO]+ of a hydroxylated PNX product (Figure S1B). Given the oxidative lability of PNX, it is unlikely that 1-hydroxyphenoxazine or 3-hydroxyphenoxazine would accumulate to a significant extent (as these are strong EDG which would further decrease E°). The hydroxylamine of PNX (PNX-NOH) was also considered, as it would provide a convenient source of PNX-NO in the absence of PNX. Interestingly, 'Unknown 1' increased as long as PNX is present, then sharply declined when PNX was depleted suggesting that it was being rapidly oxidized in the absence of the parent RTA and possibly caused the protracted increase of PNX-NO (Figure S1C). Though we were unable to prepare/isolate PNX-NOH to further corroborate the proposal, it seems reasonable based on the circumstantial evidence.[10]

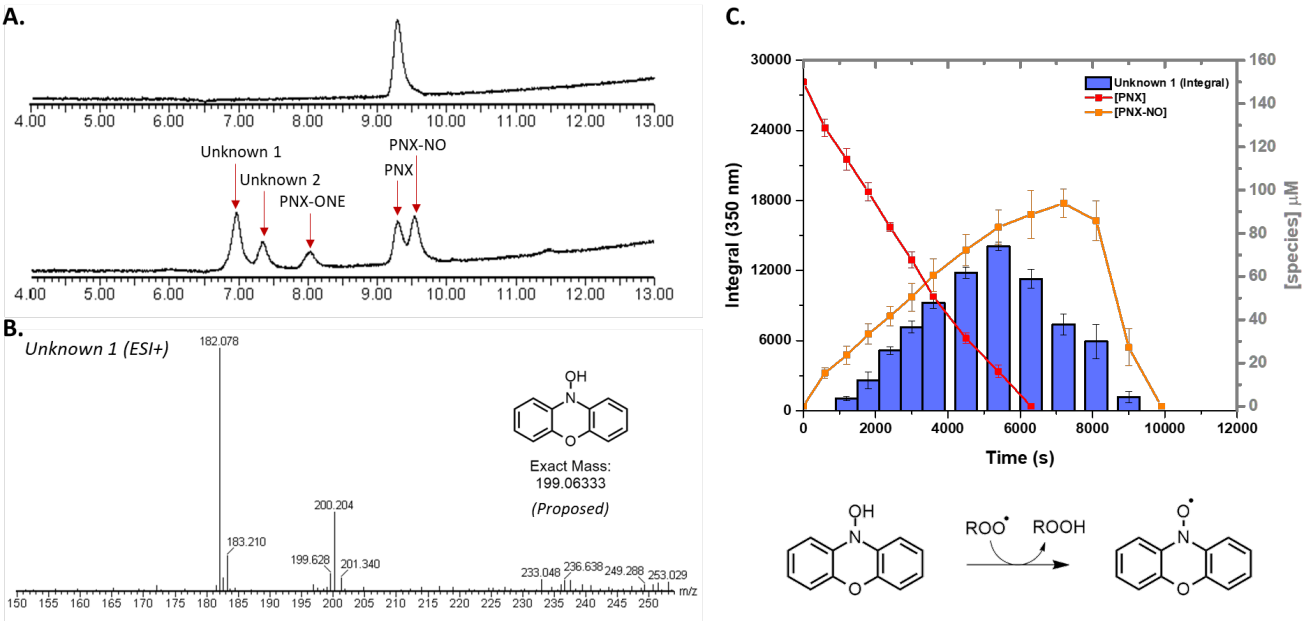



**Figure S8**. (A) *Top*: Representative UPLC-PDA trace of unoxidized PNX extracted from hexadecane (monitored at 350 nm); *Bottom*: Representative UPLC-PDA trace of PNX derived products extracted from hexadecane from an intermediate state of autoxidation (monitored at 350 nm). (B) ESI+ spectra of 'Unknown 1' (UPLC-MS). (C) The integral of 'Unknown 1' overlayed with the time-course concentrations of [PNX] and [PNX-NO].

## II. Loss of aza-PNX derivatives in *n*-hexadecane autoxidations

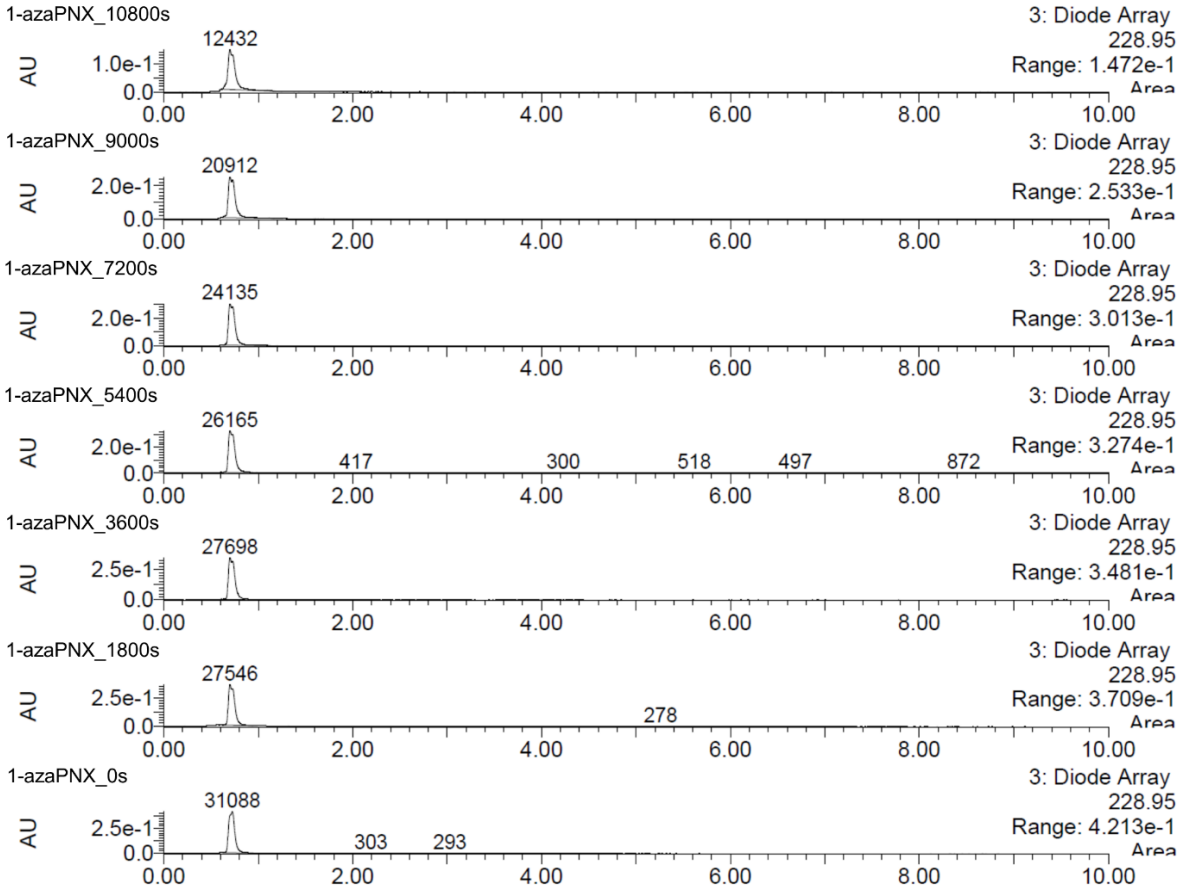



**Figure S9**. UPLC-PDA trace of 1-azaPNX extracted from hexadecane (monitored at 229 nm).

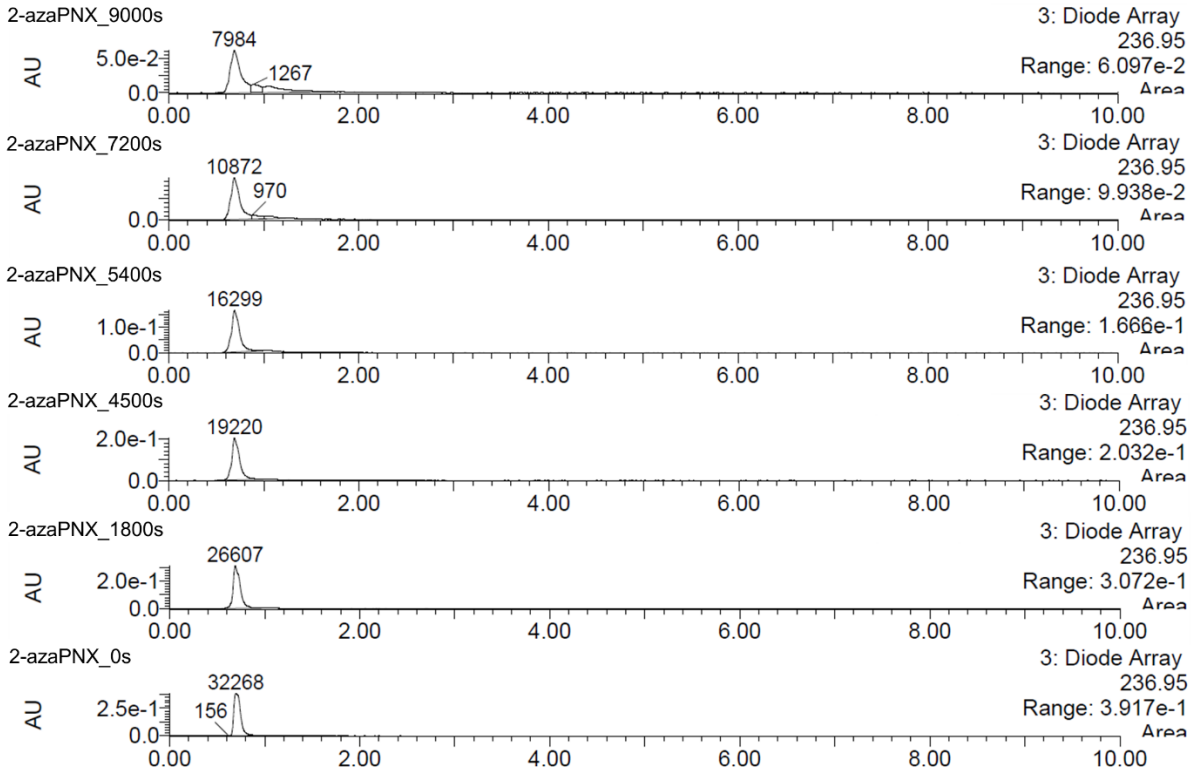



**Figure S10**. UPLC-PDA trace of 2-azaPNX extracted from hexadecane (monitored at 237 nm).

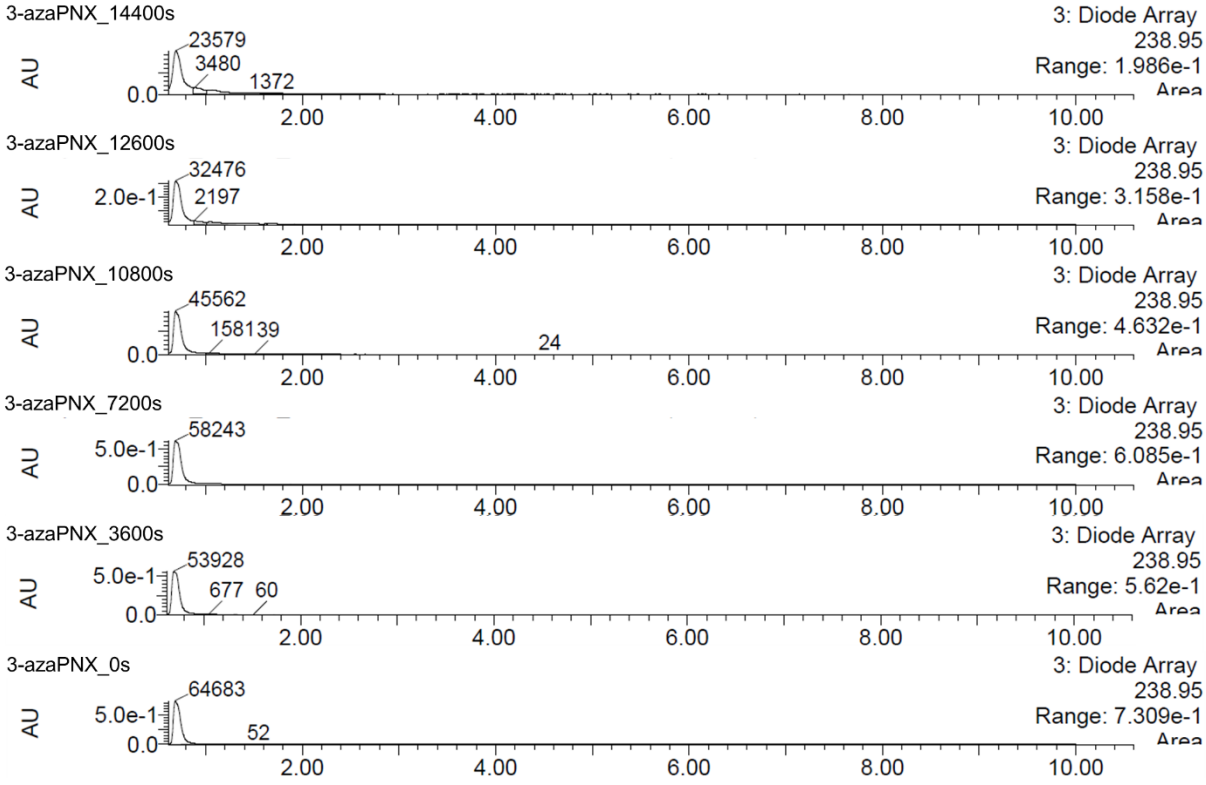



**Figure S11**. UPLC-PDA trace of 3-azaPNX extracted from hexadecane (monitored at 239 nm).

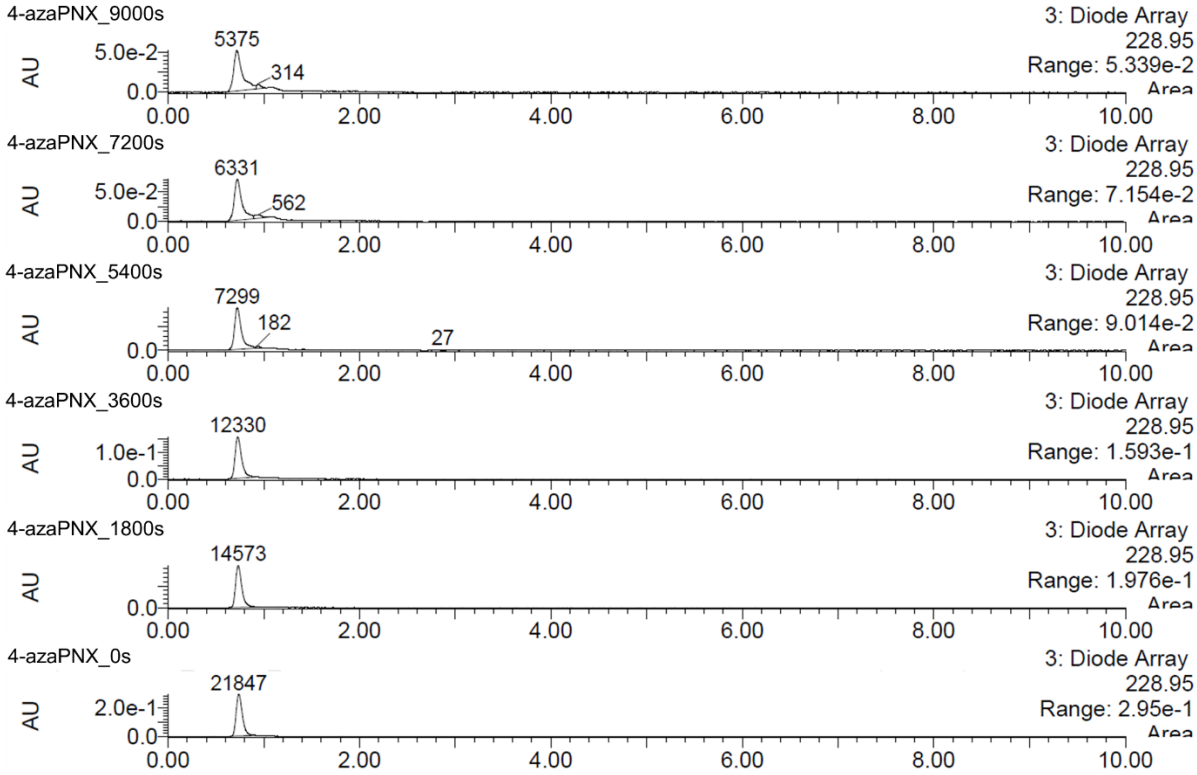



**Figure S12**. UPLC-PDA trace of 4-azaPNX extracted from hexadecane (monitored at 239 nm).

## Rate Constant and Reaction Stoichiometry Determination

$$k_{inh} = \frac{k_{\mathrm{PBD-BODIPY}}[\mathrm{PBD-BODIPY}]R_i}{n[\mathrm{RTA}]\frac{-\delta[\mathrm{PBD-BODIPY}]}{\delta t}} \qquad \text{(Eq. S1)}$$

$k_{\mathrm{PBD-BODIPY}}$ = rate constant of peroxyl radical addition to PBD-BODIPY ($M^{-1}s^{-1}$), which was determined to be 5310 $M^{-1}s^{-1}$ in 1,4-dioxane, 2720 $M^{-1}s^{-1}$ in styrene and 8283 $M^{-1}s^{-1}$ in 1-hexadecene.

[PBD-BODIPY] = dye concentration at $t$ = 0 s (M)

[RTA] = antioxidant concentration (M)

$\frac{\delta[\mathrm{PBD-BODIPY}]}{\delta t}$ = rate of dye consumption for the inhibited periods (M $s^{-1}$) which was determined from the slope of the black line as shown in Figure S13.

$n$ = stoichiometry, which was determined from Eq. S2

$$n = \frac{t_{inh} \times R_i}{[RTA]} \qquad \text{(Eq. S2)}$$

$t_{\mathrm{inh}}$ = inhibition time (s), determined from intersection of the two black lines as in Figure S13

$R_{\mathrm{i}}$ = rate of initiation (M $s^{-1}$), standardized from $t_{\mathrm{inh}}$ obtained for 2 μM PMC using $n$ = 2 in Eq. S2.

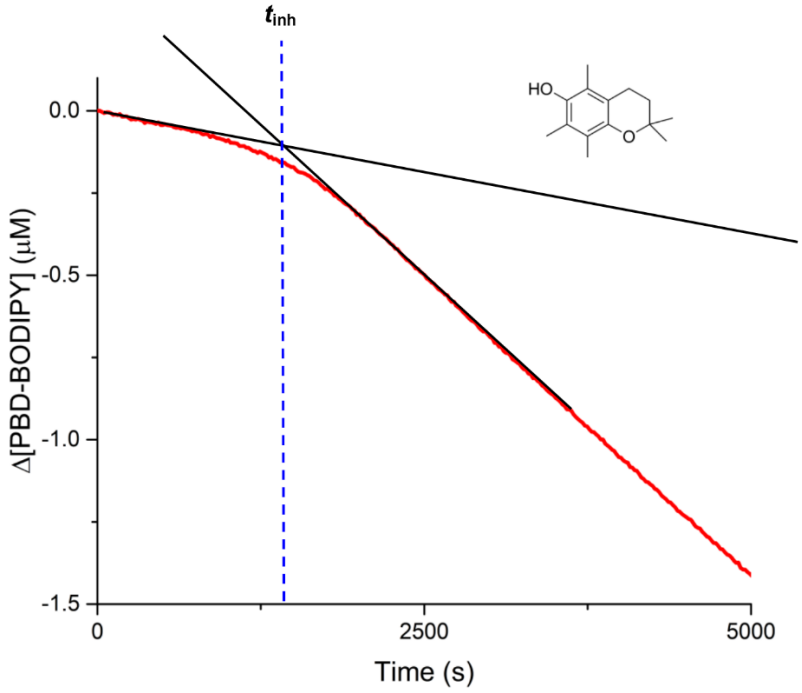



**Figure S13**. The inhibition time ($t_{\mathrm{inh}}$) of PMC (2 μM) was determined by tangential intercept between inhibited and uninhibited phases of AIBN-initiated co-autoxidation of PBD-BODIPY (10 μM) with 1,4-dioxane in PhCl at 37°C. Reaction was monitored by absorbance at 587 nm (ε = 123,023 $M^{-1}cm^{-1}$).

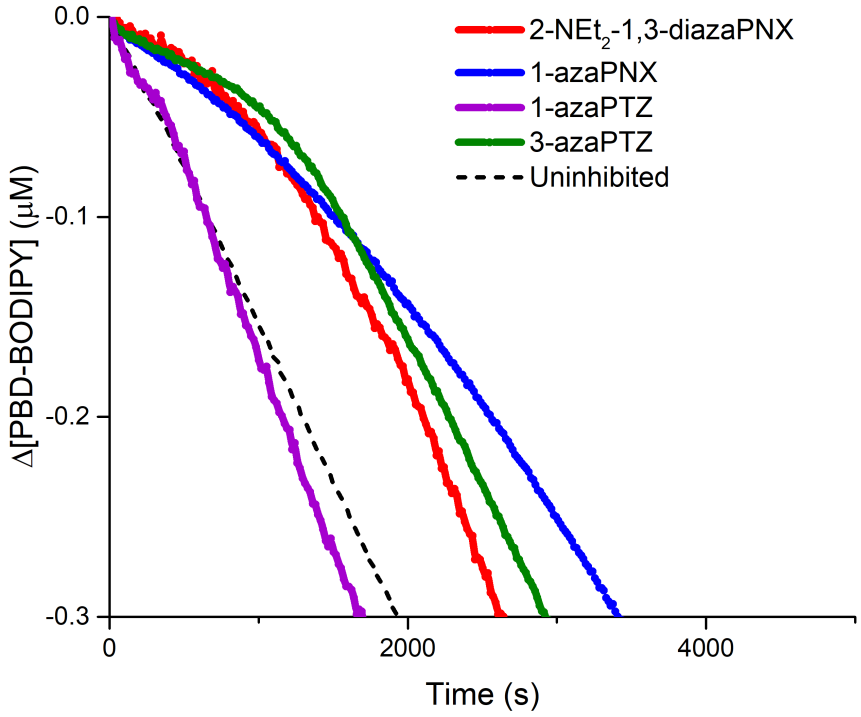



**Figure S14.** Co-autoxidation of styrene (4.3M) and PBD-BODIPY (10 μM) initiated by AIBN (6 mM) in PhCl at 37°C, monitored at 591 nm (ε= 139,000 $M^{-1}$ $cm^{-1}$) inhibited with 2 μM of 2-$NEt_2$-1,3-diazaPNX (red), 1-azaPNX (blue), 1-azaPTZ (violet) and 3-azaPTZ (green).

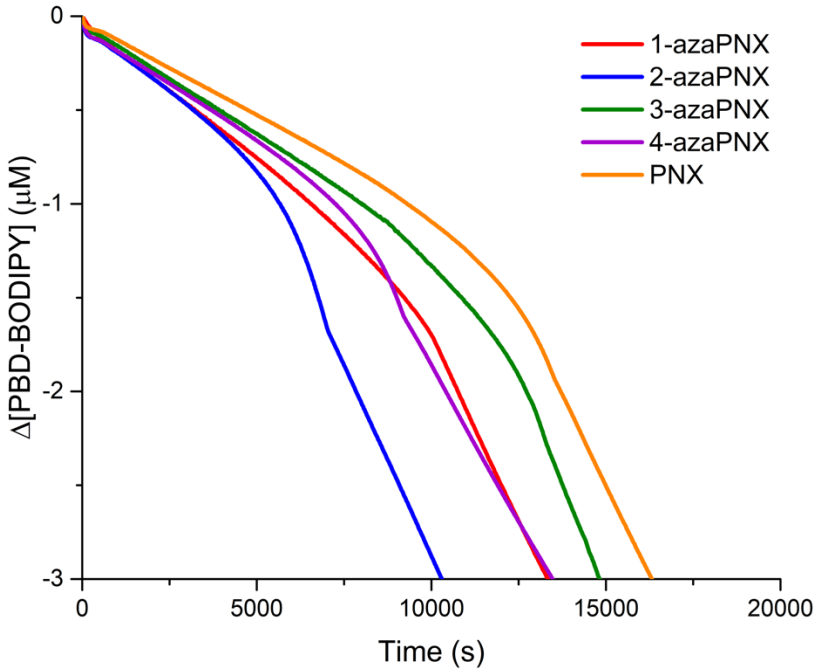



**Figure S15.** Co-autoxidation of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumyl peroxide (2 mM) in PhCl at 100°C, monitored at 587 nm (ε= 119,166 $M^{-1}$ $cm^{-1}$) inhibited with 2 μM of 1-azaPNX (red), 2-azaPNX (blue), 3-azaPNX (green), 4-azaPNX (violet) or PNX (orange).

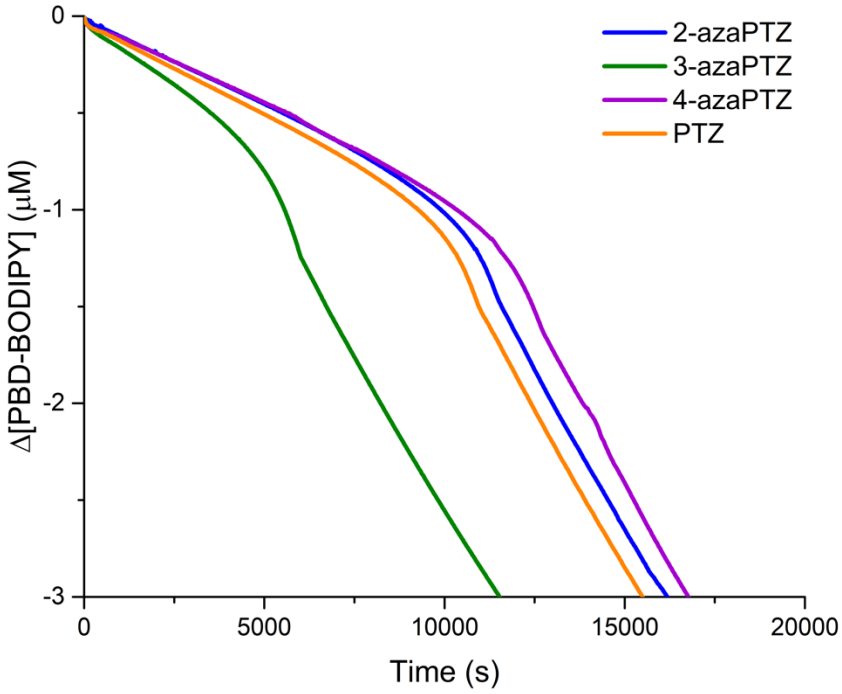



**Figure S16.** Co-autoxidation of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumyl peroxide (2 mM) in PhCl at 100°C, monitored at 587 nm (ε= 119,166 $M^{-1}$ $cm^{-1}$) inhibited with 2 μM of 2-azaPTZ (blue), 3-azaPTZ (green), 4-azaPTZ (violet) or PTZ (orange).

**Table S1** Inhibition Rate Constants and Stoichiometries of Azaphenoxazine and Azaphenothiazine RTAs in 1-Hexadecene Autoxidations initiated by DiCup (2 mM) in PhCl at 100°C.

| Compound | $k_{inh}$ ($M^{-1}s^{-1}$) | *n* |
|---|---|---|
| 1-azaPNX | $(3.6\pm0.3) \times 10^6$ | 54±1 |
| 2-azaPNX | $(4.1\pm0.1) \times 10^6$ | 31±1 |
| 3-azaPNX | $(4.7\pm0.5) \times 10^6$ | 64±2 |
| 4-azaPNX | $(4.2\pm0.2) \times 10^6$ | 42±2 |
| PNX | $(4.7\pm0.1) \times 10^6$ | 66±1 |
| 1-azaPTZ | *too slow* | - |
| 2-azaPTZ | $(5.2\pm0.3) \times 10^6$ | 57±2 |
| 3-azaPTZ | $(3.4\pm0.2) \times 10^6$ | 26±1 |
| 4-azaPTZ | $(5.0\pm0.4) \times 10^6$ | 63±3 |
| PTZ | $(4.8\pm0.1) \times 10^6$ | 52±2 |

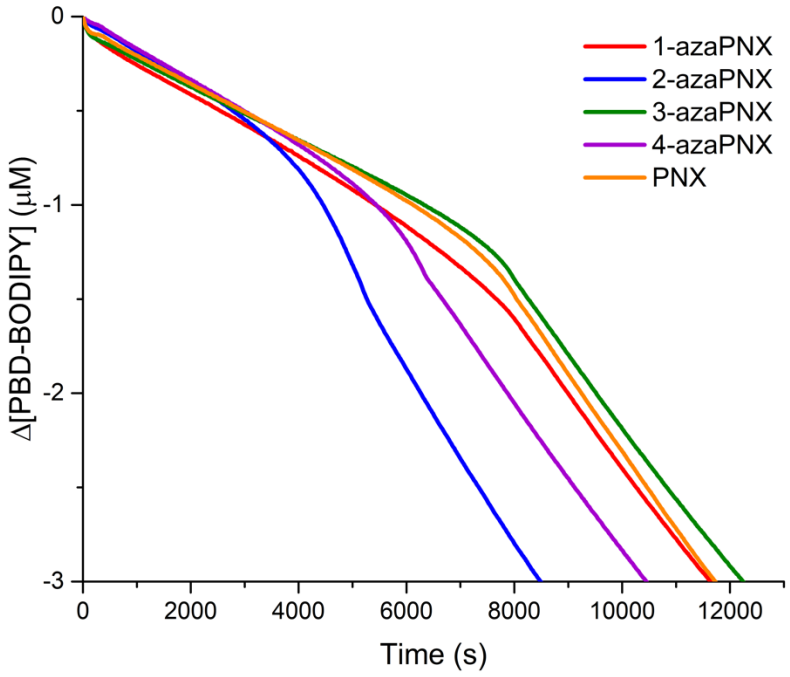



**Figure S17.** Co-autoxidation of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumyl peroxide (3 mM) in PhCl at 100°C, monitored at 587 nm ($\varepsilon$ = 119,166 $M^{-1}$ $cm^{-1}$) inhibited with 2 μM of 1-azaPNX (red), 2-azaPNX (blue), 3-azaPNX (green), 4-azaPNX (violet) or PNX (orange).

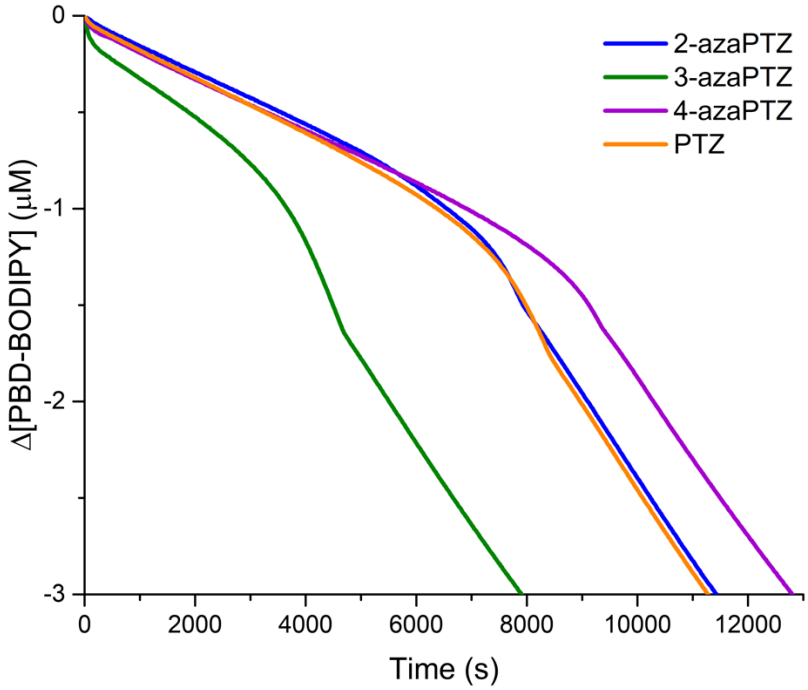



**Figure S18.** Co-autoxidation of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumyl peroxide (3 mM) in PhCl at 100°C, monitored at 587 nm ($\varepsilon$ = 119,166 $M^{-1}$ $cm^{-1}$) inhibited with 2 μM of 2-azaPTZ (blue), 3-azaPTZ (green), 4-azaPTZ (violet) or PTZ (orange).

**Table S2** Inhibition Rate Constants and Stoichiometries of Azaphenoxazine and Azaphenothiazine RTAs in 1-Hexadecene Autoxidations Initiated by DiCup (3 mM) in PhCl at 100°C.

| Compound | $k_{inh}$ ($M^{-1}s^{-1}$) | *n* |
|---|---|---|
| 1-azaPNX | $(4.7\pm0.1) \times 10^6$ | 60±2 |
| 2-azaPNX | $(4.4\pm0.1) \times 10^6$ | 29±2 |
| 3-azaPNX | $(5.4\pm0.1) \times 10^6$ | 63±3 |
| 4-azaPNX | $(4.7\pm0.1) \times 10^6$ | 48±3 |
| PNX | $(4.9\pm0.1) \times 10^6$ | 65±1 |
| 1-azaPTZ | *too slow* | - |
| 2-azaPTZ | $(5.6\pm0.1) \times 10^6$ | 60±1 |
| 3-azaPTZ | $(3.8\pm0.1) \times 10^6$ | 20±3 |
| 4-azaPTZ | $(5.7\pm0.1) \times 10^6$ | 78±1 |
| PTZ | $(5.2\pm0.1) \times 10^6$ | 62±3 |

## Inhibition Time Determination in High Temperature Autoxidations

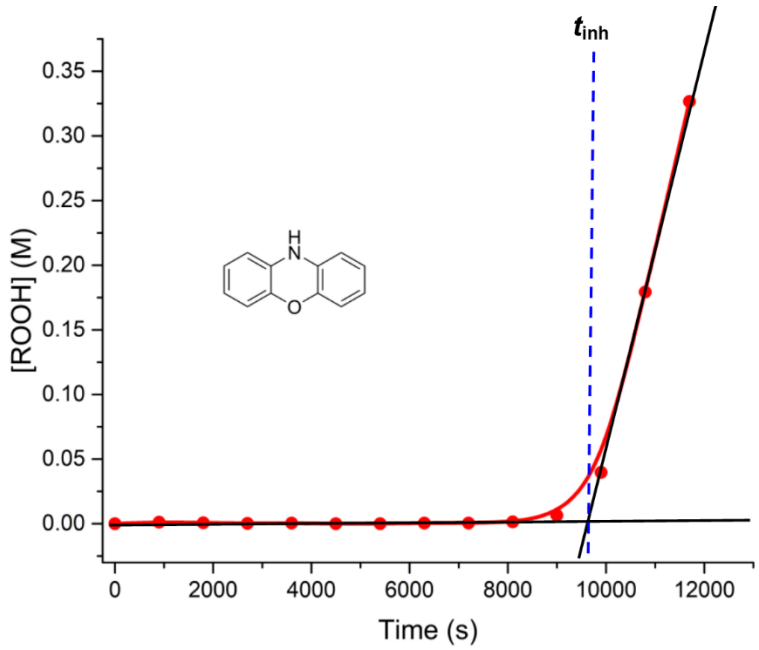



**Figure S19**. $T_{inh}$ was determined by tangential intercept between inhibited and uninhibited phases of hexadecane autoxidation at 160°C inhibited by 200 µM phenoxazine. Peroxide concentration was determined by coumarine phosphine probe ($\lambda_{ex}$ = 340 nm, $\lambda_{em}$ = 425 nm).

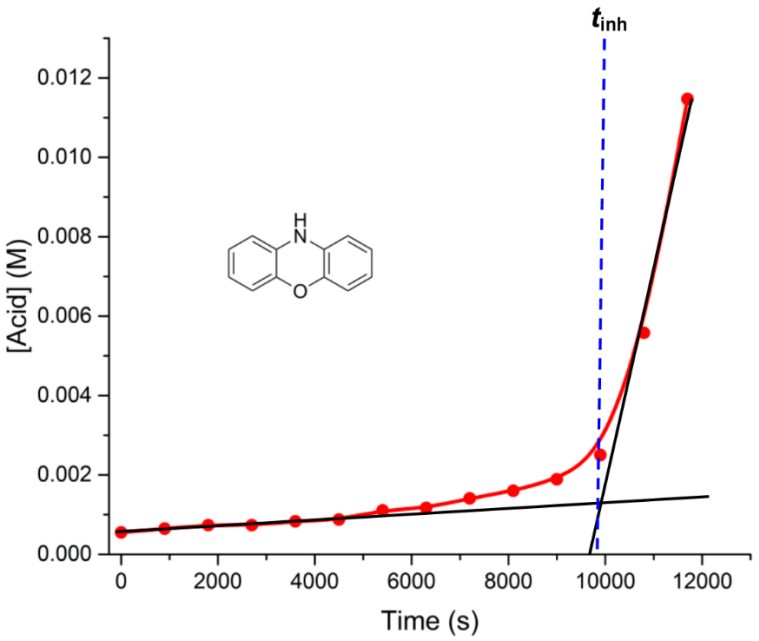



**Figure S20**. $T_{inh}$ was determined by tangential intercept between inhibited and uninhibited phases of hexadecane autoxidation at 160°C inhibited by 200 µM phenoxazine. Total acid concentration was determined by BODIPY acid probe ($\lambda_{ex}$ = 475 nm, $\lambda_{em}$ = 515 nm).

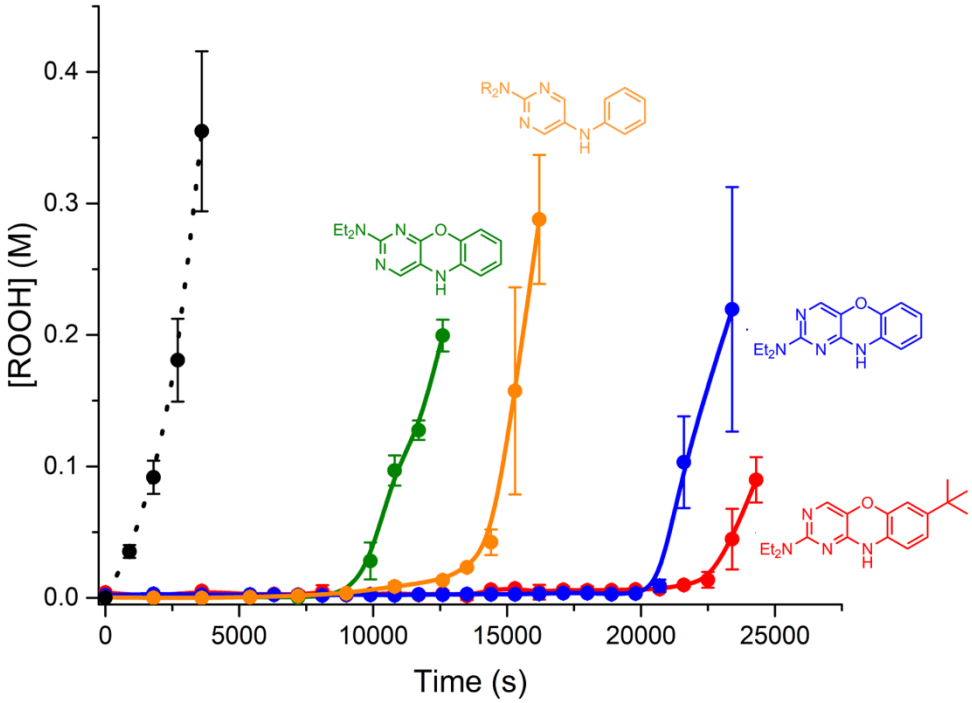



**Figure S21**. Hexadecane autoxidation inhibited by diazaphenoxazines and $N^2$,$N^2$-dihexyl-$N^5$-phenylpyrimidine-2,5-diamine (200 μM). Peroxide concentration was determined by coumarin phosphine probe ($\lambda_{ex}$ = 340 nm, $\lambda_{em}$ = 425 nm).

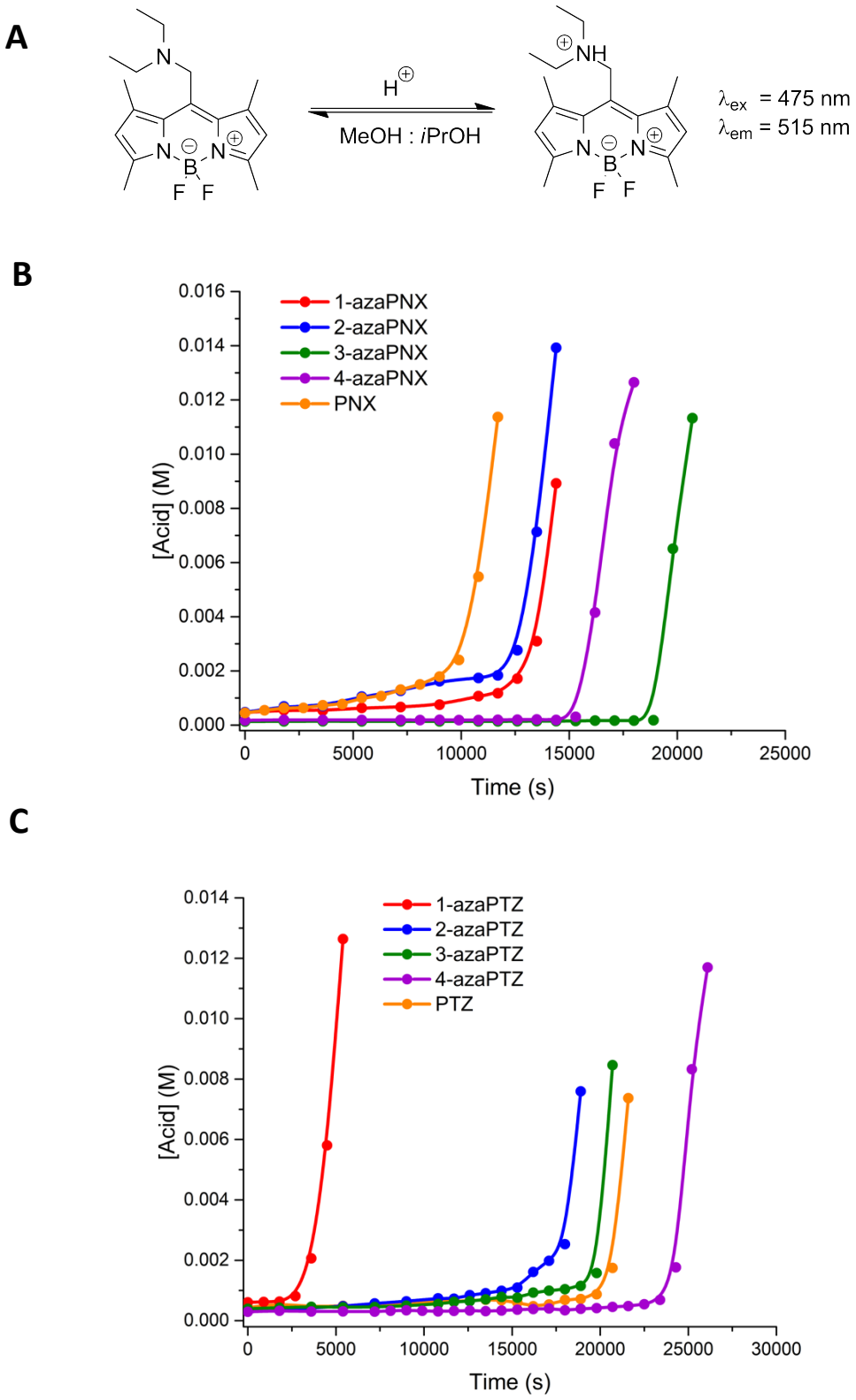



**Figure S22**. (A) BODIPY acid probe allows the quantification of acid production during hexadecane autoxidation at 160 °C. (B) Hexadecane autoxidation inhibited by 200 µM 1-azaPNX (red), 2-azaPNX (blue), 3-azaPNX (green), 4azaPNX (violet) and PNX (orange). (C) Hexadecane autoxidation inhibited by 200 µM 1-azaPTZ (red), 2-azaPTZ (blue), 3-azaPTZ (green), 4-azaPTZ (violet) and PTZ (orange). Total acid concentrations were determined by BODIPY acid probe ($\lambda_{ex}$ = 475 nm, $\lambda_{em}$ = 515 nm).

## Inhibited Autoxidation with Deuterated Phenoxazine (PNX-D) in Hexadecane

**Sample Preparation.** For the preparation of 10*D*-phenoxazine (PNX-D), 1 mmol (183mg) of commercial PNX was dissolved in a minimum of MeOD and allowed to stir at room temperature for 1 hour. The MeOD was removed under reduced pressure rendering PNX-D with ≥70% deuterium incorporation. This ~70% PNX-D was dissolved in benzene-$d_6$ to make a 30 mM stock solution. The stock solution was vortexed with $D_2O$ and the benzene-d6 layer was transferred to an NMR tube for $^1H$ NMR to ascertain deuterium incorporation (≥95%). As a control, commercial PNX was dissolved in benzene-d6 (30 mM) and vortexed with HPLC grade $H_2O$ and the benzene-d6 layer was transferred to an NMR tube for $^1H$ NMR.

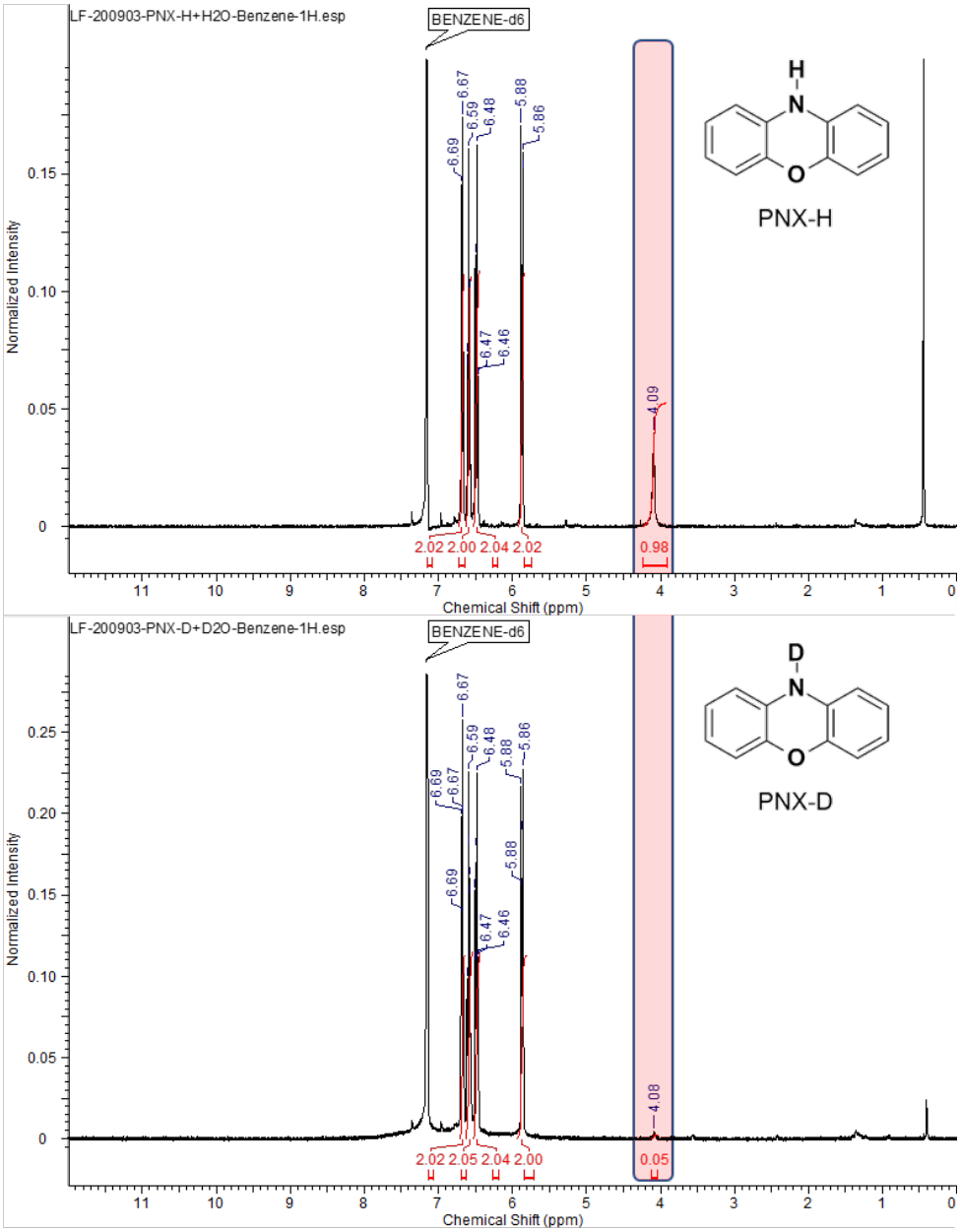



**Figure S23**. *(Top)* $^1H$-NMR (400 MHz; benzene-$d_6$) of 30mM PNX-H stock solution; *(Bottom)* $^1H$-NMR (400 MHz; benzene-$d_6$) of 30mM PNX-D stock solution.

**Autoxidation of n-Hexadecane.** The test tubes of hexadecane were continuously sparged with $N_2$ passed through a tube of anhydrous indicating Drierite® ($CaSO_4$, 8 mesh). The tubes were gradually heated to 160 ± 2 °C (heating block temperature 168 °C) and then 100 µL of either 30 mM PNX-H or PNX-D were added for a final concentration of 300 µM PNX. After the 0 s sample was taken, the $N_2$ was switched to $O_2$ (dried with $CaSO_4$) and the experiment proceeded as described in the experimental section of the main text. The concentration of PNX-H/PNX-D for the first 3000 s was determined by loss of PNX using UPLC-PDA, and [ROOH] was determined in the same manner as described in the main text.

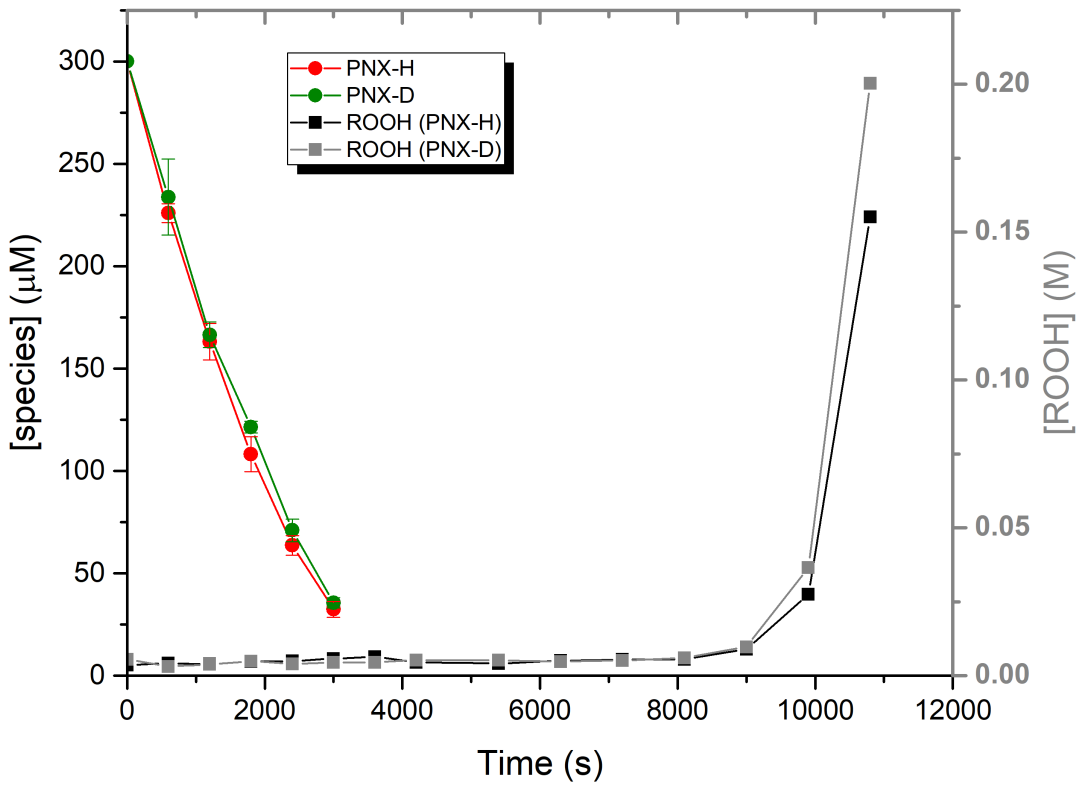
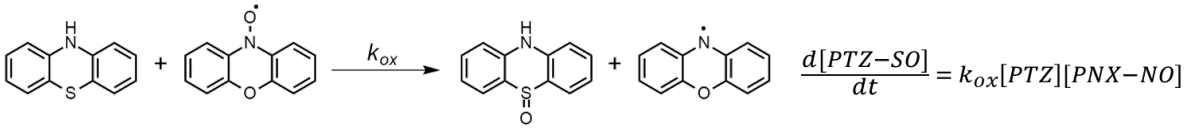



**Figure S24**. Time-course loss of PNX-H/PNX-D overlayed with [ROOH] from the autoxidation of n-hexadecane inhibited by 300 µM PNX-H/PNX-D at 160 °C.

## Kinetics of the Oxidation of Phenothiazine with Phenoxazine-N-Oxyl




**Scheme S1**. Scheme for the oxidation of PTZ by PNX-NO.

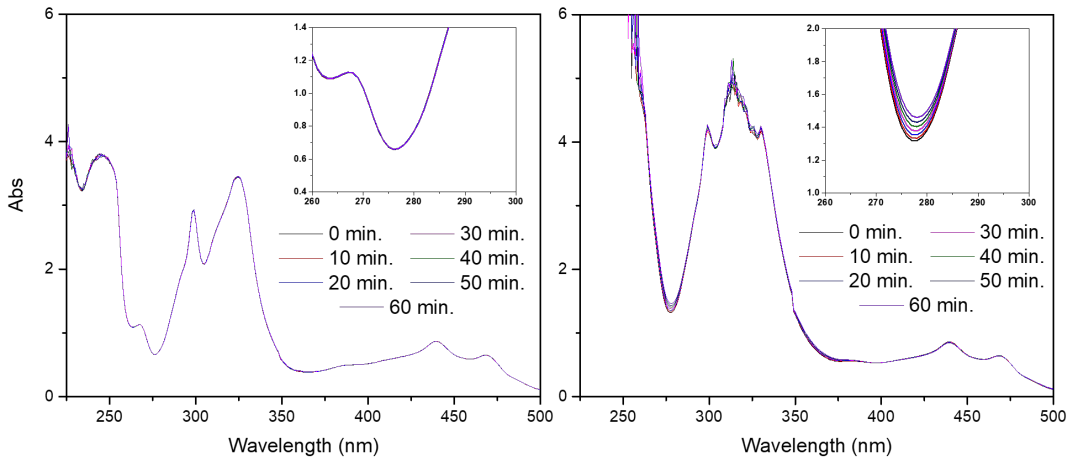



**Figure S25**. *(Left)* Kinetic UV-Vis scan (225 to 500 nm) of 300 µM PNX-NO in hexadecane at 80 °C; *(Right)* Kinetic UV-Vis scan (225 to 500 nm) of 300 µM PNX-NO with 600 µM PTZ in hexadecane at 80 °C.

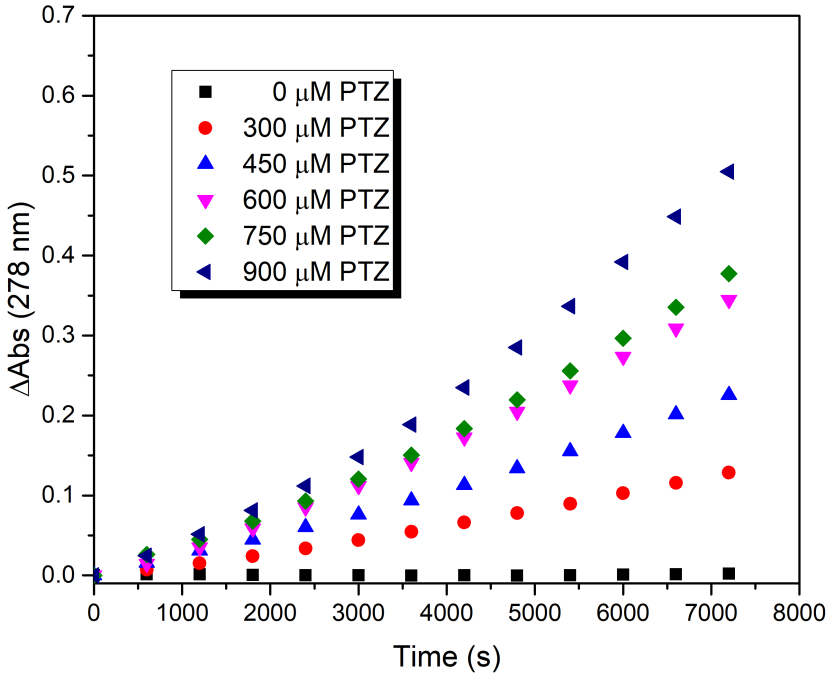



**Figure S26**. Observing the increase of absorbance at 278 nm ($\varepsilon_{278}$ = 9129 $M^{-1}$ $cm^{-1}$) with 300 µM PNX-NO at various concentrations of PTZ in hexadecane at 80 °C. *(Right)* Molar-absorptivity plot of PTZ-SO at 278 nm in hexadecane at 80 °C ($\varepsilon_{278}$ = 9129 $M^{-1}$ $cm^{-1}$).

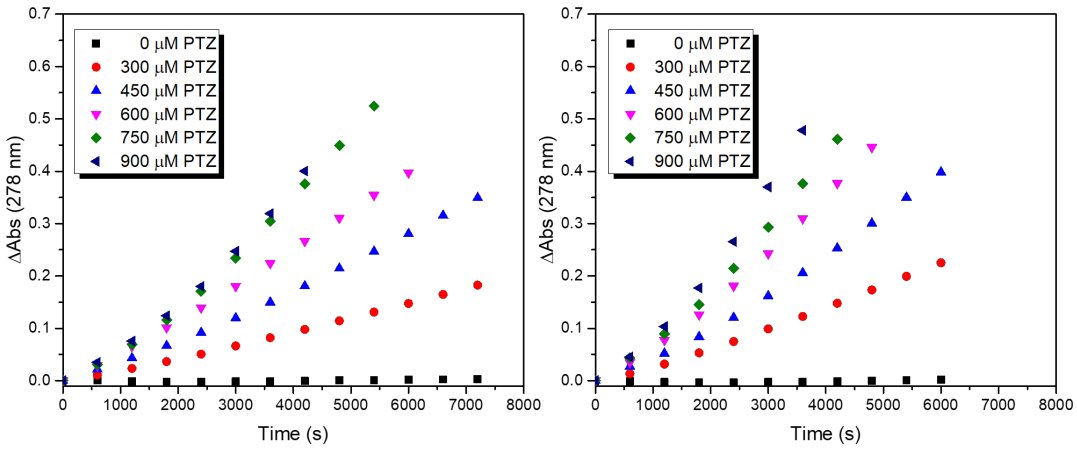



**Figure S27**. *(Left)* Observing the increase of absorbance at 278 nm ($\varepsilon_{278}$ = 9004 $M^{-1}$ $cm^{-1}$) with 300 μM PNX-NO at various concentrations of PTZ in hexadecane at 85 °C; *(Right)* Observing the increase of absorbance at 278 nm ($\varepsilon_{278}$ = 8886 $M^{-1}$ $cm^{-1}$) with 300 μM PNX-NO at various concentrations of PTZ in hexadecane at 90 °C.

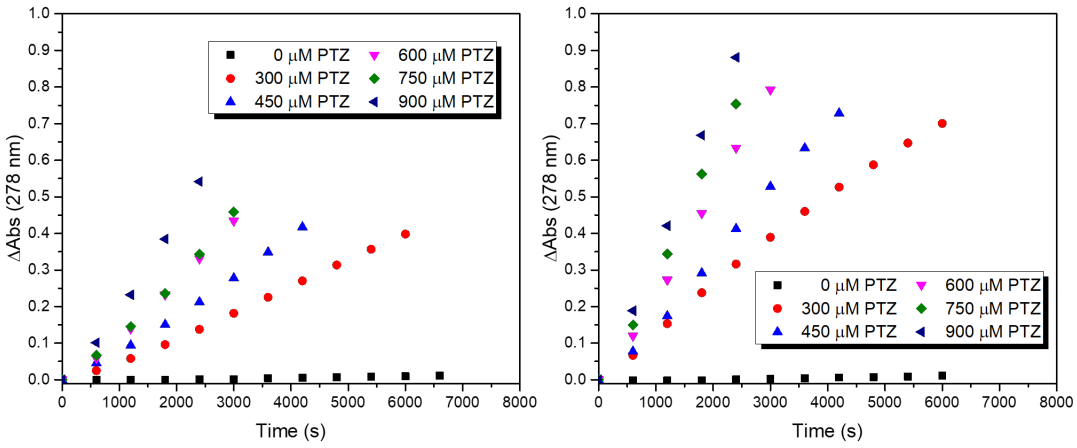



**Figure S28**. *(Left)* Observing the increase of absorbance at 278 nm ($\varepsilon_{278}$ = 8784 $M^{-1}$ $cm^{-1}$) with 300 μM PNX-NO at various concentrations of PTZ in hexadecane at 95 °C; *(Right)* Observing the increase of absorbance at 278 nm ($\varepsilon_{278}$ = 8867 $M^{-1}$ $cm^{-1}$) with 300 μM PNX-NO at various concentrations of PTZ in hexadecane at 100 °C.

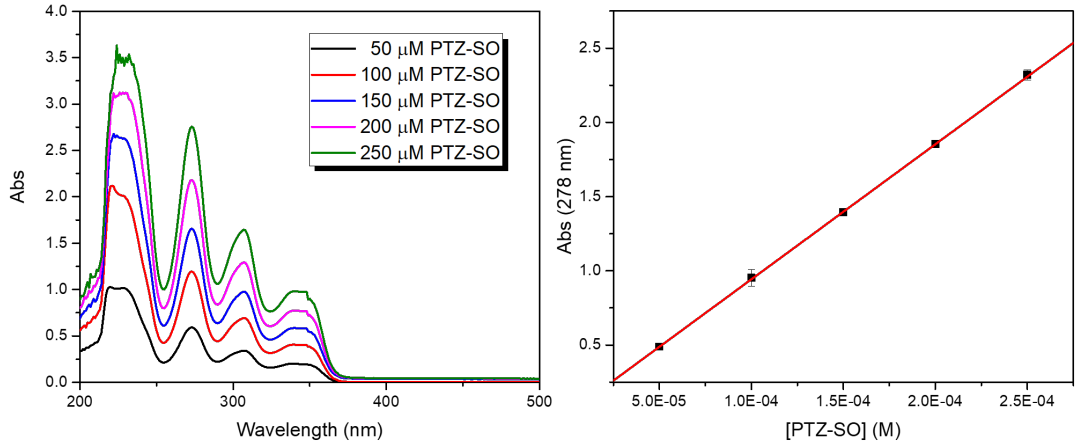



**Figure S29**. *(Left)* UV-Visible spectrum of PTZ-SO; *(Right)* Molar-absorptivity plot of PTZ-SO at 278 nm in hexadecane at 80 °C ($\varepsilon_{278}$ = 9129 $M^{-1}$ $cm^{-1}$).

| Temperature (°C) | Rate Constant ($M^{-1}$ $s^{-1}$) | Ext Coefficient (278 nm) |
|---|---|---|
| 80 | $2.41 \pm 0.26 \times 10^{-2}$ | 9129 |
| 85 | $3.94 \pm 0.48 \times 10^{-2}$ | 9004 |
| 90 | $5.70 \pm 0.54 \times 10^{-2}$ | 8886 |
| 95 | $8.21 \pm 0.51 \times 10^{-2}$ | 8784 |
| 100 | $1.60 \pm 0.04 \times 10^{-1}$ | 8667 |

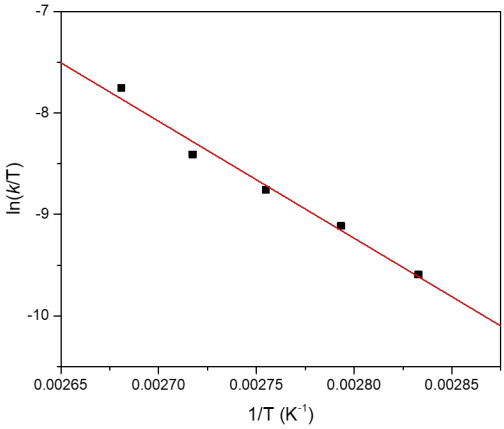



**Figure S30**. *(Left)* Table of rate constants for PTZ-SO formation ($k_{ox}$) at 80-100 °C; *(Right)* Eyring plot ($R^2$ = 0.9836, $\Delta H^{\ddagger}$ = 22.9 kcal/mol, $\Delta S^{\ddagger}$ = -1.4 cal/mol K).

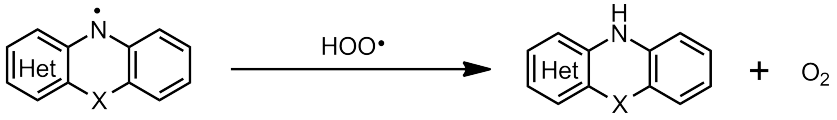
## Additional Computational Data

Geometry optimisation of reactants and products in gas phase were carried out using CBS-QB3 complete basis set method[11] as implemented in the Gaussian 16 suite of programs with Opt = Tight and Int = Ultrafine used for convergence criteria (i.e. threshold = 0.000015 and 0.000060 for maximum force and displacement, respectively). The reported CBS-QB3 enthalpy and free energy (units in Hatrees) were obtained by applying thermal corrections to the electronic energy.

**Table S3.** N-H of azaPNXz and azaPTZs as well as the O-H BDE of the corresponding hydroxyl amine.

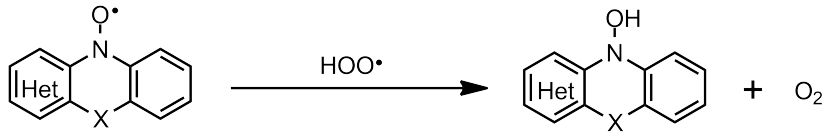
| Compound | N-H BDE (kcal/mol) | Compound | O-H BDE (kcal/mol) |
|---|---|---|---|
| 1-azaPTZ | 85.3 | 1-azaPTZOH | 80.4 |
| 2-azaPTZ | 79.0 | 2-azaPTZOH | 71.3 |
| 3-azaPTZ | 80.3 | 3-azaPTZOH | 72.0 |
| 4-azaPTZ | 77.7 | 4-azaPTZOH | 70.2 |
| PTZ | 78.7 | PTZOH | 70.7 |
| 1-azaPNX | 81.7 | 1-azaPNXOH | 74.6 |
| 2-azaPX | 75.7 | 2-azaPNXOH | 67.1 |
| 3-azaPNX | 77.4 | 3-azaPNXOH | 68.5 |
| 4-azaPNX | 75.0 | 4-azaPNXOH | 65.4 |
| PNX | 75.2 | PNXOH | 66.0 |

**Table S4.** Free energy of aminyl radical derived from azaPNX (X = O) and azaPTZ (X = S) in HAT reaction pathway



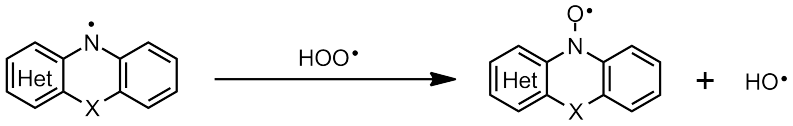

| Compound | ΔG (kcal/mol) | Compound | ΔG (kcal/mol) |
|---|---|---|---|
| 1-azaPNX | -29.7 | 1-azaPTZ | -34.1 |
| 2-azaPNX | -25.3 | 2-azaPTZ | -27.8 |
| 3-azaPNX | -27.1 | 3-azaPTZ | -29.2 |
| 4-azaPNX | -23.6 | 4-azaPTZ | -26.9 |
| PNX | -23.6 | PTZ | -27.6 |

**Table S5.** Free energy of nitroxide derived from azaPNX (X = O) and azaPTZ (X = S) in HAT reaction pathway



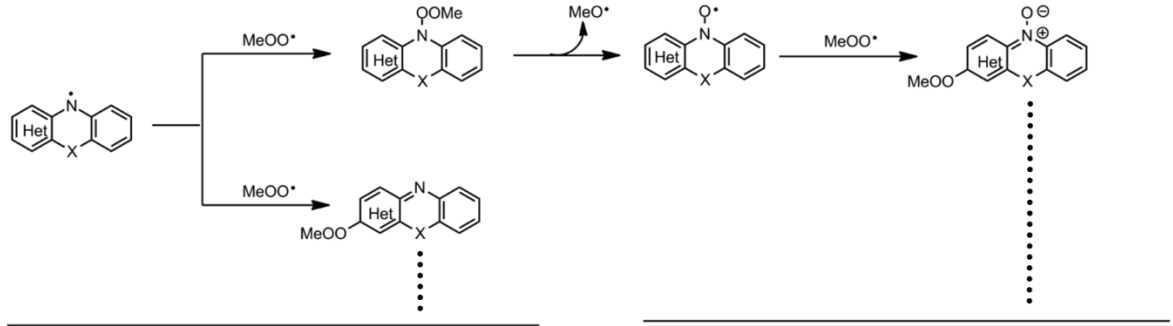

| Compound | ΔG (kcal/mol) | Compound | ΔG (kcal/mol) |
|---|---|---|---|
| 1-azaPNX | -23.7 | 1-azaPTZ | -27.7 |
| 2-azaPNX | -16.4 | 2-azaPTZ | -19.4 |
| 3-azaPNX | -17.7 | 3-azaPTZ | -20.0 |
| 4-azaPNX | -14.7 | 4-azaPTZ | -18.8 |
| PNX | -15.2 | PTZ | -19.0 |

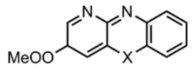
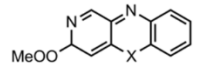
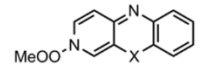
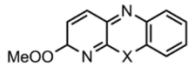
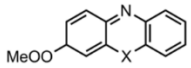
**Table S6.** Free energy of aminyl radical derived from azaPNX (X = O) and azaPTZ (X = S) in O-atom transfer reaction pathway

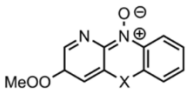
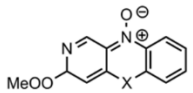
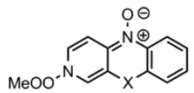
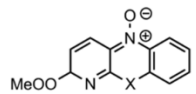
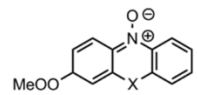



| Compound | ΔG (kcal/mol) | Compound | ΔG (kcal/mol) |
|---|---|---|---|
| 1-azaPNX | -2.7 | 1-azaPTZ | -2.7 |
| 2-azaPNX | -4.2 | 2-azaPTZ | -4.6 |
| 3-azaPNX | -5.4 | 3-azaPTZ | -5.6 |
| 4-azaPNX | -5.4 | 4-azaPTZ | -4.6 |
| PNX | -5.4 | PTZ | -5.2 |

**Table S7.** Free energy profile for radical-trapping of aminyl and nitroxide derived from azaPNX and azaPTZ.

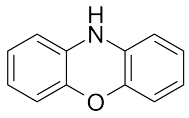



| | ΔG (kcal / mol) | |
|---|---|---|
| | azaPNX (X = O) | azaPTZ (X = S) |
|  | -15.0 | -14.6 |
|  | -14.9 | -15.6 |
|  | +4.3 | +4.2 |
|  | -18.8 | -18.1 |
|  | -14.1 | -14.1 |

| | ΔG (kcal / mol) | |
|---|---|---|
| | azaPNXO (X = O) | azaPTZO (X = S) |
|  | -7.0 | -5.3 |
|  | -7.9 | -5.4 |
|  | +13.3 | +13.4 |
|  | -11.3 | -10.8 |
|  | -6.4 | -5.7 |

## Cartesian coordinates and CBS-QB3 Energies

Phenoxazine

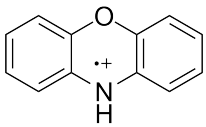


CBS-QB3 Enthalpy= -591.634775
CBS-QB3 Free Energy= -591.681608
Electronic energy= -591.823523
EE + Zero-point energy= -591.645815

0 1

| | | | |
|---|---|---|---|
| C | -3.58034600 | -0.74410900 | 0.16087500 |
| C | -3.61537400 | 0.64504600 | 0.16485300 |
| C | -2.43345800 | 1.37704400 | 0.04249000 |
| C | -1.20821900 | 0.72626400 | -0.09293200 |
| C | -1.18554300 | -0.67718200 | -0.09383800 |
| C | -2.35559200 | -1.40502000 | 0.03678600 |
| N | 0.00000000 | 1.41109700 | -0.24980300 |
| C | 1.20821900 | 0.72626400 | -0.09293200 |
| C | 1.18554300 | -0.67718200 | -0.09383800 |
| O | 0.00000000 | -1.37448800 | -0.24984400 |
| C | 2.43345800 | 1.37704400 | 0.04249000 |
| C | 3.61537400 | 0.64504600 | 0.16485300 |
| C | 3.58034600 | -0.74410900 | 0.16087500 |
| C | 2.35559200 | -1.40502000 | 0.03678600 |
| H | -4.49377300 | -1.31839200 | 0.25534500 |
| H | -4.55872200 | 1.16899200 | 0.26288100 |
| H | -2.45861900 | 2.46207600 | 0.04341700 |
| H | -2.29135500 | -2.48631200 | 0.03290700 |
| H | 0.00000000 | 2.40096500 | -0.06053500 |
| H | 2.45861900 | 2.46207600 | 0.04341800 |
| H | 4.55872100 | 1.16899200 | 0.26288100 |
| H | 4.49377300 | -1.31839200 | 0.25534500 |
| H | 2.29135500 | -2.48631200 | 0.03290700 |

Phenoxazine radical cation



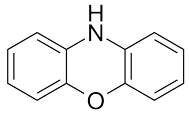
CBS-QB3 Enthalpy= -591.380411
CBS-QB3 Free Energy= -591.426865
Electronic Energy= -591.570463
EE + Zero-point energy= -591.391111

1 2

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.74501500 | 3.57042600 |
| C | 0.00000000 | -0.66342100 | 3.60671400 |
| C | 0.00000000 | -1.39773600 | 2.43843400 |
| C | 0.00000000 | -0.72542100 | 1.20504300 |
| C | 0.00000000 | 0.69010000 | 1.18125500 |
| C | 0.00000000 | 1.42366800 | 2.36288700 |
| N | 0.00000000 | -1.38605300 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 0.00000000 | -0.72542100 | -1.20504300 |
| C | 0.00000000 | 0.69010000 | -1.18125500 |
| O | 0.00000000 | 1.36629400 | 0.00000000 |
| C | 0.00000000 | -1.39773600 | -2.43843400 |
| C | 0.00000000 | -0.66342100 | -3.60671400 |
| C | 0.00000000 | 0.74501500 | -3.57042600 |
| C | 0.00000000 | 1.42366800 | -2.36288700 |
| H | 0.00000000 | 1.30469100 | 4.49712600 |
| H | 0.00000000 | -1.17517100 | 4.56059700 |
| H | 0.00000000 | -2.48148400 | 2.45973700 |
| H | 0.00000000 | 2.50464800 | 2.30985600 |
| H | 0.00000000 | -2.39981600 | 0.00000000 |
| H | 0.00000000 | -2.48148400 | -2.45973700 |
| H | 0.00000000 | -1.17517100 | -4.56059700 |
| H | 0.00000000 | 1.30469100 | -4.49712600 |
| H | 0.00000000 | 2.50464800 | -2.30985600 |

Phenoxazine (Radical Cation Geometry)

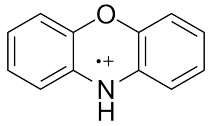



CBS-QB3 Enthalpy= -591.631531
CBS-QB3 Free Energy= -591.675354
Electronic energy= -591.819433
EE + Zero-point energy= -591.641798

0 1

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.74501500 | 3.57042600 |
| C | 0.00000000 | -0.66342100 | 3.60671400 |
| C | 0.00000000 | -1.39773600 | 2.43843400 |
| C | 0.00000000 | -0.72542100 | 1.20504300 |
| C | 0.00000000 | 0.69010000 | 1.18125500 |
| C | 0.00000000 | 1.42366800 | 2.36288700 |
| N | 0.00000000 | -1.38605300 | 0.00000000 |
| C | 0.00000000 | -0.72542100 | -1.20504300 |
| C | 0.00000000 | 0.69010000 | -1.18125500 |
| O | 0.00000000 | 1.36629400 | 0.00000000 |
| C | 0.00000000 | -1.39773600 | -2.43843400 |
| C | 0.00000000 | -0.66342100 | -3.60671400 |
| C | 0.00000000 | 0.74501500 | -3.57042600 |
| C | 0.00000000 | 1.42366800 | -2.36288700 |
| H | 0.00000000 | 1.30469100 | 4.49712600 |
| H | 0.00000000 | -1.17517100 | 4.56059700 |
| H | 0.00000000 | -2.48148400 | 2.45973700 |
| H | 0.00000000 | 2.50464800 | 2.30985600 |
| H | 0.00000000 | -2.39981600 | 0.00000000 |
| H | 0.00000000 | -2.48148400 | -2.45973700 |
| H | 0.00000000 | -1.17517100 | -4.56059700 |
| H | 0.00000000 | 1.30469100 | -4.49712600 |
| H | 0.00000000 | 2.50464800 | -2.30985600 |

Phenoxazine radical cation (Neutral PNX Geometry)

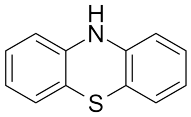


CBS-QB3 Enthalpy= -591.372766
CBS-QB3 Free Energy= -591.419268
Electronic Energy= -591.562425
EE + Zero-point energy= -591.383468

1 2

| | | | |
|---|---|---|---|
| C | -3.58034600 | -0.74410900 | 0.16087500 |
| C | -3.61537400 | 0.64504600 | 0.16485300 |
| C | -2.43345800 | 1.37704400 | 0.04249000 |
| C | -1.20821900 | 0.72626400 | -0.09293200 |
| C | -1.18554300 | -0.67718200 | -0.09383800 |
| C | -2.35559200 | -1.40502000 | 0.03678600 |
| N | 0.00000000 | 1.41109700 | -0.24980300 |
| C | 1.20821900 | 0.72626400 | -0.09293200 |
| C | 1.18554300 | -0.67718200 | -0.09383800 |
| O | 0.00000000 | -1.37448800 | -0.24984400 |
| C | 2.43345800 | 1.37704400 | 0.04249000 |
| C | 3.61537400 | 0.64504600 | 0.16485300 |
| C | 3.58034600 | -0.74410900 | 0.16087500 |
| C | 2.35559200 | -1.40502000 | 0.03678600 |
| H | -4.49377300 | -1.31839200 | 0.25534500 |
| H | -4.55872200 | 1.16899200 | 0.26288100 |
| H | -2.45861900 | 2.46207600 | 0.04341700 |
| H | -2.29135500 | -2.48631200 | 0.03290700 |
| H | 0.00000000 | 2.40096500 | -0.06053500 |
| H | 2.45861900 | 2.46207600 | 0.04341800 |
| H | 4.55872100 | 1.16899200 | 0.26288100 |
| H | 4.49377300 | -1.31839200 | 0.25534500 |
| H | 2.29135500 | -2.48631200 | 0.03290700 |

Phenothiazine



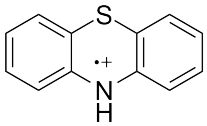
CBS-QB3 Enthalpy= -914.252455
CBS-QB3 Free Energy= -914.300126
Electronic Energy= -914.439523
EE + Zero-point Energy= -914.263843

0 1

| | | | |
|---|---|---|---|
| C | 3.68832700 | -0.36566700 | -0.51859800 |
| C | 3.56427500 | 1.01002500 | -0.34743300 |
| C | 2.33889800 | 1.56357600 | 0.01333600 |
| C | 1.22858700 | 0.74605800 | 0.24374000 |
| C | 1.36229200 | -0.64282900 | 0.08777600 |
| N | 0.00000000 | 1.29803700 | 0.63521500 |
| C | -1.22858900 | 0.74605900 | 0.24373700 |
| C | -1.36228700 | -0.64282900 | 0.08776900 |

| | | | |
|---|---|---|---|
| S | -0.00000200 | -1.71092800 | 0.51117200 |
| C | -2.33890100 | 1.56357500 | 0.01334000 |
| C | -3.56428000 | 1.01002300 | -0.34742800 |
| C | -3.68832300 | -0.36566900 | -0.51859900 |
| C | -2.57982800 | -1.18589500 | -0.31459500 |
| H | 4.63588300 | -0.80074500 | -0.81236800 |
| H | 4.41677900 | 1.65994900 | -0.50695200 |
| H | 2.23863300 | 2.63884000 | 0.12531800 |
| H | 0.00000100 | 2.30563400 | 0.69581200 |
| H | -2.23863700 | 2.63883900 | 0.12532800 |
| H | -4.41678800 | 1.65994200 | -0.50694200 |
| H | -4.63587900 | -0.80074800 | -0.81237000 |
| H | -2.66033000 | -2.25815500 | -0.45192700 |
| C | 2.57983300 | -1.18589600 | -0.31458800 |
| H | 2.66033700 | -2.25815800 | -0.45190500 |

Phenothiazine radical cation

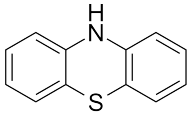



CBS-QB3 Enthalpy= -914.007226
CBS-QB3 Free Energy= -914.055519
Electronic Energy= -914.195271
EE + Zero-point energy= -914.018583

1 2

| | | | |
|---|---|---|---|
| C | -3.77286800 | -0.40794600 | 0.00000500 |
| C | -2.64985600 | -1.21220700 | 0.00000800 |
| C | -1.37014800 | -0.63521100 | 0.00000100 |
| C | -1.23653600 | 0.77542600 | -0.00000800 |
| C | -2.39356700 | 1.57808400 | -0.00000900 |
| C | -3.64143700 | 0.99300900 | -0.00000600 |
| H | -2.74879500 | -2.29131200 | 0.00001600 |
| H | -2.29118800 | 2.65774800 | -0.00001300 |
| H | -4.52578600 | 1.61764900 | -0.00001000 |
| N | 0.00000000 | 1.37779400 | 0.00000300 |
| H | 0.00000000 | 2.39089300 | 0.00000100 |
| C | 1.37014900 | -0.63521300 | -0.00000500 |
| C | 2.64985600 | -1.21220600 | -0.00001200 |
| C | 1.23653600 | 0.77542700 | 0.00000200 |
| C | 3.77286900 | -0.40794500 | -0.00000500 |
| H | 2.74879600 | -2.29131100 | -0.00002300 |
| C | 2.39356700 | 1.57808300 | 0.00001100 |
| C | 3.64143800 | 0.99300900 | 0.00000600 |
| H | 2.29118800 | 2.65774700 | 0.00001900 |
| H | 4.52578500 | 1.61765000 | 0.00001300 |
| H | -4.75689500 | -0.85910400 | 0.00001400 |
| H | 4.75689500 | -0.85910500 | -0.00000800 |
| S | -0.00000100 | -1.71120400 | 0.00000300 |

Phenothiazine (Radical Cation Geometry)

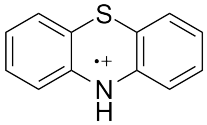


CBS-QB3 Enthalpy= -914.247221
CBS-QB3 Free Energy= -914.293231
Electronic Energy= -914.433152
EE + Zero-point Energy= -914.248165

0 1

| | | | |
|---|---|---|---|
| C | -3.77286800 | -0.40794600 | 0.00000500 |
| C | -2.64985600 | -1.21220700 | 0.00000800 |
| C | -1.37014800 | -0.63521100 | 0.00000100 |
| C | -1.23653600 | 0.77542600 | -0.00000800 |
| C | -2.39356700 | 1.57808400 | -0.00000900 |
| C | -3.64143700 | 0.99300900 | -0.00000600 |
| H | -2.74879500 | -2.29131200 | 0.00001600 |
| H | -2.29118800 | 2.65774800 | -0.00001300 |
| H | -4.52578600 | 1.61764900 | -0.00001000 |
| N | 0.00000000 | 1.37779400 | 0.00000300 |
| H | 0.00000000 | 2.39089300 | 0.00000100 |
| C | 1.37014900 | -0.63521300 | -0.00000500 |
| C | 2.64985600 | -1.21220600 | -0.00001200 |
| C | 1.23653600 | 0.77542700 | 0.00000200 |
| C | 3.77286900 | -0.40794500 | -0.00000500 |
| H | 2.74879600 | -2.29131100 | -0.00002300 |
| C | 2.39356700 | 1.57808300 | 0.00001100 |
| C | 3.64143800 | 0.99300900 | 0.00000600 |
| H | 2.29118800 | 2.65774700 | 0.00001900 |
| H | 4.52578500 | 1.61765000 | 0.00001300 |
| H | -4.75689500 | -0.85910400 | 0.00001400 |
| H | 4.75689500 | -0.85910500 | -0.00000800 |
| S | -0.00000100 | -1.71120400 | 0.00000300 |

Phenothiazine radical cation (Neutral PTZ Geometry)



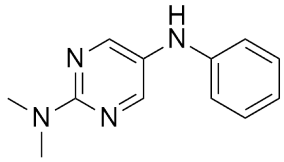
CBS-QB3 Enthalpy= -913.992395
CBS-QB3 Free Energy= -914.040504
Electronic Energy= -914.180087
EE + Zero-point energy= -914.003700

1 2

| | | | |
|---|---|---|---|
| C | 3.68832700 | -0.36566700 | -0.51859800 |
| C | 3.56427500 | 1.01002500 | -0.34743300 |
| C | 2.33889800 | 1.56357600 | 0.01333600 |
| C | 1.22858700 | 0.74605800 | 0.24374000 |
| C | 1.36229200 | -0.64282900 | 0.08777600 |

| | | | |
|---|---|---|---|
| N | 0.00000000 | 1.29803700 | 0.63521500 |
| C | -1.22858900 | 0.74605900 | 0.24373700 |
| C | -1.36228700 | -0.64282900 | 0.08776900 |
| S | -0.00000200 | -1.71092800 | 0.51117200 |
| C | -2.33890100 | 1.56357500 | 0.01334000 |
| C | -3.56428000 | 1.01002300 | -0.34742800 |
| C | -3.68832300 | -0.36566900 | -0.51859900 |
| C | -2.57982800 | -1.18589500 | -0.31459500 |
| H | 4.63588300 | -0.80074500 | -0.81236800 |
| H | 4.41677900 | 1.65994900 | -0.50695200 |
| H | 2.23863300 | 2.63884000 | 0.12531800 |
| H | 0.00000100 | 2.30563400 | 0.69581200 |
| H | -2.23863700 | 2.63883900 | 0.12532800 |
| H | -4.41678800 | 1.65994200 | -0.50694200 |
| H | -4.63587900 | -0.80074800 | -0.81237000 |
| H | -2.66033000 | -2.25815500 | -0.45192700 |
| C | 2.57983300 | -1.18589600 | -0.31458800 |
| H | 2.66033700 | -2.25815800 | -0.45190500 |

$N^2$,$N^2$-dimethyl-$N^5$-phenylpyrimidine-2,5-diamine

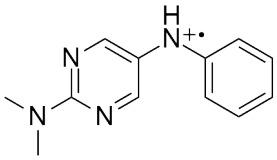


CBS-QB3 Enthalpy= -683.476910
CBS-QB3 Free Energy= -683.538002
Electronic Energy= -683.736060
EE + Zero-point energy= -683.492904

0 1

| | | | |
|---|---|---|---|
| C | 2.40300400 | 0.85181900 | 0.44191700 |
| N | 1.36442800 | -1.11181200 | -0.60944300 |
| C | 0.02365600 | -0.72661300 | -0.38647200 |
| C | -0.83583800 | -1.43596400 | 0.45440800 |
| N | -2.11474200 | -1.12569400 | 0.62440300 |
| C | -2.56968200 | -0.03888700 | -0.03459100 |
| N | -1.82541700 | 0.71944300 | -0.87139400 |
| C | -0.56202100 | 0.36031700 | -1.04367100 |
| N | -3.87362400 | 0.32269300 | 0.15719300 |
| C | -4.76959700 | -0.45385100 | 0.99679000 |
| C | -4.46953300 | 1.44870500 | -0.54137400 |
| H | 3.46707300 | 2.49515800 | 1.30362500 |
| H | 5.71545900 | 1.53511200 | 0.85361700 |
| H | 5.88305300 | -0.68215000 | -0.26637700 |
| H | 3.85027700 | -1.89188300 | -0.94516400 |
| H | 1.43300900 | 1.28010200 | 0.65972000 |
| H | 1.51863500 | -2.09628400 | -0.76343500 |
| H | -0.47058300 | -2.30480600 | 0.99979600 |
| H | 0.02739000 | 0.95927500 | -1.73390000 |
| H | -5.23335300 | 0.19353800 | 1.74963400 |
| H | -4.21100800 | -1.24164300 | 1.49233700 |
| H | -5.57005800 | -0.90336700 | 0.39538800 |
| H | -4.94380400 | 2.12596200 | 0.17777000 |
| H | -5.23962900 | 1.10531400 | -1.24396200 |
| H | -3.70096900 | 1.98361400 | -1.09036900 |

$N^2$,$N^2$-dimethyl-$N^5$-phenylpyrimidine-2,5-diamine Radical Cation

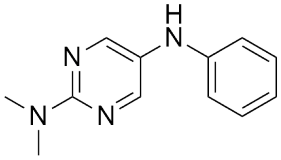


CBS-QB3 Enthalpy= -683.227841
CBS-QB3 Free Energy= -683.286603
Electronic Energy= -683.488085
EE + Zero-point energy= -683.243283

1 2

| | | | |
|---|---|---|---|
| N | -3.89472200 | 0.36695000 | -0.04066900 |
| C | -4.97135700 | -0.56206700 | 0.30832800 |
| C | -4.31660500 | 1.72827100 | -0.37612100 |
| H | 3.86534700 | 2.50340700 | 1.07505200 |
| H | 5.87214000 | 1.45992100 | 0.05928200 |
| H | 5.72160200 | -0.81432600 | -0.92526200 |
| H | 3.56549100 | -2.01701800 | -0.94060600 |
| H | 1.72219400 | 1.29680100 | 1.11652400 |
| H | 1.41690600 | -2.16464500 | 0.04425200 |
| H | -0.82456500 | -2.67348800 | 0.54114300 |
| H | 0.30782600 | 1.32680200 | -0.68438500 |
| H | -5.54979500 | -0.13926900 | 1.13339800 |
| H | -4.55793100 | -1.52244400 | 0.59377200 |
| H | -5.63260600 | -0.68258400 | -0.55403100 |
| H | -4.76816600 | 2.19190200 | 0.50540000 |
| H | -5.06902500 | 1.67896400 | -1.16664800 |
| H | -3.46442000 | 2.31218900 | -0.70438000 |

$N^2$,$N^2$-dimethyl-$N^5$-phenylpyrimidine-2,5-diamine (Radical Cation Geometry)



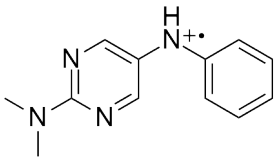
CBS-QB3 Enthalpy= -683.472602
CBS-QB3 Free Energy= -683.525991
Electronic Energy= -683.729095
EE + Zero-point energy= -683.486115

0 1

| | | | |
|---|---|---|---|
| N | -3.89472200 | 0.36695000 | -0.04066900 |
| C | -4.97135700 | -0.56206700 | 0.30832800 |
| C | -4.31660500 | 1.72827100 | -0.37612100 |
| H | 3.86534700 | 2.50340700 | 1.07505200 |
| H | 5.87214000 | 1.45992100 | 0.05928200 |
| H | 5.72160200 | -0.81432600 | -0.92526200 |
| H | 3.56549100 | -2.01701800 | -0.94060600 |
| H | 1.72219400 | 1.29680100 | 1.11652400 |
| H | 1.41690600 | -2.16464500 | 0.04425200 |
| H | -0.82456500 | -2.67348800 | 0.54114300 |
| H | 0.30782600 | 1.32680200 | -0.68438500 |
| H | -5.54979500 | -0.13926900 | 1.13339800 |
| H | -4.55793100 | -1.52244400 | 0.59377200 |

| | | | |
|---|---|---|---|
| H | -5.63260600 | -0.68258400 | -0.55403100 |
| H | -4.76816600 | 2.19190200 | 0.50540000 |
| H | -5.06902500 | 1.67896400 | -1.16664800 |
| H | -3.46442000 | 2.31218900 | -0.70438000 |

$N^2$,$N^2$-dimethyl-$N^5$-phenylpyrimidine-2,5-diamine Radical Cation (Neutral Geometry)

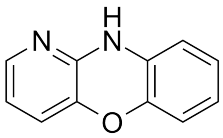


CBS-QB3 Enthalpy= -683.210184
CBS-QB3 Free Energy= -683.266638
Electronic Energy= -683.468676
EE + Zero-point energy= -683.224769

1 2

| | | | |
|---|---|---|---|
| C | 2.40300400 | 0.85181900 | 0.44191700 |
| N | 1.36442800 | -1.11181200 | -0.60944300 |
| C | 0.02365600 | -0.72661300 | -0.38647200 |
| C | -0.83583800 | -1.43596400 | 0.45440800 |
| N | -2.11474200 | -1.12569400 | 0.62440300 |
| C | -2.56968200 | -0.03888700 | -0.03459100 |
| N | -1.82541700 | 0.71944300 | -0.87139400 |
| C | -0.56202100 | 0.36031700 | -1.04367100 |
| N | -3.87362400 | 0.32269300 | 0.15719300 |
| C | -4.76959700 | -0.45385100 | 0.99679000 |
| C | -4.46953300 | 1.44870500 | -0.54137400 |
| H | 3.46707300 | 2.49515800 | 1.30362500 |
| H | 5.71545900 | 1.53511200 | 0.85361700 |
| H | 5.88305300 | -0.68215000 | -0.26637700 |
| H | 3.85027700 | -1.89188300 | -0.94516400 |
| H | 1.43300900 | 1.28010200 | 0.65972000 |
| H | 1.51863500 | -2.09628400 | -0.76343500 |
| H | -0.47058300 | -2.30480600 | 0.99979600 |
| H | 0.02739000 | 0.95927500 | -1.73390000 |
| H | -5.23335300 | 0.19353800 | 1.74963400 |
| H | -4.21100800 | -1.24164300 | 1.49233700 |
| H | -5.57005800 | -0.90336700 | 0.39538800 |
| H | -4.94380400 | 2.12596200 | 0.17777000 |
| H | -5.23962900 | 1.10531400 | -1.24396200 |
| H | -3.70096900 | 1.98361400 | -1.09036900 |

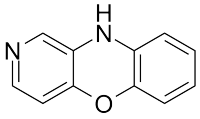
1-azaphenoxazine



CBS-QB3 Enthalpy= -607.685514
CBS-QB3 Free Energy= -607.729627
EE + Zero-point energy= -607.695522

```
0 1
 C                 -3.58828500    0.66579200    0.00016100
 C                 -3.52011500   -0.71600600    0.00012800
 N                 -2.36135100   -1.39856700    0.00001900
 C                 -1.23296100   -0.70587000   -0.00007900
 C                 -1.19718200    0.70394900   -0.00007500
 C                 -2.38908600    1.39381200    0.00006000
 N                 -0.03379800   -1.39302500   -0.00018600
 C                  1.18671400   -0.72144900   -0.00008100
 C                  1.17857400    0.68344200   -0.00008900
 O                 -0.00764100    1.40289800   -0.00024700
 C                  2.41287500   -1.38415700    0.00004700
 C                  3.60809500   -0.66357400    0.00014700
 C                  3.58697500    0.72544300    0.00014000
 C                  2.36249800    1.39895200    0.00002900
 H                 -4.54425000    1.17351100    0.00025800
 H                 -4.42144700   -1.32017900    0.00019200
 H                 -2.37340400    2.47695900    0.00006700
 H                 -0.07896600   -2.39987700   -0.00023900
 H                  2.42552600   -2.46893000    0.00006200
 H                  4.55104200   -1.19710800    0.00023400
 H                  4.51068100    1.29079500    0.00022200
 H                  2.30936600    2.48078400    0.00001800
```

2-azaphenoxazine

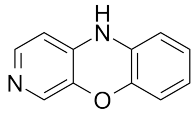



CBS-QB3 Enthalpy= -607.676678
CBS-QB3 Free Energy= -607.723416
EE + Zero-point energy= -607.853819

```
0 1
 C                 -3.56901100   -0.65549000    0.12511400
 N                 -3.61716500    0.67564800    0.13473700
 C                 -2.45851600    1.33577500    0.04149600
 C                 -1.21438400    0.71630700   -0.07068400
 C                 -1.18909000   -0.68563900   -0.07287500
 C                 -2.37991000   -1.38205500    0.02907500
 N                 -0.01296800    1.41102500   -0.20128900
 C                  1.19756400    0.72560600   -0.07500300
 C                  1.17833800   -0.67771500   -0.07380500
 O                 -0.01391900   -1.38493100   -0.19004500
 C                  2.42618000    1.37594700    0.03001600
 C                  3.60994700    0.64364900    0.12656400
 C                  3.57627300   -0.74551300    0.12456600
 C                  2.34918000   -1.40654900    0.02818600
 H                 -4.51872700   -1.17602800    0.19926800
 H                 -2.51375600    2.42261100    0.04926700
 H                 -2.37040300   -2.46464000    0.02888100
 H                 -0.01684700    2.40305200   -0.02439000
 H                  2.45154100    2.46077700    0.02911400
 H                  4.55497800    1.16804300    0.20270100
```

```
 H                  4.49169200   -1.31927000    0.19867000
 H                  2.28438200   -2.48774000    0.02681600
```

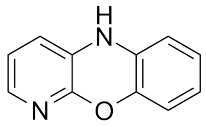
3-azaphenoxazine



CBS-QB3 Enthalpy= -607.677064
CBS-QB3 Free Energy= -607.723978
EE + Zero-point energy= -607.687993

```
0 1
 N                 -3.58346000   -0.77409300    0.11860300
 C                 -3.60062100    0.55792600    0.11651600
 C                 -2.45832200    1.35292500    0.03200300
 C                 -1.21294100    0.73393800   -0.06533900
 C                 -1.19260800   -0.66895300   -0.06475600
 C                 -2.38372500   -1.36662200    0.03308000
 N                 -0.01405200    1.41611000   -0.17342600
 C                  1.20054500    0.72679000   -0.06650000
 C                  1.17585800   -0.67654400   -0.06732900
 O                 -0.01235100   -1.37807100   -0.17984100
 C                  2.42701300    1.37954500    0.02841900
 C                  3.61286800    0.64856700    0.11499300
 C                  3.57719900   -0.74033700    0.11262300
 C                  2.35040800   -1.40287000    0.02536400
 H                 -4.57757200    1.02749300    0.18707200
 H                 -2.53636000    2.43475400    0.03585000
 H                 -2.35598300   -2.45208300    0.03575900
 H                 -0.01244900    2.41525400   -0.04562800
 H                  2.45078900    2.46450600    0.02898600
 H                  4.55842900    1.17275500    0.18377400
 H                  4.49318200   -1.31431700    0.17943400
 H                  2.28731800   -2.48411000    0.02280100
```

4-azaphenoxazine

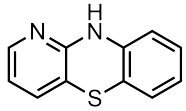


CBS-QB3 Enthalpy= -607.682321
CBS-QB3 Free Energy= -607.726865
EE + Zero-point energy= -607.692526

```
0 1
 C                 -3.48954500   -0.79815300    0.00000000
 C                 -3.61998300    0.57903700    0.00000800
 C                 -2.46105800    1.36224600    0.00000700
 C                 -1.22046300    0.73842400   -0.00000200
 C                 -1.21435700   -0.67463300   -0.00000400
 N                 -2.29263100   -1.41347500   -0.00000500
 N                 -0.01069100    1.41877600   -0.00001300
 C                  1.20114700    0.73026500   -0.00000400
```

| | | | |
|---|---|---|---|
| C | 1.16768700 | -0.67289700 | -0.00000100 |
| O | -0.02658300 | -1.37384500 | -0.00000200 |
| C | 2.43649000 | 1.37522200 | -0.00000100 |
| C | 3.62023500 | 0.63571900 | 0.00000400 |
| C | 3.57593100 | -0.75286500 | 0.00000600 |
| C | 2.34097700 | -1.40655500 | 0.00000300 |
| H | -4.35767100 | -1.44814900 | -0.00000300 |
| H | -4.59870900 | 1.04228100 | 0.00001500 |
| H | -2.52082900 | 2.44568900 | 0.00001200 |
| H | -0.00777100 | 2.42525500 | 0.00000500 |
| H | 2.46763800 | 2.45999100 | -0.00000300 |
| H | 4.57172000 | 1.15391600 | 0.00000600 |
| H | 4.49041800 | -1.33301900 | 0.00000900 |
| H | 2.26874600 | -2.48716100 | 0.00000500 |

1-azaphenothiazine

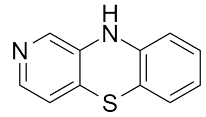



CBS-QB3 Enthalpy= -930.303076
CBS-QB3 Free Energy= -930.350471
EE + Zero-point Energy= -930.314263

0 1

| | | | |
|---|---|---|---|
| C | -3.67828700 | 0.29183200 | -0.49513300 |
| C | -3.46271800 | -1.06075100 | -0.27517800 |
| N | -2.27018700 | -1.57278100 | 0.05594600 |
| C | -1.25172600 | -0.73282400 | 0.22035200 |
| C | -1.37048500 | 0.66198800 | 0.05998100 |
| C | -2.60061000 | 1.16673800 | -0.33316600 |
| N | -0.03255800 | -1.30556000 | 0.56543900 |
| C | 1.20589300 | -0.74905300 | 0.22085900 |
| C | 1.35246400 | 0.64112800 | 0.08346600 |
| S | -0.00853100 | 1.72750800 | 0.47397900 |
| C | 2.31735600 | -1.57029600 | 0.01060500 |
| C | 3.55433000 | -1.02073100 | -0.31361500 |
| C | 3.69174100 | 0.35586200 | -0.46486500 |
| C | 2.58367600 | 1.18081400 | -0.27944500 |
| H | -4.65575300 | 0.65766200 | -0.78244500 |
| H | -4.27218500 | -1.77739800 | -0.37391600 |
| H | -2.72191500 | 2.23236900 | -0.49104700 |
| H | -0.08070300 | -2.31506500 | 0.59245700 |
| H | 2.20593500 | -2.64533800 | 0.10861100 |
| H | 4.40623700 | -1.67457000 | -0.45906300 |
| H | 4.64914600 | 0.78844400 | -0.72859200 |
| H | 2.67514400 | 2.25391600 | -0.40252200 |

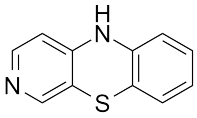
2-azaphenothiazine



CBS-QB3 Enthalpy= -930.293976
CBS-QB3 Free Energy= -930.341506
EE + Zero-point Energy= -930.305228

```
0 1
 C                  3.67350100   -0.27431200   -0.47835600
 N                  3.55935300    1.04809400   -0.33768000
 C                  2.36090900    1.53159700   -0.01408700
 C                  1.23164900    0.73949200    0.22118500
 C                  1.37003500   -0.64780200    0.07937300
 C                  2.60924700   -1.15556500   -0.29727000
 N                  0.01228300    1.30676600    0.60511500
 C                 -1.22044800    0.74786500    0.23703300
 C                 -1.35311700   -0.64141800    0.08529200
 S                  0.01346800   -1.72288300    0.47328000
 C                 -2.33699200    1.56097600    0.02287600
 C                 -3.56582100    1.00322500   -0.31828100
 C                 -3.68858500   -0.37289700   -0.48551800
 C                 -2.57471700   -1.18925800   -0.29704800
 H                  4.65472900   -0.65014300   -0.75100200
 H                  2.28260000    2.61342700    0.08382800
 H                  2.74835100   -2.22155500   -0.43228800
 H                  0.01730600    2.31535600    0.65391000
 H                 -2.23802100    2.63655800    0.13140500
 H                 -4.42243300    1.65046600   -0.46546100
 H                 -4.63892400   -0.81154000   -0.76407100
 H                 -2.65451100   -2.26186600   -0.43203500
```

3-azaphenothiazine

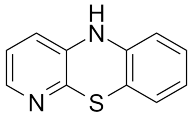


CBS-QB3 Enthalpy= -930.295644
CBS-QB3 Free Energy= -930.343142
EE + Zero-point Energy= -930.306887

```
0 1
 N                  3.69331500   -0.39651500   -0.50998200
 C                  3.56309200    0.92024800   -0.33180700
 C                  2.36859800    1.54384800    0.01217300
 C                  1.23211000    0.75921400    0.22704000
 C                  1.36546600   -0.62938300    0.07124100
 C                  2.59884300   -1.14112800   -0.32186800
 N                  0.01223000    1.32003500    0.58765700
 C                 -1.22294200    0.74997700    0.23082100
 C                 -1.35272900   -0.63995900    0.08620400
 S                  0.01519500   -1.71073400    0.48806900
 C                 -2.33767500    1.56353900    0.01483400
 C                 -3.56784700    1.00521300   -0.32166600
 C                 -3.69022600   -0.37171200   -0.48072400
```

| | | | |
|---|---|---|---|
| C | -2.57654200 | -1.18783100 | -0.29051600 |
| H | 4.45837200 | 1.51643100 | -0.48352100 |
| H | 2.32217800 | 2.62278000 | 0.11721900 |
| H | 2.70843100 | -2.21119600 | -0.47516400 |
| H | 0.00896700 | 2.32804800 | 0.64184100 |
| H | -2.23793700 | 2.63966300 | 0.11788100 |
| H | -4.42445000 | 1.65189600 | -0.47074800 |
| H | -4.64131300 | -0.81167900 | -0.75489100 |
| H | -2.65706200 | -2.26100000 | -0.41982800 |

4-azaphenothiazine

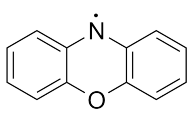


CBS-QB3 Enthalpy= -930.294716
CBS-QB3 Free Energy= -930.342472
EE + Zero-point Energy= -930.306038

0 1

| | | | |
|---|---|---|---|
| C | 3.62964200 | -0.43885100 | -0.39739500 |
| C | 3.58728900 | 0.94545100 | -0.30583600 |
| C | 2.36875800 | 1.56058500 | -0.02557500 |
| C | 1.23545800 | 0.77584900 | 0.18135900 |
| C | 1.39473800 | -0.61968200 | 0.06159800 |
| N | 2.54411000 | -1.20514600 | -0.22574900 |
| N | 0.00681700 | 1.33804200 | 0.52752000 |
| C | -1.22815200 | 0.75589800 | 0.20500900 |
| C | -1.34939200 | -0.63623600 | 0.07358100 |
| S | 0.03015600 | -1.71768400 | 0.40251600 |
| C | -2.35770700 | 1.55814100 | 0.02246100 |
| C | -3.59385900 | 0.98884300 | -0.27059800 |
| C | -3.70923100 | -0.38979200 | -0.41730700 |
| C | -2.58210300 | -1.19413400 | -0.25865700 |
| H | 4.55484600 | -0.96183800 | -0.61482700 |
| H | 4.48253700 | 1.53609500 | -0.45661400 |
| H | 2.29803200 | 2.64146000 | 0.04812000 |
| H | -0.00061900 | 2.34618800 | 0.57358200 |
| H | -2.26363800 | 2.63553400 | 0.11830200 |
| H | -4.46012800 | 1.62793400 | -0.39487000 |
| H | -4.66436700 | -0.84040500 | -0.65808300 |
| H | -2.65830100 | -2.26872300 | -0.38009500 |

Aminyl radical derived from Phenoxazine



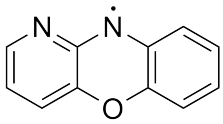
CBS-QB3 Enthalpy= -591.017452
CBS-QB3 Free Energy= -591.063557

0 2

| | | | |
|---|---|---|---|
| C | 3.57102000 | -0.70680000 | -0.00000200 |
| C | 3.58779700 | 0.69635000 | 0.00000000 |
| C | 2.40329400 | 1.40795100 | 0.00000200 |

| | | | |
|---|---|---|---|
| C | 1.15420300 | 0.74334100 | 0.00000100 |
| C | 1.17432000 | -0.67604900 | 0.00000000 |
| C | 2.36198700 | -1.39477900 | -0.00000200 |
| N | 0.00000100 | 1.46544900 | 0.00000100 |
| C | -1.15420400 | 0.74334000 | 0.00000000 |
| C | -1.17432100 | -0.67604900 | 0.00000100 |
| O | 0.00000000 | -1.38118000 | 0.00000100 |
| C | -2.40329300 | 1.40795100 | -0.00000200 |
| C | -3.58779700 | 0.69635000 | -0.00000200 |
| C | -3.57102000 | -0.70679900 | 0.00000100 |
| C | -2.36198700 | -1.39477900 | 0.00000200 |
| H | 4.50180300 | -1.26128800 | -0.00000400 |
| H | 4.53479600 | 1.22311500 | 0.00000100 |
| H | 2.38489300 | 2.49090100 | 0.00000400 |
| H | 2.32037000 | -2.47716700 | -0.00000400 |
| H | -2.38489200 | 2.49090100 | -0.00000300 |
| H | -4.53479600 | 1.22311600 | -0.00000400 |
| H | -4.50180300 | -1.26128700 | 0.00000100 |
| H | -2.32037100 | -2.47716700 | 0.00000400 |

Aminyl radical derived from 1-azaphenoxazine

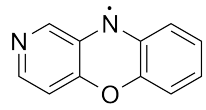



CBS-QB3 Enthalpy= -607.057788
CBS-QB3 Free Energy= -607.103681

0 2

| | | | |
|---|---|---|---|
| C | 3.55600700 | 0.65147400 | -0.00001500 |
| C | 3.47521000 | -0.75009300 | -0.00000700 |
| N | 2.34069900 | -1.43122100 | 0.00000300 |
| C | 1.17509700 | -0.74379200 | 0.00000700 |
| C | 1.18193400 | 0.67885600 | 0.00000500 |
| C | 2.37584400 | 1.38304800 | -0.00000800 |
| N | 0.02232600 | -1.45975100 | 0.00001200 |
| C | -1.13083000 | -0.73864300 | 0.00000500 |
| C | -1.16055500 | 0.68082500 | 0.00000700 |
| O | 0.01310200 | 1.38714300 | 0.00002100 |
| C | -2.37765000 | -1.40962100 | -0.00000400 |
| C | -3.56441200 | -0.70342400 | -0.00001200 |
| C | -3.55476300 | 0.70062100 | -0.00001000 |
| C | -2.35027200 | 1.39563800 | 0.00000000 |
| H | 4.51955900 | 1.14559100 | -0.00002600 |
| H | 4.38600800 | -1.34305000 | -0.00001000 |
| H | 2.35934400 | 2.46627500 | -0.00001100 |
| H | -2.35236600 | -2.49222300 | -0.00000600 |
| H | -4.50909400 | -1.23414500 | -0.00002000 |
| H | -4.48867300 | 1.24974100 | -0.00001600 |
| H | -2.31443500 | 2.47814100 | 0.00000200 |

Aminyl radical derived from 2-azaphenoxazine

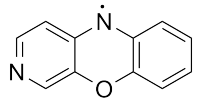


CBS-QB3 Enthalpy= -607.058525
CBS-QB3 Free Energy= -607.104440

0 2

| | | | |
|---|---|---|---|
| C | -3.55359500 | 0.61587700 | 0.00001300 |
| N | -3.58321600 | -0.72868400 | 0.00001300 |
| C | -2.42320000 | -1.36740500 | 0.00000300 |
| C | -1.15878400 | -0.72821600 | -0.00000700 |
| C | -1.17723200 | 0.68574400 | -0.00000700 |
| C | -2.38371400 | 1.36917500 | 0.00000300 |
| N | -0.01293600 | -1.46258000 | -0.00001500 |
| C | 1.14235900 | -0.74115000 | -0.00000800 |
| C | 1.16497200 | 0.67907100 | -0.00000700 |
| O | -0.01200900 | 1.39133100 | -0.00002200 |
| C | 2.39036300 | -1.40730300 | 0.00000000 |
| C | 3.57546300 | -0.69655400 | 0.00001100 |
| C | 3.56006600 | 0.70622800 | 0.00001400 |
| C | 2.35139200 | 1.39646600 | 0.00000500 |
| H | -4.51791800 | 1.11407700 | 0.00002100 |
| H | -2.43687000 | -2.45351600 | 0.00000300 |
| H | -2.39995200 | 2.45178900 | 0.00000300 |
| H | 2.37063600 | -2.49013800 | -0.00000200 |
| H | 4.52186200 | -1.22414000 | 0.00001700 |
| H | 4.49131600 | 1.25972000 | 0.00002300 |
| H | 2.31153000 | 2.47881900 | 0.00000600 |

Aminyl radical derived from 3-azaphenoxazine



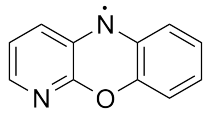
CBS-QB3 Enthalpy= -607.056324
CBS-QB3 Free Energy= -607.102218

0 2

| | | | |
|---|---|---|---|
| N | -3.56588400 | -0.73880000 | 0.00000600 |
| C | -3.56617900 | 0.60934200 | 0.00000500 |
| C | -2.42147400 | 1.38263800 | 0.00000100 |
| C | -1.15823200 | 0.75145000 | -0.00000300 |
| C | -1.17914600 | -0.66263700 | -0.00000300 |
| C | -2.38689700 | -1.35483900 | 0.00000100 |
| N | -0.00617900 | 1.47498200 | -0.00000600 |
| C | 1.14376100 | 0.74719100 | -0.00000300 |
| C | 1.16051700 | -0.67475200 | -0.00000300 |
| O | -0.01355900 | -1.37752100 | -0.00000900 |
| C | 2.39493100 | 1.40972700 | 0.00000000 |
| C | 3.57621700 | 0.69558700 | 0.00000500 |
| C | 3.55587900 | -0.70899000 | 0.00000500 |
| C | 2.34754000 | -1.39562900 | 0.00000200 |
| H | -4.54463200 | 1.07920900 | 0.00000800 |
| H | -2.45912400 | 2.46476300 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | -2.37822500 | -2.44108800 | 0.00000100 |
| H | 2.37837800 | 2.49257300 | 0.00000000 |
| H | 4.52477700 | 1.21920400 | 0.00000700 |
| H | 4.48597000 | -1.26449900 | 0.00000900 |
| H | 2.30427600 | -2.47779400 | 0.00000200 |

Aminyl radical derived from 4-azaphenoxazine

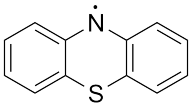


CBS-QB3 Enthalpy= -607.065308
CBS-QB3 Free Energy= -607.111128

0 2

| | | | |
|---|---|---|---|
| C | 3.46029700 | -0.76289400 | 0.00002900 |
| C | 3.57293200 | 0.63088600 | 0.00001900 |
| C | 2.41813800 | 1.39344600 | -0.00000200 |
| C | 1.16141600 | 0.75312000 | -0.00001400 |
| C | 1.19799800 | -0.67109700 | -0.00001100 |
| N | 2.28593700 | -1.40682100 | 0.00001200 |
| N | 0.01014100 | 1.47430900 | -0.00002600 |
| C | -1.14080300 | 0.74798900 | -0.00001200 |
| C | -1.15019000 | -0.67196700 | -0.00001500 |
| O | 0.02634200 | -1.37320200 | -0.00004400 |
| C | -2.39310800 | 1.40639500 | 0.00000700 |
| C | -3.57232200 | 0.68700300 | 0.00002400 |
| C | -3.54599700 | -0.71650600 | 0.00002200 |
| C | -2.33364000 | -1.39772600 | 0.00000200 |
| H | 4.34472600 | -1.39159600 | 0.00005100 |
| H | 4.55113600 | 1.09586100 | 0.00002800 |
| H | 2.43445400 | 2.47652600 | -0.00000900 |
| H | -2.38157500 | 2.48935400 | 0.00000800 |
| H | -4.52288800 | 1.20713600 | 0.00004000 |
| H | -4.47345400 | -1.27644300 | 0.00003700 |
| H | -2.28400800 | -2.47953900 | 0.00000000 |

Phenothiazine radical



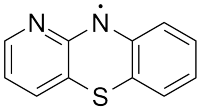
CBS-QB3 Enthalpy= -913.629550
CBS-QB3 Free Energy= -913.677602

0 2

| | | | |
|---|---|---|---|
| C | 3.77014500 | 0.36440800 | 0.00002900 |
| C | 3.62001500 | -1.03130000 | 0.00001700 |
| C | 1.18545600 | -0.79066300 | -0.00001400 |
| C | 1.36699300 | 0.62382400 | -0.00000100 |
| C | 2.64899200 | 1.18139600 | 0.00001900 |
| N | 0.00000000 | -1.44978700 | -0.00003500 |
| C | -1.18546200 | -0.79066300 | -0.00001400 |
| C | -1.36699900 | 0.62382400 | -0.00000400 |
| S | 0.00000000 | 1.72450800 | -0.00002800 |
| C | -2.36024900 | -1.59059300 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -3.62000900 | -1.03129900 | 0.00002100 |
| C | -3.77014800 | 0.36440300 | 0.00002700 |
| C | -2.64899300 | 1.18139500 | 0.00001300 |
| H | 4.75846400 | 0.80850000 | 0.00004000 |
| H | 4.49598900 | -1.66955300 | 0.00003800 |
| H | 2.76302600 | 2.26019400 | 0.00003000 |
| H | -2.21166200 | -2.66335600 | -0.00001000 |
| H | -4.49597600 | -1.66956300 | 0.00004100 |
| H | -4.75846600 | 0.80849600 | 0.00003600 |
| H | -2.76303200 | 2.26019200 | 0.00002000 |
| C | 2.36025600 | -1.59059500 | -0.00000800 |
| H | 2.21166500 | -2.66335900 | -0.00001500 |

1-azaphenothiazine radical

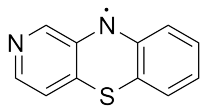


CBS-QB3 Enthalpy= -929.669635
CBS-QB3 Free Energy= -929.717546

0 2

| | | | |
|---|---|---|---|
| C | -3.74712700 | 0.31077600 | 0.00000700 |
| C | -3.50123500 | -1.07229200 | 0.00000400 |
| N | -2.29727000 | -1.61065200 | -0.00000200 |
| C | -1.20427200 | -0.79921500 | -0.00000300 |
| C | -1.37229000 | 0.62013400 | 0.00000000 |
| C | -2.65802600 | 1.16453300 | 0.00000500 |
| N | -0.01876900 | -1.44717900 | -0.00000800 |
| C | 1.16396500 | -0.78689800 | -0.00000300 |
| C | 1.35262700 | 0.62785900 | -0.00000200 |
| S | -0.01241200 | 1.72632100 | -0.00000600 |
| C | 2.33726900 | -1.59054000 | 0.00000000 |
| C | 3.59797200 | -1.03493300 | 0.00000500 |
| C | 3.75307300 | 0.36080600 | 0.00000600 |
| C | 2.63595200 | 1.18256400 | 0.00000300 |
| H | -4.76035500 | 0.69270800 | 0.00001000 |
| H | -4.33492600 | -1.77037900 | 0.00000100 |
| H | -2.79394100 | 2.24087300 | 0.00000700 |
| H | 2.18320000 | -2.66231100 | -0.00000200 |
| H | 4.47206100 | -1.67562100 | 0.00000800 |
| H | 4.74316700 | 0.80086000 | 0.00001100 |
| H | 2.75421500 | 2.26077900 | 0.00000400 |

2-azaphenothiazine radical



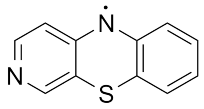
CBS-QB3 Enthalpy= -929.670669
CBS-QB3 Free Energy= -929.718509

0 2

| | | | |
|---|---|---|---|
| C | -3.74064300 | -0.26920900 | 0.00000300 |
| N | -3.60699900 | 1.07090300 | -0.00000300 |
| C | -2.37971300 | 1.55663300 | -0.00000300 |

| | | | |
|---|---|---|---|
| C | -1.18840100 | 0.77521800 | 0.00000100 |
| C | -1.37085000 | -0.63307700 | 0.00000400 |
| C | -2.66830400 | -1.14896900 | 0.00000600 |
| N | -0.01252500 | 1.44761900 | -0.00000300 |
| C | 1.17446800 | 0.78958000 | -0.00000200 |
| C | 1.35538700 | -0.62562300 | -0.00000200 |
| S | -0.01112800 | -1.73496800 | -0.00000300 |
| C | 2.34798300 | 1.58993600 | 0.00000300 |
| C | 3.60799500 | 1.03027000 | 0.00000400 |
| C | 3.75757400 | -0.36479000 | 0.00000100 |
| C | 2.63600000 | -1.18288000 | -0.00000200 |
| H | -4.75723800 | -0.64958800 | 0.00000100 |
| H | -2.25637200 | 2.63594600 | -0.00000800 |
| H | -2.84058900 | -2.21938400 | 0.00001100 |
| H | 2.19907000 | 2.66258300 | 0.00000400 |
| H | 4.48394800 | 1.66832300 | 0.00000800 |
| H | 4.74570100 | -0.80909600 | 0.00000000 |
| H | 2.75120500 | -2.26147500 | -0.00000200 |

3-azaphenothiazine radical

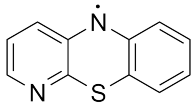



CBS-QB3 Enthalpy= -929.670189
CBS-QB3 Free Energy= -929.718019

0 2

| | | | |
|---|---|---|---|
| N | -3.76662600 | -0.39395500 | 0.00000400 |
| C | -3.60537500 | 0.94659500 | -0.00000300 |
| C | -2.37755900 | 1.57056200 | -0.00000300 |
| C | -1.18565100 | 0.80189300 | 0.00000100 |
| C | -1.36837000 | -0.60862600 | 0.00000100 |
| C | -2.66727600 | -1.13552000 | 0.00000300 |
| N | -0.00382600 | 1.46252600 | -0.00000100 |
| C | 1.17699300 | 0.79542800 | -0.00000200 |
| C | 1.35126200 | -0.62205600 | -0.00000200 |
| S | -0.01560200 | -1.71982300 | -0.00000200 |
| C | 2.35578200 | 1.59025300 | 0.00000200 |
| C | 3.61159600 | 1.02486600 | 0.00000200 |
| C | 3.75494800 | -0.37267000 | 0.00000000 |
| C | 2.63197700 | -1.18507300 | -0.00000100 |
| H | -4.52000200 | 1.53118100 | 0.00000100 |
| H | -2.28357200 | 2.64913600 | -0.00000400 |
| H | -2.80949900 | -2.21406200 | 0.00000700 |
| H | 2.21185300 | 2.66352200 | 0.00000400 |
| H | 4.49094400 | 1.65821300 | 0.00000500 |
| H | 4.74146700 | -0.82055700 | -0.00000100 |
| H | 2.74164900 | -2.26416900 | 0.00000000 |

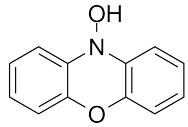
4-azaphenothiazine radical



CBS-QB3 Enthalpy= -929.673422
CBS-QB3 Free Energy= -929.721061

```
0 2
 C                  3.66343300   -0.43392700    0.00000400
 C                  3.61109700    0.96616000    0.00000300
 C                  2.37763400    1.58394100    0.00000000
 C                  1.18899900    0.81105300   -0.00000400
 C                  1.38661300   -0.60222400   -0.00000300
 N                  2.57270100   -1.20051900    0.00000300
 N                  0.00429500    1.46567300   -0.00000400
 C                 -1.17546400    0.79536800   -0.00000700
 C                 -1.34238000   -0.62229900   -0.00000500
 S                  0.03008800   -1.71912700   -0.00000200
 C                 -2.35610300    1.58638200    0.00000100
 C                 -3.61082300    1.01669200    0.00000500
 C                 -3.74861400   -0.38046500    0.00000400
 C                 -2.62128400   -1.18832900    0.00000100
 H                  4.61433200   -0.95708100    0.00001200
 H                  4.52737800    1.54417900    0.00000500
 H                  2.26789800    2.66167600    0.00000300
 H                 -2.21652200    2.66028300    0.00000400
 H                 -4.49223200    1.64728700    0.00000600
 H                 -4.73324700   -0.83260200    0.00001300
 H                 -2.72664500   -2.26790000    0.00000100
```

Hydroxylamine derived from phenoxazine

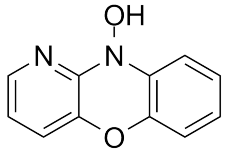


CBS-QB3 Enthalpy= -666.722969
CBS-QB3 Free Energy= -666.771773

```
0 1
 C                 -3.55749500   -0.95845700    0.22552800
 C                 -3.59554800    0.43125700    0.20163000
 C                 -2.42484900    1.16496600    0.01061600
 C                 -1.20662500    0.50812200   -0.15651800
 C                 -1.17671900   -0.89404800   -0.12615300
 C                 -2.34046100   -1.62139800    0.06594200
 N                 -0.00000100    1.20249700   -0.40984400
 C                  1.20662600    0.50812400   -0.15651400
 C                  1.17672200   -0.89404600   -0.12615400
 O                  0.00000100   -1.59227600   -0.30754300
 C                  2.42484900    1.16496800    0.01062200
 C                  3.59554800    0.43126100    0.20163300
 C                  3.55749800   -0.95845400    0.22552500
 C                  2.34046400   -1.62139600    0.06593700
```

| | | | |
|---|---|---|---|
| H | -4.46548100 | -1.53126300 | 0.36993500 |
| H | -4.53617800 | 0.95482200 | 0.32388500 |
| H | -2.44276900 | 2.24544400 | -0.02674800 |
| H | -2.27280100 | -2.70214300 | 0.08864500 |
| H | 2.44276400 | 2.24544700 | -0.02673200 |
| H | 4.53617800 | 0.95482700 | 0.32389100 |
| H | 4.46548500 | -1.53125900 | 0.36992900 |
| H | 2.27280500 | -2.70214100 | 0.08863700 |
| O | 0.00000000 | 2.53868900 | 0.02115400 |
| H | -0.00005700 | 2.51209300 | 0.99601000 |

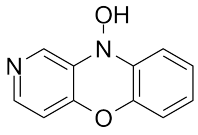
Hydroxylamine derived from 1-azaphenoxazine




CBS-QB3 Enthalpy= -682.772577
CBS-QB3 Free Energy= -682.821090
0 1

| | | | |
|---|---|---|---|
| C | -3.51995900 | -0.90170000 | -0.25361400 |
| C | -3.45804700 | 0.47866300 | -0.26386400 |
| N | -2.30904600 | 1.15814000 | -0.07684200 |
| C | -1.20653300 | 0.45883800 | 0.13594000 |
| C | -1.16112900 | -0.94845600 | 0.14666900 |
| C | -2.33619600 | -1.63499300 | -0.05753500 |
| N | -0.03532000 | 1.15861800 | 0.39260900 |
| C | 1.18544500 | 0.51487600 | 0.13463500 |
| C | 2.37619500 | 1.20189300 | -0.08213800 |
| C | 3.56159200 | 0.48884900 | -0.26857700 |
| C | 3.56204500 | -0.90069200 | -0.24347600 |
| C | 2.36498000 | -1.59283100 | -0.04160400 |
| C | 1.19060500 | -0.88912500 | 0.14890100 |
| O | 0.02087700 | -1.61076800 | 0.37139000 |
| H | -4.46334300 | -1.41011600 | -0.40441200 |
| H | -4.34432400 | 1.08201700 | -0.42443900 |
| H | -2.32569200 | -2.71801400 | -0.06144700 |
| H | 2.35744300 | 2.28232800 | -0.10081000 |
| H | 4.48530700 | 1.03126000 | -0.43117000 |
| H | 4.48292200 | -1.45319500 | -0.38414200 |
| H | 2.32713500 | -2.67513400 | -0.02928000 |
| O | -0.07437100 | 2.52642200 | 0.07221900 |
| H | -1.03491500 | 2.66639600 | -0.05555200 |

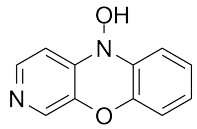
Hydroxylamine derived from 2-azaphenoxazine




CBS-QB3 Enthalpy= -682.763757
CBS-QB3 Free Energy= -682.812365
0 1

| | | | |
|---|---|---|---|
| C | -3.54140000 | -0.87396900 | 0.20711000 |
| N | -3.59475700 | 0.45771800 | 0.18688200 |
| C | -2.44815500 | 1.12265100 | 0.01086200 |
| C | -1.21089700 | 0.49694800 | -0.14900300 |
| C | -1.17733500 | -0.90349900 | -0.11356700 |
| C | -2.35947900 | -1.60105500 | 0.06841800 |
| N | -0.01289800 | 1.20016000 | -0.39481300 |
| C | 1.19692500 | 0.50798100 | -0.15301000 |
| C | 1.17235000 | -0.89368100 | -0.11576500 |
| O | -0.01005300 | -1.60175100 | -0.27083400 |
| C | 2.41586400 | 1.16743700 | -0.00332900 |
| C | 3.58940200 | 0.43598700 | 0.17677900 |
| C | 3.55504400 | -0.95377600 | 0.20635200 |
| C | 2.33752300 | -1.61978000 | 0.06378200 |
| H | -4.48476700 | -1.39384500 | 0.34315200 |
| H | -2.50023400 | 2.20458400 | -0.01464400 |
| H | -2.34475700 | -2.68297300 | 0.10159300 |
| H | 2.43073800 | 2.24788300 | -0.04356800 |
| H | 4.53039200 | 0.96161200 | 0.28610200 |
| H | 4.46581200 | -1.52403800 | 0.34178400 |
| H | 2.27180600 | -2.70044400 | 0.09189700 |
| O | -0.02302100 | 2.53463300 | 0.03881700 |
| H | -0.02987100 | 2.50756300 | 1.01356100 |

Hydroxylamine derived from 3-azaphenoxazine

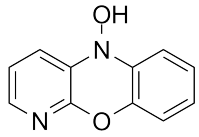



CBS-QB3 Enthalpy= -682.765798
CBS-QB3 Free Energy= -682.814291

0 1

| | | | |
|---|---|---|---|
| N | 3.52875600 | -1.00858900 | -0.27567900 |
| C | 3.54813200 | 0.32410800 | -0.31427400 |
| C | 2.42656000 | 1.12959000 | -0.12168800 |
| C | 1.20641700 | 0.51346500 | 0.13808600 |
| C | 1.17637900 | -0.88645400 | 0.16719000 |
| C | 2.34777600 | -1.59476600 | -0.04754200 |
| N | 0.01545400 | 1.20087100 | 0.42573200 |
| C | -1.19433900 | 0.51115100 | 0.14032200 |
| C | -1.16491400 | -0.89033500 | 0.17157600 |
| O | 0.01005200 | -1.57340800 | 0.42969900 |
| C | -2.39772500 | 1.16236500 | -0.11017800 |
| C | -3.56310500 | 0.42138200 | -0.30889800 |
| C | -3.52932300 | -0.96772300 | -0.26389400 |
| C | -2.32103600 | -1.62539400 | -0.03144000 |
| H | 4.51150300 | 0.78501500 | -0.51160300 |
| H | 2.49088400 | 2.20675200 | -0.17793500 |
| H | 2.31577600 | -2.67988800 | -0.02654600 |
| H | -2.40866700 | 2.24207700 | -0.15756800 |
| H | -4.49508900 | 0.93963900 | -0.49988200 |
| H | -4.43342600 | -1.54468600 | -0.41545400 |
| H | -2.25539500 | -2.70602500 | -0.00343100 |
| O | 0.02066000 | 2.54580800 | -0.00399800 |
| H | 0.01031900 | 3.04761300 | 0.82087800 |

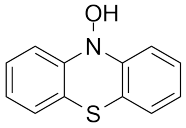
Hydroxylamine derived from 4-azaphenoxazine




CBS-QB3 Enthalpy= -682.769802
CBS-QB3 Free Energy= -682.818433

```
0 1
 C                -3.45463600   -1.01280200    0.18945600
 C                -3.58489200    0.36634800    0.18265800
 C                -2.43949700    1.14831300    0.01446400
 C                -1.21357200    0.51501200   -0.14059400
 C                -1.20083700   -0.89427700   -0.10486400
 N                -2.27124000   -1.63269000    0.05291300
 N                -0.01139300    1.20821100   -0.38522500
 C                 1.19635000    0.51089900   -0.14869800
 C                 1.15621000   -0.89027400   -0.11024200
 O                -0.02563200   -1.58956600   -0.26090100
 C                 2.41946100    1.16340800   -0.00740700
 C                 3.58859500    0.42368200    0.16947700
 C                 3.54197000   -0.96562400    0.20158400
 C                 2.31915000   -1.62288100    0.06491500
 H                -4.31681700   -1.65947300    0.31267400
 H                -4.55627400    0.82992900    0.30028500
 H                -2.48625800    2.22839500   -0.01406200
 H                 2.44267800    2.24362300   -0.05268600
 H                 4.53426400    0.94192700    0.27350400
 H                 4.44863400   -1.54302100    0.33510900
 H                 2.24450600   -2.70280600    0.09463300
 O                -0.01475700    2.54644800    0.03611800
 H                 0.02100300    2.52690600    1.01049200
```

Hydroxylamine derived from phenothiazine

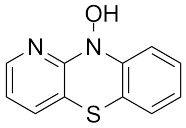



CBS-QB3 Enthalpy= -989.341723
CBS-QB3 Free Energy= -989.391562

```
0 1
 C                -3.61828300   -0.62202500   -0.65401100
 C                -2.30009400    1.36137000   -0.22763500
 C                -1.22324800    0.56811800    0.16913000
 C                -1.34752200   -0.82963100    0.14514400
 C                -2.53554000   -1.41651000   -0.28300400
 N                 0.00000000    1.12409900    0.63928400
 C                 1.22324700    0.56811900    0.16912900
 C                 1.34752400   -0.82963100    0.14514800
 S                 0.00000000   -1.83256100    0.73314300
 C                 2.30009100    1.36137100   -0.22764200
 C                 3.49467000    0.76350900   -0.62433900
 C                 3.61828500   -0.62202300   -0.65400800
 C                 2.53554400   -1.41650900   -0.28299600
 H                -4.54537600   -1.08563600   -0.96931900
```

| | | | |
|---|---|---|---|
| H | -2.19289400 | 2.43597600 | -0.21496100 |
| H | -2.60927100 | -2.49730800 | -0.31566000 |
| H | 2.19289100 | 2.43597700 | -0.21496700 |
| H | 4.32735400 | 1.39128000 | -0.91991100 |
| H | 4.54538000 | -1.08563300 | -0.96930800 |
| H | 2.60927700 | -2.49730600 | -0.31564800 |
| O | 0.00000100 | 2.53531200 | 0.59978000 |
| H | -0.00001700 | 2.78317000 | 1.53267200 |
| C | -3.49467200 | 0.76350700 | -0.62433400 |
| H | -4.32735900 | 1.39127700 | -0.91989900 |

Hydroxylamine derived from 1-azaphenothiazine

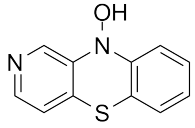



CBS-QB3 Enthalpy= -1005.391812
CBS-QB3 Free Energy= -1005.441287

0 1

| | | | |
|---|---|---|---|
| C | 3.62528300 | -0.54634100 | -0.58351000 |
| C | 3.42315900 | 0.81635300 | -0.45622300 |
| N | 2.23981700 | 1.34533500 | -0.10436100 |
| C | 1.23259200 | 0.52009600 | 0.16105500 |
| C | 1.33838600 | -0.88340500 | 0.08690000 |
| C | 2.55280200 | -1.40927700 | -0.31895200 |
| N | 0.03600500 | 1.11994000 | 0.55254300 |
| C | -1.20906000 | 0.57799400 | 0.16552100 |
| C | -1.36360600 | -0.81762600 | 0.12009800 |
| S | -0.02312500 | -1.88818900 | 0.61291500 |
| C | -2.29347600 | 1.40082000 | -0.14352300 |
| C | -3.51861000 | 0.83418500 | -0.48766700 |
| C | -3.67049400 | -0.54717600 | -0.54707100 |
| C | -2.58360800 | -1.37033800 | -0.25664800 |
| H | 4.59123100 | -0.93498500 | -0.87861800 |
| H | 4.22300900 | 1.52519100 | -0.64084300 |
| H | 2.67104100 | -2.48269500 | -0.41132700 |
| H | -2.16110700 | 2.47170300 | -0.10485000 |
| H | -4.35548700 | 1.48433300 | -0.71475600 |
| H | -4.62237200 | -0.98663200 | -0.81966000 |
| H | -2.68128000 | -2.44836500 | -0.31230000 |
| O | 0.07263900 | 2.52276500 | 0.53306100 |
| H | 0.99288800 | 2.69172200 | 0.23407400 |

Hydroxylamine derived from 2- azaphenothiazine



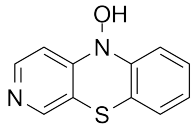

CBS-QB3 Enthalpy= -1005.382289
CBS-QB3 Free Energy= -1005.431991

0 1

| | | | |
|---|---|---|---|
| C | -3.60259300 | -0.53277800 | -0.62731600 |
| N | -3.49556600 | 0.79643900 | -0.60905500 |
| C | -2.32681800 | 1.32549700 | -0.23795800 |

| | | | |
|---|---|---|---|
| C | -1.22570000 | 0.55786100 | 0.15360800 |
| C | -1.35154900 | -0.83724800 | 0.13143500 |
| C | -2.55937600 | -1.38871600 | -0.28230100 |
| N | -0.01296500 | 1.12776600 | 0.62059300 |
| C | 1.21704200 | 0.56930900 | 0.17214500 |
| C | 1.34227300 | -0.82809400 | 0.14368900 |
| S | -0.00939000 | -1.85146900 | 0.69276200 |
| C | 2.30082200 | 1.36329500 | -0.20343100 |
| C | 3.50161600 | 0.76703400 | -0.58260900 |
| C | 3.62557600 | -0.61818700 | -0.61681200 |
| C | 2.53658700 | -1.41379700 | -0.26779100 |
| H | -4.56169200 | -0.93732700 | -0.93636300 |
| H | -2.25146400 | 2.40484200 | -0.23392100 |
| H | -2.68645600 | -2.46357700 | -0.32713700 |
| H | 2.19271100 | 2.43773300 | -0.19031400 |
| H | 4.33894000 | 1.39608600 | -0.86144400 |
| H | 4.55731000 | -1.08091000 | -0.91896700 |
| H | 2.61067200 | -2.49438500 | -0.30551300 |
| O | -0.02417000 | 2.53761300 | 0.55393200 |
| H | -0.04398500 | 2.80563100 | 1.48130500 |

Hydroxylamine derived from 3- azaphenothiazine

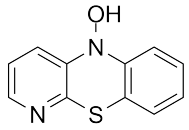



CBS-QB3 Enthalpy= -1005.384412
CBS-QB3 Free Energy= -1005.434087

0 1

| | | | |
|---|---|---|---|
| N | 3.62124300 | -0.65322600 | -0.64828500 |
| C | 3.49414400 | 0.67471900 | -0.59717100 |
| C | 2.33007400 | 1.33823600 | -0.21872500 |
| C | 1.22657800 | 0.57478100 | 0.16005200 |
| C | 1.34780500 | -0.82219100 | 0.12552400 |
| C | 2.55100400 | -1.37517000 | -0.30489800 |
| N | 0.01452800 | 1.13869800 | 0.60828500 |
| C | -1.21771800 | 0.57049700 | 0.16728100 |
| C | -1.33990800 | -0.82736500 | 0.14460500 |
| S | 0.01290400 | -1.83961200 | 0.70723400 |
| C | -2.30038300 | 1.36367300 | -0.21101200 |
| C | -3.50140800 | 0.76606000 | -0.58819100 |
| C | -3.62431700 | -0.61920300 | -0.61637100 |
| C | -2.53525900 | -1.41336700 | -0.26433900 |
| H | 4.36972600 | 1.25058800 | -0.88291900 |
| H | 2.27606100 | 2.41662200 | -0.21187700 |
| H | 2.65298900 | -2.45535700 | -0.35948800 |
| H | -2.19294000 | 2.43826000 | -0.20247600 |
| H | -4.33874300 | 1.39387700 | -0.86955100 |
| H | -4.55601900 | -1.08341600 | -0.91651800 |
| H | -2.60918700 | -2.49404800 | -0.29761000 |
| O | 0.01902100 | 2.54714300 | 0.55493500 |
| H | 0.00541000 | 2.80781100 | 1.48468900 |

Hydroxylamine derived from 4- azaphenothiazine

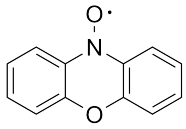



CBS-QB3 Enthalpy= -1005.383861
CBS-QB3 Free Energy= -1005.433642

0 1

| | | | |
|---|---|---|---|
| C | -3.55671700 | -0.67622400 | -0.55513200 |
| C | -3.50674200 | 0.71027100 | -0.59290500 |
| C | -2.31879300 | 1.35457800 | -0.24985200 |
| C | -1.22549900 | 0.58370100 | 0.13241900 |
| C | -1.37684700 | -0.81637200 | 0.11630400 |
| N | -2.50096800 | -1.42768700 | -0.21714800 |
| N | -0.00941900 | 1.14087500 | 0.59497100 |
| C | 1.22175600 | 0.57063300 | 0.16069200 |
| C | 1.33288700 | -0.82781800 | 0.13589200 |
| S | -0.02926100 | -1.85665000 | 0.64300000 |
| C | 2.31627100 | 1.35819200 | -0.19471300 |
| C | 3.52066200 | 0.75517200 | -0.55222300 |
| C | 3.63459400 | -0.63065300 | -0.58191000 |
| C | 2.53346700 | -1.41817000 | -0.25319800 |
| H | -4.46540400 | -1.21455600 | -0.80356300 |
| H | -4.37761400 | 1.28401900 | -0.88555200 |
| H | -2.23475400 | 2.43163500 | -0.25861600 |
| H | 2.21499900 | 2.43343200 | -0.18316600 |
| H | 4.36693000 | 1.37860500 | -0.81623700 |
| H | 4.56819800 | -1.10084800 | -0.86656900 |
| H | 2.60137000 | -2.49921500 | -0.29087000 |
| O | -0.01148100 | 2.55109600 | 0.53891000 |
| H | 0.00877700 | 2.81237900 | 1.46828700 |

Phenoxazine-*N*-oxyl



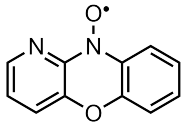

CBS-QB3 Enthalpy= -666.120319
CBS-QB3 Free Energy= -666.168856

0 2

| | | | |
|---|---|---|---|
| C | 3.58318600 | -0.92966600 | 0.00001000 |
| C | 3.61907600 | 0.46609700 | 0.00001800 |
| C | 2.43819600 | 1.19646000 | 0.00001300 |
| C | 1.21040200 | 0.52969800 | 0.00000500 |
| C | 1.17915200 | -0.87335000 | -0.00001400 |
| C | 2.36242200 | -1.59963300 | -0.00000200 |
| N | -0.00000200 | 1.25217400 | -0.00001200 |
| C | -1.21040200 | 0.52969400 | 0.00000600 |
| C | -1.17914700 | -0.87335400 | -0.00001400 |
| O | 0.00000300 | -1.57756400 | -0.00002800 |
| C | -2.43819500 | 1.19645600 | 0.00001200 |
| C | -3.61907500 | 0.46609200 | 0.00001700 |
| C | -3.58318200 | -0.92967100 | 0.00001100 |
| C | -2.36241600 | -1.59963700 | 0.00000000 |

| | | | |
|---|---|---|---|
| O | -0.00001500 | 2.52682400 | -0.00002300 |
| H | 4.50443400 | -1.49957100 | 0.00003200 |
| H | 4.56944700 | 0.98585300 | -0.00002200 |
| H | 2.42383700 | 2.27740800 | 0.00002800 |
| H | 2.30418400 | -2.68088800 | 0.00002000 |
| H | -2.42383700 | 2.27740500 | 0.00002700 |
| H | -4.56944600 | 0.98584700 | -0.00002300 |
| H | -4.50442900 | -1.49957800 | 0.00003400 |
| H | -2.30417600 | -2.68089200 | 0.00002200 |

*N*-oxyl-1-azaphenoxazine

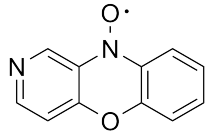


CBS-QB3 Enthalpy= -682.156178
CBS-QB3 Free Energy= -682.204647

0 2

| | | | |
|---|---|---|---|
| C | 3.57180500 | -0.87385100 | 0.00001200 |
| C | 3.51672400 | 0.51790100 | 0.00000300 |
| N | 2.37462400 | 1.20660500 | -0.00000500 |
| C | 1.23742400 | 0.52828800 | -0.00000600 |
| C | 1.18375000 | -0.87855800 | -0.00000400 |
| C | 2.37453600 | -1.58617600 | 0.00000800 |
| N | 0.02220800 | 1.25778800 | -0.00000700 |
| C | -1.19130300 | 0.52749800 | -0.00000400 |
| C | -2.41656500 | 1.19760700 | 0.00000200 |
| C | -3.60075600 | 0.47205100 | 0.00000700 |
| C | -3.57137400 | -0.92337400 | 0.00000700 |
| C | -2.35301700 | -1.59752300 | 0.00000100 |
| C | -1.16870900 | -0.87388000 | -0.00000500 |
| O | 0.01035200 | -1.58384900 | -0.00001600 |
| O | 0.01133000 | 2.52522100 | 0.00000400 |
| H | 4.52415300 | -1.38882600 | 0.00002100 |
| H | 4.42651300 | 1.10968500 | 0.00000200 |
| H | 2.34294600 | -2.66868300 | 0.00001300 |
| H | -2.39858500 | 2.27848200 | 0.00000400 |
| H | -4.54860700 | 0.99630300 | 0.00001000 |
| H | -4.49478400 | -1.48965800 | 0.00001200 |
| H | -2.29801400 | -2.67893200 | 0.00000200 |

*N*-oxyl-2-azaphenoxazine



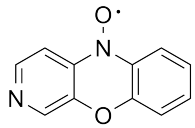
CBS-QB3 Enthalpy= -683.255215
CBS-QB3 Free Energy= -683.303401

0 2

| | | | |
|---|---|---|---|
| C | 3.56341400 | -0.84637500 | -0.00000200 |
| N | 3.61607900 | 0.49070200 | -0.00000300 |
| C | 2.46162300 | 1.15422400 | 0.00000500 |
| C | 1.21436500 | 0.51913000 | 0.00002200 |
| C | 1.17947800 | -0.88124200 | 0.00000100 |

| | | | |
|---|---|---|---|
| C | 2.37855600 | -1.57813100 | -0.00000200 |
| N | 0.01206400 | 1.25027700 | -0.00000300 |
| C | -1.20102200 | 0.52974900 | 0.00000600 |
| C | -1.17335500 | -0.87314500 | -0.00000700 |
| O | 0.01008600 | -1.58333200 | -0.00000500 |
| C | -2.42729600 | 1.19799000 | 0.00001000 |
| C | -3.60887500 | 0.46818700 | 0.00000500 |
| C | -3.57518700 | -0.92723100 | -0.00000300 |
| C | -2.35485500 | -1.59917800 | -0.00000500 |
| O | 0.02091100 | 2.52394600 | -0.00001500 |
| H | 4.51755600 | -1.36395300 | -0.00001400 |
| H | 2.48937800 | 2.23691300 | -0.00000300 |
| H | 2.37291400 | -2.66039600 | 0.00002200 |
| H | -2.41237900 | 2.27900700 | 0.00002500 |
| H | -4.55854600 | 0.98906200 | -0.00002900 |
| H | -4.49707400 | -1.49583000 | 0.00000600 |
| H | -2.29790400 | -2.68043600 | 0.00001400 |

*N*-oxyl-3-azaphenoxazine

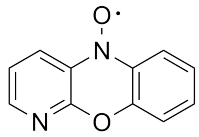


CBS-QB3 Enthalpy= -682.159211
CBS-QB3 Free Energy= -682.207525

0 2

| | | | |
|---|---|---|---|
| N | 3.57487200 | -0.96328000 | 0.00000500 |
| C | 3.59583000 | 0.37648100 | 0.00000200 |
| C | 2.45622700 | 1.16943900 | 0.00000100 |
| C | 1.21372000 | 0.53461200 | -0.00000300 |
| C | 1.18170000 | -0.86494300 | -0.00000200 |
| C | 2.38467500 | -1.56363800 | 0.00000500 |
| N | 0.01142900 | 1.25861800 | 0.00000000 |
| C | -1.20137100 | 0.53236300 | -0.00000300 |
| C | -1.16891200 | -0.87101100 | -0.00000500 |
| O | 0.01075200 | -1.57651900 | -0.00001000 |
| C | -2.42773500 | 1.19983300 | 0.00000300 |
| C | -3.60854300 | 0.46961500 | 0.00000600 |
| C | -3.57207300 | -0.92627900 | 0.00000400 |
| C | -2.35234900 | -1.59707500 | -0.00000200 |
| O | 0.01610200 | 2.53174400 | -0.00000400 |
| H | 4.57793300 | 0.83829300 | -0.00000200 |
| H | 2.49593200 | 2.24949900 | 0.00000900 |
| H | 2.36114000 | -2.64914800 | 0.00001200 |
| H | -2.41409500 | 2.28087700 | 0.00000300 |
| H | -4.55889300 | 0.98909700 | -0.00000200 |
| H | -4.49341800 | -1.49590400 | 0.00001600 |
| H | -2.29454800 | -2.67826400 | 0.00000000 |

*N*-oxyl-4-azaphenoxazine

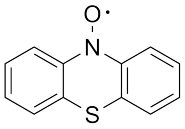


CBS-QB3 Enthalpy= -683.262588
CBS-QB3 Free Energy= -683.310653

0 2

| | | | |
|---|---|---|---|
| C | 3.47080700 | -0.98630900 | -0.00000600 |
| C | 3.60194100 | 0.39909700 | 0.00002100 |
| C | 2.45066400 | 1.17884700 | 0.00002400 |
| C | 1.21546500 | 0.53502400 | 0.00000100 |
| C | 1.20074300 | -0.87321100 | -0.00001000 |
| N | 2.28505800 | -1.61208800 | -0.00002200 |
| N | 0.01085500 | 1.25942300 | -0.00000400 |
| C | -1.19827200 | 0.53402500 | -0.00001100 |
| C | -1.15718400 | -0.86846500 | 0.00000000 |
| O | 0.02376100 | -1.57182600 | -0.00001300 |
| C | -2.42783100 | 1.19643500 | -0.00001600 |
| C | -3.60443700 | 0.45969200 | -0.00000300 |
| C | -3.56042400 | -0.93617000 | 0.00002000 |
| C | -2.33690400 | -1.60042200 | 0.00002000 |
| O | 0.01796100 | 2.53313200 | -0.00000500 |
| H | 4.34401300 | -1.63005500 | -0.00001300 |
| H | 4.58272400 | 0.85738500 | 0.00003400 |
| H | 2.46813600 | 2.25997400 | 0.00003700 |
| H | -2.41894400 | 2.27753500 | -0.00002700 |
| H | -4.55772800 | 0.97392800 | -0.00002300 |
| H | -4.47875300 | -1.51068700 | 0.00004900 |
| H | -2.27203400 | -2.68113600 | 0.00003600 |

Phenothiazine-*N*-oxyl



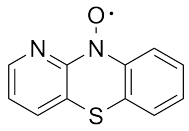
CBS-QB3 Enthalpy= -988.731654
CBS-QB3 Free Energy= -988.782591

0 2

| | | | |
|---|---|---|---|
| C | -3.77323400 | -0.58593900 | -0.18991800 |
| C | -2.40064000 | 1.39251200 | -0.06866800 |
| C | -1.24929400 | 0.59991400 | 0.03812400 |
| C | -1.37035700 | -0.79938400 | 0.03139500 |
| C | -2.63696800 | -1.37804900 | -0.08893700 |
| N | 0.00000000 | 1.26379400 | 0.15651900 |
| C | 1.24929400 | 0.59991400 | 0.03812400 |
| C | 1.37035600 | -0.79938400 | 0.03139400 |
| S | 0.00000000 | -1.89469700 | 0.22586900 |
| C | 2.40064100 | 1.39251200 | -0.06866600 |
| C | 3.65073900 | 0.80433400 | -0.17889100 |
| C | 3.77323400 | -0.58593900 | -0.18991900 |
| C | 2.63696700 | -1.37804900 | -0.08894000 |
| O | 0.00000000 | 2.53720900 | 0.27066100 |

| | | | |
|---|---|---|---|
| H | -4.74699300 | -1.05228100 | -0.27969700 |
| H | -2.27212400 | 2.46488600 | -0.05633700 |
| H | -2.72330400 | -2.45880400 | -0.10065300 |
| H | 2.27212400 | 2.46488600 | -0.05633200 |
| H | 4.53060600 | 1.43132600 | -0.25933900 |
| H | 4.74699200 | -1.05228100 | -0.27969900 |
| H | 2.72330400 | -2.45880400 | -0.10065800 |
| C | -3.65073900 | 0.80433500 | -0.17889300 |
| H | -4.53060500 | 1.43132600 | -0.25934000 |

1-azaphenothiazine-*N*-oxyl

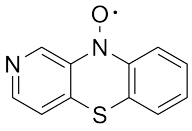


CBS-QB3 Enthalpy= -1004.768120
CBS-QB3 Free Energy= -1004.818511

0 2

| | | | |
|---|---|---|---|
| C | 3.72718000 | -0.52700700 | -0.32856000 |
| C | 3.51461900 | 0.84925400 | -0.29781600 |
| N | 2.31597200 | 1.39847900 | -0.11671700 |
| C | 1.27097500 | 0.59959000 | 0.05823000 |
| C | 1.36964100 | -0.80455500 | 0.05361300 |
| C | 2.62989300 | -1.36208700 | -0.15577000 |
| N | 0.02063500 | 1.25794800 | 0.26303600 |
| C | -1.22728100 | 0.59865100 | 0.06098600 |
| C | -1.35417400 | -0.79850600 | 0.05786200 |
| S | 0.00839800 | -1.88063200 | 0.37742300 |
| C | -2.36330000 | 1.39537800 | -0.12389600 |
| C | -3.60729100 | 0.80998400 | -0.30709600 |
| C | -3.73490400 | -0.57921800 | -0.31597700 |
| C | -2.61029100 | -1.37634300 | -0.13974100 |
| O | 0.01642100 | 2.51061000 | 0.47836900 |
| H | 4.71830000 | -0.93277500 | -0.48755000 |
| H | 4.33909800 | 1.54355600 | -0.42816600 |
| H | 2.74319800 | -2.44008300 | -0.17606600 |
| H | -2.23237100 | 2.46780800 | -0.10815700 |
| H | -4.47786500 | 1.43945300 | -0.44706200 |
| H | -4.70337500 | -1.04185800 | -0.46338400 |
| H | -2.69936400 | -2.45669800 | -0.15059400 |

2-azaphenothiazine-*N*-oxyl



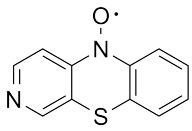
CBS-QB3 Enthalpy= -1004.771258
CBS-QB3 Free Energy= -1004.822529

0 2

| | | | |
|---|---|---|---|
| C | -3.75164400 | -0.49864500 | -0.11304300 |
| N | -3.64914900 | 0.83598500 | -0.11368700 |
| C | -2.42880900 | 1.35769700 | -0.04989500 |
| C | -1.25285600 | 0.58986200 | 0.02052600 |

| | | | |
|---|---|---|---|
| C | -1.37353700 | -0.80651700 | 0.01970100 |
| C | -2.65747100 | -1.35040600 | -0.05159900 |
| N | -0.01133700 | 1.26554100 | 0.09484300 |
| C | 1.24173100 | 0.60040500 | 0.02412700 |
| C | 1.36434900 | -0.79882400 | 0.01955400 |
| S | -0.00895400 | -1.90798700 | 0.13375300 |
| C | 2.39531200 | 1.39335400 | -0.03960300 |
| C | 3.64902200 | 0.80571900 | -0.10598900 |
| C | 3.77289800 | -0.58395000 | -0.11351300 |
| C | 2.63387600 | -1.37698200 | -0.05322900 |
| O | -0.02116500 | 2.54129000 | 0.16702500 |
| H | -4.75661400 | -0.90576400 | -0.16592600 |
| H | -2.33538400 | 2.43563000 | -0.04877800 |
| H | -2.79735900 | -2.42496900 | -0.05773600 |
| H | 2.26586300 | 2.46569600 | -0.03177400 |
| H | 4.53065600 | 1.43340500 | -0.15383500 |
| H | 4.74935900 | -1.04984000 | -0.16762200 |
| H | 2.72223500 | -2.45764700 | -0.06088500 |

3-azaphenothiazine-*N*-oxyl

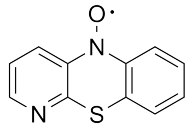



CBS-QB3 Enthalpy= -1004.772199
CBS-QB3 Free Energy= -1004.823555

0 2

| | | | |
|---|---|---|---|
| N | 3.77749600 | -0.61402500 | -0.10249500 |
| C | 3.64330900 | 0.72001500 | -0.09210900 |
| C | 2.42215700 | 1.37119500 | -0.03508800 |
| C | 1.25066800 | 0.60663700 | 0.01991700 |
| C | 1.37333400 | -0.78993600 | 0.01475600 |
| C | 2.66187400 | -1.33439500 | -0.05189400 |
| N | 0.00884000 | 1.27588100 | 0.08039200 |
| C | -1.24325300 | 0.60331700 | 0.02067500 |
| C | -1.36009300 | -0.79677600 | 0.01710800 |
| S | 0.01228500 | -1.90299500 | 0.11784100 |
| C | -2.39891100 | 1.39378300 | -0.03485700 |
| C | -3.65158700 | 0.80400500 | -0.09145700 |
| C | -3.77127000 | -0.58652300 | -0.09680500 |
| C | -2.63098100 | -1.37653700 | -0.04489600 |
| O | 0.01390300 | 2.55196000 | 0.13736700 |
| H | 4.56353400 | 1.29392000 | -0.13341800 |
| H | 2.34334400 | 2.44807300 | -0.02925400 |
| H | 2.78086400 | -2.41499100 | -0.06249500 |
| H | -2.27231300 | 2.46643000 | -0.02910400 |
| H | -4.53510600 | 1.42936800 | -0.13310100 |
| H | -4.74700000 | -1.05491000 | -0.14305700 |
| H | -2.71694400 | -2.45735000 | -0.05134400 |

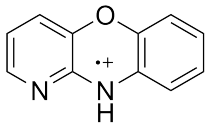
4-azaphenothiazine-*N*-oxyl



CBS-QB3 Enthalpy= -1004.774549
CBS-QB3 Free Energy= -1004.825032

```
0 2
 C                  3.67882000   -0.65148700    0.00001600
 C                  3.65150100    0.74124000    0.00001200
 C                  2.42215600    1.38304400    0.00000200
 C                  1.25225000    0.61570300   -0.00000400
 C                  1.39195200   -0.78448100   -0.00000200
 N                  2.57059200   -1.39531900    0.00000800
 N                  0.00575500    1.28227600   -0.00000800
 C                 -1.24205900    0.60376900   -0.00000400
 C                 -1.34912600   -0.79754200   -0.00000200
 S                  0.02903800   -1.90389500   -0.00001900
 C                 -2.40345900    1.38859700    0.00000300
 C                 -3.65408300    0.79219200    0.00001100
 C                 -3.76591800   -0.59906000    0.00001500
 C                 -2.61956500   -1.38221400    0.00000900
 O                  0.00930000    2.56050000   -0.00001500
 H                  4.61742000   -1.19593200    0.00002500
 H                  4.57289200    1.31000600    0.00001700
 H                  2.32540600    2.45916800   -0.00000200
 H                 -2.28166800    2.46181300   -0.00000100
 H                 -4.54209400    1.41267700    0.00001600
 H                 -4.74004500   -1.07315000    0.00002400
 H                 -2.70015700   -2.46353000    0.00001300
```

1-azaphenoxazine radical cation

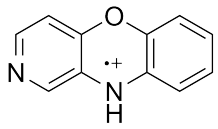


CBS-QB3 Enthalpy= -607.423185
CBS-QB3 Free Energy= -607.469293
EE + Zero-point energy= -607.433675

```
1 2
 C                 -3.56122100    0.66870800    0.00000800
 C                 -3.48986100   -0.73966600   -0.00001100
 N                 -2.34648400   -1.41231600   -0.00002000
 C                 -1.22286600   -0.69980100   -0.00001000
 C                 -1.18882900    0.71057300    0.00000900
 C                 -2.39201500    1.41024000    0.00001900
 N                 -0.02749300   -1.37477800   -0.00001900
 C                  1.17950200   -0.72350600   -0.00001000
 C                  1.16672700    0.69641400    0.00001000
 O                 -0.01026400    1.38566700    0.00001900
 C                  2.40917900   -1.40334000   -0.00001900
 C                  3.58136300   -0.67613500   -0.00000800
 C                  3.55512500    0.73339200    0.00001100
```

| | | | |
|---|---|---|---|
| C | 2.35276000 | 1.42139600 | 0.00002000 |
| H | -4.52603800 | 1.15899600 | 0.00001500 |
| H | -4.39583100 | -1.33548800 | -0.00002000 |
| H | -2.38685100 | 2.49291800 | 0.00003400 |
| H | -0.07848900 | -2.38996100 | -0.00003300 |
| H | 2.42166300 | -2.48689900 | -0.00003400 |
| H | 4.53208700 | -1.19380600 | -0.00001500 |
| H | 4.48598600 | 1.28615900 | 0.00001900 |
| H | 2.30824300 | 2.50274900 | 0.00003500 |

2-azaphenoxazine radical cation

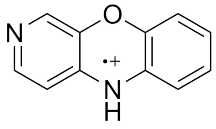


CBS-QB3 Enthalpy= -607.410294
CBS-QB3 Free Energy= -607.456623
EE + Zero-point energy= -607.420886

1 2

| | | | |
|---|---|---|---|
| C | 3.55900100 | -0.65305000 | 0.00000100 |
| N | 3.59855400 | 0.69494600 | -0.00000100 |
| C | 2.46114300 | 1.35725000 | -0.00000200 |
| C | 1.20743600 | 0.70959900 | -0.00000100 |
| C | 1.18651300 | -0.69921000 | 0.00000100 |
| C | 2.38520200 | -1.39649300 | 0.00000300 |
| N | 0.00961600 | 1.38233000 | -0.00000300 |
| C | -1.19350000 | 0.72327500 | -0.00000100 |
| C | -1.17052100 | -0.69628500 | 0.00000100 |
| O | 0.01010600 | -1.37865000 | 0.00000200 |
| C | -2.42704600 | 1.39809900 | -0.00000200 |
| C | -3.59508600 | 0.66547300 | -0.00000100 |
| C | -3.55916500 | -0.74408500 | 0.00000200 |
| C | -2.35221200 | -1.42618100 | 0.00000300 |
| H | 4.52035800 | -1.15407000 | 0.00000200 |
| H | 2.50997600 | 2.44416400 | -0.00000500 |
| H | 2.38979600 | -2.47846600 | 0.00000400 |
| H | 0.01543700 | 2.39717800 | -0.00000500 |
| H | -2.44611700 | 2.48186300 | -0.00000400 |
| H | -4.54893900 | 1.17722700 | -0.00000100 |
| H | -4.48663600 | -1.30265300 | 0.00000300 |
| H | -2.30250000 | -2.50733000 | 0.00000500 |

3-azaphenoxazine radical cation



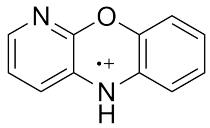
CBS-QB3 Enthalpy= -607.408227
CBS-QB3 Free Energy= -607.454535
EE + Zero-point energy= -607.418814

1 2

| | | | |
|---|---|---|---|
| N | 3.56057200 | -0.77642200 | 0.00000200 |
| C | 3.58853500 | 0.57269900 | 0.00000100 |
| C | 2.45815900 | 1.37044800 | -0.00000500 |

| | | | |
|---|---|---|---|
| C | 1.21092700 | 0.73372500 | -0.00000300 |
| C | 1.18477200 | -0.67406000 | 0.00000100 |
| C | 2.38978900 | -1.38707000 | 0.00000100 |
| N | 0.00646700 | 1.39768300 | -0.00000500 |
| C | -1.19421100 | 0.73262300 | -0.00000200 |
| C | -1.16834400 | -0.68829900 | 0.00000200 |
| O | 0.01136000 | -1.36020900 | 0.00000300 |
| C | -2.43034100 | 1.40042500 | -0.00000300 |
| C | -3.59471800 | 0.66161200 | 0.00000000 |
| C | -3.55592600 | -0.74960300 | 0.00000400 |
| C | -2.34896900 | -1.42572800 | 0.00000500 |
| H | 4.57415800 | 1.02423300 | -0.00000400 |
| H | 2.53471500 | 2.45123400 | -0.00000900 |
| H | 2.36923100 | -2.47255000 | 0.00000600 |
| H | 0.00515300 | 2.41185100 | -0.00001000 |
| H | -2.45594400 | 2.48396100 | -0.00000600 |
| H | -4.55058400 | 1.16983900 | -0.00000100 |
| H | -4.48235000 | -1.30977700 | 0.00000700 |
| H | -2.29257600 | -2.50657400 | 0.00000800 |

4-azaphenoxazine radical cation

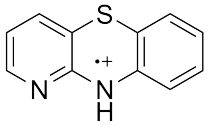


CBS-QB3 Enthalpy= -607.420135
CBS-QB3 Free Energy= -607.466365
EE + Zero-point energy= -607.430681

1 2

| | | | |
|---|---|---|---|
| C | -3.46100200 | -0.80593300 | -0.00000100 |
| C | -3.59510300 | 0.59513500 | 0.00000100 |
| C | -2.45851400 | 1.37832000 | 0.00000100 |
| C | -1.21224400 | 0.73415500 | 0.00000100 |
| C | -1.20375100 | -0.68169400 | 0.00000000 |
| N | -2.28309400 | -1.42661000 | -0.00000100 |
| N | -0.00899100 | 1.39785700 | 0.00000100 |
| C | 1.19177400 | 0.73117800 | 0.00000000 |
| C | 1.15746600 | -0.68694000 | 0.00000000 |
| O | -0.02367600 | -1.35977700 | -0.00000100 |
| C | 2.42910400 | 1.39656200 | 0.00000100 |
| C | 3.59163300 | 0.65415700 | 0.00000000 |
| C | 3.54602100 | -0.75535200 | -0.00000100 |
| C | 2.33509600 | -1.42714700 | -0.00000100 |
| H | -4.33717100 | -1.44465900 | -0.00000100 |
| H | -4.57915700 | 1.04517400 | 0.00000100 |
| H | -2.51651400 | 2.46094300 | 0.00000200 |
| H | -0.00606300 | 2.41223200 | 0.00000100 |
| H | 2.45761900 | 2.48007600 | 0.00000100 |
| H | 4.54920500 | 1.15902000 | 0.00000000 |
| H | 4.46960000 | -1.32024200 | -0.00000100 |
| H | 2.27360000 | -2.50768900 | -0.00000200 |

1-azaphenothiazine radical cation

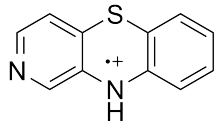


CBS-QB3 Enthalpy= -930.045996
CBS-QB3 Free Energy= -930.093932
EE + Zero-point energy= -930.057144

1 2

| | | | |
|---|---|---|---|
| C | 3.75370800 | 0.32600100 | 0.00000600 |
| C | 3.51246300 | -1.06133700 | 0.00000300 |
| N | 2.29734700 | -1.58677600 | 0.00000200 |
| C | 1.25256000 | -0.75322800 | 0.00000300 |
| C | 1.37909100 | 0.65427200 | 0.00000300 |
| C | 2.67702600 | 1.18996100 | 0.00000600 |
| N | 0.02574600 | -1.36790700 | -0.00001000 |
| C | -1.21256300 | -0.77612900 | -0.00000400 |
| C | -1.35353300 | 0.63731700 | 0.00000000 |
| S | 0.00822100 | 1.72752800 | -0.00001200 |
| C | -2.36528300 | -1.58447300 | -0.00000200 |
| C | -3.61541000 | -1.00437400 | 0.00000200 |
| C | -3.75402800 | 0.39635400 | 0.00000900 |
| C | -2.63574300 | 1.20762900 | 0.00000900 |
| H | 4.76834900 | 0.70197100 | 0.00000800 |
| H | 4.33784400 | -1.76515600 | 0.00000000 |
| H | 2.82382200 | 2.26373600 | 0.00000800 |
| H | 0.08179600 | -2.38250800 | -0.00001100 |
| H | -2.25530500 | -2.66296900 | -0.00000400 |
| H | -4.49708600 | -1.63282100 | 0.00000100 |
| H | -4.74054200 | 0.84210500 | 0.00001600 |
| H | -2.74180100 | 2.28602000 | 0.00001700 |

2-azaphenothiazine radical cation



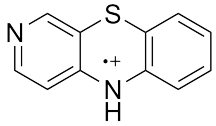
CBS-QB3 Enthalpy= -930.030794
CBS-QB3 Free Energy= -930.078929
EE + Zero-point energy= -930.042033

1 2

| | | | |
|---|---|---|---|
| C | -3.74927100 | -0.31095300 | 0.00001600 |
| N | -3.62459300 | 1.03175900 | 0.00000700 |
| C | -2.41532800 | 1.54456000 | 0.00000200 |
| C | -1.23767100 | 0.75905300 | -0.00000400 |
| C | -1.37671500 | -0.64422300 | -0.00000100 |
| C | -2.67018500 | -1.17881600 | 0.00001000 |
| N | -0.01016400 | 1.37466700 | -0.00002100 |
| C | 1.22535600 | 0.77465200 | -0.00000600 |
| C | 1.35787800 | -0.63941000 | -0.00000100 |
| S | -0.00920700 | -1.72463900 | -0.00001600 |
| C | 2.38200100 | 1.57920300 | 0.00000000 |
| C | 3.62928900 | 0.99475900 | 0.00000900 |
| C | 3.75991600 | -0.40708700 | 0.00001400 |

| | | | |
|---|---|---|---|
| C | 2.63741200 | -1.21360900 | 0.00001000 |
| H | -4.76276300 | -0.69557100 | 0.00001700 |
| H | -2.33314500 | 2.63037800 | -0.00000700 |
| H | -2.82744900 | -2.25044500 | 0.00001000 |
| H | -0.01776100 | 2.38899800 | -0.00000800 |
| H | 2.27810000 | 2.65868200 | -0.00000400 |
| H | 4.51403900 | 1.61876800 | 0.00001200 |
| H | 4.74418500 | -0.85790500 | 0.00002100 |
| H | 2.73929400 | -2.29242800 | 0.00001500 |

3-azaphenothiazine radical cation

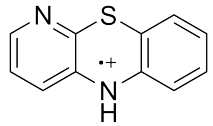


CBS-QB3 Enthalpy= -930.032531
CBS-QB3 Free Energy= -930.080662
EE + Zero-point energy= -930.043773

1 2

| | | | |
|---|---|---|---|
| N | 3.76460200 | -0.43868800 | 0.00000600 |
| C | 3.63117600 | 0.90429800 | 0.00000500 |
| C | 2.41390900 | 1.55567900 | 0.00000000 |
| C | 1.23886500 | 0.78675000 | -0.00000200 |
| C | 1.36960500 | -0.61886900 | -0.00000100 |
| C | 2.66979300 | -1.17029500 | 0.00000200 |
| N | 0.00643800 | 1.39236600 | -0.00000400 |
| C | -1.22738100 | 0.78237800 | -0.00000300 |
| C | -1.35611500 | -0.63211300 | -0.00000200 |
| S | 0.01323500 | -1.70458700 | -0.00000500 |
| C | -2.38797900 | 1.57791200 | -0.00000100 |
| C | -3.63282300 | 0.98573300 | 0.00000400 |
| C | -3.75956800 | -0.41674900 | 0.00000600 |
| C | -2.63427400 | -1.21580200 | 0.00000200 |
| H | 4.55504400 | 1.47187500 | 0.00000800 |
| H | 2.36575600 | 2.63853400 | -0.00000500 |
| H | 2.79648000 | -2.24995400 | 0.00000100 |
| H | 0.00462100 | 2.40571300 | -0.00001500 |
| H | -2.29214500 | 2.65806000 | -0.00000300 |
| H | -4.52010300 | 1.60633600 | 0.00000800 |
| H | -4.74212000 | -0.87105500 | 0.00001100 |
| H | -2.72782600 | -2.29539900 | 0.00000300 |

4-azaphenothiazine radical cation



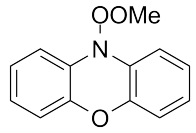
CBS-QB3 Enthalpy= -930.038535
CBS-QB3 Free Energy= -930.086504
EE + Zero-point energy= -930.049730

1 2

| | | | |
|---|---|---|---|
| C | -3.66526500 | -0.48408700 | 0.00000300 |
| C | -3.63555400 | 0.92404700 | 0.00000000 |
| C | -2.41804900 | 1.56833600 | 0.00000300 |

| | | | |
|---|---|---|---|
| C | -1.24009700 | 0.79712800 | 0.00000300 |
| C | -1.38730900 | -0.60949100 | 0.00000400 |
| N | -2.56598700 | -1.22489200 | 0.00000200 |
| N | -0.00517100 | 1.39793300 | -0.00000400 |
| C | 1.22579700 | 0.78116000 | -0.00000200 |
| C | 1.34508500 | -0.63359300 | -0.00000100 |
| S | -0.02828400 | -1.70849600 | -0.00000600 |
| C | 2.38890200 | 1.57421700 | -0.00000100 |
| C | 3.63179100 | 0.97876000 | -0.00000100 |
| C | 3.75128800 | -0.42367200 | 0.00000300 |
| C | 2.62195500 | -1.21846800 | 0.00000500 |
| H | -4.60773000 | -1.02026600 | -0.00000200 |
| H | -4.56024900 | 1.48651800 | -0.00001000 |
| H | -2.35761000 | 2.65140200 | 0.00000000 |
| H | 0.00338600 | 2.41149600 | 0.00000100 |
| H | 2.29605700 | 2.65471300 | 0.00000300 |
| H | 4.52141000 | 1.59588600 | -0.00000500 |
| H | 4.73165200 | -0.88279200 | 0.00000700 |
| H | 2.71247100 | -2.29832900 | 0.00001300 |

Methylperoxyl amine derived from phenoxazine



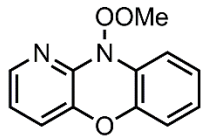

CBS-QB3 Enthalpy= -781.006447
CBS-QB3 Free Energy= -781.064040

0 1

| | | | |
|---|---|---|---|
| C | -3.57393200 | -1.46063400 | 0.22503500 |
| C | -3.61271700 | -0.08975000 | -0.02768500 |
| C | -2.43696000 | 0.61132600 | -0.27073700 |
| C | -1.21741900 | -0.06233000 | -0.26275100 |
| C | -1.17964900 | -1.43595300 | 0.00520900 |
| C | -2.35582500 | -2.13387500 | 0.24611300 |
| N | 0.00000000 | 0.60389200 | -0.54758700 |
| C | 1.21741700 | -0.06233400 | -0.26275100 |
| C | 1.17964300 | -1.43595800 | 0.00520900 |
| O | -0.00000500 | -2.14379300 | 0.03052700 |
| C | 2.43696100 | 0.61131700 | -0.27073700 |
| C | 3.61271500 | -0.08976300 | -0.02768600 |
| C | 3.57392600 | -1.46064700 | 0.22503500 |
| C | 2.35581500 | -2.13388400 | 0.24611300 |
| O | 0.00000300 | 1.86246900 | -0.75964800 |
| O | 0.00000400 | 2.69697300 | 0.78985700 |
| H | -4.48978700 | -2.00771100 | 0.41338200 |
| H | -4.55911000 | 0.43706500 | -0.03263900 |
| H | -2.43526600 | 1.67585600 | -0.45566400 |
| H | -2.29295300 | -3.19567900 | 0.44892000 |
| H | 2.43527100 | 1.67584600 | -0.45566600 |
| H | 4.55911100 | 0.43704700 | -0.03264000 |
| H | 4.48977800 | -2.00772700 | 0.41338200 |
| H | 2.29294000 | -3.19568800 | 0.44892100 |
| C | 0.00001500 | 4.03616400 | 0.42433200 |

| | | | |
|---|---|---|---|
| H | -0.89551100 | 4.32816100 | -0.14586000 |
| H | 0.00000300 | 4.61016600 | 1.36273300 |
| H | 0.89556000 | 4.32815400 | -0.14583500 |

Methylperoxylamine derived from 1-azaphenoxazine

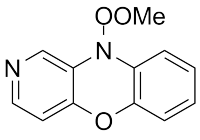



CBS-QB3 Enthalpy= -797.049036
CBS-QB3 Free Energy= -797.105167

0 1

| | | | |
|---|---|---|---|
| C | -3.21297600 | -1.92354400 | 0.21134700 |
| C | -3.38464100 | -0.57337000 | -0.05985000 |
| N | -2.36563000 | 0.26213100 | -0.30050000 |
| C | -1.14153200 | -0.22972600 | -0.28082400 |
| C | -0.85826100 | -1.58032200 | -0.00815600 |
| C | -1.91506200 | -2.43596800 | 0.24319200 |
| N | -0.05032900 | 0.62063600 | -0.57957700 |
| C | 1.26131100 | 0.18005300 | -0.26620200 |
| C | 1.46379300 | -1.17802800 | 0.00192200 |
| O | 0.41817800 | -2.08421500 | -0.00103500 |
| C | 2.34563100 | 1.05316600 | -0.25122300 |
| C | 3.62234300 | 0.56562300 | 0.01512600 |
| C | 3.82043300 | -0.78915400 | 0.26913100 |
| C | 2.73514000 | -1.66310100 | 0.26788800 |
| O | -0.25901400 | 1.89497800 | -0.75853000 |
| O | -0.39601600 | 2.61280300 | 0.68988400 |
| C | -1.43975000 | 3.53605600 | 0.51122200 |
| H | -4.06641900 | -2.56235300 | 0.40002200 |
| H | -4.37507600 | -0.13130000 | -0.08805000 |
| H | -1.70922500 | -3.47786300 | 0.45557400 |
| H | 2.16598400 | 2.10274700 | -0.43635900 |
| H | 4.46135000 | 1.25074400 | 0.02518200 |
| H | 4.81360500 | -1.16933200 | 0.47504000 |
| H | 2.85240200 | -2.72032900 | 0.47093100 |
| H | -1.53904300 | 4.03554200 | 1.48264100 |
| H | -2.37995100 | 3.03882400 | 0.25436900 |
| H | -1.19568300 | 4.29530900 | -0.24280400 |

Methoxyperoxyl amine derived from 2-azaphenoxazine



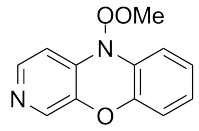

CBS-QB3 Enthalpy= -797.046594
CBS-QB3 Free Energy= -797.103842

0 1

| | | | |
|---|---|---|---|
| C | -3.49057900 | -1.50068900 | 0.20132500 |
| N | -3.59393300 | -0.19444100 | -0.06228800 |
| C | -2.46767500 | 0.48111000 | -0.29156300 |
| C | -1.20470600 | -0.11168500 | -0.27335600 |
| C | -1.11357100 | -1.47554800 | 0.01989100 |

| | | | |
|---|---|---|---|
| C | -2.28060700 | -2.18592600 | 0.26068600 |
| N | -0.02065400 | 0.60301600 | -0.56440300 |
| C | 1.22305000 | -0.01227300 | -0.27494000 |
| C | 1.23964000 | -1.38073300 | 0.01879000 |
| O | 0.08155500 | -2.13575700 | 0.06877300 |
| C | 2.41773700 | 0.70295000 | -0.30342500 |
| C | 3.61943600 | 0.04853400 | -0.05380500 |
| C | 3.63254400 | -1.31684200 | 0.22577800 |
| C | 2.43863400 | -2.03253100 | 0.26647700 |
| O | -0.07617700 | 1.87187000 | -0.74966700 |
| O | -0.11620200 | 2.64605900 | 0.78828400 |
| C | -0.27496100 | 3.99132500 | 0.46783000 |
| H | -4.42137400 | -2.03005900 | 0.37979700 |
| H | -2.54721800 | 1.54163900 | -0.49451300 |
| H | -2.22983800 | -3.24278300 | 0.48844600 |
| H | 2.37913700 | 1.76285100 | -0.51020800 |
| H | 4.54596700 | 0.60910400 | -0.07572200 |
| H | 4.56830600 | -1.82695700 | 0.41902900 |
| H | 2.41422800 | -3.09162500 | 0.49045200 |
| H | -0.30017900 | 4.52484900 | 1.42811300 |
| H | -1.21751900 | 4.19721500 | -0.05964200 |
| H | 0.56355100 | 4.39220900 | -0.12016800 |

*N*-(methoxyperoxyl)-3-azaphenoxazine



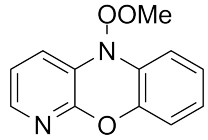

CBS-QB3 Enthalpy= -797.046254
CBS-QB3 Free Energy= -797.103457

0 1

| | | | |
|---|---|---|---|
| N | -3.55168100 | -1.51808100 | 0.23227200 |
| C | -3.58751900 | -0.20778500 | -0.03121200 |
| C | -2.45908400 | 0.56410400 | -0.28639900 |
| C | -1.21752300 | -0.06361900 | -0.27059200 |
| C | -1.16742200 | -1.43066000 | 0.01449400 |
| C | -2.35652000 | -2.10914000 | 0.25709700 |
| N | -0.01436900 | 0.61080600 | -0.55511000 |
| C | 1.21262500 | -0.04504000 | -0.27084500 |
| C | 1.18638600 | -1.41579300 | 0.01471600 |
| O | 0.01088200 | -2.13482300 | 0.05335800 |
| C | 2.42689300 | 0.63541600 | -0.29723700 |
| C | 3.60964600 | -0.05419300 | -0.05134600 |
| C | 3.58184700 | -1.42060000 | 0.22198300 |
| C | 2.36813600 | -2.10162300 | 0.25907700 |
| O | -0.03120400 | 1.88266900 | -0.74525200 |
| O | -0.03575900 | 2.65698100 | 0.77914700 |
| C | -0.05899100 | 4.01133200 | 0.45432800 |
| H | -4.57020800 | 0.25310000 | -0.03757200 |
| H | -2.52341100 | 1.62399700 | -0.48522600 |
| H | -2.31805900 | -3.17154800 | 0.47779300 |
| H | 2.42027300 | 1.69656400 | -0.50105000 |
| H | 4.55212800 | 0.47908600 | -0.07148800 |
| H | 4.50226200 | -1.95892200 | 0.41278600 |

| | | | |
|---|---|---|---|
| H | 2.31337300 | -3.16089800 | 0.47671600 |
| H | -0.96157300 | 4.30104100 | -0.10248400 |
| H | 0.83098400 | 4.33075800 | -0.10655000 |
| H | -0.06562800 | 4.54474100 | 1.41452200 |

Methylperoxyl amine derived from 4-azaphenoxazine

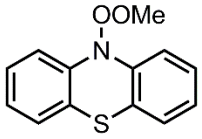



CBS-QB3 Enthalpy= -797.053176
CBS-QB3 Free Energy= -797.110429

0 1

| | | | |
|---|---|---|---|
| C | -3.45771200 | -1.52632700 | 0.22198500 |
| C | -3.59396200 | -0.16396300 | -0.01641800 |
| C | -2.44852600 | 0.58855600 | -0.26306600 |
| C | -1.22092400 | -0.05943000 | -0.26200600 |
| C | -1.19625500 | -1.43716100 | 0.01274700 |
| N | -2.27358600 | -2.15218000 | 0.24170800 |
| N | -0.01051400 | 0.60989000 | -0.55116800 |
| C | 1.20772800 | -0.05467500 | -0.26469100 |
| C | 1.16361100 | -1.42572400 | 0.01382800 |
| O | -0.01697100 | -2.13492900 | 0.05097100 |
| C | 2.42882700 | 0.61469300 | -0.28464100 |
| C | 3.60241800 | -0.08918000 | -0.03872200 |
| C | 3.55831500 | -1.45745000 | 0.22667900 |
| C | 2.33775600 | -2.12584300 | 0.25671700 |
| O | -0.02209700 | 1.87107600 | -0.76118600 |
| O | -0.04682700 | 2.69198500 | 0.78224600 |
| C | 0.00063600 | 4.03485000 | 0.42817100 |
| H | -4.32498100 | -2.14996000 | 0.41199200 |
| H | -4.57129800 | 0.30134100 | -0.00729900 |
| H | -2.48060100 | 1.65338400 | -0.44497000 |
| H | 2.43195200 | 1.67698000 | -0.48276800 |
| H | 4.55108500 | 0.43330500 | -0.05229900 |
| H | 4.47241400 | -2.00656600 | 0.41726200 |
| H | 2.26984800 | -3.18542200 | 0.46854600 |
| H | 0.92633500 | 4.30861100 | -0.10007800 |
| H | -0.86318400 | 4.35108700 | -0.17605600 |
| H | -0.02718400 | 4.59813800 | 1.37214800 |

Peroxylamine derived from phenothiazine



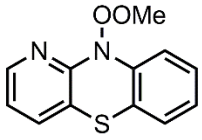

CBS-QB3 Enthalpy= -1103.622023
CBS-QB3 Free Energy= -1103.680145

0 1

| | | | |
|---|---|---|---|
| C | -3.69382800 | -1.11790700 | -0.49335400 |
| C | -3.56727200 | 0.26888300 | -0.43341800 |
| C | -2.34445900 | 0.84915800 | -0.11746000 |
| C | -1.24311200 | 0.03680100 | 0.15511800 |

| | | | |
|---|---|---|---|
| C | -1.36054600 | -1.35752900 | 0.09033500 |
| C | -2.59007300 | -1.92678500 | -0.24453600 |
| N | 0.00000000 | 0.62843400 | 0.52876700 |
| C | 1.24311200 | 0.03680300 | 0.15511800 |
| C | 1.36054700 | -1.35752800 | 0.09033400 |
| S | 0.00000200 | -2.41824600 | 0.50555200 |
| C | 2.34445900 | 0.84916100 | -0.11745800 |
| C | 3.56727300 | 0.26888800 | -0.43341600 |
| C | 3.69382900 | -1.11790200 | -0.49335500 |
| C | 2.59007400 | -1.92678100 | -0.24453800 |
| O | -0.00000100 | 1.85825200 | 0.89029700 |
| O | -0.00000200 | 2.91027000 | -0.50261800 |
| C | -0.00000500 | 4.16980200 | 0.09061000 |
| H | -4.64510200 | -1.57120500 | -0.74560600 |
| H | -4.41974600 | 0.90396700 | -0.64274500 |
| H | -2.21062500 | 1.92063100 | -0.10044100 |
| H | -2.67538900 | -3.00548600 | -0.30554200 |
| H | 2.21062500 | 1.92063300 | -0.10043800 |
| H | 4.41974700 | 0.90397300 | -0.64274100 |
| H | 4.64510300 | -1.57119800 | -0.74560900 |
| H | 2.67539300 | -3.00548200 | -0.30554600 |
| H | -0.00000200 | 4.89616700 | -0.73396000 |
| H | -0.89525300 | 4.35117200 | 0.70355100 |
| H | 0.89523800 | 4.35117300 | 0.70355700 |

Peroxylamine derived from 1-azaphenothiazine



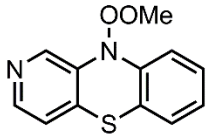

CBS-QB3 Enthalpy= -1119.665501
CBS-QB3 Free Energy= -1119.721941

0 1

| | | | |
|---|---|---|---|
| C | 3.33635900 | -1.68320600 | -0.52578700 |
| C | 3.40706700 | -0.31285400 | -0.31879600 |
| N | 2.35135000 | 0.43473300 | 0.02251600 |
| C | 1.18770400 | -0.16933600 | 0.20069500 |
| C | 1.00800600 | -1.55789500 | 0.05173000 |
| C | 2.10618500 | -2.31231900 | -0.34269700 |
| N | 0.08088900 | 0.63199700 | 0.58891500 |
| C | -1.25400400 | 0.31573900 | 0.19793100 |
| C | -1.64909900 | -1.02250900 | 0.07637900 |
| S | -0.52451100 | -2.34371600 | 0.46885800 |
| C | -2.17927800 | 1.33384200 | -0.03647900 |
| C | -3.49032900 | 1.01472700 | -0.37546100 |
| C | -3.88494800 | -0.31434400 | -0.50371400 |
| C | -2.95845600 | -1.33038400 | -0.29056200 |
| O | 0.32412200 | 1.88910000 | 0.90608100 |
| O | 0.48358100 | 2.75008400 | -0.41495900 |
| C | 1.55293100 | 3.62200000 | -0.13321900 |
| H | 4.21319300 | -2.24565200 | -0.82056600 |
| H | 4.34532200 | 0.22057900 | -0.43465700 |
| H | 1.99985600 | -3.38117100 | -0.48776500 |
| H | -1.85422400 | 2.36117100 | 0.03646500 |

| | | | |
|---|---|---|---|
| H | -4.20131200 | 1.81383800 | -0.54891400 |
| H | -4.90371700 | -0.56259600 | -0.77620400 |
| H | -3.24758700 | -2.36931300 | -0.39888700 |
| H | 1.32430900 | 4.29341500 | 0.70328300 |
| H | 1.66257500 | 4.22177300 | -1.04361600 |
| H | 2.47363900 | 3.06605000 | 0.06001800 |

Peroxylamine derived from 2-azaphenothiazine

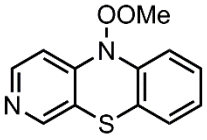



CBS-QB3 Enthalpy= -1119.662017
CBS-QB3 Free Energy= -1119.719939

0 1

| | | | |
|---|---|---|---|
| C | -3.61151800 | -1.19138300 | -0.46270500 |
| N | -3.56534400 | 0.14256000 | -0.39676600 |
| C | -2.39563100 | 0.70834000 | -0.10303900 |
| C | -1.23346600 | -0.02593200 | 0.15726700 |
| C | -1.28733800 | -1.42067300 | 0.07449900 |
| C | -2.50769200 | -2.00991600 | -0.25260100 |
| N | -0.02906500 | 0.62681200 | 0.53653500 |
| C | 1.24551200 | 0.10008700 | 0.17344000 |
| C | 1.42870300 | -1.28560800 | 0.08213000 |
| S | 0.11634900 | -2.42828500 | 0.44745600 |
| C | 2.31420600 | 0.96450600 | -0.06566000 |
| C | 3.56626700 | 0.44567900 | -0.37495800 |
| C | 3.75585000 | -0.93173700 | -0.46442300 |
| C | 2.68526500 | -1.79330000 | -0.24871000 |
| O | -0.09802700 | 1.86755000 | 0.87864500 |
| O | -0.14197200 | 2.85974100 | -0.51472400 |
| C | -0.32737800 | 4.13157000 | 0.02835800 |
| H | -4.57543600 | -1.62899000 | -0.70411500 |
| H | -2.35182100 | 1.78863800 | -0.07625800 |
| H | -2.59409900 | -3.08646700 | -0.33651400 |
| H | 2.13597400 | 2.02878200 | -0.02632200 |
| H | 4.39232900 | 1.12281700 | -0.55629000 |
| H | 4.72946400 | -1.33705200 | -0.71242100 |
| H | 2.81912100 | -2.86560900 | -0.33174200 |
| H | -1.27520200 | 4.22230900 | 0.57712400 |
| H | 0.50101700 | 4.43581900 | 0.68331500 |
| H | -0.35876200 | 4.81858200 | -0.82739900 |

Peroxylamine derived from 3-azaphenothiazine



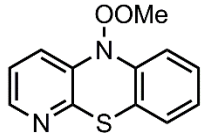

CBS-QB3 Enthalpy= -1119.663210
CBS-QB3 Free Energy= -1119.721123

0 1

| | | | |
|---|---|---|---|
| N | -3.67117200 | -1.19014300 | -0.50090100 |
| C | -3.56053900 | 0.13832200 | -0.39724000 |

| | | | |
|---|---|---|---|
| C | -2.37902500 | 0.79744200 | -0.07853200 |
| C | -1.24275400 | 0.03014800 | 0.16967000 |
| C | -1.33848300 | -1.36219300 | 0.07235200 |
| C | -2.57311400 | -1.91171200 | -0.28038100 |
| N | -0.01608600 | 0.63587600 | 0.53989700 |
| C | 1.24000100 | 0.06139900 | 0.17389400 |
| C | 1.37321800 | -1.33056200 | 0.08387400 |
| S | 0.02505900 | -2.42020800 | 0.47307000 |
| C | 2.33686800 | 0.88745000 | -0.07108500 |
| C | 3.56902700 | 0.32543900 | -0.38579400 |
| C | 3.70948900 | -1.05760600 | -0.47519200 |
| C | 2.61044900 | -1.88068200 | -0.25324400 |
| O | -0.04009000 | 1.88469600 | 0.87464800 |
| O | -0.05270000 | 2.85732900 | -0.51058900 |
| C | -0.09136900 | 4.14681400 | 0.02516300 |
| H | -4.46323800 | 0.71050700 | -0.58797700 |
| H | -2.32129700 | 1.87447500 | -0.03922300 |
| H | -2.66954100 | -2.98951100 | -0.37796900 |
| H | 2.19978300 | 1.95746900 | -0.03041900 |
| H | 4.41724500 | 0.97347600 | -0.57100000 |
| H | 4.66707000 | -1.49698000 | -0.72773100 |
| H | 2.70582800 | -2.95708100 | -0.33555400 |
| H | -0.10473100 | 4.82351600 | -0.83859100 |
| H | 0.79483300 | 4.37737000 | 0.63205100 |
| H | -0.99636600 | 4.32819600 | 0.62094800 |

Peroxylamine derived from 4-azaphenothiazine



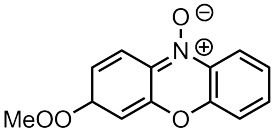

CBS-QB3 Enthalpy= -1119.664596
CBS-QB3 Free Energy= -1119.722713

0 1

| | | | |
|---|---|---|---|
| C | 3.62834500 | -1.16087100 | -0.38146600 |
| C | 3.58006200 | 0.22916700 | -0.34987400 |
| C | 2.36563100 | 0.85089900 | -0.08215800 |
| C | 1.24635300 | 0.05499100 | 0.14658900 |
| C | 1.39227900 | -1.33818500 | 0.06045200 |
| N | 2.55259600 | -1.92970000 | -0.19073500 |
| N | 0.00522200 | 0.64149000 | 0.51099600 |
| C | -1.24008400 | 0.03538800 | 0.16933800 |
| C | -1.33993400 | -1.35849400 | 0.06841400 |
| S | 0.03616500 | -2.44471100 | 0.34917200 |
| C | -2.36266700 | 0.83987100 | -0.03060600 |
| C | -3.59124500 | 0.25494300 | -0.31113500 |
| C | -3.70270200 | -1.13111100 | -0.40535900 |
| C | -2.57923800 | -1.93051400 | -0.22833800 |
| O | 0.00878100 | 1.87598800 | 0.85819700 |
| O | 0.00857900 | 2.89480000 | -0.55552300 |
| C | -0.02752600 | 4.17075000 | 0.00088500 |
| H | 4.55901100 | -1.68527500 | -0.57258600 |
| H | 4.47234900 | 0.81482100 | -0.53219400 |
| H | 2.25693600 | 1.92544700 | -0.05988000 |

| | | | |
|---|---|---|---|
| H | -2.24316200 | 1.91192800 | 0.01646300 |
| H | -4.45912000 | 0.88489700 | -0.46469000 |
| H | -4.65801700 | -1.59083500 | -0.62876200 |
| H | -2.65542300 | -3.00798400 | -0.31838300 |
| H | -0.02023800 | 4.87161700 | -0.84535500 |
| H | -0.94007200 | 4.35412300 | 0.58679300 |
| H | 0.84984000 | 4.38679100 | 0.62817000 |

3-methoxyperoxyl-*N*-oxide adduct derived from phenoxazine

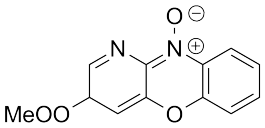



CBS-QB3 Enthalpy= -857.437512
CBS-QB3 Free Energy= -857.496181

0 1

| | | | |
|---|---|---|---|
| C | -4.48412300 | 0.15458100 | 0.58685300 |
| C | -4.32907600 | -1.22134900 | 0.40156400 |
| C | -3.09226200 | -1.75668800 | 0.05971700 |
| C | -1.99908800 | -0.90943800 | -0.09785200 |
| C | -2.15674400 | 0.46615300 | 0.08721900 |
| C | -3.39509900 | 1.00162500 | 0.42901600 |
| O | -0.80112900 | -1.46440300 | -0.42821600 |
| C | 0.29505200 | -0.64116100 | -0.59251400 |
| C | 0.15029800 | 0.78948900 | -0.41416200 |
| N | -1.02406200 | 1.33559200 | -0.08352500 |
| C | 1.47074400 | -1.19354500 | -0.92918200 |
| C | 2.71619700 | -0.38165300 | -1.08437900 |
| C | 2.49056300 | 1.09574400 | -0.94320700 |
| C | 1.30381200 | 1.62827100 | -0.61505600 |
| O | -1.19780700 | 2.57948000 | 0.08388500 |
| O | 3.78085700 | -0.84418200 | -0.21255300 |
| O | 3.33157200 | -0.68284400 | 1.16879000 |
| C | 4.38640500 | -0.02569800 | 1.84618900 |
| H | -5.45061500 | 0.56385500 | 0.85312800 |
| H | -5.17750800 | -1.88410400 | 0.52478400 |
| H | -2.94863800 | -2.81956800 | -0.08751500 |
| H | -3.46129600 | 2.07260900 | 0.55952100 |
| H | 1.54028100 | -2.26681100 | -1.05093200 |
| H | 3.19134700 | -0.59343600 | -2.05384100 |
| H | 3.35426400 | 1.73319100 | -1.09682300 |
| H | 1.15425600 | 2.69287300 | -0.49842200 |
| H | 4.05427700 | 0.02210000 | 2.88626000 |
| H | 4.54740000 | 0.98744600 | 1.46266300 |
| H | 5.31663900 | -0.59969600 | 1.78537400 |

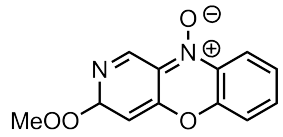
3-(methylperoxyl)-*N*-oxide adduct derived from 1-azaphenoxazine




CBS-QB3 Enthalpy= -872.142427
CBS-QB3 Free Energy= -872.201086

```
0 1
 C                -2.39648900    1.52092400   -0.63810400
 C                -2.80486300    0.12424400   -1.04346900
 C                -1.63281600   -0.78650000   -1.14912100
 C                -0.42163100   -0.38375400   -0.72785500
 C                -0.21496000    0.96960500   -0.25606400
 N                -1.22969900    1.89055300   -0.25958300
 O                 0.62986500   -1.27203200   -0.78400400
 C                 1.85216400   -0.86525800   -0.34356700
 C                 2.07348000    0.42272200    0.14727600
 N                 0.99278800    1.37899800    0.17775300
 C                 2.90079500   -1.78003700   -0.38801800
 C                 4.15931800   -1.39850800    0.06116500
 C                 4.37939100   -0.10966100    0.55432700
 C                 3.33516000    0.80358600    0.59670000
 O                 1.24124200    2.53208800    0.59972500
 O                -3.84652600   -0.35883500   -0.15410200
 O                -3.30367800   -0.36522600    1.20123700
 C                -3.50298700   -1.67459600    1.70474200
 H                -3.18522500    2.27140300   -0.62669200
 H                -3.37909700    0.16402300   -1.97953300
 H                -1.76636100   -1.79014300   -1.53182800
 H                 2.70601300   -2.77285900   -0.77320100
 H                 4.97364100   -2.11254800    0.02685900
 H                 5.36266500    0.18045700    0.90276800
 H                 3.45459500    1.81292700    0.96470700
 H                -3.15686800   -1.62260900    2.73997900
 H                -4.56257800   -1.94749300    1.68639200
 H                -2.91500500   -2.41456200    1.15243100
```

3-(methylperoxyl)-*N*-oxide adduct derived from 2-azaphenoxazine

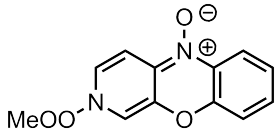



CBS-QB3 Enthalpy= -872.147382
CBS-QB3 Free Energy= -872.205591

```
0 1
 N                -2.52753100    1.00955800   -0.92160200
 C                -2.69037300   -0.43294900   -1.03375000
 C                -1.46636100   -1.27707800   -0.82838400
 C                -0.28464700   -0.72183400   -0.53561900
 C                -0.17280600    0.71205800   -0.43292100
 C                -1.37950000    1.49526700   -0.64029700
 O                 0.82685100   -1.51487800   -0.33700800
 C                 2.01354800   -0.90939000   -0.04945100
```

| | | | |
|---|---|---|---|
| C | 2.14197300 | 0.47870900 | 0.05726300 |
| N | 0.98359300 | 1.31418800 | -0.14771700 |
| C | 3.12900300 | -1.71849700 | 0.14345700 |
| C | 4.35559200 | -1.13466900 | 0.44134200 |
| C | 4.48015500 | 0.25235900 | 0.54763500 |
| C | 3.36904000 | 1.06272200 | 0.35458200 |
| O | -3.77141800 | -0.86362700 | -0.20025100 |
| O | 1.12599800 | 2.56439700 | -0.04868900 |
| O | -3.37520800 | -0.65314200 | 1.18859500 |
| C | -4.33846700 | 0.23471600 | 1.73864100 |
| H | -3.12765300 | -0.62881800 | -2.02329500 |
| H | -1.56701400 | -2.35168600 | -0.90597700 |
| H | -1.27332900 | 2.57225900 | -0.54294500 |
| H | 3.01099600 | -2.79114600 | 0.05764700 |
| H | 5.22081300 | -1.76937100 | 0.59202400 |
| H | 5.43889700 | 0.69855300 | 0.77981100 |
| H | 3.41145700 | 2.14067100 | 0.42462900 |
| H | -5.34239600 | -0.19900200 | 1.69598000 |
| H | -4.32304100 | 1.20130900 | 1.22913400 |
| H | -4.03388000 | 0.35052900 | 2.78205500 |

*N*-(methylperoxyl)-*N*-oxide adduct derived from 3-azaphenoxazine



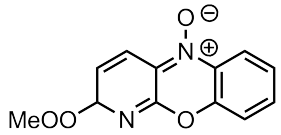

CBS-QB3 Enthalpy= -872.111979
CBS-QB3 Free Energy= -872.171597

0 1

| | | | |
|---|---|---|---|
| C | -2.24110200 | 1.48435600 | -0.36622500 |
| N | -2.51837800 | 0.14989300 | -0.62188200 |
| C | -1.50366400 | -0.80683500 | -0.55478700 |
| C | -0.22488700 | -0.42357300 | -0.32477300 |
| C | 0.10079800 | 0.95861300 | -0.12015200 |
| C | -0.97583100 | 1.90167100 | -0.14335500 |
| O | 0.74724700 | -1.38768700 | -0.29665400 |
| C | 2.04741100 | -0.98800700 | -0.09005100 |
| C | 2.38732300 | 0.35421200 | 0.10625100 |
| N | 1.36303400 | 1.35498900 | 0.09259500 |
| C | 3.03083000 | -1.96586400 | -0.07915000 |
| C | 4.35913900 | -1.59773200 | 0.13051500 |
| C | 4.69997300 | -0.26043100 | 0.32663800 |
| C | 3.71255300 | 0.71995700 | 0.31478700 |
| O | -3.74608000 | -0.23634700 | -0.69696000 |
| O | -4.28439500 | -0.56348600 | 0.94116200 |
| C | -5.58401800 | -1.01969400 | 0.76857800 |
| O | 1.68591500 | 2.57610200 | 0.28009100 |
| H | -3.11008700 | 2.12489900 | -0.37760000 |
| H | -1.80923200 | -1.82880300 | -0.70900400 |
| H | -0.74277500 | 2.94236200 | 0.02425300 |
| H | 2.74063500 | -2.99748500 | -0.23306400 |
| H | 5.12626700 | -2.36269500 | 0.14009200 |
| H | 5.73307900 | 0.02068000 | 0.48932000 |
| H | 3.92418500 | 1.76977600 | 0.46230500 |

| | | | |
|---|---|---|---|
| H | -6.24457200 | -0.26812800 | 0.31118300 |
| H | -5.63709800 | -1.95255500 | 0.18791900 |
| H | -5.96564600 | -1.23091600 | 1.77882600 |

3-(methylperoxyl)-*N*-oxide adduct derived from 4-azaphenoxazine

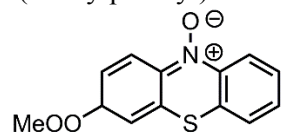



CBS-QB3 Enthalpy= -872.161631
CBS-QB3 Free Energy= -872.219619

0 1

| | | | |
|---|---|---|---|
| C | -2.21034900 | 1.89729400 | -0.25402000 |
| C | -2.66328100 | 0.49359400 | -0.54765200 |
| N | -1.63235100 | -0.52373500 | -0.57387400 |
| C | -0.42670100 | -0.20685200 | -0.34680000 |
| C | 0.05782000 | 1.13808200 | -0.08385200 |
| C | -0.92022100 | 2.19242100 | -0.04419700 |
| O | 0.48111200 | -1.24527800 | -0.34789500 |
| C | 1.80292200 | -0.98260900 | -0.15403800 |
| C | 2.28293200 | 0.30763000 | 0.07997200 |
| N | 1.35443300 | 1.39980200 | 0.12254300 |
| C | 2.69297300 | -2.05287200 | -0.19373000 |
| C | 4.04844000 | -1.82069100 | 0.00179800 |
| C | 4.52594400 | -0.52709900 | 0.23620800 |
| C | 3.64242000 | 0.54109800 | 0.27637600 |
| O | -3.63245900 | 0.19833200 | 0.46432000 |
| O | 1.79804500 | 2.55823700 | 0.35530100 |
| O | -4.49921400 | -0.85354500 | -0.04538900 |
| C | -4.24352600 | -2.02055300 | 0.72669900 |
| H | -2.97851600 | 2.66019100 | -0.22489900 |
| H | -3.19126100 | 0.45912800 | -1.50905800 |
| H | -0.56649000 | 3.19466000 | 0.15362500 |
| H | 2.30033700 | -3.04485400 | -0.37682300 |
| H | 4.73899600 | -2.65508400 | -0.02909300 |
| H | 5.58442500 | -0.35633800 | 0.38735700 |
| H | 3.96023300 | 1.55861500 | 0.45570400 |
| H | -4.96383900 | -2.75180300 | 0.35065300 |
| H | -4.43085800 | -1.83645800 | 1.78895200 |
| H | -3.22371300 | -2.37915700 | 0.57161600 |

3-(methylperoxyl)-adduct derived from phenothiazine-*N*-oxide



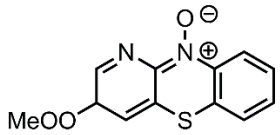

CBS-QB3 Enthalpy= -1178.715631
CBS-QB3 Free Energy= -1178.776931

0 1

| | | | |
|---|---|---|---|
| C | -2.77121700 | 0.53663000 | -0.62648600 |
| C | -0.45773900 | -0.32627700 | -0.20084600 |
| C | 0.02876300 | 1.02607800 | 0.01134300 |
| C | -0.94127800 | 2.09946900 | 0.01539500 |
| S | 0.58720300 | -1.71920100 | 0.12155700 |

| | | | |
|---|---|---|---|
| C | 2.18393300 | -0.99113200 | 0.02193800 |
| C | 2.39866400 | 0.39041000 | 0.08055100 |
| N | 1.31857700 | 1.35541400 | 0.17770900 |
| C | 3.28845000 | -1.84633300 | -0.06296500 |
| C | 4.57828400 | -1.33397900 | -0.08522100 |
| C | 4.78375900 | 0.04491500 | -0.03272600 |
| C | 3.69687100 | 0.90296900 | 0.04904800 |
| O | -3.87919000 | 0.30301200 | 0.27110800 |
| O | 1.67294500 | 2.56157800 | 0.37649600 |
| O | -4.68746200 | -0.74209100 | -0.36705400 |
| C | -5.44820500 | -1.31110800 | 0.68079000 |
| H | -3.20540900 | 0.56599500 | -1.63706500 |
| H | -0.56099800 | 3.08647100 | 0.23550600 |
| H | 3.12406700 | -2.91654300 | -0.11402900 |
| H | 5.42147600 | -2.01171500 | -0.14963700 |
| H | 5.78747700 | 0.45116600 | -0.05608000 |
| H | 3.81105600 | 1.97569500 | 0.09827600 |
| H | -6.06869300 | -2.06551900 | 0.19181800 |
| H | -6.08795600 | -0.56078500 | 1.15660400 |
| H | -4.80530400 | -1.78223800 | 1.43114500 |
| C | -1.74555900 | -0.55150000 | -0.52654200 |
| H | -2.10523700 | -1.56081300 | -0.68611500 |
| C | -2.23463000 | 1.88574800 | -0.26614000 |
| H | -2.94668600 | 2.70228500 | -0.25253300 |

3-(methylperoxyl)-adduct derived from 1-azaphenothiazine-*N*-oxide




CBS-QB3 Enthalpy= -1194.750893

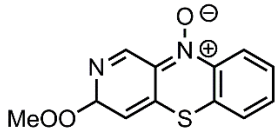
CBS-QB3 Free Energy= -1194.812273

0 1

| | | | |
|---|---|---|---|
| C | -2.13146400 | 1.79320900 | 0.09402200 |
| C | -2.70857900 | 0.47714200 | 0.55423400 |
| C | -1.71295900 | -0.62966500 | 0.40838100 |
| C | -0.42944000 | -0.37883800 | 0.08582900 |
| C | 0.01552800 | 0.99304500 | -0.08219900 |
| N | -0.89970300 | 2.01763700 | -0.16434600 |
| S | 0.64208800 | -1.72929300 | -0.31152700 |
| C | 2.21446400 | -0.97876000 | -0.07530000 |
| C | 2.39898300 | 0.40802700 | -0.03373300 |
| N | 1.30963400 | 1.36807800 | -0.16136200 |
| C | 3.33199200 | -1.81546600 | 0.02516500 |
| C | 4.60471500 | -1.27991900 | 0.16420600 |
| C | 4.77927400 | 0.10338500 | 0.21645900 |
| C | 3.67957100 | 0.94257000 | 0.11805900 |
| O | -3.87974100 | 0.26419100 | -0.24984000 |
| O | 1.64989000 | 2.57213200 | -0.29333900 |
| O | -4.71615200 | -0.66734200 | 0.51767700 |
| C | -5.69629100 | -1.11929800 | -0.39690800 |
| H | -2.83477800 | 2.61517700 | -0.02507400 |
| H | -3.06182500 | 0.57847600 | 1.59200800 |
| H | -2.07726700 | -1.64137700 | 0.53499400 |
| H | 3.19046700 | -2.88976100 | -0.00161400 |

| | | | |
|---|---|---|---|
| H | 5.45838200 | -1.94321300 | 0.23978800 |
| H | 5.76899500 | 0.52731900 | 0.33345500 |
| H | 3.77194700 | 2.01840900 | 0.14344500 |
| H | -6.32550000 | -1.79343500 | 0.18827900 |
| H | -5.24199900 | -1.66113000 | -1.23230800 |
| H | -6.29808800 | -0.28622600 | -0.77385200 |

3-(methylperoxyl)-adduct derived from 2-azaphenothiazine-*N*-oxide

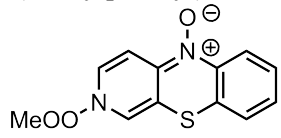



CBS-QB3 Enthalpy= -1194.754950
CBS-QB3 Free Energy= -1194.816300

0 1

| | | | |
|---|---|---|---|
| C | -2.69552800 | 0.51404700 | -0.49277700 |
| C | -0.43062400 | -0.39668800 | -0.04003500 |
| C | 0.02701900 | 0.97187300 | 0.07815200 |
| C | -1.00593100 | 2.00154900 | 0.16225400 |
| S | 0.65513700 | -1.73681800 | 0.36068000 |
| C | 2.22167300 | -0.97958100 | 0.08126500 |
| C | 2.40542000 | 0.40737300 | 0.02217900 |
| N | 1.30665200 | 1.35502000 | 0.14145200 |
| C | 3.34025400 | -1.81223800 | -0.02968700 |
| C | 4.60962300 | -1.27313400 | -0.19269100 |
| C | 4.78101300 | 0.10943800 | -0.25952900 |
| C | 3.67975000 | 0.94669800 | -0.15365800 |
| O | -3.90322800 | 0.27341100 | 0.24551300 |
| O | 1.63479800 | 2.57439400 | 0.25774900 |
| O | -4.60561000 | -0.76071500 | -0.51935800 |
| C | -5.73868300 | -1.08151100 | 0.26443600 |
| H | -2.98911000 | 0.60634500 | -1.54974700 |
| H | -0.67033500 | 2.99360100 | 0.44730100 |
| H | 3.20401600 | -2.88675700 | 0.00981600 |
| H | 5.46377000 | -1.93503100 | -0.27456400 |
| H | 5.76789800 | 0.53439200 | -0.39452500 |
| H | 3.76774200 | 2.02256900 | -0.19309000 |
| H | -6.26998800 | -1.83746700 | -0.31752600 |
| H | -6.37741200 | -0.20461300 | 0.40789300 |
| H | -5.44607200 | -1.49378900 | 1.23540500 |
| C | -1.72656800 | -0.62195400 | -0.31182900 |
| H | -2.13076800 | -1.62265900 | -0.39719400 |
| N | -2.25152600 | 1.81648600 | -0.05350100 |

*N*-(methylperoxyl)-adduct derived from 3-azaphenothiazine-*N*-oxide



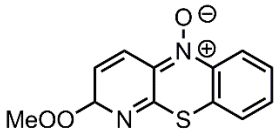

CBS-QB3 Enthalpy= -1194.726217
CBS-QB3 Free Energy= -1194.787497

0 1

| | | | |
|---|---|---|---|
| C | 2.31829800 | 1.54326000 | -0.33942500 |
| N | 2.63374000 | 0.22458200 | -0.63229400 |

| | | | |
|---|---|---|---|
| C | 1.67211600 | -0.77073500 | -0.48123700 |
| C | 0.39151900 | -0.46284800 | -0.15121300 |
| C | 0.00463600 | 0.91435200 | 0.01396800 |
| C | 1.05086800 | 1.89816600 | -0.04353600 |
| S | -0.72653000 | -1.77761200 | 0.22082500 |
| C | -2.27576400 | -0.94028100 | 0.04619300 |
| C | -2.39324000 | 0.45427000 | 0.10773700 |
| N | -1.25676800 | 1.33682600 | 0.20825900 |
| C | -3.42612900 | -1.72031100 | -0.07768700 |
| C | -4.68183500 | -1.12274600 | -0.12302400 |
| C | -4.79379600 | 0.26413700 | -0.05836600 |
| C | -3.65341700 | 1.05015300 | 0.05212400 |
| O | 3.87029000 | -0.11201400 | -0.80793200 |
| O | 4.54318300 | -0.41583400 | 0.75894300 |
| C | 5.85851000 | -0.77356600 | 0.48454100 |
| O | -1.50711000 | 2.58270600 | 0.38975500 |
| H | 3.15527700 | 2.22306700 | -0.39362800 |
| H | 2.04283800 | -1.77384400 | -0.62654900 |
| H | 0.78350300 | 2.92617400 | 0.14609000 |
| H | -3.33176500 | -2.79868600 | -0.13466600 |
| H | -5.56622500 | -1.74238800 | -0.21219900 |
| H | -5.76756700 | 0.73713700 | -0.09654300 |
| H | -3.69403400 | 2.12832000 | 0.10422600 |
| H | 6.42678000 | 0.03278400 | -0.00090500 |
| H | 6.32149700 | -0.97317800 | 1.46173300 |
| H | 5.93387800 | -1.68941900 | -0.11907100 |

3-(methylperoxyl)-adduct derived from 4-azaphenothiazine-*N*-oxide




CBS-QB3 Enthalpy= -1194.766976

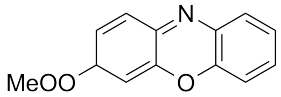
CBS-QB3 Free Energy= -1194.827412

0 1

| | | | |
|---|---|---|---|
| C | -2.27975300 | 1.96277000 | -0.24366000 |
| C | -2.79999100 | 0.58714800 | -0.53368500 |
| N | -1.81306800 | -0.47371300 | -0.52437700 |
| C | -0.57887500 | -0.21945900 | -0.31521000 |
| C | -0.02602400 | 1.10812700 | -0.09240500 |
| C | -0.97517600 | 2.19639900 | -0.05096300 |
| S | 0.45843800 | -1.65892000 | -0.27926900 |
| C | 2.06012800 | -0.97431000 | -0.07329900 |
| C | 2.31929400 | 0.39291700 | 0.07775000 |
| N | 1.27485800 | 1.39486500 | 0.08848000 |
| C | 3.13889300 | -1.86987000 | -0.06253000 |
| C | 4.43718000 | -1.41209900 | 0.09596700 |
| C | 4.68559700 | -0.04531800 | 0.24420100 |
| C | 3.63085000 | 0.85180700 | 0.23533700 |
| O | -3.80466400 | 0.34608800 | 0.45668600 |
| O | 1.65130100 | 2.59002100 | 0.27986000 |
| O | -4.70814800 | -0.66724100 | -0.06766200 |
| C | -4.57291700 | -1.81420000 | 0.76057400 |
| H | -3.00795800 | 2.76386900 | -0.20558500 |
| H | -3.30517900 | 0.56373500 | -1.50830700 |

| | | | |
|---|---|---|---|
| H | -0.58219800 | 3.18450500 | 0.13882300 |
| H | 2.94432500 | -2.92970400 | -0.18084700 |
| H | 5.25656700 | -2.12120600 | 0.10233800 |
| H | 5.69853700 | 0.31766300 | 0.36653500 |
| H | 3.77870500 | 1.91526600 | 0.34972500 |
| H | -5.31002800 | -2.51796700 | 0.36526300 |
| H | -4.81470100 | -1.57816000 | 1.80137900 |
| H | -3.56875900 | -2.23777300 | 0.68672800 |

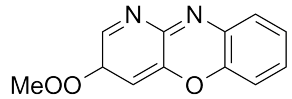
3-Methylperoxyl adduct derived from phenoxazine




CBS-QB3 Enthalpy= -781.014017
CBS-QB3 Free Energy= -781.071234
0 1

| | | | |
|---|---|---|---|
| C | -4.74049700 | -0.08935900 | 0.33541900 |
| C | -4.38504400 | -1.40760100 | 0.03980600 |
| C | -3.05538600 | -1.74651100 | -0.19915100 |
| C | -2.08475300 | -0.75543200 | -0.13880600 |
| C | -2.41798800 | 0.57690800 | 0.15694300 |
| C | -3.76107000 | 0.89377900 | 0.39295300 |
| O | -0.78300200 | -1.11331600 | -0.37409700 |
| C | 0.19087800 | -0.13941800 | -0.34447000 |
| C | -0.22325100 | 1.23087900 | -0.01807700 |
| N | -1.44794800 | 1.57656800 | 0.21947400 |
| C | 1.46222800 | -0.46642700 | -0.61166300 |
| C | 2.56265500 | 0.54919000 | -0.58220800 |
| C | 2.11293600 | 1.92983400 | -0.20305000 |
| C | 0.83322900 | 2.23284500 | 0.04229000 |
| O | 3.59119100 | 0.21474300 | 0.37519300 |
| O | 4.34514500 | -0.88955200 | -0.22306100 |
| C | 4.78340200 | -1.67935900 | 0.86654500 |
| H | -5.77707900 | 0.16564400 | 0.51971900 |
| H | -5.14595600 | -2.17801800 | -0.00525800 |
| H | -2.75692400 | -2.76179600 | -0.42982500 |
| H | -3.99968400 | 1.92594600 | 0.61955800 |
| H | 1.72414400 | -1.48822600 | -0.85473000 |
| H | 3.06348800 | 0.59139100 | -1.56097600 |
| H | 2.89077200 | 2.68171100 | -0.13563100 |
| H | 0.51722900 | 3.23758300 | 0.29689100 |
| H | 5.37486800 | -2.47519900 | 0.40784000 |
| H | 5.41504800 | -1.09874500 | 1.54656200 |
| H | 3.93901900 | -2.10725100 | 1.41605800 |

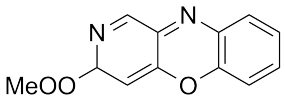
3-Methylperoxyl adduct derived from 1-azaphenoxazine




CBS-QB3 Enthalpy= -797.056194
CBS-QB3 Free Energy= -797.112905
0 1

| | | | |
|---|---|---|---|
| C | 2.64791100 | 0.37138600 | -0.98449000 |
| C | 2.26974500 | 1.68337300 | -0.33113200 |
| N | 1.11710000 | 2.03264500 | 0.08938600 |
| C | 0.04982000 | 1.13322300 | -0.03999300 |
| C | 0.28952800 | -0.19053800 | -0.63490700 |
| C | 1.49239300 | -0.56195000 | -1.09339200 |
| N | -1.10534200 | 1.52432200 | 0.37786300 |
| C | -2.16866700 | 0.63449300 | 0.25704400 |
| C | -2.00366500 | -0.64702400 | -0.29290600 |
| O | -0.77065800 | -1.05901800 | -0.72734500 |
| C | -3.44485600 | 1.01537800 | 0.69133000 |
| C | -4.51832300 | 0.14232500 | 0.57869700 |
| C | -4.32797700 | -1.12789500 | 0.02775000 |
| C | -3.06906800 | -1.52919000 | -0.41166300 |
| O | 3.80180900 | -0.18977600 | -0.32933300 |
| O | 3.44583500 | -0.40442700 | 1.07267700 |
| C | 3.76509800 | -1.75381600 | 1.36435600 |
| H | 3.08190800 | 0.58701000 | -1.97279700 |
| H | 3.09084300 | 2.38764500 | -0.19457000 |
| H | 1.63604500 | -1.53464800 | -1.54785300 |
| H | -3.55402900 | 2.00721200 | 1.11269000 |
| H | -5.50170500 | 0.44504400 | 0.91733200 |
| H | -5.16416400 | -1.81158500 | -0.06080000 |
| H | -2.89861800 | -2.50852800 | -0.84151500 |
| H | 3.55349100 | -1.85640000 | 2.43140000 |
| H | 3.14218000 | -2.44971000 | 0.79364400 |
| H | 4.82421300 | -1.95763400 | 1.17957100 |

3-(Methylperoxyl) adduct derived from 2-azaphenoxazine



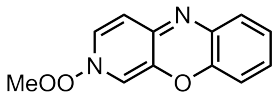

CBS-QB3 Enthalpy= -797.057505
CBS-QB3 Free Energy= -797.113393

0 1

| | | | |
|---|---|---|---|
| C | 2.45816100 | -0.36985100 | -0.57110500 |
| N | 2.32723900 | 1.07828000 | -0.44659200 |
| C | 1.17186900 | 1.59069300 | -0.29634900 |
| C | -0.09268800 | 0.84245100 | -0.20644700 |
| C | 0.02610900 | -0.60907900 | -0.23349900 |
| C | 1.21977500 | -1.19600000 | -0.38439600 |
| N | -1.20465500 | 1.48666400 | -0.08171100 |
| C | -2.36447900 | 0.71635500 | 0.02755800 |
| C | -2.31744800 | -0.68926100 | 0.02071100 |
| O | -1.12091000 | -1.35346800 | -0.09656200 |
| C | -3.60789100 | 1.34623500 | 0.15084200 |
| C | -4.77117200 | 0.59574500 | 0.26405300 |
| C | -4.70020000 | -0.79899100 | 0.25601800 |
| C | -3.47331500 | -1.44815900 | 0.13406300 |
| O | 3.39069400 | -0.85116800 | 0.39833800 |
| O | 4.72780400 | -0.52500700 | -0.07424300 |
| C | 5.27143600 | 0.42868100 | 0.82944100 |
| H | 2.89620100 | -0.55531900 | -1.56098900 |
| H | 1.07702400 | 2.67272500 | -0.20225300 |
| H | 1.31974000 | -2.27362000 | -0.40389700 |

| | | | |
|---|---|---|---|
| H | -3.62316200 | 2.42938700 | 0.15440100 |
| H | -5.72981100 | 1.09078000 | 0.35915200 |
| H | -5.60511900 | -1.38848900 | 0.34546700 |
| H | -3.39678600 | -2.52836700 | 0.12633200 |
| H | 5.30349600 | 0.03042600 | 1.84810000 |
| H | 6.29047600 | 0.58822200 | 0.46762700 |
| H | 4.70820200 | 1.36387100 | 0.79859300 |

*N*-Methylperoxyl adduct derived from 3-azaphenoxazine

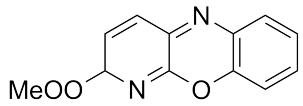



CBS-QB3 Enthalpy= -797.023241
CBS-QB3 Free Energy= -797.080535

0 1

| | | | |
|---|---|---|---|
| C | 2.17477800 | 1.58665600 | -0.27240600 |
| N | 2.40916300 | 0.25727300 | -0.57567700 |
| C | 1.37258900 | -0.67435000 | -0.54119300 |
| C | 0.10715700 | -0.26147800 | -0.30123200 |
| C | -0.21315300 | 1.13490100 | -0.04409700 |
| C | 0.92224200 | 2.03080400 | -0.03822200 |
| O | -0.89741500 | -1.18878300 | -0.30570700 |
| C | -2.18965600 | -0.74062900 | -0.08818200 |
| C | -2.44070000 | 0.62215900 | 0.14829000 |
| N | -1.42039100 | 1.57301400 | 0.17251500 |
| C | -3.20629400 | -1.67973200 | -0.11225400 |
| C | -4.52054500 | -1.26318200 | 0.10596400 |
| C | -4.79945000 | 0.08201100 | 0.34301500 |
| C | -3.76668700 | 1.01427300 | 0.36334000 |
| O | 3.63843700 | -0.16466100 | -0.66509100 |
| O | 4.14974100 | -0.54675300 | 0.88198100 |
| C | 5.42964200 | -1.06894500 | 0.68693400 |
| H | 3.06305400 | 2.20105500 | -0.26186800 |
| H | 1.65330500 | -1.69770100 | -0.73438800 |
| H | 0.73621400 | 3.07665700 | 0.16390700 |
| H | -2.96014200 | -2.71810900 | -0.29829500 |
| H | -5.32104400 | -1.99324900 | 0.08987200 |
| H | -5.82025200 | 0.40356400 | 0.51217500 |
| H | -3.95251400 | 2.06602100 | 0.54490400 |
| H | 5.79280300 | -1.32183000 | 1.69138500 |
| H | 5.42241000 | -1.98437000 | 0.08056900 |
| H | 6.11911400 | -0.33740300 | 0.24467100 |

3-Methylperoxyl adduct derived from 4-azaphenoxazine



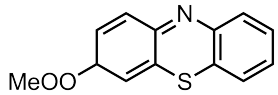

CBS-QB3 Enthalpy= -797.070676
CBS-QB3 Free Energy= -797.126381

0 1

| | | | |
|---|---|---|---|
| C | 2.62604600 | 0.39417500 | -0.91862200 |
| C | 2.39139300 | 1.72683100 | -0.25825000 |
| C | 1.17963900 | 2.11126800 | 0.15490200 |
| C | 0.04664300 | 1.21701600 | 0.00792200 |

| | | | |
|---|---|---|---|
| C | 0.36388800 | -0.10224700 | -0.58469100 |
| N | 1.49199600 | -0.49485500 | -1.00874600 |
| N | -1.13719800 | 1.56939800 | 0.39467300 |
| C | -2.16592700 | 0.64967900 | 0.24048200 |
| C | -1.92928300 | -0.62918000 | -0.28922000 |
| O | -0.66842800 | -0.99955200 | -0.67633000 |
| C | -3.47184600 | 0.98546900 | 0.62498000 |
| C | -4.50334200 | 0.06973700 | 0.48191900 |
| C | -4.24239400 | -1.19911300 | -0.04697400 |
| C | -2.95489500 | -1.55500700 | -0.43510600 |
| O | 3.75022200 | -0.27136800 | -0.34295200 |
| O | 3.42679900 | -0.55561100 | 1.05174200 |
| C | 3.45170600 | -1.97099000 | 1.18286300 |
| H | 3.00252300 | 0.56035300 | -1.93921200 |
| H | 3.26217000 | 2.36283300 | -0.14481600 |
| H | 0.98957400 | 3.07217400 | 0.61787900 |
| H | -3.63662200 | 1.97539800 | 1.03264000 |
| H | -5.51009700 | 0.33546000 | 0.78058800 |
| H | -5.04782500 | -1.91556700 | -0.15779200 |
| H | -2.72846500 | -2.53043700 | -0.84723600 |
| H | 2.68976400 | -2.43943800 | 0.55554100 |
| H | 4.44158300 | -2.36953200 | 0.94016600 |
| H | 3.23528600 | -2.14661500 | 2.23983100 |

3-Methylperoxyl adduct derived from phenothiazine



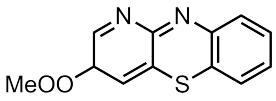

CBS-QB3 Enthalpy= -1103.625785
CBS-QB3 Free Energy= -1103.685343

0 1

| | | | |
|---|---|---|---|
| C | 2.65085200 | -0.07563000 | -0.66179200 |
| C | 1.10856900 | 1.80146600 | -0.12938200 |
| C | -0.05279400 | 0.91240000 | -0.09126500 |
| C | 0.23003700 | -0.52964500 | -0.24056600 |
| C | 1.46835800 | -0.97920200 | -0.51509500 |
| N | -1.21134100 | 1.46580000 | 0.06012900 |
| C | -2.40247400 | 0.74911200 | 0.08490200 |
| C | -2.50709600 | -0.65594900 | 0.05390000 |
| C | -3.58622600 | 1.50350300 | 0.14892100 |
| C | -4.83030400 | 0.89291600 | 0.18311100 |
| C | -4.91601200 | -0.50080100 | 0.15470600 |
| C | -3.76067900 | -1.27091200 | 0.08853200 |
| O | 3.64744800 | -0.58851300 | 0.24882200 |
| O | 4.92709300 | -0.04252500 | -0.22117300 |
| C | 5.78414000 | -0.09272800 | 0.90279700 |
| H | 3.07779200 | -0.17999600 | -1.67085300 |
| H | 0.89213900 | 2.84723600 | 0.05492200 |
| H | 1.66568000 | -2.03922800 | -0.63048500 |
| H | -3.48055000 | 2.58131600 | 0.17108800 |
| H | -5.73006500 | 1.49444500 | 0.23281700 |
| H | -5.88275000 | -0.99008400 | 0.18201400 |
| H | -3.82884600 | -2.35305000 | 0.06202500 |
| H | 5.90693000 | -1.12020700 | 1.26042400 |
| H | 6.74132700 | 0.28465800 | 0.53580700 |

| | | | |
|---|---|---|---|
| H | 5.41638000 | 0.54281800 | 1.71473300 |
| S | -1.08004400 | -1.69035900 | 0.01747800 |
| C | 2.34621800 | 1.36554900 | -0.38394600 |
| H | 3.19020500 | 2.04505900 | -0.40317700 |

3-Methylperoxyl adduct derived from 1-azaphenothiazine

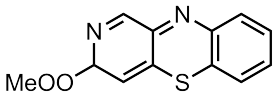



CBS-QB3 Enthalpy= -1119.667259
CBS-QB3 Free Energy= -1119.726064

0 1

| | | | |
|---|---|---|---|
| C | 2.57234100 | -0.01092200 | -0.58963400 |
| C | -0.04477400 | 0.90102300 | 0.12536100 |
| C | 0.22107700 | -0.53840000 | -0.07950100 |
| C | 1.44230300 | -0.97279600 | -0.43495500 |
| N | -1.20228400 | 1.45742400 | 0.18992900 |
| C | -2.39010400 | 0.74739500 | 0.06839900 |
| C | -2.50347700 | -0.65873800 | 0.07844500 |
| C | -3.56655000 | 1.50836800 | -0.04104900 |
| C | -4.81010500 | 0.90307100 | -0.13267000 |
| C | -4.90490900 | -0.49030000 | -0.10892500 |
| C | -3.75723200 | -1.26778300 | -0.00552400 |
| O | 3.69138400 | -0.55342900 | 0.12966600 |
| O | 4.87647200 | 0.09526700 | -0.44735300 |
| C | 5.92290000 | -0.16848000 | 0.46820300 |
| H | 2.88063100 | 0.07209000 | -1.64279800 |
| H | 1.65232500 | -2.01990300 | -0.61796600 |
| H | -3.45527400 | 2.58568100 | -0.04506300 |
| H | -5.70421600 | 1.50922200 | -0.21628400 |
| H | -5.87284100 | -0.97351100 | -0.17469900 |
| H | -3.83111400 | -2.34964500 | 0.00330000 |
| H | 6.08911700 | -1.24478400 | 0.57724700 |
| H | 6.80242900 | 0.29690700 | 0.01828600 |
| H | 5.71969700 | 0.28062400 | 1.44534700 |
| S | -1.07995700 | -1.68502000 | 0.25762100 |
| C | 2.22084900 | 1.35511100 | -0.04871200 |
| H | 3.06099800 | 2.03304400 | 0.09801800 |
| N | 1.05668500 | 1.76980200 | 0.26400600 |

3-Methylperoxyl adduct derived from 2-azaphenothiazine



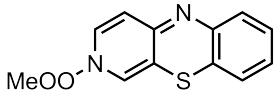

CBS-QB3 Enthalpy= -1119.670713
CBS-QB3 Free Energy= -1119.728660

0 1

| | | | |
|---|---|---|---|
| C | 2.63311600 | -0.22615300 | -0.57160600 |
| N | 2.43407800 | 1.18387600 | -0.27016800 |
| C | 1.25191800 | 1.60441500 | -0.06238900 |
| C | 0.01814800 | 0.78849300 | -0.05590300 |
| C | 0.22459400 | -0.65953600 | -0.13812200 |
| C | 1.45759500 | -1.13831800 | -0.37370900 |
| N | -1.09585900 | 1.43037200 | 0.03258900 |

| | | | |
|---|---|---|---|
| C | -2.33005000 | 0.78392400 | 0.03607300 |
| C | -2.51062600 | -0.61433100 | 0.07695300 |
| C | -3.46706400 | 1.60658200 | 0.00202300 |
| C | -4.74526500 | 1.06880200 | 0.00936400 |
| C | -4.90842100 | -0.31674800 | 0.05400900 |
| C | -3.79784900 | -1.15373900 | 0.08562900 |
| O | 3.67228000 | -0.76084600 | 0.24615500 |
| O | 4.94085500 | -0.29652900 | -0.29460700 |
| C | 5.51303300 | 0.57734200 | 0.67073900 |
| H | 2.97987400 | -0.27575500 | -1.61352100 |
| H | 1.09372000 | 2.66275500 | 0.14594100 |
| H | 1.65879700 | -2.20088300 | -0.44496900 |
| H | -3.29967700 | 2.67627200 | -0.02935300 |
| H | -5.61011200 | 1.72056300 | -0.01727400 |
| H | -5.90190600 | -0.74981400 | 0.06243300 |
| H | -3.92921100 | -2.22979500 | 0.11524800 |
| H | 5.66408300 | 0.06299700 | 1.62462100 |
| H | 6.48241300 | 0.84733500 | 0.24389100 |
| H | 4.89691600 | 1.46863300 | 0.80616600 |
| S | -1.14639400 | -1.73421600 | 0.17244500 |

*N*-Methylperoxyl adduct derived from 3-azaphenothiazine

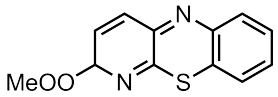



CBS-QB3 Enthalpy= -1119.637500
CBS-QB3 Free Energy= -1119.696595

0 1

| | | | |
|---|---|---|---|
| C | -2.26460700 | 1.64888700 | -0.20423800 |
| N | -2.55164000 | 0.34425900 | -0.57183400 |
| C | -1.57454200 | -0.64215300 | -0.48825500 |
| C | -0.29834600 | -0.32977600 | -0.15831400 |
| C | 0.09887700 | 1.06151600 | 0.07421400 |
| C | -1.00123200 | 2.00963200 | 0.09285000 |
| S | 0.87254400 | -1.62337000 | 0.11972000 |
| C | 2.39846300 | -0.71843300 | 0.03450400 |
| C | 2.42227500 | 0.68757600 | 0.14715300 |
| N | 1.30584800 | 1.51236400 | 0.24160000 |
| C | 3.58103200 | -1.44596400 | -0.07973200 |
| C | 4.81061500 | -0.79174800 | -0.06933700 |
| C | 4.85621300 | 0.59704300 | 0.04452000 |
| C | 3.67587200 | 1.32088400 | 0.14790300 |
| O | -3.79565600 | -0.00878200 | -0.75396600 |
| O | -4.42238500 | -0.39807200 | 0.73308600 |
| C | -5.73224400 | -0.79369400 | 0.44863400 |
| H | -3.11792000 | 2.31103100 | -0.20788700 |
| H | -1.93432100 | -1.64014700 | -0.69161800 |
| H | -0.76421100 | 3.03628600 | 0.33627600 |
| H | 3.54054100 | -2.52586000 | -0.17332600 |
| H | 5.72495600 | -1.36755100 | -0.15176400 |
| H | 5.80919900 | 1.11305000 | 0.05132100 |
| H | 3.67891700 | 2.40086200 | 0.23223100 |
| H | -6.16865500 | -1.05447200 | 1.42088400 |
| H | -6.32751700 | 0.01585400 | 0.00649400 |
| H | -5.77108600 | -1.67928900 | -0.19885800 |

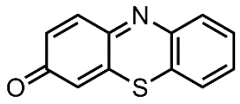
3-Methylperoxyl adduct derived from 4-azaphenothiazine




CBS-QB3 Enthalpy= -1119.677316
CBS-QB3 Free Energy= -1119.735224

```
0 1
 C                  2.79216000    0.44642600   -0.90957800
 C                  2.45335300    1.80071200   -0.35569800
 C                  1.20649700    2.12790200   -0.00525500
 C                  0.12083400    1.16203400   -0.10565000
 C                  0.54114700   -0.18392600   -0.57224200
 N                  1.71689400   -0.52096900   -0.93305700
 N                 -1.07105000    1.53744000    0.22617000
 C                 -2.17668800    0.70362800    0.19394300
 C                 -2.15441900   -0.66213900   -0.15845800
 C                 -3.40841500    1.28191300    0.55372100
 C                 -4.57586400    0.53856400    0.56381700
 C                 -4.53696000   -0.81480100    0.21300700
 C                 -3.33576600   -1.41089400   -0.14612900
 O                  3.95199700   -0.09880900   -0.28415500
 O                  3.64687700   -0.27486500    1.13295200
 C                  3.77916400   -1.66468400    1.39681100
 H                  3.16110700    0.55403800   -1.94114500
 H                  3.27469300    2.50318200   -0.26691600
 H                  0.94241400    3.10608900    0.37890300
 H                 -3.39829900    2.33129700    0.82158400
 H                 -5.51407700    1.00246400    0.84348900
 H                 -5.44514300   -1.40622000    0.21902200
 H                 -3.30851700   -2.45999500   -0.41967700
 H                  3.05346900   -2.24784900    0.82476500
 H                  4.79553900   -2.00978600    1.18342600
 H                  3.57876800   -1.75511700    2.46747800
 S                 -0.66763200   -1.48077600   -0.62267500
```

Phenothiazone

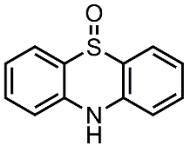



CBS-QB3 Enthalpy= -988.184974
CBS-QB3 Free Energy= -988.234788

```
0 1
 C                 -3.97028300    0.93793800    0.00004100
 C                 -4.07254400   -0.45860200    0.00002500
 C                 -2.93104800   -1.24699800    0.00000000
 C                 -1.66599800   -0.64932800   -0.00001100
 C                 -1.54413800    0.75817400    0.00000000
 C                 -2.72214200    1.53219100    0.00002800
 S                 -0.26249200   -1.69856400   -0.00004400
 C                  1.08356700   -0.56908300   -0.00000500
 C                  0.81436000    0.87966200   -0.00002600
 N                 -0.35159000    1.45237400   -0.00002200
 C                  2.35343800   -1.04536200    0.00002900
```

| | | | |
|---|---|---|---|
| C | 3.51960100 | -0.15970900 | 0.00002600 |
| C | 3.23351400 | 1.28993800 | -0.00002000 |
| C | 1.97474900 | 1.76102700 | -0.00004400 |
| O | 4.66774500 | -0.59066000 | 0.00006500 |
| H | -4.86469400 | 1.54895600 | 0.00006200 |
| H | -5.04703800 | -0.93276900 | 0.00003400 |
| H | -3.01517800 | -2.32810200 | -0.00000900 |
| H | -2.60153200 | 2.60843700 | 0.00003600 |
| H | 2.56525700 | -2.10877100 | 0.00005300 |
| H | 4.09478400 | 1.94793500 | -0.00003000 |
| H | 1.74897800 | 2.82091100 | -0.00007100 |

S-oxide derived from phenothiazine




CBS-QB3 Enthalpy= -989.366908
CBS-QB3 Free Energy= -989.416887

0 1

| | | | |
|---|---|---|---|
| C | 1.19868700 | -0.42383700 | 3.51971500 |
| C | -0.17835900 | -0.62911600 | 3.60818700 |
| C | -0.98278200 | -0.35102800 | 2.50683300 |
| C | -0.40901800 | 0.12578200 | 1.33437700 |
| C | 0.97739000 | 0.29239100 | 1.21846100 |
| C | 1.77675000 | 0.01914300 | 2.33497700 |
| S | -1.49976900 | 0.69037300 | 0.00000000 |
| C | -0.40901800 | 0.12578200 | -1.33437700 |
| C | 0.97739000 | 0.29239100 | -1.21846100 |
| N | 1.54460000 | 0.69092900 | 0.00000000 |
| C | -0.98278200 | -0.35102800 | -2.50683300 |
| C | -0.17835900 | -0.62911600 | -3.60818700 |
| C | 1.19868700 | -0.42383700 | -3.51971500 |
| C | 1.77675000 | 0.01914300 | -2.33497700 |
| O | -2.74760800 | -0.13100400 | 0.00000000 |
| H | 1.83352700 | -0.62877300 | 4.37410200 |
| H | -0.62084500 | -0.99421800 | 4.52691000 |
| H | -2.05667300 | -0.49549700 | 2.53685300 |
| H | 2.85393800 | 0.13308300 | 2.26274300 |
| H | -2.05667300 | -0.49549700 | -2.53685300 |
| H | -0.62084500 | -0.99421800 | -4.52691000 |
| H | 1.83352700 | -0.62877300 | -4.37410200 |
| H | 2.85393800 | 0.13308300 | -2.26274300 |
| H | 2.55304300 | 0.73635500 | 0.00000000 |

MeOO•
CBS-QB3 Enthalpy= -189.954731
CBS-QB3 Free Energy= -189.985244

```
0 2
 C                  1.09605600   -0.18318500    0.00000000
 O                 -0.15733400    0.54388200    0.00000000
 O                 -1.18625500   -0.27864400    0.00000000
 H                  1.87467300    0.57860400   -0.00004100
 H                  1.14887400   -0.80066900    0.89702000
 H                  1.14883600   -0.80073200   -0.89697900
```

HOO•
CBS-QB3 Enthalpy= -150.737288
CBS-QB3 Free Energy= -150.763268

```
0 2
 O                  0.05528600    0.71850700    0.00000000
 O                  0.05528600   -0.60966700    0.00000000
 H                 -0.88457400   -0.87072000    0.00000000
```

Triplet $O_2$
CBS-QB3 Enthalpy= -150.161378
CBS-QB3 Free Energy= -150.184650

```
0 3
 O                  0.00000000    0.00000000    0.60281700
 O                  0.00000000    0.00000000   -0.60281700
```

MeO•
CBS-QB3 Enthalpy= -114.870535
CBS-QB3 Free Energy= -114.897461

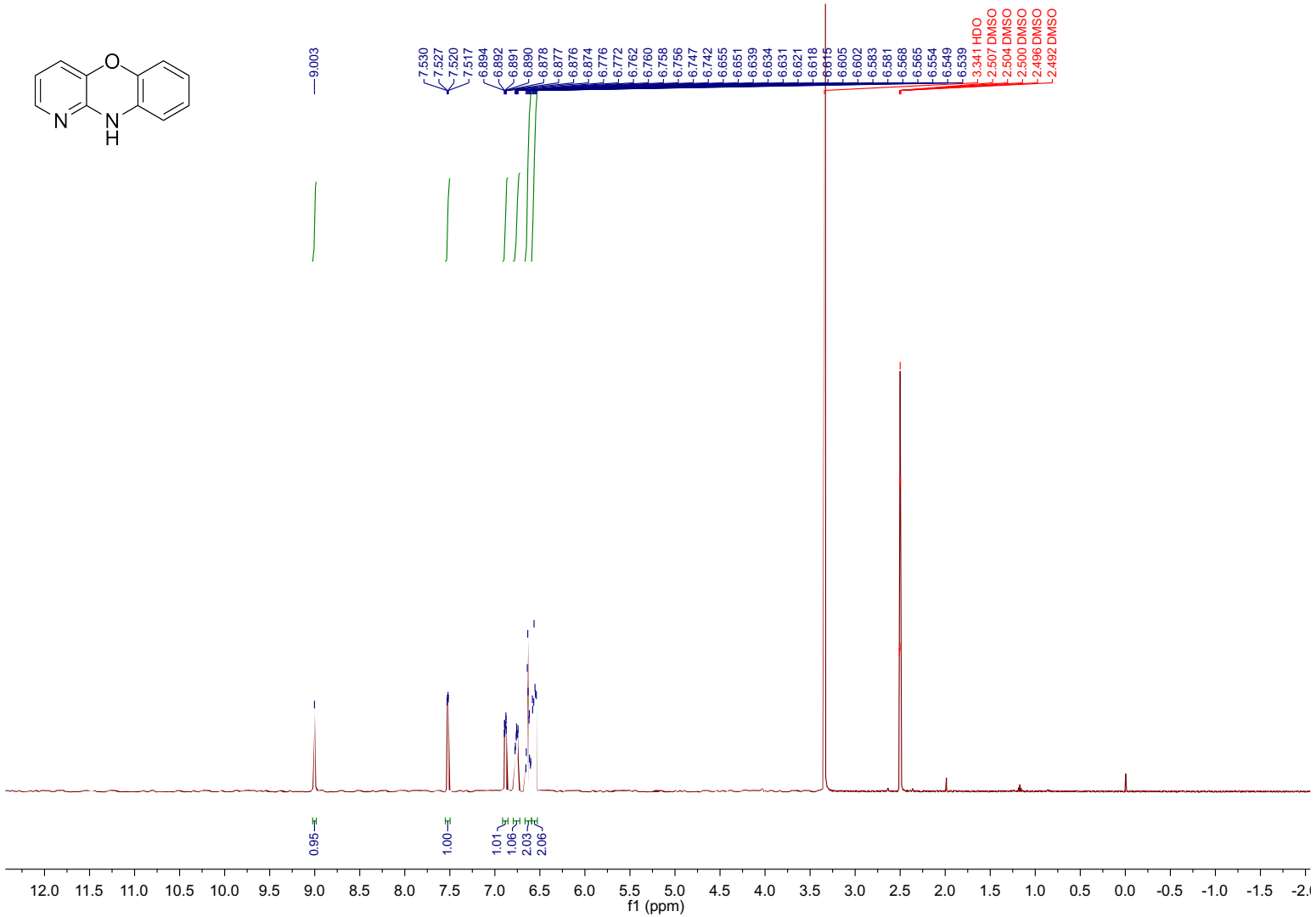
```
0 2
 C                 -0.57342700    0.00000200   -0.01405600
 O                  0.79185400    0.00000000   -0.00767900
 H                 -0.87136900   -0.00006000    1.05453800
 H                 -1.01144800   -0.90924700   -0.45443200
 H                 -1.01145200    0.90929300   -0.45434000
```

HO•
CBS-QB3 Enthalpy= -75.646409
CBS-QB3 Free Energy= -75.666640

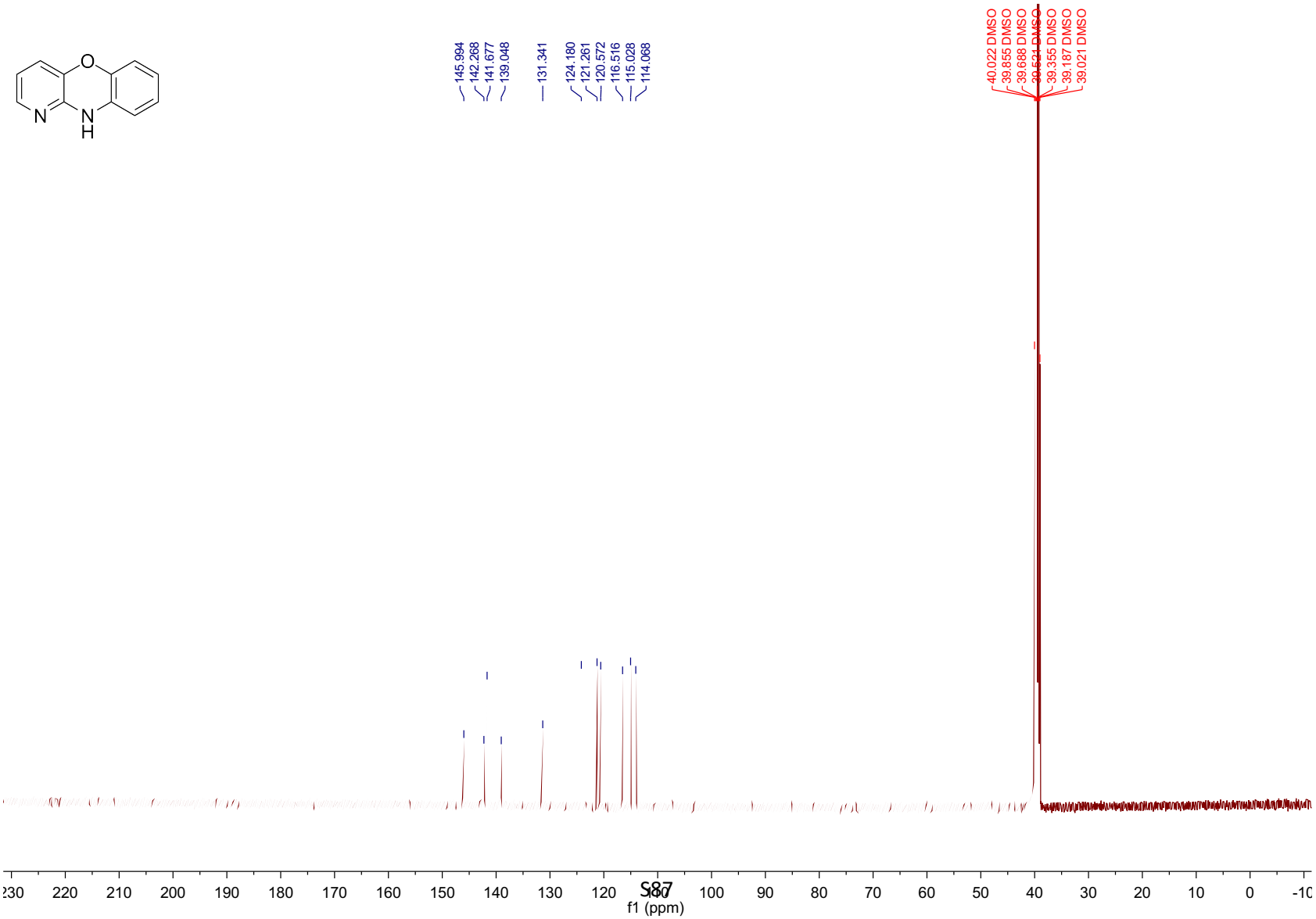
```
0 2
 O                  0.00000000    0.00000000    0.10835700
 H                  0.00000000    0.00000000   -0.86685600
```

## NMR Spectra

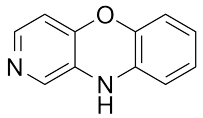
$^{1}$H-NMR of 1-azaphenoxazine



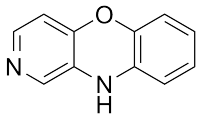
$^{13}$C-NMR of 1-azaphenoxazine



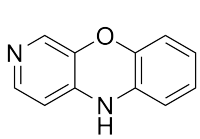
$^{1}$H-NMR of 2-azaphenoxazine



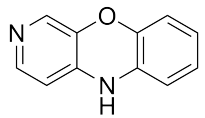
$^{13}$C-NMR of 2-azaphenoxazine



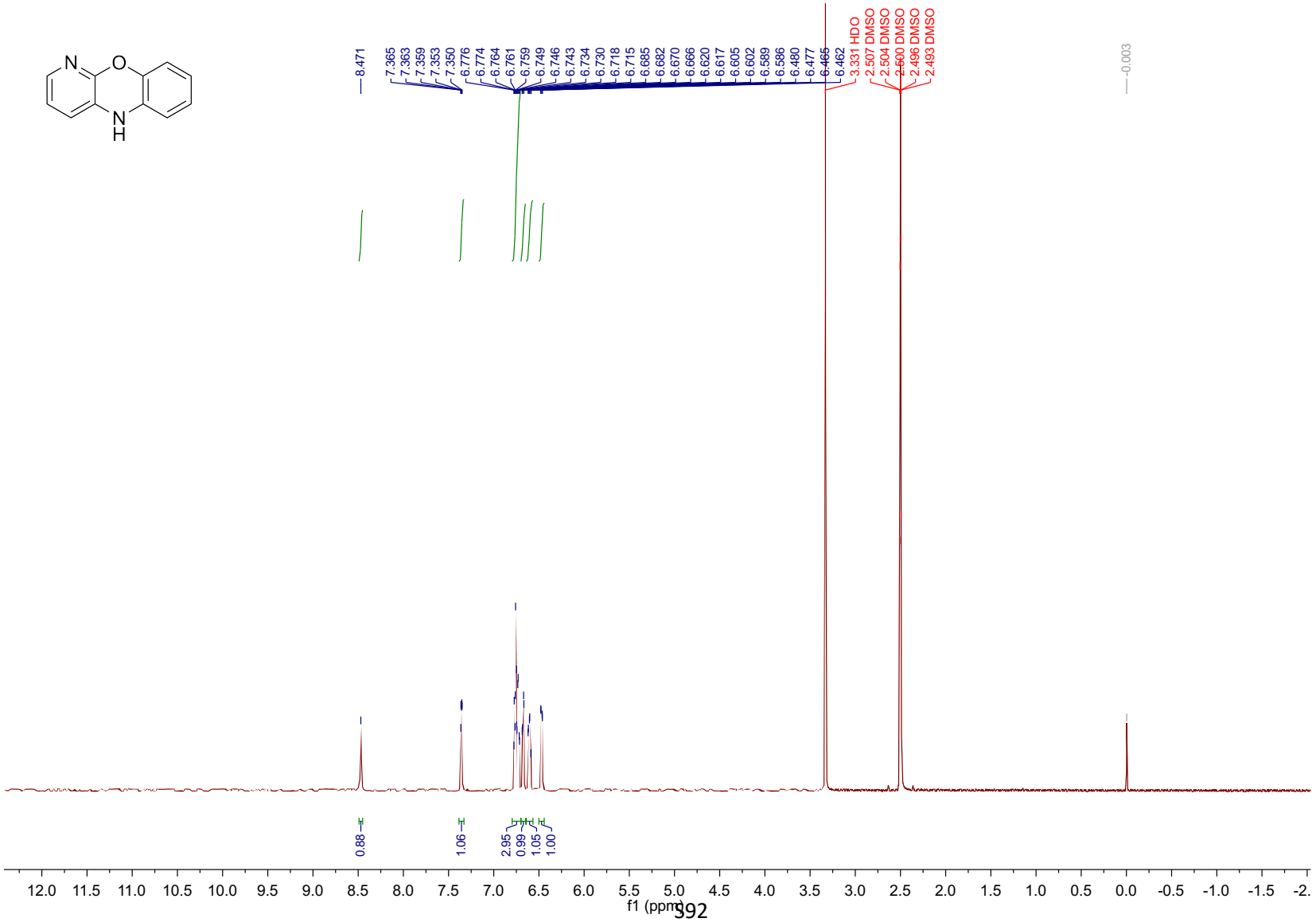
[1]H-NMR of 3-azaphenoxazine



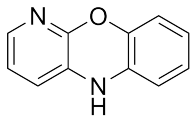
$^{13}$C-NMR of 3-azaphenoxazine



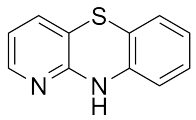
$^{1}$H-NMR of 4-azaphenoxazine



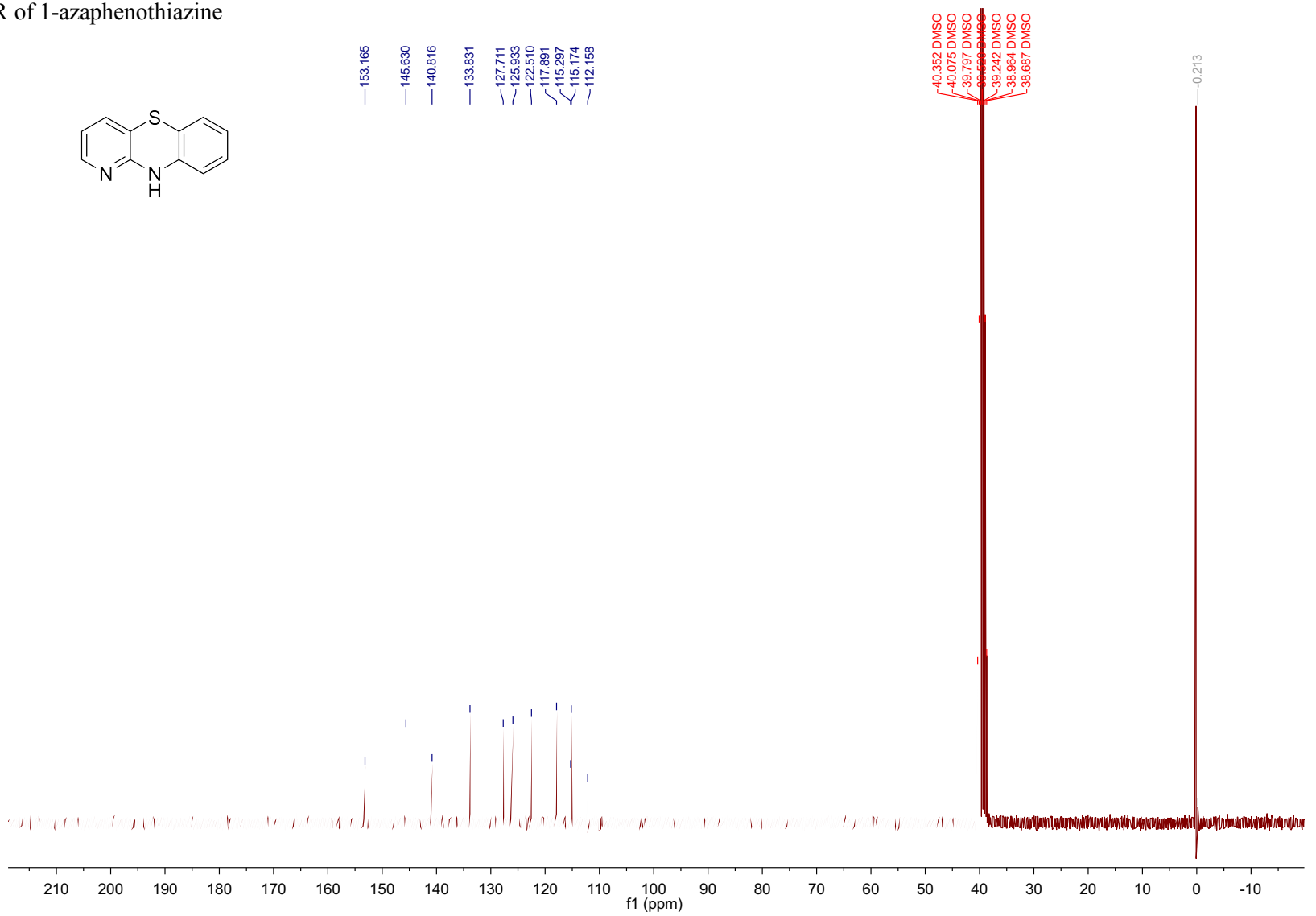
$^{13}$C-NMR of 4-azaphenoxazine



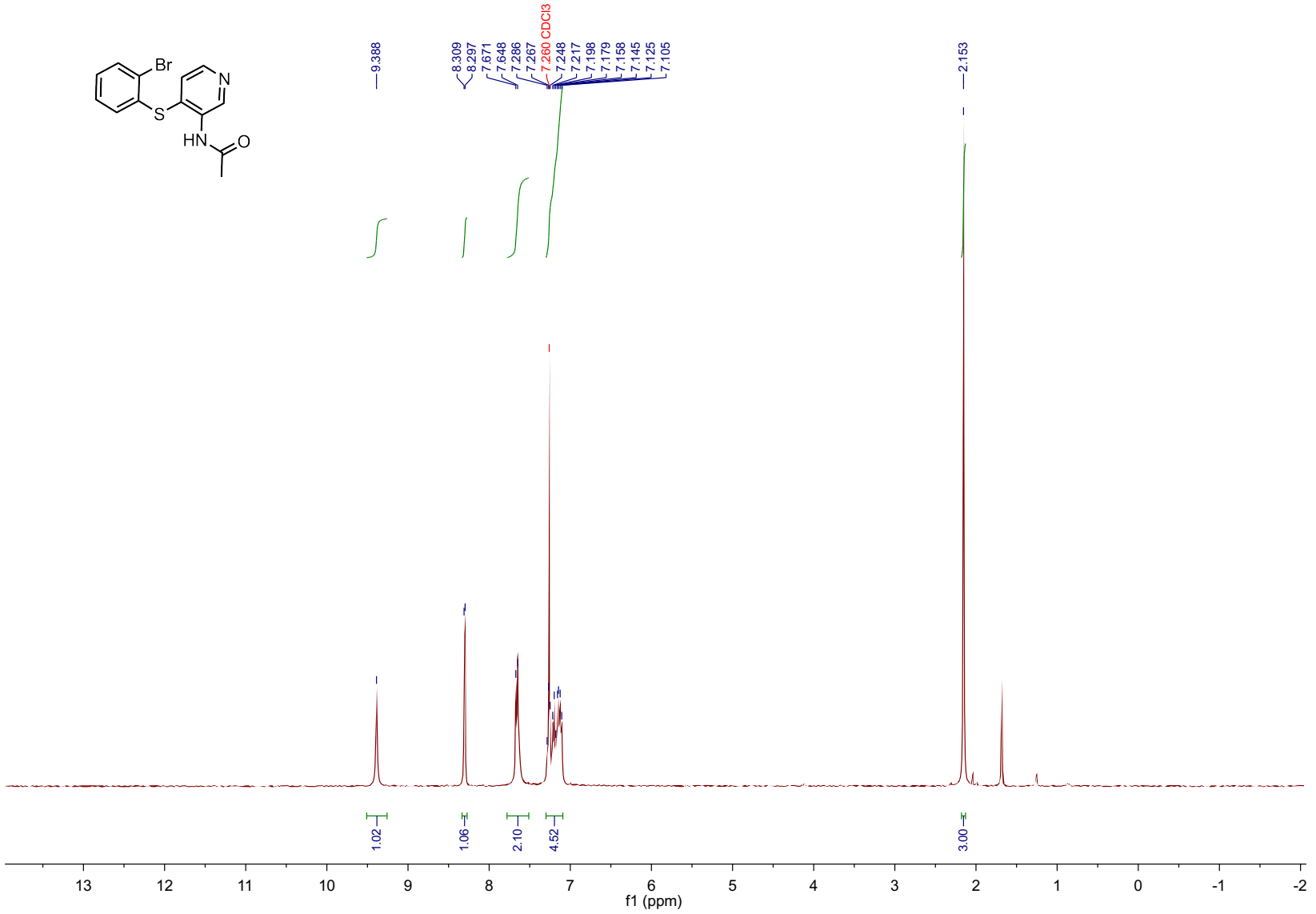
$^{1}$H-NMR of 1-azaphenothiazine



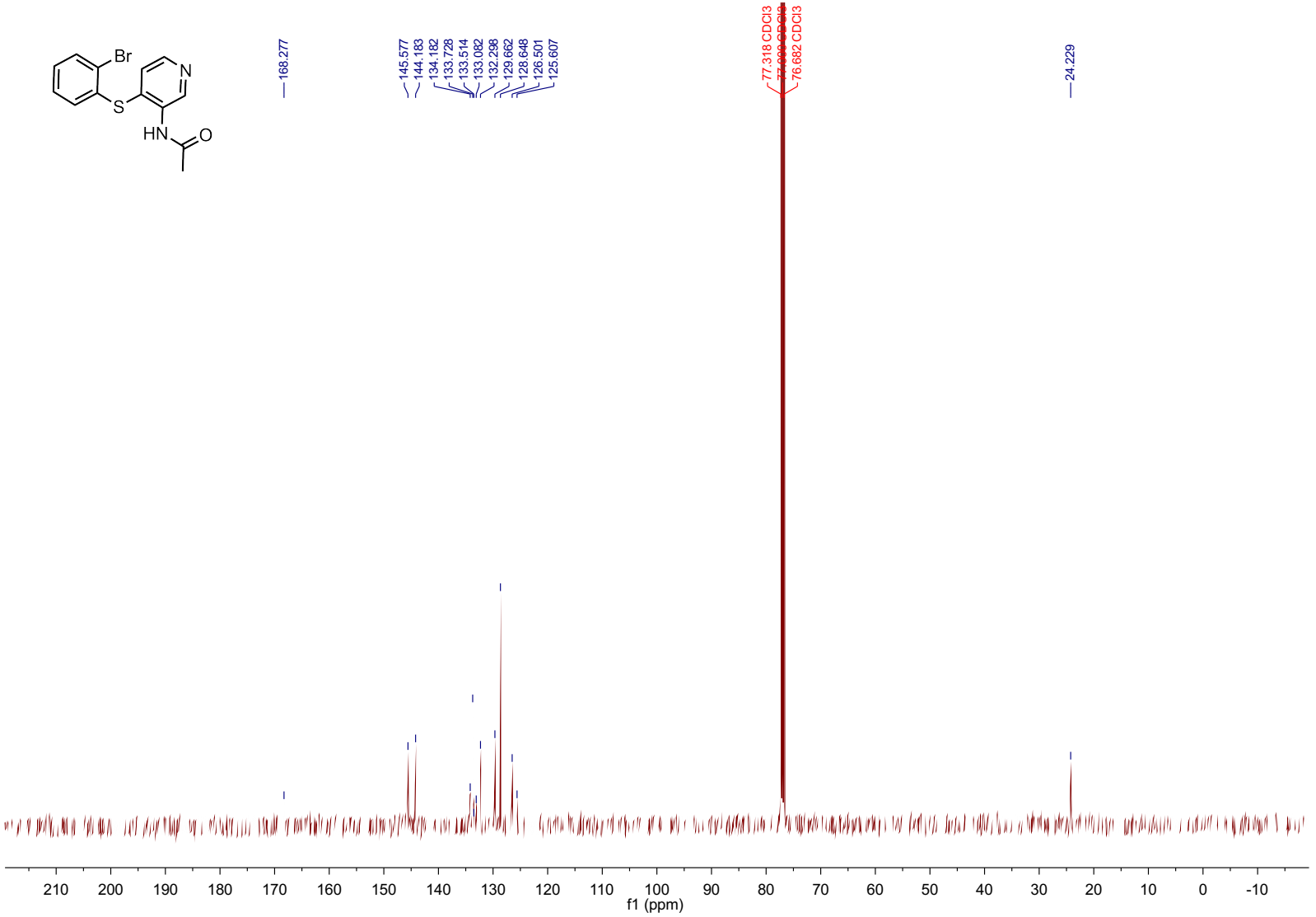
$^{13}$C-NMR of 1-azaphenothiazine



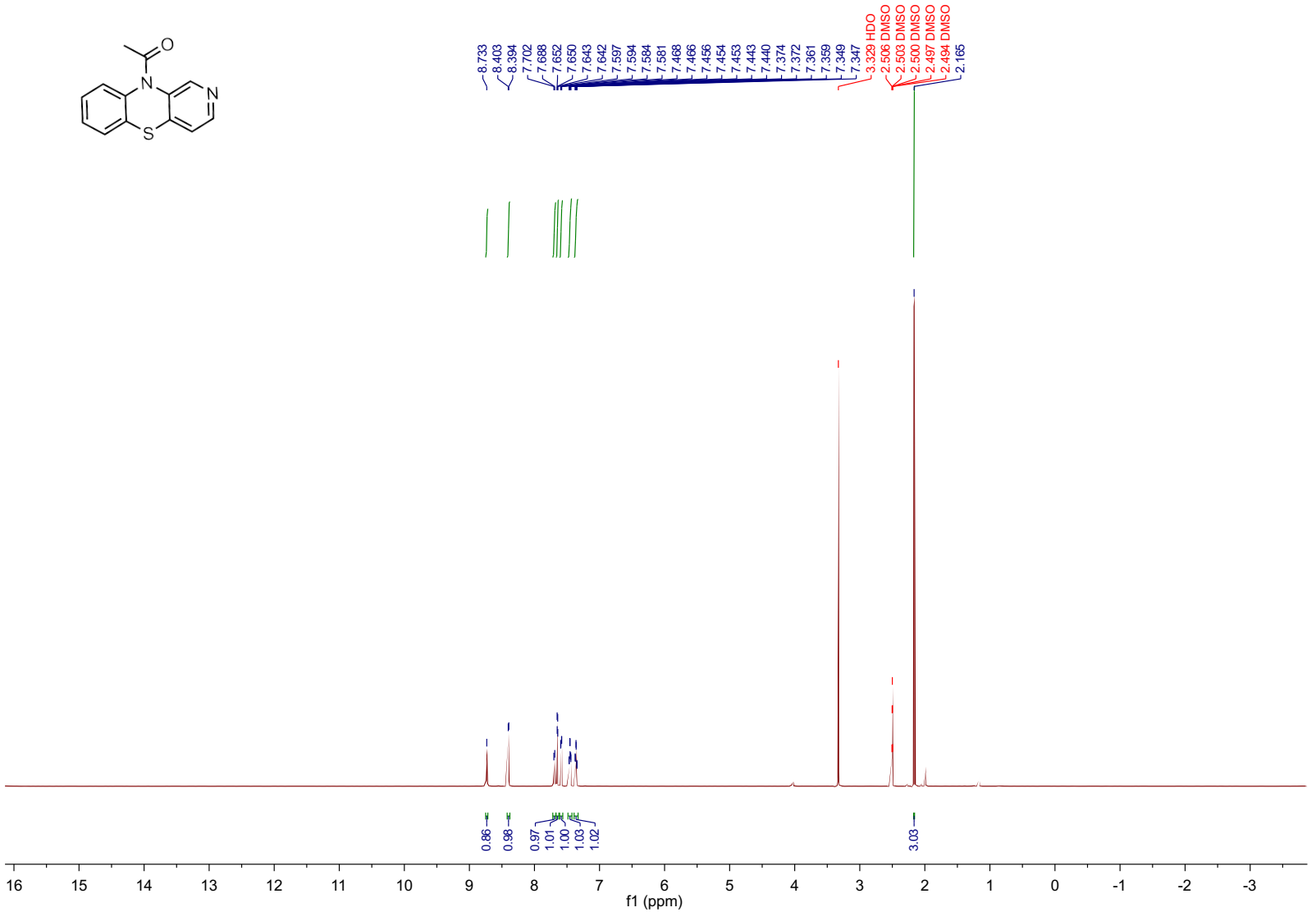
[1]H-NMR of *N*-acetyl-3-amino-4-(2'-bromophenylthio)pyridine



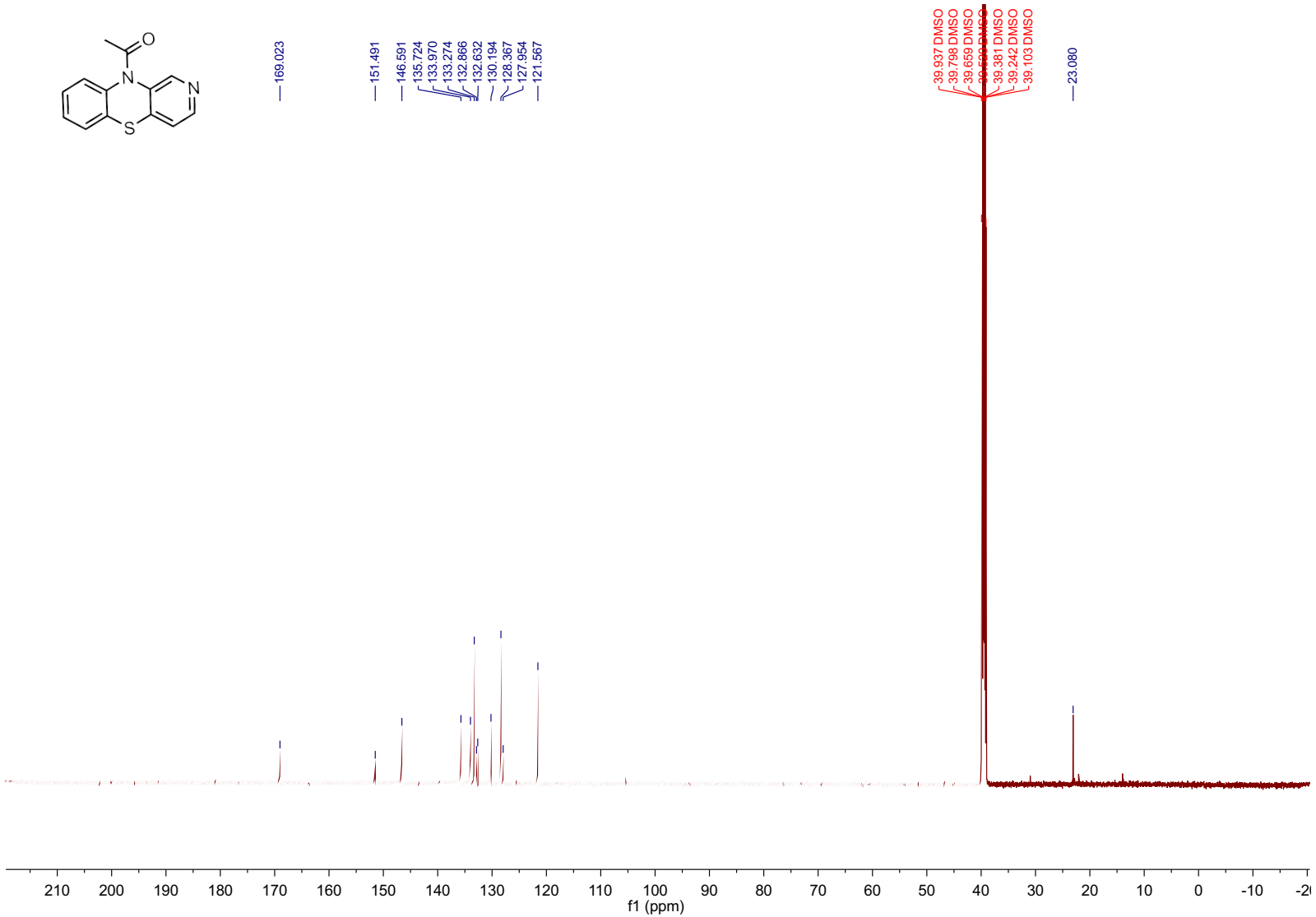
$^{13}$C-NMR of *N*-acetyl-3-amino-4-(2'-bromophenylthio)pyridine



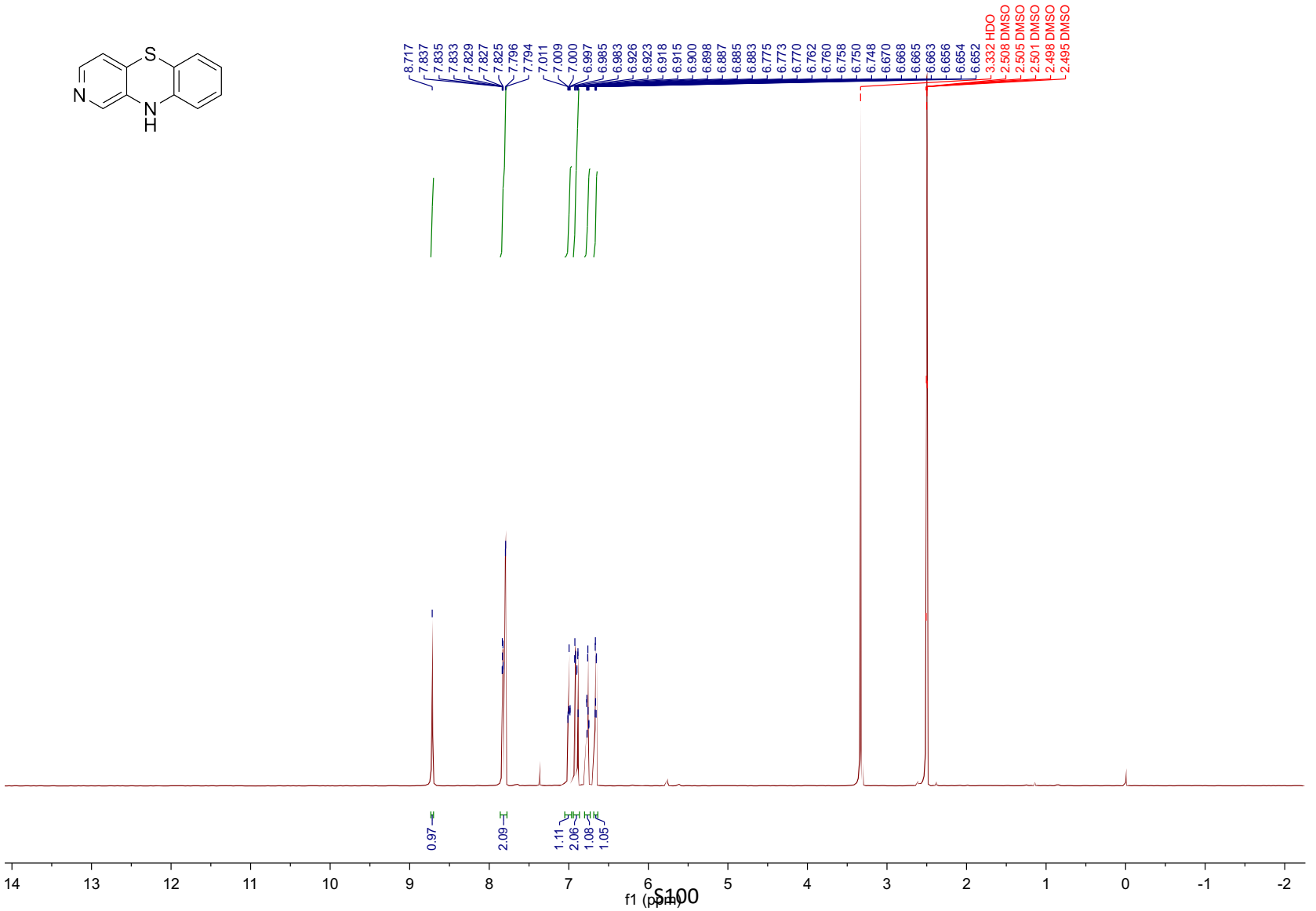
[1]H-NMR of 10-Acetyl-2-azaphenothiazine



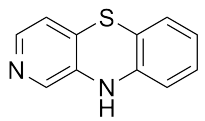
$^{13}$C-NMR of 10-Acetyl-2-azaphenothiazine



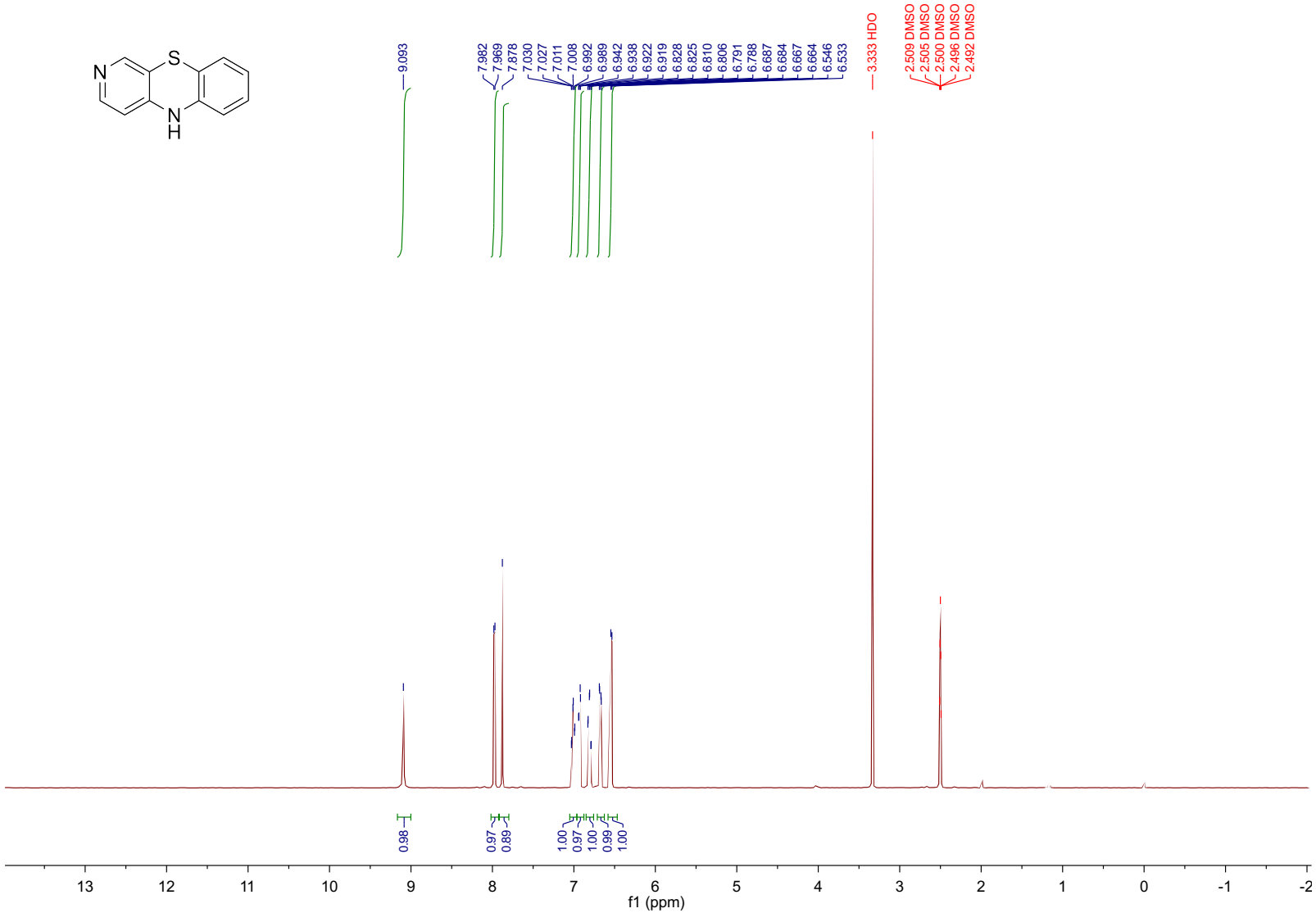
[1]H-NMR of 2-azaphenothiazine



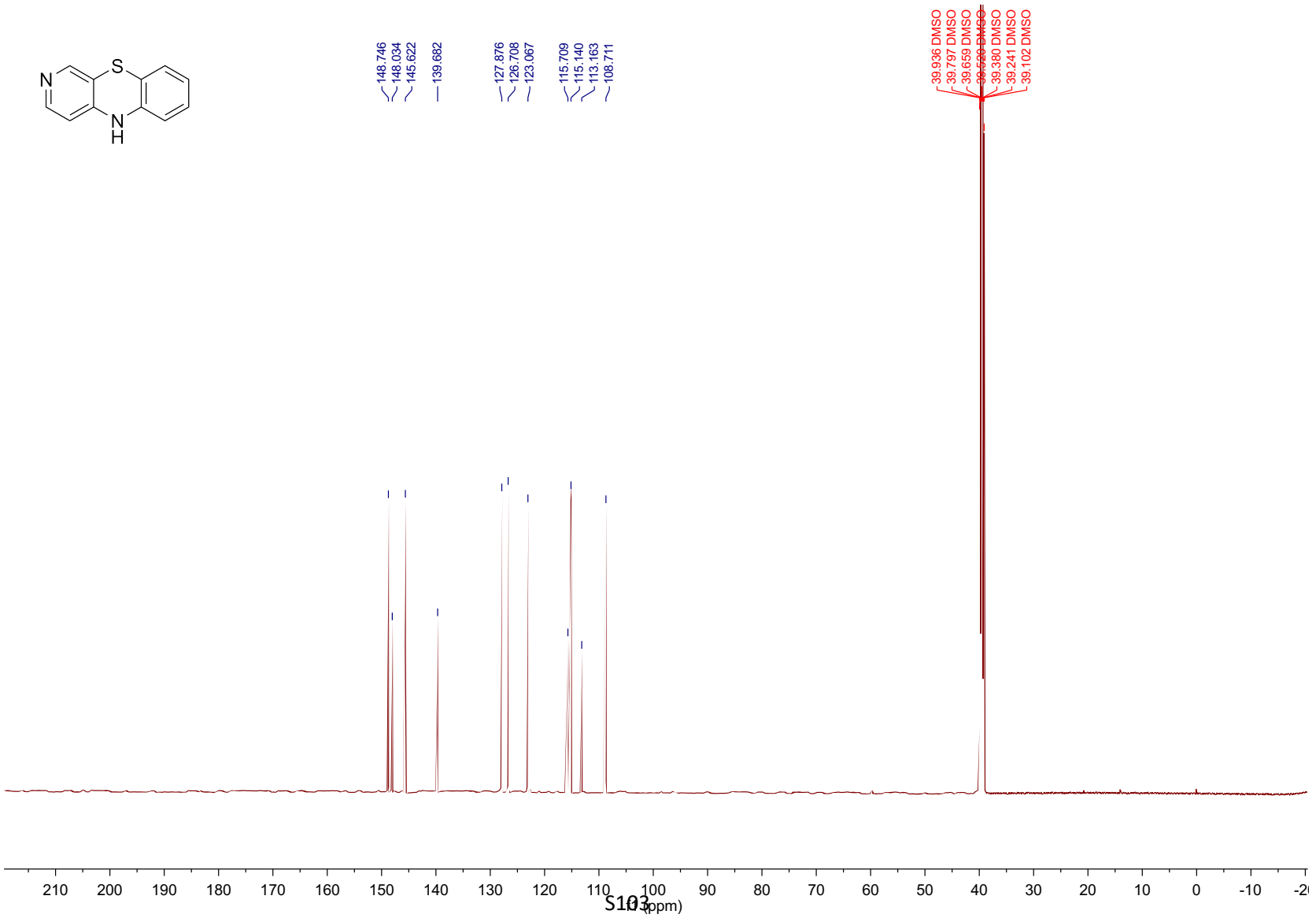
$^{13}$C-NMR of 2-azaphenothiazine



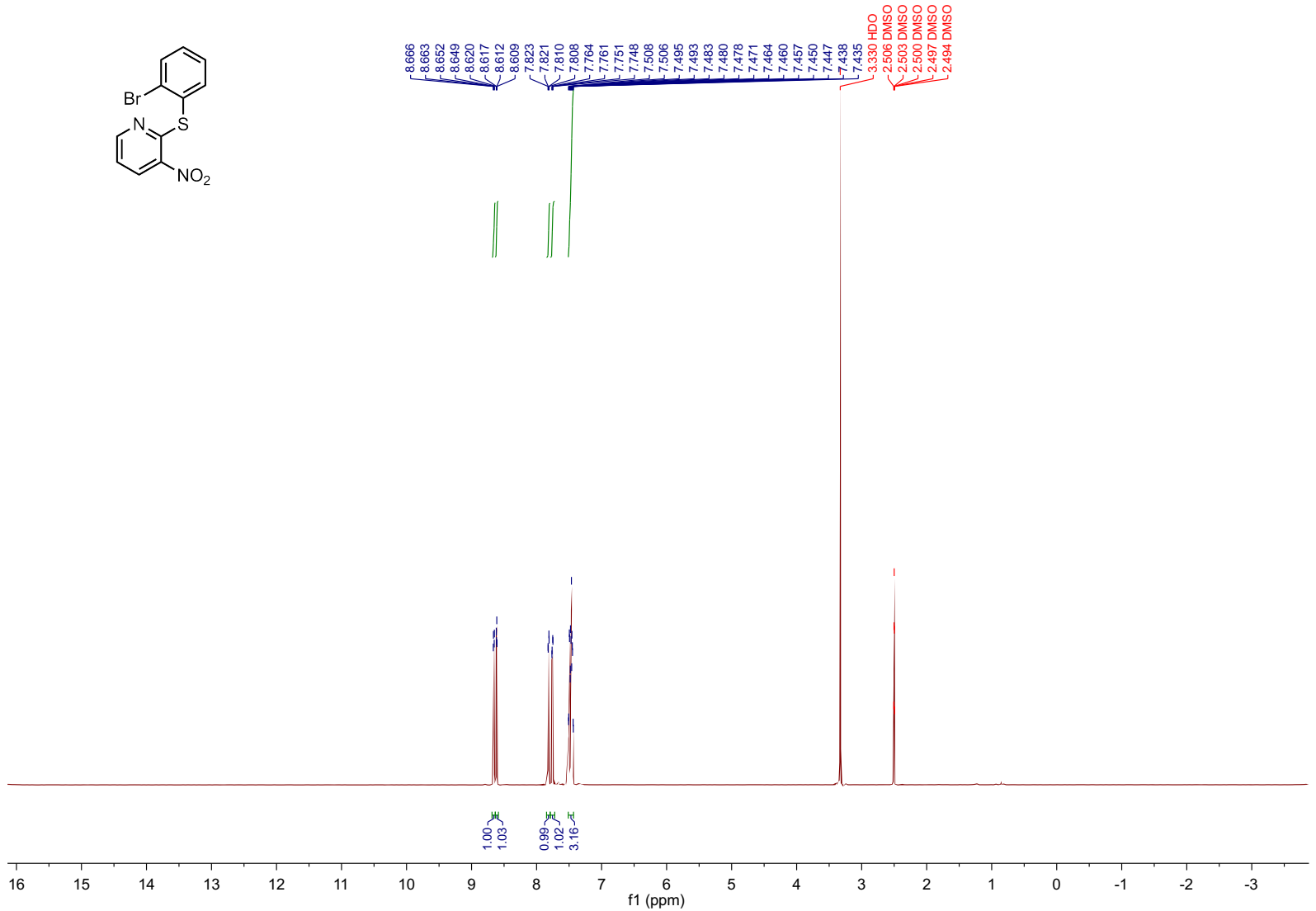
$^{1}$H-NMR of 3-azaphenothiazine



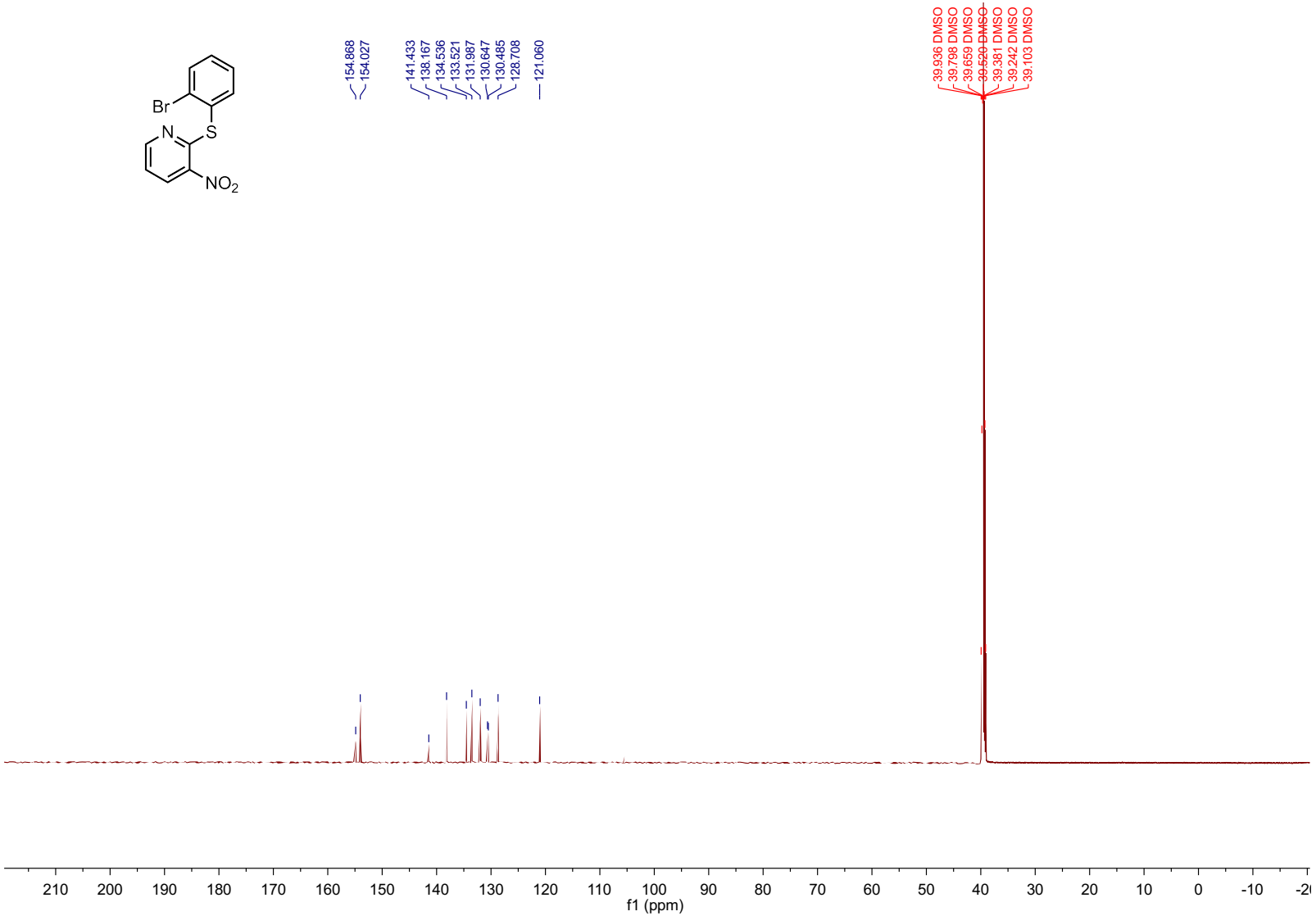
$^{13}$C-NMR of 3-azaphenothiazine



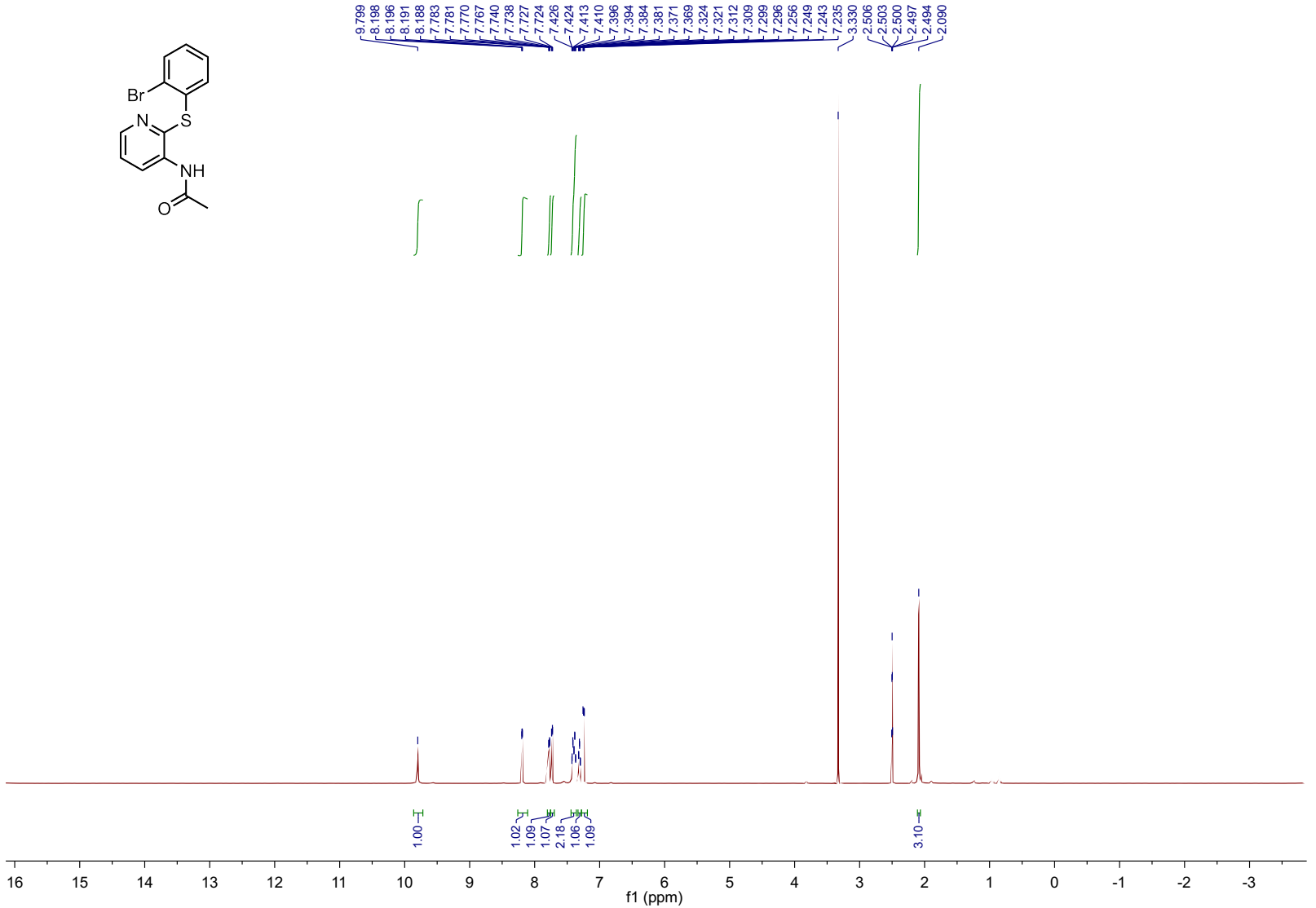
[1]H-NMR of 2'-((2-bromophenyl)thio)-3-nitropyridine.



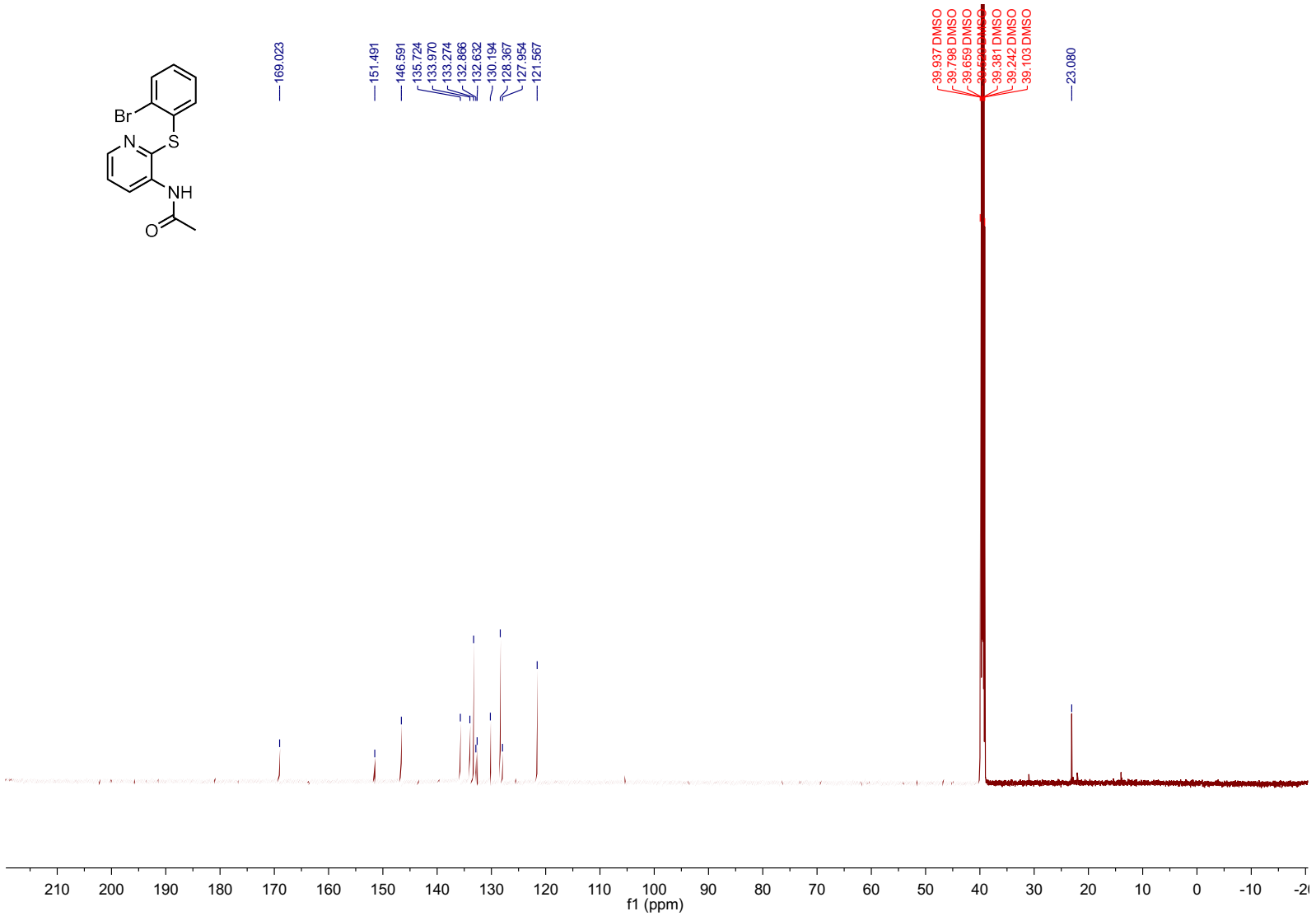
$^{13}$C-NMR of 2'-((2-bromophenyl)thio)-3-nitropyridine.



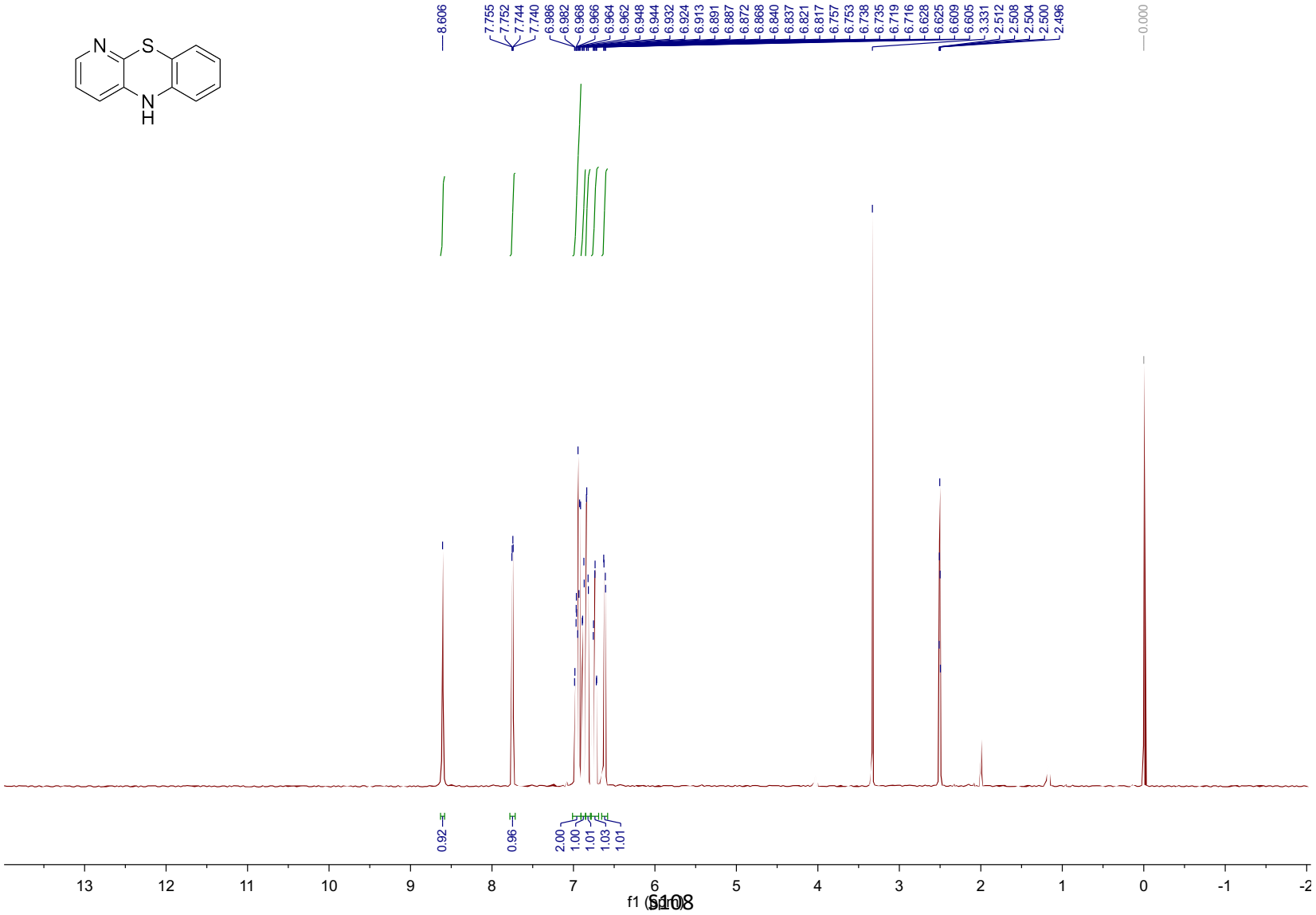
[1]H-NMR of *N*-acetyl-3-amino-2-(2'-bromophenylthio)pyridine



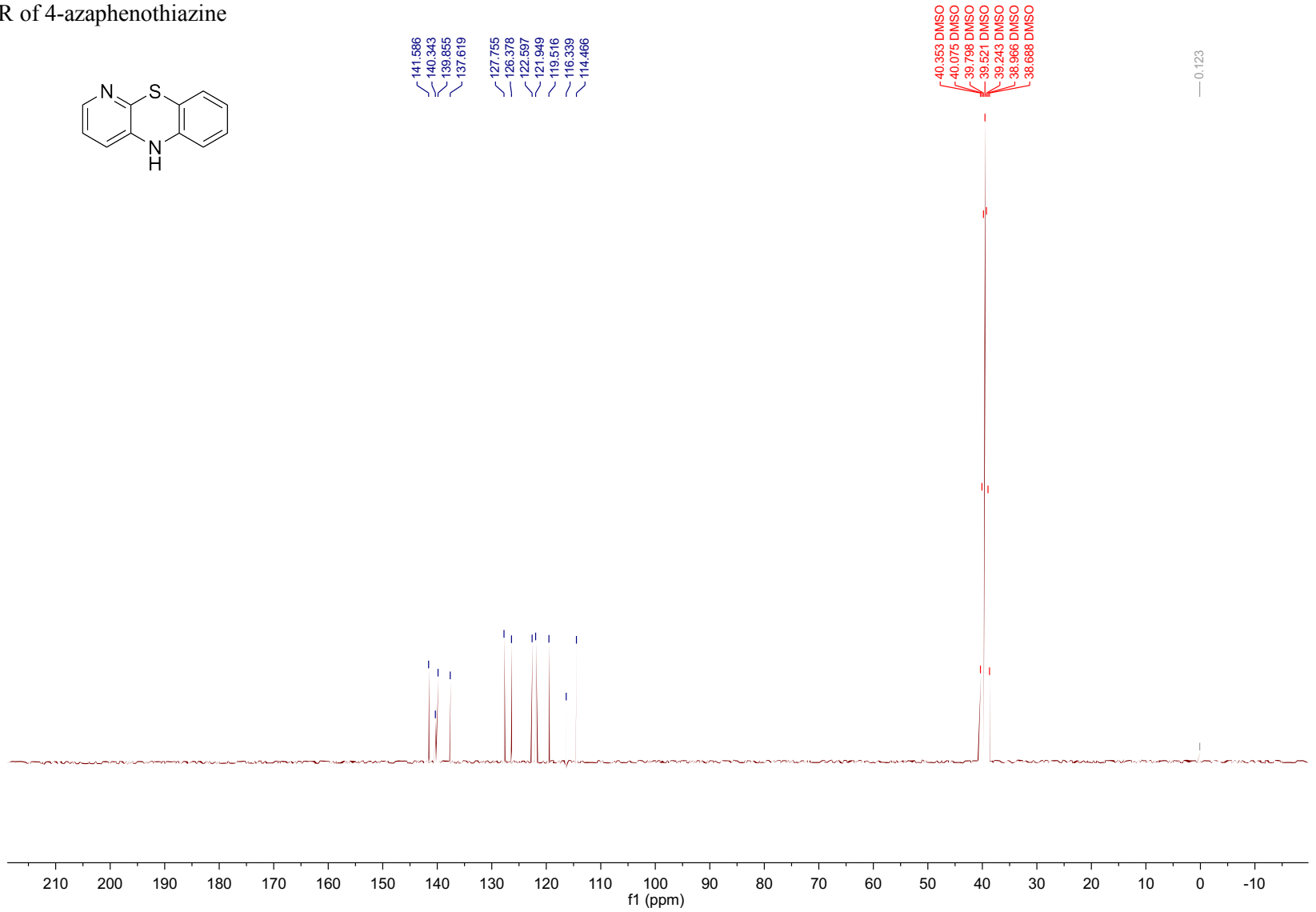
$^{13}$C-NMR of *N*-acetyl-3-amino-2-(2'-bromophenylthio)pyridine



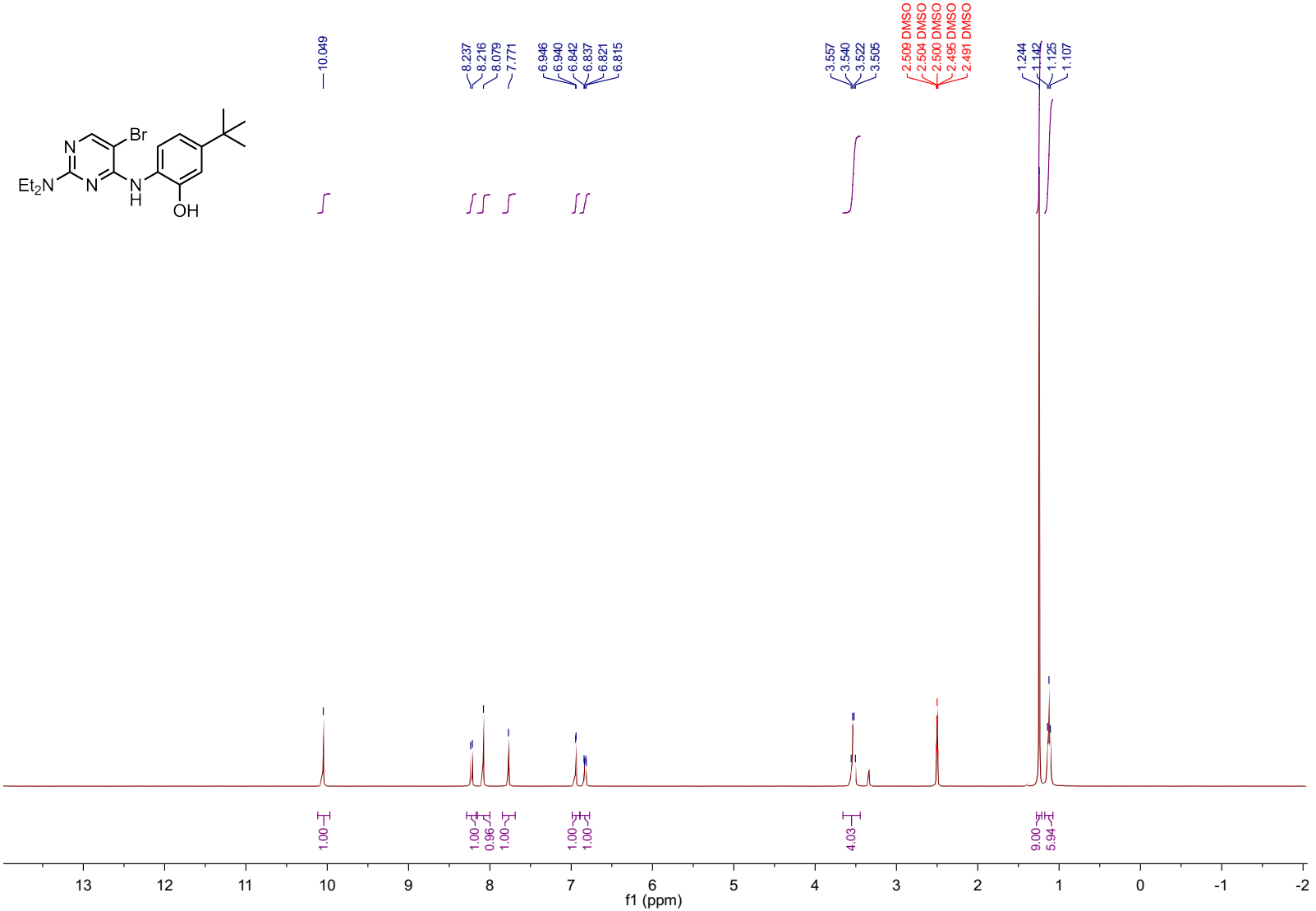
$^{1}$H-NMR of 4-azaphenothiazine



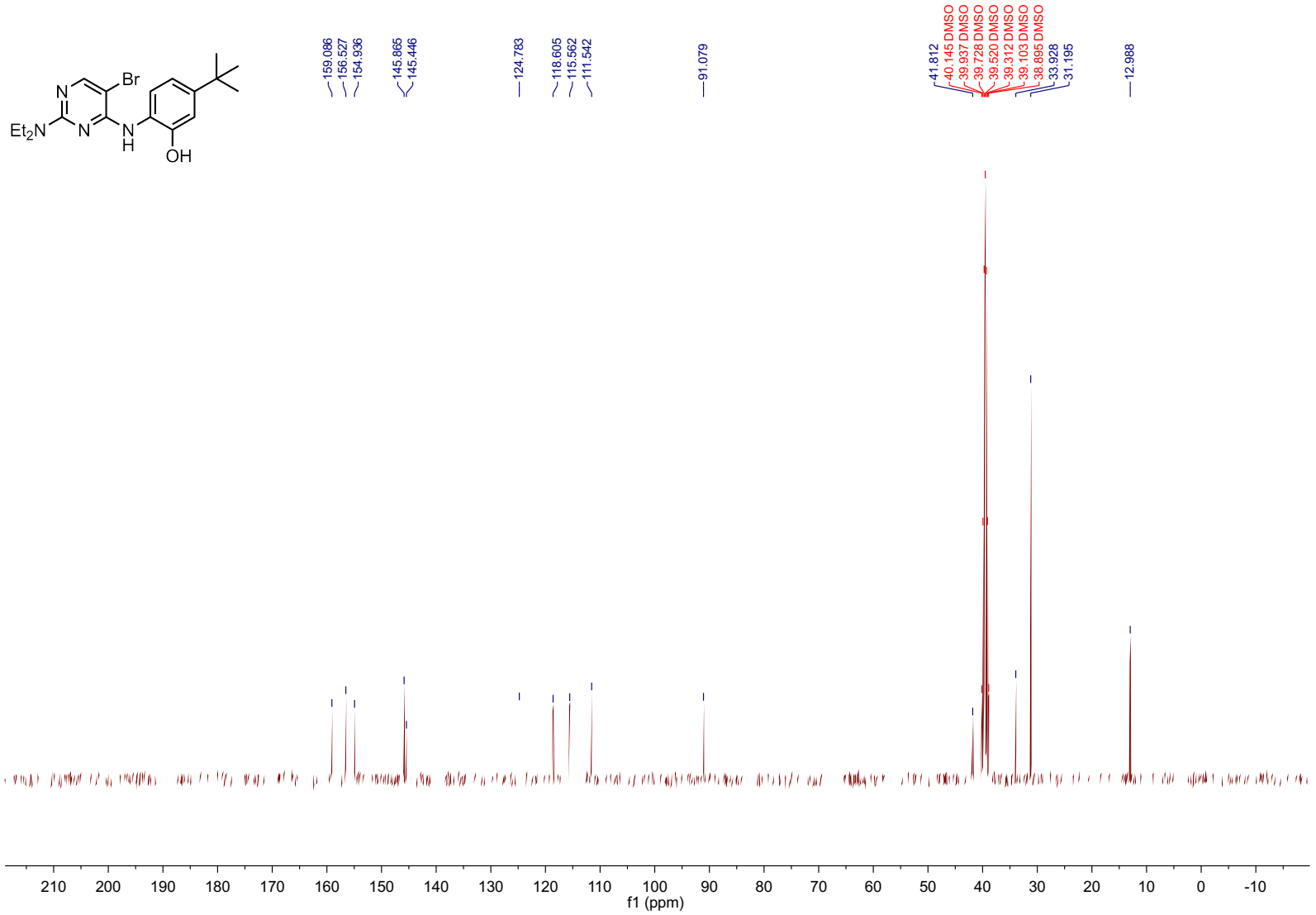
$^{13}$C-NMR of 4-azaphenothiazine



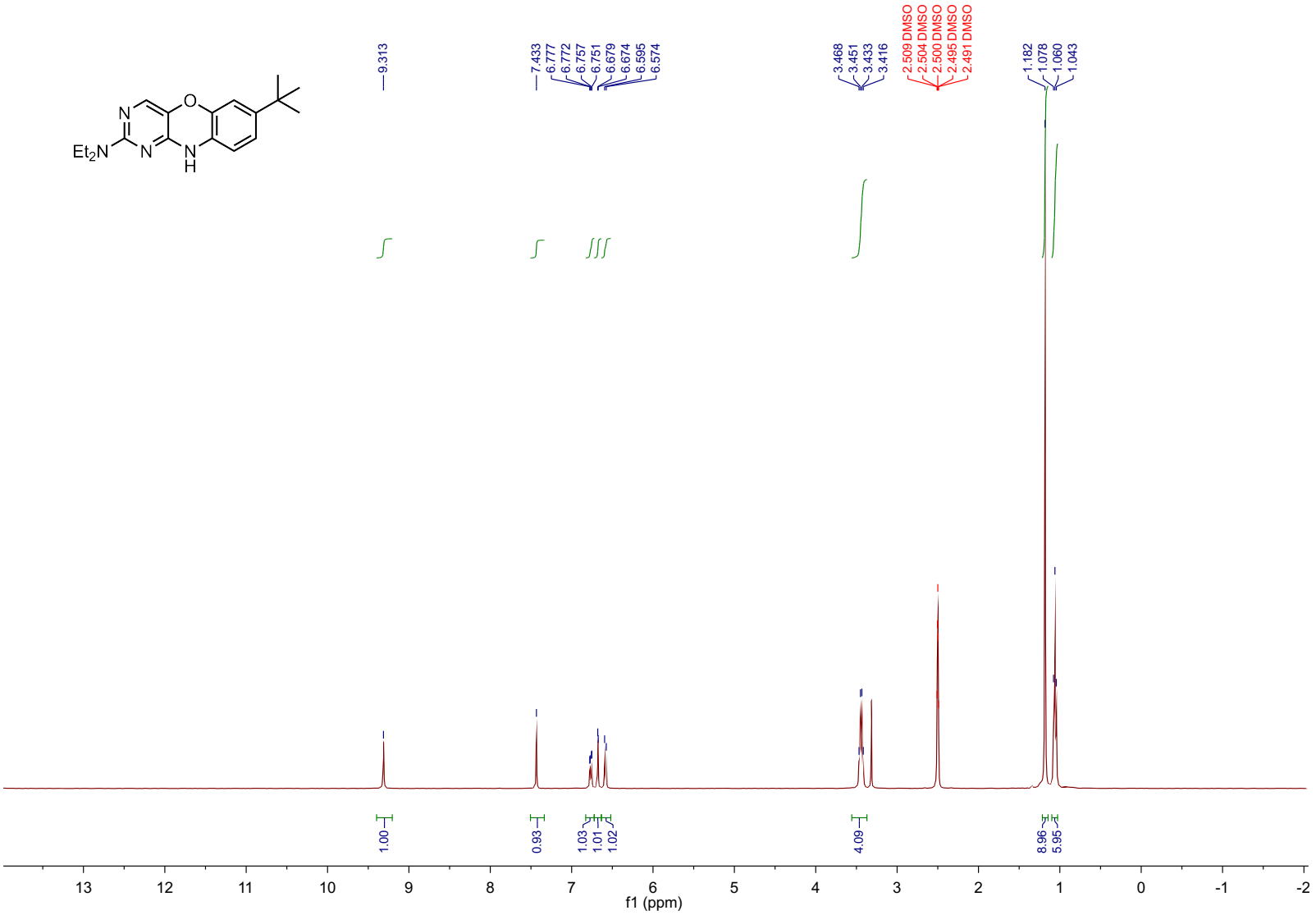
[1]H-NMR of 2-((5-bromo-2-(diethylamino)pyrimidin-4-yl)amino)-5-(*tert*-butyl)phenol



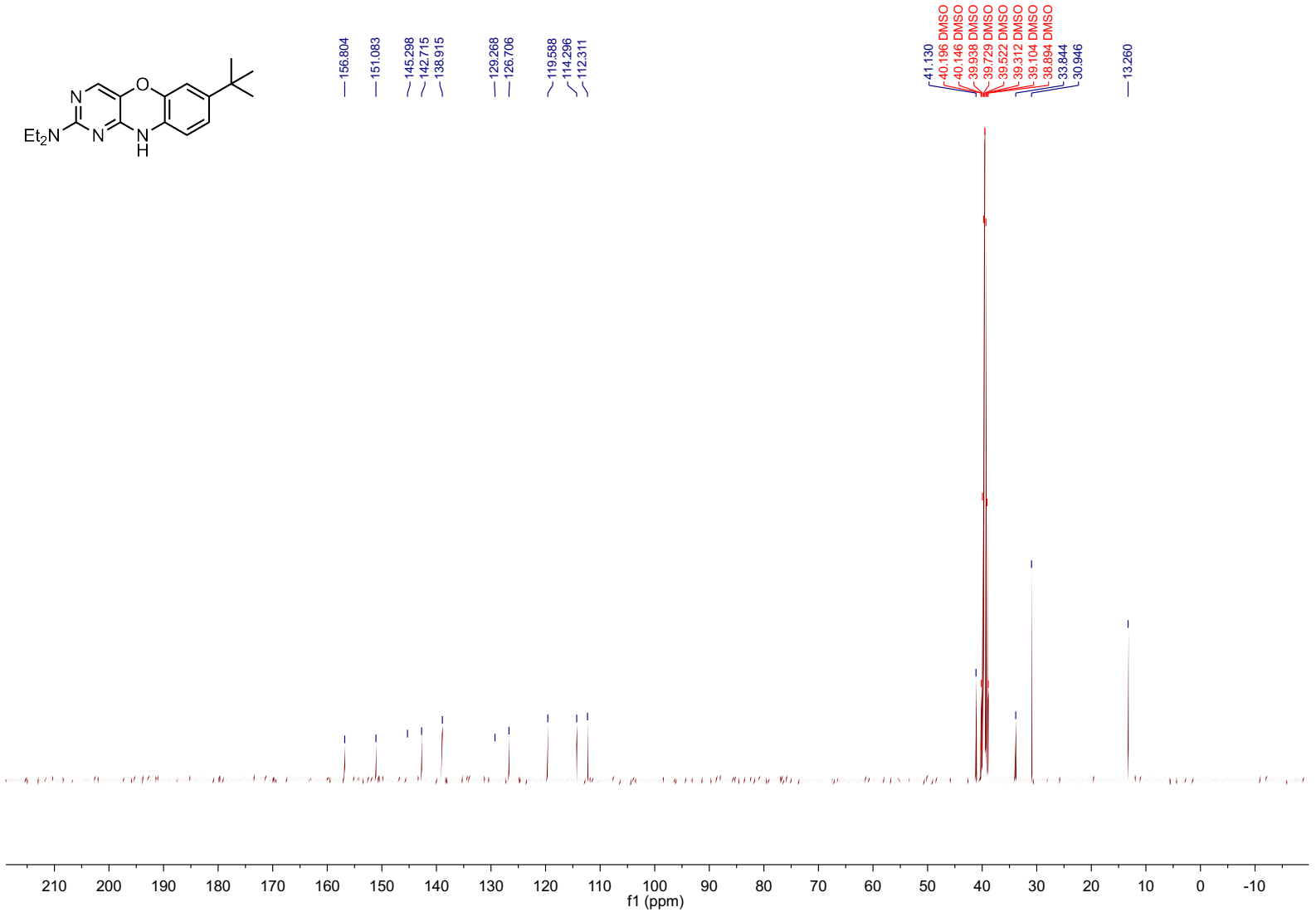
$^{13}$C-NMR of 2-((5-bromo-2-(diethylamino)pyrimidin-4-yl)amino)-5-(*tert*-butyl)phenol



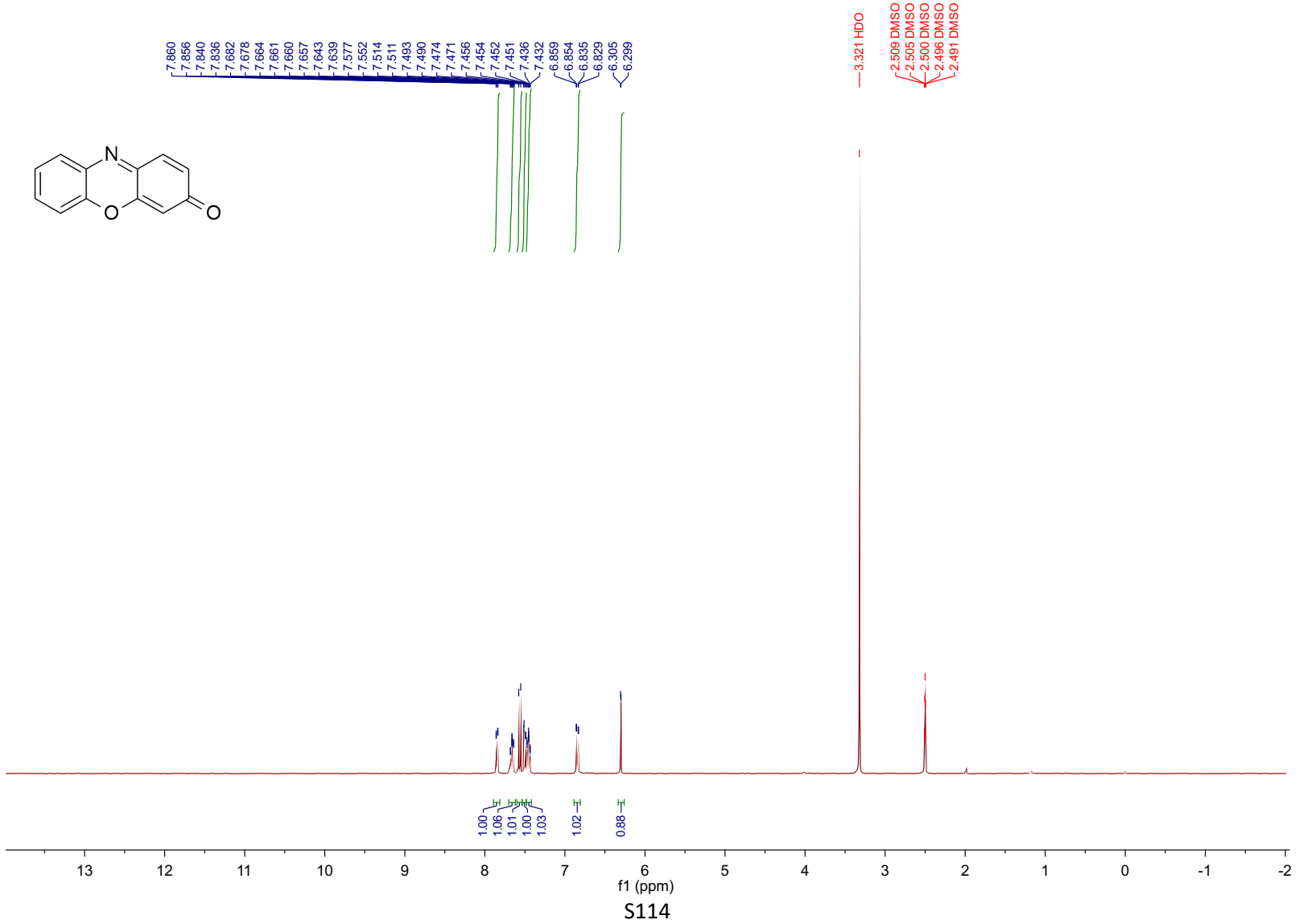
[1]H-NMR of 7-*tert*-Butyl-2-diethylamino-1,3-diazaphenoxazine



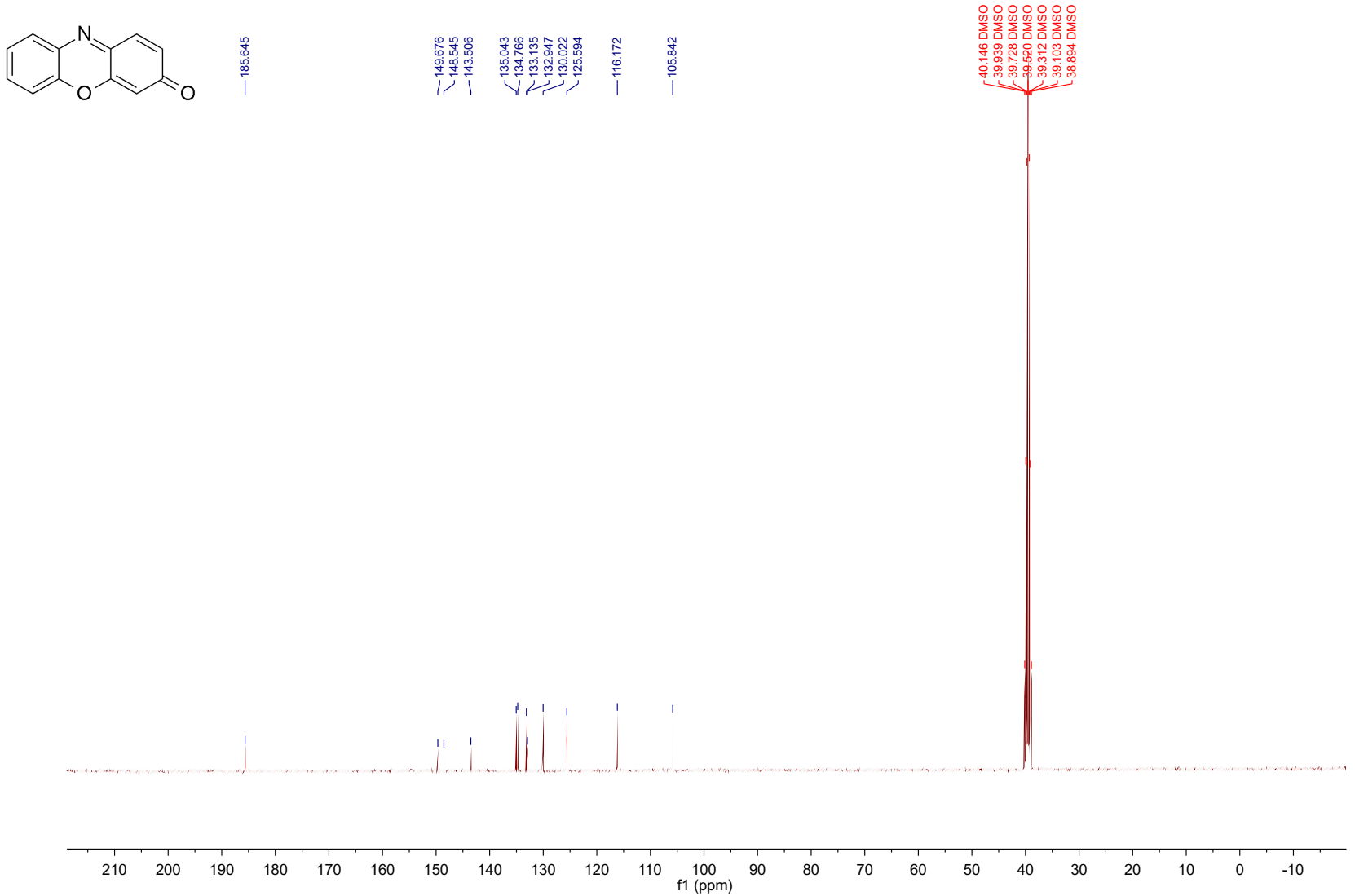
$^{13}$C-NMR of 7-*tert*-Butyl-2-diethylamino-1,3-diazaphenoxazine



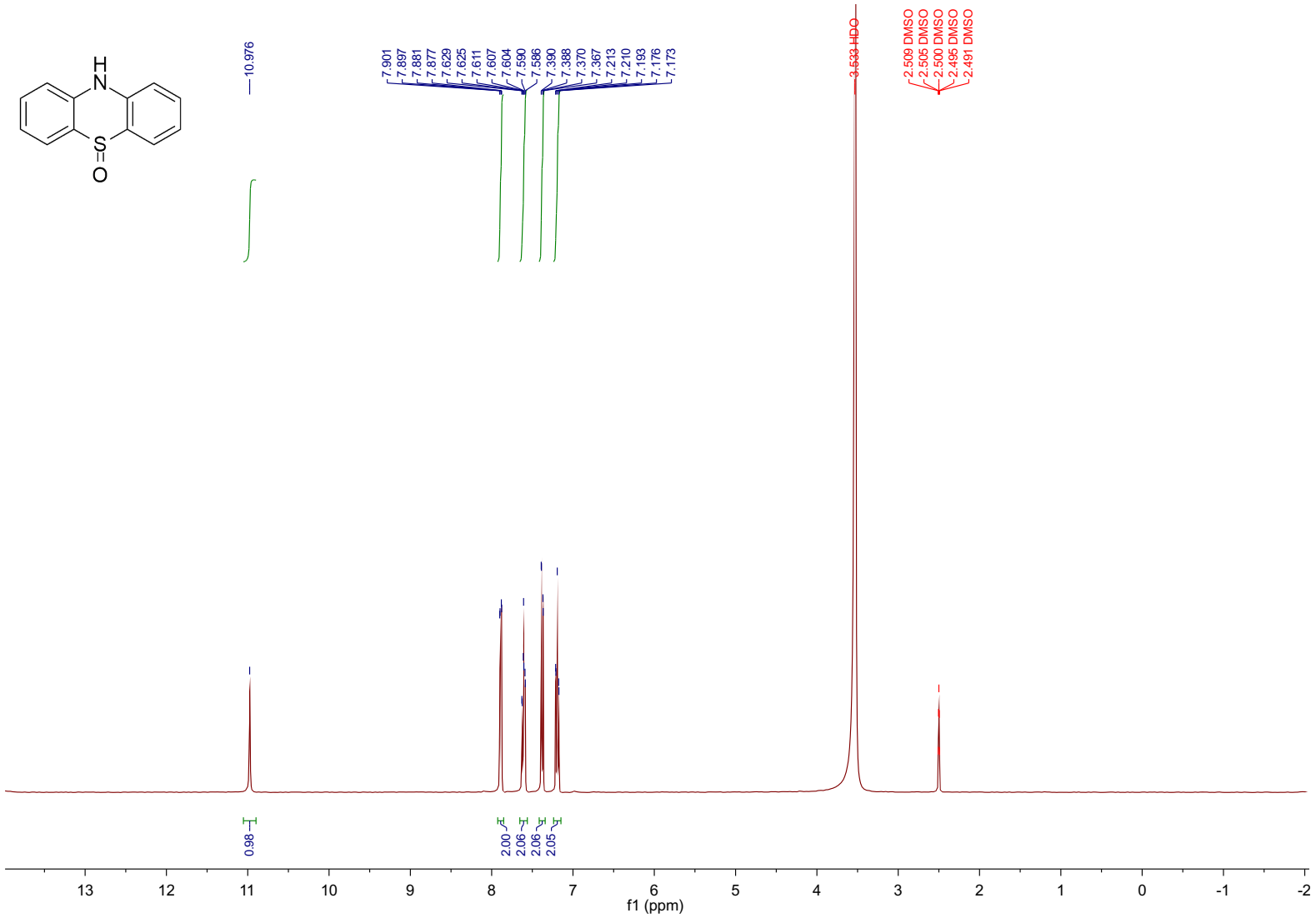
[1]H-NMR of 3*H*-phenoxazin-3-one



$^{13}$C-NMR of 3*H*-phenoxazin-3-one



[1]H-NMR of phenothiazine-5-oxide



## Notes and References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