A divergent approach to the synthesis of the yohimbinoid alkaloids venenatine and alstovenine

Terry P. Lebold,† Jessica L. Wood,† Josh Deitch,† Michael W. Lodewyk,‡ Dean J. Tantillo,‡ and Richmond Sarpong*†

†Department of Chemistry
University of California, Berkeley
Berkeley, CA 94720 (USA)
Fax: (+1) 510-642-9675
E-mail: rsarpong@berkeley.edu

‡Department of Chemistry
University of California, Davis
Davis, CA 95616 (USA)
E-mail: tantillo@chem.ucdavis.edu

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**General Experimental**

All reactions were performed in flame-dried glassware fitted with rubber septa under a nitrogen atmosphere unless otherwise specified. Microwave reactions were performed using a Biotage Initiator. Liquid reagents and solvents were transferred via syringe under nitrogen. Tetrahydrofuran (THF), diethyl ether, benzene, toluene, and triethylamine were dried over alumina under a nitrogen atmosphere in a GlassContour solvent system. Dichloromethane (DCM) was distilled over calcium hydride. All other solvents and reagents were used as received unless otherwise noted. Reaction temperatures above 23 °C were controlled by an IKA® temperature modulator. Reactions were monitored by thin layer chromatography using SiliCycle silica gel 60 F254 precoated plates (0.25 mm) which were visualized using UV light, p-anisaldehyde stain, KMnO₄ or CAM stain. Sorbent silica gel (particle size 40-63 μm) was used for flash chromatography. Preparative thin layer chromatography was carried out using Uniplate silica gel precoated plates (2.0 mm). ¹H and ¹³C NMR were recorded on Bruker AVB-400, AV-500, or AV-600 MHz spectrometers with ¹³C operating frequencies of 100, 125, and 150 MHz, respectively, in CDCl₃ or C₆D₆ at 23 °C. Chemical shifts (δ) are reported in ppm relative to the residual solvent signal (CDCl₃ δ = 7.26 for ¹H NMR and δ = 77.0 for ¹³C NMR, C₆D₆ δ = 7.16 ppm for ¹H NMR and δ = 128.06 for ¹³C NMR). Data for ¹H NMR are reported as follows: chemical shift (multiplicity, coupling constant, number of hydrogens). Multiplicity is abbreviated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad). IR spectra were recorded on a Nicolet MAGNA-IR 850 spectrometer and are reported in frequency of absorption (cm⁻¹). Mass spectral data were obtained from the Mass Spectral Facility at the University of California, Berkeley.

**Experimental Procedures and Characterization Data**

Diene 19 (2.060 g, 6.765 mmol) and enone 20 (1.375 g, 9.812 mmol) were dissolved in toluene (45 mL) and the mixture heated to 100 °C. After 16 h NMR analysis showed complete consumption of the diene. The reaction mixture was concentrated under reduced pressure to give a crude mixture that was purified by column chromatography on silica gel (hexanes→5% EtOAc/hexanes) to yield alkene 18-endo (2.553 g, 85% yield) and alkene 18-exo (117 mg, 0.263 mmol, 4% yield) as viscous pale yellow oils. Rf = 0.47 (10% EtOAc/hexanes X 2); ¹H NMR (500 MHz, CDCl₃) δ 7.33 – 7.29 (m, 2H), 7.28-7.24 (m, 3H), 5.91 (dd, J = 10.4, 4.3, 2.7 Hz, 1H), 5.70 (ddd, J = 10.4, 1.1, 1.1 Hz, 1H), 4.65 – 4.63 (m, 1H), 4.54 – 4.49 (m, 2H), 3.75 (s, 3H), 3.67 – 3.60 (m, 2H), 3.02 (ddd, J = 13.0, 6.5, 6.5 Hz, 1H), 2.52 – 2.46 (m, 1H), 2.42 – 2.36 (m, 1H), 2.29 – 2.22 (m, 1H), 2.07 – 1.98 (m, 1H), 1.91 – 1.85 (m, 1H), 0.90 (s, 9H), 0.06 (s, 6H); ¹³C NMR (150 MHz, CDCl₃) δ 212.0, 171.0, 137.9, 128.3, 128.0, 127.9, 127.6, 124.9, 73.2, 71.8, 63.8, 63.4, 54.7, 39.4, 38.7, 36.7, 25.8, 20.6, 18.2, -5.43, -5.46; IR (thin film) νmax 3031, 2953, 2859, 1753, 1727, 1598, 1497, 1455, 1360, 1254, 1231, 1189, 1111, 1088, 1069, 960, 835, 775, 737, 698, 667 cm⁻¹; HRMS (ESI) calc’d for [C₂₅H₃₆O₅SiLi]⁺: m/z 451.2492, found 451.2487.
Sulfonate 21 was prepared in two steps from alkene 18-endo without purification of alkane A or alcohol B, as both intermediates were of sufficient purity for subsequent reactions. For authenticative purposes, a small amount of alkane A and alcohol B were purified to allow full characterization.

Alkene 18-endo (1.248 g, 2.807 mmol) was dissolved in EtOAc (30 mL). 10% Pd/C (325 mg) was then added and the reaction flask was evacuated and backfilled with H₂ (3X). The reaction was carefully monitored and upon completion by NMR analysis (indicated by disappearance of olefinic protons) the reaction mixture was filtered through Celite, the filter cake washed with EtOAc, and the solvent removed under reduced pressure to produce crude alkane A as a colorless oil which was carried on without purification. Crude alkane A was dissolved in 1% HCl/MeOH (25 mL) and stirred for 30 minutes after which TLC showed complete consumption of the starting material. The reaction was poured into saturated NaHCO₃ solution and extracted with DCM (4 X 10 mL). The combined organics were dried with MgSO₄ and the solvent was removed under reduced pressure to give a crude mixture that was purified by column chromatography on silica gel (20→30% EtOAc/hexanes) to yield sulfonate 21 (1.106 g, 83% yield over three steps) as a colorless viscous oil. Rf = 0.55 (20% EtOAc/hexanes); ¹H NMR (500 MHz, CDCl₃) δ 7.36 – 7.21 (m, 5H), 5.96 – 5.88 (m, 2H), 4.57 (d, J = 11.5 Hz, 1H), 4.52 – 4.51 (m, 1H), 4.48 (d, J = 11.5 Hz, 1H), 3.72 (dd, J = 9.6, 6.1 Hz, 1H), 3.67 (s, 3H), 3.58 (dd, J = 9.5, 7.4 Hz, 1H), 2.89 – 2.81 (m, 1H), 2.37 – 2.25 (m, 1H), 2.22 – 2.11 (m, 2H), 2.00 – 1.91 (m, 1H), 1.93 – 1.84 (m, 1H), 0.89 (s, 9H), 0.05 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 210.3, 167.6, 138.3, 132.5, 128.2, 127.6, 127.5, 124.6, 71.3, 70.8, 66.8, 66.4, 52.7, 40.6, 35.5, 34.0, 26.3, 25.9, 18.3, -5.38, -5.42; IR (thin film) νmax 3031, 2953, 2929, 2894, 2857, 1755, 1738, 1730, 1462, 1433, 1399, 1249, 1211, 1101, 1061, 938, 837, 777, 735, 698 cm⁻¹; HRMS (ESI) calc’d for [C₂₅H₂₈O₇SNa]⁺: m/z 495.1453, found 495.1454.
Alcohol 22 was prepared in three steps from sulfonate 21 without purification of the intermediates. For authenticative purposes a small amount of silyl enol ether C was purified to allow full characterization. The procedure for the α-hydroxylation was adapted from: Tsui, H.-C., Paquette, L. A. Reversible charge-accelerated Oxy-Cope rearrangements. J. Org. Chem. 63, 9968-9977 (1998).

Sulfonate 21 (468 mg, 0.990 mmol) was dissolved in DCM (15 mL) and cooled to −30 °C. NEt3 (0.69 mL, 5.0 mmol) was then added followed by the dropwise addition of TBSOTf (0.27 mL, 1.2 mmol). The reaction was then allowed to warm to −10 °C. After 90 min TLC indicated that starting material remained so additional portions of NEt3 (1 mL, 7 mmol) and TBSOTf (0.27 mL, 1.2 mmol) were added. After 60 min TLC showed complete consumption of the starting material and the reaction was quenched with saturated NaHCO3 solution (5 mL). The solution was diluted with H2O and extracted with DCM (4 X 10 mL). The combined organics were concentrated to produce crude silyl enol ether C as a light yellow oil. Silyl enol ether C was dissolved in a 1:1:1 mixture of DCM/acetone/H2O (39 mL). 18-Crown-6 (100.0 mg, 0.378 mmol) and NaHCO3 (6.07 g, 72.3 mmol) were then added. Oxone (5.48 g, 8.91 mmol) was then added in portions over 5 minutes with vigorous stirring. After 60 min TLC indicated that starting material remained, so additional Oxone (2.0 g, 3.2 mmol) was added. After 30 minutes TLC showed complete consumption of the starting material and the reaction was quenched with saturated NaHCO3 solution (5 mL). The solution was then removed to produce the crude alcohol 22 which was absorbed on silica and purified by column chromatography (30→50% EtOAc/hexanes). Alcohol 22 (412 mg, 85%) was obtained as colorless viscous oil. Rf = 0.26 (40% EtOAc/hexanes; 1H NMR (500 MHz, CDCl3) δ 7.92 (d, J = 10.1 Hz, 1H), 4.94 (s, 1H), 4.84 (d, J = 10.1 Hz, 1H), 3.10 (dd, J = 12.8, 6.4 Hz, 1H), 1.84 – 1.77 (m, 1H), 1.62 – 1.42 (m, 3H); 13C NMR (150 MHz, CDCl3) δ 214.4, 170.8, 138.1, 128.2, 127.5, 127.3, 77.3, 72.0, 65.4, 63.0, 40.9, 39.2, 38.1, 26.1, 20.4, 17.3; IR (thin film) νmax 3434, 2950, 2865, 1749, 1724, 1455, 1436, 1399, 1254, 1198, 1165, 1088, 1069, 1046, 736, 698 cm⁻1; HRMS (ESI) calc’d for [C19H24O5Li]+: m/z 339.1784, found 339.1787.

Alcohol 22 was prepared in three steps from sulfonate 21 without purification of the intermediates. For authenticative purposes a small amount of silyl enol ether C was purified to allow full characterization. The procedure for the α-hydroxylation was adapted from: Tsui, H.-C., Paquette, L. A. Reversible charge-accelerated Oxy-Cope rearrangements. J. Org. Chem. 63, 9968-9977 (1998).

Sulfonate 21 (468 mg, 0.990 mmol) was dissolved in DCM (15 mL) and cooled to −30 °C. NEt3 (0.69 mL, 5.0 mmol) was then added followed by the dropwise addition of TBSOTf (0.27 mL, 1.2 mmol). The reaction was then allowed to warm to −10 °C. After 90 min TLC indicated that starting material remained so additional portions of NEt3 (1 mL, 7 mmol) and TBSOTf (0.27 mL, 1.2 mmol) were added. After 60 min TLC showed complete consumption of the starting material and the reaction was quenched with saturated NaHCO3 solution (5 mL). The solution was diluted with H2O and extracted with DCM (4 X 10 mL). The combined organics were concentrated to produce crude silyl enol ether C as a light yellow oil. Silyl enol ether C was dissolved in a 1:1:1 mixture of DCM/acetone/H2O (39 mL). 18-Crown-6 (100.0 mg, 0.378 mmol) and NaHCO3 (6.07 g, 72.3 mmol) were then added. Oxone (5.48 g, 8.91 mmol) was then added in portions over 5 minutes with vigorous stirring. After 60 min TLC indicated that starting material remained, so additional Oxone (2.0 g, 3.2 mmol) was added. After 30 minutes TLC showed complete consumption of the starting material and the reaction was quenched with H2O and extracted with EtOAc (4 X 10 mL). The combined organics were washed with H2O and brine and concentrated to produce a light yellow oil which was redissolved in 1% HCl/MeOH (10 mL). After 60 min a small amount of solid NaHCO3 was added. Solvent was then removed to produce the crude alcohol 22 which was absorbed on silica and purified by column chromatography (30→50% EtOAc/hexanes). Alcohol 22 (412 mg, 85%) was obtained as colorless viscous oil. Rf = 0.26 (40% EtOAc/hexanes; 1H NMR (500 MHz, CDCl3) δ 7.92 (d, J = 10.1 Hz, 1H), 4.94 (s, 1H), 4.84 (d, J = 10.1 Hz, 1H), 3.10 (dd, J = 12.8, 6.4 Hz, 1H), 1.84 – 1.77 (m, 1H), 1.62 – 1.42 (m, 3H); 13C NMR (150 MHz, CDCl3) δ 214.4, 170.8, 138.1, 128.2, 127.5, 127.3, 77.3, 72.0, 65.4, 63.0, 40.9, 39.2, 38.1, 26.1, 20.4, 17.3; IR (thin film) νmax 3434, 2950, 2865, 1749, 1724, 1455, 1436, 1399, 1254, 1198, 1165, 1088, 1069, 1046, 736, 698 cm⁻1; HRMS (ESI) calc’d for [C19H24O5Li]+: m/z 339.1784, found 339.1787.
= 8.0 Hz, 2H), 7.67 (t, J = 7.5 Hz, 1H), 7.57 (dd, J = 8.0, 7.5 Hz, 2H), 7.33 – 7.26 (m, 3H), 7.16 (d, J = 6.5 Hz, 2H), 4.42 (d, J = 11.0 Hz, 1H), 4.39 (s, 1H), 4.22 (d, J = 11.0 Hz, 1H), 4.00 – 3.90 (m, 3H), 3.75 (s, 3H), 3.28 (ddd, J = 13.0, 8.0, 5.0 Hz, 1H), 2.24 (ddd, J = 13.5, 13.0, 7.5 Hz, 1H), 2.14 – 2.02 (m, 3H), 1.60 – 1.42 (m, 4H); 13C NMR (150 MHz, CDCl3) δ = 212.5, 169.7, 137.3, 135.8, 133.9, 129.3, 128.4, 127.89, 127.87, 127.6, 76.5, 73.2, 72.12, 72.06, 63.1, 53.0, 37.3, 34.8, 28.8, 25.4, 16.4; IR (thin film) νmax 3430, 2951, 1758, 1726, 1622, 1448, 1404, 1361, 1256, 1187, 1095, 1047, 955, 826, 755, 689 cm−1; HRMS (ESI+) calc’d for [C25H28O8SNa]+: m/z 511.1403, found 511.1397.

**Rf** = 0.68 (40% EtOAc/hexanes); 1H NMR (600 MHz, CDCl3) δ 7.91 (d, J = 7.8 Hz, 2H), 7.66 (t, J = 7.8 Hz, 1H), 7.56 (t, J = 7.8 Hz, 2H), 7.30 – 7.21 (m, 5H), 4.73 (s, 1H), 4.49, 4.47 (ABq, J = 12.3 Hz, 2H), 4.17 (s, 1H), 3.89 (d, J = 7.2 Hz, 2H), 3.68 (s, 3H), 2.96 – 2.92 (m, 1H), 2.16 (t, J = 12.0 Hz, 1H), 2.02 – 1.92 (m, 2H), 1.84 (ddd, J = 13.2, 7.8, 3.0 Hz, 1H), 1.50 – 1.39 (m, 2H), 1.31 – 1.27 (m, 1H), 0.86 (s, 9H), 0.12 (s, 3H), 0.09 (s, 3H); 13C NMR (150 MHz, CDCl3) δ 173.8, 153.3, 139.4, 136.0, 133.7, 129.2, 128.1, 127.9, 127.0, 126.8, 102.9, 74.4, 73.2, 71.9, 61.1, 52.0, 41.1, 35.6, 27.5, 26.8, 17.82, 17.75, -4.7, -5.6; IR (thin film) νmax 2951, 2931, 2893, 2857, 1727, 1649, 1462, 1449, 1365, 1300, 1238, 1188, 1176, 1096, 1066, 1028, 961, 887, 841, 789, 734, 719, 689 cm−1.

Alcohol 22 (517 mg, 1.06 mmol) was dissolved in DCM (20 mL) and allyl alcohol (3 mL). Pb(OAc)4 (704 mg, 1.59 mmol) was then added in one portion to produce a bright orange solution. The reaction was allowed to stir for one hour after which TLC showed complete consumption of the starting material. The reaction was quenched with saturated NaHCO3 solution and water. The mixture was then filtered through a pad of Celite and washed with DCM (20 mL). The layers were then separated and the aqueous layer extracted with DCM (2 X 20 mL). The combined organics were dried with MgSO4 and the solvent was removed under reduced pressure to give a crude mixture that was purified by column chromatography on silica gel (30% EtOAc/hexanes) to yield aldehyde 17 (472 mg, 82%) as a colorless viscous oil. **Rf** = 0.29 (33% EtOAc/hexanes); 1H NMR (400 MHz, CDCl3) δ 9.62 (s, 1H), 7.84 (dd, J = 8.3, 1.3 Hz, 2H), 7.65 – 7.61 (m, 2H), 7.55 – 7.52 (m, 2H), 7.31 – 7.28 (m, 2H), 7.26 – 7.24 (m, 2H), 7.21 – 7.17 (m, 2H), 5.75 (ddt, J = 6.4 Hz, 1.2 Hz, 1H), 5.26 – 5.08 (m, 2H), 4.61 – 4.54 (m, 1H), 4.52 (d, J = 11.4 Hz, 1H), 4.48 – 4.44 (m, 1H), 4.38 (d, J = 11.3 Hz, 1H), 3.84 – 3.75 (m, 2H), 3.72 (s, 3H), 3.45 (dt, J = 6.6, 3.4 Hz, 1H), 3.07 – 3.02 (m, 1H), 2.30 (ddd, J = 12.4, 6.3, 1.8 Hz, 1H), 2.02 – 1.97 (m, 1H), 1.93 – 1.85 (m, 1H), 1.79 – 1.70 (m, 1H), 1.46 – 1.30 (m, 2H); 13C NMR (150 MHz, CDCl3) δ 201.9, 169.0, 168.1, 138.2, 135.8, 133.8, 131.2, 129.3, 128.4, 127.8, 127.6, 127.2, 119.2, 76.7, 72.2, 72.0, 66.2, 62.9, 53.3, 41.3, 37.5, 31.2, 24.8, 17.8; IR (thin film) νmax 3065, 2952, 2726, 1737, 1727, 1449, 1359, 1254, 1204, 1187, 1126, 1095, 1067, 1028, 963, 813, 755, 689 cm−1; HRMS (ESI+) calc’d for [C28H32O9SLi]+: m/z 551.1922, found 551.1927.
Aldehyde 17 (57 mg, 0.10 mmol) was dissolved in acetonitrile (4 mL). KCN (34 mg, 0.52 mmol) and MgSO₄ (210 mg) were then added and mixture stirred for 10 minutes after which tryptamine (25 mg, 0.16 mmol) was added. Upon complete consumption of the starting material by TLC analysis the reaction mixture was filtered through a sintered glass funnel and the solids washed with EtOAc. The solvent was removed under reduced pressure to produce a crude oil that was purified by column chromatography on silica gel (50% EtOAc/hexanes) to yield aminonitrile 16a (52 mg, 90%) as a colorless film. 

**R<sub>f</sub>** = 0.95 (5% MeOH/DCM); **<sup>1</sup>H NMR** (500 MHz, CDCl₃) δ 7.90 (s, 1H), 7.59 (d, J = 7.9 Hz, 1H), 7.39 – 7.25 (m, 5H), 7.18 (t, J = 7.0 Hz, 1H), 7.10 (t, J = 8.0 Hz, 1H), 7.02 (d, J = 2.4 Hz, 1H), 5.83 (m, 1H), 5.29 (dd, J = 17.2, 1.5 Hz, 1H), 5.19 (dd, J = 10.4, 1.3 Hz, 1H), 4.69 – 4.45 (m, 5H), 3.96 (s, 1H), 3.74 (s, 3H), 2.98 – 2.60 (m, 3H), 2.14 (qd, J = 13.8, 13.1, 4.2 Hz, 1H), 2.07 – 1.99 (m, 1H), 1.81 – 1.68 (m, 2H), 1.29 – 1.21 (m, 2H); **<sup>13</sup>C NMR** (100 MHz, CDCl₃) δ 169.5, 167.7, 138.8, 136.1, 131.4, 128.2, 127.4, 127.3, 127.1, 121.9, 121.6, 119.2, 118.7, 118.68, 116.5, 113.7, 111.0, 76.6, 72.3, 65.8, 62.4, 54.6, 53.7, 53.1, 35.2, 26.1, 23.1, 20.0; **IR** (thin film) ν<sub>max</sub> 3414, 3059, 3031, 2950, 2930, 2867, 1734, 1497, 1456, 1434, 1341, 1252, 1206, 1116, 1092, 1066, 1016, 943, 911, 740, 698 cm<sup>-1</sup>; **HRMS** (ESI+) calc’d for [C<sub>34</sub>H₃₈N₃O₅]<sup>+</sup>: m/z 556.2811, found 556.2813.

Aldehyde 17 (188 mg, 0.345 mmol) was dissolved in acetonitrile (6 mL). KCN (112 mg, 1.72 mmol) and MgSO₄ (500 mg) were then added and mixture stirred for 10 minutes after which 4-OMe-tryptamine (85 mg, 0.45 mmol) was added. Upon complete consumption of the starting material by TLC analysis the reaction mixture was filtered through a sintered glass funnel and the solids washed with EtOAc (10 mL). The solvent was removed under reduced pressure to produce a crude oil that was purified by column chromatography on silica gel (30% EtOAc/hexanes) to yield aminonitrile 16b (154 mg, 76%) as a colorless foam. 

**R<sub>f</sub>** = 0.28 (33% EtOAc/hexanes); **<sup>1</sup>H NMR** (500 MHz, CDCl₃) δ 7.84 (s, 1H), 7.36 – 7.31 (m, 2H), 7.30 – 7.24 (m, 3H), 7.07 (t, J = 8.0 Hz, 1H), 6.93 (d, J = 8.1 Hz, 1H), 6.86 (s, 1H), 6.46 (d, J = 7.7 Hz, 1H), 5.83 (dtt, J = 17.3, 10.5, 5.7 Hz, 1H), 5.28 (dd, J = 17.3, 1.5 Hz, 1H), 5.18 (dd, J = 10.4, 1.3 Hz, 1H), 4.68 – 4.58 (m, 2H), 4.56 – 4.43 (m, 3H), 3.97 (s, 1H), 3.91 (s, 3H), 3.74 (s, 3H), 3.06 – 2.89 (m, 3H), 2.80 – 2.56 (m, 5H), 2.26 (d, J = 14.2 Hz, 1H), 2.19 – 2.09 (m, 1H), 2.07 – 2.00 (m, 1H), 1.73 (dd, J = 35.4, 14.3 Hz, 2H), 1.29 – 1.20 (m, 1H); **<sup>13</sup>C NMR** (100 MHz, CDCl₃) δ 169.5, 167.8, 154.7, 138.8, 137.9, 131.4, 128.2, 127.3, 127.1, 122.7, 120.5, 118.7, 117.3, 116.8, 114.2, 104.3, 99.3, 76.6, 72.3, 65.8, 62.4, 57.6, 55.0, 54.7, 53.6, 53.0, 35.2, 33.6, 26.2, 25.4, 24.9, 20.0 (note: 1 sp<sup>2</sup> carbon is missing presumably due to overlap); **IR** (thin film) ν<sub>max</sub> 3409, 2951, 2837, 2252, 2220, 1735, 1616, 1587, 1548, 1507, 1455, 1436, 1362, 1255, 1207, 1118, 1066, 1028, 1017, 943, 911, 777, 734, 699 cm<sup>-1</sup>; **HRMS** (ESI+) calc’d for [C<sub>34</sub>H₄₀N₃O₆]<sup>+</sup>: m/z 586.2912, found 586.2928.
Aldehyde 17 (43 mg, 0.079 mmol) was dissolved in acetonitrile (4 mL). KCN (103 mg, 1.58 mmol) and MgSO$_4$ (150 mg) were then added and mixture stirred for 10 minutes after which 6-OMe-tryptamine (30 mg, 0.16 mmol) in acetonitrile (1.5 mL) was added. Upon complete consumption of the starting material by TLC analysis the reaction mixture was filtered through a sintered glass funnel and the solids washed with EtOAc (10 mL). The solvent was removed under reduced pressure to produce a crude oil that was purified by column chromatography on silica gel (33% EtOAc/hexanes) to yield aminonitrile 16c (40 mg, 87%) as a colorless film. R$_f$ = 0.51 (33% EtOAc/hexanes); $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.80 (s, 1H), 7.45 (d, $J$ = 8.5 Hz, 1H), 7.35 – 7.26 (m, 5H), 6.90 (s, 1H), 6.83 (d, $J$ = 2.5 Hz, 1H), 5.29 (dd, $J$ = 17.0, 1.0 Hz, 1H), 5.19 (dd, $J$ = 10.5, 1.0 Hz, 1H), 4.69 – 4.45 (m, 5H), 3.96 (s, 1H), 3.84 (s, 3H), 3.74 (s, 3H), 3.00 – 2.60 (m, 8H), 2.27 (d, $J$ = 14.1 Hz, 1H), 2.14 (qd, $J$ = 13.6, 4.1 Hz, 1H), 2.07 – 1.97 (m, 1H), 1.81 – 1.69 (m, 2H), 1.30 – 1.19 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 169.5, 167.7, 156.5, 138.8, 136.8, 131.4, 128.2, 127.3, 127.1, 121.8, 120.3, 119.3, 118.7, 116.5, 113.7, 109.2, 94.7, 76.6, 72.3, 65.8, 62.4, 56.2, 55.7, 54.6, 53.7, 53.1, 35.1, 33.5, 26.1, 25.4, 23.2, 20.1; IR (thin film) $\nu_{\text{max}}$ 3414, 2950, 1737, 1730, 1630, 1453, 1346, 1305, 1257, 1200, 1160, 1117, 1090, 1066, 943, 802, 745 cm$^{-1}$; HRMS (ESI+) calc’d for [C$_{34}$H$_{40}$N$_3$O$_6$]$^+$: m/z 586.2912, found 586.2922.

Aminonitrile 16a (26 mg, 0.047 mmol) was dissolved in 10% 1N HCl/THF (9 mL) and the reaction stirred until TLC showed complete consumption of the starting material. The reaction was quenched with saturated NaHCO$_3$. Brine solution was added and mixture extracted with DCM (4 X 10 mL). The solvent was removed under reduced pressure to produce a crude oil that was purified by column chromatography on silica gel (EtOAc→5% MeOH/DCM) to yield pentacycle 23a (21 mg, 84%) as a colorless film. R$_f$ = 0.18 (5% MeOH/DCM); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.11 (s, 1H), 7.49 (d, $J$ = 7.6 Hz, 1H), 7.41 (d, $J$ = 7.9 Hz, 1H), 7.36 – 7.26 (m, 5H), 7.21 – 7.10 (m, 2H), 5.92 (m, 1H), 5.41 – 5.23 (m, 2H), 4.76 – 4.54 (m, 3H), 4.52 – 4.40 (m, 3H), 3.59 (s, 3H), 3.33 – 3.16 (m, 2H), 3.07 – 2.93 (m, 2H), 2.83 (td, $J$ = 14.3, 4.5 Hz, 1H), 2.62 – 2.31 (m, 5H), 2.15 – 2.00 (m, 1H), 1.81 (m, 1H), 1.51 (d, $J$ = 13.2 Hz, 1H), 1.34 (d, $J$ = 13.9 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 169.7, 168.6, 138.7, 135.9, 133.2, 131.7, 128.2, 127.9, 127.3, 127.2, 121.1, 119.2, 119.1, 117.8, 111.3, 107.6, 72.2, 65.9, 62.7, 61.0, 54.6, 52.9, 51.0, 50.5, 33.9, 27.8, 25.5, 24.1, 19.7, 16.7; IR (thin film) $\nu_{\text{max}}$ 3412, 3032, 2926, 2855, 1737, 1728, 1462, 1451, 1352, 1330, 1286, 1253, 1199, 1144, 1091, 1067, 1017, 910, 737, 697 cm$^{-1}$; HRMS calc’d for [C$_{32}$H$_{37}$N$_2$O$_5$]$^+$: m/z 529.2697, found 529.2690.
Pentacycle 16b could be obtained as either the free base or HCl salt following the procedures described below.

Aminonitrile 16b (67 mg, 0.11 mmol) was dissolved in a solution of 10% 1N HCl in THF (10 mL). The reaction was allowed to stir for 28 hours after which TLC analysis showed complete consumption of the starting material. The reaction was then carefully neutralized with saturated NaHCO₃ solution and the mixture extracted with DCM (3 X 10 mL). The combined organics were dried with MgSO₄ and the solvent was removed under reduced pressure. The crude mixture was purified by column chromatography on silica gel (2% MeOH/DCM) to yield pentacycle 23b (52 mg, 0.093 mmol, 81%) as a light yellow solid. 

**Rf** = 0.37 (5% MeOH/DCM);

**1H NMR** (400 MHz, CDCl₃) δ 8.06 (s, 1H), 7.38–7.26 (m, 5H), 7.09–6.97 (m, 2H), 6.48 (dd, J = 7.1, 1.6 Hz, 1H), 5.90 (ddt, J = 16.6, 10.3, 5.9 Hz, 1H), 5.38–5.22 (m, 2H), 4.73–4.52 (m, 3H), 4.49–4.37 (m, 3H), 3.89 (s, 3H), 3.58 (s, 3H), 3.28–3.09 (m, 3H), 2.85 (d, J = 15.1 Hz, 1H), 1.51 (d, J = 12.9 Hz, 1H), 1.33 (d, J = 13.7 Hz, 1H); **13C NMR** (150 MHz, CDCl₃) δ 169.6, 168.6, 154.2, 138.7, 137.2, 131.7, 128.2, 127.6, 127.5, 121.7, 119.1, 117.9, 107.5, 104.8, 99.5, 76.7, 72.2, 65.9, 62.7, 55.2, 54.7, 52.9, 51.3, 50.4, 33.84, 33.75, 25.5, 24.1, 19.7, 18.8; **IR** (thin film) νmax 3340, 2929, 1737, 1727, 1590, 1504, 1452, 1353, 1330, 1251, 1198, 1145, 1105, 1066, 910, 734, 697 cm⁻¹; **HRMS** (ESI+) calc’d for [C₃₃H₃₈N₂O₆]⁺: m/z 559.2803, found 559.2808.

Direct concentration of the above reaction mixture leads to formation of the HCl salt of 23b. Recrystallization from MeOH with slow diffusion of hexanes yields crystals suitable for x-ray diffraction. 

**1H NMR** (500 MHz, CDCl₃) δ 12.58 (d, J = 10.0 Hz, 1H), 8.37 (s, 1H), 7.36–7.33 (m, 3H), 7.28–7.23 (m, 2H), 7.13 (dd, J = 8.5, 8.0 Hz, 1H), 7.04 (d, J = 8.5 Hz, 1H), 6.52 (d, J = 8.0 Hz, 1H), 5.83 (dddd, J = 17.5, 10.5, 5.5, 5.5 Hz, 1H), 5.30 (dd, J = 17.5, 1.5 Hz, 1H), 5.24 (dd, J = 10.5, 1.5 Hz, 1H), 4.92 (s, 3H), 4.70 (d, J = 11.5 Hz, 1H), 4.68 (dd, J = 13.0, 5.5 Hz, 1H), 4.52 (dd, J = 13.0, 5.5 Hz, 1H), 4.48 (br.s, 1 H), 4.36 (d, J = 11.5 Hz, 1H), 3.90 (s, 3H), 3.59 (s, 3H), 3.54 (dd, J = 13.0, 5.0 Hz, 1H), 3.48 (dd, J = 13.0, 5.5 Hz, 1H), 3.37–3.28 (m, 2H), 3.26–3.17 (m, 2H), 3.01 (d, J = 13.0 Hz, 1H), 2.83 (dq, J = 13.5, 4.0 Hz, 1H), 2.60 (d, J = 13.0 Hz, 1H), 2.49 (d, J = 13.0 Hz, 1H), 2.17 (d, J = 15.5 Hz, 1H), 1.77 (d, J = 13.0 Hz, 1H), 1.67 (t, J = 14.0 Hz, 1H), 1.48 (d, J = 14.0 Hz, 1H); **13C NMR** (100 MHz, CDCl₃) δ 168.6, 168.3, 154.2, 138.2, 138.0, 131.2, 128.4, 127.6, 127.5, 124.3, 123.8, 119.3, 116.8, 106.0, 105.1, 100.1, 75.7, 72.3, 66.4, 62.2, 55.8, 55.2, 53.2, 51.2, 49.2, 32.4, 31.7, 25.0, 23.0, 19.5, 17.8; **IR** (thin film) νmax 3427, 3174, 2948, 2493, 1736, 1512, 1450, 1435, 1359, 1330, 1256, 1206, 1167, 1106, 1067, 738 cm⁻¹; **HRMS** (ESI+) calc’d for [C₃₃H₃₉N₂O₆]⁺: m/z 559.2803, found 559.2811.
Aminonitrile 16c (24 mg, 0.041 mmol) was dissolved in 10% 1N HCl/THF (9 mL) and the reaction stirred until TLC showed complete consumption of the starting material. The reaction was quenched with saturated NaHCO₃. Brine solution was added and mixture extracted with DCM (4 X 10 mL). The solvent was removed under reduced pressure to produce a crude oil that was purified by column chromatography on silica gel (5% MeOH/DCM) to yield pentacycle 23c (22 mg, 96%) as a light yellow film. 

\[ R_f = 0.52 \] (10% MeOH/DCM); \[ ^1H \text{ NMR} \] (400 MHz, CDCl₃) \( \delta \) 8.05 (s, 1H), 7.39 – 7.22 (m, 6H), 6.94 (d, \( J = 2.2 \) Hz, 1H), 6.79 (dd, \( J = 8.6, 2.3 \) Hz, 1H), 5.97 – 5.82 (m, 1H), 5.40 – 5.21 (m, 2H), 4.74 – 4.40 (m, 6H), 3.86 (s, 3H), 3.60 (s, 3H), 3.39 – 3.20 (m, 2H), 3.08 – 2.80 (m, 3H), 2.68 – 2.55 (m, 2H), 2.52 – 2.31 (m, 3H), 2.15 – 2.03 (m, 1H), 1.89 – 1.71 (m, 2H), 1.56 (d, \( J = 13.3 \) Hz, 1H), 1.36 (d, \( J = 13.8 \) Hz, 1H); \[ ^13C \text{ NMR} \] (100 MHz, CDCl₃) \( \delta \) 169.5, 168.7, 156.2, 138.6, 136.8, 131.6, 130.6, 128.3, 127.3, 127.2, 122.1, 119.1, 118.3, 109.0, 107.1, 95.5, 76.5, 72.2, 66.0, 62.6, 55.8, 54.6, 53.0, 50.6, 50.0, 33.6, 33.5, 25.4, 23.8, 19.5, 16.6; \[ IR \] (thin film) \( v_{max} \) 3398, 2929, 2854, 1732, 1628, 1570, 1498, 1456, 1360, 1330, 1258, 1233, 1200, 1159, 1147, 1091, 1066, 1030, 943, 817, 738, 699 cm⁻¹; \[ HRMS \] calc’d for [C₃₃H₃₉N₂O₆]+: m/z 559.2803, found 559.2796.

A 5 mL microwave vial was charged with a stir bar, aminonitrile 16a (20 mg, 0.036 mmol), sodium iodide (14 mg, 0.095 mmol), and MeCN (3.6 mL). The vials were sealed, then evacuated and backfilled with N₂ (3X). The reaction vial was heated in the microwave at 160 °C for 1 h, then 180 °C for an additional 1 h to force complete conversion. Upon completion, the solvent was removed under reduced pressure to give a crude mixture that was purified by column chromatography on silica gel (2% MeOH/DCM) to yield pentacycle 24a (10 mg, 53%) as a yellow solid. 

\[ R_f = 0.36 \] (5% MeOH/DCM); \[ ^1H \text{ NMR} \] (600 MHz, CDCl₃) \( \delta \) 7.85 (s, 1H), 7.45 (d, \( J = 7.7 \) Hz, 1H), 7.30 (d, \( J = 8.0 \) Hz, 1H), 7.23 – 7.03 (m, 5H), 7.11 (t, \( J = 8.2 \) Hz, 1H), 7.06 (t, \( J = 7.5 \) Hz, 1H), 5.88 – 5.78 (m, 1H), 5.31 – 5.17 (m, 2H), 4.72 – 4.65 (m, 1H), 4.57 (d, \( J = 12.0 \) Hz, 1H), 4.51 – 4.44 (m, 2H), 4.36 (d, \( J = 11.9 \) Hz, 1H), 3.75 (s, 3H), 3.17 (d, \( J = 11.9 \) Hz, 1H), 3.01 – 2.93 (m, 2H), 2.89 – 2.78 (m, 2H), 2.69 (dd, \( J = 14.2, 4.3 \) Hz, 1H), 2.62 – 2.51 (m, 2H), 2.54 – 2.45 (m, 1H), 2.39 – 2.24 (m, 2H), 2.04 – 1.94 (m, 1H), 1.86 – 1.78 (m, 1H), 1.65 (d, \( J = 12.9 \) Hz, 1H), 1.31 (d, \( J = 14.3 \) Hz, 1H); \[ ^13C \text{ NMR} \] (150 MHz, CDCl₃) \( \delta \) 170.0, 168.6, 138.6, 135.9, 131.7, 128.1, 127.4, 127.24, 127.19, 121.0, 119.2, 118.5, 118.0, 110.7, 107.8, 76.4, 71.9, 65.7, 63.0, 61.5, 61.2, 53.4, 53.0, 39.5, 34.7, 27.4, 25.3, 21.7, 20.6; \[ IR \] (thin film) \( v_{max} \) 3399, 2929, 2854, 1732, 1453, 1370, 1351, 1321, 1231, 1197, 1108, 1092, 1066, 1025, 911, 738, 699 cm⁻¹; \[ HRMS \] (ESI+) calc’d for [C₃₂H₃₇N₂O₅]+: m/z 529.2697, found 529.2688.
Two separate 5 mL microwave vials were charged with a stir bar, aminonitrile 16b (19 mg in each, 0.065 mmol), sodium iodide (14 mg in each, 0.18 mmol), and MeCN (4 mL each). The vials were sealed, then evacuated and backfilled with N₂ (3X). Each reaction vial was heated in the microwave at 160 °C for 2.5 h. Upon completion, the contents of both vials were combined, and the solvent was removed under reduced pressure to give a crude mixture that was purified by column chromatography on silica gel (2% MeOH/DCM) to yield pentacycle 24b (26 mg, 72%) as a yellow solid.

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\text{R}_f = 0.48 \text{ (5\% MeOH/DCM); } ^1\text{H NMR} \ (500 \text{ MHz, CDCl}_3) \delta 7.79 (s, 1H), 7.23 - 7.13 (m, 5H), 7.01 - 6.96 (m, 1H), 6.91 (dd, \text{J} = 8.1, 2.1 \text{ Hz, 1H}), 6.44 (d, \text{J} = 8.1 \text{ Hz, 1H}), 5.88 - 5.75 (m, 1H), 5.27 (d, \text{J} = 17.1 \text{ Hz, 1H}), 5.19 (d, \text{J} = 10.5 \text{ Hz, 1H}), 4.68 (dd, \text{J} = 13.1, 5.5 \text{ Hz, 1H}), 4.56 (d, \text{J} = 11.8 \text{ Hz, 1H}), 4.49 - 4.43 (m, 2H), 4.36 (d, \text{J} = 11.8 \text{ Hz, 1H}), 3.87 (s, 3H), 3.74 (s, 3H), 3.15 - 3.07 (m, 2H), 2.99 - 2.88 (m, 2H), 2.87 - 2.76 (m, 2H), 2.53 (d, \text{J} = 12.0 \text{ Hz, 2H}), 2.51 - 2.42 (m, 1H), 2.30 (m, 2H), 1.99 (d, \text{J} = 13.5 \text{ Hz, 1H}), 1.81 (t, \text{J} = 14.4 \text{ Hz, 1H}), 1.63 (d, \text{J} = 13.1 \text{ Hz, 1H}), 1.30 (d, \text{J} = 14.5 \text{ Hz, 1H}); ^{13}\text{C NMR} \ (150 \text{ MHz, CDCl}_3) \delta 170.0, 168.6, 154.4, 138.6, 137.3, 133.5, 131.7, 128.1, 127.20, 127.19, 121.7, 118.5, 107.6, 104.3, 99.7, 76.4, 71.9, 65.7, 63.0, 61.5, 61.2, 55.3, 53.7, 52.9, 39.4, 27.5, 25.3, 23.8, 20.6, 14.1; \text{IR} \ (\text{thin film}) \nu_{\text{max}} 3397, 2936, 2800, 2752, 1733, 1618, 1596, 1569, 1457, 1435, 1256, 1105 \text{ cm}^{-1}; \text{HRMS} \text{ calc’d for } [\text{C}_{33}\text{H}_{39}\text{N}_2\text{O}_6]^+: m/z 559.2803, \text{ found 559.2797.}
\]

A 5 mL microwave vial was charged with a stir bar, aminonitrile 16c (10 mg, 0.02 mmol), sodium iodide (8.5 mg, 0.057 mmol), and MeCN (1.9 mL). The vial was sealed, then evacuated and backfilled with N₂ (3X). The reaction vial was heated in the microwave at 160 °C for 0.5 h. Upon completion, the solvent was removed under reduced pressure to give a crude mixture that was purified by column chromatography on silica gel (2% MeOH/DCM) to yield pentacycle 24c (9.1 mg, 96%) as a yellow solid.

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\text{R}_f = 0.36, \text{ (10\% MeOH/DCM);} ^1\text{H NMR} \ (600 \text{ MHz, CDCl}_3) \delta 7.73 (s, 1H), 7.39 - 7.31 (m, 2H), 7.24 - 7.15 (m, 4H), 6.83 (d, \text{J} = 2.2 \text{ Hz, 1H}), 6.73 (dd, \text{J} = 8.6, 2.3 \text{ Hz, 1H}), 5.83 (m, 1H), 5.31 - 5.17 (m, 2H), 4.73 - 4.65 (m, 1H), 4.57 (d, \text{J} = 12.0 \text{ Hz, 1H}), 4.53 - 4.41 (m, 2H), 4.36 (d, \text{J} = 12.1 \text{ Hz, 1H}), 3.83 (s, 3H), 3.74 (s, 3H), 3.14 (d, \text{J} = 11.5 \text{ Hz, 1H}), 3.02 - 2.88 (m, 3H), 2.87 - 2.77 (m, 2H), 2.69 - 2.60 (m, 1H), 2.61 - 2.43 (m, 3H), 2.40 - 2.22 (m, 2H), 1.99 (d, \text{J} = 15.2 \text{ Hz, 1H}), 1.86 - 1.77 (m, 1H), 1.31 (d, \text{J} = 15.4 \text{ Hz, 1H}); ^{13}\text{C NMR} \ (100 \text{ MHz, CDCl}_3) \delta 170.0, 168.6, 155.8, 138.6, 136.7, 134.2, 131.7, 128.5, 128.3, 128.1, 127.6, 127.2, 122.0, 118.5, 118.4, 108.5, 107.6, 95.1, 76.4, 71.9, 65.7, 62.9, 61.5, 61.2, 55.8, 53.4, 52.9, 39.5, 34.7, 27.5, 25.3, 21.8, 20.6; \text{IR} \ (\text{thin film}) \nu_{\text{max}} 3397, 2931, 2800, 2752, 1733, 1630, 1498, 1457, 1345, 1263, 1229, 1198, 1154, 1107, 1067, 1028, 910, 734, 699 \text{ cm}^{-1}; \text{HRMS} \ (\text{ESI}+) \text{ calc’d for } [\text{C}_{33}\text{H}_{39}\text{N}_2\text{O}_6]^+: m/z 559.2803, \text{ found 559.2792.}
A 4 mL vial was charged with pentacycle 23b (9 mg, 0.02 mmol), Pd(OAc)₂ (2.4 mg, 0.01 mmol), PPh₃·PS (2.8 mg, 3 mmol/g, 0.008 mmol), EtOH (0.5 mL) and H₂O (0.1 mL). The vial was purged with N₂ for 5 min, then sealed with Teflon tape, and heated to 70 °C in a heating block. Upon complete consumption of starting material (by TLC), the reaction mixture was filtered through a plug of Celite, rinsed with DCM (2 mL). The combined organics were dried with MgSO₄ and the solvent was removed under reduced pressure to give a crude mixture that was purified by column chromatography on silica gel (1% MeOH/DCM→10% MeOH/DCM) to yield monoester 29 (3.1 mg, 41%) as a white solid and enoate 30 (1.1 mg, 19%).

\[ R_f = 0.3 \text{ (10\% MeOH/DCM)} \]

**1H NMR** (500 MHz, CDCl₃) δ 8.28 (s, 1H), 7.40–7.25 (m, 5H), 7.12–7.01 (m, 2H), 6.49 (d, J = 7.5 Hz, 1H), 4.71 (s, 1H), 4.65 (d, J = 11.9 Hz, 1H), 4.36 (d, J = 11.9 Hz, 1H), 4.18 (s, 1H), 3.89 (s, 3H), 3.66 (s, 3H), 3.51–3.30 (m, 2H), 3.27–3.04 (m, 3H), 2.93–2.78 (m, 2H), 2.53–2.37 (m, 3H), 2.26–2.16 (m, 1H), 2.06 (m, 1H), 1.63–1.61 (m, 1H) 1.44 (d, J = 14.0 Hz , 1H), 1.37–1.26 (m, 1H);

**13C NMR** (150 MHz, CDCl₃) δ 172.8, 154.3, 138.6, 137.8, 128.3, 127.5, 127.4, 123.1, 117.2, 106.6, 104.9, 100.0, 73.4, 71.4, 55.2, 51.6, 50.8, 49.4, 49.2, 35.9, 29.7, 29.0, 28.1, 24.1, 19.7, 18.3 (note: 1 sp² carbon is missing presumably due to overlap);

**IR** (thin film) ν max 3431, 2929, 1731, 1508, 1436, 1353, 1300, 1257, 1208, 1106, 1066, 910, 731, 667, 643 cm⁻¹;

**HRMS** (ESI⁺) calc’d for [C₂₉H₃₅N₂O₄]+: m/z 475.2597, found 475.2591.

Pale yellow solid. \[ R_f = 0.3 \text{ (10\% MeOH/DCM)} \];

**1H NMR** (500 MHz, CDCl₃) δ 7.98 (s, 1H), 7.07–6.95 (m, 3H), 6.47 (d, J = 7.5 Hz 1H), 3.89 (s, 3H), 3.78 (s, 3H), 3.24–3.09 (m, 2H), 3.09–2.95 (m, 2H), 2.95–2.83 (m, 1H), 2.61 (s, 1H), 2.53 (m, 1H), 2.38–2.06 (m, 6H), 1.94–1.81 (br s, 1H), 1.66–1.56 (m, 1H);

**13C NMR** (150 MHz, CDCl₃) δ 167.6, 154.4, 140.5, 137.2, 128.2, 127.3, 121.9, 117.8, 107.8, 104.6, 99.7, 64.4, 60.4, 55.3, 54.5, 52.2, 51.6, 33.1, 30.7, 19.1, 14.2, 13.7; **IR** (thin film) ν max 2925, 2851, 1701, 1635, 1559, 1512, 1437, 1358, 1334, 1251, 1211, 1129, 1108, 778, 738, 700 cm⁻¹; **HRMS** (ESI⁺) calc’d for [C₂₂H₂₇N₂O₃]+: m/z 367.2022, found 367.2018.

A flame-dried 4 mL vial was charged with monoester 29 (15 mg, 0.032 mmol) and DCM (1.9 mL). The reaction flask was cooled to –78 °C in a dry ice/acetone bath under N₂. A 1M solution of BBr₃ in DCM (160 μL, 0.16 mmol, 5 equiv) was added dropwise over 5 mins. The light yellow solution became dark brown and heterogeneous with the addition of BBr₃. Upon complete consumption of starting material (by TLC), the reaction mixture was quenched by the addition of sat. aq. NaHCO₃ (3 mL). The aq. layer was extracted with DCM (3 X 5 mL), then the combined organics were washed with brine, dried with MgSO₄ and the solvent was removed under reduced pressure to give a crude mixture that was purified by preparative TLC on silica gel (5% MeOH/DCM) to yield venenatine 9 (6.9 mg, 56%) as a white solid. \[ R_f = 0.10 \text{ (10\% MeOH/DCM)} \];

**1H NMR** (500 MHz, CDCl₃) δ 8.13 (s, 1H), 6.99 (dd, J = 7.5, 8.0 Hz, 1H), 9.94 (d, J = 8.0 Hz, 1H), 6.44 (d, J = 7.5 Hz, 1H), 4.32 (s, 1H), 4.29 (s, 1H),
3.86 (s, 3H), 3.80 (s, 3H), 3.25 – 3.10 (m, 3H), 3.00 (dd, $J = 11.5, 3.5$ Hz, 1H), 2.82-2.73 (m, 2H), 2.50 (dd, $J = 11.5, 2.0$ Hz, 1H), 2.45 (br.s, 1H), 2.34 (dq, $J = 12.5, 3.0$ Hz, 1H), 2.21 (br.s, 1H), 2.08-1.98 (m, 2H), 1.83 (d, $J = 14.0$ Hz, 1H), 1.55 (d, $J = 12.5$ Hz, 1H), 1.43 (tt, $J = 13.5, 3.5$ Hz, 1H), 1.32 (dd, $J = 13.5, 3.5$ Hz, 1H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 175.0, 154.2, 137.0, 131.0, 121.6, 117.8, 107.7, 104.4, 99.5, 65.8, 55.2, 54.2, 51.8, 51.4, 50.6, 49.5, 36.7, 32.0, 31.1, 25.8, 19.8, 18.9; IR (thin film) $\nu_{\text{max}}$ 3390, 2951, 1717, 1622, 1437, 1262, 1107 cm$^{-1}$; HRMS (ESI+) calc’d for [C$_{22}$H$_{29}$N$_2$O$_4$]$^+$: $m/z$ 385.2122, found 385.2127.

| This Work | Isolated$^a$ | Computational |
|-----------|-------------|---------------|
| 175.0     | 174.7       | 178.2         |
| 154.2     | 155.1       | 152.5         |
| 137.0     | 137.1       | 134.4         |
| 131.0     | 130.6       | 131.2         |
| 121.6     | 121.5       | 118.9         |
| 117.8     | 117.6       | 115.9         |
| 107.7     | 107.1       | 107.1         |
| 104.4     | 105.7       | 102.7         |
| 99.5      | 104.3       | 96.8          |
| 65.8      | 67.1        | 67.0          |
| 55.2      | 54.9        | 54.4          |
| 54.2      | 53.8        | 51.9          |
| 51.8      | 51.9        | 51.5          |
| 51.4      | 51.5        | 51.3          |
| 50.6      | 50.8        | 50.9          |
| 49.5      | 50.7        | 50.7          |
| 36.7      | 39.7        | 38.5          |
| 32.0      | 32.0        | 32.7          |
| 31.1      | 31.6        | 32.3          |
| 25.8      | 31.0        | 25.9          |
| 19.8      | 22.8        | 21.2          |
| 18.9      | 18.7        | 20.6          |

$^a$ Chatterjee, A., Roy, D. J., Mukhopadhyay S. 16-epivenenatine and 16-epialstovenine, new stereomers from Alstonia venenata. Phytochemistry 20, 1981-1985 (1981).
Procedures for the deallylation/decarboxylation sequence were adapted from: (a) Kunz, H., Waldmann, H. Synthesis of the Glycopeptide Partial Sequence A80–A84 of Human Fibroblast Interferon. Helv. Chim. Acta 68, 618-622 (1985). (b) Deziel, R. Mild palladium (O)-catalyzed deprotection of allyl esters. A useful application in the synthesis of carbapenems and other β-lactam derivatives. Tetrahedron Lett. 28, 4371-4372 (1987).

A 5 mL microwave vial was charged with pentacycle 24b (14 mg, 0.025 mmol), Pd2dba3•CHCl3 (1.8 mg, 2.0 μmol), MeCN (2 mL) and pyrrolidine (20 μL, 0.2 mmol). The vial was sealed, then evacuated and backfilled with N2 (3X) and heated to 70 °C in an oil bath. Upon complete consumption of starting material (by TLC), the solvent was removed under reduced pressure to give a crude mixture that was purified by preparative TLC on silica gel (2% MeOH/DCM → 5% MeOH/DCM) to yield monoester 31 (7.7 mg) as a white solid. Rf = 0.36 (10% MeOH/DCM);

**1H NMR** (600 MHz, CDCl3) δ 7.83 (s, 1H), 7.23 (m, 5H), 6.98 (t, J = 7.7 Hz, 1H), 6.90 (d, J = 7.8 Hz, 1H), 6.44 (d, J = 7.8 Hz, 1H), 4.53 (d, J = 12.4 Hz, 1H), 4.34 (d, J = 12.5 Hz, 1H), 4.17 (br s, 1H), 3.87 (s, 3H), 3.67 (s, 3H), 3.18 – 3.05 (m, 2H), 3.00 – 2.90 (m, 2H), 2.97 (d, J = 11.4 Hz, 1H), 2.60 – 2.53 (m, 1H), 2.51 – 2.43 (m, 1H), 2.42 – 2.35 (m, 1H), 2.35 – 2.20 (m, 3H), 2.10 (d, J = 13.6 Hz, 1H), 1.67 (d, J = 13.6 Hz, 1H); 13C NMR (150 MHz, CDCl3) δ 173.0, 154.4, 138.9, 137.3, 133.8, 128.1, 127.6, 127.2, 121.7, 107.5, 104.3, 99.7, 73.6, 71.1, 61.8, 61.1, 55.3, 54.0, 51.4, 50.2, 39.7, 36.0, 28.5, 28.4, 23.8, 21.1; IR (thin film) νmax 3377, 2929, 2796, 2749, 1732, 1597, 1557, 1479, 1456, 1353, 1254, 1105, 733, 680 cm−1; HRMS (ESI+) calc’d for [C29H35N2O4]+: m/z 475.2591, found 475.2581.

A flame dried 4 mL vial was charged with monoester 31 (7.7 mg, 0.016 mmol) and DCM (1 mL), then cooled to –78 °C in a dry ice/acetone bath under N2. A 1M solution of BBr3 in DCM (60 μL, 60 μmol) was added dropwise over 5 min. The light yellow solution became bright orange-red. Upon complete consumption of starting material (by TLC), the reaction mixture was quenched by the addition of sat. aq. NaHCO3 (3 mL). The aq. layer was extracted with DCM (3 X 5 mL), then the combined organics were washed with brine, dried with MgSO4 and the solvent was removed under reduced pressure to give a crude mixture that was purified by preparative TLC on silica gel (5% MeOH/DCM) to yield alstovenine 12 (4.3 mg, 44% over 2 steps) as a white solid. Rf = 0.41 (10% MeOH/DCM);

**1H NMR** (600 MHz, CDCl3) δ 7.68 (s, 1H), 6.99 (t, J = 7.8 Hz, 1H), 6.90 (d, J = 7.8 Hz, 1H), 6.45 (d, J = 7.8 Hz, 1H), 4.27 (s, 1H), 3.87 (s, 1H), 3.83 (s, 1H), 3.38 (s, 1H), 3.13 – 3.06 (m, 1H), 3.03 (d, J = 10.8 Hz, 1H), 2.97 – 2.91 (m, 2H), 2.87 (d, J = 11.4 Hz, 1H), 2.62 – 2.59 (m, 1H), 2.55 (d, dd, J = 11.4, 3.6 Hz, 1H), 2.47 (dt, J = 11.4, 4.2 Hz, 1H) 2.42 – 2.30 (m, 3H), 1.98 (dd, J = 14.4, 1.2 Hz, 1H), 1.74 (d, J = 11.4 Hz, 1H), 1.46 (t, J = 14.4 Hz, 1H), 1.33 (d, J = 11.4 Hz, 1H) (note: OH proton is missing); 13C NMR (150 MHz, CDCl3) δ 175.7, 154.5, 137.3, 133.1, 121.9, 117.6, 108.1, 104.2, 99.8, 65.7, 61.6, 60.8, 55.3, 53.7, 51.9, 49.7, 37.6, 36.8, 31.8, 29.4, 23.8, 20.5; IR (thin film) νmax 3389, 2928, 2798, 2750, 1722, 1711, 1620, 1597, 1435, 1456, 1353, 1105, 733, 680 cm−1; HRMS (ESI+) calc’d for [C22H29N2O4]+: m/z 385.2122, found 385.2125.
| This Work | Isolation* | Computational |
|-----------|------------|---------------|
| 175.7     | 175.4      | 178.1         |
| 154.5     | 154.3      | 152.4         |
| 137.3     | 137.3      | 134.6         |
| 133.1     | 132.5      | 132.6         |
| 121.9     | 121.8      | 119.9         |
| 117.6     | -          | 115.2         |
| 108.1     | 107.8      | 107.2         |
| 104.2     | 104.1      | 101.2         |
| 99.8      | 99.6       | 96.4          |
| 65.7      | 66.8       | 67.1          |
| 61.6      | 61.1       | 59.7          |
| 60.8      | 59.7       | 59.4          |
| 55.3      | 55.1       | 52.0          |
| 53.7      | 53.0       | 51.7          |
| 51.9      | 52.2       | 51.3          |
| 49.7      | 51.7       | 50.3          |
| 37.6      | 40.4       | 39.9          |
| 36.8      | 36.5       | 38.4          |
| 31.8      | 34.1       | 31.6          |
| 29.4      | 31.4       | 30.3          |
| 23.8      | 23.6       | 25.0          |
| 20.5      | 23.1       | 22.4          |

* Chatterjee, A., Roy, D. J., Mukhopadhyay S. 16-epivenenatine and 16-epialstovenine, new stereomers from Alstonia venenata. Phytochemistry 20, 1981-1985 (1981).
**Supercritical Fluid Chromatography (SFC) Data**

**Analysis Summary:**

The following SFC separation (conditions listed below) yielded 410mg of 18-endo-peak-1 (chemical purity >99%, ee >99%) and 435mg of 18-endo-peak-2 (chemical purity >99%, ee >99%). Peaks-1 and 2 were ‘re-worked’ to improve ee%. Samples may contain residual solvent. Chromatograms are included in this report.

**Preparative Method:**

OD-H (3 x 15 cm)  
10% 1:1 hep:iPOH(0.1%DEA)/CO₂, 100 bar  
60 mL/min, 254 nm.  
inj vol.: 0.5 mL, 15 mg/mL ethanol

**Analytical Method:**

OD-H (15 x 0.46 cm)  
10% 1:1 hep:iPOH(DEA)/CO₂, 100 bar  
3 mL/min, 220 and 254 nm

Sample: 18-endo
Sample: **18-endo** (peak-1)

| Index  | Time (min) | Area (%) |
|--------|------------|----------|
| Peak-1 | 2.93       | 100.00   |
| Peak-2 |            |          |
| Total  |            | 100.00   |
Sample: 18-endo (peak-2)

| Index  | Time (min) | Area (%) |
|--------|------------|----------|
| Peak-1 | 3.21       | 0.147    |
| Peak-2 | 3.47       | 99.843   |
| Total  |            | 100.00   |
\[ ^1H \text{ and } ^{13}C \text{ NMR Spectra} \]

[Diagram of the NMR spectra for compounds 18-endo]
24c

BnO
CO₂Me
CO₂allyl
H
H
H
N
N
H
OMe

24c

BnO
CO₂Me
CO₂allyl
H
H
H
N
N
H
OMe
9: venenatine

9: venenatine
\[^1\text{H}\] irradiated
\[^1\text{H}\] nOe observed

\[\text{E} = \text{CO}_2\text{Me}\]

9. venenatine
Crystallographic Data

A colorless plate 0.20 x 0.12 x 0.03 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 1.0°. Data collection was 97.6% complete to 67.00° in θ. A total of 26646 reflections were collected covering the indices, -11<=h<=11, -12<=k<=12, -18<=l<=19. 5546 reflections were found to be symmetry independent, with an R_{int} of 0.0274. Indexing and unit cell refinement indicated a primitive, triclinic lattice. The space group was found to be P-1 (No. 2). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-2008) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97.
Table 1. Crystal data and structure refinement for sarpong21.

| Property                        | Value                          |
|---------------------------------|--------------------------------|
| X-ray ID                        | sarpong21                      |
| Sample/notebook ID              | JWX-073B                       |
| Empirical formula               | C34 H39 N3 O6                  |
| Formula weight                  | 585.68                         |
| Temperature                     | 100(2) K                       |
| Wavelength                      | 1.54178 Å                      |
| Crystal system                  | Triclinic                      |
| Space group                     | P-1                            |
| Unit cell dimensions            | a = 9.7555(8) Å, α = 92.716(5)° |
|                                 | b = 10.4051(9) Å, β = 100.872(4)° |
|                                 | c = 15.9353(15) Å, γ = 99.935(4)° |
| Volume                          | 1559.3(2) Å³                   |
| Z                               | 2                              |
| Density (calculated)            | 1.247 Mg/m³                    |
| Absorption coefficient          | 0.696 mm⁻¹                     |
| F(000)                          | 624                            |
| Crystal size                    | 0.20 x 0.12 x 0.03 mm³         |
| Crystal color/habit             | colorless plate                |
| Theta range for data collection | 2.83 to 68.30°                 |
| Index ranges                    | -11<=h<=11, -12<=k<=12, -18<=l<=19 |
| Reflections collected           | 26646                          |
| Independent reflections         | 5546 [R(int) = 0.0274]          |
| Completeness to theta = 67.00°  | 97.6 %                         |
| Absorption correction           | Semi-empirical from equivalents|
| Max. and min. transmission      | 0.9794 and 0.8734              |
| Refinement method               | Full-matrix least-squares on F² |
| Data / restraints / parameters  | 5546 / 0 / 390                 |
| Goodness-of-fit on F²           | 1.021                          |
| Final R indices [I>2sigma(I)]   | R1 = 0.0430, wR2 = 0.1128      |
| R indices (all data)            | R1 = 0.0506, wR2 = 0.1188      |
| Largest diff. peak and hole     | 0.781 and -0.224 e.Å⁻³        |
Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\AA^2 \times 10^3$) for sarpong21. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized $U^j$ tensor.

|        | x    | y    | z    | $U(\text{eq})$ |
|--------|------|------|------|----------------|
| C(1)   | -159(2) | 3386(2) | 6298(1) | 22(1)          |
| C(2)   | 404(2)  | 4200(2)  | 7168(1)  | 21(1)          |
| C(3)   | 838(2)  | 3346(1)  | 7909(1)  | 20(1)          |
| C(4)   | 2179(2) | 2772(2)  | 7875(1)  | 21(1)          |
| C(5)   | 2507(2) | 1952(1)  | 8636(1)  | 20(1)          |
| C(6)   | 10(2)   | 1425(2)  | 8698(1)  | 23(1)          |
| C(7)   | -403(2) | 2224(2)  | 7941(1)  | 22(1)          |
| C(8)   | -864(2) | 1381(2)  | 7086(1)  | 25(1)          |
| C(9)   | -1298(2) | 2210(2)  | 6349(1)  | 25(1)          |
| C(10)  | 1027(2) | 2957(2)  | 5161(1)  | 32(1)          |
| C(11)  | 2390(2) | 2593(2)  | 5010(1)  | 29(1)          |
| C(12)  | 3684(2) | 3426(2)  | 5341(1)  | 35(1)          |
| C(13)  | 4952(2) | 3070(2)  | 5242(1)  | 36(1)          |
| C(14)  | 4941(2) | 1874(2)  | 4813(1)  | 36(1)          |
| C(15)  | 3674(2) | 1052(2)  | 4475(1)  | 37(1)          |
| C(16)  | 2401(2) | 1417(2)  | 4575(1)  | 34(1)          |
| C(17)  | 1638(2) | 5289(2)  | 7089(1)  | 21(1)          |
| C(18)  | 2359(2) | 6942(2)  | 6207(1)  | 29(1)          |
| C(19)  | 2151(2) | 8212(2)  | 6589(1)  | 36(1)          |
| C(20)  | 1206(3) | 8380(2)  | 7022(1)  | 53(1)          |
| C(21)  | -751(2) | 4947(2)  | 7368(1)  | 24(1)          |
| C(22)  | -1277(2) | 6406(2)  | 8392(2)  | 44(1)          |
| C(23)  | 2936(2) | 2839(2)  | 9449(1)  | 23(1)          |
| C(24)  | 1595(2) | 51(2)    | 9358(1)  | 22(1)          |
| C(25)  | 2916(2) | -548(2)  | 9341(1)  | 22(1)          |
| C(26)  | 3075(2) | -1614(2) | 9938(1)  | 22(1)          |
| C(27)  | 2890(2) | -2915(2) | 9694(1)  | 26(1)          |
| C(28)  | 3633(2) | -2754(2) | 11117(1) | 24(1)          |
| C(29)  | 4115(2) | -2989(2) | 11971(1) | 28(1)          |
| C(30)  | 4523(2) | -1920(2) | 12560(1) | 29(1)          |
| C(31)  | 4447(2) | -642(2)  | 12326(1) | 27(1)          |
| C(32)  | 3960(2) | -421(2)  | 11482(1) | 22(1)          |
| C(33)  | 3550(2) | -1485(2) | 10854(1) | 21(1)          |
| C(34)  | 4425(2) | 1897(2)  | 11793(1) | 32(1)          |
| N(1)   | 1311(1) | 909(1)   | 8661(1)  | 20(1)          |
| N(2)   | 3210(2) | 3526(1)  | 10061(1) | 29(1)          |
| N(3)   | 3201(2) | -3607(1) | 10397(1) | 28(1)          |
| O(1)   | 1063(1) | 3001(1)  | 6057(1)  | 23(1)          |
| O(2)   | 2718(1) | 5631(1)  | 7609(1)  | 26(1)          |
| O(3)   | 1316(1) | 5861(1)  | 6353(1)  | 24(1)          |
| O(4)   | -1855(1) | 4972(1)  | 6892(1)  | 34(1)          |
| O(5)   | -317(1)  | 5613(1)  | 8135(1)  | 32(1)          |
| O(6)   | 3855(1) | 782(1)   | 11194(1) | 26(1)          |
Table 3. Bond lengths [Å] and angles [°] for sarppong21.

| Bond                  | Length/Angle          |
|-----------------------|-----------------------|
| C(1)-O(1)             | 1.4327(18)            |
| C(1)-C(9)             | 1.521(2)              |
| C(1)-C(2)             | 1.543(2)              |
| C(1)-H(1)             | 1.0000                |
| C(2)-C(17)            | 1.532(2)              |
| C(2)-C(21)            | 1.546(2)              |
| C(2)-C(3)             | 1.552(2)              |
| C(3)-C(4)             | 1.538(2)              |
| C(3)-C(7)             | 1.540(2)              |
| C(3)-H(3)             | 1.0000                |
| C(4)-C(5)             | 1.533(2)              |
| C(4)-H(4A)            | 0.9900                |
| C(4)-H(4B)            | 0.9900                |
| C(5)-N(1)             | 1.4579(19)            |
| C(5)-H(5)             | 1.0000                |
| C(6)-N(1)             | 1.4708(19)            |
| C(6)-H(6A)            | 0.9900                |
| C(6)-H(6B)            | 0.9900                |
| C(7)-C(8)             | 1.532(2)              |
| C(7)-H(7)             | 1.0000                |
| C(8)-C(9)             | 1.529(2)              |
| C(8)-H(8A)            | 0.9900                |
| C(8)-H(8B)            | 0.9900                |
| C(9)-H(9A)            | 0.9900                |
| C(9)-H(9B)            | 0.9900                |
| C(10)-O(1)            | 1.419(2)              |
| C(10)-C(11)           | 1.502(2)              |
| C(10)-H(10A)          | 0.9900                |
| C(10)-H(10B)          | 0.9900                |
| C(11)-C(16)           | 1.381(3)              |
| C(11)-C(12)           | 1.397(3)              |
| C(12)-C(13)           | 1.385(3)              |
| C(12)-H(12)           | 0.9500                |
| C(13)-C(14)           | 1.388(3)              |
| C(13)-H(13)           | 0.9500                |
| C(14)-C(15)           | 1.375(3)              |
| C(14)-H(14)           | 0.9500                |
| C(15)-C(16)           | 1.394(3)              |
| C(15)-H(15)           | 0.9500                |
| C(16)-H(16)           | 0.9500                |
| C(17)-O(2)            | 1.198(2)              |
| N(3)-H(3A)            | 0.8800                |

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O(1)-C(1)-C(9) 111.83(12)
O(1)-C(1)-C(2) 105.35(12)
C(9)-C(1)-C(2) 112.51(13)
O(1)-C(1)-H(1) 109.0
C(9)-C(1)-H(1) 109.0
C(2)-C(1)-H(1) 109.0
C(17)-C(2)-C(1) 109.58(12)
C(17)-C(2)-C(21) 103.94(12)
C(1)-C(2)-C(21) 108.84(13)
C(17)-C(2)-C(3) 111.48(12)
C(1)-C(2)-C(3) 112.51(12)
C(21)-C(2)-C(3) 110.12(12)
C(4)-C(3)-C(7) 109.18(12)
C(4)-C(3)-C(2) 114.96(12)
C(7)-C(3)-C(2) 110.01(12)
C(4)-C(3)-H(3) 107.5
C(7)-C(3)-H(3) 107.5
C(2)-C(3)-H(3) 107.5
C(5)-C(4)-C(3) 110.43(12)
C(5)-C(4)-H(4A) 109.6
C(3)-C(4)-H(4A) 109.6
C(5)-C(4)-H(4B) 109.6
C(3)-C(4)-H(4B) 109.6
H(4A)-C(4)-H(4B) 108.1
N(1)-C(5)-C(23) 112.21(12)
N(1)-C(5)-C(4) 111.47(12)
C(23)-C(5)-C(4) 109.11(12)
N(1)-C(5)-H(5) 108.0
C(23)-C(5)-H(5) 108.0
C(4)-C(5)-H(5) 108.0
N(1)-C(6)-C(7) 112.24(12)
N(1)-C(6)-H(6A) 109.2
C(7)-C(6)-H(6A) 109.2
N(1)-C(6)-H(6B) 109.2
C(7)-C(6)-H(6B) 109.2
H(6A)-C(6)-H(6B) 107.9
C(6)-C(7)-C(8) 112.51(13)
C(6)-C(7)-C(3) 109.62(13)
C(8)-C(7)-C(3) 111.02(13)
C(6)-C(7)-H(7) 107.8
C(8)-C(7)-H(7) 107.8
C(3)-C(7)-H(7) 107.8
C(9)-C(8)-C(7) 110.91(13)
C(9)-C(8)-H(8A) 109.5
C(7)-C(8)-H(8A) 109.5
C(9)-C(8)-H(8B) 109.5
C(7)-C(8)-H(8B) 109.5
H(8A)-C(8)-H(8B) 108.0
C(1)-C(9)-C(8) 113.16(13)
C(1)-C(9)-H(9A) 108.9
C(8)-C(9)-H(9A) 108.9
C(1)-C(9)-H(9B) 108.9
C(8)-C(9)-H(9B) 108.9
H(9A)-C(9)-H(9B) 107.8
O(1)-C(10)-C(11) 107.79(13)
O(1)-C(10)-H(10A) 110.1
| Bond                  | Angle  |
|----------------------|--------|
| C(11)-C(10)-H(10A)   | 110.1  |
| O(1)-C(10)-H(10B)    | 110.1  |
| C(11)-C(10)-H(10B)   | 110.1  |
| H(10A)-C(10)-H(10B)  | 108.5  |
| C(16)-C(11)-C(12)    | 118.69(17) |
| C(16)-C(11)-C(10)    | 121.20(17) |
| C(12)-C(11)-C(10)    | 120.07(16) |
| C(13)-C(12)-C(11)    | 120.52(17) |
| C(13)-C(12)-H(12)    | 119.7  |
| C(11)-C(12)-H(12)    | 119.7  |
| C(12)-C(13)-C(14)    | 119.92(18) |
| C(12)-C(13)-H(13)    | 120.0  |
| C(14)-C(13)-H(13)    | 120.0  |
| C(15)-C(14)-C(13)    | 120.13(17) |
| C(15)-C(14)-H(14)    | 119.9  |
| C(13)-C(14)-H(14)    | 119.9  |
| C(14)-C(15)-C(16)    | 119.72(17) |
| C(14)-C(15)-H(15)    | 120.1  |
| C(16)-C(15)-H(15)    | 120.1  |
| C(11)-C(16)-C(15)    | 121.01(17) |
| C(11)-C(16)-H(16)    | 119.5  |
| C(15)-C(16)-H(16)    | 119.5  |
| O(2)-C(17)-O(3)      | 123.88(14) |
| O(2)-C(17)-C(2)      | 126.12(14) |
| O(3)-C(17)-C(2)      | 109.96(13) |
| O(3)-C(18)-C(19)     | 111.94(15) |
| O(3)-C(18)-H(18A)    | 109.2  |
| C(19)-C(18)-H(18A)   | 109.2  |
| O(3)-C(18)-H(18B)    | 109.2  |
| C(19)-C(18)-H(18B)   | 109.2  |
| H(18A)-C(18)-H(18B)  | 107.9  |
| C(20)-C(19)-C(18)    | 126.64(19) |
| C(20)-C(19)-H(19)    | 116.7  |
| C(18)-C(19)-H(19)    | 116.7  |
| C(19)-C(20)-H(20A)   | 120.0  |
| C(19)-C(20)-H(20B)   | 120.0  |
| H(20A)-C(20)-H(20B)  | 120.0  |
| O(4)-C(21)-O(5)      | 124.51(15) |
| O(4)-C(21)-C(2)      | 125.38(15) |
| O(5)-C(21)-C(2)      | 110.04(14) |
| O(5)-C(22)-H(22A)    | 109.5  |
| O(5)-C(22)-H(22B)    | 109.5  |
| H(22A)-C(22)-H(22B)  | 109.5  |
| O(5)-C(22)-H(22C)    | 109.5  |
| H(22A)-C(22)-H(22C)  | 109.5  |
| H(22B)-C(22)-H(22C)  | 109.5  |
| N(2)-C(23)-C(5)      | 177.31(17) |
| N(1)-C(24)-C(25)     | 112.83(12) |
| N(1)-C(24)-H(24A)    | 109.0  |
| C(25)-C(24)-H(24A)   | 109.0  |
| N(1)-C(24)-H(24B)    | 109.0  |
| C(25)-C(24)-H(24B)   | 109.0  |
| H(24A)-C(24)-H(24B)  | 107.8  |
| C(26)-C(25)-C(24)    | 113.72(13) |
| C(26)-C(25)-H(25A)   | 108.8  |
| C(24)-C(25)-H(25A)   | 108.8  |
C(26)-C(25)-H(25B) 108.8
C(24)-C(25)-H(25B) 108.8
H(25A)-C(25)-H(25B) 107.7
C(27)-C(26)-C(33) 106.03(14)
C(27)-C(26)-C(25) 125.52(15)
C(33)-C(26)-C(25) 128.29(14)
C(26)-C(27)-N(3) 110.42(15)
C(26)-C(27)-H(27) 124.8
N(3)-C(27)-H(27) 124.8
N(3)-C(28)-C(29) 130.02(15)
N(3)-C(28)-C(33) 107.14(14)
C(29)-C(28)-C(33) 122.82(16)
C(30)-C(29)-C(28) 116.96(15)
C(30)-C(29)-H(29) 121.5
C(28)-C(29)-H(29) 121.5
C(29)-C(30)-C(31) 121.99(16)
C(29)-C(30)-H(30) 119.0
C(31)-C(30)-H(30) 119.0
C(32)-C(31)-C(30) 120.61(16)
C(32)-C(31)-H(31) 119.7
C(30)-C(31)-H(31) 119.7
C(32)-C(31)-C(33) 121.73(16)
O(6)-C(32)-C(31) 124.74(15)
O(6)-C(32)-C(33) 115.83(14)
C(31)-C(32)-C(33) 119.42(15)
C(32)-C(33)-C(28) 118.19(15)
C(32)-C(33)-C(26) 134.48(14)
C(28)-C(33)-C(26) 107.29(14)
C(32)-C(34)-H(34A) 109.5
O(6)-C(34)-H(34A) 109.5
H(34A)-C(34)-H(34B) 109.5
H(34A)-C(34)-H(34C) 109.5
H(34B)-C(34)-H(34C) 109.5
C(5)-N(1)-C(6) 111.76(12)
C(5)-N(1)-C(24) 113.70(12)
C(6)-N(1)-C(24) 110.24(12)
C(28)-N(3)-C(27) 109.10(13)
C(28)-N(3)-H(3A) 125.5
C(27)-N(3)-H(3A) 125.5
C(10)-O(1)-C(1) 113.86(12)
C(17)-O(3)-C(18) 116.25(12)
C(21)-O(5)-C(22) 116.00(15)
C(32)-O(6)-C(34) 117.26(13)

Symmetry transformations used to generate equivalent atoms:
A colorless plate 0.08 x 0.06 x 0.04 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 1.0°. Data collection was 98.4% complete to 67.00° in θ. A total of 51705 reflections were collected covering the indices, -13<=h<=13, -30<=k<=25, -13<=l<=14. 5881 reflections were found to be symmetry independent, with an R_{int} of 0.0423. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P2(1)/c (No. 14). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-2008) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97.

ORTEP representation of 23b - HCl
Table 1. Crystal data and structure refinement for sarpong26.

| Property                              | Value                        |
|---------------------------------------|------------------------------|
| X-ray ID                              | sarpong26                    |
| Sample/notebook ID                    | TL5-127-2                    |
| Empirical formula                     | C33 H39 Cl N2 O6             |
| Formula weight                        | 595.11                       |
| Temperature                           | 100(2) K                     |
| Wavelength                            | 1.54178 Å                    |
| Crystal system                        | Monoclinic                   |
| Space group                           | P2(1)/c                      |
| Unit cell dimensions                  | a = 11.4692(6) Å, b = 25.8682(13) Å, c = 12.3901(6) Å |
| Volume                                | 3316.5(3) Å^3               |
| Z                                      | 4                            |
| Density (calculated)                  | 1.192 Mg/m^3                 |
| Absorption coefficient                | 1.375 mm^{-1}                |
| F(000)                                | 1264                         |
| Crystal size                          | 0.08 x 0.06 x 0.04 mm^3      |
| Crystal color/habit                    | colorless plate              |
| Theta range for data collection       | 3.42 to 67.89°               |
| Index ranges                          | -13<=h<=13, -30<=k<=25, -13<=l<=14 |
| Reflections collected                 | 51705                        |
| Independent reflections               | 5881 [R(int) = 0.0423]       |
| Completeness to theta = 67.00°        | 98.4 %                       |
| Absorption correction                 | Semi-empirical from equivalents |
| Max. and min. transmission            | 0.9470 and 0.8979            |
| Refinement method                     | Full-matrix least-squares on F^2 |
| Data / restraints / parameters        | 5881 / 0 / 382               |
| Goodness-of-fit on F^2                | 1.145                        |
| Final R indices [I>2sigma(I)]         | R1 = 0.0879, wR2 = 0.2262    |
| R indices (all data)                  | R1 = 0.0923, wR2 = 0.2292    |
| Largest diff. peak and hole           | 1.115 and -0.419 eÅ^{-3}     |
Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\AA^2 \times 10^3$) for sarpong26. $U_{eq}$ is defined as one third of the trace of the orthogonalized $U^i$ tensor.

|          | x      | y      | z      | $U_{eq}$ |
|----------|--------|--------|--------|----------|
| C(1)     | 4679(4)| 1682(2)| 6988(4)| 28(1)    |
| C(2)     | 5332(4)| 2183(2)| 6860(4)| 30(1)    |
| C(3)     | 5172(4)| 2235(2)| 5573(4)| 34(1)    |
| C(4)     | 3762(4)| 2223(2)| 4691(4)| 32(1)    |
| C(5)     | 3120(4)| 1722(2)| 4794(4)| 31(1)    |
| C(6)     | 1724(4)| 1660(2)| 3901(4)| 32(1)    |
| C(7)     | -560(4)| 1920(2)| 3264(4)| 37(1)    |
| C(8)     | -1011(4)| 1364(2)| 3236(4)| 34(1)    |
| C(9)     | -558(4)| 1172(2)| 4504(4)| 30(1)    |
| C(10)    | -867(4)| 708(2) | 4974(4)| 30(1)    |
| C(11)    | -1675(4)| 283(2) | 4465(4)| 29(1)    |
| C(12)    | -1774(4)| -101(2)| 5177(4)| 33(1)    |
| C(13)    | -992(4)| -80(2) | 6441(4)| 33(1)    |
| C(14)    | -172(4)| 323(2) | 6964(4)| 33(1)    |
| C(15)    | -123(4)| 719(2) | 6224(4)| 27(1)    |
| C(16)    | 318(4) | 1432(2)| 5452(4)| 29(1)    |
| C(17)    | 951(4) | 1941(2)| 5428(4)| 31(1)    |
| C(18)    | 2344(4)| 2009(2)| 6313(4)| 28(1)    |
| C(19)    | 3251(4)| 1637(2)| 6078(4)| 28(1)    |
| C(20)    | 5434(4)| 1212(2)| 6836(3)| 28(1)    |
| C(21)    | 7523(5)| 901(2) | 7287(5)| 44(1)    |
| C(22)    | 4889(4)| 1635(2)| 8294(4)| 27(1)    |
| C(23)    | 4283(5)| 1181(2)| 9634(4)| 36(1)    |
| C(24)    | 5416(5)| 859(2) | 10353(4)| 45(1) |
| C(25)    | 6249(6)| 655(2) | 9999(5)| 58(2)    |
| C(26)    | 5618(4)| 3022(2)| 7688(4)| 31(1)    |
| C(27)    | 4934(4)| 3494(2)| 7814(4)| 29(1)    |
| C(28)    | 5628(4)| 3869(2)| 8649(4)| 32(1)    |
| C(29)    | 5037(5)| 4319(2)| 8737(4)| 37(1)    |
| C(30)    | 3749(5)| 4410(2)| 8003(4)| 40(1)    |
| C(31)    | 3059(5)| 4034(2)| 7166(4)| 40(1)    |
| C(32)    | 3637(4)| 3581(2)| 7065(4)| 32(1)    |
| C(33)    | -3142(4)| -142(2)| 2680(4)| 36(1)    |
| N(1)     | 814(3) | 2001(1)| 4160(3)| 31(1)    |
| N(2)     | 605(3) | 1164(1)| 6499(3)| 28(1)    |
| O(1)     | 4963(3)| 820(1) | 6336(3)| 36(1)    |
| O(2)     | 6703(3)| 1307(1)| 7382(3)| 39(1)    |
| O(3)     | 5675(3)| 1876(1)| 9117(3)| 37(1)    |
| O(4)     | 4127(3)| 1268(1)| 8418(2)| 33(1)    |
| O(5)     | 4739(3)| 2612(1)| 7157(2)| 28(1)    |
| O(6)     | -2363(3)| 299(1) | 3235(3)| 32(1)    |
| Cl(1)    | 1087(1)| 3178(1)| 3887(1)| 38(1)    |
Table 3. Bond lengths [Å] and angles [°] for sarpong26.

| Bond | Distance Å | Bond | Distance Å |
|------|------------|------|------------|
| C(1)-C(22) | 1.533(5) | C(17)-H(17) | 1.0000 |
| C(1)-C(2) | 1.539(6) | C(18)-C(19) | 1.534(5) |
| C(1)-C(19) | 1.541(6) | C(18)-H(18A) | 0.9900 |
| C(1)-C(20) | 1.550(5) | C(18)-H(18B) | 0.9900 |
| C(2)-O(5) | 1.431(5) | C(19)-H(19) | 1.0000 |
| C(2)-C(3) | 1.530(6) | C(20)-O(1) | 1.190(5) |
| C(2)-H(2) | 1.0000 | C(20)-O(2) | 1.336(5) |
| C(3)-C(4) | 1.512(6) | C(21)-O(2) | 1.448(5) |
| C(3)-H(3A) | 0.9900 | C(21)-H(21A) | 0.9800 |
| C(3)-H(3B) | 0.9900 | C(21)-H(21B) | 0.9800 |
| C(4)-C(5) | 1.524(6) | C(21)-H(21C) | 0.9800 |
| C(4)-H(4A) | 0.9900 | C(22)-O(3) | 1.203(5) |
| C(4)-H(4B) | 0.9900 | C(22)-O(4) | 1.343(5) |
| C(5)-C(6) | 1.512(6) | C(23)-O(4) | 1.457(5) |
| C(5)-C(19) | 1.548(5) | C(23)-C(24) | 1.476(7) |
| C(5)-H(5) | 1.0000 | C(23)-H(23A) | 0.9900 |
| C(6)-N(1) | 1.503(5) | C(23)-H(23B) | 0.9900 |
| C(6)-H(6A) | 0.9900 | C(24)-C(25) | 0.9500 |
| C(6)-H(6B) | 0.9900 | C(24)-H(24) | 0.9500 |
| C(7)-N(1) | 1.501(6) | C(25)-H(25A) | 0.9500 |
| C(7)-C(8) | 1.522(6) | C(25)-H(25B) | 0.9500 |
| C(7)-H(7A) | 0.9900 | C(26)-O(5) | 1.415(5) |
| C(7)-H(7B) | 0.9900 | C(26)-C(27) | 1.495(6) |
| C(8)-C(9) | 1.511(6) | C(26)-H(26A) | 0.9900 |
| C(8)-H(8A) | 0.9900 | C(26)-H(26B) | 0.9900 |
| C(8)-H(8B) | 0.9900 | C(27)-C(28) | 1.391(6) |
| C(9)-C(16) | 1.351(6) | C(27)-C(32) | 1.391(6) |
| C(9)-C(10) | 1.443(6) | C(28)-C(29) | 1.376(6) |
| C(10)-C(11) | 1.401(6) | C(28)-H(28) | 0.9500 |
| C(10)-C(15) | 1.410(6) | C(29)-C(30) | 1.380(7) |
| C(11)-C(12) | 1.365(6) | C(29)-H(29) | 0.9500 |
| C(11)-O(6) | 1.382(5) | C(30)-C(31) | 1.392(7) |
| C(12)-C(13) | 1.431(6) | C(30)-H(30) | 0.9500 |
| C(12)-H(12) | 0.9500 | C(31)-C(32) | 1.379(6) |
| C(13)-C(14) | 1.366(6) | C(31)-H(31) | 0.9500 |
| C(13)-H(13) | 0.9500 | C(32)-H(32) | 0.9500 |
| C(14)-C(15) | 1.391(6) | C(33)-O(6) | 1.430(5) |
| C(14)-H(14) | 0.9500 | C(33)-H(33A) | 0.9800 |
| C(15)-N(2) | 1.376(5) | C(33)-H(33B) | 0.9800 |
| C(16)-N(2) | 1.381(5) | C(33)-H(33C) | 0.9800 |
| C(16)-C(17) | 1.509(6) | N(1)-H(1) | 0.9300 |
| C(17)-C(18) | 1.508(6) | N(2)-H(2A) | 0.8800 |
| C(17)-N(1) | 1.518(5) | | |
C(22)-C(1)-C(2) 108.3(3)
C(22)-C(1)-C(19) 113.6(3)
C(2)-C(1)-C(19) 113.5(3)
C(22)-C(1)-C(20) 103.0(3)
C(2)-C(1)-C(20) 108.9(3)
C(19)-C(1)-C(20) 108.9(3)
O(5)-C(2)-C(3) 110.0(3)
O(5)-C(2)-C(1) 108.6(3)
C(3)-C(2)-C(1) 109.7(3)
O(5)-C(2)-H(2) 109.5
C(3)-C(2)-H(2) 109.5
C(1)-C(2)-H(2) 109.5
C(4)-C(3)-C(2) 111.2(3)
C(4)-C(3)-H(3A) 109.4
C(2)-C(3)-H(3A) 109.4
C(4)-C(3)-H(3B) 109.4
H(3A)-C(3)-H(3B) 108.0
C(3)-C(4)-C(5) 111.2(4)
C(3)-C(4)-H(4A) 109.4
C(5)-C(4)-H(4A) 109.4
C(3)-C(4)-H(4B) 109.4
C(5)-C(4)-H(4B) 109.4
H(4A)-C(4)-H(4B) 108.0
C(6)-C(5)-C(4) 115.2(4)
C(6)-C(5)-C(19) 109.9(3)
C(4)-C(5)-C(19) 111.7(3)
C(6)-C(5)-H(5) 106.5
C(4)-C(5)-H(5) 106.5
C(19)-C(5)-H(5) 106.5
N(1)-C(6)-C(5) 113.4(3)
N(1)-C(6)-H(6A) 108.9
C(5)-C(6)-H(6A) 108.9
N(1)-C(6)-H(6B) 108.9
C(5)-C(6)-H(6B) 108.9
H(6A)-C(6)-H(6B) 107.7
N(1)-C(7)-C(8) 112.8(3)
N(1)-C(7)-H(7A) 109.0
C(8)-C(7)-H(7A) 109.0
N(1)-C(7)-H(7B) 109.0
C(8)-C(7)-H(7B) 109.0
H(7A)-C(7)-H(7B) 107.8
C(9)-C(8)-C(7) 109.0(4)
C(9)-C(8)-H(8A) 109.9
C(7)-C(8)-H(8A) 109.9
C(9)-C(8)-H(8B) 109.9
C(7)-C(8)-H(8B) 109.9
H(8A)-C(8)-H(8B) 108.3
C(16)-C(9)-C(10) 106.5(4)
C(16)-C(9)-C(8) 122.3(4)
C(10)-C(9)-C(8) 131.2(4)
C(11)-C(10)-C(15) 118.6(4)
C(11)-C(10)-C(9) 134.6(4)
C(15)-C(10)-C(9) 106.9(4)
C(12)-C(11)-O(6) 124.5(4)
C(12)-C(11)-C(10) 120.3(4)
O(6)-C(11)-C(10) 115.2(4)
C(11)-C(12)-C(13) 119.5(4)
C(11)-C(12)-H(12) 120.2
C(13)-C(12)-H(12) 120.2
C(14)-C(13)-C(12) 115.2(4)
C(14)-C(13)-H(13) 120.2
C(12)-C(13)-H(13) 120.2
C(13)-C(14)-C(15) 119.5(4)
C(13)-C(14)-H(14) 120.2
C(15)-C(14)-H(14) 120.2
N(2)-C(15)-C(14) 115.2(4)
N(2)-C(15)-C(10) 107.6(3)
C(14)-C(15)-C(10) 122.2(4)
C(9)-C(16)-N(2) 110.6(4)
C(9)-C(16)-C(17) 126.9(4)
N(2)-C(16)-C(17) 122.4(4)
C(18)-C(17)-C(16) 117.1(4)
C(18)-C(17)-N(1) 110.2(3)
C(16)-C(17)-N(1) 105.9(3)
C(18)-C(17)-H(17) 107.8
C(16)-C(17)-H(17) 107.8
N(1)-C(17)-H(17) 107.8
C(17)-C(18)-C(19) 112.5(3)
C(17)-C(18)-H(18A) 109.1
C(19)-C(18)-H(18A) 109.1
C(17)-C(18)-H(18B) 109.1
C(19)-C(18)-H(18B) 109.1
H(18A)-C(18)-H(18B) 107.8
C(18)-C(19)-C(1) 114.0(3)
C(18)-C(19)-C(5) 109.5(3)
C(1)-C(19)-C(5) 110.1(3)
C(18)-C(19)-H(19) 107.7
C(1)-C(19)-H(19) 107.7
C(5)-C(19)-H(19) 107.7
O(1)-C(20)-O(2) 124.7(4)
O(1)-C(20)-C(1) 125.4(4)
O(2)-C(20)-C(1) 109.8(3)
O(2)-C(21)-H(21A) 109.5
O(2)-C(21)-H(21B) 109.5
H(21A)-C(21)-H(21B) 109.5
O(2)-C(21)-H(21C) 109.5
H(21A)-C(21)-H(21C) 109.5
O(3)-C(22)-O(4) 123.7(4)
O(3)-C(22)-C(1) 124.9(4)
O(4)-C(22)-C(1) 111.2(3)
O(4)-C(23)-C(24) 113.3(4)
O(4)-C(23)-H(23A) 108.9
C(24)-C(23)-H(23A) 108.9
O(4)-C(23)-H(23B) 108.9
C(24)-C(23)-H(23B) 108.9
H(23A)-C(23)-H(23B) 107.7
C(25)-C(24)-C(23) 126.9(5)
C(25)-C(24)-H(24) 116.6
C(23)-C(24)-H(24) 116.6
C(24)-C(25)-H(25A) 120.0
| Bond                  | Angle (°)  |
|-----------------------|------------|
| C(24)-C(25)-H(25B)   | 120.0      |
| H(25A)-C(25)-H(25B)  | 120.0      |
| O(5)-C(26)-C(27)     | 111.1(3)   |
| O(5)-C(26)-H(26A)    | 109.4      |
| C(27)-C(26)-H(26A)   | 109.4      |
| O(5)-C(26)-H(26B)    | 109.4      |
| C(27)-C(26)-H(26B)   | 109.4      |
| H(26A)-C(26)-H(26B)  | 108.0      |
| C(28)-C(27)-C(32)    | 119.2(4)   |
| C(28)-C(27)-C(26)    | 119.3(4)   |
| C(32)-C(27)-C(26)    | 121.4(4)   |
| C(29)-C(28)-C(27)    | 120.5(4)   |
| C(29)-C(28)-H(28)    | 119.8      |
| C(27)-C(28)-H(28)    | 119.8      |
| C(28)-C(29)-C(30)    | 121.0(4)   |
| C(28)-C(29)-H(29)    | 119.5      |
| C(30)-C(29)-H(29)    | 119.5      |
| C(29)-C(30)-C(31)    | 118.4(4)   |
| C(29)-C(30)-H(30)    | 120.8      |
| C(31)-C(30)-H(30)    | 120.8      |
| C(32)-C(31)-C(30)    | 121.3(4)   |
| C(32)-C(31)-H(31)    | 119.3      |
| C(30)-C(31)-H(31)    | 119.3      |
| C(31)-C(32)-C(27)    | 119.7(4)   |
| C(31)-C(32)-H(32)    | 120.2      |
| C(27)-C(32)-H(32)    | 120.2      |
| O(6)-C(33)-H(33A)    | 109.5      |
| O(6)-C(33)-H(33B)    | 109.5      |
| H(33A)-C(33)-H(33B)  | 109.5      |
| O(6)-C(33)-H(33C)    | 109.5      |
| H(33A)-C(33)-H(33C)  | 109.5      |
| H(33B)-C(33)-H(33C)  | 109.5      |
| C(7)-N(1)-C(6)       | 111.3(3)   |
| C(7)-N(1)-C(17)      | 111.0(3)   |
| C(6)-N(1)-C(17)      | 112.9(3)   |
| C(7)-N(1)-H(1)       | 107.1      |
| C(6)-N(1)-H(1)       | 107.1      |
| C(17)-N(1)-H(1)      | 107.1      |
| C(15)-N(2)-C(16)     | 108.4(3)   |
| C(15)-N(2)-H(2A)     | 125.8      |
| C(16)-N(2)-H(2A)     | 125.8      |
| C(20)-O(2)-C(21)     | 115.5(4)   |
| C(22)-O(4)-C(23)     | 115.6(3)   |
| C(26)-O(5)-C(2)      | 112.2(3)   |
| C(11)-O(6)-C(33)     | 116.6(3)   |

Symmetry transformations used to generate equivalent atoms:
Table 4. Anisotropic displacement parameters (Å² x 10³) for sarpong26. The anisotropic displacement factor exponent takes the form: -2π² [ h²a*²U¹¹ + ... + 2 h k a* b* U¹² ]

|      | U¹¹  | U¹²  | U¹³  | U¹²  | U¹²  | U¹²  |
|------|------|------|------|------|------|------|
| C(1) | 33(2)| 29(2)| 29(2)| -1(2)| 19(2)| 0(2) |
| C(2) | 32(2)| 26(2)| 38(2)| -1(2)| 21(2)| 0(2) |
| C(3) | 41(2)| 30(2)| 38(2)|  1(2)| 25(2)| 1(2) |
| C(4) | 43(2)| 32(2)| 26(2)|  0(2)| 21(2)| 2(2) |
| C(5) | 37(2)| 30(2)| 29(2)| -1(2)| 19(2)| 2(2) |
| C(6) | 42(2)| 32(2)| 26(2)| -2(2)| 18(2)| 0(2) |
| C(7) | 40(2)| 36(2)| 33(2)|  5(2)| 13(2)| 6(2) |
| C(8) | 32(2)| 36(2)| 28(2)|  0(2)|  7(2)| 5(2) |
| C(9) | 30(2)| 29(2)| 33(2)| -1(2)| 16(2)| 4(2) |
| C(10)| 33(2)| 29(2)| 34(2)| -1(2)| 20(2)| 5(2) |
| C(11)| 29(2)| 28(2)| 36(2)| -3(2)| 19(2)| 4(2) |
| C(12)| 33(2)| 31(2)| 38(2)| -5(2)| 17(2)| 3(2) |
| C(13)| 33(2)| 31(2)| 40(2)|  4(2)| 23(2)| 7(2) |
| C(14)| 32(2)| 35(2)| 34(2)|  1(2)| 18(2)| 5(2) |
| C(15)| 21(2)| 31(2)| 31(2)|  1(2)| 13(2)| 4(2) |
| C(16)| 32(2)| 27(2)| 32(2)|  1(2)| 16(2)| 5(2) |
| C(17)| 39(2)| 27(2)| 33(2)| -1(2)| 22(2)| 4(2) |
| C(18)| 35(2)| 26(2)| 29(2)|  1(2)| 19(2)| 2(2) |
| C(19)| 37(2)| 23(2)| 30(2)| -3(2)| 20(2)| 0(2) |
| C(20)| 34(2)| 31(2)| 25(2)|  2(2)| 19(2)| 4(2) |
| C(21)| 39(3)| 44(3)| 52(3)| -7(2)| 21(2)| 4(2) |
| C(22)| 31(2)| 25(2)| 29(2)| -2(2)| 17(2)| 4(2) |
| C(23)| 47(3)| 40(2)| 27(2)|  4(2)| 21(2)| 1(2) |
| C(24)| 52(3)| 46(3)| 36(2)|  6(2)| 19(2)| 3(2) |
| C(25)| 56(3)| 67(4)| 59(3)| 24(3)| 32(3)| 2(3) |
| C(26)| 25(2)| 37(2)| 30(2)| -5(2)| 11(2)| -1(2) |
| C(27)| 33(2)| 31(2)| 27(2)|  2(2)| 17(2)| -1(2) |
| C(28)| 33(2)| 35(2)| 32(2)| -1(2)| 18(2)| -8(2) |
| C(29)| 51(3)| 28(2)| 38(2)| -4(2)| 24(2)| -11(2) |
| C(30)| 47(3)| 30(2)| 51(3)|  4(2)| 28(2)| 4(2) |
| C(31)| 36(2)| 40(3)| 42(3)|  6(2)| 15(2)| 7(2) |
| C(32)| 34(2)| 34(2)| 30(2)| -1(2)| 16(2)| -2(2) |
| C(33)| 36(2)| 32(2)| 35(2)| -5(2)| 13(2)| -2(2) |
| N(1) | 35(2)| 28(2)| 30(2)|  2(1)| 14(2)| 2(2) |
| N(2) | 29(2)| 30(2)| 25(2)|  1(1)| 11(1)| 3(1) |
| O(1) | 43(2)| 30(2)| 42(2)| -1(1)| 25(2)| 5(1) |
| O(2) | 36(2)| 38(2)| 46(2)| -7(1)| 20(1)| 7(1) |
| O(3) | 46(2)| 35(2)| 33(2)| -4(1)| 21(2)| -3(1) |
| O(4) | 36(2)| 39(2)| 26(1)|  3(1)| 14(1)| -2(1) |
| O(5) | 29(1)| 26(1)| 33(2)| -1(1)| 16(1)| 1(1) |
| O(6) | 32(2)| 29(2)| 32(2)| -2(1)| 12(1)| 1(1) |
| Cl(1)| 45(1)| 34(1)| 34(1)|  6(1)| 17(1)| 2(1) |
Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\AA^2 \times 10^3$) for sarpong26.

|      | x     | y     | z     | U(eq) |
|------|-------|-------|-------|-------|
| H(2) | 6273  | 2172  | 7419  | 36    |
| H(3A)| 5562  | 2565  | 5487  | 40    |
| H(3B)| 5635  | 1949  | 5394  | 40    |
| H(4A)| 3688  | 2258  | 3868  | 38    |
| H(4B)| 3309  | 2520  | 4844  | 38    |
| H(5) | 3608  | 1434  | 4633  | 37    |
| H(6A)| 1645  | 1742  | 3092  | 39    |
| H(6B)| 1464  | 1295  | 3900  | 39    |
| H(7A)| -646  | 2015  | 2460  | 45    |
| H(7B)| -1129 | 2152  | 3459  | 45    |
| H(8A)| -1966 | 1348  | 2815  | 41    |
| H(8B)| -651  | 1143  | 2800  | 41    |
| H(12)| -2357 | -380  | 4836  | 40    |
| H(13)| -1046 | -354  | 6929  | 39    |
| H(14)| 348   | 332   | 7803  | 39    |
| H(17)| 438   | 2222  | 5574  | 37    |
| H(18A)| 2424 | 1950  | 7131  | 34    |
| H(18B)| 2613 | 2369  | 6270  | 34    |
| H(19)| 2961  | 1277  | 6124  | 33    |
| H(21A)| 7429 | 590   | 7695  | 67    |
| H(21B)| 8425 | 1015  | 7661  | 67    |
| H(21C)| 7269 | 822   | 6442  | 67    |
| H(23A)| 3495 | 1011  | 9602  | 43    |
| H(23B)| 4370 | 1520  | 10036 | 43    |
| H(24)| 5562  | 791   | 11155 | 54    |
| H(25A)| 6147 | 711   | 9205  | 70    |
| H(25B)| 6949 | 453   | 10537 | 70    |
| H(26A)| 6073 | 3104  | 7188  | 38    |
| H(26B)| 6272 | 2914  | 8486  | 38    |
| H(28)| 6515  | 3814  | 9162  | 39    |
| H(29)| 5523  | 4572  | 9311  | 44    |
| H(30)| 3343  | 4721  | 8067  | 48    |
| H(31)| 2172  | 4091  | 6655  | 48    |
| H(32)| 3152  | 3330  | 6486  | 39    |
| H(33A)| -2591 | -450  | 2849  | 53    |
| H(33B)| -3585 | -88   | 1813  | 53    |
| H(33C)| -3784 | -192  | 2996  | 53    |
| H(1)| 1026  | 2341  | 4080  | 37    |
| H(2A)| 1160  | 1260  | 7220  | 33    |
Table 4. Anisotropic displacement parameters (Å²x 10³) for sarpong21. The anisotropic displacement factor exponent takes the form: -2π² [ h²a² U₁₁ + ... + 2hkak*b*U₁₂ ]

|     | U₁₁  | U₂₂  | U₃₃  | U₁₂  | U₁₃  | U₂₃  |
|-----|------|------|------|------|------|------|
| C(1)| 20(1)| 24(1)| 24(1)| 3(1) | 0(1) | 8(1) |
| C(2)| 20(1)| 20(1)| 23(1)| 2(1) | 3(1) | 7(1) |
| C(3)| 20(1)| 20(1)| 21(1)| 3(1) | 4(1) | 6(1) |
| C(4)| 18(1)| 21(1)| 23(1)| 5(1) | 4(1) | 5(1) |
| C(5)| 19(1)| 19(1)| 23(1)| 2(1) | 4(1) | 6(1) |
| C(6)| 19(1)| 23(1)| 29(1)| 6(1) | 7(1) | 6(1) |
| C(7)| 18(1)| 22(1)| 29(1)| 6(1) | 6(1) | 7(1) |
| C(8)| 20(1)| 20(1)| 33(1)| 4(1) | 2(1) | 3(1) |
| C(9)| 21(1)| 25(1)| 28(1)| 2(1) | -2(1)| 5(1) |
| C(10)| 34(1)| 42(1)| 21(1)| 0(1) | 0(1) | 16(1)|
| C(11)| 33(1)| 35(1)| 21(1)| 6(1) | 4(1) | 12(1)|
| C(12)| 41(1)| 29(1)| 34(1)| 3(1) | 5(1) | 9(1) |
| C(13)| 33(1)| 35(1)| 39(1)| 9(1) | 5(1) | 1(1) |
| C(14)| 34(1)| 40(1)| 38(1)| 10(1)| 15(1)| 10(1)|
| C(15)| 39(1)| 35(1)| 40(1)| -2(1)| 15(1)| 7(1) |
| C(16)| 31(1)| 36(1)| 33(1)| -3(1)| 6(1) | 4(1) |
| C(17)| 23(1)| 20(1)| 22(1)| 2(1) | 4(1) | 8(1) |
| C(18)| 26(1)| 28(1)| 30(1)| 9(1) | 2(1) | 0(1) |
| C(19)| 33(1)| 26(1)| 42(1)| 4(1) | -8(1)| 3(1) |
| C(20)| 81(2)| 35(1)| 43(1)| 0(1) | -2(1)| 22(1)|
| C(21)| 25(1)| 20(1)| 31(1)| 7(1) | 9(1) | 6(1) |
| C(22)| 43(1)| 37(1)| 60(1)| -6(1)| 24(1)| 16(1)|
| C(23)| 22(1)| 21(1)| 28(1)| 9(1) | 5(1) | 6(1) |
| C(24)| 21(1)| 20(1)| 26(1)| 5(1) | 5(1) | 4(1) |
| C(25)| 24(1)| 20(1)| 23(1)| 3(1) | 5(1) | 7(1) |
| C(26)| 19(1)| 22(1)| 27(1)| 4(1) | 5(1) | 6(1) |
| C(27)| 27(1)| 22(1)| 30(1)| 2(1) | 4(1) | 6(1) |
| C(28)| 17(1)| 23(1)| 34(1)| 7(1) | 7(1) | 6(1) |
| C(29)| 20(1)| 29(1)| 37(1)| 16(1)| 8(1) | 8(1) |
| C(30)| 21(1)| 41(1)| 28(1)| 14(1)| 6(1) | 9(1) |
| C(31)| 21(1)| 33(1)| 27(1)| 3(1) | 5(1) | 6(1) |
| C(32)| 16(1)| 24(1)| 27(1)| 5(1) | 5(1) | 7(1) |
| C(33)| 15(1)| 22(1)| 28(1)| 6(1) | 6(1) | 5(1) |
| C(34)| 38(1)| 25(1)| 33(1)| -3(1)| -2(1)| 10(1)|
| N(1)| 18(1)| 19(1)| 25(1)| 5(1) | 5(1) | 5(1) |
| N(2)| 38(1)| 21(1)| 28(1)| 3(1) | 4(1) | 7(1) |
| N(3)| 30(1)| 17(1)| 37(1)| 6(1) | 6(1) | 6(1) |
| O(1)| 22(1)| 27(1)| 20(1)| 2(1) | 1(1) | 9(1) |
| O(2)| 25(1)| 24(1)| 27(1)| 4(1) | -1(1)| 2(1) |
| O(3)| 23(1)| 23(1)| 24(1)| 6(1) | 2(1) | 3(1) |
| O(4)| 24(1)| 35(1)| 44(1)| 6(1) | 2(1) | 14(1) |
| O(5)| 32(1)| 33(1)| 36(1)| -4(1)| 10(1)| 14(1) |
| O(6)| 29(1)| 20(1)| 27(1)| 0(1) | 0(1) | 7(1) |
Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\AA^2 \times 10^3$) for sarpong21.

|     | x     | y     | z     | U(eq) |
|-----|-------|-------|-------|-------|
| H(1)| -561  | 3957  | 5866  | 27    |
| H(3)| 1027  | 3912  | 8458  | 24    |
| H(4A)| 2034 | 2217  | 7332  | 25    |
| H(4B)| 2993 | 3492  | 7888  | 25    |
| H(5)| 3334  | 1537  | 8564  | 24    |
| H(6A)| 157  | 1985  | 9239  | 28    |
| H(6B)| -778 | 687   | 8701  | 28    |
| H(7)| -1226 | 2624  | 8041  | 26    |
| H(8A)| -71  | 961   | 6976  | 30    |
| H(8B)| -1675| 680   | 7119  | 30    |
| H(9A)| -1514| 1654  | 5801  | 30    |
| H(9B)| -2176| 2520  | 6420  | 30    |
| H(10A)| 930 | 3822  | 4948  | 38    |
| H(10B)| 207 | 2300  | 4853  | 38    |
| H(12)| 3694  | 4244  | 5636  | 42    |
| H(13)| 5827  | 3643  | 5467  | 44    |
| H(14)| 5811  | 1623  | 4754  | 43    |
| H(15)| 3666  | 240   | 4174  | 44    |
| H(16)| 1527  | 847   | 4339  | 41    |
| H(18A)| 2298| 6988  | 5582  | 35    |
| H(18B)| 3320| 6791  | 6460  | 35    |
| H(19)| 2783  | 8974  | 6502  | 43    |
| H(20A)| 548 | 7649  | 7127  | 64    |
| H(20B)| 1164| 9236  | 7238  | 64    |
| H(22A)| -1412| 7075  | 7987  | 66    |
| H(22B)| -872| 6830  | 8969  | 66    |
| H(22C)| -2194| 5847  | 8393  | 66    |
| H(24A)| 762  | -663  | 9311  | 26    |
| H(24B)| 1719| 563   | 9916  | 26    |
| H(25A)| 2874| -911  | 8749  | 26    |
| H(25B)| 3767| 153   | 9497  | 26    |
| H(27)| 2588  | -3290 | 9120  | 32    |
| H(29)| 4157  | -3850 | 12135 | 33    |
| H(30)| 4866  | -2046 | 13143 | 35    |
| H(31)| 4733  | 74    | 12751 | 32    |
| H(34A)| 3894| 1869  | 12257 | 49    |
| H(34B)| 4348| 2697  | 11501 | 49    |
| H(34C)| 5427| 1890  | 12030 | 49    |
| H(3A)| 3133  | -4463 | 10386 | 34    |
**Computational Data**

**General**

Calculations (geometry optimization, frequency, and NMR chemical shift) were performed on venenatine (9), venenatine – HCl salt (9-HCl) alstovenine (12), 16-epi-alstovenine (13), and 9-methoxy-3-epi-α-yohimbine (8).

Candidate conformers for each system were identified via systematic conformational searches performed as described below with the MMFF94 force field in Spartan’10. Quantum mechanical calculations were performed with GAUSSIAN09. Geometries were optimized in the gas-phase using the B3LYP/6-31+G(d,p) level of theory. Frequency calculations (at 298.15 K) at the same level of theory were used to confirm the nature of all stationary points as minima and also provided values for computed free energies. NMR single point calculations (GIAO) were performed as described below on these geometries at the mPW1PW91/6-311+G(d,p) level of theory in an implicit chloroform solvent continuum (SMD method).

**Conformational Search and Analysis of NMR data**

For each system, systematic conformation searches were performed in two major stages: first to locate conformers of the ring system, and second to locate conformers of the hydroxyl and ester substituents on each ring conformer. The candidate conformers located via the systematic force field searches in Spartan’10 were first refined in GAUSSIAN09 at the B3LYP/6-31G(d) level of theory (optimizations only, no frequency calculations); unique conformers within a 20 kcal/mol electronic energy window were then further refined with optimizations and frequency calculations at the B3LYP/6-31+G(d,p) level of theory. In some cases the intermediate B3LYP/6-31G(d) optimizations were bypassed. Ring system conformers within a 10 kcal/mol free energy window at the B3LYP/6-31+G(d,p) level of theory were carried through to the second stage where conformations of the hydroxyl and ester substituents were analyzed using the same approach. In the end, all unique conformers within a 3 kcal/mol free energy window at the B3LYP/6-31+G(d,p) level of theory were included in the subsequent NMR calculations.

Boltzmann-weighted averaging of the computed chemical shifts based on the relative computed free energies at 298.15 K of each conformer was performed, using the equation below to determine relative populations.

\[
P_i = \frac{e^{-\frac{(E_i - E_j)}{RT}}}{\sum_j e^{-\frac{(E_i - E_j)}{RT}}} P_i = \text{population of conformer } i \text{ relative to lowest energy conformer } j
\]

\[
E_i, E_j = \text{computed free energies (in J/mol)}
\]

\[
R = \text{molar gas constant (8.314510 J mol}^{-1} \text{ K}^{-1})
\]

\[
T = 298.15 \text{ K}
\]

The relative populations were then converted to Boltzmann-weighting factors by means of a set of linear equations.
Empirical scaling of computed NMR chemical shifts

Computed chemical shifts are commonly scaled empirically in order to remove systematic error that results from a variety of sources. The scaling factors themselves are generally determined by comparison of computed NMR data with known experimental chemical shifts for large databases of molecules. These factors (slope and intercept from a best fit line) are specific for each level of theory used computationally. We have generated numerous such scaling factors for $^1$H and $^{13}$C chemical shifts utilizing a database originally compiled by Rablen and co-workers and have made them available on our web site at http://cheshirenmr.info.

One of our preferred methods for obtaining high quality computed chemical shifts at reasonable costs is to use mPW1PW91/6-311+G(2d,p) NMR calculations (with the SMD chloroform continuum model) on B3LYP/6-31+G(d,p) geometries. After scaling, this method produces average errors (CMAD’S) of 0.11-0.15 ppm for $^1$H and 1.8-2.5 ppm for $^{13}$C on diverse sets of small organic molecules. Details and numerous references on linear regression methods applied to computed chemical shifts can be found in our review paper.7

The specific scaling factors used in this study are given below and are applied to the computed NMR isotropic shielding constants by way of the equation shown.

\[
\delta = b - \sigma - m
\]

\[\sigma = \text{computed isotropic shielding constant}\]

\[m = \text{slope, } b = \text{intercept}\]


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Venenatine (9) $^{13}$C computed NMR data (ppm)

|     | Computed | Exp. a | Abs. Dev. a | Exp. b | Abs. Dev. b |
|-----|----------|--------|-------------|--------|-------------|
| C2  | 131.23   | 130.62 | 0.61        | 131.0  | 0.23        |
| C3  | 54.37    | 53.82  | 0.55        | 55.2   | 0.83        |
| C5  | 51.50    | 50.77  | 0.73        | 51.8   | 0.30        |
| C6  | 20.57    | 18.74  | 1.83        | 18.9   | 1.67        |
| C7  | 107.12   | 107.10 | 0.02        | 107.7  | 0.58        |
| C8  | 115.92   | 117.56 | 1.64        | 117.8  | 1.88        |
| C9  | 152.54   | 155.06 | 2.52        | 154.2  | 1.66        |
| C10 | 96.81    | 104.29 | 7.48        | 99.5   | 2.69        |
| C11 | 118.93   | 121.49 | 2.56        | 121.6  | 2.67        |
| C12 | 102.67   | 105.66 | 2.99        | 104.4  | 1.73        |
| C13 | 134.42   | 137.07 | 2.65        | 137.0  | 2.58        |
| C14 | 25.92    | 30.96  | 5.04        | 25.8   | 0.12        |
| C15 | 32.67    | 32.02  | 0.65        | 32.0   | 0.67        |
| C16 | 50.91    | 51.86  | 0.95        | 50.6   | 0.31        |
| C17 | 66.95    | 67.14  | 0.19        | 65.8   | 1.15        |
| C18 | 32.27    | 31.61  | 0.66        | 31.1   | 1.17        |
| C19 | 21.22    | 22.77  | 1.55        | 19.8   | 1.42        |
| C20 | 38.48    | 39.74  | 1.26        | 36.7   | 1.78        |
| C21 | 50.65    | 50.68  | 0.03        | 49.5   | 1.15        |
| C22 | 178.16   | 174.67 | 3.49        | 175.0  | 3.16        |
| C23 | 51.26    | 51.46  | 0.20        | 51.4   | 0.14        |
| C24 | 51.88    | 54.94  | 3.06        | 54.2   | 2.32        |

MAD: **1.85**

aPhytochemistry, **1981**, 20, 1981-1985, C14 and C19 assignments swapped

bThis work
Venenate – HCl salt (9-HCl) $^{13}$C computed NMR data (ppm)

|   | Computed | Exp. | Abs. Dev. |
|---|----------|------|-----------|
| C2 | 126.18   | 130.62 | 4.44      |
| C3 | 55.42    | 53.82  | 1.60      |
| C5 | 49.77    | 50.77  | 1.00      |
| C6 | 19.51    | 18.74  | 0.77      |
| C7 | 107.09   | 107.10 | 0.01      |
| C8 | 116.09   | 117.56 | 1.47      |
| C9 | 152.11   | 155.06 | 2.95      |
| C10| 97.71    | 104.29 | 6.58      |
| C11| 121.44   | 121.49 | 0.05      |
| C12| 100.97   | 105.66 | 4.69      |
| C13| 135.08   | 137.07 | 1.99      |
| C14| 24.13    | 30.96  | 6.83      |
| C15| 30.47    | 32.02  | 1.55      |
| C16| 50.75    | 51.86  | 1.11      |
| C17| 67.72    | 67.14  | 0.58      |
| C18| 33.15    | 31.61  | 1.54      |
| C19| 21.89    | 22.77  | 0.88      |
| C20| 37.26    | 39.74  | 2.48      |
| C21| 47.77    | 50.68  | 2.91      |
| C22| 175.22   | 174.67 | 0.55      |
| C23| 51.35    | 51.46  | 0.11      |
| C24| 52.13    | 54.94  | 2.81      |

MAD: 2.13

*Phytochemistry, **1981**, 20, 1981-1985, C14 and C19 assignments swapped
Alstovenine (12) $^{13}$C computed NMR data (ppm)

|     | Computed | Exp. | Abs. Dev. | Exp. | Abs. Dev. |
|-----|----------|------|-----------|------|-----------|
| C2  | 132.55   | 132.50 | 0.05 | 133.1 | 0.55 |
| C3  | 59.36    | 59.70  | 0.34 | 60.7  | 1.34 |
| C5  | 51.97    | 55.10  | 3.13 | 55.3  | 3.33 |
| C6  | 25.01    | 23.60  | 1.41 | 23.8  | 1.21 |
| C7  | 107.22   | 107.80 | 0.58 | 108.1 | 0.88 |
| C8  | 115.22   | --     | --    | 117.6 | 2.38 |
| C9  | 152.35   | 154.30 | 1.95 | 154.5 | 2.15 |
| C10 | 96.38    | 99.60  | 3.22 | 99.8  | 3.42 |
| C11 | 119.85   | 121.80 | 1.95 | 121.9 | 2.05 |
| C12 | 101.21   | 104.10 | 2.89 | 104.2 | 2.99 |
| C13 | 134.56   | 137.30 | 2.74 | 137.3 | 2.74 |
| C14 | 30.25    | 31.40  | 1.15 | 29.4  | 0.85 |
| C15 | 39.85    | 40.40  | 0.55 | 37.6  | 2.25 |
| C16 | 50.34    | 61.70  | 11.36 | 49.7 | 0.64 |
| C17 | 67.05    | 66.80  | 0.25 | 65.7  | 1.35 |
| C18 | 31.59    | 34.10  | 2.51 | 31.3  | 0.29 |
| C19 | 22.36    | 23.10  | 0.74 | 20.5  | 1.86 |
| C20 | 38.36    | 36.50  | 1.86 | 36.8  | 1.56 |
| C21 | 59.73    | 61.10  | 1.37 | 61.6  | 1.87 |
| C22 | 178.10   | 175.40 | 2.70 | 175.7 | 2.40 |
| C23 | 51.28    | 52.20  | 0.92 | 51.9  | 0.62 |
| C24 | 51.65    | 53.00  | 1.35 | 53.7  | 2.05 |

$^a$Phytochemistry, 1981, 20, 1981-1985

$^b$This work

MAD: 2.05  1.76

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16-epi-alstovenine (13) $^{13}$C computed NMR data (ppm)

|       | Computed | Exp.\(^a\) | Abs. Dev.\(^a\) |
|-------|----------|------------|-----------------|
| C2    | 132.82   | 134.03     | 1.21            |
| C3    | 59.34    | 60.49      | 1.15            |
| C5    | 51.74    | 52.76      | 1.02            |
| C6    | 25.14    | 24.26      | 0.88            |
| C7    | 107.10   | 106.29     | 0.81            |
| C8    | 115.05   | 117.15     | 2.10            |
| C9    | 152.32   | 154.16     | 1.84            |
| C10   | 96.52    | 99.34      | 2.82            |
| C11   | 119.91   | 121.34     | 1.43            |
| C12   | 101.30   | 105.13     | 3.83            |
| C13   | 134.37   | 137.88     | 3.51            |
| C14   | 33.72    | 32.89      | 0.83            |
| C15   | 37.95    | 36.32      | 1.63            |
| C16   | 52.43    | 51.46      | 0.97            |
| C17   | 68.56    | 67.03      | 1.53            |
| C18   | 30.99    | 32.80      | 1.81            |
| C19   | 21.58    | 23.36      | 1.78            |
| C20   | 33.93    | 34.88      | 0.95            |
| C21   | 59.29    | 61.43      | 2.14            |
| C22   | 175.13   | 173.25     | 1.88            |
| C23   | 50.97    | 53.12      | 2.15            |
| C24   | 51.78    | 55.43      | 3.65            |

\(^a\)Phytochemistry, \textbf{1981}, 20, 1981-1985.

MAD: \textbf{1.81}
9-methoxy-3-epi-α-yohimbine (8) $^{13}$C computed NMR data (ppm)

|   | Computed | Exp. | Abs. Dev. |
|---|----------|------|-----------|
| C2 | 130.91   | 130.00 | 0.91     |
| C3 | 54.15    | 53.80 | 0.35      |
| C5 | 51.41    | 51.30 | 0.11      |
| C6 | 20.62    | 18.50 | 2.12      |
| C7 | 107.39   | 108.20 | 0.81     |
| C8 | 115.56   | 117.90 | 2.34     |
| C9 | 152.70   | 154.00 | 1.30      |
| C10| 96.90    | 99.80 | 2.90      |
| C11| 119.23   | 122.10 | 2.87     |
| C12| 103.23   | 104.30 | 1.07      |
| C13| 134.71   | 136.90 | 2.19      |
| C14| 24.26    | 24.30 | 0.04      |
| C15| 33.23    | 32.40 | 0.83      |
| C16| 55.09    | 53.90 | 1.19      |
| C17| 65.58    | 66.00 | 0.42      |
| C18| 32.96    | 33.30 | 0.34      |
| C19| 25.19    | 23.70 | 1.49      |
| C20| 37.84    | 35.90 | 1.94      |
| C21| 49.97    | 49.60 | 0.37      |
| C22| 176.74   | 174.50 | 2.24     |
| C23| 51.12    | 55.20 | 4.08      |
| C24| 51.88    | 51.90 | 0.02      |

**MAD:** 1.36

*a* Chem. Pharm. Bull., 2004, 3, 359-361.
### Energies, coordinates, and NMR isotropic shielding constants

venenatine (9), conformer 1

Sum of electronic and thermal free energies = \(-1265.26599\) H

| Center Number | Atomic Number | Coordinates (Angstroms) | X  | Y  | Z  |
|---------------|---------------|------------------------|----|----|----|
| 1             | 7             | 1.213487               | 1.176565 | 0.890635 |
| 2             | 6             | 1.020165               | -0.196080 | 0.837514 |
| 3             | 6             | -0.229924              | -0.938406 | 1.257648 |
| 4             | 7             | -0.230712              | -2.286647 | 0.653449 |
| 5             | 6             | 1.043245               | -2.972308 | 0.919033 |
| 6             | 6             | 2.287207               | -2.299213 | 0.283996 |
| 7             | 6             | 2.182170               | -0.805327 | 0.424486 |
| 8             | 6             | 3.141309               | 0.243701  | 0.188638 |
| 9             | 6             | 4.484549               | 0.274445  | -0.248753 |
| 10            | 6             | 5.137265               | 1.501035  | -0.365991 |
| 11            | 6             | 4.465738               | 2.704722  | -0.052203 |
| 12            | 6             | 3.146314               | 2.716998  | 0.379294  |
| 13            | 6             | 2.503163               | 1.475310  | 0.493123  |
| 14            | 6             | -1.567007              | -0.220229 | 0.998496  |
| 15            | 6             | -1.971014              | -0.214122 | -0.487044 |
| 16            | 6             | -3.357547              | 0.439730  | -0.775298 |
| 17            | 6             | -4.575954              | -0.410300 | -0.330447 |
| 18            | 6             | -4.466635              | -1.833713 | -0.881717 |
| 19            | 6             | -3.124309              | -2.499283 | -0.546859 |
| 20            | 6             | -1.942374              | -1.654282 | -1.053205 |
| 21            | 6             | -0.569541              | -2.282186 | -0.775538 |
| 22            | 6             | -3.443294              | 1.854636  | -0.232173 |
| 23            | 6             | -2.631296              | 4.072834  | -0.449749 |
| 24            | 6             | 6.400031               | -0.970547 | -0.974302 |
| 25            | 8             | 5.050552               | -0.941169 | -0.530422 |
| 26            | 8             | -4.708288              | -0.499864 | 1.087295  |
| 27            | 8             | -4.160163              | 2.222704  | 0.685757  |
| 28            | 8             | -2.617058              | 2.697119  | -0.884532 |
| 29            | 1             | 0.517710               | 1.856284  | 1.150725  |
| 30            | 1             | -0.173926              | -1.959829 | 2.345965  |
| 31            | 1             | 0.953561               | -4.008048 | 0.571661  |
| 32            | 1             | 1.168078               | -3.007798 | 2.008548  |
| 33            | 1             | 2.383776               | -2.578895 | -0.774281 |
| 34            | 1             | 3.192442               | -2.677802 | 0.772220  |
| 35            | 1             | 6.167031               | 1.550167  | -0.698202 |
| 36            | 1             | 5.005049               | 3.641954  | -0.153218 |
| 37            | 1             | 2.639233               | 3.646503  | 0.620340  |
| 38            | 1             | -1.506332              | 0.805735  | 1.386454  |
| 39            | 1             | -2.338467              | -0.717731 | 1.589182  |
| 40            | 1             | -1.224787              | 0.372313  | -1.039190 |
| 41            | 1             | -3.423695              | 0.535661  | -1.868386 |
| 42            | 1             | -5.479931              | 0.061949  | -0.746661 |
| 43            | 1             | -4.596707              | -1.791724 | -1.972437 |
| 44            | 1             | -5.302004              | -2.417992 | -0.481162 |
| 45            | 1             | -3.082002              | -3.492177 | -1.012307 |
| 46            | 1             | -3.042682              | -2.658321 | 0.532207  |
| 47            | 1             | -2.034524              | -1.579544 | -2.148187 |
| 48            | 1             | 0.182201               | -1.743838 | -1.380489 |
| 49            | 1             | 0.568206               | -3.325805 | -1.13974  |
| 50            | 1             | -1.891677              | 4.578430  | -1.069450 |
| 51            | 1             | -2.367238              | 4.143381  | 0.608067  |
| 52            | 1             | -3.622612              | 4.506646  | -0.599572 |
| 53            | 1             | 7.078982               | -0.555146 | -0.218754 |
| 54            | 1             | 6.523548               | -0.420057 | -1.915636 |
| 55            | 1             | 6.638398               | -2.022905 | -1.136183 |
| 56            | 1             | -4.788549              | 0.410347  | 1.415646  |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 48.8082             |
| C3      | 129.2013            |
| C5      | 132.202             |
| C6      | 165.3658            |
| C7      | 73.6688             |
| C8      | 64.1538             |
| C9      | 25.8295             |
| C10     | 84.4953             |
| C11     | 61.3757             |
| C12     | 78.3122             |
| C13     | 45.0674             |
| C14     | 159.4591            |
| C15     | 152.019             |
| C16     | 132.863             |
| C17     | 116.0144            |
| C18     | 152.6971            |
| C19     | 164.5188            |
| C20     | 145.8592            |
| C21     | 133.9814            |
| C22     | -1.6539             |
| C23     | 132.5075            |
| C24     | 131.8571            |
venenatine (9), conformer 2

Sum of electronic and thermal free energies = -1265.262794 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|------------------------|
|               |               | X          | Y          | Z          |
| 1             | 7             | 1.163722   | 1.177230   | 0.883055   |
| 2             | 6             | 1.098891   | -0.207526  | 0.874169   |
| 3             | 6             | -0.082680  | -1.044692  | 1.307438   |
| 4             | 7             | -0.004706  | -2.377300  | 0.669653   |
| 5             | 6             | 1.313231   | -2.983011  | 0.918969   |
| 6             | 6             | 2.519429   | -2.209050  | 0.320747   |
| 7             | 6             | 2.302528   | -0.726523  | 0.458667   |
| 8             | 6             | 3.158822   | 0.396191   | 0.171608   |
| 9             | 6             | 4.488073   | 0.534198   | -0.286082  |
| 10            | 6             | 5.020925   | 1.809979   | -0.465529  |
| 11            | 6             | 4.241447   | 2.957908   | -0.193325  |
| 12            | 6             | 2.933059   | 2.864783   | 0.261193   |
| 13            | 6             | 2.410947   | 1.574700   | 0.439558   |
| 14            | 6             | -1.455977  | -0.403839  | 1.076684   |
| 15            | 6             | -1.800173  | -0.325904  | -0.421411  |
| 16            | 6             | -3.160132  | 0.329097   | -0.755477  |
| 17            | 6             | -4.387218  | -0.522157  | -0.370089  |
| 18            | 6             | -4.251934  | -1.949250  | -0.926603  |
| 19            | 6             | -2.909774  | -2.616637  | -0.587338  |
| 20            | 6             | -1.726488  | -1.742365  | -1.040551  |
| 21            | 6             | -0.345452  | -2.357365  | -0.759873  |
| 22            | 6             | -3.252190  | 1.774029   | -0.274950  |
| 23            | 6             | -4.658304  | 3.670219   | -0.093056  |
| 24            | 6             | 6.507238   | -0.554473  | -0.90254   |
| 25            | 8             | 5.164980   | -0.635095  | -0.523749  |
| 26            | 8             | -4.499055  | -0.506247  | 1.062256   |
| 27            | 8             | -2.330518  | 2.427585   | 0.176991   |
| 28            | 8             | -4.481544  | 2.293561   | -0.477346  |
| 29            | 1             | 0.373345   | 1.792521   | 1.011025   |
| 30            | 1             | 0.004936   | -1.224463  | 2.389901   |
| 31            | 1             | 1.297762   | -4.010128  | 0.535828   |
| 32            | 1             | 1.431671   | -3.047795  | 2.007837   |
| 33            | 1             | 2.663340   | -2.470952  | -0.736828  |
| 34            | 1             | 3.436932   | -2.528276  | 0.528917   |
| 35            | 1             | 6.037775   | 1.941016   | -0.815181  |
| 36            | 1             | 4.687642   | 3.936522   | -0.344634  |
| 37            | 1             | 2.342084   | 3.750987   | 0.471370   |
| 38            | 1             | -1.476673  | 0.592900   | 1.525660   |
| 39            | 1             | -2.202823  | -0.993144  | 1.610287   |
| 40            | 1             | -1.030492  | 0.288361   | -0.906391  |
| 41            | 1             | -3.208991  | 0.410131   | -1.853307  |
| 42            | 1             | -5.279184  | -0.499664  | -0.800829  |
| 43            | 1             | -4.371422  | -1.895301  | -2.018630  |
| 44            | 1             | -5.090568  | -2.554599  | -0.557029  |
| 45            | 1             | -2.854141  | -3.593630  | -1.083683  |
| 46            | 1             | -2.844899  | -2.811531  | 0.487240   |
| 47            | 1             | -1.797746  | -1.636290  | -2.134927  |
| 48            | 1             | 0.397499   | -1.797409  | -1.355506  |
| 49            | 1             | 0.324726   | -3.958755  | -1.114636  |
| 50            | 1             | -3.978767  | 4.314930   | -0.652790  |
| 51            | 1             | -4.467290  | 3.790531   | 0.978457   |
| 52            | 1             | -5.696031  | 3.905730   | -0.324988  |
| 53            | 1             | 7.148369   | -0.042478  | -0.251109  |
| 54            | 1             | 6.517893   | -0.036608  | -1.945936  |
| 55            | 1             | 6.845497   | -1.585168  | -1.098972  |
| 56            | 1             | -5.344620  | -0.900541  | 1.311505   |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 47.6405             |
| C3      | 128.8528            |
| C5      | 132.3662            |
| C6      | 165.3193            |
| C7      | 73.3022             |
| C8      | 64.9024             |
| C9      | 25.8694             |
| C10     | 84.565              |
| C11     | 61.2457             |
| C12     | 78.2111             |
| C13     | 44.6407             |
| C14     | 160.5346            |
| C15     | 154.3091            |
| C16     | 132.893             |
| C17     | 113.8008            |
| C18     | 149.4938            |
| C19     | 164.9703            |
| C20     | 145.5844            |
| C21     | 134.0752            |
| C22     | 3.1019              |
| C23     | 133.0294            |
| C24     | 132.0341            |
venenatine (9), conformer 3

Sum of electronic and thermal free energies = -1265.263914 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 7             | 1.171332    | 1.248225    | 0.769015    |
| 2             | 6             | 1.084626    | -0.133898   | 0.850762    |
| 3             | 6             | -0.118718   | -0.931092   | 1.302803    |
| 4             | 7             | -0.042332   | -2.296981   | 0.742604    |
| 5             | 6             | 1.255983    | -2.907076   | 1.070317    |
| 6             | 6             | 2.493995    | -2.185035   | 0.472481    |
| 7             | 6             | 2.292172    | -0.694519   | 0.506925    |
| 8             | 6             | 3.173073    | 0.394656    | 0.169973    |
| 9             | 6             | 4.516458    | 0.483375    | -0.258366   |
| 10            | 6             | 5.071782    | 1.736724    | -0.512384   |
| 11            | 6             | 4.301501    | 2.910473    | -0.344318   |
| 12            | 6             | 2.980436    | 2.865903    | 0.079565    |
| 13            | 6             | 2.436099    | 1.598035    | 0.333928    |
| 14            | 6             | -1.483313   | -0.296153   | 1.002464    |
| 15            | 6             | -1.805813   | -0.309535   | -0.501607   |
| 16            | 6             | -3.175164   | 0.323658    | -0.865330   |
| 17            | 6             | -4.408221   | -0.541287   | -0.501906   |
| 18            | 6             | -4.232760   | -1.976542   | -1.008145   |
| 19            | 6             | -2.901437   | -2.613924   | -0.585495   |
| 20            | 6             | -1.711805   | -1.754148   | -1.045729   |
| 21            | 6             | -0.336688   | -2.347400   | -0.696244   |
| 22            | 6             | -3.247480   | 1.769663    | -0.387997   |
| 23            | 6             | -4.658619   | 3.528231    | 0.365559    |
| 24            | 6             | 6.539765    | -0.676061   | -0.811576   |
| 25            | 8             | 5.182922    | -0.707676   | -0.390555   |
| 26            | 8             | -4.644790   | -0.602800   | 0.910287    |
| 27            | 8             | -4.305080   | 2.536177    | -0.351750   |
| 28            | 8             | -4.500497   | 2.146935    | -0.025893   |
| 29            | 1             | 0.388921    | 1.883182    | 0.821781    |
| 30            | 1             | -0.059463   | -1.049436   | 2.395432    |
| 31            | 1             | 1.235904    | -3.953236   | 0.743522    |
| 32            | 1             | 1.336144    | -2.914239   | 2.164597    |
| 33            | 1             | 2.675249    | -2.514501   | -0.559995   |
| 34            | 1             | 3.387362    | -2.480479   | 1.035138    |
| 35            | 1             | 6.099345    | 1.830244    | -0.842144   |
| 36            | 1             | 4.765030    | 3.870208    | -0.553250   |
| 37            | 1             | 2.396119    | 3.771876    | 0.208308    |
| 38            | 1             | -1.496475   | 0.729479    | 1.388703    |
| 39            | 1             | -2.246104   | -0.844766   | 1.558675    |
| 40            | 1             | -1.041036   | 0.289002    | -1.01561    |
| 41            | 1             | -3.192271   | 0.412493    | -1.964510   |
| 42            | 1             | -5.298585   | -0.104730   | -0.990574   |
| 43            | 1             | -4.296134   | -1.957731   | -2.105430   |
| 44            | 1             | -5.081782   | -2.567890   | -0.648943   |
| 45            | 1             | -2.820166   | -3.614407   | -1.028785   |
| 46            | 1             | -2.875928   | -2.752759   | 0.499370    |
| 47            | 1             | -1.752544   | -1.700058   | -2.145336   |
| 48            | 1             | 0.424296    | -1.814581   | -1.293983   |
| 49            | 1             | 0.303649    | -3.401703   | -0.998731   |
| 50            | 1             | -4.368050   | 4.188032    | -0.454610   |
| 51            | 1             | -4.042748   | 3.747666    | 1.240476    |
| 52            | 1             | -5.716886   | 3.643504    | 0.597549    |
| 53            | 1             | 7.165237    | -0.121073   | -0.100592   |
| 54            | 1             | 6.641436    | -0.229551   | -1.809093   |
| 55            | 1             | 6.866547    | -1.716624   | -0.845854   |
| 56            | 1             | -4.957453   | 0.267991    | 1.190717    |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 47.9366             |
| C3      | 129.1879            |
| C5      | 132.3413            |
| C6      | 165.1666            |
| C7      | 73.3564             |
| C8      | 64.6853             |
| C9      | 25.8497             |
| C10     | 84.5691             |
| C11     | 60.9992             |
| C12     | 78.0521             |
| C13     | 44.4221             |
| C14     | 160.3549            |
| C15     | 153.7286            |
| C16     | 130.9901            |
| C17     | 116.5857            |
| C18     | 152.2444            |
| C19     | 165.1108            |
| C20     | 145.6378            |
| C21     | 134.1385            |
| C22     | 2.9491              |
| C23     | 132.5005            |
| C24     | 131.9325            |
venenatine (9), conformer 4

Sum of electronic and thermal free energies = -1265.263983 H

| Center Number | Atomic Number | Coordinates (Angstroms) | X  | Y  | Z   |
|---------------|---------------|-------------------------|----|----|-----|
| 1             | 7             | -1.494416 0.760799 -1.389913 |
| 2             | 6             | -1.181260 -0.353144 -0.625696 |
| 3             | 6             | 0.175291 -0.990060 -0.584707 |
| 4             | 7             | 0.211516 -1.987646 0.498205 |
| 5             | 6             | -1.002736 -2.806721 0.582054 |
| 6             | 6             | -2.222437 -1.970036 0.958769 |
| 7             | 6             | -2.289533 -0.763845 0.068849 |
| 8             | 6             | -3.352965 0.147562 -0.269543 |
| 9             | 6             | -4.707794 0.269016 0.110584 |
| 10            | 6             | -5.478238 1.299627 -0.426648 |
| 11            | 6             | -4.912474 2.215889 -1.342304 |
| 12            | 6             | -3.584733 2.131463 -1.739661 |
| 13            | 6             | -2.822216 1.090194 -1.190121 |
| 14            | 6             | 1.319589 0.045886 -0.382414 |
| 15            | 6             | 2.412097 -0.482952 0.571936 |
| 16            | 6             | 3.735376 0.341975 0.545680 |
| 17            | 6             | 4.624346 0.108644 -0.703556 |
| 18            | 6             | 4.849611 -1.388111 -0.927900 |
| 19            | 6             | 3.537076 -2.181797 -0.964121 |
| 20            | 6             | 2.721170 -1.976639 0.325027 |
| 21            | 6             | 1.410518 -2.815430 0.356480 |
| 22            | 6             | 3.472939 1.820185 0.771338 |
| 23            | 6             | 2.777882 3.451289 2.345895 |
| 24            | 6             | -6.516420 -0.579591 1.434610 |
| 25            | 8             | -5.165094 -0.664425 1.004018 |
| 26            | 8             | 4.066092 0.647552 -1.901728 |
| 27            | 8             | 3.576952 2.696478 -0.074686 |
| 28            | 8             | 3.093083 2.077126 2.036195 |
| 29            | 1             | -0.858115 1.257660 -1.992797 |
| 30            | 1             | 0.346449 -1.505579 -1.556154 |
| 31            | 1             | -0.828479 -3.579455 1.338835 |
| 32            | 1             | -1.193835 -3.328286 -0.379042 |
| 33            | 1             | -2.172629 -1.675905 2.015334 |
| 34            | 1             | -3.135908 -2.579824 0.853000 |
| 35            | 1             | -6.519622 1.413397 -0.151415 |
| 36            | 1             | 5.541296 3.006108 -1.741829 |
| 37            | 1             | -3.159122 2.840373 -2.443442 |
| 38            | 1             | 0.901178 0.964252 0.045427 |
| 39            | 1             | 1.751334 0.304345 -1.352505 |
| 40            | 1             | 2.011567 -0.402055 1.586785 |
| 41            | 1             | 4.319608 0.004018 1.413017 |
| 42            | 1             | 5.597572 0.588991 -0.514245 |
| 43            | 1             | 5.488447 -1.769600 -0.119143 |
| 44            | 1             | 5.405828 -1.512632 -1.863125 |
| 45            | 1             | 3.754978 -3.249486 -1.093757 |
| 46            | 1             | 2.947263 -1.876872 -1.837110 |
| 47            | 1             | 3.353422 -2.311968 1.160083 |
| 48            | 1             | 1.431466 -3.513163 1.200310 |
| 49            | 1             | 1.349494 -3.430871 -0.565348 |
| 50            | 1             | 3.648543 4.087802 2.173344 |
| 51            | 1             | 2.500155 3.451731 3.399100 |
| 52            | 1             | 1.947460 3.798550 1.727079 |
| 53            | 1             | -7.212760 -0.694659 0.594186 |
| 54            | 1             | -6.714744 0.372630 1.942923 |
| 55            | 1             | -6.658254 -1.401923 2.137594 |
| 56            | 1             | 3.921513 1.593722 -1.733839 |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 44.5215             |
| C3      | 129.8354            |
| C5      | 132.8169            |
| C6      | 160.1434            |
| C7      | 74.3357             |
| C8      | 66.2911             |
| C9      | 26.0676             |
| C10     | 84.9963             |
| C11     | 60.4375             |
| C12     | 79.2983             |
| C13     | 44.4491             |
| C14     | 155.7834            |
| C15     | 150.7355            |
| C16     | 134.9913            |
| C17     | 116.0425            |
| C18     | 152.2445            |
| C19     | 160.1417            |
| C20     | 147.5705            |
| C21     | 125.2858            |
| C22     | -1.8161             |
| C23     | 132.5809            |
| C24     | 132.0068            |
venenatine – HCl salt (9-HCl), conformer 1

Sum of electronic and thermal free energies = -1726.085995 H

| Center Number | Atomic Number | Coordinates (Angstroms) | X  | Y  | Z  |
|---------------|---------------|-------------------------|----|----|----|
| 1             | 7             | -1.378848               | 1.097762 | -1.090939 |
| 2             | 6             | -1.083263               | -0.206722 | -0.731113 |
| 3             | 6             | 0.235054                | -0.880296 | -0.991243 |
| 4             | 7             | 0.317626                | -2.105588 | -0.112891 |
| 5             | 6             | -0.935552               | -2.935341 | -0.218892 |
| 6             | 6             | -2.186139               | -2.216798 | 0.301572  |
| 7             | 6             | -2.193163               | -0.791596 | -0.170784 |
| 8             | 6             | -3.232648               | 0.204816  | -0.169947 |
| 9             | 6             | -4.577325               | 0.223571  | 0.263573  |
| 10            | 6             | -5.326777               | 1.387102  | 0.099427  |
| 11            | 6             | -4.750897               | 2.534059  | -0.492988 |
| 12            | 6             | -3.434050               | 2.594429  | -0.930899 |
| 13            | 6             | -2.691936               | 1.376337  | -0.758839 |
| 14            | 6             | 1.491285                | -0.009527 | -0.816935 |
| 15            | 6             | 1.749990                | 0.359252  | 0.654393  |
| 16            | 6             | 2.973794                | 1.293816  | 0.890212  |
| 17            | 6             | 4.347374                | 0.614133  | 0.665060  |
| 18            | 6             | 4.438230                | -0.684636 | 1.470776  |
| 19            | 6             | 3.261140                | -1.636234 | 1.210851  |
| 20            | 6             | 1.918371                | -0.933805 | 1.487375  |
| 21            | 6             | 0.684800                | -1.830616 | 1.314430  |
| 22            | 6             | 2.858806                | 2.591241  | 0.107799  |
| 23            | 6             | 1.662208                | 4.629350  | -0.106577 |
| 24            | 6             | -6.394449               | -0.982619 | 1.258292  |
| 25            | 8             | -5.04052                | -0.936619 | 0.821366  |
| 26            | 8             | 4.588342                | 0.299909  | -0.702567 |
| 27            | 8             | 3.579852                | 2.930446  | -0.816083 |
| 28            | 8             | 1.842801                | 3.358189  | 0.553539  |
| 29            | 1             | -0.746093               | 1.742712  | -1.535725 |
| 30            | 1             | 0.258226                | -1.285283 | -2.011877 |
| 31            | 1             | -0.737141               | -3.867881 | 0.314029  |
| 32            | 1             | -1.028692               | -3.182782 | -1.279297 |
| 33            | 1             | -2.247375               | -2.270305 | 1.396740  |
| 34            | 1             | -3.065521               | -2.755621 | -0.066244 |
| 35            | 1             | -6.360053               | 1.429632  | 0.421040  |
| 36            | 1             | -5.365240               | 3.422118  | -0.606928 |
| 37            | 1             | -3.003832               | 3.439786  | -1.388576 |
| 38            | 1             | 1.372556                | 0.888004  | -1.435672 |
| 39            | 1             | 2.345312                | -0.546679 | -1.235044 |
| 40            | 1             | 0.868350                | 0.893983  | 1.031687  |
| 41            | 1             | 2.930650                | 1.582923  | 1.949949  |
| 42            | 1             | 5.124622                | 1.307322  | 1.023069  |
| 43            | 1             | 4.479720                | -0.425325 | 2.538437  |
| 44            | 1             | 5.384663                | -1.174581 | 1.221442  |
| 45            | 1             | 3.348050                | -2.511926 | 1.865174  |
| 46            | 1             | 3.305063                | -2.023448 | 0.188371  |
| 47            | 1             | 1.910466                | -0.645424 | 2.549879  |
| 48            | 1             | -0.176661               | -1.360878 | 1.797534  |
| 49            | 1             | 0.852524                | -2.809092 | 1.774650  |
| 50            | 1             | 0.790971                | 5.078958  | 0.368073  |
| 51            | 1             | 1.493691                | 4.484880  | -1.176288 |
| 52            | 1             | 2.545501                | 5.256418  | 0.033549  |
| 53            | 1             | -7.086866               | -0.811227 | 0.425035  |
| 54            | 1             | -6.582870               | -0.245203 | 2.048260  |
| 55            | 1             | -6.545417               | -1.987075 | 1.655644  |
| 56            | 1             | 4.573944                | 1.137540  | -1.192057 |
| 57            | 1             | 1.091111                | -2.765631 | -0.595988 |
| 58            | 17            | 2.061495                | -3.889226 | -1.559727 |
# Supplementary Information

| Nucleus | Isotropic shielding |
|---------|----------------------|
| C2      | 54.674               |
| C3      | 129.5075             |
| C5      | 133.7712             |
| C6      | 166.2318             |
| C7      | 74.1582              |
| C8      | 64.76                |
| C9      | 26.1242              |
| C10     | 83.8962              |
| C11     | 58.5074              |
| C12     | 80.9207              |
| C13     | 44.6748              |
| C14     | 159.9608             |
| C15     | 153.3416             |
| C16     | 133.6882             |
| C17     | 116.7531             |
| C18     | 153.6965             |
| C19     | 163.3266             |
| C20     | 147.1667             |
| C21     | 135.8696             |
| C22     | -0.5124              |
| C23     | 132.5143             |
| C24     | 131.4524             |
venenatine – HCl salt (9-HCl), conformer 2

Sum of electronic and thermal free energies = -1726.087139 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 7             | -1.288005   | 1.171891   | -1.027843   |
| 2             | 6             | -1.151476   | -0.181629  | -0.771234   |
| 3             | 6             | 0.093723    | -0.974703  | -1.043603   |
| 4             | 7             | 0.073101    | -2.191560  | -0.148294   |
| 5             | 6             | -1.229364   | -2.934800  | -0.292680   |
| 6             | 6             | -2.457277   | -2.123472  | 0.150895    |
| 7             | 6             | -2.323542   | -0.685392  | -0.263025   |
| 8             | 6             | -3.243076   | 0.419727   | -0.179423   |
| 9             | 6             | -4.581122   | 0.556946   | 0.251934    |
| 10            | 6             | -5.183624   | 1.812502   | 0.205531    |
| 11            | 6             | -4.466099   | 2.935535   | -0.267260   |
| 12            | 6             | -3.152647   | 2.839696   | -0.704947   |
| 13            | 6             | -2.559253   | 1.569168   | -0.657742   |
| 14            | 6             | 1.407988    | -0.213250  | -0.867901   |
| 15            | 6             | 1.605071    | 0.212404   | 0.597407    |
| 16            | 6             | 2.824999    | 1.122116   | 0.861532    |
| 17            | 6             | 4.182688    | 0.408608   | 0.706489    |
| 18            | 6             | 4.206385    | -0.879039  | 1.546614    |
| 19            | 6             | 3.007191    | -1.808130  | 1.297870    |
| 20            | 6             | 1.677956    | -1.050934  | 1.486004    |
| 21            | 6             | 0.418002    | -1.913622  | 1.287060    |
| 22            | 6             | 2.733455    | 2.439461   | 0.096672    |
| 23            | 6             | 3.846330    | 4.467186   | -0.412085   |
| 24            | 6             | -6.543004   | -0.514142  | 1.117373    |
| 25            | 8             | -5.187379   | -0.589735  | 0.692551    |
| 26            | 8             | 4.370464    | 0.163331   | -0.691819   |
| 27            | 8             | 1.761538    | 2.819738   | -0.53436    |
| 28            | 8             | 3.839591    | 3.187498   | 0.253386    |
| 29            | 1             | -0.523373   | 1.802291   | -1.231400   |
| 30            | 1             | 0.075556    | -1.389517  | -2.059607   |
| 31            | 1             | -1.125493   | -3.866206  | 0.268738    |
| 32            | 1             | -1.287955   | -3.200077  | -1.351354   |
| 33            | 1             | -2.603421   | -2.197047  | 1.236810    |
| 34            | 1             | -3.344756   | -2.587319  | -0.29336    |
| 35            | 1             | -6.208500   | 1.947235   | 0.529122    |
| 36            | 1             | -4.966918   | 3.898333   | -0.287664   |
| 37            | 1             | -2.610991   | 3.706376   | -1.069990   |
| 38            | 1             | 1.398209    | 0.654481   | -1.530543   |
| 39            | 1             | 2.226834    | -0.847879  | -1.208814   |
| 40            | 1             | 0.720946    | 0.787319   | 0.900535    |
| 41            | 1             | 2.777320    | 1.421638   | 1.920433    |
| 42            | 1             | 4.970805    | 1.084654   | 1.063277    |
| 43            | 1             | 4.238487    | -0.583710  | 2.605743    |
| 44            | 1             | 5.144905    | -1.414863  | 1.353273    |
| 45            | 1             | 3.049165    | -2.648106  | 2.001501    |
| 46            | 1             | 3.066549    | -2.256285  | 0.301177    |
| 47            | 1             | 1.630647    | -0.726381  | 2.537322    |
| 48            | 1             | -0.439404   | -1.410524  | 1.741967    |
| 49            | 1             | 0.540263    | -2.893056  | 1.759598    |
| 50            | 1             | 3.030893    | 5.092753   | -0.041832   |
| 51            | 1             | 3.739375    | 4.331123   | -1.490413   |
| 52            | 1             | 4.812447    | 4.910247   | -0.173337   |
| 53            | 1             | -7.197090   | -0.178981  | 0.302905    |
| 54            | 1             | -6.654862   | 0.159837   | 1.975866    |
| 55            | 1             | -6.820411   | -1.527018  | 1.412502    |
| 56            | 1             | 5.189541    | -0.331847  | -0.823826   |
| 57            | 1             | 0.824901    | -2.892087  | -0.578055   |
| 58            | 17            | 1.876269    | -4.081191  | -1.422823   |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 53.3544             |
| C3      | 127.7252            |
| C5      | 134.221             |
| C6      | 165.9212            |
| C7      | 73.6855             |
| C8      | 64.1154             |
| C9      | 26.3883             |
| C10     | 83.5614             |
| C11     | 58.6217             |
| C12     | 80.0836             |
| C13     | 44.2352             |
| C14     | 161.3569            |
| C15     | 154.8073            |
| C16     | 133.3262            |
| C17     | 114.2423            |
| C18     | 150.6656            |
| C19     | 163.5373            |
| C20     | 147.276             |
| C21     | 136.3758            |
| C22     | 2.5512              |
| C23     | 132.4943            |
| C24     | 131.662             |

![Molecular structure diagram]

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venenatine – HCl salt (9-HCl), conformer 3

Sum of electronic and thermal free energies = -1726.085870 H

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---------------|---------------|---------------------------|---|---|
| 1             | 7             | -1.283800                 | 1.221268 | -0.969673 |
| 2             | 6             | -1.144034                 | -0.140553 | -0.754404 |
| 3             | 6             | 0.106090                  | -0.924178 | -1.038554 |
| 4             | 7             | 0.076810                  | -2.167233 | -0.182733 |
| 5             | 6             | -1.220793                 | -2.909278 | -0.368171 |
| 6             | 6             | -2.458352                 | -2.116719 | 0.080674  |
| 7             | 6             | -2.322021                 | -0.665605 | -0.282622 |
| 8             | 6             | 3.247714                  | 0.432191  | -0.174237 |
| 9             | 6             | -4.592865                 | 0.548401  | 0.241190  |
| 10            | 6             | 5.199305                  | 1.802936  | 0.232955  |
| 11            | 6             | -4.478675                 | 2.945295  | -0.185511 |
| 12            | 6             | -3.158586                 | 2.870099  | -0.606876 |
| 13            | 6             | -2.561783                 | 1.600360  | -0.597321 |
| 14            | 6             | 1.418838                  | -0.167346 | -0.823448 |
| 15            | 6             | 1.597875                  | 0.212666  | 0.656323  |
| 16            | 6             | 2.817847                  | 1.120251  | 0.944811  |
| 17            | 6             | 4.188643                  | 0.405068  | 0.843323  |
| 18            | 6             | 4.176192                  | -0.900857 | 1.645811  |
| 19            | 6             | 2.933068                  | -1.823200 | 1.316158  |
| 20            | 6             | 1.659298                  | 1.076834  | 1.506015  |
| 21            | 6             | 0.401828                  | -1.932224 | 1.263877  |
| 22            | 6             | 2.723632                  | 2.418496  | 0.149933  |
| 23            | 6             | 3.923038                  | 4.276907  | -0.718110 |
| 24            | 6             | -6.563233                 | -0.561209 | 1.036278  |
| 25            | 8             | -5.201088                 | -0.615806 | 0.629052  |
| 26            | 8             | 4.530977                  | 0.039359  | -0.510775 |
| 27            | 8             | 1.687288                  | 2.916499  | -0.251343 |
| 28            | 8             | 3.928617                  | 2.998950  | -0.042575 |
| 29            | 1             | -0.518670                 | 1.865587  | -1.115451 |
| 30            | 1             | 0.099558                  | -1.306147 | -2.067535 |
| 31            | 1             | -1.120667                 | -3.856633 | 0.166469  |
| 32            | 1             | -1.261852                 | -3.144329 | -1.434715 |
| 33            | 1             | -2.622899                 | -2.225263 | 1.169050  |
| 34            | 1             | -3.335532                 | -2.567500 | -0.395569 |
| 35            | 1             | -6.229389                 | 1.921981  | 0.545884  |
| 36            | 1             | -4.982524                 | 3.907223  | -0.176569 |
| 37            | 1             | -2.614651                 | 3.751861  | -0.930033 |
| 38            | 1             | 1.405948                  | 0.720440  | -1.461994 |
| 39            | 1             | 2.244802                  | -0.788247 | -1.176496 |
| 40            | 1             | 0.712031                  | 0.780659  | 0.965068  |
| 41            | 1             | 2.727814                  | 1.446133  | 1.994734  |
| 42            | 1             | 4.955126                  | 1.066101  | 1.266969  |
| 43            | 1             | 4.150605                  | -0.637370 | 2.713105  |
| 44            | 1             | 5.124082                  | -1.417754 | 1.466201  |
| 45            | 1             | 3.018592                  | -2.694551 | 1.981382  |
| 46            | 1             | 3.086721                  | -2.222764 | 0.301570  |
| 47            | 1             | 1.596836                  | -0.783856 | 2.565785  |
| 48            | 1             | -0.462236                 | -1.443888 | 1.722822  |
| 49            | 1             | 0.519446                  | -2.925083 | 1.708604  |
| 50            | 1             | 3.331084                  | 4.998965  | -0.151997 |
| 51            | 1             | 3.505337                  | 4.173024  | -1.721795 |
| 52            | 1             | 4.976742                  | 4.582955  | -0.762455 |
| 53            | 1             | -7.206541                 | -0.198163 | 0.225225  |
| 54            | 1             | -6.690527                 | 0.079567  | 1.917685  |
| 55            | 1             | -6.840561                 | -1.585496 | 1.288981  |
| 56            | 1             | 4.830765                  | 0.906039  | -0.939919 |
| 57            | 1             | 0.833250                  | -2.860923 | -0.630884 |
| 58            | 17            | 1.841573                  | -4.032812 | -1.516677 |
Nucleus | Isotropic shielding
---|---
C2 | 53.4775
C3 | 128.0602
C5 | 134.1002
C6 | 166.0597
C7 | 73.3278
C8 | 64.072
C9 | 26.2202
C10 | 83.4474
C11 | 58.716
C12 | 79.6663
C13 | 43.8179
C14 | 161.64
C15 | 154.3061
C16 | 131.1761
C17 | 117.0109
C18 | 152.7694
C19 | 163.6546
C20 | 147.312
C21 | 136.4254
C22 | 2.7456
C23 | 132.1534
C24 | 131.5968
venenatine – HCl salt (9-HCl), conformer 4

Sum of electronic and thermal free energies = -1726.083219 H

| Center Number | Atomic Number | Coordinates (Angstroms) | X    | Y    | Z    |
|---------------|---------------|-------------------------|------|------|------|
| 1             | 7             | -1.509131               | 1.392054 | -1.077039 |
| 2             | 6             | -1.234524               | 0.074873 | -0.744813 |
| 3             | 6             | 0.124724                | -0.540625 | -0.867351 |
| 4             | 7             | 0.114752                | -1.884266 | -0.191053 |
| 5             | 6             | -1.136593               | -2.680973 | -0.439182 |
| 6             | 6             | -2.370555               | -1.978387 | 0.131867  |
| 7             | 6             | -2.375955               | -0.544019 | -0.306042 |
| 8             | 6             | -3.422445               | 0.443693 | -0.349777 |
| 9             | 6             | -4.795942               | 0.434954 | -0.019203 |
| 10            | 6             | -5.539458               | 1.602899 | -0.179863 |
| 11            | 6             | -4.929220               | 2.780360 | -0.668903 |
| 12            | 6             | -3.583756               | 2.827637 | -1.006529 |
| 13            | 6             | -2.847436               | 1.645802 | -0.836346 |
| 14            | 6             | 1.258995                | 0.322155 | -0.273454 |
| 15            | 6             | 2.482500                | -0.515668 | 0.183960 |
| 16            | 6             | 3.803446                | 0.267345 | 0.157836 |
| 17            | 6             | 4.416895                | 0.493628 | -1.258903 |
| 18            | 6             | 4.491820                | -0.827834 | -2.026987 |
| 19            | 6             | 3.148403                | -1.570570 | -2.054586 |
| 20            | 6             | 2.634538                | -1.827033 | -0.623280 |
| 21            | 6             | 1.336802                | -2.673484 | -0.567250 |
| 22            | 6             | 3.719380                | 1.570459 | 0.931762 |
| 23            | 6             | 3.538820                | 2.523106 | 3.097212 |
| 24            | 6             | -6.654005               | -0.806018 | 0.847521 |
| 25            | 8             | -5.291256               | -0.753440 | 0.441817 |
| 26            | 8             | 3.651603                | 1.409601 | -2.043399 |
| 27            | 8             | 3.622015                | 2.681295 | 0.426512 |
| 28            | 8             | 3.721498                | 1.365059 | 2.253986 |
| 29            | 1             | -0.835212               | 2.076599 | -1.381246 |
| 30            | 1             | 0.344646                | -0.743060 | -1.925855 |
| 31            | 1             | -0.980223               | -3.649977 | 0.040793 |
| 32            | 1             | -1.224750               | -2.825723 | -1.522258 |
| 33            | 1             | -2.359378               | -2.054510 | 1.225616 |
| 34            | 1             | -3.263161               | -2.504901 | -0.219819 |
| 35            | 1             | -6.593307               | 1.626106 | 0.068888 |
| 36            | 1             | 5.538875                | 3.672098 | -0.779971 |
| 37            | 1             | 3.125164                | 3.738139 | -1.379380 |
| 38            | 1             | 0.867660                | 0.869811 | 0.590267 |
| 39            | 1             | 1.550811                | 1.048030 | -1.035537 |
| 40            | 1             | 2.296967                | -0.801355 | 1.224947 |
| 41            | 1             | 4.550857                | -0.353104 | 0.706789 |
| 42            | 1             | 5.437990                | 0.888287 | -1.140027 |
| 43            | 1             | 5.253367                | -1.463184 | -1.554806 |
| 44            | 1             | 4.835505                | -0.614560 | -3.044483 |
| 45            | 1             | 3.267601                | -2.526648 | -2.580061 |
| 46            | 1             | 2.425185                | -0.982189 | -2.631254 |
| 47            | 1             | 3.403232                | -2.422810 | -0.113121 |
| 48            | 1             | 1.415832                | -3.451033 | 0.194756 |
| 49            | 1             | 1.139262                | -3.144239 | -1.536681 |
| 50            | 1             | 4.354210                | 3.233594 | 2.944865 |
| 51            | 1             | 3.542850                | 2.136466 | 4.115429 |
| 52            | 1             | 2.585720                | 3.006184 | 2.872710 |
| 53            | 1             | -7.328830               | -0.597008 | 0.007975 |
| 54            | 1             | -6.852839               | -0.098591 | 1.661809 |
| 55            | 1             | -6.819983               | -1.823977 | 1.202386 |
| 56            | 1             | 3.602951                | 2.232157 | -1.525829 |
| 57            | 1             | 0.165560                | -1.771510 | 0.919058 |
| 58            | 17            | 0.320628                | -1.942076 | 2.710010 |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 52.1567             |
| C3      | 130.4228            |
| C5      | 132.3832            |
| C6      | 163.1832            |
| C7      | 74.7322             |
| C8      | 65.0686             |
| C9      | 25.9254             |
| C10     | 83.854              |
| C11     | 58.4262             |
| C12     | 80.062              |
| C13     | 43.678              |
| C14     | 158.4554            |
| C15     | 152.5591            |
| C16     | 136.0204            |
| C17     | 115.9209            |
| C18     | 152.7106            |
| C19     | 158.9347            |
| C20     | 149.1928            |
| C21     | 128.199             |
| C22     | -1.2742             |
| C23     | 132.3201            |
| C24     | 131.5326            |
alstovenine (12), conformer 1

Sum of electronic and thermal free energies = -1265.27218 H

| Center Number | Atomic Number | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|-------------------------|-------|-------|-------|
| 1             | 7             | 1.439374                | 1.490559 | -0.423238 |
| 2             | 6             | 1.200681                | 0.133819 | -0.586392 |
| 3             | 6             | -0.122309               | -0.458244 | -0.977821 |
| 4             | 7             | -0.070707               | -1.911438 | -0.748702 |
| 5             | 6             | 1.152763                | -2.527195 | -1.276472 |
| 6             | 6             | 2.396573                | -2.060470 | -0.507539 |
| 7             | 6             | 2.359945                | -0.566551 | -0.372946 |
| 8             | 6             | 3.374692                | 0.399364 | -0.039373 |
| 9             | 6             | 4.745740                | 0.317525 | 0.290545 |
| 10            | 6             | 5.451660                | 1.487049 | 0.569857 |
| 11            | 6             | 4.805537                | 2.743494 | 0.524574 |
| 12            | 6             | 3.460537                | 2.865923 | 0.202905 |
| 13            | 6             | 2.763954                | 1.680751 | -0.076449 |
| 14            | 6             | -1.310740               | 0.144310 | -0.205233 |
| 15            | 6             | -2.633264               | -0.514088 | -0.643144 |
| 16            | 6             | -3.904469               | -0.000202 | 0.101068 |
| 17            | 6             | -4.035496               | -0.498577 | 1.563177 |
| 18            | 6             | -3.902361               | -2.021956 | 1.618731 |
| 19            | 6             | -2.625464               | -2.528505 | 0.933965 |
| 20            | 6             | -2.544068               | -2.054672 | -0.528224 |
| 21            | 6             | -1.282494               | -2.558787 | -1.249088 |
| 22            | 6             | -4.032431               | 1.508858 | 0.011265 |
| 23            | 6             | -4.499861               | 3.334748 | -1.430288 |
| 24            | 6             | 6.654972                | -1.084788 | 0.651577 |
| 25            | 8             | 5.283241                | -0.942892 | 0.309869 |
| 26            | 8             | -3.054341               | 0.058230 | 2.434476 |
| 27            | 8             | -3.847180               | 2.294694 | 0.927901 |
| 28            | 8             | -4.372255               | 1.911551 | -1.229353 |
| 29            | 1             | 0.744364                | 2.218274 | -0.460171 |
| 30            | 1             | -0.291011               | -0.260307 | -2.062934 |
| 31            | 1             | 1.276937                | -2.298563 | -2.354744 |
| 32            | 1             | 1.045177                | -3.613253 | -1.187670 |
| 33            | 1             | 3.298724                | -2.386869 | -1.036017 |
| 34            | 1             | 2.420462                | -2.538147 | 0.481091 |
| 35            | 1             | 6.503269                | 1.450977 | 0.827045 |
| 36            | 1             | 5.385265                | 3.633872 | 0.749597 |
| 37            | 1             | 2.972913                | 3.835590 | 0.171064 |
| 38            | 1             | -1.359129               | 1.223490 | -0.403910 |
| 39            | 1             | -1.144936               | 0.020532 | 0.867121 |
| 40            | 1             | -2.777319               | -0.272239 | -1.705745 |
| 41            | 1             | -4.762710               | -0.409192 | -0.449869 |
| 42            | 1             | -5.038828               | -0.217342 | 1.921778 |
| 43            | 1             | -4.784887               | -2.463574 | 1.134687 |
| 44            | 1             | -3.925776               | -2.327520 | 2.670247 |
| 45            | 1             | -2.605975               | -3.625556 | 0.959269 |
| 46            | 1             | -1.745301               | -2.186657 | 1.485651 |
| 47            | 1             | -3.406694               | -2.477507 | -1.066888 |
| 48            | 1             | -1.399542               | -2.392604 | -2.342155 |
| 49            | 1             | -1.182756               | -3.636737 | -1.096798 |
| 50            | 1             | -4.774945               | 3.453936 | -2.477553 |
| 51            | 1             | -3.552358               | 3.836090 | -1.219741 |
| 52            | 1             | -5.274970               | 3.741973 | -0.777290 |
| 53            | 1             | 6.855298                | -0.710935 | 1.663725 |
| 54            | 1             | 7.301819                | -0.561026 | -0.063846 |
| 55            | 1             | 6.863595                | -2.155048 | 0.612660 |
| 56            | 1             | -3.141658               | 1.029340 | 2.373662 |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 46.9257             |
| C3      | 124.0244            |
| C5      | 131.7747            |
| C6      | 160.1914            |
| C7      | 73.5286             |
| C8      | 65.1842             |
| C9      | 26.0791             |
| C10     | 85.0317             |
| C11     | 60.2032             |
| C12     | 80.01               |
| C13     | 44.8093             |
| C14     | 154.6347            |
| C15     | 144.5527            |
| C16     | 133.6465            |
| C17     | 115.8723            |
| C18     | 153.3528            |
| C19     | 162.898             |
| C20     | 146.2299            |
| C21     | 123.5542            |
| C22     | -1.3426             |
| C23     | 132.4986            |
| C24     | 132.1374            |
alstovenine (12), conformer 2

Sum of electronic and thermal free energies = -1265.267873 H

| Center Number | Atomic Number | Coordinates (Ångstroms) |
|---------------|---------------|-------------------------|
| 1             | 7             | 1.494169 1.459343 -0.582484 |
| 2             | 6             | 1.293818 0.086166 -0.614854 |
| 3             | 6             | -0.001637 -0.571538 -0.985290 |
| 4             | 7             | 0.072942 -1.994082 -0.607297 |
| 5             | 6             | 1.326283 -2.629014 -1.031594 |
| 6             | 6             | 2.534072 -2.055529 -0.276438 |
| 7             | 6             | 2.461526 -0.556662 -0.296576 |
| 8             | 6             | 3.442714 0.464761 -0.036053 |
| 9             | 6             | 4.805397 0.455159 0.335330 |
| 10            | 6             | 5.475265 1.665689 0.508871 |
| 11            | 6             | 4.801006 2.893166 0.315013 |
| 12            | 6             | 3.463276 2.945213 -0.052492 |
| 13            | 6             | 2.802745 1.719402 -0.223720 |
| 14            | 6             | -1.226490 0.082419 -0.320373 |
| 15            | 6             | -2.517640 -0.639209 -0.757486 |
| 16            | 6             | -3.836827 -0.094978 -0.155032 |
| 17            | 6             | -4.035221 -0.413767 1.340607 |
| 18            | 6             | -3.844029 -1.915373 1.603461 |
| 19            | 6             | -2.533686 -2.468127 1.026897 |
| 20            | 6             | -2.404961 -2.158667 -0.476221 |
| 21            | 6             | -1.106550 -2.711123 -1.085440 |
| 22            | 6             | -4.095101 1.372187 -0.483741 |
| 23            | 6             | -5.573245 3.193436 -0.157689 |
| 24            | 6             | 6.742396 -0.850384 0.870271 |
| 25            | 8             | 5.373356 -0.782264 0.499982 |
| 26            | 8             | -3.105425 0.391252 2.082260 |
| 27            | 8             | -3.432746 2.058731 -1.236123 |
| 28            | 8             | -5.220399 1.823948 0.115339 |
| 29            | 1             | 0.786747 2.158123 -0.744593 |
| 30            | 1             | -0.132919 -0.490860 -2.089797 |
| 31            | 1             | 1.481096 -2.550547 -2.123120 |
| 32            | 1             | 1.240609 -3.703323 -0.836183 |
| 33            | 1             | 3.459809 -2.411773 -0.741184 |
| 34            | 1             | 2.535636 -2.430599 0.755977 |
| 35            | 1             | 6.519937 1.684446 0.794672 |
| 36            | 1             | 5.353097 3.817342 0.458893 |
| 37            | 1             | 2.953841 3.892593 -0.200727 |
| 38            | 1             | -1.294156 1.130401 -0.626960 |
| 39            | 1             | -1.102781 0.059806 0.761494 |
| 40            | 1             | -2.598543 -0.509244 -1.845910 |
| 41            | 1             | -4.654547 -0.629076 -0.664984 |
| 42            | 1             | -5.056737 -0.125332 1.618136 |
| 43            | 1             | -4.699389 -2.445856 1.160051 |
| 44            | 1             | -3.898546 -2.097877 2.685197 |
| 45            | 1             | -2.496502 -3.554168 1.180423 |
| 46            | 1             | -1.678109 -2.048587 1.564171 |
| 47            | 1             | -3.237481 -2.661398 -0.994128 |
| 48            | 1             | -1.180566 -2.665661 -2.193254 |
| 49            | 1             | -0.997369 -3.768253 -0.816014 |
| 50            | 1             | -5.374825 3.340304 -1.228282 |
| 51            | 1             | -4.780226 3.863944 0.181582 |
| 52            | 1             | -6.492731 3.372246 0.399227 |
| 53            | 1             | -6.918044 -0.372549 1.842691 |
| 54            | 1             | 7.385963 -0.381899 0.114565 |
| 55            | 1             | 6.980831 -1.912873 0.940922 |
| 56            | 1             | -3.306948 0.312432 3.023455 |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 46.1839             |
| C3      | 123.6361            |
| C5      | 131.6351            |
| C6      | 160.0053            |
| C7      | 74.7009             |
| C8      | 64.9666             |
| C9      | 25.5893             |
| C10     | 84.7143             |
| C11     | 61.4916             |
| C12     | 78.3088             |
| C13     | 44.401              |
| C14     | 156.0238            |
| C15     | 146.8179            |
| C16     | 133.046             |
| C17     | 113.1501            |
| C18     | 149.4935            |
| C19     | 163.8666            |
| C20     | 144.5434            |
| C21     | 124.4232            |
| C22     | 3.191               |
| C23     | 132.9066            |
| C24     | 131.9224            |
alstovenine (12), conformer 3

Sum of electronic and thermal free energies = -1265.269559 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X  | Y  | Z  |
| 1             | 7             | 1.465857 | 1.409281 | -0.676507 |
| 2             | 6             | 1.237931 | 0.041924 | -0.642073 |
| 3             | 6             | -0.063819 | -0.611288 | -1.002653 |
| 4             | 7             | -0.017256 | -2.022213 | -0.584425 |
| 5             | 6             | 1.238252 | -2.685810 | -0.949837 |
| 6             | 6             | 2.430750 | -2.104728 | -0.179234 |
| 7             | 6             | 2.386617 | -0.607489 | -0.269184 |
| 8             | 6             | 3.384370 | 0.406972 | -0.046011 |
| 9             | 6             | 4.739841 | 0.389747 | 0.351119 |
| 10            | 6             | 5.432815 | 1.594138 | 0.468042 |
| 11            | 6             | 4.789231 | 2.822262 | 0.192748 |
| 12            | 6             | 3.458996 | 2.881541 | -0.200083 |
| 13            | 6             | 2.775116 | 1.661904 | -0.313230 |
| 14            | 6             | -1.287837 | 0.068441 | -0.361140 |
| 15            | 6             | -2.583417 | -0.646899 | -0.786961 |
| 16            | 6             | -3.887864 | -0.050662 | -0.186726 |
| 17            | 6             | -4.117662 | -0.378788 | 1.308273 |
| 18            | 6             | -3.988531 | -1.886446 | 1.545737 |
| 19            | 6             | -2.672153 | -2.463427 | 1.008171 |
| 20            | 6             | -2.499167 | -2.162723 | -0.491630 |
| 21            | 6             | -1.195518 | -0.737687 | -1.068877 |
| 22            | 6             | -4.031696 | 1.418417 | -0.566155 |
| 23            | 6             | -4.554915 | 3.616925 | 0.175703 |
| 24            | 6             | 6.635199 | -0.923571 | 1.004084 |
| 25            | 8             | 5.276696 | -0.847244 | 0.595641 |
| 26            | 8             | -3.188731 | 0.272530 | 2.179610 |
| 27            | 8             | -3.893318 | 1.851386 | -1.691578 |
| 28            | 8             | -4.355004 | 2.220217 | 0.483847 |
| 29            | 1             | 0.787507 | 2.112242 | -0.920917 |
| 30            | 1             | -0.190515 | -0.555593 | -2.109274 |
| 31            | 1             | 1.427670 | -2.608481 | -2.039647 |
| 32            | 1             | 1.130214 | -3.753347 | -0.718148 |
| 33            | 1             | 3.364742 | -2.495777 | -0.596647 |
| 34            | 1             | 2.390418 | -2.433864 | 0.867809 |
| 35            | 1             | 6.472589 | 1.607209 | 0.771285 |
| 36            | 1             | 5.359139 | 3.741273 | 0.293539 |
| 37            | 1             | 2.973197 | 3.829694 | -0.410154 |
| 38            | 1             | -1.332588 | 1.115182 | -0.688620 |
| 39            | 1             | -1.170770 | 0.064463 | 0.725087 |
| 40            | 1             | -2.667377 | -0.524841 | -1.877947 |
| 41            | 1             | -4.716009 | -0.535639 | -0.727494 |
| 42            | 1             | -5.138074 | -0.066490 | 1.573772 |
| 43            | 1             | -4.838206 | -2.384409 | 1.057567 |
| 44            | 1             | -4.083265 | -2.071005 | 2.621130 |
| 45            | 1             | -2.659285 | -3.549820 | 1.163413 |
| 46            | 1             | -1.827197 | -2.056911 | 1.571534 |
| 47            | 1             | -3.327064 | -2.653445 | -1.027565 |
| 48            | 1             | -1.248513 | -2.714103 | -2.178418 |
| 49            | 1             | -1.101699 | -3.789534 | -0.775482 |
| 50            | 1             | -4.824947 | 4.086497 | 1.121042 |
| 51            | 1             | -5.357106 | 3.730242 | -0.556373 |
| 52            | 1             | -3.636844 | 4.051553 | -0.225709 |
| 53            | 1             | 6.798450 | -0.393820 | 1.951284 |
| 54            | 1             | 7.307030 | -0.514375 | 0.238708 |
| 55            | 1             | 6.846732 | -1.985086 | 1.141846 |
| 56            | 1             | -3.354805 | 1.223297 | 2.117711 |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 46.7368             |
| C3      | 123.7459            |
| C5      | 131.8664            |
| C6      | 160.0717            |
| C7      | 74.2956             |
| C8      | 64.7845             |
| C9      | 25.6666             |
| C10     | 84.6357             |
| C11     | 61.4055             |
| C12     | 78.7577             |
| C13     | 44.4986             |
| C14     | 154.7727            |
| C15     | 144.0527            |
| C16     | 131.2231            |
| C17     | 116.8815            |
| C18     | 152.2512            |
| C19     | 163.9968            |
| C20     | 144.5202            |
| C21     | 124.4169            |
| C22     | 2.5826              |
| C23     | 132.6936            |
| C24     | 131.8174            |
16-epi-alstovenine (13), conformer 1

Sum of electronic and thermal free energies = -1265.268541 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 7             | 1.821298    | 1.650656    | -0.350311   |
| 2             | 6             | 1.433271    | 0.330090    | -0.519810   |
| 3             | 6             | 0.033653    | -0.113033   | -0.833147   |
| 4             | 7             | -0.051251   | -1.569621   | -0.634654   |
| 5             | 6             | 1.064963    | -2.292475   | -1.255941   |
| 6             | 6             | 2.398763    | -1.975883   | -0.564566   |
| 7             | 6             | 2.525394    | -0.490224   | -0.396991   |
| 8             | 6             | 3.654649    | 0.358994    | -0.117962   |
| 9             | 6             | 5.029175    | 0.130968    | 0.114740    |
| 10            | 6             | 5.869397    | 1.215937    | 0.361888    |
| 11            | 6             | 5.354934    | 2.532536    | 0.379668    |
| 12            | 6             | 4.011056    | 2.793115    | 0.154398    |
| 13            | 6             | 3.178597    | 1.696763    | -0.093586   |
| 14            | 6             | -1.034661   | 0.589506    | 0.024052    |
| 15            | 6             | -2.443037   | 0.078233    | -0.331672   |
| 16            | 6             | -3.559172   | 0.761305    | 0.521251    |
| 17            | 6             | -3.713649   | 0.182861    | 1.943523    |
| 18            | 6             | -3.713132   | -1.350918   | 1.974103    |
| 19            | 6             | -2.535669   | -1.962940   | 1.204346    |
| 20            | 6             | -2.507372   | -1.465197   | -0.251817   |
| 21            | 6             | -1.353695   | -0.073425   | -1.065246   |
| 22            | 6             | -4.887619   | 0.730796    | -0.220594   |
| 23            | 6             | -6.067402   | 1.608326    | -2.081122   |
| 24            | 6             | 6.805721    | -1.465936   | 0.308611    |
| 25            | 8             | 5.433819    | -1.177984   | 0.077955    |
| 26            | 8             | -2.625640   | 0.736458    | 2.706876    |
| 27            | 8             | -5.859585   | 0.058651    | 0.066957    |
| 28            | 8             | -4.867926   | 1.568723    | -1.283710   |
| 29            | 1             | 1.206033    | 2.447850    | -0.343691   |
| 30            | 1             | -0.180939   | 0.127386    | -1.901451   |
| 31            | 1             | 1.141593    | -2.048262   | -2.35200    |
| 32            | 1             | 0.851701    | -3.364008   | -1.182315   |
| 33            | 1             | 3.225099    | -2.376526   | -1.161602   |
| 34            | 1             | 2.440362    | -2.482214   | 0.409198    |
| 35            | 1             | 6.926627    | 1.066760    | 0.544277    |
| 36            | 1             | 6.037435    | 3.354151    | 0.576474    |
| 37            | 1             | 3.625110    | 3.813133    | 0.170148    |
| 38            | 1             | -0.999721   | 1.671761    | -0.160109   |
| 39            | 1             | -0.812733   | 0.436507    | 1.082277    |
| 40            | 1             | -2.623203   | 0.362923    | -1.37066    |
| 41            | 1             | -3.294503   | 1.820279    | 0.627917    |
| 42            | 1             | -4.662796   | 0.546094    | 2.359564    |
| 43            | 1             | -4.662453   | -1.691697   | 1.544928    |
| 44            | 1             | -3.705323   | -1.683925   | 3.021513    |
| 45            | 1             | -2.623291   | -3.056833   | 1.211160    |
| 46            | 1             | -1.588075   | -1.722957   | 1.696504    |
| 47            | 1             | -3.441354   | -1.792898   | -0.732814   |
| 48            | 1             | -1.523348   | -1.870253   | -2.144452   |
| 49            | 1             | -1.356236   | -3.162524   | -0.941757   |
| 50            | 1             | -6.282648   | 0.620968    | -2.496749   |
| 51            | 1             | -5.862501   | 2.324703    | -2.876178   |
| 52            | 1             | -6.916418   | 1.935242    | -1.476122   |
| 53            | 1             | 6.895803    | -2.550593   | 0.236241    |
| 54            | 1             | 7.120729    | -1.138961   | 1.307792    |
| 55            | 1             | -7.446301   | -0.993304   | -0.446928   |
| 56            | 1             | -2.687238   | 0.405672    | 3.612614    |
| Nucleus | Isotropic shielding |
|---------|----------------------|
| C2      | 46.6148              |
| C3      | 124.0653             |
| C5      | 131.9455             |
| C6      | 160.0885             |
| C7      | 73.7864              |
| C8      | 65.5739              |
| C9      | 26.1516              |
| C10     | 84.847               |
| C11     | 60.0077              |
| C12     | 79.8808              |
| C13     | 45.1488              |
| C14     | 151.239              |
| C15     | 145.61               |
| C16     | 132.6854             |
| C17     | 114.8558             |
| C18     | 153.0301             |
| C19     | 163.5496             |
| C20     | 150.6942             |
| C21     | 123.8091             |
| C22     | 1.8758               |
| C23     | 132.8651             |
| C24     | 131.9658             |
16-epi-alstovenine (13), conformer 2

Sum of electronic and thermal free energies = -1265.267551 \text{H}

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 7             | -1.878887   | -1.584504   | -0.654010   |
| 2             | 6             | -1.508976   | -0.248592   | -0.611117   |
| 3             | 6             | -0.126274   | 0.261856    | -0.896318   |
| 4             | 7             | -0.046951   | 1.667462    | -0.464082   |
| 5             | 6             | -1.195333   | 2.465233    | -0.909712   |
| 6             | 6             | -2.493829   | 2.016334    | -0.224943   |
| 7             | 6             | -2.602612   | 0.522267    | -0.309990   |
| 8             | 6             | -3.712786   | -0.378860   | -0.138347   |
| 9             | 6             | -5.079001   | -0.214290   | 0.180493    |
| 10            | 6             | -5.900288   | -1.337637   | 0.268505    |
| 11            | 6             | -5.374648   | -2.630376   | 0.042840    |
| 12            | 6             | -4.038120   | -2.833975   | -0.273277   |
| 13            | 6             | -3.224765   | -1.694216   | -0.359589   |
| 14            | 6             | 0.980288    | -0.551385   | -0.201456   |
| 15            | 6             | 2.372179    | 0.026876    | -0.522745   |
| 16            | 6             | 3.513694    | -0.761924   | 0.165877    |
| 17            | 6             | 3.721781    | -0.410478   | 1.662060    |
| 18            | 6             | 3.748005    | 1.104966    | 1.900124    |
| 19            | 6             | 2.531935    | 1.819177    | 1.296337    |
| 20            | 6             | 2.427575    | 1.542093    | -0.213785   |
| 21            | 6             | 1.231523    | 2.253494    | -0.865269   |
| 22            | 6             | 4.824914    | -0.629858   | -0.607863   |
| 23            | 6             | 7.057486    | -1.414399   | -0.767565   |
| 24            | 6             | -6.857100   | 1.299069    | 0.721324    |
| 25            | 8             | -5.495315   | 1.075657    | 0.384294    |
| 26            | 8             | 2.664842    | -1.045181   | 2.374426    |
| 27            | 8             | 5.014271    | 0.072096    | -1.581075   |
| 28            | 8             | 5.784623    | -1.434392   | -0.092019   |
| 29            | 1             | -1.256571   | -2.361308   | -0.807130   |
| 30            | 1             | 0.050847    | 0.202827    | -1.995981   |
| 31            | 1             | -1.317590   | 2.403487    | -2.010375   |
| 32            | 1             | -0.988400   | 3.512802    | -0.666843   |
| 33            | 1             | -3.349703   | 2.502182    | -0.705700   |
| 34            | 1             | -2.491638   | 2.348580    | 0.822848    |
| 35            | 1             | -6.951065   | -1.237402   | 0.511757    |
| 36            | 1             | -6.042423   | -3.483365   | 0.120423    |
| 37            | 1             | -3.643523   | -3.830794   | -0.445377   |
| 38            | 1             | 0.944218    | -1.593208   | -0.549421   |
| 39            | 1             | 0.794093    | -0.566206   | 0.874685    |
| 40            | 1             | 2.525337    | -0.079855   | -1.604940   |
| 41            | 1             | 3.275264    | -1.834184   | 0.147687    |
| 42            | 1             | 4.670755    | -0.851502   | 1.990099    |
| 43            | 1             | 4.671790    | 1.506596    | 1.458913    |
| 44            | 1             | 3.819082    | 1.295488    | 2.980115    |
| 45            | 1             | 2.621008    | 2.899991    | 1.464101    |
| 46            | 1             | 1.615546    | 1.497627    | 1.800865    |
| 47            | 1             | 3.332302    | 1.941772    | -0.691473   |
| 48            | 1             | 1.352962    | 2.226311    | -1.968776   |
| 49            | 1             | 1.229950    | 3.309223    | -0.570141   |
| 50            | 1             | 6.942117    | -1.734576   | -1.805795   |
| 51            | 1             | 7.687955    | -2.112059   | -0.217037   |
| 52            | 1             | 7.484399    | -0.408834   | -0.748411   |
| 53            | 1             | -6.961396   | 2.378234    | 0.844452    |
| 54            | 1             | -7.124149   | 0.797777    | 1.660438    |
| 55            | 1             | -7.528851   | 0.957099    | -0.076469   |
| 56            | 1             | 2.741362    | -0.847253   | 3.315534    |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 46.0778             |
| C3      | 123.8138            |
| C5      | 131.9817            |
| C6      | 159.9601            |
| C7      | 73.8903             |
| C8      | 64.7252             |
| C9      | 25.9024             |
| C10     | 84.9716             |
| C11     | 61.0382             |
| C12     | 79.6218             |
| C13     | 44.5976             |
| C14     | 151.9381            |
| C15     | 148.9824            |
| C16     | 132.2275            |
| C17     | 112.466             |
| C18     | 152.1709            |
| C19     | 164.4993            |
| C20     | 149.9014            |
| C21     | 124.2177            |
| C22     | 2.9715              |
| C23     | 132.8374            |
| C24     | 132.0572            |
16-epi-alstovenine (13), conformer 3

Sum of electronic and thermal free energies = -1265.266627 H

| Center Number | Atomic Number | Coordinates (Angstroms) | X     | Y    | Z     |
|---------------|---------------|-------------------------|-------|------|-------|
| 1             | 7             | 1.824374 1.669203 -0.321762 |
| 2             | 6             | 1.436278 0.352869 -0.524023 |
| 3             | 6             | 0.037700 -0.082283 -0.851833 |
| 4             | 7             | -0.048076 -1.544562 -0.702897 |
| 5             | 6             | 1.076098 -2.249284 -1.332267 |
| 6             | 6             | 2.408544 -1.952380 -0.615399 |
| 7             | 6             | 2.526332 -0.471432 -0.410165 |
| 8             | 6             | 3.654570 0.370198 -0.105010 |
| 9             | 6             | 5.026772 0.133952 0.134016 |
| 10            | 6             | 5.867043 1.212263 0.408061 |
| 11            | 6             | 5.355038 2.529339 0.446899 |
| 12            | 6             | 4.013508 2.802794 0.217285 |
| 13            | 6             | 3.180711 1.707788 -0.057353 |
| 14            | 6             | -1.029033 0.582295 0.037190 |
| 15            | 6             | -2.440811 0.083451 -0.326333 |
| 16            | 6             | -3.553827 0.723008 0.564816 |
| 17            | 6             | -3.734398 0.055275 1.955063 |
| 18            | 6             | -3.746651 -1.475660 1.883036 |
| 19            | 6             | -2.557362 -2.043835 1.093203 |
| 20            | 6             | -2.506164 -1.462824 0.330989 |
| 21            | 6             | -1.346902 -2.031478 -1.164731 |
| 22            | 6             | -4.870954 0.751354 -0.196718 |
| 23            | 6             | -6.053884 1.820877 -1.952836 |
| 24            | 6             | 6.796686 -1.471945 0.315757 |
| 25            | 8             | 5.427913 -1.174768 0.075727 |
| 26            | 8             | -2.743321 0.548268 2.870816 |
| 27            | 8             | -5.824196 0.018552 -0.014075 |
| 28            | 8             | -4.864344 1.717985 -1.145654 |
| 29            | 1             | 1.215356 2.471230 -0.325626 |
| 30            | 1             | -0.184123 0.198515 -1.908172 |
| 31            | 1             | 1.165453 -1.974164 -2.402598 |
| 32            | 1             | 0.861638 -3.322200 -1.291462 |
| 33            | 1             | 3.234491 -2.383181 -2.11302 |
| 34            | 1             | 2.429160 -2.483497 0.345514 |
| 35            | 1             | 6.922470 1.057550 0.595940 |
| 36            | 1             | 6.037803 3.345488 0.664032 |
| 37            | 1             | 3.629692 3.817939 0.250237 |
| 38            | 1             | -0.998846 1.671756 -0.093048 |
| 39            | 1             | -0.775699 0.383946 1.081761 |
| 40            | 1             | -2.621841 0.421461 -1.355838 |
| 41            | 1             | -3.279784 1.769256 0.742837 |
| 42            | 1             | -4.686194 0.398096 2.371301 |
| 43            | 1             | -4.681357 -1.779343 1.399634 |
| 44            | 1             | -3.765630 -1.872122 2.905247 |
| 45            | 1             | -2.647869 -3.135718 1.036459 |
| 46            | 1             | -1.604638 -1.855920 1.605333 |
| 47            | 1             | -3.437052 -1.758911 -0.836403 |
| 48            | 1             | -1.509505 -1.780534 -2.234443 |
| 49            | 1             | -1.347879 -3.124858 -1.090377 |
| 50            | 1             | -5.865672 2.643788 -2.641797 |
| 51            | 1             | -6.922633 2.033075 -1.325347 |
| 52            | 1             | -6.225648 0.890644 -2.499928 |
| 53            | 1             | 6.887704 -2.555354 0.224323 |
| 54            | 1             | 7.101566 -1.164604 1.324161 |
| 55            | 1             | 7.446720 -0.987766 -0.424092 |
| 56            | 1             | -1.967981 -0.026670 2.845733 |
Nuclear Isotropic Shielding

| Nucleus | Isotropic Shielding |
|---------|---------------------|
| C2      | 47.3713             |
| C3      | 124.0948            |
| C5      | 132.1273            |
| C6      | 160.0684            |
| C7      | 73.5574             |
| C8      | 65.6835             |
| C9      | 26.1342             |
| C10     | 84.6868             |
| C11     | 59.6667             |
| C12     | 79.7853             |
| C13     | 45.0457             |
| C14     | 150.416             |
| C15     | 146.3818            |
| C16     | 130.3556            |
| C17     | 115.2736            |
| C18     | 155.2437            |
| C19     | 164.3094            |
| C20     | 151.2175            |
| C21     | 123.8634            |
| C22     | 1.9792              |
| C23     | 132.9268            |
| C24     | 131.9119            |
16-epi-alstovenine (13), conformer 4

Sum of electronic and thermal free energies = -1265.266106 H

| Center Number | Atomic Number | Coordinates (Ångstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z               |
| 1             | 7             | 1.885375    | 1.598361    | -0.647894      |
| 2             | 6             | 1.512916    | 0.262320    | -0.618162      |
| 3             | 6             | 0.129951    | -0.243807   | -0.909184      |
| 4             | 7             | 0.047203    | -1.654821   | -0.496153      |
| 5             | 6             | 1.199079    | -2.448450   | -0.943045      |
| 6             | 6             | 2.492179    | -2.007324   | -0.243997      |
| 7             | 6             | 2.603182    | -0.512782   | -0.315927      |
| 8             | 6             | 3.714438    | 0.384801    | -0.133008      |
| 9             | 6             | 5.078510    | 0.213849    | 0.192137       |
| 10            | 6             | 5.902031    | 1.334457    | 0.291271       |
| 11            | 6             | 5.380874    | 2.629824    | 0.070557       |
| 12            | 6             | 4.046752    | 2.839534    | -0.251213      |
| 13            | 6             | 3.230934    | 1.702384    | -0.348524      |
| 14            | 6             | -0.973930   | 0.555489    | -0.194088      |
| 15            | 6             | -2.369959   | -0.013695   | -0.516010      |
| 16            | 6             | -3.509045   | 0.759871    | 0.194459       |
| 17            | 6             | -3.740755   | 0.353655    | 1.685967       |
| 18            | 6             | -3.782942   | -1.169699   | 1.857858       |
| 19            | 6             | -2.558762   | -1.867240   | 1.243991       |
| 20            | 6             | -2.429397   | -1.539548   | -0.253735      |
| 21            | 6             | -1.229519   | -2.234093   | -0.915392      |
| 22            | 6             | -4.812983   | 0.658469    | -0.593323      |
| 23            | 6             | 7.030936    | 1.483455    | -0.758339      |
| 24            | 6             | 6.849514    | -1.308636   | 0.730827       |
| 25            | 8             | 5.489316    | -1.078194   | 0.389916       |
| 26            | 8             | 2.771213    | 0.966118    | 2.543558       |
| 27            | 8             | -2.013428   | -0.47319    | -1.562715      |
| 28            | 8             | -5.756835   | 1.484689    | -0.084928      |
| 29            | 1             | 1.271937    | 2.377702    | -0.822581      |
| 30            | 1             | -0.054940   | -0.164608   | -2.005751      |
| 31            | 1             | 1.328698    | -2.374158   | -2.041645      |
| 32            | 1             | 0.994444    | -3.498259   | -0.713238      |
| 33            | 1             | 3.351426    | -2.489296   | -0.722315      |
| 34            | 1             | 2.418187    | -2.436333   | 0.800660       |
| 35            | 1             | 6.951120    | 1.230084    | 0.539837       |
| 36            | 1             | 6.050461    | 3.480449    | 0.157254       |
| 37            | 1             | 3.655892    | 3.838596    | -0.418731      |
| 38            | 1             | 0.939705    | 1.606724    | -0.509898      |
| 39            | 1             | -0.754420   | 0.544244    | 0.877377       |
| 40            | 1             | 2.521198    | 0.122382    | -1.594659      |
| 41            | 1             | -3.264853   | 1.829812    | 0.220964       |
| 42            | 1             | -6.89885    | 0.788106    | 2.007852       |
| 43            | 1             | -6.691564   | -1.550034   | 1.371224       |
| 44            | 1             | -3.876274   | -1.397812   | 2.925964       |
| 45            | 1             | -2.654389   | -2.952252   | 1.374655       |
| 46            | 1             | -1.636066   | -1.589118   | 1.770004       |
| 47            | 1             | -3.330912   | -1.917545   | -0.752717      |
| 48            | 1             | -1.345600   | -2.183123   | -2.018160      |
| 49            | 1             | -1.227576   | -3.295808   | -0.643403      |
| 50            | 1             | -7.647265   | 2.196488    | -0.211622      |
| 51            | 1             | -7.476309   | 0.486115    | -0.731012      |
| 52            | 1             | -6.911399   | 1.794042    | -1.799011      |
| 53            | 1             | 6.949468    | -2.388937   | 0.846697       |
| 54            | 1             | 7.114116    | -0.814844   | 1.674451       |
| 55            | 1             | 7.525069    | -0.963277   | -0.062126      |
| 56            | 1             | -1.970692   | 0.426510    | 2.564485       |
Nucleus | Isotropic shielding
---|---
C2 | 46.6817
C3 | 123.7971
C5 | 132.1134
C6 | 160.0117
C7 | 73.5803
C8 | 64.8873
C9 | 25.8718
C10 | 84.8479
C11 | 60.6638
C12 | 79.6521
C13 | 44.599
C14 | 150.9263
C15 | 149.2805
C16 | 129.8669
C17 | 112.5867
C18 | 154.6679
C19 | 165.3754
C20 | 150.5327
C21 | 124.4524
C22 | 2.9403
C23 | 132.8521
C24 | 132.0026
16-epi-alstovenine (13), conformer 5

Sum of electronic and thermal free energies = -1265.267365 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 7             | 1.821744    | 1.656694    | -0.333786   |
| 2             | 6             | 1.434895    | 0.336968    | -0.514938   |
| 3             | 6             | 0.036098    | -0.104312   | -0.833426   |
| 4             | 7             | -0.046653   | -1.563678   | -0.664665   |
| 5             | 6             | 1.075145    | -2.275363   | -1.287992   |
| 6             | 6             | 2.402162    | -1.967201   | -0.580033   |
| 7             | 6             | 2.527436    | -0.483228   | -0.397051   |
| 8             | 6             | 3.655928    | 0.364895    | -0.111303   |
| 9             | 6             | 5.030384    | 0.135835    | 0.121253    |
| 10            | 6             | 5.870249    | 1.219837    | 0.374154    |
| 11            | 6             | 5.355684    | 2.536196    | 0.398143    |
| 12            | 6             | 4.011700    | 2.802853    | 0.174108    |
| 13            | 6             | 3.179549    | 1.702270    | -0.079105   |
| 14            | 6             | -1.033007   | 0.574191    | 0.042847    |
| 15            | 6             | -2.440691   | 0.072540    | -0.330672   |
| 16            | 6             | -3.559850   | 0.736448    | 0.534254    |
| 17            | 6             | -3.721899   | 0.117029    | 1.948167    |
| 18            | 6             | -3.723894   | -1.412359   | 1.935937    |
| 19            | 6             | -2.540872   | -2.002747   | 1.157312    |
| 20            | 6             | -2.504526   | -1.472341   | -0.286833   |
| 21            | 6             | -1.346768   | -2.060810   | -1.109348   |
| 22            | 6             | -4.881172   | 0.727506    | -0.221032   |
| 23            | 6             | -6.080875   | 1.733339    | -2.003398   |
| 24            | 6             | 6.806269    | -1.462163   | 0.311994    |
| 25            | 8             | 5.435107    | -1.172472   | 0.078097    |
| 26            | 8             | -2.643154   | 0.533168    | 2.803434    |
| 27            | 8             | -5.823438   | -0.013055   | -0.016671   |
| 28            | 8             | -4.891137   | 1.672677    | -1.191967   |
| 29            | 1             | 1.210503    | 2.456689    | -0.347049   |
| 30            | 1             | 0.183231    | 0.160083    | -1.895324   |
| 31            | 1             | 1.161019    | -2.015352   | -2.362866   |
| 32            | 1             | 0.862403    | -3.347966   | -1.231562   |
| 33            | 1             | 3.234494    | -2.361473   | -1.172832   |
| 34            | 1             | 2.433235    | -2.483349   | 0.388836    |
| 35            | 1             | 6.927356    | 1.069901    | 0.556531    |
| 36            | 1             | 6.038072    | 3.356961    | 0.598638    |
| 37            | 1             | 3.625727    | 3.817617    | 0.194854    |
| 38            | 1             | -0.996063   | 1.661815    | -0.110172   |
| 39            | 1             | -0.811421   | 0.384339    | 1.095560    |
| 40            | 1             | -2.615114   | 0.382790    | -1.370427   |
| 41            | 1             | -3.294130   | 1.795775    | 0.652038    |
| 42            | 1             | -4.673201   | 0.465310    | 2.372213    |
| 43            | 1             | -4.667454   | -1.739026   | 1.485763    |
| 44            | 1             | -3.715017   | -1.757807   | 2.975408    |
| 45            | 1             | -2.630068   | -3.096384   | 1.136255    |
| 46            | 1             | -1.598319   | -1.776909   | 1.664970    |
| 47            | 1             | -3.435829   | -1.787990   | -0.780257   |
| 48            | 1             | -1.512730   | -1.836663   | -2.185095   |
| 49            | 1             | -1.348078   | -3.151984   | -1.007317   |
| 50            | 1             | 5.906205    | 2.541611    | -2.712929   |
| 51            | 1             | 6.954861    | 1.945260    | -1.383049   |
| 52            | 1             | 6.234181    | 0.786468    | -2.526725   |
| 53            | 1             | 6.899906    | -2.546505   | 0.235063    |
| 54            | 1             | 7.117859    | -1.139852   | 1.313704    |
| 55            | 1             | 7.449474    | -0.986477   | -0.439354   |
| 56            | 1             | -2.740495   | 1.473168    | 3.002915    |
Nucleus  Isotropic shielding

C2  46.9186
C3  123.9854
C5  132.1062
C6  160.0912
C7  73.5599
C8  65.5575
C9  26.1139
C10 84.7923
C11 59.9206
C12 80.0242
C13 45.1771
C14 150.7378
C15 145.6352
C16 129.2897
C17 115.3353
C18 155.5207
C19 163.3123
C20 151.0117
C21 123.7218
C22 2.3563
C23 132.9204
C24 131.9456
16-epi-alstovenine (13), conformer 6

Sum of electronic and thermal free energies = -1265.267026 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X   | Y   | Z   |
| 1             | 7             | 1.876063 | 1.589108 | -0.650529 |
| 2             | 6             | 1.508257 | 0.252031 | -0.613303 |
| 3             | 6             | 0.126743 | -0.259734 | -0.901062 |
| 4             | 7             | 0.050723 | -1.669365 | -0.485642 |
| 5             | 6             | 1.203838 | -2.459978 | -0.930621 |
| 6             | 6             | 2.495785 | -2.012242 | -0.232794 |
| 7             | 6             | 2.602334 | -0.517626 | -0.311510 |
| 8             | 6             | 3.710952 | 0.384811  | -0.136248 |
| 9             | 6             | 5.076630 | 0.221226  | 0.185653  |
| 10            | 6             | 5.896738 | 1.345347  | 0.275653  |
| 11            | 6             | 5.370613 | 2.637608  | 0.049003  |
| 12            | 6             | 4.034401 | 2.840293  | -0.269221 |
| 13            | 6             | 3.222159 | 1.699850  | -0.356877 |
| 14            | 6             | -0.981582| 0.538926  | -0.191253 |
| 15            | 6             | -2.372692| -0.035222 | -0.524052 |
| 16            | 6             | -3.511969| 0.746638  | 0.176156  |
| 17            | 6             | -3.724012| 0.364246  | 1.676340  |
| 18            | 6             | -3.755706| -1.150827 | 1.880315  |
| 19            | 6             | -2.534838| -1.852148 | 1.270188  |
| 20            | 6             | -2.425276| -1.555935 | -0.235384 |
| 21            | 6             | -1.225750| 2.254095  | -0.894430 |
| 22            | 6             | -4.827665| 0.631109  | -0.588648 |
| 23            | 6             | -7.025148| 1.508428  | -0.772456 |
| 24            | 6             | 6.854110 | -1.290762 | 0.732299  |
| 25            | 8             | 5.493386 | -1.068069 | 0.389725  |
| 26            | 8             | -2.662429| 0.877919  | 2.492500  |
| 27            | 8             | -5.065949| -0.131709 | -1.503096 |
| 28            | 8             | -5.737983| 1.522016  | -0.123608 |
| 29            | 1             | 1.258955 | 2.364183  | -0.830144 |
| 30            | 1             | -0.054987| -0.185524 | 1.999321  |
| 31            | 1             | 1.333882 | -2.389245 | -2.029894 |
| 32            | 1             | 0.998163 | -3.509843 | -0.697213 |
| 33            | 1             | 3.356838 | -2.493877 | -0.708351 |
| 34            | 1             | 2.484700 | -2.345972 | 0.813474  |
| 35            | 1             | 6.946994 | 1.245911  | 0.521394  |
| 36            | 1             | 6.037608 | 3.491083  | 0.127893  |
| 37            | 1             | 3.639476 | 3.836988  | 0.441926  |
| 38            | 1             | -0.94462 | 1.587985  | -0.518829 |
| 39            | 1             | -0.795167| 0.526235  | 0.885482  |
| 40            | 1             | -2.522886| 0.087224  | -1.605137 |
| 41            | 1             | -3.271190| 1.819701  | 0.161576  |
| 42            | 1             | -4.674278| 0.797339  | 2.011739  |
| 43            | 1             | -4.673516| -1.540675 | 1.418754  |
| 44            | 1             | -3.826639| -1.348994 | 2.955301  |
| 45            | 1             | -2.624576| -2.935442 | 1.420929  |
| 46            | 1             | -1.623702| -1.537484 | 1.787547  |
| 47            | 1             | -3.327439| -1.948956 | -0.721780 |
| 48            | 1             | -1.345540| -2.214861 | -1.997944 |
| 49            | 1             | -1.221763| -3.312876 | -0.611145 |
| 50            | 1             | -6.918359| 1.744796  | -1.833803 |
| 51            | 1             | -7.613433| 2.272383  | -0.264932 |
| 52            | 1             | -7.490455| 0.527023  | -0.669357 |
| 53            | 1             | 6.958356 | -2.369876 | 0.855541  |
| 54            | 1             | 7.116737 | -0.789593 | 1.672660  |
| 55            | 1             | 7.528774 | -0.948191 | -0.062733 |
| 56            | 1             | -2.739722| 1.839445  | 2.542693  |
Nucleus | Isotropic shielding
---|---
C2 | 46.2541
C3 | 123.8133
C5 | 132.1181
C6 | 159.9807
C7 | 73.6554
C8 | 64.7146
C9 | 25.8264
C10 | 84.9226
C11 | 60.9916
C12 | 79.8162
C13 | 44.6437
C14 | 151.296
C15 | 148.4234
C16 | 128.9427
C17 | 112.56
C18 | 154.8609
C19 | 164.3613
C20 | 150.2003
C21 | 124.2628
C22 | 3.0723
C23 | 132.8771
C24 | 132.0304
16-epi-alstovenine (13), conformer 7

Sum of electronic and thermal free energies = -1265.264693 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X  | Y  | Z   |
| 1             | 7             | 1.745961 | 1.630964 | -0.149165 |
| 2             | 6             | 1.443593 | 0.311916 | -0.452994 |
| 3             | 6             | 0.079446 | -0.182058 | -0.837752 |
| 4             | 7             | 0.080155 | -1.653310 | -0.783801 |
| 5             | 6             | 1.250963 | -2.245768 | -1.442733 |
| 6             | 6             | 2.548627 | -1.918193 | -0.690438 |
| 7             | 6             | 2.581716 | -0.449882 | -0.382999 |
| 8             | 6             | 3.651858 | 0.435259 | -0.000772 |
| 9             | 6             | 5.034174 | 0.268748 | 0.238814 |
| 10            | 6             | 5.801836 | 1.374496 | 0.602261 |
| 11            | 6             | 5.207359 | 2.650619 | 0.730196 |
| 12            | 6             | 3.853431 | 2.855754 | 0.502185 |
| 13            | 6             | 3.094303 | 1.739777 | 0.137219 |
| 14            | 6             | -1.046266 | 0.367413 | -0.058025 |
| 15            | 6             | -2.410533 | -0.195621 | -0.375159 |
| 16            | 6             | -3.589395 | 0.354147 | 0.503507 |
| 17            | 6             | -4.191190 | -0.703117 | 1.439721 |
| 18            | 6             | -3.093581 | -1.565292 | 2.062027 |
| 19            | 6             | -2.339719 | -2.386025 | 0.989880 |
| 20            | 6             | -2.374248 | -1.738909 | -0.418028 |
| 21            | 6             | -1.183921 | -2.197525 | -1.277735 |
| 22            | 6             | -4.667573 | 0.933885 | -0.394740 |
| 23            | 6             | -5.462086 | 2.907870 | -1.435702 |
| 24            | 6             | 6.904158 | -1.228039 | 0.316205 |
| 25            | 6             | 5.519432 | -1.003903 | 0.089077 |
| 26            | 6             | -4.931123 | 0.030756 | 2.426670 |
| 27            | 6             | -5.539805 | 0.29387 | -0.949190 |
| 28            | 6             | -4.512073 | 2.266767 | -0.561611 |
| 29            | 1             | 1.088376 | 2.392573 | -0.108728 |
| 30            | 1             | -0.136677 | 0.152103 | -1.879642 |
| 31            | 1             | 1.333621 | -1.895559 | -2.491370 |
| 32            | 1             | 1.102386 | -3.30029 | -1.475702 |
| 33            | 1             | 3.409953 | -2.211561 | -1.300082 |
| 34            | 1             | 2.601077 | -2.509933 | 0.233286 |
| 35            | 1             | 6.863227 | 1.272585 | 0.792623 |
| 36            | 1             | 5.835216 | 3.489604 | 1.015396 |
| 37            | 1             | 3.405834 | 3.839919 | 0.602567 |
| 38            | 1             | -1.075409 | 1.462593 | -0.012226 |
| 39            | 1             | -0.824893 | 0.113912 | 1.100598 |
| 40            | 1             | -2.570790 | 0.142054 | -1.408617 |
| 41            | 1             | -3.213212 | 1.164661 | 1.136447 |
| 42            | 1             | -4.882282 | -1.313633 | 0.861672 |
| 43            | 1             | -3.534392 | -2.232964 | 2.812480 |
| 44            | 1             | -2.408142 | -0.903214 | 2.605575 |
| 45            | 1             | -2.778547 | -3.388343 | 0.912360 |
| 46            | 1             | -1.298747 | -2.522422 | 1.298787 |
| 47            | 1             | -3.286197 | -2.069658 | -0.931475 |
| 48            | 1             | -1.361968 | -1.908759 | -2.334561 |
| 49            | 1             | -1.15433 | -3.291256 | -1.253016 |
| 50            | 1             | -5.183676 | 3.961361 | -1.443327 |
| 51            | 1             | -6.476471 | 2.779439 | -1.051087 |
| 52            | 1             | -5.403168 | 2.484227 | -2.441291 |
| 53            | 1             | 7.184997 | -0.982373 | 1.348245 |
| 54            | 1             | 7.522643 | -0.644498 | -0.377584 |
| 55            | 1             | 7.067463 | -2.292344 | 0.140082 |
| 56            | 1             | -5.496756 | -0.582044 | 2.913855 |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 47.2704             |
| C3      | 124.5893            |
| C5      | 132.2003            |
| C6      | 159.9431            |
| C7      | 73.4507             |
| C8      | 65.6936             |
| C9      | 26.486              |
| C10     | 84.9033             |
| C11     | 59.4044             |
| C12     | 79.7138             |
| C13     | 45.1283             |
| C14     | 148.2935            |
| C15     | 143.0634            |
| C16     | 130.7744            |
| C17     | 113.5415            |
| C18     | 155.4724            |
| C19     | 162.425             |
| C20     | 154.3355            |
| C21     | 125.863             |
| C22     | -0.1214             |
| C23     | 132.635             |
| C24     | 132.0439            |
16-epi-alstovenine (13), conformer 8

Sum of electronic and thermal free energies = -1265.2664 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X                       |
| 1             | 7             | 1.725836                |
| 2             | 6             | 1.427999                |
| 3             | 6             | 0.068428                |
| 4             | 7             | 0.071103                |
| 5             | 6             | 1.250686                |
| 6             | 6             | 2.538343                |
| 7             | 6             | 2.566759                |
| 8             | 6             | 3.632713                |
| 9             | 6             | 5.013533                |
| 10            | 6             | 5.777004                |
| 11            | 6             | 5.179645                |
| 12            | 6             | 3.826900                |
| 13            | 6             | 3.072063                |
| 14            | 6             | -1.066254               |
| 15            | 6             | -2.429842               |
| 16            | 6             | -3.599114               |
| 17            | 6             | -4.326488               |
| 18            | 6             | -3.299864               |
| 19            | 6             | -2.400477               |
| 20            | 6             | -2.391814               |
| 21            | 6             | -1.185430               |
| 22            | 6             | -4.599733               |
| 23            | 6             | -4.879551               |
| 24            | 6             | 6.883740                |
| 25            | 6             | 5.501429                |
| 26            | 6             | -5.167439               |
| 27            | 6             | -5.812736               |
| 28            | 6             | -4.002099               |
| 29            | 1             | 1.066342                |
| 30            | 1             | -0.140872               |
| 31            | 1             | 1.345887                |
| 32            | 1             | 1.104182                |
| 33            | 1             | 3.407540                |
| 34            | 1             | 2.579053                |
| 35            | 1             | 6.837189                |
| 36            | 1             | 5.804212                |
| 37            | 1             | 3.377156                |
| 38            | 1             | -1.096177               |
| 39            | 1             | -0.856784               |
| 40            | 1             | -2.593404               |
| 41            | 1             | -3.172980               |
| 42            | 1             | -4.939314               |
| 43            | 1             | -3.830651               |
| 44            | 1             | -2.698209               |
| 45            | 1             | -2.741726               |
| 46            | 1             | -1.374844               |
| 47            | 1             | -3.289261               |
| 48            | 1             | -1.345259               |
| 49            | 1             | -1.118698               |
| 50            | 1             | -4.221026               |
| 51            | 1             | -5.492020               |
| 52            | 1             | -5.531548               |
| 53            | 1             | 7.153247                |
| 54            | 1             | 7.509625                |
| 55            | 1             | 7.048975                |
| 56            | 1             | -5.877929               |
### Nucleus Isotropic shielding

| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 47.2447             |
| C3      | 124.4546            |
| C5      | 132.2413            |
| C6      | 159.9178            |
| C7      | 73.4184             |
| C8      | 65.6331             |
| C9      | 26.407              |
| C10     | 84.7847             |
| C11     | 59.3475             |
| C12     | 79.562              |
| C13     | 45.1552             |
| C14     | 147.7851            |
| C15     | 144.6787            |
| C16     | 128.2265            |
| C17     | 116.2419            |
| C18     | 158.1884            |
| C19     | 163.0869            |
| C20     | 153.1978            |
| C21     | 125.8321            |
| C22     | -1.718              |
| C23     | 132.4063            |
| C24     | 132.0077            |
16-epi-alstovenine (13), conformer 9

Sum of electronic and thermal free energies = -1265.26502 H

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---------------|---------------|---------------------------|---|---|
| 1             | 7             | 1.824659                  | 1.635944 | -0.388839 |
| 2             | 6             | 1.524743                  | 0.288524 | -0.525850 |
| 3             | 6             | 0.167451                  | -0.250168 | -0.872508 |
| 4             | 7             | 0.164441                  | -1.704364 | -0.640964 |
| 5             | 6             | 1.350790                  | -2.372159 | -1.190541 |
| 6             | 6             | 2.627939                  | -1.953324 | -0.488448 |
| 7             | 6             | 2.658225                  | -0.457723 | -0.329246 |
| 8             | 6             | 3.722281                  | 0.469375 | -0.041010 |
| 9             | 6             | 5.097628                  | 0.335336 | 0.252719 |
| 10            | 6             | 5.860723                  | 1.478955 | 0.485324 |
| 11            | 6             | 5.268484                  | 2.761182 | 0.429042 |
| 12            | 6             | 3.921055                  | 2.935008 | 0.143566 |
| 13            | 6             | 3.166562                  | 1.775343 | -0.088428 |
| 14            | 6             | -0.974047                 | 0.399864 | -0.067665 |
| 15            | 6             | -2.331196                 | -0.207755 | -0.465634 |
| 16            | 6             | -3.524219                 | 0.433937 | 0.297688 |
| 17            | 6             | -4.143394                 | -0.493823 | 1.393237 |
| 18            | 6             | -3.043064                 | -1.276670 | 2.099015 |
| 19            | 6             | -2.304860                 | -2.232597 | 1.140200 |
| 20            | 6             | -2.296968                 | -1.746050 | -0.331340 |
| 21            | 6             | -1.087946                 | -2.302696 | -1.10749 |
| 22            | 6             | -4.611676                 | 0.906971 | -0.659520 |
| 23            | 6             | -6.684320                 | 2.075657 | -0.800790 |
| 24            | 6             | 6.957622                  | -1.138864 | 0.582832 |
| 25            | 8             | 5.581503                  | -0.946114 | 0.285448 |
| 26            | 8             | -4.843472                 | 0.252034 | 2.383828 |
| 27            | 8             | -4.667517                 | 0.705200 | -1.854242 |
| 28            | 8             | -5.581144                 | 1.601121 | 0.001899 |
| 29            | 1             | 1.171889                  | 2.397419 | -0.477804 |
| 30            | 1             | -0.031051                 | -0.044360 | -1.950070 |
| 31            | 1             | 1.463542                  | -2.153633 | -2.271639 |
| 32            | 1             | 1.200184                  | -3.452381 | -1.093976 |
| 33            | 1             | 3.505084                  | -2.321742 | -0.991113 |
| 34            | 1             | 2.651118                  | -2.424275 | 0.543501 |
| 35            | 1             | 6.916915                  | 1.402520 | 0.713037 |
| 36            | 1             | 5.892538                  | 3.630123 | 0.615951 |
| 37            | 1             | 3.474721                  | 3.924035 | 0.102745 |
| 38            | 1             | -0.994402                 | 1.480333 | -0.265890 |
| 39            | 1             | -0.768461                 | 0.269475 | 1.000549 |
| 40            | 1             | -2.478461                 | 0.010286 | -1.529675 |
| 41            | 1             | -3.179699                 | 1.322974 | 0.842980 |
| 42            | 1             | -4.836641                 | -1.203918 | 0.911425 |
| 43            | 1             | -3.491493                 | -1.826816 | 2.932470 |
| 44            | 1             | -2.350990                 | -0.552567 | 2.546316 |
| 45            | 1             | -2.775214                 | -3.223374 | 1.169665 |
| 46            | 1             | -1.274044                 | -2.364791 | 1.483230 |
| 47            | 1             | -3.195586                 | -2.132854 | -0.830682 |
| 48            | 1             | -1.237190                 | -2.138297 | -2.18863 |
| 49            | 1             | -1.023637                 | -3.386023 | -0.946920 |
| 50            | 1             | -7.337720                 | 2.607160 | -0.109667 |
| 51            | 1             | -7.208040                 | 1.235345 | -1.261783 |
| 52            | 1             | -6.319927                 | 2.746486 | -1.581499 |
| 53            | 1             | -7.208839                 | -0.753326 | 1.579077 |
| 54            | 1             | -7.599663                 | -0.657364 | -0.165745 |
| 55            | 1             | -7.120076                 | -2.217519 | 0.560032 |
| 56            | 1             | -5.468318                 | 0.838278 | 1.932144 |
Nucleus  Isotropic shielding

C2  47.0015
C3  124.5904
C5  132.0999
C6  160.0721
C7  73.4066
C8  65.5469
C9  26.1755
C10 85.0218
C11 60.0907
C12 80.1687
C13 45.0406
C14 148.5738
C15 148.2051
C16 128.7134
C17 113.9037
C18 157.6917
C19 162.6636
C20 154.7469
C21 125.9116
C22  1.066
C23 132.1996
C24 132.0952
16-epi-alstovenine (13), conformer 10

Sum of electronic and thermal free energies = -1265.264201 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|------------------------|
|               |               | X          | Y          | Z          |
| 1             | 7             | 1.738940   | 1.520160   | -0.529266  |
| 2             | 6             | 1.470101   | 0.160007   | -0.572951  |
| 3             | 6             | 0.139971   | -0.434508  | -0.932925  |
| 4             | 7             | 0.151894   | -1.866822  | -0.591898  |
| 5             | 6             | 1.377320   | -2.548865  | -1.028020  |
| 6             | 6             | 2.605562   | -2.044665  | -0.258269  |
| 7             | 6             | 2.605034   | -0.544085  | -0.262418  |
| 8             | 6             | 3.637153   | 0.425327   | 0.001082   |
| 9             | 6             | 4.998367   | 0.342922   | 0.369835   |
| 10            | 6             | 5.729500   | 1.516840   | 0.547120   |
| 11            | 6             | 5.118322   | 2.777946   | 0.360423   |
| 12            | 6             | 3.784548   | 2.901076   | -0.002638  |
| 13            | 6             | 3.061956   | 1.711330   | -0.177283  |
| 14            | 6             | -1.038385  | 0.231923   | -0.205268  |
| 15            | 6             | -2.392702  | -0.409319  | -0.565145  |
| 16            | 6             | -3.520945  | 0.200056   | 0.322750   |
| 17            | 6             | -4.597585  | -0.856734  | 0.671473   |
| 18            | 6             | -3.970033  | -1.998973  | 1.492139   |
| 19            | 6             | -2.562038  | -2.412775  | 0.989703   |
| 20            | 6             | -2.340978  | -1.956641  | -0.462485  |
| 21            | 6             | -1.057192  | -2.508618  | -1.102398  |
| 22            | 6             | -4.178053  | 1.392051   | -0.350994  |
| 23            | 6             | -5.057816  | 3.564310   | -0.013568  |
| 24            | 6             | 6.863903   | -1.063590  | 0.903095   |
| 25            | 8             | 5.500798   | -0.921964  | 0.527153   |
| 26            | 8             | -5.725857  | -0.287897  | 1.334255   |
| 27            | 8             | -4.526635  | 1.430393   | -1.51435   |
| 28            | 8             | -4.351148  | 2.421179   | 0.508879   |
| 29            | 1             | 1.079646   | 2.257804   | -0.71058   |
| 30            | 1             | -0.021397  | -0.312691  | -2.028956  |
| 31            | 1             | 1.540746   | -2.411826  | -2.116029  |
| 32            | 1             | 1.241793   | -3.621361  | -0.853915  |
| 33            | 1             | 3.516637   | -2.438300  | -0.71298   |
| 34            | 1             | 2.581747   | -2.431254  | 0.769429   |
| 35            | 1             | 6.774314   | 1.480813   | 0.830580   |
| 36            | 1             | 5.718134   | 3.671689   | 0.507109   |
| 37            | 1             | 3.324527   | 3.874414   | -0.144042  |
| 38            | 1             | -1.076527  | 1.301382   | -0.452620  |
| 39            | 1             | -0.851647  | 0.157890   | 0.872761   |
| 40            | 1             | -2.625033  | -0.158336  | -1.607228  |
| 41            | 1             | -3.093441  | 0.550758   | 1.271367   |
| 42            | 1             | -5.015622  | -1.242343  | -0.263450  |
| 43            | 1             | -4.661675  | -2.848266  | 1.472890   |
| 44            | 1             | -3.913911  | -1.672293  | 2.539674   |
| 45            | 1             | -2.443111  | -3.499952  | 1.063206   |
| 46            | 1             | -1.781643  | -1.980974  | 1.625068   |
| 47            | 1             | -3.166138  | -2.361313  | -1.064981  |
| 48            | 1             | -1.127605  | -2.394881  | -2.204965  |
| 49            | 1             | -0.989280  | -3.583085  | -0.898237  |
| 50            | 1             | -5.096377  | 4.280963   | 0.806350   |
| 51            | 1             | -6.064949  | 3.275067   | -0.322547  |
| 52            | 1             | -4.524812  | 3.984302   | -0.869814  |
| 53            | 1             | 7.059882   | -0.599269  | 1.877960   |
| 54            | 1             | 7.53585   | -0.626957  | 0.151280   |
| 55            | 1             | 7.045261   | -2.137264  | 0.970292   |
| 56            | 1             | -5.435442  | 0.108245   | 2.168145   |
| Nucleus | Isotropic shielding |
|---------|----------------------|
| C2      | 47.1472              |
| C3      | 125.1631             |
| C5      | 131.9466             |
| C6      | 160.0728             |
| C7      | 73.7504              |
| C8      | 65.0404              |
| C9      | 25.6128              |
| C10     | 84.7088              |
| C11     | 60.8574              |
| C12     | 79.1592              |
| C13     | 44.426               |
| C14     | 149.9412             |
| C15     | 146.1026             |
| C16     | 126.774              |
| C17     | 112.0614             |
| C18     | 151.4939             |
| C19     | 160.3979             |
| C20     | 152.0942             |
| C21     | 125.6352             |
| C22     | -0.3952              |
| C23     | 132.7747             |
| C24     | 131.9308             |
9-methoxy-3-epi-α-yohimbine (8), conformer 1

Sum of electronic and thermal free energies = -1265.267083 H

| Center Number | Atomic Number | Coordinates (Angstroms) | X    | Y    | Z    |
|---------------|--------------|-------------------------|------|------|------|
| 1             | 7            | 1.245195                | 1.182956 | 0.885441 |
| 2             | 6            | 1.075121                | -0.193792 | 0.872465 |
| 3             | 6            | -0.149831               | -0.949236 | 1.339670 |
| 4             | 7            | -0.148037               | -2.305778 | 0.750404 |
| 5             | 6            | 1.140742                | -2.970577 | 1.004828 |
| 6             | 6            | 2.363572                | -2.289522 | 0.337782 |
| 7             | 6            | 2.237140                | -0.794693 | 0.447888 |
| 8             | 6            | 3.170343                | 0.263804  | 0.156818 |
| 9             | 6            | 4.501132                | 0.304764  | -0.316512 |
| 10            | 6            | 5.126145                | 1.538823  | -0.491221 |
| 11            | 6            | 4.439408                | 2.739344  | -0.98937  |
| 12            | 6            | 3.132399                | 2.741339  | 0.268692  |
| 13            | 6            | 2.516826                | 1.492210  | 0.440145  |
| 14            | 6            | -1.502788               | -0.254715 | 1.105153  |
| 15            | 6            | -1.934937               | -0.267507 | -0.375970 |
| 16            | 6            | -3.333917               | 0.367226  | -0.620725 |
| 17            | 6            | -4.498163               | -0.499844 | -0.090912 |
| 18            | 6            | -4.416889               | -1.912526 | -0.664245 |
| 19            | 6            | -3.057158               | -2.570586 | -0.396598 |
| 20            | 6            | -1.896709               | -1.711590 | -0.930246 |
| 21            | 6            | -0.512189               | -2.322532 | -0.670153 |
| 22            | 6            | -3.430300               | 1.791247  | -0.096264 |
| 23            | 6            | -2.495805               | 3.968639  | -0.184862 |
| 24            | 6            | 6.420408                | -0.927530 | -1.053317 |
| 25            | 8            | 5.083115                | -0.908582 | -0.572944 |
| 26            | 8            | -5.762674               | 0.043829  | -0.464631 |
| 27            | 8            | -4.299471               | 2.212402  | 0.649019  |
| 28            | 8            | -2.441126               | 2.579092  | -0.569190 |
| 29            | 1            | 0.530706                | 1.858992  | 1.101119  |
| 30            | 1            | -0.061590               | -1.090162 | 2.428063  |
| 31            | 1            | 1.058757                | -4.011885 | 0.672950  |
| 32            | 1            | 1.285573                | -2.989838 | 2.092239  |
| 33            | 1            | 2.448199                | -2.588218 | -0.716239 |
| 34            | 1            | 3.282066                | -2.644585 | 0.818793  |
| 35            | 1            | 6.145668                | 1.596502  | -0.852336 |
| 36            | 1            | 4.957135                | 3.682663  | -0.345629 |
| 37            | 1            | 2.614338                | 3.668669  | 0.49057   |
| 38            | 1            | -1.453966               | 0.774278  | 1.480829  |
| 39            | 1            | -2.242681               | -0.768468 | 1.722171  |
| 40            | 1            | -1.206364               | 0.325187  | -0.942329 |
| 41            | 1            | -3.466771               | 0.446201  | -1.710882 |
| 42            | 1            | -4.437081               | -0.551550 | 1.006195  |
| 43            | 1            | -4.599994               | -1.849131 | -1.748095 |
| 44            | 1            | -5.232898               | -2.508596 | -0.243952 |
| 45            | 1            | -3.024763               | -3.556401 | -0.876873 |
| 46            | 1            | -2.925806               | -2.751647 | 0.676270  |
| 47            | 1            | -2.011341               | -1.647145 | -2.022880 |
| 48            | 1            | 0.223985                | -1.784908 | -1.293397 |
| 49            | 1            | 0.505811                | -3.370302 | -0.994921 |
| 50            | 1            | 3.428027                | 4.420942  | -0.530663 |
| 51            | 1            | 1.638902                | 4.435918  | -0.669101 |
| 52            | 1            | 2.432370                | 4.068027  | 0.901429  |
| 53            | 1            | 6.507293                | -0.405596 | -2.014736 |
| 54            | 1            | 6.674515                | -1.979967 | -1.188192 |
| 55            | 1            | 7.111498                | 0.475680  | -0.330558 |
| 56            | 1            | 5.857580                | 0.885838  | 0.006110  |
Nucleus | Isotropic shielding
--- | ---
C2 | 49.1851
C3 | 129.3655
C5 | 132.2462
C6 | 165.378
C7 | 73.3985
C8 | 64.6323
C9 | 25.5462
C10 | 84.3759
C11 | 61.0935
C12 | 77.3693
C13 | 44.6506
C14 | 161.3355
C15 | 151.6821
C16 | 128.3407
C17 | 117.7612
C18 | 152.2023
C19 | 160.4639
C20 | 146.5103
C21 | 134.7604
C22 | -0.0829
C23 | 132.6586
C24 | 131.8373
9-methoxy-3-epi-α-yohimbine (8), conformer 2

Sum of electronic and thermal free energies = -1265.264413 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               | X             | Y                        | Z                        |
| 1             | 1.271532      | 1.146346                 | 0.983541                 |
| 2             | 1.125273      | -0.229540                | 0.885107                 |
| 3             | -0.078762     | -1.030515                | 1.329354                 |
| 4             | -0.055568     | -2.361818                | 0.687587                 |
| 5             | 1.256173      | -3.002402                | 0.873698                 |
| 6             | 2.439420      | -2.262899                | 0.198510                 |
| 7             | 2.287524      | -0.779835                | 0.397100                 |
| 8             | 3.197978      | 0.311842                 | 0.162430                 |
| 9             | 4.518071      | 0.407837                 | -0.332228                |
| 10            | 5.123654      | 1.660272                 | -0.424287                |
| 11            | 4.426825      | 2.825266                 | -0.029692                |
| 12            | 3.128017      | 2.773518                 | 0.457753                 |
| 13            | 2.532283      | 1.506306                 | 0.545667                 |
| 14            | -1.443567     | -0.343981                | 1.138347                 |
| 15            | -1.897275     | -0.309753                | -0.33042                 |
| 16            | -3.300898     | 0.324408                 | -0.570178                |
| 17            | -4.441630     | -0.544451                | -0.021560                |
| 18            | -4.364702     | -1.967910                | -0.586326                |
| 19            | -2.991032     | -2.620241                | -0.361716                |
| 20            | -1.859021     | -1.739205                | -0.925383                |
| 21            | -0.459616     | -2.335769                | -0.724524                |
| 22            | -3.384242     | 1.731466                 | -0.002110                |
| 23            | -3.312339     | 4.037818                 | -0.535930                |
| 24            | 6.434650      | -0.736902                | -1.204967                |
| 25            | 5.110306      | -0.774569                | -0.691513                |
| 26            | -5.659373     | 0.104497                 | -0.417994                |
| 27            | -3.517869     | 2.010671                 | 1.174494                 |
| 28            | -3.248416     | 2.665685                 | -0.969168                |
| 29            | 0.573612      | 1.787559                 | 1.324853                 |
| 30            | 0.023874      | -1.215777                | 2.410067                 |
| 31            | 1.190218      | -4.031864                | 0.502929                 |
| 32            | 1.435593      | -3.059608                | 1.954617                 |
| 33            | 2.490242      | -2.505112                | -0.872119                |
| 34            | 3.382194      | -2.622195                | 0.626438                 |
| 35            | 6.135203      | 1.759635                 | -0.798582                |
| 36            | 4.929398      | 3.784358                 | -0.113387                |
| 37            | 2.600875      | 3.673859                 | 0.758638                 |
| 38            | -1.410934     | 0.665905                 | 1.558775                 |
| 39            | -2.170440     | -0.887083                | 1.749021                 |
| 40            | -1.173834     | 0.298097                 | -0.893931                |
| 41            | -3.445295     | 0.403353                 | -1.625364                |
| 42            | -4.381578     | -0.561511                | 1.074939                 |
| 43            | -4.585539     | -1.908981                | -1.660675                |
| 44            | -5.156230     | -2.580477                | -0.134634                |
| 45            | -2.967588     | -3.597853                | -0.864568                |
| 46            | -2.822754     | -2.817746                | 0.697049                 |
| 47            | -2.011547     | -1.653814                | -2.011719                |
| 48            | 0.247937      | -1.763871                | -1.350813                |
| 49            | 0.444553      | 3.371529                 | -1.086298                |
| 50            | 2.505715      | 4.256771                 | 0.168344                 |
| 51            | 4.272314      | 4.237657                 | -0.054326                |
| 52            | 3.203214      | 4.633217                 | -1.441898                |
| 53            | 6.489575      | -0.142500                | -2.125901                |
| 54            | 6.690011      | -1.772226                | -1.425761                |
| 55            | 7.138687      | -0.330543                | 0.467556                 |
| 56            | -6.394512     | -0.271668                | 0.082462                 |
Nucleus | Isotropic shielding
---|---
C2 | 49.0453
C3 | 129.0419
C5 | 132.4834
C6 | 165.3312
C7 | 73.1494
C8 | 64.4867
C9 | 26.1361
C10 | 84.4111
C11 | 60.9077
C12 | 78.9103
C13 | 45.4165
C14 | 161.7544
C15 | 150.6399
C16 | 129.2277
C17 | 115.1401
C18 | 148.9023
C19 | 160.6593
C20 | 146.8711
C21 | 134.7125
C22 | 1.8842
C23 | 133.1265
C24 | 131.9679
9-methoxy-3-epi-α-yohimbine (8), conformer 3

Sum of electronic and thermal free energies = -1265.26566 H

| Center Number | Atomic Number | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|--------------------------|-------|-------|-------|
| 1             | 7             | 1.189820 1.236405 0.780959 |
| 2             | 6             | 1.127553 -0.145997 0.884711 |
| 3             | 6             | -0.048563 -0.957341 1.380122 |
| 4             | 7             | 0.027564 -2.325726 0.826678 |
| 5             | 6             | 1.342208 -2.917201 1.125048 |
| 6             | 6             | 2.555661 -2.182159 0.493515 |
| 7             | 6             | 2.333296 -0.694237 0.516658 |
| 8             | 6             | 3.187763 0.402722 0.138690 |
| 9             | 6             | 4.517537 0.504061 -0.327246 |
| 10            | 6             | 5.045239 1.761066 -0.618878 |
| 11            | 6             | 4.260861 2.925376 -0.450712 |
| 12            | 6             | 2.953045 2.868274 0.010921 |
| 13            | 6             | 2.436591 1.596964 0.303325 |
| 14            | 6             | -1.428042 -0.340956 1.111881 |
| 15            | 6             | -1.786256 -0.363613 -0.384461 |
| 16            | 6             | -3.169736 0.268384 -0.700552 |
| 17            | 6             | -4.361131 -0.608872 -0.238912 |
| 18            | 6             | -4.209833 -2.039458 -0.762819 |
| 19            | 6             | -2.858743 -2.677750 -0.417034 |
| 20            | 6             | -1.693418 -1.809610 -0.920833 |
| 21            | 6             | -0.303040 -2.387598 -0.604949 |
| 22            | 6             | -3.183439 1.720533 -0.225525 |
| 23            | 6             | -4.485654 3.532870 0.605264 |
| 24            | 6             | 6.542545 -0.634071 -0.917230 |
| 25            | 8             | 5.198697 -0.678693 -0.458732 |
| 26            | 8             | -5.609992 -0.137859 -0.745514 |
| 27            | 8             | -2.213001 2.453071 -0.221252 |
| 28            | 8             | -4.403571 2.152419 0.184659 |
| 29            | 1             | 0.395125 1.857449 0.822991 |
| 30            | 1             | 0.044725 -1.066894 2.471289 |
| 31            | 1             | 1.327557 -3.965042 0.803891 |
| 32            | 1             | 1.448977 -2.917827 2.170531 |
| 33            | 1             | 2.719269 -2.518662 -0.539552 |
| 34            | 1             | 3.465338 -2.459155 1.039082 |
| 35            | 1             | 6.061828 1.864765 -0.978229 |
| 36            | 1             | 4.702821 3.888152 -0.690041 |
| 37            | 1             | 2.357998 3.767147 0.139600 |
| 38            | 1             | -1.446410 0.683097 1.500121 |
| 39            | 1             | -2.159960 -0.907758 1.695563 |
| 40            | 1             | -1.038624 0.238966 -0.912303 |
| 41            | 1             | -2.565954 0.339086 -1.796694 |
| 42            | 1             | -4.393311 -0.625772 0.861639 |
| 43            | 1             | -4.338526 -2.003680 -1.853436 |
| 44            | 1             | -5.040338 -2.631202 -0.370336 |
| 45            | 1             | -2.797794 -3.671592 -0.877533 |
| 46            | 1             | -2.770682 -2.838826 0.663308 |
| 47            | 1             | -1.769382 -1.764153 -2.017963 |
| 48            | 1             | 0.437771 -1.851939 -1.224127 |
| 49            | 1             | -0.268160 -3.443359 -0.901452 |
| 50            | 1             | -5.526797 3.687166 0.886429 |
| 51            | 1             | -4.202437 4.194092 -0.216107 |
| 52            | 1             | -3.824721 3.707595 1.456222 |
| 53            | 1             | 6.607910 -0.204704 -1.925156 |
| 54            | 1             | 6.884562 -1.669947 -0.942034 |
| 55            | 1             | 7.179178 -0.056413 -0.234881 |
| 56            | 1             | -5.742750 0.759757 -0.410340 |
| Nucleus | Isotropic shielding |
|---------|----------------------|
| C2      | 48.2352              |
| C3      | 129.1505             |
| C5      | 132.4893             |
| C6      | 164.9661             |
| C7      | 73.0073              |
| C8      | 64.7114              |
| C9      | 25.8728              |
| C10     | 84.5353              |
| C11     | 60.7328              |
| C12     | 78.1717              |
| C13     | 44.2867              |
| C14     | 161.6507             |
| C15     | 152.0416             |
| C16     | 128.741              |
| C17     | 117.4381             |
| C18     | 150.9009             |
| C19     | 161.1491             |
| C20     | 146.3082             |
| C21     | 134.8359             |
| C22     | 1.4997               |
| C23     | 132.5502             |
| C24     | 131.922              |
9-methoxy-3-epi-α-yohimbine (8), conformer 4

Sum of electronic and thermal free energies = -1265.262583 H

| Center Number | Atomic Number | Coordinates (Å) |
|---------------|---------------|-----------------|
|               |               | X               |
| 1             | 7             | 1.251758        |
| 2             | 6             | 1.116661        |
| 3             | 6             | -0.104425       |
| 4             | 7             | -0.063277       |
| 5             | 6             | 1.226862        |
| 6             | 6             | 2.464839        |
| 7             | 6             | 2.504027        |
| 8             | 6             | 3.219245        |
| 9             | 6             | 4.562016        |
| 10            | 6             | 5.159003        |
| 11            | 6             | 4.431928        |
| 12            | 6             | 3.112924        |
| 13            | 6             | 2.526689        |
| 14            | 6             | -1.461516       |
| 15            | 6             | -1.847021       |
| 16            | 6             | -3.244723       |
| 17            | 6             | -4.416070       |
| 18            | 6             | -4.278262       |
| 19            | 6             | -2.925922       |
| 20            | 6             | -1.761614       |
| 21            | 6             | -0.376160       |
| 22            | 6             | 3.300434        |
| 23            | 6             | -4.024204       |
| 24            | 6             | 6.536496        |
| 25            | 8             | 5.183874        |
| 26            | 8             | -5.602199       |
| 27            | 8             | -3.928490       |
| 28            | 8             | 3.928490        |
| 29            | 1             | 0.510277        |
| 30            | 1             | -0.042082       |
| 31            | 1             | 1.175790        |
| 32            | 1             | 1.328674        |
| 33            | 1             | 2.605575        |
| 34            | 1             | 3.366992        |
| 35            | 1             | 6.186552        |
| 36            | 1             | 4.927442        |
| 37            | 1             | 2.561603        |
| 38            | 1             | -1.443693       |
| 39            | 1             | -2.213061       |
| 40            | 1             | -1.114402       |
| 41            | 1             | -3.320084       |
| 42            | 1             | -4.453597       |
| 43            | 1             | -4.396873       |
| 44            | 1             | -5.103655       |
| 45            | 1             | -2.855222       |
| 46            | 1             | -2.844131       |
| 47            | 1             | -1.839076       |
| 48            | 1             | 0.371670        |
| 49            | 1             | -0.339850       |
| 50            | 1             | -4.572046       |
| 51            | 1             | -4.563414       |
| 52            | 1             | -3.029416       |
| 53            | 1             | 6.641871        |
| 54            | 1             | -6.824657       |
| 55            | 1             | -7.189618       |
| 56            | 1             | -6.376078       |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 49.1543             |
| C3      | 129.5149            |
| C5      | 132.4203            |
| C6      | 165.0108            |
| C7      | 73.4889             |
| C8      | 64.6312             |
| C9      | 25.664              |
| C10     | 84.6674             |
| C11     | 60.5679             |
| C12     | 78.5382             |
| C13     | 44.6886             |
| C14     | 160.3327            |
| C15     | 149.3103            |
| C16     | 128.228             |
| C17     | 116.7666            |
| C18     | 148.8889            |
| C19     | 160.9079            |
| C20     | 146.6507            |
| C21     | 134.8288            |
| C22     | 1.8219              |
| C23     | 133.3752            |
| C24     | 131.8904            |
9-methoxy-3-epi-α-yohimbine (8), conformer 5

Sum of electronic and thermal free energies = -1265.263463 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 7             | 1.281691    | 1.136437    | 1.015083    |
| 2             | 6             | 1.158193    | -0.239711   | 0.893997    |
| 3             | 6             | -0.029135   | -1.067459   | 1.332890    |
| 4             | 7             | 0.007979    | -2.385525   | 0.664420    |
| 5             | 6             | 1.330983    | -3.009584   | 0.826395    |
| 6             | 6             | 2.497649    | -2.238452   | 0.157163    |
| 7             | 6             | 2.324146    | -0.761809   | 0.384420    |
| 8             | 6             | 3.213407    | 0.349281    | 0.159496    |
| 9             | 6             | 4.526617    | 0.476549    | -0.346265   |
| 10            | 6             | 5.109671    | 1.740658    | -0.422659   |
| 11            | 6             | 4.396951    | 2.886526    | -0.001115   |
| 12            | 6             | 3.104262    | 2.804021    | 0.498222    |
| 13            | 6             | 2.531224    | 1.525369    | 0.570139    |
| 14            | 6             | -1.403225   | -0.394502   | 1.166076    |
| 15            | 6             | -1.859163   | -0.331994   | -0.303620   |
| 16            | 6             | -3.266721   | 0.291404    | -0.535299   |
| 17            | 6             | -4.399775   | -0.590001   | 0.038421    |
| 18            | 6             | -4.321483   | -2.004919   | -0.546197   |
| 19            | 6             | -2.937014   | -2.649378   | -0.370325   |
| 20            | 6             | -1.815281   | -1.750477   | -0.922335   |
| 21            | 6             | -0.409669   | -2.339834   | -0.74269    |
| 22            | 6             | -3.82009    | 1.710178    | -0.005750   |
| 23            | 6             | -3.788317   | 3.967226    | -0.598488   |
| 24            | 6             | 6.454843    | -0.619840   | -1.254641   |
| 25            | 8             | 5.135547    | -0.689202   | -0.731653   |
| 26            | 8             | -5.680753   | 0.005517    | -0.188379   |
| 27            | 8             | -3.266252   | 2.043876    | 1.158138    |
| 28            | 8             | -3.627295   | 2.592532    | -1.001281   |
| 29            | 1             | 0.574206    | 1.759799    | 1.370292    |
| 30            | 1             | 0.084765    | -1.272710   | 2.408767    |
| 31            | 1             | 1.277758    | -4.032221   | 0.435190    |
| 32            | 1             | 1.520125    | -3.085905   | 1.904412    |
| 33            | 1             | 2.545055    | -2.459699   | -0.918164   |
| 34            | 1             | 3.448863    | -2.591017   | 0.571896    |
| 35            | 1             | 6.115633    | 1.863916    | -0.804851   |
| 36            | 1             | 4.882231    | 3.855439    | -0.073045   |
| 37            | 1             | 2.564894    | 3.689681    | 0.820198    |
| 38            | 1             | -1.385578   | 0.605271    | 1.607914    |
| 39            | 1             | -2.119591   | -0.963764   | 1.765257    |
| 40            | 1             | -1.136461   | 0.288522    | -0.852394   |
| 41            | 1             | -3.415894   | 0.345204    | -1.621623   |
| 42            | 1             | -4.313482   | -0.623132   | 1.128631    |
| 43            | 1             | -4.559016   | -1.942357   | -1.620427   |
| 44            | 1             | -5.102140   | -2.621000   | -0.086233   |
| 45            | 1             | -2.915989   | -3.615273   | -0.890159   |
| 46            | 1             | -2.753622   | -2.870874   | 0.866340    |
| 47            | 1             | -1.975544   | -1.648040   | -2.006458   |
| 48            | 1             | 0.287080    | -1.752113   | -1.367922   |
| 49            | 1             | 0.389573    | -3.369494   | -1.121653   |
| 50            | 1             | 3.993783    | 4.516052    | -1.517055   |
| 51            | 1             | 2.875049    | 4.336288    | -0.125434   |
| 52            | 1             | 4.619892    | 4.060149    | 0.103727    |
| 53            | 1             | 6.735172    | -1.646504   | -1.495292   |
| 54            | 1             | 7.157884    | -0.213972   | -0.515968   |
| 55            | 1             | 6.492186    | -0.009800   | -2.165623   |
| 56            | 1             | 5.864619    | -0.001033   | -1.138510   |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 49.1509             |
| C3      | 128.8644            |
| C5      | 132.5121            |
| C6      | 165.2324            |
| C7      | 72.9405             |
| C8      | 64.5278             |
| C9      | 26.1742             |
| C10     | 84.4529             |
| C11     | 60.8728             |
| C12     | 79.1596             |
| C13     | 45.5936             |
| C14     | 162.1698            |
| C15     | 150.6254            |
| C16     | 125.8853            |
| C17     | 113.8715            |
| C18     | 148.1466            |
| C19     | 159.9817            |
| C20     | 146.7331            |
| C21     | 134.7906            |
| C22     | 2.0259              |
| C23     | 133.0295            |
| C24     | 132.0046            |
9-methoxy-3-epi-α-yohimbine (8), conformer 6

Sum of electronic and thermal free energies = -1265.2624 H

| Center Number | Atomic Number | Coordinates (Å)         |
|---------------|---------------|-------------------------|
|               |               | X          | Y          | Z          |
| 1             | 7             | 1.263112   | 1.307303   | 0.710982   |
| 2             | 6             | 1.123818   | -0.067184  | 0.838916   |
| 3             | 6             | -0.098134  | -0.802841  | 1.344691   |
| 4             | 7             | -0.058531  | -2.205224  | 0.880340   |
| 5             | 6             | 1.233787   | -2.820817  | 1.224248   |
| 6             | 6             | 2.465439   | -2.176147  | 0.537093   |
| 7             | 6             | 2.507451   | -0.680013  | 0.501082   |
| 8             | 6             | 3.224248   | 0.363852   | 0.121504   |
| 9             | 6             | 4.564400   | 0.387776   | -0.325601  |
| 10            | 6             | 5.165106   | 1.611734   | -0.616448  |
| 11            | 6             | 4.444515   | 2.818936   | -0.467092  |
| 12            | 6             | 3.127900   | 2.837947   | -0.028430  |
| 13            | 6             | 2.537636   | 1.598725   | 0.261756   |
| 14            | 6             | -1.454983  | -0.155944  | 1.014227   |
| 15            | 6             | -1.846493  | -0.304260  | -0.466762  |
| 16            | 6             | -3.248222  | 0.282980   | -0.822131  |
| 17            | 6             | -4.419767  | -0.553597  | -0.270706  |
| 18            | 6             | -4.288675  | -2.020307  | -0.691952  |
| 19            | 6             | -2.926171  | -2.619462  | -0.317611  |
| 20            | 6             | -1.767429  | -1.789400  | -0.893202  |
| 21            | 6             | -0.379752  | -2.348883  | -0.545910  |
| 22            | 6             | -3.333977  | 1.758640   | -0.460561  |
| 23            | 6             | -3.975747  | 3.34863    | 1.172164   |
| 24            | 6             | 6.530177   | -0.865350  | -0.881117  |
| 25            | 8             | 5.179992   | -0.831385  | -0.439543  |
| 26            | 8             | 5.675640   | 0.000775   | -0.680644  |
| 27            | 8             | -2.960280  | 2.658340   | -1.189063  |
| 28            | 8             | 3.827836   | 1.971931   | 0.777261   |
| 29            | 1             | 0.532738   | 1.988036   | 0.844078   |
| 30            | 1             | -0.035655  | -0.846318  | 2.442919   |
| 31            | 1             | 1.179902   | -3.888280  | 0.981343   |
| 32            | 1             | 1.344898   | -2.743871  | 2.313084   |
| 33            | 1             | 2.592901   | -2.569242  | -0.481082  |
| 34            | 1             | 3.373317   | -2.464966  | 1.079015   |
| 35            | 1             | 6.190809   | 1.656857   | -0.961668  |
| 36            | 1             | 4.943071   | 3.753972   | -0.704887  |
| 37            | 1             | 2.581634   | 3.769743   | 0.081852   |
| 38            | 1             | -1.434842  | 0.900770   | 1.304432   |
| 39            | 1             | -2.205561  | -0.623611  | 1.658571   |
| 40            | 1             | -1.113179  | 0.251832   | -1.665735  |
| 41            | 1             | -3.317034  | 0.267079   | -1.918452  |
| 42            | 1             | -4.440982  | -0.482851  | 0.820341   |
| 43            | 1             | -4.419298  | -2.081991  | -1.784672  |
| 44            | 1             | -5.109172  | -2.591569  | -0.243650  |
| 45            | 1             | -2.859093  | -3.648087  | -0.688174  |
| 46            | 1             | -2.831090  | -2.686746  | 0.776636   |
| 47            | 1             | -1.854037  | -1.824030  | -1.989877  |
| 48            | 1             | 0.363486   | -1.849855  | -1.192310  |
| 49            | 1             | 0.344354   | -3.419824  | -0.781488  |
| 50            | 1             | -4.644313  | 3.868938   | 0.482424   |
| 51            | 1             | -3.006411  | 3.853776   | 1.180062   |
| 52            | 1             | -4.404073  | 3.318724   | 2.173582   |
| 53            | 1             | 6.631660   | -0.446625  | -1.890437  |
| 54            | 1             | 6.813362   | -1.918936  | -0.695895  |
| 55            | 1             | 7.189534   | -0.320261  | -0.193719  |
| 56            | 1             | -5.790926  | -0.161185  | -1.627697  |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 49.1612             |
| C3      | 129.5777            |
| C5      | 132.4169            |
| C6      | 165.1313            |
| C7      | 73.6266             |
| C8      | 64.7815             |
| C9      | 25.546              |
| C10     | 84.5577             |
| C11     | 60.5837             |
| C12     | 78.4637             |
| C13     | 44.7865             |
| C14     | 160.4155            |
| C15     | 149.0144            |
| C16     | 124.1561            |
| C17     | 115.6442            |
| C18     | 148.8136            |
| C19     | 160.1749            |
| C20     | 146.4441            |
| C21     | 134.8237            |
| C22     | 2.0682              |
| C23     | 133.2879            |
| C24     | 131.865             |
9-methoxy-3-epi-α-yohimbine (8), conformer 7

Sum of electronic and thermal free energies = -1265.265227 H

| Center Number | Atomic Number | Coordinates (Ångstroms) |
|---------------|---------------|-------------------------|
| X             | Y             | Z                       |
|---------------|---------------|-------------------------|
| 1             | 7             | -1.548243               | 0.792004 | -1.376276 |
| 2             | 6             | -1.251765               | -0.316984 | -0.597418 |
| 3             | 6             | 0.099940                | -0.962185 | -0.533798 |
| 4             | 7             | 0.116646                | -1.963124 | 0.544731  |
| 5             | 6             | -1.110290               | -2.763303 | 0.633237  |
| 6             | 6             | -2.332320               | -1.908717 | 0.992164  |
| 7             | 6             | -2.571201               | -0.713744 | 0.086452  |
| 8             | 6             | -3.425504               | 0.198519  | -0.276730 |
| 9             | 6             | -4.786364               | 0.326463  | 0.079452  |
| 10            | 6             | -5.544448               | 1.354372  | -0.479994 |
| 11            | 6             | -4.960701               | 2.260759  | -1.394045 |
| 12            | 6             | -3.627085               | 2.168665  | -1.769285 |
| 13            | 6             | -2.877326               | 1.129794  | -1.198107 |
| 14            | 6             | 1.238391                | 0.066398  | -0.288631 |
| 15            | 6             | 2.389312                | -0.524190 | 0.560166  |
| 16            | 6             | 3.724649                | 0.262246  | 0.413094  |
| 17            | 6             | 4.406788                | 0.044822  | -0.954055 |
| 18            | 6             | 4.613230                | -1.445340 | -1.216302 |
| 19            | 6             | 3.298329                | -2.229345 | -1.108210 |
| 20            | 6             | 2.622342                | -2.020303 | 0.260020  |
| 21            | 6             | 1.297608                | -2.821096 | 0.413019  |
| 22            | 6             | 3.550262                | 1.743294  | 0.709271  |
| 23            | 6             | 2.865090                | 3.335014  | 2.327599  |
| 24            | 6             | -6.622161               | -0.512817 | 1.371718  |
| 25            | 8             | -5.261150               | -0.598491 | 0.971846  |
| 26            | 8             | 5.684302                | 0.676757  | -1.007339 |
| 27            | 8             | 3.834586                | 2.651922  | -0.054820 |
| 28            | 8             | 3.049961                | 1.957349  | 1.940659  |
| 29            | 1             | -0.902598               | 1.281424  | -1.974995 |
| 30            | 1             | 0.288453                | -1.467180 | -1.507525 |
| 31            | 1             | -0.948642               | -3.528903 | 1.400063  |
| 32            | 1             | -1.302225               | -3.294824 | -0.321114 |
| 33            | 1             | -2.275636               | -1.601024 | 2.044960  |
| 34            | 1             | -3.241535               | -2.510127 | 0.889134  |
| 35            | 1             | -6.589956               | 1.473497  | -0.223318 |
| 36            | 1             | -5.580373               | 3.049314  | -1.810719 |
| 37            | 1             | -3.188033               | 2.869611  | -2.472770 |
| 38            | 1             | 0.828543                | 0.933176  | 0.240856  |
| 39            | 1             | 1.602394                | 0.428878  | -1.257106 |
| 40            | 1             | 2.080705                | -0.448007 | 1.601068  |
| 41            | 1             | 4.413186                | -0.118293 | 1.181551  |
| 42            | 1             | 3.766254                | 0.461569  | -1.745248 |
| 43            | 1             | 5.341065                | -1.825971 | -0.486590 |
| 44            | 1             | 5.065011                | -1.569090 | -2.206349 |
| 45            | 1             | 3.489438                | -3.298621 | -1.261809 |
| 46            | 1             | 2.615854                | -1.925407 | -1.914104 |
| 47            | 1             | 3.324048                | -2.391634 | 1.017720  |
| 48            | 1             | 1.341611                | -3.453137 | 0.306652  |
| 49            | 1             | 1.185784                | -3.503739 | -0.454780 |
| 50            | 1             | 2.462315                | 3.297932  | 3.339025  |
| 51            | 1             | 2.164876                | 3.829556  | 1.650621  |
| 52            | 1             | 3.820136                | 3.864955  | 2.309358  |
| 53            | 1             | -7.299004               | -0.635208 | 0.516581  |
| 54            | 1             | -6.833175               | 0.442628  | 1.686552  |
| 55            | 1             | -6.778233               | -1.330228 | 2.077214  |
| 56            | 1             | 5.526315                | 1.632556  | -0.971615 |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 45.2163             |
| C3      | 131.0675            |
| C5      | 133.0258            |
| C6      | 160.3705            |
| C7      | 74.1816             |
| C8      | 66.2516             |
| C9      | 26.0547             |
| C10     | 84.9033             |
| C11     | 60.2484             |
| C12     | 79.3563             |
| C13     | 44.5507             |
| C14     | 157.155             |
| C15     | 150.3261            |
| C16     | 129.3689            |
| C17     | 117.0343            |
| C18     | 152.6679            |
| C19     | 154.7569            |
| C20     | 148.151             |
| C21     | 126.0104            |
| C22     | 0.5437              |
| C23     | 132.658             |
| C24     | 132.0095            |
9-methoxy-3-epi-α-yohimbine (8), conformer 8

Sum of electronic and thermal free energies = -1265.26251 H

| Center Number | Atomic Number | Coordinates (Angstroms) |
|---------------|---------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 7             | -1.576019   | 0.803569   | -1.350717   |
| 2             | 6             | -1.285665   | -0.310566  | -0.577434   |
| 3             | 6             | 0.060130    | -0.969473  | -0.524985   |
| 4             | 7             | 0.075333    | -1.963807  | 0.560009    |
| 5             | 6             | -1.154295   | -2.759457  | 0.652542    |
| 6             | 6             | -2.374342   | -1.901119  | 1.008880    |
| 7             | 6             | -2.406432   | -0.703241  | 0.106847    |
| 8             | 6             | -3.453904   | 0.220613   | -0.246137   |
| 9             | 6             | -4.812397   | 0.357607   | 0.115086    |
| 10            | 6             | -5.562063   | 1.399200   | -0.430074   |
| 11            | 6             | -4.971823   | 2.310462   | -1.335241   |
| 12            | 6             | -3.640665   | 2.208559   | -1.716607   |
| 13            | 6             | -2.899659   | 1.155303   | -1.160541   |
| 14            | 6             | 1.210006    | 0.050446   | -0.302836   |
| 15            | 6             | 2.364561    | -0.539497  | 0.541399    |
| 16            | 6             | 3.711661    | 0.233945   | 0.393463    |
| 17            | 6             | 4.409452    | -0.008578  | -0.951140   |
| 18            | 6             | 4.554959    | -1.505379  | -1.245449   |
| 19            | 6             | 3.218980    | -2.252798  | -1.136890   |
| 20            | 6             | 2.577293    | -2.039824  | 0.246063    |
| 21            | 6             | 1.250172    | -2.829160  | 0.429942    |
| 22            | 6             | 3.504150    | 1.724029   | 0.617375    |
| 23            | 6             | 3.457051    | 3.439583   | 2.250449    |
| 24            | 6             | -6.651772   | -0.476872  | 1.405471    |
| 25            | 8             | -5.293837   | -0.573053  | 0.998544    |
| 26            | 8             | 5.697662    | 0.620649   | -0.851291   |
| 27            | 8             | 3.185960    | 2.528147   | -0.237406   |
| 28            | 8             | 3.671536    | 2.054308   | 1.916653    |
| 29            | 1             | -0.915344   | 1.319816   | -1.909514   |
| 30            | 1             | 0.229582    | -1.484569  | -1.497140   |
| 31            | 1             | -0.994852   | -3.523530  | 1.421468    |
| 32            | 1             | -1.347400   | -3.293333  | -0.300467   |
| 33            | 1             | -2.320077   | -1.595474  | 2.062423    |
| 34            | 1             | -3.285084   | -2.499705  | 0.902273    |
| 35            | 1             | -6.605536   | 1.527577   | -0.168667   |
| 36            | 1             | 5.584471    | 3.110659   | -1.739969   |
| 37            | 1             | -3.196504   | 2.913239   | -2.413067   |
| 38            | 1             | 0.814223    | 0.929308   | 0.214815    |
| 39            | 1             | 1.570684    | 0.404130   | -1.274970   |
| 40            | 1             | 2.064930    | -0.457764  | 1.591057    |
| 41            | 1             | 4.384848    | -0.124203  | 1.181149    |
| 42            | 1             | 3.828629    | 0.479841   | -1.744508   |
| 43            | 1             | 5.274190    | -1.920761  | -0.527009   |
| 44            | 1             | 4.993495    | -1.638097  | -2.242778   |
| 45            | 1             | 3.378040    | -3.324653  | -1.308132   |
| 46            | 1             | 2.533059    | -1.917665  | -1.926939   |
| 47            | 1             | 3.295227    | -2.417607  | 0.987183    |
| 48            | 1             | 1.302573    | -3.445240  | 1.334359    |
| 49            | 1             | 1.124946    | -3.527403  | -0.423815   |
| 50            | 1             | 3.650678    | 3.512822   | 3.320221    |
| 51            | 1             | 2.429000    | 3.732597   | 2.023553    |
| 52            | 1             | 4.144926    | 4.075236   | 1.688149    |
| 53            | 1             | -7.333916   | -0.582646  | 0.552257    |
| 54            | 1             | -6.850279   | 0.475384   | 1.913525    |
| 55            | 1             | -6.813772   | -1.300222  | 2.102875    |
| 56            | 1             | 6.017255    | 0.832630   | -1.736490   |
| Nucleus | Isotropic shielding |
|---------|---------------------|
| C2      | 45.0656             |
| C3      | 131.0934            |
| C5      | 132.9705            |
| C6      | 160.4794            |
| C7      | 74.3618             |
| C8      | 66.2012             |
| C9      | 25.979              |
| C10     | 84.9411             |
| C11     | 60.3405             |
| C12     | 79.2987             |
| C13     | 44.4336             |
| C14     | 156.3815            |
| C15     | 150.752             |
| C16     | 131.2475            |
| C17     | 114.947             |
| C18     | 149.8265            |
| C19     | 155.2184            |
| C20     | 148.9931            |
| C21     | 126.0309            |
| C22     | 2.4732              |
| C23     | 133.1016            |
| C24     | 132.048             |