

Controlling Rates and Reversibilities of Elimination Reactions of Hydroxybenzylammoniums by Tuning Dearomatization Energies

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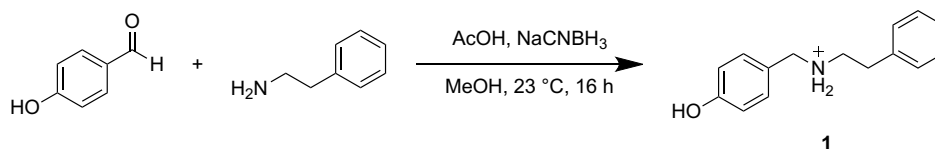
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General Experimental Information

Unless specifically mentioned, all solvents were purchased as ACS grade solvents and used without any further purification. Anhydrous solvents used were either freshly distilled or passed through activated alumina columns. Reagents were purchased at the highest commercial quality from Sigma-Aldrich, Fisher Scientific, Oakwood Chemical, or Combi-Blocks and were used without further purification, unless otherwise stated. Yields refer to isolated material, unless otherwise stated. Reactions were monitored by reverse-phase high performance liquid chromatography (HPLC), liquid chromatography/mass spectrometry (LC/MS), and/or thin layer chromatography (TLC). Analytical HPLC was carried out on a Agilent 1260 Infinity II HPLC system equipped with an autosampler and a UV detector using a Poroshell 120 2.7 μm C18 120 \AA column (Analytical: 2.7 μm , 4.6 \times 100 mm) with monitoring at $\lambda = 220$ and 254 nm and with a flow rate of 0.8 mL/min. TLC was performed using Millipore Sigma silica plates (60F-254), using short-wave UV light as the visualizing agent. NMR spectra were recorded on Bruker AV400, AV500, and NEO600 instruments and are calibrated using residual undeuterated solvent. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Flash column chromatography was performed on a Biotage Isolera One 3.0 autocolumn instrument. All silica chromatography unless specifically was carried out on the Biotage using KP-Sil high-performance columns repacked using the Silicycle silica (P60, particle size 40–63 μm , column sizes described in each experimental procedure). Preparative HPLC was performed on Agilent 1290 Infinity II system with an open bed sampler/fraction collector equipped with a UV detector using a Luna 5 μm C18 100A column (5 μm , 250 \times 21.2 mm). Electrospray ionization (ESI) mass spectra were obtained using an Agilent 6545 QTOF-ESI in tandem with a 1260 Infinity LC. Direct Analysis in Real Time (DART) mass spectra were obtained using Thermo Exactive Plus Orbitrap with IonSense ID-CUBE DART source. IR spectra were obtained using PerkinElmer Spectrum ONE FT-IR Spectrometer.

Experimental Procedures and Characterization Data

Compound 1



General Procedure A (reductive amination with phenethylamine):

To a solution of 4-hydroxybenzaldehyde (100 mg, 1 equiv, 819 μmol) in methanol (2 mL) was added acetic acid (246 mg, 234 μL , 5 equiv, 4.09 mmol) and 2-phenylethan-1-amine (149 mg, 154 μL , 1.5 equiv, 1.23 mmol). The reaction was stirred at 23 °C for one hour and sodium cyanoborohydride (154 mg, 3 equiv, 2.46 mmol) was added. The reaction was stirred for another 15 hours until LC/MS showed near full conversion. The crude reaction mixture was then purified on preparative HPLC (C18, 5-40% MeCN gradient against water with 0.1% TFA additive over 15 minutes) to afford **1** (191 mg, 68% yield) as its TFA salt.

Physical State: White solid

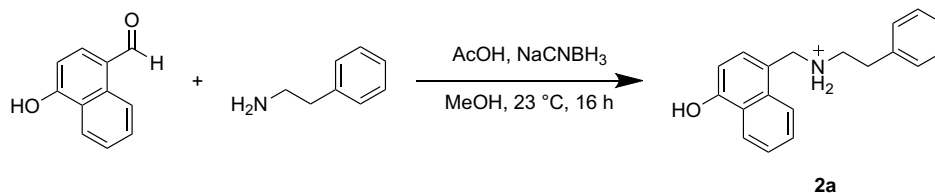
¹H NMR (500 MHz, CD₃CN): δ 8.45 (br s, 2H), 7.36 – 7.19 (m, 7H), 6.86 – 6.79 (m, 2H), 4.05 (s, 2H), 3.16 (s, 3H), 3.01 – 2.93 (m, 2H).

¹³C NMR (126 MHz, CD₃CN): δ 159.00, 137.82, 132.63, 129.74, 129.71, 127.96, 122.97, 116.52, 51.54, 48.96, 32.64.

HRMS (ESI/Q-TOF): [M+H]⁺ calculated for C₁₅H₁₈NO⁺ 228.1383, found 228.1395.

IR (Film): 3188, 2003, 1444, 1268, 1145 cm⁻¹.

Compound 2a



Following General Procedure A using 4-hydroxy-1-naphthaldehyde (50 mg, 290 μmol) afforded **2a** (65 mg, 166 μmol , 57% yield).

Physical State: White solid

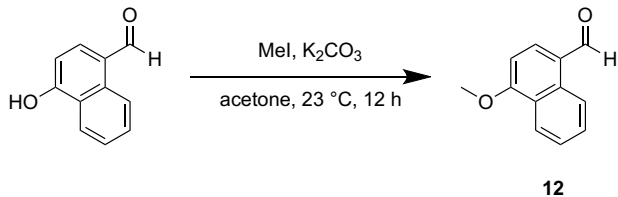
¹H NMR (500 MHz, CD₃CN): δ 8.47 (br s, 2H), 8.26 (dd, $J = 8.3, 1.4$ Hz, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.60 (ddd, $J = 8.4, 6.8, 1.4$ Hz, 1H), 7.53 (ddd, $J = 8.0, 6.7, 1.1$ Hz, 1H), 7.47 (d, $J = 7.8$ Hz, 1H), 7.36 – 7.28 (m, 2H), 7.29 – 7.17 (m, 3H), 6.91 (d, $J = 7.7$ Hz, 1H), 4.55 (s, 2H), 3.32 – 3.23 (m, 2H), 3.03 – 2.95 (m, 2H).

¹³C NMR (126 MHz, CD₃CN): δ 155.57, 137.80, 133.61, 131.77, 129.74, 129.70, 128.21, 127.97, 126.15, 125.92, 123.94, 123.75, 118.86, 108.44, 49.46, 48.93, 32.61.

HRMS (ESI/Q-TOF): $[M+H]^+$ calculated for C₁₉H₂₀NO⁺ 278.1539, found 278.1526.

IR (Film): 3031, 2818, 1671, 1584, 1521, 1386, 1357, 1285, 1058, 1020 cm⁻¹.

Compound 12



To a solution of 4-hydroxy-1-naphthaldehyde (100 mg, 1 equiv, 581 μ mol) in acetone (5 mL) was added potassium carbonate (161 mg, 2 equiv, 1.16 mmol) and iodomethane (124 mg, 55 μ L, 1.5 equiv, 581 μ mol). The reaction was stirred at 23 °C for 12 hours. The solids were filtered off, and the solution was concentrated under reduced pressure directly on to silica gel (5 g). The crude product was then purified by flash column chromatography (25 g silica gel, 0-40% EtOAc gradient against hexanes over 10 column volumes) to afford **12** (88 mg, 81% yield).

Physical State: Orange solid

TLC (UV): R_f 0.33 (1:4 EtOAc:Hexanes)

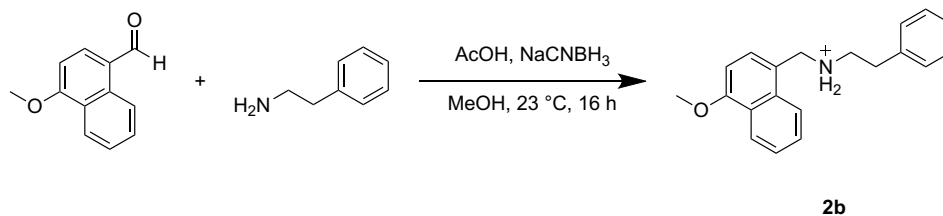
¹H NMR (400 MHz, CDCl₃): δ 10.21 (s, 1H), 9.35 – 9.28 (m, 1H), 8.38 – 8.30 (m, 1H), 7.93 (d, J = 8.1 Hz, 1H), 7.75 – 7.68 (m, 1H), 7.58 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 6.93 (d, J = 8.0 Hz, 1H), 4.10 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 192.51, 161.11, 139.86, 132.16, 129.78, 126.65, 125.78, 125.30, 125.12, 122.61, 103.16, 56.24.

HRMS (DART): [M+H]⁺ calculated for C₁₂H₁₁O₂⁺ 187.0681, found 187.0597.

IR (Film): 2969, 1737, 1572, 1512, 1429, 1365, 1217, 1094, 1059, 1028 cm⁻¹.

Compound 2b



Following General Procedure A using **12** (50 mg, 269 μ mol) afforded **2b** (57 mg, 52% yield).

Physical State: White solid

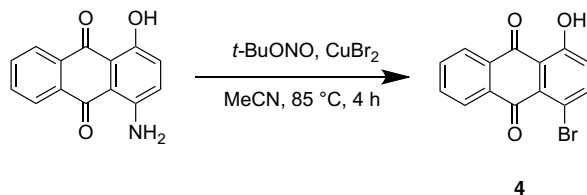
¹H NMR (500 MHz, CD₃CN): δ 8.66 (br s, 2H), 8.29 (ddd, J = 8.4, 1.6, 0.7 Hz, 1H), 8.04 (dt, J = 8.6, 1.0 Hz, 1H), 7.66 – 7.53 (m, 3H), 7.35 – 7.29 (m, 2H), 7.29 – 7.18 (m, 3H), 6.93 (d, J = 8.0 Hz, 1H), 4.56 (s, 2H), 4.00 (s, 3H), 3.29 (dd, J = 9.9, 6.5 Hz, 2H), 3.00 – 2.93 (m, 2H).

¹³C NMR (126 MHz, CD₃CN): δ 157.63, 137.85, 133.22, 131.55, 129.74, 129.71, 128.35, 127.96, 126.64, 126.56, 124.04, 123.42, 119.92, 104.44, 56.40, 49.56, 48.82, 32.61.

HRMS (ESI/Q-TOF): [M+H]⁺ calculated for C₂₀H₂₄NO⁺ 294.1952, found 294.1936.

IR (Film): 3031, 1670, 1584, 1517, 1462, 1417, 1394, 1278, 1231, 1095, 1025 cm⁻¹.

Compound 4



To a solution of 1-amino-4-hydroxyanthraquinone (3.000 g, 1 equiv, 12.54 mmol) in MeCN (50 mL) was added copper (II) bromide (5.602 g, 2 equiv, 25.08 mmol). The mixture was heated to 85 °C, and *tert*-Butyl nitrite (2.586 g, 2.99 mL, 2 equiv, 25.08 mmol) in 20 mL MeCN was added slowly over 10 minutes. The reaction was stirred at 85 °C for 4 hours. The reaction content was then poured into 100 mL 1 M HCl and extracted with DCM (3 x 100 mL). The combined organic layers were dried with anhydrous MgSO₄ and concentrated under reduced pressure directly on to silica gel (10 g). The crude product was then purified by flash column chromatography (100 g silica gel, 0-40% EtOAc gradient against hexanes over 15 column volumes) to afford **4** (2.336 g, 7.71 mmol, 62% yield).

Physical State: Orange solid

TLC (UV): R_f 0.73 (1:2 EtOAc:Hexanes)

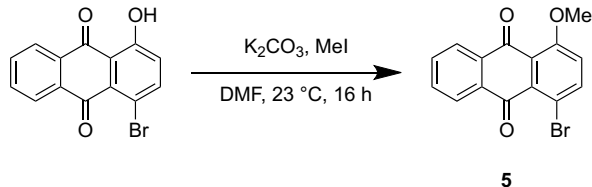
¹H NMR (600 MHz, CDCl₃): δ 13.30 (s, 1H), 8.33 – 8.28 (m, 2H), 7.90 (d, *J* = 9.0 Hz, 1H), 7.83 (dtd, *J* = 20.1, 7.4, 1.5 Hz, 2H), 7.17 (d, *J* = 9.0 Hz, 1H).

¹³C NMR (151 MHz, CDCl₃): δ 188.30, 181.43, 163.18, 144.08, 135.31, 134.28, 134.21, 132.25, 130.20, 127.98, 126.77, 125.37, 117.92, 113.34.

HRMS (DART): [M-H]⁻ calculated for C₁₄H₆BrO₃⁻ 300.9506, found 300.9502.

IR (Film): 2969, 2354, 1738, 1571, 1435, 1365, 1216, 1093, 1027 cm⁻¹.

Compound 5



To a solution of 1-bromo-4-hydroxyanthraquinone **4** (1.180 g, 1 equiv, 3.893 mmol) in DMF (20 mL) was added potassium carbonate (1.614 g, 3 equiv, 11.68 mmol) and iodomethane (2.763 g, 5 equiv, 19.46 mmol). The reaction was stirred at 23 °C for 16 hours. The reaction content was poured into 100 mL 1 M HCl and extracted with EtOAc (3 x 50 mL). The combined organic layers were dried with anhydrous $MgSO_4$ and concentrated under reduced pressure directly on to silica gel (10 g). The crude product was then purified by flash column chromatography (50 g silica gel, 0-50% EtOAc gradient against hexanes over 15 column volumes) to afford **5** (895 mg, 2.82 mmol, 73% yield).

Physical State: Yellow solid

TLC (UV): R_f 0.33 (1:2 EtOAc:Hexanes)

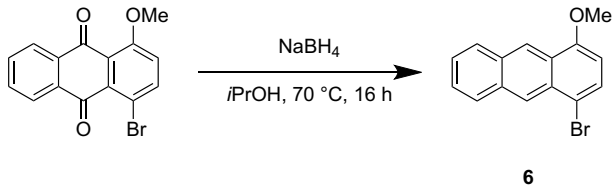
1H NMR (500 MHz, $CDCl_3$): δ 8.20 – 8.14 (m, 2H), 7.94 (d, $J = 9.0$ Hz, 1H), 7.78 – 7.70 (m, 2H), 7.18 (d, $J = 9.1$ Hz, 1H), 4.04 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 183.00, 182.38, 160.04, 141.94, 134.38, 134.10, 133.68, 133.50, 132.96, 126.89, 126.72, 124.21, 118.61, 112.82, 56.99.

HRMS (DART): $[M+H]^+$ calculated for $C_{15}H_{10}BrO_3^+$ 316.9808, found 316.9804.

IR (Film): 3019, 2363, 1712, 1365, 1226, 1092 cm^{-1} .

Compound 6



A solution of 1-bromo-4-methoxyanthracene-9,10-dione **5** (1.000 g, 1 equiv, 3.153 mmol) was dissolved in isopropanol (30 mL) and cooled to 0 °C. Sodium borohydride (1.193 g, 10 equiv, 31.53 mmol) was added slowly. The reaction was stirred at 70 °C for 16 hours. The reaction content was poured into 100 mL 1 M HCl and extracted with DCM (3 x 50 mL). The combined organic layers were dried with anhydrous MgSO₄ and concentrated under reduced pressure directly on to silica gel (5 g). The crude product was then purified by flash column chromatography (25 g silica gel, 1% DCM isocratic against hexanes) to afford **6** (421 mg, 1.47 mmol, 47% yield).

Physical State: Light yellow solid

TLC (UV): R_f 0.56 (1:9 EtOAc:Hexanes)

¹H NMR (500 MHz, CDCl₃): δ 8.87 (s, 1H), 8.73 (s, 1H), 8.07 (t, *J* = 9.1 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.59 – 7.47 (m, 2H), 6.60 (d, *J* = 7.9 Hz, 1H), 4.07 (s, 3H).

¹³C NMR (126 MHz, CDCl₃): δ 155.56, 132.63, 131.57, 130.53, 128.93, 128.65, 128.53, 126.50, 126.13, 126.07, 125.78, 122.02, 113.48, 102.20, 55.89.

HRMS (DART): [M+H]⁺ calculated for C₁₅H₁₂BrO⁺ 287.0066, found 287.0071.

IR (Film): 3011, 2970, 1426, 2158, 2028, 1738, 1435, 1365, 1227, 1216, 1092 cm⁻¹.

Compound 7



1-bromo-4-methoxyanthracene **6** (60.0 mg, 1 equiv, 209 μmol) was dissolved in anhydrous DCM (5 mL) and cooled to 0 °C under argon. Boron tribromide (209 mg, 836 μL , 1 molar, 4 equiv, 836 μmol) was added slowly over 5 minutes. The reaction was stirred at 23 °C for 16 hours. The reaction content was poured into 20 mL 1 M HCl and extracted with DCM (3 x 25 mL). The combined organic layers were dried with anhydrous MgSO₄ and concentrated under reduced pressure directly on to silica gel (5 g). The crude product was then purified by flash column chromatography (25 g silica gel, 0-30% EtOAc gradient against hexanes over 15 column volumes) to afford **7** (37.3 mg, 137 μmol , 65% yield).

Physical State: Brown solid

TLC (UV): R_f 0.37 (1:2 EtOAc:Hexanes)

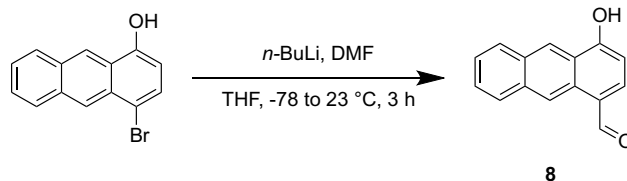
¹H NMR (500 MHz, CDCl₃): δ 8.81 (s, 1H), 8.75 (s, 1H), 8.08 (t, $J = 7.9$ Hz, 2H), 7.60 (d, $J = 7.7$ Hz, 1H), 7.53 (tt, $J = 7.7, 5.5$ Hz, 2H), 6.65 (d, $J = 7.8$ Hz, 1H), 5.39 (s, 1H).

¹³C NMR (126 MHz, CDCl₃): δ 151.52, 132.74, 131.57, 130.69, 128.75, 128.62, 128.58, 126.63, 126.30, 124.72, 121.85, 106.70.

HRMS (DART): [M-H]⁻ calculated for C₁₄H₉BrO⁻ 270.9764, found 270.9757.

IR (Film): 3003, 2969, 2364, 1737, 1434m 1365, 1228, 1226, 1092 cm⁻¹.

Compound 8



4-bromoanthracen-1-ol **7** (35.0 mg, 1 equiv, 128 μmol) was dissolved in anhydrous THF (5 mL) and cooled to $-78\text{ }^{\circ}\text{C}$ under argon. *n*-butyllithium (20.5 mg, 320 μL , 1.8 molar in hexanes, 2.5 equiv, 178 μmol) was added slowly over 5 minutes. The reaction was stirred at $-78\text{ }^{\circ}\text{C}$ for one hour. Then, anhydrous DMF (46.8 mg, 49.6 μL , 5 equiv, 641 μmol) was added and this was allowed to stir at $-78\text{ }^{\circ}\text{C}$ for one hour and at $23\text{ }^{\circ}\text{C}$ for another hour. The reaction content was poured into 10 mL saturated NH_4Cl solution and extracted with DCM (3 x 25 mL). The combined organic layers were dried with anhydrous MgSO_4 and concentrated under reduced pressure directly on to silica gel (1 g). The crude product was then purified by flash column chromatography (10 g silica gel, 0-40% EtOAc gradient against hexanes over 20 column volumes) to afford **8** (15.3 mg, 68.8 μmol , 54% yield).

Physical State: Yellow solid

TLC (UV): R_f 0.24 (1:2 EtOAc:Hexanes)

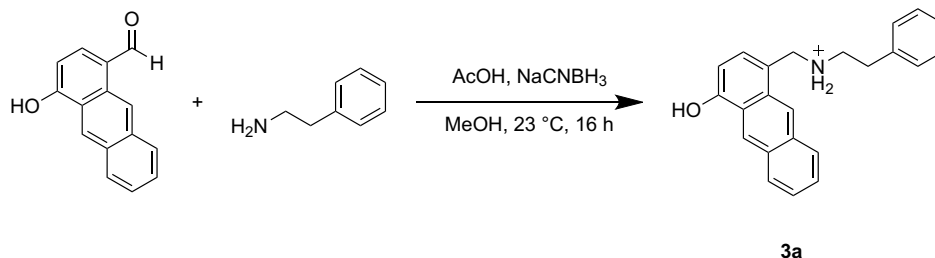
^1H NMR (500 MHz, Acetone): δ 10.59 (s, 1H), 10.19 (s, 1H), 10.01 (s, 1H), 9.00 (s, 1H), 8.22 – 8.12 (m, 2H), 8.04 (d, $J = 7.7$ Hz, 1H), 7.60 (dddd, $J = 17.9, 8.0, 6.6, 1.4$ Hz, 2H), 7.08 (d, $J = 7.7$ Hz, 1H).

^{13}C NMR (126 MHz, Acetone): δ 192.63, 160.83, 143.41, 134.73, 132.15, 130.11, 129.70, 129.62, 127.84, 127.10, 125.49, 125.17, 125.06, 123.08, 106.21.

HRMS (DART): $[\text{M}-\text{H}]^-$ calculated for $\text{C}_{15}\text{H}_9\text{O}_2^-$ 221.0608, found 221.0601.

IR (Film): 3454, 3017, 2970, 2513, 2158, 1977, 1736, 1435, 1366, 1228, 1216, 1092 cm^{-1} .

Compound 3a



Following General Procedure A using 4-hydroxyanthracene-1-carbaldehyde **8** (50 mg, 225 μmol) afforded **3a** (23 mg, 52.8 μmol , 24% yield).

Physical State: Yellow solid

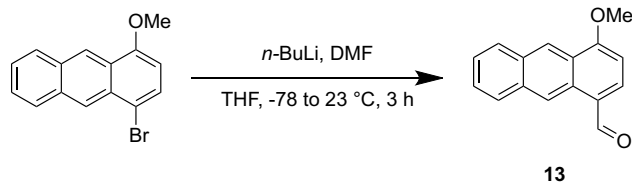
^1H NMR (500 MHz, CD_3CN): δ 8.90 (s, 1H), 8.65 (s, 1H), 8.35 (br s, 2H), 8.15 – 8.06 (m, 2H), 7.62 – 7.52 (m, 2H), 7.50 (d, $J = 7.5$ Hz, 1H), 7.32 (dd, $J = 8.5, 6.4$ Hz, 2H), 7.28 – 7.20 (m, 3H), 6.85 (d, $J = 7.4$ Hz, 1H), 4.69 (s, 2H), 3.34 (t, $J = 8.0$ Hz, 2H), 3.05 – 2.98 (m, 2H).

^{13}C NMR (126 MHz, CD_3CN): δ 155.69, 137.75, 133.04, 131.91, 131.81, 131.35, 129.75, 129.71, 129.40, 129.03, 127.99, 127.42, 126.80, 125.40, 123.02, 122.79, 118.87, 105.82, 49.63, 49.57, 32.61.

HRMS (ESI/Q-TOF): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{23}\text{H}_{22}\text{NO}^+$ 328.1696, found 328.1774.

IR (Film): 3459, 3014, 2969, 2360, 2335, 1738, 1433, 1365, 1227, 1216, 1140, 1092 cm^{-1} .

Compound 13



1-bromo-4-methoxyanthracene **6** (150 mg, 1 equiv, 522 μmol) was dissolved in anhydrous THF (5 mL) and cooled to $-78\text{ }^{\circ}\text{C}$ under argon. *n*-butyllithium (36.8 mg, 230 μL , 2.5 molar in hexanes, 1.1 equiv, 178 μmol) was added slowly over 5 minutes. The reaction was stirred at $-78\text{ }^{\circ}\text{C}$ for one hour. Then, anhydrous DMF (191 mg, 202 μL , 5 equiv, 2.61 mmol) was added and this was allowed to stir at $-78\text{ }^{\circ}\text{C}$ for one hour and at $23\text{ }^{\circ}\text{C}$ for another hour. The reaction content was poured into 10 mL saturated NH_4Cl solution and extracted with DCM (3 x 25 mL). The combined organic layers were dried with anhydrous MgSO_4 and concentrated under reduced pressure directly on to silica gel (1 g). The crude product was then purified by flash column chromatography (10 g silica gel, 0-20% EtOAc gradient against hexanes over 15 column volumes) to afford **13** (72.1 mg, 305 μmol , 58% yield).

Physical State: Green solid

TLC (UV): R_f 0.19 (1:9 EtOAc:Hexanes)

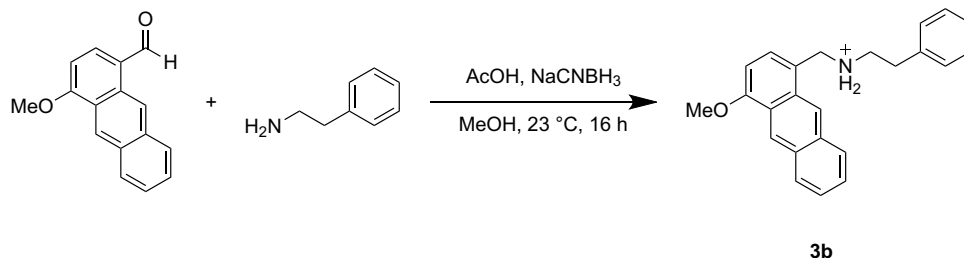
^1H NMR (500 MHz, CDCl_3): δ 10.21 (s, 1H), 9.97 (s, 1H), 8.91 (s, 1H), 8.16 – 8.03 (m, 2H), 7.94 (d, $J = 7.9$ Hz, 1H), 7.55 (dq, $J = 8.1, 6.6, 1.5$ Hz, 2H), 6.86 (d, $J = 7.9$ Hz, 1H), 4.19 (s, 3H).

^{13}C NMR (126 MHz, CDCl_3): δ 192.53, 161.48, 141.99, 133.85, 131.46, 129.10, 128.77, 128.66, 126.87, 126.33, 125.52, 124.81, 124.56, 122.00, 100.93, 56.25.

HRMS (DART): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{16}\text{H}_{13}\text{O}_2^+$ 237.0910, found 237.0906.

IR (Film): 3189, 2959, 2497, 2156, 2004, 1541, 1369, 1269, 1222, 1162, 1033, 1004 cm^{-1} .

Compound 3b



Following General Procedure A using 4-hydroxyanthracene-1-carbaldehyde **13** (70 mg, 296 μmol) afforded **3b** (135 mg, quant. yield).

Physical State: Yellow solid

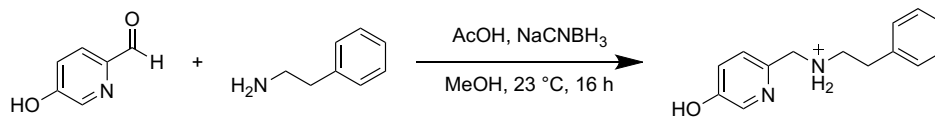
¹H NMR (500 MHz, CD₃CN): δ 8.90 (d, $J = 5.5$ Hz, 1H), 8.68 (d, $J = 5.8$ Hz, 1H), 8.15 – 8.07 (m, 2H), 7.57 (ddd, $J = 15.1, 7.7, 4.0$ Hz, 3H), 7.30 (q, $J = 6.9$ Hz, 2H), 7.26 – 7.18 (m, 3H), 6.84 (d, $J = 7.6$ Hz, 1H), 4.69 (d, $J = 5.7$ Hz, 2H), 4.08 (d, $J = 6.3$ Hz, 3H), 3.34 (dd, $J = 9.7, 6.6$ Hz, 2H), 3.02 (dd, $J = 9.6, 6.5$ Hz, 2H).

¹³C NMR (126 MHz, CD₃CN): δ 157.75, 137.95, 133.04, 131.98, 131.44, 131.03, 129.72, 129.70, 129.40, 129.06, 127.93, 127.46, 126.95, 125.79, 123.00, 122.67, 120.11, 102.14, 56.52, 49.57, 49.35, 32.66.

HRMS (ESI/Q-TOF): $[M+H]^+$ calculated for C₂₄H₂₄NO⁺ 342.1852, found 342.1869.

IR (Film): 3383, 3204, 3010, 2312, 1681, 1275, 1261, 1183, 1014 cm⁻¹.

Compound 9



9

Following General Procedure A using 5-hydroxypicolinaldehyde (50 mg, 406 μ mol) afforded **9** (11.4 mg, 8% yield).

Physical State: White solid

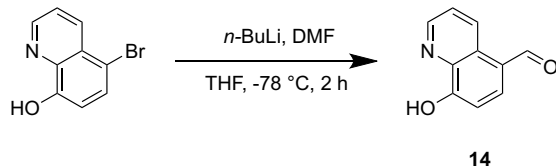
¹H NMR (500 MHz, CD₃CN): δ 8.19 – 8.14 (m, 1H), 7.42 – 7.22 (m, 7H), 4.26 (s, 3H), 3.31 (t, J = 7.8 Hz, 2H), 3.02 (t, J = 7.8 Hz, 2H).

¹³C NMR (126 MHz, CD₃CN): δ 155.22, 141.14, 137.39, 137.14, 129.86, 129.81, 128.23, 125.95, 125.91, 50.61, 49.75, 32.60.

HRMS (ESI/Q-TOF): [M+H]⁺ calculated for C₁₄H₁₇NO⁺ 229.1335, found 229.1354.

IR (Film): 3439, 3012, 2969, 2365, 2157, 1977, 1737, 1570, 1435, 1365, 1228, 1216, 1140, 1092, 1010 cm⁻¹.

Compound 14



A solution of 5-bromoquinolin-8-ol (300 mg, 1 equiv, 1.34 mmol) in anhydrous THF (20 mL) was cooled to $-78\text{ }^{\circ}\text{C}$ under argon. *n*-butyllithium (189 mg, 1.18 mL, 2.5 M in hexanes, 2.2 equiv, 2.95 mmol) was added slowly over 5 minutes. The reaction was allowed to stir at $-78\text{ }^{\circ}\text{C}$ for one hour. Then anhydrous DMF (294 mg, 311 μL , 3 equiv, 4.02 mmol) was added, and the reaction was allowed to stir at $-78\text{ }^{\circ}\text{C}$ for another hour. The reaction was then quenched with water (50 mL) and extracted with DCM (3 x 50 mL). The combined organic layers were dried with anhydrous MgSO_4 and concentrated under reduced pressure directly on to silica gel (5 g). The crude product was then purified by flash column chromatography (50 g silica gel, 10-80% EtOAc gradient against hexanes over 15 column volumes) to afford **14** (100 mg, 577 μmol , 43% yield).

Physical State: Pale yellow solid

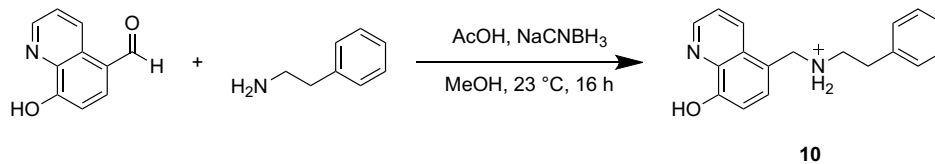
^1H NMR (400 MHz, CDCl_3): δ 10.14 (s, 1H), 9.68 (dd, $J = 8.7, 1.6$ Hz, 1H), 8.86 (dd, $J = 4.2, 1.6$ Hz, 1H), 8.00 (d, $J = 7.9$ Hz, 1H), 7.66 (dd, $J = 8.6, 4.2$ Hz, 1H), 7.28 (d, $J = 7.9$ Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3): δ 192.16, 157.99, 148.86, 140.58, 137.99, 134.94, 126.75, 124.86, 123.73, 109.15.

HRMS (DART): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{10}\text{H}_8\text{NO}_2^+$ 174.0550, found 174.0548.

IR (Film): 3201, 2314, 1503, 1275, 1143 cm^{-1} .

Compound 10



Following General Procedure A using **14** (46 mg, 263 μmol) afforded **10** (45 mg, 89 μmol , 34% yield).

Physical State: Yellow solid

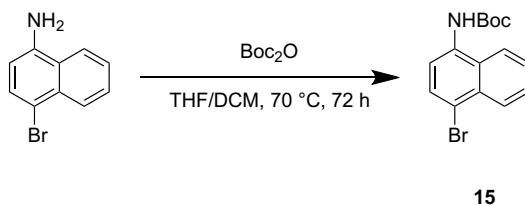
^1H NMR (500 MHz, CD_3CN): δ 8.93 (dd, $J = 4.4, 1.3$ Hz, 1H), 8.73 (d, $J = 8.6$ Hz, 1H), 7.74 (dd, $J = 8.7, 4.4$ Hz, 1H), 7.66 (d, $J = 8.0$ Hz, 1H), 7.39 – 7.32 (m, 2H), 7.32 – 7.25 (m, 3H), 7.03 (d, $J = 7.8$ Hz, 1H), 4.58 (s, 2H), 3.38 (t, $J = 8.1$ Hz, 2H), 3.04 (t, $J = 8.2$ Hz, 3H).

^{13}C NMR (126 MHz, CD_3CN): δ 137.66, 133.90, 129.79, 129.73, 128.49, 128.05, 123.44, 111.69, 50.01, 48.17, 32.67.

HRMS (ESI/Q-TOF): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{18}\text{H}_{19}\text{N}_2\text{O}^+$ 279.1492, found 279.1483.

IR (Film): 3338, 3009, 2987, 2315, 1682, 1276, 1261, 1198 cm^{-1} .

Compound 15



To a solution of 4-bromonaphthalen-1-amine (1.000 g, 1 equiv, 4.503 mmol) in THF (20 mL) and DCM (40 mL) was added di-*tert*-butyl dicarbonate (1.081 g, 1.14 mL, 1.1 equiv, 4.953 mmol). The reaction was refluxed at 70 °C for 72 hours. The reaction mixture was then concentrated under reduced pressure directly on to silica gel (5 g). The crude product was then purified by flash column chromatography (50 g silica gel, 0-40% EtOAc gradient against hexanes over 10 column volumes) to afford **15** (1.345 g, 4.174 mmol, 93% yield).

Physical State: White solid

TLC (UV): R_f 0.61 (1:4 EtOAc:Hexanes)

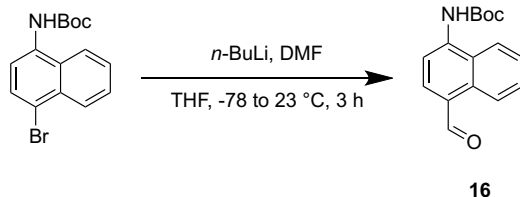
$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 8.28 – 8.25 (m, 1H), 7.89 – 7.86 (m, 1H), 7.77 (q, $J = 8.5$ Hz, 2H), 7.63 – 7.55 (m, 2H), 6.83 (s, 1H), 1.56 (s, 9H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3): δ 153.35, 146.89, 133.10, 132.36, 129.95, 128.25, 127.43, 126.95, 120.98, 85.34, 81.19, 28.49, 27.57.

HRMS (DART): $[M+H]^+$ calculated for $\text{C}_{15}\text{H}_{17}\text{BrNO}_2^+$ 322.0437, found 322.0404.

IR (Film): 2986, 2313, 1688, 1534, 1491, 1364, 1328, 1273, 1260, 1155, 1001 cm^{-1} .

Compound 16



A solution of tert-butyl (4-bromonaphthalen-1-yl)carbamate **15** (500 mg, 1 equiv, 1.55 mmol) in anhydrous THF (20 mL) was cooled to -78 °C under argon. *n*-butyllithium (348 mg, 2.17 mL, 2.5 M in hexanes, 3.5 equiv, 5.43 mmol) was added slowly over 5 minutes. The reaction was allowed to stir at -78 °C for one hour. Then anhydrous DMF (709 mg, 751 μ L, 6.25 equiv, 9.70 mmol) was added, and the reaction was allowed to stir at -78 °C for one hour and at 23 °C for another hour. The reaction was then quenched with water (50 mL) and extracted with EtOAc (3 x 50 mL). The combined organic layers were dried with anhydrous MgSO₄ and concentrated under reduced pressure directly on to silica gel (5 g). The crude product was then purified by flash column chromatography (50 g silica gel, 0-40% EtOAc gradient against hexanes over 15 column volumes) to afford **16** (261 mg, 962 μ mol, 62% yield).

Physical State: Light yellow solid

TLC (UV): R_f 0.43 (1:4 EtOAc:Hexanes)

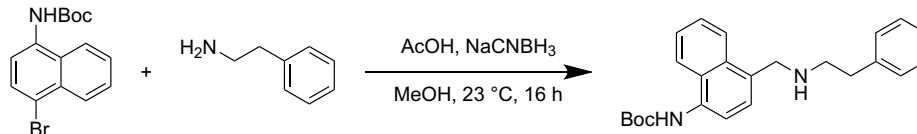
¹H NMR (500 MHz, CDCl₃): δ 10.25 (s, 1H), 9.42 (ddd, *J* = 8.6, 1.3, 0.6 Hz, 1H), 8.33 (d, *J* = 8.1 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.89 (dt, *J* = 8.4, 0.9 Hz, 1H), 7.71 (ddd, *J* = 8.4, 6.9, 1.2 Hz, 1H), 7.63 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.31 (s, 1H), 1.58 (s, 9H).

¹³C NMR (126 MHz, CDCl₃): δ 192.76, 152.44, 139.57, 138.82, 131.69, 129.15, 127.13, 126.74, 126.30, 124.47, 119.74, 114.10, 82.00, 28.44.

HRMS (DART): [M+H]⁺ calculated for C₁₆H₁₈NO₃⁺ 272.1281, found 272.1285.

IR (Film): 3216, 2986, 2315, 1682, 1576, 1524, 1505, 1458, 1392, 1363, 1330, 1261, 1216, 1146, 1085, 1060 cm⁻¹.

Compound 17



17

To solution of tert-butyl (4-formylnaphthalen-1-yl)carbamate **16** (250 mg, 1 equiv, 921 μ mol) in methanol (5 mL) was added acetic acid (55.3 mg, 52.7 μ L, 1 equiv, 921 μ mol), 2-phenylethan-1-amine (223 mg, 232 μ L, 2 equiv, 1.84 mmol), and sodium cyanoborohydride (174 mg, 3 equiv, 2.76 mmol). The reaction was allowed to stir at 23 °C for 16 hours. The reaction was then concentrated under reduced pressure directly on to silica gel (5 g). The crude product was then purified by flash column chromatography (50 g silica gel, 10-60% EtOAc gradient against hexanes over 15 column volumes) to afford **17** (253 mg, 671 μ mol, 73% yield).

Physical State: White solid

TLC (UV): R_f 0.72 (2:1 EtOAc:Hexanes)

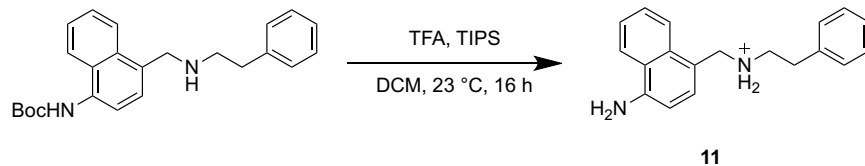
¹H NMR (600 MHz, CD₃CN): δ 8.18 – 8.13 (m, 1H), 8.00 – 7.96 (m, 1H), 7.57 – 7.44 (m, 4H), 7.42 (d, J = 7.6 Hz, 1H), 7.30 – 7.16 (m, 5H), 4.17 (s, 2H), 2.92 (t, J = 7.2 Hz, 2H), 2.80 (t, J = 7.2 Hz, 2H), 1.51 (s, 9H).

¹³C NMR (151 MHz, CD₃CN): δ 155.14, 141.71, 134.64, 133.94, 133.28, 129.66, 129.29, 129.23, 126.83, 126.77, 126.70, 126.52, 125.64, 123.44, 121.30, 80.42, 51.91, 51.86, 36.94, 28.51.

HRMS (DART): [M+H]⁺ calculated for C₂₄H₂₉N₂O₂⁺ 377.2224, found 377.2226.

IR (Film): 3340, 3202, 2678, 2357, 2120, 1274 cm⁻¹.

Compound 11



To solution of tert-butyl (4-((phenethylamino)methyl)naphthalen-1-yl)carbamate **17** (253 mg, 1 equiv, 671 μmol) in DCM (5 mL) was added triisopropylsilane (117 mg, 151 μL , 1.1 equiv, 738 μmol) and trifluoroacetic acid (7.68 g, 5.17 mL, 100 equiv, 67.1 mmol). The reaction was allowed to stir at 23 °C for 16 hours. The reaction was then purified on preparative HPLC (C18, 5-40% MeCN gradient against water with 0.1% TFA additive over 15 minutes) to afford **11** (216 mg, 428 μmol , 64% yield).

Physical State: Beige solid

^1H NMR (500 MHz, CD_3CN): δ 8.02 – 7.88 (m, 3H), 7.58 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.51 (ddd, J = 8.2, 6.8, 1.2 Hz, 1H), 7.40 (d, J = 7.8 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.29 – 7.20 (m, 3H), 6.74 (d, J = 7.8 Hz, 1H), 4.52 (s, 2H), 3.00 – 2.94 (m, 2H).

^{13}C NMR (126 MHz, CD_3CN): δ 146.89, 137.67, 133.32, 132.34, 129.76, 129.70, 128.02, 127.81, 125.66, 124.37, 124.06, 123.26, 115.81, 108.36, 49.50, 49.41, 32.57.

HRMS (ESI/Q-TOF): $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{19}\text{H}_{21}\text{N}_2^+$ 277.1699, found 277.1749.

IR (Film): 3382, 2674, 2314, 2121, 1794, 1682, 1415, 1275, 1189, 1014 cm^{-1} .

Phenethylamine Release Studies

General Release Study Procedure

The phenethylamine conjugate was first dissolved in MeOH as a 10 mM solution. Each aliquot was diluted to a final concentration of 5 mM with 0.1 M Tris buffer (pH 7.4). Then it was immediately analyzed on the analytical HPLC to determine the amount of phenethylamine release using a phenethylamine standard curve (254 nm area under the curve (AUC) vs. concentration). Each sample was prepared immediately prior to the first injection to ensure a consistent starting point across the three separate repeats.

Phenethylamine Standard Curve

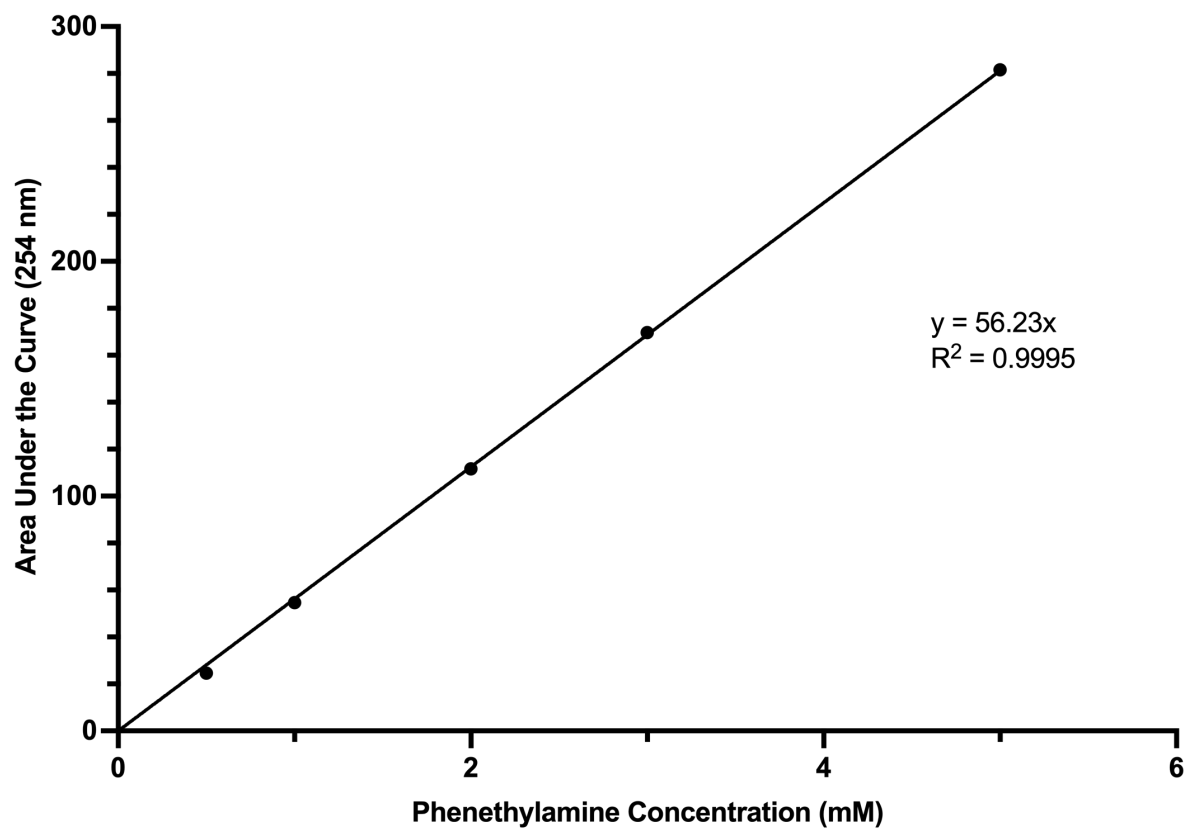


Figure S1. Phenethylamine Standard Curve – $n = 3$, error bars represent standard deviation but are smaller than the size of the markers. Area under the curve measured with 4.00 μL injections.

Phenethylamine Release From 1

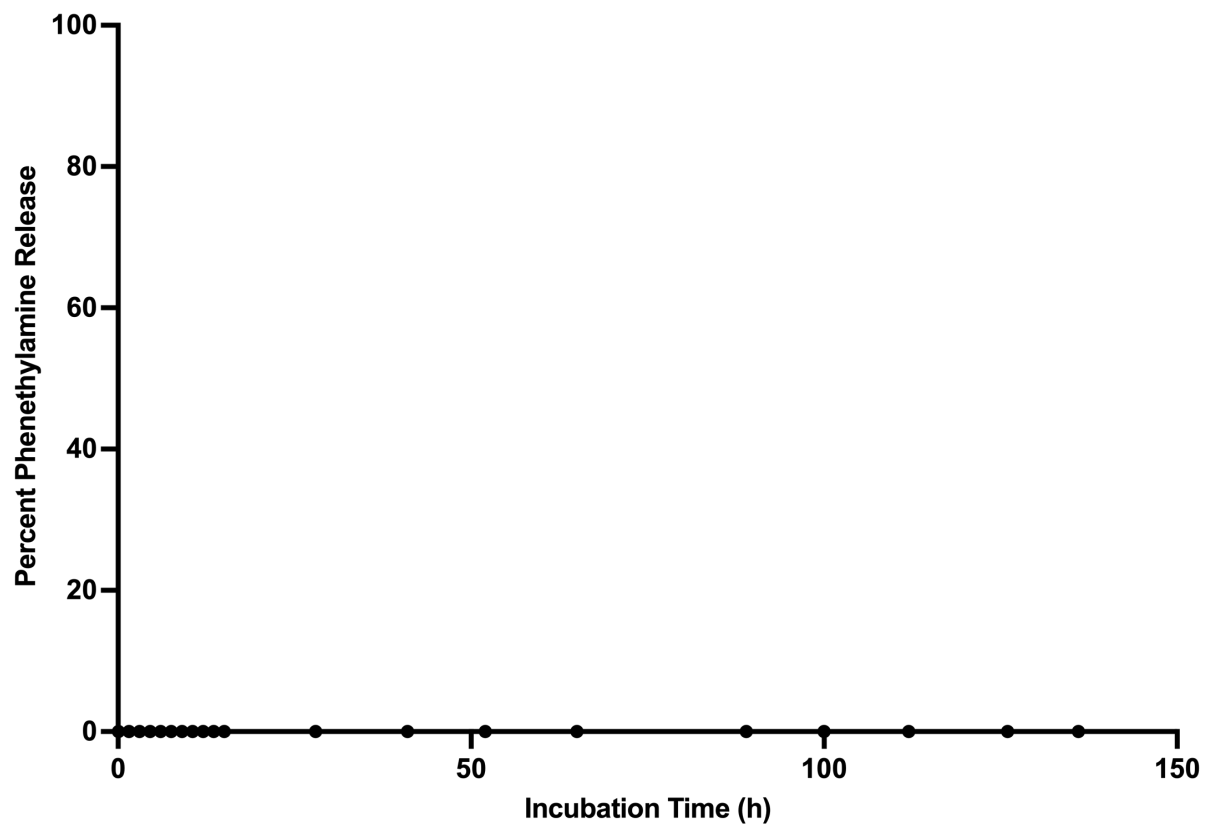


Figure S2. Phenethylamine release from 1 – $n = 3$, error bars represent standard deviation but are smaller than the size of the markers.

Phenethylamine Release From 2a

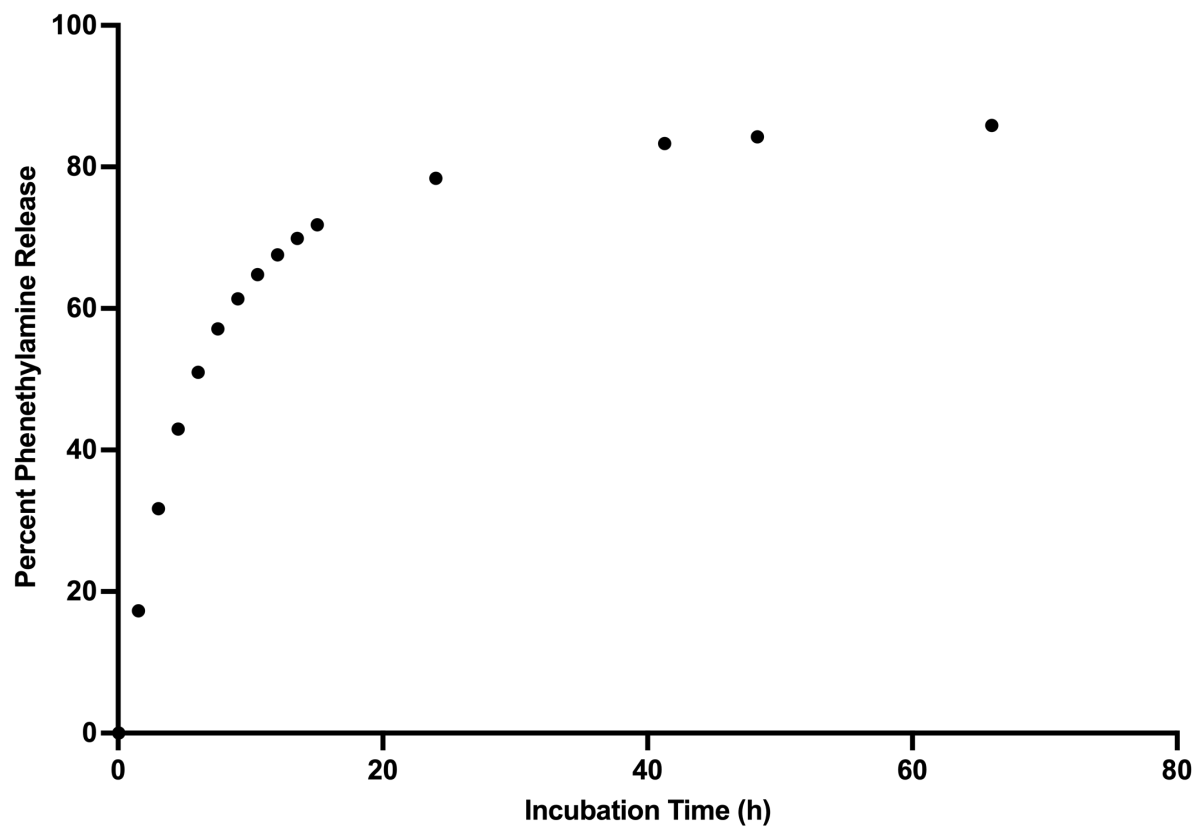


Figure S3. Phenethylamine release from **2a** – $n = 3$, error bars represent standard deviation but are smaller than the size of the markers.

Phenethylamine Release From 2b

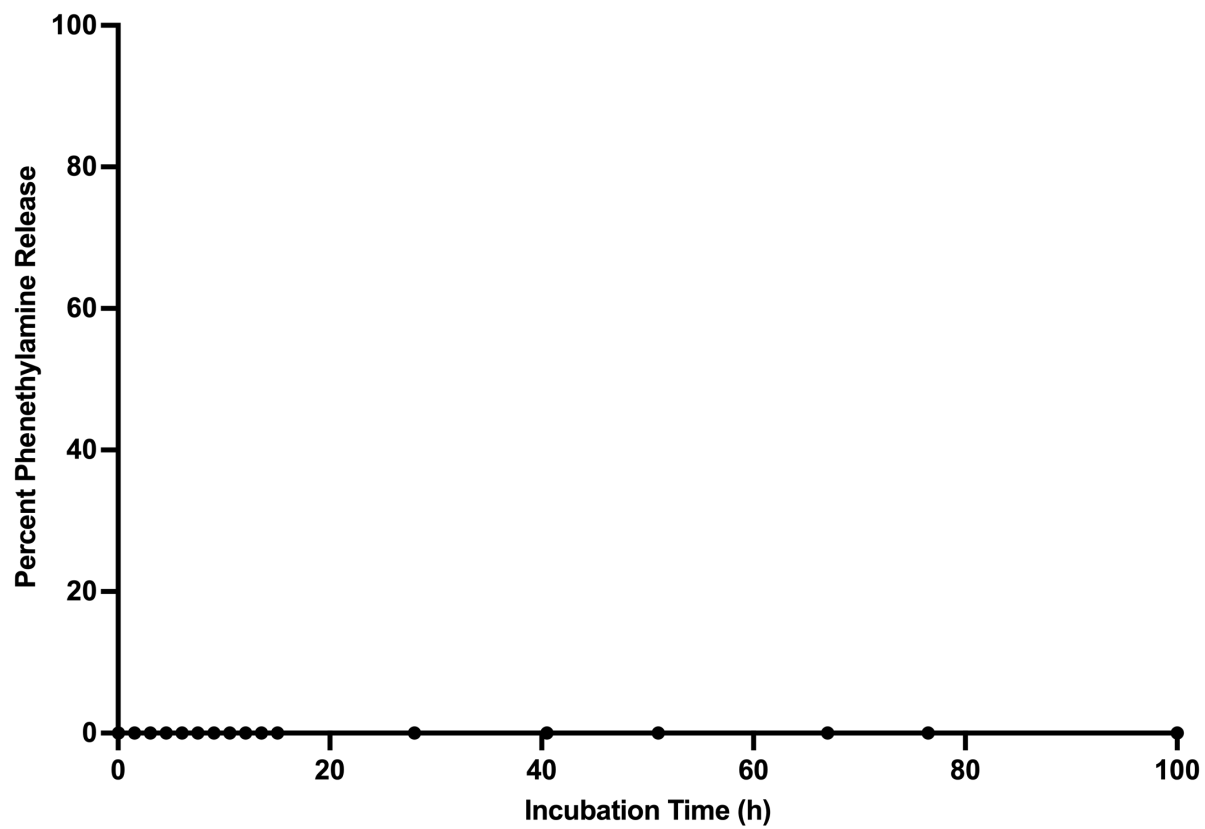


Figure S4. Phenethylamine release from **2b** – $n = 3$, error bars represent standard deviation but are smaller than the size of the markers.

Phenethylamine Release From 3a

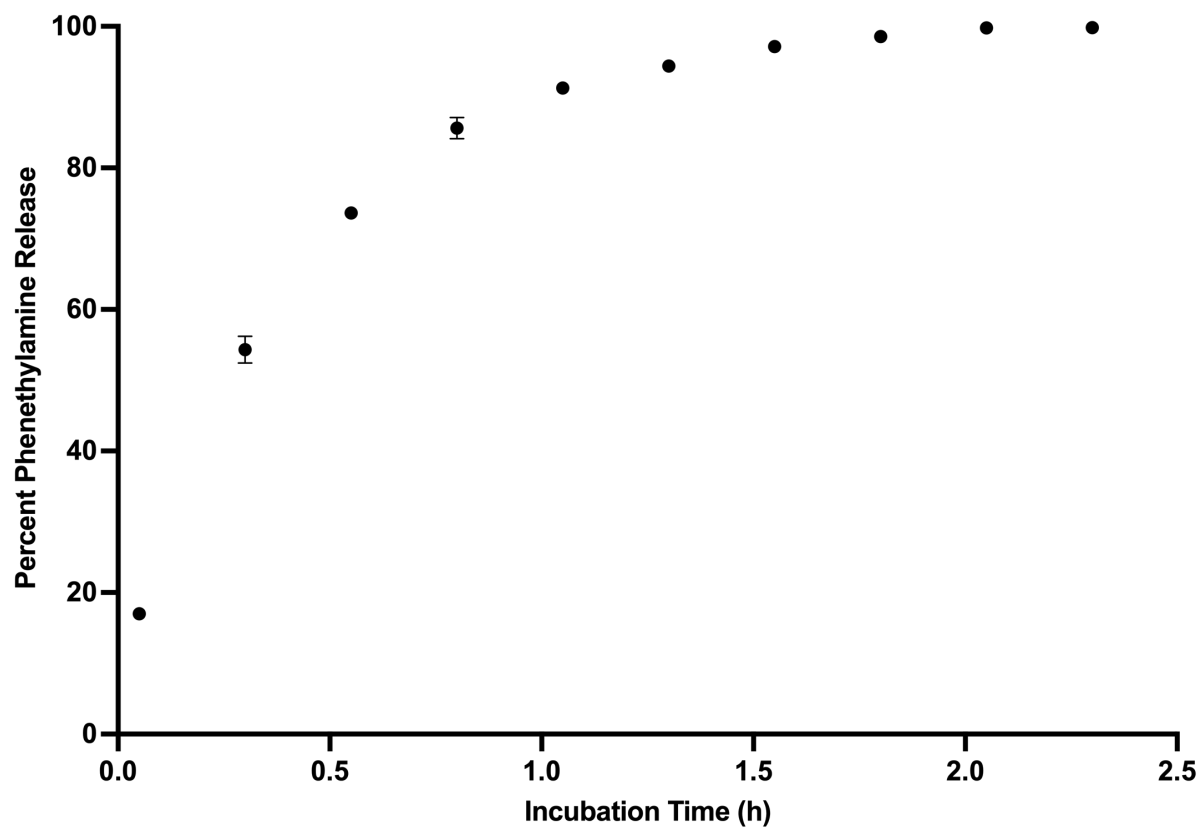


Figure S5. Phenethylamine release from **3a** – $n = 3$, error bars represent standard deviation but some are smaller than the size of the markers.

Phenethylamine Release From 3b

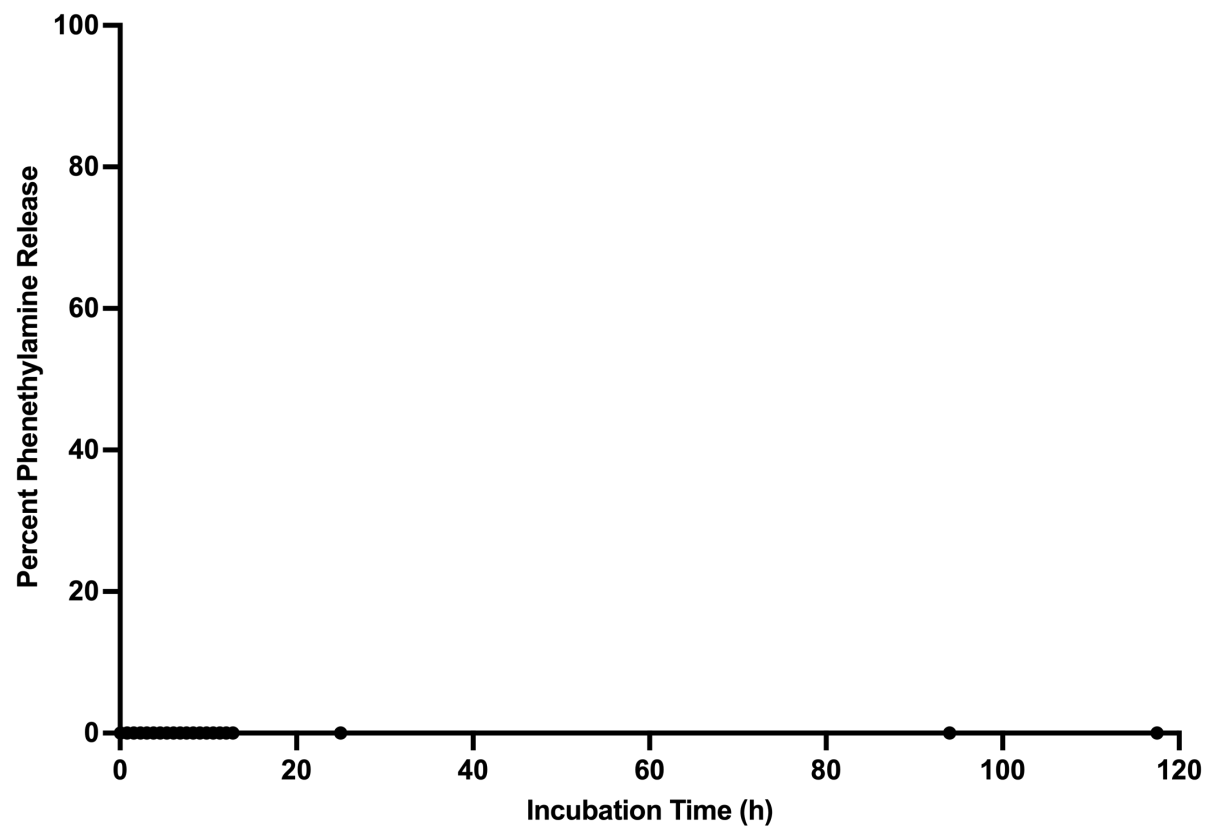


Figure S6. Phenethylamine release from **3b** – $n = 3$, error bars represent standard deviation but are smaller than the size of the markers.

Phenethylamine Release From 9

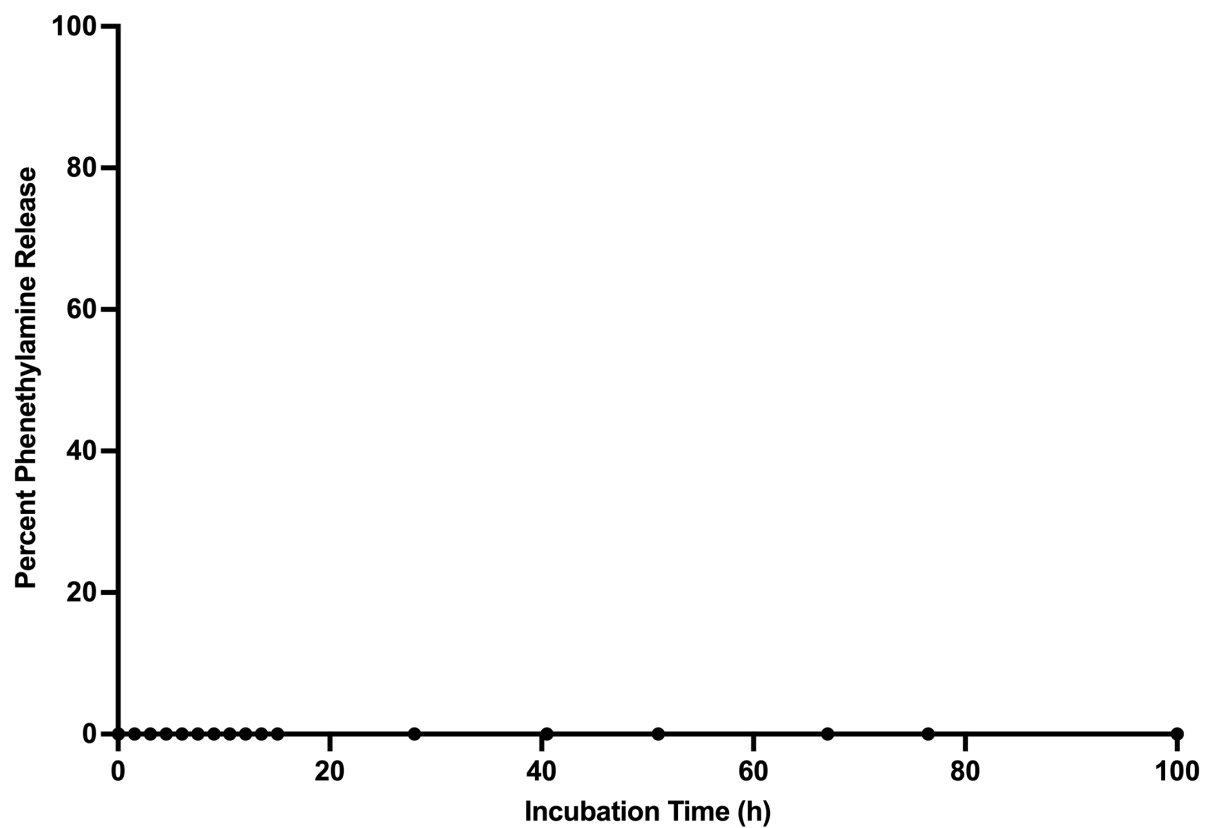


Figure S7. Phenethylamine release from **9** – $n = 3$, error bars represent standard deviation but are smaller than the size of the markers.

Phenethylamine Release From 10

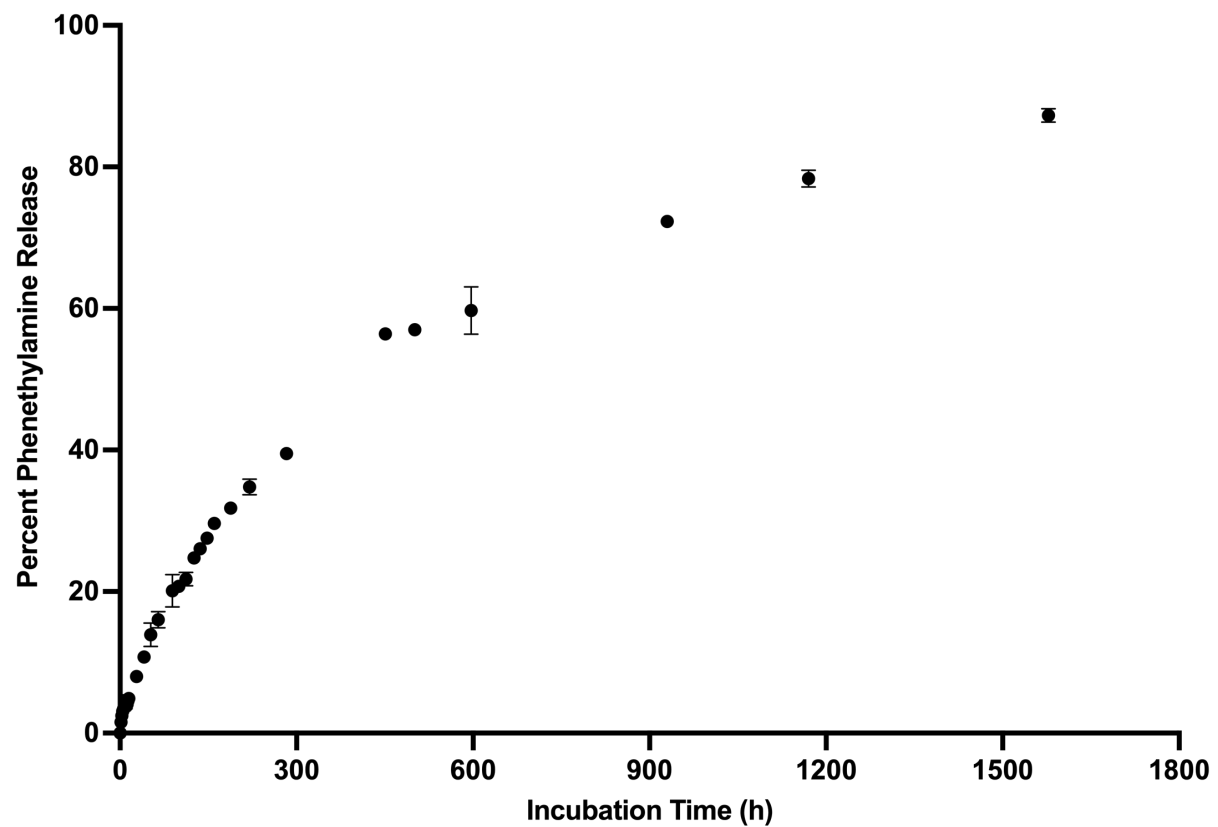


Figure S8. Phenethylamine release from **10** – $n = 3$, error bars represent standard deviation but some are smaller than the size of the markers.

Phenethylamine Release From 11

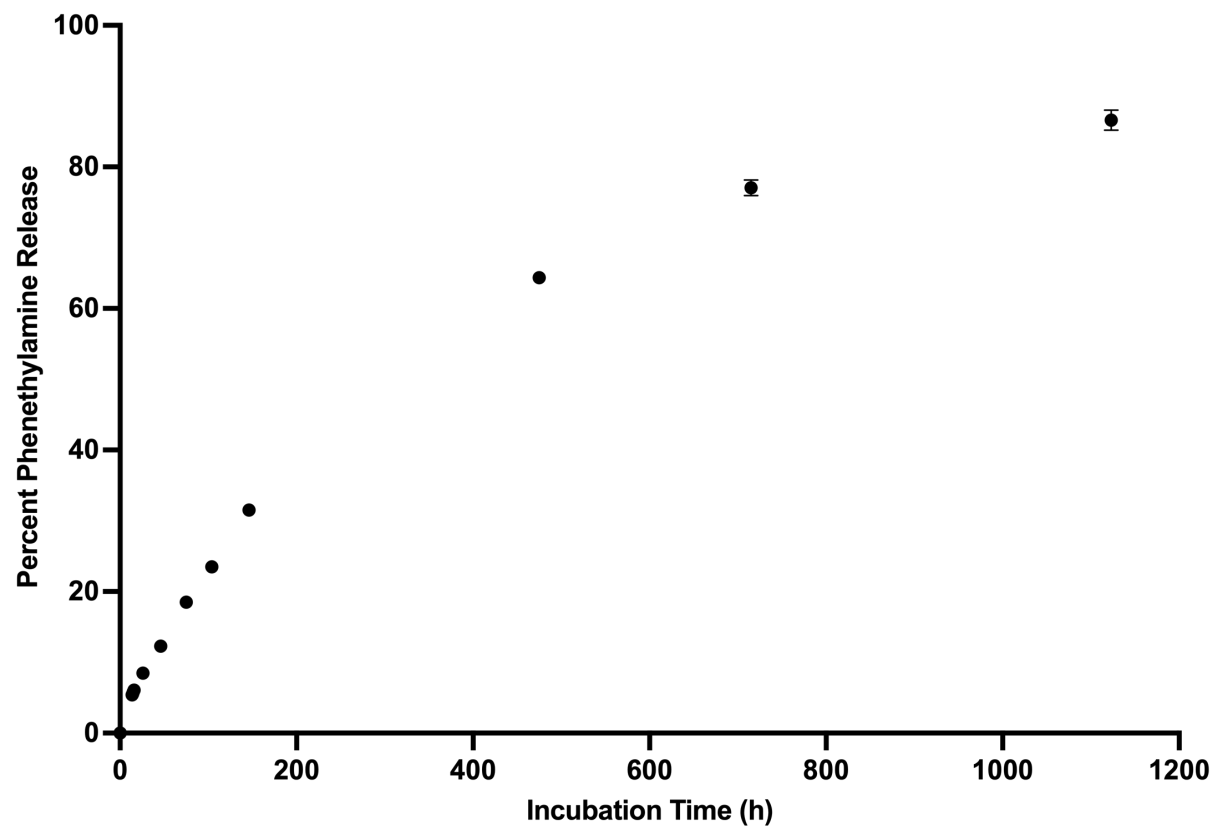


Figure S9. Phenethylamine release from **11** – $n = 3$, error bars represent standard deviation but some are smaller than the size of the markers.

NMR Spectra

Compound 1 ¹H NMR

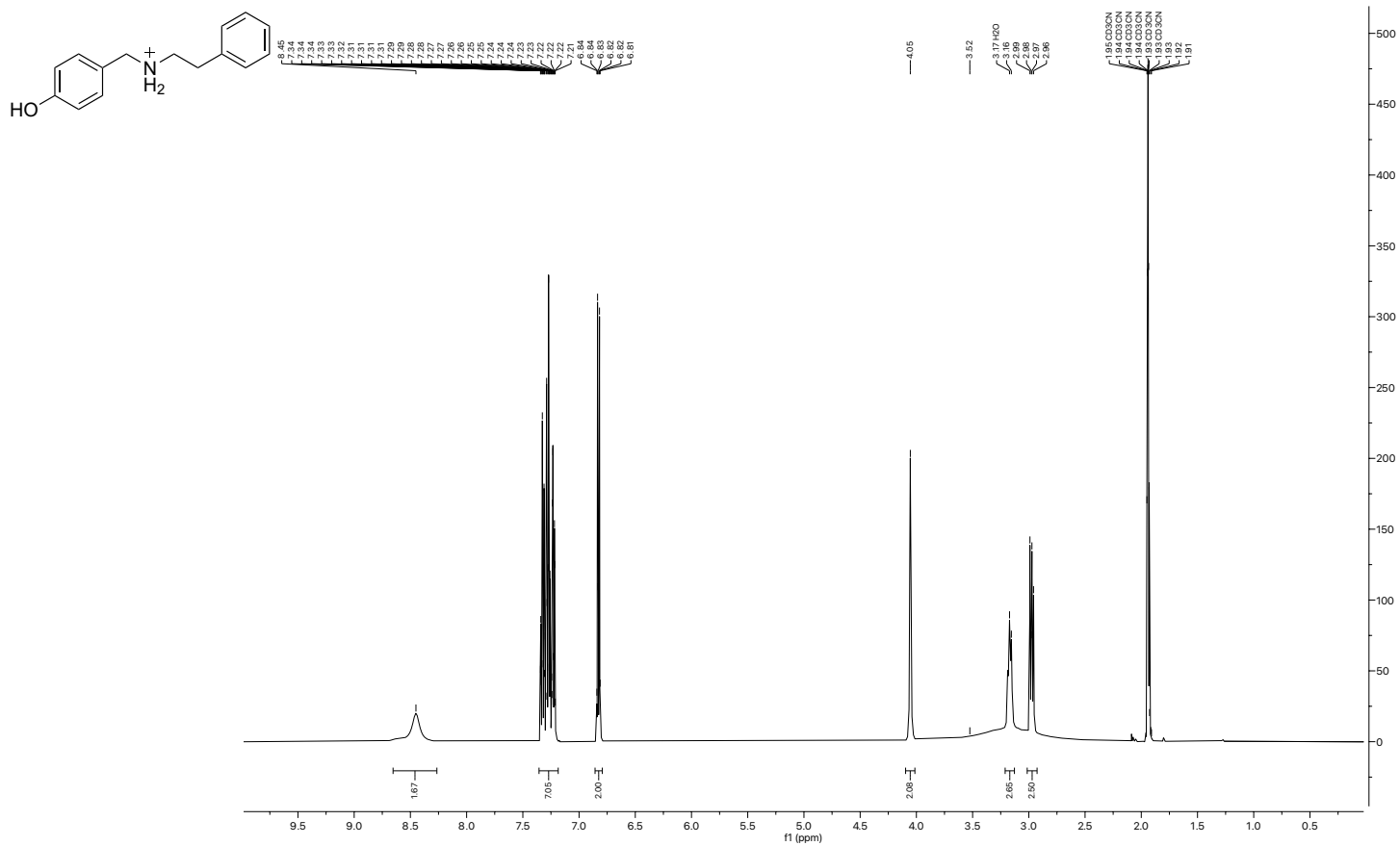


Figure S10. ¹H NMR of 1 in CD₃CN at 298 K.

Compound 1 ¹³C NMR

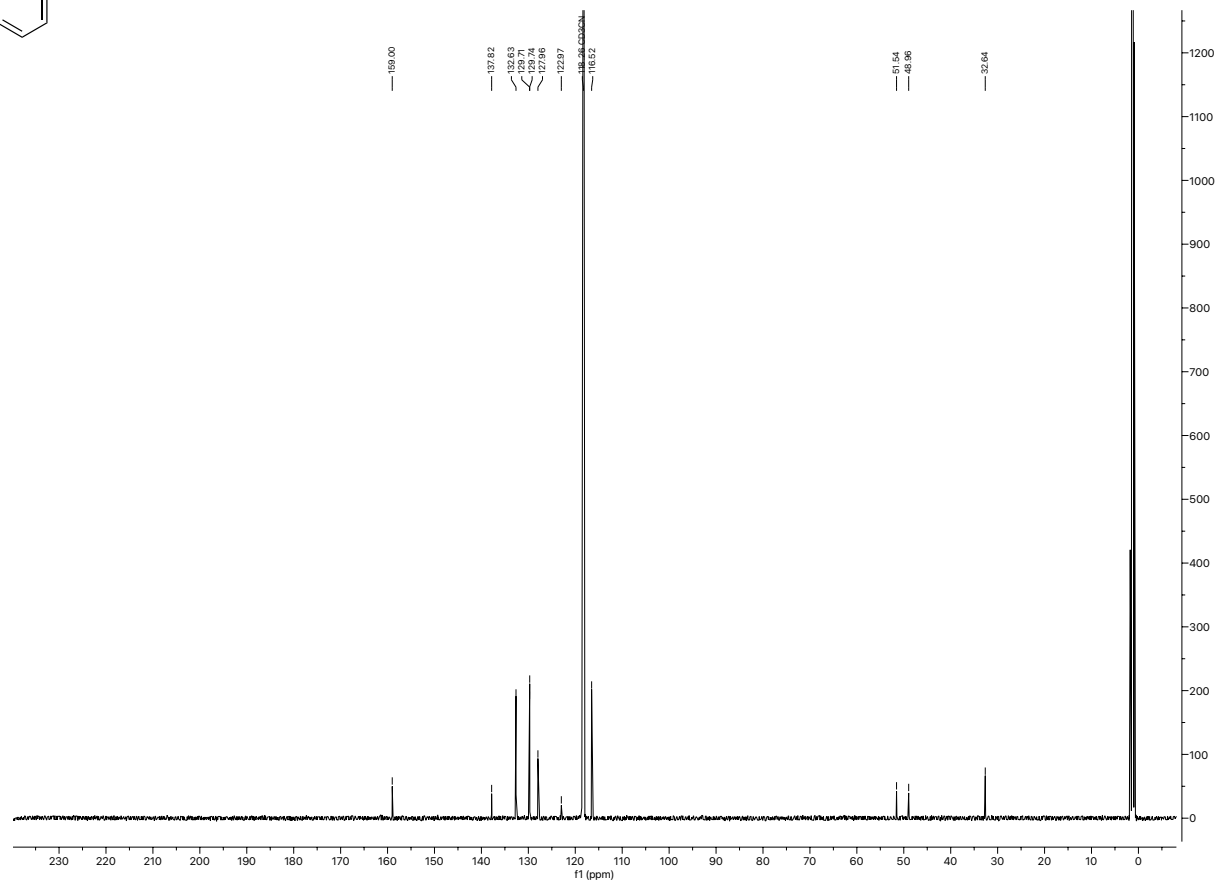
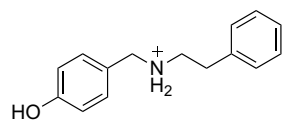


Figure S11. ¹³C NMR of 1 in CD₃CN at 298 K.

Compound 2a ¹H NMR

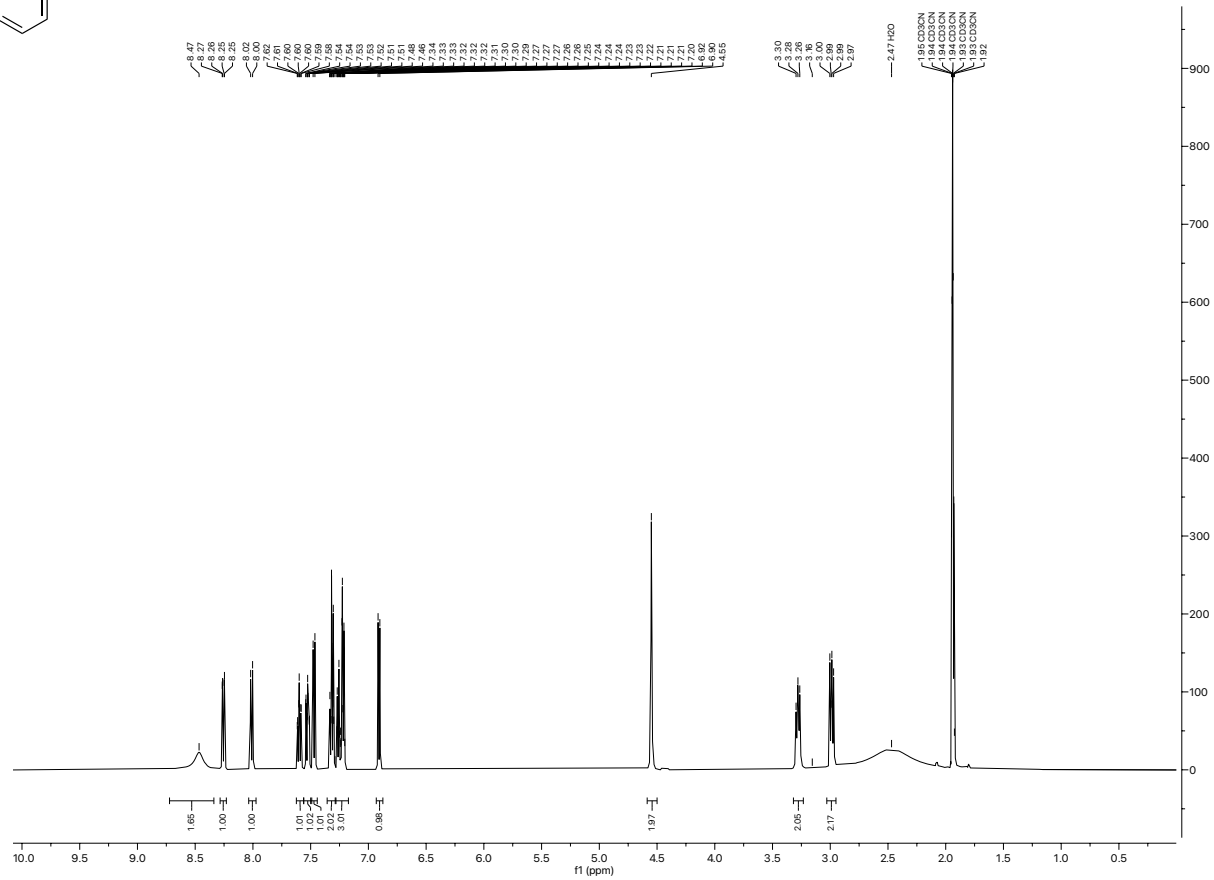
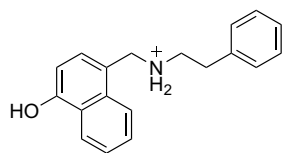
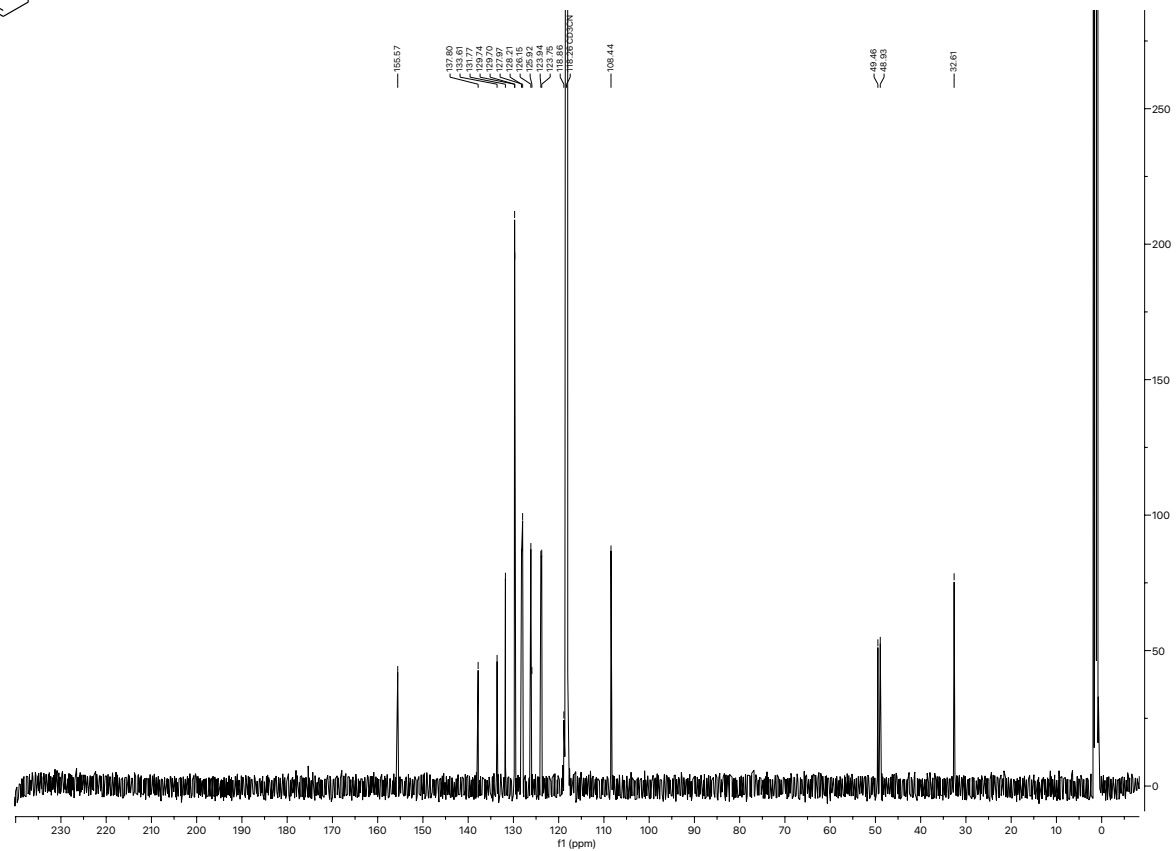
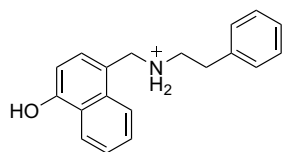


Figure S12. ¹H NMR of 2a in CD₃CN at 298 K.

Compound 2a ¹³C NMR



Compound 12 ¹H NMR

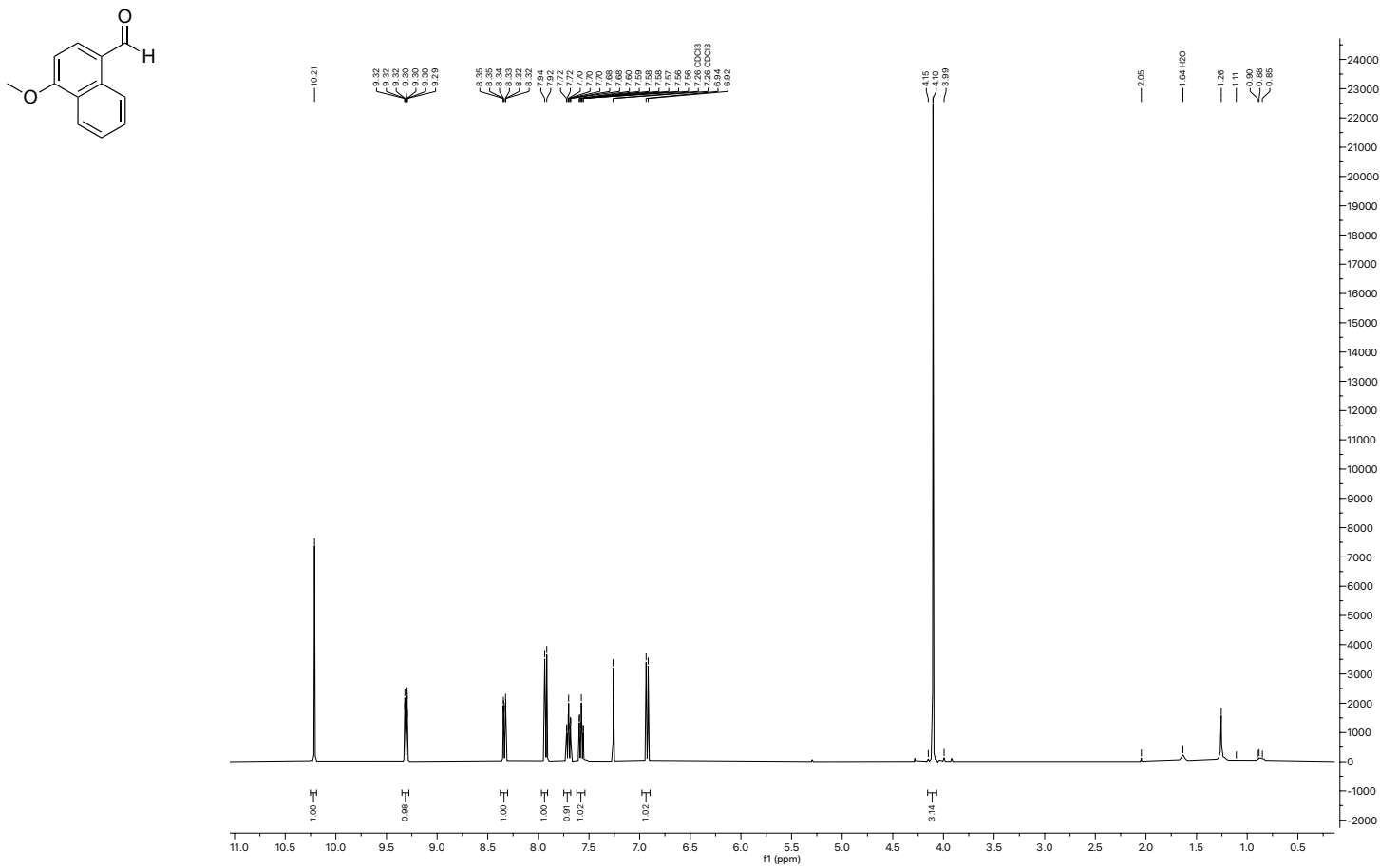


Figure S14. ¹H NMR of 12 in CDCl₃ at 298 K.

Compound 12 ¹³C NMR

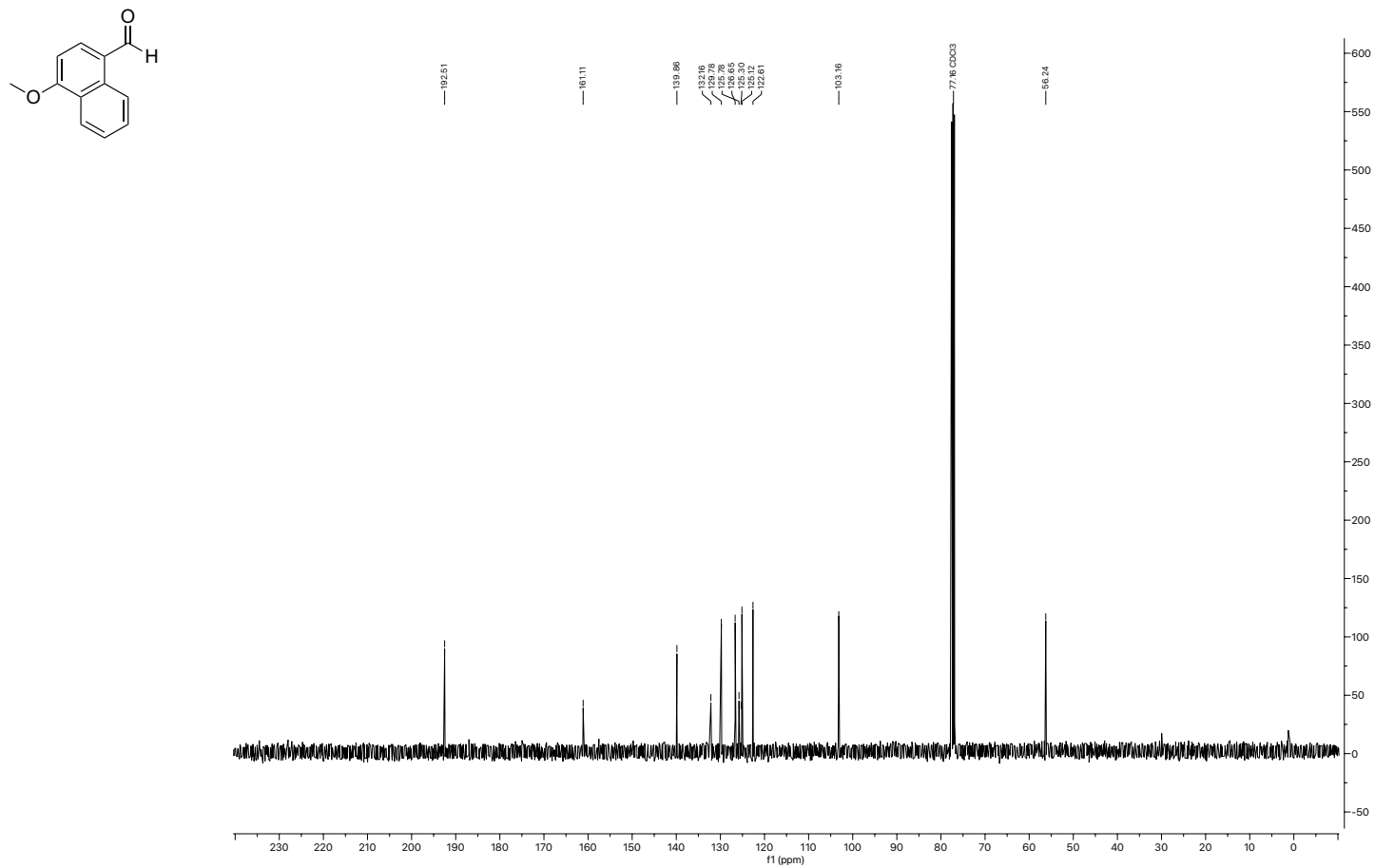


Figure S15. ¹³C NMR of 12 in CDCl₃ at 298 K.

Compound 2b ¹³C NMR

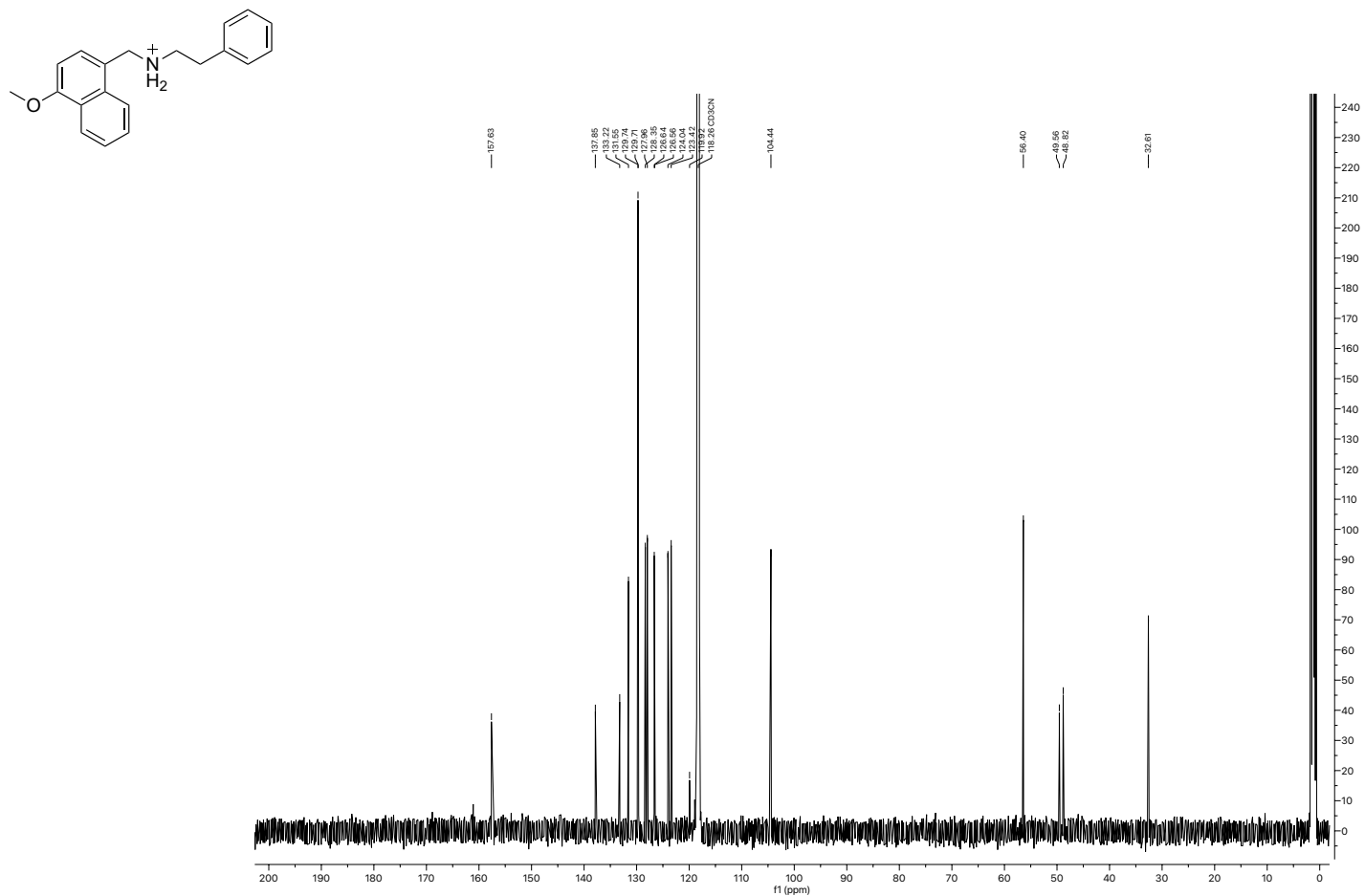


Figure S17. ¹³C NMR of 2b in CD₃CN at 298 K.

Compound 4 ¹H NMR

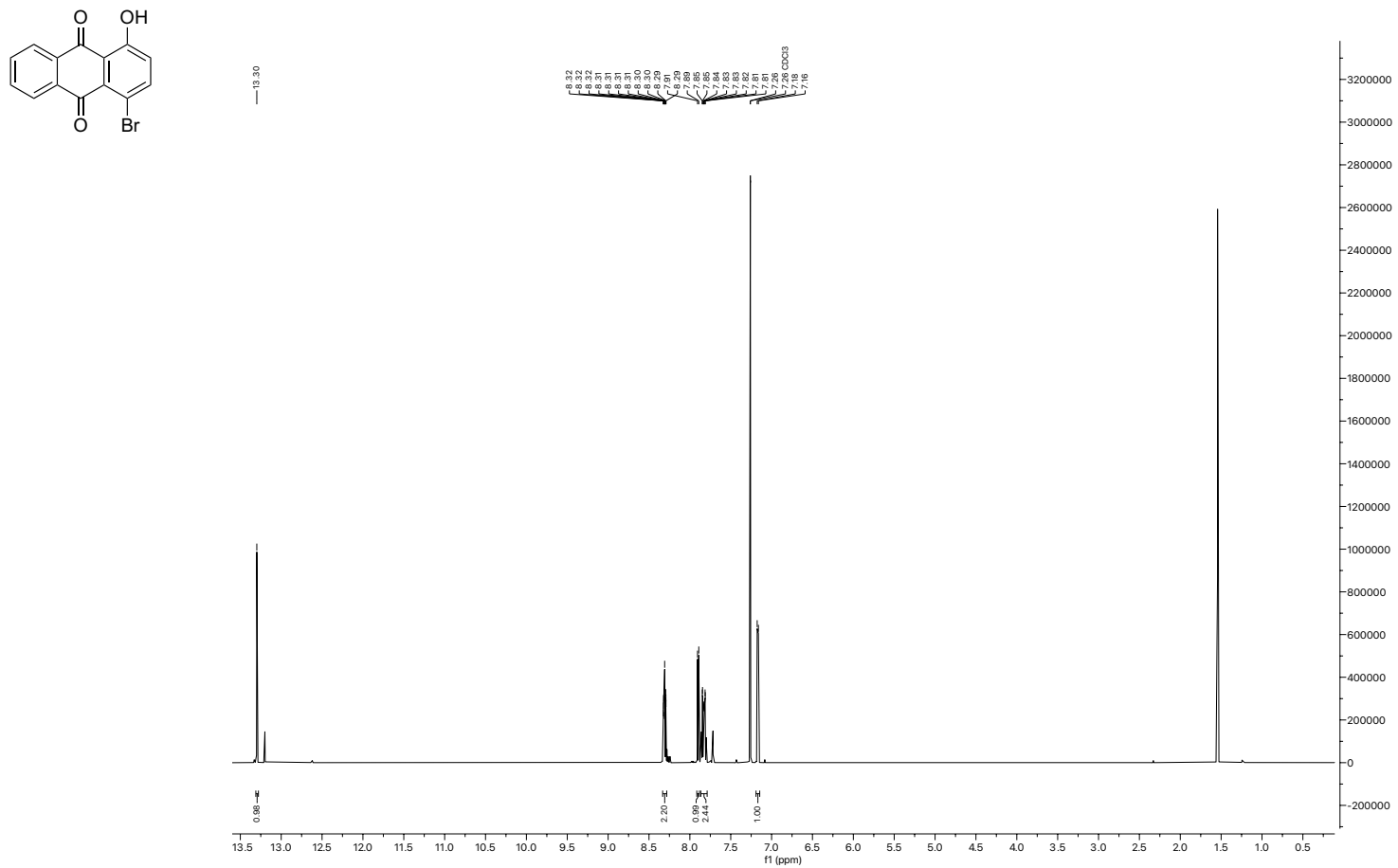


Figure S18. ¹H NMR of 4 in CDCl₃ at 298 K.

Compound 4 ¹³C NMR

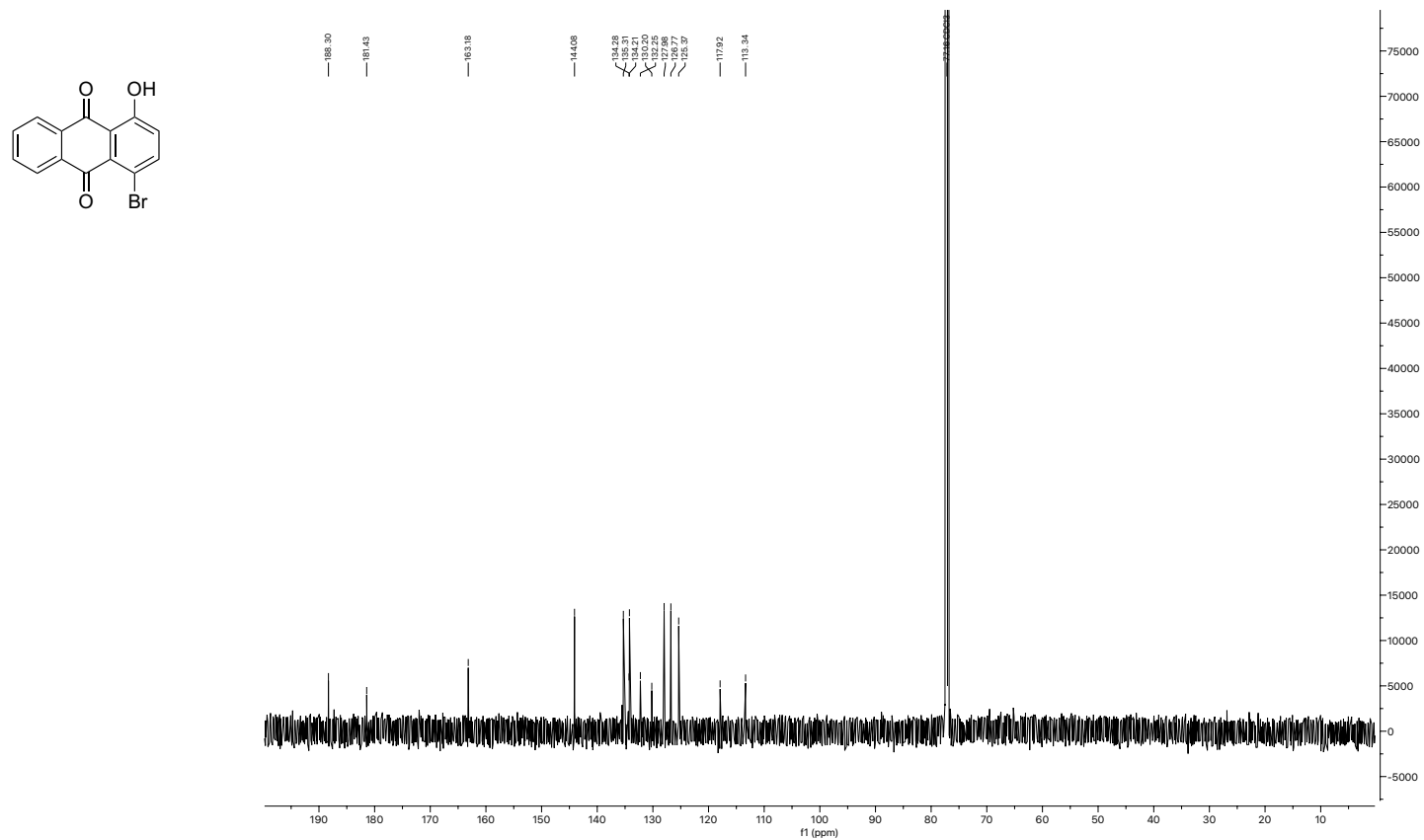


Figure S19. ¹³C NMR of 4 in CDCl₃ at 298 K.

Compound 5 ¹H NMR

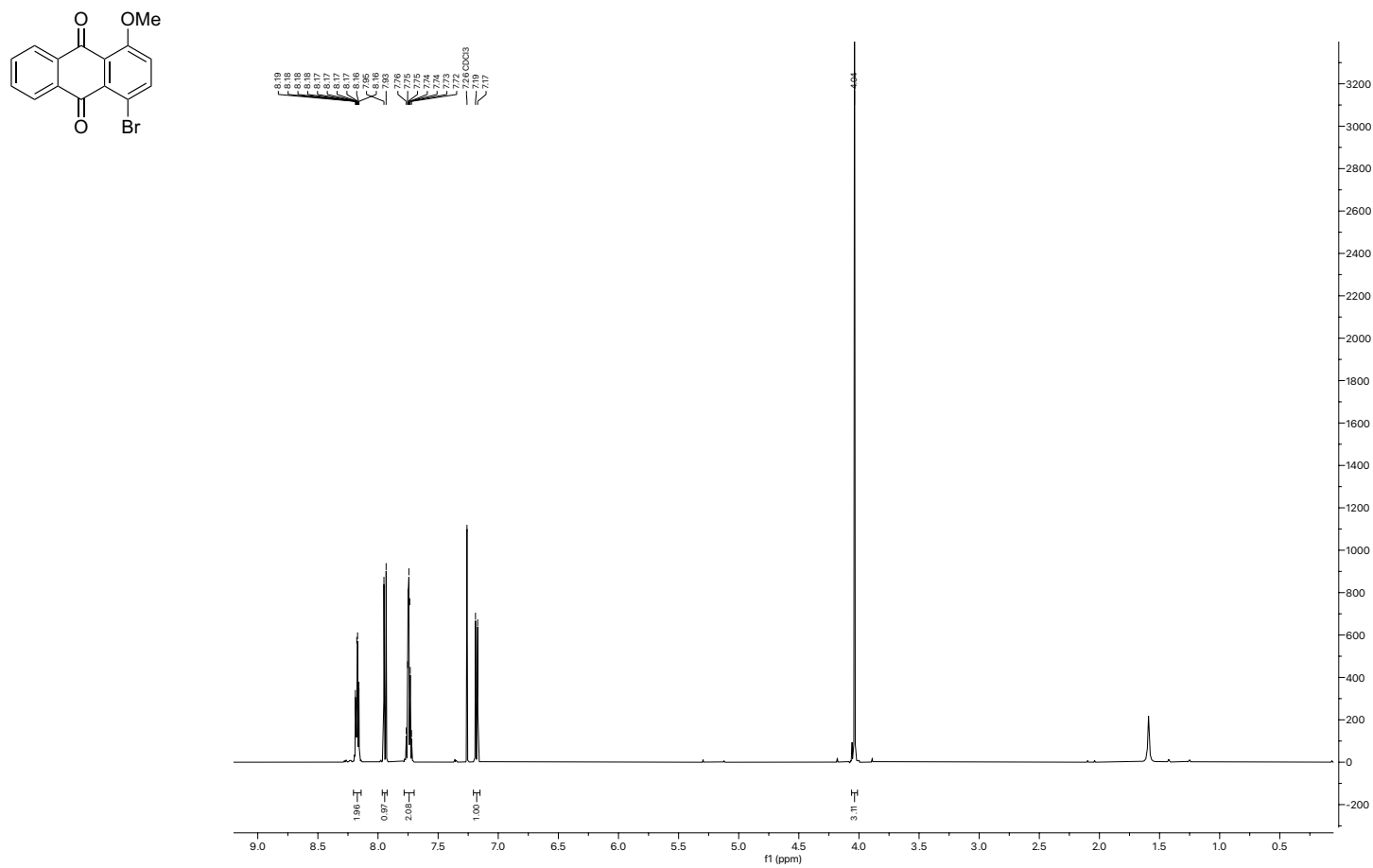


Figure S20. ¹H NMR of 5 in CDCl₃ at 298 K.

Compound 5 ¹³C NMR

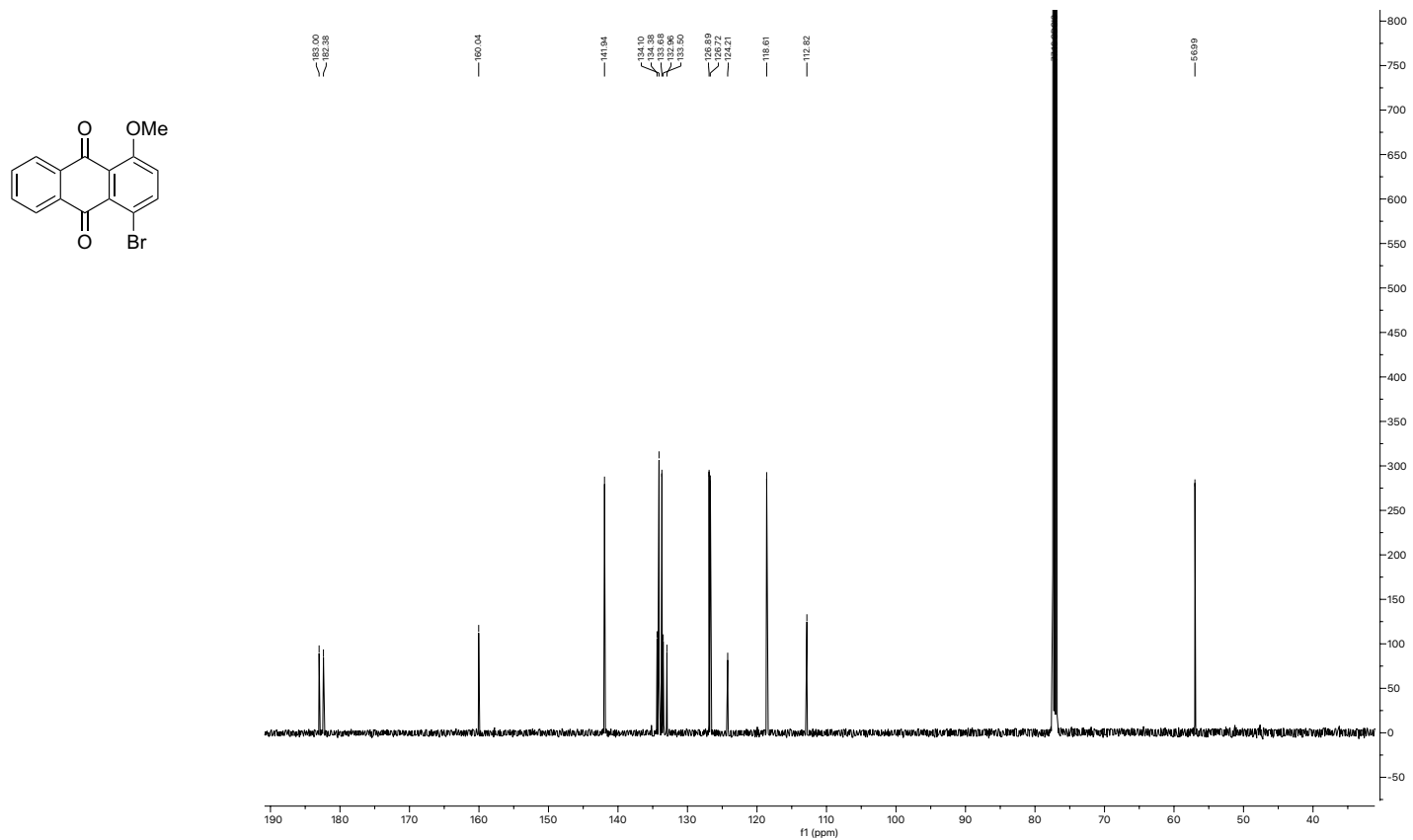


Figure S21. ¹³C NMR of 5 in CDCl₃ at 298 K.

Compound 6 ¹H NMR

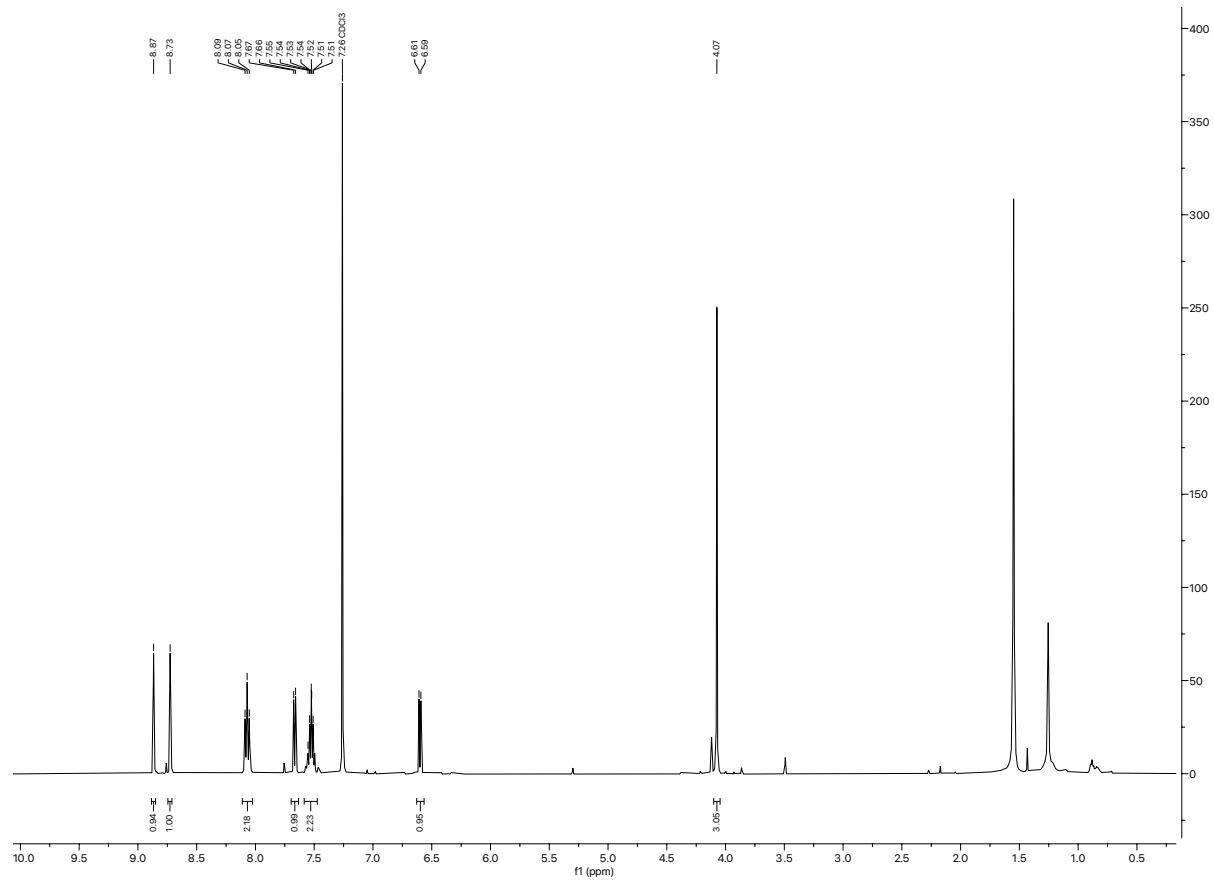
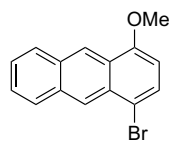


Figure S22. ¹H NMR of 6 in CDCl₃ at 298 K.

Compound 7 ^1H NMR

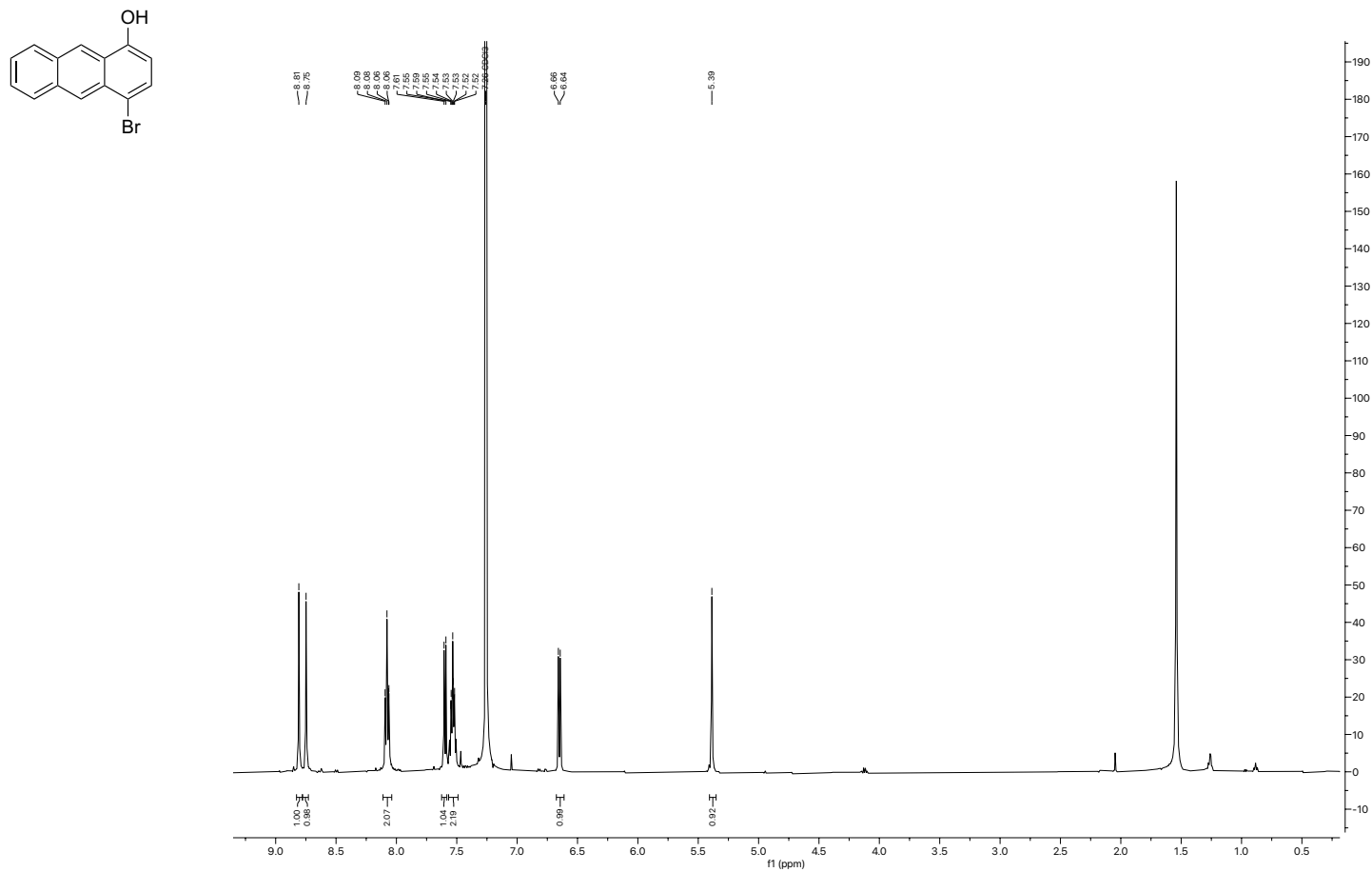


Figure S24. ^1H NMR of 7 in CDCl₃ at 298 K.

Compound 7 ¹³C NMR

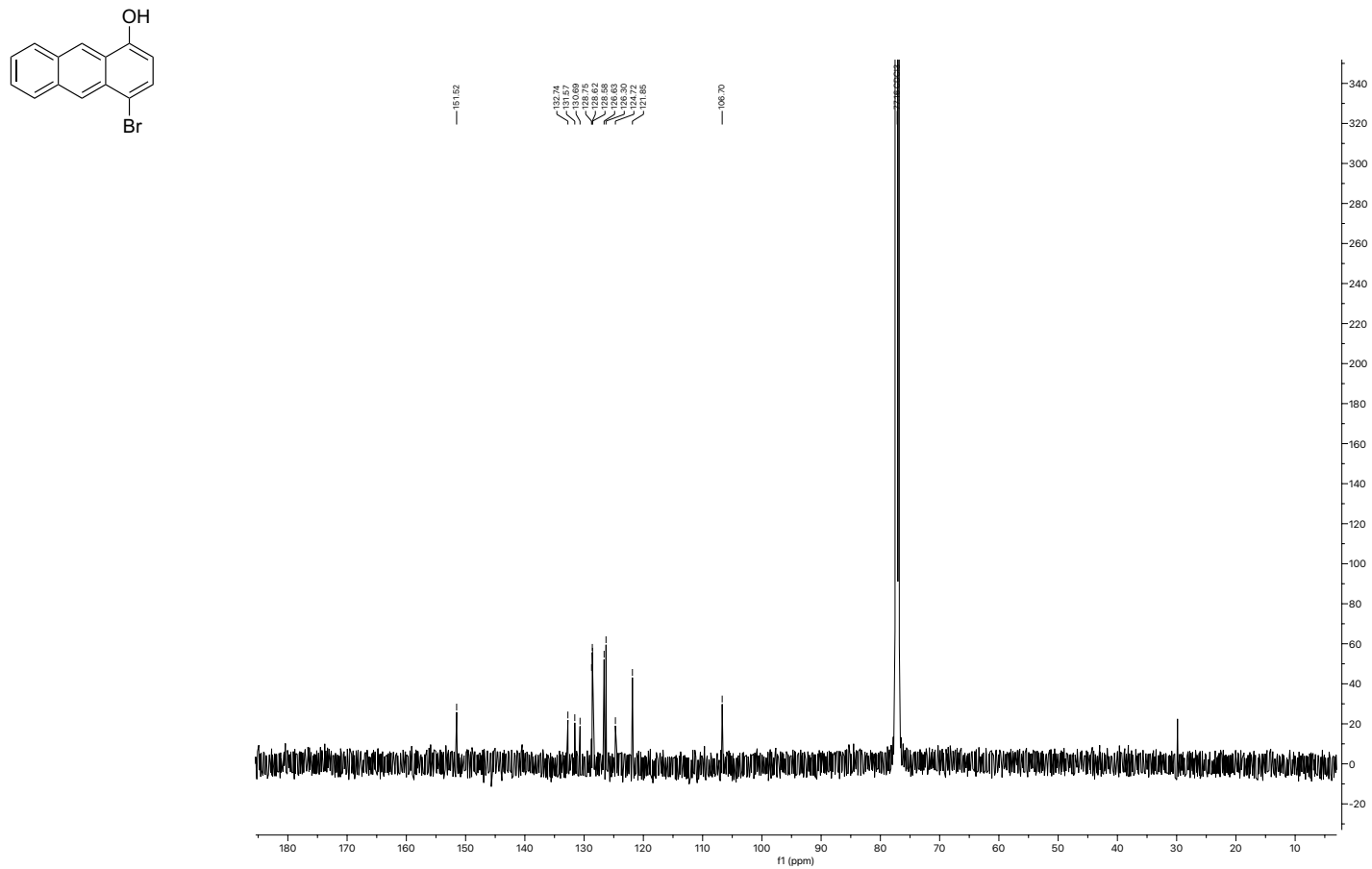
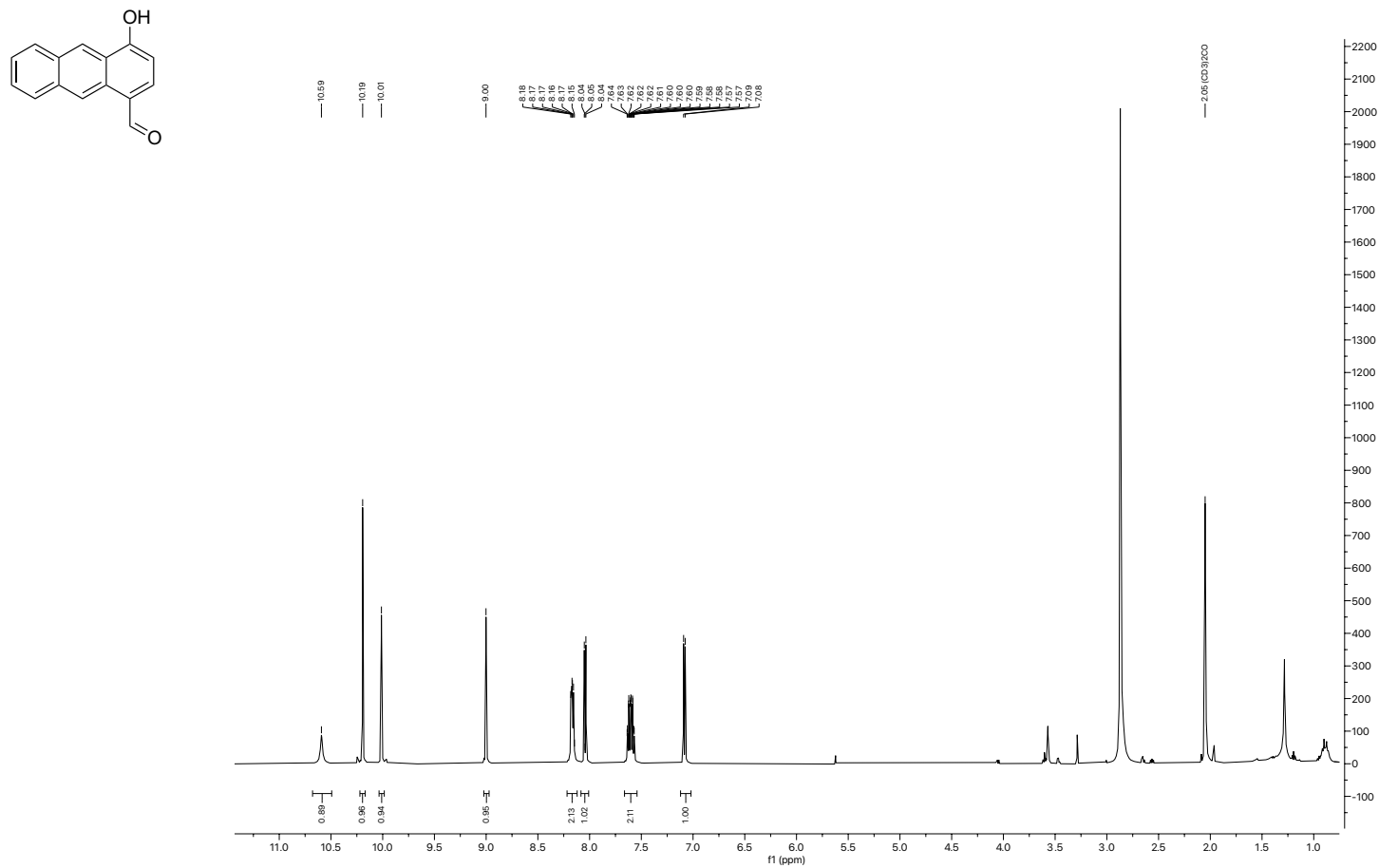


Figure S25. ¹³C NMR of 7 in CDCl₃ at 298 K.

Compound 8 ¹H NMR



Compound 8 ¹³C NMR

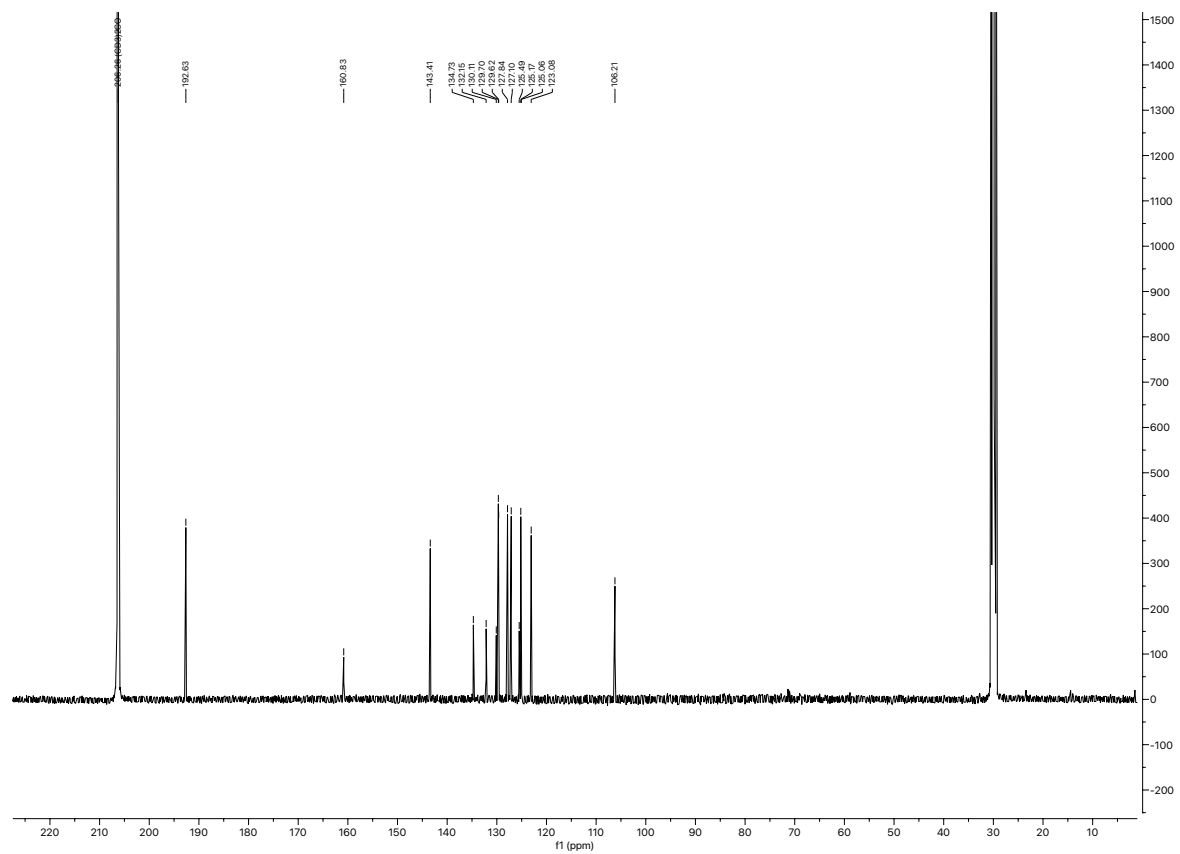
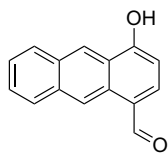


Figure S27. ¹³C NMR of 8 in acetone-d₆ at 298 K.

Compound 3a ¹H NMR

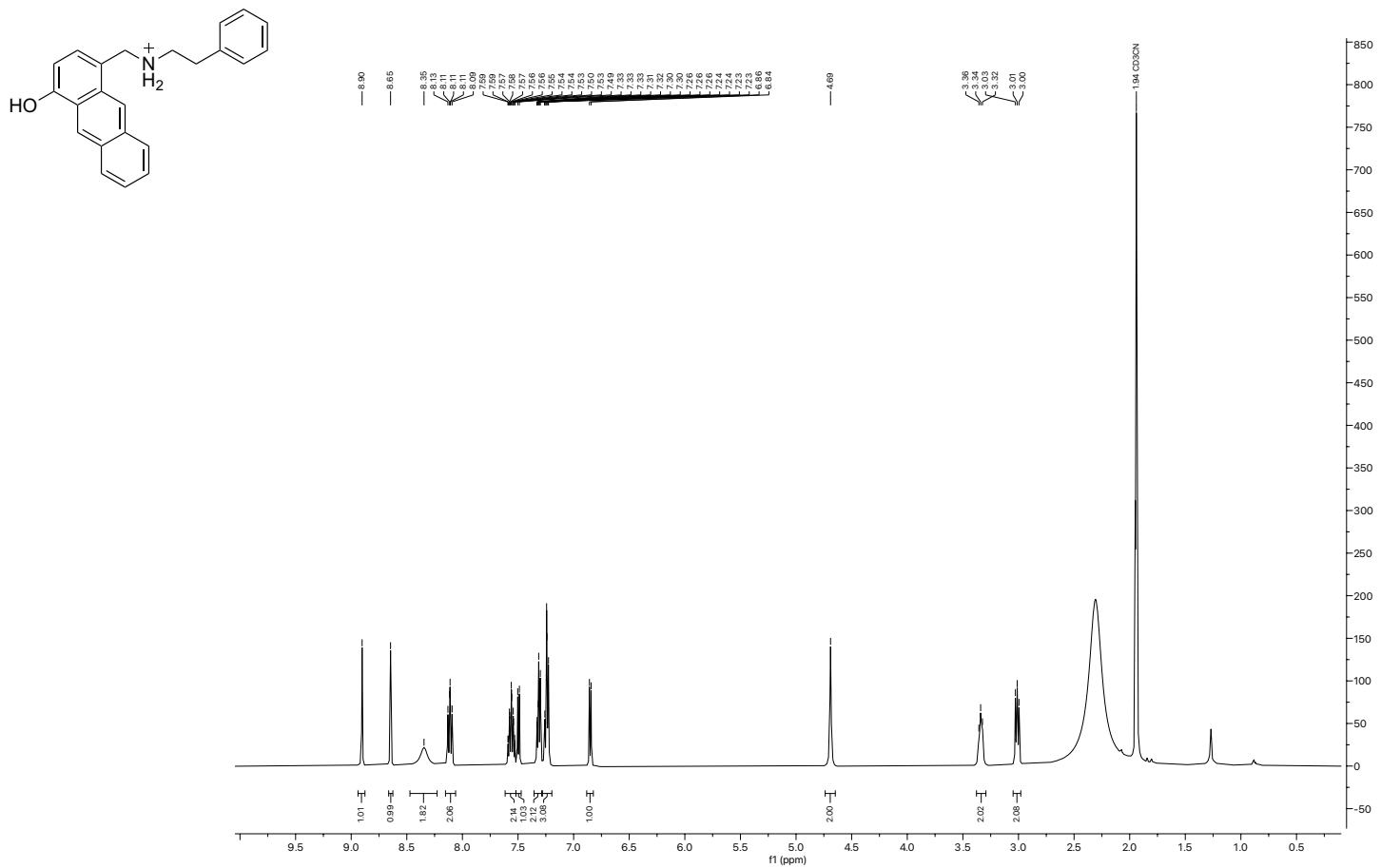


Figure S28. ¹H NMR of 3a in CD₃CN at 298 K.

Compound 3a ¹³C NMR

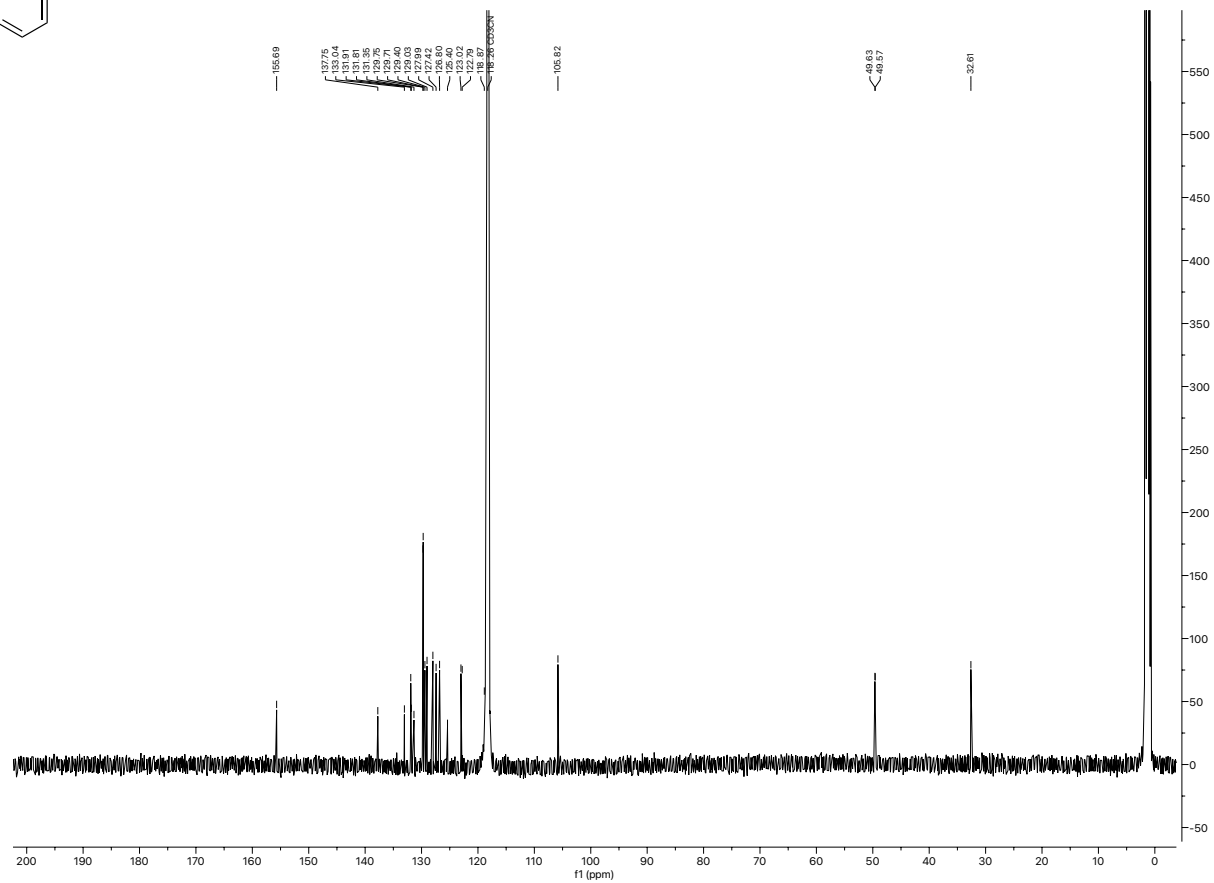
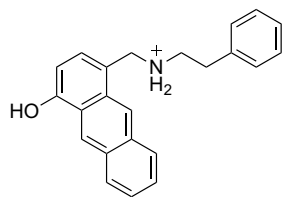


Figure S29. ¹³C NMR of 3a in CD₃CN at 298 K.

Compound 13 ¹³C NMR

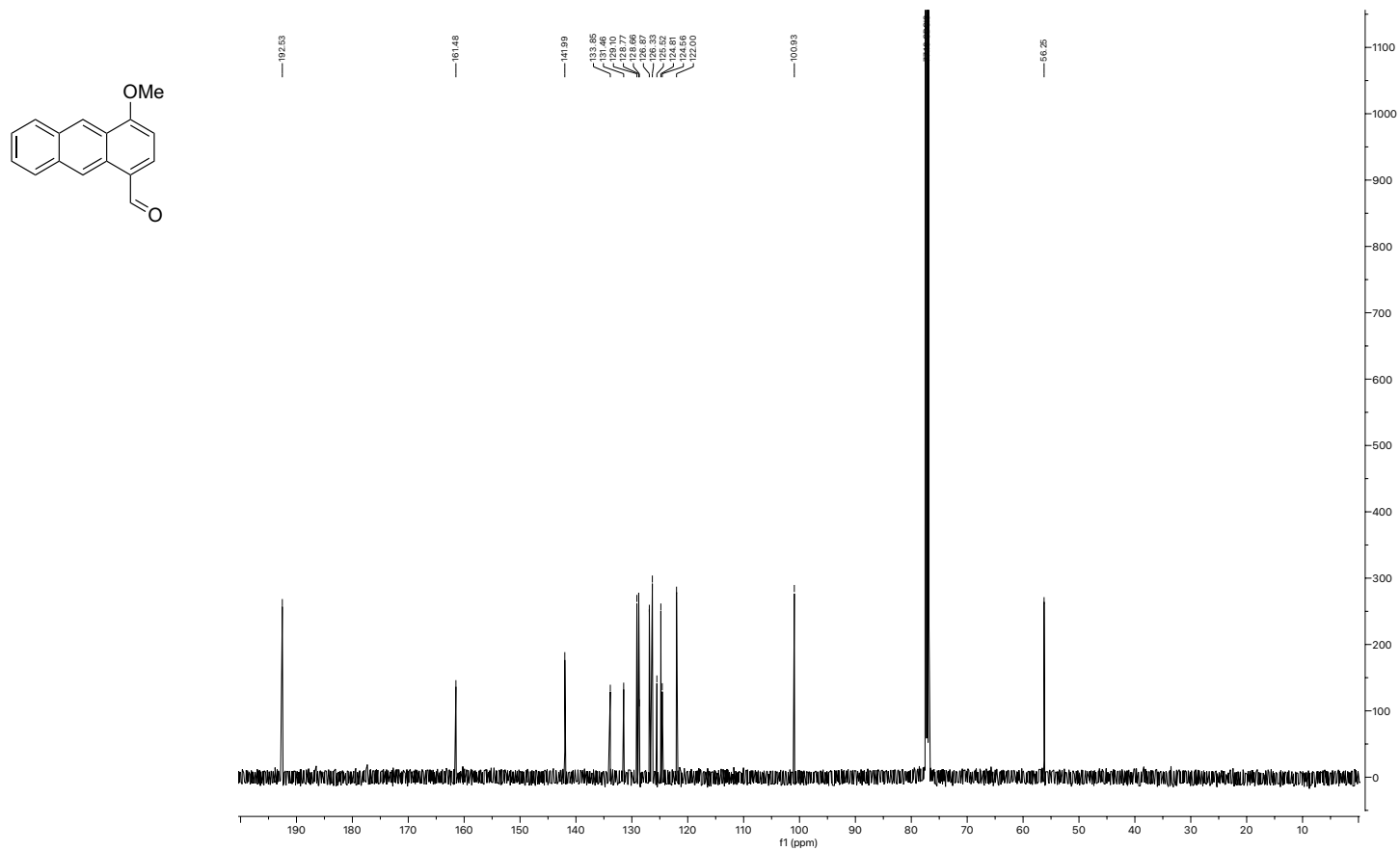


Figure S31. ¹³C NMR of 13 in CDCl₃ at 298 K.

Compound 3b ¹H NMR

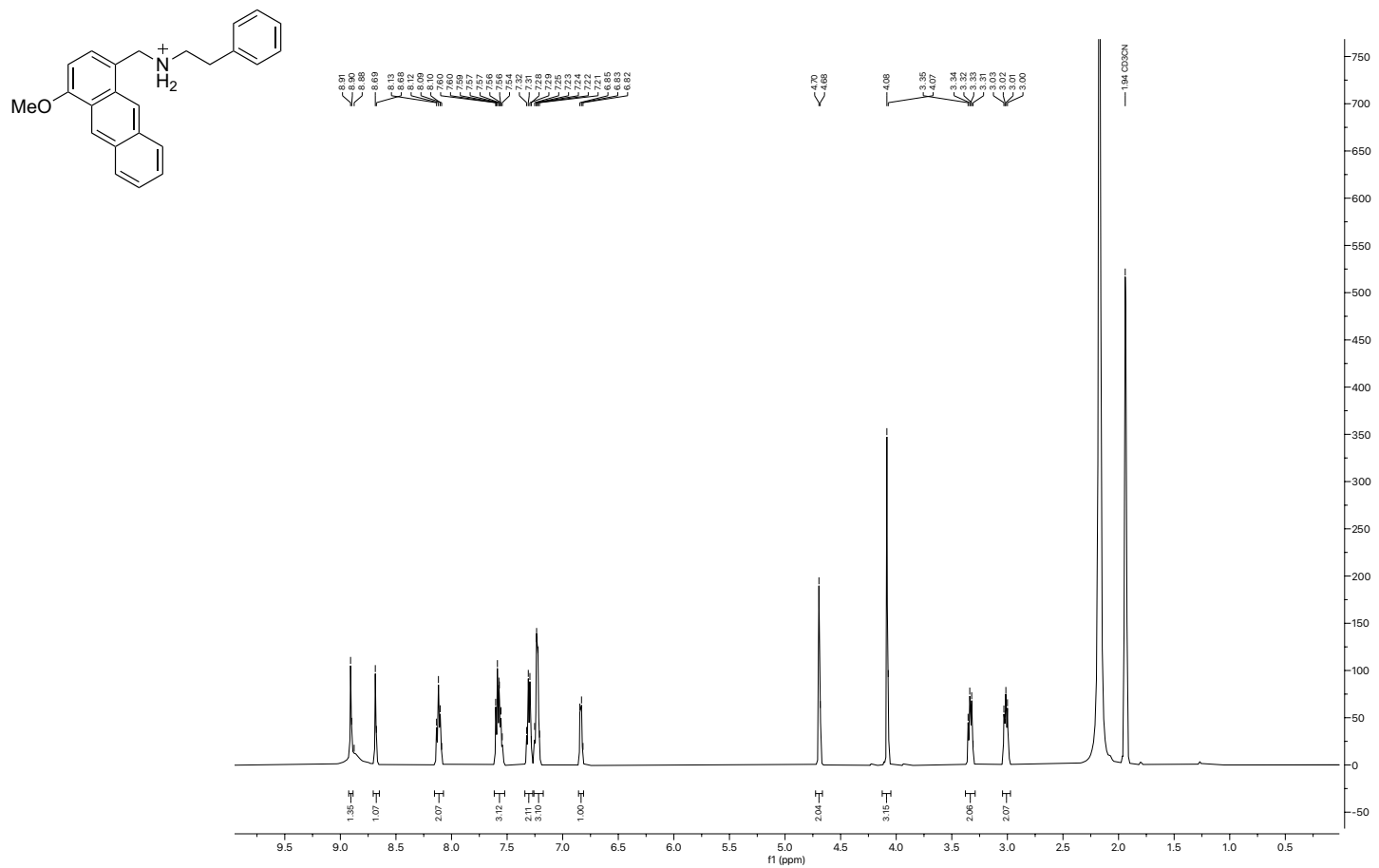


Figure S32. ¹H NMR of 3b in CD₃CN at 298 K.

Compound 3b ¹³C NMR

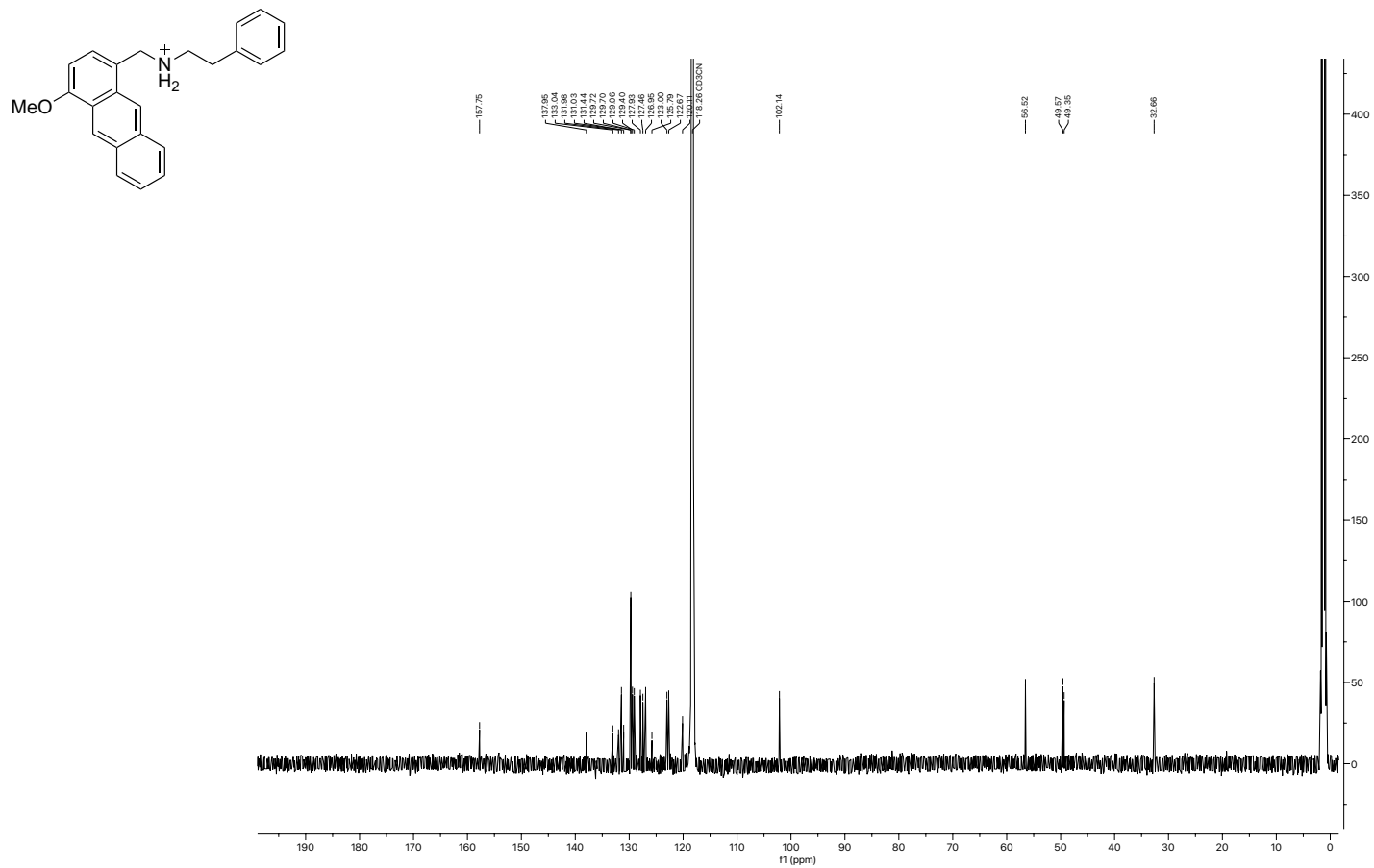


Figure S33. ¹³C NMR of 3b in CD₃CN at 298 K.

Compound 9 ¹H NMR

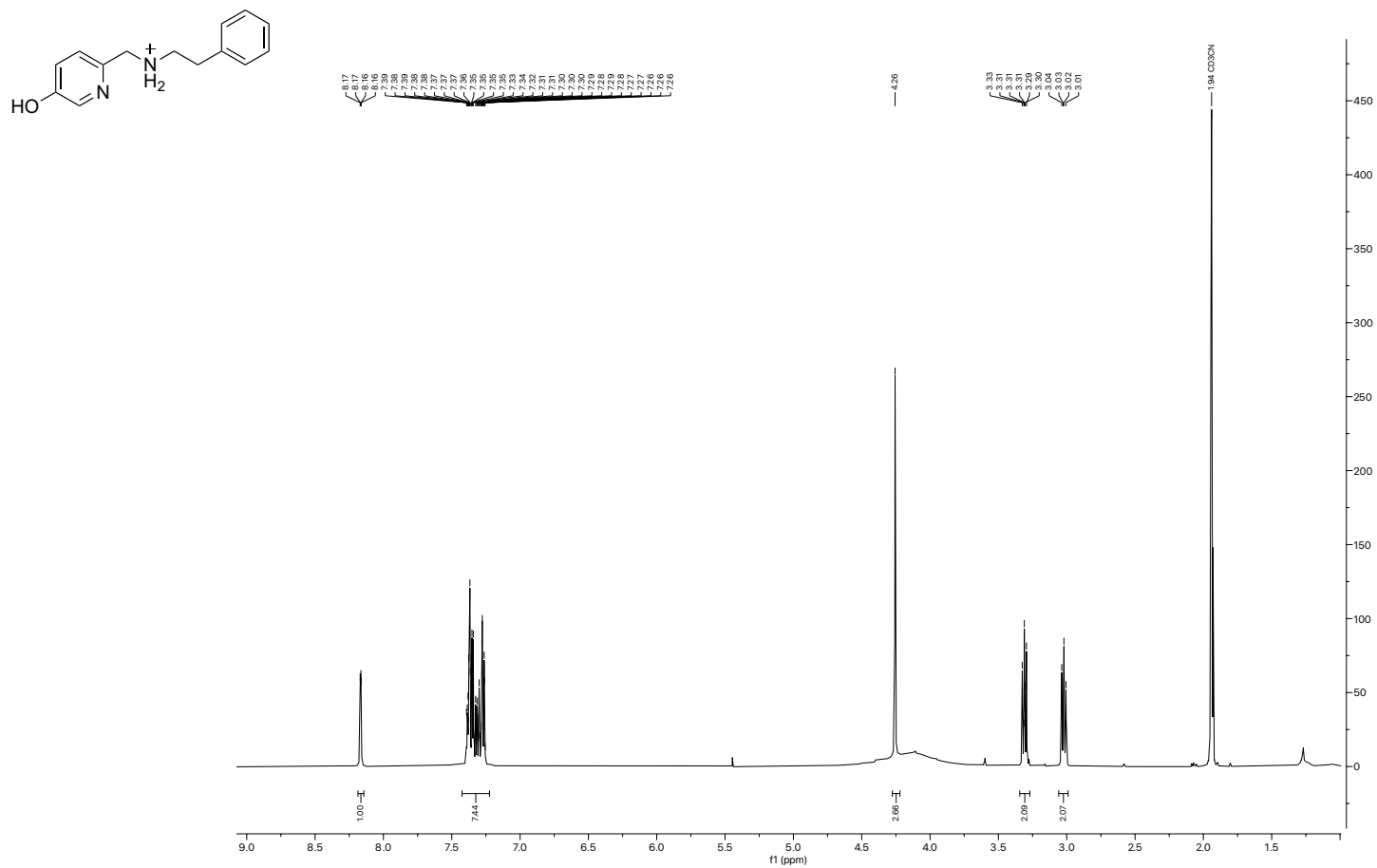


Figure S34. ¹H NMR of 9 in CD₃CN at 298 K.

Compound 9 ¹³C NMR

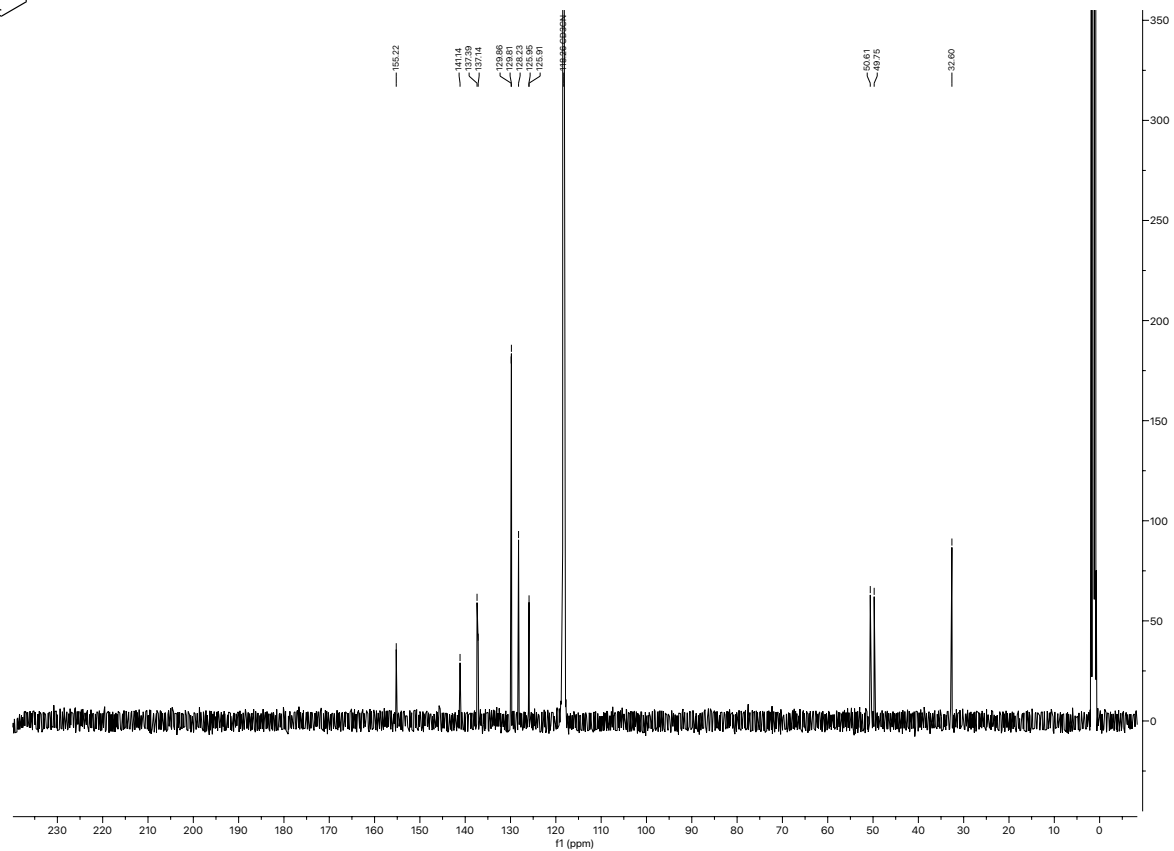
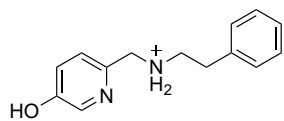


Figure S35. ¹³C NMR of 9 in CD₃CN at 298 K.

Compound 14 ¹H NMR

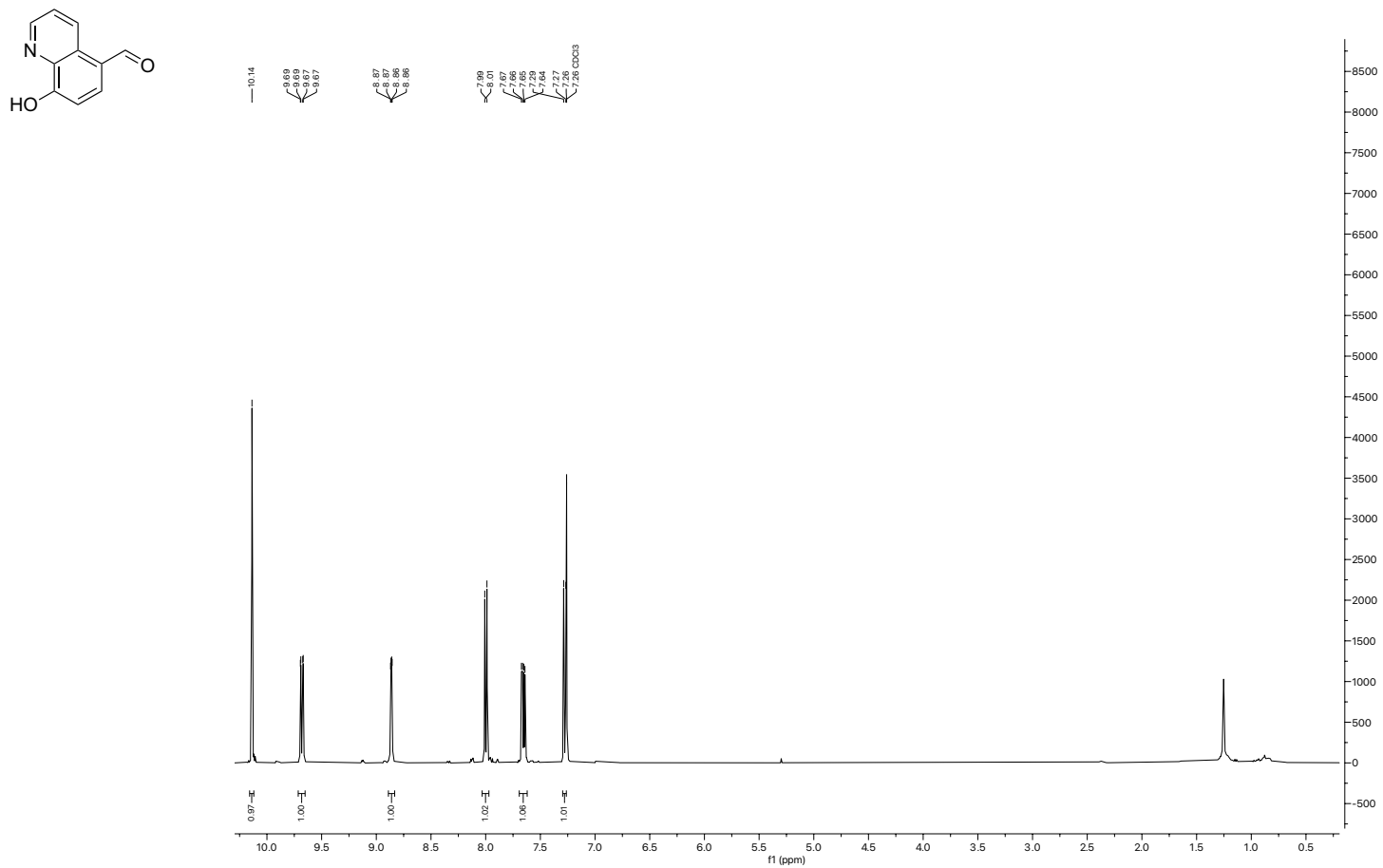


Figure S36. ¹H NMR of 14 in CDCl₃ at 298 K.

Compound 14 ¹³C NMR

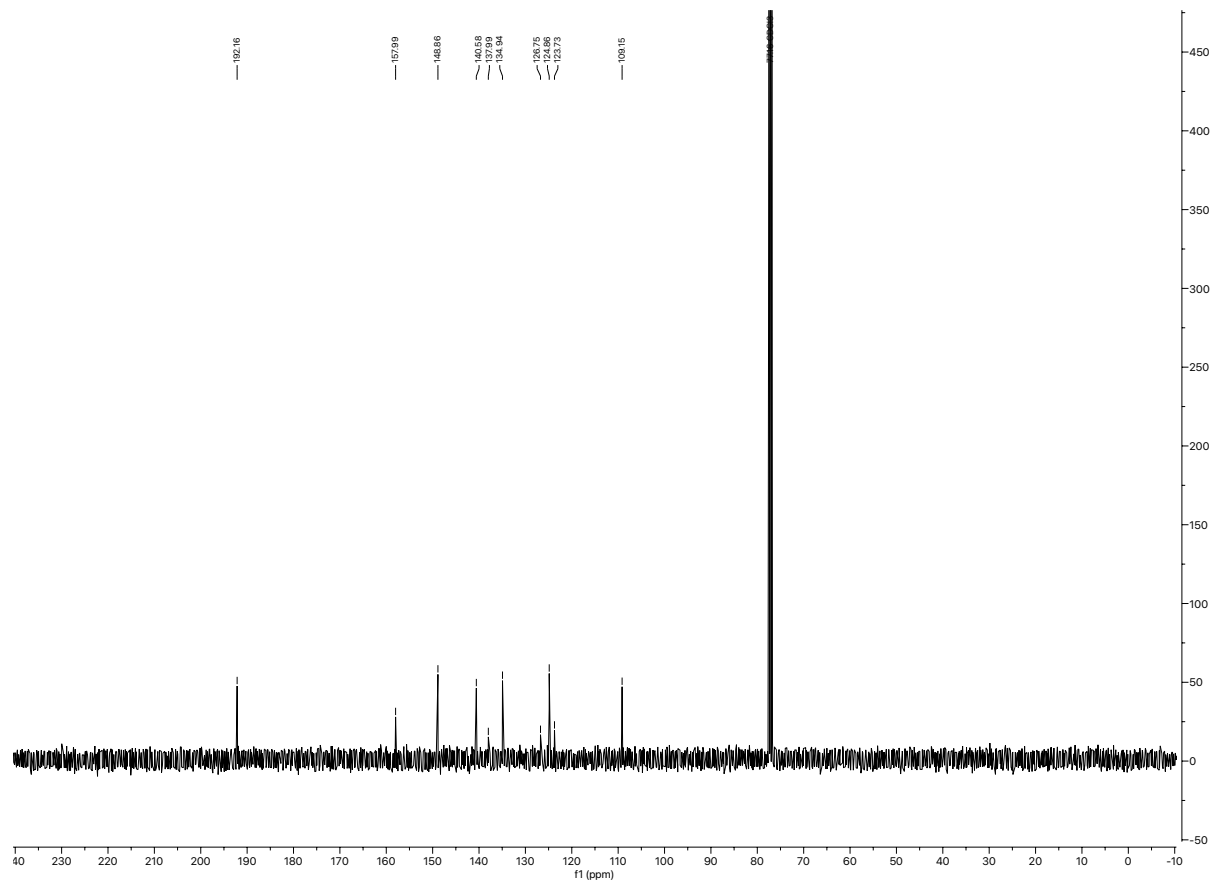
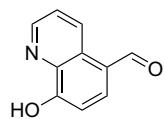


Figure S37. ¹³C NMR of 14 in CDCl₃ at 298 K.

Compound 10 ¹H NMR

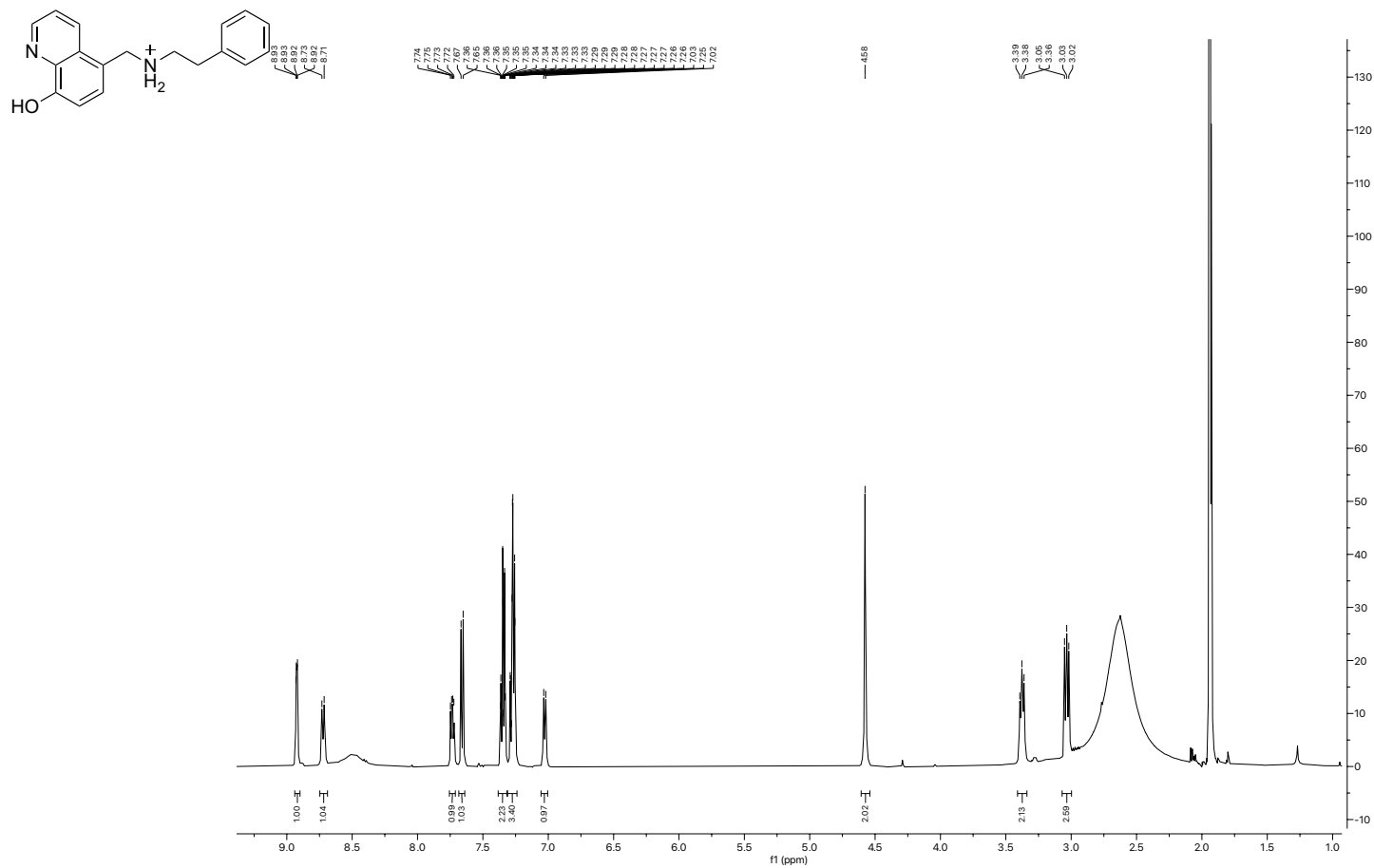


Figure S38. ¹H NMR of **10** in CD₃CN at 298 K.

Compound 10 ¹³C NMR

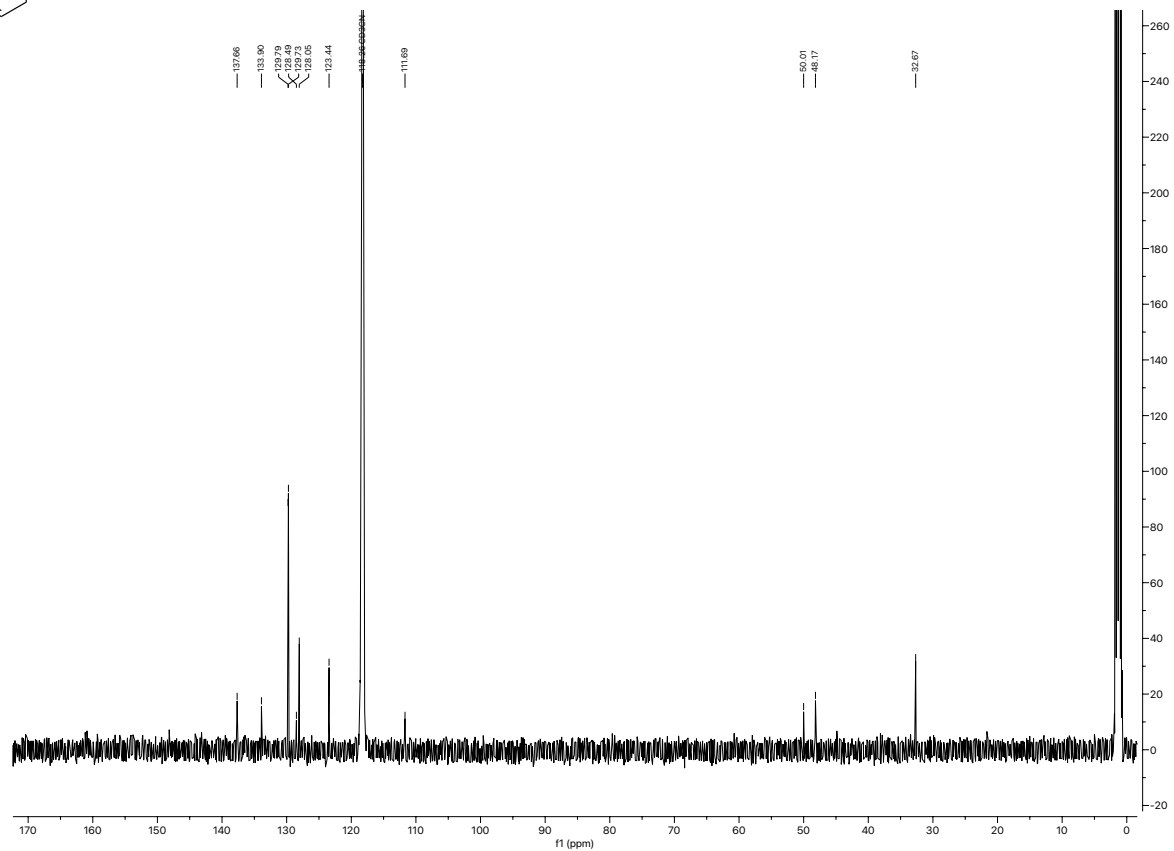
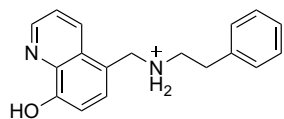


Figure S39. ¹³C NMR of 10 in CD₃CN at 298 K.

Compound 15 ¹³C NMR

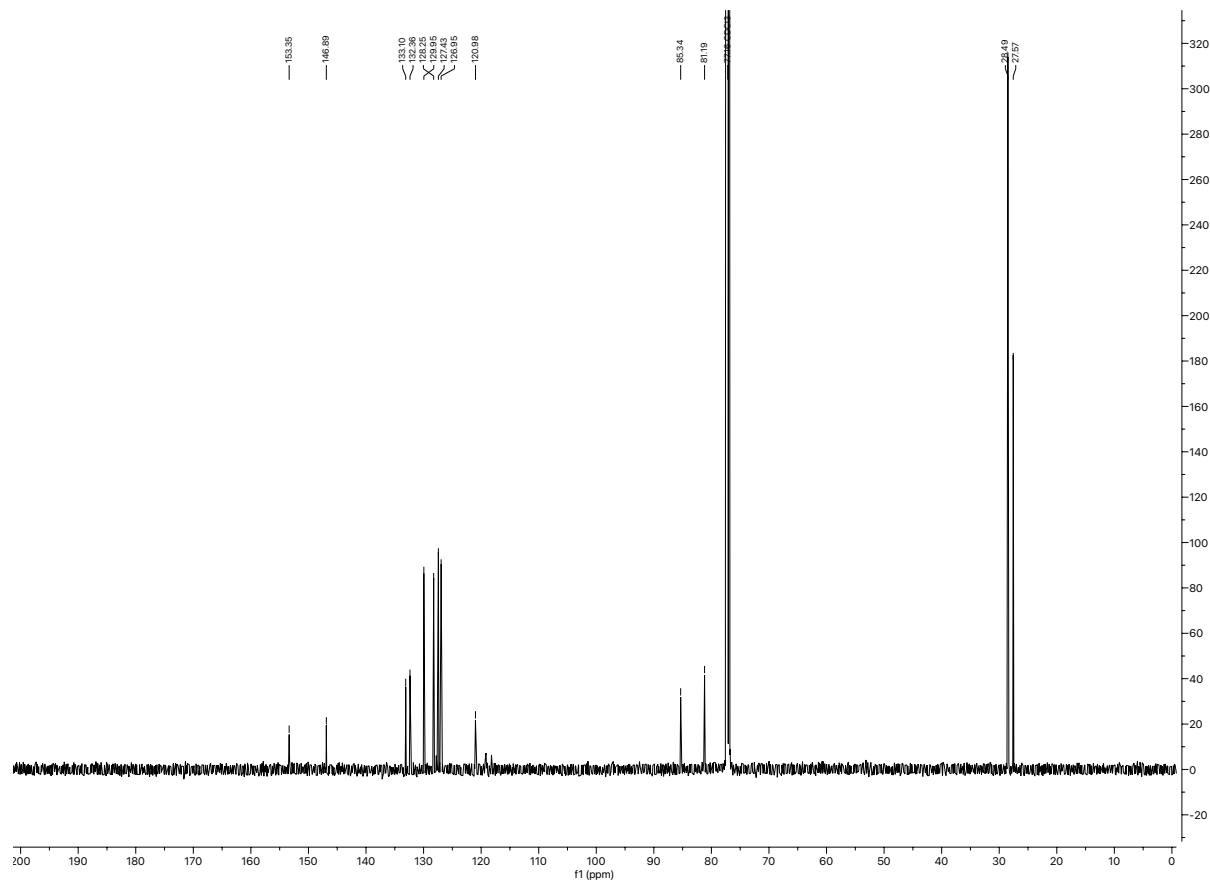
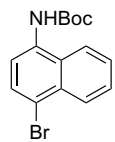


Figure S41. ¹³C NMR of 15 in CDCl₃ at 298 K.

Compound 16 ¹H NMR

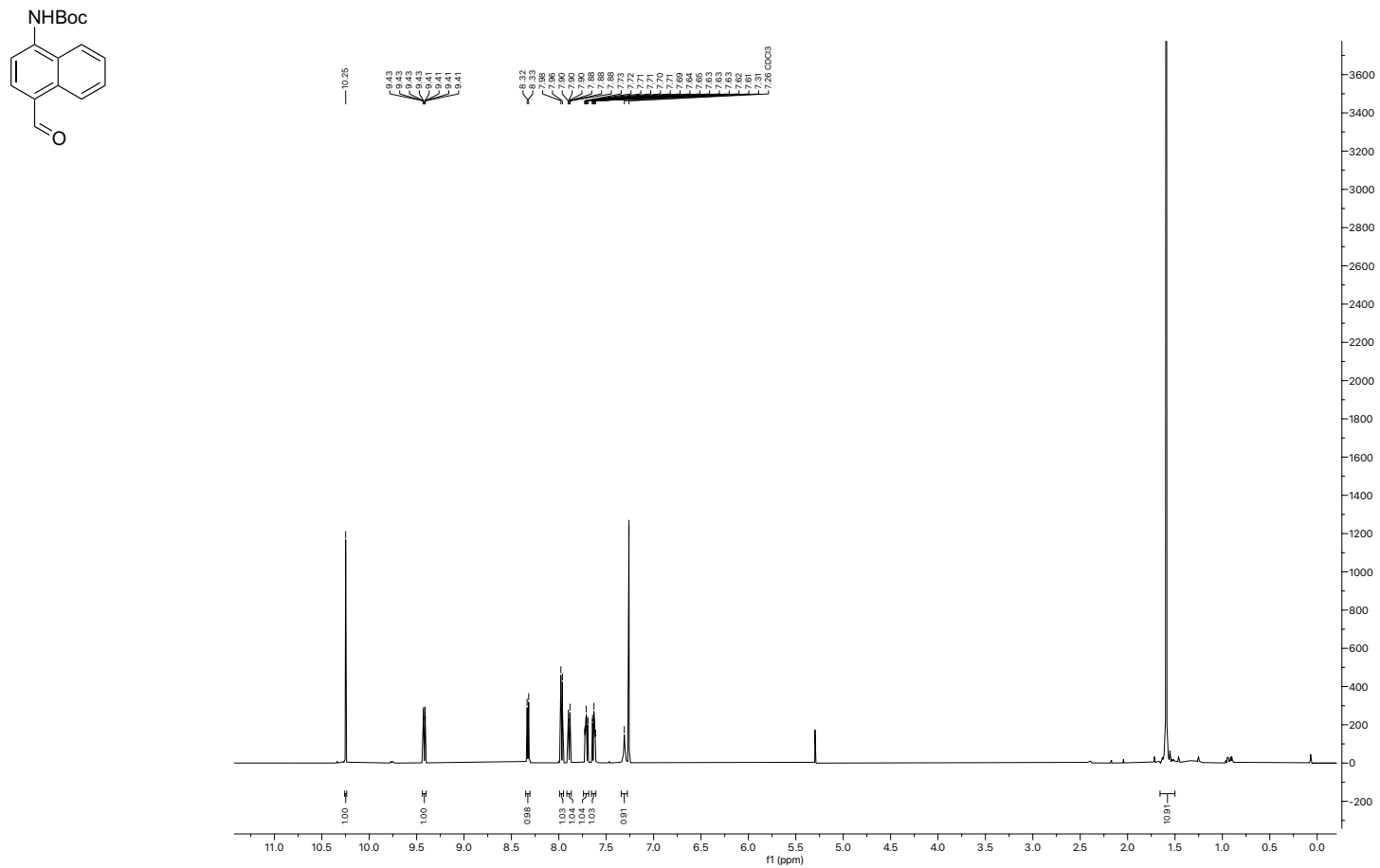


Figure S42. ¹H NMR of 16 in CDCl₃ at 298 K.

Compound 16 ¹³C NMR

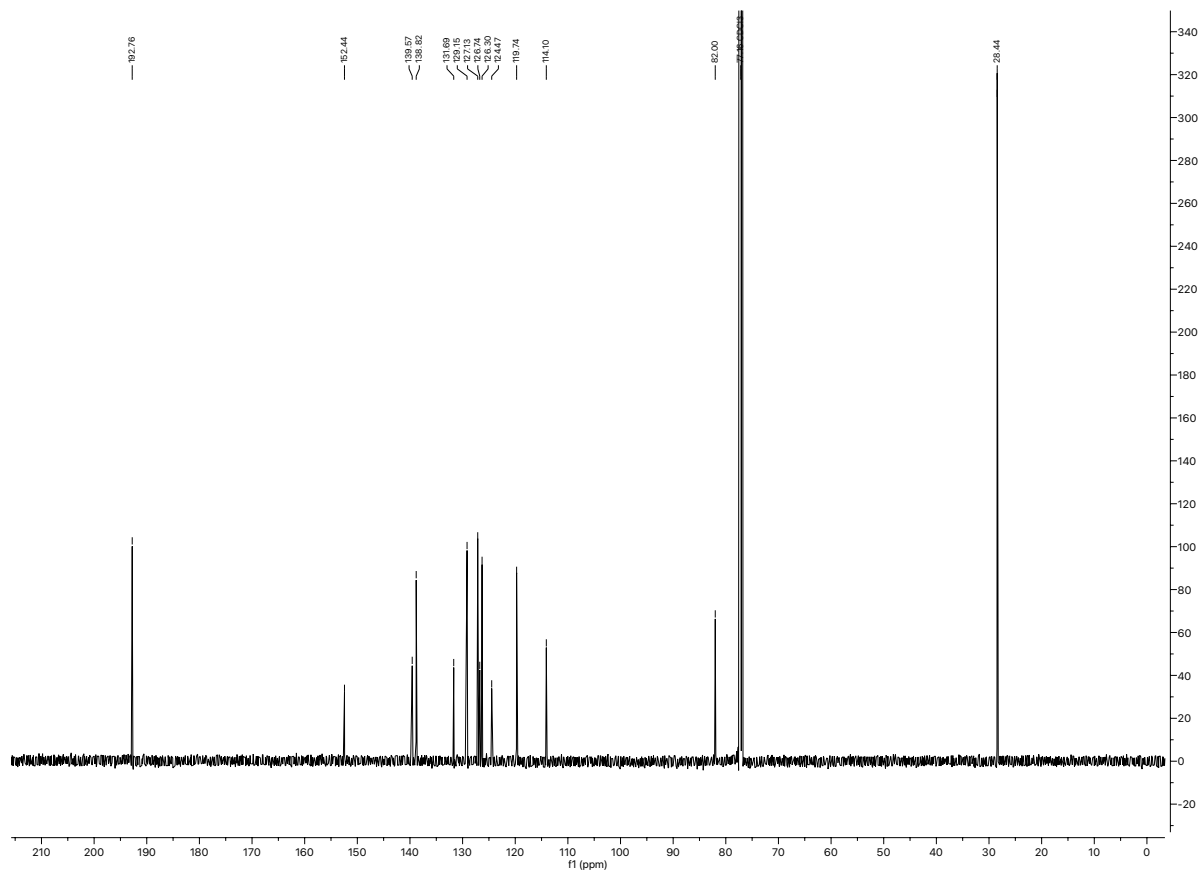
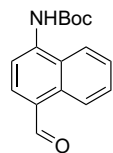


Figure S43. ¹³C NMR of 16 in CDCl₃ at 298 K.

Compound 17 ¹H NMR

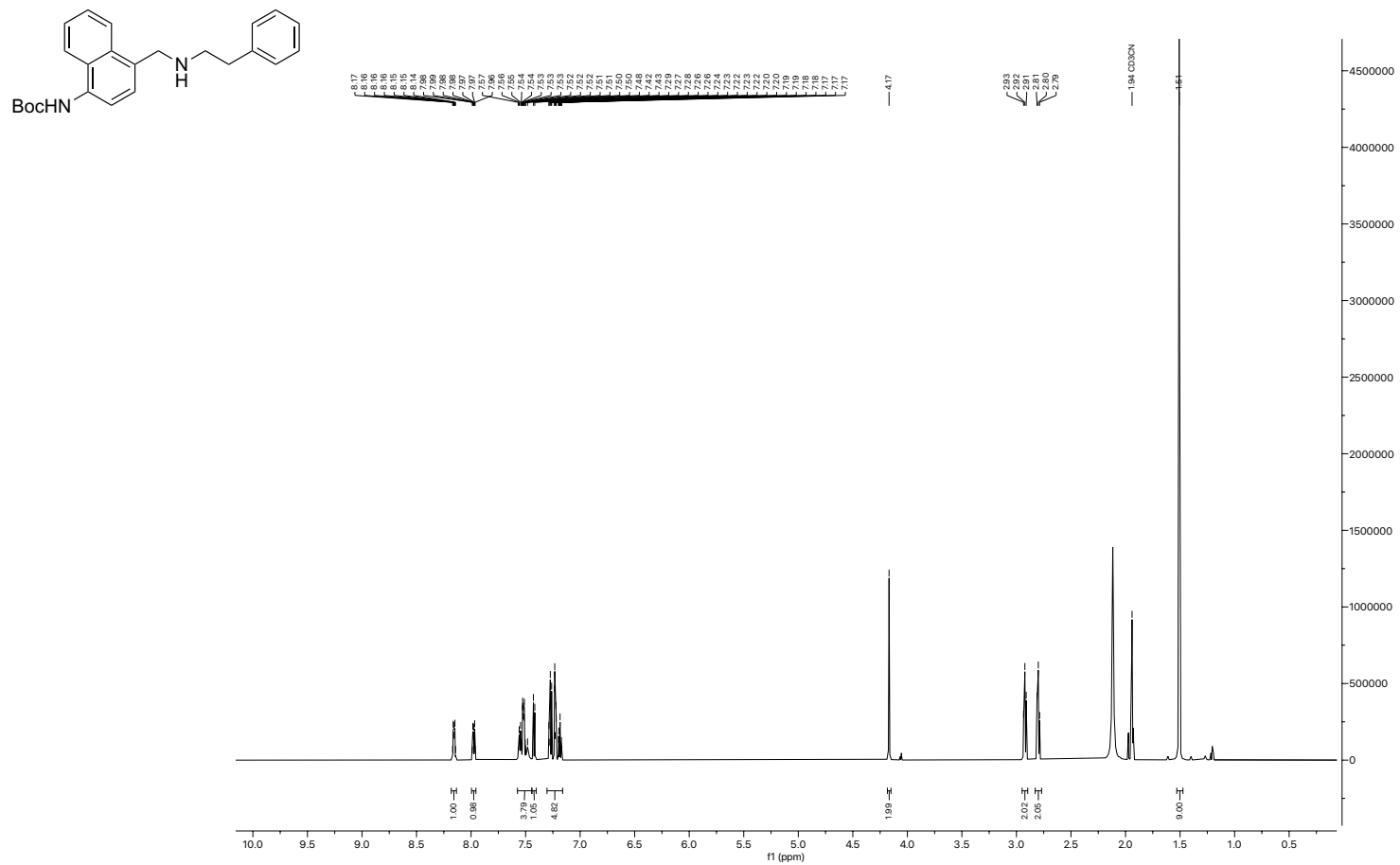


Figure S44. ¹H NMR of 17 in CD₃CN at 298 K.

Compound 17 ¹³C NMR

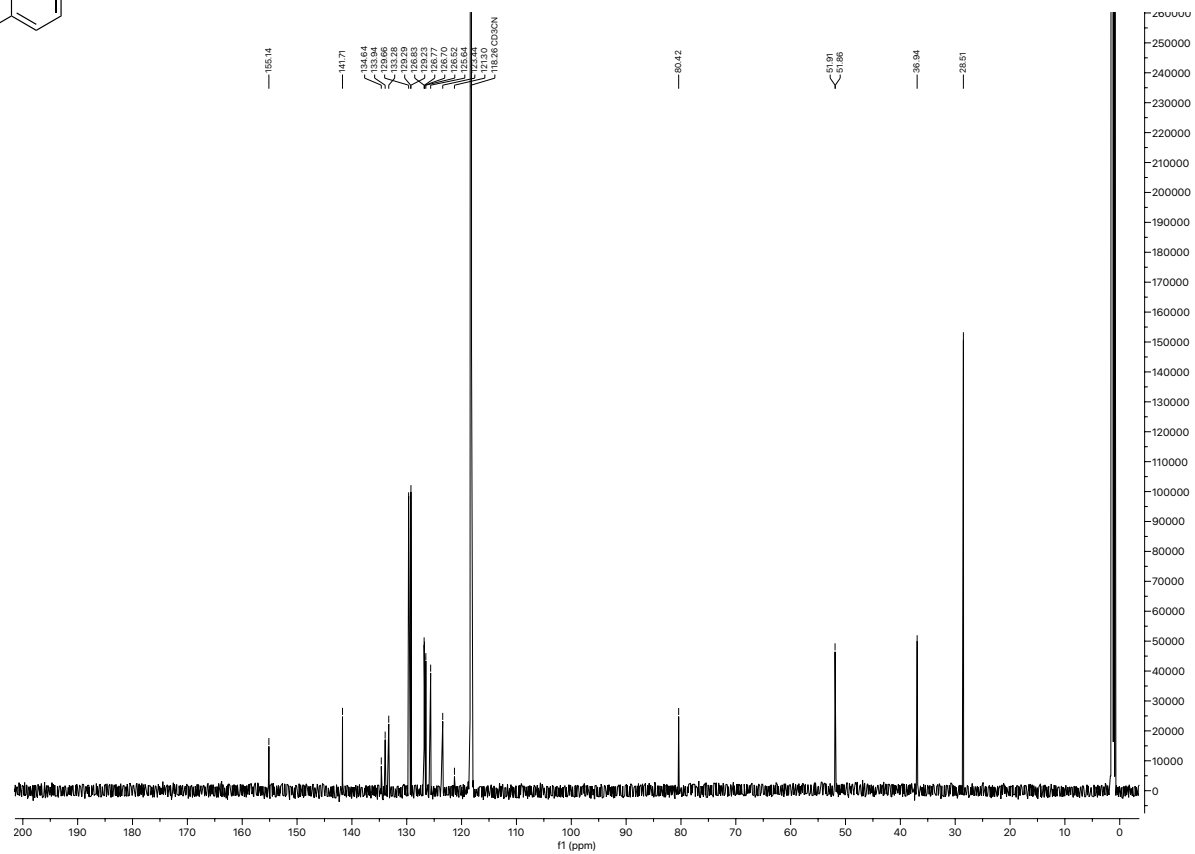
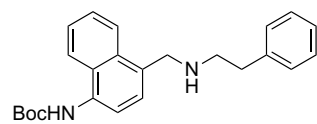


Figure S45. ¹³C NMR of 17 in CD₃CN at 298 K.

Compound 11 ¹³C NMR

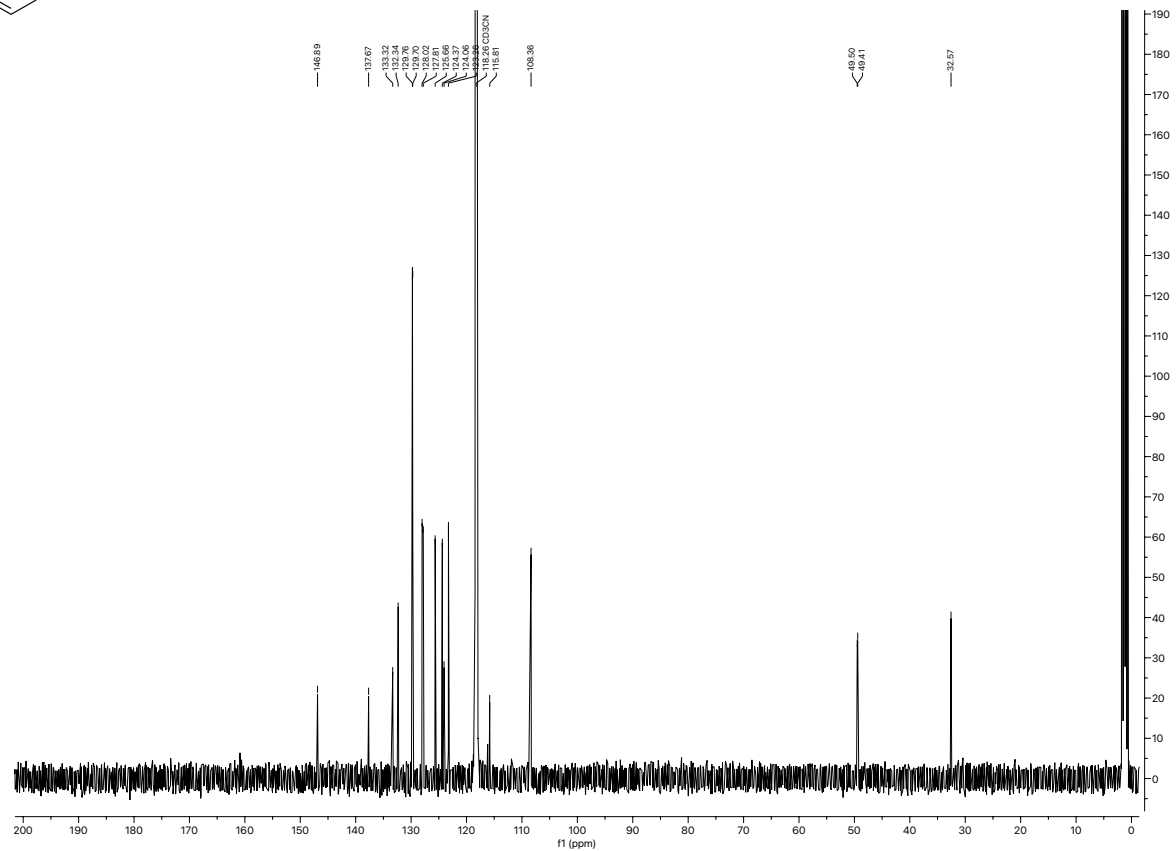
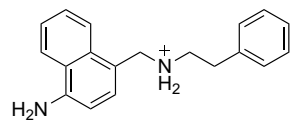


Figure S47. ¹³C NMR of 11 in CD₃CN at 298 K.

General Computational Details

All calculations were carried out with the Gaussian 16 software package.¹ Ground state geometries were optimized in water with the CPCM solvation model² using the B3LYP functional^{3,4} with the D3 correction for dispersion.⁵ The 6-31+G(d,p) basis set was used for all atoms in the system. Frequency calculations were carried out at the same level of theory to ensure that stationary points were truly minima or saddle points on the potential energy surface. Thermal corrections to free energies were calculated using Grimme's quasi-rigid rotor-harmonic oscillator approximation at 298K⁶ using the Goodvibes program.⁷ Single point energy calculations were performed with the M06-2X functional⁸ and the aug-cc-pVTZ basis set⁹ for all atoms in the system, and solvation effects were incorporated with the CPCM solvation model in water. Conformational searches were carried out using the CREST conformer-rotamer ensemble sampling tool,^{10,11} version 2.7.1 with XTB version 6.2 RC2 (SAW190805).¹²⁻¹⁴ All transition states were verified using intrinsic reaction coordinate (IRC) calculations. Images of molecular structures were rendered in CYLview.¹⁵

pK_a calculations for hydroxybenzylammoniums and azabenzylammoniums were performed using the online platform <https://xundrug.cn/molgpka>.¹⁶

Computed pK_a Values

Aromatic Scaffolds

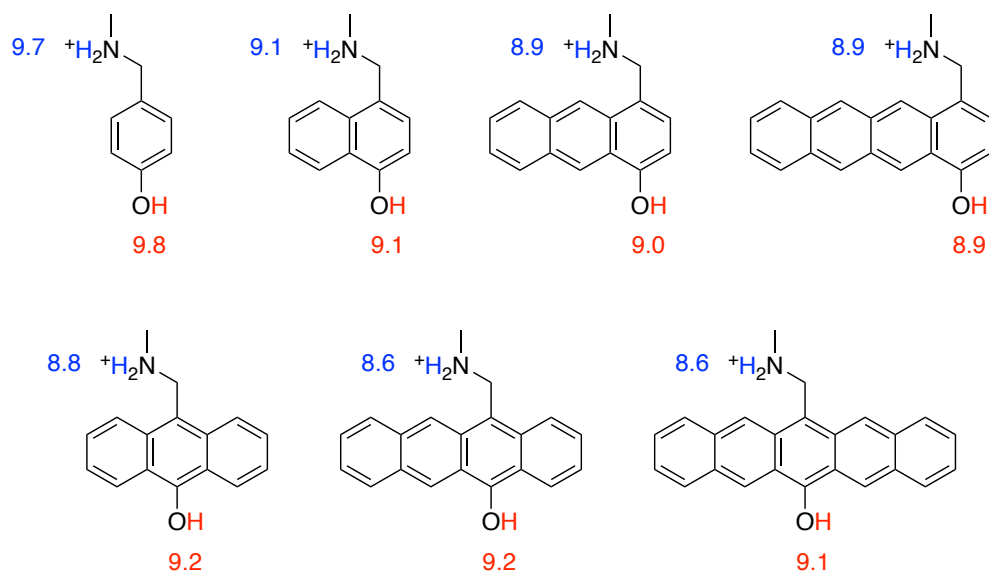


Figure S48. pK_a values calculated for protons for the scaffolds presented in **Figure 2** of the main text.

Heteroaromatic/Aza Scaffolds

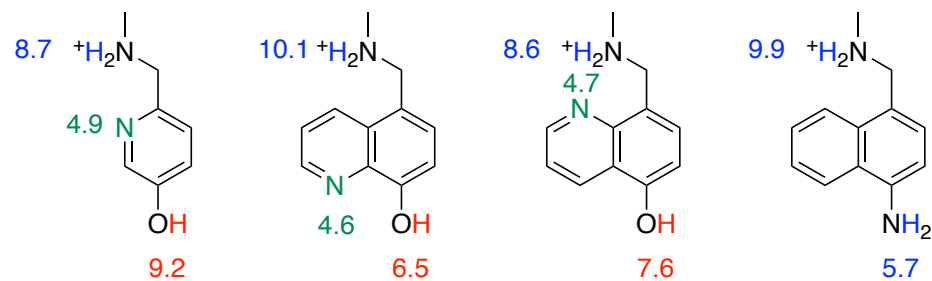


Figure S49. pK_a values calculated for protons for the scaffolds presented in **Figure 4** of the main text.

Computed Energies – Benzylammoniums (Primary Amine)

1,4-Benzene

Table S1. Computed energies for the 1,4-benzene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-441.484423	0.180642	-441.293415	0.045677	0.044651	-441.339092	-441.338066	-441.403709
TS1	-441.465476	0.175166	-441.279194	0.047794	0.046345	-441.326988	-441.325539	-441.374575
Int2	-345.584159	0.108939	-345.467851	0.037885	0.037763	-345.505736	-345.505614	-345.526779
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

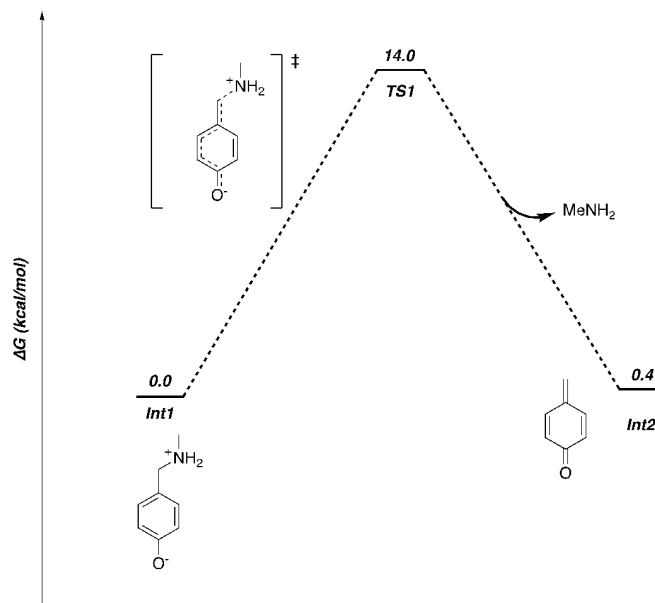


Figure S50. Free energy diagram for the 1,4-benzene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

1,4-Naphthalene

Table S2. Computed energies for the 1,4-naphthalene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-595.14508	0.227673	-594.90455	0.051131	0.050151	-594.955681	-594.954701	-595.041926
TS1	-595.130081	0.223254	-594.89347	0.053052	0.051337	-594.946522	-594.944807	-595.017629
Int2	-499.251416	0.15627	-499.085268	0.044211	0.043721	-499.129479	-499.128988	-499.172606
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

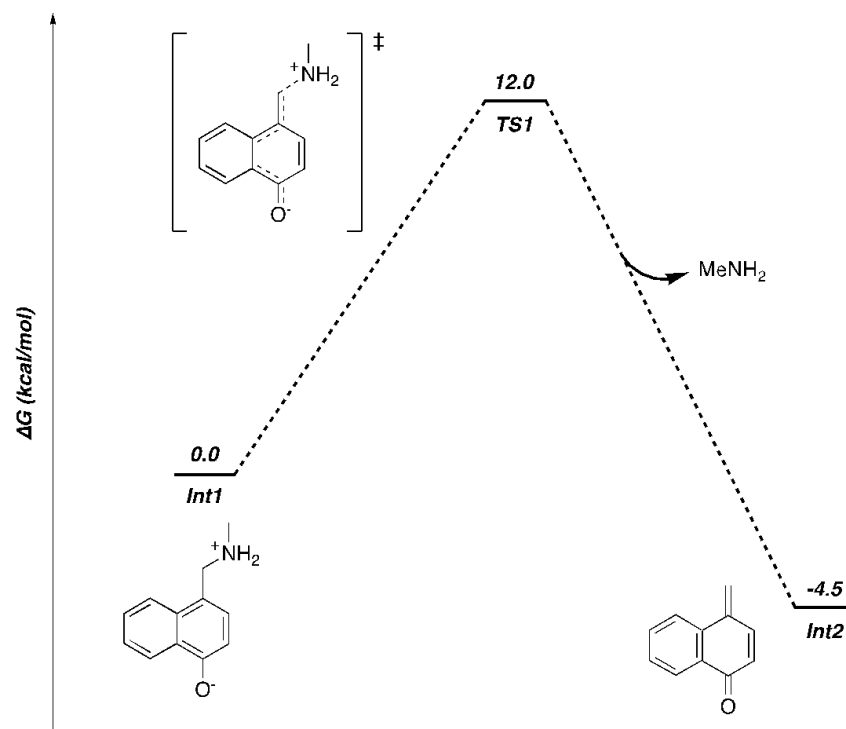


Figure S51. Free energy diagram for the 1,4-naphthalene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

1,4-Anthracene

Table S3. Computed energies for the 1,4-anthracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-748.799677	0.274412	-748.509849	0.0568	0.055505	-748.566649	-748.565355	-748.672681
TS1	-748.78589	0.269819	-748.499993	0.059699	0.057187	-748.559693	-748.55718	-748.649846
Int2	-652.908802	0.202923	-652.693312	0.050647	0.049596	-652.743958	-652.742908	-652.806198
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

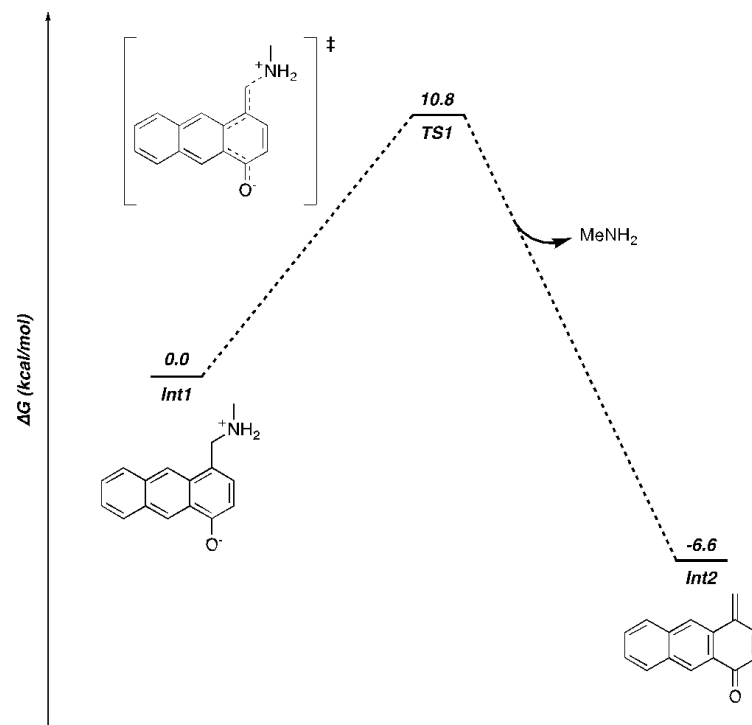


Figure S52. Free energy diagram for the 1,4-anthracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

9,10-Anthracene

Table S4. Computed energies for the 9,10-anthracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-748.799596	0.274685	-748.50947	0.057092	0.055471	-748.566562	-748.564941	-748.674229
TS1	-748.789214	0.271064	-748.502361	0.058492	0.056328	-748.560853	-748.558689	-748.656592
Int2	-652.916461	0.203493	-652.700574	0.050018	0.049228	-652.750592	-652.749801	-652.816691
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

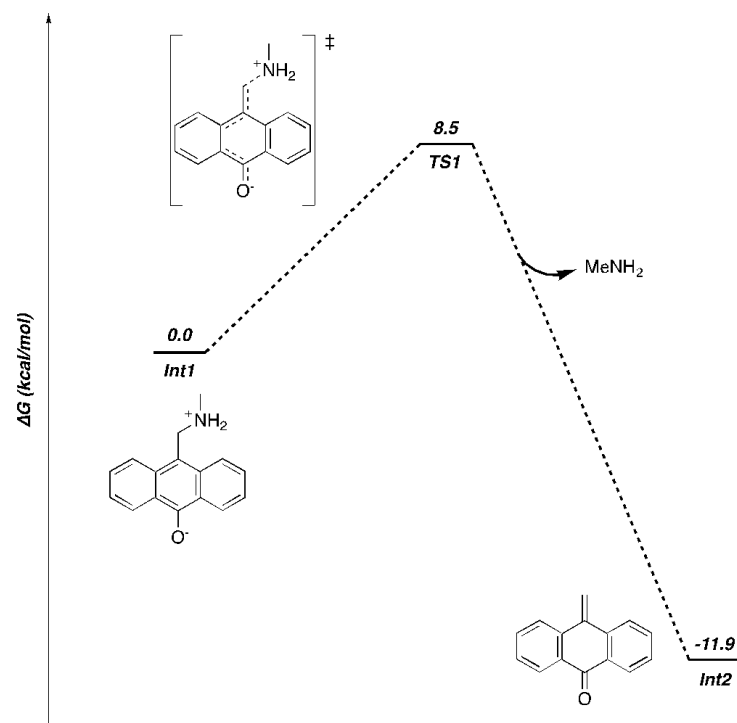


Figure S53. Free energy diagram for the 9,10-anthracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

1,4-Tetracene

Table S5. Computed energies for the 1,4-tetracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-902.450795	0.320428	-902.111979	0.064537	0.061872	-902.176516	-902.173851	-902.29865
TS1	-902.437274	0.316506	-902.102057	0.065263	0.062512	-902.16732	-902.164569	-902.276777
Int2	-806.561034	0.249392	-806.296349	0.056989	0.055338	-806.353338	-806.351687	-806.433807
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

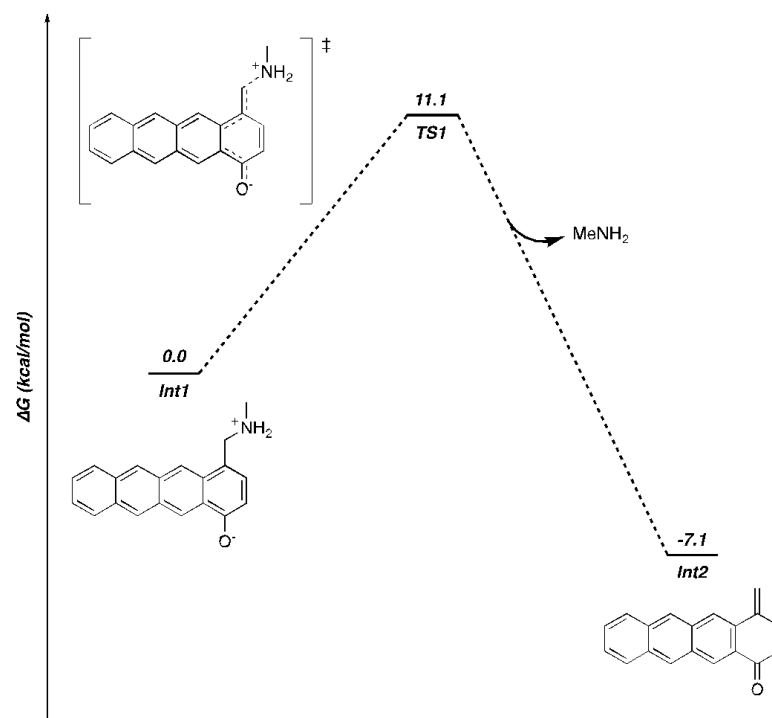


Figure S54. Free energy diagram for the 1,4-tetracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

5,12-Tetracene

Table S6. Computed energies for the 5,12-tetracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-902.45398	0.321028	-902.11464	0.063926	0.061523	-902.17857	-902.17617	-902.30371
TS1	-902.44431	0.317596	-902.10821	0.064715	0.061958	-902.17293	-902.17017	-902.28817
Int2	-806.57408	0.250112	-806.30889	0.056158	0.054868	-806.36505	-806.36376	-806.45053
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

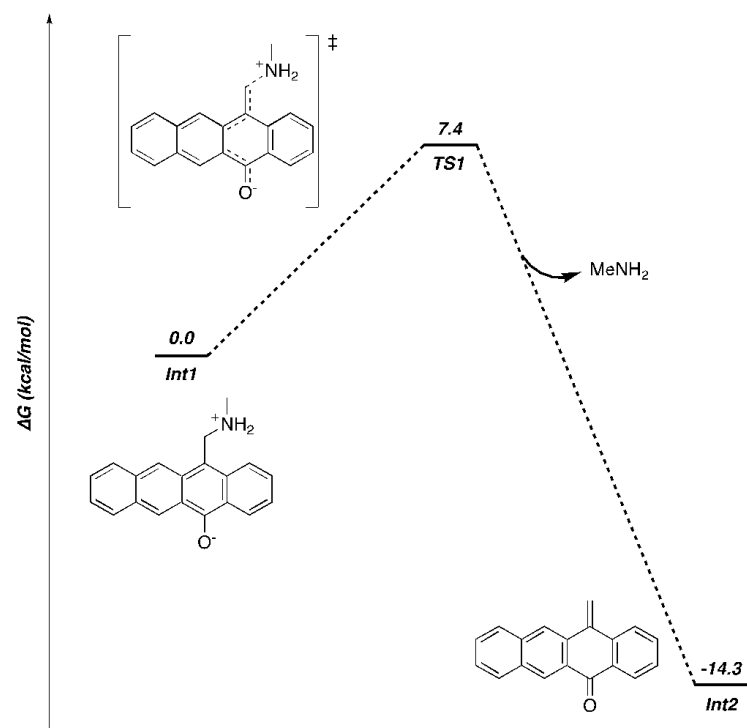


Figure S55. Free energy diagram for the 5,12-tetracene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

6,13-Pentacene

Table S7. Computed energies for the 6,13-pentacene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-1056.107499	0.367446	-1055.719115	0.069603	0.066717	-1055.788718	-1055.785832	-1055.933759
TS1	-1056.09938	0.364342	-1055.713883	0.070522	0.067328	-1055.784405	-1055.781211	-1055.919905
Int2	-960.231831	0.296763	-959.917305	0.062203	0.060382	-959.979508	-959.977686	-960.08449
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

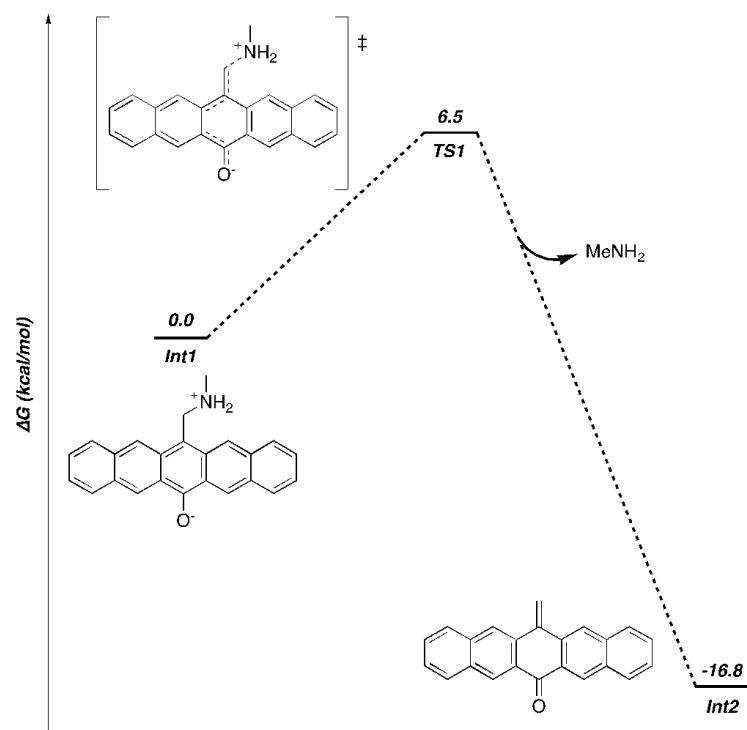


Figure S56. Free energy diagram for the 6,13-pentacene hydroxybenzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

8-Hydroxyquinoline

Table S8. Computed energies for the 8-hydroxyquinoline benzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-611.181023	0.215831	-610.952376	0.051504	0.050206	-611.00388	-611.002582	-611.08325
TS1	-611.164908	0.211101	-610.940458	0.053316	0.051434	-610.993774	-610.991892	-611.05811
Int2	-515.284486	0.144401	-515.130319	0.044084	0.043566	-515.174403	-515.173885	-515.21201
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

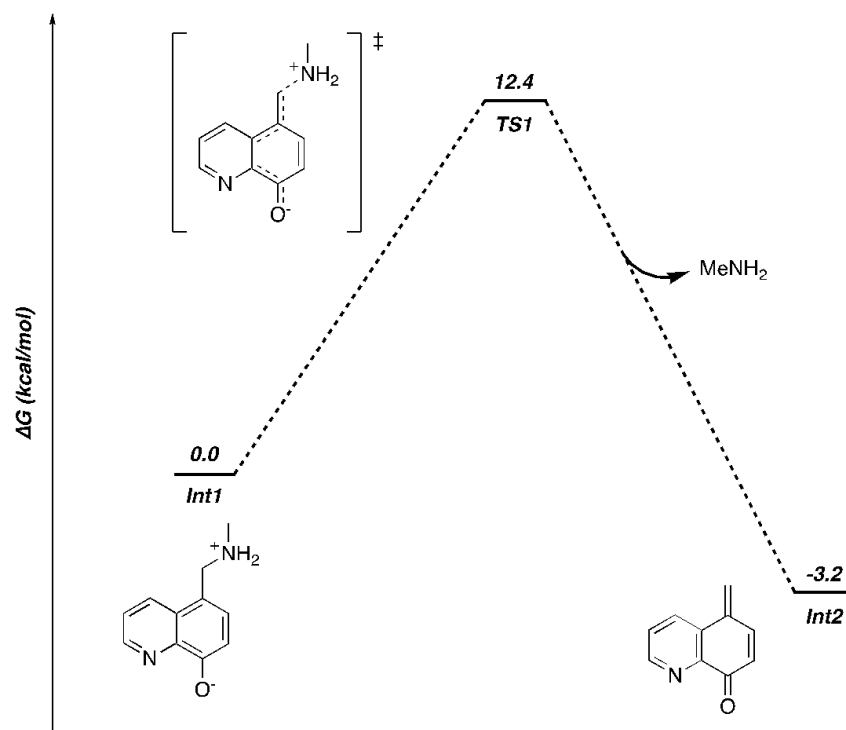


Figure S57. Free energy diagram for the 8-hydroxyquinoline benzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

5-Hydroxyquinoline

Table S9. Computed energies for the 5-hydroxyquinoline benzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-611.195362	0.215481	-610.967323	0.050378	0.049485	-611.017701	-611.016807	-611.097251
TS1	-611.171011	0.210683	-610.946842	0.053789	0.051759	-611.000631	-610.998601	-611.064188
Int2	-515.290251	0.144528	-515.136033	0.043701	0.043418	-515.179733	-515.179451	-515.217369
Methylamine	-95.87827	0.064024	-95.809891	0.027277	0.027279	-95.837168	-95.83717	-95.849641

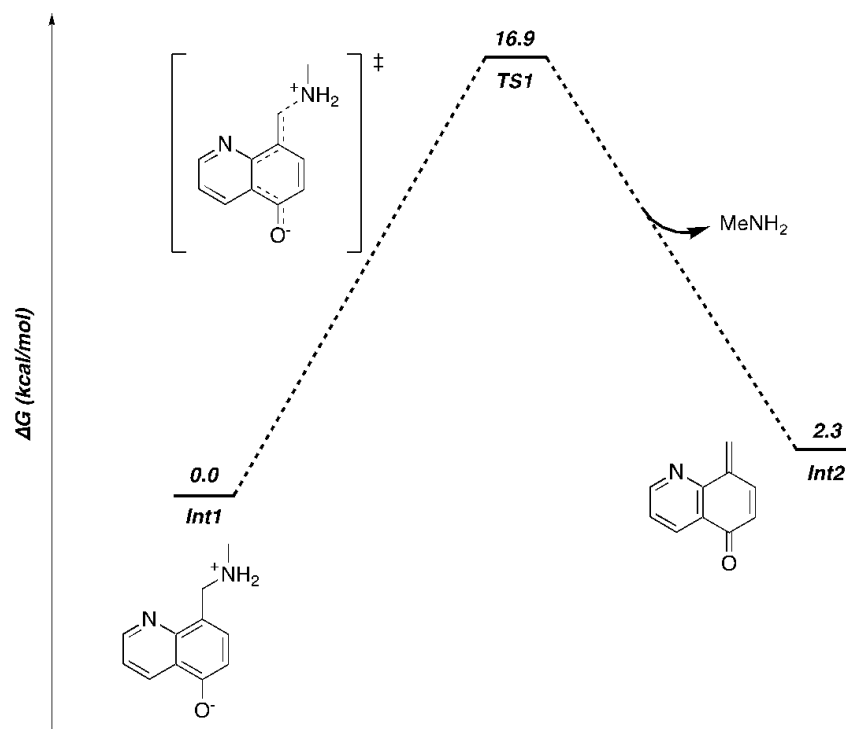


Figure S58. Free energy diagram for the 1,5-quinoline benzylammonium calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

Computed Energies – Benzylammoniums (Secondary and Tertiary Amine)

1,4-Naphthalene (Secondary Amine)

Table S10. Computed energies for the 1,4-naphthalene hydroxybenzylammonium (Secondary amine) calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-634.460077	0.255856	-634.190192	0.053651	0.05234	-634.243842	-634.242531	-634.345018
TS1	-634.444081	0.250817	-634.178453	0.057209	0.054657	-634.235662	-634.23311	-634.318325
Int2	-499.251416	0.15627	-499.085268	0.044211	0.043721	-499.129479	-499.128988	-499.172606
Dimethylamine	-135.188628	0.092395	-135.090937	0.030717	0.030723	-135.121654	-135.121659	-135.147284

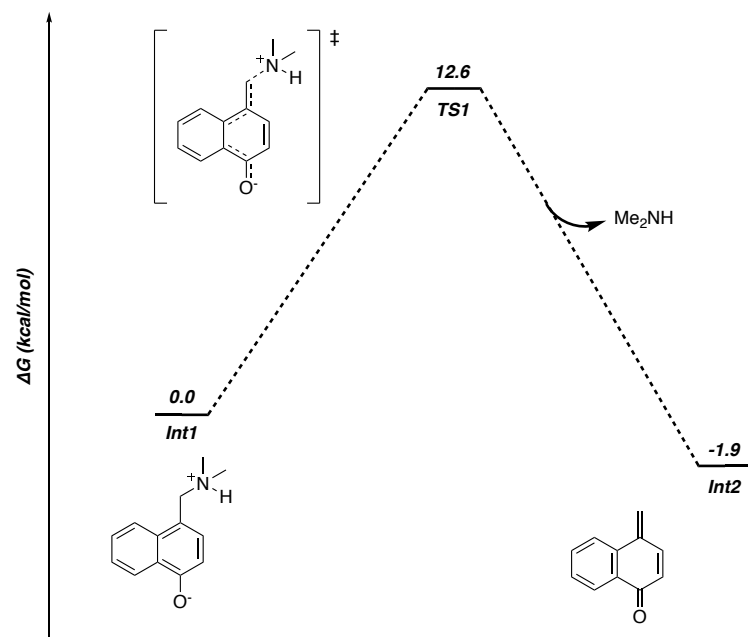


Figure S59. Free energy diagram for the 1,4-naphthalene hydroxybenzylammonium (Secondary amine) calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

1,4-Naphthalene (Tertiary Amine)

Table S11. Computed energies for the 1,4-naphthalene hydroxybenzylammonium (Tertiary amine) calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
Int1	-673.771674	0.284006	-673.472732	0.054928	0.053797	-673.52766	-673.52653	-673.645981
TS1	-673.760536	0.278821	-673.4659	0.058244	0.056141	-673.524143	-673.52204	-673.623001
Int2	-499.251416	0.15627	-499.085268	0.044211	0.043721	-499.129479	-499.128988	-499.172606
Trimethylamine	-174.502343	0.120291	-174.375783	0.033462	0.033472	-174.409245	-174.409254	-174.44907

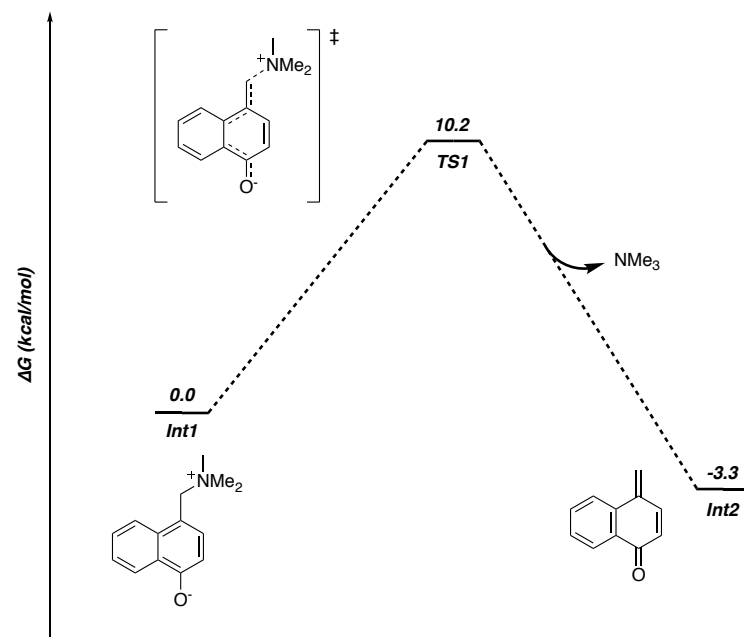


Figure S60. Free energy diagram for the 1,4-naphthalene hydroxybenzylammonium (Tertiary amine) calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory.

Computed Energies – Isomerization

1,4-Hydroxyanthraldehyde

Table S12. Computed energies for the isomers of the 1,4-hydroxyanthraldehyde calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
HA	-728.154897	0.207604	-727.933629	0.052679	0.051855	-727.986308	-727.985483	-728.057741
AA	-728.137868	0.20697	-727.917068	0.054255	0.05253	-727.971323	-727.969598	-728.037803
AE	-728.141269	0.207846	-727.919649	0.053849	0.052407	-727.973498	-727.972056	-728.043536

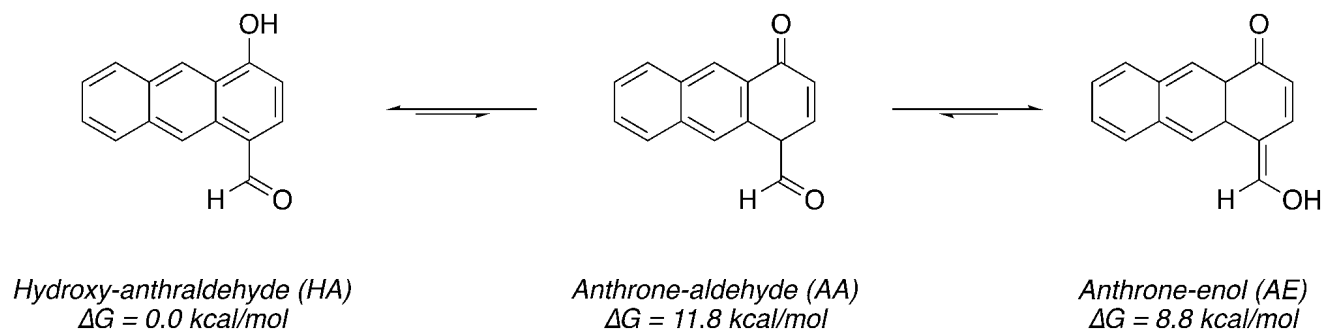


Figure S61. Free energies for the isomers of the 1,4-hydroxyanthraldehyde calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

9,10-Hydroxyanthraldehyde

Table S13. Computed energies for the isomers of the 9,10-hydroxyanthraldehyde calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
HA	-728.145769	0.207438	-727.924355	0.053989	0.052617	-727.978344	-727.976972	-728.048799
AA	-728.152361	0.207596	-727.931059	0.053811	0.052275	-727.984871	-727.983335	-728.053731
AE	-728.147042	0.208643	-727.924971	0.052163	0.05139	-727.977134	-727.976361	-728.052157

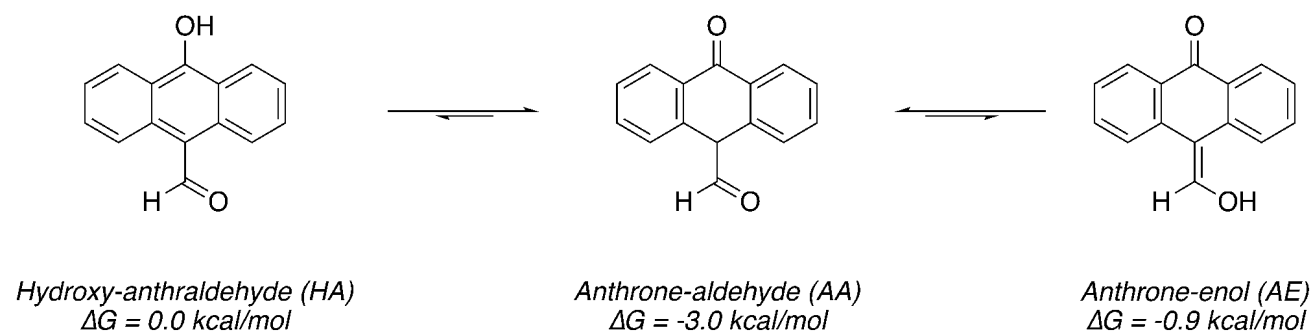


Figure S62. Free energies for the isomers of the 9,10-hydroxyanthraldehyde calculated at the M06-2X/aug-cc-pVTZ, CPCM(Water)//B3LYP-D3/6-31+G(d,p), CPCM(Water) level of theory. All units are in Hartrees.

Calculated Coordinates – Benzylammoniums (Primary Amine)

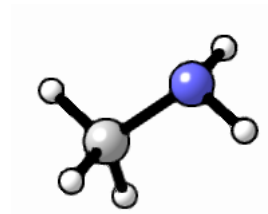
Methylamine

Methylamine

Charge: 0 Multiplicity: 1

Negative Frequency: None

H	1.14990800	-0.81308700	0.34071300
N	0.75418900	0.00000000	-0.12535400
H	1.14990600	0.81308800	0.34071200
C	-0.71079700	0.00000000	0.01700100
H	-1.12251900	0.88310600	-0.48189300
H	-1.12252600	-0.88307400	-0.48194600
H	-1.06931500	-0.00002900	1.05788800



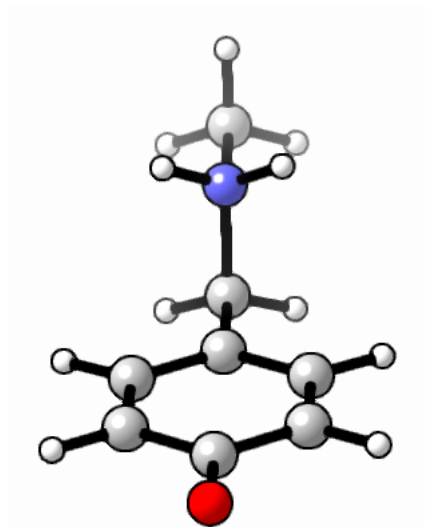
1,4-Benzene

Int1

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	0.42530700	1.20654900	-0.31070700
C	1.77916000	1.21523200	-0.00327500
C	-0.28707900	0.00004600	-0.46981100
C	2.53232600	-0.00002000	0.17259100
C	1.77911800	-1.21523800	-0.00333800
C	0.42526600	-1.20649200	-0.31077600
H	2.30861100	-2.15913000	0.10652500
H	-0.09837600	-2.15364600	-0.43734100
C	-1.75263200	0.00007900	-0.74347500
H	-2.08705400	0.89008500	-1.28129400
H	-2.08706500	-0.88980700	-1.28148900
H	-2.27558100	-0.81541800	1.11710400
H	-2.27554900	0.81513800	1.11730800
C	-4.04970900	-0.00001700	0.38818400
H	-4.32942600	0.89419400	-0.16762800
H	-4.32945400	-0.89407800	-0.16785900
H	-4.52200300	-0.00013600	1.36994900
N	-2.56192800	-0.00006600	0.56692100
O	3.78855900	-0.00005000	0.45881300
H	-0.09830600	2.15372700	-0.43721600
H	2.30868700	2.15909900	0.10663500

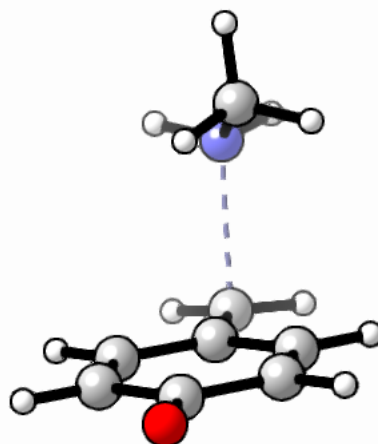


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -92.09

C	0.35295000	1.33706700	-0.42075800
C	1.60140100	0.94504600	-0.80413000
C	-0.37166300	0.64746300	0.61939600
C	2.26684300	-0.19829700	-0.18615800
C	1.52057000	-0.89256600	0.85850000
C	0.27154300	-0.49061600	1.23021000
H	2.00096600	-1.74659500	1.32753900
H	-0.26663800	-1.02888600	2.00728200
C	-1.64716500	1.02929500	0.97909000
H	-2.14719900	0.56806400	1.82224100
H	-2.08263100	1.94457900	0.59686700
H	-3.98676900	-0.40824600	0.12706900
H	-3.45407400	0.51795300	-1.12586400
C	-2.43255800	-1.27444100	-0.94049600
H	-2.99773200	-1.83523100	-1.69608400
H	-1.50052400	-0.92083000	-1.39136300
H	-2.17129900	-1.95188100	-0.12325800
N	-3.16288200	-0.12837100	-0.39776500
O	3.41934500	-0.56490200	-0.53611400
H	-0.12320900	2.18954000	-0.90025400
H	2.14300400	1.47165000	-1.58484000

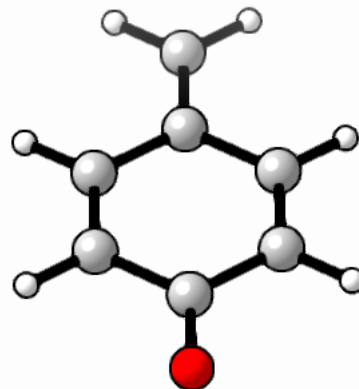


Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	-0.64362900	-1.24785800	-0.00001300
C	0.70931200	-1.25308400	-0.00000600
C	1.47899600	0.00000000	0.00001700
O	2.72412700	0.00000000	0.00000300
C	0.70931200	1.25308400	0.00001400
C	-0.64362900	1.24785800	0.00000700
C	-1.40226100	0.00000000	-0.00000500
C	-2.75822400	0.00000000	-0.00001100
H	-3.32304500	0.92724100	-0.00000400
H	-3.32304800	-0.92723900	-0.00002000
H	-1.20025700	2.18135000	0.00001000
H	1.27715900	2.17837800	0.00001900
H	1.27716000	-2.17837800	-0.00001500
H	-1.20025500	-2.18135100	-0.00002600

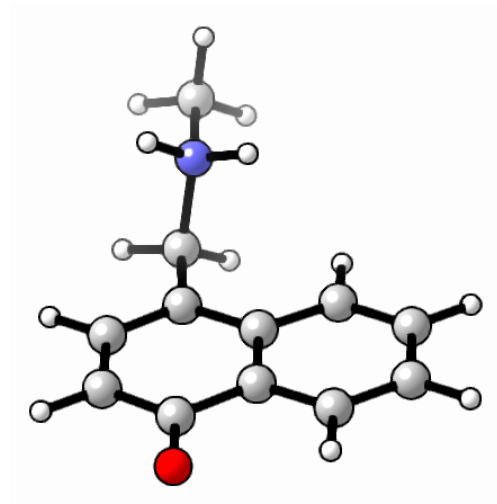


1,4-Naphthalene

Int1

Charge: 0 Multiplicity: 1
Negative Frequency: None

C	0.75195800	2.73033800	-0.17142600
C	-0.17915300	1.72290400	-0.35151600
C	0.17892200	0.34531400	-0.25670200
C	1.55138600	0.03333000	0.02907200
C	2.47800300	1.08607800	0.20686800
C	2.09858000	2.41474000	0.11480800
H	0.44245800	3.76881300	-0.25303600
H	-1.20200300	2.00519900	-0.58569600
C	-0.76657300	-0.72162800	-0.42864400
C	2.01732400	-1.36276200	0.13834300
H	3.50739800	0.81608400	0.42096000
H	2.82664200	3.20808700	0.25808100
C	1.02167600	-2.36214400	-0.05213300
C	-0.31041400	-2.03673800	-0.31747200
H	1.32621400	-3.40351500	0.01392500
H	-1.02640500	-2.84727200	-0.44967200
C	-2.21107000	-0.45701100	-0.68039500
H	-2.40592400	0.36008500	-1.37915900
H	-2.73416400	-1.34674000	-1.03515200
H	-2.82494300	-0.81261700	1.29153700
H	-2.45565700	0.75183800	1.02339300
C	-4.39642100	0.26374500	0.44626600
H	-4.81851000	0.51950600	1.41769400
H	-4.48930700	1.10500300	-0.23963300
H	-4.89332600	-0.61485100	0.03623800
N	-2.94266300	-0.05201000	0.61619300
O	3.24260800	-1.63531700	0.38809600

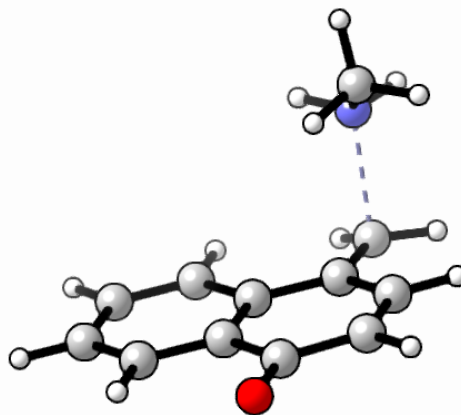


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -200.87

C	-1.30721600	2.63423600	-0.08833000
C	-0.19784600	1.88731600	-0.45775000
C	-0.21863400	0.47145100	-0.42684100
C	-1.41334600	-0.16671200	0.01458100
C	-2.53027200	0.61066700	0.38431500
C	-2.48818600	1.99570600	0.33529200
H	-1.25918300	3.71895000	-0.12430100
H	0.69929800	2.40942700	-0.77275200
C	0.93180400	-0.34200100	-0.81296800
C	-1.50687300	-1.64440300	0.10660400
H	-3.42482100	0.09169600	0.71289300
H	-3.35438000	2.58348200	0.62428900
C	-0.32427000	-2.38847900	-0.25441500
C	0.81916600	-1.76044400	-0.67477400
H	-0.37474200	-3.47099500	-0.18304000
H	1.68754800	-2.36192200	-0.93628800
C	2.13787100	0.19886100	-1.25088900
H	2.90726300	-0.47225000	-1.61621800
H	2.20867500	1.21578200	-1.61427000
O	-2.56374800	-2.21217300	0.48708600
H	4.31763100	0.71826500	0.17386600
H	3.09926300	1.69274500	0.70394700
C	3.05173400	-0.20099500	1.54359200
H	3.38936000	-1.19875200	1.25403200
H	3.53630300	0.08221200	2.48462400
H	1.96973000	-0.23858900	1.69710100
N	3.34063500	0.73659000	0.45556200

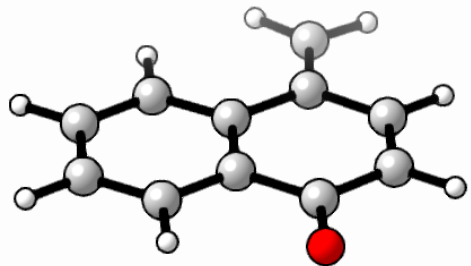


Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	2.61095500	0.93255000	-0.00018600
C	1.34823700	1.51755100	-0.00022400
C	0.18201400	0.72926200	-0.00004100
C	0.32777000	-0.68026100	0.00008300
C	1.60834500	-1.25980600	0.00013200
C	2.74691600	-0.46372300	0.00001600
H	3.73303400	-0.91751500	0.00005300
H	1.68403100	-2.34190600	0.00024100
C	-0.86150600	-1.57486100	0.00005700
O	-0.74936800	-2.81177100	0.00025800
C	-2.17798800	-0.93698700	-0.00029700
C	-2.31294200	0.40787600	-0.00033800
C	-1.17621300	1.32368300	-0.00000600
C	-1.42284400	2.65547200	0.00047600
H	-0.63932200	3.40385000	0.00093000
H	-2.44314500	3.02543700	0.00046600
H	-3.30536000	0.85130200	-0.00054100
H	-3.04058100	-1.59584500	-0.00046900
H	1.27633500	2.59924700	-0.00043800
H	3.49348700	1.56506000	-0.00033800



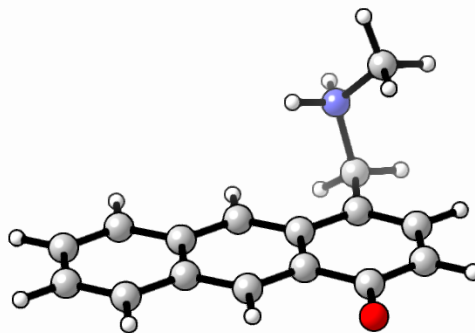
1,4-Anthracene

Int1

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	1.75461200	-0.80626900	-0.21629400
C	0.38677100	-1.02677700	-0.45666600
C	-0.57050300	0.00148400	-0.38067500
C	-0.10664000	1.33481800	-0.04358900
C	1.24722600	1.55189500	0.19534500
C	2.20216300	0.52042000	0.12393100
H	0.09143800	-2.03641400	-0.73146900
C	-1.97621300	-0.20756100	-0.61604300
C	-1.04814300	2.48154300	0.04582500
H	1.56469200	2.56038000	0.44422000
C	-2.41058700	2.18334600	-0.21797200
C	-2.83567300	0.88524300	-0.52460900
H	-3.13069500	2.99578600	-0.17038900
H	-3.89775300	0.72111700	-0.70309600
C	-2.52051700	-1.56180700	-0.90305400
H	-3.54782000	-1.52292700	-1.26861500
H	-1.92383300	-2.14433500	-1.61001500
H	-2.83911900	-3.39973900	0.10033400
H	-1.63256000	-2.50842100	0.75525000
C	-3.50958200	-1.95136300	1.42987000
H	-3.44956800	-2.62117200	2.28702200
H	-3.20569000	-0.94358400	1.70743700
H	-4.52029600	-1.94203800	1.02256400
N	-2.57837400	-2.44643900	0.36820800
O	-0.62651900	3.64970800	0.34208400
C	2.72601200	-1.85422200	-0.29772200
H	2.39345300	-2.85681200	-0.55553500
C	4.05617400	-1.60338600	-0.05460300
H	4.78145700	-2.40957800	-0.11984000
C	4.49749300	-0.28965800	0.28428500
H	5.55185000	-0.11023600	0.47305400
C	3.59151400	0.74215300	0.37004900
H	3.92056500	1.74621700	0.62648500

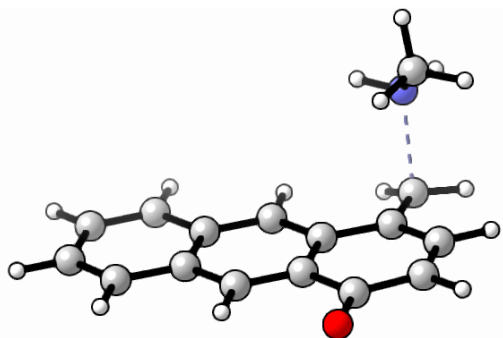


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -231.78

C	1.76673900	-0.77707800	-0.26240900
C	0.40373100	-1.00612900	-0.54447700
C	-0.55344000	0.00742200	-0.47309600
C	-0.11968900	1.32348600	-0.07158800
C	1.22050100	1.56035000	0.20728700
C	2.19150000	0.54249100	0.12110200
H	0.11225200	-2.01422600	-0.82230600
C	-1.96927700	-0.21589000	-0.76531200
C	-1.09118100	2.44360300	0.06837700
H	1.51592800	2.56186800	0.50559800
C	-2.47356200	2.13151900	-0.18709800
C	-2.86951400	0.87239500	-0.56709300
H	-3.19618900	2.93434000	-0.07528100
H	-3.92630700	0.68814900	-0.75152700
C	-2.47805900	-1.45091600	-1.16987200
H	-3.52176700	-1.50903400	-1.45951800
H	-1.84175200	-2.20619100	-1.61420000
O	-0.71241900	3.59589900	0.40143100
C	3.57058400	0.77299300	0.40634500
H	3.88377400	1.77285300	0.69558400
C	4.48737700	-0.24989800	0.31818600
H	5.53499800	-0.06564600	0.53682300
C	4.06773300	-1.55770600	-0.06001500
H	4.80171700	-2.35573700	-0.12514500
C	2.74506500	-1.81481300	-0.34148400
H	2.42736500	-2.81350900	-0.63000000
H	-3.49515600	-3.36549800	0.28771900
H	-1.90696500	-3.18267000	0.68473600
C	-3.15016300	-1.84540700	1.66519900
H	-3.20068300	-2.41322300	2.60037900
H	-2.41063500	-1.04716000	1.77044900
H	-4.12234400	-1.38734800	1.47029100
N	-2.77784900	-2.68324200	0.52151800

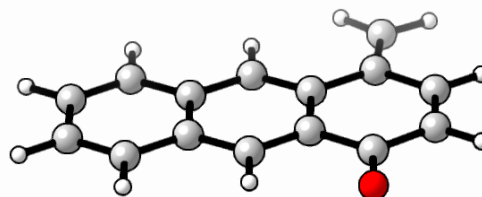


Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	-1.56731900	0.72849000	0.00004300
C	-0.32026700	1.39859000	0.00015300
C	0.88507200	0.71305000	0.00003300
C	0.85182400	-0.72374500	0.00008400
C	-0.35851500	-1.39756200	-0.00006800
C	-1.59000800	-0.70657800	-0.00013000
C	-2.84387000	-1.38235700	-0.00025900
C	-4.02262900	-0.66913600	-0.00022700
C	-4.00116300	0.75233600	-0.00004200
C	-2.80404400	1.43532400	0.00009900
H	-2.78931400	2.52174300	0.00024100
H	-4.93846800	1.30057600	-0.00001500
H	-4.97519100	-1.19011300	-0.00033100
H	-2.85402600	-2.46878100	-0.00038000
H	-0.35020300	-2.48315100	-0.00003900
C	2.11068100	-1.51919200	0.00063700
O	2.10232000	-2.76064200	-0.00035100
C	3.36996600	-0.77482200	0.00111400
C	3.39755700	0.57668000	0.00087800
C	2.19697900	1.40762500	-0.00008900
C	2.35045000	2.75311600	-0.00148200
H	1.51661600	3.44517500	-0.00277100
H	3.34262400	3.19275900	-0.00146400
H	4.35378600	1.09385200	0.00116800
H	4.28333900	-1.36127800	0.00156200
H	-0.33601000	2.48344600	0.00037700

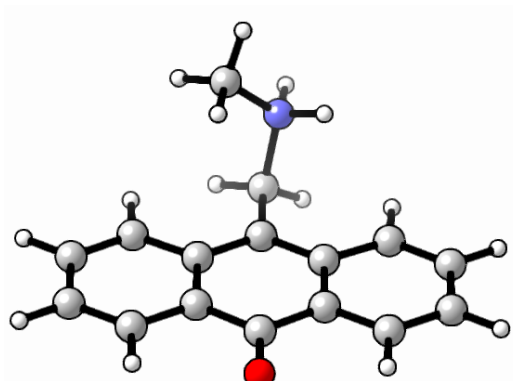


9,10-Anthracene

Int1

Charge: 0 Multiplicity: 1
Negative Frequency: None

C	3.71358500	0.34816500	-0.25766400
C	2.49207000	0.95819600	-0.45921000
C	1.25225500	0.24862100	-0.32061800
C	1.34759400	-1.14161500	0.03784300
C	2.61728700	-1.73645800	0.23915700
C	3.78965900	-1.01906200	0.10148300
H	4.62492000	0.92798200	-0.37858100
H	2.49493500	2.00473300	-0.74722100
C	-0.01847200	0.86685300	-0.51632100
C	0.15405000	-1.96394900	0.20147100
H	2.63789900	-2.78758600	0.50911800
H	4.75401700	-1.49158300	0.26264100
C	-1.12851700	-1.30244100	-0.00890300
C	-1.20645500	0.09358700	-0.35463200
C	-0.07886600	2.31771400	-0.84611300
H	0.70619500	2.64224600	-1.53163500
H	-1.02897900	2.63828500	-1.26871800
H	1.01950100	2.96519000	0.82856600
H	0.19482400	4.18937600	0.11788600
C	-0.95219700	3.07740900	1.44553100
H	-1.02256500	2.02884500	1.72921900
H	-0.68428300	3.69096100	2.30499600
H	-1.89295500	3.41748900	1.01471000
N	0.11875700	3.20984800	0.40826100
O	0.22855900	-3.19133400	0.51468600
C	-2.52546000	0.63396900	-0.51938200
H	-2.65582600	1.67959100	-0.77363400
C	-3.65991800	-0.13482800	-0.36462300
H	-4.63595000	0.32352600	-0.50187600
C	-2.31450300	-2.06368500	0.14328800
H	-2.20268600	-3.11131300	0.40384500
C	-3.56624100	-1.50746600	-0.02782800
H	-4.46404500	-2.10606600	0.09450400

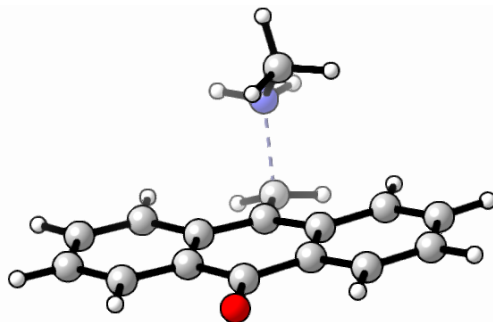


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -302.86

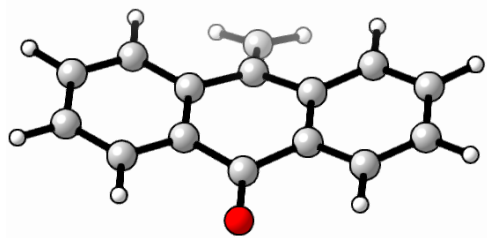
C	-3.71391700	0.26896100	-0.19837800
C	-2.50633500	0.89947400	-0.44360000
C	-1.26626600	0.20335500	-0.36842600
C	-1.32174800	-1.17389500	0.00025300
C	-2.56639500	-1.79896500	0.24239900
C	-3.75543300	-1.09876700	0.14516800
H	-4.63627600	0.83952700	-0.26511400
H	-2.52205400	1.95527700	-0.68900100
C	0.00449800	0.84797200	-0.64187300
C	-0.09690400	-1.97048500	0.14857100
H	-2.55953500	-2.84930000	0.51447200
H	-4.70511000	-1.58841200	0.33817800
C	1.18227400	-1.26971500	-0.02320700
C	1.22866900	0.10824000	-0.39243900
C	0.04554700	2.17576400	-1.10540000
H	0.97033900	2.56080900	-1.51586100
H	-0.82914200	2.59912600	-1.58387100
O	-0.14135600	-3.19301900	0.43012600
C	2.52007300	0.69911000	-0.50392300
H	2.61750100	1.74865700	-0.75675300
C	2.37822700	-1.99261100	0.19429800
H	2.29197500	-3.03847600	0.46970100
C	3.61707000	-1.39151400	0.06871900
H	4.52830300	-1.95558900	0.24296100
C	3.67746700	-0.02599900	-0.28233200
H	4.64099500	0.46790300	-0.37450400
H	0.51105200	4.30944900	0.11785300
H	-0.97930300	3.74794500	0.52435100
C	0.53927000	2.88771100	1.63835000
H	0.32708700	3.50835400	2.51364900
H	0.08959300	1.90093700	1.77569400
H	1.61734700	2.76398600	1.52941400
N	-0.00407300	3.48030600	0.40696400



Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None



C	-3.67902800	0.65114600	-0.33255400
C	-2.49336800	1.37030500	-0.21084800
C	-1.26626800	0.71591400	0.00785200
C	-1.26657200	-0.69659700	0.07130300
C	-2.47125900	-1.41344900	-0.04051100
C	-3.67469600	-0.74872500	-0.23918500
H	-4.60059500	-1.30716500	-0.33429200
H	-2.43483700	-2.49573200	0.02074500
C	0.00000000	-1.45266500	0.22846200
O	0.00000000	-2.67396600	0.43067100
C	1.26657200	-0.69659700	0.07130200
C	2.47125900	-1.41344900	-0.04051100
C	3.67469600	-0.74872500	-0.23918500
C	3.67902800	0.65114600	-0.33255400
C	2.49336800	1.37030500	-0.21084800
C	1.26626800	0.71591400	0.00785200
C	0.00000000	1.46597600	0.19485300
C	0.00000000	2.75368100	0.60250500
H	-0.91870100	3.29506800	0.79404800
H	0.91870200	3.29506800	0.79404700
H	2.52253200	2.44987800	-0.30725300
H	4.60999500	1.18127700	-0.50973100
H	4.60059500	-1.30716500	-0.33429300
H	2.43483700	-2.49573200	0.02074500
H	-2.52253200	2.44987800	-0.30725400
H	-4.60999400	1.18127700	-0.50973100

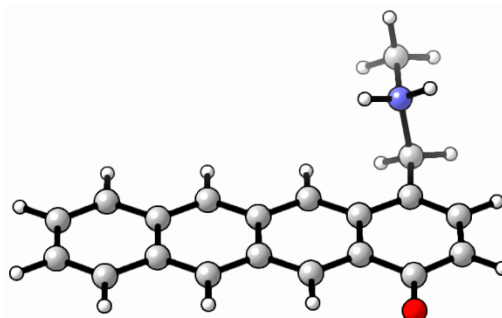
1,4-Tetracene

Int1

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	-0.71765100	0.35085600	-0.20924500
C	0.63085800	0.75110100	-0.36022200
C	1.69978900	-0.14849500	-0.27298700
C	1.39462500	-1.55216400	-0.01913700
C	0.07858600	-1.95236800	0.13185300
C	-1.00736600	-1.04559400	0.04961300
H	0.81051200	1.80249100	-0.56984500
C	3.08030300	0.24283000	-0.41466800
C	2.47622800	-2.57386200	0.07659500
H	-0.11687000	-3.00439100	0.31888000
C	3.79997400	-2.09127100	-0.08383200
C	4.06693100	-0.73456300	-0.31110700
H	4.61646100	-2.80559400	-0.02472700
H	5.10700400	-0.42732500	-0.41734400
C	3.45998300	1.66785000	-0.61279900
H	4.49346700	1.77826300	-0.94499000
H	2.81355800	2.21440900	-1.30430300
H	2.44842400	2.30137800	1.11895700
H	4.03577700	2.03227900	1.36984100
C	3.63878900	3.92469400	0.59096800
H	3.58563200	4.37584500	1.58117500
H	4.63154800	4.06275200	0.16366200
H	2.88234300	4.35696100	-0.06316300
N	3.37582800	2.45633100	0.71212700
O	2.19051600	-3.79816500	0.29000800
C	-1.79292300	1.26036700	-0.30104700
H	-1.58268200	2.30970000	-0.49653700
C	-3.11901100	0.84807300	-0.14691200
C	-3.40594400	-0.55101700	0.11500400
C	-2.34460900	-1.45656800	0.20556500
H	-2.55436300	-2.50610900	0.40012100
C	-4.22041600	1.76458100	-0.23825900
H	-4.00788300	2.81243900	-0.43463200
C	-5.51279200	1.33398700	-0.08213600
H	-6.33464200	2.04054600	-0.15411800
C	-4.77301800	-0.95601400	0.27111700
H	-4.98359100	-2.00446500	0.46691400
C	-5.79470400	-0.04604900	0.17638700
H	-6.82540000	-0.36642300	0.29666800

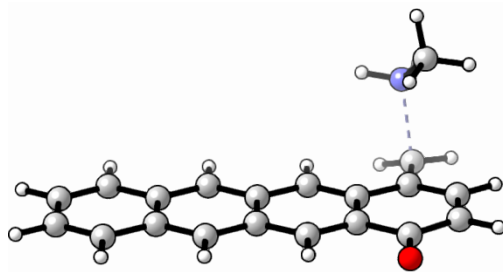


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -242.30

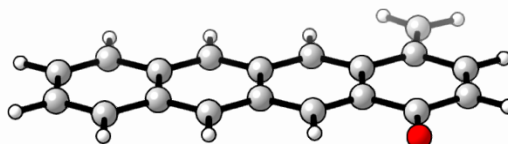
C	0.78170500	-0.40514600	-0.32092300
C	-0.54517800	-0.85069400	-0.55772100
C	-1.64210200	-0.00229800	-0.47727400
C	-1.41189400	1.38293800	-0.10886100
C	-0.12775100	1.83572600	0.12569000
C	1.00100600	0.98227200	0.02821400
H	-0.68027200	-1.89826200	-0.80859000
C	-3.01413300	-0.44780200	-0.72368700
C	-2.54850000	2.33737800	0.04244000
H	0.01187800	2.87735000	0.39883500
C	-3.86845000	1.80354100	-0.16454500
C	-4.06747400	0.48885400	-0.51299800
H	-4.70729600	2.48225200	-0.04345300
H	-5.08652800	0.13649500	-0.66199500
C	-3.33350900	-1.75543200	-1.09730400
H	-4.36281500	-1.97999800	-1.35624200
H	-2.59912100	-2.40241000	-1.56150800
O	-2.34833100	3.54152200	0.34383500
C	2.31020100	1.43755500	0.26567800
H	2.46771500	2.48111400	0.52826600
C	3.41103500	0.57924800	0.17262300
C	3.19394900	-0.81183400	-0.17626800
C	1.89173100	-1.26632100	-0.41206900
H	1.73280700	-2.30994700	-0.67378500
C	4.75151300	1.02838600	0.41156100
H	4.91033200	2.07148500	0.67268200
C	5.81239200	0.16453800	0.31358600
H	6.82292500	0.51733600	0.49700800
C	4.33278000	-1.67912800	-0.26761200
H	4.17159300	-2.72168800	-0.52923100
C	5.59898400	-1.20793100	-0.03070000
H	6.45145300	-1.87692600	-0.10355600
H	-3.95429600	-3.79755300	0.38077900
H	-2.42758600	-3.30935800	0.76148300
C	-3.89626800	-2.22240100	1.73869500
H	-3.82738600	-2.77760200	2.68006600
H	-3.32344700	-1.29544800	1.82643300
H	-4.94033200	-1.96357100	1.54937100
N	-3.37902800	-2.98773300	0.60023000



Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None



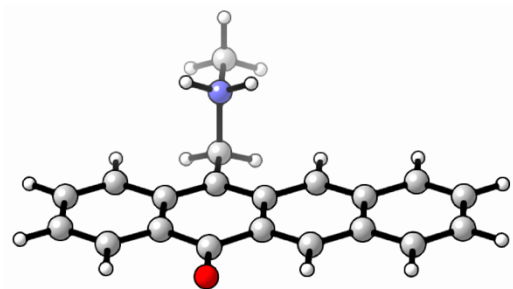
C	0.40988400	0.71896900	0.00026100
C	1.63007100	1.41220700	0.00070900
C	2.85657100	0.73318300	0.00043900
C	4.10900300	1.42794800	0.00084900
C	5.29570900	0.73849000	0.00056200
C	5.30597000	-0.69071600	-0.00015500
C	4.12819300	-1.39485700	-0.00055700
C	2.86727500	-0.71534800	-0.00028200
C	1.64937700	-1.40774400	-0.00067900
C	0.42227800	-0.72619200	-0.00041800
C	-0.82395900	-1.40781400	-0.00064200
C	-2.02330500	-0.72753100	-0.00044700
C	-2.04671600	0.71974200	-0.00014300
C	-0.84378100	1.39552100	0.00044500
H	-0.82127100	2.48035400	0.00118400
C	-3.35567300	1.42029900	-0.00026300
C	-3.50565700	2.76659200	-0.00259000
H	-2.66991800	3.45644700	-0.00495100
H	-4.49665500	3.20873600	-0.00233400
C	-4.55950100	0.59364000	0.00174500
C	-4.54091100	-0.75824700	0.00191500
C	-3.28786600	-1.51301600	-0.00009400
O	-3.29108600	-2.75491600	-0.00046500
H	-5.45887700	-1.33753000	0.00314600
H	-5.51324400	1.11553300	0.00276700
H	-0.83955500	-2.49335500	-0.00087800
H	1.65283200	-2.49488900	-0.00118200
H	4.13334500	-2.48148900	-0.00110000
H	6.25588300	-1.21673400	-0.00037600
H	6.23837200	1.27753300	0.00087800
H	4.10127700	2.51455900	0.00139300
H	1.62474100	2.49940200	0.00123600

5,12-Tetracene

Int1

Charge: 0 Multiplicity: 1
Negative Frequency: None

C	2.69915000	0.46822900	-0.16130700
C	1.41562000	1.01617300	-0.29607400
C	0.23594400	0.23630100	-0.23689200
C	0.40615900	-1.18684200	-0.00556800
C	1.68290600	-1.73195100	0.12649500
C	2.84710600	-0.95102500	0.05493600
H	1.35860700	2.08932500	-0.45288000
C	-1.07802100	0.78316400	-0.38277900
C	-0.75342200	-2.08508100	0.10050200
H	1.76263900	-2.80211900	0.29424200
C	-2.06961600	-1.47170100	-0.00109500
C	-2.21732800	-0.05687800	-0.23242700
C	-1.24502000	2.23798100	-0.63660000
H	-0.42087200	2.68296500	-1.19479800
H	-2.16580300	2.49415900	-1.15995400
H	-2.08150400	2.66851900	1.24160400
H	-0.46014200	2.82504300	1.22257900
C	-1.45045400	4.52030800	0.52509900
H	-0.59346500	4.89030600	-0.03693900
H	-2.37301400	4.71893200	-0.01963800
H	-1.48490300	4.98303400	1.51094800
N	-1.30567200	3.03973800	0.68645300
O	-0.60395500	-3.32698400	0.28295000
C	3.88629300	1.26960000	-0.22777400
H	3.78561700	2.34005400	-0.39000200
C	5.13018300	0.70147200	-0.09178100
H	6.01888100	1.32422300	-0.14612800
C	5.27280800	-0.70400600	0.12075800
H	6.26491800	-1.13297400	0.22552600
C	4.15703100	-1.50463700	0.19192100
H	4.25415600	-2.57547300	0.35415200
C	-3.56425100	0.43844700	-0.29137900
H	-3.74850500	1.49608600	-0.44896100
C	-4.65774300	-0.39026600	-0.15013800
H	-5.65684200	0.03495000	-0.20184000
C	-3.21510600	-2.29450300	0.13663700
H	-3.05020400	-3.35400100	0.30623200
C	-4.49497500	-1.78139600	0.06572300
H	-5.36180700	-2.42564600	0.17754800

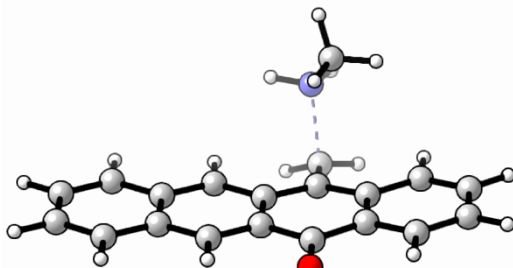


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -336.52

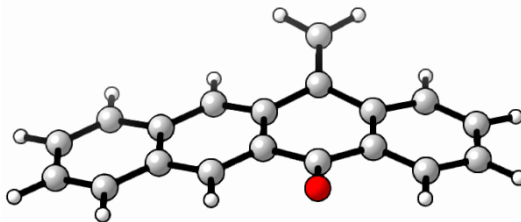
C	-2.72483200	0.48183600	-0.22831100
C	-1.45324000	1.04549500	-0.44289300
C	-0.26919200	0.29391800	-0.38459400
C	-0.39577500	-1.10544100	-0.05643400
C	-1.64873300	-1.67420600	0.15444000
C	-2.83358900	-0.92132700	0.07519600
H	-1.41605600	2.10902300	-0.65376700
C	1.04223800	0.87183900	-0.62700700
C	0.79613700	-1.96525000	0.08024400
H	-1.69810900	-2.73212700	0.39431800
C	2.10649300	-1.31882300	-0.04473000
C	2.22111000	0.06776700	-0.37121900
C	1.15600500	2.20679800	-1.06430700
H	2.10906700	2.55248800	-1.44524300
H	0.31699500	2.66401300	-1.57660500
O	0.68683900	-3.19105900	0.31481000
C	-4.12405600	-1.49115900	0.29422200
H	-4.19376500	-2.55168900	0.52259000
C	-5.25734900	-0.71464200	0.21912100
H	-6.23582200	-1.15472700	0.38660200
C	-5.15231400	0.67614100	-0.07847900
H	-6.05459300	1.27856500	-0.13412100
C	-3.92448000	1.25788000	-0.29469300
H	-3.85027800	2.31839500	-0.52168300
C	3.54258200	0.59861100	-0.43816500
H	3.69441300	1.64961400	-0.65498000
C	3.26329400	-2.10350600	0.17195300
H	3.12283700	-3.15218100	0.41276100
C	4.65984100	-0.18665800	-0.21759800
H	5.64656800	0.26503500	-0.27527600
C	4.53112600	-1.55872000	0.08881100
H	5.41171600	-2.16949500	0.26249200
H	1.62013400	4.30373000	0.16434600
H	0.12324600	3.74746300	0.55076600
C	1.62364100	2.86834300	1.67315000
H	1.40341200	3.48486900	2.54896300
H	1.16562000	1.88368600	1.79607500
H	2.70222800	2.73981800	1.57609400
N	1.09774900	3.47409000	0.43942100



Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None



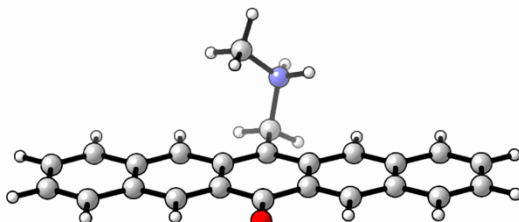
C	-2.59612200	0.71158000	-0.09507800
C	-1.36324000	1.40596300	-0.01752300
C	-0.15805100	0.74374300	0.15418600
C	-0.16812000	-0.68870700	0.21581000
C	-1.36372700	-1.38686900	0.15582900
C	-2.59999100	-0.72055100	0.00447900
C	-3.83833900	-1.42043200	-0.06897400
C	-5.02108600	-0.73314600	-0.23466600
C	-5.01775400	0.68452500	-0.33755400
C	-3.83518200	1.39030100	-0.27158500
H	-3.83473900	2.47401000	-0.34970900
H	-5.95745000	1.21253100	-0.46940900
H	-5.96208700	-1.27192200	-0.28940800
H	-3.83333000	-2.50428700	0.00681300
H	-1.33909500	-2.47074900	0.21174700
C	1.10169600	-1.45270900	0.30100000
O	1.11016500	-2.67185000	0.51404100
C	2.35867700	-0.70409800	0.05050900
C	3.54453700	-1.42912700	-0.16230800
C	4.73461500	-0.77195300	-0.44926100
C	4.74409700	0.62855800	-0.52977700
C	3.57782000	1.35623700	-0.30813800
C	2.36667700	0.70944300	0.00058400
C	1.12792200	1.46963200	0.29998800
C	1.17532200	2.73649200	0.76461900
H	2.11336500	3.25762400	0.91539900
H	0.27768400	3.27649300	1.04263700
H	3.60663300	2.43671600	-0.39538200
H	5.66292900	1.15268700	-0.77513600
H	5.64501900	-1.33701200	-0.62259100
H	3.50399000	-2.51168000	-0.10820800
H	-1.38272800	2.48709100	-0.11191000

6,13-Pentacene

Int1

Charge: 0 Multiplicity: 1

Negative Frequency: None



C	3.73633200	0.32888600	-0.24584400
C	2.52000900	1.00746600	-0.40900100
C	1.25792600	0.37346700	-0.29113700
C	1.27763700	-1.04665600	0.01504500
C	2.48596800	-1.72132100	0.17981400
C	3.72989700	-1.08084500	0.06251100
H	2.58538800	2.06365700	-0.65273600
C	0.01684100	1.06318900	-0.45077500
C	0.02957500	-1.80639900	0.15593800
H	2.44848800	-2.78268700	0.40734700
C	-1.22418000	-1.06043000	-0.00648700
C	-1.22092000	0.36457400	-0.29707300
C	0.04048500	2.51908800	-0.74701500
H	0.83769800	2.81103300	-1.43402300
H	-0.89311900	2.90686000	-1.15070900
H	1.19835800	3.06829800	0.92484000
H	0.43835100	4.35432900	0.25206000
C	-0.75625100	3.28373200	1.57173700
H	-1.67784400	3.69592900	1.16302300
H	-0.89184000	2.23410300	1.82662000
H	-0.43979400	3.85405200	2.44443300
N	0.30770500	3.37521800	0.52377500
O	0.03505300	-3.03918200	0.40934700
C	5.00462100	0.98530700	-0.37202700
H	5.02280900	2.04708400	-0.60559300
C	6.17892500	0.29140200	-0.20175600
H	7.13048400	0.80649700	-0.30118300
C	6.16798000	-1.10336500	0.10541700
H	7.10732000	-1.63219400	0.23606600
C	4.97013400	-1.76752900	0.23287300
H	4.94852600	-2.82959400	0.46535500
C	-2.49120600	0.98122700	-0.40909800
H	-2.56653300	2.04409100	-0.61152500
C	-3.69797300	0.28388900	-0.26627600
C	-2.42521700	-1.75508400	0.13597600
H	-2.37383500	-2.81807400	0.35268900
C	-3.67620300	-1.13175400	0.01444600
C	-4.97425500	0.92759200	-0.38518500
H	-5.00391500	1.99382600	-0.59627700

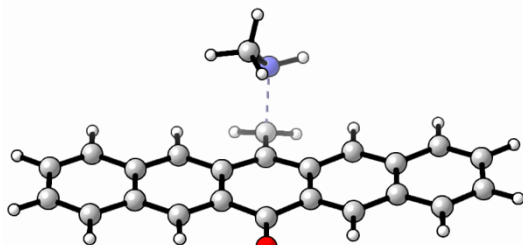
C	-4.90922500	-1.83723500	0.16177000
H	-4.87599500	-2.90345500	0.37313000
C	-6.11413700	-1.18532400	0.04016700
H	-7.04773700	-1.72818600	0.15353700
C	-6.14061700	0.21611700	-0.23693100
H	-7.09802000	0.72139200	-0.33078700

TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -358.30

C	-3.70438400	0.30120100	-0.21600700
C	-2.49110400	0.98452200	-0.41533400
C	-1.23988700	0.34649200	-0.37719200
C	-1.24185100	-1.06999900	-0.09122300
C	-2.43749800	-1.75648300	0.10415500
C	-3.68630700	-1.11430300	0.04788000
H	-2.55451800	2.05291200	-0.59306500
C	0.01295100	1.04156400	-0.61609000
C	0.01851100	-1.82873300	0.01192700
H	-2.38922200	-2.82111100	0.31218800
C	1.27599800	-1.06501600	-0.08673200
C	1.26576000	0.35035200	-0.37505900
C	0.01750900	2.38832100	-1.04047100
H	0.89682800	2.76961700	-1.54831300
H	-0.89888900	2.80134200	-1.44565000
O	0.02111900	-3.06461000	0.19835900
C	-4.91845200	-1.80558600	0.25071000
H	-4.89026100	-2.87428100	0.44828200
C	-6.11821500	-1.13397900	0.19816300
H	-7.05231800	-1.66559000	0.35274800
C	-6.13962900	0.26883800	-0.05909300
H	-7.09293500	0.78850300	-0.09691500
C	-4.97055000	0.96606000	-0.25893200
H	-4.99411000	2.03506000	-0.45497500
C	2.51091400	1.00035200	-0.40172000
H	2.56619500	2.06919300	-0.57963900
C	2.47504000	-1.74201500	0.11615500
H	2.43422500	-2.80674900	0.32537500
C	3.72907400	0.32615200	-0.19617900
C	3.71958300	-1.08951400	0.06658800
C	4.95540600	-1.77160100	0.27659800
H	4.93401600	-2.84052700	0.47363200
C	6.15063500	-1.09109000	0.23133800
H	7.08763300	-1.61597800	0.39122900
C	6.16330100	0.31162200	-0.02517300
H	7.11290300	0.83837300	-0.05732500
C	4.99007400	1.00037400	-0.23132700
H	5.00687400	2.06960300	-0.42677900
H	1.13515700	3.84060800	0.55640300
H	-0.32204700	4.48773200	0.16517300
C	-0.41816100	3.06224400	1.67997500

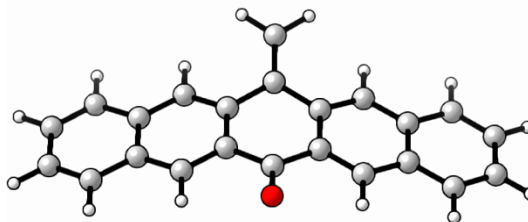


H	-0.14115900	3.65977000	2.55240800
H	-1.50389200	3.02030600	1.59086500
H	-0.03858600	2.04429000	1.79761200
N	0.14612100	3.62645300	0.44173300

Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None



C	3.67450800	0.70012600	-0.17889100
C	2.45686000	1.40414600	-0.00273700
C	1.26348800	0.75065500	0.25844800
C	1.26559800	-0.68261800	0.31295000
C	2.44721500	-1.38973400	0.15780300
C	3.67374600	-0.73253400	-0.08641500
C	4.89649800	-1.44227600	-0.25870100
C	6.06901900	-0.76404100	-0.51187100
C	6.06996600	0.65399200	-0.60755100
C	4.90203000	1.36924000	-0.44744700
H	4.90527200	2.45329100	-0.52044100
H	7.00119500	1.17498300	-0.80904400
H	6.99826900	-1.31034300	-0.64148600
H	4.88801300	-2.52644300	-0.18776800
H	2.41810100	-2.47365400	0.21119100
C	0.00000000	-1.43851200	0.49387100
O	0.00000000	-2.65464200	0.72195500
C	-1.26559800	-0.68261800	0.31295000
C	-2.44721500	-1.38973400	0.15780300
C	-3.67374600	-0.73253400	-0.08641500
C	-4.89649800	-1.44227600	-0.25870200
C	-6.06901900	-0.76404100	-0.51187200
C	-6.06996700	0.65399200	-0.60755100
C	-4.90203100	1.36924000	-0.44744600
C	-3.67450800	0.70012600	-0.17889000
C	-2.45686000	1.40414600	-0.00273600
C	-1.26348800	0.75065600	0.25844800
C	0.00000000	1.48711300	0.51141600
C	0.00000100	2.73636600	1.02251900
H	-0.92126000	3.25827200	1.25477900
H	0.92126200	3.25827100	1.25477800
H	-2.47620200	2.48581300	-0.09199900
H	-4.90527300	2.45329200	-0.52043900
H	-7.00119500	1.17498400	-0.80904300
H	-6.99826900	-1.31034300	-0.64148700
H	-4.88801300	-2.52644300	-0.18777000
H	-2.41810100	-2.47365400	0.21119000
H	2.47620100	2.48581300	-0.09200100

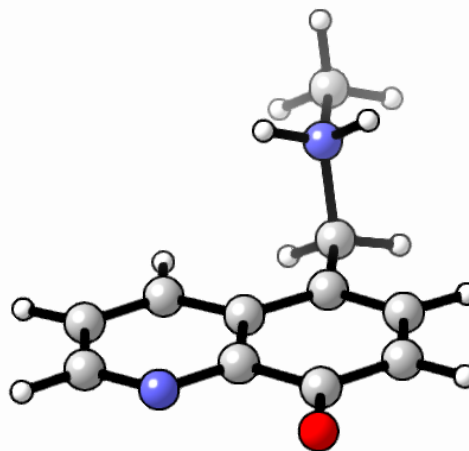
8-Hydroxyquinoline

Int1

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	-0.88902200	2.70905100	-0.14494800
C	-0.19985400	0.37953700	-0.25190800
C	-1.56834900	0.03560500	0.03523900
C	-2.19889600	2.26346700	0.13421300
H	-0.67344100	3.77107900	-0.20807600
C	0.77711800	-0.65124300	-0.44005100
C	-1.99306800	-1.38076100	0.14117500
H	-2.99879400	2.98529900	0.29082900
C	-0.96107900	-2.34181000	-0.06934500
C	0.35714700	-1.98003700	-0.34288900
H	-1.23526800	-3.39185900	-0.01143800
H	1.09215900	-2.77015600	-0.49185400
C	2.21374500	-0.34659700	-0.69370100
H	2.73593600	-1.19372500	-1.14142100
H	2.38823900	0.53177500	-1.31824000
H	2.50168300	0.70489600	1.10898800
H	2.86831000	-0.87743300	1.22604600
C	4.42435500	0.26585300	0.44179200
H	4.50434900	1.16310000	-0.17077500
H	4.86998300	0.43479800	1.42154500
H	4.90739500	-0.57521800	-0.05441600
N	2.97322700	-0.06019400	0.61801000
O	-3.19684500	-1.70779000	0.40010400
C	0.10029800	1.76782900	-0.33508300
H	1.10920000	2.10220800	-0.55808100
N	-2.52599400	0.98193500	0.21900300

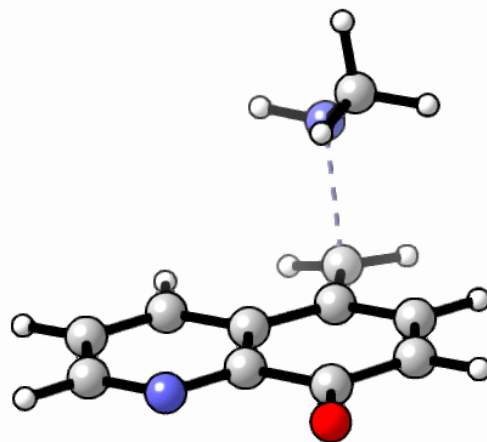


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -169.80

C	1.31800000	-2.61440400	-0.06916000
C	0.22302100	-0.48494000	-0.43407700
C	1.42320000	0.12938700	0.02224800
C	2.45946700	-1.90639700	0.34897800
H	1.32062700	-3.69950500	-0.08078000
C	-0.91616600	0.33465500	-0.83584100
C	1.52945100	1.61712600	0.12083700
H	3.35451900	-2.44267000	0.65752600
C	0.35459000	2.36610600	-0.26490300
C	-0.78830600	1.75388100	-0.70178700
H	0.41631200	3.44790100	-0.19360500
H	-1.64538700	2.36439200	-0.97784600
C	-2.11618500	-0.19980500	-1.28203300
H	-2.88416500	0.46922000	-1.65252700
H	-2.20414000	-1.22781300	-1.60693400
O	2.57286200	2.18140300	0.52115900
N	2.51267900	-0.58015800	0.39724600
C	0.20087700	-1.89854200	-0.45790600
H	-0.68910600	-2.42984800	-0.77670900
H	-4.35021200	-0.61215300	0.19751500
H	-3.19347900	-1.66663700	0.71174700
C	-3.01382600	0.21763400	1.55562900
H	-3.28169100	1.23735300	1.26881800
H	-3.50978400	-0.02829300	2.50181100
H	-1.93084800	0.18100600	1.70373200
N	-3.37414900	-0.69589700	0.46933500

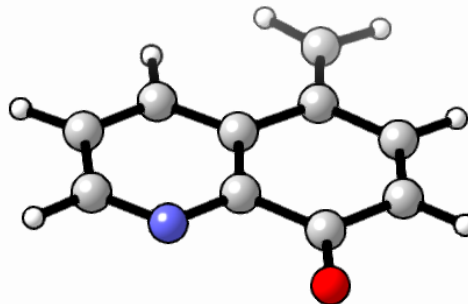


Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	-2.60891400	0.86872300	-0.00003300
C	-1.37518800	1.49980500	-0.00004300
C	-0.19742900	0.72889200	-0.00000700
C	-0.35038700	-0.67696100	0.00001600
N	-1.55048600	-1.28968500	0.00003000
C	-2.64615200	-0.53403800	0.00001100
H	-3.59883500	-1.05838800	0.00002900
C	0.85232300	-1.57660100	0.00001400
O	0.74825800	-2.80917900	0.00002300
C	2.16214100	-0.92548800	-0.00003900
C	2.29376100	0.42001800	-0.00004800
C	1.15513000	1.33050300	-0.00000100
C	1.38483900	2.66483300	0.00007200
H	0.59227400	3.40364600	0.00013700
H	2.40039400	3.04722800	0.00007200
H	3.28467000	0.86631300	-0.00007800
H	3.02804900	-1.57986300	-0.00006400
H	-1.32981200	2.58278900	-0.00008500
H	-3.53015300	1.44137400	-0.00006200



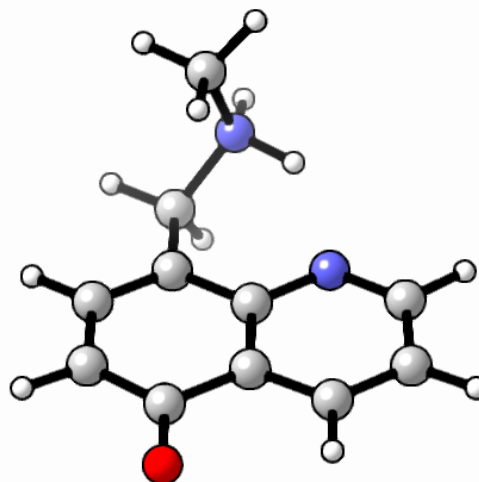
5-Hydroxyquinoline

Int1

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	0.18682000	2.60644000	-0.21625500
C	0.02512300	0.28352900	-0.29802200
C	1.41775400	0.14275700	0.01188500
C	2.16914600	1.31810800	0.18324300
C	1.56561600	2.56146600	0.06433700
H	-0.32621400	3.56300700	-0.29337900
C	-0.79088300	-0.86743700	-0.48429100
C	2.04131800	-1.18591600	0.15252300
H	3.22605900	1.22357100	0.41329400
H	2.12479100	3.48185300	0.19479700
C	1.15709700	-2.29022200	-0.01776700
C	-0.19748600	-2.11976700	-0.32066700
H	1.56681500	-3.29063400	0.09240800
H	-0.81630200	-3.00685300	-0.44666600
C	-2.22135700	-0.71947000	-0.90686200
H	-2.31972700	-0.28700800	-1.90843500
H	-2.75699200	-1.67046800	-0.88231500
H	-2.37075400	1.11651600	-0.05505800
H	-3.87949500	0.46891900	-0.40568100
C	-3.11833300	-0.18585000	1.41323800
H	-3.61224700	0.60717500	1.97427500
H	-3.71595000	-1.09734300	1.43693900
H	-2.12707400	-0.37744200	1.82209800
N	-2.96430500	0.25569500	-0.00324800
O	3.28544000	-1.30637300	0.41666400
N	-0.56217000	1.52400000	-0.39157400

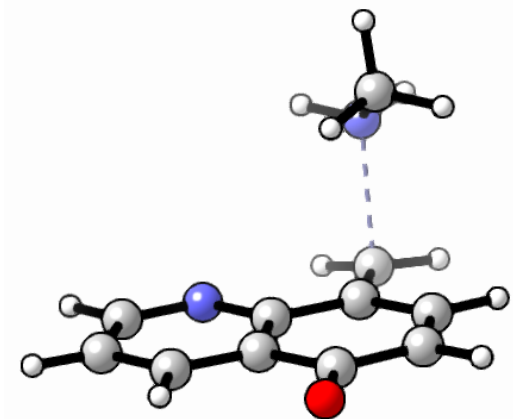


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -133.08

C	-1.09844000	2.59232100	-0.15005100
C	-0.21772900	0.47835800	-0.44877700
C	-1.41291000	-0.12120300	0.02893400
C	-2.47116600	0.71680800	0.41771500
C	-2.32119500	2.09174000	0.33000300
H	-0.94501300	3.66688000	-0.22918100
C	0.90017100	-0.36607100	-0.86207200
C	-1.55204600	-1.59504600	0.13004600
H	-3.38805800	0.26535600	0.78267000
H	-3.11435700	2.77177700	0.62193900
C	-0.40273000	-2.37739100	-0.27220900
C	0.74314100	-1.78591100	-0.72741400
H	-0.48594200	-3.45728700	-0.19720400
H	1.58543300	-2.41132500	-1.01510200
C	2.08938600	0.16921700	-1.31501200
H	2.86619400	-0.48375300	-1.69463000
H	2.16005000	1.21878800	-1.56347600
H	4.37286100	0.43047600	0.28313200
H	3.29953500	1.60993400	0.69903700
C	2.90816800	-0.21056700	1.60778700
H	3.39978900	0.00529600	2.56453300
H	1.83233900	-0.04858900	1.72129200
H	3.06366800	-1.26393800	1.36094100
N	3.39915100	0.61731400	0.50580900
O	-2.61088900	-2.11996000	0.54791000
N	-0.07733600	1.82590500	-0.52737200

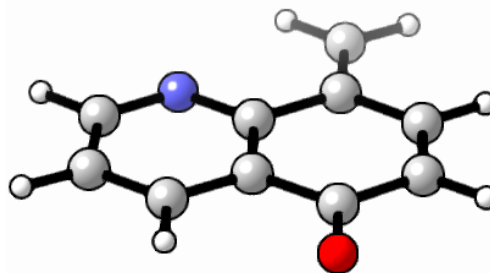


Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	2.52864100	0.87850000	0.00009200
N	1.33626100	1.47729200	0.00005400
C	0.23238700	0.70284000	-0.00003400
C	0.30482300	-0.70697000	-0.00009600
C	1.56969500	-1.31417600	-0.00004400
C	2.70243300	-0.51399800	0.00004400
H	3.69945100	-0.94072600	0.00007200
H	1.63493100	-2.39701300	-0.00009800
C	-0.92634500	-1.54279000	-0.00027000
O	-0.86528900	-2.78209300	0.00009800
C	-2.20671900	-0.83613400	-0.00000600
C	-2.27137300	0.51584100	0.00004300
C	-1.09038400	1.36957900	-0.00001500
C	-1.22055600	2.71605600	0.00001900
H	-0.35159900	3.36339800	0.00000400
H	-2.20232600	3.17871700	0.00005300
H	-3.23915000	1.01037700	0.00015100
H	-3.10289600	-1.44813500	0.00009500
H	3.39446300	1.53659200	0.00016500



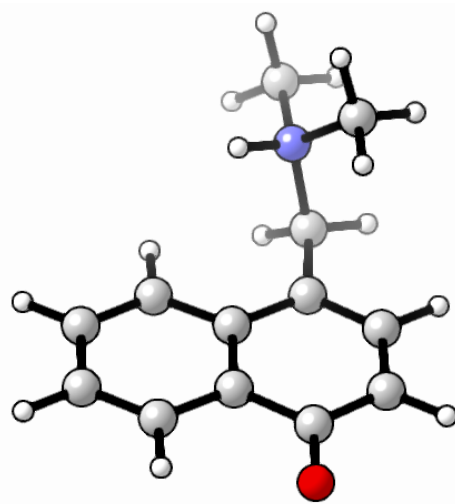
Calculated Coordinates – Benzylammoniums (Benzylammoniums (Secondary and Tertiary Amine))

1,4-Naphthalene (Secondary Amine)

Int1

Charge: 0 Multiplicity: 1
Negative Frequency: None

C	-1.14094300	2.74689300	-0.06782800
C	-0.16927700	1.80927800	-0.36987100
C	-0.44024900	0.40896800	-0.33192100
C	-1.77089500	-0.00019200	0.02233000
C	-2.73998400	0.98283000	0.32642600
C	-2.44339000	2.33510400	0.29054900
H	-0.89780400	3.80514500	-0.11095700
H	0.81454000	2.16719200	-0.66088900
C	0.55068800	-0.58774000	-0.62604700
C	-2.15133400	-1.42542000	0.07140600
H	-3.73509500	0.63936300	0.59130000
H	-3.20300000	3.07367900	0.53028400
C	-1.11814500	-2.35040900	-0.24975500
C	0.17375300	-1.93137600	-0.57377600
H	-1.35952600	-3.41007200	-0.23166700
H	0.92385000	-2.68948500	-0.79586100
C	1.95989800	-0.22101700	-0.93343000
H	2.51967400	-1.05798800	-1.35533200
H	2.05792600	0.63240600	-1.60867800
H	2.21326600	0.93759000	0.78235700
C	4.09848100	0.76617800	-0.02293200
H	4.59684700	1.09793900	0.88775000
H	4.68543600	-0.01260300	-0.51068700
H	3.95567000	1.60822600	-0.69968600
N	2.75904500	0.19658000	0.33277300
O	-3.33931700	-1.78480800	0.38282600
C	2.87699000	-0.92279700	1.32209900
H	1.87756500	-1.27776700	1.56643600
H	3.45983300	-1.72336600	0.86542200
H	3.37848100	-0.54964500	2.21468500

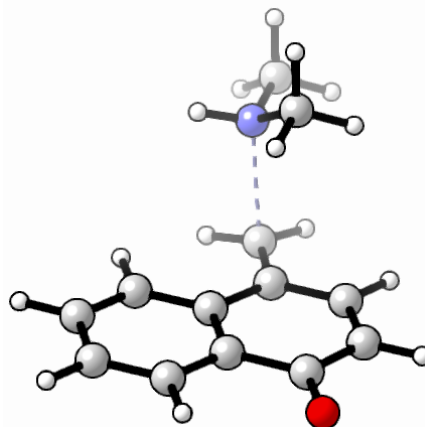


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -101.71

C	-1.50757300	2.69295600	-0.09605400
C	-0.45708900	1.87235800	-0.48326500
C	-0.57243600	0.46276600	-0.44554600
C	-1.79695200	-0.09282700	0.02026600
C	-2.85305100	0.75654000	0.40758100
C	-2.71956100	2.13590100	0.35172300
H	-1.38800000	3.77186400	-0.13702500
H	0.46735600	2.33181200	-0.81587300
C	0.51844000	-0.42812800	-0.84777300
C	-1.98494300	-1.56187100	0.12100600
H	-3.77370400	0.29961700	0.75529600
H	-3.53917800	2.78066400	0.65448300
C	-0.85834400	-2.38701500	-0.25549400
C	0.31342500	-1.84037700	-0.69950400
H	-0.98133000	-3.46291300	-0.17479900
H	1.13607400	-2.49766700	-0.97337800
C	1.74326200	0.02410600	-1.30196800
H	2.47912300	-0.69284900	-1.64876700
H	1.90416600	1.04570500	-1.61943800
H	2.88127500	1.44499900	0.69715000
C	2.63846300	-0.40486900	1.54876600
H	3.19696800	-0.24338200	2.48160800
H	1.57443800	-0.23772500	1.73466600
H	2.77043500	-1.44565300	1.23710000
N	3.08387600	0.47422700	0.47293700
O	-3.06706300	-2.05850700	0.52010900
C	4.48412900	0.31366200	0.08406000
H	5.17773100	0.50402600	0.91613900
H	4.64178200	-0.71084200	-0.26791500
H	4.71560800	1.00160000	-0.73346700

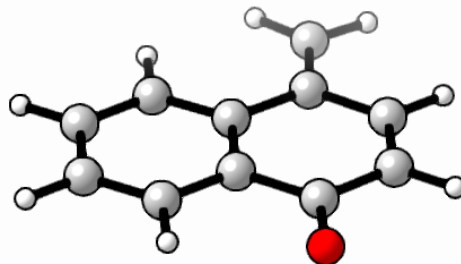


Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	2.61095500	0.93255000	-0.00018600
C	1.34823700	1.51755100	-0.00022400
C	0.18201400	0.72926200	-0.00004100
C	0.32777000	-0.68026100	0.00008300
C	1.60834500	-1.25980600	0.00013200
C	2.74691600	-0.46372300	0.00001600
H	3.73303400	-0.91751500	0.00005300
H	1.68403100	-2.34190600	0.00024100
C	-0.86150600	-1.57486100	0.00005700
O	-0.74936800	-2.81177100	0.00025800
C	-2.17798800	-0.93698700	-0.00029700
C	-2.31294200	0.40787600	-0.00033800
C	-1.17621300	1.32368300	-0.00000600
C	-1.42284400	2.65547200	0.00047600
H	-0.63932200	3.40385000	0.00093000
H	-2.44314500	3.02543700	0.00046600
H	-3.30536000	0.85130200	-0.00054100
H	-3.04058100	-1.59584500	-0.00046900
H	1.27633500	2.59924700	-0.00043800
H	3.49348700	1.56506000	-0.00033800

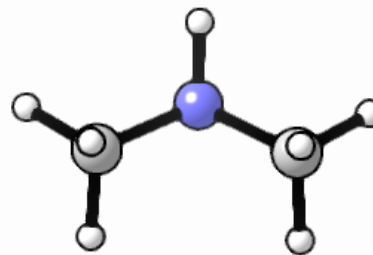


Dimethylamine

Charge: 0 Multiplicity: 1

Negative Frequency: None

H	-0.00000100	1.32742000	0.52598600
N	0.00000000	0.57066300	-0.15367800
C	-1.21724500	-0.22491400	0.02020300
H	-2.09653600	0.42176000	-0.05665800
H	-1.26039100	-0.75818500	0.98689100
H	-1.27783300	-0.97512000	-0.77657000
C	1.21724500	-0.22491400	0.02020300
H	1.26040500	-0.75816100	0.98690400
H	1.27781600	-0.97514100	-0.77655100
H	2.09653700	0.42175400	-0.05669200



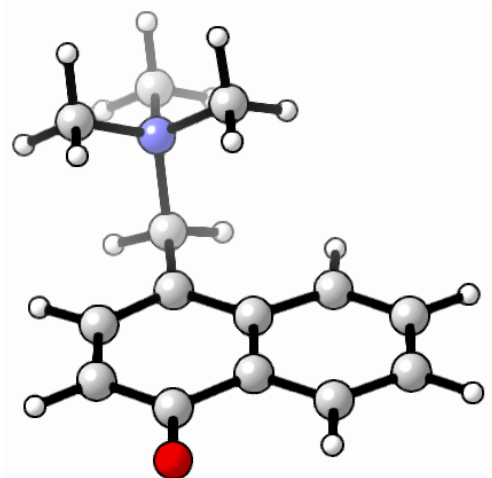
1,4-Naphthalene (Tertiary Amine)

Int1

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	1.61555900	2.68581300	-0.19179500
C	0.56261000	1.83070400	-0.46011300
C	0.69578200	0.41406000	-0.36031700
C	1.98442900	-0.09899400	0.01749000
C	3.03959700	0.80208800	0.29255200
C	2.87250200	2.17252200	0.19753400
H	1.47111800	3.75898500	-0.28420700
H	-0.38392600	2.26433200	-0.76356900
C	-0.37805800	-0.50418400	-0.63664400
C	2.24282400	-1.54852600	0.11415900
H	3.99700600	0.37841300	0.57901500
H	3.69654300	2.84686400	0.41263400
C	1.14735600	-2.39233700	-0.22484200
C	-0.09599700	-1.87419400	-0.58297700
H	1.30393100	-3.46760400	-0.19903100
H	-0.89054400	-2.57578000	-0.83298200
C	-1.75025200	-0.06307300	-1.00593700
H	-1.78124700	0.91281600	-1.49201500
H	-2.24070500	-0.78470800	-1.66259100
C	-4.07763100	0.56442400	-0.36199700
H	-4.44224600	-0.16256100	-1.08764300
H	-4.79422300	0.66842100	0.45296900
H	-3.92303200	1.52876900	-0.84575400
N	-2.76726400	0.08172600	0.19474200
O	3.38647900	-1.99958400	0.46637600
C	-2.26039300	1.06645100	1.20938100
H	-1.28846100	0.73067500	1.56633800
H	-2.16878000	2.04442500	0.74010700
H	-2.97116200	1.11527900	2.03455300
C	-2.97200500	-1.24779600	0.86433600
H	-3.32871500	-1.96538300	0.12568000
H	-2.02338100	-1.58111200	1.28059400
H	-3.71109800	-1.12899100	1.65670500

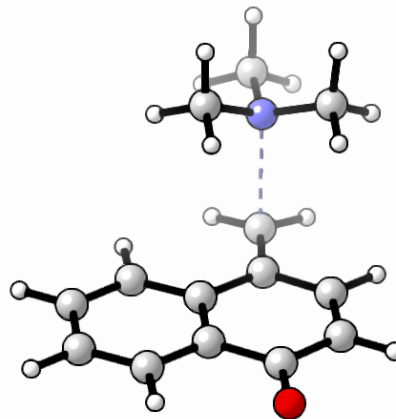


TS1

Charge: 0 Multiplicity: 1

Negative Frequency: -67.56

C	1.63641600	2.69027700	0.23721000
C	0.63248700	1.81487400	0.62545700
C	0.78672300	0.41433900	0.49968300
C	2.00940200	-0.07324100	-0.03979900
C	3.01806300	0.83127600	-0.43037800
C	2.84223600	2.20006500	-0.29766600
H	1.48576200	3.76044400	0.34669600
H	-0.28670200	2.22502700	1.02850600
C	-0.25531300	-0.53661400	0.90391800
C	2.25181900	-1.52833500	-0.20469200
H	3.93747700	0.42472000	-0.83842200
H	3.62537100	2.88780100	-0.60230900
C	1.18898800	-2.41581900	0.21580700
C	0.01731300	-1.93645600	0.72887700
H	1.35977800	-3.48256000	0.10623200
H	-0.75746100	-2.63831400	1.02967700
C	-1.48938100	-0.15860100	1.39378100
H	-2.16569200	-0.91171800	1.78143000
H	-1.71366200	0.86066200	1.67961800
O	3.32703800	-1.96405900	-0.68339100
C	-3.10314000	-1.22967000	-0.90499500
H	-3.73426500	-1.22879700	-1.80760900
H	-2.11408800	-1.61577300	-1.16857000
H	-3.55172500	-1.89567600	-0.16312700
N	-2.96131000	0.11137500	-0.34284100
C	-4.20868200	0.63524200	0.21098600
H	-4.97816000	0.77073500	-0.56581700
H	-4.59254800	-0.05750900	0.96521700
H	-4.01966900	1.60147100	0.68708500
C	-2.31813700	1.03075600	-1.28066400
H	-2.20758800	2.01357600	-0.81667600
H	-1.32415700	0.65071400	-1.53185600
H	-2.90256300	1.13949900	-2.20820200

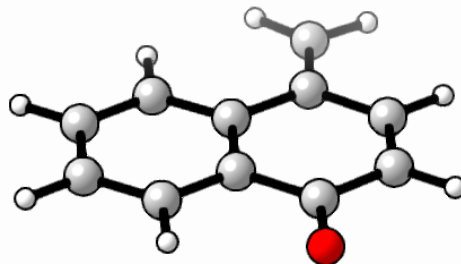


Int2

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	2.61095500	0.93255000	-0.00018600
C	1.34823700	1.51755100	-0.00022400
C	0.18201400	0.72926200	-0.00004100
C	0.32777000	-0.68026100	0.00008300
C	1.60834500	-1.25980600	0.00013200
C	2.74691600	-0.46372300	0.00001600
H	3.73303400	-0.91751500	0.00005300
H	1.68403100	-2.34190600	0.00024100
C	-0.86150600	-1.57486100	0.00005700
O	-0.74936800	-2.81177100	0.00025800
C	-2.17798800	-0.93698700	-0.00029700
C	-2.31294200	0.40787600	-0.00033800
C	-1.17621300	1.32368300	-0.00000600
C	-1.42284400	2.65547200	0.00047600
H	-0.63932200	3.40385000	0.00093000
H	-2.44314500	3.02543700	0.00046600
H	-3.30536000	0.85130200	-0.00054100
H	-3.04058100	-1.59584500	-0.00046900
H	1.27633500	2.59924700	-0.00043800
H	3.49348700	1.56506000	-0.00033800

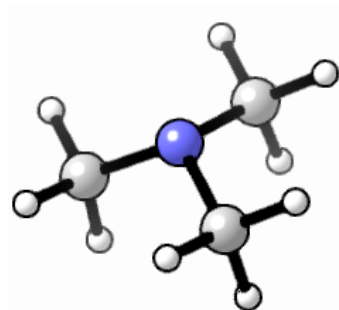


Trimethylamine

Charge: 0 Multiplicity: 1

Negative Frequency: None

C	1.30494500	0.48189600	0.06224000
N	-0.00001800	0.00003800	-0.38598500
C	-1.06982700	0.88910400	0.06243700
H	-2.03267000	0.53557200	-0.31993900
H	-0.89851100	1.90038600	-0.31992500
H	-1.13832100	0.94595700	1.16695200
C	-0.23511000	-1.37101300	0.06227800
H	-0.25048700	-1.45883900	1.16679200
H	0.55268200	-2.02798800	-0.31986300
H	-1.19644200	-1.72832000	-0.32037700
H	1.38856200	0.51271400	1.16676000
H	1.48029400	1.49253400	-0.32005300
H	2.09497100	-0.17220900	-0.32018300



Calculated Coordinates – Isomerization

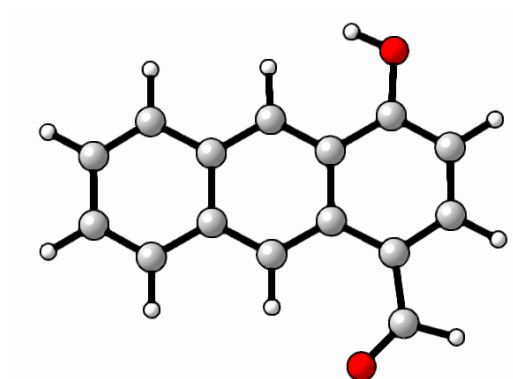
1,4-Hydroxyanthraldehyde

Hydroxy-aldehyde

Charge: 0 Multiplicity: 1

Negative Frequency: None

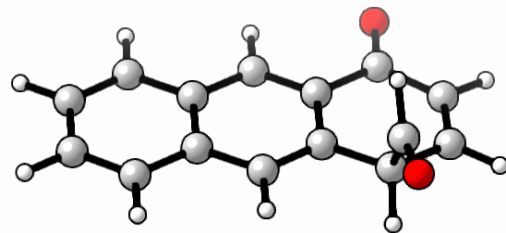
C	3.11305200	-1.28378800	0.00002600
C	1.84886600	-1.83785900	-0.00002000
C	0.66871100	-1.00529100	0.00000600
C	-0.61831300	-1.55452200	-0.00005100
C	-1.76775600	-0.75079100	-0.00002400
C	-3.08657900	-1.30419800	-0.00008600
C	-4.18763700	-0.48344000	-0.00006100
C	-4.03209300	0.93549600	0.00003000
C	-2.78001400	1.50078700	0.00009300
C	-1.60858600	0.68025300	0.00006700
C	-0.31665900	1.23360400	0.00012600
C	0.83461100	0.43656000	0.00009600
C	2.17802000	0.98296000	0.00015700
C	3.26188500	0.11325300	0.00010000
H	4.26785300	0.52486200	0.00013300
C	2.51192800	2.40633300	0.00027100
O	1.73415800	3.36306900	-0.00038800
H	3.60343300	2.60063500	-0.00048700
H	-0.20683600	2.31005500	0.00019800
H	-2.66029900	2.58065500	0.00016300
H	-4.91486700	1.56778900	0.00005000
H	-5.18579800	-0.91064400	-0.00011100
H	-3.20151800	-2.38470600	-0.00015300
H	-0.77099300	-2.63080200	-0.00012100
O	1.77925400	-3.19108700	-0.00010900
H	0.86726400	-3.51222300	-0.00007700
H	3.97784300	-1.93761900	0.00000200



Anthrone-aldehyde

Charge: 0 Multiplicity: 1

Negative Frequency: None

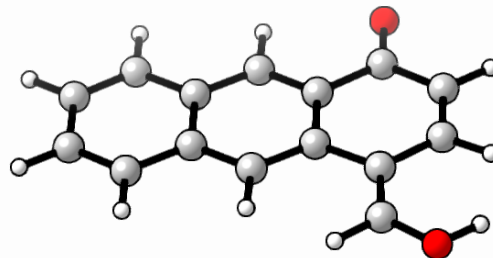


C	3.05007300	1.34526800	-0.32183400
C	3.22857200	0.03818500	-0.58025200
C	2.13017200	-0.98057300	-0.47902000
C	0.74293500	-0.39378800	-0.31604300
C	-0.36202900	-1.21868900	-0.39927700
C	-1.67629800	-0.71871600	-0.20980200
C	-2.82445300	-1.55419400	-0.30003100
C	-4.08604900	-1.03366700	-0.10404500
C	-4.26155800	0.34569500	0.18925500
C	-3.17036700	1.18163800	0.28138400
C	-1.85290100	0.67572500	0.08562500
C	-0.70976800	1.50348400	0.16802800
C	0.56434700	0.99445600	-0.02605600
C	1.73535700	1.91039500	0.02671900
O	1.62206400	3.10613900	0.32446800
H	-0.82461900	2.56180200	0.38149600
H	-3.29887400	2.23723300	0.50386500
H	-5.26268300	0.73777600	0.33996200
H	-4.95595100	-1.67976900	-0.17373900
H	-2.69146900	-2.60883600	-0.52437200
H	-0.23161600	-2.27578200	-0.61767300
C	2.42969200	-1.84266500	0.76046900
O	2.76065200	-3.00949400	0.70810600
H	2.31735900	-1.31525300	1.72751700
H	2.16945600	-1.65482300	-1.34169900
H	4.21525900	-0.34026800	-0.83453300
H	3.87506000	2.04944400	-0.37214700

Anthrone-enol

Charge: 0 Multiplicity: 1

Negative Frequency: None



C	2.87198700	1.59598000	-0.00015400
C	3.15959400	0.26935200	-0.00016900
C	2.15178400	-0.76531800	-0.00002600
C	2.50564700	-2.08792600	0.00000100
O	3.73928900	-2.61436400	-0.00000100
H	4.43876100	-1.94262300	0.00033000
H	1.76843100	-2.88132800	-0.00002000
C	0.73090500	-0.34874500	0.00004000
C	-0.33138400	-1.24688000	0.00010100
C	-1.67957500	-0.82264500	0.00005800
C	-2.76326900	-1.75009100	0.00007300
C	-4.06666800	-1.30527700	-0.00000600
C	-4.35743100	0.08804500	-0.00010000
C	-3.33489000	1.00980200	-0.00010500
C	-1.97440900	0.58262500	-0.00002300
C	-0.89584800	1.48939400	-0.00001000
C	0.42305500	1.05750900	0.00002500
C	1.50035100	2.08258000	0.00006400
O	1.24781900	3.30243100	0.00022400
H	-1.08902200	2.55770800	-0.00002200
H	-3.54899400	2.07517900	-0.00017100
H	-5.39148500	0.41917900	-0.00017000
H	-4.88360600	-2.02081100	0.00000100
H	-2.54443700	-2.81448100	0.00014300
H	-0.15552400	-2.31721300	0.00018100
H	4.20978500	-0.01244000	-0.00036200
H	3.66013000	2.34186500	-0.00029400

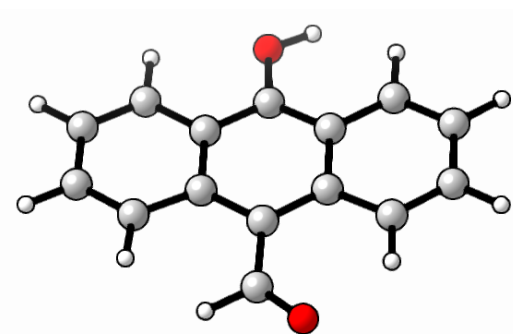
9,10-Hydroxyanthraldehyde

Hydroxy-aldehyde

Charge: 0 Multiplicity: 1

Negative Frequency: None

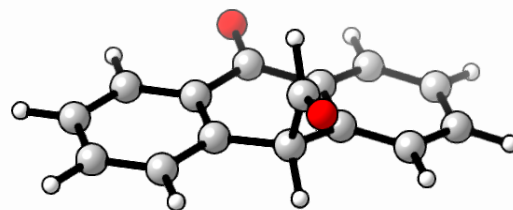
C	-3.78670600	-0.68916500	-0.02716000
C	-2.63558200	-1.43367800	0.02534000
C	-1.35416800	-0.80127900	0.02464000
C	-0.17957500	-1.58536700	0.04531100
C	1.10912400	-1.00227700	-0.00328200
C	2.28478400	-1.81215300	-0.03689900
C	3.53709500	-1.25046300	-0.06357900
C	3.66401500	0.16122000	-0.05537400
C	2.55319000	0.97419400	-0.03073000
C	1.22645100	0.43671900	-0.01062000
C	0.05114900	1.25580800	0.01635500
C	-1.24323200	0.63376300	-0.00778700
C	-2.47612000	1.36085200	-0.09124400
C	-3.69634700	0.72561600	-0.09515300
H	-4.60346700	1.31884600	-0.16228300
H	-2.47151700	2.43895200	-0.17508200
C	0.11269400	2.71233100	0.13301400
O	1.10943100	3.44023200	0.04192500
H	-0.84817500	3.20247000	0.35213100
H	2.67306300	2.04674300	-0.03479200
H	4.65284600	0.60989800	-0.07423600
H	4.41991400	-1.88061300	-0.09345000
H	2.21274800	-2.89593500	-0.05197200
O	-0.36749800	-2.92287000	0.09793500
H	0.46771300	-3.40631400	0.15506900
H	-2.68172700	-2.51541500	0.05896400
H	-4.75750900	-1.17426300	-0.03020900



Anthrone-aldehyde

Charge: 0 Multiplicity: 1

Negative Frequency: None

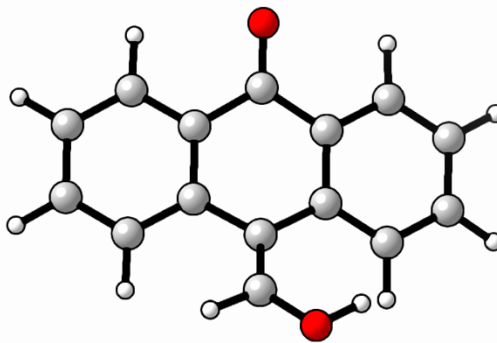


C	-3.68330600	-0.95674100	-0.21748600
C	-2.48280600	-1.58623600	0.09274200
C	-1.27145800	-0.87305100	0.04981800
C	-1.27372700	0.48806500	-0.30942900
C	-2.48984400	1.11588000	-0.61363000
C	-3.68538600	0.39943900	-0.57507500
H	-4.61868200	0.89536700	-0.82350100
H	-2.49525900	2.16789400	-0.88456400
C	0.00000000	1.30308800	-0.29151700
C	1.27372700	0.48806500	-0.30942900
C	2.48984400	1.11588100	-0.61363000
C	3.68538700	0.39944100	-0.57507500
C	3.68330700	-0.95673900	-0.21748500
C	2.48280800	-1.58623500	0.09274200
C	1.27145900	-0.87305100	0.04981800
C	0.00000000	-1.58654400	0.34305900
O	0.00000000	-2.74417100	0.77430300
H	2.45716100	-2.63568000	0.36566400
H	4.61454900	-1.51350300	-0.18627700
H	4.61868200	0.89537000	-0.82350000
H	2.49525900	2.16789500	-0.88456400
C	0.00000000	2.11054000	1.01589500
O	-0.00000400	3.32399000	1.06367600
H	0.00000100	1.49529900	1.93716700
H	0.00000000	2.02717100	-1.11155600
H	-2.45715900	-2.63568100	0.36566500
H	-4.61454800	-1.51350500	-0.18627800

Anthrone-enol

Charge: 0 Multiplicity: 1

Negative Frequency: None



C	-3.48492100	-1.33284100	-0.30606500
C	-2.23965400	-1.85283900	0.02948900
C	-1.10807000	-1.02331000	0.09997000
C	-1.22633500	0.36821500	-0.14125700
C	-2.48760800	0.86754600	-0.52982900
C	-3.59987700	0.03115700	-0.60667600
H	-4.55509500	0.44184800	-0.91927200
H	-2.59338500	1.90065800	-0.84663700
C	-0.04412900	1.22883000	0.02012600
C	-0.10593700	2.51480200	0.46534600
O	-1.19507300	3.23113300	0.81330600
H	-1.99971900	2.68714600	0.80437000
H	0.79417900	3.09275200	0.63908600
C	1.28233000	0.59507400	-0.11657600
C	2.44645000	1.32606700	-0.43012400
C	3.68859700	0.70274200	-0.49216600
C	3.81043400	-0.67491200	-0.24773300
C	2.67253900	-1.41537400	0.04192000
C	1.40843400	-0.79895600	0.10012700
C	0.21631300	-1.63532000	0.36851100
O	0.31893400	-2.81450100	0.73785700
H	2.73197200	-2.48395300	0.21928800
H	4.78136400	-1.15716300	-0.30088500
H	4.56696000	1.28853400	-0.74662600
H	2.37820300	2.38541800	-0.65396200
H	-2.11364600	-2.91200400	0.22735600
H	-4.35311700	-1.98158400	-0.36239900

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