Supporting Information for

Total synthesis and isolation of citrinalin and cyclopiamine congeners

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Supporting Information Layout

I. General Experimental for the synthesis of compounds 14-31, 33-36, 2 and 6

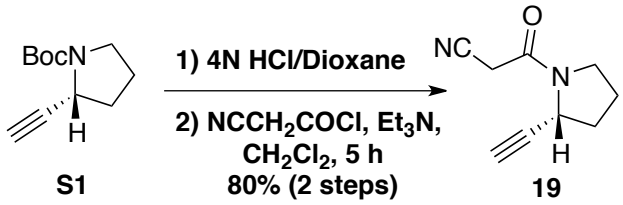
Unless otherwise noted, all reactions were carried out under an atmosphere of nitrogen, and all reagents were purchased from commercial suppliers and used without further purification. All reactions were carried out in flame-dried glassware under a positive pressure of nitrogen in dry solvents using standard Schlenk techniques. Tetrahydrofuran (THF), diethyl ether (Et_2O), benzene, toluene (PhMe), methanol (MeOH) and triethylamine (Et_3N) were dried over alumina under an argon atmosphere in a GlassContour solvent system. Dichloromethane (CH_2Cl_2) was distilled over calcium hydride under a nitrogen atmosphere. All other solvents and reagents were used as received unless otherwise noted. Reaction temperatures above room temperature (RT), 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 (254 nm), *p*-anisaldehyde stain, $KMnO_4$ or CAM stain. Sorbtech silica gel (particle size 40-63 μm) was used for flash chromatography. Melting points were recorded on a Mel-Temp II Laboratory Devices, USA. Optical rotation was recorded on a Perkin Elmer Polarimeter 241 at the D line (1.0 dm path length). ^1H and ^{13}C NMR were recorded on Bruker AVB-400, AV-500, DRX-500 or AV-600 MHz spectrometers with ^{13}C operating frequencies of 100, 125, 125, and 150 MHz, respectively, in $CDCl_3$, DMF-d_7, $(CD_3)_2SO$ or C_6D_6 at 23 °C. Chemical shifts (δ) are reported in ppm relative to the residual solvent signal ($CDCl_3$ δ = 7.26 for ^1H NMR and δ = 77.16 for ^{13}C NMR; DMF-d_7 δ = 8.02 for ^1H NMR and δ = 163.15 for ^{13}C NMR $(CD_3)_2SO$ δ = 2.50 for ^1H NMR and δ = 39.52 for ^{13}C NMR; C_6D_6 δ = 7.16 for ^1H NMR and δ = 128.06 for ^{13}C 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.

II. General Experimental for the synthesis of indole oxidation catalyst 32

Dichloromethane (CH_2Cl_2) was dried in a Seca Solvent Purification System by Glass Contour. Normal phase flash chromatography was performed using Dynamic Adsorbents silica gel (particle size 32-63 μm). Reversed phase chromatography used C-18 silica and was performed on a Biotage Isolera One purification system. Products were analyzed by thin-layer chromatography using EMD Millipore silica gel 60 F254 precoated plates (0.25 mm thickness) and were visualized by irradiation with UV light (254 nm) or staining with $KMnO_4$. Optical rotation was recorded on a Perkin Elmer Polarimeter 341 at the D line (1.0 dm path length). ^1H and ^{13}C NMR were recorded on an Agilent DD2 600 MHz spectrometer, equipped with a cold probe, with a ^{13}C operating frequency of 150 MHz. Spectra were recorded in $CDCl_3$ at ambient temperature and chemical shifts (δ) are reported in ppm relative to the residual solvent signal ($CDCl_3$ δ = 7.26 for ^1H NMR and δ = 77.16 for ^{13}C 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), p (pentet), dt (doublet of triplets), td (triplet of doublets), m (multiplet). IR spectrum was recorded on a Nicolet 6700 FT-IR spectrometer and is reported in frequency of absorption (cm^{-1}). High resolution mass spectra were acquired from the Mass Spectrometry Facility at the Keck Center of Yale University.

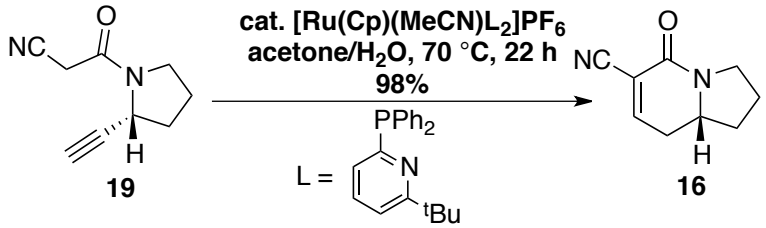
All reactions were performed at ambient temperature (21 °C). Boc-*trans*-4-benyloxy-D-proline (Boc-DHyp(Bn)-OH) was prepared from Boc-*trans*-4-hydroxy-D-proline by a method reported in the literature.[35]

III. Experimental Procedures and Characterization Data for compounds 14-36, 2 and 6

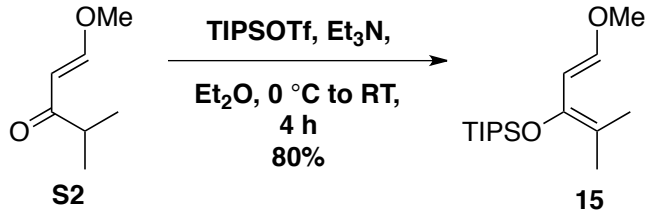


S1 19

(*R*)-3-(2-ethynylpyrrolidin-1-yl)-3-oxopropanenitrile (19). To a flask charged with known **(*R*)-*tert*-**butyl 2-ethynylpyrrolidine-1-carboxylate[36] (**S1**) (500 mg, 2.56 mmol) was added 4 N HCl/dioxane (12.8 mL, 51.2 mmol) drop-wise at 0 °C. The resulting brown mixture was stirred for 10 min at the same temperature then warmed to room temperature for 1 h. The solvent was removed *in vacuo* and excess HCl/dioxane was azeotroped off with diethyl ether (4 x 10 mL) then ethyl acetate (3 x 10 mL) then placed *in vacuo* overnight. The resulting beige crystals were suspended in dichloromethane (8.5 mL) and triethylamine (1.0 mL, 7.10 mmol) was added drop-wise at 0 °C, followed by the drop-wise addition of cyanoacetylchloride (727 mg, 7.10 mmol) as a solution in dichloromethane (2 mL). The resulting red solution was stirred at the same temperature for 2 h and then warmed to room temperature for 3 h, at which time saturated aqueous $NaHCO_3$ (10 mL) was added and volatiles removed *in vacuo*. The resulting aqueous solution was extracted with ethyl acetate (3 x 10 mL) and the combined organic extracts were dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The resulting red oil was purified by silica gel chromatography (1:2 hexanes:ethyl acetate) to yield the title compound (330 mg, 2.03 mmol, 80%) as a yellow solid. m.p. 88–89 °C; TLC (hexanes:EtOAc, 1:2 v/v): R_f=0.34; ^{1}H NMR (600 MHz, $CDCl_3$, mixture of amide conformers 1.4:1) δ = 4.75–4.60 (s, 0.4H), 4.52–4.38 (d, J = 6.4 Hz, 0.6H), 3.78–3.53 (m, 2H), 3.50–3.36 (m, 2H), 2.56–2.42 (m, 0.4H), 2.30–2.10 (m, 2H), 2.10–1.98 (m, 2H), 1.98–1.85 (m, 0.6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 160.4, 159.9, 114.0, 113.7, 82.1, 81.4, 73.4, 70.7, 48.4, 48.1, 46.7, 46.6, 34.0, 32.0, 25.8, 25.6, 24.6, 22.8; IR (NaCl, thin film) ν_{max}: 3276, 2955, 2883, 2262, 1655, 1437 cm^{-1}; HRMS (ESI) (*m/z*) $[M]^+$ calcd for $C_9H_{11}N_2O$, 163.0866; found, 163.0866.

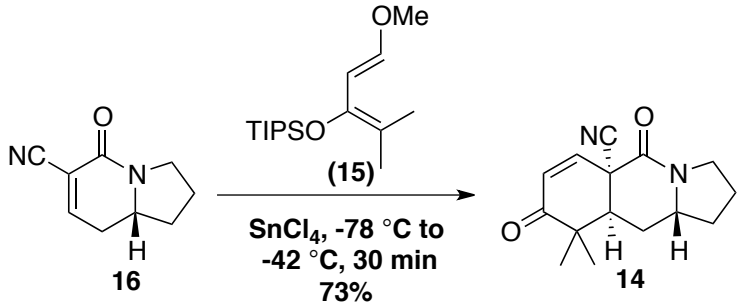


(*R*)-5-oxo-1,2,3,5,8,8a-hexahydroindolizine-6-carbonitrile (16). This procedure was adapted from a known procedure.[16] To a Schlenk flask charged with (*R*)-3-(2-ethynylpyrrolidin-1-yl)-3-oxopropanenitrile (**19**) (750 mg, 4.62 mmol) and a stir bar in an inert atmosphere glovebox was added acetonitrilebis[2-diphenylphosphino-6-*t*-butylpyridine]cyclopentadienylruthenium(II) hexafluorophosphate (367 mg, 370 μmol). A degassed (via three cycles of freeze, pump, thaw) mixture of acetone (9.6 mL) and water (400 μL) was added under a nitrogen atmosphere via syringe. The resulting yellow solution was stirred at 70 °C for 22 h, at which time the reaction was diluted with ethyl acetate (10 mL) and concentrated *in vacuo*. The resulting yellow oil was purified by silica chromatography (1:4 hexanes:ethyl acetate) to yield the title compound (732 mg, 4.53 mmol, 98%) as a yellow solid. m.p.: 85–87 °C; TLC (hexanes:EtOAc, 1:4 v/v); R_f=0.19; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.35–7.30 (dd, *J* = 6.8, 2.3 Hz, 1H), 3.80–3.72 (m, 1H), 3.68–3.61 (ddd, *J* = 12.0, 9.4, 2.3 Hz, 1H), 3.50–3.42 (m, 1H), 2.78–2.69 (m, 1H), 2.37–2.22 (m, 2H), 2.09–2.01 (m, 1H), 1.87–1.77 (m, 1H), 1.71–1.61 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 157.1, 152.2, 114.6, 114.2, 55.8, 44.6, 33.2, 31.0, 22.7; IR (NaCl, thin film) ν_{max}: 3046, 2980, 2235, 1661, 1606 cm^{-1}; HRMS (ESI) (*m/z*) $[M]^+$ calcd for $C_9H_{11}N_2O$, 163.0866; found, 163.0865.



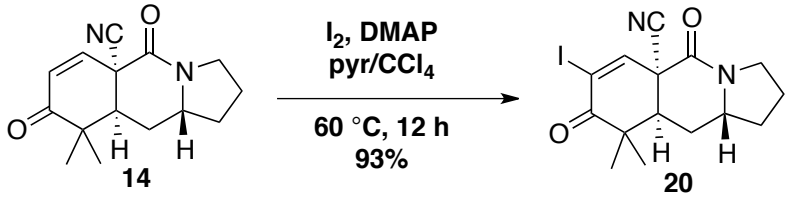
(*E*)-triisopropyl((1-methoxy-4-methylpenta-1,3-dien-3-yl)oxy)silane (15). This procedure was adapted from a known procedure.[13] A solution of (*E*)-1-methoxy-4-methylpent-1-en-3-one[13] (**S2**) (2.00 g, 15.6 mmol) in diethyl ether (78 mL) was cooled to 0 °C. Triethylamine (13.0 mL, 93.7 mmol) was added quickly, followed by the drop-wise addition of triisopropylsilyl trifluoromethanesulfonate (8.4 mL, 31.2 mmol). After 10 minutes the solution was warmed to room temperature and allowed to stir for an additional 4 h, at which point two distinct layers were formed. The viscous bottom layer was removed and the top layer was diluted with hexanes (50 mL). This solution was washed with saturated aqueous

$NaHCO_3$ (1 x 100 mL), and the aqueous layer was extracted with diethyl ether (3 x 100 mL). The combined organic layers were washed with brine (1 x 200 mL), dried over Na_2SO_4, filtered and concentrated *in vacuo.* The crude orange oil was purified by filtration through a plug of silica gel (12 mL SiO_2, 100% pentanes) to yield the title compound (3.55 g, 12.5 mmol, 80%) as a yellow oil. TLC (hexanes:EtOAc, 16:1 v/v); R_f=0.49; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 6.65 (d, *J* = 12.5 Hz, 1H), 5.54 (d, *J* = 12.5 Hz, 1H), 3.60 (s, 3H), 1.71 (s, 3H), 1.67 (s, 3H), 1.23–1.16 (m, 3H), 1.14–1.09 (m, 18H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 149.4, 140.8, 110.4, 101.4, 56.4, 19.4, 18.6, 18.1, 13.7; IR (NaCl, thin film) ν_{max}: 2946, 2360, 1717, 1656 cm^{-1}; HRMS (ESI) (*m/z*) $[M]^+$ calcd for $C_{16}H_{33}O_2Si$, 285.2244; found, 285.2248

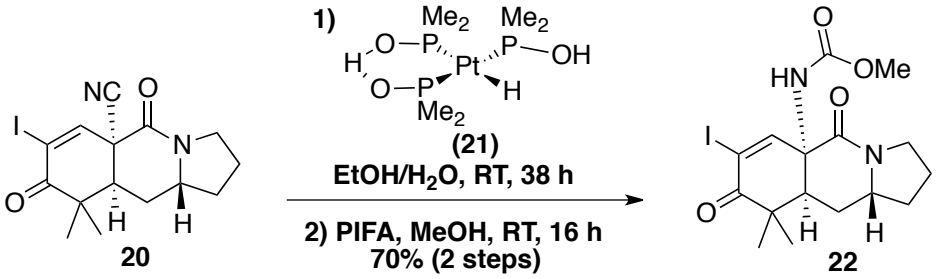


(5a*R*,9a*S*,10a*R*)-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinoline-5a-carbonitrile (14). A round-bottom flask charged with (*R*)-5-oxo-1,2,3,5,8,8a-hexahydroindolizine-6-carbonitrile (**16**) (2.09 g, 12.9 mmol), (*E*)-triisopropyl((1-methoxy-4-methylpenta-1,3-dien-3-yl)oxy)silane (**15**) (7.35 g, 25.8 mmol) and dichloromethane (130 mL) was cooled to -78 °C. Tin tetrachloride (1.0 M in CH_2Cl_2, 15.5 mL, 15.5 mmol) was added drop-wise, and the solution was immediately warmed to -42 °C. After 30 minutes the solution was warmed to room temperature and stirred for 15 minutes, after which time saturated aqueous $NaHCO_3$ (130 mL) was slowly added. The resulting mixture was stirred vigorously for 1 h then vacuum filtered through a fritted funnel and the volatiles removed *in vacuo*. The aqueous layer was extracted with ethyl acetate (3 x 150 mL), and the combined organic extracts were dried over Na_2SO_4, filtered and concentrated *in vacuo*. The brown oil was purified by silica gel chromatography (1:2 hexanes:ethyl acetate) to yield the title compound (2.42 g, 9.37 mmol, 73%) as a yellow solid. m.p.: 113–115 °C; TLC (hexanes:EtOAc, 1:4 v/v); R_f=0.38; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.78 (d, *J* = 10.0 Hz, 1H), 6.21 (d, *J* = 10.0 Hz, 1H), 3.75–3.61 (m, 1H), 3.55–3.42 (m, 2H), 2.78 (dd, *J* = 7.9, 2.4 Hz, 1H), 2.29 (ddd, *J* = 14.8, 4.3, 2.4 Hz, 1H), 2.24–2.15 (m, 1H), 2.07–1.97 (m, 1H), 1.91 (ddd, *J* = 14.8, 11.6, 7.9 Hz, 1H), 1.86–1.75 (m, 1H), 1.60–1.46 (m, 1H), 1.44 (s, 3H),

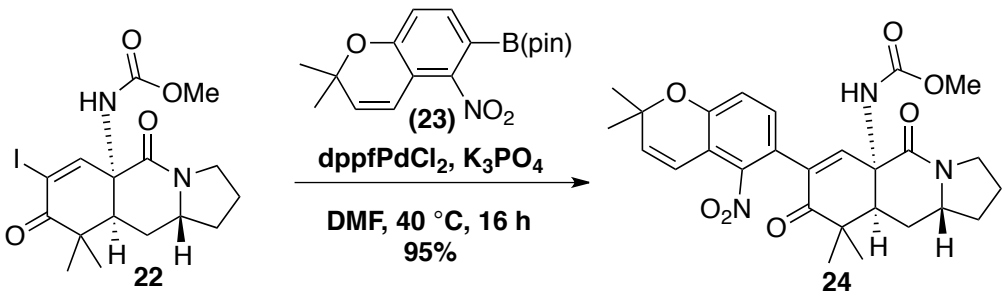
1.19 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 200.5, 161.4, 138.3, 129.7, 118.2, 55.7, 46.2, 45.9, 45.4, 45.3, 34.1, 30.0, 25.3, 22.4, 22.3; IR (NaCl, thin film) ν_{max}: 2976, 2887, 2359, 2341, 1675, 1568, 1443 cm^{-1}; HRMS (ESI) (*m/z*) $[M]^+$ calcd for $C_{15}H_{19}O_2N_2$, 259.1441; found, 259.1444.



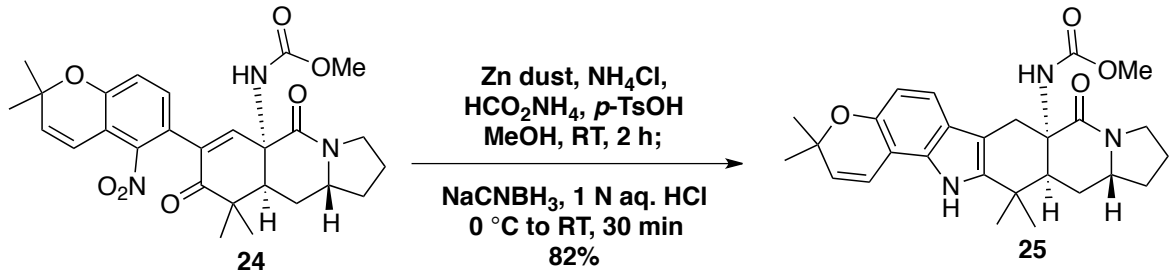
(5a*S*,9a*S*,10a*R*)-7-iodo-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinoline-5a-carbonitrile (20). Iodine (383 mg, 1.51 mmol) and 4-dimethylaminopyridine (185 mg, 1.51 mmol) were added sequentially to a solution of (5a*R*,9a*S*,10a*R*)-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinoline-5a-carbonitrile (**14**) (130 mg, 0.503 mmol) in a mixture of pyridine (630 µL) and CCl_4 (630 µL). The resulting dark brown mixture was stirred at 60 ºC in the dark for 12 h and then cooled to room temperature. The reaction mixture was poured into saturated aqueous $Na_2S_2O_3$ (60 mL) and the aqueous layer was extracted with 50% EtOAc/Hex (5 x 40 mL). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (4:1 to 1:1 hexanes:ethyl acetate), using 10 mL silica gel, afforded the title compound (179 mg, 0.466 mmol, 93%) as a colorless foam. TLC (hexanes:EtOAc, 1:4 v/v); R_f=0.54; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.49 (s, 1H), 3.72–3.61 (m, 1H), 3.56–3.46 (m, 1H), 3.45–3.36 (m, 1H), 2.83 (dd, *J* = 8.0, 2.1 Hz, 1H), 2.33–2.14 (m, 2H), 2.08–1.97 (m, 1H), 1.95–1.76 (m, 2H), 1.58–1.51 (m, 1H), 1.49 (s, 3H), 1.24 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 194.8, 160.3, 145.0, 117.2, 105.5, 55.6, 48.7, 46.4, 46.0, 45.6, 34.2, 30.1, 25.8, 23.0, 22.5; IR (NaCl, thin film) ν_{max}: 2976, 1692, 1678, 1666, 1659, 1442, 1110, 736; HRMS-ESI calcd for $C_{15}H_{18}N_2O_2I$ ($[M+H]^+$): 385.0408, found 385.0407.



methyl ((5a*R*,9a*S*,10a*R*)-7-iodo-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinolin-5a-yl)carbamate (22). $(Me_2POH)_2Pt(H)(Me_2PO)$[19] (**21**) (208 mg, 484 μmol) was added in one portion to a solution of (5a*S*,9a*S*,10a*R*)-7-iodo-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinoline-5a-carbonitrile (**20**) (930 mg, 2.42 mmol) in a mixture of H_2O (2.42 mL) and EtOH (9.68 mL). The resulting suspension was stirred at room temperature for 38 h. The reaction mixture was subsequently diluted with CH_2Cl_2 and passed through a short column containing silica and anhyd. Na_2SO_4. Further purification of the filtrate via silica gel chromatography (2% to 10% MeOH/CH_2Cl_2), using 40 mL silica gave the carboxamide as a creamy orange foam, which was used in the next step without further purification. The carboxamide prepared above was dissolved in MeOH (24 mL) and the flask was placed in a room temperature water bath. [Bis(trifluoroacetoxy)iodo]benzene (PIFA) was added in one portion and the mixture stirred at room temperature for 16 h. The reaction mixture was subsequently poured into saturated aqueous $NaHCO_3$ (60 mL) and the aqueous layer was extracted with EtOAc (3 x 100 mL). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (2% to 5% MeOH/CH_2Cl_2), using 40 mL silica, gave the title compound (730 mg, 1.69 mmol, 70%, 2 steps) as an orange foam. TLC (hexanes:EtOAc, 1:4 v/v); R_f=0.40; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.15 (s, 1H), 5.20 (s, 1H), 3.71 (s, 3H), 3.63–3.55 (m, 1H), 3.50–3.41 (m, 1H), 3.23–3.13 (m, 1H), 3.10–3.01 (m, 1H), 2.21–2.14 (m, 1H), 2.14–2.07 (m, 1H), 1.99–1.90 (m, 1H), 1.85–1.70 (m, 2H), 1.51–1.43 (m, 1H), 1.39 (s, 3H), 1.24 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 197.4, 166.3, 156.5, 149.6, 108.1, 104.9, 67.8, 62.5, 55.2, 52.6, 46.6, 45.0, 34.1, 30.9, 29.4, 23.8, 23.0; IR (NaCl, thin film) ν_{max}: 3294, 2972, 1725, 1692, 1658, 1624, 1109; HRMS-ESI calcd for $C_{15}H_{20}N_2O_2I$ ($[M+H]^+$): 433.0619, found 433.0620.



methyl ((5a*S*,9a*S*,10a*R*)-7-(2,2-dimethyl-5-nitro-2*H*-chromen-6-yl)-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinolin-5a-yl)carbamate (24). A flask was charged with methyl ((5a*R*,9a*S*,10a*R*)-7-iodo-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinolin-5a-yl)carbamate (**22**) (659 mg, 1.53 mmol), 2-(2,2-dimethyl-5-nitro-2*H*-chromen-6-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane[21] (**23**) (760 mg, 2.29 mmol), $dppfPdCl_2$ (125 mg, 153 μmol) and K_3PO_4 (1.22 g, 5.74 mmol). *N,N*-dimethylformamide (15.3 mL) was added and the mixture degassed by purging with N_2 (3x). The resulting brown mixture was stirred at 40 ºC. After 16 h, the reaction mixture was cooled to room temperature, poured into saturated aqueous NH_4Cl (120 mL) and the aqueous layer extracted with EtOAc (3 x 100 mL). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (4:1 to 1:4 hexanes:ethyl acetate), using 100 mL silica yielded the title compound (739 mg, 1.45 mmol, 95%) as a brown foam. TLC (hexanes:EtOAc, 1:4 v/v); R_f=0.19; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.91 (d, *J* = 8.3 Hz, 1H), 6.87 (d, *J* = 8.3 Hz, 1H), 6.42 (s, 1H), 6.38 (d, *J* = 10.2 Hz, 1H), 5.82 (d, *J* = 10.2 Hz, 1H), 5.48 (s, 1H), 3.70 (s, 3H), 3.63–3.54 (m, 1H), 3.53–3.43 (m, 1H), 3.35–3.21 (m, 1H), 3.02–2.93 (m, 1H), 2.23–2.15 (m, 1H), 2.14–2.05 (m, 1H), 1.98–1.89 (m, 1H), 1.85–1.72 (m, 2H), 1.50–1.44 (m, 1H), 1.45 (s, 6H), 1.43 (s, 3H), 1.19 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 201.3, 167.3, 156.9, 154.2, 146.9, 139.9, 136.6, 134.4, 131.0, 121.4, 119.4, 116.6, 114.7, 77.0, 60.0, 55.0, 52.5, 46.6, 46.3, 44.5, 34.1, 31.5, 29.9, 27.9, 23.2, 23.0; IR (NaCl, thin film) ν_{max}: 2975, 1725, 1652, 1530, 1361, 1281; HRMS-ESI calcd for $C_{27}H_{31}N_3O_7Na$ ($[M+Na]^+$): 532.2054, found 532.2052.



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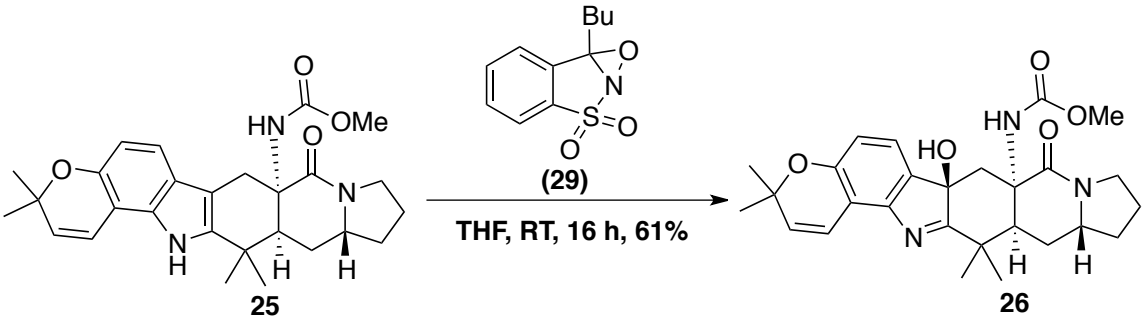
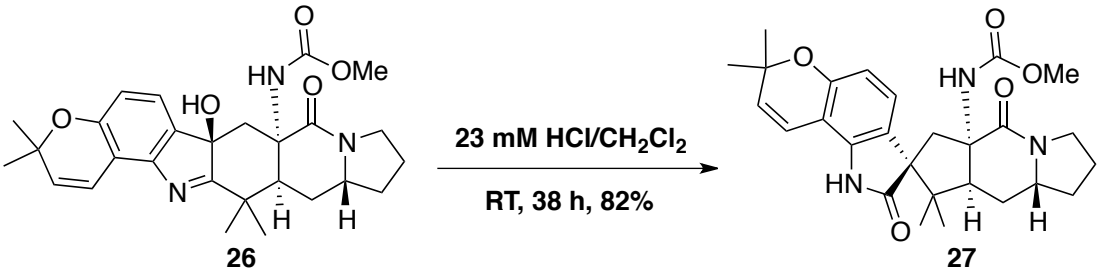
methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-8-oxo-3,7,7a,8,10,11,12,12a,13,13a,14,15-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (25). Zinc dust was freshly activated by sequential washing with 0.1 M aq. HCl (3 x 10 mL) and H_2O (10 mL). The solid was collected by filtration and washed with EtOH (2 x 10 mL) and Et_2O (2 x 10 mL), then dried under high vacuum to give a soft blue-gray solid, which was ground to a powder. A separate flask was charged with methyl ((5a*S*,9a*S*,10a*R*)-7-(2,2-dimethyl-5-nitro-2*H*-chromen-6-yl)-9,9-dimethyl-5,8-dioxo-1,2,3,5,5a,8,9,9a,10,10a-decahydropyrrolo[1,2-*b*]isoquinolin-5a-yl)carbamate (**24**) (120 mg, 236 μmol), NH_4Cl (25.2 mg, 472 μmol), HCO_2NH_4 (74.4 mg, 1.18 mmol) and *p*-TsOH·H_2O (449 mg, 2.36 mmol). MeOH (47 mL) was then added and the mixture stirred at room temperature for 5 minutes to ensure complete dissolution of all salts. The above activated zinc dust (77.0 mg, 1.18 mmol) was then added in one portion and the mixture stirred rapidly at room temperature. After 1 h, more NH_4Cl (25.2 mg), HCO_2NH_4 (74.4 mg) and activated zinc dust (77.0 mg) were added sequentially and the reaction mixture stirred at room temperature another 1 h. The reaction mixture above was cooled to 0 ºC and adjusted to pH 2 by the addition of 1 M aq. HCl. $NaCNBH_3$ (29.7 mg, 472 μmol) was added in one portion at 0 ºC and allowed to stir at room temperature for 30 min. The resulting reaction mixture was subsequently quenched by the addition of saturated aqueous $NaHCO_3$ (60 mL), at which point the MeOH was removed *in vacuo*. The resulting aqueous mixture was extracted with EtOAc (3 x 30 mL) and the combined organic extracts dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (1% MeOH/CH_2Cl_2 to 5% MeOH/CH_2Cl_2), using 20 mL silica afforded the title compound (90.4 mg, 195 μmol, 83%) as an off-white foam. TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.15; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.71 (s, 1H), 7.12 (d, *J* = 8.4 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 1H), 6.60 (d, *J* = 9.7 Hz, 1H), 5.69 (d, *J* = 9.7 Hz, 1H), 4.93 (s, 1H), 4.02–3.92 (m, 1H), 3.61 (s, 3H), 3.55–3.47 (m, 1H), 3.33–3.24 (m, 1H), 3.14–3.02 (m, 2H), 2.81 (d, *J* = 16.7 Hz, 1H), 2.15–2.04 (m, 1H), 2.04–1.87 (m, 3H), 1.85–1.74 (m, 1H), 1.74–1.63 (m, 1H), 1.48 (s, 3H), 1.46 (s, 6H), 1.34 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 170.8, 156.4, 148.7, 138.6, 132.7, 129.9, 121.9, 117.8, 117.3, 110.3, 105.3, 102.7,

75.7, 59.6, 54.7, 52.0, 44.8, 39.4, 34.5, 33.2, 30.1, 28.7, 28.1, 27.5, 27.3, 25.5, 22.0; IR (NaCl, thin film) ν_{max}: 3311, 1718, 1639, 1507, 1457, 1267, 1188, 1119, 754; HRMS-ESI calcd for $C_{27}H_{34}N_3O_4$ ([M+H]$^+$): 464.2544, found 464.2543.



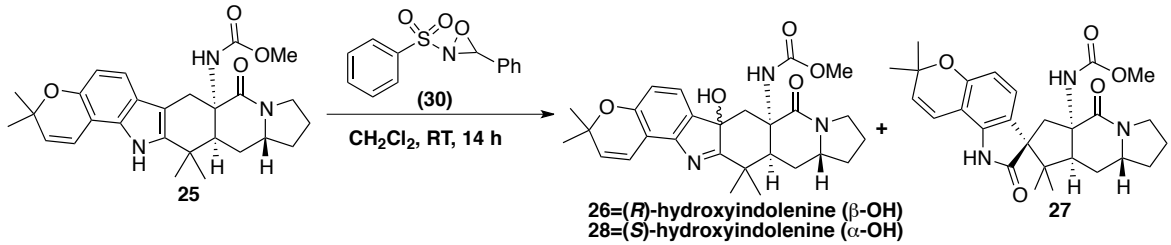
25 26

methyl ((6b*R*,7a*S*,12a*R*,13a*S*)-6b-hydroxy-3,3,14,14-tetramethyl-8-oxo-3,6b,7,7a,8,10,11,12,12a,13,13a,14-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (26). A solution of known saccharin-derived oxaziridine[37] (**29**) (177 mg, 738 μmol) in THF (6.2 mL) was added drop-wise to a stirring solution of methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-8-oxo-3,7,7a,8,10,11,12,12a,13,13a,14,15-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**25**) (114 mg, 246 μmol) in THF (6.2 mL). The reaction mixture was stirred at room temperature for 16 h. Solvent was removed *in vacuo* at ambient temperature (25 ºC). NMR analysis of the crude mixture indicated a ca. 8:1:1 mixture of (*R*)-hydroxylindolenine (**26**): (*S*)-hydroxylindolenine (**28**): (*S*)-spiroxindole (**27**) products. Purification of the crude mixture by silica gel chromatography (1% MeOH/CH_2Cl_2 to 2% MeOH/CH_2Cl_2 to 5% MeOH/CH_2Cl_2), using 10 mL silica, afforded the title compound (71.9 mg, 150 μmol, 61%) as an orange oil. TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.18; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.06 (d, *J* = 7.9 Hz, 1H), 6.96 (d, *J* = 9.8 Hz, 1H), 6.55 (d, *J* = 7.9 Hz, 1H), 5.69 (d, *J* = 9.8 Hz, 1H), 4.84 (s, 1H), 3.87–3.72 (m, 2H), 3.49 (s, 3H), 3.42–3.30 (m, 1H), 3.30 (d, *J* = 14.5 Hz, 1H), 3.18 (s, 1H), 3.04–2.95 (m, 1H), 2.35–2.24 (m, 1H), 2.20–2.05 (m, 3H), 2.01–1.95 (m, 2H), 1.88–1.74 (m, 1H), 1.50 (s, 3H), 1.49 (s, 3H), 1.43 (s, 3H), 1.41 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 188.9, 168.9, 155.1, 154.3, 149.0, 133.7, 131.3, 121.3, 118.2, 114.9, 113.2, 82.1, 76.3, 59.2, 57.5, 52.0, 46.3, 45.3, 42.0, 40.7, 34.5, 28.0, 27.9, 27.9, 25.7, 23.3, 22.4; IR (NaCl, thin film) ν_{max}: 3313, 2973, 1725, 1635, 1459, 1246, 1112, 752; HRMS-ESI calcd for $C_{27}H_{34}N_3O_5$ ([M+H]$^+$): 480.2493, found 480.2492.

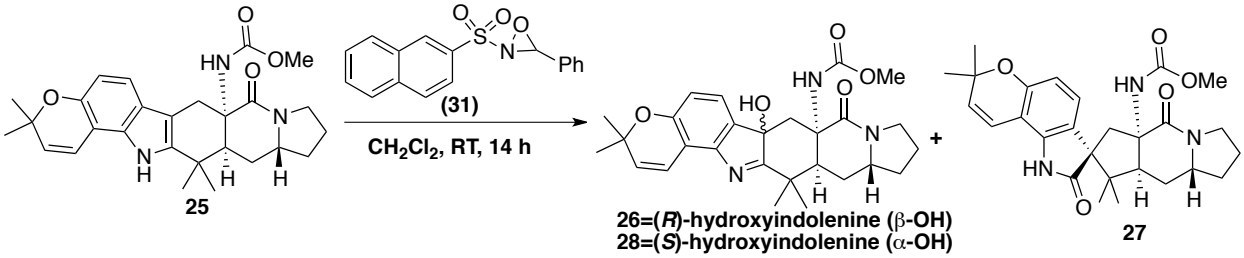


26 27

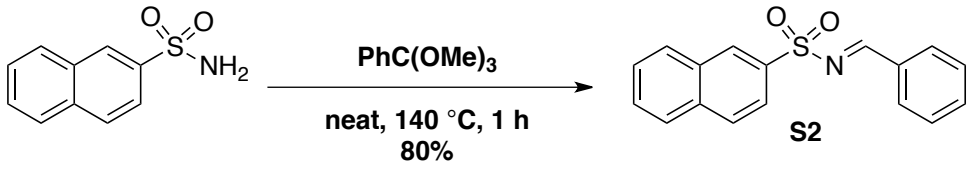
methyl ((3'*S*,5a*S*,8a*S*,9a*R*)-7',7',8,8-tetramethyl-2',5-dioxo-1,2,2',3,5,5a,6,7',8,8a,9,9a-dodecahydro-1'*H*-spiro[cyclopenta[*f*]indolizine-7,3'-pyrano[2,3-*g*]indol]-5a-yl)carbamate (27). A flask was charged with methyl ((6b*R*,7a*S*,12a*R*,13a*S*)-6b-hydroxy-3,3,14,14-tetramethyl-8-oxo-3,6b,7,7a,8,10,11,12,12a,13,13a,14-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**26**) (75.0 mg, 156 μmol). 23 mM HCl/CH_2Cl_2 (15.6 mL, prepared from AcCl/MeOH) was added and the resulting pale yellow solution was allowed to stir at room temperature for 38 h. Solvent was subsequently removed *in vacuo* and the resulting residue purified by silica gel chromatography (1% $MeOH/CH_2Cl_2$ to 2% $MeOH/CH_2Cl_2$ to 5% $MeOH/CH_2Cl_2$), using 10 mL silica. The fractions containing the product were concentrated *in vacuo* to yield the title compound (61.3 mg, 128 μmol, 82%) as a pale brown solid. X-ray quality crystals were obtained from slow evaporation of a concentrated solution in 5% $MeOH/CH_2Cl_2$. m.p.: 305–307 ºC (decomp). TLC ($MeOH:CH_2Cl_2$, 1:19 v/v); R_f=0.15; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.25 (s, 1H), 7.34 (d, *J* = 8.3 Hz, 1H), 6.46 (d, *J* = 8.3 Hz, 1H), 6.31 (d, *J* = 9.8 Hz, 1H), 5.69 (d, *J* = 9.8 Hz, 1H), 5.56 (s, 1H), 3.84–3.68 (m, 2H), 3.65 (s, 3H), 3.49–3.39 (m, 1H), 2.99–2.91 (m, 2H), 2.55–2.42 (m, 1H), 2.18–2.08 (m, 1H), 2.07–1.95 (m, 3H), 1.89–1.73 (m, 1H), 1.66–1.51 (m, 1H), 1.47 (s, 3H), 1.42 (s, 3H), 1.22 (s, 3H), 0.74 (s, 3H); ^{13}C NMR (150 MHz, 20% D_3OD-$CDCl_3$) δ = 180.2, 171.0, 157.0, 152.5, 137.0, 130.7, 126.5, 123.9, 116.6, 109.4, 105.5, 76.1, 62.6, 61.5, 57.7, 55.4, 52.1, 51.3, 47.0, 45.6, 34.7, 27.9, 27.4, 26.5, 25.6, 23.2, 22.5; IR (NaCl, thin film) ν_{max}: 2967, 1729, 1688, 1457, 1250; HRMS-ESI calcd for $C_{27}H_{34}N_3O_5$ ($[M+H]^+$): 480.2493, found 480.2493.



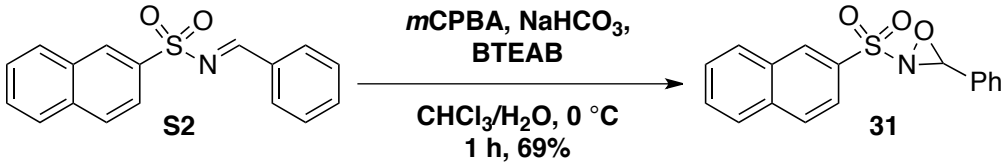
A solution of the Davis oxaziridine[26] (**30**) (3.38 mg, 12.9 μmol) in CH_2Cl_2 (100 μL) was added dropwise to a 0 ºC stirring solution of methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-8-oxo-3,7,7a,8,10,11,12,12a,13,13a,14,15-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**25**) (2.0 mg, 4.31 μmol) in CH_2Cl_2 (116 μL). The reaction mixture was stirred at room temperature for 14 h, at which point TLC indicated complete consumption of starting material. The crude mixture was passed through a quick plug of silica (1 mL) (1% MeOH/CH_2Cl_2 to 5% MeOH/CH_2Cl_2) to remove sulfonamide-based byproducts. Analysis of the combined fractions by ^{1}H NMR indicated a ca. 4:1 mixture of ((*S*)-spiroxindole (**27**) + (*R*)-hydroxylindolenine (**26**)): (*S*)-hydroxylindolenine (**28**).



A solution of the napthyl oxaziridine (**31**) (10.1 mg, 10.8 μmol) in CH_2Cl_2 (200 μL) was added dropwise to a 0 ºC stirring solution of methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-8-oxo-3,7,7a,8,10,11,12,12a,13,13a,14,15-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**25**) (5.0 mg, 3.24 μmol) in CH_2Cl_2 (340 μL). The reaction mixture was stirred at room temperature for 14 h, at which point TLC indicated complete consumption of starting material. The crude mixture was passed through a quick plug of silica (1 mL) (1% MeOH/CH_2Cl_2 to 5% MeOH/CH_2Cl_2) to remove sulfonamide-based byproducts. Analysis of the combined fractions by ^{1}H NMR indicated a ca. 1:1 mixture of ((*S*)-spiroxindole (**27**) + (*R*)-hydroxylindolenine (**26**)): (*S*)-hydroxylindolenine (**28**).

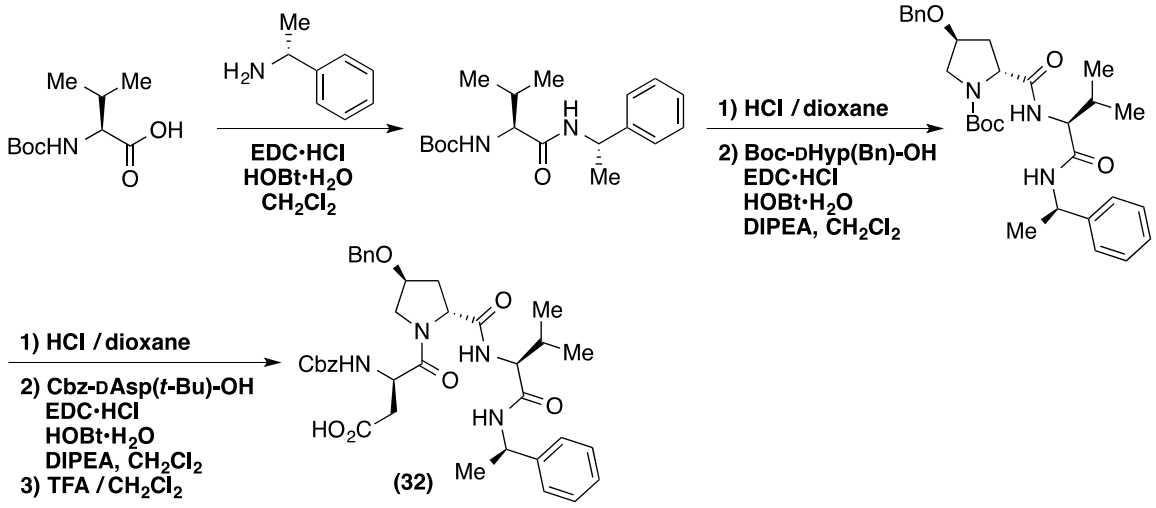


(*E*)-*N*-benzylidenenaphthalene-2-sulfonamide (S2). Following the general procedure reported by Davis,[26] a neat mixture of naphthalene-2-sulfonamide (1.04 g, 5.00 mmol) and benzaldehyde dimethylacetal (750 μL, 5.00 mmol) was stirred at 150 ºC under a slight flow of N_2 for 1 h. The reaction solution was allowed to cool to room temperature and the resulting pale yellow solid recrystallized from CH_2Cl_2/Hex. Collection of the solid by vacuum filtration afforded the title compound (1.22 g, 4.11 mmol, 83%) as a colorless solid. TLC (hexanes:EtOAc, 4:1 v/v); R_f=0.19; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 9.11 (s, 1H), 8.61 (s, 1H), 8.01–7.88 (m, 6H), 7.69–7.57 (m, 3H), 7.50–7.44 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.5, 135.2, 135.0, 135.0, 132.3, 132.3, 132.1, 131.3, 129.6, 129.4, 129.4, 129.2, 129.1, 127.9, 127.6, 122.9; IR (NaCl, thin film) ν_{max}: 1597, 1575, 1450, 1348, 1320, 1155, 1130, 1073, 860, 818, 788, 756, 672, 639; HRMS-ESI calcd for $C_{77}H_{14}NO_2S_1$ ($[M+H]^+$): 296.0740, found 296.0741.



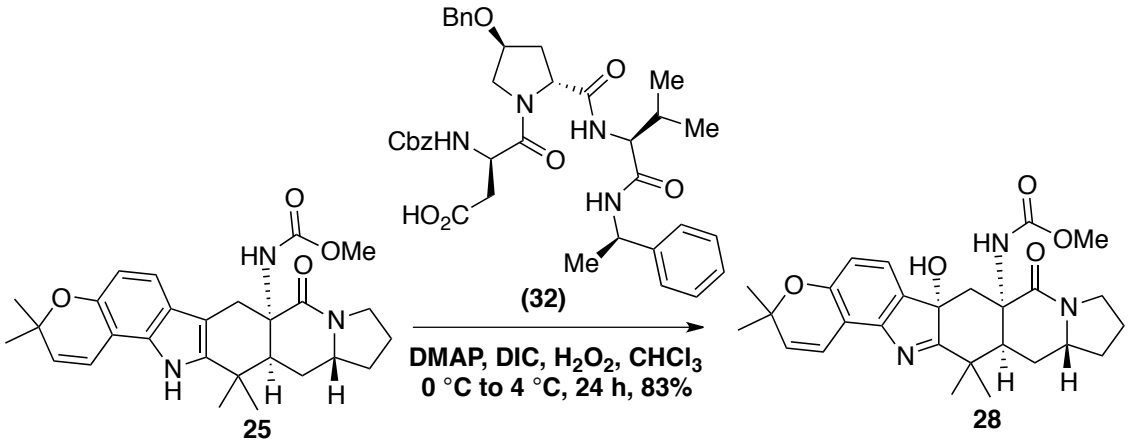
2-(naphthalen-2-ylsulfonyl)-3-phenyl-1,2-oxaziridine (31). Following the procedure reported by Davis,[26] a mixture of the (*E*)-*N*-benzylidenenaphthalene-2-sulfonamide (**S2**) (300 mg, 1.02 mmol), benzyltriethylammonium bromide (30.5 mg, 1.12 mmol) and saturated aqueous $NaHCO_3$ (3.0 mL) was stirred vigorously at 0 ºC. A solution of *m*CPBA (193 mg, 1.12 mmol) in CH_2Cl_2 (3.0 mL) was then added drop-wise over 30 min, after which the cloudy mixture was stirred another 30 min at 0 ºC. The reaction mixture was subsequently diluted with EtOAc (60 mL) and washed with H_2O, 10% aq. $Na_2S_2O_3$, and brine. The combined organic extracts were concentrated *in vacuo* and the resulting residue purified by silica gel chromatography (10% EtOAc/Hex), using 10 mL silica to yield the title compound

(220 mg, 707 μmol, 69%) as a colorless solid. TLC (hexanes:EtOAc, 4:1 v/v); R_f=0.31; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.64 (s, 1H), 8.11–7.93 (m, 4H), 7.78–7.60 (m, 2H), 7.51–7.36 (m, 5H), 5.54 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 136.1, 132.1, 131.8, 131.6, 131.5, 130.6, 130.0, 129.8, 129.8, 128.8, 128.3, 128.2, 128.0, 76.5; IR (NaCl, thin film) ν_{max}: 1348, 1240, 1167, 747; HRMS-ESI calcd for $C_{17}H_{13}NO_3NaS$ ($[M+Na]^+$): 334.0508, found 334.0520.



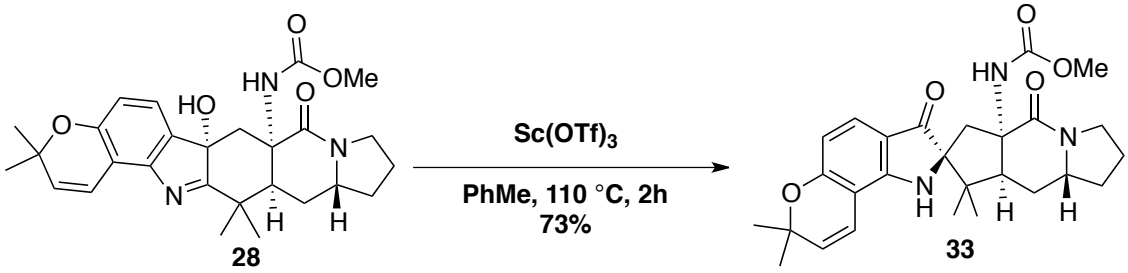
Cbz-DAsp-DHyp(Bn)-Val-(*R*)-Mba (32). *N*-Boc-valine (300 mg, 1.38 mmol), EDC•HCl (291 mg, 1.52 mmol), and HOBt•H_2O (232 mg, 1.52 mmol) were suspended in CH_2Cl_2 (7 mL). (*R*)-α-methylbenzylamine (328 μL, 2.60 mmol) was added and the reaction mixture was stirred vigorously. After 4 h, the reaction was diluted with EtOAc (90 mL) and washed with aqueous citric acid (10% w/w, 30 mL), water (30 mL), saturated aqueous $NaHCO_3$ (30 mL), then brine (90 mL). The organic portion was dried over $MgSO_4$ and filtered, then concentrated *in vacuo*. The resulting solid was dissolved in 4.0 M HCl/dioxane (2.8 mL). After 45 min, the mixture was concentrated under a stream of N_2, then *in vacuo*. The residue was dissolved in CH_2Cl_2 with Boc-DHyp(Bn)-OH[35] (488 mg, 1.52 mmol), EDC•HCl (291 mg, 1.52 mmol), and HOBt•H_2O (232 mg, 1.52 mmol). Diisopropylethylamine (262 μL, 1.52 mmol) was added, then the resulting suspension was stirred for 12 h. The work-up procedure and Boc removal were conducted as described previously. To the resulting solid were added Cbz-DAsp(*t*-Bu)-OH (491 mg, 1.52 mmol), EDC•HCl (291 mg, 1.52 mmol), and HOBt•H_2O (232 mg, 1.52 mmol), followed by CH_2Cl_2 (7 mL). Diisopropylethylamine (262 μL, 1.52 mmol) was added, then the resulting suspension was stirred vigorously. After 12 h, the

reaction was processed as before, then the resulting oil was dissolved in a 1:1 mixture of trifluoroacetic acid and CH_2Cl_2 (9 mL total volume). After 1 h, the solution was concentrated under a stream of N_2, then *in vacuo*. Initial purification was conducted by silica gel chromatography (150 mL of silica, 2 column volumes of 1%, 2%, then 5% MeOH/CH_2Cl_2, all buffered with 1% AcOH). The resulting red oil was purified further by C-18 silica chromatography (120 grams C-18 silica, 5% MeOH/H_2O for 1 CV, 5% to 50% MeOH/H_2O over 2 CV, 50% to 100% MeOH/H_2O over 9 CV, then 100% MeOH for 1 CV) to give the title compound as a white solid (536 mg, 58% yield). TLC (10% MeOH/CH_2Cl_2 with 1% AcOH buffer); R_f =0.54; $[\alpha]_D^{20}$ +23.0° (c = 1.0, MeOH); ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.37–7.25 (m, 14H), 7.23–7.19 (m, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 5.52 (d, *J* = 9.2 Hz, 1H), 5.10 (p, *J* = 7.2 Hz, 1H), 5.08–4.93 (m, 2H), 4.86 (td, *J* = 8.8, 5.3 Hz, 1H), 4.67 (t, *J* = 7.2 Hz, 1H), 4.52–4.37 (m, 2H), 4.09–4.01 (m, 3H), 3.68–3.62 (m, 1H), 2.75 (**AB**X, J_{AX} = 5.4 Hz, J_{BX} = 8.4 Hz, J_{AB} = 16.2 Hz, ν_{AB} = 93.0 Hz, 2H), 2.30 (dt, *J* = 11.8, 5.6 Hz, 1H), 2.23–2.09 (m, 2H), 1.46 (d, *J* = 6.9 Hz, 3H), 0.94 (d, *J* = 6.7 Hz, 3H), 0.90 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 173.0, 171.8, 171.2, 171.0, 155.6, 143.1, 137.7, 136.1, 128.6, 128.6, 128.5, 128.3, 128.0, 127.9, 127.7, 127.3, 126.1, 76.5, 71.0, 67.2, 59.7, 59.49, 52.3, 49.2, 49.1, 37.5, 35.2, 29.7, 22.1, 19.5, 18.4; IR (NaCl, thin film) ν_{max}: 3274, 2931, 1720, 1655, 1616, 1524, 1432, 1313, 1281, 1238, 1201, 1131, 1075, 1053; HRMS (ESI) (*m/z*) $[M+H]^+$ calculated for $C_{37}H_{45}N_4O_8$, 673.3232; found, 673.3213; $[M+Na]^+$ calculated for $C_{37}H_{44}N_4NaO_8$, 695.3051; found, 695.2994.



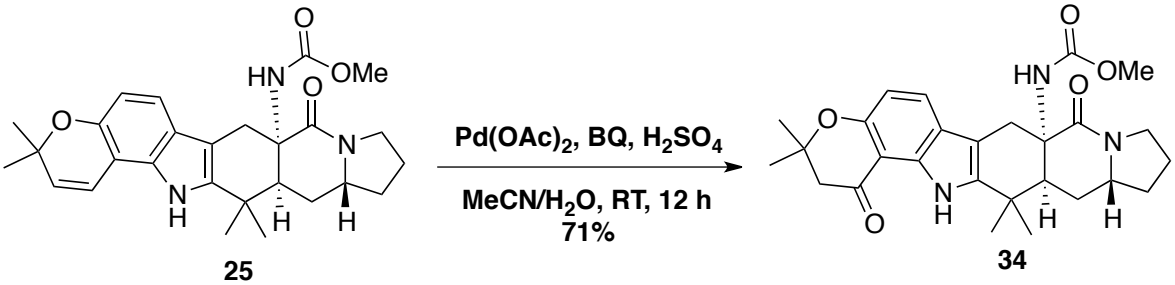
methyl ((6b*S*,7a*S*,12a*R*,13a*S*)-6b-hydroxy-3,3,14,14-tetramethyl-8-oxo-3,6b,7,7a,8,10,11,12,12a,13,13a,14-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (28). *N,N*-diisopropyl carbodiimide (25.4 μL, 162 μmol) was added drop-wise to a 0 ºC stirring solution of methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-8-oxo-

3,7,7a,8,10,11,12,12a,13,13a,14,15-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**25**) (50.0 mg, 108 μmol), the peptide acid (**32**) (14.5 mg, 21.6 μmol) and 4-dimethylaminopyridine (13.2 mg, 108 μmol) in $CHCl_3$ (2.2 mL). 30% aq. H_2O_2 (27.6 μL, 270 μmol) was then added and the mixture stirred at 0 ºC for 5 minutes and then allowed to stand in the fridge (4 ºC) overnight. After 24 h, saturated aqueous $Na_2S_2O_3$ (1 mL) and saturated aqueous $NaHCO_3$ was added and the aqueous layer extracted with EtOAc) (3 x 2 mL). The combined organic extracts were concentrated *in vacuo*. Purification of resulting residue by silica gel chromatography (1% MeOH/CH_2Cl_2 to 2% MeOH/CH_2Cl_2 to 5% MeOH/CH_2Cl_2), using 20 mL silica, afforded the title compound (42.8 mg, 89.2 μmol, 83%) as an orange oil. TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.19; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.05 (d, *J* = 7.9 Hz, 1H), 6.99 (d, *J* = 9.9 Hz, 1H), 6.82 (s, 1H), 6.58 (d, *J* = 7.9 Hz, 1H), 5.74 (d, *J* = 9.9 Hz, 1H), 3.95–3.81 (m, 1H), 3.68 (s, 3H), 3.26–3.11 (m, 3H), 2.79 (s, 1H), 2.66 (d, *J* = 15.2 Hz, 1H), 2.06–1.83 (m, 4H), 1.78 (d, *J* = 15.2 Hz, 1H), 1.73 (s, 3H), 1.56–1.51 (m, 1H) 1.45 (s, 3H), 1.44 (s, 3H), 1.36 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 187.8, 169.6, 155.5, 154.7, 148.2, 133.3, 131.7, 121.7, 117.9, 114.7, 113.5, 82.7, 76.6, 59.8, 54.5, 52.0, 45.2, 44.8, 42.3, 41.8, 41.2, 32.9, 28.2, 28.1, 27.0, 26.7, 24.7, 23.6, 22.1; IR (NaCl, thin film) ν_{max}: 3392, 2972, 1717, 1637, 1508, 1455, 1270; HRMS-ESI calcd for $C_{27}H_{34}N_3O_5$ ($[M+H]^+$): 480.2493, found 480.2492.



methyl ((2'*S*,5a*S*,8a*S*,9a*R*)-7',7',8,8-tetramethyl-3',5-dioxo-1,2,3,3',5,5a,6,7',8,8a,9,9a-dodecahydro-1'*H*-spiro[cyclopenta[*f*]indolizine-7,2'-pyrano[2,3-*g*]indol]-5a-yl)carbamate (33). Following Movassaghi's protocol,[29] $Sc(OTf)_3$ (41.0 mg, 83.4 μmol) was added in one portion to a solution of methyl ((6b*S*,7a*S*,12a*R*,13a*S*)-6b-hydroxy-3,3,14,14-tetramethyl-8-oxo-3,6b,7,7a,8,10,11,12,12a,13,13a,14-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**28**) (20.0 mg, 41.7 μmol) in toluene (8.3 mL)

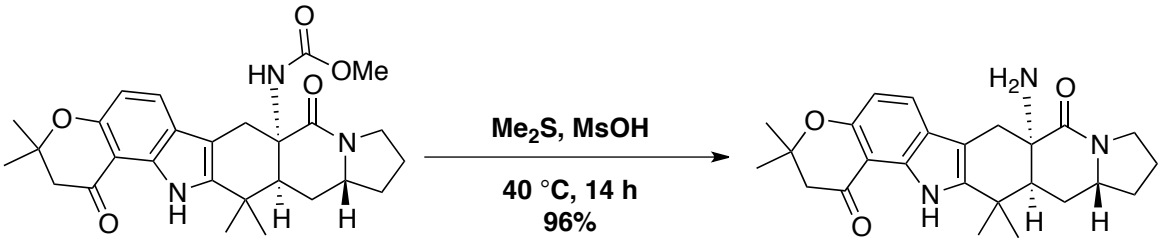
under N_2. The resulting solution was heated to 110 ºC for 2 h, then cooled to room temperature. Saturated aqueous $NaHCO_3$ (10 mL) was added and the aqueous layer extracted with EtOAc (3 x 10 mL) and the combined organic extracts dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (1% MeOH/CH_2Cl_2 to 10% MeOH/CH_2Cl_2), using 5 mL silica afforded the title compound (14.5 mg, 30.2 µmol, 73%) as a yellow-orange oil. TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.17; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.29 (d, *J* = 8.5 Hz, 1H), 6.38 (d, *J* = 9.9 Hz, 1H), 6.26–6.19 (m, 2H), 5.53 (d, *J* = 9.9 Hz, 1H), 5.13 (s, 1H), 3.88–3.75 (m, 1H), 3.72–3.63 (m, 1H), 3.59 (s, 3H), 3.42–3.31 (m, 1H), 3.15–3.06 (m, 1H), 2.51 (d, *J* = 15.2 Hz, 1H), 2.31–2.18 (m, 1H), 2.14 (d, *J* = 15.2 Hz, 1H), 2.10–2.05 (m, 1H), 2.03–1.96 (m, 2H), 1.85–1.69 (m, 1H), 1.65–1.50 (m, 1H), 1.45 (s, 3H), 1.41 (s, 3H), 1.14 (s, 3H), 0.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 203.5, 170.1, 161.1, 157.9, 156.5, 128.0, 125.9, 115.7, 114.1, 109.9, 104.0, 77.7, 77.3, 60.0, 58.1, 53.6, 52.0, 49.5, 45.7, 44.8, 42.2, 34.8, 28.5, 28.3, 25.7, 23.6, 22.7, 22.6, 22.2; IR (NaCl, thin film) ν_{max}: 3350, 2971, 1726, 1631, 1602, 1503, 1445, 1317, 1253, 1113; HRMS-ESI calcd for $C_{27}H_{34}N_3O_5$ ($[M+H]^+$): 480.2493, found 480.2494.



25 **34**

methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-1,8-dioxo-1,2,3,7,7a,8,10,11,12,12a,13,13a,14,15-tetradecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (34). A flask was charged with $Pd(OAc)_2$ (50.4 mg, 224 µmol) and *p*-benzoquinone (91.0 mg, 842 µmol, recrystallized from CH_2Cl_2/Hex). The flask was fitted with a septum, purged with N_2 (3x) and then MeCN (13.4 mL) and H_2O (4.06 mL) added via syringe to give an orange solution. H_2SO_4 (60.0 µL, 95% wt in H_2O) was then added via syringe and the resulting pale yellow solution was stirred at room temperature for 5 min. In a separate flask, methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-8-oxo-3,7,7a,8,10,11,12,12a,13,13a,14,15-dodecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**25**) (260 mg, 561 µmol) was dissolved in MeCN (13.4 mL) under an N_2

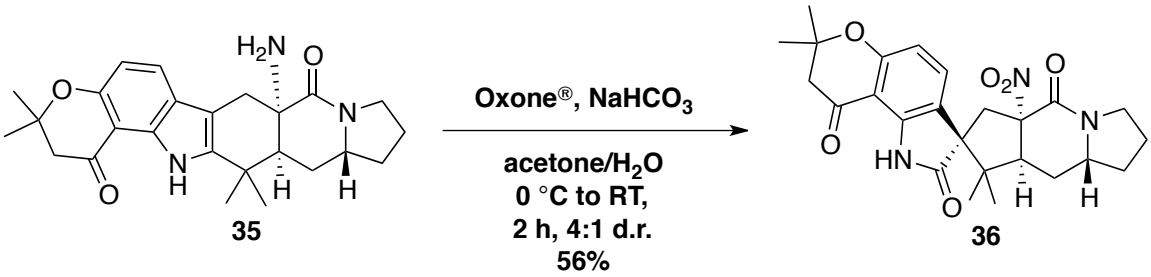
atmosphere. To this was added, drop-wise, the catalyst-containing solution prepared above and the resulting dark red mixture was stirred at room temperature. After 12 h, TLC analysis indicated complete consumption of starting material. The resulting dark brown reaction mixture was poured into saturated aqueous $NaHCO_3$ (120 mL) and the aqueous layer extracted with EtOAc (3 x 100 mL). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (1% MeOH/CH_2Cl_2 to 2% MeOH/CH_2Cl_2 to 5% MeOH/CH_2Cl_2), using 50 mL silica, afforded the title compound (190 mg, 396 μmol, 71%) as a brown foam. TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.14; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 9.73 (s, 1H), 7.47 (d, *J* = 8.5 Hz, 1H), 6.63 (d, *J* = 8.5 Hz, 1H), 4.94 (s, 1H), 4.00–3.89 (m, 1H), 3.59 (s, 3H), 3.53–3.44 (m, 1H), 3.32–3.21 (m, 1H), 3.11–3.01 (m, 2H), 2.82 (d, *J* = 16.6 Hz, 1H), 2.74 (s, 2H), 2.13–2.03 (m, 1H), 2.02–1.83 (m, 3H), 1.82–1.72 (m, 1H), 1.72–1.63 (m, 1H), 1.52–1.43 (m, 9H), 1.35 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 194.2, 170.6, 157.6, 156.4, 139.8, 134.0, 126.9, 121.5, 110.0, 105.3, 102.6, 79.6, 59.6, 54.7, 52.0, 48.8, 44.8, 39.3, 34.5, 33.1, 30.1, 28.5, 28.0, 26.7, 26.6, 25.5, 22.0; IR (NaCl, thin film) ν_{max}: 3443, 2970, 1729, 1655, 1619, 1581, 1458, 1370, 1289, 1210; HRMS-ESI calcd for $C_{27}H_{34}N_3O_5$ ($[M+H]^+$): 480.2493, found 480.2492.



34 **35**

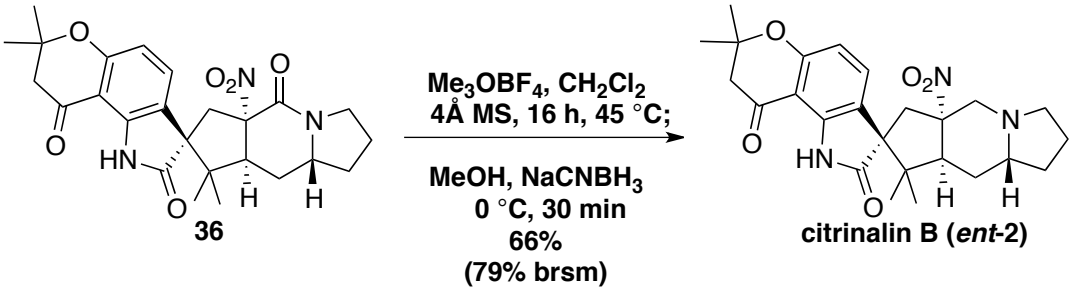
(7a*S*,12a*R*,13a*S*)-7a-amino-3,3,14,14-tetramethyl-2,3,7,7a,11,12,12a,13,13a,14-decahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazole-1,8(10*H*,15*H*)-dione (35). Dimethylsulfide (400 μL, 5.42 mmol) was added to a solution of methyl ((7a*S*,12a*R*,13a*S*)-3,3,14,14-tetramethyl-1,8-dioxo-1,2,3,7,7a,8,10,11,12,12a,13,13a,14,15-tetradecahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazol-7a-yl)carbamate (**34**) (130 mg, 271 μmol) in MsOH (5.4 mL). The reaction mixture was stirred at 40 ºC for 14 h. After cooling to room temperature, the resulting dark red reaction mixture was slowly added to a 0 ºC stirring mixture of EtOAc (100 mL) and saturated aqueous $NaHCO_3$ (100 mL). The aqueous layer was extracted with EtOAc (4 x 100 mL) and the combined organic extracts were dried

with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (2% MeOH/CH_2Cl_2 to 5% MeOH/CH_2Cl_2), using 40 mL silica, afforded the title compound (110 mg, 261 μmol, 96%) as a yellow foam. TLC (MeOH:CH_2Cl_2, 1:9 v/v); R_f=0.17; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 9.72 (s, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 6.63 (d, *J* = 8.4 Hz, 1H), 3.86–3.74 (m, 1H), 3.59–3.49 (m, 1H), 3.40–3.29 (m, 1H), 2.96 (d, *J* = 15.8 Hz, 1H), 2.76 (br s, 2H), 2.69 (d, *J* = 15.8 Hz, 1H), 2.19 (s, 2H), 2.07–1.83 (m, 5H), 1.83–1.73 (m, 1H), 1.66 (s, 3H), 1.59–1.51 (m, 1H), 1.49 (s, 3H), 1.48 (s, 3H), 1.36 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ = 194.2, 173.7, 157.5, 138.8, 134.2, 127.2, 122.2, 109.7, 105.3, 104.7, 79.5, 57.6, 54.3, 48.8, 44.9, 44.8, 34.9, 34.4, 30.8, 30.4, 28.2, 26.8, 26.7, 26.6, 22.0; IR (NaCl, thin film) ν_{max}: 3443, 3372, 2971, 1652, 1579, 1459, 1370, 1285, 1209; HRMS-ESI calcd for $C_{25}H_{32}N_3O_3$ ([M+H]$^+$): 422.2438, found 422.2442.



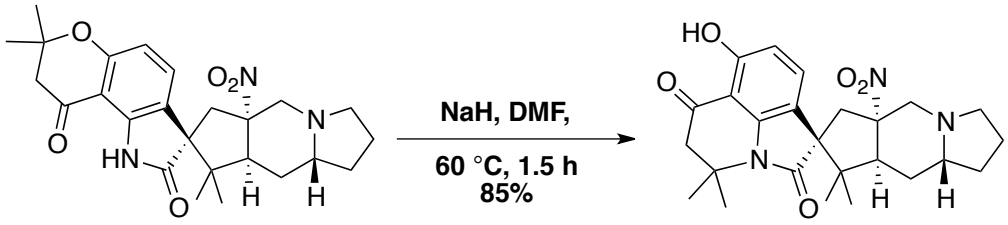
(3'*R*,5a*S*,8a*S*,9a*R*)-7',7',8,8-tetramethyl-5a-nitro-2,3,5a,6,7',8,8a,8',9,9a-decahydro-1'*H*-spiro[cyclopenta[*f*]indolizine-7,3'-pyrano[2,3-*g*]indole]-2',5,9'(1*H*)-trione (36). A saturated aqueous solution of $NaHCO_3$ (3.0 mL) was added to a solution of (7a*S*,12a*R*,13a*S*)-7a-amino-3,3,14,14-tetramethyl-2,3,7,7a,11,12,12a,13,13a,14-decahydroindolizino[6,7-*h*]pyrano[3,2-*a*]carbazole-1,8(10*H*,15*H*)-dione (**35**) (40.0 mg, 95.0 μmol) in acetone (4.0 mL) at 0 ºC, resulting in precipitate formation. A solution of Oxone® (145 mg, 950 μmol) in deionized water (2.00 mL) was added drop-wise and the mixture was warmed to room temperature by allowing the ice bath to expire. After 2 h, the resulting mixture was diluted with deionized water (40 mL) and extracted with ethyl acetate (3 x 40 mL). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (1% MeOH/CH_2Cl_2), using 10 mL silica, afforded the title compound (25 mg, 53.5 μmol, 56%) as a yellow foam and ca. 4:1 mixture of diastereomers. X-ray quality crystals of the major diastereomer were obtained from slow evaporation of a dilute solution in 5% MeOH/Et_2O. m.p.: 174–176 ºC; TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.38; ^{1}H NMR (500 MHz, $CDCl_3$, major diastereomer) δ = 9.30 (s, 1H), 7.14

(d, *J* = 8.3 Hz, 1H), 6.52 (d, *J* = 8.3 Hz, 1H), 3.87–3.83 (m, 1H), 3.79–3.66 (m, 2H), 3.61 (d, *J* = 16.6 Hz, 1H), 3.55–3.49 (m, 1H), 2.71 (s, 2H), 2.65 (d, *J* = 16.6 Hz, 1H), 2.44–2.36 (m, 1H), 2.26–2.15 (m, 2H), 2.10–2.03 (m, 1H), 1.90–1.79 (m, 1H), 1.65–1.55 (m, 1H), 1.48 (s, 3H), 1.47 (s, 3H), 1.15 (s, 3H), 0.91 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, major diastereomer) δ = 193.7, 180.7, 163.3, 159.7, 143.3, 132.6, 118.7, 109.8, 105.2, 93.9, 79.7, 59.3, 57.9, 50.2, 49.7, 48.8, 45.9, 40.0, 35.0, 26.9, 26.8, 25.6, 22.8, 22.5, 22.2; IR (NaCl, thin film) ν_{max}: 3402, 2976, 1724, 1652, 1619, 1555, 1463, 1374, 1320, 1257, 1216; HRMS-ESI calcd for $C_{25}H_{29}N_3O_6Na$ ([M+Na]$^+$): 490.1949, found 490.1954.



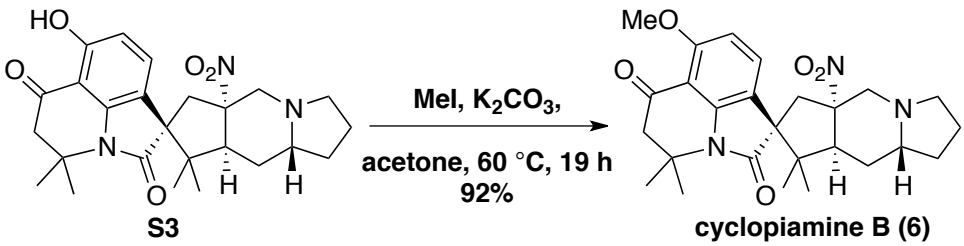
***ent*-Citrinalin B (*ent*-2).** A Schlenk tube was charged with (3'*R*,5a*S*,8a*S*,9a*R*)-7',7',8,8-tetramethyl-5a-nitro-2,3,5a,6,7',8,8a,8',9,9a-decahydro-1'*H*-spiro[cyclopenta[*f*]indolizine-7,3'-pyrano[2,3-*g*]indole]-2',5,9'(1*H*)-trione (**36**) (10.0 mg, 21.4 μmol), Me_3OBF_4 (38.0 mg, 257 μmol) and activated 4 Å MS (100 mg). CH_2Cl_2 (1.5 mL) was added via syringe and the mixture was stirred at 45 ºC for 16 h. After cooling to 0 ºC, anhydrous MeOH (1.5 mL) was added drop-wise followed by $NaCNBH_3$ (20.0 mg, 321 μmol) in one portion. After 5 min, more $NaCNBH_3$ (15.0 mg, 241 μmol) was added in one portion and the reaction mixture stirred at 0 ºC for 30 min. The resulting reaction mixture was subsequently quenched by the addition of saturated aqueous $NaHCO_3$ (3.0 mL) and extracted with EtOAc (4 x 3.0 mL). The combined organic extracts dried with Na_2SO_4, filtered and concentrated *in vacuo*. The reaction mixture was subsequently diluted with CH_2Cl_2 and passed through a short column containing silica (2 mL) with 1% MeOH/CH_2Cl_2. The fractions containing the product were collected and concentrated *in vacuo*. Further purification of the filtrate via silica gel chromatography (1% to 2% MeOH/toluene), using 5 mL silica, afforded the title compound (6.4 mg, 14.1 μmol, 66% (79% brsm)) as a yellow oil. X-ray quality crystals of the HCl salt were obtained from a supersaturated solution of a 2:1 mixture of ethyl acetate and methanol. m.p.: 238–240 ºC (HCl salt, decomp). TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.38; $[\alpha]_D^{25}$ -125° (c = 2.53, MeOH); ^{1}H NMR (600 MHz, DMSO-d_6) δ = 10.12 (s, 1H), 7.51 (d, *J* = 8.3 Hz, 1H), 6.53 (d, *J* = 8.3 Hz, 1H), 3.67–3.59 (m, 2H), 2.93–2.85 (m, 1H), 2.84–2.78 (m, 1H),

2.78–2.72 (m, 1H), 2.71–2.60 (m, 3H), 2.00–1.81 (m, 4H), 1.75–1.60 (m, 3H), 1.40 (s, 3H), 1.38 (s, 3H), 1.25–1.15 (m, 1H), 0.98 (s, 3H), 0.70 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ = 192.6, 182.4, 158.7, 142.8, 132.7, 119.5, 108.8, 104.9, 94.6, 79.2, 64.1, 61.2, 58.3, 52.9, 48.7, 48.0, 43.9, 41.4, 30.9, 26.8, 26.3, 26.0, 22.9, 22.7, 20.8; IR (NaCl, thin film) ν_{max}: 3402, 2972, 2936, 1725, 1673, 1619, 1594, 1542, 1464, 1372, 1323; HRMS-ESI calcd for $C_{25}H_{32}O_5N_3$ ([M+H$^+$]): 454.2336, found 454.2344.



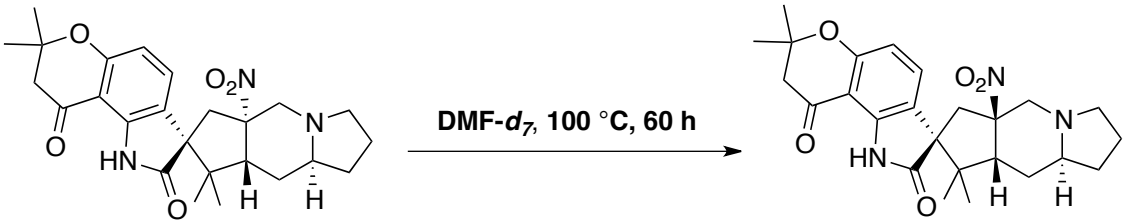
citrinalin B (*ent*-2) **S3**

(1'*R*,5a*S*,8a*S*,9a*R*)-7'-hydroxy-4',4',8,8-tetramethyl-5a-nitro-1,2,3,4',5,5a,5',6,8,8a,9,9a-dodecahydrospiro[cyclopenta[*f*]indolizine-7,1'-pyrrolo[3,2,1-*ij*]quinoline]-2',6'-dione (S3). To a solution of *ent*-citrinalin B (*ent*-**2**) (5.0 mg, 11.0 μmol) in anhydrous DMF (1.0 mL) was added NaH (1.32 mg, 33.0 μmol) as a solution in anhydrous DMF (100 μL) under an N_2 atmosphere. The resulting yellow solution was stirred at 60 ºC for 1.5 h. The reaction mixture was cooled to room temperature, poured into saturated aqueous NH_4Cl (1.0 mL) and the aqueous layer extracted with CH_2Cl_2 (4 x 1.0 mL). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (1% MeOH/CH_2Cl_2 to 2% MeOH/CH_2Cl_2), using 2 mL silica, afforded the title compound (4.3 mg, 9.35 μmol, 85%) as a yellow oil. TLC (MeOH:CH_2Cl_2, 1:19 v/v); R_f=0.35; ^{1}H NMR (600 MHz, $CDCl_3$) δ = 10.59 (s, 1H), 7.20 (d, *J* = 8.3 Hz, 1H), 6.48 (d, *J* = 8.3 Hz, 1H), 3.88 (d, *J* = 12.6 Hz, 1H), 3.81–3.77 (m, 1H), 3.00–2.94 (m, 1H), 2.88 (d, *J* = 15.8 Hz, 1H), 2.83 (d, *J* = 16.9 Hz, 1H), 2.56 (d, *J* = 16.9 Hz, 1H), 2.48 (d, *J* = 12.6 Hz, 1H), 2.38 (d, *J* = 15.8 Hz, 1H), 2.06–1.99 (m, 1H), 1.99–1.88 (m, 3H), 1.86–1.76 (m, 2H), 1.73 (s, 3H), 1.71–1.60 (m, 2H), 1.41 (s, 3H), 1.03 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 196.9, 181.1, 159.8, 147.6, 133.4, 116.4, 108.4, 104.2, 94.7, 65.5, 62.0, 61.6, 57.2, 53.7, 51.5, 49.6, 44.6, 43.2, 31.6, 27.5, 26.8, 24.1, 23.9, 23.2, 21.3; IR (NaCl, thin film) ν_{max}: 2970, 2937, 1717, 1651, 1605, 1542, 1487, 1370, 1242; HRMS-ESI calcd for $C_{25}H_{32}O_5N_3$ ([M+H$^+$]): 454.2336, found 454.2333.



S3 **cyclopiamine B (6)**

Cyclopiamine B (6). To a flame-dried vial containing (1'*R*,5a*S*,8a*S*,9a*R*)-7'-hydroxy-4',4',8,8-tetramethyl-5a-nitro-1,2,3,4',5,5a,5',6,8,8a,9,9a-dodecahydrospiro[cyclopenta[*f*]indolizine-7,1'-pyrrolo[3,2,1-*ij*]quinoline]-2',6'-dione (**S3**) (4.2 mg, 9.3 μmol) and K_2CO_3 (6.4 mg, 46 μmol) was added anhydrous acetone (1.0 mL) via syringe under an N_2 atmosphere. Iodomethane (0.7 μL, 11 μmol) was added as a solution in anhydrous acetone (100 μL) and the resulting mixture was heated to 60 ºC for 19 h. The reaction mixture was cooled to room temperature, poured into saturated aqueous $NaHCO_3$ (1.0 mL) and the aqueous layer extracted with CH_2Cl_2 (4 x 1.0 mL). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification of the resulting residue by flash chromatography (1% MeOH/CH_2Cl_2 to 2% MeOH/CH_2Cl_2), using 2 mL silica, afforded the title compound (4.0 mg, 8.6 μmol, 92%) as a yellow oil. X-ray quality crystals were obtained from a supersaturated solution of a 2:1 mixture of ethyl acetate and methanol. m.p.: 241–243 ºC (lit.[9] 245–246 ºC); TLC (MeOH:CH_2Cl_2, 1:19 v/v): R_f=0.37; $[\alpha]_D^{25}$ -97.9° (c = 1.90, MeOH); ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.22 (d, *J* = 8.3 Hz, 1H), 6.50 (d, *J* = 8.3 Hz, 1H), 3.93 (s, 3H), 3.92–3.88 (m, 1H), 3.85–3.81 (m, 1H), 3.02–2.96 (m, 1H), 2.93 (d, *J* = 15.8 Hz, 1H), 2.80 (d, *J* = 15.3 Hz, 1H), 2.55–2.48 (m, 2H), 2.39 (d, *J* = 15.8 Hz, 1H), 2.07–2.01 (m, 1H), 2.01–1.88 (m, 3H), 1.87–1.79 (m, 2H), 1.71 (s, 3H), 1.70–1.54 (m, 2H), 1.41 (s, 3H), 1.04 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 190.5, 180.3, 159.1, 149.1, 131.2, 118.6, 107.6, 103.4, 94.7, 65.5, 62.0, 60.7, 56.9, 56.3, 53.7, 53.6, 49.7, 44.6, 43.2, 31.6, 27.5, 26.6, 23.9, 23.8, 23.2, 21.3; IR (NaCl, thin film) ν_{max}: 2968, 2936, 1715, 1688, 1610, 1541, 1488, 1456, 1367, 1248; HRMS-ESI calcd for $C_{26}H_{34}O_5N_3$ ([M+H$^+$]): 468.2493, found 468.2497.



citrinalin A (1) citrinalin B (2)

Conversion of citrinalin A (1) to citrinalin B (2). An NMR tube was charged with a degassed (freeze, pump, thaw) solution of citrinalin A (**1**) (0.3 mg, 0.066 μmol) in DMF-d_7 (300 μL). The resulting solution was heated to 100 ºC. After 20 h, NMR shows ca. 1:1 ratio of citrinalin A (**1**) : citrinalin B (**2**) with complete conversion to citrinalin B (**2**) after 60 h. See **Figure S22** (below) for NMR studies.

IV. ^{1}H & ^{13}C NMR spectra for compounds 14-36, 2 and 6

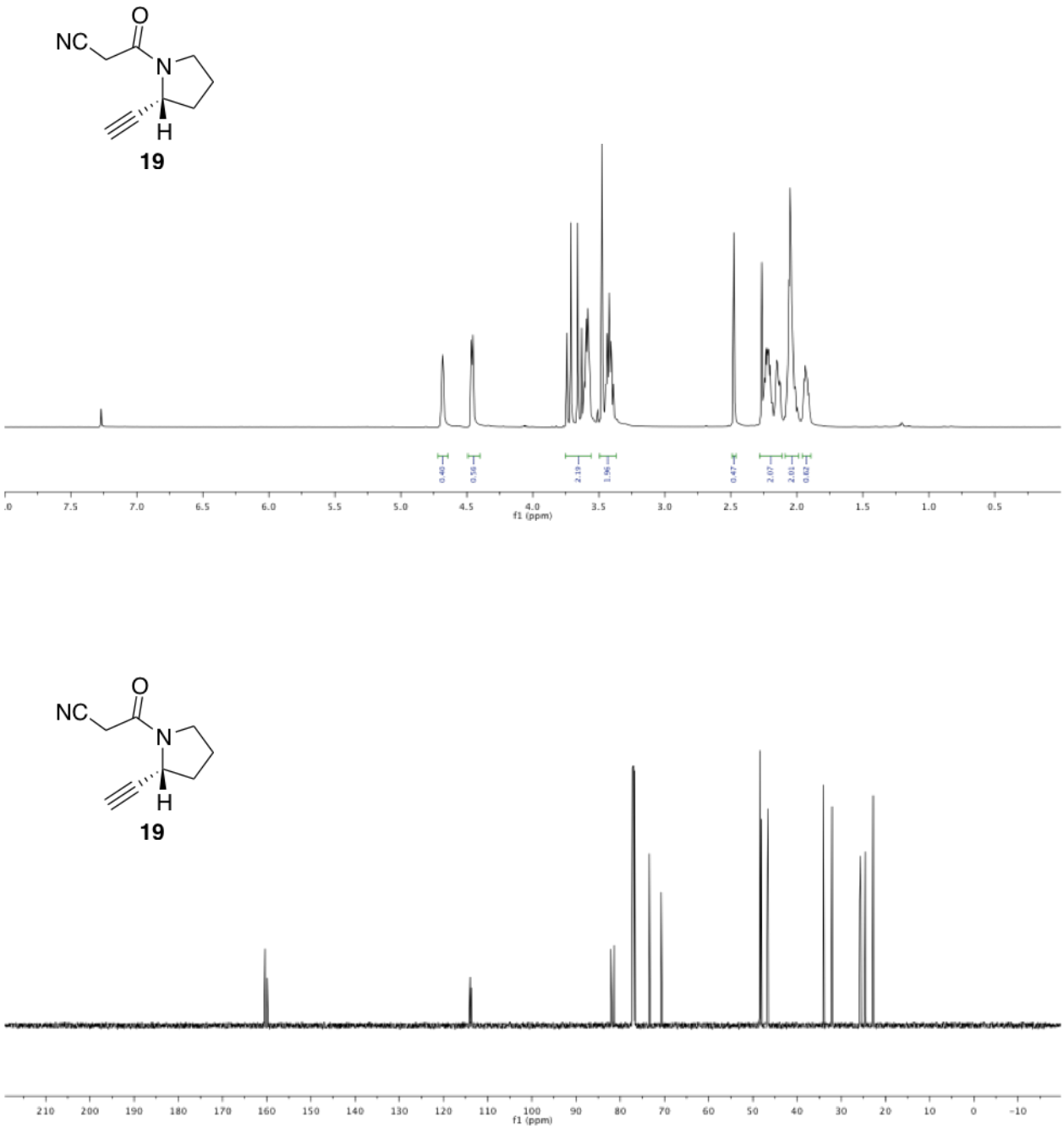
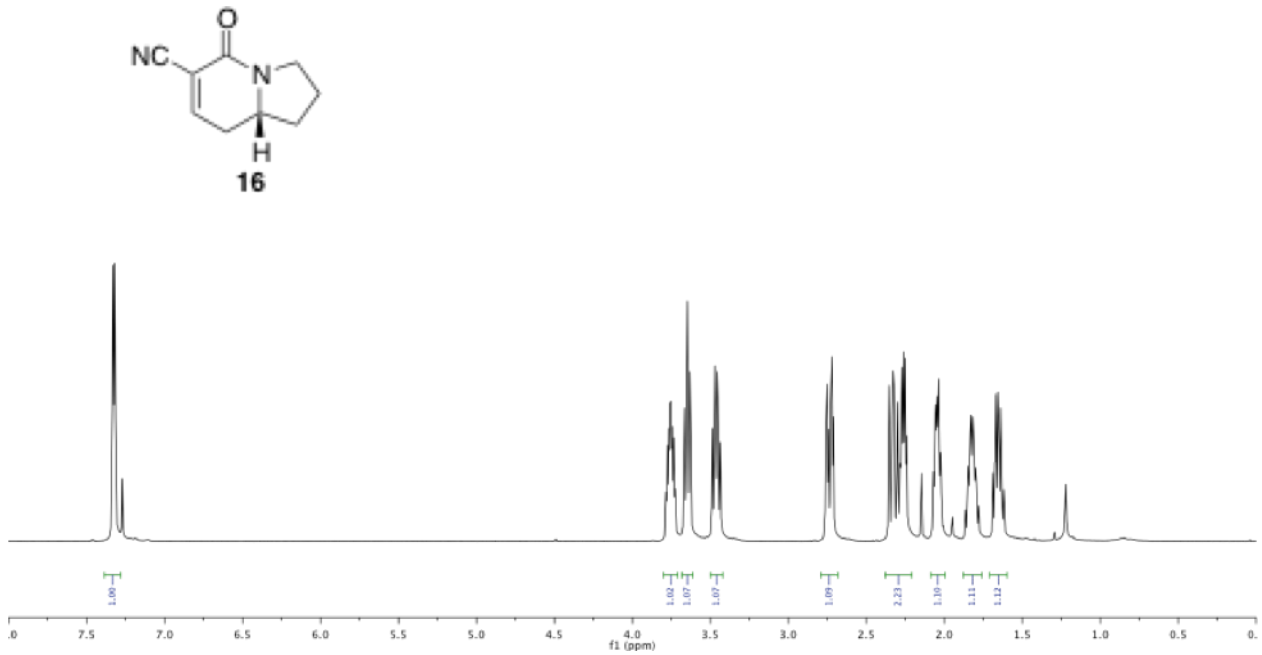


Figure S1. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **19**



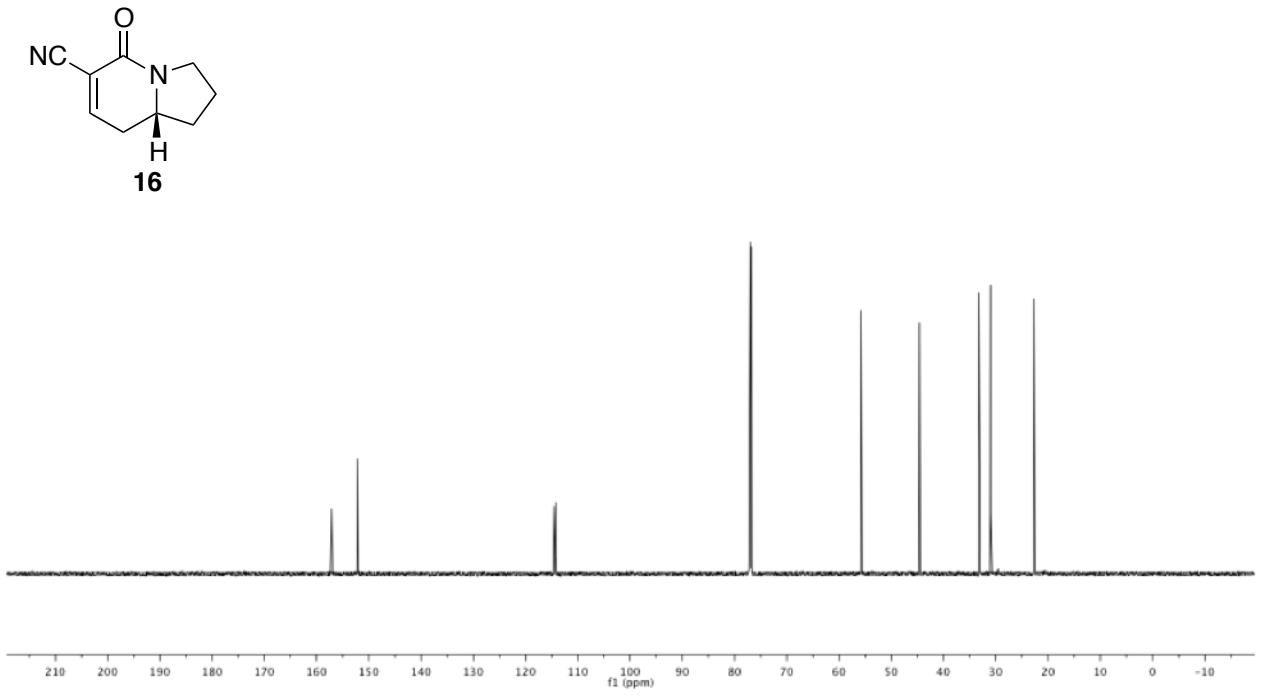


Figure S2. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **16**

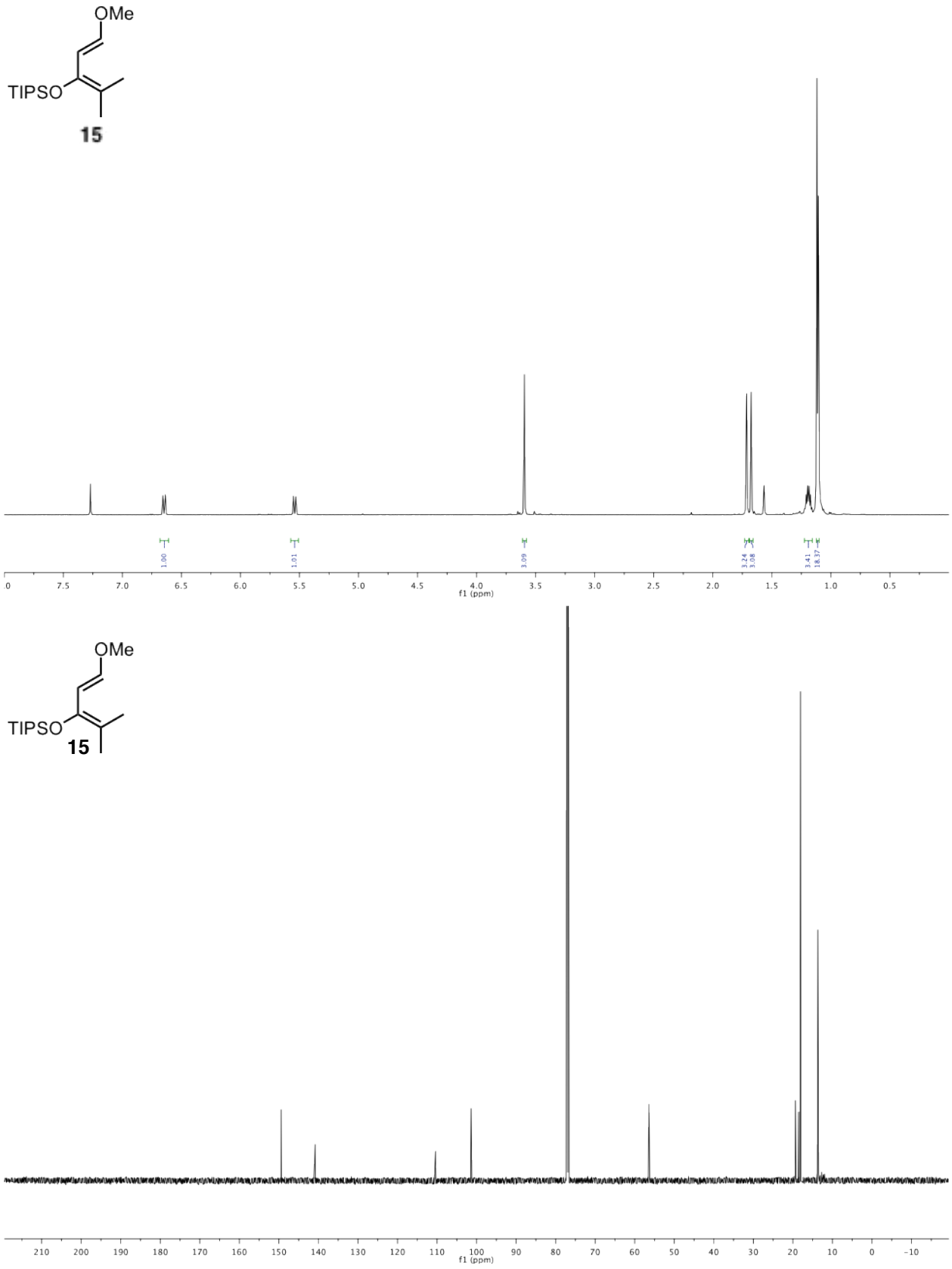


Figure S3. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **15**

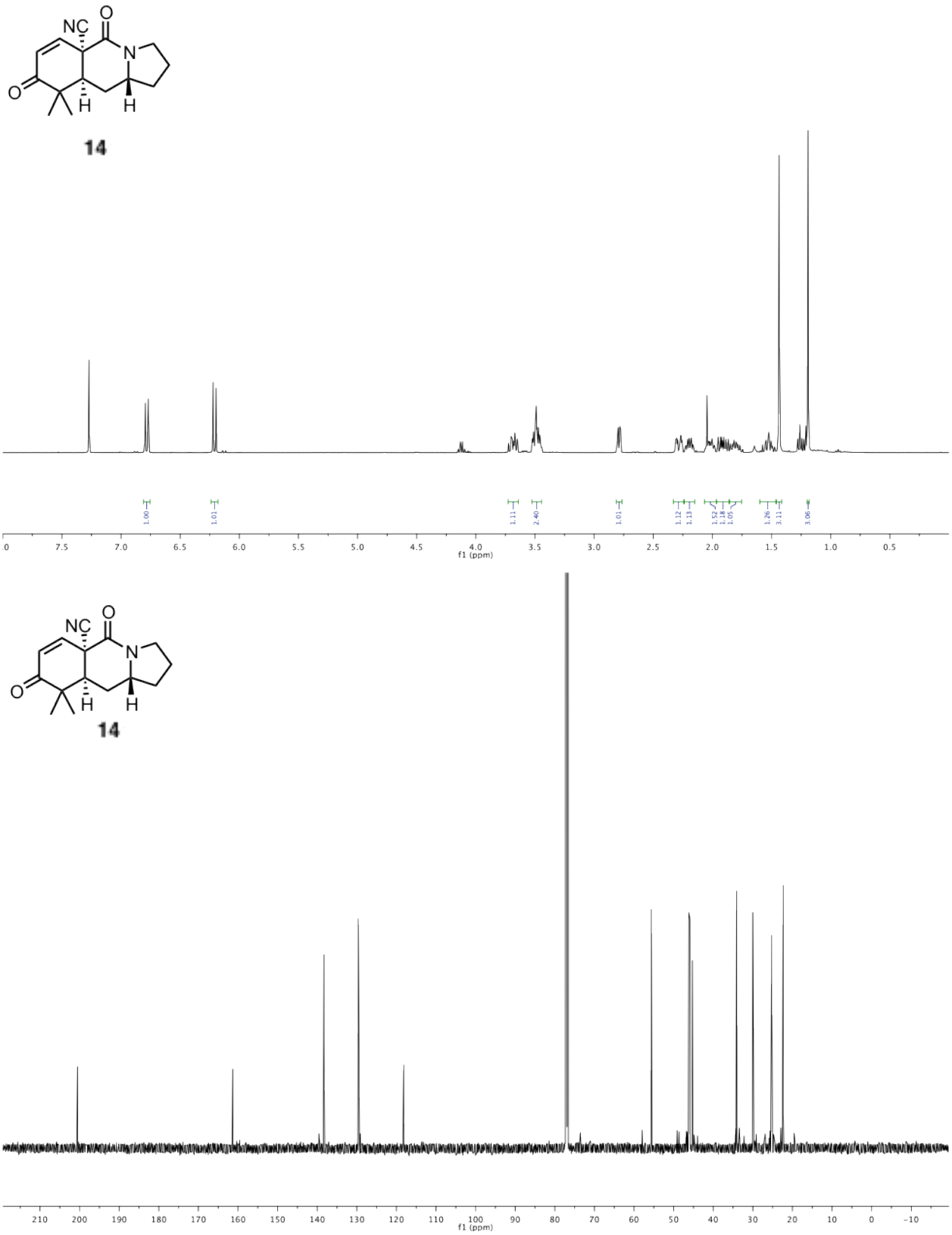
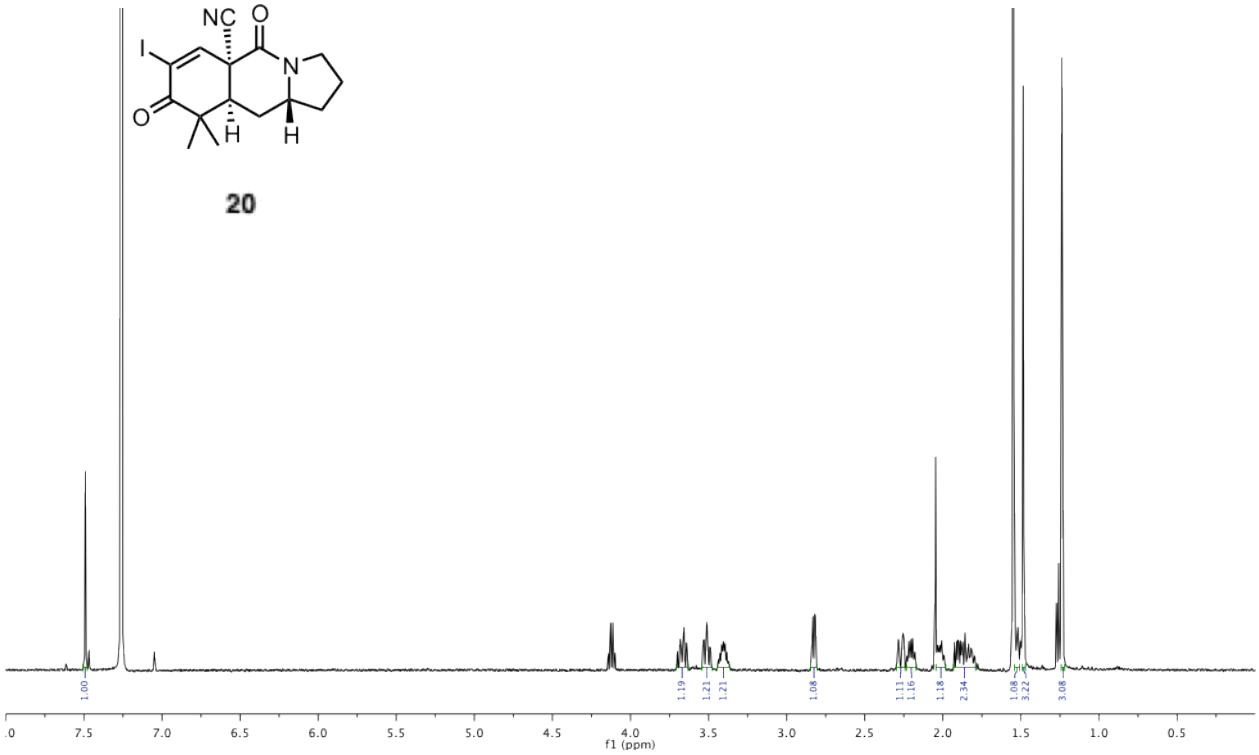


Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **14**



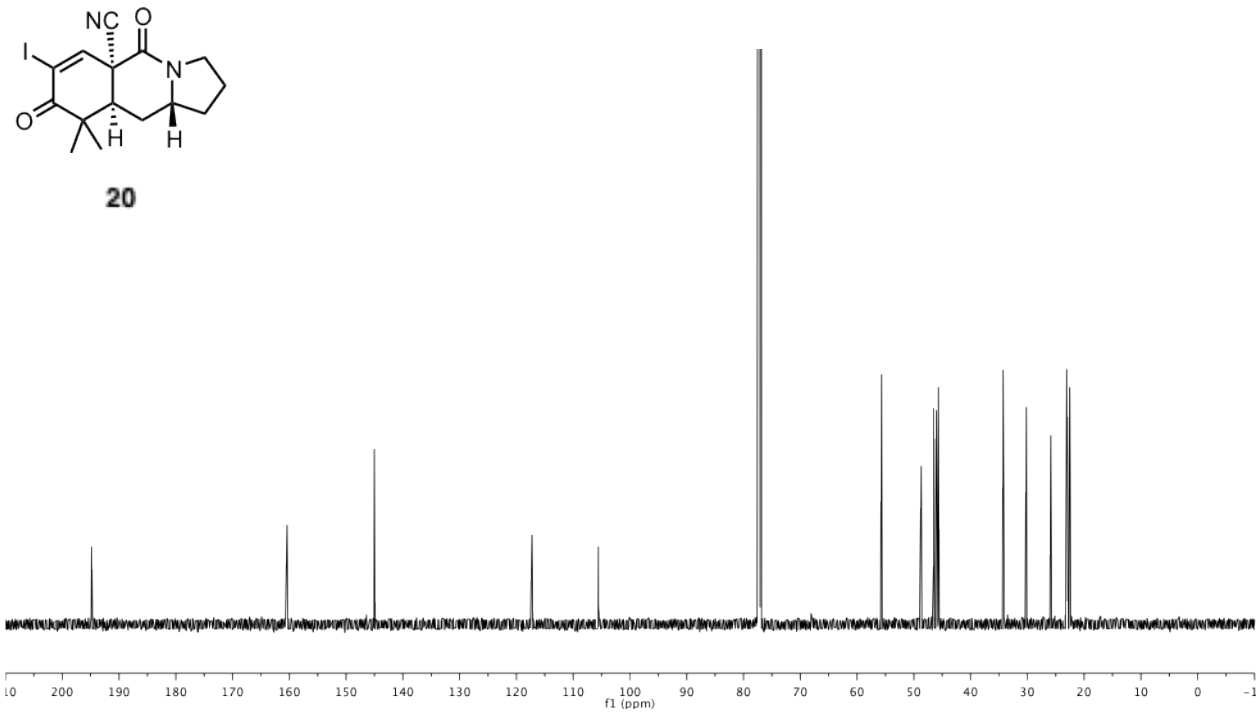


Figure S5. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **20**

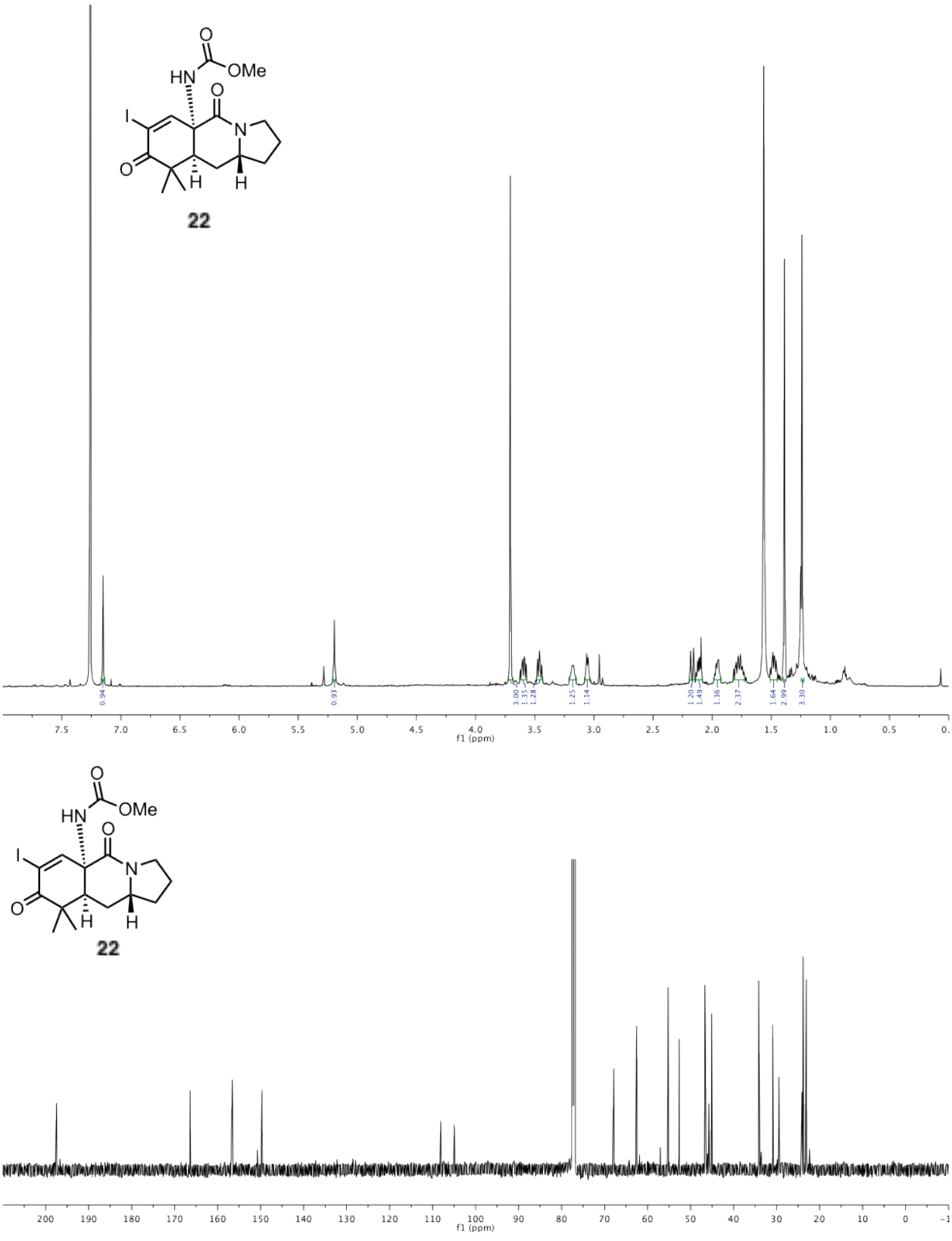


Figure S6. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **22**

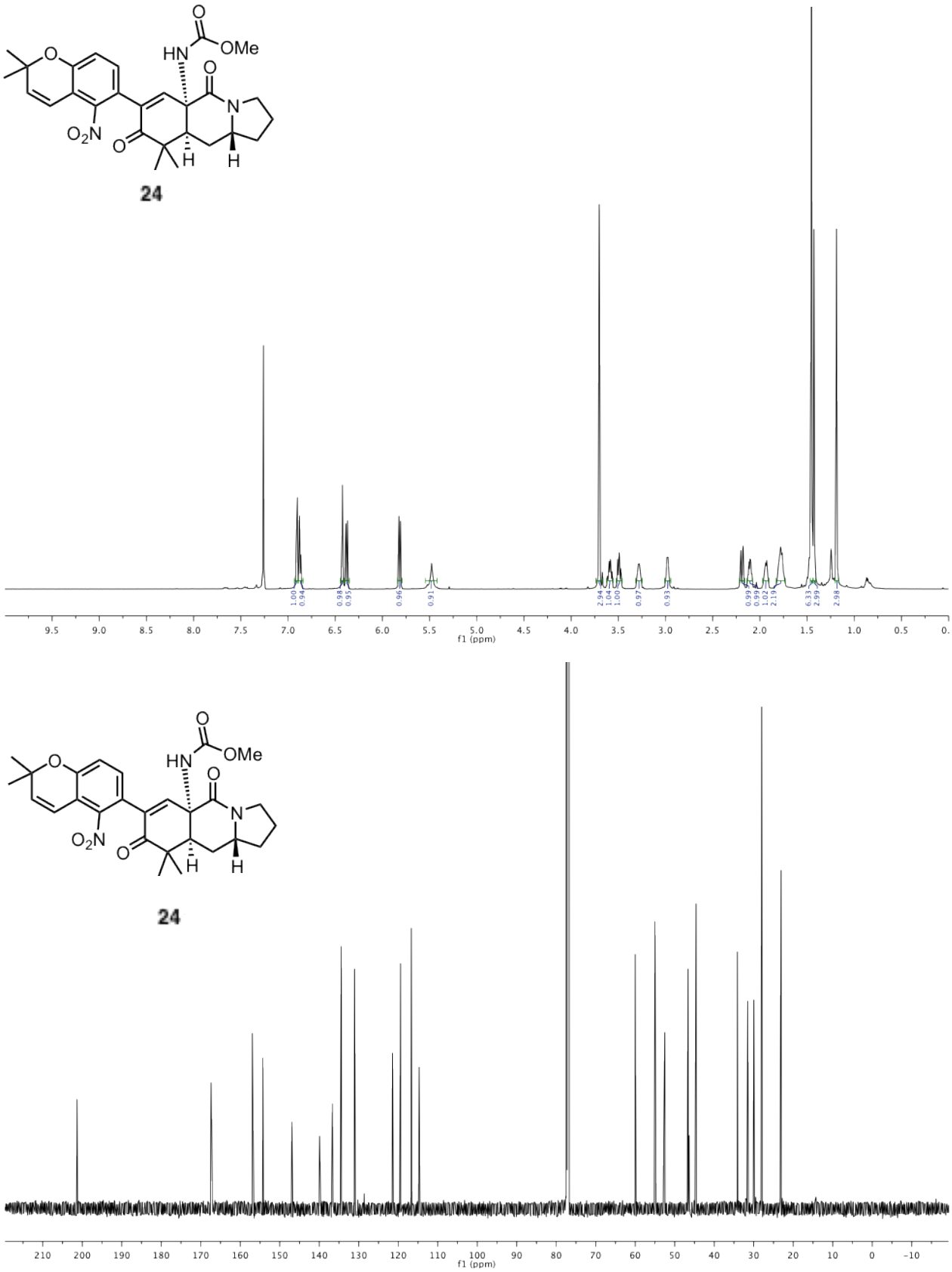


Figure S7. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **24**

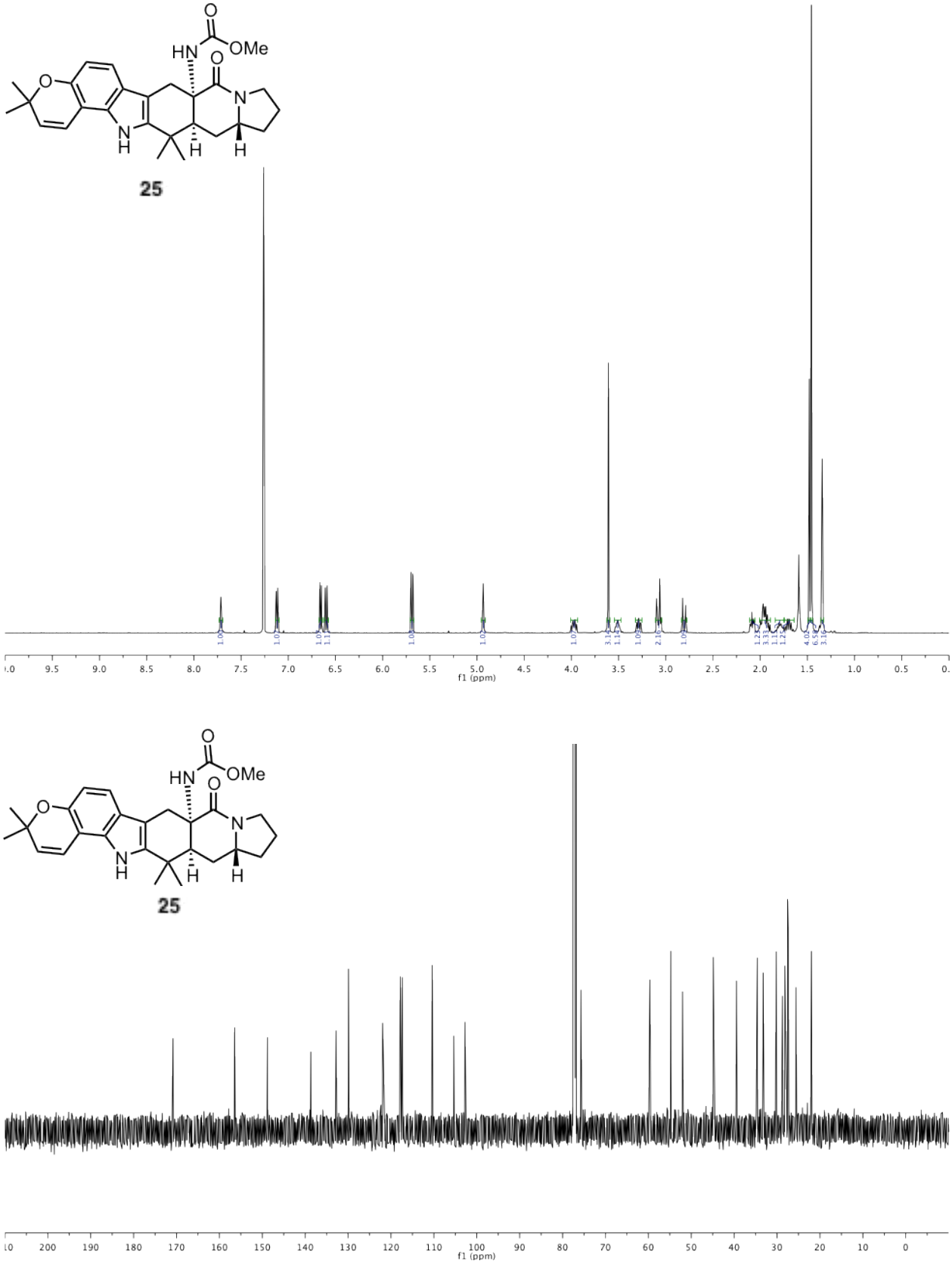


Figure S8. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **25**

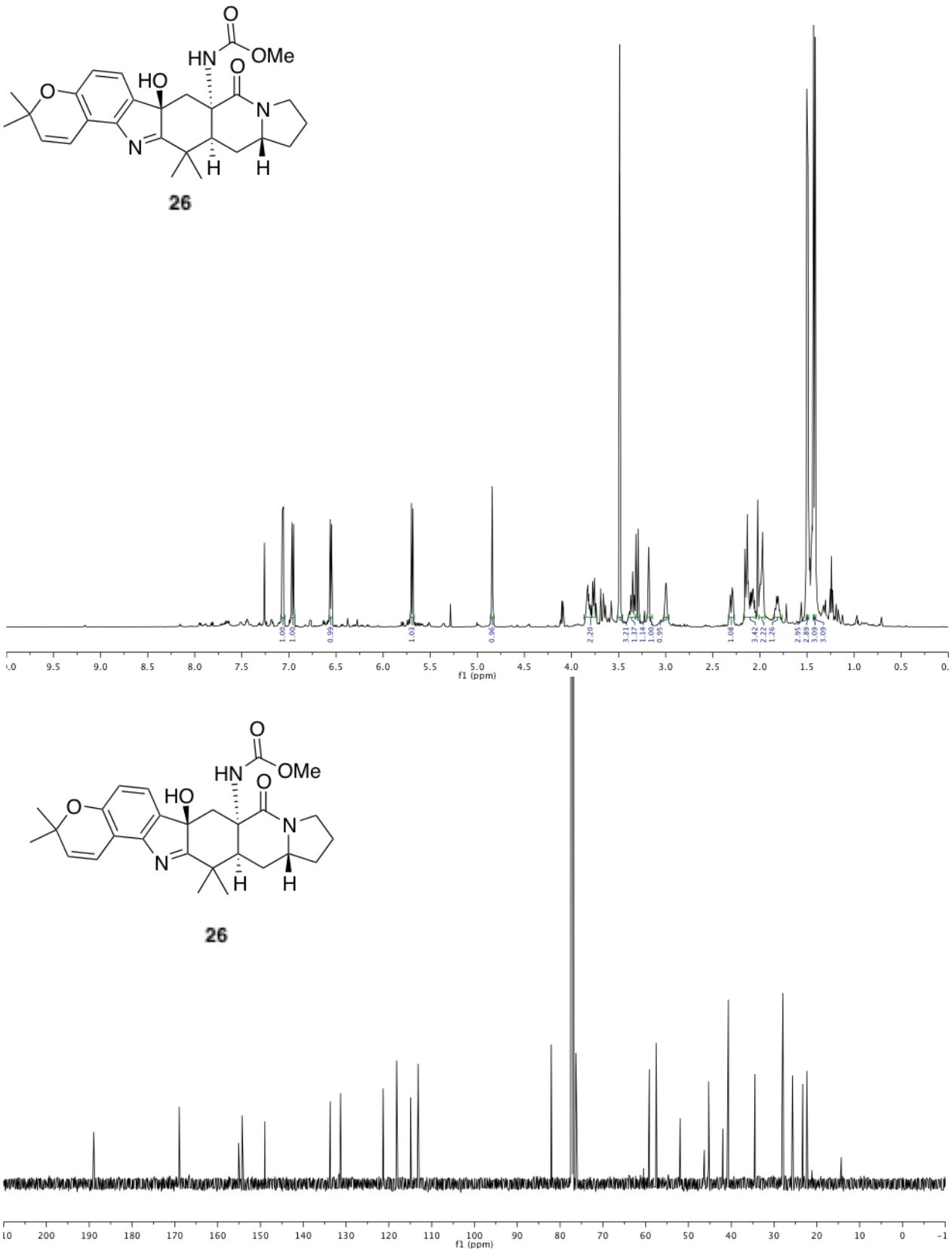


Figure S9. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **26**

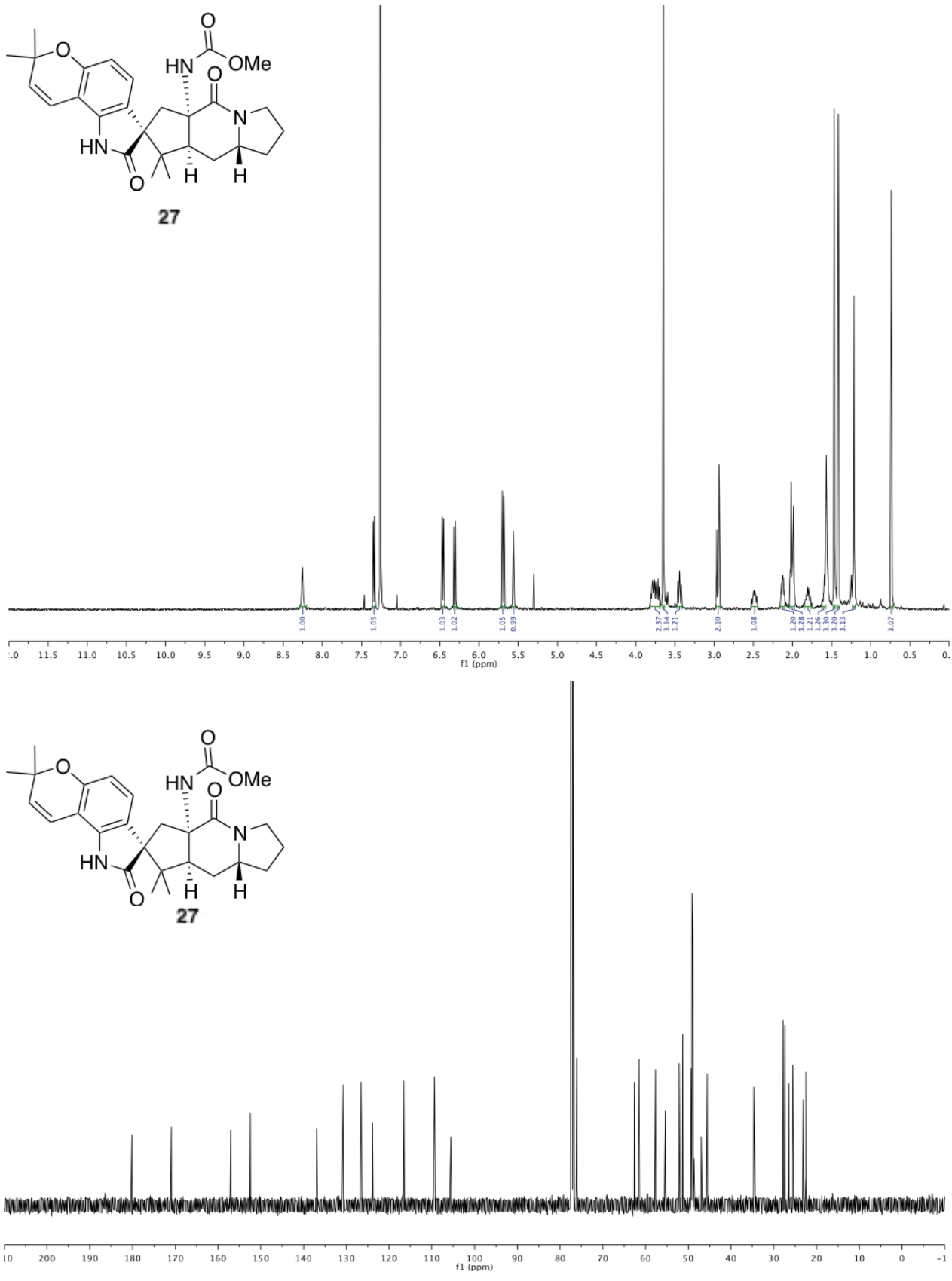


Figure S10. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, 20% $CD_3OD/CDCl_3$) spectrum of **27**

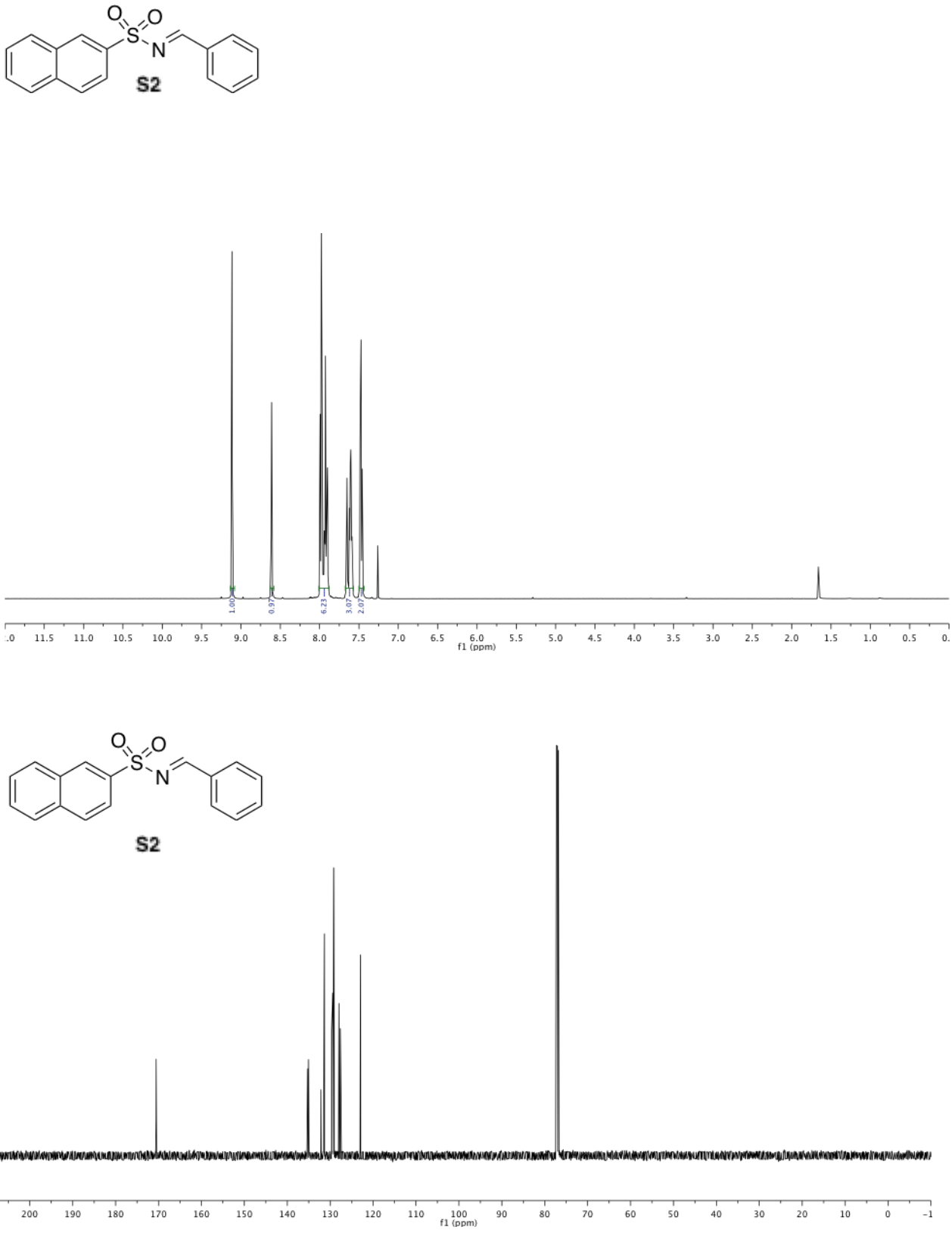


Figure S11. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **S2**

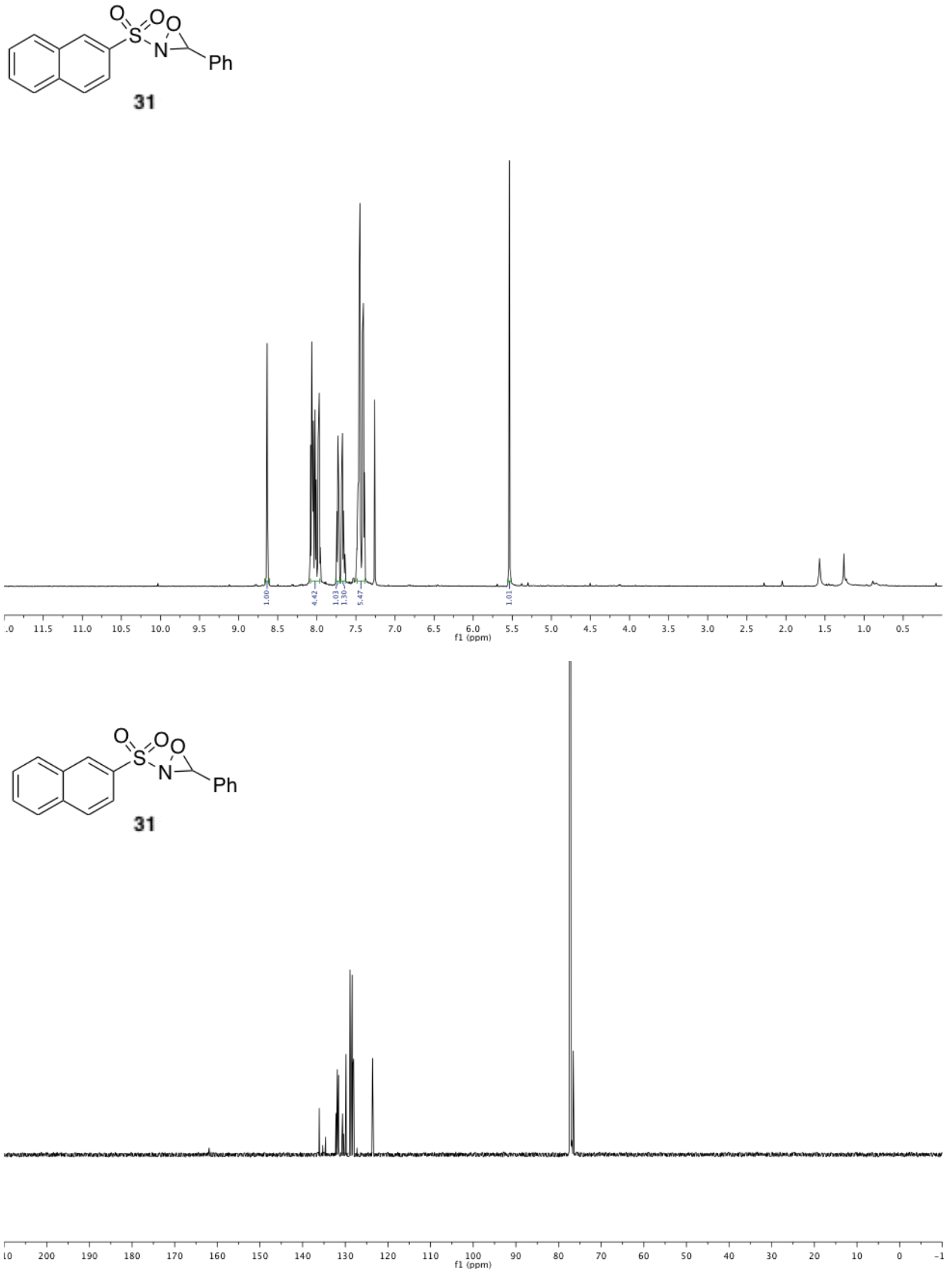


Figure S12. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **31**

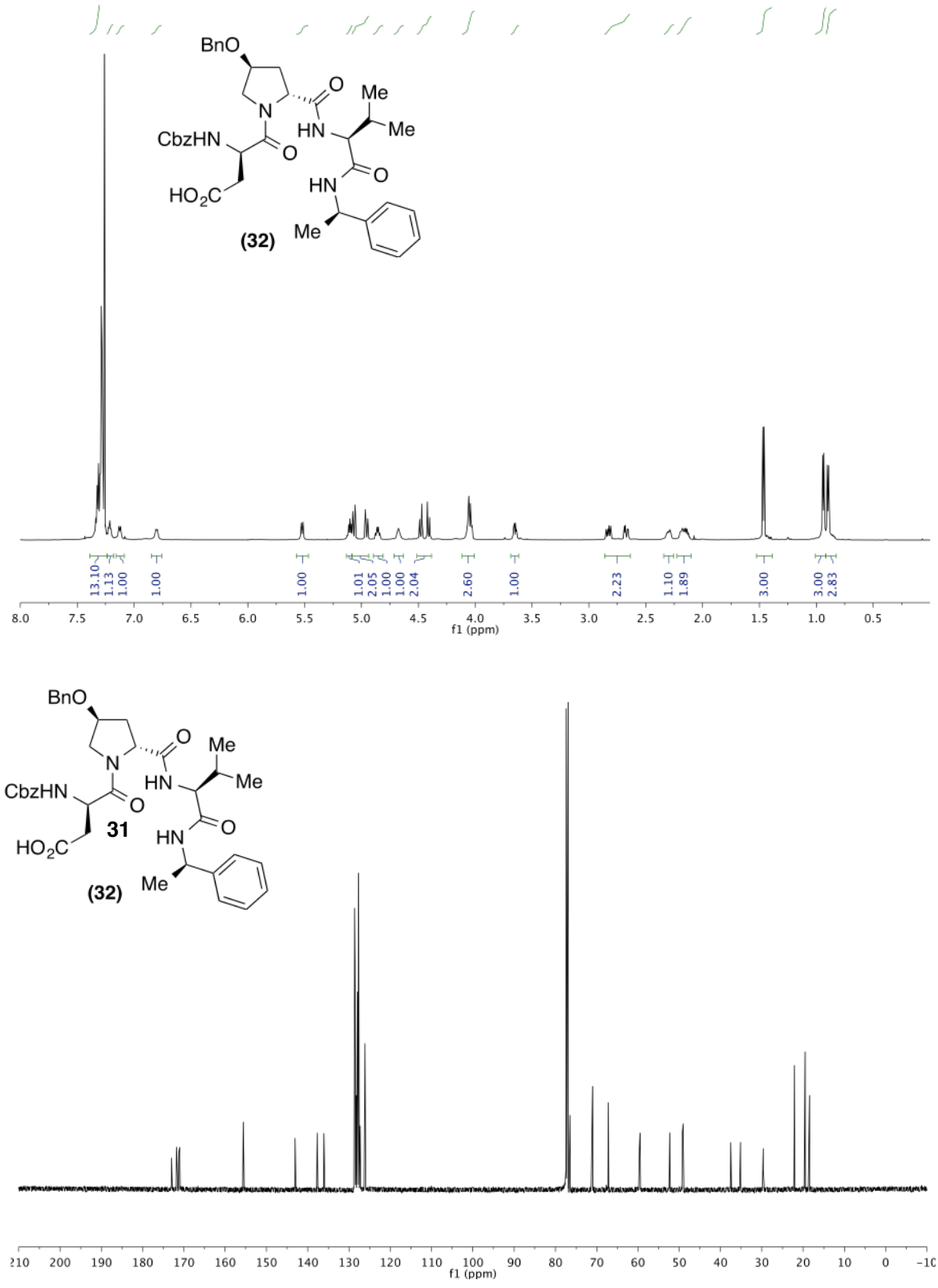


Figure S13. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **32**

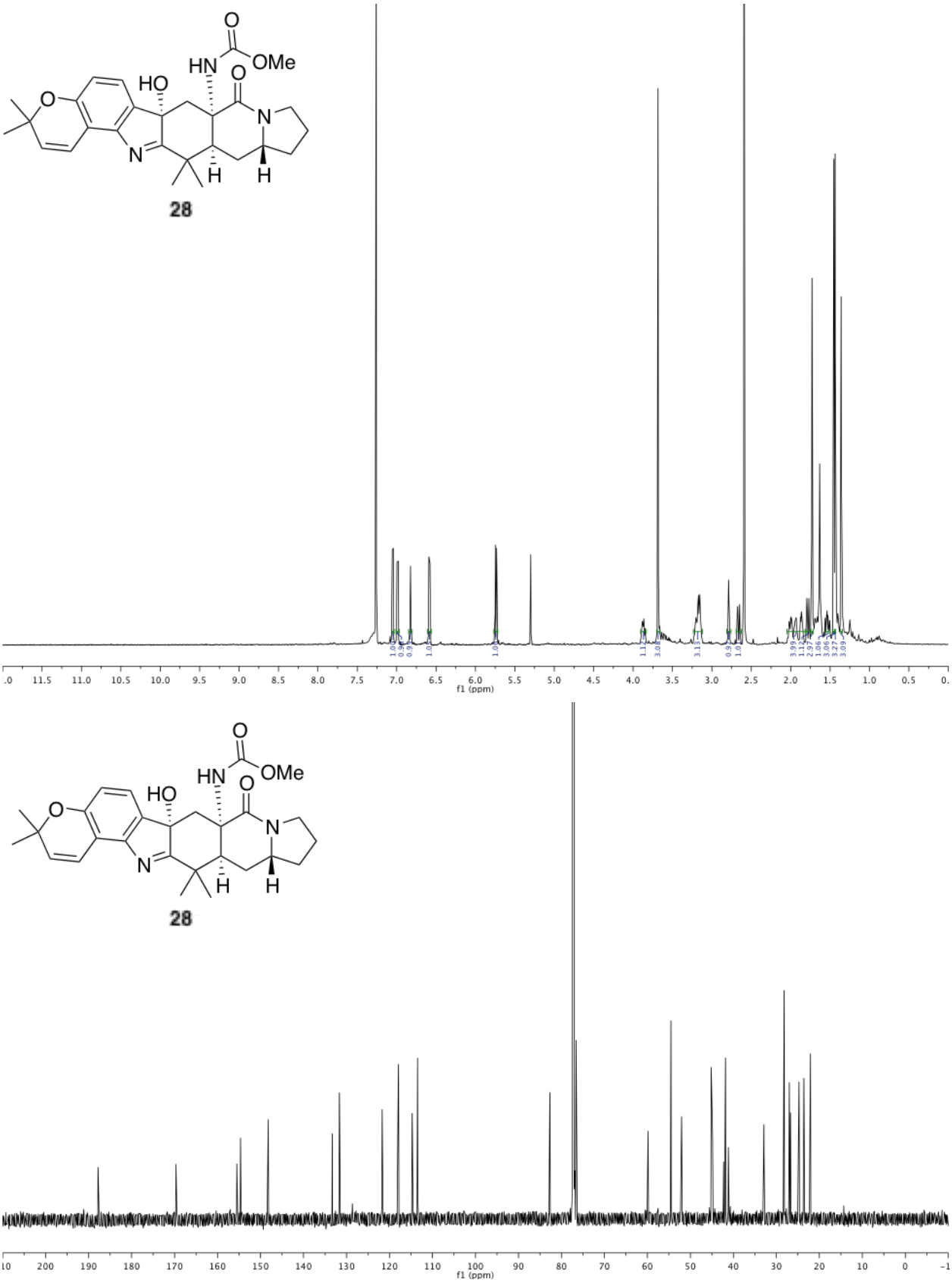


Figure S14. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **28**

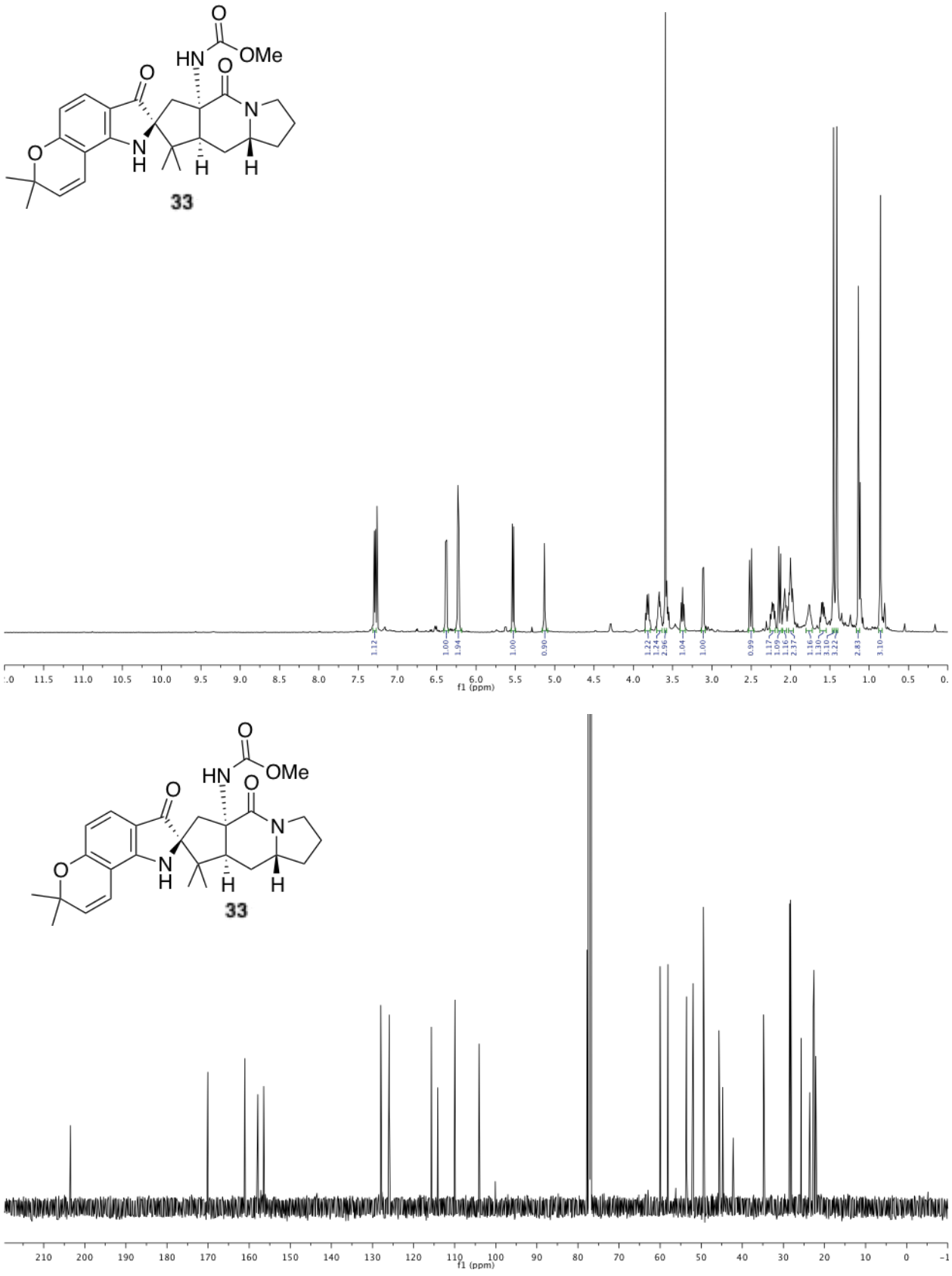


Figure S15. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **33**

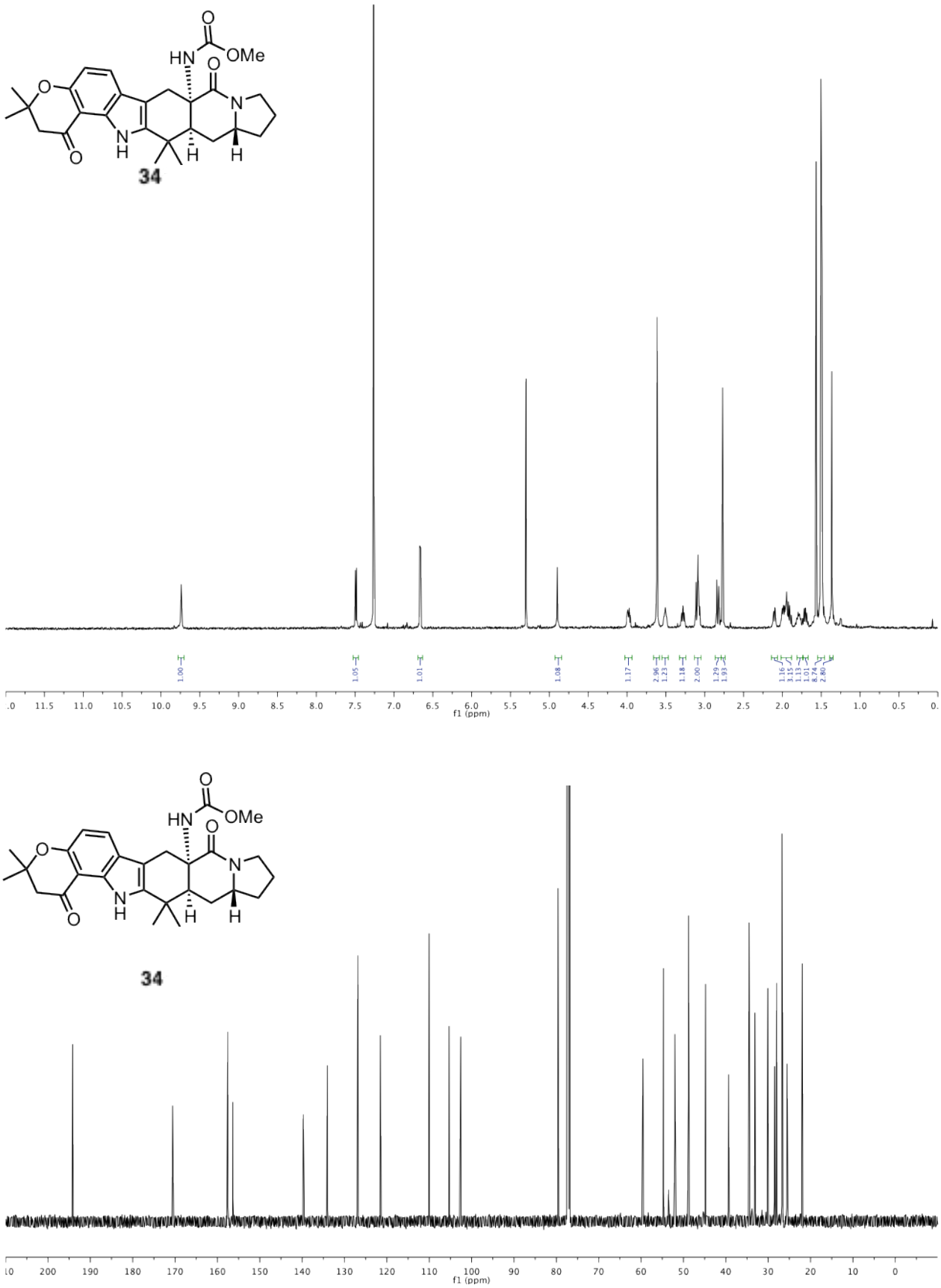


Figure S16. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **34**

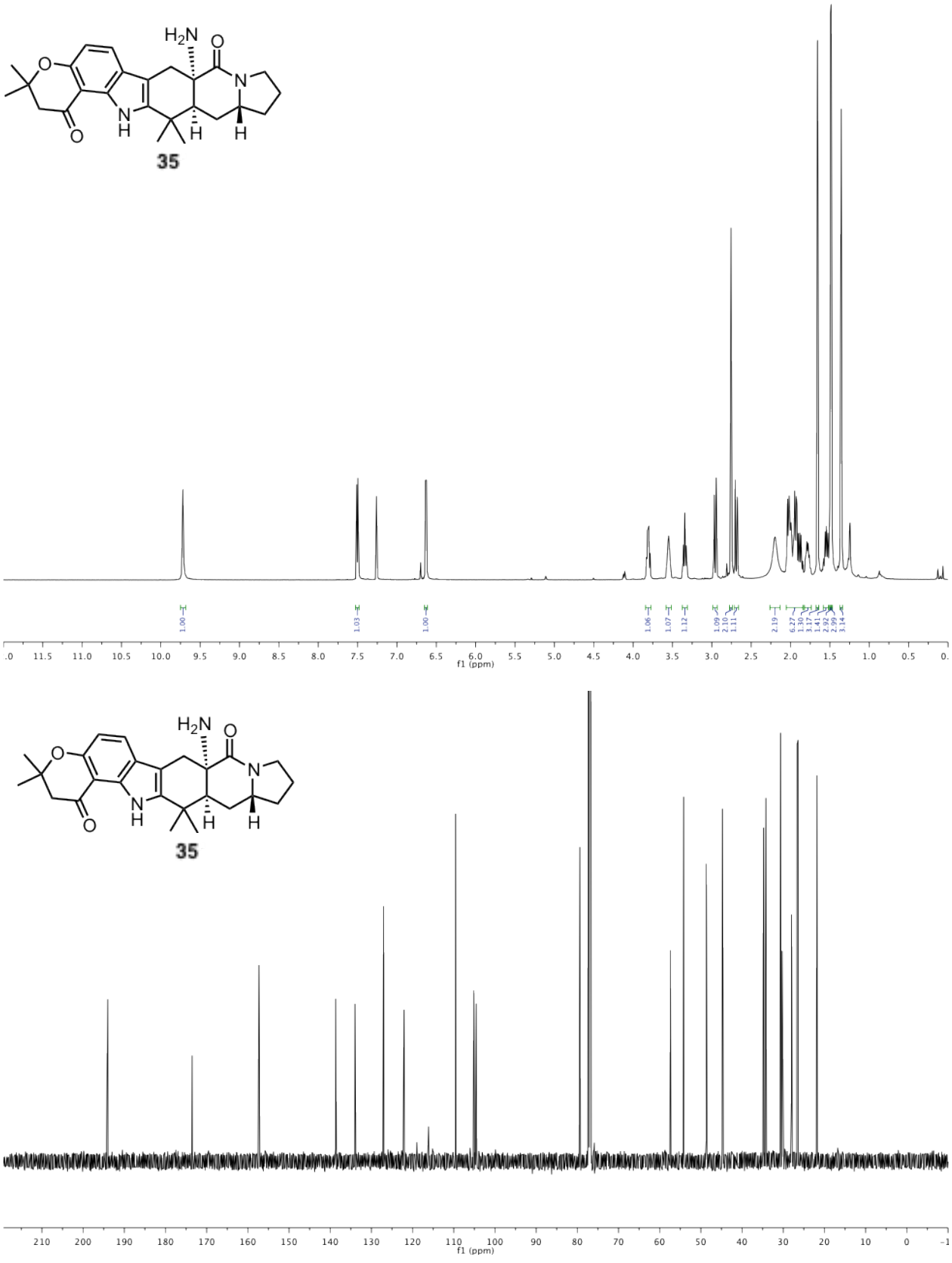
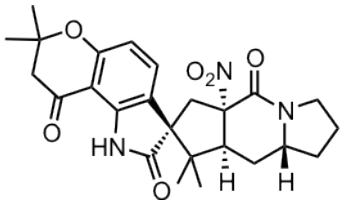
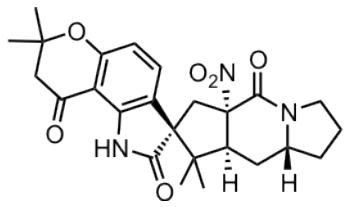


Figure S17. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **35**

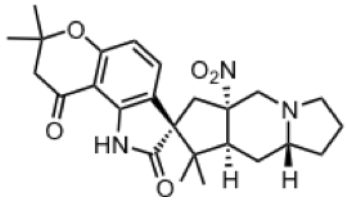


36

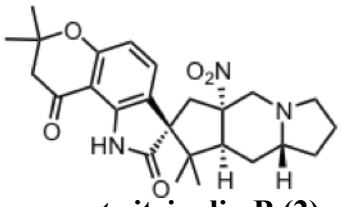


36

Figure S18. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **36**



***ent*-citrinalin B (2)**



***ent*-citrinalin B (2)**

Figure S19. Synthetic ^{1}H NMR (600 MHz, DMSO-d_6) and ^{13}C NMR (150 MHz, DMSO-d_6)) spectrum of ***ent*-Citrinalin B (2)**

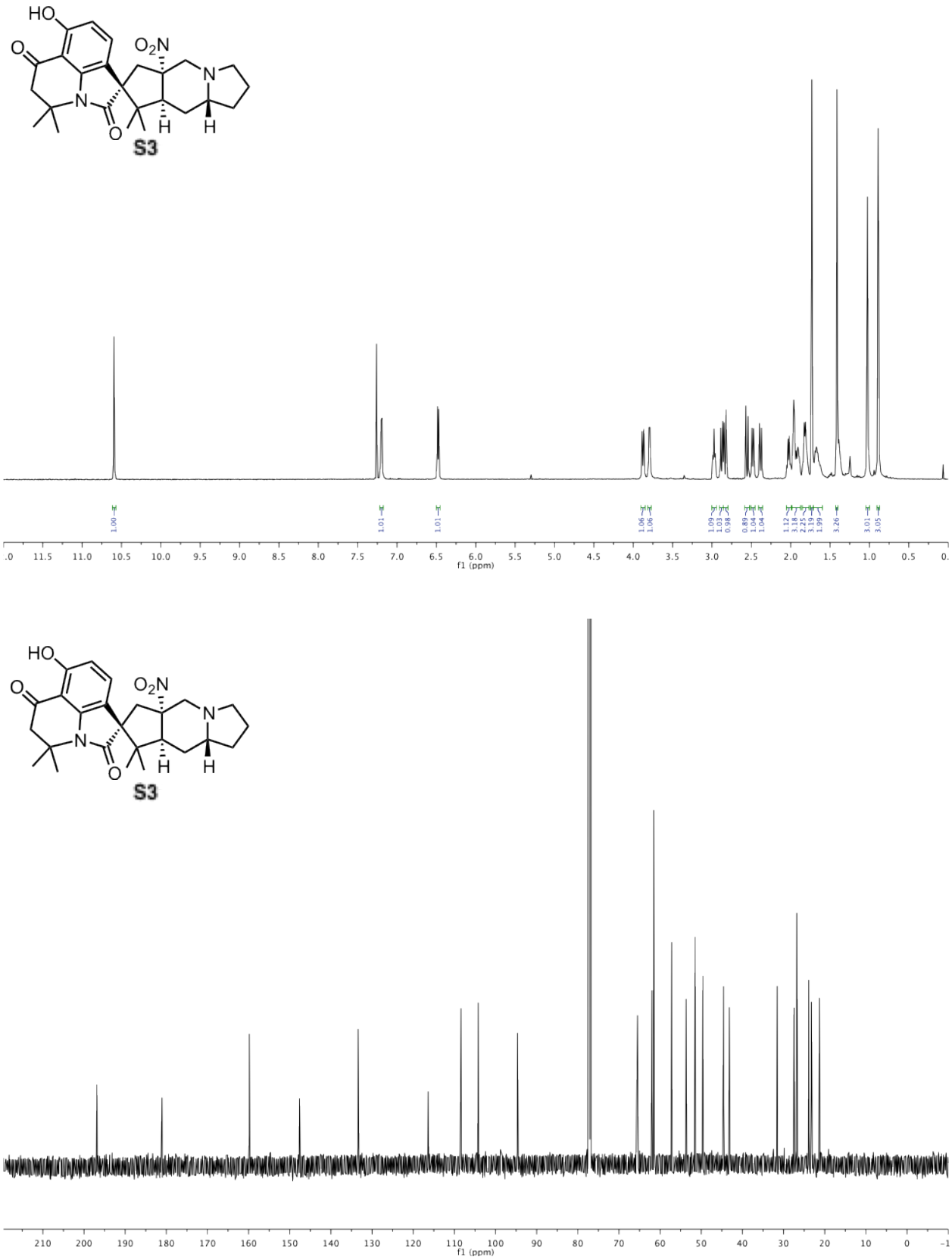
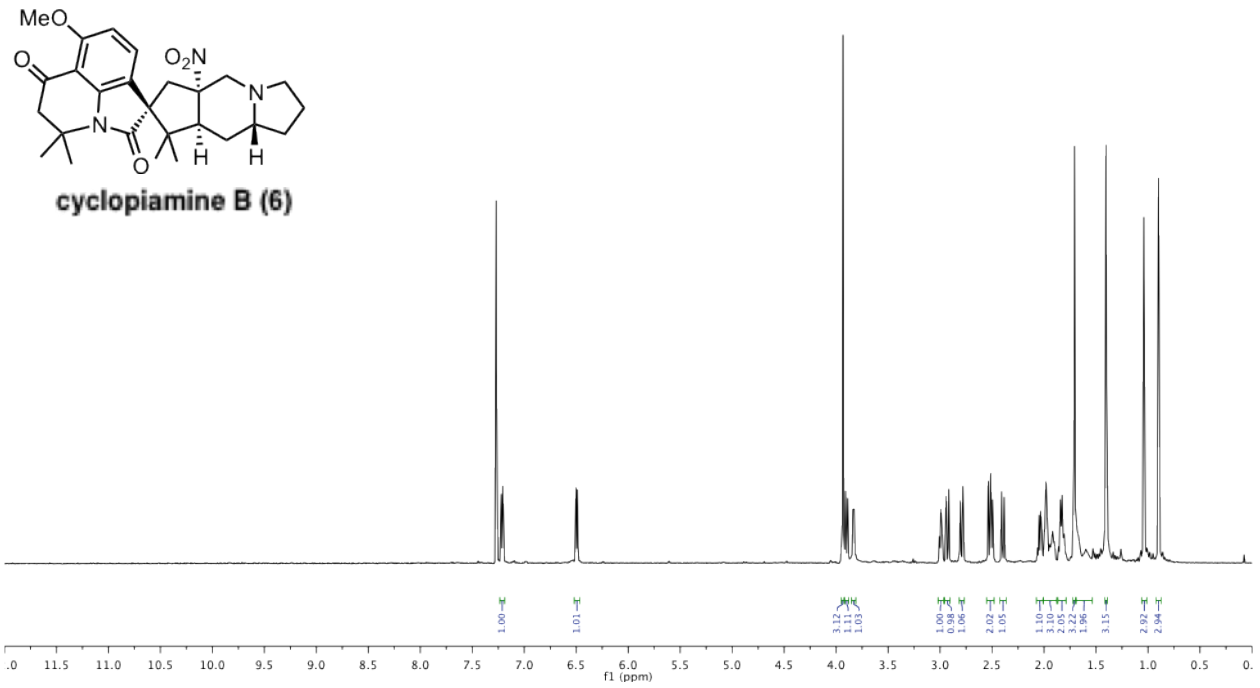


Figure S20. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **S3**



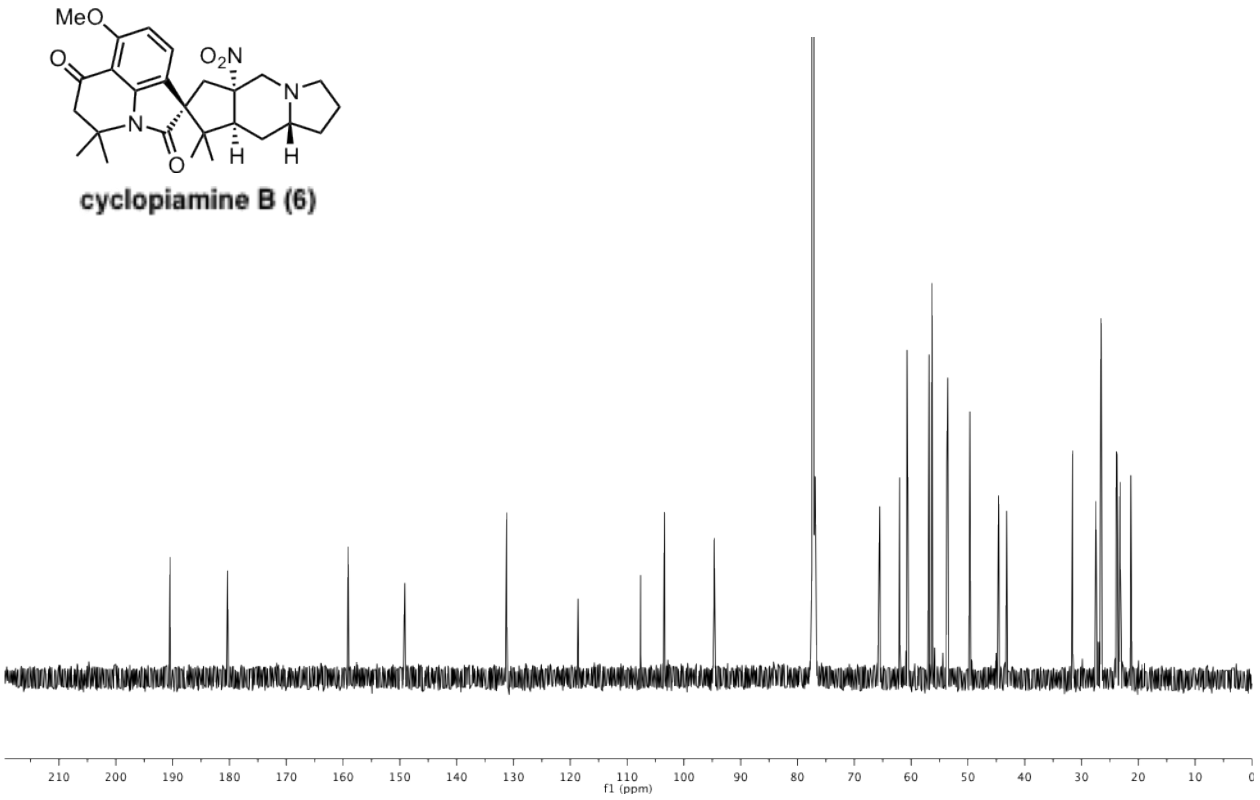


Figure S21. ^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **cyclopiamine B (6)**

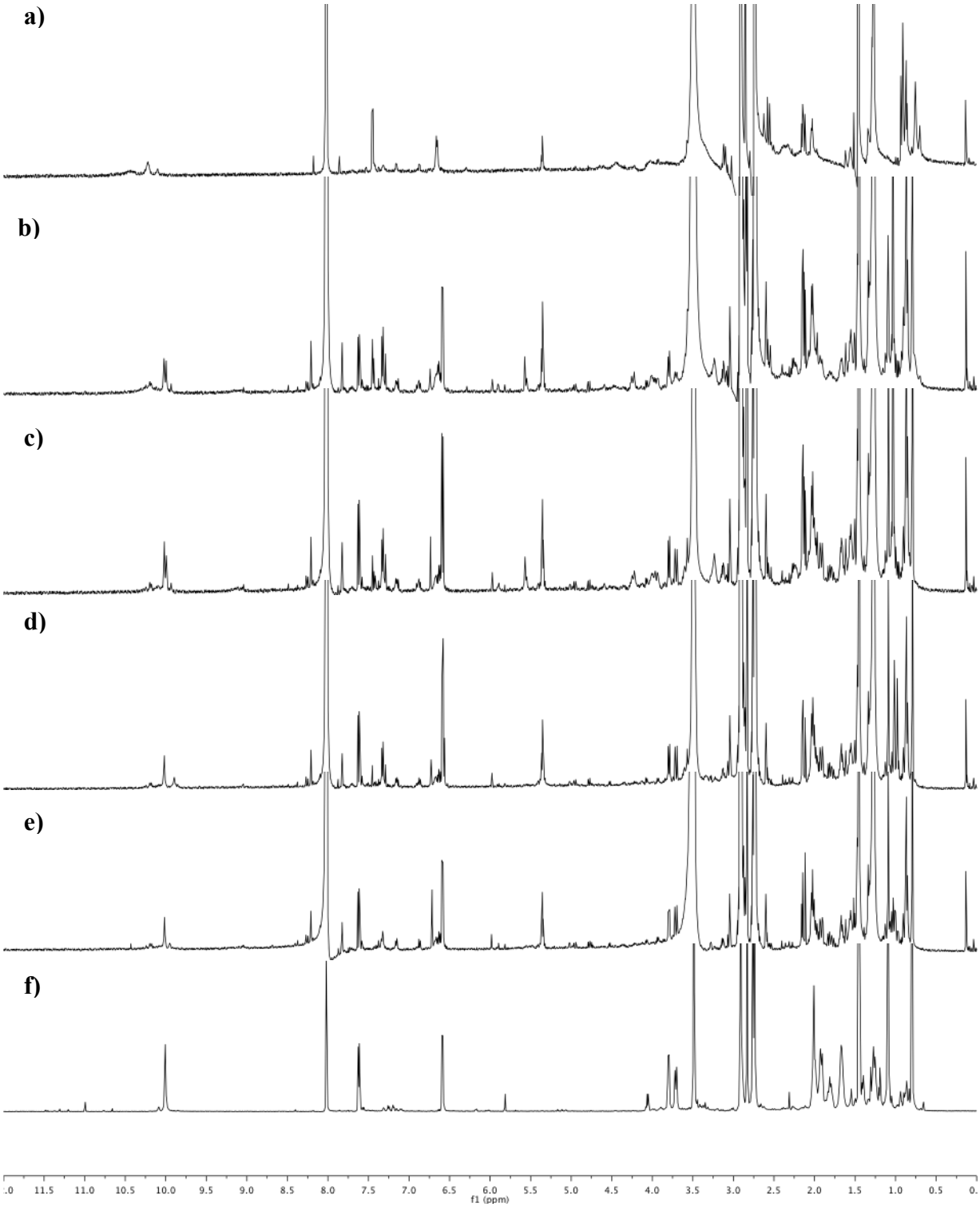


Figure S22. Conversion of citrinalin A (1) to citrinalin B (2). Solution (**a**) was prepared as follows: To a NMR tube was charged with a degassed (freeze, pump, thaw) solution of citrinalin A (**1**) (0.3 mg, 0.066 μmol) in DMF-d_7 (300 μL). **a)** ^{1}H (600 MHz) spectra of citrinalin A (**1**) in DMF-d_7. **b)** ^{1}H (500 MHz) spectra of solution (**a**) after heating at 100 °C for 20 h in DMF-d_7. **c)** ^{1}H (500 MHz) spectra of solution (**a**) after heating at 100 °C for 35 h in DMF-d_7. **d)** ^{1}H (500 MHz) spectra of solution (**a**) after heating at 100 °C for 60 h in DMF-d_7. **e)** ^{1}H (500 MHz) spectra of solution (**a**) post-heating, 11 days at room temperature in DMF-d_7. **f)** ^{1}H (600 MHz) spectra of *ent*-citrinalin B (*ent*-**2**) in DMF-d_7.

V. General Experimental for the isolation of compounds 2, 37 and 38

Optical rotations were measured using a Jasco P-1010 Polarimeter with sodium light (589 nm). NMR spectra were recorded on a Bruker AV-600 spectrometer with a 5 mm CPTCI cryoprobe. ^{1}H and ^{13}C chemical shifts are referenced to the residual methanol-d_4 signal at δ 3.35 ppm (^{1}H) and δ 49.3 ppm (^{13}C) and to the residual acetone-d_6 signal at δ 2.04 ppm (^{1}H) and δ 29.8 ppm (^{13}C), respectively. Solvents used for extraction and chromatography were HPLC-grade solvents. HPLC separations were performed either with a Waters quaternary pump 600, double beam UV detector 2487, and data module 746, or with a Waters 600E system controller connected to a Waters 996 photodiode array detector, on which the UV spectra have been recorded. HPLC-UV-ESI-MS analyses were performed using a Waters Alliance 2695 coupled on-line with a Waters 2996 photodiode array detector, followed by a Micromass ZQ2000 mass spectrometry detector with an electrospray interface. The photodiode array scanned the samples at λ_{max} 254 nm. The ESI-MS detector was optimized using the following conditions: capillary voltage: 3.00 kV; source block temperature: 100 ^{o}C; desolvation temperature: 350 ^{o}C; voltage cone: 25 V; electrospray: positive mode; detection range: 200-550 Da with total ion count extracting acquisition. Cone and desolvation gas flow were at 50 and 350 L/h, respectively. Nitrogen Peak Scientific N110DR was used as a nitrogen source. Data acquisition and processing were performed using Empower 2.0. HPLC-HRMS analyses were performed using a Thermo Scientifc Accela 1250 High Speed LC quaternary pump coupled on-line with a Thermo Scientifc LTQ Orbitrap Velos high resolution mass spectrometer with an electrospray interface. The HRMS detector was optimized using the following conditions: capillary voltage: 3.70 kV; capillary temperature: 400 ^{o}C; desolvation temperature: 500 ^{o}C; electrospray: positive mode; detection range: 200-600 Da with total ion count extracting acquisition. Data acquisition and processing were performed using Xcalibur software.

VI. Isolation and Biofeeding Experimental Procedures for compounds 2, 37 and 38

Small scale incorporation experiments with ^{13}C-labeled precursors

Small scale incorporation experiments of [U-^{13}C]ornithine, [U-^{13}C]proline, [2-*indole*-^{13}C]tryptophan, and [U-$^{13}C_6$]anthranilic acid were performed in 50 mL of sterilized and modified MF fermentation media (consisting of glucose 20 g/L, yeast extract 5 g/L, and beef extract 0.3 g/L) prepared in artificial sea water (ASW: $CaCl_2$ 0.27 g/L; $MgCl_2$ 1.94 g/L; KCl 0.12 g/L; NaCl 6.0 g/L; Na_2HPO_4 0.03 g/L; $NaSO_4$ 0.64 g/L; $NaHCO_3$ 0.034 g/L; KBr 0,020 g/L; $SrCl_2$ 0.008 g/L; H_3BO_3 0.006 g/L) in 250 mL Schott flasks. The incorporation experiment of [1-$^{13}C_1$]glucose was performed in 50 mL of sterilized and modified MF fermentation media (soluble starch 10 g/L, yeast extract 5 g/L, and beef extract 0.3 g/L), in ASW added to 250 mL Schott flasks. Cultures were prepared in duplicates for each incorporation experiment. An inoculum of 10^5 spores of *P. citrinum* F53 was added to each Schott flask, followed by incubation at 28 ^{o}C during 28 days. ^{13}C-Labeled precursors ([1-$^{13}C_1$]glucose, [U-$^{13}C_5$]proline, [U-$^{13}C_5$]ornithine, [indole-2-$^{13}C_1$]tryptophan, and [U-$^{13}C_6$]anthranilic acid) were added in a final concentration of 1 mg/mL on the sixth day of microbial growth. A separate culture in identical culture conditions but without the addition of any labeled precursor was incubated as a control.

Cultures were harvested after 28 days of growth and filtered through a bed of celite. The liquid media of each growth experiment using distinct ^{13}C-labeled precursors were separately subjected to a reverse-phase solid phase extraction using a C_{18} cartridge (5 g) eluted with 100% H_2O (fraction 1, discarded), 1:1 MeOH/H_2O (fraction 2, F2) and 100% MeOH (fraction 3, F3). Fractions F2 and F3 were collected, dried *in vacuo* and weighed. Aliquots of 2 mg of each F2 and F3 were analyzed by HPLC-UV-ESI-MS using a reversed-phase C_{18} column (Waters X-Terra® MS, 50 x 2.1 mm, 3.5 µm) and gradient elution (starting at 90% H_2O containing 0.1% formic acid, followed by linear gradient during 12 minutes to 100% 1:1 MeOH/MeCN, remaining in this final eluting condition for 5 min). The flow rate was 0.5 mL/min.

Fractions F3 collected from the growth experiments using [1-$^{13}C_1$]glucose, [U-$^{13}C_5$]ornithine, and [U-$^{13}C_6$]anthranilic acid showed good incorporation rates by HPLC-UV-ESI-MS into citrinalin A (**1**), citrinalin B (**2**), and 17-hydroxycitrinalin B (**37**) by measuring the $[M+H]^+$ signals intensity for each ion species detected which showed incorporation, relative to the

control experiment. Incorporation experiments using [1-$^{13}C_1$]glucose, [U-$^{13}C_5$]ornithine, and [U-$^{13}C_6$]anthranilic acid were subsequently performed in a larger scale.

Larger scale incorporation experiments with ^{13}C-labeled precursors

A total volume of 2 liters of culture media was distributed in 20 Schott flasks with 100 mL each. Each Schott flask was inoculated with 10^5 spores of *P. citrinum* F53, followed by incubation at 28 ^{o}C. Larger scale growth experiments were performed using [U-$^{13}C_5$]ornithine, [U-$^{13}C_6$]anthranilic acid (both in glucose 20 g/L, yeast extract 5 g/L, and beef extract 0.3 g/L), and [1-$^{13}C_1$]glucose (in soluble starch 10 g/L, yeast extract 5 g/L, and beef extract 0.3 g/L). ^{13}C-labeled precursors were added at a final concentration of 1 mg/mL on the sixth day of microbial growth. Cultures were harvested after 28 days of fermentation and filtered through a bed of celite. Liquid media of identical growth experiments were subjected to a reverse-phase solid phase extraction using a C_{18} cartridge (5 g) eluted with 100% H_2O (fraction 1, discarded), 1:1 MeOH/H_2O (fraction 2, F2) and 100% MeOH (fraction 3, F3). Fractions F2 and F3 were collected, pooled, dried *in vacuo* and weighed. A total amount of crude F3 fractions for each ^{13}C-labeled precursor experiment were obtained: 42 mg of crude F3 using [1-$^{13}C_1$]glucose, 49.4 mg of crude F3 using [U-$^{13}C_5$]ornithine, and 90 mg of crude F3 using [U-$^{13}C_6$]anthranilic acid.

Each of these crude fractions were first fractionated by HPLC-UV using a reverse-phase C_{18} analytical column (Inertsil EP, 4.6 x 250 mm, 5 mm), with a gradient elution starting at 80% H_2O containing 0.1% of TFA, followed by a linear gradient for 20 minutes until 100% 1:1 MeOH/MeCN, maintaining this final condition for 5 min. The flow rate was 1 mL/min, monitored at λ_{max} 254 nm. The resulting fractions of interest were then purified by HPLC-UV using a reversed-phase C_{18} column (InertSustain, 4.6 x 250 mm, 5 μm) with 1:1 MeOH/(0.05% TFA/ H_2O) as eluent to yield 17-hydroxycitrinalin B (**37**). The ^{13}C-labeled feeding experiment using [U-$^{13}C_5$]ornithine yielded 1.2 mg of **37**, [U-$^{13}C_6$]anthranilic acid gave 0.7 mg of **37**, and [1-$^{13}C_1$]glucose gave 2.4 mg of **37**.

A *P. citrinum* F53 "control" growth experiment (with no ^{13}C-labeled precursor added) in a 3 L culture (in glucose 20 g/L, yeast extract 5 g/L, and beef extract 0.3 g/L) gave, after medium filtration and solid phase extraction, 139.2 mg of a crude fraction. This fraction was separated by HPLC-UV using a reverse-phase C_{18} analytical column (Inertsil EP, 4.6 x 250 mm, 5 mm), with a gradient elution starting at 80% H_2O containing 0.1% of TFA, followed by a linear gradient for 20 minutes until 100% 1:1 MeOH/MeCN, maintaining this final condition

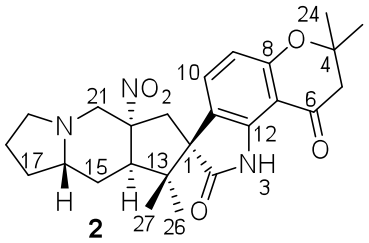
for 5 min. The flow rate was 1 mL/min, monitored at λ_{max} 254 nm. An yet impure citrinalin B containing fraction (4 mg) was purified by reversed-phase HPLC using a C_{18} InertSustain column (4.6 x 250 mm, 5 μm) with 11:9 (0.05% TFA/ H_2O)/MeOH as eluent to yield 2.3 mg of citrinalin B (**2**) and 0.9 mg of citrinalin C (**38**).

Summary of incorporation results:

The incorporation results are readily interpreted (Figure 6B; see Supporting Information, Table S3). [U-^{13}C]ornithine is incorporated intact at C16, C17, C18 and C19 (see **37** for numbering). Incorporation of > 2 % was seen at the aromatic carbons C7, C8, C9, C10, C11 and C12 when **37** was isolated from *P. citrinum* F53 grown in culture medium enriched with [U-^{13}C]anthranilic acid. These results indicate that both L-ornithine and anthranilic acid, probably via tryptophan (Trp),[38] are biosynthetic precursors to **37**. When [1-^{13}C]glucose was administered, significant levels of incorporation were observed throughout **37**, most likely due to metabolic scrambling. Higher incorporation rates of [1-^{13}C]glucose at C14, C24, C25, C26 and C27 indicate that the formation of the isoprene moieties likely proceeds via the mevalonate pathway, as seen in the majority of isoprene-bearing fungal metabolites.[39] The significant incorporation of [1-^{13}C]glucose into C23 can be explained by the formation of Trp from the condensation between the indole C3 and serine C3, the latter of which is biosynthezised from glucose C1.[40]

VII. Characterization Data, 1D and 2D NMR Spectra for compounds 2, 37 and 38

Citrinalin B (**2**): NMR (MeOH-d_4) see Table S1; HRESI(+)MS *m*/*z* 454.2285 corresponding to the molecular formula $C_{25}H_{32}N_3O_5$.



2

Table S1. NMR data for citrinalin B (**2**) recorded in MeOH-d_4

Position	$^{13}C/^{15}N$ (δ)	^{1}H mult (δ)
1	60.3	
2	183.6	
3	n.o.	
4	80.6	
5	49.5	2.77 (d, 16.8); 2.74 (d, 16.8)
6	194.7	
7	106.7	
8	161.2	
9	111.0	6.59 (d, 8.4)
10	133.7	7.40 (d, 8.4)
11	119.9	
12	144.3	
13	50.7	
14	46.8	3.90 (d, 10.1)
15	25.6	2.34 (bd, 16.0); 2.22 (m)
16	65.8	3.22 (m)
17	29.8	2.39 (m); 1.71 (m)
18	20.7	2.16 (m); 2.10 (m)

19	54.9	3.62 (m); 3.06 (m)
20	n.o.	
21	61.0	4.43 (d, 14.1); 3.60 (d, 14.1)
22	93.6	
22-NO_2	-486.1	
23	42.4	3.12 (d, 16.1); 2.64 (d, 16.1)
24	26.7*	1.45 (s)
25	26.6*	1.44 (s)
26	22.7	1.15 (s)
27	22.6	0.86 (s)

[a]The ^{15}N assignments were not calibrated with an external standard. The value has an accuracy of about 1 ppm in reference to CH_3NO_2 on the basis of ^{15}NHSQC and ^{15}NlrHMQC correlations. n.o. = not observed. *Within a column these signals are interchangeable.

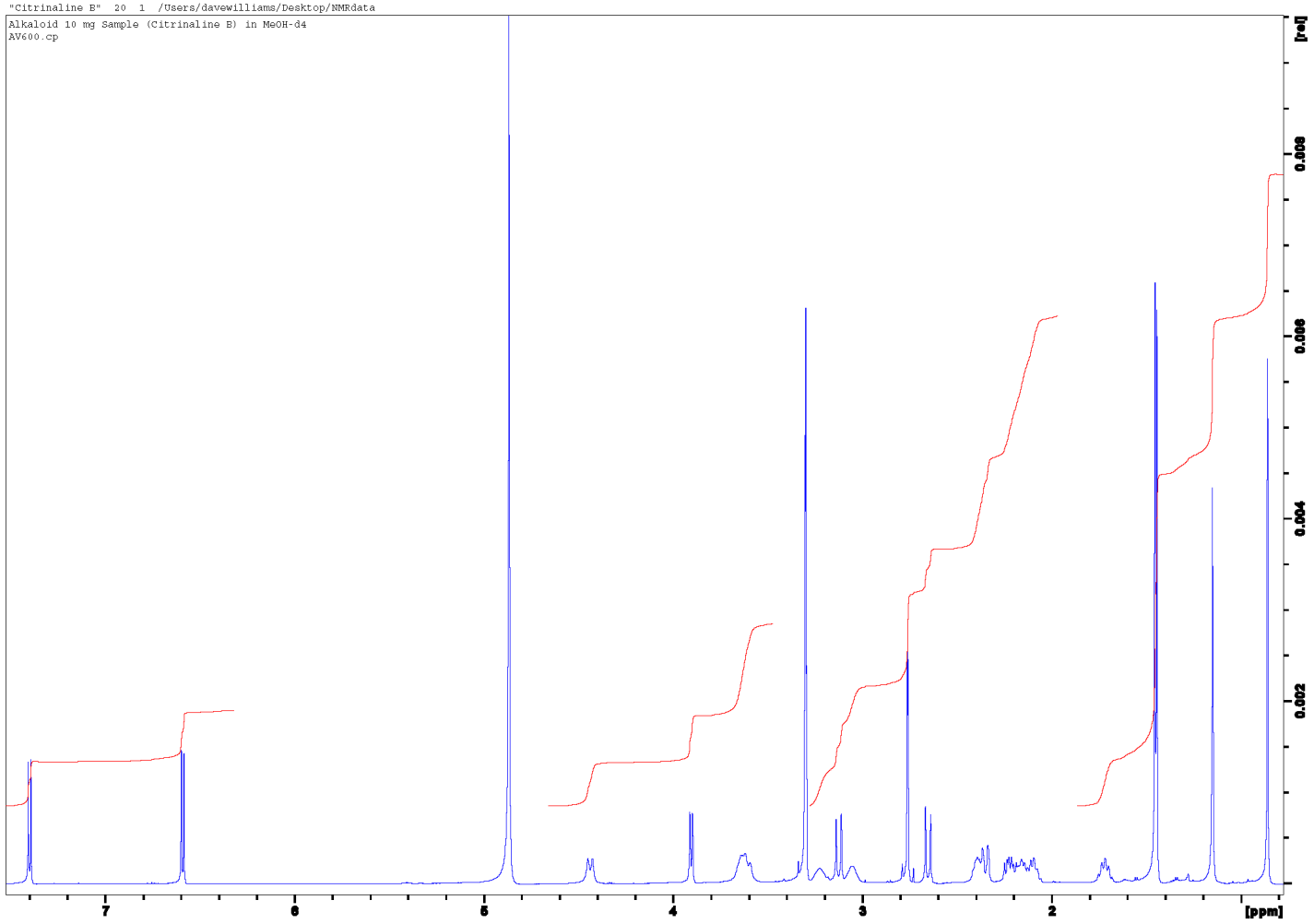


Figure S23. ^{1}H NMR spectrum (MeOH-d_4) for citrinalin B (**2**).

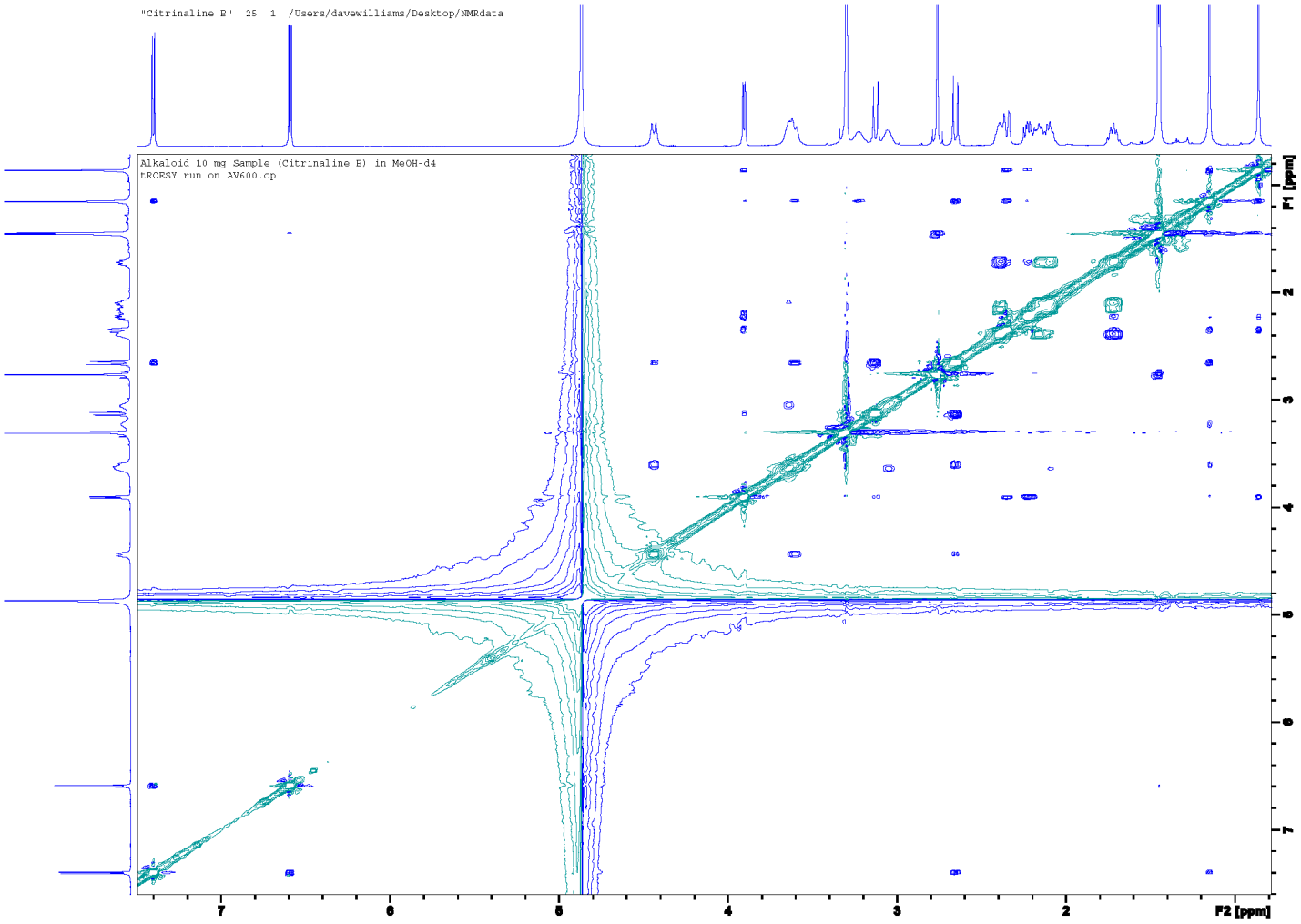
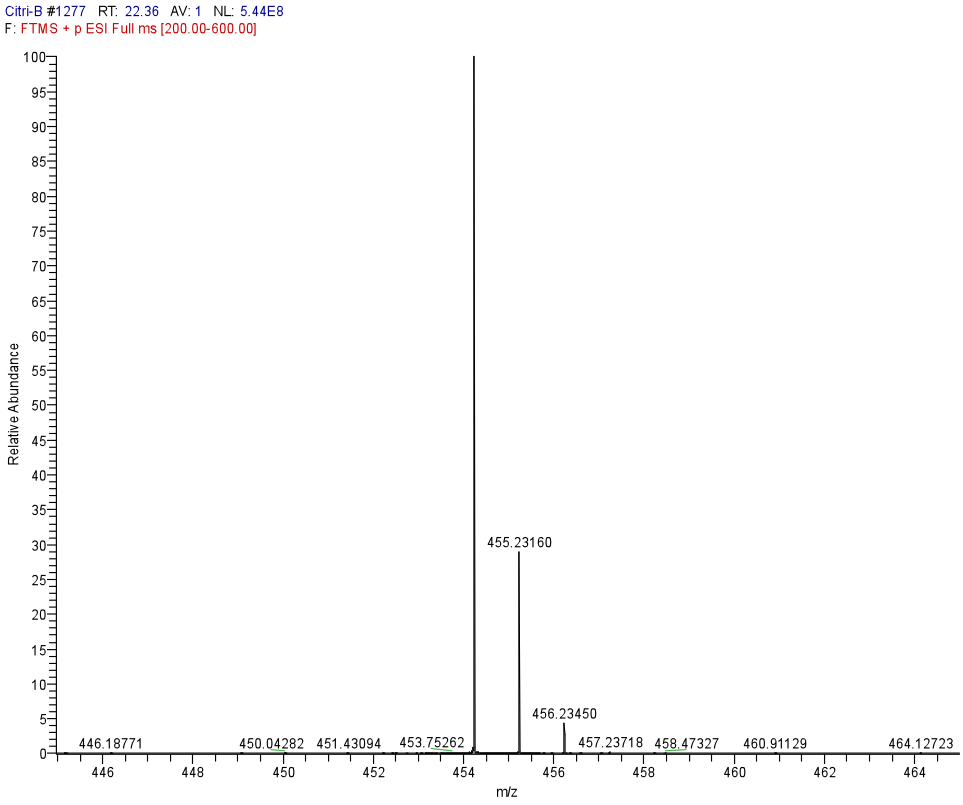
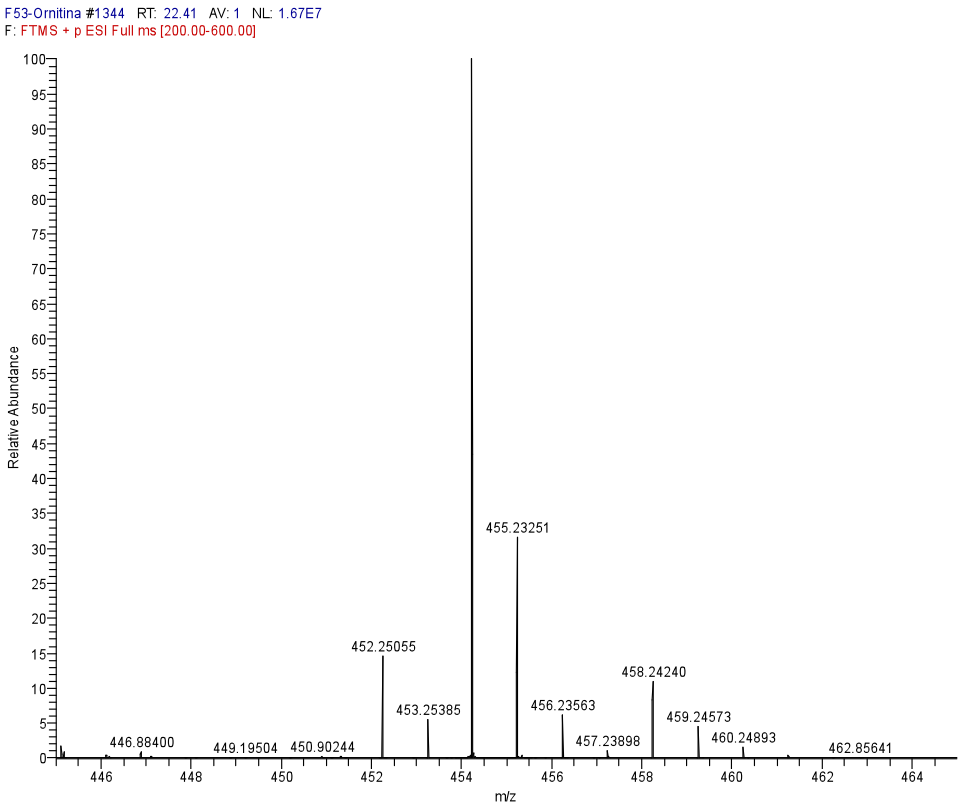


Figure S24. tROESY spectrum (MeOH-d_4) for citrinalin B (**2**).

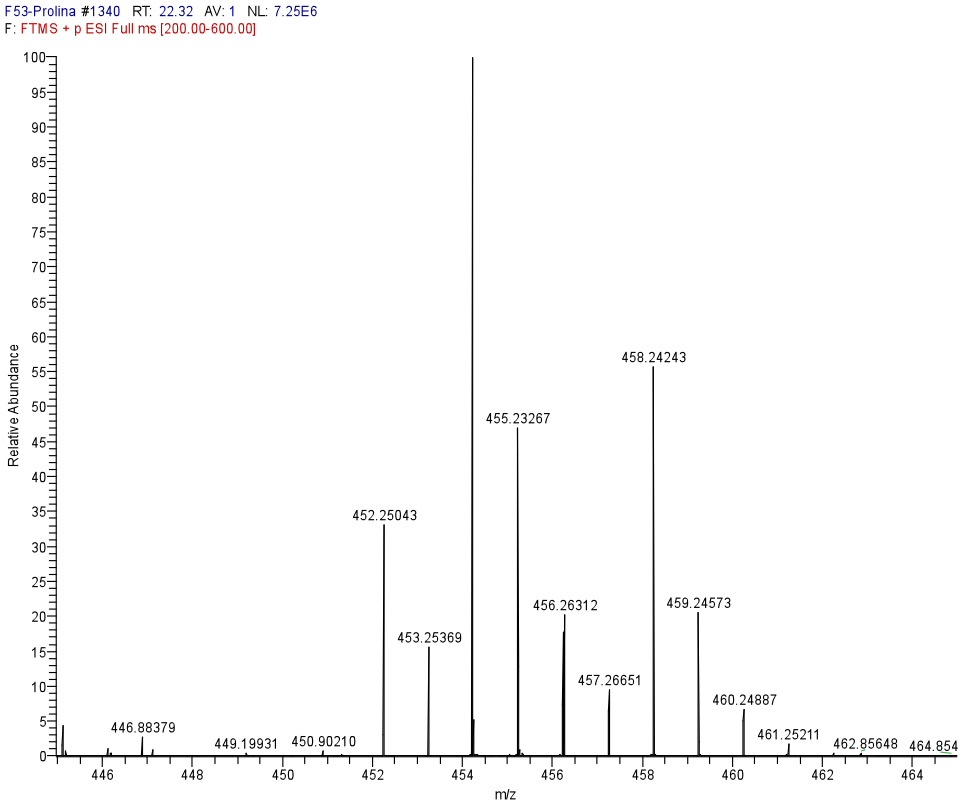
(A)


Citri-B #1277 RT: 22.36 AV: 1 NL: 5.44E8
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
455.23160
456.23450
446.18771
450.04282
451.43094
453.75262
457.23718
458.47327
460.91129
464.12723

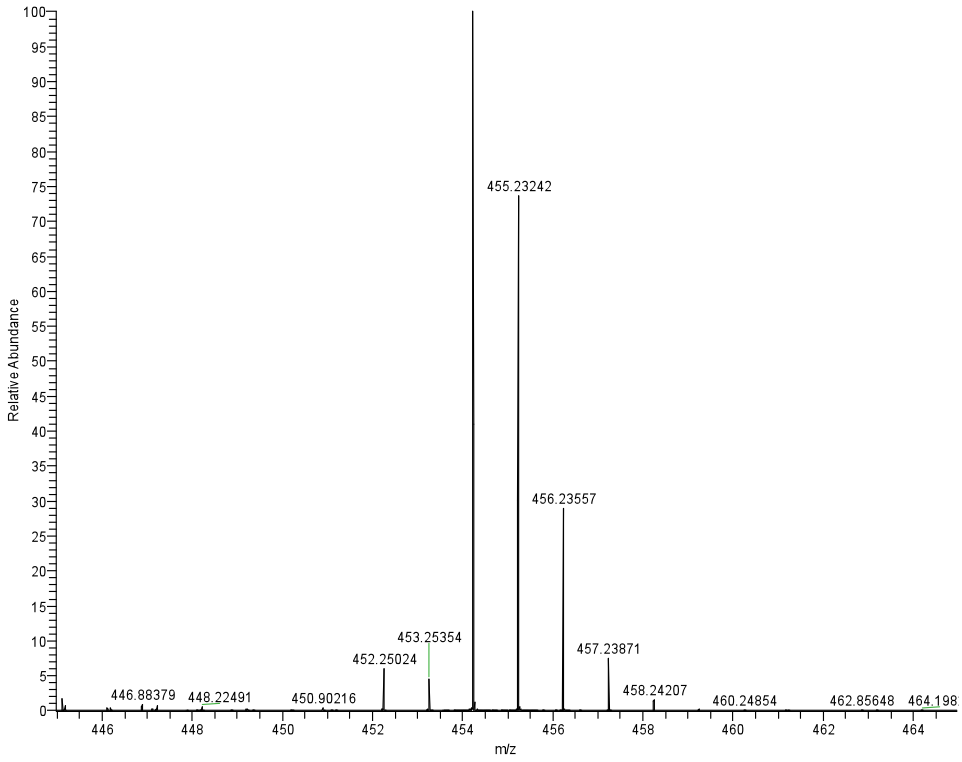
(B)


F53-Ornitina #1344 RT: 22.41 AV: 1 NL: 1.67E7
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
455.23251
452.25055
458.24240
453.25385
456.23563
459.24573
460.24893
446.88400
449.19504
450.90244
457.23898
462.85641

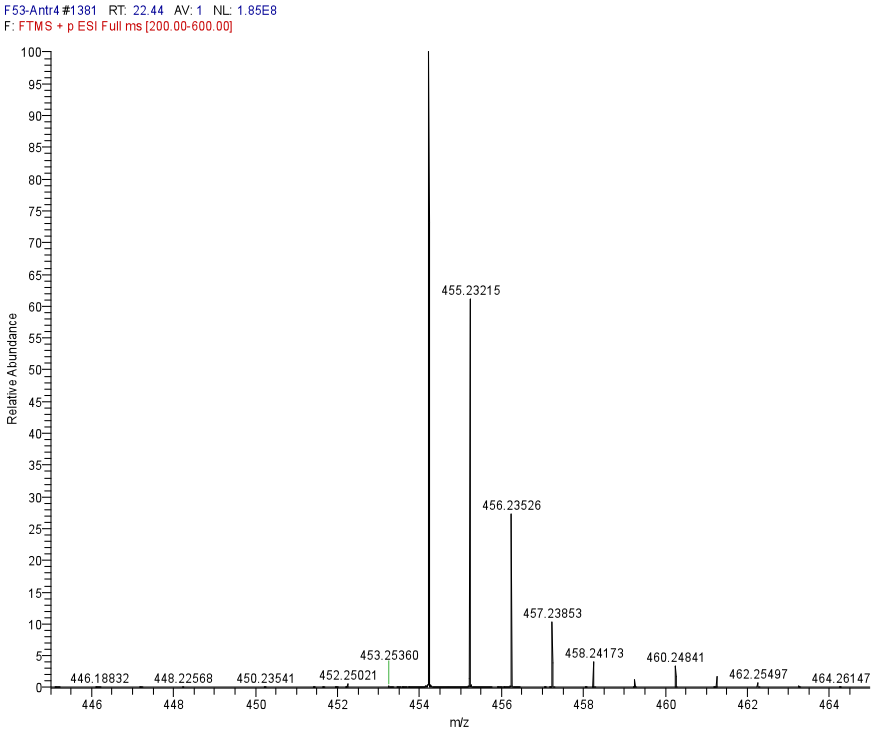
(C)


F53-Prolina #1340 RT: 22.32 AV: 1 NL: 7.25E6
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
458.24243
455.23267
452.25043
456.26312
459.24573
453.25369
457.26651
460.24887
461.25211
446.88379
449.19931
450.90210
462.85648
464.854

(D)


F53-Gli7 #1353 RT: 22.55 AV: 1 NL: 1.39E7
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
455.23242
456.23557
453.25354
452.25024
457.23871
458.24207
446.88379
448.22491
450.90216
460.24854
462.85648
464.198

(**E**)



(**F**)

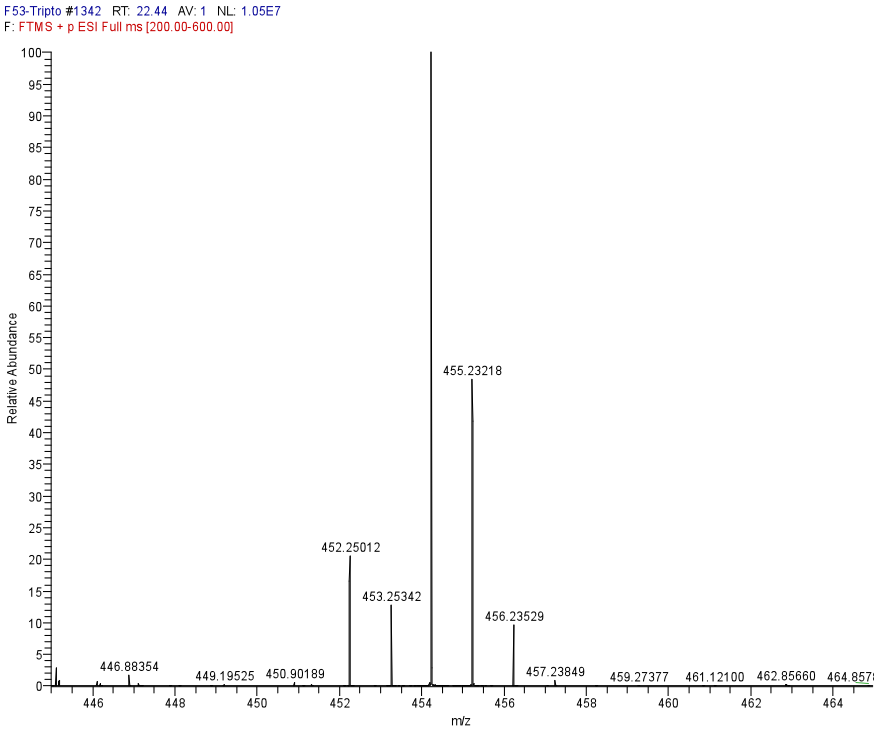
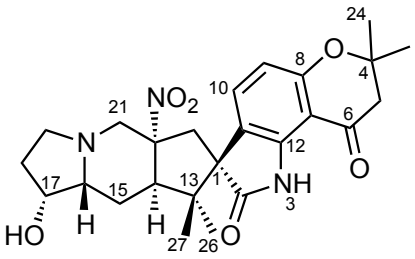


Figure S25. HRMS(ESI$^+$) spectrum of citrinalin B (**A**), ([U-$^{13}C_5$]ornithine)-citrinalin B (**B**), ([U-$^{13}C_5$]proline)-citrinalin B (**C**), ([1-$^{13}C_1$]glucose)-citrinalin B (**D**), ([U-$^{13}C_6$]anthranilic acid)-citrinalin B (**E**), and ([2-indole-$^{13}C_1$]tryptophan)-citrinalin B (**F**).

17-Hydroxycitrinalin B (37): $[\alpha]_D$ +76.9 degrees (*c* 1.6, MeOH); UV (1:1 MeOH/(0.05% TFA/ H_2O)) λmax 208, 235, 265, 280(sh), 359 nm; NMR (MeOH-d_4) see Table S2; (+)-HRESIMS $[M+H]^+$ *m/z* 470.2229 (calcd for $C_{25}H_{32}N_3O_6$, 470.2291).



[a]The ^{15}N assignments were not calibrated with an external standard. The value has an accuracy of about 1 ppm in reference to CH_3NO_2 on the basis of ^{15}NHSQC and ^{15}NlrHMQC correlations. [b]Multiplicity not determined due to overlapping signals/chemical shifts determined from 2D data. n.o. = not observed. *Within a column these signals are interchangeable.

Table S2. NMR data for 17-hydroxycitrinalin B (**37**) recorded in MeOH-d_4

Position	$^{13}C/^{15}N$[a] (δ)	δ ^1H mult (*J* in Hz)
1	60.3	
2	184.2	
3	n.o	
4	80.9	
5	49.0	2.77 (d, *J*=16.8); 2.75 (d, *J*=16.8)
6	195.0	
7	107.0	
8	161.5	
9	111.3	6.60 (d, *J*=8.4)
10	133.9	7.38 (d, *J*=8.4)
11	120.2	
12	144.6	
13	51.0	
14	45.9	3.99 (d, *J*=8.7)
15	20.0	2.60 (ddd, *J*=8.7, 13.5,15.6) 2.10 (dd, *J*=3.9, 15.6)
16	69.4	3.20 (bd, *J*=13.5)
17	70.1	4.47 (dd, *J*=3.2, 5.4)
18	32.5	2.48 (m) 2.00 (dt, *J*=8.7, 13.0)
19	54.2	3.76 (m) 3.12[b]
20	-319.5	
21	61.0	4.40 (d, *J*=14.5); 3.70 (d, *J*=14.5)
22	93.7	
22-NO_2	-486.5	
23	43.2	3.08 (d, *J*=16.1); 2.67 (d, *J*=16.1)
24	27.0*	1.45 (s)*

25	26.9*	1.44 (s)*
26	23.0	1.15 (s)
27	23.0	0.88 (s)

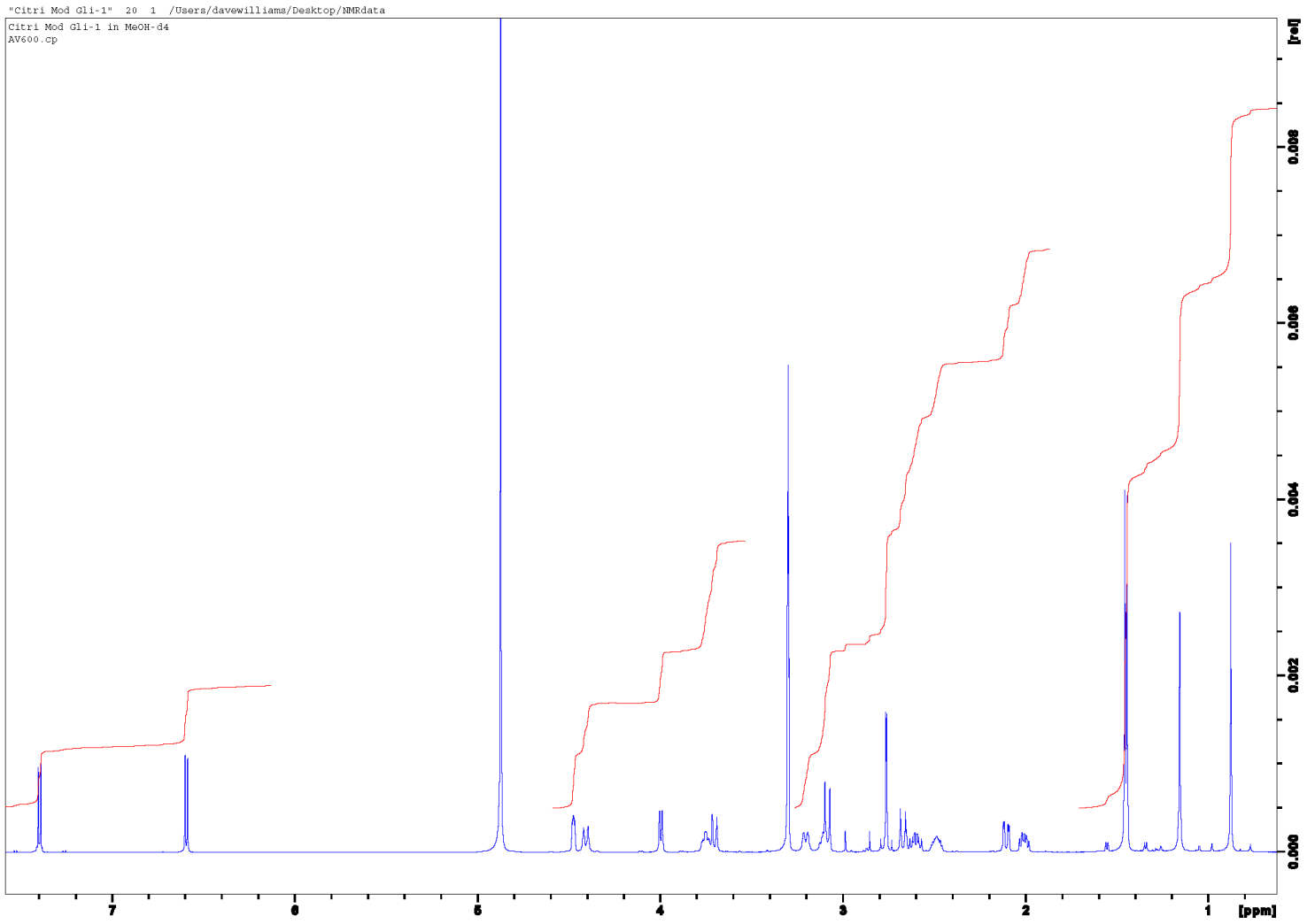


Figure S26. ^{1}H NMR spectrum (600 MHz, MeOH-d_4) for 17-hydroxycitrinalin B (**37**).

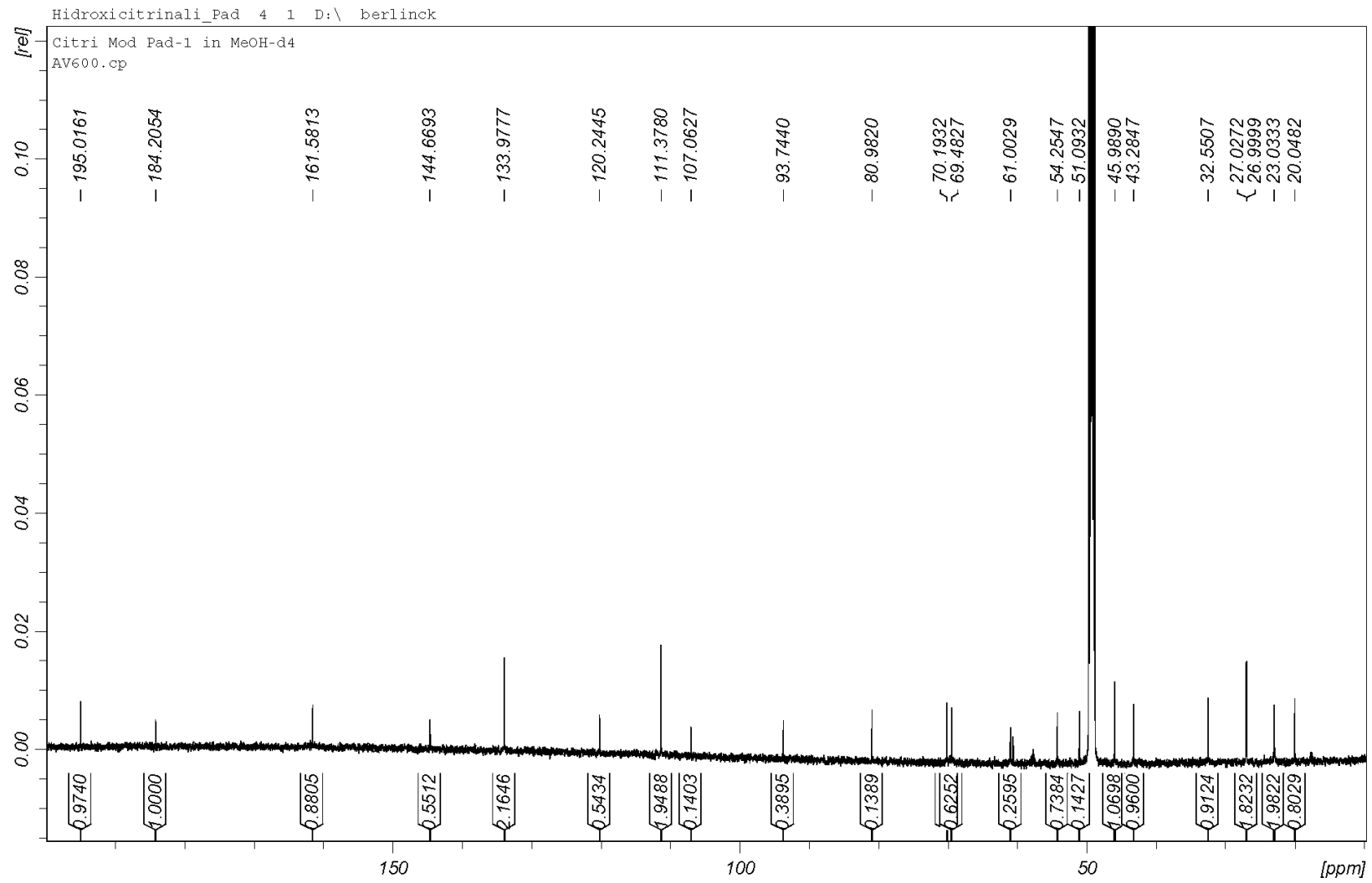


Figure S27. ^{13}C NMR spectrum (150 MHz, MeOH-d_4) for 17-hydroxycitrinalin B (**37**).

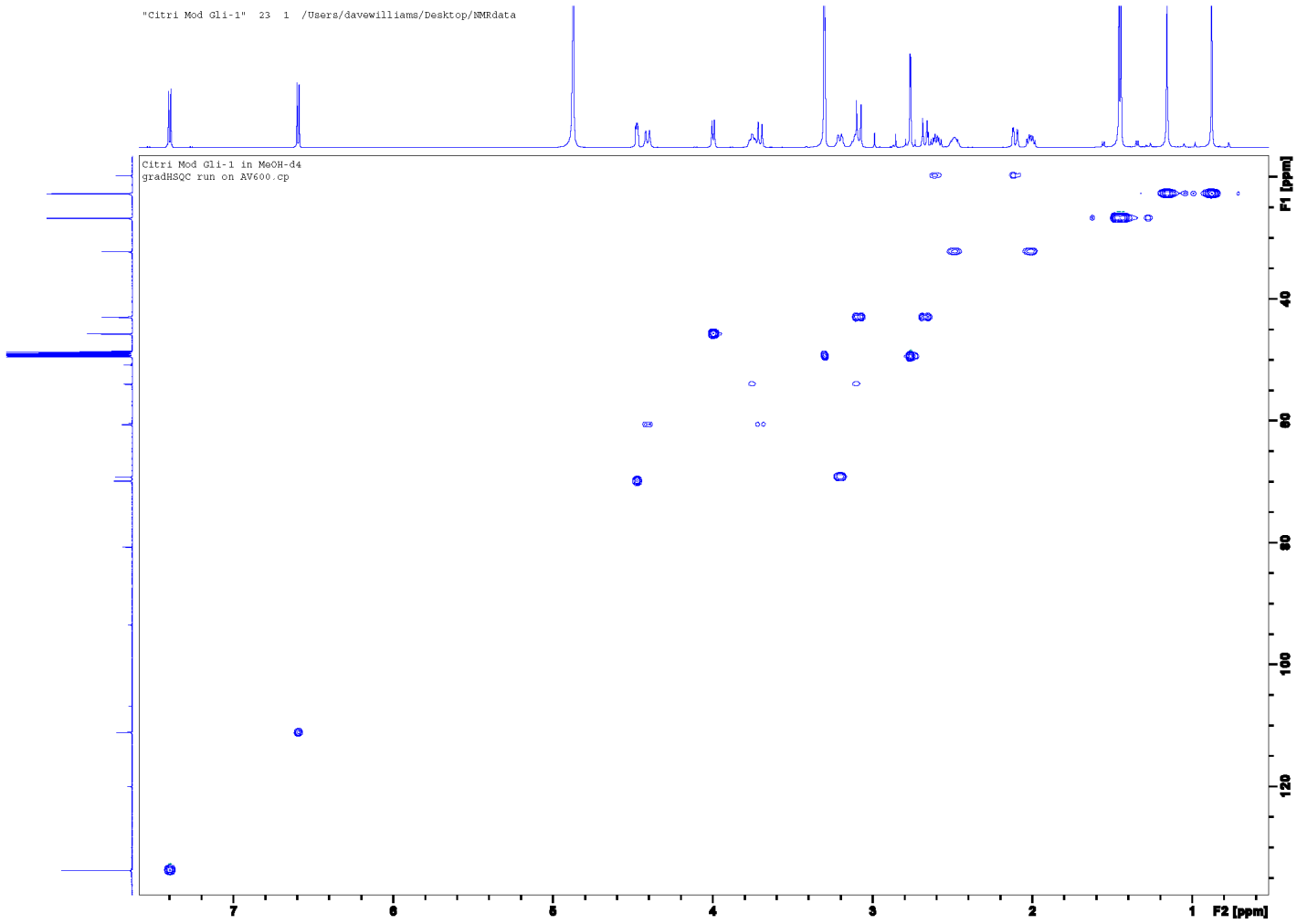


Figure S28. gHSQC spectrum (MeOH-d_4) for 17-hydroxycitrinalin B (**37**).

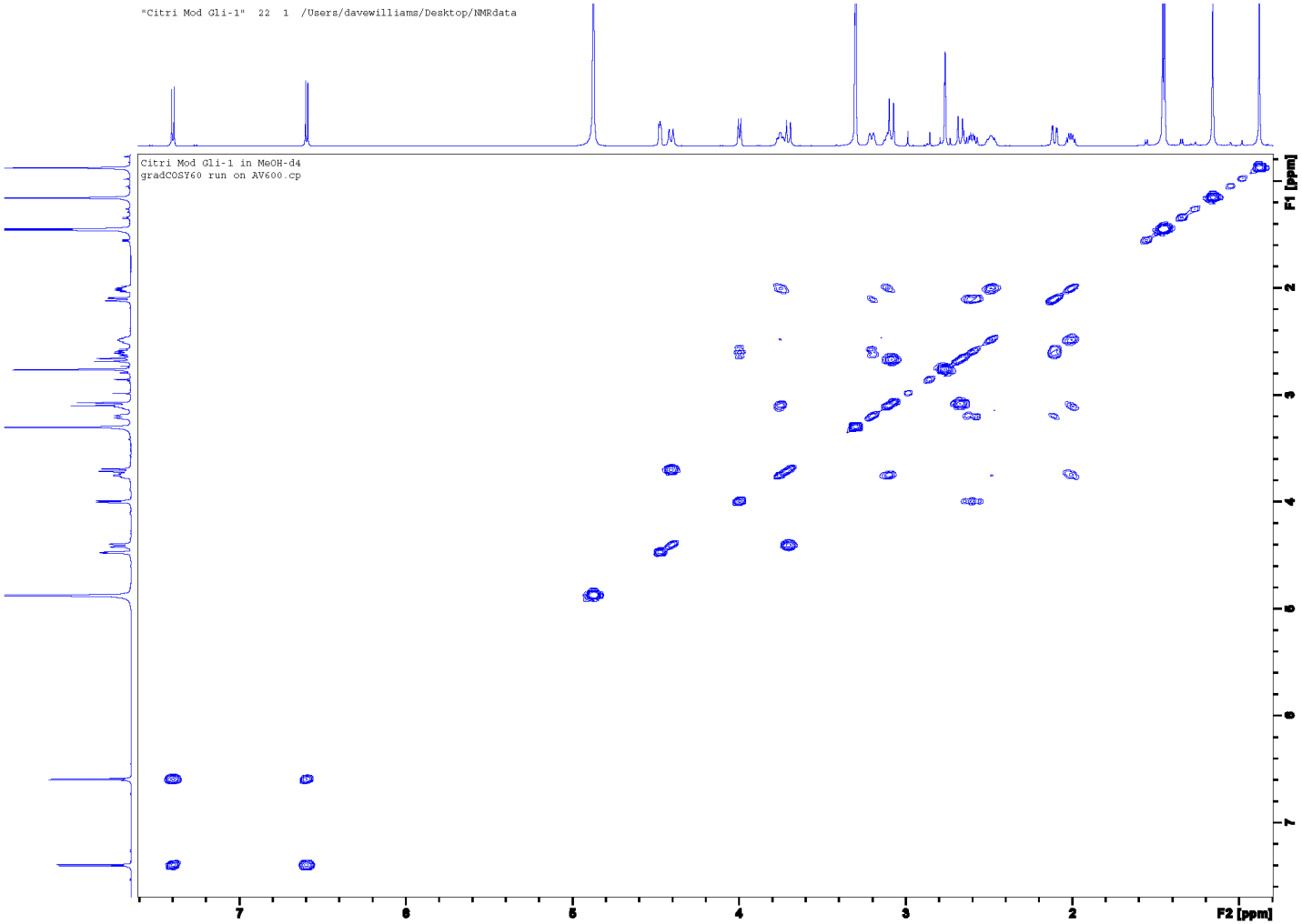


Figure S29. gCOSY60 spectrum (MeOH-d_4) for 17-hydroxycitrinalin B (**37**).

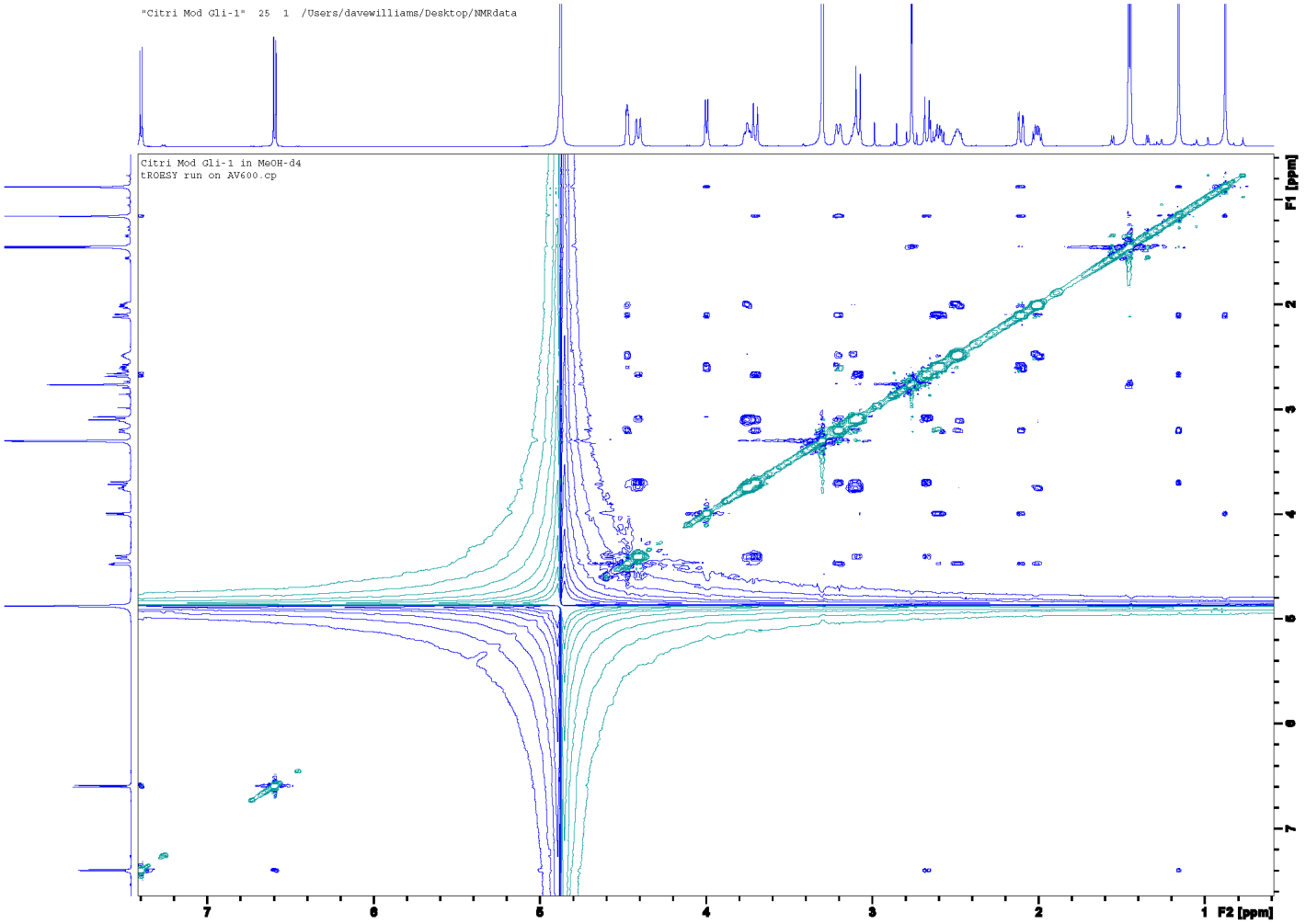


Figure S30. tROESY spectrum (MeOH-d_4) for 17-hydroxycitrinalin B (**37**).

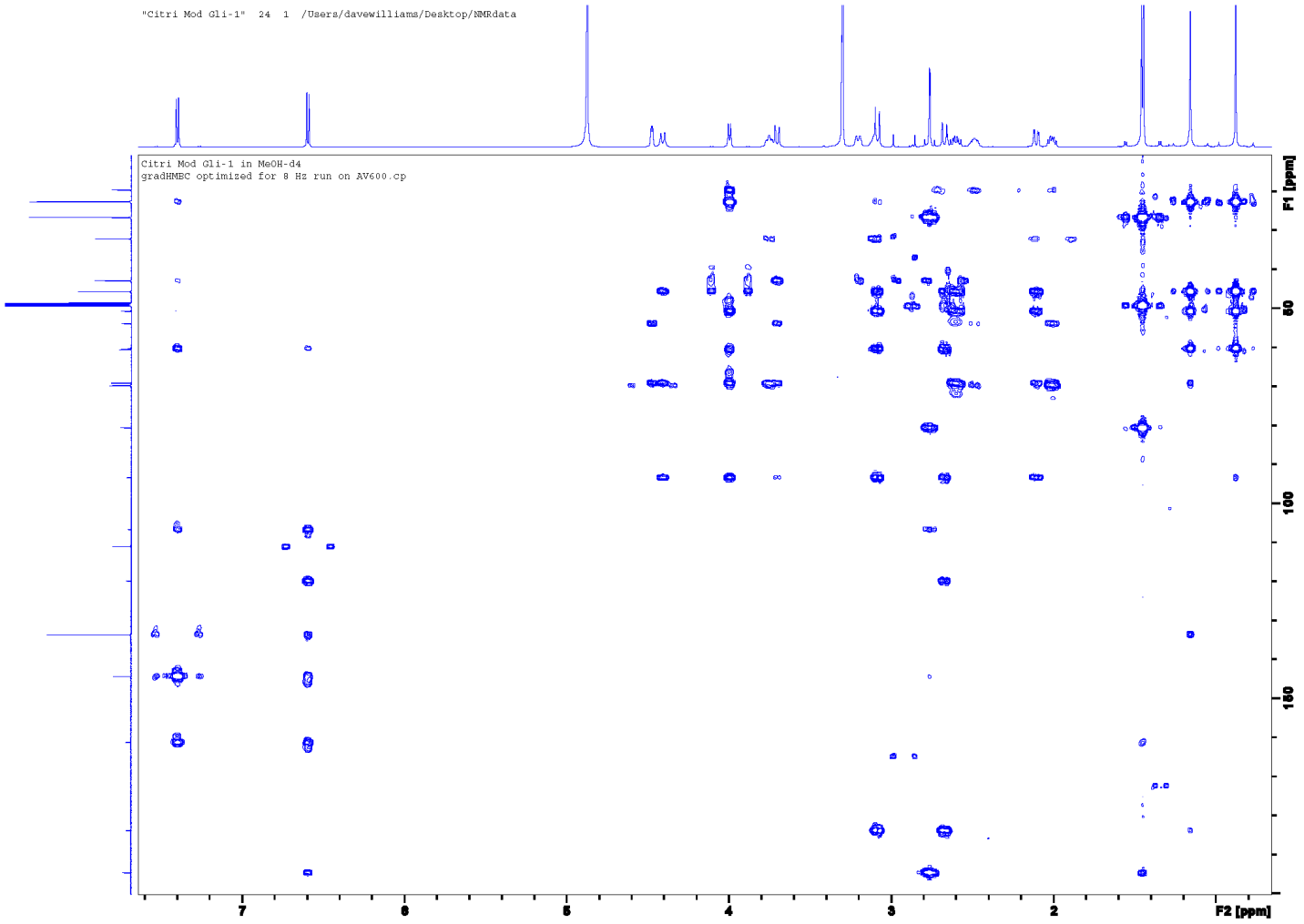


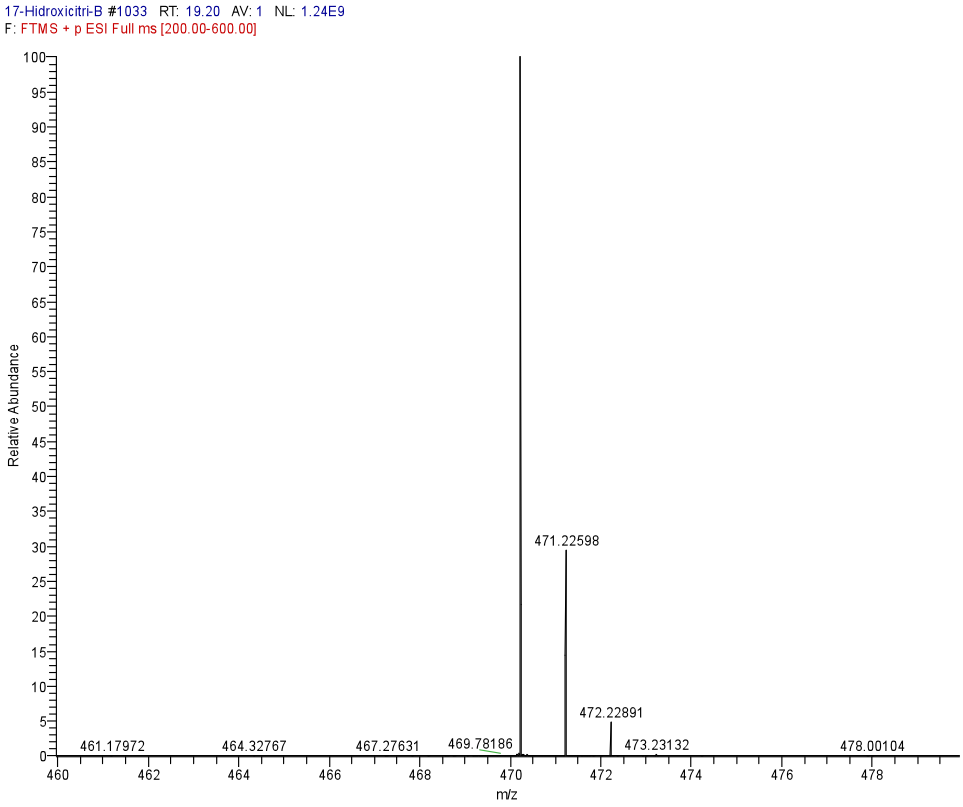
Figure S31. gHMBC spectrum (MeOH-d_4) for 17-hydroxycitrinalin B (**37**)

Table S3. ^{13}C-labeled precursor incorporation rates (%) for 17-hydroxycitrinalin B (**37**)

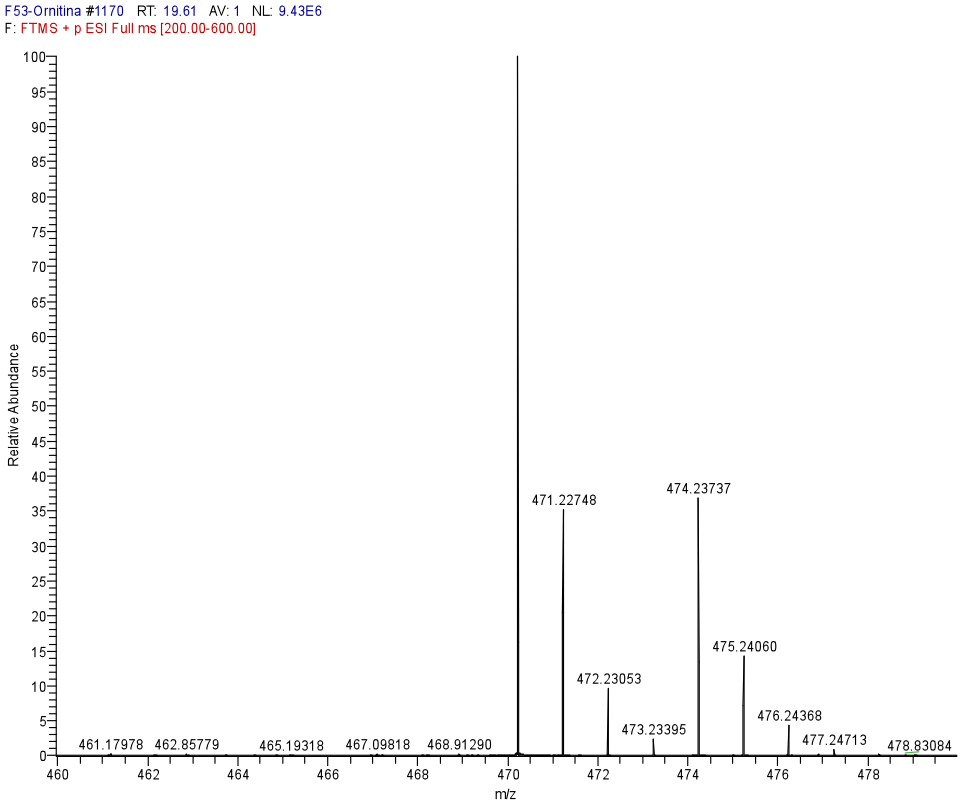
Position	δC	"Cold" (37)	[1-$^{13}C_1$]Glu	[U-$^{13}C_5$]Orn	[U-$^{13}C_6$] AntA
1	60.3	n.o.	n.o.	n.o.	n.o.
2	184.2	1.10	1.10	1.10	1.10
3	-	-	-	-	-
4	80.9	1.10	8.36	6.56	9.38
5	49.0	n.o.	n.o.	n.o.	n.o.
6	195.0	1.10	1.23	1.71	1.07
7	107.0	1.10	2.52	2.55	4.28
8	161.5	1.10	0.99	1.18	2.04
9	111.3	1.10	1.76	1.34	4.66
10	133.9	1.10	7.71	1.22	5.95
11	120.2	1.10	1.24	1.35	2.58
12	144.6	1.10	4.82	1.12	3.27
13	51.0	n.o.	n.o.	n.o.	n.o.
14	45.9	1.10	15.71	2.79	4.37
15	20.0	1.10	6.61	2.61	5.51
16	69.4	1.10	13.77	124	21.83
17	70.1	1.10	8.22	84.7	13.93
18	32.5	1.10	11.58	71.94	5.12
19	54.2	1.10	5.14	92	7.32
20	-	-	-	-	-
21	61.0	1.10	18.73	7.53	2.02
22	93.7	1.10	2.20	2.14	n.o.
23	43.2	1.10	15.33	3.05	3.53
24	27.0	1.10	10.48	2.80	4.14
25	26.9	1.10	9.94	2.22	3.83
26	23.0	1.10	17.88	4.21	6.17
27	23.0	1.10	17.88	4.21	6.17

n.o. = not observed.

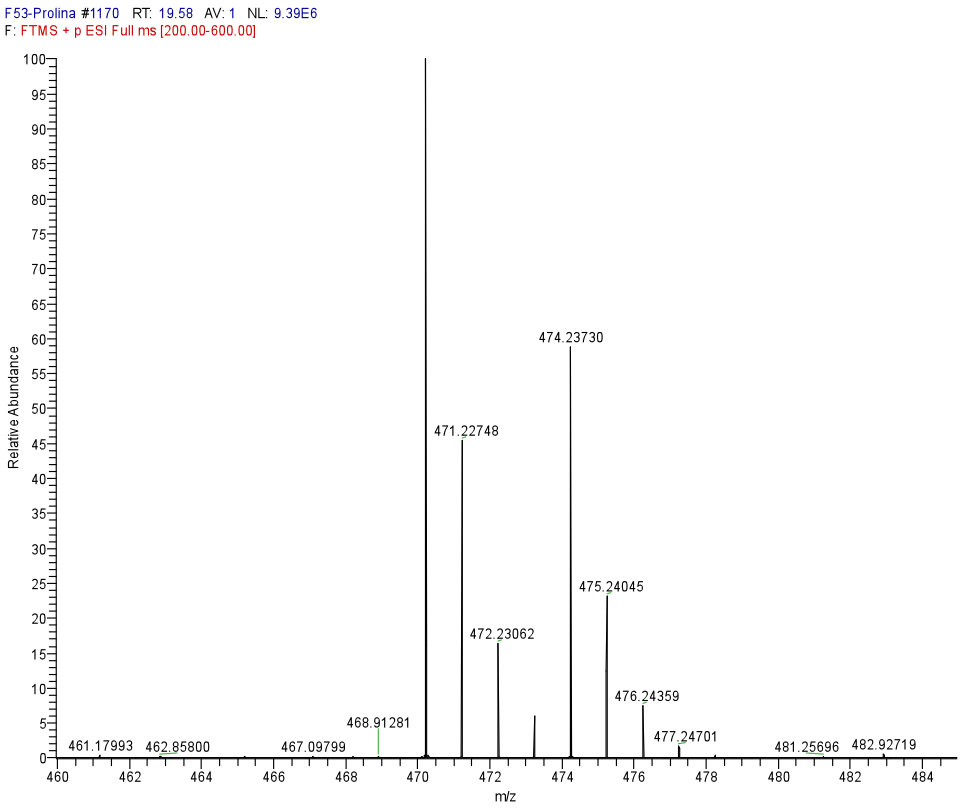
(A)


17-Hidroxicitri-B #1033 RT: 19.20 AV: 1 NL: 1.24E9
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
471.22598
472.22891
461.17972
464.32767
467.27631
469.78186
473.23132
478.00104

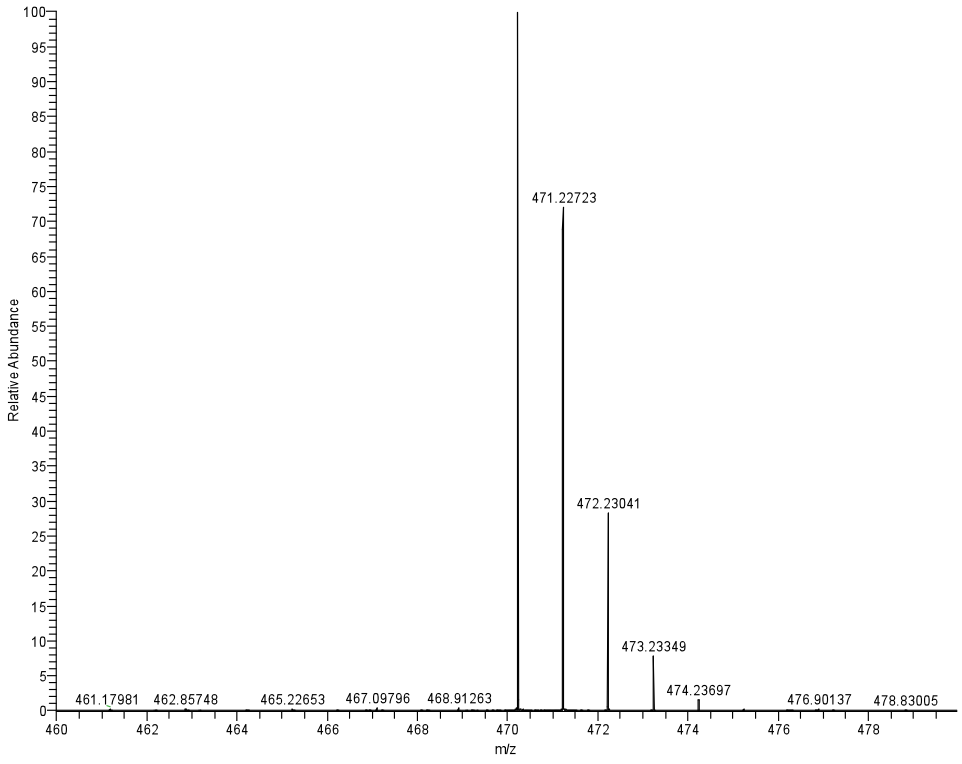
(B)

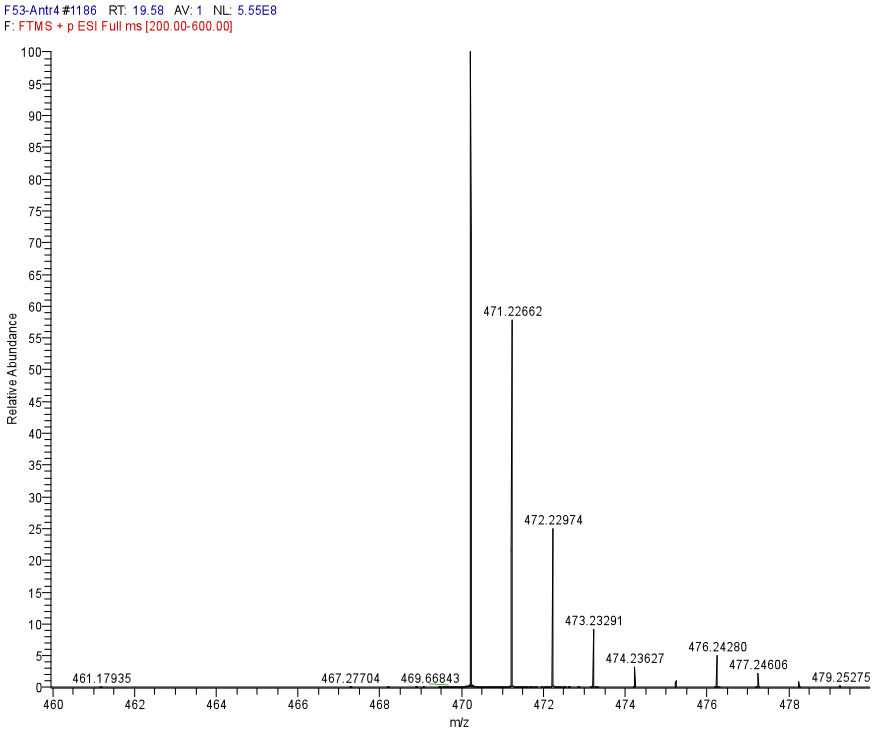

F53-Ornitina #1170 RT: 19.61 AV: 1 NL: 9.43E6
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
471.22748
474.23737
475.24060
472.23053
476.24368
473.23395
477.24713
461.17978
462.85779
465.19318
467.09818
468.91290
478.83084

(C)


F53-Prolina #1170 RT: 19.58 AV: 1 NL: 9.39E6
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
474.23730
471.22748
475.24045
472.23062
476.24359
468.91281
477.24701
461.17993
462.85800
467.09799
481.25696
482.92719

(D)


F53-Gli7 #1179 RT: 19.77 AV: 1 NL: 7.28E6
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
471.22723
472.23041
473.23349
474.23697
461.17981
462.85748
465.22653
467.09796
468.91263
476.90137
478.83005



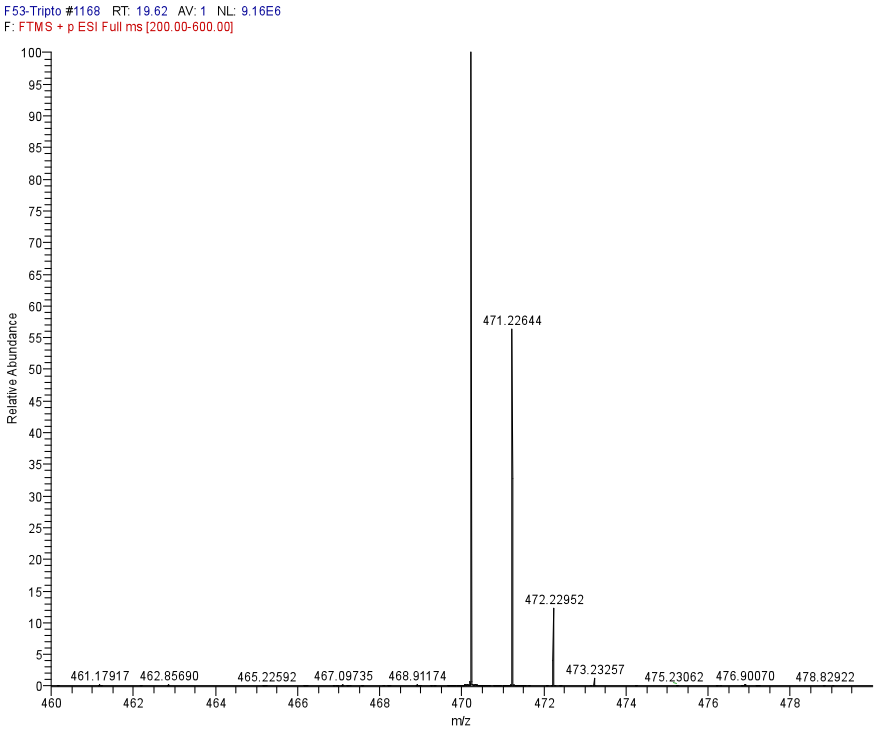


Figure S32. HRMS(ESI$^+$) spectrum of 17-hydroxycitrinalin B (**A**), ([U-$^{13}C_5$]ornithine)-17-hydroxycitrinalin B (**B**), ([U-$^{13}C_5$]proline)-17-hydroxycitrinalin B (**C**), ([1-$^{13}C_1$]glucose)-17-hydroxycitrinalin B (**D**), ([U-$^{13}C_6$]anthranilic acid)-17-hydroxycitrinalin B (**E**), and ([2-indole-$^{13}C_1$]tryptophan)- 17-hydroxycitrinalin B (**F**).

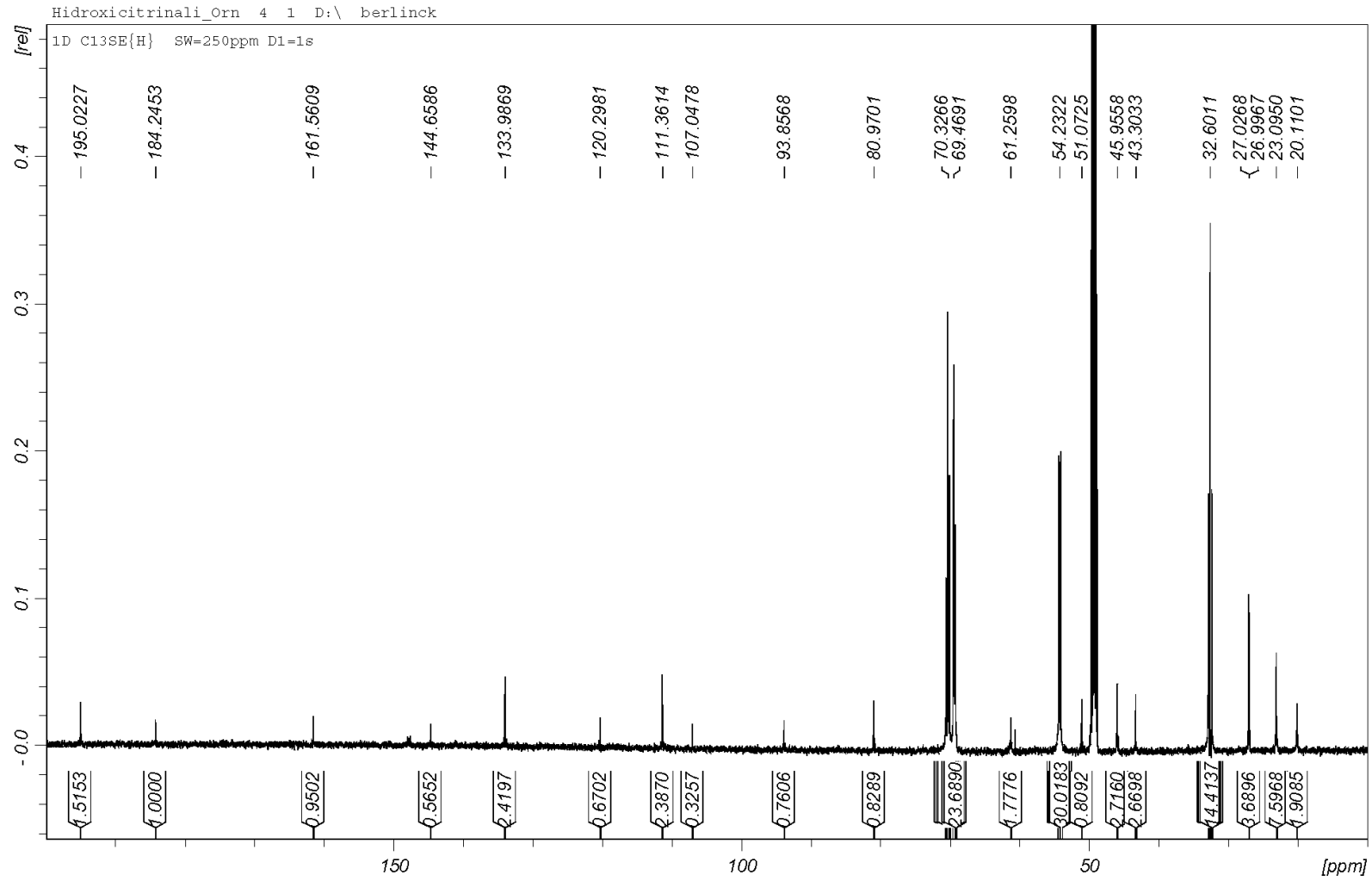


Figure S33. ^{13}C NMR spectrum (MeOH-d_4) for [U-$^{13}C_5$]ornithine labeled 17-hydroxycitrinalin B (**37**).

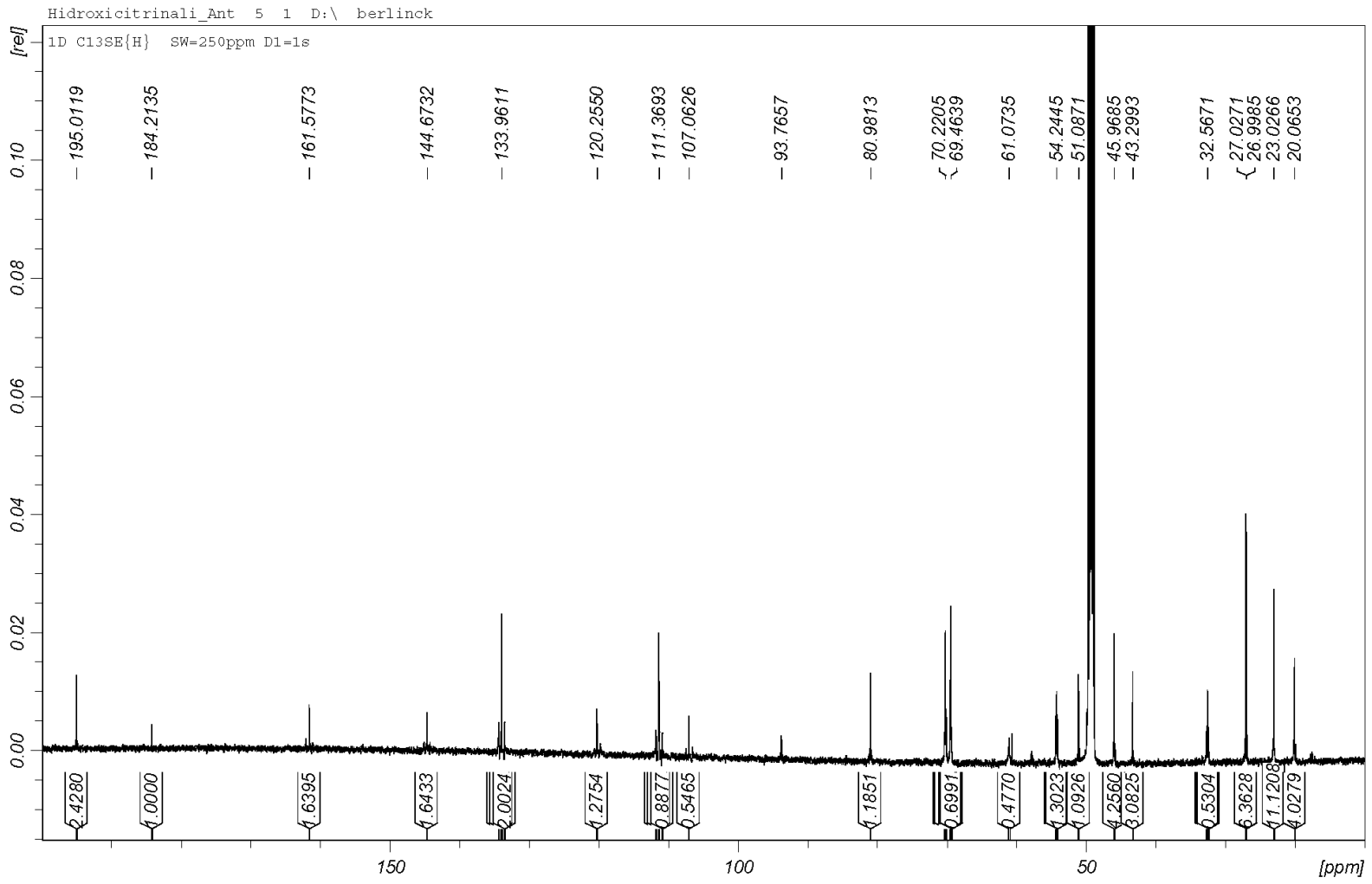


Figure S34. ^{13}C NMR spectrum (MeOH-d_4) for [U-$^{13}C_6$]anthranilic acid labeled 17-hydroxycitrinalin B (**37**).

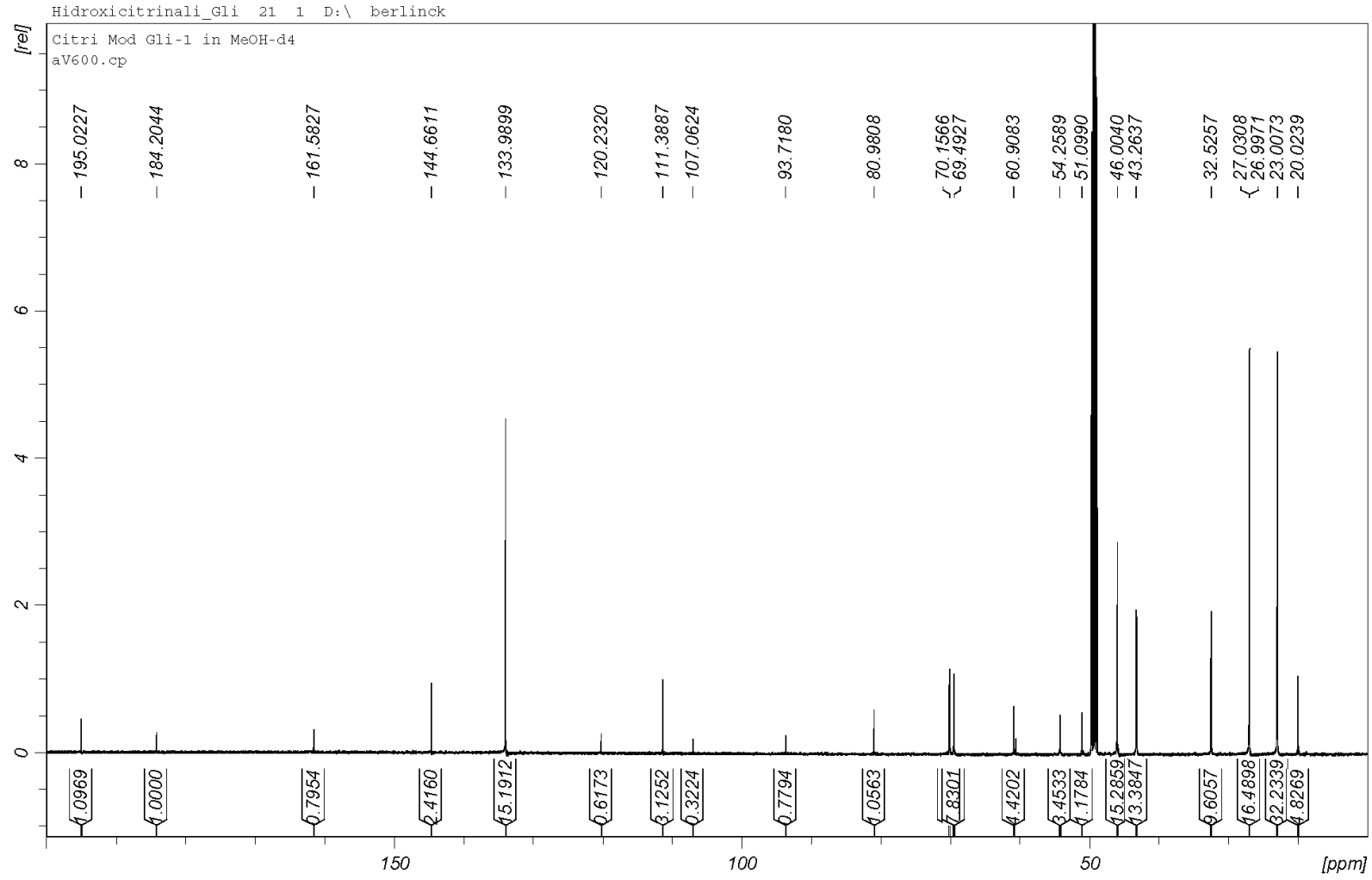
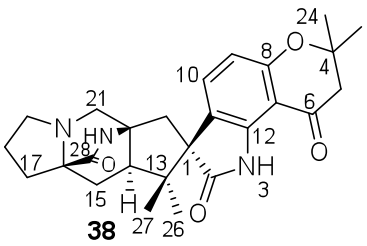


Figure S35. ^{13}C NMR spectrum (MeOH-d_4) for [1-$^{13}C_1$]glucose labeled 17-hydroxycitrinalin B (**37**).

Citrinalin C (**38**): [α]D +40.8 degrees (c. 0.6, MeOH); UV (11:9 (0.05% TFA/ H2O)/MeOH) λmax 208, 231, 265, 284 (sh), 355 nm; NMR (acetone-d_6) see Table S4; (+)-HRESIMS $[M+H]^+$ m/z 450.2329 (calcd for C26H32N3O4, 450.2393).



38

[a]The ^{15}N assignments were not calibrated with an external standard. The value has an accuracy of about 1 ppm in reference to CH_3NO_2 on the basis of ^{15}NHSQC and ^{15}NlrHMQC correlations. n.o. = not observed. *Within a column these signals are interchangeable.

Table S4. NMR data for citrinalin C (**38**) recorded in acetone-d_6

Position	$^{13}C/^{15}N$ (δ)	δ ^1H mult (*J* in Hz)[a]
1	62.5	
2	183.0	
3	-246.3	9.48 (bs)
4	80.2	
5	49.1	2.81 (d, 16.8); 2.76 (d, 16.8)
6	194	
7	105.9	
8	160.5	
9	110.2	6.56 (d, 8.4)
10	133.6	7.49 (d, 8.4)
11	121.6	
12	143.9	
13	47.2	
14	48.7	3.46 (t, 8.5)
15	28.7	2.50 (dd, 8.5, 13.4); 1.93 (dd, 8.5, 13.4)
16	72.3	
17	26.1	2.80[b]
		1.83 (m)
18	23.2	2.15 (m)
19	54.2	3.84 (m)
		2.75[b]
20	-311.5	
21	62.7	4.01 (bd, 9.6)
		3.22 (bd, 9.6)
22	62.6	8.18 (bs)
23	39.2	2.53 (d, 15.6); 2.40 (d, 15.6)
24	26.7*	1.45 (s)
25	26.9*	1.48 (s)
26	20.8	1.09 (s)

27	22.8	0.78 (s)
28	168.3	
28-NH	-249.9	

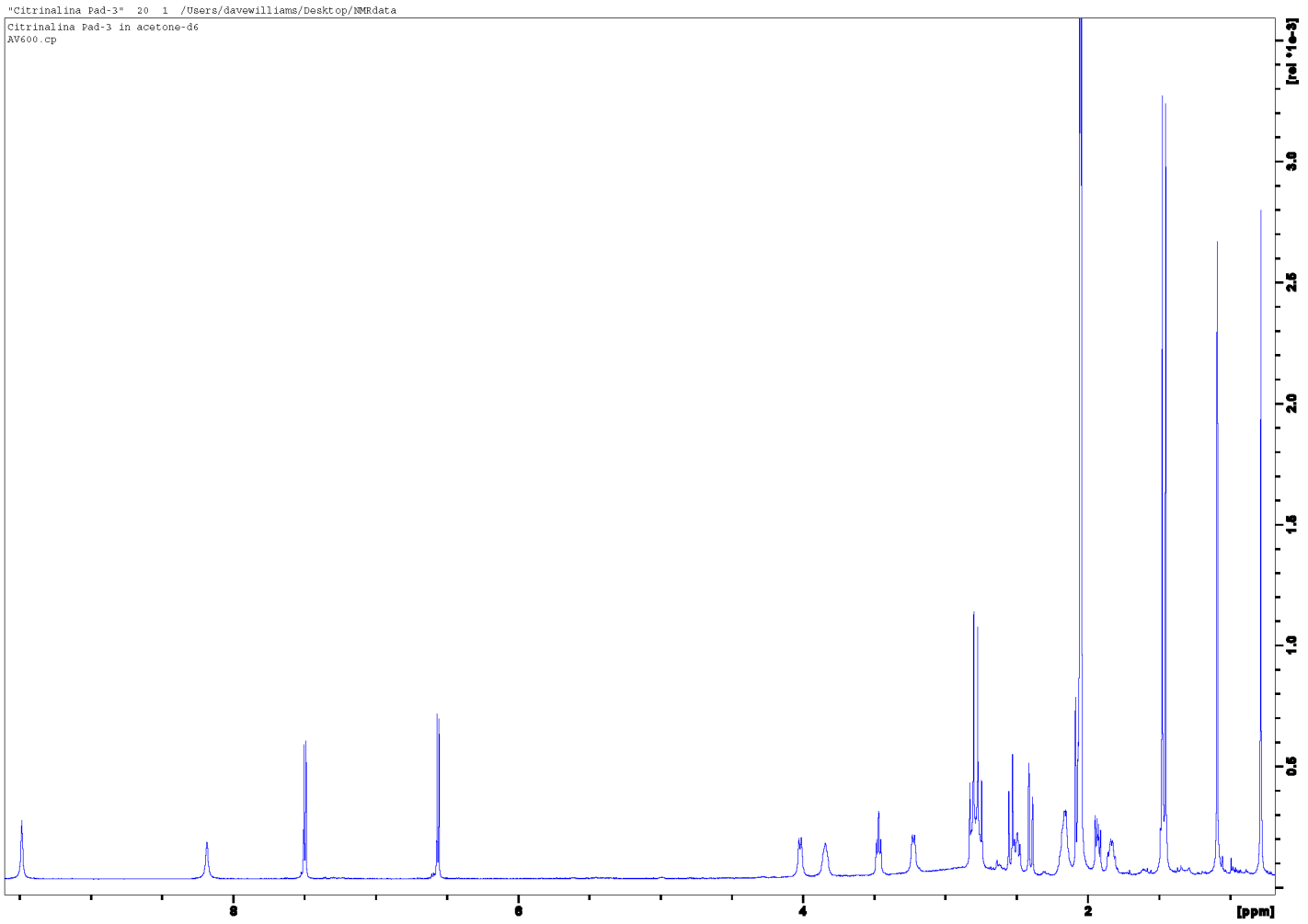


Figure S36. ^{1}H NMR spectrum (600 MHz, acetone-d_6) for citrinalin C (**38**).

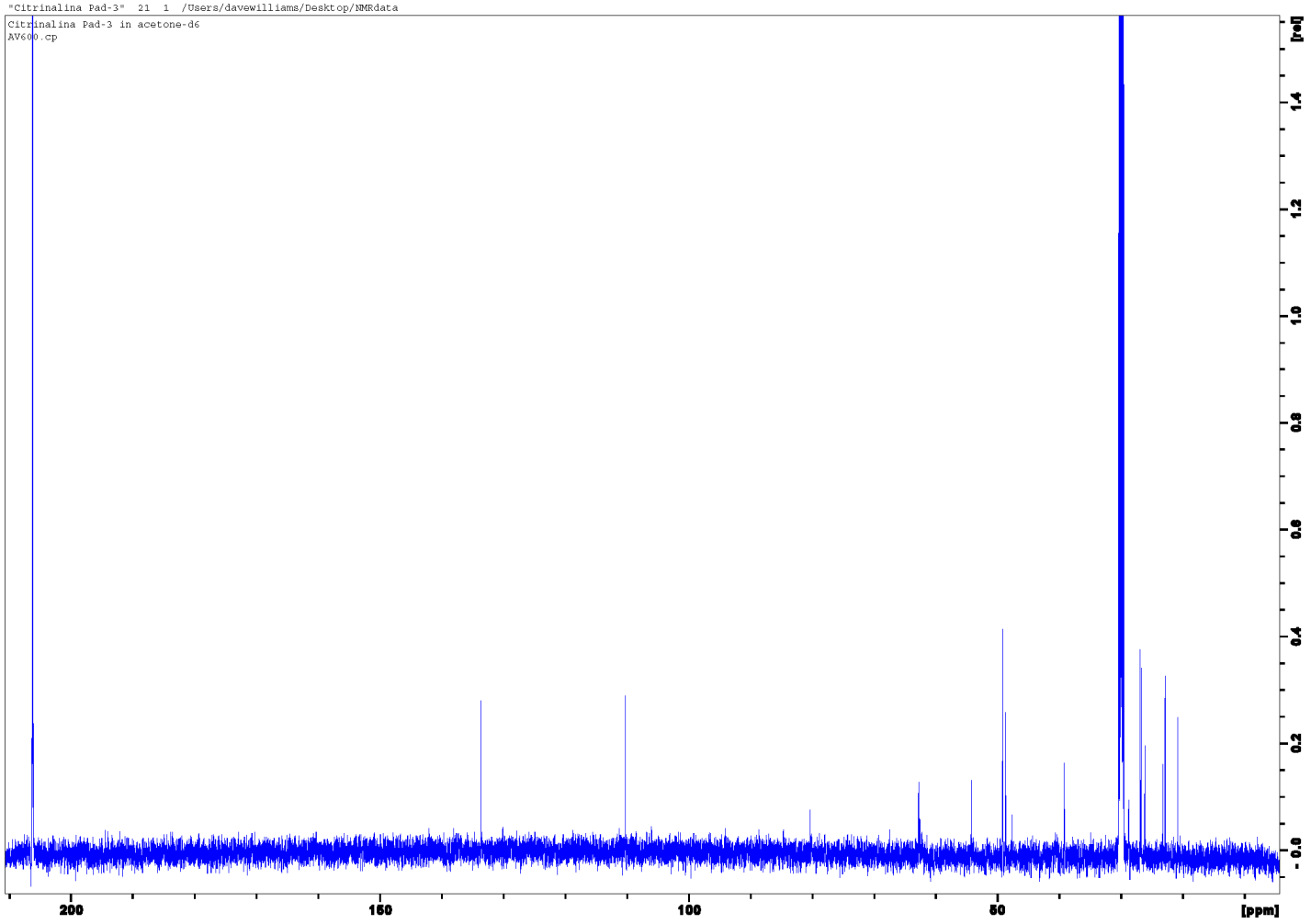


Figure S37. ^{13}C NMR spectrum (150 MHz, acetone-d_6) for citrinalin C (**38**).

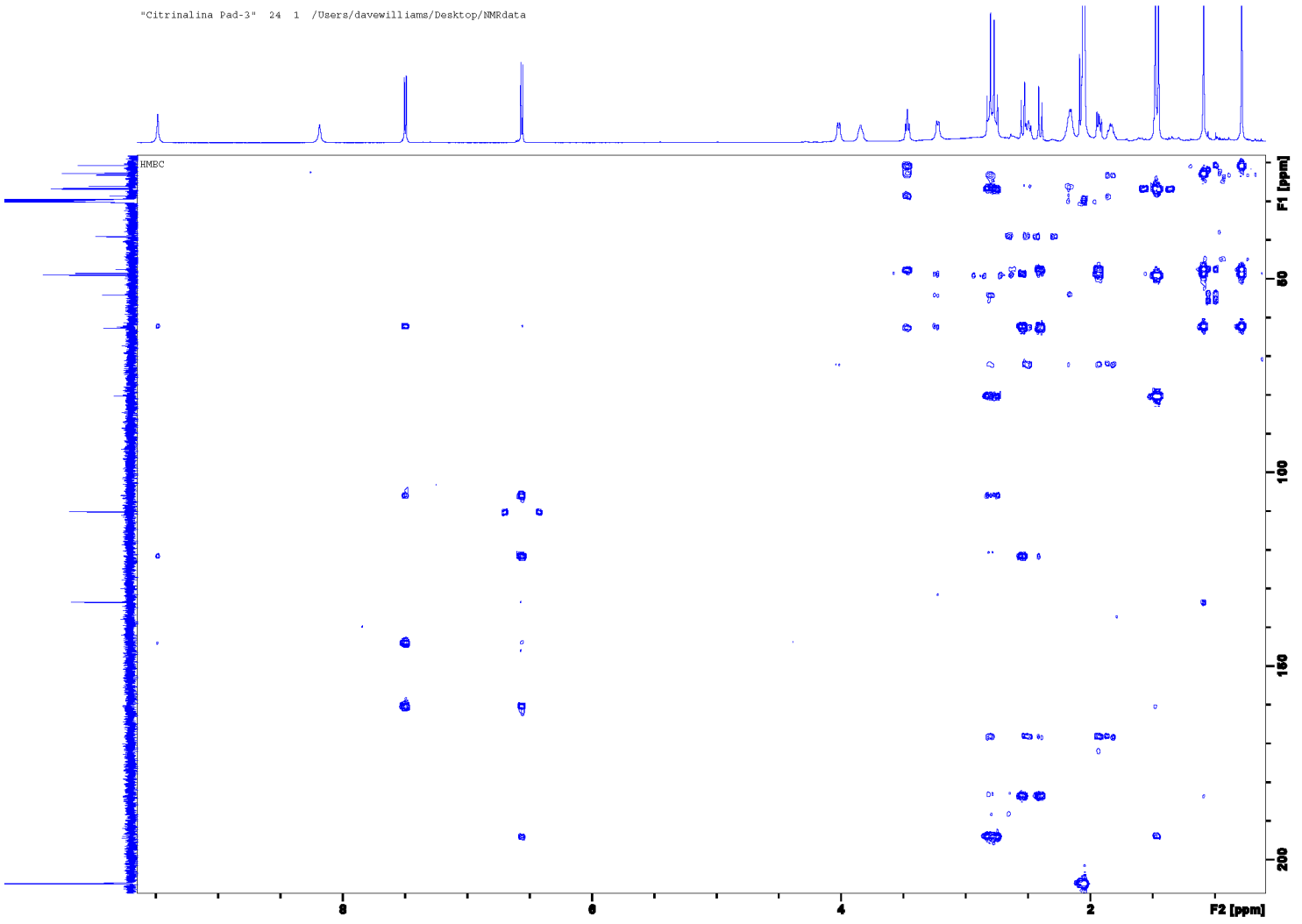


Figure S38. gHMBC spectrum (acetone-d_6) for citrinalin C (**38**).

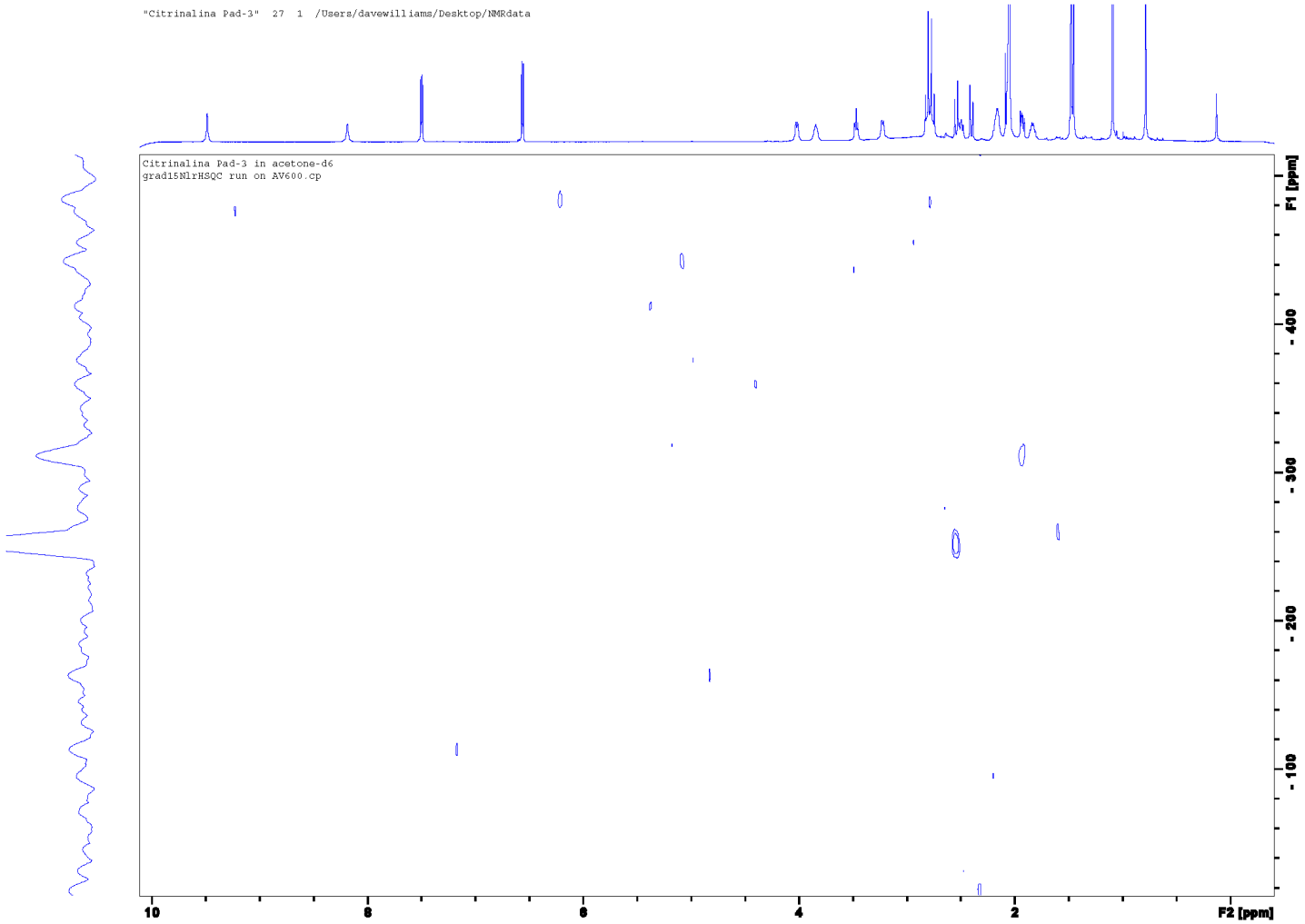


Figure S39. g^{15}NlrHMQC spectrum (acetone-d_6) for citrinalin C (**38**).

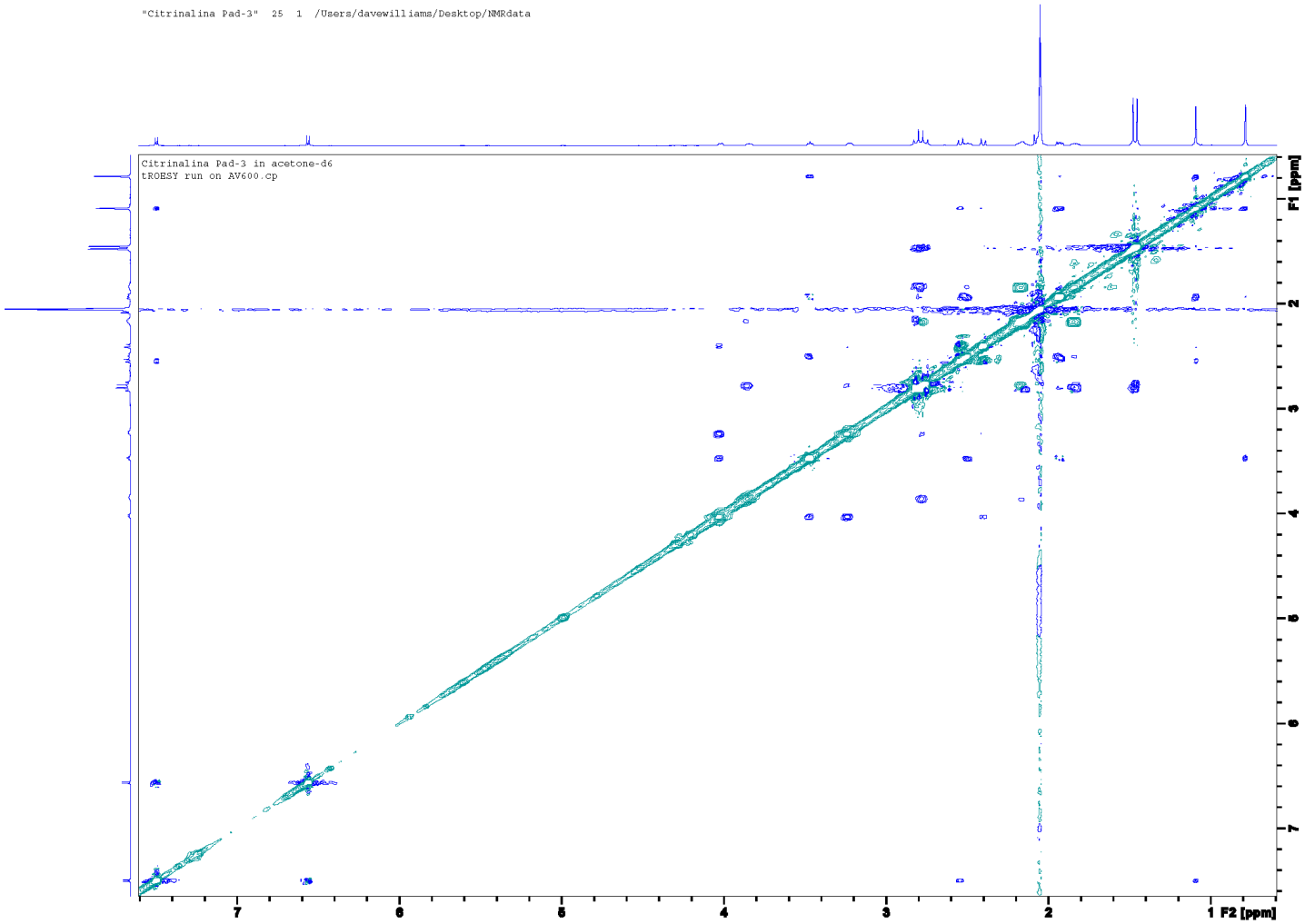


Figure S40. tROESY spectrum (acetone-d_6) for citrinalin C (**38**).

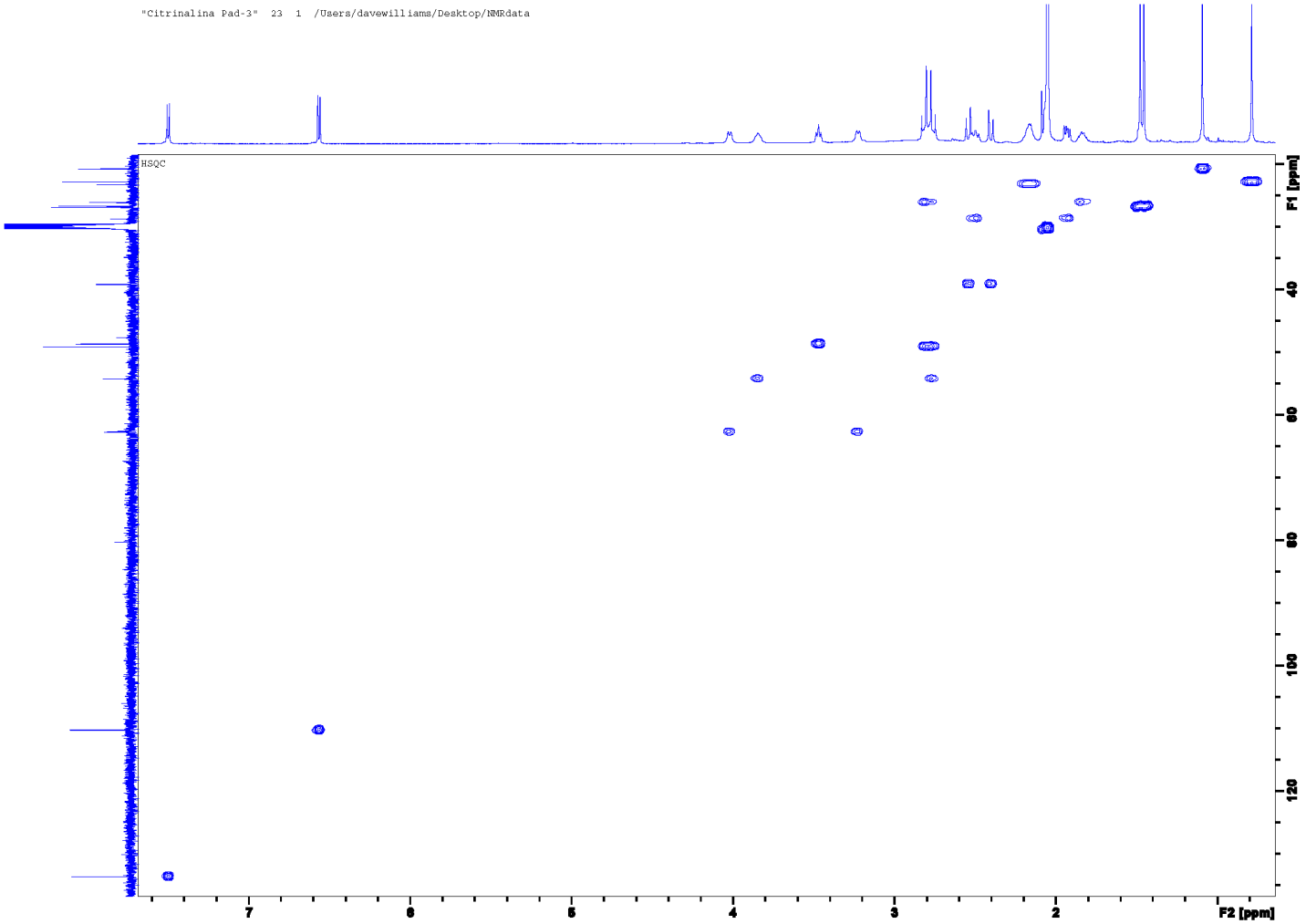


Figure S41. gHSQC spectrum (acetone-d_6) for citrinalin C (**38**).

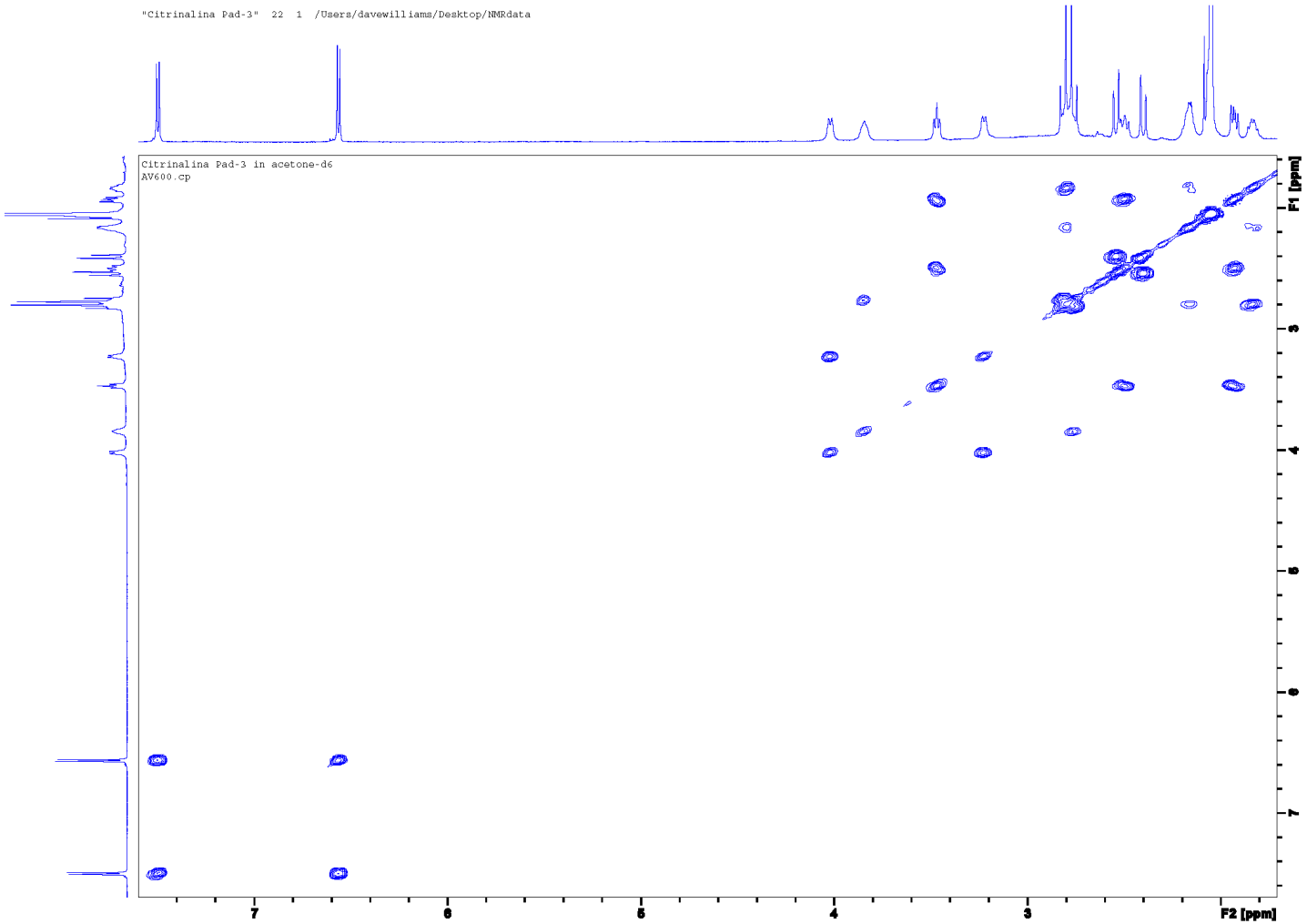
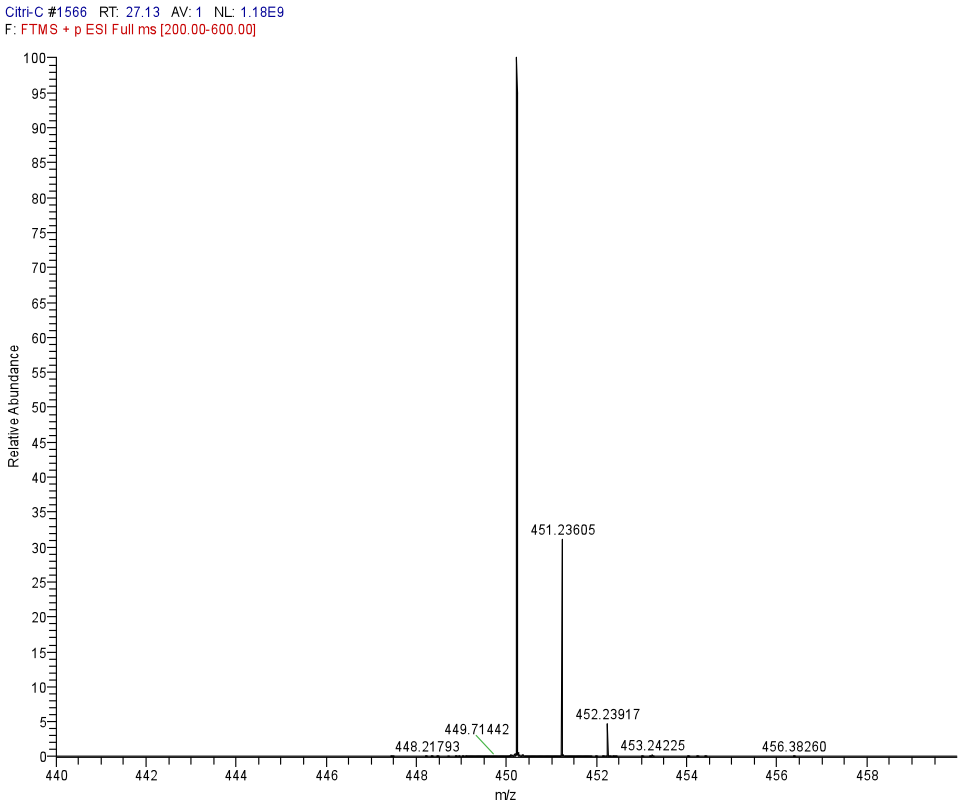
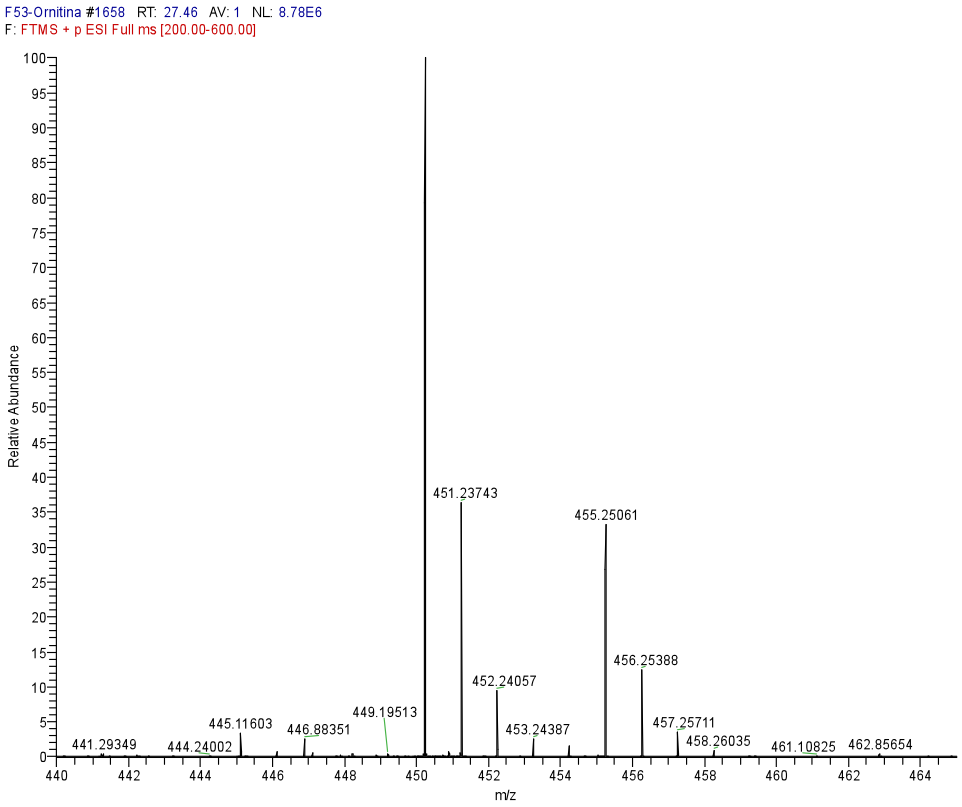


Figure S42. gCOSY60 spectrum (acetone-d_6) for citrinalin C (**38**)

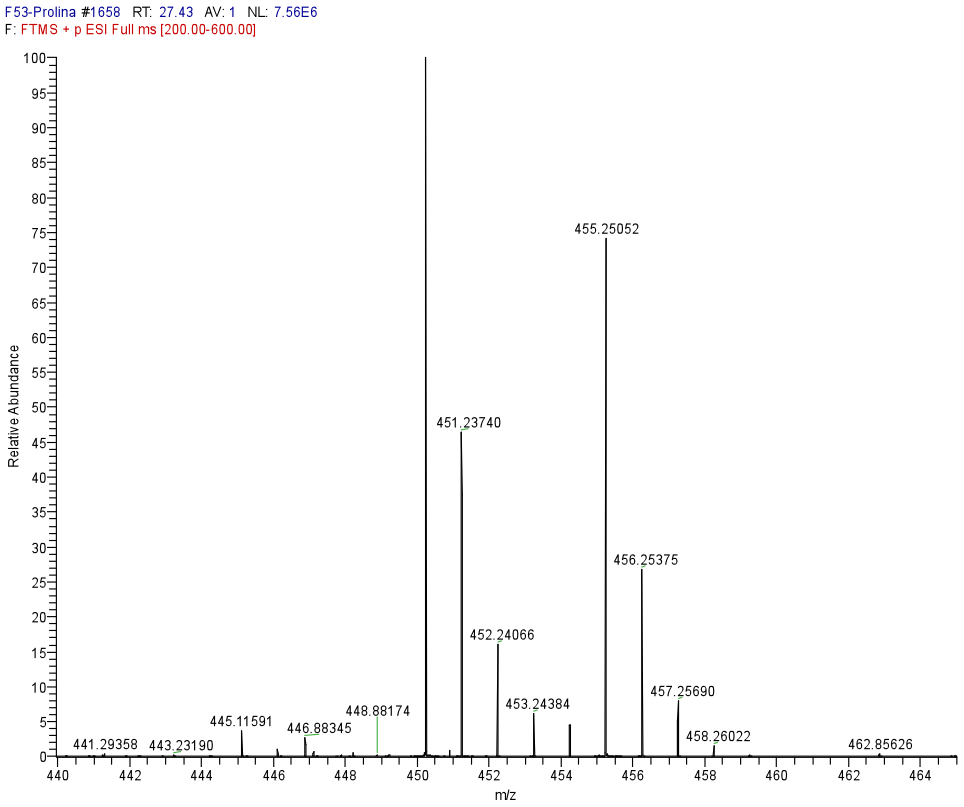
(A)


Citri-C #1566 RT: 27.13 AV: 1 NL: 1.18E9
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
451.23605
449.71442
448.21793
452.23917
453.24225
456.38260

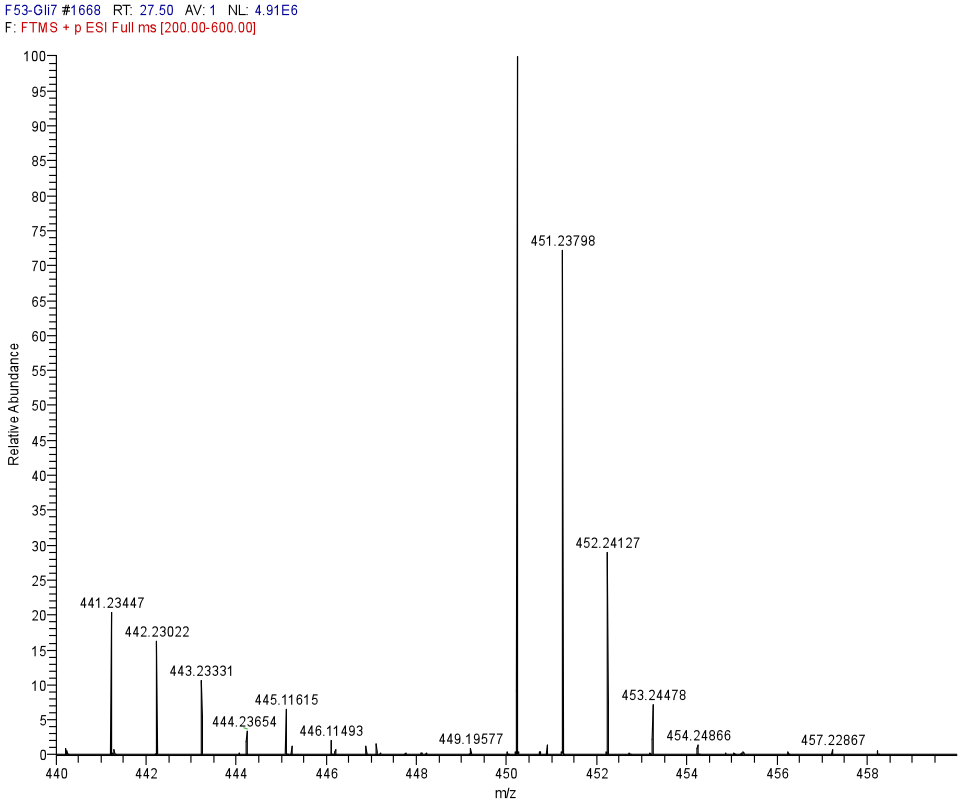
(B)

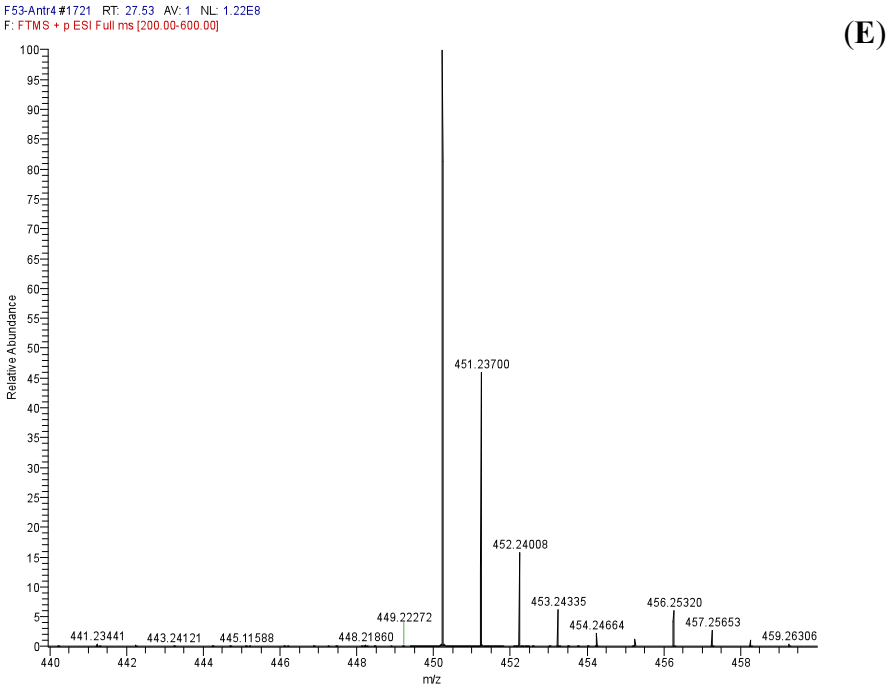

F53-Ornitina #1658 RT: 27.46 AV: 1 NL: 8.78E6
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
451.23743
455.25061
456.25388
452.24057
449.19513
445.11603
446.88351
453.24387
457.25711
458.26035
441.29349
444.24002
461.10825
462.85654

(C)


F53-Prolina #1658 RT: 27.43 AV: 1 NL: 7.56E6
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
455.25052
451.23740
456.25375
452.24066
457.25690
453.24384
458.26022
448.88174
445.11591
446.88345
441.29358
443.23190
462.85626

(D)


F53-Gli7 #1668 RT: 27.50 AV: 1 NL: 4.91E6
F: FTMS + p ESI Full ms [200.00-600.00]
Relative Abundance
m/z
451.23798
452.24127
441.23447
442.23022
443.23331
453.24478
445.11615
444.23654
446.11493
449.19577
454.24866
457.22867



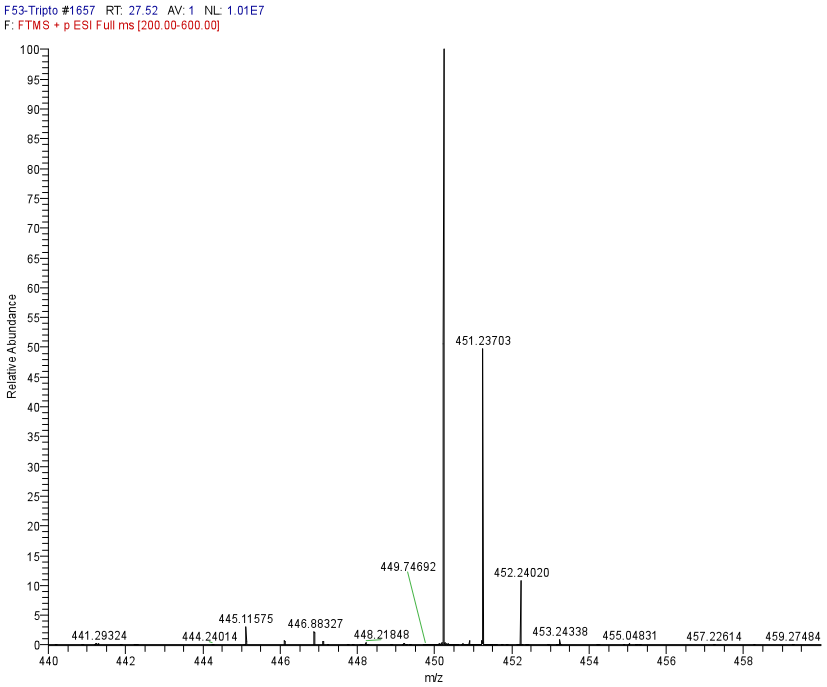
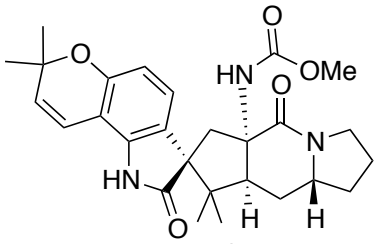


Figure S43. HRMS(ESI$^+$) spectrum of citrinalin C (**A**), ([U-$^{13}C_5$]ornithine)-citrinalin C (**B**), ([U-$^{13}C_5$]proline)-citrinalin C (**C**), ([1-$^{13}C_1$]glucose)-citrinalin C (**D**), ([U-$^{13}C_6$]anthranilic acid)-citrinalin C (**E**), and ([2-indole-$^{13}C_1$]tryptophan)-citrinalin C (**F**).

VIII. Crystallographic Data for compounds 27, 36, *ent*-2•HCl and 6



27

A colorless rod 0.070 x 0.050 x 0.040 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 omgea scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 1.0°. Data collection was 100.0% complete to 67.000° in θ. A total of 43987 reflections were collected covering the indices, -14<=*h*<=14, -15<=*k*<=15, -22<=*l*<=22. 5221 reflections were found to be symmetry independent, with an R_{int} of 0.0234. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P 21 21 21 (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-2011) 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-2012). 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-2012. Absolute stereochemistry was unambiguously determined to be *R* at C5 and *S* at C1, C3 and C10, respectively. CCDC 984480 (**27**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

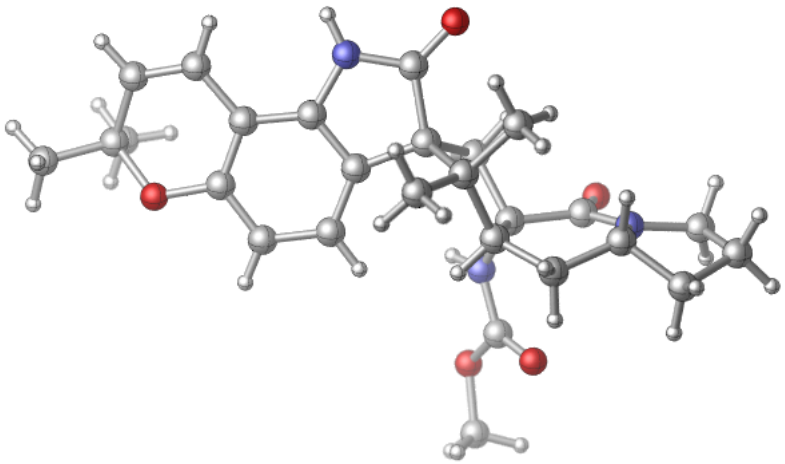


Figure S44. ORTEP representation of **27**

Table 1. Crystal data and structure refinement for sarpong41.

X-ray ID	sarpong41	
Sample/notebook ID	PG7-196B	
Empirical formula	C28 H34 Cl3 N3 O5	
Formula weight	598.93	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 12.3041(9) Å	α= 90°.
	b = 12.6161(9) Å	β= 90°.
	c = 18.4443(14) Å	γ = 90°.
Volume	2863.1(4) $Å^3$	
Z	4	
Density (calculated)	1.389 Mg/m^3	
Absorption coefficient	3.255 mm^{-1}	
F(000)	1256	
Crystal size	0.070 x 0.050 x 0.040 mm^3	
Crystal color/habit	colorless rod	
Theta range for data collection	4.246 to 68.125°.	
Index ranges	-14<=h<=14, -15<=k<=15, -22<=l<=22	
Reflections collected	43987	
Independent reflections	5221 [R(int) = 0.0234]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.817	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5221 / 0 / 357	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0604, wR2 = 0.1713	
R indices (all data)	R1 = 0.0610, wR2 = 0.1720	
Absolute structure parameter	0.010(9)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.962 and -0.724 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sarpong41. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5700(4)	12046(4)	1337(3)	18(1)
C(2)	5237(4)	11847(4)	553(2)	19(1)
C(3)	4962(4)	10637(4)	579(3)	19(1)
C(4)	4171(4)	10241(4)	-2(3)	23(1)
C(5)	2985(4)	10380(4)	186(3)	25(1)
C(6)	2191(5)	9645(5)	-210(3)	34(1)
C(7)	1175(5)	9688(4)	261(4)	37(1)
C(8)	1606(4)	9761(4)	1033(3)	30(1)
C(9)	3411(4)	10158(3)	1506(3)	19(1)
C(10)	4626(4)	10381(4)	1371(2)	18(1)
C(11)	4941(4)	11374(4)	1815(3)	19(1)
C(12)	6910(4)	11817(4)	1425(3)	20(1)
C(13)	7541(4)	10914(4)	1308(3)	23(1)
C(14)	8661(4)	10952(4)	1445(3)	26(1)
C(15)	9140(4)	11881(4)	1693(3)	24(1)
C(16)	10715(4)	12655(5)	2297(3)	31(1)
C(17)	10142(4)	13717(5)	2234(3)	31(1)
C(18)	9099(4)	13769(4)	2031(3)	26(1)
C(19)	8538(4)	12802(4)	1810(3)	22(1)
C(20)	7426(4)	12732(4)	1672(3)	21(1)
C(21)	5635(4)	13207(4)	1612(2)	20(1)
C(22)	6051(4)	12080(4)	-52(3)	25(1)
C(23)	4230(4)	12549(4)	408(3)	21(1)
C(24)	5199(4)	8492(4)	1375(3)	21(1)
C(25)	5921(5)	6771(5)	1469(3)	34(1)
C(26)	11902(5)	12731(6)	2077(4)	39(1)
C(27)	10594(6)	12211(6)	3052(3)	42(2)
C(28)	7858(5)	8463(5)	-773(3)	34(1)
N(1)	2741(3)	10119(3)	941(2)	23(1)
N(2)	6660(3)	13551(3)	1764(2)	22(1)
N(3)	5239(3)	9471(3)	1670(2)	19(1)
O(1)	3092(3)	9995(3)	2131(2)	24(1)
O(2)	10245(3)	11886(3)	1780(2)	28(1)
O(3)	4815(3)	13725(3)	1716(2)	22(1)
O(4)	4749(3)	8252(3)	817(2)	29(1)
O(5)	5772(3)	7808(3)	1787(2)	26(1)
Cl(1)	6634(1)	8280(1)	-285(1)	43(1)
Cl(2)	8362(2)	9729(2)	-626(2)	78(1)
Cl(3)	7648(2)	8215(3)	-1692(1)	74(1)

Table 3. Bond lengths [Å] and angles [°] for sarpong41.

C(1)-C(12)	1.525(6)	C(15)-C(19)	1.395(8)
C(1)-C(11)	1.539(6)	C(16)-O(2)	1.477(6)
C(1)-C(21)	1.553(7)	C(16)-C(27)	1.509(8)
C(1)-C(2)	1.574(6)	C(16)-C(26)	1.519(8)
C(2)-C(22)	1.528(6)	C(16)-C(17)	1.519(8)
C(2)-C(23)	1.547(6)	C(17)-C(18)	1.338(8)
C(2)-C(3)	1.564(6)	C(17)-H(17)	0.9500
C(3)-C(4)	1.530(6)	C(18)-C(19)	1.460(7)
C(3)-C(10)	1.553(6)	C(18)-H(18)	0.9500
C(3)-H(3)	1.0000	C(19)-C(20)	1.394(7)
C(4)-C(5)	1.510(7)	C(20)-N(2)	1.409(6)
C(4)-H(4A)	0.9900	C(21)-O(3)	1.217(6)
C(4)-H(4B)	0.9900	C(21)-N(2)	1.363(6)
C(5)-N(1)	1.463(7)	C(22)-H(22A)	0.9800
C(5)-C(6)	1.532(7)	C(22)-H(22B)	0.9800
C(5)-H(5)	1.0000	C(22)-H(22C)	0.9800
C(6)-C(7)	1.524(9)	C(23)-H(23A)	0.9800
C(6)-H(6A)	0.9900	C(23)-H(23B)	0.9800
C(6)-H(6B)	0.9900	C(23)-H(23C)	0.9800
C(7)-C(8)	1.521(9)	C(24)-O(4)	1.207(6)
C(7)-H(7A)	0.9900	C(24)-O(5)	1.348(6)
C(7)-H(7B)	0.9900	C(24)-N(3)	1.351(6)
C(8)-N(1)	1.477(7)	C(25)-O(5)	1.446(6)
C(8)-H(8A)	0.9900	C(25)-H(25A)	0.9800
C(8)-H(8B)	0.9900	C(25)-H(25B)	0.9800
C(9)-O(1)	1.235(6)	C(25)-H(25C)	0.9800
C(9)-N(1)	1.329(6)	C(26)-H(26A)	0.9800
C(9)-C(10)	1.541(6)	C(26)-H(26B)	0.9800
C(10)-N(3)	1.480(6)	C(26)-H(26C)	0.9800
C(10)-C(11)	1.545(6)	C(27)-H(27A)	0.9800
C(11)-H(11A)	0.9900	C(27)-H(27B)	0.9800
C(11)-H(11B)	0.9900	C(27)-H(27C)	0.9800
C(12)-C(13)	1.395(7)	C(28)-Cl(2)	1.735(7)
C(12)-C(20)	1.394(7)	C(28)-Cl(3)	1.744(6)
C(13)-C(14)	1.402(7)	C(28)-Cl(1)	1.770(6)
C(13)-H(13)	0.9500	C(28)-H(28)	1.0000
C(14)-C(15)	1.389(8)	N(2)-H(2)	0.8800
C(14)-H(14)	0.9500	N(3)-H(3A)	0.8800
C(15)-O(2)	1.369(6)		

C(12)-C(1)-C(11)	115.3(4)	C(10)-C(3)-C(2)	106.8(4)
C(12)-C(1)-C(21)	101.2(4)	C(4)-C(3)-H(3)	106.2
C(11)-C(1)-C(21)	107.5(4)	C(10)-C(3)-H(3)	106.2
C(12)-C(1)-C(2)	114.9(4)	C(2)-C(3)-H(3)	106.2
C(11)-C(1)-C(2)	102.6(4)	C(5)-C(4)-C(3)	114.6(4)
C(21)-C(1)-C(2)	115.6(4)	C(5)-C(4)-H(4A)	108.6
C(22)-C(2)-C(23)	106.8(4)	C(3)-C(4)-H(4A)	108.6
C(22)-C(2)-C(3)	110.6(4)	C(5)-C(4)-H(4B)	108.6
C(23)-C(2)-C(3)	113.0(4)	C(3)-C(4)-H(4B)	108.6
C(22)-C(2)-C(1)	113.7(4)	H(4A)-C(4)-H(4B)	107.6
C(23)-C(2)-C(1)	111.0(4)	N(1)-C(5)-C(4)	113.0(4)
C(3)-C(2)-C(1)	101.9(4)	N(1)-C(5)-C(6)	100.7(4)
C(4)-C(3)-C(10)	114.9(4)	C(4)-C(5)-C(6)	115.9(5)
C(4)-C(3)-C(2)	115.8(4)	N(1)-C(5)-H(5)	109.0

C(4)-C(5)-H(5)	109.0	C(17)-C(18)-C(19)	119.4(5)
C(6)-C(5)-H(5)	109.0	C(17)-C(18)-H(18)	120.3
C(7)-C(6)-C(5)	103.3(5)	C(19)-C(18)-H(18)	120.3
C(7)-C(6)-H(6A)	111.1	C(20)-C(19)-C(15)	116.1(5)
C(5)-C(6)-H(6A)	111.1	C(20)-C(19)-C(18)	124.6(5)
C(7)-C(6)-H(6B)	111.1	C(15)-C(19)-C(18)	119.3(5)
C(5)-C(6)-H(6B)	111.1	C(19)-C(20)-C(12)	124.0(5)
H(6A)-C(6)-H(6B)	109.1	C(19)-C(20)-N(2)	126.0(5)
C(8)-C(7)-C(6)	104.4(4)	C(12)-C(20)-N(2)	110.0(4)
C(8)-C(7)-H(7A)	110.9	O(3)-C(21)-N(2)	124.3(4)
C(6)-C(7)-H(7A)	110.9	O(3)-C(21)-C(1)	126.9(4)
C(8)-C(7)-H(7B)	110.9	N(2)-C(21)-C(1)	108.7(4)
C(6)-C(7)-H(7B)	110.9	C(2)-C(22)-H(22A)	109.5
H(7A)-C(7)-H(7B)	108.9	C(2)-C(22)-H(22B)	109.5
N(1)-C(8)-C(7)	104.0(5)	H(22A)-C(22)-H(22B)	109.5
N(1)-C(8)-H(8A)	111.0	C(2)-C(22)-H(22C)	109.5
C(7)-C(8)-H(8A)	111.0	H(22A)-C(22)-H(22C)	109.5
N(1)-C(8)-H(8B)	111.0	H(22B)-C(22)-H(22C)	109.5
C(7)-C(8)-H(8B)	111.0	C(2)-C(23)-H(23A)	109.5
H(8A)-C(8)-H(8B)	109.0	C(2)-C(23)-H(23B)	109.5
O(1)-C(9)-N(1)	121.9(5)	H(23A)-C(23)-H(23B)	109.5
O(1)-C(9)-C(10)	119.3(4)	C(2)-C(23)-H(23C)	109.5
N(1)-C(9)-C(10)	118.8(4)	H(23A)-C(23)-H(23C)	109.5
N(3)-C(10)-C(9)	107.0(4)	H(23B)-C(23)-H(23C)	109.5
N(3)-C(10)-C(11)	107.7(4)	O(4)-C(24)-O(5)	124.1(4)
C(9)-C(10)-C(11)	107.9(4)	O(4)-C(24)-N(3)	126.1(4)
N(3)-C(10)-C(3)	112.0(4)	O(5)-C(24)-N(3)	109.8(4)
C(9)-C(10)-C(3)	116.6(4)	O(5)-C(25)-H(25A)	109.5
C(11)-C(10)-C(3)	105.2(4)	O(5)-C(25)-H(25B)	109.5
C(1)-C(11)-C(10)	107.2(4)	H(25A)-C(25)-H(25B)	109.5
C(1)-C(11)-H(11A)	110.3	O(5)-C(25)-H(25C)	109.5
C(10)-C(11)-H(11A)	110.3	H(25A)-C(25)-H(25C)	109.5
C(1)-C(11)-H(11B)	110.3	H(25B)-C(25)-H(25C)	109.5
C(10)-C(11)-H(11B)	110.3	C(16)-C(26)-H(26A)	109.5
H(11A)-C(11)-H(11B)	108.5	C(16)-C(26)-H(26B)	109.5
C(13)-C(12)-C(20)	118.3(4)	H(26A)-C(26)-H(26B)	109.5
C(13)-C(12)-C(1)	132.9(5)	C(16)-C(26)-H(26C)	109.5
C(20)-C(12)-C(1)	108.8(4)	H(26A)-C(26)-H(26C)	109.5
C(12)-C(13)-C(14)	119.4(5)	H(26B)-C(26)-H(26C)	109.5
C(12)-C(13)-H(13)	120.3	C(16)-C(27)-H(27A)	109.5
C(14)-C(13)-H(13)	120.3	C(16)-C(27)-H(27B)	109.5
C(15)-C(14)-C(13)	120.4(5)	H(27A)-C(27)-H(27B)	109.5
C(15)-C(14)-H(14)	119.8	C(16)-C(27)-H(27C)	109.5
C(13)-C(14)-H(14)	119.8	H(27A)-C(27)-H(27C)	109.5
O(2)-C(15)-C(14)	117.6(5)	H(27B)-C(27)-H(27C)	109.5
O(2)-C(15)-C(19)	120.3(5)	Cl(2)-C(28)-Cl(3)	111.7(4)
C(14)-C(15)-C(19)	121.9(4)	Cl(2)-C(28)-Cl(1)	110.1(3)
O(2)-C(16)-C(27)	108.3(5)	Cl(3)-C(28)-Cl(1)	110.2(3)
O(2)-C(16)-C(26)	104.2(4)	Cl(2)-C(28)-H(28)	108.2
C(27)-C(16)-C(26)	111.4(5)	Cl(3)-C(28)-H(28)	108.2
O(2)-C(16)-C(17)	110.4(4)	Cl(1)-C(28)-H(28)	108.2
C(27)-C(16)-C(17)	110.6(5)	C(9)-N(1)-C(5)	127.7(4)
C(26)-C(16)-C(17)	111.8(5)	C(9)-N(1)-C(8)	120.5(4)
C(18)-C(17)-C(16)	120.7(5)	C(5)-N(1)-C(8)	111.8(4)
C(18)-C(17)-H(17)	119.7	C(21)-N(2)-C(20)	111.1(4)
C(16)-C(17)-H(17)	119.7	C(21)-N(2)-H(2)	124.4

C(20)-N(2)-H(2)	124.4
C(24)-N(3)-C(10)	122.8(4)
C(24)-N(3)-H(3A)	118.6
C(10)-N(3)-H(3A)	118.6
C(15)-O(2)-C(16)	117.9(4)
C(24)-O(5)-C(25)	114.6(4)

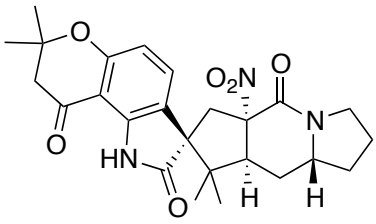
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sarpong41. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	13(2)	22(2)	20(2)	0(2)	1(2)	1(2)
C(2)	16(2)	20(2)	21(2)	1(2)	0(2)	1(2)
C(3)	17(2)	18(2)	23(2)	-1(2)	0(2)	2(2)
C(4)	29(3)	21(2)	18(2)	-1(2)	-3(2)	1(2)
C(5)	29(3)	16(2)	30(3)	2(2)	-14(2)	0(2)
C(6)	38(3)	31(3)	33(3)	9(2)	-21(2)	-11(2)
C(7)	30(3)	25(3)	56(4)	9(3)	-17(3)	-5(2)
C(8)	16(2)	27(3)	48(3)	-8(2)	-4(2)	-1(2)
C(9)	20(2)	12(2)	25(2)	0(2)	0(2)	2(2)
C(10)	15(2)	21(2)	19(2)	-2(2)	-4(2)	1(2)
C(11)	14(2)	20(2)	22(2)	-2(2)	-1(2)	0(2)
C(12)	15(2)	23(2)	22(2)	1(2)	0(2)	3(2)
C(13)	19(2)	27(2)	24(2)	-4(2)	1(2)	1(2)
C(14)	22(2)	29(3)	27(2)	-1(2)	0(2)	9(2)
C(15)	15(2)	35(3)	21(2)	1(2)	0(2)	-1(2)
C(16)	21(3)	40(3)	32(3)	-7(2)	-4(2)	-2(2)
C(17)	23(3)	38(3)	31(3)	-5(2)	-4(2)	-10(2)
C(18)	22(2)	26(2)	28(2)	-4(2)	3(2)	-1(2)
C(19)	19(2)	29(2)	19(2)	2(2)	-2(2)	-3(2)
C(20)	20(2)	22(2)	19(2)	0(2)	3(2)	1(2)
C(21)	21(2)	21(2)	18(2)	3(2)	-2(2)	-1(2)
C(22)	21(2)	27(3)	26(2)	3(2)	4(2)	-2(2)
C(23)	18(2)	17(2)	28(2)	1(2)	-2(2)	1(2)
C(24)	20(2)	20(2)	22(2)	4(2)	6(2)	1(2)
C(25)	48(3)	24(3)	28(3)	1(2)	6(2)	17(2)
C(26)	19(3)	53(4)	46(3)	-10(3)	-4(2)	-2(2)
C(27)	40(3)	55(4)	31(3)	1(3)	-6(3)	5(3)
C(28)	32(3)	44(3)	28(3)	1(2)	2(2)	1(2)
N(1)	15(2)	20(2)	35(2)	-3(2)	-2(2)	2(2)
N(2)	19(2)	19(2)	26(2)	-1(2)	-4(2)	0(2)
N(3)	17(2)	21(2)	20(2)	2(2)	-5(2)	2(2)
O(1)	19(2)	23(2)	29(2)	4(1)	1(1)	1(1)
O(2)	15(2)	39(2)	31(2)	-6(2)	-1(1)	2(2)
O(3)	18(2)	22(2)	27(2)	-3(1)	-1(1)	4(1)
O(4)	38(2)	20(2)	28(2)	1(1)	-6(2)	0(2)
O(5)	29(2)	21(2)	27(2)	1(1)	-1(2)	11(1)
Cl(1)	47(1)	38(1)	44(1)	5(1)	16(1)	6(1)
Cl(2)	46(1)	41(1)	146(2)	-21(1)	1(1)	-13(1)
Cl(3)	47(1)	146(2)	31(1)	-18(1)	2(1)	-11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sarpong41.

	x	y	z	U(eq)
H(3)	5662	10255	492	23
H(4A)	4321	10623	-460	27
H(4B)	4312	9479	-88	27
H(5)	2772	11133	92	30
H(6A)	2039	9905	-706	41
H(6B)	2481	8914	-239	41
H(7A)	727	10316	140	44
H(7B)	729	9042	196	44
H(8A)	1182	10278	1320	36
H(8B)	1577	9062	1276	36
H(11A)	4284	11785	1944	23
H(11B)	5317	11164	2267	23
H(13)	7214	10280	1137	28
H(14)	9094	10340	1369	31
H(17)	10527	14351	2341	37
H(18)	8728	14430	2030	31
H(22A)	5727	11899	-521	37
H(22B)	6709	11655	23	37
H(22C)	6240	12834	-45	37
H(23A)	4438	13298	437	31
H(23B)	3670	12398	771	31
H(23C)	3945	12397	-77	31
H(25A)	5211	6432	1402	50
H(25B)	6369	6335	1791	50
H(25C)	6283	6843	998	50
H(26A)	12235	12026	2099	59
H(26B)	12284	13210	2409	59
H(26C)	11953	13006	1581	59
H(27A)	9821	12099	3158	63
H(27B)	10899	12712	3404	63
H(27C)	10981	11534	3086	63
H(28)	8404	7941	-588	41
H(2)	6822	14200	1902	26
H(3A)	5647	9572	2056	23



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A colorless plate 0.060 x 0.040 x 0.010 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 20 seconds per frame using a scan width of 2.0°. Data collection was 99.9% complete to 67.000° in θ. A total of 31636 reflections were collected covering the indices, -8<=*h*<=5, -13<=*k*<=13, -35<=*l*<=35. 4203 reflections were found to be symmetry independent, with an R_{int} of 0.0441. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P 21 21 21 (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT) 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-2013). 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-2013. Absolute stereochemistry was unambiguously determined to be *R* at C1 and C15, and *S* at C13 and C20, respectively. CCDC 984479 (**36**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

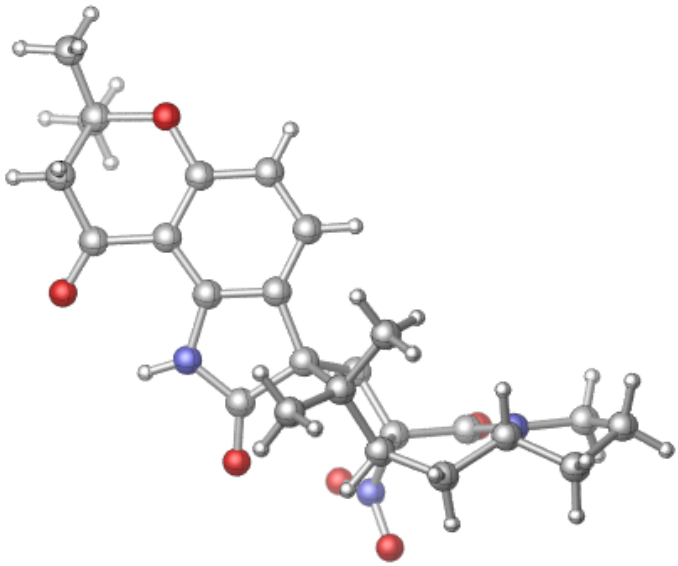


Figure S45. ORTEP representation of **36**

Table 1. Crystal data and structure refinement for sarpong52.

X-ray ID	sarpong52	
Sample/notebook ID	EM04-013C	
Empirical formula	C25 H29 N3 O6	
Formula weight	467.51	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.8459(5) Å	a= 90°.
	b = 11.5478(9) Å	b= 90°.
	c = 29.618(2) Å	g = 90°.
Volume	2341.5(3) $Å^3$	
Z	4	
Density (calculated)	1.326 Mg/m^3	
Absorption coefficient	0.787 mm^{-1}	
F(000)	992	
Crystal size	0.060 x 0.040 x 0.010 mm^3	
Crystal color/habit	colorless plate	
Theta range for data collection	2.984 to 68.243°.	
Index ranges	-8<=h<=5, -13<=k<=13, -35<=l<=35	
Reflections collected	31636	
Independent reflections	4203 [R(int) = 0.0441]	
Completeness to theta = 67.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.781	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4203 / 0 / 311	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0359, wR2 = 0.0750	
R indices (all data)	R1 = 0.0422, wR2 = 0.0773	
Absolute structure parameter	-0.06(8)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.154 and -0.171 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sarpong52. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8956(4)	1404(2)	8450(1)	21(1)
C(2)	9980(4)	554(2)	8755(1)	21(1)
C(3)	10758(4)	-540(2)	8678(1)	24(1)
C(4)	11738(4)	-1111(2)	9021(1)	27(1)
C(5)	11898(4)	-618(2)	9446(1)	27(1)
C(6)	13375(5)	-716(3)	10190(1)	43(1)
C(7)	11796(5)	113(3)	10345(1)	41(1)
C(8)	11233(4)	981(3)	9991(1)	34(1)
C(9)	11152(4)	492(2)	9536(1)	26(1)
C(10)	10249(4)	1060(2)	9176(1)	24(1)
C(11)	8869(4)	2494(2)	8754(1)	24(1)
C(12)	6836(4)	1084(2)	8283(1)	23(1)
C(13)	6540(4)	1934(2)	7877(1)	22(1)
C(14)	5061(4)	1597(2)	7508(1)	25(1)
C(15)	5859(4)	758(2)	7163(1)	26(1)
C(16)	4706(4)	621(3)	6725(1)	38(1)
C(17)	6251(5)	76(3)	6415(1)	44(1)
C(18)	8123(4)	730(2)	6528(1)	28(1)
C(19)	9054(4)	1822(2)	7193(1)	21(1)
C(20)	8601(3)	2192(2)	7684(1)	20(1)
C(21)	10065(4)	1644(2)	8009(1)	21(1)
C(22)	13596(7)	-1723(3)	10516(1)	69(1)
C(23)	15290(5)	-90(3)	10107(1)	61(1)
C(24)	6741(4)	-195(2)	8153(1)	27(1)
C(25)	5282(4)	1292(3)	8646(1)	32(1)
N(1)	9535(3)	2184(2)	9171(1)	28(1)
N(2)	7771(3)	1145(2)	6990(1)	22(1)
N(3)	8890(3)	3502(2)	7650(1)	25(1)
O(1)	12779(3)	-1277(2)	9768(1)	38(1)
O(2)	10782(3)	1977(2)	10078(1)	46(1)
O(3)	8275(3)	3451(2)	8651(1)	30(1)
O(4)	10400(3)	3942(2)	7781(1)	35(1)
O(5)	7576(3)	4040(2)	7460(1)	33(1)
O(6)	10580(3)	2167(2)	7018(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for sarpong52.

C(1)-C(2)	1.508(3)	C(15)-N(2)	1.475(3)
C(1)-C(21)	1.535(3)	C(15)-C(16)	1.526(4)
C(1)-C(11)	1.549(3)	C(15)-H(15)	1.0000
C(1)-C(12)	1.578(4)	C(16)-C(17)	1.536(4)
C(2)-C(10)	1.387(3)	C(16)-H(16A)	0.9900
C(2)-C(3)	1.390(3)	C(16)-H(16B)	0.9900
C(3)-C(4)	1.384(4)	C(17)-C(18)	1.525(4)
C(3)-H(3)	0.9500	C(17)-H(17A)	0.9900
C(4)-C(5)	1.387(4)	C(17)-H(17B)	0.9900
C(4)-H(4)	0.9500	C(18)-N(2)	1.469(3)
C(5)-O(1)	1.362(3)	C(18)-H(18A)	0.9900
C(5)-C(9)	1.405(4)	C(18)-H(18B)	0.9900
C(6)-O(1)	1.463(3)	C(19)-O(6)	1.232(3)
C(6)-C(7)	1.515(5)	C(19)-N(2)	1.321(3)
C(6)-C(23)	1.516(5)	C(19)-C(20)	1.549(3)
C(6)-C(22)	1.521(5)	C(20)-C(21)	1.526(3)
C(7)-C(8)	1.500(4)	C(20)-N(3)	1.530(3)
C(7)-H(7A)	0.9900	C(21)-H(21A)	0.9900
C(7)-H(7B)	0.9900	C(21)-H(21B)	0.9900
C(8)-O(2)	1.219(3)	C(22)-H(22A)	0.9800
C(8)-C(9)	1.462(4)	C(22)-H(22B)	0.9800
C(9)-C(10)	1.397(4)	C(22)-H(22C)	0.9800
C(10)-N(1)	1.387(3)	C(23)-H(23A)	0.9800
C(11)-O(3)	1.217(3)	C(23)-H(23B)	0.9800
C(11)-N(1)	1.364(3)	C(23)-H(23C)	0.9800
C(12)-C(24)	1.528(4)	C(24)-H(24A)	0.9800
C(12)-C(25)	1.531(3)	C(24)-H(24B)	0.9800
C(12)-C(13)	1.565(3)	C(24)-H(24C)	0.9800
C(13)-C(14)	1.539(4)	C(25)-H(25A)	0.9800
C(13)-C(20)	1.551(3)	C(25)-H(25B)	0.9800
C(13)-H(13)	1.0000	C(25)-H(25C)	0.9800
C(14)-C(15)	1.511(4)	N(1)-H(1)	0.8800
C(14)-H(14A)	0.9900	N(3)-O(4)	1.216(3)
C(14)-H(14B)	0.9900	N(3)-O(5)	1.229(3)

C(2)-C(1)-C(21)	113.4(2)	O(1)-C(6)-C(23)	108.3(3)
C(2)-C(1)-C(11)	101.40(19)	C(7)-C(6)-C(23)	111.4(3)
C(21)-C(1)-C(11)	111.6(2)	O(1)-C(6)-C(22)	103.4(2)
C(2)-C(1)-C(12)	117.6(2)	C(7)-C(6)-C(22)	111.1(3)
C(21)-C(1)-C(12)	103.31(18)	C(23)-C(6)-C(22)	112.4(3)
C(11)-C(1)-C(12)	109.7(2)	C(8)-C(7)-C(6)	113.2(2)
C(10)-C(2)-C(3)	118.7(2)	C(8)-C(7)-H(7A)	108.9
C(10)-C(2)-C(1)	109.0(2)	C(6)-C(7)-H(7A)	108.9
C(3)-C(2)-C(1)	132.1(2)	C(8)-C(7)-H(7B)	108.9
C(4)-C(3)-C(2)	119.8(2)	C(6)-C(7)-H(7B)	108.9
C(4)-C(3)-H(3)	120.1	H(7A)-C(7)-H(7B)	107.8
C(2)-C(3)-H(3)	120.1	O(2)-C(8)-C(9)	123.3(3)
C(3)-C(4)-C(5)	120.6(2)	O(2)-C(8)-C(7)	123.2(2)
C(3)-C(4)-H(4)	119.7	C(9)-C(8)-C(7)	113.3(2)
C(5)-C(4)-H(4)	119.7	C(10)-C(9)-C(5)	116.4(2)
O(1)-C(5)-C(4)	116.3(2)	C(10)-C(9)-C(8)	122.7(2)
O(1)-C(5)-C(9)	122.5(2)	C(5)-C(9)-C(8)	120.9(2)
C(4)-C(5)-C(9)	121.2(2)	C(2)-C(10)-N(1)	109.8(2)
O(1)-C(6)-C(7)	109.8(2)	C(2)-C(10)-C(9)	123.2(2)

N(1)-C(10)-C(9)	127.1(2)
O(3)-C(11)-N(1)	125.2(2)
O(3)-C(11)-C(1)	127.2(2)
N(1)-C(11)-C(1)	107.5(2)
C(24)-C(12)-C(25)	107.4(2)
C(24)-C(12)-C(13)	114.0(2)
C(25)-C(12)-C(13)	110.5(2)
C(24)-C(12)-C(1)	110.2(2)
C(25)-C(12)-C(1)	112.5(2)
C(13)-C(12)-C(1)	102.30(19)
C(14)-C(13)-C(20)	112.7(2)
C(14)-C(13)-C(12)	118.1(2)
C(20)-C(13)-C(12)	106.57(19)
C(14)-C(13)-H(13)	106.2
C(20)-C(13)-H(13)	106.2
C(12)-C(13)-H(13)	106.2
C(15)-C(14)-C(13)	113.9(2)
C(15)-C(14)-H(14A)	108.8
C(13)-C(14)-H(14A)	108.8
C(15)-C(14)-H(14B)	108.8
C(13)-C(14)-H(14B)	108.8
H(14A)-C(14)-H(14B)	107.7
N(2)-C(15)-C(14)	111.2(2)
N(2)-C(15)-C(16)	101.3(2)
C(14)-C(15)-C(16)	117.1(2)
N(2)-C(15)-H(15)	109.0
C(14)-C(15)-H(15)	109.0
C(16)-C(15)-H(15)	109.0
C(15)-C(16)-C(17)	101.2(2)
C(15)-C(16)-H(16A)	111.5
C(17)-C(16)-H(16A)	111.5
C(15)-C(16)-H(16B)	111.5
C(17)-C(16)-H(16B)	111.5
H(16A)-C(16)-H(16B)	109.3
C(18)-C(17)-C(16)	104.2(2)
C(18)-C(17)-H(17A)	110.9
C(16)-C(17)-H(17A)	110.9
C(18)-C(17)-H(17B)	110.9
C(16)-C(17)-H(17B)	110.9
H(17A)-C(17)-H(17B)	108.9
N(2)-C(18)-C(17)	103.2(2)
N(2)-C(18)-H(18A)	111.1
C(17)-C(18)-H(18A)	111.1
N(2)-C(18)-H(18B)	111.1
C(17)-C(18)-H(18B)	111.1
H(18A)-C(18)-H(18B)	109.1
O(6)-C(19)-N(2)	124.3(2)
O(6)-C(19)-C(20)	118.4(2)
N(2)-C(19)-C(20)	117.2(2)
C(21)-C(20)-N(3)	111.6(2)
C(21)-C(20)-C(19)	110.31(19)
N(3)-C(20)-C(19)	100.58(18)
C(21)-C(20)-C(13)	106.62(19)
N(3)-C(20)-C(13)	109.39(19)
C(19)-C(20)-C(13)	118.4(2)
C(20)-C(21)-C(1)	106.6(2)
C(20)-C(21)-H(21A)	110.4
C(1)-C(21)-H(21A)	110.4
C(20)-C(21)-H(21B)	110.4
C(1)-C(21)-H(21B)	110.4
H(21A)-C(21)-H(21B)	108.6
C(6)-C(22)-H(22A)	109.5
C(6)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(6)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(6)-C(23)-H(23A)	109.5
C(6)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(6)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(12)-C(24)-H(24A)	109.5
C(12)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(12)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(12)-C(25)-H(25A)	109.5
C(12)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(12)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(11)-N(1)-C(10)	111.9(2)
C(11)-N(1)-H(1)	124.1
C(10)-N(1)-H(1)	124.1
C(19)-N(2)-C(18)	120.5(2)
C(19)-N(2)-C(15)	127.7(2)
C(18)-N(2)-C(15)	111.7(2)
O(4)-N(3)-O(5)	123.9(2)
O(4)-N(3)-C(20)	120.1(2)
O(5)-N(3)-C(20)	115.9(2)
C(5)-O(1)-C(6)	118.3(2)

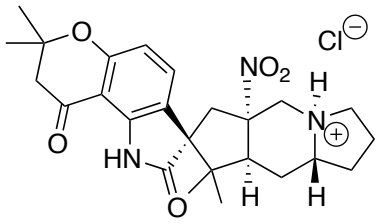
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sarpong52. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	19(1)	18(1)	24(1)	-1(1)	2(1)	0(1)
C(2)	18(1)	21(1)	23(1)	0(1)	2(1)	-3(1)
C(3)	26(1)	22(1)	24(1)	-1(1)	0(1)	-2(1)
C(4)	32(1)	18(1)	30(1)	-2(1)	-2(1)	2(1)
C(5)	28(1)	26(2)	28(1)	4(1)	-7(1)	-2(1)
C(6)	59(2)	36(2)	35(2)	-5(1)	-24(2)	8(2)
C(7)	56(2)	40(2)	27(1)	-4(1)	-10(1)	-3(2)
C(8)	36(2)	35(2)	30(1)	-4(1)	-5(1)	2(1)
C(9)	27(1)	26(2)	26(1)	-1(1)	-2(1)	0(1)
C(10)	21(1)	23(1)	26(1)	-2(1)	2(1)	0(1)
C(11)	22(1)	22(2)	29(1)	-3(1)	1(1)	0(1)
C(12)	19(1)	25(1)	25(1)	1(1)	1(1)	-1(1)
C(13)	19(1)	21(1)	27(1)	1(1)	3(1)	2(1)
C(14)	17(1)	28(2)	30(1)	3(1)	0(1)	1(1)
C(15)	20(1)	30(2)	27(1)	2(1)	-2(1)	-2(1)
C(16)	29(2)	52(2)	31(1)	1(1)	-6(1)	-5(2)
C(17)	44(2)	61(2)	28(1)	-9(1)	-4(1)	-6(2)
C(18)	32(2)	30(2)	23(1)	2(1)	0(1)	3(1)
C(19)	18(1)	19(1)	25(1)	5(1)	1(1)	4(1)
C(20)	19(1)	14(1)	27(1)	0(1)	0(1)	1(1)
C(21)	16(1)	22(1)	26(1)	1(1)	1(1)	-1(1)
C(22)	116(4)	49(2)	42(2)	-3(2)	-40(2)	17(2)
C(23)	48(2)	59(2)	75(3)	-23(2)	-28(2)	13(2)
C(24)	26(1)	28(2)	28(1)	4(1)	-5(1)	-7(1)
C(25)	22(1)	45(2)	30(1)	5(1)	4(1)	-2(1)
N(1)	36(1)	23(1)	26(1)	-8(1)	-2(1)	6(1)
N(2)	22(1)	23(1)	23(1)	2(1)	1(1)	1(1)
N(3)	26(1)	23(1)	26(1)	1(1)	4(1)	-1(1)
O(1)	55(1)	29(1)	30(1)	-1(1)	-17(1)	5(1)
O(2)	66(2)	38(1)	34(1)	-13(1)	-11(1)	14(1)
O(3)	35(1)	22(1)	34(1)	-3(1)	0(1)	5(1)
O(4)	37(1)	28(1)	38(1)	1(1)	-3(1)	-14(1)
O(5)	36(1)	23(1)	40(1)	7(1)	1(1)	8(1)
O(6)	22(1)	33(1)	30(1)	3(1)	6(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sarpong52.

	x	y	z	U(eq)
H(3)	10617	-895	8390	29
H(4)	12306	-1847	8964	32
H(7A)	10625	-338	10432	50
H(7B)	12260	531	10616	50
H(13)	6059	2678	8010	27
H(14A)	3902	1246	7654	30
H(14B)	4626	2308	7351	30
H(15)	6016	-19	7307	31
H(16A)	4255	1378	6608	45
H(16B)	3567	102	6766	45
H(17A)	6398	-762	6478	53
H(17B)	5897	179	6093	53
H(18A)	9273	211	6517	34
H(18B)	8330	1384	6318	34
H(21A)	11171	2177	8065	26
H(21B)	10584	913	7882	26
H(22A)	12380	-2171	10524	104
H(22B)	13878	-1425	10819	104
H(22C)	14671	-2222	10417	104
H(23A)	16260	-640	9992	91
H(23B)	15758	247	10391	91
H(23C)	15088	527	9885	91
H(24A)	6933	-673	8423	41
H(24B)	7767	-367	7932	41
H(24C)	5461	-366	8020	41
H(25A)	3998	1065	8529	48
H(25B)	5262	2115	8727	48
H(25C)	5590	829	8914	48
H(1)	9515	2642	9408	34



ent-Citrinalin B•HCl (*ent*-**2**•HCl)

A colorless plate 0.040 x 0.030 x 0.010 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 20 seconds per frame using a scan width of 2.0°. Data collection was 98.4% complete to 67.000° in θ. A total of 17934 reflections were collected covering the indices, -30<=*h*<=25, -8<=*k*<=8, -19<=*l*<=19. 4686 reflections were found to be symmetry independent, with an R_{int} of 0.0572. Indexing and unit cell refinement indicated a C-centered, monoclinic lattice. The space group was found to be C 2 (No. 5). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT) 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-2013). 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-2013. Absolute stereochemistry was unambiguously determined to be *R* at N2, C1, C18, and *S* at C13 and C20, respectively. CCDC 984477 (*ent*-**2**•HCl) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

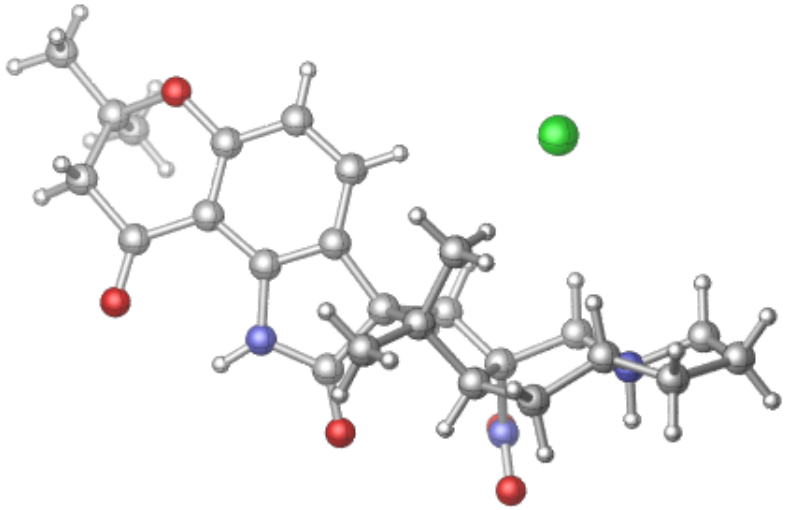


Figure S46. ORTEP representation of *ent*-citrinalin B•HCl (*ent*-**2**•HCl)

Table 1. Crystal data and structure refinement for sarpong75.

X-ray ID	sarpong75	
Sample/notebook ID	EM05-080D-F3	
Empirical formula	C50 H63 Cl N6 O10	
Formula weight	943.51	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C 2	
Unit cell dimensions	a = 25.8379(8) Å	α= 90°.
	b = 6.7742(2) Å	β= 112.251(2)°.
	c = 16.2191(5) Å	γ = 90°.
Volume	2627.45(14) $Å^3$	
Z	2	
Density (calculated)	1.193 Mg/m^3	
Absorption coefficient	1.131 mm^{-1}	
F(000)	1004	
Crystal size	0.040 x 0.030 x 0.010 mm^3	
Crystal color/habit	colorless plate	
Theta range for data collection	2.944 to 68.356°.	
Index ranges	-30<=h<=25, -8<=k<=8, -19<=l<=19	
Reflections collected	17934	
Independent reflections	4686 [R(int) = 0.0572]	
Completeness to theta = 67.000°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.822	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4686 / 1 / 307	
Goodness-of-fit on F^2	1.092	
Final R indices [I>2sigma(I)]	R1 = 0.0931, wR2 = 0.2547	
R indices (all data)	R1 = 0.1077, wR2 = 0.2701	
Absolute structure parameter	-0.014(18)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.355 and -0.276 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sarpong75. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8290(3)	7996(11)	4427(6)	40(2)
C(2)	8170(3)	7126(11)	3505(5)	37(2)
C(3)	8527(3)	6179(10)	3152(5)	37(2)
C(4)	8302(4)	5364(12)	2307(6)	45(2)
C(5)	7734(4)	5512(12)	1804(5)	45(2)
C(6)	6961(5)	4100(20)	621(6)	63(3)
C(7)	6608(5)	5830(20)	668(7)	67(3)
C(8)	6779(4)	6715(15)	1585(6)	54(2)
C(9)	7369(3)	6444(13)	2127(6)	44(2)
C(10)	7609(3)	7212(11)	3005(5)	40(2)
C(11)	7682(3)	8414(11)	4350(5)	36(2)
C(12)	8609(3)	6705(11)	5224(5)	38(2)
C(13)	8863(3)	8120(12)	6004(6)	42(2)
C(14)	9472(4)	7543(11)	6555(6)	43(2)
C(15)	10405(4)	8769(18)	7613(7)	62(3)
C(16)	10682(4)	10800(17)	7816(7)	59(2)
C(17)	10257(4)	12266(16)	7152(7)	57(2)
C(18)	9798(3)	10946(12)	6517(5)	40(2)
C(19)	9208(3)	11802(12)	6106(5)	40(2)
C(20)	8765(3)	10248(11)	5619(5)	38(2)
C(21)	8626(3)	10002(12)	4620(5)	36(2)
C(22)	6839(6)	3620(30)	-360(7)	95(5)
C(23)	6875(5)	2308(16)	1110(8)	70(3)
C(24)	8286(3)	11755(11)	4092(5)	40(2)
C(25)	9155(3)	9794(11)	4387(5)	36(2)
N(1)	7327(2)	8092(9)	3493(5)	37(1)
N(2)	9804(3)	9193(11)	7106(5)	47(2)
N(3)	8572(3)	7928(11)	6668(5)	46(2)
O(1)	7542(3)	4663(10)	978(4)	57(2)
O(2)	6454(3)	7636(11)	1822(5)	57(2)
O(3)	7542(2)	9026(8)	4933(4)	44(1)
O(4)	8455(5)	6300(13)	6834(6)	93(3)
O(5)	8488(4)	9380(12)	7033(5)	80(3)
Cl(1)	10000	5013(4)	5000	43(1)

Table 3. Bond lengths [Å] and angles [°] for sarpong75.

C(1)-C(12)	1.520(11)	C(15)-C(16)	1.527(17)
C(1)-C(2)	1.526(11)	C(15)-H(15A)	0.9900
C(1)-C(11)	1.553(11)	C(15)-H(15B)	0.9900
C(1)-C(21)	1.579(11)	C(16)-C(17)	1.567(14)
C(2)-C(10)	1.369(11)	C(16)-H(16A)	0.9900
C(2)-C(3)	1.411(11)	C(16)-H(16B)	0.9900
C(3)-C(4)	1.385(12)	C(17)-C(18)	1.529(12)
C(3)-H(3)	0.9500	C(17)-H(17A)	0.9900
C(4)-C(5)	1.386(13)	C(17)-H(17B)	0.9900
C(4)-H(4)	0.9500	C(18)-N(2)	1.521(11)
C(5)-O(1)	1.367(10)	C(18)-C(19)	1.529(11)
C(5)-C(9)	1.392(12)	C(18)-H(18)	1.0000
C(6)-O(1)	1.441(13)	C(19)-C(20)	1.535(11)
C(6)-C(7)	1.506(17)	C(19)-H(19A)	0.9900
C(6)-C(23)	1.511(17)	C(19)-H(19B)	0.9900
C(6)-C(22)	1.535(14)	C(20)-C(21)	1.531(10)
C(7)-C(8)	1.507(15)	C(20)-H(20)	1.0000
C(7)-H(7A)	0.9900	C(21)-C(24)	1.531(11)
C(7)-H(7B)	0.9900	C(21)-C(25)	1.556(10)
C(8)-O(2)	1.219(11)	C(22)-H(22A)	0.9800
C(8)-C(9)	1.455(13)	C(22)-H(22B)	0.9800
C(9)-C(10)	1.419(12)	C(22)-H(22C)	0.9800
C(10)-N(1)	1.396(10)	C(23)-H(23A)	0.9800
C(11)-O(3)	1.206(9)	C(23)-H(23B)	0.9800
C(11)-N(1)	1.363(11)	C(23)-H(23C)	0.9800
C(12)-C(13)	1.524(11)	C(24)-H(24A)	0.9800
C(12)-H(12A)	0.9900	C(24)-H(24B)	0.9800
C(12)-H(12B)	0.9900	C(24)-H(24C)	0.9800
C(13)-N(3)	1.535(10)	C(25)-H(25A)	0.9800
C(13)-C(14)	1.536(11)	C(25)-H(25B)	0.9800
C(13)-C(20)	1.553(10)	C(25)-H(25C)	0.9800
C(14)-N(2)	1.485(12)	N(1)-H(1)	0.8800
C(14)-H(14A)	0.9900	N(2)-H(2)	1.0000
C(14)-H(14B)	0.9900	N(3)-O(4)	1.200(11)
C(15)-N(2)	1.484(13)	N(3)-O(5)	1.208(10)

C(12)-C(1)-C(2)	117.0(6)	O(1)-C(6)-C(7)	109.4(9)
C(12)-C(1)-C(11)	112.3(6)	O(1)-C(6)-C(23)	109.9(9)
C(2)-C(1)-C(11)	99.7(6)	C(7)-C(6)-C(23)	112.7(9)
C(12)-C(1)-C(21)	104.2(6)	O(1)-C(6)-C(22)	104.3(9)
C(2)-C(1)-C(21)	114.8(6)	C(7)-C(6)-C(22)	109.1(10)
C(11)-C(1)-C(21)	108.8(6)	C(23)-C(6)-C(22)	111.1(12)
C(10)-C(2)-C(3)	119.2(7)	C(6)-C(7)-C(8)	113.8(8)
C(10)-C(2)-C(1)	109.9(6)	C(6)-C(7)-H(7A)	108.8
C(3)-C(2)-C(1)	130.7(7)	C(8)-C(7)-H(7A)	108.8
C(4)-C(3)-C(2)	119.2(7)	C(6)-C(7)-H(7B)	108.8
C(4)-C(3)-H(3)	120.4	C(8)-C(7)-H(7B)	108.8
C(2)-C(3)-H(3)	120.4	H(7A)-C(7)-H(7B)	107.7
C(3)-C(4)-C(5)	120.5(8)	O(2)-C(8)-C(9)	124.3(9)
C(3)-C(4)-H(4)	119.8	O(2)-C(8)-C(7)	122.3(9)
C(5)-C(4)-H(4)	119.8	C(9)-C(8)-C(7)	113.3(8)
O(1)-C(5)-C(4)	117.1(8)	C(5)-C(9)-C(10)	116.3(7)
O(1)-C(5)-C(9)	120.9(8)	C(5)-C(9)-C(8)	122.3(8)
C(4)-C(5)-C(9)	122.0(7)	C(10)-C(9)-C(8)	121.3(8)

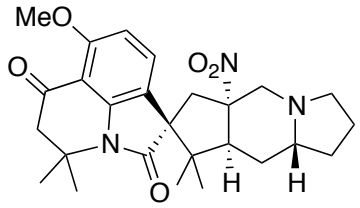
C(2)-C(10)-N(1)	110.3(7)
C(2)-C(10)-C(9)	122.7(7)
N(1)-C(10)-C(9)	127.0(7)
O(3)-C(11)-N(1)	124.6(7)
O(3)-C(11)-C(1)	126.5(7)
N(1)-C(11)-C(1)	108.8(6)
C(1)-C(12)-C(13)	105.6(6)
C(1)-C(12)-H(12A)	110.6
C(13)-C(12)-H(12A)	110.6
C(1)-C(12)-H(12B)	110.6
C(13)-C(12)-H(12B)	110.6
H(12A)-C(12)-H(12B)	108.8
C(12)-C(13)-N(3)	111.0(6)
C(12)-C(13)-C(14)	110.2(7)
N(3)-C(13)-C(14)	103.7(7)
C(12)-C(13)-C(20)	107.3(6)
N(3)-C(13)-C(20)	108.2(6)
C(14)-C(13)-C(20)	116.4(6)
N(2)-C(14)-C(13)	113.0(6)
N(2)-C(14)-H(14A)	109.0
C(13)-C(14)-H(14A)	109.0
N(2)-C(14)-H(14B)	109.0
C(13)-C(14)-H(14B)	109.0
H(14A)-C(14)-H(14B)	107.8
N(2)-C(15)-C(16)	104.5(8)
N(2)-C(15)-H(15A)	110.8
C(16)-C(15)-H(15A)	110.8
N(2)-C(15)-H(15B)	110.8
C(16)-C(15)-H(15B)	110.8
H(15A)-C(15)-H(15B)	108.9
C(15)-C(16)-C(17)	105.9(8)
C(15)-C(16)-H(16A)	110.6
C(17)-C(16)-H(16A)	110.6
C(15)-C(16)-H(16B)	110.6
C(17)-C(16)-H(16B)	110.6
H(16A)-C(16)-H(16B)	108.7
C(18)-C(17)-C(16)	104.8(8)
C(18)-C(17)-H(17A)	110.8
C(16)-C(17)-H(17A)	110.8
C(18)-C(17)-H(17B)	110.8
C(16)-C(17)-H(17B)	110.8
H(17A)-C(17)-H(17B)	108.9
N(2)-C(18)-C(19)	109.9(6)
N(2)-C(18)-C(17)	102.3(7)
C(19)-C(18)-C(17)	117.6(7)
N(2)-C(18)-H(18)	108.9
C(19)-C(18)-H(18)	108.9
C(17)-C(18)-H(18)	108.9
C(18)-C(19)-C(20)	113.0(6)
C(18)-C(19)-H(19A)	109.0
C(20)-C(19)-H(19A)	109.0
C(18)-C(19)-H(19B)	109.0
C(20)-C(19)-H(19B)	109.0
H(19A)-C(19)-H(19B)	107.8
C(21)-C(20)-C(19)	116.7(6)
C(21)-C(20)-C(13)	105.2(6)
C(19)-C(20)-C(13)	117.0(6)
C(21)-C(20)-H(20)	105.6
C(19)-C(20)-H(20)	105.6
C(13)-C(20)-H(20)	105.6
C(20)-C(21)-C(24)	111.2(6)
C(20)-C(21)-C(25)	113.1(6)
C(24)-C(21)-C(25)	107.7(6)
C(20)-C(21)-C(1)	101.2(6)
C(24)-C(21)-C(1)	113.6(6)
C(25)-C(21)-C(1)	110.0(6)
C(6)-C(22)-H(22A)	109.5
C(6)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(6)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(6)-C(23)-H(23A)	109.5
C(6)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(6)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(21)-C(25)-H(25A)	109.5
C(21)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(21)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(11)-N(1)-C(10)	110.6(6)
C(11)-N(1)-H(1)	124.7
C(10)-N(1)-H(1)	124.7
C(15)-N(2)-C(14)	115.7(7)
C(15)-N(2)-C(18)	105.0(7)
C(14)-N(2)-C(18)	110.1(6)
C(15)-N(2)-H(2)	108.6
C(14)-N(2)-H(2)	108.6
C(18)-N(2)-H(2)	108.6
O(4)-N(3)-O(5)	122.1(7)
O(4)-N(3)-C(13)	117.8(7)
O(5)-N(3)-C(13)	120.0(7)
C(5)-O(1)-C(6)	116.2(7)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sarpong75. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	53(4)	24(3)	48(4)	-2(3)	24(4)	3(3)
C(2)	45(4)	30(3)	41(4)	-1(3)	21(3)	-5(3)
C(3)	45(4)	26(3)	44(4)	-2(3)	23(3)	2(3)
C(4)	59(5)	35(4)	50(5)	1(3)	31(4)	6(4)
C(5)	65(5)	39(4)	39(4)	0(3)	27(4)	0(4)
C(6)	63(6)	83(7)	37(5)	-19(5)	11(4)	-2(5)
C(7)	64(6)	86(8)	46(5)	6(5)	14(4)	9(5)
C(8)	56(5)	62(6)	45(4)	8(4)	22(4)	8(4)
C(9)	46(4)	48(4)	43(4)	3(4)	23(4)	-1(3)
C(10)	52(4)	28(3)	44(4)	5(3)	24(4)	2(3)
C(11)	45(4)	29(3)	39(4)	1(3)	20(3)	-2(3)
C(12)	44(4)	31(4)	48(4)	1(3)	28(3)	0(3)
C(13)	42(4)	38(4)	51(5)	3(4)	24(4)	1(3)
C(14)	53(4)	30(4)	53(5)	10(3)	28(4)	12(3)
C(15)	60(6)	73(7)	55(6)	12(5)	24(5)	16(5)
C(16)	51(5)	71(6)	50(5)	6(5)	11(4)	18(5)
C(17)	53(5)	58(6)	54(5)	-11(4)	15(4)	-3(4)
C(18)	39(4)	44(4)	35(4)	4(3)	14(3)	0(3)
C(19)	45(4)	40(4)	36(4)	3(3)	16(3)	10(3)
C(20)	45(4)	29(4)	44(4)	2(3)	21(3)	1(3)
C(21)	45(4)	31(3)	39(4)	0(3)	22(3)	-2(3)
C(22)	91(8)	137(14)	43(6)	-29(7)	11(6)	1(9)
C(23)	62(6)	49(5)	81(7)	-15(5)	7(5)	-13(4)
C(24)	48(4)	32(4)	41(4)	5(3)	19(3)	1(3)
C(25)	38(3)	32(3)	42(4)	4(3)	18(3)	-7(3)
N(1)	29(3)	32(3)	54(4)	4(3)	19(3)	0(2)
N(2)	52(4)	39(3)	53(4)	0(3)	24(3)	3(3)
N(3)	62(4)	40(4)	47(4)	4(3)	34(3)	4(3)
O(1)	80(4)	59(4)	36(3)	-9(3)	25(3)	-4(3)
O(2)	55(3)	63(4)	56(4)	0(3)	23(3)	7(3)
O(3)	53(3)	34(3)	57(3)	-2(3)	34(3)	-3(2)
O(4)	164(9)	68(5)	85(6)	-29(4)	90(6)	-57(6)
O(5)	139(7)	61(5)	77(5)	6(4)	83(6)	15(5)
Cl(1)	43(1)	34(1)	57(2)	0	25(1)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sarpong75.

	x	y	z	U(eq)
H(3)	8918	6102	3490	44
H(4)	8539	4699	2070	54
H(7A)	6213	5397	468	81
H(7B)	6630	6861	251	81
H(12A)	8906	5955	5115	45
H(12B)	8354	5760	5344	45
H(14A)	9474	6425	6949	52
H(14B)	9651	7091	6146	52
H(15A)	10562	7971	7252	75
H(15B)	10458	8048	8170	75
H(16A)	11040	10793	7726	71
H(16B)	10756	11184	8440	71
H(17A)	10101	13184	7473	68
H(17B)	10441	13044	6822	68
H(18)	9916	10491	6027	47
H(19A)	9203	12857	5681	48
H(19B)	9110	12408	6584	48
H(20)	8411	10708	5672	46
H(22A)	6970	4703	-630	142
H(22B)	6435	3444	-679	142
H(22C)	7033	2398	-397	142
H(23A)	6956	2653	1733	104
H(23B)	7127	1249	1084	104
H(23C)	6487	1860	830	104
H(24A)	7948	11910	4221	60
H(24B)	8182	11517	3454	60
H(24C)	8512	12960	4264	60
H(25A)	9396	10951	4608	54
H(25B)	9042	9701	3740	54
H(25C)	9360	8600	4668	54
H(1)	6969	8396	3277	45
H(2)	9630	9605	7535	56



cyclopiamine B (6)

A colorless blade 0.050 x 0.040 x 0.020 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 100.0% complete to 67.000° in θ. A total of 43571 reflections were collected covering the indices, -12<=*h*<=12, -16<=*k*<=16, -19<=*l*<=19. 4544 reflections were found to be symmetry independent, with an R_{int} of 0.0179. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P 21 21 21 (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT) 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-2013). 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-2013. Absolute stereochemistry was unambiguously determined to be *R* at C1 and C8, and *S* at C3 and C10, respectively. CCDC 984478 (cyclopiamine B (**6**)) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

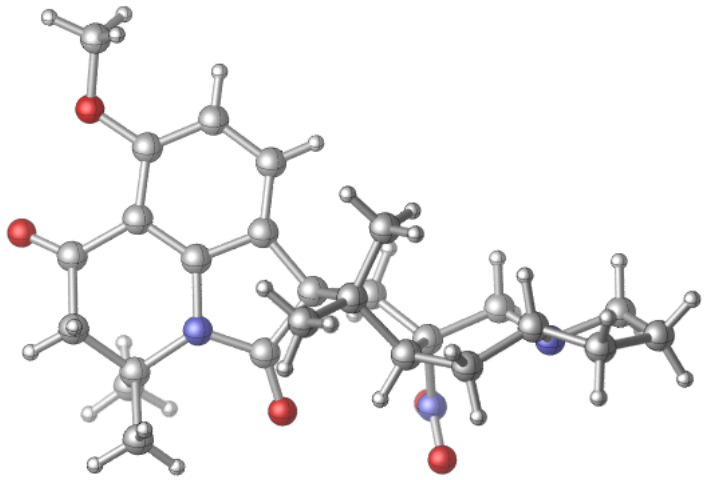


Figure S47. ORTEP representation of **cyclopiamine B (6)**

Table 1. Crystal data and structure refinement for sarpong70.

X-ray ID	sarpong70	
Sample/notebook ID	EM05-028B	
Empirical formula	C27 H37 N3 O6	
Formula weight	499.59	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 10.7754(6) Å	α= 90°.
	b = 14.1165(8) Å	β= 90°.
	c = 16.3912(9) Å	γ = 90°.
Volume	2493.3(2) $Å^3$	
Z	4	
Density (calculated)	1.331 Mg/m^3	
Absorption coefficient	0.769 mm^{-1}	
F(000)	1072	
Crystal size	0.050 x 0.040 x 0.020 mm^3	
Crystal color/habit	colorless blade	
Theta range for data collection	4.133 to 68.289°.	
Index ranges	-12<=h<=12, -16<=k<=16, -19<=l<=19	
Reflections collected	43571	
Independent reflections	4544 [R(int) = 0.0179]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.881	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4544 / 0 / 332	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0304, wR2 = 0.0886	
R indices (all data)	R1 = 0.0306, wR2 = 0.0887	
Absolute structure parameter	-0.02(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.235 and -0.332 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sarpong70. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9601(2)	6235(2)	3390(1)	16(1)
C(2)	10240(2)	5593(1)	2751(1)	16(1)
C(3)	11251(2)	6206(2)	2348(1)	16(1)
C(4)	11254(2)	6108(2)	1411(1)	18(1)
C(5)	11985(2)	6819(2)	134(1)	24(1)
C(6)	12356(2)	7825(2)	-123(2)	30(1)
C(7)	11953(3)	8457(2)	596(2)	29(1)
C(8)	11333(2)	7780(2)	1194(1)	21(1)
C(9)	11465(2)	8024(2)	2091(1)	21(1)
C(10)	11068(2)	7229(2)	2675(1)	17(1)
C(11)	9720(2)	7255(2)	3009(1)	18(1)
C(12)	8740(2)	7404(2)	2344(1)	22(1)
C(13)	9572(2)	8039(2)	3646(1)	24(1)
C(14)	8314(2)	5973(2)	3662(1)	16(1)
C(15)	7227(2)	5771(2)	3251(1)	18(1)
C(16)	6142(2)	5571(2)	3685(1)	18(1)
C(17)	6149(2)	5537(1)	4538(1)	16(1)
C(18)	7259(2)	5705(1)	4974(1)	16(1)
C(19)	7439(2)	5631(2)	5866(1)	18(1)
C(20)	8550(2)	6189(2)	6176(1)	22(1)
C(21)	9768(2)	6004(2)	5713(1)	18(1)
C(22)	10322(2)	6189(2)	4199(1)	17(1)
C(23)	8294(2)	5942(1)	4515(1)	16(1)
C(24)	3948(2)	5496(2)	4599(1)	22(1)
C(25)	10741(2)	6734(2)	5977(2)	28(1)
C(26)	10225(2)	4995(2)	5868(1)	27(1)
C(27)	15124(3)	7835(2)	1748(2)	44(1)
N(1)	11951(2)	6868(1)	1031(1)	19(1)
N(2)	12545(2)	5849(1)	2601(1)	21(1)
N(3)	9480(2)	6118(1)	4830(1)	16(1)
O(1)	13359(2)	6430(1)	2744(1)	27(1)
O(2)	12720(2)	4990(1)	2605(1)	29(1)
O(3)	5127(1)	5358(1)	4989(1)	19(1)
O(4)	6783(1)	5175(1)	6320(1)	26(1)
O(5)	11446(1)	6198(1)	4276(1)	24(1)
O(6)	14649(2)	7307(2)	1098(1)	45(1)

Table 3. Bond lengths [Å] and angles [°] for sarpong70.

C(1)-C(14)	1.503(3)	C(14)-C(15)	1.381(3)
C(1)-C(22)	1.539(3)	C(14)-C(23)	1.399(3)
C(1)-C(2)	1.547(3)	C(15)-C(16)	1.397(3)
C(1)-C(11)	1.575(3)	C(15)-H(15)	0.9500
C(2)-C(3)	1.541(3)	C(16)-C(17)	1.398(3)
C(2)-H(2A)	0.9900	C(16)-H(16)	0.9500
C(2)-H(2B)	0.9900	C(17)-O(3)	1.351(3)
C(3)-N(2)	1.540(3)	C(17)-C(18)	1.413(3)
C(3)-C(4)	1.541(3)	C(18)-C(23)	1.386(3)
C(3)-C(10)	1.554(3)	C(18)-C(19)	1.480(3)
C(4)-N(1)	1.451(3)	C(19)-O(4)	1.212(3)
C(4)-H(4A)	0.9900	C(19)-C(20)	1.520(3)
C(4)-H(4B)	0.9900	C(20)-C(21)	1.539(3)
C(5)-N(1)	1.473(3)	C(20)-H(20A)	0.9900
C(5)-C(6)	1.534(3)	C(20)-H(20B)	0.9900
C(5)-H(5A)	0.9900	C(21)-N(3)	1.488(3)
C(5)-H(5B)	0.9900	C(21)-C(26)	1.528(3)
C(6)-C(7)	1.541(4)	C(21)-C(25)	1.533(3)
C(6)-H(6A)	0.9900	C(22)-O(5)	1.217(3)
C(6)-H(6B)	0.9900	C(22)-N(3)	1.380(3)
C(7)-C(8)	1.523(3)	C(23)-N(3)	1.400(3)
C(7)-H(7A)	0.9900	C(24)-O(3)	1.435(3)
C(7)-H(7B)	0.9900	C(24)-H(24A)	0.9800
C(8)-N(1)	1.474(3)	C(24)-H(24B)	0.9800
C(8)-C(9)	1.516(3)	C(24)-H(24C)	0.9800
C(8)-H(8)	1.0000	C(25)-H(25A)	0.9800
C(9)-C(10)	1.536(3)	C(25)-H(25B)	0.9800
C(9)-H(9A)	0.9900	C(25)-H(25C)	0.9800
C(9)-H(9B)	0.9900	C(26)-H(26A)	0.9800
C(10)-C(11)	1.553(3)	C(26)-H(26B)	0.9800
C(10)-H(10)	1.0000	C(26)-H(26C)	0.9800
C(11)-C(13)	1.530(3)	C(27)-O(6)	1.397(4)
C(11)-C(12)	1.533(3)	C(27)-H(27A)	0.9800
C(12)-H(12A)	0.9800	C(27)-H(27B)	0.9800
C(12)-H(12B)	0.9800	C(27)-H(27C)	0.9800
C(12)-H(12C)	0.9800	N(2)-O(1)	1.223(3)
C(13)-H(13A)	0.9800	N(2)-O(2)	1.227(3)
C(13)-H(13B)	0.9800	O(6)-H(6)	0.8400
C(13)-H(13C)	0.9800		

C(14)-C(1)-C(22)	101.52(16)	C(2)-C(3)-C(4)	112.26(17)
C(14)-C(1)-C(2)	117.90(18)	N(2)-C(3)-C(10)	108.99(17)
C(22)-C(1)-C(2)	109.52(17)	C(2)-C(3)-C(10)	106.52(16)
C(14)-C(1)-C(11)	114.68(17)	C(4)-C(3)-C(10)	115.30(17)
C(22)-C(1)-C(11)	109.79(17)	N(1)-C(4)-C(3)	111.26(17)
C(2)-C(1)-C(11)	103.39(16)	N(1)-C(4)-H(4A)	109.4
C(3)-C(2)-C(1)	106.04(16)	C(3)-C(4)-H(4A)	109.4
C(3)-C(2)-H(2A)	110.5	N(1)-C(4)-H(4B)	109.4
C(1)-C(2)-H(2A)	110.5	C(3)-C(4)-H(4B)	109.4
C(3)-C(2)-H(2B)	110.5	H(4A)-C(4)-H(4B)	108.0
C(1)-C(2)-H(2B)	110.5	N(1)-C(5)-C(6)	103.73(19)
H(2A)-C(2)-H(2B)	108.7	N(1)-C(5)-H(5A)	111.0
N(2)-C(3)-C(2)	109.96(16)	C(6)-C(5)-H(5A)	111.0
N(2)-C(3)-C(4)	103.74(16)	N(1)-C(5)-H(5B)	111.0

C(6)-C(5)-H(5B)	111.0	C(15)-C(16)-C(17)	120.8(2)
H(5A)-C(5)-H(5B)	109.0	C(15)-C(16)-H(16)	119.6
C(5)-C(6)-C(7)	104.59(18)	C(17)-C(16)-H(16)	119.6
C(5)-C(6)-H(6A)	110.8	O(3)-C(17)-C(16)	123.36(19)
C(7)-C(6)-H(6A)	110.8	O(3)-C(17)-C(18)	116.38(18)
C(5)-C(6)-H(6B)	110.8	C(16)-C(17)-C(18)	120.25(19)
C(7)-C(6)-H(6B)	110.8	C(23)-C(18)-C(17)	116.60(19)
H(6A)-C(6)-H(6B)	108.9	C(23)-C(18)-C(19)	116.57(19)
C(8)-C(7)-C(6)	104.68(19)	C(17)-C(18)-C(19)	126.81(19)
C(8)-C(7)-H(7A)	110.8	O(4)-C(19)-C(18)	124.7(2)
C(6)-C(7)-H(7A)	110.8	O(4)-C(19)-C(20)	121.98(19)
C(8)-C(7)-H(7B)	110.8	C(18)-C(19)-C(20)	113.37(18)
C(6)-C(7)-H(7B)	110.8	C(19)-C(20)-C(21)	114.77(17)
H(7A)-C(7)-H(7B)	108.9	C(19)-C(20)-H(20A)	108.6
N(1)-C(8)-C(9)	109.43(18)	C(21)-C(20)-H(20A)	108.6
N(1)-C(8)-C(7)	103.43(19)	C(19)-C(20)-H(20B)	108.6
C(9)-C(8)-C(7)	116.09(19)	C(21)-C(20)-H(20B)	108.6
N(1)-C(8)-H(8)	109.2	H(20A)-C(20)-H(20B)	107.6
C(9)-C(8)-H(8)	109.2	N(3)-C(21)-C(26)	109.24(17)
C(7)-C(8)-H(8)	109.2	N(3)-C(21)-C(25)	110.19(18)
C(8)-C(9)-C(10)	114.31(18)	C(26)-C(21)-C(25)	111.05(19)
C(8)-C(9)-H(9A)	108.7	N(3)-C(21)-C(20)	106.45(17)
C(10)-C(9)-H(9A)	108.7	C(26)-C(21)-C(20)	110.54(19)
C(8)-C(9)-H(9B)	108.7	C(25)-C(21)-C(20)	109.27(18)
C(10)-C(9)-H(9B)	108.7	O(5)-C(22)-N(3)	125.3(2)
H(9A)-C(9)-H(9B)	107.6	O(5)-C(22)-C(1)	126.21(19)
C(9)-C(10)-C(11)	117.61(18)	N(3)-C(22)-C(1)	108.48(17)
C(9)-C(10)-C(3)	115.40(17)	C(18)-C(23)-C(14)	124.16(19)
C(11)-C(10)-C(3)	105.20(16)	C(18)-C(23)-N(3)	125.28(19)
C(9)-C(10)-H(10)	105.9	C(14)-C(23)-N(3)	110.42(18)
C(11)-C(10)-H(10)	105.9	O(3)-C(24)-H(24A)	109.5
C(3)-C(10)-H(10)	105.9	O(3)-C(24)-H(24B)	109.5
C(13)-C(11)-C(12)	108.34(18)	H(24A)-C(24)-H(24B)	109.5
C(13)-C(11)-C(10)	110.81(17)	O(3)-C(24)-H(24C)	109.5
C(12)-C(11)-C(10)	113.38(17)	H(24A)-C(24)-H(24C)	109.5
C(13)-C(11)-C(1)	112.47(17)	H(24B)-C(24)-H(24C)	109.5
C(12)-C(11)-C(1)	110.57(17)	C(21)-C(25)-H(25A)	109.5
C(10)-C(11)-C(1)	101.22(16)	C(21)-C(25)-H(25B)	109.5
C(11)-C(12)-H(12A)	109.5	H(25A)-C(25)-H(25B)	109.5
C(11)-C(12)-H(12B)	109.5	C(21)-C(25)-H(25C)	109.5
H(12A)-C(12)-H(12B)	109.5	H(25A)-C(25)-H(25C)	109.5
C(11)-C(12)-H(12C)	109.5	H(25B)-C(25)-H(25C)	109.5
H(12A)-C(12)-H(12C)	109.5	C(21)-C(26)-H(26A)	109.5
H(12B)-C(12)-H(12C)	109.5	C(21)-C(26)-H(26B)	109.5
C(11)-C(13)-H(13A)	109.5	H(26A)-C(26)-H(26B)	109.5
C(11)-C(13)-H(13B)	109.5	C(21)-C(26)-H(26C)	109.5
H(13A)-C(13)-H(13B)	109.5	H(26A)-C(26)-H(26C)	109.5
C(11)-C(13)-H(13C)	109.5	H(26B)-C(26)-H(26C)	109.5
H(13A)-C(13)-H(13C)	109.5	O(6)-C(27)-H(27A)	109.5
H(13B)-C(13)-H(13C)	109.5	O(6)-C(27)-H(27B)	109.5
C(15)-C(14)-C(23)	117.93(19)	H(27A)-C(27)-H(27B)	109.5
C(15)-C(14)-C(1)	133.48(19)	O(6)-C(27)-H(27C)	109.5
C(23)-C(14)-C(1)	108.59(18)	H(27A)-C(27)-H(27C)	109.5
C(14)-C(15)-C(16)	120.2(2)	H(27B)-C(27)-H(27C)	109.5
C(14)-C(15)-H(15)	119.9	C(4)-N(1)-C(5)	114.03(17)
C(16)-C(15)-H(15)	119.9	C(4)-N(1)-C(8)	109.50(16)

C(5)-N(1)-C(8)	103.52(17)
O(1)-N(2)-O(2)	123.5(2)
O(1)-N(2)-C(3)	118.84(18)
O(2)-N(2)-C(3)	117.59(18)
C(22)-N(3)-C(23)	109.69(17)
C(22)-N(3)-C(21)	126.81(17)
C(23)-N(3)-C(21)	121.99(17)
C(17)-O(3)-C(24)	116.84(16)
C(27)-O(6)-H(6)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sarpong70. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(1)	20(1)	14(1)	0(1)	-2(1)	-1(1)
C(2)	16(1)	17(1)	15(1)	-1(1)	1(1)	1(1)
C(3)	15(1)	18(1)	16(1)	1(1)	0(1)	1(1)
C(4)	21(1)	19(1)	14(1)	-1(1)	1(1)	1(1)
C(5)	28(1)	29(1)	16(1)	3(1)	1(1)	0(1)
C(6)	34(1)	34(1)	22(1)	5(1)	3(1)	-7(1)
C(7)	37(1)	24(1)	25(1)	4(1)	2(1)	-7(1)
C(8)	22(1)	20(1)	22(1)	4(1)	-1(1)	-2(1)
C(9)	22(1)	20(1)	22(1)	-2(1)	1(1)	-5(1)
C(10)	17(1)	18(1)	15(1)	-2(1)	0(1)	-3(1)
C(11)	16(1)	18(1)	18(1)	-1(1)	0(1)	0(1)
C(12)	19(1)	23(1)	23(1)	4(1)	0(1)	1(1)
C(13)	26(1)	22(1)	24(1)	-4(1)	5(1)	-1(1)
C(14)	15(1)	17(1)	17(1)	2(1)	1(1)	0(1)
C(15)	18(1)	21(1)	16(1)	0(1)	0(1)	-1(1)
C(16)	14(1)	20(1)	19(1)	0(1)	-2(1)	-1(1)
C(17)	15(1)	15(1)	18(1)	0(1)	1(1)	1(1)
C(18)	14(1)	15(1)	18(1)	-1(1)	0(1)	2(1)
C(19)	14(1)	23(1)	17(1)	0(1)	1(1)	4(1)
C(20)	20(1)	30(1)	16(1)	-4(1)	1(1)	1(1)
C(21)	15(1)	26(1)	13(1)	-1(1)	-2(1)	-1(1)
C(22)	16(1)	20(1)	16(1)	-2(1)	0(1)	-1(1)
C(23)	14(1)	16(1)	18(1)	-2(1)	-2(1)	2(1)
C(24)	13(1)	32(1)	22(1)	5(1)	0(1)	-1(1)
C(25)	23(1)	39(1)	22(1)	-7(1)	-1(1)	-8(1)
C(26)	23(1)	34(1)	23(1)	3(1)	-2(1)	6(1)
C(27)	39(2)	56(2)	37(2)	-6(1)	2(1)	-9(1)
N(1)	19(1)	21(1)	16(1)	0(1)	1(1)	-1(1)
N(2)	18(1)	29(1)	15(1)	3(1)	2(1)	3(1)
N(3)	13(1)	21(1)	15(1)	-2(1)	-1(1)	0(1)
O(1)	16(1)	39(1)	27(1)	4(1)	-1(1)	-3(1)
O(2)	27(1)	27(1)	33(1)	4(1)	3(1)	10(1)
O(3)	12(1)	27(1)	17(1)	2(1)	0(1)	0(1)
O(4)	19(1)	40(1)	19(1)	7(1)	2(1)	-2(1)
O(5)	13(1)	38(1)	20(1)	1(1)	0(1)	0(1)
O(6)	34(1)	58(1)	42(1)	-11(1)	3(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sarpong70.

	x	y	z	U(eq)
H(2A)	10614	5032	3018	19
H(2B)	9632	5373	2339	19
H(4A)	11625	5491	1258	21
H(4B)	10389	6118	1208	21
H(5A)	11162	6648	-90	29
H(5B)	12605	6350	-54	29
H(6A)	11924	8013	-631	36
H(6B)	13263	7868	-213	36
H(7A)	12680	8768	850	34
H(7B)	11363	8950	413	34
H(8)	10432	7725	1056	25
H(9A)	10960	8594	2207	25
H(9B)	12343	8186	2202	25
H(10)	11621	7286	3162	20
H(12A)	7914	7426	2593	32
H(12B)	8777	6880	1953	32
H(12C)	8902	8003	2060	32
H(13A)	9629	8658	3379	36
H(13B)	10231	7982	4056	36
H(13C)	8762	7978	3913	36
H(15)	7217	5768	2671	22
H(16)	5392	5457	3397	21
H(20A)	8679	6034	6759	26
H(20B)	8354	6873	6141	26
H(24A)	3925	6126	4348	33
H(24B)	3284	5446	5005	33
H(24C)	3830	5012	4178	33
H(25A)	11520	6615	5686	42
H(25B)	10883	6681	6566	42
H(25C)	10443	7373	5848	42
H(26A)	9566	4544	5730	40
H(26B)	10446	4925	6445	40
H(26C)	10955	4869	5529	40
H(27A)	15954	8067	1607	66
H(27B)	15175	7435	2235	66
H(27C)	14577	8375	1857	66
H(6)	13924	7131	1209	67

IX. General Experimental Procedures for computational data

Molecular mechanics conformational searches and density functional theory (DFT) calculations (geometry optimization, frequency, and NMR chemical shift) were performed on citrinalin A (**1**), revised citrinalin B (**2**), and originally-proposed citrinalin B (**3**). In addition, conformational searches and DFT geometry optimization and frequency calculations were performed on cyclopiamine A (**4**), and cyclopiamine B (**6**). For the citrinalin NMR calculations, various protonation states were examined, including neutral, protonated, and TFA salt forms as detailed below.

Candidate conformers for each system were identified via systematic conformational searches performed as described below with the MMFF94 force field in Spartan'10.[41] DFT calculations were performed with GAUSSIAN09.[42] Geometries were optimized in the gas-phase using the B3LYP/6-31+G(d,p)[43] 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)[44] were performed as described below on these geometries at the mPW1PW91/6-311+G(2d,p)[45] level of theory in an implicit chloroform solvent continuum (SMD[46] method). DMF solvent single point calculations (SMD method) were also performed for the neutral forms of (**1**), (**2**), (**4**), and (**6**). The lowest energy conformers of each system under this method were then re-optimized with DMF solvent.

Conformational Search and Analysis of NMR data

For each natural product, systematic MMFF94 conformational searches were conducted in Spartan'10 where all rotatable and foldable atoms were given at least three degrees of freedom. These searches located between four and 13 candidate conformers per system, generally lying with a 15 kcal/mol energy window (MMFF94 energies). All candidates were then refined in GAUSSIAN09 with B3LYP/6-31+G(d,p) gas phase optimization and frequency calculations. NMR single points calculations in chloroform solvent were then performed at the mPW1PW91/6-311+G(2d,p) level of theory on the B3LYP/6-31+G(d,p) geometries.

Boltzmann-weighted averaging of the computed chemical shifts based on the relative computed B3LYP free energies at 298.15 K of each conformer was performed, using the equation below to determine relative populations.

$$\frac{P_i}{P_j} = e^{\frac{-(E_i - E_j)}{RT}}$$

P_i = population of conformer i relative to lowest energy conformer j
E_i, E_j = computed free energies (in J/mol)
R = molar gas constant (8.314510 J mol^{-1} K^{-1})
T = 298.15 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.[12]

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.

	^{1}H	^{13}C
Slope	-1.0936	-1.0533
Intercept	31.8018	186.5242

$$\delta = \frac{b - \sigma}{-m}$$

δ = computed chemical shift relative to TMS
σ = computed isotropic shielding constant
m = slope, b = intercept

DP4 Probability Analysis

For further support of the citrinalin B structural reassignment, we utilized the DP4 probability analysis of Smith and Goodman.[47] This analysis is more advanced than simple CMAD comparisons and has proven utility is assigning the spectra of closely related diastereomers.

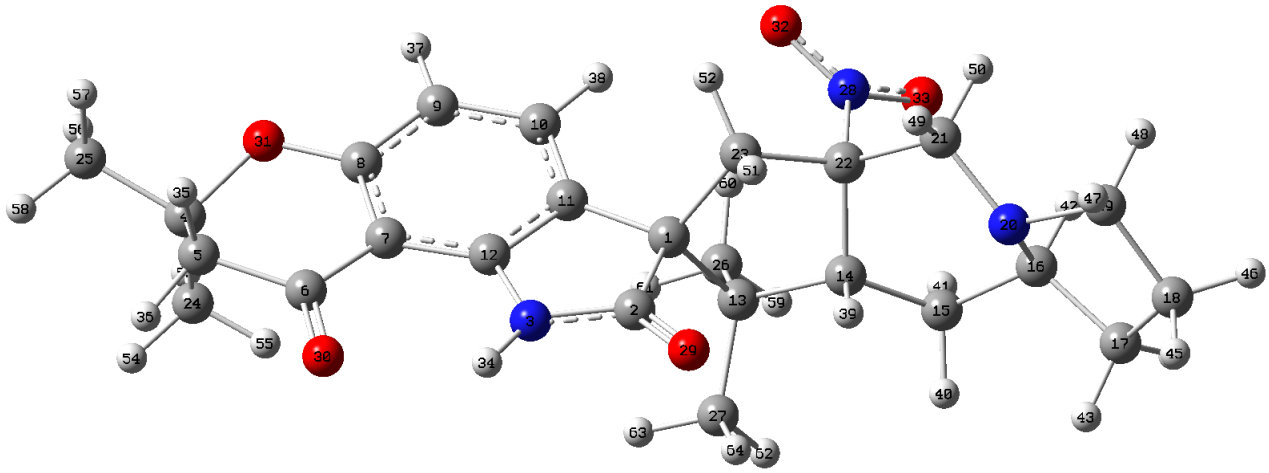
X. Computational Data

Table S5. Citrinalin A (1) neutral form computed NMR data compared to TFA salt form experimental data for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation.

^{13}C			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
C1	C1	61.52	57.5	4.0	58.3	3.2
C2	C2	181.61	182.9	1.3	182.4	0.8
C4	C4	81.02	79.3	1.7	79.2	1.8
C5	C5	47.66	48.0	0.3	48.0	0.3
C6	C6	192.51	192.6	0.1	192.6	0.1
C7	C7	102.16	105.2	3.0	104.9	2.7
C8	C8	157.72	158.8	1.1	158.7	1.0
C9	C9	107.27	109.6	2.3	108.8	1.5
C10	C10	133.81	132.4	1.4	132.7	1.1
C11	C11	121.39	120.9	0.5	119.5	1.9
C12	C12	142.34	142.6	0.3	142.8	0.5
C13	C13	50.23	46.1	4.1	48.7	1.5
C14	C14	51.08	45.8	5.3	43.9	7.2
C15	C15	25.22	19.8	5.4	26.8	1.6
C16	C16	58.16	61.1	2.9	61.3	3.1
C17	C17	32.28	26.1	6.2	30.9	1.4
C18	C18	22.80	20.0	2.8	20.8	2.0
C19	C19	52.05	55.5	3.4	52.9	0.8
C21	C21	60.39	55.4	5.0	64.1	3.7
C22	C22	100.68	92.4	8.3	94.6	6.1
C23	C23	45.78	41.0	4.8	41.3	4.5
C24	C24	24.35	25.8	1.5	26.0	1.7
C25	C25	25.02	26.5	1.5	26.3	1.3
C26	C26	20.53	20.3	0.2	22.7	2.2
C27	C27	22.15	23.4	1.3	22.9	0.8
			CMAD:	**2.7 ppm**	**CMAD:**	**2.1 ppm**

* TFA salt data from Ref. 10 .



^{1}H			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
N3	H34	8.65	10.35		10.10	
C5	H35	2.64	2.84	0.2	2.80	0.2
C5	H36	2.64	2.75	0.1	2.74	0.1
C9	H37	6.37	6.61	0.2	6.53	0.2
C10	H38	7.26	7.34	0.1	7.51	0.3
C14	H39	3.22	2.89	0.3	3.63	0.4
C15	H40	1.48	1.88	0.4	1.71	0.2
C15	H41	2.11	2.39	0.3	1.83	0.3
C16	H42	3.08	4.19	1.1	1.92	1.2
C17	H43	1.48	1.93	0.5	1.22	0.3
C17	H44	2.01	2.24	0.2	1.90	0.1
C18	H45	1.88	2.19	0.3	1.63	0.2
C18	H46	1.66	2.05	0.4	1.63	0.0
C19	H47	2.82	3.50	0.7	2.87	0.0
C19	H48	2.23	3.24	1.0	1.96	0.3
N20	H65	0.00	9.41		n.o	
C21	H49	3.15	4.19	1.0	3.61	0.5
C21	H50	2.58	3.53	1.0	2.68	0.1
C23	H51	2.42	2.43	0.0	2.61	0.2
C23	H52	3.27	3.19	0.1	2.65	0.6
C24	avg(53-55)	1.34	1.38	0.0	1.37	0.0
C25	avg(56-58)	1.34	1.41	0.1	1.39	0.0
C26	avg(59-61)	0.64	0.62	0.0	0.69	0.1
C27	avg(62-64)	0.86	0.83	0.0	0.97	0.1
			CMAD:	**0.37 ppm**	**CMAD:**	**0.24 ppm**

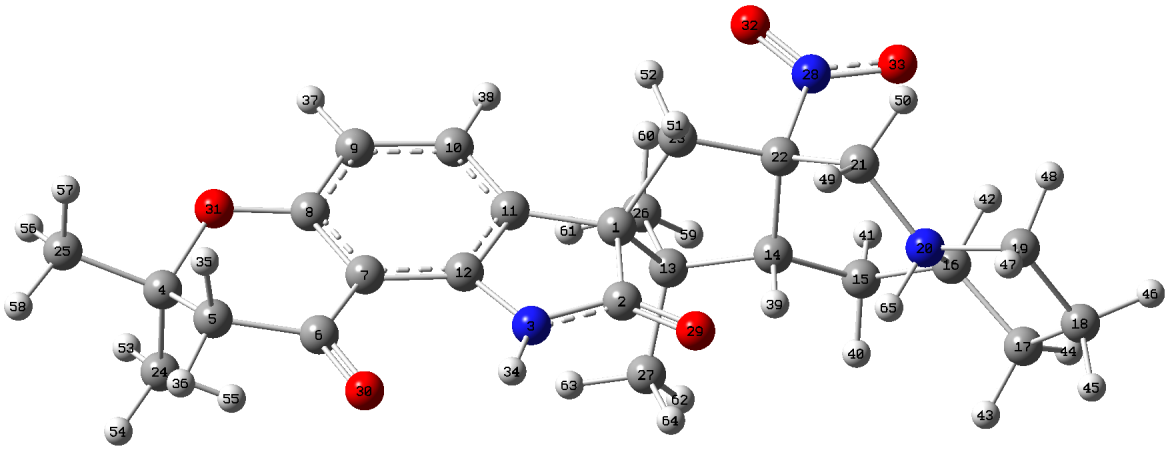
* TFA salt data from Ref. 10.

Table S6. Citrinalin A (1) H^+ form computed NMR data compared to TFA salt form experimental data for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation.

^{13}C			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
C1	C1	63.39	57.5	5.9	58.3	5.1
C2	C2	181.87	182.9	1.0	182.4	0.5
C4	C4	83.21	79.3	3.9	79.2	4.0
C5	C5	47.35	48.0	0.7	48.0	0.7
C6	C6	193.11	192.6	0.5	192.6	0.5
C7	C7	103.05	105.2	2.2	104.9	1.9
C8	C8	158.64	158.8	0.2	158.7	0.1
C9	C9	109.37	109.6	0.2	108.8	0.6
C10	C10	132.47	132.4	0.1	132.7	0.2
C11	C11	116.38	120.9	4.5	119.5	3.1
C12	C12	142.61	142.6	0.0	142.8	0.2
C13	C13	50.41	46.1	4.3	48.7	1.7
C14	C14	48.95	45.8	3.2	43.9	5.1
C15	C15	22.55	19.8	2.7	26.8	4.3
C16	C16	67.99	61.1	6.9	61.3	6.7
C17	C17	26.80	26.1	0.7	30.9	4.1
C18	C18	22.61	20.0	2.6	20.8	1.8
C19	C19	55.45	55.5	0.1	52.9	2.5
C21	C21	58.22	55.4	2.8	64.1	5.9
C22	C22	99.55	92.4	7.2	94.6	5.0
C23	C23	41.42	41.0	0.4	41.3	0.1
C24	C24	24.43	25.8	1.4	26.0	1.6
C25	C25	24.82	26.5	1.7	26.3	1.5
C26	C26	17.54	20.3	2.8	22.7	5.2
C27	C27	20.67	23.4	2.7	22.9	2.2
			CMAD:	**2.3 ppm**	**CMAD:**	**2.6 ppm**

* TFA salt data from Ref. 10.



^{1}H			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
N3	H34	9.04	10.35		10.10	
C5	H35	2.73	2.84	0.1	2.80	0.1
C5	H36	2.73	2.75	0.0	2.74	0.0
C9	H37	6.55	6.61	0.1	6.53	0.0
C10	H38	7.43	7.34	0.1	7.51	0.1
C14	H39	4.00	2.89	1.1	3.63	0.4
C15	H40	1.89	1.88	0.0	1.71	0.2
C15	H41	2.02	2.39	0.4	1.83	0.2
C16	H42	4.17	4.19	0.0	1.92	2.2
C17	H43	2.21	1.93	0.3	1.22	1.0
C17	H44	2.21	2.24	0.0	1.90	0.3
C18	H45	2.34	2.19	0.2	1.63	0.7
C18	H46	2.25	2.05	0.2	1.63	0.6
C19	H47	3.36	3.50	0.1	2.87	0.5
C19	H48	3.36	3.24	0.1	1.96	1.4
N20	H65	7.41	9.41		n.o	
C21	H49	3.59	4.19	0.6	3.61	0.0
C21	H50	3.54	3.53	0.0	2.68	0.9
C23	H51	2.13	2.43	0.3	2.61	0.5
C23	H52	3.46	3.19	0.3	2.65	0.8
C24	avg(53-55)	1.39	1.38	0.0	1.37	0.0
C25	avg(56-58)	1.38	1.41	0.0	1.39	0.0
C26	avg(59-61)	0.99	0.62	0.4	0.69	0.3
C27	avg(62-64)	0.79	0.83	0.0	0.97	0.2
			CMAD:	**0.20 ppm**	**CMAD:**	**0.47 ppm**

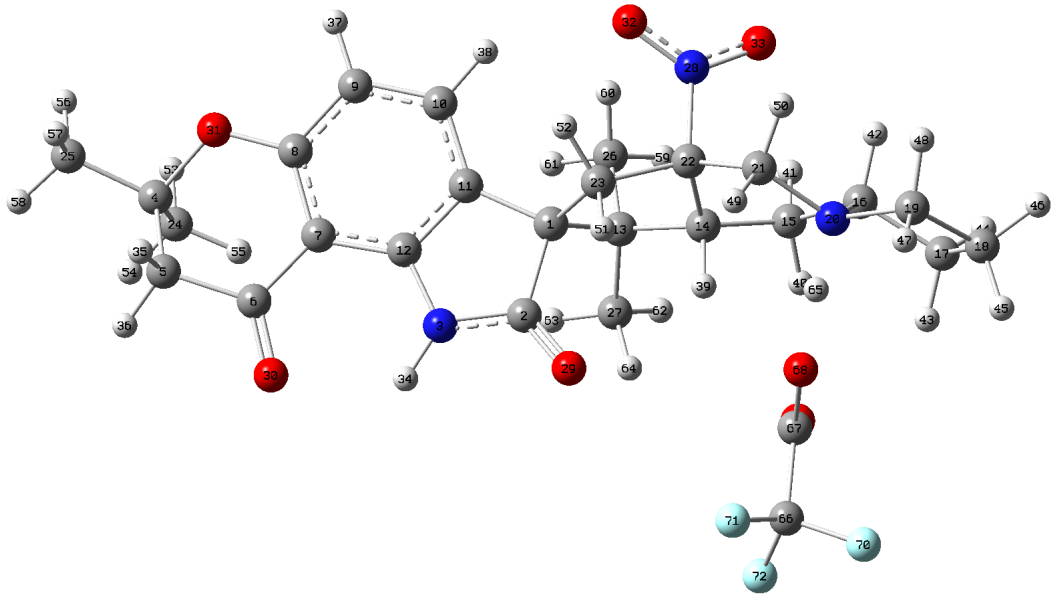
* TFA salt data from Ref. 10.

Table S7. Citrinalin A (1) TFA salt form computed NMR data compared to TFA salt form experimental data for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation.

^{13}C			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
C1	C1	61.58	57.5	4.1	58.3	3.3
C2	C2	181.84	182.9	1.1	182.4	0.6
C4	C4	81.84	79.3	2.5	79.2	2.6
C5	C5	47.67	48.0	0.3	48.0	0.3
C6	C6	192.76	192.6	0.2	192.6	0.2
C7	C7	102.48	105.2	2.7	104.9	2.4
C8	C8	158.34	158.8	0.5	158.7	0.4
C9	C9	107.84	109.6	1.8	108.8	1.0
C10	C10	133.01	132.4	0.6	132.7	0.3
C11	C11	119.74	120.9	1.2	119.5	0.2
C12	C12	142.61	142.6	0.0	142.8	0.2
C13	C13	50.89	46.1	4.8	48.7	2.2
C14	C14	49.50	45.8	3.7	43.9	5.6
C15	C15	22.79	19.8	3.0	26.8	4.0
C16	C16	58.97	61.1	2.1	61.3	2.3
C17	C17	31.29	26.1	5.2	30.9	0.4
C18	C18	21.88	20.0	1.9	20.8	1.1
C19	C19	54.26	55.5	1.2	52.9	1.4
C21	C21	55.93	55.4	0.5	64.1	8.2
C22	C22	96.57	92.4	4.2	94.6	2.0
C23	C23	43.61	41.0	2.6	41.3	2.3
C24	C24	24.76	25.8	1.0	26.0	1.2
C25	C25	24.62	26.5	1.9	26.3	1.7
C26	C26	18.24	20.3	2.1	22.7	4.5
C27	C27	21.47	23.4	1.9	22.9	1.4
			CMAD:	**2.0 ppm**	**CMAD:**	**2.0 ppm**

* TFA salt data from Ref. 10.



^{1}H			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
N3	H34	8.73	10.35		10.10	
C5	H35	2.66	2.84	0.2	2.80	0.1
C5	H36	2.71	2.75	0.0	2.74	0.0
C9	H37	6.44	6.61	0.2	6.53	0.1
C10	H38	7.33	7.34	0.0	7.51	0.2
C14	H39	3.23	2.89	0.3	3.63	0.4
C15	H40	1.65	1.88	0.2	1.71	0.1
C15	H41	2.27	2.39	0.1	1.83	0.4
C16	H42	4.01	4.19	0.2	1.92	2.1
C17	H43	2.12	1.93	0.2	1.22	0.9
C17	H44	1.97	2.24	0.3	1.90	0.1
C18	H45	2.10	2.19	0.1	1.63	0.5
C18	H46	1.91	2.05	0.1	1.63	0.3
C19	H47	3.30	3.50	0.2	2.87	0.4
C19	H48	3.01	3.24	0.2	1.96	1.0
N20	H65	16.75	9.41		n.o	
C21	H49	3.15	4.19	1.0	3.61	0.5
C21	H50	3.97	3.53	0.4	2.68	1.3
C23	H51	2.25	2.43	0.2	2.61	0.4
C23	H52	3.68	3.19	0.5	2.65	1.0
C24	avg(53-55)	1.37	1.38	0.0	1.37	0.0
C25	avg(56-58)	1.36	1.41	0.1	1.39	0.0
C26	avg(59-61)	0.66	0.62	0.0	0.69	0.0
C27	avg(62-64)	0.83	0.83	0.0	0.97	0.1
			CMAD:	**0.21 ppm**	**CMAD:**	**0.45 ppm**

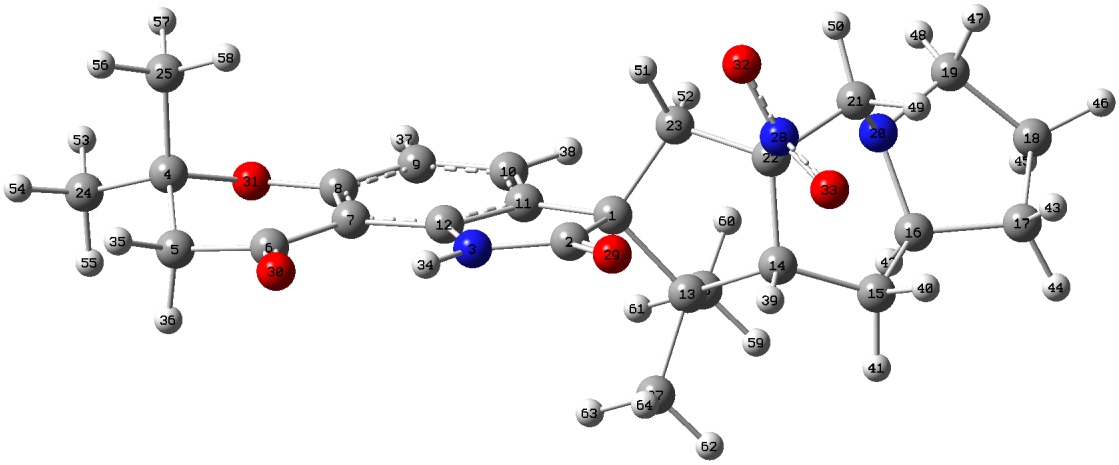
* TFA salt data from Ref. 10.

Table S8. Revised Citrinalin B (2) neutral form computed NMR data compared to TFA salt form experimental data for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation.

^{13}C			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
C1	C1	61.21	57.5	3.7	58.3	2.9
C2	C2	179.87	182.9	3.0	182.4	2.5
C4	C4	81.67	79.3	2.4	79.2	2.5
C5	C5	47.60	48.0	0.4	48.0	0.4
C6	C6	192.70	192.6	0.1	192.6	0.1
C7	C7	101.78	105.2	3.4	104.9	3.1
C8	C8	158.12	158.8	0.7	158.7	0.6
C9	C9	106.63	109.6	3.0	108.8	2.2
C10	C10	131.90	132.4	0.5	132.7	0.8
C11	C11	118.86	120.9	2.0	119.5	0.6
C12	C12	143.53	142.6	0.9	142.8	0.7
C13	C13	53.06	46.1	7.0	48.7	4.4
C14	C14	46.44	45.8	0.6	43.9	2.5
C15	C15	28.01	19.8	8.2	26.8	1.2
C16	C16	60.18	61.1	0.9	61.3	1.1
C17	C17	31.75	26.1	5.6	30.9	0.8
C18	C18	22.25	20.0	2.3	20.8	1.5
C19	C19	52.74	55.5	2.8	52.9	0.2
C21	C21	63.84	55.4	8.4	64.1	0.3
C22	C22	98.23	92.4	5.8	94.6	3.6
C23	C23	44.77	41.0	3.8	41.3	3.5
C24	C24	24.32	25.8	1.5	26.0	1.7
C25	C25	25.43	26.5	1.1	26.3	0.9
C26	C26	22.80	20.3	2.5	22.7	0.1
C27	C27	21.77	23.4	1.6	22.9	1.1
			CMAD:	**2.9 ppm**	**CMAD:**	**1.6 ppm**

* TFA salt data from Ref. 10.



^{1}H			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
N3	H34	8.67	10.35		10.10	
C5	H35	2.70	2.84	0.1	2.80	0.1
C5	H36	2.68	2.75	0.1	2.74	0.1
C9	H37	6.36	6.61	0.2	6.53	0.2
C10	H38	7.13	7.34	0.2	7.51	0.4
C14	H39	3.79	2.89	0.9	3.63	0.2
C15	H40	1.74	1.88	0.1	1.71	0.0
C15	H41	1.79	2.39	0.6	1.83	0.0
C16	H42	2.03	4.19	2.2	1.92	0.1
C17	H43	1.33	1.93	0.6	1.22	0.1
C17	H44	1.80	2.24	0.4	1.90	0.1
C18	H45	1.75	2.19	0.4	1.63	0.1
C18	H46	1.62	2.05	0.4	1.63	0.0
C19	H47	2.73	3.50	0.8	2.87	0.1
C19	H48	2.09	3.24	1.1	1.96	0.1
N20	H65	0.00	9.41		n.o	
C21	H49	3.48	4.19	0.7	3.61	0.1
C21	H50	2.55	3.53	1.0	2.68	0.1
C23	H51	2.71	2.43	0.3	2.61	0.1
C23	H52	2.50	3.19	0.7	2.65	0.1
C24	avg(53-55)	1.35	1.38	0.0	1.37	0.0
C25	avg(56-58)	1.37	1.41	0.0	1.39	0.0
C26	avg(59-61)	1.02	0.62	0.4	0.69	0.3
C27	avg(62-64)	0.83	0.83	0.0	0.97	0.1
			CMAD:	**0.52 ppm**	**CMAD:**	**0.12 ppm**

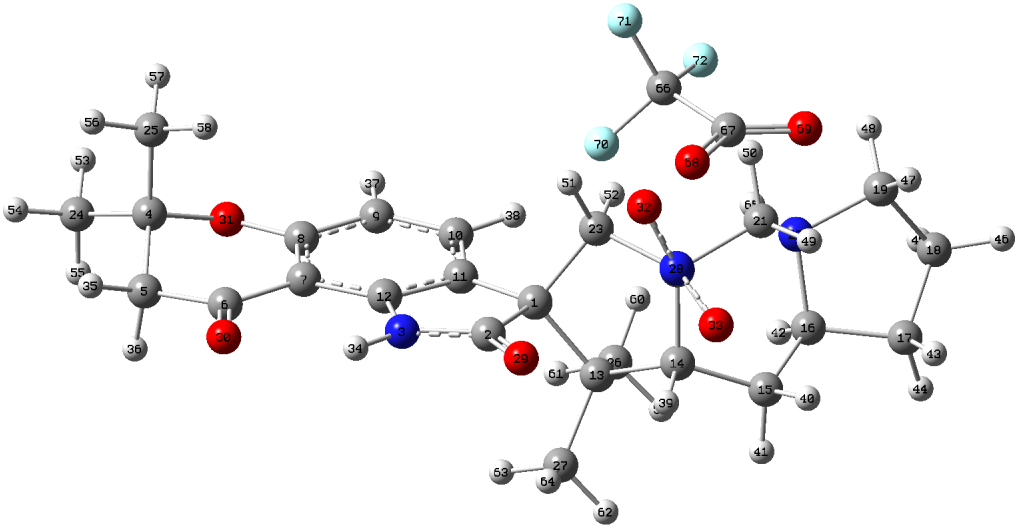
* TFA salt data from Ref. 10.

Table S9. Revised Citrinalin B (2) TFA salt form computed NMR data compared to TFA salt form experimental data for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation.

^{13}C			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
C1	C1	61.53	57.5	4.0	58.3	3.2
C2	C2	179.36	182.9	3.5	182.4	3.0
C4	C4	81.77	79.3	2.5	79.2	2.6
C5	C5	47.52	48.0	0.5	48.0	0.5
C6	C6	192.74	192.6	0.1	192.6	0.1
C7	C7	102.26	105.2	2.9	104.9	2.6
C8	C8	158.47	158.8	0.3	158.7	0.2
C9	C9	107.29	109.6	2.3	108.8	1.5
C10	C10	132.89	132.4	0.5	132.7	0.2
C11	C11	118.55	120.9	2.4	119.5	1.0
C12	C12	143.19	142.6	0.6	142.8	0.4
C13	C13	54.35	46.1	8.3	48.7	5.7
C14	C14	46.99	45.8	1.2	43.9	3.1
C15	C15	24.19	19.8	4.4	26.8	2.6
C16	C16	58.71	61.1	2.4	61.3	2.6
C17	C17	31.24	26.1	5.1	30.9	0.3
C18	C18	22.77	20.0	2.8	20.8	2.0
C19	C19	51.55	55.5	4.0	52.9	1.4
C21	C21	55.70	55.4	0.3	64.1	8.4
C22	C22	95.37	92.4	3.0	94.6	0.8
C23	C23	44.30	41.0	3.3	41.3	3.0
C24	C24	26.12	25.8	0.3	26.0	0.1
C25	C25	23.63	26.5	2.9	26.3	2.7
C26	C26	22.38	20.3	2.1	22.7	0.3
C27	C27	22.40	23.4	1.0	22.9	0.5
			CMAD:	**2.4 ppm**	**CMAD:**	**2.0 ppm**

* TFA salt data from Ref. 10.



^{1}H			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
N3	H34	8.70	10.35		10.10	
C5	H35	2.62	2.84	0.2	2.80	0.2
C5	H36	2.74	2.75	0.0	2.74	0.0
C9	H37	6.38	6.61	0.2	6.53	0.2
C10	H38	7.30	7.34	0.0	7.51	0.2
C14	H39	3.95	2.89	1.1	3.63	0.3
C15	H40	2.21	1.88	0.3	1.71	0.5
C15	H41	1.91	2.39	0.5	1.83	0.1
C16	H42	3.28	4.19	0.9	1.92	1.4
C17	H43	1.80	1.93	0.1	1.22	0.6
C17	H44	2.05	2.24	0.2	1.90	0.2
C18	H45	1.95	2.19	0.2	1.63	0.3
C18	H46	1.94	2.05	0.1	1.63	0.3
C19	H47	2.71	3.50	0.8	2.87	0.2
C19	H48	3.38	3.24	0.1	1.96	1.4
N20	H65	15.29	9.41		n.o	
C21	H49	3.40	4.19	0.8	3.61	0.2
C21	H50	3.05	3.53	0.5	2.68	0.4
C23	H51	2.98	2.43	0.5	2.61	0.4
C23	H52	2.88	3.19	0.3	2.65	0.2
C24	avg(53-55)	1.42	1.38	0.0	1.37	0.0
C25	avg(56-58)	1.32	1.41	0.1	1.39	0.1
C26	avg(59-61)	1.10	0.62	0.5	0.69	0.4
C27	avg(62-64)	0.90	0.83	0.1	0.97	0.1
			CMAD:	**0.35 ppm**	**CMAD:**	**0.34 ppm**

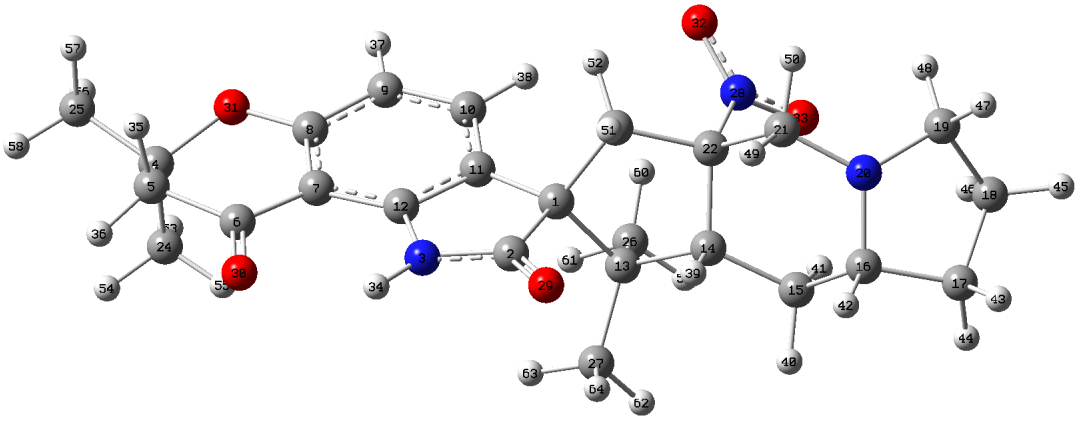
* TFA salt data from Ref. 10.

Table S10. Original Citrinalin B (3) neutral form computed NMR data compared to TFA salt form experimental data for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation.

^{13}C			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
C1	C1	61.01	57.5	3.5	58.3	2.7
C2	C2	181.85	182.9	1.1	182.4	0.6
C4	C4	81.17	79.3	1.9	79.2	2.0
C5	C5	47.62	48.0	0.4	48.0	0.4
C6	C6	192.86	192.6	0.3	192.6	0.3
C7	C7	102.13	105.2	3.1	104.9	2.8
C8	C8	157.92	158.8	0.9	158.7	0.8
C9	C9	106.96	109.6	2.6	108.8	1.8
C10	C10	133.01	132.4	0.6	132.7	0.3
C11	C11	121.78	120.9	0.9	119.5	2.3
C12	C12	142.91	142.6	0.3	142.8	0.1
C13	C13	52.27	46.1	6.2	48.7	3.6
C14	C14	56.38	45.8	10.6	43.9	12.5
C15	C15	28.81	19.8	9.0	26.8	2.0
C16	C16	58.51	61.1	2.6	61.3	2.8
C17	C17	32.74	26.1	6.6	30.9	1.8
C18	C18	25.60	20.0	5.6	20.8	4.8
C19	C19	52.76	55.5	2.7	52.9	0.1
C21	C21	59.70	55.4	4.3	64.1	4.4
C22	C22	94.42	92.4	2.0	94.6	0.2
C23	C23	42.28	41.0	1.3	41.3	1.0
C24	C24	24.78	25.8	1.0	26.0	1.2
C25	C25	24.84	26.5	1.7	26.3	1.5
C26	C26	20.88	20.3	0.6	22.7	1.8
C27	C27	21.39	23.4	2.0	22.9	1.5
			CMAD:	**2.9 ppm**	**CMAD:**	**2.1 ppm**

* TFA salt data from Ref. 10.



^{1}H			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
N3	H34	8.67	10.35		10.10	
C5	H35	2.66	2.84	0.2	2.80	0.1
C5	H36	2.67	2.75	0.1	2.74	0.1
C9	H37	6.35	6.61	0.3	6.53	0.2
C10	H38	7.11	7.34	0.2	7.51	0.4
C14	H39	2.64	2.89	0.3	3.63	1.0
C15	H40	1.25	1.88	0.6	1.71	0.5
C15	H41	2.39	2.39	0.0	1.83	0.6
C16	H42	3.08	4.19	1.1	1.92	1.2
C17	H43	2.14	1.93	0.2	1.22	0.9
C17	H44	1.78	2.24	0.5	1.90	0.1
C18	H45	1.70	2.19	0.5	1.63	0.1
C18	H46	2.24	2.05	0.2	1.63	0.6
C19	H47	3.13	3.50	0.4	2.87	0.3
C19	H48	2.93	3.24	0.3	1.96	1.0
N20	H65	0.00	9.41		n.o	
C21	H49	3.26	4.19	0.9	3.61	0.4
C21	H50	3.59	3.53	0.1	2.68	0.9
C23	H51	2.12	2.43	0.3	2.61	0.5
C23	H52	3.35	3.19	0.2	2.65	0.7
C24	avg(53-55)	1.36	1.38	0.0	1.37	0.0
C25	avg(56-58)	1.36	1.41	0.1	1.39	0.0
C26	avg(59-61)	0.63	0.62	0.0	0.69	0.1
C27	avg(62-64)	0.85	0.83	0.0	0.97	0.1
			CMAD:	**0.29 ppm**	**CMAD:**	**0.44 ppm**

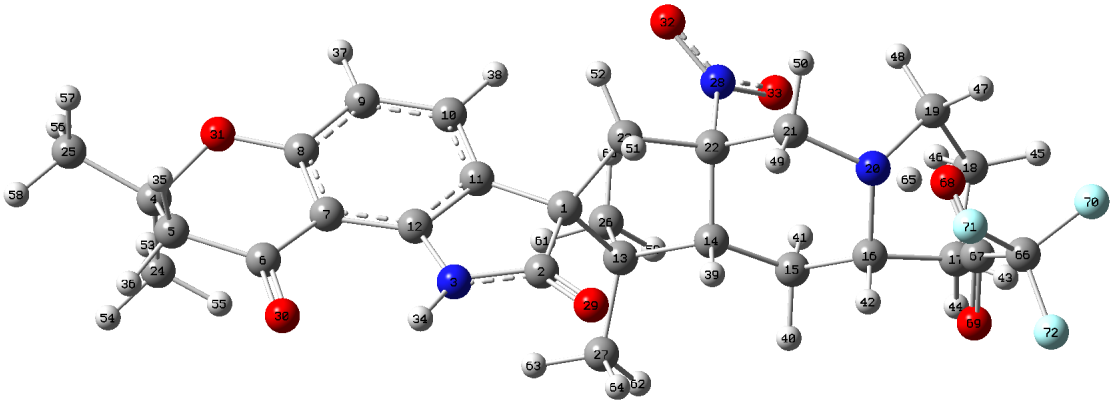
* TFA salt data from Ref. 10.

Table S11. Original Citrinalin B (3) TFA salt form computed NMR data compared to TFA salt form experimental data for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation.

^{13}C			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
C1	C1	60.52	57.5	3.0	58.3	2.2
C2	C2	181.33	182.9	1.6	182.4	1.1
C4	C4	82.09	79.3	2.8	79.2	2.9
C5	C5	47.38	48.0	0.6	48.0	0.6
C6	C6	192.61	192.6	0.0	192.6	0.0
C7	C7	102.76	105.2	2.4	104.9	2.1
C8	C8	158.49	158.8	0.3	158.7	0.2
C9	C9	107.18	109.6	2.4	108.8	1.6
C10	C10	132.87	132.4	0.5	132.7	0.2
C11	C11	120.07	120.9	0.8	119.5	0.6
C12	C12	142.72	142.6	0.1	142.8	0.1
C13	C13	51.02	46.1	4.9	48.7	2.3
C14	C14	51.93	45.8	6.1	43.9	8.0
C15	C15	24.17	19.8	4.4	26.8	2.6
C16	C16	61.46	61.1	0.4	61.3	0.2
C17	C17	32.49	26.1	6.4	30.9	1.6
C18	C18	24.56	20.0	4.6	20.8	3.8
C19	C19	53.43	55.5	2.1	52.9	0.5
C21	C21	54.54	55.4	0.9	64.1	9.6
C22	C22	93.41	92.4	1.0	94.6	1.2
C23	C23	43.13	41.0	2.1	41.3	1.8
C24	C24	24.77	25.8	1.0	26.0	1.2
C25	C25	24.86	26.5	1.6	26.3	1.4
C26	C26	19.87	20.3	0.4	22.7	2.8
C27	C27	21.87	23.4	1.5	22.9	1.0
			CMAD:	**2.1 ppm**	**CMAD:**	**2.0 ppm**

* TFA salt data from Ref. 10.



^{1}H			Citrinalin A*		Citrinalin B*	
Expt. #s	**Comp #**	**Comp.**	**Expt.**	**Abs. Dev.**	**Expt.**	**Abs. Dev.**
N3	H34	8.70	10.35		10.10	
C5	H35	2.68	2.84	0.2	2.80	0.1
C5	H36	2.67	2.75	0.1	2.74	0.1
C9	H37	6.40	6.61	0.2	6.53	0.1
C10	H38	7.15	7.34	0.2	7.51	0.4
C14	H39	2.84	2.89	0.0	3.63	0.8
C15	H40	1.61	1.88	0.3	1.71	0.1
C15	H41	2.44	2.39	0.1	1.83	0.6
C16	H42	4.18	4.19	0.0	1.92	2.3
C17	H43	2.18	1.93	0.3	1.22	1.0
C17	H44	1.89	2.24	0.4	1.90	0.0
C18	H45	1.90	2.19	0.3	1.63	0.3
C18	H46	2.36	2.05	0.3	1.63	0.7
C19	H47	3.16	3.50	0.3	2.87	0.3
C19	H48	2.85	3.24	0.4	1.96	0.9
N20	H65	16.98	9.41		n.o	
C21	H49	3.08	4.19	1.1	3.61	0.5
C21	H50	3.21	3.53	0.3	2.68	0.5
C23	H51	2.21	2.43	0.2	2.61	0.4
C23	H52	3.47	3.19	0.3	2.65	0.8
C24	avg(53-55)	1.38	1.38	0.0	1.37	0.0
C25	avg(56-58)	1.36	1.41	0.0	1.39	0.0
C26	avg(59-61)	0.71	0.62	0.1	0.69	0.0
C27	avg(62-64)	0.89	0.83	0.1	0.97	0.1
			CMAD:	**0.23 ppm**	**CMAD**	**0.46 ppm**

* TFA salt data from Ref. 10.

Table S12. Summary of NMR data comparison for Citrinalin A and Citrinalin B

Values in ppm relative to $CHCl_3$. CMAD = corrected mean absolute deviation. Comparisons are between the computed values for each structure and the experimental values reported for TFA salt forms of Citrinalin A and B (Ref. 10)

Structure	^{13}C CMAD		^{13}C largest outlier		^{1}H CMAD		^{1}H largest outlier	
	CitA	CitB	CitA	CitB	CitA	CitB	CitA	CitB
(**1**) Neutral	2.7	2.1	8.3	7.2	0.37	0.24	1.1	1.2
(**1**) H^+ form	2.3	2.6	7.2	6.7	0.20	0.47	1.1	2.2
(**1**) TFA salt	**2.0**	2.0	**5.2**	8.2	**0.21**	0.45	**1.0**	2.1
(**2**) Neutral	2.9	**1.6**	8.4	**4.4**	0.52	**0.12**	2.2	**0.38**
(**2**) TFA salt	2.4	2.0	8.3	8.4	0.35	0.34	1.1	1.4
(**3**) Neutral	2.9	2.1	10.6	12.5	0.29	0.44	1.1	1.2
(**3**) TFA salt	2.1	2.0	6.4	9.6	0.23	0.46	1.1	2.3

The values we believe represent the best match to experimental data are shown in bold blue text. Specifically, the computed TFA salt form of citrinalin A (**1**) is the best match for the experimental data of this compound. The computed neutral form of revised citrinalin B (**2**) is the best match for the experimental data of this compound. These conclusions are supported by comparison of all data above, but are most apparent in the ^{13}C and ^{1}H largest outliers, as well as the ^{1}H CMAD values. In addition, these conclusions are supported by DP4 analyses as described below.

DP4 Analysis

DP4 analysis was utilized to compare the computed and experimental data for the various forms of citrinalin A and citrinalin B. Specifically, the experimental data for both compounds were compared to computed data for neutral and TFA salt forms of structures (**1**), (**2**), and (**3**). The combined ^{1}H and ^{13}C results from this DP4 analysis show a 100% probability that citrinalin A corresponds to the TFA salt form of (**1**), and a 100% probability that citrinalin B corresponds to the neutral form of (**2**). Note that DP4 is known to somewhat overestimate the confidence levels of very closely related assignments, and that the conclusions are only valid within the structures included in the analysis.

Energies, coordinates, and NMR isotropic shielding constants

Citrinalin A (**1**) neutral form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.252797 H (rel E = "0" kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7629095 H (rel E = 5.56 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.273842	-0.284603	-0.210014
2	6	0.078417	-1.782168	-0.443912
3	7	1.449909	-1.912686	-0.348301
4	6	6.171271	0.291891	0.144338
5	6	5.877356	-1.030973	-0.581309
6	6	4.440760	-1.494518	-0.420348
7	6	3.454274	-0.425884	-0.278539
8	6	3.860293	0.934075	-0.238856
9	6	2.916338	1.963842	-0.230036
10	6	1.546785	1.666208	-0.227265
11	6	1.108881	0.343492	-0.210510
12	6	2.070411	-0.675071	-0.259355
13	6	-1.113502	-0.140099	1.168789
14	6	-2.560918	-0.185803	0.612996
15	6	-3.775280	0.040319	1.521260
16	6	-5.067328	0.060774	0.659191
17	6	-6.208403	-0.866642	1.115049
18	6	-6.978322	-1.216471	-0.189503
19	6	-6.110387	-0.625863	-1.324601
20	7	-4.801834	-0.429876	-0.706420
21	6	-3.881320	0.382785	-1.488439
22	6	-2.558640	0.627711	-0.698228
23	6	-1.245816	0.181252	-1.353422
24	6	6.131188	0.132648	1.670803
25	6	7.502396	0.886434	-0.308792
26	6	-0.778541	1.159431	1.930712
27	6	-0.870031	-1.301445	2.155188
28	7	-2.511158	2.160095	-0.431641
29	8	-0.700267	-2.691064	-0.678855
30	8	4.138791	-2.689621	-0.463213
31	8	5.172789	1.288642	-0.246884
32	8	-1.600622	2.828550	-0.921392
33	8	-3.418224	2.639391	0.243533
34	1	1.969282	-2.775003	-0.473462
35	1	6.052032	-0.901680	-1.658806
36	1	6.545785	-1.824888	-0.236753
37	1	3.264147	2.990739	-0.224418
38	1	0.830201	2.480478	-0.244772
39	1	-2.678723	-1.203185	0.220357
40	1	-3.821770	-0.782450	2.244213
41	1	-3.696262	0.970402	2.088720
42	1	-5.443979	1.098687	0.615033
43	1	-5.789478	-1.772869	1.565042
44	1	-6.842142	-0.386288	1.866779
45	1	-7.084913	-2.299206	-0.299054
46	1	-7.984225	-0.787187	-0.204892
47	1	-6.029830	-1.282659	-2.197978
48	1	-6.535473	0.338117	-1.669302
49	1	-3.652439	-0.150551	-2.417554
50	1	-4.332659	1.351190	-1.771074
51	1	-1.477058	-0.678381	-1.987627
52	1	-0.802363	0.959084	-1.973404
53	1	6.305150	1.099322	2.151703

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     54          1             6.911017   -0.563222    1.996477
     55          1             5.168263   -0.254900    2.015790
     56          1             7.679768    1.845554    0.186536
     57          1             7.503156    1.051025   -1.390180
     58          1             8.323984    0.208580   -0.057012
     59          1            -1.463394    1.270486    2.777202
     60          1            -0.844276    2.068452    1.333656
     61          1             0.236639    1.110491    2.334148
     62          1            -1.430997   -1.125087    3.078956
     63          1             0.188708   -1.366591    2.429941
     64          1            -1.182534   -2.266315    1.749574
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.018	61.24		H34	22.333	8.66
C2	-4.8469	181.68		H35	28.7614	2.78
C4	100.9472	81.25		H36	29.1273	2.45
C5	136.4587	47.53		H37	24.838	6.37
C6	-16.2812	192.54		H38	23.8281	7.29
C7	78.5138	102.54		H39	28.2209	3.27
C8	20.3576	157.76		H40	30.2053	1.46
C9	73.5565	107.25		H41	29.6921	1.93
C10	45.2788	134.10		H42	28.449	3.07
C11	58.5212	121.52		H43	30.2957	1.38
C12	36.8702	142.08		H44	29.4999	2.10
C13	133.4746	50.36		H45	29.7711	1.86
C14	131.8796	51.88		H46	29.9608	1.68
C15	159.2799	25.87		H47	28.6802	2.85
C16	125.5617	57.88		H48	29.4856	2.12
C17	151.2426	33.50		H49	28.2647	3.23
C18	162.5085	22.80		H50	29.1314	2.44
C19	132.1349	51.64		H51	29.1454	2.43
C21	122.7971	60.50		H52	28.0406	3.44
C22	79.8183	101.30		H53	30.6319	1.07
C23	138.1856	45.89		H54	30.6583	1.05
C24	163.7253	21.64		H55	29.9755	1.67
C25	157.2202	27.82		H56	30.0855	1.57
C26	165.1589	20.28		H57	30.2345	1.43
C27	162.8823	22.45		H58	30.3379	1.34
				H59	30.9486	0.78
				H60	31.1259	0.62
				H61	31.4989	0.28
				H62	30.8044	0.91
				H63	31.0326	0.70
				H64	30.674	1.03

Citrinalin A (**1**) neutral form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.252665 H (rel E = 0.08 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7717631 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.269538	-0.281451	-0.103830
2	6	0.091641	-1.762803	-0.414891
3	7	1.455481	-1.907045	-0.254897
4	6	6.189825	0.316199	-0.205350
5	6	5.867642	-1.094321	0.316407
6	6	4.440375	-1.521941	0.027793
7	6	3.455493	-0.442399	0.040651
8	6	3.864078	0.910541	0.173270
9	6	2.923357	1.942775	0.208633
10	6	1.554273	1.654021	0.128650
11	6	1.112758	0.337146	0.015071
12	6	2.073153	-0.681203	-0.053632
13	6	-1.185468	-0.222647	1.232112
14	6	-2.599426	-0.222112	0.593978
15	6	-3.861385	-0.046175	1.446208
16	6	-5.103239	0.035724	0.516817
17	6	-6.270900	-0.911124	0.849130
18	6	-6.961556	-1.183232	-0.517428
19	6	-6.035795	-0.516896	-1.560593
20	7	-4.762805	-0.368993	-0.860710
21	6	-3.797770	0.486629	-1.536620
22	6	-2.521141	0.673245	-0.659626
23	6	-1.174495	0.262456	-1.267417
24	6	7.500822	0.835810	0.378952
25	6	6.210641	0.368816	-1.739378
26	6	-0.891086	1.021284	2.096586
27	6	-1.001839	-1.448199	2.151534
28	7	-2.485299	2.185231	-0.292449
29	8	-0.674949	-2.649797	-0.751593
30	8	4.142336	-2.704609	-0.155090
31	8	5.175429	1.254968	0.278204
32	8	-1.544910	2.877422	-0.682874
33	8	-3.429227	2.625998	0.358068
34	1	1.977903	-2.763661	-0.403293
35	1	6.551824	-1.834711	-0.106987
36	1	5.994585	-1.116131	1.408133
37	1	3.274073	2.965804	0.285321
38	1	0.842364	2.472483	0.131048
39	1	-2.698104	-1.211534	0.131055
40	1	-3.948723	-0.911792	2.113074
41	1	-3.810980	0.846355	2.074064
42	1	-5.472946	1.077018	0.516575
43	1	-5.881925	-1.843436	1.271665
44	1	-6.948964	-0.471351	1.586909
45	1	-7.048781	-2.257721	-0.700703
46	1	-7.969752	-0.761727	-0.564494
47	1	-5.908301	-1.111046	-2.472385
48	1	-6.442623	0.470403	-1.858546
49	1	-3.518532	0.011639	-2.483400
50	1	-4.230486	1.473526	-1.782046
51	1	-1.371795	-0.553546	-1.967355
52	1	-0.695571	1.075821	-1.810779
53	1	7.695262	1.854150	0.030057
54	1	8.333014	0.196992	0.067267

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     55          1             7.458227    0.847121    1.471866
     56          1             5.261908    0.038443   -2.172456
     57          1             7.002090   -0.280385   -2.127435
     58          1             6.403780    1.391304   -2.075847
     59          1            -1.624949    1.083281    2.906304
     60          1            -0.916560    1.968001    1.557865
     61          1             0.097588    0.937347    2.556108
     62          1            -1.608550   -1.326089    3.054892
     63          1             0.040724   -1.541919    2.475399
     64          1            -1.299374   -2.381688    1.668635
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.7606	61.49		H34	22.3498	8.64
C2	-4.6749	181.52		H35	29.1058	2.47
C4	101.5836	80.64		H36	28.6758	2.86
C5	136.1999	47.78		H37	24.8235	6.38
C6	-16.1242	192.39		H38	23.8039	7.31
C7	79.4985	101.61		H39	28.2405	3.26
C8	20.5311	157.59		H40	30.2219	1.44
C9	73.5268	107.28		H41	29.7194	1.90
C10	45.2321	134.14		H42	28.4696	3.05
C11	57.8938	122.12		H43	30.2046	1.46
C12	36.5331	142.40		H44	29.5491	2.06
C13	134.3227	49.56		H45	29.7434	1.88
C14	131.8831	51.88		H46	29.9613	1.68
C15	159.3371	25.81		H47	28.7087	2.83
C16	125.7441	57.70		H48	29.504	2.10
C17	151.2359	33.50		H49	28.287	3.21
C18	162.5007	22.81		H50	29.1746	2.40
C19	132.2103	51.56		H51	29.1708	2.41
C21	122.916	60.39		H52	28.0414	3.44
C22	80.5239	100.63		H53	30.1171	1.54
C23	137.9899	46.08		H54	30.3975	1.28
C24	157.5836	27.48		H55	30.199	1.47
C25	163.6055	21.76		H56	30.0258	1.62
C26	165.2952	20.15		H57	30.7569	0.96
C27	162.9566	22.37		H58	30.5989	1.10
				H59	30.9589	0.77
				H60	31.105	0.64
				H61	31.4512	0.32
				H62	30.8483	0.87
				H63	31.0759	0.66
				H64	30.7242	0.99

Citrinalin A (**1**) neutral form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.251517 H (rel E = 0.80 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7656904 H (rel E = 3.81 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.276556	-0.037349	-0.093140
2	6	-0.022859	-1.556226	-0.324775
3	7	1.341217	-1.764076	-0.300190
4	6	6.203119	0.144107	0.023954
5	6	5.799982	-1.152138	-0.697962
6	6	4.345238	-1.527995	-0.484636
7	6	3.431569	-0.401745	-0.300457
8	6	3.921984	0.929897	-0.262189
9	6	3.043082	2.014822	-0.201669
10	6	1.659469	1.798645	-0.149222
11	6	1.140631	0.505590	-0.138050
12	6	2.037493	-0.567062	-0.231226
13	6	-1.071427	0.171514	1.290451
14	6	-2.518525	-0.062470	0.778755
15	6	-3.760363	0.059553	1.661550
16	6	-5.014230	-0.335596	0.848932
17	6	-5.295057	-1.858668	0.703516
18	6	-6.162068	-1.960217	-0.580170
19	6	-6.198675	-0.499446	-1.129235
20	7	-5.051087	0.204791	-0.537195
21	6	-3.823925	0.008810	-1.325247
22	6	-2.645641	0.641423	-0.577821
23	6	-1.239026	0.500689	-1.208293
24	6	6.215449	-0.026279	1.549486
25	6	7.547820	0.662216	-0.479589
26	6	-0.819728	1.569441	1.887278
27	6	-0.687940	-0.861189	2.367186
28	7	-2.987766	2.161561	-0.535842
29	8	-0.857897	-2.428591	-0.507942
30	8	3.967837	-2.701432	-0.521246
31	8	5.251344	1.204087	-0.318236
32	8	-2.964723	2.734573	-1.624281
33	8	-3.263481	2.711153	0.524261
34	1	1.803309	-2.656484	-0.439315
35	1	5.941227	-1.025702	-1.780764
36	1	6.430735	-1.988397	-0.383957
37	1	3.452329	3.018680	-0.192435
38	1	0.999826	2.659742	-0.114191
39	1	-2.491740	-1.113455	0.462827
40	1	-3.678936	-0.621146	2.517509
41	1	-3.876844	1.071495	2.049929
42	1	-5.883574	0.110943	1.349498
43	1	-5.803860	-2.250525	1.590294
44	1	-4.362986	-2.423874	0.593133
45	1	-5.713090	-2.645931	-1.305639
46	1	-7.171537	-2.329210	-0.373991
47	1	-7.115988	0.004251	-0.801474
48	1	-6.163923	-0.440743	-2.220930
49	1	-3.556686	-1.048329	-1.496154
50	1	-3.964704	0.483589	-2.300356
51	1	-1.274262	-0.192644	-2.053241
52	1	-0.890600	1.456482	-1.601097
53	1	6.471228	0.922730	2.029021
54	1	6.961852	-0.773428	1.837593

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      55          1             5.244858   -0.354715    1.932412
      56          1             7.800600    1.605168    0.013841
      57          1             7.515397    0.834784   -1.559177
      58          1             8.337329   -0.064493   -0.264330
      59          1            -1.530457    1.754938    2.698110
      60          1            -0.936565    2.384571    1.172711
      61          1             0.189510    1.626922    2.305660
      62          1            -1.222274   -0.643390    3.298028
      63          1             0.383593   -0.812914    2.591354
      64          1            -0.933835   -1.885135    2.072703
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.0789	62.13		H34	22.3277	8.66
C2	-4.7874	181.63		H35	28.7187	2.82
C4	100.8166	81.37		H36	29.0891	2.48
C5	136.2704	47.71		H37	24.8657	6.34
C6	-16.405	192.66		H38	24.042	7.10
C7	78.2767	102.77		H39	28.4346	3.08
C8	20.0005	158.09		H40	30.0342	1.62
C9	73.6076	107.20		H41	28.6059	2.92
C10	46.8852	132.57		H42	28.3468	3.16
C11	60.5266	119.62		H43	30.0307	1.62
C12	36.1048	142.81		H44	29.826	1.81
C13	132.711	51.09		H45	29.7099	1.91
C14	136.3713	47.61		H46	30.0898	1.57
C15	162.618	22.70		H47	28.8011	2.74
C16	123.4959	59.84		H48	28.879	2.67
C17	157.917	27.16		H49	28.6767	2.86
C18	162.5375	22.77		H50	28.313	3.19
C19	129.7668	53.88		H51	29.1069	2.46
C21	123.1346	60.18		H52	28.9572	2.60
C22	82.1942	99.05		H53	30.6101	1.09
C23	139.0961	45.03		H54	30.6701	1.03
C24	163.6177	21.75		H55	29.9471	1.70
C25	157.2928	27.75		H56	30.1175	1.54
C26	163.6212	21.74		H57	30.238	1.43
C27	164.1609	21.23		H58	30.3742	1.31
				H59	30.4532	1.23
				H60	30.6712	1.03
				H61	31.2423	0.51
				H62	30.6871	1.02
				H63	31.0888	0.65
				H64	30.8531	0.87

Citrinalin A (**1**) neutral form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.251269 H (rel E = 0.96 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7655076 H (rel E = 3.93 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.272500	-0.041223	0.029200
2	6	-0.012391	-1.550184	-0.253942
3	7	1.347892	-1.766678	-0.168663
4	6	6.203170	0.171775	-0.321264
5	6	5.817945	-1.214324	0.222400
6	6	4.358236	-1.557946	-0.009288
7	6	3.439979	-0.420790	0.029727
8	6	3.932939	0.905435	0.141489
9	6	3.056175	1.991361	0.213334
10	6	1.670969	1.781691	0.187222
11	6	1.147184	0.494171	0.089050
12	6	2.043891	-0.578137	-0.009622
13	6	-1.145437	0.115156	1.373070
14	6	-2.560520	-0.091486	0.769996
15	6	-3.851716	0.000979	1.583595
16	6	-5.057593	-0.355993	0.684486
17	6	-5.334585	-1.870694	0.464014
18	6	-6.124122	-1.917557	-0.872134
19	6	-6.124413	-0.436652	-1.364437
20	7	-5.010815	0.237315	-0.679544
21	6	-3.740612	0.064129	-1.401430
22	6	-2.608768	0.665702	-0.563732
23	6	-1.166891	0.550691	-1.115167
24	6	7.563268	0.616077	0.210372
25	6	6.168559	0.216451	-1.855160
26	6	-0.924312	1.485721	2.039803
27	6	-0.825537	-0.963233	2.425625
28	7	-2.954164	2.183637	-0.482446
29	8	-0.839265	-2.408883	-0.520288
30	8	3.982316	-2.721256	-0.169168
31	8	5.264323	1.171936	0.193389
32	8	-2.879697	2.795797	-1.546986
33	8	-3.277546	2.695205	0.583225
34	1	1.812424	-2.655992	-0.318266
35	1	6.440993	-1.995965	-0.220659
36	1	5.983888	-1.238168	1.308814
37	1	3.468539	2.991849	0.278457
38	1	1.014082	2.644389	0.230321
39	1	-2.517735	-1.129376	0.414807
40	1	-3.820946	-0.712849	2.415656
41	1	-3.988145	0.997178	2.004968
42	1	-5.953272	0.076124	1.150003
43	1	-4.399265	-2.436161	0.387565
44	1	-5.896635	-2.293471	1.303107
45	1	-5.634932	-2.576788	-1.596145
46	1	-7.144954	-2.289548	-0.740625
47	1	-6.026059	-0.335487	-2.449133
48	1	-7.057605	0.058868	-1.070774
49	1	-3.466003	-0.987084	-1.595044
50	1	-3.823318	0.574793	-2.364897
51	1	-1.149724	-0.100310	-1.993841
52	1	-0.795679	1.523693	-1.438807
53	1	7.803294	1.619866	-0.151891
54	1	8.344505	-0.071316	-0.128579

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      55          1             7.562913    0.633985    1.304012
      56          1             6.410105    1.223853   -2.205507
      57          1             5.185839   -0.057853   -2.249875
      58          1             6.903944   -0.481134   -2.268649
      59          1            -1.678657    1.641188    2.816856
      60          1            -1.000258    2.329591    1.353724
      61          1             0.060256    1.521038    2.515251
      62          1            -1.411619   -0.782248    3.332899
      63          1             0.231617   -0.929025    2.711856
      64          1            -1.056529   -1.972684    2.074342
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	120.9649	62.24		H34	22.3595	8.63
C2	-4.6931	181.54		H35	29.1181	2.45
C4	101.1598	81.04		H36	28.6777	2.86
C5	136.2237	47.75		H37	24.8577	6.35
C6	-16.422	192.67		H38	24.0778	7.06
C7	79.2528	101.84		H39	28.4355	3.08
C8	20.4746	157.64		H40	30.0553	1.60
C9	73.3795	107.42		H41	28.6302	2.90
C10	46.9175	132.54		H42	28.3688	3.14
C11	60.3183	119.82		H43	29.8031	1.83
C12	36.1979	142.72		H44	30.051	1.60
C13	132.4628	51.33		H45	29.7031	1.92
C14	136.2006	47.78		H46	30.1096	1.55
C15	162.8285	22.50		H47	28.8428	2.71
C16	123.6123	59.73		H48	28.8464	2.70
C17	157.8895	27.19		H49	28.6942	2.84
C18	162.6506	22.67		H50	28.3324	3.17
C19	129.8478	53.81		H51	29.1515	2.42
C21	123.1125	60.20		H52	29.0613	2.51
C22	81.2076	99.99		H53	30.1244	1.53
C23	139.3234	44.81		H54	30.3897	1.29
C24	157.4935	27.56		H55	30.2052	1.46
C25	163.6341	21.73		H56	30.608	1.09
C26	163.3694	21.98		H57	30.0299	1.62
C27	164.5093	20.90		H58	30.7459	0.97
				H59	30.4685	1.22
				H60	30.617	1.08
				H61	31.2008	0.55
				H62	30.706	1.00
				H63	31.1533	0.59
				H64	30.9135	0.81

Citrinalin A (**1**) neutral form, conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.248397 H (rel E = 2.76 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7586802 H (rel E = 8.21 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.350502	-0.122529	-0.240780
2	6	-0.064484	-1.631595	-0.482682
3	7	1.297677	-1.825291	-0.375048
4	6	6.106895	0.160971	0.207026
5	6	5.763947	-1.139621	-0.537590
6	6	4.306030	-1.539926	-0.401829
7	6	3.366137	-0.430070	-0.259426
8	6	3.831505	0.909927	-0.196296
9	6	2.933811	1.980852	-0.185082
10	6	1.552683	1.744126	-0.203687
11	6	1.057468	0.441623	-0.210625
12	6	1.972872	-0.617691	-0.261153
13	6	-1.207751	0.044151	1.118840
14	6	-2.645761	-0.008357	0.535721
15	6	-3.875332	0.197771	1.421774
16	6	-5.180629	0.171582	0.542941
17	6	-6.186769	-0.901432	0.983386
18	6	-5.659377	-2.177080	0.294337
19	6	-5.061426	-1.669465	-1.036492
20	7	-4.941329	-0.208404	-0.856469
21	6	-3.937580	0.525515	-1.593980
22	6	-2.618332	0.810362	-0.771326
23	6	-1.276582	0.403878	-1.396261
24	6	6.040620	-0.013288	1.730875
25	6	7.468244	0.701448	-0.223209
26	6	-0.887962	1.360237	1.857228
27	6	-0.974097	-1.098102	2.128308
28	7	-2.626934	2.334391	-0.505952
29	8	-0.882168	-2.503496	-0.732679
30	8	3.950895	-2.719472	-0.463785
31	8	5.158149	1.205679	-0.183890
32	8	-1.734681	3.041348	-0.978728
33	8	-3.576858	2.780347	0.135104
34	1	1.779520	-2.708945	-0.501973
35	1	5.959744	-1.007212	-1.611090
36	1	6.390917	-1.966560	-0.192791
37	1	3.326802	2.991030	-0.161302
38	1	0.873087	2.590116	-0.218572
39	1	-2.731805	-1.028687	0.140436
40	1	-3.907455	-0.613160	2.159525
41	1	-3.826767	1.137702	1.977167
42	1	-5.623740	1.172374	0.561701
43	1	-7.182803	-0.645717	0.605431
44	1	-6.252348	-0.997764	2.071725
45	1	-4.876860	-2.640410	0.905661
46	1	-6.438389	-2.929525	0.142423
47	1	-5.725295	-1.882183	-1.886026
48	1	-4.096971	-2.153519	-1.248279
49	1	-3.673054	-0.046939	-2.487631
50	1	-4.351244	1.482468	-1.934716
51	1	-1.464435	-0.409995	-2.100980
52	1	-0.812708	1.224886	-1.940317
53	1	6.250584	0.939482	2.224944
54	1	6.785112	-0.746204	2.057937

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      55          1             5.057393   -0.362037    2.059610
      56          1             7.680574    1.646782    0.284681
      57          1             7.490193    0.877019   -1.302632
      58          1             8.256388   -0.013932    0.031517
      59          1            -1.595667    1.496497    2.680880
      60          1            -0.933787    2.251738    1.232346
      61          1             0.115677    1.317389    2.289429
      62          1            -1.542325   -0.905170    3.044173
      63          1             0.082578   -1.158368    2.411969
      64          1            -1.283280   -2.071023    1.738748
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.8357	61.41		H34	22.2903	8.70
C2	-5.3343	182.15		H35	28.7201	2.82
C4	100.8504	81.34		H36	29.0964	2.47
C5	136.3371	47.65		H37	24.8098	6.39
C6	-16.4803	192.73		H38	23.8277	7.29
C7	78.4019	102.65		H39	28.8904	2.66
C8	20.2811	157.83		H40	30.2943	1.38
C9	73.4408	107.36		H41	29.7379	1.89
C10	45.5875	133.80		H42	27.6948	3.76
C11	58.7173	121.34		H43	29.5822	2.03
C12	36.3741	142.55		H44	30.0072	1.64
C13	132.8156	50.99		H45	29.5752	2.04
C14	129.8563	53.80		H46	29.8994	1.74
C15	158.6829	26.43		H47	28.4365	3.08
C16	128.5496	55.04		H48	28.4784	3.04
C17	149.608	35.05		H49	27.962	3.51
C18	161.6703	23.60		H50	28.0568	3.42
C19	130.7048	52.99		H51	29.3248	2.26
C21	123.3826	59.95		H52	27.8865	3.58
C22	82.1004	99.14		H53	30.605	1.09
C23	137.8685	46.19		H54	30.6442	1.06
C24	163.7143	21.66		H55	29.9514	1.69
C25	157.1841	27.86		H56	30.0808	1.57
C26	165.8984	19.58		H57	30.2151	1.45
C27	163.47	21.89		H58	30.3393	1.34
				H59	30.896	0.83
				H60	31.0518	0.69
				H61	31.469	0.30
				H62	30.7314	0.98
				H63	31.034	0.70
				H64	30.7443	0.97

Citrinalin A (**1**) neutral form, conformer 6

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.248634 H (rel E = 2.61 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7621818 H (rel E = 6.01 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.344933	-0.093377	-0.124107
2	6	-0.062290	-1.596999	-0.402070
3	7	1.290161	-1.810822	-0.231157
4	6	6.135108	0.161518	-0.139111
5	6	5.732773	-1.224362	0.392665
6	6	4.288903	-1.579764	0.088851
7	6	3.362005	-0.449835	0.075212
8	6	3.839037	0.881197	0.201016
9	6	2.953338	1.962067	0.213968
10	6	1.572489	1.744328	0.116671
11	6	1.064984	0.450928	0.008735
12	6	1.970761	-0.616885	-0.036277
13	6	-1.277664	0.037363	1.187331
14	6	-2.678628	-0.008816	0.519934
15	6	-3.960789	0.159290	1.335579
16	6	-5.209978	0.130289	0.378481
17	6	-6.217971	-0.973491	0.729245
18	6	-5.621075	-2.220463	0.044329
19	6	-4.955356	-1.667036	-1.235092
20	7	-4.878197	-0.208284	-1.013075
21	6	-3.845055	0.561980	-1.668774
22	6	-2.583541	0.847167	-0.759423
23	6	-1.196900	0.484734	-1.311537
24	6	7.463615	0.619172	0.457345
25	6	6.178164	0.196136	-1.673257
26	6	-1.009350	1.338263	1.970947
27	6	-1.094042	-1.127794	2.180234
28	7	-2.639238	2.364239	-0.453635
29	8	-0.873771	-2.450366	-0.726145
30	8	3.930607	-2.746926	-0.084569
31	8	5.164800	1.157277	0.321114
32	8	-1.734881	3.101568	-0.850773
33	8	-3.635857	2.773616	0.139221
34	1	1.767295	-2.697057	-0.356872
35	1	6.382701	-2.003983	-0.013843
36	1	5.844030	-1.240788	1.486160
37	1	3.356499	2.965833	0.286920
38	1	0.904488	2.599453	0.103682
39	1	-2.730397	-1.017860	0.091927
40	1	-4.022079	-0.667267	2.053919
41	1	-3.961301	1.087934	1.911444
42	1	-5.673730	1.121661	0.395086
43	1	-7.193680	-0.728666	0.295196
44	1	-6.349355	-1.098409	1.808673
45	1	-4.866799	-2.681865	0.691553
46	1	-6.372099	-2.985254	-0.172867
47	1	-5.562762	-1.871137	-2.127902
48	1	-3.969732	-2.125971	-1.399620
49	1	-3.515895	0.017428	-2.558267
50	1	-4.255073	1.520276	-2.010135
51	1	-1.322120	-0.288861	-2.073098
52	1	-0.708260	1.340013	-1.775132
53	1	7.714009	1.622909	0.101843
54	1	8.266157	-0.063855	0.162105

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      55          1             7.408275    0.643275    1.549498
      56          1             6.428618    1.203332   -2.017848
      57          1             5.219133   -0.089510   -2.115340
      58          1             6.939528   -0.497707   -2.043874
      59          1            -1.772101    1.460652    2.746364
      60          1            -1.012291    2.240861    1.360119
      61          1            -0.037973    1.286420    2.470600
      62          1            -1.709753   -0.957902    3.069545
      63          1            -0.053406   -1.193171    2.517093
      64          1            -1.379825   -2.091714    1.751994
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.5347	61.70		H34	22.296	8.69
C2	-5.148	181.97		H35	29.0994	2.47
C4	101.1747	81.03		H36	28.6602	2.87
C5	136.0139	47.95		H37	24.7853	6.42
C6	-16.4018	192.65		H38	23.8337	7.29
C7	79.1727	101.92		H39	28.8612	2.69
C8	20.4987	157.62		H40	30.3065	1.37
C9	73.1847	107.60		H41	29.7346	1.89
C10	45.7259	133.67		H42	27.634	3.81
C11	58.5139	121.53		H43	29.5712	2.04
C12	36.3165	142.60		H44	29.9774	1.67
C13	133.084	50.74		H45	29.5628	2.05
C14	130.0535	53.61		H46	29.8925	1.75
C15	158.4388	26.66		H47	28.4437	3.07
C16	128.5148	55.07		H48	28.4495	3.07
C17	149.6149	35.04		H49	27.9557	3.52
C18	161.7068	23.56		H50	28.0985	3.39
C19	130.6929	53.01		H51	29.3133	2.28
C21	123.4055	59.92		H52	27.8062	3.65
C22	82.4662	98.79		H53	30.1091	1.55
C23	138.2106	45.87		H54	30.3778	1.30
C24	157.3648	27.68		H55	30.1952	1.47
C25	163.5689	21.79		H56	30.5825	1.11
C26	166.2559	19.24		H57	29.9897	1.66
C27	163.7648	21.61		H58	30.7489	0.96
				H59	30.9022	0.82
				H60	31.0052	0.73
				H61	31.3868	0.38
				H62	30.7467	0.96
				H63	31.1153	0.63
				H64	30.8185	0.90

Citrinalin A (**1**) neutral form, conformer 1

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1511.287902 H (rel E = 1.22 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.245860	-0.115385	-0.168663
2	6	0.039777	-1.627856	-0.394495
3	7	1.401184	-1.815433	-0.332651
4	6	6.235088	0.168233	0.121535
5	6	5.865698	-1.122311	-0.624376
6	6	4.419162	-1.525798	-0.444981
7	6	3.475713	-0.421873	-0.277050
8	6	3.942650	0.919077	-0.215914
9	6	3.041135	1.988575	-0.179432
10	6	1.660488	1.750782	-0.170034
11	6	1.164791	0.448296	-0.175690
12	6	2.081678	-0.608155	-0.245975
13	6	-1.077508	0.080218	1.195897
14	6	-2.512107	-0.121612	0.645764
15	6	-3.754677	-0.053122	1.544597
16	6	-5.024481	-0.094471	0.656370
17	6	-6.172359	-1.002555	1.141914
18	6	-6.851257	-1.524151	-0.156728
19	6	-6.013962	-0.919363	-1.300713
20	7	-4.715347	-0.648342	-0.680098
21	6	-3.840454	0.190754	-1.497578
22	6	-2.587218	0.648465	-0.681346
23	6	-1.192453	0.414596	-1.304187
24	6	6.222051	-0.020205	1.642191
25	6	7.578462	0.710498	-0.352044
26	6	-0.839111	1.470880	1.815149
27	6	-0.737737	-0.962046	2.275885
28	7	-2.803012	2.187497	-0.512701
29	8	-0.773572	-2.520831	-0.603762
30	8	4.062778	-2.709538	-0.499936
31	8	5.264104	1.220377	-0.227740
32	8	-2.345924	2.933079	-1.381136
33	8	-3.494053	2.590190	0.420605
34	1	1.870103	-2.705157	-0.466344
35	1	6.022092	-0.979620	-1.703434
36	1	6.512542	-1.944114	-0.305830
37	1	3.427390	3.002083	-0.153731
38	1	0.986125	2.600617	-0.156243
39	1	-2.506588	-1.150634	0.269304
40	1	-3.739758	-0.925493	2.207965
41	1	-3.767652	0.838833	2.174200
42	1	-5.412103	0.934263	0.541977
43	1	-5.768377	-1.835924	1.726334
44	1	-6.864751	-0.453719	1.787574
45	1	-6.824213	-2.617537	-0.193066
46	1	-7.899079	-1.219906	-0.233408
47	1	-5.901408	-1.586653	-2.162132
48	1	-6.477535	0.019220	-1.661689
49	1	-3.510345	-0.385783	-2.367289
50	1	-4.381843	1.072931	-1.883904
51	1	-1.276649	-0.323554	-2.104549
52	1	-0.796032	1.326487	-1.748337
53	1	6.466079	0.921716	2.142963
54	1	6.971914	-0.765929	1.925433
55	1	5.249831	-0.364872	2.008386
56	1	7.816869	1.648292	0.159846
57	1	7.567434	0.892007	-1.431292
58	1	8.370212	-0.011801	-0.130260

59	1	-1.576818	1.652604	2.603215
60	1	-0.904754	2.294233	1.101302
61	1	0.152884	1.519175	2.273514
62	1	-1.286876	-0.735263	3.196071
63	1	0.330427	-0.936974	2.520292
64	1	-1.000624	-1.980634	1.976445

Citrinalin A (**1**) neutral form, conformer 2

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1511.287254 H (rel E = 1.63 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.241007	-0.152008	-0.046807
2	6	0.065492	-1.644401	-0.357468
3	7	1.421991	-1.834157	-0.226834
4	6	6.239239	0.229598	-0.241262
5	6	5.878128	-1.170767	0.277099
6	6	4.436748	-1.550422	0.019181
7	6	3.481790	-0.443686	0.050854
8	6	3.937164	0.895569	0.186305
9	6	3.028309	1.957312	0.248837
10	6	1.649882	1.713883	0.188902
11	6	1.164261	0.413485	0.066661
12	6	2.090033	-0.633473	-0.025304
13	6	-1.154610	-0.052163	1.276858
14	6	-2.556835	-0.182089	0.627853
15	6	-3.848031	-0.149125	1.457856
16	6	-5.064680	-0.089347	0.500225
17	6	-6.262609	-0.992099	0.856963
18	6	-6.876351	-1.407273	-0.510629
19	6	-5.959958	-0.750730	-1.561772
20	7	-4.692907	-0.558867	-0.852296
21	6	-3.751935	0.310375	-1.558686
22	6	-2.539678	0.680875	-0.641367
23	6	-1.117228	0.455838	-1.199177
24	6	7.575327	0.697625	0.322992
25	6	6.232854	0.298707	-1.772123
26	6	-0.933250	1.276282	2.023945
27	6	-0.899557	-1.186845	2.285068
28	7	-2.733259	2.209027	-0.378090
29	8	-0.729255	-2.521409	-0.676296
30	8	4.093383	-2.726879	-0.150766
31	8	5.255906	1.199622	0.271839
32	8	-2.223923	2.999423	-1.174918
33	8	-3.457141	2.564945	0.549374
34	1	1.902349	-2.712603	-0.390476
35	1	6.536474	-1.922495	-0.166460
36	1	6.024020	-1.205626	1.366539
37	1	3.407843	2.970444	0.329996
38	1	0.969688	2.558537	0.219611
39	1	-2.546652	-1.181467	0.177865
40	1	-3.890855	-1.069172	2.051672
41	1	-3.876932	0.692802	2.152586
42	1	-5.417048	0.956320	0.436863
43	1	-5.916978	-1.873674	1.407043
44	1	-6.977590	-0.465418	1.496439
45	1	-6.872489	-2.496054	-0.619715
46	1	-7.910514	-1.070343	-0.626199
47	1	-5.814463	-1.361660	-2.459412
48	1	-6.378970	0.222843	-1.882408
49	1	-3.383524	-0.215566	-2.444844
50	1	-4.249130	1.230359	-1.914684
51	1	-1.171125	-0.238534	-2.040236
52	1	-0.682469	1.381659	-1.572574
53	1	7.800474	1.713337	-0.017419
54	1	8.375857	0.034955	-0.020328
55	1	7.562394	0.688067	1.417364
56	1	5.266482	0.006637	-2.195178
57	1	6.993538	-0.377485	-2.175502
58	1	6.463095	1.315299	-2.105390

59	1	-1.711329	1.404247	2.783207
60	1	-0.947674	2.159665	1.383146
61	1	0.031940	1.266569	2.538745
62	1	-1.503653	-1.026110	3.184474
63	1	0.150547	-1.202772	2.598227
64	1	-1.156834	-2.171120	1.883719

Citrinalin A (**1**) neutral form, conformer 3

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1511.289853 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.279131	-0.106230	-0.115635
2	6	0.004767	-1.616014	-0.357315
3	7	1.367723	-1.800368	-0.326127
4	6	6.203009	0.197432	0.040413
5	6	5.825397	-1.096117	-0.696235
6	6	4.383018	-1.502919	-0.492933
7	6	3.439622	-0.401298	-0.309967
8	6	3.903504	0.941131	-0.258840
9	6	2.999681	2.008024	-0.205507
10	6	1.620241	1.766017	-0.165188
11	6	1.129120	0.461888	-0.157979
12	6	2.047141	-0.591722	-0.250359
13	6	-1.069554	0.077789	1.279054
14	6	-2.522534	-0.117340	0.767760
15	6	-3.754112	-0.003231	1.666382
16	6	-5.033958	-0.311008	0.856002
17	6	-5.369792	-1.813091	0.640026
18	6	-6.246329	-1.828503	-0.639975
19	6	-6.249760	-0.345925	-1.116698
20	7	-5.071698	0.300110	-0.506503
21	6	-3.859889	0.074371	-1.315802
22	6	-2.639939	0.626072	-0.567148
23	6	-1.252210	0.436685	-1.221491
24	6	6.213820	0.013678	1.561701
25	6	7.537686	0.741812	-0.454866
26	6	-0.793988	1.454887	1.910961
27	6	-0.704927	-0.982694	2.333331
28	7	-2.922078	2.158162	-0.473388
29	8	-0.810435	-2.511164	-0.549927
30	8	4.028662	-2.687577	-0.540354
31	8	5.223738	1.245883	-0.296974
32	8	-2.845297	2.783251	-1.534437
33	8	-3.239440	2.678325	0.591438
34	1	1.835682	-2.688709	-0.471625
35	1	5.964185	-0.955784	-1.778034
36	1	6.479308	-1.915539	-0.386028
37	1	3.383298	3.022740	-0.189388
38	1	0.943246	2.613684	-0.137704
39	1	-2.518829	-1.158193	0.418293
40	1	-3.682833	-0.732634	2.481600
41	1	-3.829767	0.986663	2.117689
42	1	-5.880533	0.137491	1.391331
43	1	-5.887757	-2.222562	1.513297
44	1	-4.457134	-2.401979	0.498303
45	1	-5.818965	-2.487079	-1.402905
46	1	-7.264955	-2.177728	-0.444160
47	1	-7.148383	0.163048	-0.748099
48	1	-6.225530	-0.235477	-2.204567
49	1	-3.648188	-0.987828	-1.514964
50	1	-3.990533	0.572228	-2.280461
51	1	-1.330655	-0.272694	-2.049591
52	1	-0.880027	1.372265	-1.638814
53	1	6.467295	0.956855	2.055409
54	1	6.967241	-0.732097	1.835223
55	1	5.247149	-0.328502	1.944544
56	1	7.780873	1.681734	0.050804
57	1	7.510348	0.920078	-1.534386
58	1	8.334634	0.022350	-0.242685

59	1	-1.508180	1.633518	2.721069
60	1	-0.873132	2.286727	1.210581
61	1	0.211054	1.478600	2.343029
62	1	-1.222578	-0.762358	3.273241
63	1	0.370366	-0.971177	2.544989
64	1	-0.987463	-1.994872	2.029998

Citrinalin A (**1**) neutral form, conformer 4

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1511.288186 H (rel E = 1.05 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.273774	-0.103169	0.028709
2	6	0.012470	-1.599441	-0.283815
3	7	1.370663	-1.798866	-0.190150
4	6	6.202937	0.225381	-0.331911
5	6	5.843373	-1.171695	0.196313
6	6	4.392307	-1.539544	-0.019813
7	6	3.447948	-0.424583	0.031191
8	6	3.917489	0.911240	0.151529
9	6	3.018846	1.980397	0.234641
10	6	1.637446	1.747835	0.210314
11	6	1.138680	0.451013	0.103698
12	6	2.053359	-0.603340	-0.009054
13	6	-1.154037	0.012458	1.375944
14	6	-2.570733	-0.143698	0.760007
15	6	-3.860194	-0.064480	1.577811
16	6	-5.081306	-0.334959	0.668376
17	6	-5.400230	-1.827111	0.372640
18	6	-6.176880	-1.793743	-0.969960
19	6	-6.153956	-0.293284	-1.385045
20	7	-5.023557	0.329196	-0.668994
21	6	-3.756806	0.138857	-1.400294
22	6	-2.598426	0.662205	-0.543350
23	6	-1.164652	0.517749	-1.104087
24	6	7.555691	0.682427	0.200826
25	6	6.160428	0.294217	-1.862088
26	6	-0.911013	1.349769	2.098260
27	6	-0.866359	-1.109042	2.390139
28	7	-2.898398	2.186688	-0.399725
29	8	-0.796352	-2.473600	-0.574827
30	8	4.034177	-2.714022	-0.172224
31	8	5.240317	1.204418	0.203589
32	8	-2.796037	2.851274	-1.434084
33	8	-3.240434	2.666361	0.676551
34	1	1.839732	-2.681997	-0.361163
35	1	6.482026	-1.929337	-0.265692
36	1	6.019482	-1.208553	1.281237
37	1	3.407996	2.990723	0.304306
38	1	0.964874	2.597943	0.256433
39	1	-2.548372	-1.166229	0.361177
40	1	-3.845500	-0.828345	2.363770
41	1	-3.966607	0.905195	2.065668
42	1	-5.963033	0.095173	1.160042
43	1	-4.479164	-2.412681	0.280178
44	1	-5.983011	-2.265706	1.189098
45	1	-5.687588	-2.418553	-1.723957
46	1	-7.204830	-2.155262	-0.867270
47	1	-6.055414	-0.138648	-2.463340
48	1	-7.077999	0.198759	-1.058465
49	1	-3.526721	-0.913381	-1.629181
50	1	-3.821728	0.678051	-2.349036
51	1	-1.172819	-0.123701	-1.989479
52	1	-0.765254	1.482556	-1.417133
53	1	7.783297	1.694708	-0.147957
54	1	8.342159	0.010710	-0.157172
55	1	7.565892	0.676513	1.295255
56	1	6.392776	1.308394	-2.201267
57	1	5.181105	0.011923	-2.261359
58	1	6.904212	-0.389672	-2.283519

59	1	-1.675614	1.493629	2.868348
60	1	-0.937696	2.219056	1.440731
61	1	0.063410	1.338092	2.596150
62	1	-1.446903	-0.939648	3.303497
63	1	0.191810	-1.117253	2.675273
64	1	-1.130486	-2.099781	2.008984

Citrinalin A (**1**) H^+ form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.626178 H (rel E = 4.86 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.211651	0.240070	-0.103006
2	6	-0.070991	-1.308695	-0.270603
3	7	1.255111	-1.613519	-0.248107
4	6	6.255392	-0.107064	0.077791
5	6	5.742000	-1.368198	-0.637919
6	6	4.266272	-1.622311	-0.412936
7	6	3.446097	-0.416886	-0.247584
8	6	4.044800	0.868445	-0.221349
9	6	3.251707	2.026505	-0.188036
10	6	1.859147	1.928379	-0.151822
11	6	1.239322	0.675276	-0.133429
12	6	2.046823	-0.462910	-0.193911
13	6	-1.038696	0.585832	1.222151
14	6	-2.450463	0.217392	0.699039
15	6	-3.743470	0.353838	1.507440
16	6	-4.908841	-0.251321	0.682217
17	6	-5.799479	-1.320001	1.315697
18	6	-6.465131	-2.051051	0.115495
19	6	-5.622356	-1.670904	-1.126773
20	7	-4.387011	-1.011753	-0.554488
21	6	-3.532465	-0.221438	-1.527696
22	6	-2.565771	0.718199	-0.770703
23	6	-1.103493	0.772167	-1.268209
24	6	6.260099	-0.269900	1.602722
25	6	7.630538	0.303109	-0.439285
26	6	-0.877014	2.052432	1.661049
27	6	-0.644576	-0.309966	2.411872
28	7	-3.200979	2.155257	-0.841897
29	8	-0.990858	-2.115308	-0.428546
30	8	3.779909	-2.753714	-0.429331
31	8	5.382442	1.032263	-0.258308
32	8	-2.470679	3.131888	-0.878159
33	8	-4.432144	2.213880	-0.840009
34	1	1.661236	-2.539820	-0.355413
35	1	5.883264	-1.257774	-1.722682
36	1	6.307750	-2.250414	-0.326963
37	1	3.743987	2.992292	-0.188478
38	1	1.272047	2.841147	-0.137592
39	1	-2.320950	-0.857204	0.544377
40	1	-3.635397	-0.186009	2.453602
41	1	-3.984834	1.392665	1.750323
42	1	-5.517648	0.545952	0.255777
43	1	-5.193525	-2.013164	1.911544
44	1	-6.531070	-0.868613	1.989477
45	1	-6.482189	-3.132003	0.268983
46	1	-7.498047	-1.727899	-0.029207
47	1	-5.318063	-2.514136	-1.749329
48	1	-6.116266	-0.925968	-1.753467
49	1	-2.962211	-0.958807	-2.094141
50	1	-4.205251	0.319046	-2.191663
51	1	-0.963077	0.191473	-2.183398
52	1	-0.836760	1.804579	-1.490920
53	1	6.588994	0.658284	2.077525
54	1	6.950675	-1.068634	1.890192
55	1	5.270432	-0.525732	1.993341
56	1	7.962919	1.221978	0.051381
57	1	7.603746	0.476173	-1.518708
58	1	8.360708	-0.484173	-0.229429

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     59          1           -1.604353    2.283799    2.447063
     60          1           -1.020944    2.771679    0.855018
     61          1            0.116752    2.210832    2.087290
     62          1           -1.196525   -0.017686    3.311052
     63          1            0.419789   -0.191669    2.637587
     64          1           -0.836776   -1.371479    2.227228
     65          1           -3.784428   -1.766682   -0.207376
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	118.0836	64.98		H34	21.7978	9.15
C2	-5.6554	182.45		H35	28.6285	2.90
C4	98.8611	83.23		H36	28.9883	2.57
C5	136.6883	47.31		H37	24.64	6.55
C6	-17.0939	193.31		H38	23.7019	7.41
C7	77.7833	103.24		H39	27.4436	3.99
C8	19.098	158.95		H40	29.9269	1.71
C9	70.8986	109.77		H41	29.905	1.73
C10	46.8873	132.57		H42	26.7537	4.62
C11	64.1887	116.14		H43	29.9042	1.74
C12	36.6014	142.33		H44	29.1241	2.45
C13	133.3469	50.49		H45	29.4143	2.18
C14	132.4506	51.34		H46	29.2686	2.32
C15	162.8908	22.44		H47	27.8591	3.61
C16	114.4883	68.39		H48	28.3542	3.15
C17	154.9504	29.98		H49	27.6358	3.81
C18	162.8774	22.45		H50	27.6376	3.81
C19	130.6688	53.03		H51	29.5508	2.06
C21	122.2298	61.04		H52	27.8356	3.63
C22	81.9113	99.32		H53	30.5262	1.17
C23	141.0683	43.16		H54	30.6344	1.07
C24	163.7284	21.64		H55	29.9271	1.71
C25	157.4826	27.57		H56	30.0566	1.60
C26	168.5821	17.03		H57	30.1839	1.48
C27	164.4428	20.96		H58	30.3306	1.35
				H59	30.9205	0.81
				H60	30.0746	1.58
				H61	30.9528	0.78
				H62	30.7142	0.99
				H63	30.9945	0.74
				H64	31.0565	0.68
				H65	26.4164	4.92

Citrinalin A (**1**) H^+ form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.62609 H (rel E = 4.54 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.206858	0.235512	0.028016
2	6	-0.060452	-1.312299	-0.144338
3	7	1.262384	-1.620099	-0.057133
4	6	6.258400	-0.091615	-0.272470
5	6	5.753033	-1.405869	0.347740
6	6	4.276362	-1.642587	0.111227
7	6	3.452233	-0.428529	0.080925
8	6	4.051344	0.855802	0.128228
9	6	3.259082	2.014586	0.150032
10	6	1.866164	1.918921	0.125510
11	6	1.244548	0.667367	0.079615
12	6	2.052487	-0.471459	0.043126
13	6	-1.107306	0.572819	1.307323
14	6	-2.488818	0.213130	0.701079
15	6	-3.827241	0.354122	1.430701
16	6	-4.944240	-0.242121	0.534903
17	6	-5.879716	-1.304880	1.111814
18	6	-6.473197	-2.033601	-0.127612
19	6	-5.558911	-1.649945	-1.317076
20	7	-4.354240	-1.004517	-0.669802
21	6	-3.431745	-0.221978	-1.587328
22	6	-2.517888	0.719576	-0.771437
23	6	-1.029185	0.781226	-1.180971
24	6	7.639630	0.277495	0.258818
25	6	6.244061	-0.135044	-1.805369
26	6	-0.965608	2.034243	1.769325
27	6	-0.786051	-0.335702	2.508986
28	7	-3.152969	2.154040	-0.874341
29	8	-0.971982	-2.115572	-0.357726
30	8	3.793164	-2.770268	0.005202
31	8	5.389648	1.017417	0.161484
32	8	-2.426601	3.133397	-0.831249
33	8	-4.380041	2.208996	-0.976942
34	1	1.670593	-2.547119	-0.147449
35	1	6.318274	-2.259755	-0.034698
36	1	5.900891	-1.377130	1.436805
37	1	3.752510	2.979520	0.171853
38	1	1.280788	2.832807	0.125350
39	1	-2.355831	-0.861433	0.549987
40	1	-3.779523	-0.188701	2.380097
41	1	-4.077072	1.393750	1.662002
42	1	-5.521797	0.559417	0.074305
43	1	-5.317884	-2.001136	1.745903
44	1	-6.649663	-0.847767	1.737299
45	1	-6.497663	-3.114955	0.022243
46	1	-7.496278	-1.711699	-0.332366
47	1	-5.226040	-2.490633	-1.928385
48	1	-6.011116	-0.896090	-1.964390
49	1	-2.824879	-0.965372	-2.105709
50	1	-4.054936	0.315032	-2.300506
51	1	-0.832947	0.213760	-2.094163
52	1	-0.751549	1.816905	-1.372848
53	1	7.967411	1.231516	-0.163127
54	1	8.366749	-0.491237	-0.019310
55	1	7.625350	0.366886	1.348607
56	1	5.249316	-0.360348	-2.202079
57	1	6.930286	-0.908755	-2.163159
58	1	6.566825	0.827453	-2.210959
59	1	-1.735888	2.260761	2.514732
60	1	-1.060609	2.762620	0.964286

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     61          1             0.002662    2.183240    2.253561
     62          1            -1.391293   -0.051779    3.375999
     63          1             0.262764   -0.221251    2.799958
     64          1            -0.967632   -1.394925    2.302275
     65          1            -3.782304   -1.766324   -0.287923
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	118.0186	65.04		H34	21.8098	9.14
C2	-5.6091	182.41		H35	29.0214	2.54
C4	98.7141	83.37		H36	28.5955	2.93
C5	136.6481	47.35		H37	24.6331	6.55
C6	-17.1697	193.38		H38	23.7142	7.40
C7	78.2858	102.76		H39	27.3701	4.05
C8	19.3554	158.71		H40	29.9208	1.72
C9	70.6576	110.00		H41	29.9293	1.71
C10	47.0235	132.44		H42	26.8121	4.56
C11	64.093	116.23		H43	29.921	1.72
C12	36.6129	142.32		H44	29.1575	2.42
C13	133.6224	50.22		H45	29.4062	2.19
C14	132.0746	51.69		H46	29.2775	2.31
C15	162.8615	22.46		H47	27.8369	3.63
C16	114.5196	68.36		H48	28.3425	3.16
C17	155.1553	29.78		H49	27.6052	3.84
C18	163.0547	22.28		H50	27.5714	3.87
C19	130.7171	52.98		H51	29.5172	2.09
C21	122.3891	60.89		H52	27.8443	3.62
C22	81.8738	99.35		H53	30.0602	1.59
C23	140.9674	43.25		H54	30.3337	1.34
C24	157.5302	27.53		H55	30.1566	1.50
C25	163.7139	21.66		H56	30.0252	1.62
C26	168.4379	17.17		H57	30.6799	1.03
C27	164.741	20.68		H58	30.54	1.15
				H59	30.9339	0.79
				H60	29.9734	1.67
				H61	30.897	0.83
				H62	30.7373	0.97
				H63	30.9922	0.74
				H64	31.0808	0.66
				H65	26.4437	4.90

Citrinalin A (**1**) H^+ form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.633327 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.273297	0.173135	-0.069519
2	6	-0.102001	-1.369894	-0.244596
3	7	1.233127	-1.648208	-0.226374
4	6	6.203937	-0.027692	0.007685
5	6	5.706123	-1.304771	-0.690320
6	6	4.240490	-1.590522	-0.437377
7	6	3.396278	-0.403231	-0.263363
8	6	3.966332	0.895517	-0.255497
9	6	3.148611	2.035744	-0.214960
10	6	1.759180	1.906103	-0.155114
11	6	1.167739	0.640223	-0.120217
12	6	1.999057	-0.481351	-0.187065
13	6	-1.081044	0.483135	1.278302
14	6	-2.509836	0.170888	0.764275
15	6	-3.781990	0.336520	1.586624
16	6	-4.920610	-0.436499	0.892412
17	6	-4.896737	-1.975921	1.009648
18	6	-5.445138	-2.532318	-0.333142
19	6	-5.883693	-1.299301	-1.136578
20	7	-4.990160	-0.187376	-0.634367
21	6	-3.675915	-0.106543	-1.400523
22	6	-2.631871	0.744276	-0.670994
23	6	-1.192922	0.686770	-1.226719
24	6	6.241617	-0.180744	1.533159
25	6	7.559247	0.410609	-0.538158
26	6	-0.884211	1.927831	1.774919
27	6	-0.694865	-0.463413	2.430669
28	7	-3.145149	2.225821	-0.701997
29	8	-1.007895	-2.186433	-0.399988
30	8	3.780391	-2.732940	-0.439902
31	8	5.299297	1.089195	-0.318249
32	8	-2.351369	3.142710	-0.787680
33	8	-4.373129	2.393933	-0.628168
34	1	1.656872	-2.565551	-0.339625
35	1	5.825705	-1.199176	-1.778167
36	1	6.296870	-2.171963	-0.383540
37	1	3.618908	3.012313	-0.228892
38	1	1.151923	2.805593	-0.136283
39	1	-2.441076	-0.900601	0.544409
40	1	-3.656445	-0.103673	2.581624
41	1	-4.062918	1.383274	1.734934
42	1	-5.886759	-0.060735	1.242741
43	1	-5.510727	-2.277855	1.861437
44	1	-3.885517	-2.346412	1.194571
45	1	-4.668908	-3.087258	-0.866399
46	1	-6.287840	-3.212572	-0.195127
47	1	-6.910417	-1.002967	-0.907640
48	1	-5.777682	-1.391457	-2.219027
49	1	-3.268228	-1.115046	-1.490397
50	1	-3.927724	0.272586	-2.394315
51	1	-1.133591	0.032306	-2.100752
52	1	-0.882249	1.681719	-1.542421
53	1	6.557953	0.757797	1.996025
54	1	6.955863	-0.961578	1.811850
55	1	5.265697	-0.456813	1.944025
56	1	7.879293	1.340323	-0.059819
57	1	7.507876	0.575787	-1.617945
58	1	8.311638	-0.357944	-0.337518
59	1	-1.605426	2.146672	2.570307
60	1	-1.004704	2.683516	0.998887

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      61          1             0.113573    2.045336    2.205085
      62          1            -1.229128   -0.188249    3.346040
      63          1             0.374416   -0.378494    2.648557
      64          1            -0.915939   -1.512107    2.212070
      65          1            -5.411272    0.738535   -0.764941
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	119.7353	63.41		H34	21.9042	9.05
C2	-5.0505	181.88		H35	28.6332	2.90
C4	98.9252	83.17		H36	29.0008	2.56
C5	136.675	47.33		H37	24.6483	6.54
C6	-16.8575	193.09		H38	23.6731	7.43
C7	77.6449	103.37		H39	27.4242	4.00
C8	19.2919	158.77		H40	29.7198	1.90
C9	71.4805	109.22		H41	29.589	2.02
C10	46.9582	132.50		H42	27.2433	4.17
C11	64	116.32		H43	29.3146	2.27
C12	36.2881	142.63		H44	29.4507	2.15
C13	133.4698	50.37		H45	29.237	2.35
C14	134.7593	49.14		H46	29.3449	2.25
C15	162.7072	22.61		H47	28.0538	3.43
C16	114.9185	67.98		H48	28.2186	3.28
C17	158.3201	26.78		H49	27.8633	3.60
C18	162.662	22.65		H50	27.9226	3.55
C19	128.1231	55.45		H51	29.484	2.12
C21	125.1779	58.24		H52	28.0275	3.45
C22	81.7701	99.45		H53	30.5299	1.16
C23	142.8094	41.50		H54	30.6398	1.06
C24	163.676	21.69		H55	29.9085	1.73
C25	157.4767	27.58		H56	30.0609	1.59
C26	168.1224	17.47		H57	30.1773	1.49
C27	164.5088	20.90		H58	30.3321	1.34
				H59	30.9257	0.80
				H60	30.2019	1.46
				H61	31.0302	0.71
				H62	30.7747	0.94
				H63	30.9965	0.74
				H64	30.9751	0.76
				H65	23.7139	7.40

Citrinalin A (**1**) H^+ form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.633211 H (rel E = 0.07 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.269472	0.168024	0.036978
2	6	-0.091342	-1.372203	-0.155594
3	7	1.240892	-1.653532	-0.074482
4	6	6.201040	-0.012451	-0.316030
5	6	5.728241	-1.340787	0.299674
6	6	4.255495	-1.609044	0.070957
7	6	3.404249	-0.413904	0.051308
8	6	3.975089	0.883367	0.099994
9	6	3.157916	2.024160	0.130699
10	6	1.767099	1.896976	0.116219
11	6	1.172838	0.632691	0.070232
12	6	2.005237	-0.489078	0.023117
13	6	-1.144245	0.455174	1.348329
14	6	-2.544766	0.154288	0.756741
15	6	-3.856372	0.302940	1.517983
16	6	-4.960119	-0.450724	0.750497
17	6	-4.942837	-1.992178	0.828647
18	6	-5.443162	-2.511766	-0.547460
19	6	-5.829737	-1.255995	-1.343231
20	7	-4.954864	-0.163485	-0.770672
21	6	-3.603994	-0.073512	-1.468861
22	6	-2.594225	0.757419	-0.670772
23	6	-1.129328	0.704708	-1.155376
24	6	7.576042	0.385176	0.211038
25	6	6.180961	-0.048623	-1.849068
26	6	-0.972975	1.890352	1.880202
27	6	-0.817835	-0.512328	2.501569
28	7	-3.100501	2.241700	-0.698059
29	8	-0.988901	-2.183993	-0.372151
30	8	3.797877	-2.747089	-0.037372
31	8	5.309952	1.074660	0.126905
32	8	-2.300901	3.156743	-0.734980
33	8	-4.330034	2.413624	-0.673821
34	1	1.667534	-2.570758	-0.175650
35	1	6.309583	-2.179853	-0.091342
36	1	5.882410	-1.315173	1.387933
37	1	3.629766	2.999807	0.152835
38	1	1.161478	2.797644	0.124396
39	1	-2.463907	-0.912257	0.517758
40	1	-3.780823	-0.161376	2.507128
41	1	-4.143076	1.346485	1.677500
42	1	-5.942111	-0.082440	1.062833
43	1	-3.939361	-2.369657	1.039782
44	1	-5.587179	-2.314936	1.649801
45	1	-4.654454	-3.068733	-1.059686
46	1	-6.301433	-3.180670	-0.458592
47	1	-5.668542	-1.324436	-2.420594
48	1	-6.864589	-0.955645	-1.161177
49	1	-3.196122	-1.081869	-1.559783
50	1	-3.804384	0.327317	-2.465889
51	1	-1.028891	0.064722	-2.036390
52	1	-0.800612	1.703922	-1.437491
53	1	7.879361	1.349157	-0.206547
54	1	8.319578	-0.364642	-0.075221
55	1	7.564874	0.467601	1.301421
56	1	6.481121	0.922719	-2.251012
57	1	5.189442	-0.293197	-2.242406
58	1	6.882046	-0.805560	-2.213905

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      59          1            -1.734162    2.095730    2.641124
      60          1            -1.053110    2.660476    1.113083
      61          1             0.001217    1.998784    2.363277
      62          1            -1.399149   -0.253294    3.392652
      63          1             0.238633   -0.432089    2.776160
      64          1            -1.027276   -1.556818    2.253470
      65          1            -5.363293    0.768608   -0.898379
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	119.7716	63.37		H34	21.9275	9.03
C2	-5.0335	181.86		H35	29.0272	2.54
C4	98.8253	83.26		H36	28.5976	2.93
C5	136.6218	47.38		H37	24.6377	6.55
C6	-16.9182	193.14		H38	23.6803	7.43
C7	78.3688	102.68		H39	27.4224	4.00
C8	19.5695	158.50		H40	29.749	1.88
C9	71.1413	109.54		H41	29.5946	2.02
C10	47.0381	132.43		H42	27.2481	4.16
C11	63.8707	116.45		H43	29.454	2.15
C12	36.336	142.59		H44	29.3178	2.27
C13	133.3718	50.46		H45	29.2435	2.34
C14	135.1995	48.73		H46	29.3289	2.26
C15	162.8486	22.48		H47	28.2009	3.29
C16	114.8943	68.00		H48	28.0227	3.46
C17	158.2685	26.83		H49	27.882	3.58
C18	162.7604	22.56		H50	27.9333	3.54
C19	128.1124	55.46		H51	29.4665	2.14
C21	125.2381	58.18		H52	27.9998	3.48
C22	81.5406	99.67		H53	30.061	1.59
C23	142.9899	41.33		H54	30.3328	1.34
C24	157.5335	27.52		H55	30.1552	1.51
C25	163.6613	21.71		H56	30.5349	1.16
C26	167.9611	17.62		H57	30.0046	1.64
C27	165.0334	20.40		H58	30.6741	1.03
				H59	30.9535	0.78
				H60	30.1685	1.49
				H61	31.0014	0.73
				H62	30.8006	0.92
				H63	31.0525	0.69
				H64	31.0296	0.71
				H65	23.68	7.42

Citrinalin A (**1**) H^+ form, conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.623463 H (rel E = 6.19 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.281852	0.249970	-0.139635
2	6	-0.117399	-1.269972	-0.464314
3	7	1.212170	-1.563822	-0.434385
4	6	6.186406	-0.046236	0.149998
5	6	5.701987	-1.233012	-0.700361
6	6	4.225619	-1.524712	-0.532265
7	6	3.387438	-0.351431	-0.260766
8	6	3.969084	0.930841	-0.091573
9	6	3.160812	2.071082	0.041380
10	6	1.769226	1.954767	0.036069
11	6	1.164869	0.699845	-0.085137
12	6	1.987919	-0.417807	-0.242998
13	6	-1.150063	0.445685	1.189939
14	6	-2.556965	0.163825	0.597527
15	6	-3.854388	0.354091	1.375038
16	6	-5.077536	-0.095267	0.525083
17	6	-5.904884	-1.234280	1.126288
18	6	-5.117491	-2.508751	0.778551
19	6	-4.563484	-2.252750	-0.631588
20	7	-4.668909	-0.727580	-0.851811
21	6	-3.504905	-0.127950	-1.667971
22	6	-2.618150	0.783143	-0.825574
23	6	-1.140900	0.904930	-1.265213
24	6	6.166726	-0.364128	1.650116
25	6	7.564611	0.430204	-0.297590
26	6	-0.984192	1.849378	1.799573
27	6	-0.799435	-0.585231	2.279622
28	7	-3.286625	2.196372	-0.832134
29	8	-1.022074	-2.063127	-0.728616
30	8	3.754099	-2.653594	-0.674258
31	8	5.304917	1.112028	-0.083776
32	8	-2.612280	3.177427	-0.565265
33	8	-4.490880	2.235672	-1.099866
34	1	1.631720	-2.470268	-0.625914
35	1	5.862432	-1.010706	-1.765076
36	1	6.273021	-2.136236	-0.469742
37	1	3.640459	3.037186	0.149335
38	1	1.170724	2.855457	0.128655
39	1	-2.496536	-0.904573	0.368982
40	1	-3.815847	-0.235535	2.296016
41	1	-4.006164	1.397217	1.670713
42	1	-5.685124	0.768508	0.264548
43	1	-6.903217	-1.259380	0.673253
44	1	-6.041561	-1.095338	2.201495
45	1	-4.293125	-2.659432	1.481455
46	1	-5.740638	-3.404864	0.808745
47	1	-5.148934	-2.730519	-1.419873
48	1	-3.517751	-2.538508	-0.743676
49	1	-2.899103	-0.971491	-1.997348
50	1	-3.935566	0.379706	-2.529737
51	1	-0.962141	0.440369	-2.238748
52	1	-0.882335	1.960017	-1.352852
53	1	6.474447	0.514424	2.223290
54	1	6.862940	-1.179927	1.867589
55	1	5.173840	-0.670234	1.993546
56	1	7.877258	1.297656	0.290156
57	1	7.553317	0.713203	-1.353870
58	1	8.301543	-0.366121	-0.157032

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     59          1            -1.717094    1.993462    2.600927
     60          1            -1.117188    2.658361    1.081752
     61          1             0.006026    1.946983    2.251180
     62          1            -1.386748   -0.399553    3.184948
     63          1             0.254907   -0.496921    2.559735
     64          1            -0.981790   -1.616656    1.963370
     65          1            -5.496802   -0.575737   -1.428464
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	117.8477	65.20		H34	21.8421	9.11
C2	-5.1868	182.01		H35	28.6439	2.89
C4	98.8969	83.19		H36	28.9835	2.58
C5	136.8847	47.13		H37	24.6249	6.56
C6	-16.8998	193.13		H38	23.7349	7.38
C7	77.2945	103.70		H39	27.7777	3.68
C8	19.0105	159.03		H40	29.9938	1.65
C9	71.4667	109.23		H41	29.8781	1.76
C10	46.8623	132.59		H42	26.8183	4.56
C11	64.3697	115.97		H43	29.432	2.17
C12	36.4265	142.50		H44	29.574	2.04
C13	133.5717	50.27		H45	29.3278	2.26
C14	130.974	52.74		H46	29.4271	2.17
C15	160.4934	24.71		H47	27.5975	3.84
C16	113.8041	69.04		H48	27.6259	3.82
C17	149.8246	34.84		H49	27.3098	4.11
C18	160.923	24.31		H50	27.1448	4.26
C19	121.6389	61.60		H51	29.4585	2.14
C21	120.6853	62.51		H52	28.1339	3.35
C22	82.8616	98.42		H53	30.5093	1.18
C23	141.2152	43.02		H54	30.5801	1.12
C24	163.8799	21.50		H55	29.9465	1.70
C25	157.4873	27.57		H56	30.041	1.61
C26	168.4912	17.12		H57	30.1924	1.47
C27	164.5148	20.90		H58	30.3147	1.36
				H59	30.7784	0.94
				H60	29.7276	1.90
				H61	30.9048	0.82
				H62	30.6289	1.07
				H63	30.9562	0.77
				H64	30.9824	0.75
				H65	26.0176	5.29

Citrinalin A (**1**) H^+ form, conformer 6

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.623063 H (rel E = 6.44 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.278093	0.243092	-0.037165
2	6	-0.109966	-1.272806	-0.379110
3	7	1.213319	-1.580067	-0.284116
4	6	6.198240	-0.007038	-0.165991
5	6	5.685456	-1.384978	0.286993
6	6	4.219297	-1.602716	-0.022094
7	6	3.385526	-0.397293	0.053670
8	6	3.970413	0.877540	0.261751
9	6	3.166425	2.021866	0.384227
10	6	1.775812	1.920389	0.304493
11	6	1.167792	0.677734	0.102367
12	6	1.988084	-0.444853	-0.033993
13	6	-1.210669	0.422618	1.251470
14	6	-2.587694	0.159868	0.585787
15	6	-3.921522	0.347158	1.298973
16	6	-5.101709	-0.084951	0.382019
17	6	-5.961630	-1.229809	0.923046
18	6	-5.162559	-2.502061	0.594485
19	6	-4.538688	-2.226503	-0.782441
20	7	-4.626569	-0.697462	-0.982639
21	6	-3.420983	-0.090604	-1.729747
22	6	-2.573850	0.802349	-0.829172
23	6	-1.075492	0.925083	-1.191073
24	6	7.557590	0.308403	0.449586
25	6	6.235039	0.121113	-1.693842
26	6	-1.068712	1.814392	1.893311
27	6	-0.919240	-0.628690	2.339398
28	7	-3.236071	2.218570	-0.845694
29	8	-1.005725	-2.052391	-0.706844
30	8	3.750289	-2.714787	-0.266594
31	8	5.305255	1.042062	0.358524
32	8	-2.572962	3.191595	-0.526450
33	8	-4.424593	2.268228	-1.174927
34	1	1.633205	-2.488534	-0.464175
35	1	6.270519	-2.187661	-0.169381
36	1	5.798671	-1.476996	1.376647
37	1	3.649145	2.981719	0.528136
38	1	1.182073	2.825120	0.387093
39	1	-2.522940	-0.905083	0.343523
40	1	-3.931881	-0.254567	2.212892
41	1	-4.082958	1.387095	1.600277
42	1	-5.692920	0.785010	0.104797
43	1	-6.936166	-1.243434	0.420416
44	1	-6.151241	-1.107280	1.992163
45	1	-4.374805	-2.667800	1.335081
46	1	-5.789921	-3.395626	0.579281
47	1	-5.087237	-2.688455	-1.605930
48	1	-3.489931	-2.515697	-0.847996
49	1	-2.802619	-0.931461	-2.042078
50	1	-3.806156	0.433276	-2.603214
51	1	-0.849711	0.479703	-2.163844
52	1	-0.808298	1.980488	-1.242863
53	1	7.889470	1.306199	0.149577
54	1	8.301183	-0.419167	0.110812
55	1	7.507145	0.273659	1.541508
56	1	6.562005	1.124925	-1.977531
57	1	5.256155	-0.064256	-2.146665
58	1	6.940232	-0.603506	-2.112386

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     59          1            -1.843434    1.950026    2.655927
     60          1            -1.157689    2.636491    1.183691
     61          1            -0.104227    1.897089    2.400068
     62          1            -1.547251   -0.453044    3.219068
     63          1             0.121228   -0.553174    2.670471
     64          1            -1.093920   -1.653475    1.997958
     65          1            -5.423804   -0.532360   -1.597538
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	117.7221	65.32		H34	21.8632	9.09
C2	-5.1703	181.99		H35	29.0708	2.50
C4	98.4912	83.58		H36	28.5915	2.94
C5	136.8423	47.17		H37	24.6364	6.55
C6	-17.1363	193.35		H38	23.7771	7.34
C7	78.283	102.76		H39	27.7936	3.66
C8	19.4957	158.57		H40	30.0192	1.63
C9	71.1009	109.58		H41	29.8731	1.76
C10	47.1322	132.34		H42	26.8472	4.53
C11	64.3357	116.00		H43	29.4436	2.16
C12	36.5084	142.42		H44	29.554	2.06
C13	133.2655	50.56		H45	29.3144	2.27
C14	130.8669	52.84		H46	29.4345	2.16
C15	160.4704	24.74		H47	27.5809	3.86
C16	113.7014	69.14		H48	27.5831	3.86
C17	149.8261	34.84		H49	27.2845	4.13
C18	160.855	24.37		H50	27.1108	4.29
C19	121.6166	61.62		H51	29.4326	2.17
C21	120.7766	62.42		H52	28.1082	3.38
C22	82.681	98.59		H53	30.025	1.62
C23	141.3317	42.91		H54	30.2861	1.39
C24	157.2136	27.83		H55	30.1358	1.52
C25	163.7663	21.61		H56	30.5325	1.16
C26	168.2095	17.39		H57	30.0861	1.57
C27	164.6224	20.79		H58	30.6697	1.04
				H59	30.8267	0.89
				H60	29.7187	1.90
				H61	30.8621	0.86
				H62	30.6785	1.03
				H63	30.9778	0.75
				H64	31.0277	0.71
				H65	26.0055	5.30

Citrinalin A (**1**) TFA salt form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.066764 H (rel E = 0.80 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.640616	-0.391347	-0.189372
2	6	-0.654081	1.158296	-0.350109
3	7	-1.964528	1.580785	-0.244108
4	6	-7.060685	0.446311	0.123434
5	6	-6.472609	1.700648	-0.542507
6	6	-4.973051	1.831746	-0.347776
7	6	-4.245148	0.566813	-0.252583
8	6	-4.940356	-0.670731	-0.278609
9	6	-4.245544	-1.882618	-0.318433
10	6	-2.844768	-1.892845	-0.300873
11	6	-2.127129	-0.701027	-0.221942
12	6	-2.840912	0.506157	-0.219342
13	6	0.130709	-0.780318	1.178831
14	6	1.565278	-1.012638	0.630420
15	6	2.677335	-1.533337	1.550337
16	6	3.921754	-1.927325	0.728967
17	6	5.297384	-1.477543	1.234671
18	6	6.207182	-1.500914	-0.027119
19	6	5.242204	-1.655818	-1.226220
20	7	3.897656	-1.322754	-0.658209
21	6	2.743949	-1.720684	-1.517736
22	6	1.407198	-1.734102	-0.726197
23	6	0.220268	-0.993160	-1.357534
24	6	-7.010240	0.530086	1.655340
25	6	-8.481632	0.175354	-0.364238
26	6	-0.479886	-2.019164	1.866559
27	6	0.131072	0.354771	2.224413
28	7	1.044057	-3.245484	-0.558238
29	8	0.308804	1.875998	-0.549099
30	8	-4.416360	2.931288	-0.329536
31	8	-6.297241	-0.728677	-0.304377
32	8	-0.001156	-3.667709	-1.044131
33	8	1.852264	-3.953445	0.039610
34	1	-2.279841	2.541880	-0.323715
35	1	-6.650681	1.655039	-1.626245
36	1	-6.958093	2.607252	-0.171034
37	1	-4.810460	-2.806992	-0.361407
38	1	-2.325727	-2.843828	-0.354444
39	1	1.892388	-0.013512	0.313625
40	1	2.933980	-0.729512	2.244652
41	1	2.356631	-2.404973	2.126477
42	1	3.921593	-3.010036	0.574571
43	1	5.224090	-0.465840	1.642655
44	1	5.658709	-2.140027	2.025568
45	1	6.783135	-0.576766	-0.108973
46	1	6.916936	-2.332085	-0.008401
47	1	5.454523	-0.978117	-2.055641
48	1	5.214995	-2.685679	-1.598639
49	1	2.683611	-0.983401	-2.322038
50	1	2.952322	-2.699151	-1.959529
51	1	0.625766	-0.169762	-1.951243
52	1	-0.369495	-1.634121	-2.011020
53	1	-7.399117	-0.393383	2.093460
54	1	-7.623400	1.366309	2.006157
55	1	-5.991410	0.682886	2.022901
56	1	-8.870898	-0.741614	0.087744
57	1	-8.500651	0.059878	-1.451770
58	1	-9.140416	1.004726	-0.088705

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    59          1             0.150833   -2.320397    2.708630
    60          1            -0.606457   -2.887220    1.219819
    61          1            -1.465449   -1.774208    2.271280
    62          1             0.615283    0.010355    3.143866
    63          1            -0.893946    0.638938    2.486477
    64          1             0.667191    1.241642    1.881613
    65          1             3.908168   -0.162508   -0.616913
    66          6             4.236478    3.432912   -0.124590
    67          6             3.931730    1.934281    0.177262
    68          8             4.044963    1.182589   -0.854579
    69          8             3.665778    1.609289    1.334888
    70          9             5.584256    3.608623   -0.238015
    71          9             3.680012    3.851346   -1.280894
    72          9             3.808384    4.251022    0.853528
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.7382	61.51		H34	22.3392	8.65
C2	-3.5726	180.47		H35	28.7133	2.82
C4	101.4231	80.79		H36	29.0907	2.48
C5	136.3396	47.64		H37	24.7743	6.43
C6	-16.5535	192.80		H38	23.7708	7.34
C7	77.7075	103.31		H39	28.2501	3.25
C8	19.9764	158.12		H40	29.1655	2.41
C9	73.8777	106.94		H41	29.7651	1.86
C10	46.2932	133.13		H42	27.402	4.02
C11	59.7784	120.33		H43	29.3447	2.25
C12	35.7744	143.12		H44	29.5686	2.04
C13	132.8944	50.92		H45	29.564	2.05
C14	131.4652	52.27		H46	29.6973	1.92
C15	162.7934	22.53		H47	28.284	3.22
C16	121.7646	61.48		H48	29.1604	2.42
C17	155.6062	29.35		H49	28.0163	3.46
C18	163.2107	22.13		H50	28.6713	2.86
C19	131.6124	52.13		H51	29.174	2.40
C21	125.3092	58.12		H52	28.0344	3.44
C22	81.3869	99.82		H53	30.5888	1.11
C23	138.2902	45.79		H54	30.7083	1.00
C24	163.8456	21.53		H55	29.9562	1.69
C25	157.3391	27.71		H56	30.1108	1.55
C26	166.4199	19.09		H57	30.2044	1.46
C27	162.289	23.01		H58	30.363	1.32
				H59	30.9237	0.80
				H60	31.0819	0.66
				H61	31.3353	0.43
				H62	30.7714	0.94
				H63	31.0411	0.70
				H64	30.6801	1.03
				H65	12.8575	17.32

Citrinalin A (**1**) TFA salt form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.066347 H (rel E = 1.06 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.642709	-0.400471	-0.061639
2	6	-0.664436	1.150662	-0.207498
3	7	-1.967534	1.571299	-0.029588
4	6	-7.070946	0.452300	-0.246033
5	6	-6.463073	1.683405	0.446114
6	6	-4.970988	1.820359	0.205273
7	6	-4.244551	0.556142	0.088045
8	6	-4.941898	-0.679816	0.059794
9	6	-4.250191	-1.891402	-0.021777
10	6	-2.849862	-1.902726	-0.063422
11	6	-2.128993	-0.710863	-0.025076
12	6	-2.841623	0.495943	0.024007
13	6	0.190781	-0.796916	1.267648
14	6	1.599525	-1.020393	0.653130
15	6	2.754294	-1.544635	1.517117
16	6	3.962341	-1.923776	0.635813
17	6	5.357922	-1.471327	1.081410
18	6	6.208346	-1.481223	-0.221124
19	6	5.189593	-1.630291	-1.375637
20	7	3.870871	-1.308953	-0.743936
21	6	2.681394	-1.708748	-1.551989
22	6	1.382585	-1.732665	-0.700693
23	6	0.165220	-0.991854	-1.271368
24	6	-8.478772	0.166002	0.269533
25	6	-7.060093	0.589613	-1.774822
26	6	-0.382476	-2.042911	1.974777
27	6	0.234013	0.331089	2.320412
28	7	1.032915	-3.246467	-0.526598
29	8	0.286599	1.870699	-0.450195
30	8	-4.417846	2.920768	0.161120
31	8	-6.298169	-0.737908	0.118508
32	8	-0.035755	-3.668090	-0.959047
33	8	1.873925	-3.956518	0.021513
34	1	-2.285440	2.533469	-0.077507
35	1	-6.960274	2.601599	0.122031
36	1	-6.606311	1.597045	1.532520
37	1	-4.817662	-2.814209	-0.064216
38	1	-2.334762	-2.853488	-0.149040
39	1	1.910850	-0.018367	0.329802
40	1	3.037675	-0.746113	2.207191
41	1	2.463822	-2.423476	2.098219
42	1	3.960950	-3.005288	0.472818
43	1	5.299850	-0.463338	1.500976
44	1	5.757832	-2.138670	1.849357
45	1	6.777136	-0.554539	-0.322110
46	1	6.920837	-2.310007	-0.241656
47	1	5.360269	-0.944333	-2.207867
48	1	5.150081	-2.656950	-1.755701
49	1	2.581485	-0.968421	-2.349518
50	1	2.874290	-2.684323	-2.006857
51	1	0.540983	-0.163361	-1.877588
52	1	-0.451656	-1.630547	-1.901762
53	1	-8.880795	-0.735328	-0.202301
54	1	-9.143330	1.004354	0.038689
55	1	-8.469513	0.014587	1.352781
56	1	-6.049929	0.749637	-2.163021
57	1	-7.676539	1.440998	-2.080560
58	1	-7.465583	-0.315928	-2.234702

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    59          1             0.285995   -2.343453    2.787508
    60          1            -0.530973   -2.909121    1.330107
    61          1            -1.351013   -1.806277    2.423007
    62          1             0.760504   -0.017606    3.214686
    63          1            -0.779134    0.608983    2.630761
    64          1             0.750739    1.222573    1.960301
    65          1             3.876187   -0.148624   -0.696531
    66          6             4.209447    3.443346   -0.194307
    67          6             3.925669    1.940636    0.107439
    68          8             3.994673    1.197584   -0.934465
    69          8             3.715902    1.604588    1.273461
    70          9             5.552966    3.630971   -0.336939
    71          9             3.624130    3.863058   -1.335681
    72          9             3.796449    4.252806    0.797412
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.789	61.46		H34	22.3604	8.63
C2	-3.4945	180.40		H35	29.1081	2.46
C4	100.7105	81.47		H36	28.6741	2.86
C5	136.0607	47.91		H37	24.7881	6.41
C6	-16.7472	192.98		H38	23.7816	7.33
C7	78.1574	102.88		H39	28.1847	3.31
C8	19.9973	158.10		H40	29.1766	2.40
C9	73.4467	107.35		H41	29.7771	1.85
C10	45.9746	133.44		H42	27.3934	4.03
C11	59.3994	120.69		H43	29.3953	2.20
C12	35.5881	143.30		H44	29.5577	2.05
C13	132.4462	51.34		H45	29.6033	2.01
C14	131.9122	51.85		H46	29.7065	1.92
C15	163.021	22.31		H47	28.2935	3.21
C16	121.7144	61.53		H48	29.1378	2.44
C17	155.7651	29.20		H49	28.0255	3.45
C18	163.3271	22.02		H50	28.6619	2.87
C19	131.563	52.18		H51	29.1279	2.44
C21	125.4298	58.00		H52	28.0515	3.43
C22	81.4831	99.72		H53	30.107	1.55
C23	138.4713	45.62		H54	30.3557	1.32
C24	157.1944	27.85		H55	30.2082	1.46
C25	163.6595	21.71		H56	29.9735	1.67
C26	166.0967	19.39		H57	30.7302	0.98
C27	162.4209	22.88		H58	30.5948	1.10
				H59	30.9073	0.82
				H60	31.0608	0.68
				H61	31.3115	0.45
				H62	30.8269	0.89
				H63	31.094	0.65
				H64	30.7278	0.98
				H65	12.8145	17.36

Citrinalin A (**1**) TFA salt form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.068038 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.171252	0.578979	-0.066901
2	6	-1.765801	1.846532	-0.746689
3	7	-3.131229	1.687119	-0.813247
4	6	-7.374798	-1.282529	-0.049364
5	6	-7.235394	-0.186073	-1.117807
6	6	-5.951697	0.612653	-0.987633
7	6	-4.809215	-0.128943	-0.454512
8	6	-4.952766	-1.478184	-0.037488
9	6	-3.840665	-2.231315	0.352700
10	6	-2.566696	-1.651068	0.369093
11	6	-2.394986	-0.312619	0.017755
12	6	-3.514064	0.413782	-0.406581
13	6	-0.506921	1.000249	1.340841
14	6	0.923238	1.344901	0.849458
15	6	2.043880	1.730975	1.810149
16	6	3.284086	2.178085	1.012662
17	6	3.202751	3.604051	0.407222
18	6	3.936072	3.537169	-0.957000
19	6	4.547332	2.130535	-1.000040
20	7	3.642385	1.272988	-0.156099
21	6	2.516230	0.722938	-0.989690
22	6	1.308282	0.254549	-0.169274
23	6	0.007127	0.044682	-0.959301
24	6	-7.583201	-0.696332	1.353901
25	6	-8.489131	-2.263465	-0.404670
26	6	-0.546727	-0.138170	2.381012
27	6	-1.184772	2.223090	1.989686
28	7	1.720895	-1.090631	0.508674
29	8	-1.142513	2.814166	-1.159124
30	8	-5.875352	1.785480	-1.360125
31	8	-6.158640	-2.100388	-0.035400
32	8	1.131778	-2.123304	0.200841
33	8	2.643521	-1.038002	1.315183
34	1	-3.785105	2.346772	-1.222175
35	1	-7.223661	-0.648088	-2.115201
36	1	-8.085387	0.501171	-1.088260
37	1	-3.986902	-3.266096	0.641016
38	1	-1.714957	-2.259917	0.654730
39	1	0.766541	2.212346	0.192668
40	1	1.732202	2.582703	2.425979
41	1	2.304824	0.914872	2.484253
42	1	4.162714	2.112948	1.662002
43	1	3.669071	4.317496	1.092477
44	1	2.164200	3.921910	0.276053
45	1	3.233199	3.687049	-1.782185
46	1	4.712409	4.299637	-1.058204
47	1	5.529406	2.097116	-0.521401
48	1	4.640962	1.687775	-1.992658
49	1	2.156495	1.512827	-1.655040
50	1	2.963515	-0.079807	-1.585044
51	1	0.055084	0.623115	-1.885577
52	1	-0.130761	-1.001753	-1.223106
53	1	-7.632014	-1.501904	2.091741
54	1	-8.522044	-0.134672	1.390330
55	1	-6.773927	-0.017458	1.638314
56	1	-8.549333	-3.058647	0.344046
57	1	-8.304173	-2.721291	-1.380623
58	1	-9.452377	-1.745007	-0.437902

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    59          1             0.070780    0.131736    3.243878
    60          1            -0.195568   -1.101252    2.011743
    61          1            -1.568668   -0.282153    2.742230
    62          1            -0.728339    2.429876    2.963403
    63          1            -2.246973    2.025531    2.170131
    64          1            -1.100747    3.124892    1.378209
    65          1             4.326176    0.428317    0.190542
    66          6             6.762497   -2.210075   -0.337177
    67          6             5.566474   -1.226114   -0.514744
    68          8             5.414237   -0.434331    0.473473
    69          8             4.915925   -1.276162   -1.566044
    70          9             7.940787   -1.531714   -0.414790
    71          9             6.734265   -2.828616    0.865444
    72          9             6.791401   -3.168087   -1.282402
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.1681	61.10		H34	22.2799	8.71
C2	-5.4551	182.26		H35	28.6368	2.89
C4	100.8022	81.38		H36	28.9493	2.61
C5	136.1312	47.84		H37	24.7554	6.44
C6	-16.3692	192.62		H38	23.792	7.32
C7	78.6713	102.39		H39	28.4524	3.06
C8	19.4782	158.59		H40	30.0233	1.63
C9	73.3171	107.48		H41	28.9489	2.61
C10	46.2495	133.17		H42	27.6381	3.81
C11	60.0362	120.09		H43	29.4147	2.18
C12	36.3092	142.61		H44	29.6039	2.01
C13	132.4011	51.38		H45	29.5452	2.06
C14	135.8915	48.07		H46	29.7397	1.89
C15	163.4035	21.95		H47	28.4324	3.08
C16	123.7582	59.59		H48	28.6335	2.90
C17	155.527	29.43		H49	28.7957	2.75
C18	164.3403	21.06		H50	26.6725	4.69
C19	129.0138	54.60		H51	29.4437	2.16
C21	129.7775	53.87		H52	27.8224	3.64
C22	86.0422	95.40		H53	30.5449	1.15
C23	141.5531	42.69		H54	30.6509	1.05
C24	163.9631	21.42		H55	30.0936	1.56
C25	157.4875	27.57		H56	30.1007	1.56
C26	166.7347	18.79		H57	30.1932	1.47
C27	163.6391	21.73		H58	30.3751	1.30
				H59	31.0973	0.64
				H60	31.12	0.62
				H61	31.2537	0.50
				H62	30.778	0.94
				H63	31.0018	0.73
				H64	30.8288	0.89
				H65	13.6699	16.58

Citrinalin A (**1**) TFA salt form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.067742 H (rel E = 0.19 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.183772	0.579496	0.076634
2	6	-1.753490	1.801646	-0.701752
3	7	-3.123608	1.679080	-0.732769
4	6	-7.336784	-1.401089	-0.398150
5	6	-7.354596	0.135327	-0.332085
6	6	-5.999563	0.757110	-0.611310
7	6	-4.851638	-0.032070	-0.165107
8	6	-5.029273	-1.337657	0.362037
9	6	-3.936336	-2.081883	0.818212
10	6	-2.645323	-1.541911	0.770416
11	6	-2.433834	-0.257152	0.270954
12	6	-3.536887	0.460601	-0.206576
13	6	-0.464933	1.100262	1.420223
14	6	0.948224	1.384503	0.848800
15	6	2.107198	1.847113	1.726478
16	6	3.306676	2.227798	0.837699
17	6	3.189708	3.601841	0.124592
18	6	3.827712	3.419018	-1.275950
19	6	4.461373	2.023540	-1.231055
20	7	3.612565	1.231399	-0.271871
21	6	2.452678	0.602083	-0.998265
22	6	1.287537	0.205368	-0.083346
23	6	-0.048710	-0.076098	-0.791178
24	6	-8.607723	-1.995705	0.202377
25	6	-7.109768	-1.912456	-1.827374
26	6	-0.473685	0.047055	2.546579
27	6	-1.106270	2.379018	1.993647
28	7	1.741359	-1.073322	0.690421
29	8	-1.111298	2.709443	-1.210693
30	8	-5.887418	1.868547	-1.132861
31	8	-6.256645	-1.909998	0.452970
32	8	1.142049	-2.130127	0.511275
33	8	2.708080	-0.947340	1.434716
34	1	-3.765570	2.321984	-1.184808
35	1	-8.085942	0.549017	-1.031673
36	1	-7.650253	0.452632	0.678024
37	1	-4.108571	-3.084517	1.192763
38	1	-1.810248	-2.147813	1.107121
39	1	0.772689	2.190749	0.123093
40	1	1.818926	2.746670	2.282757
41	1	2.401079	1.090017	2.453696
42	1	4.216191	2.214444	1.446206
43	1	2.146311	3.919458	0.039512
44	1	3.706294	4.362776	0.716446
45	1	3.065120	3.478749	-2.058825
46	1	4.578342	4.180005	-1.503287
47	1	4.514278	1.496786	-2.184810
48	1	5.465908	2.044804	-0.800490
49	1	2.055102	1.328102	-1.712878
50	1	2.879814	-0.247616	-1.541079
51	1	-0.033078	0.379884	-1.784337
52	1	-0.208202	-1.145111	-0.916138
53	1	-8.562101	-3.088352	0.182853
54	1	-9.482567	-1.674779	-0.371510
55	1	-8.732198	-1.673105	1.240066
56	1	-7.062054	-3.004920	-1.830413
57	1	-6.180935	-1.527060	-2.258269
58	1	-7.935791	-1.598884	-2.473604

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    59          1             0.181806    0.375887    3.359625
    60          1            -0.146141   -0.945262    2.237407
    61          1            -1.480742   -0.056165    2.959575
    62          1            -0.614062    2.654376    2.932239
    63          1            -2.163830    2.211181    2.224418
    64          1            -1.033026    3.229826    1.311422
    65          1             4.320205    0.425126    0.103646
    66          6             6.780581   -2.210110   -0.374429
    67          6             5.560705   -1.256293   -0.555694
    68          8             5.437788   -0.411856    0.391483
    69          8             4.863254   -1.379826   -1.570687
    70          9             7.944038   -1.509626   -0.467678
    71          9             6.770442   -2.812414    0.837408
    72          9             6.825045   -3.180835   -1.306074
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.9135	61.34		H34	22.2422	8.74
C2	-5.1324	181.96		H35	29.1761	2.40
C4	100.4709	81.70		H36	28.6879	2.85
C5	136.3873	47.60		H37	24.7365	6.46
C6	-16.7178	192.95		H38	23.7316	7.38
C7	78.4146	102.64		H39	28.248	3.25
C8	19.6971	158.38		H40	30.0205	1.63
C9	72.2878	108.45		H41	28.9862	2.57
C10	46.4306	133.00		H42	27.5596	3.88
C11	59.9776	120.14		H43	29.6266	1.99
C12	36.7933	142.15		H44	29.3459	2.25
C13	132.8344	50.97		H45	29.5283	2.08
C14	135.44	48.50		H46	29.7117	1.91
C15	162.5472	22.76		H47	28.5626	2.96
C16	123.8819	59.47		H48	28.4741	3.04
C17	155.1727	29.76		H49	28.7833	2.76
C18	164.1907	21.20		H50	26.6157	4.74
C19	128.763	54.84		H51	29.409	2.19
C21	129.3879	54.24		H52	27.7603	3.70
C22	85.8783	95.55		H53	30.1124	1.54
C23	141.9218	42.34		H54	30.3495	1.33
C24	157.6958	27.37		H55	30.2135	1.45
C25	163.8332	21.54		H56	30.5778	1.12
C26	166.9748	18.56		H57	30.0295	1.62
C27	163.8042	21.57		H58	30.6424	1.06
				H59	31.0689	0.67
				H60	30.998	0.73
				H61	31.1869	0.56
				H62	30.8575	0.86
				H63	31.0686	0.67
				H64	30.8448	0.88
				H65	13.8745	16.39

Citrinalin A (**1**) TFA salt form, conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.06748 H (rel E = 0.35 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.210590	0.236463	0.002693
2	6	-1.378939	-0.286819	-1.455007
3	7	-2.714421	-0.545313	-1.657470
4	6	-7.604451	-0.797539	0.191748
5	6	-7.039533	-1.645655	-0.959974
6	6	-5.641581	-1.230109	-1.376885
7	6	-4.806868	-0.690032	-0.303441
8	6	-5.330876	-0.516237	1.004054
9	6	-4.505038	-0.114389	2.059615
10	6	-3.149044	0.150516	1.832706
11	6	-2.609680	0.036796	0.551801
12	6	-3.444985	-0.398079	-0.484194
13	6	-0.673040	1.749297	-0.039861
14	6	0.846371	1.466022	-0.176655
15	6	1.875185	2.595012	-0.212298
16	6	3.326275	2.036156	-0.287926
17	6	4.119024	2.502445	-1.515508
18	6	3.624781	1.580429	-2.651321
19	6	3.305369	0.239407	-1.960726
20	7	3.385327	0.531247	-0.473603
21	6	2.529437	-0.331451	0.406471
22	6	1.172096	0.306110	0.786738
23	6	-0.076902	-0.592380	0.703584
24	6	-7.893664	0.645196	-0.244548
25	6	-8.844867	-1.446174	0.800106
26	6	-1.049792	2.543853	1.226662
27	6	-1.205129	2.543853	-1.248765
28	7	1.351167	0.809188	2.261156
29	8	-0.492889	-0.452535	-2.281957
30	8	-5.230741	-1.392231	-2.527769
31	8	-6.633257	-0.764312	1.290289
32	8	0.606259	0.392431	3.143114
33	8	2.272892	1.596556	2.459582
34	1	-3.123152	-0.915766	-2.509558
35	1	-6.978807	-2.696872	-0.644214
36	1	-7.696161	-1.606757	-1.833402
37	1	-4.936144	-0.012805	3.049107
38	1	-2.524855	0.443754	2.670840
39	1	0.916383	0.962948	-1.147318
40	1	1.674542	3.213545	-1.093986
41	1	1.798490	3.245851	0.661967
42	1	3.849846	2.245771	0.644720
43	1	5.188049	2.349519	-1.337555
44	1	3.957591	3.563650	-1.724123
45	1	2.722157	1.988724	-3.117749
46	1	4.372999	1.462559	-3.438570
47	1	4.037375	-0.545689	-2.162385
48	1	2.314521	-0.140766	-2.215465
49	1	2.372475	-1.266775	-0.130023
50	1	3.120295	-0.571090	1.292228
51	1	0.153414	-1.484979	0.117794
52	1	-0.386816	-0.917428	1.694991
53	1	-8.254261	1.228097	0.607518
54	1	-8.663820	0.653831	-1.022351
55	1	-7.003493	1.137554	-0.646944
56	1	-9.210259	-0.851533	1.642278
57	1	-8.616597	-2.453133	1.160861
58	1	-9.640918	-1.514163	0.052259

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    59          1          -0.513308    3.498224    1.236108
    60          1          -0.829728    2.028592    2.161616
    61          1          -2.118952    2.772657    1.223027
    62          1          -0.851422    3.579159   -1.202545
    63          1          -2.299933    2.577579   -1.236307
    64          1          -0.885139    2.121034   -2.204740
    65          1           4.459784    0.254359   -0.185737
    66          6           7.393599   -1.786506    0.329635
    67          6           5.933877   -1.328014    0.030633
    68          8           5.771283   -0.062922    0.147706
    69          8           5.101029   -2.175119   -0.299866
    70          9           8.230663   -1.364615   -0.655506
    71          9           7.852305   -1.272415    1.495237
    72          9           7.507977   -3.125134    0.407187
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.4123	61.82		H34	22.2283	8.75
C2	-4.87	181.71		H35	28.6866	2.85
C4	101.2389	80.97		H36	29.0281	2.54
C5	136.1742	47.80		H37	24.7129	6.48
C6	-16.4544	192.70		H38	23.876	7.25
C7	78.8732	102.20		H39	28.1298	3.36
C8	19.9474	158.15		H40	30.1602	1.50
C9	72.9056	107.87		H41	29.5546	2.05
C10	46.6416	132.80		H42	27.2316	4.18
C11	61.0642	119.11		H43	29.45	2.15
C12	36.5129	142.42		H44	29.8972	1.74
C13	133.4248	50.41		H45	29.4497	2.15
C14	133.8784	49.98		H46	29.6839	1.94
C15	161.6768	23.59		H47	27.8192	3.64
C16	125.9356	57.52		H48	28.2473	3.25
C17	150.9696	33.75		H49	27.9224	3.55
C18	162.6107	22.70		H50	28.0921	3.39
C19	129.2836	54.34		H51	29.2771	2.31
C21	125.9472	57.51		H52	27.6616	3.79
C22	84.3777	96.98		H53	30.5458	1.15
C23	140.1333	44.04		H54	30.6169	1.08
C24	163.715	21.65		H55	29.9319	1.71
C25	157.2757	27.77		H56	30.0728	1.58
C26	168.0014	17.59		H57	30.2074	1.46
C27	164.2448	21.15		H58	30.3518	1.33
				H59	31.0322	0.70
				H60	30.8373	0.88
				H61	31.3252	0.44
				H62	30.7891	0.93
				H63	31.0379	0.70
				H64	30.8852	0.84
				H65	13.3458	16.88

Citrinalin A (**1**) TFA salt form, conformer 6

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.067971 H (rel E = 0.04 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.221503	0.419750	0.029389
2	6	-1.391752	0.124213	-1.491357
3	7	-2.731597	-0.065169	-1.736072
4	6	-7.476808	-1.269103	0.096033
5	6	-7.193223	-0.630939	-1.274188
6	6	-5.712372	-0.538697	-1.589723
7	6	-4.844136	-0.324057	-0.431374
8	6	-5.373402	-0.341835	0.885075
9	6	-4.551272	-0.103155	1.991572
10	6	-3.188250	0.162949	1.813674
11	6	-2.634092	0.196800	0.534228
12	6	-3.469050	-0.067895	-0.557985
13	6	-0.618209	1.895493	0.215635
14	6	0.889650	1.567975	0.051889
15	6	1.965641	2.640949	0.205618
16	6	3.392013	2.038344	0.040955
17	6	4.206436	2.653747	-1.103711
18	6	3.672251	1.942024	-2.365096
19	6	3.305663	0.522170	-1.889766
20	7	3.386157	0.577791	-0.374347
21	6	2.483968	-0.371070	0.359635
22	6	1.151926	0.260315	0.828135
23	6	-0.134726	-0.556589	0.605230
24	6	-8.926765	-1.051328	0.519499
25	6	-7.111390	-2.759462	0.122573
26	6	-0.977745	2.513312	1.581683
27	6	-1.097795	2.881403	-0.867952
28	7	1.337875	0.525599	2.362417
29	8	-0.503150	0.055023	-2.329361
30	8	-5.286560	-0.592956	-2.745117
31	8	-6.687750	-0.580134	1.122992
32	8	0.549853	0.038174	3.167320
33	8	2.307150	1.209264	2.681858
34	1	-3.142717	-0.292808	-2.635696
35	1	-7.693195	-1.182837	-2.074662
36	1	-7.587545	0.395041	-1.286056
37	1	-4.987495	-0.144460	2.983165
38	1	-2.566919	0.320625	2.689462
39	1	0.955644	1.218252	-0.984074
40	1	1.801876	3.405794	-0.561440
41	1	1.907292	3.140141	1.175708
42	1	3.921888	2.080651	0.992518
43	1	5.267472	2.427874	-0.958191
44	1	4.092928	3.740649	-1.143915
45	1	2.783424	2.451902	-2.751258
46	1	4.411371	1.922026	-3.169298
47	1	4.013725	-0.245274	-2.209613
48	1	2.305291	0.216420	-2.201114
49	1	2.293558	-1.204487	-0.315972
50	1	3.054517	-0.769746	1.200061
51	1	0.060898	-1.362739	-0.105253
52	1	-0.472450	-1.009675	1.535520
53	1	-9.100984	-1.477334	1.511803
54	1	-9.604040	-1.536896	-0.189816
55	1	-9.163504	0.015946	0.555004
56	1	-7.286307	-3.169581	1.120964
57	1	-6.063057	-2.928636	-0.140243
58	1	-7.730392	-3.310286	-0.592660

59	1	-0.407693	3.436241	1.730080
60	1	-0.783375	1.861569	2.433335
61	1	-2.037914	2.779362	1.606796
62	1	-0.710237	3.884397	-0.661392
63	1	-2.190854	2.952959	-0.866510
64	1	-0.772979	2.594565	-1.871459
65	1	4.444600	0.209653	-0.131671
66	6	7.273237	-2.026491	0.046894
67	6	5.838249	-1.458341	-0.173269
68	8	5.737708	-0.220540	0.140421
69	8	4.964049	-2.203883	-0.620864
70	9	8.163802	-1.404549	-0.769368
71	9	7.691003	-1.833094	1.321627
72	9	7.350805	-3.345618	-0.206245

Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.0263	62.18		H34	22.2038	8.78
C2	-5.2028	182.02		H35	29.0584	2.51
C4	98.7544	83.33		H36	28.6958	2.84
C5	136.5522	47.44		H37	24.7837	6.42
C6	-16.4993	192.75		H38	23.7711	7.34
C7	78.7664	102.30		H39	28.1732	3.32
C8	19.8393	158.25		H40	30.2247	1.44
C9	72.6797	108.08		H41	29.6254	1.99
C10	46.5988	132.84		H42	27.1823	4.22
C11	61.0845	119.09		H43	29.5113	2.09
C12	36.0847	142.82		H44	29.8112	1.82
C13	133.3305	50.50		H45	29.4271	2.17
C14	133.4825	50.36		H46	29.7034	1.92
C15	161.8999	23.38		H47	27.8439	3.62
C16	125.8351	57.62		H48	28.2692	3.23
C17	150.7924	33.92		H49	27.9543	3.52
C18	162.6187	22.70		H50	28.048	3.43
C19	129.2515	54.37		H51	29.3151	2.27
C21	125.9299	57.53		H52	27.6817	3.77
C22	84.4344	96.92		H53	29.9835	1.66
C23	139.7856	44.37		H54	30.3001	1.37
C24	156.5322	28.47		H55	30.2333	1.43
C25	163.7016	21.67		H56	30.6279	1.07
C26	168.2336	17.36		H57	29.9831	1.66
C27	163.8259	21.55		H58	30.5978	1.10
				H59	30.9786	0.75
				H60	30.8171	0.90
				H61	31.2344	0.52
				H62	30.7698	0.94
				H63	31.071	0.67
				H64	30.922	0.80
				H65	13.3371	16.88

Revised Citrinalin B (**2**) neutral form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.256505 H (rel E = 4.38 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.771543 H (rel E = 5.13 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.331006	0.362018	0.163852
2	6	-0.178444	1.823439	0.311833
3	7	-1.558733	1.783522	0.390505
4	6	-6.022850	-0.819827	-0.398202
5	6	-5.867340	0.418166	0.500464
6	6	-4.488257	1.046006	0.413444
7	6	-3.392889	0.106758	0.177539
8	6	-3.656098	-1.265132	-0.073790
9	6	-2.610281	-2.172384	-0.260170
10	6	-1.279421	-1.737224	-0.188730
11	6	-0.978135	-0.402246	0.071233
12	6	-2.043210	0.498302	0.220777
13	6	1.323363	0.006904	1.360719
14	6	2.664330	0.683224	0.886619
15	6	4.000787	0.109822	1.399323
16	6	4.459306	-1.200392	0.732401
17	6	5.978010	-1.433060	0.671428
18	6	6.075852	-2.549235	-0.379344
19	6	4.973917	-2.176330	-1.400354
20	7	3.994385	-1.318214	-0.679476
21	6	3.793084	-0.032882	-1.334441
22	6	2.626378	0.737599	-0.665132
23	6	1.239729	0.232359	-1.082987
24	6	-7.283349	-1.605009	-0.045160
25	6	-6.001068	-0.453345	-1.888657
26	6	1.426501	-1.520158	1.535767
27	6	0.869333	0.592496	2.711696
28	7	2.860991	2.188637	-1.166778
29	8	0.493447	2.838986	0.361555
30	8	-4.314729	2.254841	0.581245
31	8	-4.924050	-1.751678	-0.132468
32	8	2.389248	2.494509	-2.258711
33	8	3.602736	2.904217	-0.501939
34	1	-2.165095	2.591331	0.483231
35	1	-6.616996	1.175981	0.257068
36	1	-6.022083	0.128272	1.549451
37	1	-2.849374	-3.208767	-0.470176
38	1	-0.486840	-2.460027	-0.352621
39	1	2.618321	1.718675	1.228902
40	1	4.759241	0.882550	1.227494
41	1	3.958465	-0.033590	2.485175
42	1	4.026500	-2.049577	1.275213
43	1	6.489277	-0.524751	0.325814
44	1	6.406646	-1.710803	1.640122
45	1	5.858213	-3.518757	0.083592
46	1	7.061570	-2.623405	-0.848028
47	1	5.408285	-1.620941	-2.242373
48	1	4.480584	-3.063359	-1.814571
49	1	4.697691	0.601468	-1.320612
50	1	3.538120	-0.208114	-2.384311
51	1	0.857797	0.762232	-1.957009
52	1	1.333250	-0.826204	-1.342724
53	1	-7.359795	-2.501272	-0.667628
54	1	-8.171864	-0.988643	-0.213618

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      55          1            -7.264902   -1.913088    1.004225
      56          1            -6.845688    0.201050   -2.126973
      57          1            -6.080303   -1.358417   -2.497415
      58          1            -5.081475    0.069320   -2.167557
      59          1             2.135403   -1.751999    2.335820
      60          1             1.764595   -2.029943    0.629876
      61          1             0.461590   -1.933853    1.839746
      62          1             1.585027    0.324781    3.497188
      63          1            -0.103792    0.183349    3.006774
      64          1             0.796409    1.682678    2.687915
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.9143	61.34		H34	22.3318	8.66
C2	-2.1649	179.14		H35	29.1181	2.45
C4	100.0357	82.11		H36	28.6658	2.87
C5	136.4888	47.50		H37	24.8341	6.37
C6	-16.6188	192.86		H38	23.981	7.15
C7	78.6068	102.46		H39	27.8488	3.61
C8	19.9902	158.10		H40	29.5367	2.07
C9	74.084	106.75		H41	29.6216	1.99
C10	46.7149	132.73		H42	28.5399	2.98
C11	60.6758	119.48		H43	30.2685	1.40
C12	35.6014	143.28		H44	30.0333	1.62
C13	129.3391	54.29		H45	30.0645	1.59
C14	133.7064	50.14		H46	29.7947	1.84
C15	159.2439	25.90		H47	29.1992	2.38
C16	126.0013	57.46		H48	28.3964	3.11
C17	153.0543	31.78		H49	28.7584	2.78
C18	158.6537	26.46		H50	28.9681	2.59
C19	130.368	53.31		H51	28.5078	3.01
C21	125.528	57.91		H52	28.759	2.78
C22	81.1046	100.08		H53	30.0849	1.57
C23	142.5227	41.77		H54	30.3248	1.35
C24	156.8318	28.19		H55	30.2193	1.45
C25	163.5823	21.78		H56	30.6757	1.03
C26	164.0068	21.38		H57	30.6166	1.08
C27	162.5423	22.77		H58	29.9837	1.66
				H59	30.7259	0.98
				H60	29.7859	1.84
				H61	30.9848	0.75
				H62	30.6705	1.03
				H63	31.2527	0.50
				H64	30.7359	0.97

Revised Citrinalin B (**2**) neutral form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.257232 H (rel E = 3.92 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7717631 H (rel E = 4.99 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.329889	0.352729	0.091883
2	6	-0.156232	1.811978	0.317414
3	7	-1.539291	1.801935	0.309590
4	6	-6.045721	-0.819170	-0.136992
5	6	-5.843320	0.669084	-0.464214
6	6	-4.468555	1.182594	-0.076264
7	6	-3.390595	0.198756	-0.162012
8	6	-3.667244	-1.149383	-0.509970
9	6	-2.630942	-2.066075	-0.703382
10	6	-1.297823	-1.668907	-0.528462
11	6	-0.986449	-0.368784	-0.137112
12	6	-2.039605	0.544846	0.017596
13	6	1.237338	-0.117907	1.313364
14	6	2.616606	0.561307	0.976668
15	6	3.901298	-0.074640	1.544393
16	6	4.420663	-1.318517	0.790054
17	6	5.974829	-1.434170	0.703632
18	6	6.254068	-2.066713	-0.685920
19	6	4.839411	-2.307508	-1.279621
20	7	3.928530	-1.370362	-0.607670
21	6	3.861105	-0.047026	-1.214630
22	6	2.681334	0.727184	-0.568313
23	6	1.310068	0.294717	-1.105049
24	6	-6.096479	-1.073554	1.376195
25	6	-7.288951	-1.374070	-0.827461
26	6	1.307542	-1.655728	1.376061
27	6	0.711110	0.372868	2.676200
28	7	2.990386	2.197808	-0.949584
29	8	0.533307	2.803359	0.482578
30	8	-4.281971	2.360738	0.235144
31	8	-4.937578	-1.592898	-0.701782
32	8	2.596077	2.596135	-2.042476
33	8	3.713067	2.838139	-0.192703
34	1	-2.133421	2.616911	0.418529
35	1	-5.947490	0.821406	-1.547829
36	1	-6.602427	1.285039	0.025645
37	1	-2.879282	-3.082799	-0.986312
38	1	-0.511717	-2.397239	-0.699134
39	1	2.563810	1.570949	1.388160
40	1	4.671582	0.703860	1.513654
41	1	3.763795	-0.315978	2.604490
42	1	4.044204	-2.227431	1.274354
43	1	6.369550	-2.039985	1.525512
44	1	6.440997	-0.446331	0.784269
45	1	6.829125	-1.380236	-1.315772
46	1	6.825541	-2.997642	-0.620949
47	1	4.506337	-3.327644	-1.048256
48	1	4.789382	-2.183869	-2.365380
49	1	4.787695	0.539955	-1.095373
50	1	3.673197	-0.152954	-2.287477
51	1	0.993476	0.899114	-1.956586
52	1	1.393900	-0.743762	-1.437837
53	1	-6.202214	-2.144357	1.571552
54	1	-6.953487	-0.553515	1.816051
55	1	-5.192759	-0.719053	1.880327
56	1	-7.396629	-2.442012	-0.616074
57	1	-7.220295	-1.241464	-1.911007
58	1	-8.183896	-0.857234	-0.467289
59	1	1.977194	-1.958325	2.186644

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      60          1             1.683887   -2.100762    0.451954
      61          1             0.323610   -2.073888    1.604281
      62          1             1.372999    0.030922    3.479787
      63          1            -0.284513   -0.037684    2.880201
      64          1             0.657204    1.463115    2.733087
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.0217	61.24		H34	22.3457	8.65
C2	-2.3475	179.31		H35	28.6447	2.89
C4	101.5964	80.63		H36	29.0645	2.50
C5	136.163	47.81		H37	24.8547	6.35
C6	-16.0973	192.37		H38	23.9996	7.13
C7	79.3917	101.71		H39	27.8624	3.60
C8	19.9327	158.16		H40	29.6705	1.95
C9	74.7888	106.08		H41	29.4726	2.13
C10	46.8112	132.64		H42	28.5506	2.97
C11	60.9073	119.26		H43	29.7302	1.89
C12	35.2316	143.63		H44	30.0945	1.56
C13	130.1661	53.51		H45	29.7742	1.85
C14	133.292	50.54		H46	30.0359	1.61
C15	157.7296	27.34		H47	28.6303	2.90
C16	125.188	58.23		H48	28.7479	2.79
C17	153.1378	31.70		H49	28.8477	2.70
C18	160.5653	24.64		H50	29.0235	2.54
C19	129.4443	54.19		H51	28.4656	3.05
C21	127.8139	55.74		H52	28.7677	2.77
C22	81.4733	99.73		H53	30.564	1.13
C23	142.0604	42.21		H54	30.6932	1.01
C24	163.6022	21.76		H55	29.9576	1.69
C25	157.4181	27.63		H56	30.0919	1.56
C26	164.6773	20.74		H57	30.1626	1.50
C27	162.6151	22.70		H58	30.354	1.32
				H59	30.7265	0.98
				H60	29.7551	1.87
				H61	31.0461	0.69
				H62	30.661	1.04
				H63	31.2077	0.54
				H64	30.727	0.98

Revised Citrinalin B (**2**) neutral form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.25701 H (rel E = 4.06 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7717582 H (rel E = 5.00 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.328959	0.347357	0.164266
2	6	-0.167000	1.816055	0.281927
3	7	-1.548016	1.790703	0.354073
4	6	-6.033303	-0.788422	-0.398805
5	6	-5.869199	0.465713	0.475689
6	6	-4.484599	1.079889	0.379242
7	6	-3.396794	0.126672	0.165610
8	6	-3.671371	-1.247750	-0.058518
9	6	-2.633181	-2.168024	-0.222347
10	6	-1.298714	-1.743411	-0.154902
11	6	-0.986633	-0.405991	0.077804
12	6	-2.043809	0.506960	0.205956
13	6	1.307753	0.003083	1.374600
14	6	2.657592	0.657625	0.899752
15	6	3.978763	0.088079	1.453250
16	6	4.469527	-1.219686	0.793719
17	6	6.019021	-1.339393	0.643117
18	6	6.236015	-2.078457	-0.704382
19	6	4.797205	-2.392126	-1.195212
20	7	3.908088	-1.405715	-0.565665
21	6	3.789681	-0.146601	-1.289899
22	6	2.637911	0.677302	-0.654877
23	6	1.244447	0.190148	-1.074564
24	6	-7.301442	-1.555730	-0.033894
25	6	-6.004412	-0.451727	-1.896147
26	6	1.400589	-1.520961	1.581051
27	6	0.848976	0.618595	2.710753
28	7	2.911720	2.107652	-1.187937
29	8	0.514646	2.825975	0.312962
30	8	-4.301089	2.290390	0.522689
31	8	-4.943437	-1.724260	-0.111555
32	8	2.461935	2.397085	-2.293682
33	8	3.661624	2.822504	-0.530978
34	1	-2.147400	2.605626	0.427964
35	1	-6.611986	1.224829	0.215879
36	1	-6.028288	0.197715	1.529836
37	1	-2.880990	-3.206401	-0.411365
38	1	-0.511715	-2.476306	-0.299555
39	1	2.614006	1.701680	1.215384
40	1	4.736961	0.864995	1.304848
41	1	3.902648	-0.050983	2.537578
42	1	4.125166	-2.079822	1.379939
43	1	6.453383	-1.880518	1.489774
44	1	6.485807	-0.348826	0.625698
45	1	6.758255	-1.434624	-1.419649
46	1	6.832559	-2.989574	-0.597567
47	1	4.688058	-2.372340	-2.283544
48	1	4.493560	-3.389627	-0.851445
49	1	4.713427	0.456977	-1.280522
50	1	3.543942	-0.355693	-2.335566
51	1	0.875945	0.716317	-1.956572
52	1	1.322286	-0.872587	-1.321201
53	1	-7.383676	-2.463407	-0.638837
54	1	-8.184321	-0.935458	-0.216970

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      55          1            -7.288325   -1.843184    1.021399
      56          1            -6.088827   -1.368120   -2.486993
      57          1            -5.080002    0.058215   -2.182563
      58          1            -6.843237    0.204276   -2.149977
      59          1             2.113274   -1.739553    2.381963
      60          1             1.734646   -2.050709    0.685855
      61          1             0.434801   -1.922108    1.899094
      62          1             1.554451    0.356834    3.507411
      63          1            -0.131266    0.226136    3.004852
      64          1             0.788988    1.709026    2.666948
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.765	61.48		H34	22.3074	8.68
C2	-2.3552	179.32		H35	29.1357	2.44
C4	100.0431	82.10		H36	28.6735	2.86
C5	136.5271	47.47		H37	24.85	6.36
C6	-16.6609	192.90		H38	23.9852	7.15
C7	78.3864	102.66		H39	27.8874	3.58
C8	20.0352	158.06		H40	29.6392	1.98
C9	74.0463	106.78		H41	29.507	2.10
C10	46.848	132.61		H42	28.5727	2.95
C11	60.6865	119.47		H43	29.7484	1.88
C12	35.6784	143.21		H44	30.1538	1.51
C13	129.692	53.96		H45	29.791	1.84
C14	132.8471	50.96		H46	30.0733	1.58
C15	157.8767	27.20		H47	28.7729	2.77
C16	125.2493	58.17		H48	28.7101	2.83
C17	153.0642	31.77		H49	28.7811	2.76
C18	161.0534	24.18		H50	29.0374	2.53
C19	129.6485	54.00		H51	28.4737	3.04
C21	127.6289	55.91		H52	28.7676	2.77
C22	81.414	99.79		H53	30.0866	1.57
C23	142.0314	42.24		H54	30.3211	1.35
C24	156.8501	28.17		H55	30.2159	1.45
C25	163.5918	21.77		H56	30.6195	1.08
C26	164.4295	20.98		H57	29.9895	1.66
C27	162.563	22.75		H58	30.6817	1.02
				H59	30.8457	0.87
				H60	29.6695	1.95
				H61	31.0622	0.68
				H62	30.6769	1.03
				H63	31.2603	0.50
				H64	30.7504	0.96

Revised Citrinalin B (**2**) neutral form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.263485 H (rel E = "0" kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7797189 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.210056	0.344095	0.002743
2	6	-0.255095	1.757429	0.461852
3	7	-1.636956	1.743058	0.530685
4	6	-6.180871	-0.765620	-0.137614
5	6	-5.979535	0.755564	-0.230253
6	6	-4.585920	1.198326	0.176285
7	6	-3.520154	0.239217	-0.111788
8	6	-3.822855	-1.033980	-0.661524
9	6	-2.803346	-1.907601	-1.048618
10	6	-1.461218	-1.544177	-0.872784
11	6	-1.121939	-0.324182	-0.292380
12	6	-2.159893	0.550945	0.060444
13	6	1.122711	-0.324495	1.126503
14	6	2.492290	0.389073	0.872147
15	6	3.758050	-0.173069	1.564934
16	6	4.569269	-1.157251	0.720856
17	6	6.004941	-1.441270	1.200160
18	6	6.804786	-1.709798	-0.109013
19	6	5.783152	-1.478440	-1.244270
20	7	4.776916	-0.617157	-0.626902
21	6	3.537200	-0.475220	-1.353418
22	6	2.606306	0.550122	-0.664062
23	6	1.161928	0.477360	-1.217942
24	6	-6.170671	-1.260437	1.315448
25	6	-7.456206	-1.199609	-0.855453
26	6	1.180525	-1.854863	0.951605
27	6	0.610740	-0.044125	2.551977
28	7	3.228037	1.931713	-1.011029
29	8	0.444265	2.722418	0.714698
30	8	-4.376086	2.311356	0.662538
31	8	-5.102998	-1.439862	-0.866010
32	8	3.140549	2.287026	-2.186981
33	8	3.803177	2.560649	-0.134435
34	1	-2.219229	2.535169	0.781101
35	1	-6.126641	1.079461	-1.270318
36	1	-6.712882	1.286521	0.382803
37	1	-3.072042	-2.864605	-1.481373
38	1	-0.690589	-2.236288	-1.196706
39	1	2.355445	1.402883	1.253537
40	1	4.409786	0.675662	1.796066
41	1	3.488204	-0.635674	2.521956
42	1	4.028282	-2.124056	0.645749
43	1	6.404095	-0.565915	1.722664
44	1	6.037227	-2.285198	1.895912
45	1	7.641431	-1.011533	-0.197895
46	1	7.217049	-2.722162	-0.147234
47	1	6.213906	-0.999038	-2.129257
48	1	5.339184	-2.443208	-1.564318
49	1	3.731530	-0.145145	-2.378606
50	1	2.992631	-1.438404	-1.417302
51	1	0.924977	1.343567	-1.837483
52	1	1.060031	-0.403383	-1.858704
53	1	-6.273085	-2.348995	1.340125
54	1	-7.006888	-0.820275	1.868051

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      55          1            -5.245815   -0.989665    1.832967
      56          1            -7.565318   -2.287305   -0.814571
      57          1            -7.431077   -0.893895   -1.905383
      58          1            -8.330459   -0.744950   -0.379361
      59          1             1.914054   -2.279585    1.643398
      60          1             1.462689   -2.168375   -0.056985
      61          1             0.212314   -2.305302    1.187043
      62          1             1.246739   -0.544197    3.290221
      63          1            -0.405182   -0.433654    2.684199
      64          1             0.606892    1.023597    2.786948
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.1803	61.09		H34	22.2846	8.70
C2	-2.9665	179.90		H35	28.6699	2.86
C4	100.7548	81.43		H36	29.0264	2.54
C5	136.4204	47.57		H37	24.8404	6.37
C6	-16.3284	192.58		H38	23.9999	7.13
C7	79.5423	101.57		H39	27.6902	3.76
C8	20.1081	157.99		H40	29.9122	1.73
C9	74.336	106.51		H41	29.8461	1.79
C10	47.6385	131.86		H42	29.5894	2.02
C11	61.2013	118.98		H43	30.3388	1.34
C12	35.4106	143.46		H44	29.7963	1.83
C13	130.5638	53.13		H45	29.9159	1.72
C14	137.9744	46.09		H46	30.0356	1.61
C15	156.8951	28.13		H47	28.7976	2.75
C16	123.1441	60.17		H48	29.5173	2.09
C17	153.0333	31.80		H49	28.0354	3.44
C18	163.3585	21.99		H50	29.0366	2.53
C19	130.9495	52.76		H51	28.8371	2.71
C21	119.2335	63.88		H52	29.0414	2.52
C22	83.1432	98.15		H53	30.6003	1.10
C23	139.259	44.87		H54	30.6346	1.07
C24	163.8641	21.51		H55	30.0182	1.63
C25	156.7429	28.27		H56	30.0571	1.60
C26	162.6762	22.64		H57	30.2289	1.44
C27	163.5216	21.84		H58	30.3148	1.36
				H59	30.5512	1.14
				H60	30.497	1.19
				H61	30.9989	0.73
				H62	30.5884	1.11
				H63	31.2005	0.55
				H64	30.841	0.88

Revised Citrinalin B (**2**) neutral form, conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.263207 H (rel E = 0.17 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7796297 H (rel E = 0.06 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.206833	0.309299	0.086207
2	6	-0.267618	1.760819	0.391509
3	7	-1.643868	1.732406	0.532314
4	6	-6.185681	-0.684905	-0.394828
5	6	-5.978430	0.447110	0.624989
6	6	-4.588271	1.053403	0.565210
7	6	-3.520422	0.123247	0.199393
8	6	-3.821646	-1.207691	-0.190617
9	6	-2.802399	-2.108573	-0.509449
10	6	-1.461251	-1.707346	-0.439461
11	6	-1.122462	-0.413145	-0.051349
12	6	-2.161866	0.483072	0.238554
13	6	1.192862	-0.197034	1.233023
14	6	2.530888	0.499412	0.814589
15	6	3.845580	0.050036	1.498881
16	6	4.629973	-1.022432	0.741340
17	6	6.094837	-1.225390	1.173010
18	6	6.836146	-1.620785	-0.138861
19	6	5.747003	-1.566863	-1.231821
20	7	4.753082	-0.653237	-0.673195
21	6	3.472121	-0.626672	-1.339173
22	6	2.559189	0.464735	-0.732984
23	6	1.089144	0.304218	-1.192811
24	6	-7.453044	-1.479134	-0.090330
25	6	-6.194554	-0.163451	-1.838406
26	6	1.276911	-1.735958	1.250175
27	6	0.749758	0.253141	2.637979
28	7	3.132491	1.800181	-1.286081
29	8	0.421067	2.761383	0.485305
30	8	-4.382155	2.234087	0.852780
31	8	-5.100705	-1.660867	-0.260658
32	8	2.983984	1.995733	-2.492995
33	8	3.728866	2.550790	-0.527465
34	1	-2.230694	2.539016	0.716615
35	1	-6.716970	1.241125	0.484998
36	1	-6.111959	0.049986	1.641213
37	1	-3.070747	-3.111554	-0.821420
38	1	-0.692134	-2.423835	-0.709580
39	1	2.391873	1.551322	1.072066
40	1	4.490205	0.931330	1.578663
41	1	3.640443	-0.287770	2.521776
42	1	4.105165	-1.998071	0.815976
43	1	6.499018	-0.292124	1.578317
44	1	6.180893	-1.988528	1.952433
45	1	7.633433	-0.905601	-0.358629
46	1	7.291884	-2.613334	-0.080077
47	1	6.112905	-1.200236	-2.196321
48	1	5.315127	-2.575599	-1.394277
49	1	3.600737	-0.428685	-2.407692
50	1	2.947460	-1.598302	-1.245053
51	1	0.801786	1.084535	-1.899119
52	1	0.970836	-0.649875	-1.714797
53	1	-7.563219	-2.305860	-0.798181
54	1	-8.332565	-0.832989	-0.172090

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     55          1           -7.415645   -1.893118    0.921455
     56          1           -7.033924    0.523737   -1.984895
     57          1           -6.303420   -0.998225   -2.536430
     58          1           -5.273641    0.373116   -2.084745
     59          1            2.052882   -2.057171    1.951289
     60          1            1.516826   -2.170502    0.276187
     61          1            0.332401   -2.169800    1.589918
     62          1            1.431731   -0.143720    3.397515
     63          1           -0.250459   -0.130068    2.870092
     64          1            0.737778    1.341653    2.739193
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.8676	61.38		H34	22.3587	8.63
C2	-2.8936	179.83		H35	29.077	2.49
C4	100.147	82.01		H36	28.6595	2.87
C5	136.3518	47.63		H37	24.8422	6.36
C6	-16.6154	192.86		H38	24.008	7.13
C7	79.0282	102.05		H39	27.6221	3.82
C8	19.7899	158.29		H40	29.8766	1.76
C9	74.0348	106.80		H41	29.8506	1.78
C10	47.5205	131.97		H42	29.5936	2.02
C11	61.5019	118.69		H43	30.352	1.33
C12	35.2531	143.61		H44	29.8937	1.74
C13	130.7273	52.97		H45	29.8519	1.78
C14	137.131	46.89		H46	30.0133	1.64
C15	157.1703	27.87		H47	28.8389	2.71
C16	123.0989	60.21		H48	29.5152	2.09
C17	153.1569	31.68		H49	27.9406	3.53
C18	162.7478	22.57		H50	28.9811	2.58
C19	130.9838	52.73		H51	28.8302	2.72
C21	119.3099	63.81		H52	29.1028	2.47
C22	82.9285	98.35		H53	30.0659	1.59
C23	139.4981	44.65		H54	30.2944	1.38
C24	156.9548	28.07		H55	30.2147	1.45
C25	163.7635	21.61		H56	30.6694	1.04
C26	162.2784	23.02		H57	30.5873	1.11
C27	163.6929	21.68		H58	30.0484	1.60
				H59	30.7227	0.99
				H60	30.4335	1.25
				H61	30.9542	0.78
				H62	30.6701	1.03
				H63	31.2654	0.49
				H64	30.8221	0.90

Revised Citrinalin B (**2**) neutral form, conformer 6

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.24546 H (rel E = 11.31 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7621818 H (rel E = 11.00 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.386860	0.837696	-0.030499
2	6	-0.273015	2.225462	-0.286235
3	7	-1.648614	2.059774	-0.201551
4	6	-5.809086	-1.109070	-0.025532
5	6	-5.767621	0.272460	-0.698148
6	6	-4.472670	1.022781	-0.444088
7	6	-3.288128	0.182659	-0.276815
8	6	-3.398184	-1.232489	-0.299973
9	6	-2.257764	-2.037880	-0.274731
10	6	-0.985971	-1.452924	-0.194195
11	6	-0.835205	-0.071925	-0.113358
12	6	-1.991696	0.719718	-0.178372
13	6	1.177568	0.827974	1.394029
14	6	2.560431	0.157000	1.042721
15	6	2.547982	-1.380640	1.204803
16	6	3.639929	-2.147444	0.461854
17	6	5.101470	-2.090619	0.976471
18	6	5.928515	-2.493995	-0.275923
19	6	4.884543	-2.506930	-1.442743
20	7	3.702597	-1.762136	-0.963864
21	6	3.920293	-0.321679	-1.128326
22	6	2.842029	0.536401	-0.423483
23	6	1.472403	0.532321	-1.107581
24	6	-5.878146	-1.002245	1.504404
25	6	-6.958767	-1.954268	-0.567878
26	6	0.400131	0.084753	2.497291
27	6	1.426137	2.253739	1.947993
28	7	3.499498	1.951336	-0.526635
29	8	0.282355	3.277947	-0.532619
30	8	-4.431455	2.255016	-0.439467
31	8	-4.602654	-1.856555	-0.386918
32	8	3.354692	2.557703	-1.581064
33	8	4.215728	2.325484	0.400469
34	1	-2.331141	2.792424	-0.364474
35	1	-5.856993	0.150536	-1.786929
36	1	-6.605890	0.893739	-0.371014
37	1	-2.376559	-3.114640	-0.317798
38	1	-0.118419	-2.105780	-0.199291
39	1	3.343127	0.572100	1.681926
40	1	2.598142	-1.626430	2.270761
41	1	1.595352	-1.777582	0.847140
42	1	3.340573	-3.205267	0.468263
43	1	5.254184	-2.768805	1.821691
44	1	5.365661	-1.084522	1.319204
45	1	6.737901	-1.782721	-0.465384
46	1	6.391421	-3.478708	-0.160661
47	1	5.263961	-2.071209	-2.371309
48	1	4.572006	-3.533800	-1.662914
49	1	4.902320	-0.001575	-0.743548
50	1	3.900005	-0.091646	-2.198382
51	1	1.446518	1.241722	-1.936382
52	1	1.317973	-0.469195	-1.518531
53	1	-5.862379	-2.000826	1.950166
54	1	-6.804515	-0.502236	1.804833

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     55          1            -5.039585   -0.430348    1.912053
     56          1            -6.951225   -2.947136   -0.108640
     57          1            -6.871733   -2.074212   -1.651600
     58          1            -7.917391   -1.475874   -0.344391
     59          1             0.982831    0.088020    3.425367
     60          1             0.157453   -0.949769    2.253907
     61          1            -0.543254    0.600796    2.703552
     62          1             2.062411    2.179131    2.835942
     63          1             0.484325    2.720353    2.253630
     64          1             1.906999    2.928740    1.243838
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.3174	61.91		H34	22.5322	8.48
C2	-2.8673	179.81		H35	28.7356	2.80
C4	101.0173	81.18		H36	29.1347	2.44
C5	136.2817	47.70		H37	24.8815	6.33
C6	-16.3597	192.61		H38	23.7477	7.36
C7	79.02	102.06		H39	28.3156	3.19
C8	20.3881	157.73		H40	29.6733	1.95
C9	74.7199	106.15		H41	29.3823	2.21
C10	47.3268	132.15		H42	28.5368	2.99
C11	55.1206	124.75		H43	30.1176	1.54
C12	35.9675	142.94		H44	29.7383	1.89
C13	128.0048	55.56		H45	29.6924	1.93
C14	138.421	45.67		H46	29.9041	1.74
C15	158.2426	26.85		H47	28.883	2.67
C16	123.0783	60.23		H48	28.7255	2.81
C17	160.6817	24.53		H49	29.1713	2.41
C18	160.8706	24.36		H50	28.8823	2.67
C19	129.8558	53.80		H51	28.1703	3.32
C21	130.4214	53.26		H52	28.7729	2.77
C22	77.1241	103.86		H53	30.6112	1.09
C23	141.9421	42.33		H54	30.635	1.07
C24	163.8679	21.51		H55	30.0057	1.64
C25	156.8133	28.21		H56	30.0716	1.58
C26	162.5906	22.72		H57	30.236	1.43
C27	155.3837	29.56		H58	30.3003	1.37
				H59	30.8803	0.84
				H60	30.8249	0.89
				H61	31.5308	0.25
				H62	30.743	0.97
				H63	31.1511	0.59
				H64	29.9257	1.72

Revised Citrinalin B (**2**) neutral form, conformer 7

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.245622 H (rel E = 11.21 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7622415 H (rel E = 10.97 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.378418	0.810714	0.026923
2	6	-0.283257	2.180230	-0.310866
3	7	-1.654529	2.037037	-0.153091
4	6	-5.817290	-1.124788	-0.285442
5	6	-5.811077	0.311273	0.264780
6	6	-4.497991	1.032817	0.022715
7	6	-3.308961	0.182652	0.055656
8	6	-3.430419	-1.227631	0.159039
9	6	-2.295993	-2.040333	0.211259
10	6	-1.017475	-1.465511	0.177832
11	6	-0.853041	-0.086342	0.094636
12	6	-2.005453	0.708873	0.009339
13	6	1.257377	0.911108	1.395666
14	6	2.627936	0.234981	1.003933
15	6	2.654284	-1.285710	1.285874
16	6	3.716504	-2.092827	0.542794
17	6	5.202996	-1.975527	0.970542
18	6	5.971559	-2.443942	-0.296795
19	6	4.863776	-2.577986	-1.394384
20	7	3.691788	-1.822566	-0.908916
21	6	3.857189	-0.396574	-1.205057
22	6	2.803509	0.494635	-0.504275
23	6	1.391406	0.401617	-1.086577
24	6	-7.006842	-1.917224	0.250292
25	6	-5.782773	-1.152070	-1.819851
26	6	0.565848	0.234579	2.595347
27	6	1.510952	2.374600	1.838072
28	7	3.411983	1.908578	-0.774566
29	8	0.267730	3.202307	-0.669736
30	8	-4.449640	2.253469	-0.142471
31	8	-4.642722	-1.840528	0.218245
32	8	3.200452	2.402094	-1.875563
33	8	4.158488	2.391073	0.075095
34	1	-2.338311	2.762104	-0.341066
35	1	-6.624096	0.900671	-0.167710
36	1	-5.966611	0.283616	1.352564
37	1	-2.424922	-3.115426	0.264676
38	1	-0.155527	-2.125515	0.199545
39	1	3.443267	0.711009	1.553812
40	1	2.769702	-1.446071	2.362891
41	1	1.690450	-1.724050	1.016120
42	1	3.438118	-3.151019	0.649722
43	1	5.414757	-2.595605	1.847128
44	1	5.464399	-0.945655	1.235624
45	1	6.739695	-1.720786	-0.586442
46	1	6.478672	-3.400590	-0.139359
47	1	4.567052	-3.626477	-1.510432
48	1	5.177168	-2.213164	-2.376608
49	1	4.852319	-0.021060	-0.914867
50	1	3.762242	-0.258095	-2.286684
51	1	1.294619	1.014846	-1.984150
52	1	1.227463	-0.640544	-1.374303
53	1	-6.978266	-2.945339	-0.122432
54	1	-7.944860	-1.456376	-0.074513

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      55          1           -6.990944   -1.945330    1.343654
      56          1           -5.750679   -2.186223   -2.174066
      57          1           -4.911120   -0.624713   -2.218346
      58          1           -6.680064   -0.673083   -2.224543
      59          1            1.207926    0.309342    3.480173
      60          1            0.326382   -0.817425    2.440599
      61          1           -0.371041    0.750663    2.828486
      62          1            2.190572    2.367796    2.696571
      63          1            0.577642    2.848545    2.158821
      64          1            1.947747    3.005596    1.067858
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.4994	61.73		H34	22.5044	8.50
C2	-2.7011	179.65		H35	29.1407	2.43
C4	99.952	82.19		H36	28.6719	2.86
C5	136.4255	47.56		H37	24.8941	6.32
C6	-16.4461	192.70		H38	23.7494	7.36
C7	79.2139	101.88		H39	28.39	3.12
C8	20.359	157.75		H40	29.6832	1.94
C9	74.5574	106.30		H41	29.4464	2.15
C10	47.277	132.20		H42	28.5653	2.96
C11	55.5418	124.35		H43	30.1274	1.53
C12	35.8354	143.06		H44	29.7166	1.91
C13	128.6058	54.99		H45	29.7303	1.89
C14	138.6494	45.45		H46	29.9991	1.65
C15	158.4007	26.70		H47	28.821	2.73
C16	123.4503	59.88		H48	28.9433	2.61
C17	160.4865	24.72		H49	29.1541	2.42
C18	161.3404	23.91		H50	28.8853	2.67
C19	129.8717	53.78		H51	28.2277	3.27
C21	130.2533	53.42		H52	28.7093	2.83
C22	77.4892	103.52		H53	30.0517	1.60
C23	141.5947	42.66		H54	30.3023	1.37
C24	156.7632	28.25		H55	30.2298	1.44
C25	163.6908	21.68		H56	30.6044	1.09
C26	162.0643	23.22		H57	30.0479	1.60
C27	155.4153	29.53		H58	30.6259	1.08
				H59	30.8972	0.83
				H60	30.778	0.94
				H61	31.6391	0.15
				H62	30.7372	0.97
				H63	31.198	0.55
				H64	29.8199	1.81

Revised Citrinalin B (**2**) neutral form, conformer 8

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.257344 H (rel E = 3.85 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7729435 H (rel E = 4.25 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.210280	0.266938	0.006551
2	6	-0.206845	1.635151	0.620925
3	7	-1.587685	1.654764	0.705057
4	6	-6.211863	-0.635360	-0.170157
5	6	-5.965748	0.880492	-0.103953
6	6	-4.555873	1.236565	0.330743
7	6	-3.522154	0.282954	-0.069869
8	6	-3.867693	-0.915582	-0.747526
9	6	-2.878716	-1.772901	-1.236853
10	6	-1.524793	-1.469220	-1.039796
11	6	-1.144107	-0.327644	-0.338111
12	6	-2.151580	0.535272	0.117694
13	6	1.119039	-0.543028	1.035886
14	6	2.506452	0.153588	0.835657
15	6	3.762785	-0.521975	1.431189
16	6	4.509065	-1.515706	0.510995
17	6	5.961889	-1.783547	0.991133
18	6	6.882463	-1.128352	-0.077540
19	6	5.940677	-0.227030	-0.890183
20	7	4.690676	-0.993699	-0.850472
21	6	3.494029	-0.514824	-1.488540
22	6	2.600756	0.484584	-0.674419
23	6	1.148068	0.505485	-1.209176
24	6	-6.205011	-1.280870	1.222739
25	6	-7.505563	-0.954407	-0.914977
26	6	1.128806	-2.047384	0.698242
27	6	0.635756	-0.402645	2.491756
28	7	3.238870	1.874951	-0.882593
29	8	0.524728	2.546215	0.966949
30	8	-4.308315	2.284756	0.930208
31	8	-5.161291	-1.260349	-0.977834
32	8	3.105559	2.382108	-1.996622
33	8	3.894484	2.369290	0.029409
34	1	-2.142467	2.432424	1.046524
35	1	-6.112791	1.317791	-1.101690
36	1	-6.677049	1.364340	0.570995
37	1	-3.180210	-2.670274	-1.765181
38	1	-0.777555	-2.145174	-1.442936
39	1	2.409545	1.120597	1.334434
40	1	4.459855	0.279432	1.699398
41	1	3.504581	-1.025463	2.371523
42	1	3.940895	-2.451947	0.441550
43	1	6.123561	-1.345474	1.981723
44	1	6.160484	-2.855517	1.079165
45	1	7.310002	-1.896117	-0.729661
46	1	7.710000	-0.568305	0.367496
47	1	5.864957	0.769647	-0.429502
48	1	6.264000	-0.093948	-1.928513
49	1	3.736430	-0.064915	-2.456613
50	1	2.853845	-1.382746	-1.692070
51	1	0.923948	1.437590	-1.729389
52	1	1.012181	-0.298758	-1.938769
53	1	-6.345459	-2.361801	1.134197
54	1	-7.019899	-0.873211	1.829478

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     55          1            -5.266505   -1.098646    1.754443
     56          1            -7.645522   -2.036847   -0.987848
     57          1            -7.480387   -0.540066   -1.926883
     58          1            -8.362270   -0.528782   -0.383430
     59          1             1.843616   -2.566877    1.343062
     60          1             1.405916   -2.260893   -0.337767
     61          1             0.146073   -2.490264    0.881892
     62          1             1.267505   -0.995581    3.161630
     63          1            -0.389214   -0.775645    2.599552
     64          1             0.666885    0.633837    2.837909
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.452	61.78		H34	22.2362	8.75
C2	-2.9746	179.91		H35	28.7069	2.83
C4	100.3751	81.79		H36	29.0952	2.47
C5	136.4631	47.53		H37	24.8186	6.39
C6	-16.474	192.72		H38	23.9691	7.16
C7	78.7145	102.35		H39	27.4445	3.98
C8	20.2117	157.89		H40	29.4074	2.19
C9	74.0548	106.78		H41	30.2615	1.41
C10	47.3439	132.14		H42	28.2212	3.27
C11	60.7236	119.43		H43	30.1498	1.51
C12	35.6334	143.25		H44	29.4628	2.14
C13	130.6162	53.08		H45	30.0145	1.63
C14	136.3045	47.68		H46	30.0172	1.63
C15	160.6624	24.55		H47	28.4579	3.06
C16	129.6249	54.02		H48	28.9625	2.60
C17	153.0989	31.73		H49	27.4845	3.95
C18	159.7423	25.43		H50	27.8674	3.60
C19	136.4389	47.55		H51	28.8479	2.70
C21	122.4963	60.79		H52	29.2178	2.36
C22	89.8352	91.79		H53	30.6206	1.08
C23	137.6435	46.41		H54	30.6935	1.01
C24	163.7018	21.67		H55	29.9684	1.68
C25	156.6415	28.37		H56	30.0514	1.60
C26	162.8906	22.44		H57	30.2426	1.43
C27	163.0724	22.26		H58	30.2916	1.38
				H59	30.4118	1.27
				H60	30.4349	1.25
				H61	30.9096	0.82
				H62	30.5427	1.15
				H63	31.1788	0.57
				H64	30.8048	0.91

Revised Citrinalin B (**2**) neutral form, conformer 9

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.257369 H (rel E = 3.84 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7729365 H (rel E = 4.26 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.207814	0.195242	0.088054
2	6	-0.209512	1.599637	0.614777
3	7	-1.584257	1.599153	0.768750
4	6	-6.221486	-0.488059	-0.437774
5	6	-5.959590	0.461572	0.742648
6	6	-4.550259	1.024489	0.748959
7	6	-3.521910	0.125834	0.225439
8	6	-3.876065	-1.119016	-0.357163
9	6	-2.893904	-1.997257	-0.822368
10	6	-1.538058	-1.659597	-0.711145
11	6	-1.148007	-0.451363	-0.137827
12	6	-2.150772	0.427301	0.298081
13	6	1.186498	-0.511227	1.128883
14	6	2.540317	0.209025	0.813331
15	6	3.843330	-0.383392	1.397803
16	6	4.583675	-1.415467	0.516443
17	6	6.062184	-1.605124	0.952123
18	6	6.916317	-0.983349	-0.189469
19	6	5.910238	-0.170442	-1.018728
20	7	4.694151	-0.979730	-0.882247
21	6	3.455290	-0.590588	-1.500892
22	6	2.555090	0.430266	-0.720601
23	6	1.080632	0.353071	-1.186853
24	6	-7.513585	-1.275863	-0.237776
25	6	-6.230314	0.253626	-1.781429
26	6	1.230860	-2.034982	0.899649
27	6	0.763803	-0.279438	2.591802
28	7	3.124259	1.825028	-1.058102
29	8	0.516602	2.550062	0.848208
30	8	-4.298315	2.139855	1.209059
31	8	-5.171781	-1.510208	-0.477412
32	8	2.912790	2.248183	-2.194861
33	8	3.808369	2.403851	-0.219840
34	1	-2.139020	2.388420	1.082180
35	1	-6.672273	1.290762	0.744988
36	1	-6.090219	-0.086860	1.686314
37	1	-3.202398	-2.931211	-1.278290
38	1	-0.797997	-2.353483	-1.096634
39	1	2.434880	1.206655	1.244909
40	1	4.523649	0.456314	1.576199
41	1	3.643736	-0.825024	2.382512
42	1	4.043297	-2.370343	0.532098
43	1	6.302910	-2.662710	1.093180
44	1	6.245587	-1.104487	1.908632
45	1	7.736762	-0.366392	0.188336
46	1	7.349455	-1.773775	-0.809954
47	1	5.811443	0.849659	-0.617737
48	1	6.189597	-0.091274	-2.075154
49	1	3.641049	-0.201828	-2.507251
50	1	2.843066	-1.494181	-1.616340
51	1	0.798659	1.224125	-1.779712
52	1	0.944149	-0.521438	-1.830464
53	1	-7.666872	-1.972696	-1.066960
54	1	-8.368545	-0.594022	-0.195084

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      55          1            -7.476253   -1.848877    0.693182
      56          1            -6.382345   -0.456049   -2.599441
      57          1            -5.292759    0.788145   -1.959682
      58          1            -7.043787    0.985904   -1.800582
      59          1             1.995103   -2.483277    1.541166
      60          1             1.461865   -2.316013   -0.131743
      61          1             0.274747   -2.492624    1.167821
      62          1             1.444186   -0.802164    3.272321
      63          1            -0.241912   -0.675567    2.772945
      64          1             0.774328    0.779799    2.862384
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.7327	61.51		H34	22.3001	8.69
C2	-2.8661	179.80		H35	29.1035	2.47
C4	100.7297	81.45		H36	28.6602	2.87
C5	136.2124	47.77		H37	24.8267	6.38
C6	-16.3797	192.63		H38	24.0256	7.11
C7	79.3286	101.77		H39	27.4483	3.98
C8	19.9066	158.18		H40	29.4379	2.16
C9	74.3633	106.48		H41	30.2781	1.39
C10	47.7896	131.71		H42	28.3045	3.20
C11	61.1625	119.02		H43	29.4791	2.12
C12	35.2544	143.61		H44	30.1672	1.49
C13	129.996	53.67		H45	29.9937	1.65
C14	136.4375	47.55		H46	30.0009	1.65
C15	160.8996	24.33		H47	28.4263	3.09
C16	129.4227	54.21		H48	28.9861	2.57
C17	153.0678	31.76		H49	27.5478	3.89
C18	159.7458	25.42		H50	27.9125	3.56
C19	136.5577	47.44		H51	28.7988	2.75
C21	122.4273	60.85		H52	29.2161	2.36
C22	89.9974	91.64		H53	30.0571	1.60
C23	137.8392	46.22		H54	30.3204	1.35
C24	157.0683	27.96		H55	30.2006	1.46
C25	163.5529	21.81		H56	30.5986	1.10
C26	163.1284	22.21		H57	29.9212	1.72
C27	163.204	22.14		H58	30.7157	0.99
				H59	30.3852	1.30
				H60	30.4837	1.21
				H61	30.9298	0.80
				H62	30.5583	1.14
				H63	31.2663	0.49
				H64	30.8842	0.84

Revised Citrinalin B (**2**) neutral form, conformer 10

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.251877 H (rel E = 7.28 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1511.7680149 H (rel E = 7.34 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.220267	-0.098530	0.037336
2	6	-0.043595	1.316997	0.623884
3	7	-1.413264	1.500482	0.687228
4	6	-6.266105	-0.252738	-0.177181
5	6	-5.841391	1.224396	-0.149887
6	6	-4.403964	1.421818	0.295881
7	6	-3.487261	0.341824	-0.067136
8	6	-3.966713	-0.825025	-0.717614
9	6	-3.080989	-1.804139	-1.174793
10	6	-1.702243	-1.656447	-0.970138
11	6	-1.194305	-0.552992	-0.287366
12	6	-2.098142	0.435726	0.129911
13	6	1.077661	-0.967050	1.064143
14	6	2.559651	-0.484065	0.785579
15	6	3.643035	-1.560941	1.017034
16	6	5.031388	-1.260451	0.422317
17	6	5.901713	-0.199413	1.118540
18	6	6.856236	0.230870	-0.008830
19	6	5.964490	0.218770	-1.266103
20	7	4.944440	-0.813019	-0.988227
21	6	3.626015	-0.670546	-1.555694
22	6	2.585528	0.079877	-0.662379
23	6	1.149023	-0.009380	-1.199204
24	6	-6.347263	-0.853220	1.233157
25	6	-7.581739	-0.437566	-0.928871
26	6	0.864537	-2.467917	0.779950
27	6	0.688301	-0.722109	2.534792
28	7	3.039441	1.563892	-0.687561
29	8	0.785413	2.133159	0.983473
30	8	-4.040148	2.448088	0.873576
31	8	-5.289985	-1.020868	-0.954243
32	8	2.774628	2.200666	-1.707718
33	8	3.714493	1.995750	0.238696
34	1	-1.877707	2.340547	1.015371
35	1	-5.922651	1.646128	-1.161715
36	1	-6.497359	1.809340	0.500597
37	1	-3.480852	-2.672921	-1.685361
38	1	-1.038275	-2.425064	-1.352361
39	1	2.756109	0.357905	1.451835
40	1	3.756626	-1.747207	2.091492
41	1	3.319295	-2.509189	0.579087
42	1	5.586255	-2.213608	0.453819
43	1	5.293035	0.648280	1.444206
44	1	6.426930	-0.607476	1.988894
45	1	7.667687	-0.499315	-0.114495
46	1	7.309637	1.211433	0.161204
47	1	5.519618	1.208059	-1.429409
48	1	6.536306	-0.037349	-2.167689
49	1	3.697250	-0.173261	-2.527600
50	1	3.188186	-1.662015	-1.741739
51	1	0.903984	0.818407	-1.865828
52	1	1.046801	-0.933553	-1.778472
53	1	-6.608386	-1.913523	1.173546
54	1	-7.116686	-0.337943	1.816966

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     55          1            -5.399147   -0.761257    1.770850
     56          1            -7.849340   -1.497420   -0.972132
     57          1            -7.498264   -0.059956   -1.952037
     58          1            -8.386426    0.102831   -0.420756
     59          1             1.460406   -3.075613    1.465563
     60          1             1.136483   -2.760089   -0.240125
     61          1            -0.181787   -2.737193    0.942451
     62          1             1.301999   -1.346157    3.193871
     63          1            -0.358976   -0.992381    2.713781
     64          1             0.834908    0.319222    2.831860
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.633	60.66		H34	22.2944	8.69
C2	-1.7049	178.70		H35	28.7082	2.83
C4	99.7669	82.37		H36	29.1329	2.44
C5	136.5874	47.41		H37	24.8788	6.33
C6	-16.2163	192.48		H38	24.1148	7.03
C7	78.19	102.85		H39	27.7547	3.70
C8	20.0769	158.02		H40	29.8617	1.77
C9	74.9446	105.93		H41	29.7722	1.86
C10	46.9222	132.54		H42	27.9786	3.50
C11	60.4074	119.73		H43	29.2212	2.36
C12	35.4303	143.45		H44	30.0416	1.61
C13	129.4958	54.14		H45	30.0115	1.64
C14	138.8979	45.22		H46	29.9475	1.70
C15	161.6333	23.63		H47	28.8419	2.71
C16	125.901	57.55		H48	28.8064	2.74
C17	152.4004	32.40		H49	27.9895	3.49
C18	159.4202	25.73		H50	28.3434	3.16
C19	132.5238	51.27		H51	28.6486	2.88
C21	123.9497	59.41		H52	29.3478	2.24
C22	83.8663	97.46		H53	30.6138	1.09
C23	139.7269	44.43		H54	30.6202	1.08
C24	163.7153	21.65		H55	29.9332	1.71
C25	156.9226	28.10		H56	30.0582	1.59
C26	163.183	22.16		H57	30.2636	1.41
C27	162.7765	22.55		H58	30.2833	1.39
				H59	30.6517	1.05
				H60	30.5427	1.15
				H61	30.9495	0.78
				H62	30.6466	1.06
				H63	31.1316	0.61
				H64	30.5686	1.13

Revised Citrinalin B (**2**) neutral form, conformer 4

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1511.302593 H (rel E = 0.30 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.214416	0.334979	0.013936
2	6	-0.249546	1.746129	0.468560
3	7	-1.624018	1.734611	0.547059
4	6	-6.189762	-0.762308	-0.151701
5	6	-5.972895	0.756157	-0.230332
6	6	-4.585981	1.190004	0.188210
7	6	-3.517139	0.234654	-0.096844
8	6	-3.820326	-1.038396	-0.651138
9	6	-2.797564	-1.911266	-1.038718
10	6	-1.454979	-1.551126	-0.863787
11	6	-1.118725	-0.330364	-0.281307
12	6	-2.155137	0.541547	0.075428
13	6	1.129567	-0.343394	1.131493
14	6	2.500582	0.371022	0.880218
15	6	3.762967	-0.212630	1.561855
16	6	4.579398	-1.163408	0.688131
17	6	6.005660	-1.480110	1.168772
18	6	6.805980	-1.733230	-0.142691
19	6	5.798950	-1.441925	-1.276912
20	7	4.806308	-0.568747	-0.640487
21	6	3.561800	-0.427882	-1.369216
22	6	2.604654	0.559879	-0.655928
23	6	1.161772	0.457440	-1.208636
24	6	-6.215061	-1.270566	1.293291
25	6	-7.452827	-1.173274	-0.899327
26	6	1.187941	-1.870963	0.943162
27	6	0.627882	-0.074698	2.561477
28	7	3.187598	1.964149	-0.976492
29	8	0.450628	2.723553	0.707316
30	8	-4.373939	2.305428	0.680052
31	8	-5.095528	-1.444073	-0.864732
32	8	3.060527	2.373968	-2.133377
33	8	3.793777	2.578507	-0.104144
34	1	-2.198740	2.532771	0.797660
35	1	-6.105112	1.090667	-1.269385
36	1	-6.716408	1.277336	0.378533
37	1	-3.060426	-2.869506	-1.474409
38	1	-0.683806	-2.240363	-1.191337
39	1	2.365920	1.375455	1.284546
40	1	4.414223	0.623417	1.840534
41	1	3.480256	-0.715237	2.493539
42	1	4.030662	-2.116609	0.561061
43	1	6.416810	-0.622912	1.713703
44	1	6.018879	-2.339754	1.845559
45	1	7.666105	-1.059805	-0.206781
46	1	7.185878	-2.756849	-0.208482
47	1	6.247534	-0.952277	-2.147405
48	1	5.327943	-2.381996	-1.622206
49	1	3.752487	-0.079778	-2.389039
50	1	3.032398	-1.393935	-1.446151
51	1	0.902043	1.299806	-1.851136
52	1	1.077560	-0.445848	-1.817365
53	1	-6.335093	-2.358186	1.308686
54	1	-7.060084	-0.822948	1.826457
55	1	-5.300827	-1.015469	1.838525
56	1	-7.582614	-2.259842	-0.869632
57	1	-7.407947	-0.852993	-1.944932
58	1	-8.327573	-0.709825	-0.432573
59	1	1.929609	-2.296718	1.626029
60	1	1.454206	-2.175381	-0.072021

61	1	0.223828	-2.324087	1.190986
62	1	1.271721	-0.581436	3.288536
63	1	-0.386868	-0.465418	2.698392
64	1	0.624736	0.990918	2.810655

Revised Citrinalin B (**2**) neutral form, conformer 5

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = H (rel E = kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.210446	0.301357	0.089508
2	6	-0.262755	1.746771	0.407075
3	7	-1.630791	1.720748	0.558073
4	6	-6.190492	-0.679622	-0.402539
5	6	-5.975944	0.441863	0.625321
6	6	-4.589059	1.043528	0.577117
7	6	-3.517991	0.121376	0.202664
8	6	-3.820295	-1.204555	-0.209148
9	6	-2.798697	-2.100748	-0.542107
10	6	-1.456524	-1.704734	-0.467979
11	6	-1.120447	-0.415365	-0.059523
12	6	-2.157569	0.475007	0.246223
13	6	1.192858	-0.231014	1.228904
14	6	2.534321	0.471553	0.829028
15	6	3.843653	-0.006625	1.505042
16	6	4.634073	-1.041974	0.706720
17	6	6.089180	-1.280892	1.147649
18	6	6.838667	-1.638738	-0.170109
19	6	5.764345	-1.522884	-1.272049
20	7	4.781143	-0.601999	-0.691618
21	6	3.498306	-0.568046	-1.365281
22	6	2.559493	0.482835	-0.721777
23	6	1.093338	0.301800	-1.186430
24	6	-7.454612	-1.472781	-0.092636
25	6	-6.210788	-0.150818	-1.840413
26	6	1.275544	-1.769144	1.214222
27	6	0.751865	0.190646	2.641643
28	7	3.100755	1.848348	-1.229817
29	8	0.425652	2.757088	0.495033
30	8	-4.378796	2.222733	0.887452
31	8	-5.095564	-1.658685	-0.284380
32	8	2.909939	2.120123	-2.418200
33	8	3.736254	2.567474	-0.464976
34	1	-2.209993	2.532075	0.747020
35	1	-6.718925	1.231679	0.486447
36	1	-6.108845	0.038422	1.639535
37	1	-3.062334	-3.100516	-0.870770
38	1	-0.687037	-2.415061	-0.751779
39	1	2.397501	1.513534	1.122853
40	1	4.489664	0.868129	1.639560
41	1	3.623871	-0.394352	2.506053
42	1	4.099258	-2.010877	0.718518
43	1	6.502475	-0.369304	1.593599
44	1	6.152916	-2.074500	1.898213
45	1	7.654697	-0.932766	-0.352605
46	1	7.272256	-2.642634	-0.145663
47	1	6.148652	-1.135788	-2.221360
48	1	5.307591	-2.511742	-1.468534
49	1	3.629210	-0.339492	-2.427350
50	1	2.986246	-1.543937	-1.299602
51	1	0.787372	1.067371	-1.900598
52	1	0.994655	-0.662077	-1.691589
53	1	-7.576822	-2.296151	-0.803679
54	1	-8.329965	-0.820365	-0.170168
55	1	-7.418672	-1.885167	0.920572
56	1	-7.056868	0.531560	-1.970847
57	1	-6.324253	-0.979918	-2.545613
58	1	-5.296571	0.395346	-2.093917

59	1	2.063402	-2.100445	1.897478
60	1	1.492830	-2.184728	0.227216
61	1	0.337258	-2.207650	1.566214
62	1	1.433500	-0.227304	3.390521
63	1	-0.250415	-0.192840	2.864352
64	1	0.744228	1.277179	2.773281

Revised Citrinalin B (**2**) TFA salt form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.077583 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.271075	-1.292610	0.138712
2	6	1.022495	-2.625946	-0.130432
3	7	2.374460	-2.370899	-0.050355
4	6	6.286799	1.095600	-0.148088
5	6	6.395599	-0.343598	0.381742
6	6	5.138170	-1.159648	0.144648
7	6	3.889633	-0.400354	0.188009
8	6	3.903368	1.013616	0.315129
9	6	2.711219	1.739745	0.389055
10	6	1.477266	1.078187	0.351386
11	6	1.425404	-0.312207	0.248641
12	6	2.628946	-1.019002	0.137759
13	6	-0.687064	-1.463852	1.402522
14	6	-1.947025	-2.169829	0.769200
15	6	-3.325151	-1.957674	1.426197
16	6	-4.023037	-0.622325	1.139017
17	6	-5.539084	-0.600368	1.374394
18	6	-6.028462	0.535704	0.466489
19	6	-5.204058	0.341011	-0.804331
20	7	-3.854185	-0.168282	-0.320188
21	6	-3.299021	-1.200457	-1.238362
22	6	-1.968160	-1.820150	-0.744264
23	6	-0.714564	-0.979577	-1.013568
24	6	7.417195	1.970220	0.387959
25	6	6.233797	1.141443	-1.681495
26	6	-0.977839	-0.093077	2.042754
27	6	-0.083021	-2.355764	2.506394
28	7	-1.950323	-3.132617	-1.602526
29	8	0.520397	-3.715410	-0.357569
30	8	5.177683	-2.380833	-0.021614
31	8	5.066265	1.713058	0.376653
32	8	-1.456389	-3.068467	-2.721158
33	8	-2.545556	-4.103903	-1.148425
34	1	3.113157	-3.052521	-0.188471
35	1	7.246004	-0.863935	-0.067270
36	1	6.561527	-0.319585	1.468171
37	1	2.760068	2.820455	0.458041
38	1	0.567416	1.668903	0.380179
39	1	-1.751670	-3.242025	0.824169
40	1	-3.975605	-2.774211	1.090831
41	1	-3.243934	-2.065660	2.513414
42	1	-3.566414	0.179971	1.720047
43	1	-5.985254	-1.558045	1.076522
44	1	-5.772915	-0.439144	2.430420
45	1	-5.803410	1.515323	0.898189
46	1	-7.100540	0.488559	0.257920
47	1	-5.637735	-0.422706	-1.456558
48	1	-5.040891	1.265024	-1.360416
49	1	-4.048720	-1.989521	-1.342959
50	1	-3.154836	-0.726757	-2.213077
51	1	-0.301752	-1.181205	-2.003467
52	1	-0.976396	0.081199	-0.974232
53	1	7.301932	2.998813	0.034065
54	1	8.384525	1.591208	0.043880
55	1	7.413314	1.978843	1.481723
56	1	7.160320	0.737909	-2.102292
57	1	6.119368	2.174894	-2.020082
58	1	5.400068	0.555551	-2.079362

59	1	-1.694442	-0.205119	2.863341
60	1	-1.360873	0.651285	1.341932
61	1	-0.061413	0.309393	2.481484
62	1	-0.777088	-2.428399	3.351642
63	1	0.846122	-1.920225	2.890155
64	1	0.125353	-3.370216	2.158313
65	1	-3.183799	0.706875	-0.334884
66	6	-1.851588	4.210667	-0.324698
67	6	-2.846544	3.009576	-0.275859
68	8	-2.261761	1.878437	-0.405801
69	8	-4.046775	3.242645	-0.129228
70	9	-0.859329	4.058773	0.595739
71	9	-1.255332	4.293936	-1.541195
72	9	-2.443135	5.391453	-0.081901

Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.4898	61.74		H34	22.3635	8.63
C2	-2.0658	179.04		H35	29.0611	2.51
C4	100.0642	82.08		H36	28.6686	2.86
C5	136.4545	47.54		H37	24.8173	6.39
C6	-16.7609	193.00		H38	23.4957	7.59
C7	79.2141	101.88		H39	27.6258	3.82
C8	19.7247	158.36		H40	29.4633	2.14
C9	72.935	107.84		H41	29.4876	2.12
C10	44.9434	134.41		H42	27.9289	3.54
C11	61.2803	118.90		H43	30.0097	1.64
C12	36.0348	142.87		H44	29.3485	2.24
C13	129.4762	54.16		H45	29.4028	2.19
C14	135.0717	48.85		H46	29.747	1.88
C15	159.321	25.83		H47	29.0216	2.54
C16	123.8606	59.49		H48	27.482	3.95
C17	151.0134	33.71		H49	28.8379	2.71
C18	159.7808	25.39		H50	28.2353	3.26
C19	126.4908	56.99		H51	28.4377	3.08
C21	129.3736	54.26		H52	27.9844	3.49
C22	82.667	98.60		H53	30.0185	1.63
C23	143.0544	41.27		H54	30.2474	1.42
C24	156.5986	28.41		H55	30.2394	1.43
C25	163.7213	21.65		H56	30.6162	1.08
C26	162.7772	22.55		H57	30.5791	1.12
C27	161.3321	23.92		H58	30.0078	1.64
				H59	30.7248	0.98
				H60	29.6707	1.95
				H61	31.0734	0.67
				H62	30.6622	1.04
				H63	31.3259	0.44
				H64	30.7035	1.00
				H65	15.8917	14.55

Revised Citrinalin B (**2**) TFA salt form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.074245 H (rel E = 2.09 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.236710	-1.202965	0.011023
2	6	0.904923	-2.470344	-0.591991
3	7	2.267080	-2.259762	-0.608488
4	6	6.379555	0.837175	0.341688
5	6	6.322142	-0.269684	-0.723641
6	6	5.059780	-1.108064	-0.642662
7	6	3.871358	-0.396869	-0.174582
8	6	3.954351	0.958565	0.239643
9	6	2.803445	1.680039	0.570088
10	6	1.547029	1.062883	0.528331
11	6	1.432990	-0.284102	0.183652
12	6	2.591853	-0.977833	-0.186613
13	6	-0.592472	-1.603209	1.311839
14	6	-1.927506	-2.162187	0.686523
15	6	-3.223460	-2.092911	1.511316
16	6	-3.904906	-0.720052	1.606317
17	6	-5.404780	-0.793714	1.997816
18	6	-6.177707	-0.397912	0.728018
19	6	-5.248372	0.617510	0.072864
20	7	-3.864442	0.041509	0.275033
21	6	-3.446309	-0.764417	-0.911991
22	6	-2.101732	-1.504508	-0.710244
23	6	-0.851006	-0.648031	-0.940023
24	6	6.543369	0.265307	1.756915
25	6	7.478549	1.849814	0.029590
26	6	-0.775099	-0.376675	2.227660
27	6	0.093936	-2.695202	2.157228
28	7	-2.226171	-2.612195	-1.810190
29	8	0.342751	-3.486976	-0.966708
30	8	5.040509	-2.288014	-0.999986
31	8	5.140567	1.616887	0.296260
32	8	-1.817067	-2.349215	-2.932579
33	8	-2.837381	-3.631045	-1.501263
34	1	2.960465	-2.912271	-0.959202
35	1	6.339331	0.185879	-1.723886
36	1	7.191200	-0.929443	-0.651699
37	1	2.902230	2.721642	0.853621
38	1	0.668010	1.654541	0.764111
39	1	-1.749484	-3.222118	0.497072
40	1	-3.928920	-2.806716	1.068617
41	1	-3.043647	-2.443221	2.533927
42	1	-3.366138	-0.080188	2.304005
43	1	-5.616543	-0.084054	2.803885
44	1	-5.670377	-1.790696	2.360438
45	1	-6.332223	-1.263304	0.073790
46	1	-7.160152	0.029996	0.943033
47	1	-5.267491	1.577654	0.595615
48	1	-5.407794	0.808136	-0.988001
49	1	-4.235520	-1.490845	-1.120569
50	1	-3.371647	-0.060456	-1.744429
51	1	-0.552453	-0.639858	-1.989453
52	1	-1.072071	0.382889	-0.652124
53	1	6.538303	1.076434	2.490374
54	1	7.494566	-0.270531	1.837564
55	1	5.740895	-0.433453	2.010812
56	1	7.479299	2.651374	0.773945
57	1	7.323936	2.295221	-0.957313
58	1	8.457881	1.361436	0.044279

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    59          1           -1.401722   -0.638093    3.086786
    60          1           -1.209096    0.493971    1.731791
    61          1            0.194008   -0.073227    2.631953
    62          1           -0.511181   -2.922946    3.042346
    63          1            1.069759   -2.348758    2.515123
    64          1            0.236811   -3.625983    1.603146
    65          1           -3.182922    0.903371    0.361979
    66          6           -1.853276    4.229203   -0.531993
    67          6           -2.566876    2.842930   -0.566422
    68          8           -2.351937    2.139882    0.481072
    69          8           -3.251363    2.552918   -1.551258
    70          9           -2.352783    5.001975    0.466312
    71          9           -0.520901    4.086415   -0.300339
    72          9           -1.988556    4.914140   -1.679577
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.6246	61.61		H34	22.4049	8.59
C2	-1.967	178.95		H35	28.6713	2.86
C4	101.5322	80.69		H36	28.9818	2.58
C5	136.2481	47.73		H37	24.8096	6.39
C6	-16.372	192.63		H38	23.7708	7.34
C7	78.7415	102.33		H39	27.8336	3.63
C8	19.5876	158.49		H40	29.447	2.15
C9	73.8326	106.99		H41	29.4478	2.15
C10	45.2745	134.10		H42	27.6792	3.77
C11	61.8102	118.40		H43	29.3711	2.22
C12	36.0655	142.84		H44	29.857	1.78
C13	130.001	53.66		H45	29.7179	1.91
C14	134.6324	49.27		H46	29.7009	1.92
C15	158.0446	27.04		H47	28.4476	3.07
C16	126.5776	56.91		H48	28.4588	3.06
C17	150.7595	33.95		H49	28.7413	2.80
C18	161.7979	23.47		H50	27.6827	3.77
C19	126.9096	56.60		H51	28.4503	3.06
C21	131.2449	52.48		H52	28.5219	3.00
C22	83.3668	97.94		H53	30.5692	1.13
C23	143.5379	40.81		H54	30.6494	1.05
C24	163.8499	21.53		H55	30.0351	1.62
C25	157.5642	27.49		H56	30.1125	1.54
C26	162.7282	22.59		H57	30.2033	1.46
C27	162.3438	22.96		H58	30.3901	1.29
				H59	30.7149	0.99
				H60	29.7418	1.88
				H61	30.9998	0.73
				H62	30.5764	1.12
				H63	31.2374	0.52
				H64	30.6181	1.08
				H65	15.4915	14.91

Revised Citrinalin B (**2**) TFA salt form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.075705 H (rel E = 1.18 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.289386	-1.250012	0.150186
2	6	1.028179	-2.606278	-0.025693
3	7	2.382069	-2.360956	0.050653
4	6	6.338237	1.046031	-0.216785
5	6	6.421119	-0.357985	0.404499
6	6	5.156657	-1.172311	0.201759
7	6	3.917536	-0.396780	0.178747
8	6	3.947348	1.021951	0.215279
9	6	2.763279	1.764936	0.227363
10	6	1.521749	1.116487	0.217810
11	6	1.453672	-0.276891	0.204305
12	6	2.650023	-1.002714	0.153027
13	6	-0.676451	-1.328679	1.417247
14	6	-1.940188	-2.063619	0.824979
15	6	-3.319298	-1.789114	1.450624
16	6	-3.996402	-0.461647	1.076172
17	6	-5.525926	-0.445602	1.325693
18	6	-6.169462	-0.480778	-0.070530
19	6	-5.180532	0.320682	-0.910491
20	7	-3.819717	-0.120274	-0.412453
21	6	-3.269491	-1.223461	-1.251796
22	6	-1.949119	-1.819064	-0.707849
23	6	-0.688824	-1.004355	-1.024276
24	6	7.471710	1.938867	0.281477
25	6	6.309564	0.994236	-1.750622
26	6	-0.958620	0.083369	1.964738
27	6	-0.085623	-2.151069	2.580287
28	7	-1.934693	-3.185392	-1.476029
29	8	0.515982	-3.702752	-0.185947
30	8	5.182525	-2.402026	0.114700
31	8	5.117863	1.710295	0.247764
32	8	-1.432990	-3.199379	-2.593050
33	8	-2.540990	-4.119610	-0.962810
34	1	3.114514	-3.058025	-0.033202
35	1	7.270396	-0.915915	0.000850
36	1	6.573373	-0.267829	1.489466
37	1	2.824522	2.847209	0.229192
38	1	0.619751	1.719650	0.199468
39	1	-1.757604	-3.131682	0.954918
40	1	-3.979639	-2.616953	1.163783
41	1	-3.252464	-1.824936	2.543625
42	1	-3.529917	0.368997	1.601864
43	1	-5.804475	0.477527	1.841668
44	1	-5.833297	-1.287243	1.953030
45	1	-6.260625	-1.508533	-0.441132
46	1	-7.166794	-0.034108	-0.088538
47	1	-5.241343	0.156127	-1.988108
48	1	-5.247397	1.390815	-0.696503
49	1	-4.026024	-2.009901	-1.315032
50	1	-3.105736	-0.814477	-2.251898
51	1	-0.273192	-1.268654	-1.998129
52	1	-0.945170	0.058452	-1.052577
53	1	7.377096	2.944140	-0.139131
54	1	8.439100	1.525720	-0.020619
55	1	7.449771	2.017386	1.372254
56	1	6.213276	2.004843	-2.156968
57	1	5.474935	0.393473	-2.123777
58	1	7.237380	0.553473	-2.129104

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    59          1           -1.686311    0.032114    2.781100
    60          1           -1.328432    0.782756    1.212303
    61          1           -0.043517    0.506029    2.387046
    62          1           -0.780614   -2.155930    3.427727
    63          1            0.849754   -1.703506    2.933732
    64          1            0.108349   -3.189600    2.301842
    65          1           -3.153942    0.754750   -0.498507
    66          6           -1.977617    4.273799   -0.269114
    67          6           -2.849122    2.985238   -0.154786
    68          8           -2.278538    1.953301   -0.649242
    69          8           -3.957571    3.065400    0.381037
    70          9           -0.772672    4.094601    0.341679
    71          9           -1.725945    4.577843   -1.566044
    72          9           -2.553637    5.348327    0.294479
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.6753	61.57		H34	22.3486	8.64
C2	-2.0723	179.05		H35	29.0646	2.50
C4	100.6494	81.53		H36	28.6612	2.87
C5	136.3497	47.63		H37	24.8385	6.37
C6	-16.7494	192.98		H38	23.5348	7.56
C7	79.3416	101.76		H39	27.723	3.73
C8	19.824	158.26		H40	29.5306	2.08
C9	72.9737	107.80		H41	29.5421	2.07
C10	44.9717	134.39		H42	27.5542	3.88
C11	61.386	118.80		H43	29.3081	2.28
C12	35.9991	142.91		H44	29.9032	1.74
C13	129.2905	54.34		H45	29.7142	1.91
C14	135.9658	48.00		H46	29.648	1.97
C15	158.5335	26.57		H47	28.8562	2.69
C16	125.5461	57.89		H48	27.2667	4.15
C17	151.5306	33.22		H49	28.7172	2.82
C18	161.54	23.72		H50	28.3089	3.19
C19	128.477	55.11		H51	28.4003	3.11
C21	130.8921	52.82		H52	28.1178	3.37
C22	83.7003	97.62		H53	30.0267	1.62
C23	143.0408	41.28		H54	30.2636	1.41
C24	156.7742	28.24		H55	30.206	1.46
C25	163.8116	21.56		H56	30.548	1.15
C26	162.542	22.77		H57	30.0621	1.59
C27	161.3544	23.90		H58	30.6575	1.05
				H59	30.6794	1.03
				H60	29.8569	1.78
				H61	31.082	0.66
				H62	30.6634	1.04
				H63	31.3429	0.42
				H64	30.6699	1.03
				H65	15.6769	14.74

Revised Citrinalin B (**2**) TFA salt form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.076304 H (rel E = 0.80 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.225583	-0.000557	0.013015
2	6	1.447399	-1.460335	0.509183
3	7	2.810566	-1.678269	0.577250
4	6	7.711967	-0.003801	-0.162275
5	6	7.250884	-1.469426	-0.213484
6	6	5.805002	-1.654468	0.207738
7	6	4.917817	-0.534041	-0.105381
8	6	5.431358	0.653784	-0.688048
9	6	4.573790	1.679507	-1.096128
10	6	3.190374	1.555658	-0.910089
11	6	2.650194	0.425819	-0.299075
12	6	3.525663	-0.604366	0.075306
13	6	0.437153	0.840328	1.111338
14	6	-1.028460	0.332640	0.891905
15	6	-2.187023	1.115439	1.556853
16	6	-2.805522	2.191437	0.669388
17	6	-4.115493	2.835604	1.145962
18	6	-4.820874	3.279240	-0.170238
19	6	-3.946940	2.699739	-1.306885
20	7	-3.181293	1.616201	-0.647752
21	6	-1.989847	1.197630	-1.387727
22	6	-1.176718	0.113863	-0.637319
23	6	0.261600	-0.003630	-1.202776
24	6	7.798006	0.522267	1.277169
25	6	9.036798	0.185958	-0.896066
26	6	0.609143	2.352815	0.871555
27	6	0.915644	0.542827	2.544531
28	7	-1.942135	-1.215994	-0.912030
29	8	0.593614	-2.284326	0.785602
30	8	5.408768	-2.700485	0.724870
31	8	6.760051	0.828535	-0.904286
32	8	-1.862240	-1.667400	-2.052901
33	8	-2.616999	-1.698122	-0.013138
34	1	3.251994	-2.550422	0.849546
35	1	7.332921	-1.841897	-1.244376
36	1	7.885915	-2.102116	0.412620
37	1	4.999929	2.564985	-1.553950
38	1	2.548753	2.362140	-1.250770
39	1	-1.046119	-0.670189	1.322090
40	1	-2.975562	0.403995	1.820501
41	1	-1.843651	1.566781	2.495014
42	1	-2.070801	2.994968	0.480477
43	1	-4.719274	2.097591	1.680979
44	1	-3.924915	3.672548	1.823616
45	1	-5.837715	2.881124	-0.219475
46	1	-4.894362	4.366652	-0.257021
47	1	-4.523145	2.301492	-2.147187
48	1	-3.254174	3.463358	-1.698789
49	1	-2.272551	0.818722	-2.374778
50	1	-1.331033	2.067964	-1.543766
51	1	0.374900	-0.890503	-1.827431
52	1	0.479666	0.858375	-1.839540
53	1	8.088249	1.576607	1.273125
54	1	8.548745	-0.042648	1.838853
55	1	6.843886	0.429554	1.804156
56	1	9.331390	1.239369	-0.883316
57	1	8.951207	-0.136708	-1.937629
58	1	9.823923	-0.400019	-0.411590

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    59          1           -0.029417    2.914206    1.559948
    60          1            0.353341    2.665539   -0.145142
    61          1            1.640577    2.658266    1.066972
    62          1            0.368583    1.159646    3.265382
    63          1            1.979381    0.781694    2.655691
    64          1            0.763646   -0.503620    2.822614
    65          1           -4.387775    0.433471   -0.595389
    66          6           -6.930912   -1.600999   -0.089517
    67          6           -5.762777   -0.645126    0.278134
    68          8           -5.176468   -0.189601   -0.808627
    69          8           -5.511491   -0.370456    1.430878
    70          9           -7.951733   -0.886305   -0.628377
    71          9           -6.558010   -2.530163   -0.989194
    72          9           -7.398168   -2.230919    0.996979
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.7784	61.47		H34	22.2473	8.74
C2	-2.429	179.39		H35	28.6954	2.84
C4	98.8563	83.23		H36	29.1013	2.47
C5	136.9278	47.09		H37	24.9061	6.31
C6	-16.1239	192.39		H38	24.0528	7.09
C7	78.024	103.01		H39	27.5392	3.90
C8	19.767	158.32		H40	29.1218	2.45
C9	74.9537	105.92		H41	29.7962	1.83
C10	47.6004	131.89		H42	29.2858	2.30
C11	61.4719	118.72		H43	29.6866	1.93
C12	35.217	143.65		H44	29.857	1.78
C13	129.8306	53.82		H45	29.8458	1.79
C14	138.0395	46.03		H46	29.9035	1.74
C15	159.4587	25.70		H47	28.6883	2.85
C16	120.5849	62.60		H48	29.5109	2.09
C17	155.7649	29.20		H49	27.8088	3.65
C18	164.0716	21.32		H50	29.0113	2.55
C19	130.1799	53.49		H51	28.7022	2.83
C21	119.0285	64.08		H52	29.0678	2.50
C22	83.7858	97.54		H53	30.6193	1.08
C23	138.2292	45.85		H54	30.5386	1.16
C24	163.5709	21.79		H55	29.8802	1.76
C25	156.5439	28.46		H56	30.0155	1.63
C26	163.0092	22.32		H57	30.2815	1.39
C27	163.7637	21.61		H58	30.2593	1.41
				H59	30.6711	1.03
				H60	30.4894	1.20
				H61	30.8218	0.90
				H62	30.5776	1.12
				H63	31.12	0.62
				H64	30.8067	0.91
				H65	16.9467	13.58

Revised Citrinalin B (**2**) TFA salt form, conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.076437 H (rel E = 0.72 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.229395	0.064590	0.176874
2	6	1.462341	-1.386573	0.692824
3	7	2.826684	-1.579436	0.802941
4	6	7.667404	-0.168165	-0.569015
5	6	7.316287	-1.079953	0.618295
6	6	5.841602	-1.433110	0.678413
7	6	4.933777	-0.392618	0.194027
8	6	5.441606	0.791899	-0.399727
9	6	4.579083	1.804374	-0.829246
10	6	3.193875	1.661799	-0.672878
11	6	2.655228	0.517352	-0.088318
12	6	3.537214	-0.496556	0.313875
13	6	0.382103	0.897088	1.237320
14	6	-1.065289	0.363707	0.961674
15	6	-2.261716	1.135796	1.570494
16	6	-2.858651	2.193233	0.646913
17	6	-4.195997	2.823248	1.062888
18	6	-4.852082	3.245172	-0.285487
19	6	-3.924965	2.665902	-1.379520
20	7	-3.172547	1.599830	-0.678462
21	6	-1.946256	1.191075	-1.364876
22	6	-1.147430	0.128724	-0.570016
23	6	0.314075	0.031807	-1.075650
24	6	9.065402	0.425283	-0.417932
25	6	7.517741	-0.893393	-1.913466
26	6	0.536716	2.411575	0.997633
27	6	0.807397	0.614904	2.690439
28	7	-1.878657	-1.216500	-0.861858
29	8	0.615483	-2.224239	0.948679
30	8	5.447713	-2.502363	1.147236
31	8	6.773815	0.994185	-0.566309
32	8	-1.742880	-1.679151	-1.992933
33	8	-2.583803	-1.699511	0.013019
34	1	3.274791	-2.440589	1.097894
35	1	7.900373	-2.003771	0.589405
36	1	7.562062	-0.565421	1.558037
37	1	5.001862	2.687666	-1.294311
38	1	2.548700	2.456754	-1.033089
39	1	-1.086427	-0.635443	1.400259
40	1	-3.050047	0.415932	1.811160
41	1	-1.962582	1.602441	2.516148
42	1	-2.128275	3.005442	0.479588
43	1	-4.811551	2.081797	1.579455
44	1	-4.045199	3.668772	1.739914
45	1	-5.861113	2.833821	-0.372438
46	1	-4.935222	4.330691	-0.386237
47	1	-4.461355	2.251617	-2.238199
48	1	-3.226810	3.434866	-1.750785
49	1	-2.183470	0.796716	-2.357859
50	1	-1.295002	2.069735	-1.505259
51	1	0.468399	-0.858537	-1.686453
52	1	0.542139	0.891794	-1.711705
53	1	9.283310	1.102107	-1.249216
54	1	9.815571	-0.371539	-0.413957
55	1	9.147381	0.987788	0.516563
56	1	8.220031	-1.731282	-1.968307
57	1	7.733475	-0.205294	-2.735549
58	1	6.508627	-1.291864	-2.053901

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     59          1           -0.137816    2.964162    1.658277
     60          1            0.315021    2.716486   -0.029413
     61          1            1.553995    2.736255    1.232016
     62          1            0.221532    1.225703    3.385445
     63          1            1.861512    0.872806    2.842862
     64          1            0.662340   -0.432636    2.967839
     65          1           -4.361846    0.400145   -0.660813
     66          6           -6.886414   -1.675501   -0.235365
     67          6           -5.750883   -0.695315    0.168513
     68          8           -5.131046   -0.238377   -0.898864
     69          8           -5.549033   -0.406670    1.327533
     70          9           -7.894911   -0.985758   -0.827167
     71          9           -6.459725   -2.609790   -1.105467
     72          9           -7.389158   -2.299276    0.838775
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.9438	61.31		H34	22.2924	8.70
C2	-2.3635	179.33		H35	29.0776	2.49
C4	100.8035	81.38		H36	28.6668	2.87
C5	136.4187	47.57		H37	24.7988	6.40
C6	-16.3883	192.64		H38	24.0166	7.12
C7	77.1225	103.86		H39	27.5271	3.91
C8	19.588	158.49		H40	29.1199	2.45
C9	74.6858	106.18		H41	29.798	1.83
C10	47.736	131.76		H42	29.2715	2.31
C11	61.2709	118.91		H43	29.6795	1.94
C12	35.2228	143.64		H44	29.8252	1.81
C13	129.7087	53.94		H45	29.8393	1.79
C14	137.9161	46.15		H46	29.884	1.75
C15	159.4763	25.68		H47	28.7007	2.84
C16	120.5027	62.68		H48	29.5034	2.10
C17	155.6402	29.32		H49	27.7843	3.67
C18	163.8793	21.50		H50	29.0038	2.56
C19	130.1364	53.53		H51	28.6735	2.86
C21	118.9227	64.18		H52	29.0874	2.48
C22	83.7786	97.55		H53	30.1015	1.55
C23	138.0149	46.05		H54	30.359	1.32
C24	157.1414	27.90		H55	30.201	1.46
C25	163.5968	21.77		H56	30.6622	1.04
C26	163.0105	22.32		H57	30.6507	1.05
C27	163.7231	21.65		H58	30.0317	1.62
				H59	30.6821	1.02
				H60	30.4842	1.20
				H61	30.8327	0.89
				H62	30.5813	1.12
				H63	31.1679	0.58
				H64	30.8157	0.90
				H65	16.9256	13.60

Revised Citrinalin B (**2**) TFA salt form, conformer 6

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.066627 H (rel E = 6.87 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.085655	-1.553949	-0.420500
2	6	0.870303	-2.404941	-1.465566
3	7	2.220249	-2.173514	-1.258547
4	6	6.014933	0.801062	0.781092
5	6	6.074071	0.075211	-0.572565
6	6	4.892251	-0.847017	-0.809149
7	6	3.638649	-0.422781	-0.188280
8	6	3.590437	0.746863	0.615437
9	6	2.370286	1.246868	1.076789
10	6	1.176535	0.574930	0.783402
11	6	1.189773	-0.616635	0.060760
12	6	2.417393	-1.072633	-0.437661
13	6	-0.552206	-2.525626	0.717243
14	6	-2.003301	-1.954115	0.925755
15	6	-2.087392	-0.878372	2.027163
16	6	-3.371686	-0.057520	2.039774
17	6	-4.717009	-0.720539	2.378342
18	6	-5.776260	0.218146	1.730988
19	6	-4.970692	1.206004	0.849629
20	7	-3.613673	0.578622	0.699353
21	6	-3.609311	-0.386364	-0.439862
22	6	-2.414111	-1.373444	-0.445349
23	6	-1.125675	-0.820839	-1.065313
24	6	6.213678	-0.161546	1.960267
25	6	7.019113	1.949776	0.836820
26	6	0.283768	-2.550461	2.010419
27	6	-0.664190	-3.998982	0.249869
28	7	-3.018092	-2.510590	-1.349236
29	8	0.409703	-3.142492	-2.314929
30	8	4.985057	-1.846242	-1.525822
31	8	4.710094	1.449608	0.925281
32	8	-2.832787	-2.439672	-2.554032
33	8	-3.731006	-3.346800	-0.793930
34	1	2.967533	-2.563365	-1.823914
35	1	6.065984	0.816674	-1.383948
36	1	6.998251	-0.501290	-0.668700
37	1	2.363001	2.170363	1.644274
38	1	0.244106	1.030295	1.103965
39	1	-2.682800	-2.768221	1.187782
40	1	-1.976987	-1.356849	3.005090
41	1	-1.256322	-0.174172	1.938655
42	1	-3.221880	0.791256	2.717773
43	1	-4.840562	-0.811372	3.460509
44	1	-4.778747	-1.729684	1.960016
45	1	-6.496960	-0.350641	1.137783
46	1	-6.347084	0.767930	2.483412
47	1	-5.390654	1.401759	-0.136903
48	1	-4.815339	2.167416	1.344729
49	1	-4.540280	-0.955897	-0.398089
50	1	-3.604428	0.219129	-1.350373
51	1	-1.146722	-0.931113	-2.151085
52	1	-1.068052	0.248676	-0.846658
53	1	6.125352	0.382353	2.904931
54	1	7.209085	-0.614522	1.911626
55	1	5.475513	-0.968760	1.957277
56	1	6.934720	2.482553	1.788471
57	1	6.836835	2.660900	0.026060
58	1	8.039509	1.565166	0.743418

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    59          1           -0.193560   -3.201201    2.752117
    60          1            0.434084   -1.568251    2.460389
    61          1            1.274707   -2.966740    1.804226
    62          1           -1.218312   -4.568421    1.003306
    63          1            0.326880   -4.451505    0.153821
    64          1           -1.163165   -4.124785   -0.709544
    65          1           -2.842610    1.379801    0.524415
    66          6           -1.307212    4.309235   -0.954136
    67          6           -2.207352    3.066496   -0.682153
    68          8           -1.862088    2.411410    0.364841
    69          8           -3.135453    2.820256   -1.455338
    70          9           -1.370169    5.186687    0.080114
    71          9           -0.007648    3.943399   -1.094197
    72          9           -1.662333    4.972069   -2.067438
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.647	61.59		H34	22.4524	8.55
C2	-2.5254	179.48		H35	28.6845	2.85
C4	100.9014	81.29		H36	29.0989	2.47
C5	136.4238	47.56		H37	24.8604	6.35
C6	-16.4659	192.72		H38	23.4395	7.65
C7	78.9447	102.13		H39	28.2687	3.23
C8	20.4418	157.68		H40	29.4928	2.11
C9	74.3795	106.47		H41	29.3024	2.29
C10	46.7223	132.73		H42	27.9977	3.48
C11	56.074	123.85		H43	29.5888	2.02
C12	36.2705	142.65		H44	29.3611	2.23
C13	129.1715	54.45		H45	29.5926	2.02
C14	137.3237	46.71		H46	29.5364	2.07
C15	160.389	24.81		H47	28.5315	2.99
C16	124.4618	58.92		H48	28.5324	2.99
C17	160.5186	24.69		H49	29.0947	2.48
C18	163.8199	21.56		H50	27.7971	3.66
C19	130.8507	52.86		H51	27.8705	3.59
C21	135.552	48.39		H52	28.8263	2.72
C22	79.0086	102.07		H53	30.6442	1.06
C23	143.1806	41.15		H54	30.6796	1.03
C24	163.605	21.76		H55	29.8479	1.79
C25	156.789	28.23		H56	30.0619	1.59
C26	163.3736	21.98		H57	30.2555	1.41
C27	154.9411	29.98		H58	30.3245	1.35
				H59	31.0708	0.67
				H60	30.8595	0.86
				H61	31.2793	0.48
				H62	30.9028	0.82
				H63	31.1011	0.64
				H64	30.1617	1.50
				H65	13.8852	16.38

Revised Citrinalin B (**2**) TFA salt form, conformer 7

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.067439 H (rel E = 6.37 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.021077	-1.620840	-0.333544
2	6	0.807218	-2.518233	-1.338309
3	7	2.156214	-2.361743	-1.066324
4	6	5.961312	0.858563	0.499550
5	6	6.127232	-0.650622	0.254530
6	6	4.886211	-1.294803	-0.335320
7	6	3.618369	-0.710905	0.100427
8	6	3.597148	0.466547	0.893292
9	6	2.386994	1.029254	1.305395
10	6	1.172533	0.424011	0.956397
11	6	1.152453	-0.752035	0.209284
12	6	2.374941	-1.274091	-0.233706
13	6	-0.736171	-2.550264	0.765493
14	6	-2.161636	-1.895540	0.892187
15	6	-2.249756	-0.818313	1.991235
16	6	-3.486088	0.071038	1.931687
17	6	-4.883911	-0.519354	2.178384
18	6	-5.847398	0.483614	1.479689
19	6	-4.934955	1.428369	0.656730
20	7	-3.608692	0.726112	0.584196
21	6	-3.589975	-0.232907	-0.560214
22	6	-2.457999	-1.290789	-0.498083
23	6	-1.106036	-0.814362	-1.040384
24	6	7.083897	1.403124	1.378854
25	6	5.857929	1.646392	-0.813610
26	6	0.022540	-2.621268	2.103888
27	6	-0.907847	-4.015901	0.291699
28	7	-3.073848	-2.391414	-1.438274
29	8	0.348307	-3.229839	-2.210557
30	8	4.955390	-2.266414	-1.091222
31	8	4.741643	1.089487	1.277893
32	8	-2.810551	-2.337075	-2.629224
33	8	-3.869674	-3.180224	-0.927812
34	1	2.906641	-2.797768	-1.591895
35	1	6.976884	-0.850205	-0.404043
36	1	6.326798	-1.153713	1.211344
37	1	2.404241	1.956460	1.866454
38	1	0.253289	0.927977	1.239879
39	1	-2.900874	-2.669817	1.109726
40	1	-2.221741	-1.302280	2.972260
41	1	-1.378656	-0.159669	1.952628
42	1	-3.333359	0.906828	2.625060
43	1	-5.079635	-0.614749	3.249423
44	1	-4.974144	-1.518753	1.742261
45	1	-6.563846	-0.037841	0.839756
46	1	-6.428193	1.060929	2.203316
47	1	-4.756510	2.377240	1.168080
48	1	-5.283097	1.650646	-0.352056
49	1	-4.554596	-0.744724	-0.581257
50	1	-3.489709	0.375064	-1.463565
51	1	-1.071959	-0.916784	-2.126550
52	1	-0.997394	0.248581	-0.809828
53	1	6.927938	2.467265	1.578380
54	1	8.049134	1.281899	0.877510
55	1	7.116942	0.873126	2.335231
56	1	5.700774	2.707488	-0.601448
57	1	5.030763	1.296199	-1.437931
58	1	6.783080	1.539254	-1.388882

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    59          1           -0.532401   -3.243581    2.815401
    60          1            0.202327   -1.649198    2.564881
    61          1            0.998731   -3.092608    1.953625
    62          1           -1.533978   -4.549631    1.014190
    63          1            0.058724   -4.525848    0.249815
    64          1           -1.361073   -4.115476   -0.693168
    65          1           -2.783612    1.483905    0.465699
    66          6           -0.979799    4.330941   -0.861476
    67          6           -1.945986    3.120268   -0.689197
    68          8           -1.741402    2.459629    0.390645
    69          8           -2.798177    2.909184   -1.554562
    70          9           -1.222267    5.270342    0.089691
    71          9            0.315384    3.949619   -0.730025
    72          9           -1.104813    4.927789   -2.058783
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.6397	61.60		H34	22.5181	8.49
C2	-2.2718	179.24		H35	29.0501	2.52
C4	100.1602	81.99		H36	28.6872	2.85
C5	135.9845	47.98		H37	24.818	6.39
C6	-16.8014	193.03		H38	23.6012	7.50
C7	78.2044	102.84		H39	28.3167	3.19
C8	20.05	158.05		H40	29.509	2.10
C9	73.6155	107.19		H41	29.3203	2.27
C10	46.8766	132.58		H42	28.0278	3.45
C11	55.6433	124.26		H43	29.6226	1.99
C12	36.3525	142.57		H44	29.3886	2.21
C13	129.0626	54.55		H45	29.5872	2.02
C14	137.7445	46.31		H46	29.5143	2.09
C15	160.5183	24.69		H47	28.563	2.96
C16	124.4573	58.93		H48	28.6029	2.92
C17	160.6169	24.60		H49	29.1475	2.43
C18	163.7627	21.61		H50	27.7521	3.70
C19	131.1397	52.58		H51	27.8548	3.61
C21	135.5134	48.43		H52	28.8743	2.68
C22	79.2768	101.82		H53	30.072	1.58
C23	142.9864	41.33		H54	30.3684	1.31
C24	156.918	28.11		H55	30.2256	1.44
C25	163.4599	21.90		H56	30.6236	1.08
C26	163.5251	21.83		H57	29.9461	1.70
C27	154.8449	30.08		H58	30.6993	1.01
				H59	31.0062	0.73
				H60	30.8873	0.84
				H61	31.3164	0.44
				H62	30.9358	0.79
				H63	31.1142	0.63
				H64	30.1216	1.54
				H65	13.8988	16.37

Revised Citrinalin B (**2**) TFA salt form, conformer 8

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.077199 H (rel E = 0.24 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.146750	-0.831778	-0.093481
2	6	1.955986	-2.082137	-0.551312
3	7	3.293289	-1.744016	-0.537133
4	6	7.060264	1.815169	0.189743
5	6	7.147332	0.599820	-0.748261
6	6	5.963902	-0.340050	-0.617914
7	6	4.696089	0.300833	-0.266447
8	6	4.639429	1.693292	0.002097
9	6	3.414383	2.331015	0.223445
10	6	2.224606	1.592658	0.210146
11	6	2.243491	0.214906	-0.002399
12	6	3.477892	-0.398937	-0.255284
13	6	0.345400	-1.160680	1.242882
14	6	-0.861512	-1.977922	0.672404
15	6	-2.059359	-2.275576	1.598064
16	6	-3.174277	-1.223778	1.634777
17	6	-4.505452	-1.751964	2.189031
18	6	-5.192315	-2.440622	0.981073
19	6	-4.572087	-1.794672	-0.279372
20	7	-3.580396	-0.789316	0.254200
21	6	-2.459543	-0.370928	-0.627107
22	6	-1.231588	-1.307383	-0.672690
23	6	0.030727	-0.526791	-1.128623
24	6	7.217256	1.417231	1.663709
25	6	8.072208	2.889079	-0.200215
26	6	-0.069677	0.132501	1.971167
27	6	1.164402	-2.007237	2.234724
28	7	-1.569386	-2.395607	-1.733990
29	8	1.508499	-3.169780	-0.874487
30	8	6.063534	-1.546687	-0.847516
31	8	5.755291	2.463654	0.021715
32	8	-1.542954	-2.048581	-2.909465
33	8	-1.906783	-3.508330	-1.339216
34	1	4.057132	-2.354418	-0.809178
35	1	7.167666	0.944796	-1.791751
36	1	8.067951	0.036159	-0.574485
37	1	3.407546	3.399616	0.405561
38	1	1.287882	2.116914	0.371044
39	1	-0.439648	-2.946705	0.397962
40	1	-2.490260	-3.229954	1.278372
41	1	-1.707723	-2.429687	2.624553
42	1	-2.850332	-0.320260	2.158234
43	1	-4.351703	-2.432792	3.030859
44	1	-5.109207	-0.910597	2.541167
45	1	-6.275307	-2.301861	1.011032
46	1	-5.002043	-3.517335	0.980782
47	1	-4.064550	-2.530877	-0.901190
48	1	-5.281582	-1.238473	-0.895434
49	1	-2.862133	-0.185194	-1.625460
50	1	-2.131228	0.594296	-0.235564
51	1	0.318841	-0.795837	-2.145324
52	1	-0.178436	0.546103	-1.138565
53	1	7.107430	2.297948	2.302540
54	1	8.209631	0.987325	1.832524
55	1	6.473170	0.675646	1.968844
56	1	7.970736	3.762196	0.450774
57	1	7.916829	3.209080	-1.234480
58	1	9.090660	2.500593	-0.103284

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    59          1           -0.701329   -0.107533    2.831690
    60          1           -0.620454    0.837447    1.341852
    61          1            0.810418    0.652004    2.358400
    62          1            0.589278   -2.190950    3.148474
    63          1            2.077598   -1.479123    2.530189
    64          1            1.444603   -2.978087    1.817417
    65          1           -4.172185    0.180916    0.416713
    66          6           -5.963557    3.223048   -0.312495
    67          6           -5.247424    1.846333   -0.458215
    68          8           -4.820720    1.383660    0.659045
    69          8           -5.138306    1.346859   -1.579071
    70          9           -6.932500    3.181774    0.633805
    71          9           -5.074547    4.181788    0.061075
    72          9           -6.536535    3.631134   -1.458271
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.9698	61.29		H34	22.2548	8.73
C2	-2.7775	179.72		H35	28.6728	2.86
C4	101.3425	80.87		H36	29.064	2.50
C5	136.5999	47.40		H37	24.8271	6.38
C6	-15.9615	192.24		H38	23.997	7.14
C7	79.3701	101.73		H39	27.3185	4.10
C8	19.391	158.67		H40	29.4316	2.17
C9	73.6623	107.15		H41	29.8796	1.76
C10	47.394	132.09		H42	28.0726	3.41
C11	61.9614	118.26		H43	29.8443	1.79
C12	35.613	143.27		H44	29.5662	2.04
C13	128.7321	54.87		H45	29.7852	1.84
C14	138.1157	45.96		H46	29.5283	2.08
C15	163.2609	22.09		H47	28.7406	2.80
C16	127.031	56.48		H48	28.0689	3.41
C17	154.9863	29.94		H49	27.5616	3.88
C18	164.0452	21.34		H50	28.458	3.06
C19	137.9585	46.11		H51	28.5922	2.93
C21	130.0816	53.59		H52	29.0241	2.54
C22	89.9511	91.68		H53	30.6135	1.09
C23	137.9513	46.11		H54	30.6939	1.01
C24	163.5773	21.79		H55	29.9267	1.71
C25	157.457	27.60		H56	30.0858	1.57
C26	163.2453	22.10		H57	30.2108	1.45
C27	164.094	21.29		H58	30.3766	1.30
				H59	30.6457	1.06
				H60	30.5615	1.13
				H61	30.7832	0.93
				H62	30.5421	1.15
				H63	31.0137	0.72
				H64	30.6572	1.05
				H65	13.6103	16.63

Revised Citrinalin B (**2**) TFA salt form, conformer 9

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.077171 H (rel E = 0.26 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.144924	-0.863950	-0.002309
2	6	-1.961500	-2.088244	0.510763
3	7	-3.299789	-1.766952	0.420553
4	6	-7.010033	1.897928	0.097867
5	6	-7.214947	0.403673	-0.202034
6	6	-5.996267	-0.438247	0.125457
7	6	-4.709490	0.230632	-0.073223
8	6	-4.653547	1.605428	-0.420286
9	6	-3.427172	2.236967	-0.651355
10	6	-2.232460	1.513686	-0.547501
11	6	-2.246101	0.159730	-0.215379
12	6	-3.484078	-0.447381	0.036823
13	6	-0.284451	-1.279943	-1.275947
14	6	0.900750	-2.043161	-0.595602
15	6	2.139009	-2.398529	-1.444239
16	6	3.243977	-1.338534	-1.517417
17	6	4.601761	-1.886698	-1.980718
18	6	5.263716	-2.456067	-0.697720
19	6	4.564314	-1.750895	0.487180
20	7	3.589976	-0.796978	-0.158569
21	6	2.431112	-0.326380	0.643976
22	6	1.210013	-1.270969	0.710193
23	6	-0.076880	-0.473240	1.054429
24	6	-8.110149	2.745573	-0.534741
25	6	-6.897154	2.171357	1.603591
26	6	0.156608	-0.039823	-2.079013
27	6	-1.056774	-2.201184	-2.238803
28	7	1.512598	-2.272710	1.862938
29	8	-1.518267	-3.144508	0.929856
30	8	-6.092527	-1.612998	0.484447
31	8	-5.775962	2.355925	-0.550319
32	8	1.440193	-1.836648	3.006445
33	8	1.868770	-3.410096	1.567952
34	1	-4.068658	-2.367046	0.700829
35	1	-8.075938	0.008583	0.343762
36	1	-7.417128	0.271811	-1.274465
37	1	-3.422054	3.292752	-0.897062
38	1	-1.295429	2.035216	-0.714897
39	1	0.471648	-2.991906	-0.268079
40	1	2.564420	-3.319856	-1.033132
41	1	1.831859	-2.637029	-2.468766
42	1	2.930365	-0.481242	-2.118534
43	1	4.486592	-2.640192	-2.764815
44	1	5.202635	-1.067740	-2.386229
45	1	6.339764	-2.268866	-0.695372
46	1	5.121317	-3.537656	-0.625466
47	1	4.031120	-2.459407	1.119674
48	1	5.229512	-1.148362	1.109180
49	1	2.792070	-0.063493	1.640914
50	1	2.111935	0.603963	0.169249
51	1	-0.406901	-0.671931	2.074611
52	1	0.122772	0.599959	0.995231
53	1	-7.927696	3.807614	-0.347224
54	1	-9.082545	2.480313	-0.108563
55	1	-8.146959	2.586451	-1.616311
56	1	-6.714612	3.235249	1.778067
57	1	-6.083282	1.602617	2.062841
58	1	-7.828355	1.891204	2.106090

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    59          1             0.830591   -0.338447   -2.887502
    60          1             0.672982    0.714219   -1.478303
    61          1            -0.705808    0.442165   -2.546451
    62          1            -0.447048   -2.436349   -3.117704
    63          1            -1.964235   -1.705247   -2.600223
    64          1            -1.342048   -3.146565   -1.769494
    65          1             4.178416    0.163962   -0.368192
    66          6             5.883599    3.288334    0.217403
    67          6             5.199706    1.903194    0.425518
    68          8             4.822071    1.359667   -0.672511
    69          8             5.062692    1.474185    1.572490
    70          9             6.848885    3.233397   -0.731014
    71          9             4.967815    4.207780   -0.191026
    72          9             6.450369    3.758599    1.342431
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.6546	61.59		H34	22.2125	8.77
C2	-2.6349	179.58		H35	29.0397	2.53
C4	100.2443	81.91		H36	28.721	2.82
C5	136.2332	47.75		H37	24.833	6.37
C6	-16.7924	193.03		H38	23.9949	7.14
C7	78.6075	102.45		H39	27.2943	4.12
C8	19.5659	158.51		H40	29.3777	2.22
C9	73.204	107.58		H41	29.8883	1.75
C10	47.5611	131.93		H42	28.0743	3.41
C11	62.2099	118.02		H43	29.8621	1.77
C12	35.621	143.27		H44	29.5452	2.06
C13	129.0483	54.57		H45	29.808	1.82
C14	138.3386	45.75		H46	29.5755	2.04
C15	163.3979	21.96		H47	28.7533	2.79
C16	126.8329	56.67		H48	28.0514	3.43
C17	155.0097	29.92		H49	27.5566	3.88
C18	164.3745	21.03		H50	28.4345	3.08
C19	138.0162	46.05		H51	28.5739	2.95
C21	129.9812	53.68		H52	29.0211	2.54
C22	89.963	91.67		H53	30.0785	1.58
C23	137.5908	46.46		H54	30.3324	1.34
C24	157.193	27.85		H55	30.2172	1.45
C25	163.7196	21.65		H56	30.5878	1.11
C26	162.9379	22.39		H57	30.004	1.64
C27	163.866	21.51		H58	30.7055	1.00
				H59	30.6857	1.02
				H60	30.5274	1.17
				H61	30.7788	0.94
				H62	30.5278	1.16
				H63	31.0754	0.66
				H64	30.6922	1.01
				H65	13.6554	16.59

Revised Citrinalin B (**2**) TFA salt form, conformer 10

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.073967 H (rel E = 2.27 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.150797	-0.607398	0.152597
2	6	1.837366	-1.913173	-0.342738
3	7	3.190641	-1.666113	-0.445607
4	6	7.240719	1.620259	-0.046248
5	6	7.163615	0.408827	-0.989005
6	6	5.935230	-0.450204	-0.753359
7	6	4.748302	0.275401	-0.298350
8	6	4.810485	1.667887	-0.032119
9	6	3.654191	2.388962	0.282334
10	6	2.419054	1.735026	0.367859
11	6	2.324997	0.358081	0.168581
12	6	3.489522	-0.338482	-0.183269
13	6	0.381929	-0.877908	1.521864
14	6	-0.970718	-1.538548	1.036102
15	6	-2.178261	-1.285493	1.964454
16	6	-3.559701	-1.572161	1.366240
17	6	-3.996521	-3.023210	1.126428
18	6	-5.076355	-2.882476	0.039244
19	6	-4.510090	-1.809921	-0.897088
20	7	-3.743135	-0.876251	0.015152
21	6	-2.522665	-0.237846	-0.562040
22	6	-1.218140	-1.039532	-0.413101
23	6	0.011717	-0.199643	-0.812262
24	6	7.491843	1.202079	1.408970
25	6	8.289271	2.624033	-0.518142
26	6	0.170189	0.451665	2.275344
27	6	1.145110	-1.825866	2.465915
28	7	-1.345618	-2.236691	-1.415346
29	8	1.294529	-2.975555	-0.592531
30	8	5.933604	-1.660723	-0.983843
31	8	5.974954	2.359014	-0.104800
32	8	-1.211152	-1.965425	-2.604377
33	8	-1.662359	-3.338718	-0.985517
34	1	3.888444	-2.331371	-0.762552
35	1	7.113991	0.758689	-2.029890
36	1	8.056202	-0.216023	-0.898188
37	1	3.735570	3.455574	0.457996
38	1	1.537358	2.324781	0.597089
39	1	-0.798990	-2.613881	0.967288
40	1	-2.076223	-1.884812	2.875939
41	1	-2.190710	-0.242412	2.289807
42	1	-4.300885	-1.096247	2.018136
43	1	-3.165823	-3.633540	0.766253
44	1	-4.381581	-3.468504	2.048491
45	1	-6.020965	-2.542987	0.478555
46	1	-5.269190	-3.816279	-0.494761
47	1	-3.835077	-2.243893	-1.634424
48	1	-5.261978	-1.216123	-1.420813
49	1	-2.737434	0.013353	-1.602106
50	1	-2.389018	0.706773	-0.027956
51	1	0.266383	-0.324960	-1.865230
52	1	-0.215947	0.860282	-0.662393
53	1	7.498786	2.083931	2.055581
54	1	8.462033	0.702180	1.493100
55	1	6.725613	0.512229	1.774662
56	1	8.303318	3.497722	0.139830
57	1	8.071019	2.960907	-1.535578
58	1	9.282908	2.165576	-0.506771

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    59          1           -0.367346    0.282254    3.211740
    60          1           -0.392676    1.195927    1.701687
    61          1            1.134632    0.890174    2.540045
    62          1            0.583341   -1.965577    3.395992
    63          1            2.119886   -1.404596    2.736274
    64          1            1.303643   -2.810971    2.020253
    65          1           -4.432747    0.002645    0.231226
    66          6           -6.278455    3.076294   -0.205680
    67          6           -5.433579    1.793891   -0.474563
    68          8           -5.239000    1.092707    0.580167
    69          8           -5.025961    1.579133   -1.617699
    70          9           -7.446698    2.782109    0.414651
    71          9           -5.596594    3.932367    0.601894
    72          9           -6.578462    3.743950   -1.334067
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.4315	60.85		H34	22.3294	8.66
C2	-1.69	178.69		H35	28.6722	2.86
C4	100.9178	81.27		H36	28.9784	2.58
C5	136.0503	47.92		H37	24.8487	6.36
C6	-16.111	192.38		H38	24.1257	7.02
C7	78.7454	102.32		H39	27.6299	3.81
C8	19.4229	158.64		H40	29.6558	1.96
C9	74.454	106.40		H41	29.7258	1.90
C10	46.8354	132.62		H42	27.8723	3.59
C11	62.3563	117.88		H43	28.952	2.61
C12	35.4987	143.38		H44	29.7247	1.90
C13	129.2965	54.33		H45	29.888	1.75
C14	140.2948	43.89		H46	29.7421	1.88
C15	163.0839	22.25		H47	29.2563	2.33
C16	124.4411	58.94		H48	28.1737	3.32
C17	153.8461	31.02		H49	27.8578	3.61
C18	159.3893	25.76		H50	28.6838	2.85
C19	132.4437	51.34		H51	28.5211	3.00
C21	129.2489	54.38		H52	29.1574	2.42
C22	85.5687	95.85		H53	30.615	1.09
C23	138.528	45.57		H54	30.6679	1.04
C24	163.5886	21.77		H55	29.9184	1.72
C25	157.1943	27.85		H56	30.1014	1.55
C26	163.9024	21.48		H57	30.2366	1.43
C27	162.9963	22.34		H58	30.3823	1.30
				H59	30.6492	1.05
				H60	30.703	1.00
				H61	30.727	0.98
				H62	30.6427	1.06
				H63	31.0619	0.68
				H64	30.5119	1.18
				H65	13.714	16.54

Originally-Proposed Citrinalin B (**3**) neutral form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.255374 H (rel E = 0.06 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.219446	0.444343	-0.261299
2	6	-0.249965	1.883732	-0.615827
3	7	-1.626187	1.917832	-0.505599
4	6	-6.162547	-0.586479	0.245713
5	6	-5.970145	0.677784	-0.607867
6	6	-4.575331	1.266109	-0.496969
7	6	-3.508136	0.295817	-0.261873
8	6	-3.807327	-1.081340	-0.089597
9	6	-2.785969	-2.030345	0.004177
10	6	-1.444156	-1.629100	-0.043206
11	6	-1.109750	-0.281134	-0.157779
12	6	-2.147981	0.651227	-0.286141
13	6	1.113519	0.488542	1.083207
14	6	2.524681	0.658915	0.456734
15	6	3.802510	0.693825	1.297552
16	6	4.989601	1.042744	0.356014
17	6	6.375552	0.767153	0.966959
18	6	6.694589	-0.672629	0.519476
19	6	6.089172	-0.752934	-0.891040
20	7	5.013817	0.248555	-0.878406
21	6	3.805854	0.099863	-1.636961
22	6	2.561829	-0.282378	-0.763228
23	6	1.181066	-0.069149	-1.395078
24	6	-6.140193	-0.274428	1.748676
25	6	-7.440944	-1.326082	-0.140842
26	6	0.968145	-0.798683	1.920135
27	6	0.764981	1.669517	2.009942
28	7	2.748150	-1.773013	-0.422394
29	8	0.452130	2.826661	-0.943777
30	8	-4.367642	2.471741	-0.653193
31	8	-5.087577	-1.535830	-0.049093
32	8	2.107122	-2.609432	-1.064420
33	8	3.593003	-2.074398	0.420309
34	1	-2.213016	2.722856	-0.697365
35	1	-6.128261	0.429958	-1.667088
36	1	-6.700890	1.446225	-0.341117
37	1	-3.052929	-3.075704	0.110779
38	1	-0.669272	-2.387738	0.003330
39	1	2.475193	1.644419	-0.033592
40	1	3.722761	1.485054	2.053709
41	1	3.980593	-0.251583	1.812761
42	1	4.884922	2.108501	0.092982
43	1	7.109451	1.465897	0.549021
44	1	6.379625	0.889802	2.054660
45	1	7.766713	-0.890887	0.529412
46	1	6.196846	-1.393182	1.175976
47	1	6.840154	-0.500922	-1.657105
48	1	5.712713	-1.757458	-1.113575
49	1	3.523657	1.053817	-2.110777
50	1	3.956354	-0.627852	-2.440661
51	1	1.273606	0.702905	-2.164828
52	1	0.803913	-0.973694	-1.868015
53	1	-6.240774	-1.199252	2.323602
54	1	-6.972512	0.388094	2.007059
55	1	-5.211330	0.218527	2.049840
56	1	-7.542947	-2.241910	0.448579
57	1	-7.424315	-1.596967	-1.200433
58	1	-8.314795	-0.694083	0.045516
59	1	1.726586	-0.807724	2.709130
60	1	1.080856	-1.721382	1.350116

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      61          1            -0.013953   -0.831480    2.400431
      62          1             1.365040    1.613005    2.924235
      63          1            -0.287548    1.631570    2.312486
      64          1             0.955798    2.638284    1.541833
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.219	61.05		H34	22.2953	8.69
C2	-5.0388	181.87		H35	28.7253	2.81
C4	100.5806	81.59		H36	29.1595	2.42
C5	136.7496	47.26		H37	24.8599	6.35
C6	-16.7137	192.95		H38	24.0161	7.12
C7	78.2074	102.83		H39	28.9941	2.57
C8	20.2299	157.88		H40	30.4501	1.24
C9	73.9027	106.92		H41	29.2257	2.36
C10	46.2044	133.22		H42	28.4299	3.08
C11	57.9309	122.08		H43	29.4797	2.12
C12	36.1436	142.77		H44	29.8416	1.79
C13	131.5601	52.18		H45	29.9847	1.66
C14	126.4964	56.99		H46	29.3172	2.27
C15	156.3791	28.62		H47	28.4	3.11
C16	125.3178	58.11		H48	28.5692	2.96
C17	152.0906	32.69		H49	28.2751	3.22
C18	159.6607	25.50		H50	27.8559	3.61
C19	130.842	52.86		H51	29.4997	2.10
C21	123.732	59.61		H52	28.1406	3.35
C22	86.2378	95.21		H53	30.6248	1.08
C23	141.6607	42.59		H54	30.6818	1.02
C24	163.7668	21.61		H55	29.9748	1.67
C25	156.8771	28.15		H56	30.0849	1.57
C26	164.3667	21.04		H57	30.2169	1.45
C27	163.742	21.63		H58	30.3258	1.35
				H59	30.95	0.78
				H60	31.0864	0.65
				H61	31.38	0.39
				H62	30.7575	0.95
				H63	31.0257	0.71
				H64	30.6865	1.02

Originally-Proposed Citrinalin B (**3**) neutral form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.255466 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.210875	0.390315	-0.184099
2	6	-0.243569	1.800381	-0.657820
3	7	-1.612525	1.879178	-0.495510
4	6	-6.198238	-0.595874	-0.054439
5	6	-5.957099	0.886336	0.276995
6	6	-4.563504	1.357984	-0.095484
7	6	-3.513563	0.348871	0.030866
8	6	-3.835666	-0.997076	0.346573
9	6	-2.832115	-1.958043	0.494335
10	6	-1.485339	-1.600238	0.344720
11	6	-1.127641	-0.286077	0.050439
12	6	-2.150616	0.655331	-0.126199
13	6	1.162082	0.544072	1.110216
14	6	2.539433	0.672294	0.404529
15	6	3.855566	0.801612	1.173184
16	6	4.986425	1.084227	0.143614
17	6	6.406737	0.882737	0.701367
18	6	6.727147	-0.586989	0.366774
19	6	6.050943	-0.801532	-0.997017
20	7	4.963797	0.187620	-1.019199
21	6	3.720180	-0.044302	-1.696266
22	6	2.533730	-0.375267	-0.726453
23	6	1.114025	-0.254968	-1.298302
24	6	-7.466760	-1.114589	0.617655
25	6	-6.234560	-0.846954	-1.568507
26	6	1.068118	-0.676225	2.047531
27	6	0.840543	1.791773	1.954477
28	7	2.782390	-1.826607	-0.272053
29	8	0.461662	2.689995	-1.106486
30	8	-4.341045	2.523278	-0.431866
31	8	-5.121155	-1.402196	0.524196
32	8	2.160983	-2.732195	-0.834413
33	8	3.656488	-2.031865	0.569547
34	1	-2.188294	2.680216	-0.731381
35	1	-6.692327	1.524094	-0.221165
36	1	-6.068820	1.039213	1.359800
37	1	-3.117210	-2.981110	0.712055
38	1	-0.727022	-2.370759	0.440415
39	1	2.450006	1.608267	-0.169404
40	1	3.798568	1.657601	1.857304
41	1	4.077193	-0.089765	1.762478
42	1	4.847427	2.121285	-0.204052
43	1	7.105395	1.551107	0.184865
44	1	6.465550	1.101816	1.772261
45	1	7.801921	-0.790221	0.339293
46	1	6.276129	-1.251794	1.110024
47	1	6.757148	-0.613664	-1.821649
48	1	5.677715	-1.825747	-1.106737
49	1	3.392416	0.862917	-2.228438
50	1	3.843534	-0.832668	-2.445579
51	1	1.145069	0.406932	-2.168898
52	1	0.726718	-1.218402	-1.623800
53	1	-7.602713	-2.178560	0.402691
54	1	-8.340954	-0.571052	0.245998
55	1	-7.409316	-0.985968	1.702364
56	1	-6.368667	-1.913975	-1.766873
57	1	-5.313272	-0.519159	-2.058897
58	1	-7.069134	-0.301333	-2.020380

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     59          1             1.862653   -0.620711    2.798184
     60          1             1.165950   -1.637780    1.542300
     61          1             0.109798   -0.680653    2.574494
     62          1             1.477532    1.813907    2.844990
     63          1            -0.198427    1.770241    2.302209
     64          1             1.001538    2.721470    1.402898
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.219	61.05		H34	22.2953	8.69
C2	-5.0388	181.87		H35	28.7253	2.81
C4	100.5806	81.59		H36	29.1595	2.42
C5	136.7496	47.26		H37	24.8599	6.35
C6	-16.7137	192.95		H38	24.0161	7.12
C7	78.2074	102.83		H39	28.9941	2.57
C8	20.2299	157.88		H40	30.4501	1.24
C9	73.9027	106.92		H41	29.2257	2.36
C10	46.2044	133.22		H42	28.4299	3.08
C11	57.9309	122.08		H43	29.4797	2.12
C12	36.1436	142.77		H44	29.8416	1.79
C13	131.5601	52.18		H45	29.9847	1.66
C14	126.4964	56.99		H46	29.3172	2.27
C15	156.3791	28.62		H47	28.4	3.11
C16	125.3178	58.11		H48	28.5692	2.96
C17	152.0906	32.69		H49	28.2751	3.22
C18	159.6607	25.50		H50	27.8559	3.61
C19	130.842	52.86		H51	29.4997	2.10
C21	123.732	59.61		H52	28.1406	3.35
C22	86.2378	95.21		H53	30.6248	1.08
C23	141.6607	42.59		H54	30.6818	1.02
C24	163.7668	21.61		H55	29.9748	1.67
C25	156.8771	28.15		H56	30.0849	1.57
C26	164.3667	21.04		H57	30.2169	1.45
C27	163.742	21.63		H58	30.3258	1.35
				H59	30.95	0.78
				H60	31.0864	0.65
				H61	31.38	0.39
				H62	30.7575	0.95
				H63	31.0257	0.71
				H64	30.6865	1.02

Originally-Proposed Citrinalin B (**3**) neutral form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.242523 H (rel E = 5.67 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.266491	0.405914	-0.163319
2	6	-0.154788	1.896068	-0.327936
3	7	-1.531991	1.956083	-0.257880
4	6	-6.148770	-0.477902	0.077965
5	6	-5.909065	0.885619	-0.589452
6	6	-4.496591	1.406342	-0.392905
7	6	-3.463837	0.378120	-0.285669
8	6	-3.808170	-0.998975	-0.306676
9	6	-2.818304	-1.984128	-0.327621
10	6	-1.463676	-1.625911	-0.295685
11	6	-1.085132	-0.286489	-0.221704
12	6	-2.092946	0.688055	-0.238343
13	6	1.083577	0.230219	1.228006
14	6	2.534649	0.366376	0.703190
15	6	3.758277	0.142901	1.590385
16	6	5.022131	0.571388	0.793392
17	6	6.218295	-0.416786	0.774465
18	6	6.986646	-0.050183	-0.525060
19	6	6.092922	1.034793	-1.203246
20	7	4.744104	0.898496	-0.632543
21	6	3.938708	-0.085815	-1.371636
22	6	2.596288	-0.384952	-0.643224
23	6	1.289134	0.060418	-1.308450
24	6	-6.128846	-0.380883	1.610198
25	6	-7.447896	-1.112596	-0.412361
26	6	0.797368	-1.112926	1.931591
27	6	0.771577	1.336120	2.258238
28	7	2.574044	-1.933626	-0.454900
29	8	0.583055	2.852017	-0.498282
30	8	-4.249548	2.614756	-0.380827
31	8	-5.103152	-1.411441	-0.344200
32	8	1.655642	-2.585745	-0.950799
33	8	3.504328	-2.440677	0.167855
34	1	-2.090693	2.797886	-0.349122
35	1	-6.067191	0.792946	-1.673242
36	1	-6.616333	1.633415	-0.220230
37	1	-3.118822	-3.025169	-0.366274
38	1	-0.711789	-2.406199	-0.334130
39	1	2.606543	1.407351	0.363007
40	1	3.671283	0.756975	2.492712
41	1	3.838470	-0.897491	1.912867
42	1	5.383670	1.519160	1.214912
43	1	6.835460	-0.313125	1.673082
44	1	5.856013	-1.448137	0.741560
45	1	7.989589	0.339116	-0.324465
46	1	7.107594	-0.927463	-1.168705
47	1	6.466145	2.036590	-0.958095
48	1	6.060465	0.955530	-2.293974
49	1	3.724883	0.343090	-2.356287
50	1	4.473909	-1.032156	-1.539323
51	1	1.512374	0.975770	-1.863223
52	1	0.892997	-0.679372	-2.002890
53	1	-6.942732	0.264200	1.956465
54	1	-5.187873	0.035500	1.981257
55	1	-6.262405	-1.373757	2.048817
56	1	-7.584865	-2.098579	0.041280
57	1	-7.432618	-1.231723	-1.499599
58	1	-8.301718	-0.483979	-0.140775

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     59          1             1.482981   -1.227457    2.777625
     60          1             0.905351   -1.992711    1.298980
     61          1            -0.221015   -1.124012    2.329984
     62          1             1.320289    1.142277    3.185855
     63          1            -0.294253    1.344575    2.512220
     64          1             1.050351    2.330263    1.902135
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.1209	61.14		H34	22.2508	8.73
C2	-4.6414	181.49		H35	28.7651	2.78
C4	101.1077	81.09		H36	29.1229	2.45
C5	136.5481	47.45		H37	24.8318	6.37
C6	-16.4139	192.67		H38	23.7836	7.33
C7	77.9402	103.09		H39	28.1644	3.33
C8	20.3462	157.77		H40	29.7852	1.84
C9	73.695	107.12		H41	29.5632	2.05
C10	45.1856	134.18		H42	28.1665	3.32
C11	58.9504	121.12		H43	29.7071	1.92
C12	36.6564	142.28		H44	29.5976	2.02
C13	133.7533	50.10		H45	29.9504	1.69
C14	131.0019	52.71		H46	29.6324	1.98
C15	164.3457	21.06		H47	28.8251	2.72
C16	123.3524	59.97		H48	28.9046	2.65
C17	155.4907	29.46		H49	28.5316	2.99
C18	161.2338	24.01		H50	28.5872	2.94
C19	132.531	51.26		H51	29.1067	2.46
C21	126.5326	56.96		H52	28.1881	3.30
C22	77.3425	103.66		H53	30.6643	1.04
C23	138.5652	45.53		H54	29.9738	1.67
C24	163.7633	21.61		H55	30.6315	1.07
C25	157.2709	27.77		H56	30.0727	1.58
C26	165.4154	20.04		H57	30.2247	1.44
C27	162.3908	22.91		H58	30.3409	1.34
				H59	31.0657	0.67
				H60	31.0798	0.66
				H61	31.5158	0.26
				H62	30.7313	0.98
				H63	30.9994	0.73
				H64	30.5753	1.12

Originally-Proposed Citrinalin B (**3**) neutral form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1511.242912 H (rel E = 7.88 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.261640	0.409237	-0.048374
2	6	-0.171181	1.874331	-0.348468
3	7	-1.542735	1.946826	-0.209414
4	6	-6.153971	-0.512148	-0.278256
5	6	-5.918631	0.909200	0.259155
6	6	-4.507293	1.410946	0.012178
7	6	-3.469801	0.382057	0.040250
8	6	-3.812772	-0.990387	0.156807
9	6	-2.822370	-1.973761	0.208987
10	6	-1.468109	-1.616977	0.155477
11	6	-1.089617	-0.279470	0.052090
12	6	-2.099397	0.689831	-0.026508
13	6	1.172286	0.383032	1.294580
14	6	2.584683	0.443041	0.658130
15	6	3.867059	0.312157	1.477964
16	6	5.072363	0.635611	0.551799
17	6	6.263465	-0.358381	0.564594
18	6	6.940523	-0.149498	-0.817925
19	6	6.001624	0.856951	-1.554280
20	7	4.695665	0.797783	-0.879997
21	6	3.840648	-0.259319	-1.441393
22	6	2.549830	-0.455782	-0.593328
23	6	1.203265	-0.070600	-1.215143
24	6	-7.452807	-1.101159	0.266438
25	6	-6.129906	-0.557473	-1.812500
26	6	0.929390	-0.868524	2.164131
27	6	0.937107	1.601634	2.212065
28	7	2.532665	-1.972737	-0.230722
29	8	0.553639	2.803099	-0.663596
30	8	-4.265109	2.608983	-0.152823
31	8	-5.107322	-1.400410	0.230283
32	8	1.586770	-2.667442	-0.601472
33	8	3.494010	-2.415909	0.393488
34	1	-2.106428	2.776786	-0.358652
35	1	-6.627638	1.616969	-0.178963
36	1	-6.076297	0.917139	1.347023
37	1	-3.122525	-3.013467	0.275541
38	1	-0.717518	-2.399265	0.167943
39	1	2.633362	1.437633	0.196757
40	1	3.843266	1.026512	2.307410
41	1	3.968805	-0.684915	1.911675
42	1	5.462939	1.622493	0.834441
43	1	6.941128	-0.157771	1.401041
44	1	5.899423	-1.383719	0.675531
45	1	7.954642	0.253071	-0.732634
46	1	7.018014	-1.095802	-1.362996
47	1	6.390747	1.877378	-1.452485
48	1	5.894120	0.653048	-2.623835
49	1	3.561489	0.051131	-2.453774
50	1	4.361539	-1.224322	-1.530778
51	1	1.392511	0.775669	-1.881189
52	1	0.757332	-0.877929	-1.794443
53	1	-7.584985	-2.126238	-0.091849
54	1	-8.307608	-0.504199	-0.066461
55	1	-7.440680	-1.116071	1.360106
56	1	-6.263254	-1.586571	-2.157755
57	1	-5.187168	-0.178680	-2.218000
58	1	-6.941652	0.053825	-2.219671

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     59          1             1.679476   -0.903537    2.961095
     60          1             0.975198   -1.815280    1.627913
     61          1            -0.053828   -0.814683    2.640077
     62          1             1.539105    1.501458    3.121344
     63          1            -0.111019    1.656909    2.526772
     64          1             1.204263    2.545466    1.731889
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.0425	61.22		H34	22.2788	8.71
C2	-4.5353	181.39		H35	29.1206	2.45
C4	101.3846	80.83		H36	28.6799	2.85
C5	136.474	47.52		H37	24.8327	6.37
C6	-16.3222	192.58		H38	23.7347	7.38
C7	78.8326	102.24		H39	28.214	3.28
C8	20.3914	157.72		H40	29.8027	1.83
C9	73.6521	107.16		H41	29.6032	2.01
C10	45.091	134.27		H42	28.1935	3.30
C11	58.0429	121.98		H43	29.7614	1.87
C12	36.2759	142.64		H44	29.6558	1.96
C13	134.3254	49.56		H45	29.969	1.68
C14	130.8419	52.86		H46	29.6502	1.97
C15	164.6174	20.80		H47	28.8603	2.69
C16	123.3635	59.96		H48	28.9399	2.62
C17	155.7478	29.22		H49	28.5097	3.01
C18	161.4693	23.79		H50	28.5461	2.98
C19	132.5662	51.23		H51	29.1575	2.42
C21	126.685	56.81		H52	28.191	3.30
C22	78.2069	102.83		H53	30.0955	1.56
C23	137.9497	46.12		H54	30.3867	1.29
C24	157.5726	27.49		H55	30.1963	1.47
C25	163.7031	21.67		H56	30.5998	1.10
C26	165.5457	19.92		H57	30.0336	1.62
C27	162.1698	23.12		H58	30.7165	0.99
				H59	31.0608	0.68
				H60	31.0668	0.67
				H61	31.4449	0.33
				H62	30.7396	0.97
				H63	31.0162	0.72
				H64	30.5951	1.10

Originally-Proposed Citrinalin B (**3**) TFA salt form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.072321 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.136872	-0.052168	0.049426
2	6	-1.209912	1.444861	0.470207
3	7	-2.540494	1.798527	0.536143
4	6	-7.578663	0.591121	-0.203085
5	6	-6.979043	2.003958	-0.289699
6	6	-5.523695	2.059115	0.136756
7	6	-4.749106	0.848596	-0.137693
8	6	-5.371425	-0.296619	-0.699679
9	6	-4.614959	-1.408705	-1.082976
10	6	-3.228663	-1.419712	-0.885710
11	6	-2.589204	-0.335647	-0.286322
12	6	-3.358626	0.784540	0.055499
13	6	-0.510925	-0.911997	1.263453
14	6	0.993197	-0.832731	0.889343
15	6	2.076805	-1.567750	1.674343
16	6	3.460542	-1.097182	1.188471
17	6	4.624253	-2.001630	1.609617
18	6	4.686203	-3.082599	0.514689
19	6	4.328351	-2.335620	-0.777841
20	7	3.619201	-1.069263	-0.330791
21	6	2.453001	-0.599674	-1.145757
22	6	1.064611	-1.025585	-0.636547
23	6	-0.117775	-0.182244	-1.140231
24	6	-7.717171	0.113004	1.248910
25	6	-8.914560	0.509154	-0.937037
26	6	-1.061014	-2.352771	1.306026
27	6	-0.772765	-0.291447	2.649741
28	7	0.861222	-2.506405	-1.089579
29	8	-0.265625	2.183523	0.696133
30	8	-5.028163	3.075704	0.626742
31	8	-6.709382	-0.346826	-0.920380
32	8	0.062732	-2.749904	-1.989344
33	8	1.557294	-3.364733	-0.549413
34	1	-2.895782	2.719549	0.771580
35	1	-7.020291	2.354791	-1.330594
36	1	-7.552706	2.711617	0.314958
37	1	-5.122504	-2.255102	-1.531657
38	1	-2.660487	-2.285315	-1.211278
39	1	1.233226	0.237361	0.984594
40	1	2.010035	-1.296610	2.734076
41	1	1.975700	-2.651463	1.601792
42	1	3.634044	-0.067637	1.516737
43	1	5.544206	-1.409561	1.634073
44	1	4.464918	-2.417537	2.608691
45	1	5.671518	-3.551077	0.448667
46	1	3.951995	-3.870862	0.704282
47	1	5.215005	-2.012142	-1.330582
48	1	3.689036	-2.918822	-1.438158
49	1	2.476518	0.493561	-1.112270
50	1	2.626485	-0.895252	-2.183741
51	1	0.256015	0.810663	-1.403748
52	1	-0.580158	-0.614770	-2.025141
53	1	-8.102116	-0.910291	1.270012
54	1	-8.415549	0.758347	1.791105
55	1	-6.760495	0.132983	1.778940
56	1	-9.307837	-0.510875	-0.898030
57	1	-8.797707	0.794560	-1.986461
58	1	-9.643171	1.179666	-0.471026

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    59          1           -0.478634   -2.947779    2.016703
    60          1           -1.044625   -2.873505    0.348533
    61          1           -2.098375   -2.348798    1.651016
    62          1           -0.376072   -0.946116    3.432735
    63          1           -1.848159   -0.190064    2.831400
    64          1           -0.308637    0.690884    2.764556
    65          1            4.397495   -0.229722   -0.532832
    66          6            6.818925    2.468711   -0.514196
    67          6            5.814430    1.398341    0.010991
    68          8            5.257985    0.740887   -0.940911
    69          8            5.654979    1.276157    1.224179
    70          9            7.837334    1.880235   -1.193442
    71          9            6.213276    3.334103   -1.364518
    72          9            7.364214    3.194211    0.478004
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.8238	60.48		H34	22.3083	8.68
C2	-4.4909	181.35		H35	28.6777	2.86
C4	100.0736	82.07		H36	29.0892	2.48
C5	136.7603	47.25		H37	24.8141	6.39
C6	-16.1341	192.40		H38	24.0194	7.12
C7	78.4429	102.61		H39	28.7116	2.83
C8	19.4225	158.64		H40	30.0304	1.62
C9	73.9401	106.89		H41	29.1239	2.45
C10	46.5485	132.89		H42	27.2789	4.14
C11	60.1153	120.01		H43	29.37	2.22
C12	36.1558	142.76		H44	29.7279	1.90
C13	132.7438	51.06		H45	29.7274	1.90
C14	131.7578	51.99		H46	29.2239	2.36
C15	161.0172	24.22		H47	28.3423	3.16
C16	121.8164	61.43		H48	28.686	2.85
C17	152.3418	32.45		H49	28.4331	3.08
C18	160.67	24.55		H50	28.2786	3.22
C19	130.2819	53.40		H51	29.3887	2.21
C21	129.0803	54.54		H52	28.0116	3.47
C22	87.958	93.58		H53	30.5664	1.13
C23	141.0221	43.20		H54	30.6068	1.09
C24	163.7368	21.63		H55	29.923	1.72
C25	157.1899	27.85		H56	30.0399	1.61
C26	165.6007	19.86		H57	30.2293	1.44
C27	163.4292	21.93		H58	30.315	1.36
				H59	30.8941	0.83
				H60	31.0002	0.73
				H61	31.1796	0.57
				H62	30.71	1.00
				H63	30.9639	0.77
				H64	30.8031	0.91
				H65	13.2247	16.99

Originally-Proposed Citrinalin B (**3**) TFA salt form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.072294 H (rel E = 0.02 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.139070	-0.121474	0.191534
2	6	-1.221127	1.359836	0.663007
3	7	-2.553984	1.688224	0.787433
4	6	-7.516299	0.759483	-0.575739
5	6	-7.072662	1.632338	0.609985
6	6	-5.570895	1.840918	0.662505
7	6	-4.771454	0.713958	0.180787
8	6	-5.393928	-0.414386	-0.413643
9	6	-4.635417	-1.506016	-0.848125
10	6	-3.243899	-1.504958	-0.690737
11	6	-2.598100	-0.420723	-0.098464
12	6	-3.372130	0.676827	0.301564
13	6	-0.452667	-1.006902	1.353456
14	6	1.034115	-0.890468	0.924774
15	6	2.156794	-1.631866	1.645695
16	6	3.514624	-1.124559	1.125102
17	6	4.705155	-2.024906	1.473567
18	6	4.737983	-3.070391	0.343799
19	6	4.327006	-2.287067	-0.910391
20	7	3.615990	-1.046194	-0.397547
21	6	2.413172	-0.568602	-1.153031
22	6	1.051013	-1.033206	-0.608044
23	6	-0.162937	-0.194419	-1.039016
24	6	-8.964315	0.303788	-0.417576
25	6	-7.303254	1.467163	-1.920791
26	6	-0.975280	-2.458370	1.374843
27	6	-0.670672	-0.432792	2.767244
28	7	0.853124	-2.501176	-1.103028
29	8	-0.281476	2.108031	0.876409
30	8	-5.071240	2.868608	1.124058
31	8	-6.739505	-0.484449	-0.578128
32	8	0.023817	-2.728050	-1.978987
33	8	1.583570	-3.364981	-0.620025
34	1	-2.915049	2.593687	1.069252
35	1	-7.565913	2.607754	0.584696
36	1	-7.361358	1.142466	1.550755
37	1	-5.143877	-2.339616	-1.319119
38	1	-2.675276	-2.352992	-1.058856
39	1	1.261131	0.180063	1.044622
40	1	2.124842	-1.395066	2.715216
41	1	2.068704	-2.714300	1.543007
42	1	3.686439	-0.103520	1.479777
43	1	5.618497	-1.422103	1.481406
44	1	4.589750	-2.473236	2.464559
45	1	5.724316	-3.526885	0.227761
46	1	4.017720	-3.871008	0.534761
47	1	5.190161	-1.932086	-1.480668
48	1	3.673935	-2.857407	-1.568459
49	1	2.421928	0.523053	-1.082944
50	1	2.552606	-0.826591	-2.206080
51	1	0.184047	0.813224	-1.282649
52	1	-0.650686	-0.606524	-1.919951
53	1	-9.250702	-0.347627	-1.248322
54	1	-9.634066	1.169189	-0.408650
55	1	-9.095238	-0.249645	0.516752
56	1	-7.586909	0.802725	-2.741680
57	1	-6.261020	1.766847	-2.064965
58	1	-7.922522	2.368248	-1.972924

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    59          1           -0.356644   -3.060508    2.047929
    60          1           -0.983098   -2.953261    0.403596
    61          1           -1.999226   -2.484550    1.756743
    62          1           -0.231437   -1.102504    3.513995
    63          1           -1.739717   -0.357916    2.993515
    64          1           -0.220523    0.554570    2.894018
    65          1            4.373821   -0.189375   -0.601016
    66          6            6.724689    2.571947   -0.579932
    67          6            5.755737    1.468754   -0.055832
    68          8            5.208232    0.805527   -1.008844
    69          8            5.611739    1.330606    1.157617
    70          9            7.751450    2.019293   -1.276401
    71          9            6.085946    3.429142   -1.414380
    72          9            7.260523    3.301913    0.414102
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	122.734	60.56		H34	22.2606	8.72
C2	-4.4559	181.31		H35	29.0693	2.50
C4	100.0507	82.10		H36	28.676	2.86
C5	136.4765	47.51		H37	24.7995	6.40
C6	-16.5847	192.83		H38	23.9517	7.18
C7	78.1173	102.92		H39	28.6704	2.86
C8	19.7517	158.33		H40	30.0566	1.60
C9	73.3044	107.49		H41	29.1379	2.44
C10	46.6028	132.84		H42	27.1809	4.23
C11	59.9911	120.13		H43	29.4573	2.14
C12	36.233	142.68		H44	29.7447	1.88
C13	132.8347	50.97		H45	29.7184	1.90
C14	131.903	51.86		H46	29.2212	2.36
C15	161.115	24.12		H47	28.3543	3.15
C16	121.7544	61.49		H48	28.6856	2.85
C17	152.2679	32.52		H49	28.4267	3.09
C18	160.6387	24.58		H50	28.2961	3.21
C19	130.2097	53.46		H51	29.3782	2.22
C21	129.0687	54.55		H52	28.0098	3.47
C22	88.32	93.23		H53	30.0875	1.57
C23	141.1604	43.07		H54	30.3526	1.33
C24	157.0425	27.99		H55	30.1983	1.47
C25	163.5757	21.79		H56	30.6191	1.08
C26	165.5813	19.88		H57	30.0342	1.62
C27	163.5526	21.81		H58	30.6353	1.07
				H59	30.9133	0.81
				H60	30.9573	0.77
				H61	31.1998	0.55
				H62	30.7221	0.99
				H63	30.9843	0.75
				H64	30.811	0.91
				H65	13.2429	16.97

Originally-Proposed Citrinalin B (**3**) TFA salt form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.063284 H (rel E = 5.67 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.651480	-0.352592	-0.171145
2	6	-0.697202	1.189646	-0.390201
3	7	-2.017025	1.587247	-0.309086
4	6	-7.089034	0.358088	0.088482
5	6	-6.525484	1.593902	-0.631135
6	6	-5.030256	1.766843	-0.436250
7	6	-4.275183	0.523711	-0.282087
8	6	-4.942862	-0.728888	-0.255343
9	6	-4.221593	-1.925971	-0.237851
10	6	-2.821073	-1.904736	-0.216157
11	6	-2.130582	-0.694732	-0.190723
12	6	-2.870176	0.495516	-0.241829
13	6	0.127770	-0.678540	1.205118
14	6	1.572339	-0.883996	0.672628
15	6	2.650709	-1.470723	1.577365
16	6	4.029336	-1.450877	0.876041
17	6	4.889111	-2.738417	0.962348
18	6	5.465535	-2.962462	-0.455429
19	6	5.266400	-1.617304	-1.158190
20	7	3.975530	-1.081015	-0.611313
21	6	2.791539	-1.461296	-1.464688
22	6	1.465004	-1.600961	-0.691126
23	6	0.214519	-0.972626	-1.325793
24	6	-7.047527	0.511601	1.615254
25	6	-8.501488	0.034298	-0.391459
26	6	-0.441723	-1.911384	1.937632
27	6	0.091598	0.491010	2.212420
28	7	1.243238	-3.136424	-0.524962
29	8	0.251549	1.918863	-0.615148
30	8	-4.497717	2.877999	-0.465014
31	8	-6.297910	-0.817933	-0.282966
32	8	0.136407	-3.617416	-0.745750
33	8	2.221492	-3.801245	-0.183857
34	1	-2.352917	2.537137	-0.429113
35	1	-6.696976	1.495647	-1.712462
36	1	-7.032800	2.505216	-0.302945
37	1	-4.766412	-2.863326	-0.239115
38	1	-2.279354	-2.844325	-0.221871
39	1	1.910249	0.122752	0.390781
40	1	2.721192	-0.860253	2.481330
41	1	2.401300	-2.490189	1.881385
42	1	4.588413	-0.608571	1.289907
43	1	5.685910	-2.594343	1.698334
44	1	4.292497	-3.594749	1.281140
45	1	6.518717	-3.255552	-0.450652
46	1	4.905325	-3.749168	-0.970072
47	1	6.043353	-0.896682	-0.885884
48	1	5.216053	-1.664380	-2.248225
49	1	2.691298	-0.646268	-2.186114
50	1	3.023635	-2.377481	-2.008872
51	1	0.541064	-0.170265	-1.991765
52	1	-0.353515	-1.694725	-1.910829
53	1	-7.679754	1.349473	1.925962
54	1	-6.033922	0.702063	1.979725
55	1	-7.419202	-0.399373	2.092726
56	1	-8.872411	-0.869801	0.100042
57	1	-8.513310	-0.129923	-1.472789
58	1	-9.179170	0.860562	-0.155273

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    59          1             0.196999   -2.152920    2.793438
    60          1            -0.527604   -2.805609    1.321299
    61          1            -1.436896   -1.687789    2.331150
    62          1             0.583061    0.193621    3.144345
    63          1            -0.942601    0.751013    2.463255
    64          1             0.600789    1.382466    1.841576
    65          1             4.060227    0.057349   -0.675885
    66          6             4.318735    3.633709   -0.027527
    67          6             4.041480    2.113576    0.176862
    68          8             4.268209    1.417522   -0.873381
    69          8             3.679037    1.724540    1.289680
    70          9             5.661907    3.854181   -0.083733
    71          9             3.787111    4.099438   -1.178889
    72          9             3.832712    4.385572    0.977200
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.1487	62.07		H34	22.2952	8.69
C2	-4.1046	180.98		H35	28.7017	2.83
C4	101.1174	81.08		H36	29.068	2.50
C5	136.2089	47.77		H37	24.7308	6.47
C6	-16.6022	192.84		H38	23.5034	7.59
C7	78.1553	102.88		H39	28.4022	3.11
C8	20.0982	158.00		H40	29.3325	2.26
C9	73.5541	107.25		H41	30.0426	1.61
C10	45.8906	133.52		H42	27.0145	4.38
C11	59.7325	120.37		H43	29.2869	2.30
C12	35.5248	143.36		H44	29.5461	2.06
C13	132.6259	51.17		H45	29.68	1.94
C14	129.9752	53.69		H46	29.3985	2.20
C15	160.6073	24.61		H47	28.5594	2.96
C16	122.2679	61.00		H48	28.7096	2.83
C17	152.1142	32.67		H49	27.9214	3.55
C18	160.6294	24.58		H50	28.2928	3.21
C19	129.9588	53.70		H51	29.1262	2.45
C21	123.9089	59.45		H52	28.1704	3.32
C22	79.8632	101.26		H53	30.6833	1.02
C23	136.9654	47.05		H54	29.8995	1.74
C24	163.7611	21.61		H55	30.5826	1.11
C25	157.2018	27.84		H56	30.1077	1.55
C26	166.0622	19.43		H57	30.22	1.45
C27	161.8637	23.41		H58	30.3589	1.32
				H59	31.0685	0.67
				H60	30.7556	0.96
				H61	31.3052	0.45
				H62	30.7229	0.99
				H63	30.9852	0.75
				H64	30.6525	1.05
				H65	13.5712	16.67

Originally-Proposed Citrinalin B (**3**) TFA salt form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -2038.063189 H (rel E = 5.73 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.649397	-0.343337	-0.038831
2	6	-0.706521	1.201440	-0.237251
3	7	-2.020588	1.596769	-0.084711
4	6	-7.094336	0.344121	-0.283865
5	6	-6.521416	1.617804	0.359324
6	6	-5.031583	1.781496	0.121761
7	6	-4.273491	0.531774	0.061135
8	6	-4.940188	-0.721177	0.080468
9	6	-4.218901	-1.917946	0.053086
10	6	-2.818647	-1.896861	0.017283
11	6	-2.127743	-0.686868	0.007490
12	6	-2.869194	0.503341	0.006176
13	6	0.191147	-0.680261	1.299139
14	6	1.608894	-0.887115	0.700155
15	6	2.726856	-1.478748	1.552764
16	6	4.070850	-1.461253	0.786775
17	6	4.926766	-2.753555	0.824399
18	6	5.453647	-2.958270	-0.616248
19	6	5.215022	-1.609076	-1.299997
20	7	3.947384	-1.083662	-0.692895
21	6	2.729390	-1.472461	-1.491671
22	6	1.435608	-1.597025	-0.660736
23	6	0.166772	-0.949290	-1.236036
24	6	-8.498093	0.045124	0.235591
25	6	-7.076903	0.417584	-1.816944
26	6	-0.346092	-1.915885	2.051839
27	6	0.204600	0.483171	2.314640
28	7	1.201687	-3.129787	-0.491115
29	8	0.229262	1.934100	-0.501589
30	8	-4.504960	2.892337	0.035687
31	8	-6.294930	-0.810310	0.134655
32	8	0.084187	-3.597908	-0.684572
33	8	2.180994	-3.806172	-0.177154
34	1	-2.361095	2.548570	-0.170147
35	1	-7.038839	2.509077	-0.005766
36	1	-6.669687	1.573450	1.447571
37	1	-4.763864	-2.855182	0.048253
38	1	-2.278353	-2.836253	-0.024134
39	1	1.936506	0.119885	0.407444
40	1	2.840808	-0.869503	2.453053
41	1	2.489261	-2.498127	1.866488
42	1	4.653909	-0.624072	1.177586
43	1	5.747931	-2.624791	1.535913
44	1	4.335880	-3.611379	1.149288
45	1	6.509507	-3.239133	-0.652510
46	1	4.885370	-3.747655	-1.117982
47	1	5.999335	-0.885836	-1.057657
48	1	5.116621	-1.649377	-2.387037
49	1	2.602464	-0.668940	-2.221741
50	1	2.937039	-2.398111	-2.029613
51	1	0.476792	-0.136623	-1.897580
52	1	-0.428813	-1.655226	-1.813409
53	1	-8.876111	-0.883665	-0.201564
54	1	-9.180705	0.857625	-0.032021
55	1	-8.491867	-0.062477	1.324075
56	1	-7.455055	-0.516947	-2.240718
57	1	-6.068852	0.588501	-2.205990
58	1	-7.713807	1.238555	-2.161387

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    59          1             0.332219   -2.160907    2.875469
    60          1            -0.462137   -2.808401    1.437784
    61          1            -1.321356   -1.692865    2.492532
    62          1             0.736961    0.178135    3.221301
    63          1            -0.816193    0.744441    2.614196
    64          1             0.699148    1.375666    1.926933
    65          1             4.022496    0.056700   -0.759311
    66          6             4.305464    3.630478   -0.121534
    67          6             4.042000    2.109577    0.094511
    68          8             4.213784    1.415016   -0.967302
    69          8             3.741630    1.718034    1.224678
    70          9             5.645651    3.855389   -0.219998
    71          9             3.736898    4.092764   -1.256261
    72          9             3.848373    4.381863    0.896922
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Nucleus	Isotropic	Shift		Nucleus	Isotropic	Shift
C1	121.3548	61.87		H34	22.3059	8.68
C2	-4.0108	180.89		H35	29.0933	2.48
C4	100.7736	81.41		H36	28.656	2.88
C5	136.0892	47.88		H37	24.7423	6.45
C6	-16.7548	192.99		H38	23.5129	7.58
C7	78.2734	102.77		H39	28.3905	3.12
C8	20.0803	158.02		H40	29.3241	2.27
C9	73.2621	107.53		H41	30.0234	1.63
C10	45.9237	133.48		H42	27.0584	4.34
C11	59.6035	120.50		H43	29.2936	2.29
C12	35.5448	143.34		H44	29.5278	2.08
C13	132.3711	51.41		H45	29.6409	1.98
C14	130.0817	53.59		H46	29.451	2.15
C15	160.7247	24.49		H47	28.5529	2.97
C16	122.473	60.81		H48	28.7094	2.83
C17	152.3232	32.47		H49	27.8872	3.58
C18	160.7295	24.49		H50	28.2857	3.22
C19	130.1352	53.53		H51	29.0746	2.49
C21	124.1384	59.23		H52	28.1888	3.30
C22	80.4145	100.74		H53	30.1125	1.54
C23	137.1568	46.87		H54	30.3602	1.32
C24	157.2329	27.81		H55	30.1891	1.47
C25	163.6808	21.69		H56	30.5869	1.11
C26	165.9473	19.54		H57	29.9919	1.65
C27	161.8314	23.44		H58	30.7223	0.99
				H59	31.0693	0.67
				H60	30.7763	0.94
				H61	31.3251	0.44
				H62	30.7288	0.98
				H63	31.0415	0.70
				H64	30.6779	1.03
				H65	13.4964	16.74

Cyclopiamine A (**4**) neutral form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.516076 H (rel E = "0" kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0532933 H (rel E = 1.74 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.005468	-0.041538	-0.083457
2	6	0.490770	1.426703	-0.235996
3	7	1.859876	1.466897	-0.017204
4	6	2.753767	2.644610	-0.197631
5	6	4.095694	2.285900	0.479372
6	6	4.706439	0.935280	0.100080
7	6	3.730255	-0.172003	0.015860
8	6	4.044199	-1.562358	-0.055417
9	6	3.016740	-2.511197	-0.145800
10	6	1.668804	-2.117450	-0.154648
11	6	1.328761	-0.775896	-0.060098
12	6	2.369399	0.160829	0.006796
13	6	-0.903714	-0.179260	1.252146
14	6	-2.318867	-0.002308	0.642966
15	6	-3.584489	-0.178699	1.490702
16	6	-4.836000	-0.074310	0.576544
17	6	-5.936639	0.901438	1.031431
18	6	-6.622013	1.366273	-0.284412
19	6	-5.744939	0.774022	-1.411120
20	7	-4.479750	0.461595	-0.751174
21	6	-3.584339	-0.377458	-1.534957
22	6	-2.318208	-0.753657	-0.704885
23	6	-0.950458	-0.374517	-1.284516
24	6	2.168651	3.886861	0.493213
25	6	2.945668	2.898891	-1.705909
26	6	-0.694689	-1.531899	1.963454
27	6	-0.621768	0.918419	2.298130
28	6	5.734460	-3.258023	-0.077907
29	8	-0.213674	2.384805	-0.520782
30	8	5.913902	0.825455	-0.061023
31	8	5.354921	-1.886194	-0.026054
32	7	-2.392762	-2.296355	-0.511162
33	8	-3.355351	-2.736985	0.111534
34	8	-1.517973	-3.007581	-1.005466
35	1	3.950022	2.270929	1.569150
36	1	4.835884	3.058688	0.259353
37	1	3.250803	-3.565279	-0.217689
38	1	0.900138	-2.876233	-0.256670
39	1	-2.347481	1.037384	0.294852
40	1	-3.593887	-1.134027	2.020276
41	1	-3.607201	0.616140	2.245254
42	1	-5.273728	-1.082552	0.464998
43	1	-5.484577	1.755008	1.547686
44	1	-6.633938	0.425877	1.727906
45	1	-7.652412	1.008198	-0.364011
46	1	-6.651651	2.457866	-0.342161
47	1	-6.215797	-0.141687	-1.821545
48	1	-5.583848	1.464799	-2.246389
49	1	-4.089563	-1.296447	-1.883830
50	1	-3.278122	0.180787	-2.426377
51	1	-0.539440	-1.149332	-1.930188
52	1	-1.092530	0.532748	-1.876926
53	1	1.242984	4.210815	0.017686
54	1	2.901148	4.698613	0.438273

55	1	1.964541	3.682932	1.549200
56	1	3.623074	3.744888	-1.860006
57	1	1.986838	3.134604	-2.175502
58	1	3.376818	2.025663	-2.205991
59	1	-0.799509	-2.403615	1.318154
60	1	-1.419876	-1.632910	2.777102
61	1	0.304519	-1.575899	2.405352
62	1	-0.837187	1.919957	1.917957
63	1	0.422412	0.886697	2.628025
64	1	-1.243729	0.753228	3.184189
65	1	5.407956	-3.726326	-1.014145
66	1	5.329856	-3.816489	0.774878
67	1	6.823631	-3.257879	-0.031371

Cyclopiamine A (**4**) neutral form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.514201 H (rel E = 1.17 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0512846 H (rel E = 3.00 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.007333	-0.047341	-0.109411
2	6	0.478093	1.427725	-0.249576
3	7	1.864055	1.459398	-0.247628
4	6	2.748426	2.657608	-0.180254
5	6	4.127922	2.235401	-0.736881
6	6	4.710737	0.929590	-0.196499
7	6	3.732653	-0.175417	-0.109778
8	6	4.047853	-1.565008	-0.054993
9	6	3.020858	-2.518075	-0.081621
10	6	1.673305	-2.125296	-0.114826
11	6	1.331510	-0.780095	-0.112399
12	6	2.372864	0.157698	-0.149415
13	6	-0.892477	-0.210002	1.229432
14	6	-2.312015	-0.018787	0.634694
15	6	-3.571833	-0.209218	1.487654
16	6	-4.829754	-0.080746	0.585113
17	6	-5.921106	0.893361	1.064896
18	6	-6.615952	1.381156	-0.237604
19	6	-5.749331	0.805192	-1.380956
20	7	-4.480769	0.476079	-0.735928
21	6	-3.595589	-0.354399	-1.539708
22	6	-2.323576	-0.746731	-0.726512
23	6	-0.959664	-0.361410	-1.311652
24	6	2.863024	3.096933	1.292820
25	6	2.208250	3.808103	-1.046200
26	6	-0.688892	-1.575885	1.918049
27	6	-0.597091	0.861620	2.299464
28	6	5.741919	-3.256272	-0.009843
29	8	-0.259267	2.397920	-0.355792
30	8	5.900615	0.842331	0.071511
31	8	5.359918	-1.884163	-0.016860
32	7	-2.397461	-2.292575	-0.558235
33	8	-3.362962	-2.743526	0.052547
34	8	-1.517597	-2.995069	-1.055978
35	1	4.854444	3.029262	-0.549106
36	1	4.046564	2.113685	-1.826601
37	1	3.254373	-3.574750	-0.078323
38	1	0.906359	-2.891161	-0.149432
39	1	-2.339416	1.027083	0.306811
40	1	-3.581376	-1.175806	1.996439
41	1	-3.585624	0.569012	2.259533
42	1	-5.274600	-1.084200	0.458908
43	1	-5.459929	1.736854	1.589546
44	1	-6.614485	0.410837	1.760494
45	1	-7.647685	1.026357	-0.314624
46	1	-6.643819	2.473597	-0.277382
47	1	-6.227163	-0.101084	-1.804197
48	1	-5.591268	1.509941	-2.205097
49	1	-4.107124	-1.266664	-1.896732
50	1	-3.295745	0.215362	-2.426086
51	1	-0.553663	-1.129091	-1.968928
52	1	-1.106665	0.551770	-1.893771
53	1	1.880302	3.374086	1.684619
54	1	3.523401	3.966227	1.374536

55	1	3.276651	2.298476	1.917313
56	1	2.960307	4.603559	-1.073526
57	1	1.276397	4.212065	-0.652325
58	1	2.028469	3.472798	-2.072359
59	1	-0.811252	-2.438312	1.264068
60	1	-1.407914	-1.678713	2.736804
61	1	0.312805	-1.636297	2.351907
62	1	-0.829949	1.870832	1.954630
63	1	0.455489	0.829193	2.603548
64	1	-1.194565	0.662294	3.195236
65	1	5.401440	-3.770231	-0.916859
66	1	5.352368	-3.773182	0.875367
67	1	6.831648	-3.252292	0.020736

Cyclopiamine A (**4**) neutral form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.514065 H (rel E = 1.26 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0560677 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.009526	-0.260893	0.012344
2	6	0.367442	1.242299	-0.147303
3	7	1.738051	1.390978	0.003704
4	6	2.527374	2.638163	-0.203963
5	6	3.920947	2.385022	0.413415
6	6	4.620098	1.089786	-0.002843
7	6	3.733172	-0.093435	-0.041123
8	6	4.154218	-1.454635	-0.119211
9	6	3.202911	-2.483834	-0.152386
10	6	1.829335	-2.196408	-0.103160
11	6	1.386638	-0.885599	-0.009731
12	6	2.351576	0.130736	0.007761
13	6	-0.849514	-0.478575	1.357576
14	6	-2.263622	-0.155338	0.803520
15	6	-3.542296	-0.252293	1.635723
16	6	-4.744413	0.235594	0.795994
17	6	-4.943689	1.775461	0.699918
18	6	-5.752734	1.969036	-0.610929
19	6	-5.845929	0.531950	-1.213196
20	7	-4.756388	-0.250976	-0.610228
21	6	-3.493295	-0.084010	-1.346477
22	6	-2.371929	-0.797651	-0.584514
23	6	-0.939580	-0.692432	-1.158820
24	6	1.875929	3.827097	0.520963
25	6	2.634663	2.913439	-1.716806
26	6	-0.682395	-1.907526	1.907994
27	6	-0.461747	0.494032	2.486664
28	6	5.973934	-3.008482	-0.222089
29	8	-0.420954	2.147443	-0.388562
30	8	5.822059	1.077324	-0.226661
31	8	5.485983	-1.671788	-0.150997
32	7	-2.780515	-2.301540	-0.616290
33	8	-3.121018	-2.878142	0.410190
34	8	-2.740432	-2.832986	-1.725095
35	1	3.823075	2.353201	1.508108
36	1	4.586320	3.216052	0.168308
37	1	3.517082	-3.516920	-0.222594
38	1	1.124261	-3.020291	-0.152858
39	1	-2.177111	0.904837	0.531027
40	1	-3.720869	-1.272539	1.975355
41	1	-3.462450	0.388160	2.522354
42	1	-5.653029	-0.183648	1.247835
43	1	-5.467796	2.158780	1.581498
44	1	-3.981151	2.296668	0.648012
45	1	-6.748095	2.386149	-0.429530
46	1	-5.239207	2.653180	-1.293838
47	1	-6.798099	0.066157	-0.932229
48	1	-5.777949	0.508860	-2.304652
49	1	-3.619682	-0.515024	-2.343610
50	1	-3.172593	0.965195	-1.467015
51	1	-0.622147	-1.641209	-1.592399
52	1	-0.913771	0.047549	-1.963336
53	1	0.910520	4.083140	0.084680
54	1	2.541832	4.692759	0.445646

55	1	1.729669	3.601525	1.582147
56	1	3.236106	3.811157	-1.891909
57	1	1.641501	3.074676	-2.144662
58	1	3.112568	2.079671	-2.241231
59	1	-0.811423	-2.688502	1.158429
60	1	-1.425969	-2.091281	2.689336
61	1	0.310055	-2.026288	2.352709
62	1	-0.650378	1.538528	2.222526
63	1	0.596596	0.386410	2.748822
64	1	-1.041975	0.268262	3.387653
65	1	5.638346	-3.505807	-1.139864
66	1	5.662674	-3.594126	0.651298
67	1	7.060226	-2.918361	-0.233250

Cyclopiamine A (**4**) neutral form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.512384 H (rel E = 2.32 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0541211 H (rel E = 1.22 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.010631	-0.263883	-0.017349
2	6	0.358994	1.245478	-0.161859
3	7	1.736450	1.383493	-0.230816
4	6	2.525519	2.648912	-0.196284
5	6	3.911212	2.335579	-0.806780
6	6	4.616340	1.081071	-0.291603
7	6	3.732468	-0.098190	-0.167053
8	6	4.158339	-1.458124	-0.118489
9	6	3.209180	-2.489029	-0.089216
10	6	1.835143	-2.201288	-0.065352
11	6	1.388003	-0.887884	-0.065663
12	6	2.350614	0.127183	-0.152007
13	6	-0.837991	-0.506539	1.329286
14	6	-2.257820	-0.173935	0.794281
15	6	-3.529367	-0.288303	1.634885
16	6	-4.736812	0.220301	0.815276
17	6	-4.932770	1.762214	0.751851
18	6	-5.751956	1.984236	-0.548225
19	6	-5.853481	0.560049	-1.178883
20	7	-4.760935	-0.237248	-0.600754
21	6	-3.503547	-0.058050	-1.343646
22	6	-2.377929	-0.789479	-0.604873
23	6	-0.949926	-0.679331	-1.189719
24	6	2.662391	3.098372	1.271687
25	6	1.863904	3.750926	-1.040465
26	6	-0.677499	-1.945174	1.857305
27	6	-0.436934	0.441168	2.475761
28	6	5.982361	-3.009985	-0.149266
29	8	-0.447825	2.165343	-0.216065
30	8	5.818343	1.087762	-0.069207
31	8	5.491151	-1.672622	-0.139630
32	7	-2.791901	-2.291635	-0.664998
33	8	-3.123141	-2.889708	0.352086
34	8	-2.765212	-2.798670	-1.785619
35	1	4.579555	3.184600	-0.646133
36	1	3.798213	2.206122	-1.892817
37	1	3.524921	-3.524032	-0.083383
38	1	1.134170	-3.028954	-0.044911
39	1	-2.172933	0.890922	0.543519
40	1	-3.707857	-1.315336	1.953584
41	1	-3.441162	0.332610	2.534532
42	1	-5.643109	-0.205976	1.265206
43	1	-5.448824	2.128934	1.645155
44	1	-3.969208	2.281729	0.702812
45	1	-6.744837	2.399773	-0.350298
46	1	-5.242401	2.681086	-1.221237
47	1	-6.804407	0.090623	-0.899778
48	1	-5.794376	0.559020	-2.271121
49	1	-3.639179	-0.468147	-2.348368
50	1	-3.181432	0.992965	-1.445073
51	1	-0.636245	-1.624239	-1.634514
52	1	-0.928789	0.066751	-1.989165
53	1	1.677246	3.299353	1.701877
54	1	3.256057	4.016361	1.328436
55	1	3.160327	2.335599	1.878899
56	1	2.550300	4.602074	-1.097097

57	1	0.919749	4.081766	-0.609769
58	1	1.671587	3.399415	-2.058927
59	1	-0.821376	-2.715118	1.099283
60	1	-1.418169	-2.130863	2.640911
61	1	0.315333	-2.079766	2.296354
62	1	-0.635308	1.489884	2.240917
63	1	0.626378	0.331219	2.717811
64	1	-0.999454	0.188250	3.380714
65	1	5.639502	-3.554402	-1.037335
66	1	5.681209	-3.551111	0.755613
67	1	7.068285	-2.917991	-0.173841

Cyclopiamine A (**4**) neutral form, conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.51124 H (rel E = 3.03 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0490599 H (rel E = 4.40 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.062388	-0.168134	-0.104591
2	6	0.345894	1.322069	-0.255678
3	7	1.707007	1.436527	-0.018498
4	6	2.542315	2.657336	-0.196809
5	6	3.889809	2.375408	0.504833
6	6	4.575640	1.054560	0.149220
7	6	3.659814	-0.103277	0.065866
8	6	4.045448	-1.476504	0.016770
9	6	3.069421	-2.478325	-0.077101
10	6	1.703585	-2.154379	-0.112699
11	6	1.294935	-0.830956	-0.039890
12	6	2.284109	0.158792	0.031723
13	6	-1.003040	-0.344884	1.198318
14	6	-2.403434	-0.181624	0.547651
15	6	-3.688331	-0.366066	1.356826
16	6	-4.941708	-0.231283	0.414399
17	6	-5.921885	0.863276	0.860365
18	6	-5.302200	2.148047	0.271556
19	6	-4.646770	1.683335	-1.048237
20	7	-4.610557	0.210812	-0.947531
21	6	-3.604305	-0.532505	-1.672635
22	6	-2.349651	-0.931760	-0.799246
23	6	-0.958567	-0.566503	-1.332870
24	6	1.882279	3.874601	0.471012
25	6	2.745425	2.906037	-1.704450
26	6	-0.795960	-1.710269	1.884628
27	6	-0.762682	0.734257	2.272608
28	6	5.821694	-3.082521	0.036636
29	8	-0.405680	2.240437	-0.556631
30	8	5.789032	1.006430	0.004251
31	8	5.370336	-1.731823	0.069563
32	7	-2.452382	-2.465062	-0.618362
33	8	-3.455516	-2.890905	-0.048550
34	8	-1.576085	-3.194314	-1.086827
35	1	3.727829	2.364410	1.592291
36	1	4.592218	3.183373	0.287333
37	1	3.358641	-3.519643	-0.132045
38	1	0.976013	-2.952521	-0.218965
39	1	-2.413934	0.860887	0.204619
40	1	-3.715254	-1.333017	1.865220
41	1	-3.722474	0.408861	2.132080
42	1	-5.428477	-1.209733	0.354276
43	1	-6.905630	0.674966	0.416656
44	1	-6.043112	0.905161	1.947372
45	1	-6.039812	2.940252	0.115229
46	1	-4.539955	2.545692	0.950844
47	1	-5.243698	1.977631	-1.922702
48	1	-3.648124	2.127370	-1.173229
49	1	-4.044909	-1.445239	-2.092018
50	1	-3.260646	0.074850	-2.514696
51	1	-0.513130	-1.376233	-1.908303
52	1	-1.066917	0.301653	-1.987512
53	1	0.949800	4.146278	-0.023693
54	1	2.573001	4.722424	0.420013

55	1	1.670290	3.670734	1.525494
56	1	3.382484	3.783132	-1.856681
57	1	1.783776	3.089301	-2.191348
58	1	3.227437	2.050543	-2.188427
59	1	-0.854705	-2.565189	1.211479
60	1	-1.553635	-1.847363	2.662520
61	1	0.184151	-1.745227	2.368337
62	1	-0.987339	1.740780	1.910418
63	1	0.275609	0.713091	2.621582
64	1	-1.398320	0.539916	3.142797
65	1	5.534581	-3.575348	-0.899877
66	1	5.433908	-3.653788	0.888704
67	1	6.908508	-3.024890	0.099283

Cyclopiamine A (**4**) neutral form, conformer 6

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.509371 H (rel E = 4.21 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0470844 H (rel E = 5.64 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.055561	-0.205614	-0.146602
2	6	0.321918	1.294258	-0.291511
3	7	1.701943	1.414926	-0.261558
4	6	2.506667	2.668435	-0.190635
5	6	3.923757	2.327908	-0.707430
6	6	4.574934	1.068230	-0.136022
7	6	3.667631	-0.096728	-0.060973
8	6	4.067812	-1.463199	0.018434
9	6	3.103230	-2.479610	-0.017204
10	6	1.734749	-2.172392	-0.083976
11	6	1.310701	-0.851453	-0.107590
12	6	2.291229	0.149298	-0.134985
13	6	-0.975531	-0.407820	1.164528
14	6	-2.382127	-0.206608	0.539735
15	6	-3.658916	-0.372506	1.365978
16	6	-4.921446	-0.201062	0.442358
17	6	-5.877955	0.902104	0.917601
18	6	-5.246502	2.186460	0.339950
19	6	-4.607979	1.731725	-0.991784
20	7	-4.600116	0.257224	-0.916618
21	6	-3.618820	-0.492602	-1.668627
22	6	-2.363154	-0.937237	-0.818695
23	6	-0.967340	-0.605405	-1.366932
24	6	2.555597	3.133777	1.277919
25	6	1.916140	3.769935	-1.086816
26	6	-0.784276	-1.796412	1.808779
27	6	-0.698641	0.630690	2.270022
28	6	5.864625	-3.042866	0.124245
29	8	-0.473422	2.216611	-0.421363
30	8	5.760096	1.060644	0.164109
31	8	5.396073	-1.698119	0.087964
32	7	-2.505595	-2.471719	-0.662158
33	8	-3.504913	-2.878377	-0.072014
34	8	-1.666003	-3.217734	-1.169310
35	1	4.593530	3.168606	-0.512536
36	1	3.877798	2.188437	-1.797059
37	1	3.402790	-3.519240	0.005110
38	1	1.017665	-2.985488	-0.122093
39	1	-2.373771	0.840569	0.213451
40	1	-3.701499	-1.342969	1.866650
41	1	-3.664274	0.396563	2.147858
42	1	-5.425366	-1.170086	0.372477
43	1	-6.870335	0.735582	0.484539
44	1	-5.984202	0.929503	2.006633
45	1	-5.975806	2.989441	0.200294
46	1	-4.473772	2.566422	1.017472
47	1	-5.204065	2.052176	-1.857590
48	1	-3.601703	2.158541	-1.114276
49	1	-4.083759	-1.386658	-2.102124
50	1	-3.271608	0.124760	-2.501934
51	1	-0.541049	-1.437822	-1.924078
52	1	-1.058937	0.246724	-2.044996
53	1	1.547899	3.355285	1.640594
54	1	3.159385	4.042962	1.362884

55	1	3.000471	2.370661	1.924589
56	1	2.615187	4.612492	-1.105834
57	1	0.949691	4.116401	-0.722684
58	1	1.786766	3.410876	-2.112563
59	1	-0.859748	-2.631326	1.112595
60	1	-1.541738	-1.943825	2.584854
61	1	0.195799	-1.859811	2.289412
62	1	-0.931428	1.650246	1.954963
63	1	0.350617	0.592584	2.584663
64	1	-1.305841	0.403019	3.152297
65	1	5.580048	-3.589631	-0.782837
66	1	5.487745	-3.571633	1.007855
67	1	6.950788	-2.968418	0.180063

Cyclopiamine A (**4**) neutral form, conformer 1

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1550.551259 H (rel E = 0.10 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.037914	-0.176296	-0.057602
2	6	0.437903	1.317792	-0.203940
3	7	1.806800	1.431912	-0.022058
4	6	2.636892	2.658255	-0.204053
5	6	3.998991	2.369907	0.464635
6	6	4.674835	1.056664	0.088897
7	6	3.767681	-0.102919	0.010166
8	6	4.153792	-1.478373	-0.051752
9	6	3.176475	-2.480236	-0.122003
10	6	1.810093	-2.155647	-0.121806
11	6	1.399555	-0.833370	-0.042031
12	6	2.387543	0.158731	0.007235
13	6	-0.859020	-0.377612	1.266317
14	6	-2.260241	-0.086517	0.671951
15	6	-3.538402	-0.140384	1.521200
16	6	-4.770154	-0.001552	0.590294
17	6	-5.900420	0.926366	1.080050
18	6	-6.498667	1.551648	-0.212631
19	6	-5.645103	0.968806	-1.355630
20	7	-4.385489	0.604987	-0.702744
21	6	-3.519887	-0.235145	-1.529076
22	6	-2.318739	-0.787435	-0.692677
23	6	-0.894442	-0.585046	-1.252571
24	6	2.001961	3.868180	0.496926
25	6	2.808400	2.929029	-1.710043
26	6	-0.708544	-1.797774	1.843528
27	6	-0.518427	0.610427	2.395504
28	6	5.914091	-3.108666	-0.087258
29	8	-0.322271	2.245535	-0.459156
30	8	5.893950	1.011517	-0.069250
31	8	5.478755	-1.743523	-0.031665
32	7	-2.604481	-2.321340	-0.611849
33	8	-3.333956	-2.743526	0.282902
34	8	-2.159372	-3.037418	-1.510885
35	1	3.860521	2.345790	1.555232
36	1	4.687179	3.187212	0.237725
37	1	3.463526	-3.522079	-0.180284
38	1	1.086489	-2.960789	-0.198236
39	1	-2.194150	0.957695	0.346075
40	1	-3.613699	-1.059467	2.105894
41	1	-3.511728	0.698606	2.225826
42	1	-5.192752	-1.006435	0.407394
43	1	-5.491067	1.706332	1.730729
44	1	-6.643355	0.371144	1.660782
45	1	-7.556030	1.306032	-0.346986
46	1	-6.416579	2.642582	-0.186466
47	1	-6.136054	0.073594	-1.784658
48	1	-5.468550	1.674510	-2.174663
49	1	-4.086314	-1.072818	-1.973921
50	1	-3.133171	0.364114	-2.359159
51	1	-0.527164	-1.483379	-1.746221
52	1	-0.916559	0.210095	-2.000612
53	1	1.079113	4.179362	0.006928
54	1	2.712852	4.700273	0.467215
55	1	1.784399	3.642685	1.545995
56	1	3.431787	3.817099	-1.856870
57	1	1.838102	3.108030	-2.182419
58	1	3.290028	2.086231	-2.217428

59	1	-0.782051	-2.592663	1.099017
60	1	-1.483676	-1.973395	2.596395
61	1	0.261963	-1.906539	2.336615
62	1	-0.722015	1.649405	2.120718
63	1	0.535420	0.527242	2.684036
64	1	-1.118084	0.380114	3.282744
65	1	5.591093	-3.589634	-1.017010
66	1	5.547576	-3.677615	0.774287
67	1	7.003801	-3.065930	-0.059470

Cyclopiamine A (**4**) neutral form, conformer 2

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1550.548727 H (rel E = 1.69 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.040191	-0.187854	-0.098230
2	6	0.425744	1.310830	-0.247136
3	7	1.806294	1.421511	-0.245662
4	6	2.622466	2.669595	-0.178016
5	6	4.026140	2.325581	-0.725823
6	6	4.676504	1.054158	-0.198492
7	6	3.769597	-0.104905	-0.109520
8	6	4.159716	-1.478456	-0.050946
9	6	3.185281	-2.485316	-0.064119
10	6	1.818493	-2.164103	-0.091081
11	6	1.403999	-0.840280	-0.100510
12	6	2.389973	0.154149	-0.147300
13	6	-0.840884	-0.393902	1.235123
14	6	-2.249061	-0.099203	0.658668
15	6	-3.517166	-0.150472	1.522507
16	6	-4.758358	0.002568	0.606177
17	6	-5.875092	0.938809	1.111124
18	6	-6.482602	1.572481	-0.173225
19	6	-5.647525	0.984436	-1.327195
20	7	-4.383412	0.609497	-0.689649
21	6	-3.533649	-0.235302	-1.527593
22	6	-2.325562	-0.796617	-0.706856
23	6	-0.906107	-0.601738	-1.283366
24	6	2.700349	3.120720	1.291650
25	6	2.036346	3.784191	-1.057695
26	6	-0.692863	-1.815790	1.809500
27	6	-0.481960	0.586851	2.366378
28	6	5.926880	-3.101575	-0.017064
29	8	-0.360566	2.246097	-0.356008
30	8	5.878812	1.031110	0.059308
31	8	5.486177	-1.736959	-0.020565
32	7	-2.619104	-2.329485	-0.628064
33	8	-3.344191	-2.749787	0.271120
34	8	-2.185183	-3.045985	-1.532323
35	1	4.697464	3.164127	-0.528153
36	1	3.958749	2.204383	-1.816741
37	1	3.474415	-3.528153	-0.052058
38	1	1.097967	-2.974840	-0.103993
39	1	-2.182968	0.944963	0.334613
40	1	-3.592672	-1.072378	2.102748
41	1	-3.476337	0.684157	2.231731
42	1	-5.191764	-0.997994	0.424909
43	1	-5.452043	1.713761	1.759064
44	1	-6.616171	0.388455	1.698833
45	1	-7.543680	1.336862	-0.295795
46	1	-6.390090	2.662553	-0.145753
47	1	-6.150951	0.093931	-1.751605
48	1	-5.474871	1.689963	-2.147214
49	1	-4.111354	-1.068582	-1.966135
50	1	-3.153360	0.362408	-2.361728
51	1	-0.545395	-1.506472	-1.770189
52	1	-0.931899	0.183871	-2.041699
53	1	1.702391	3.346412	1.678873
54	1	3.311131	4.026337	1.369499
55	1	3.151407	2.348426	1.923868
56	1	2.762798	4.602248	-1.103107
57	1	1.098951	4.170953	-0.658519
58	1	1.861696	3.427292	-2.077838

59	1	-0.789879	-2.611882	1.069087
60	1	-1.456760	-1.980694	2.576195
61	1	0.284020	-1.935065	2.287015
62	1	-0.707683	1.624944	2.109848
63	1	0.581365	0.515275	2.622637
64	1	-1.051369	0.336373	3.267917
65	1	5.598530	-3.627198	-0.920479
66	1	5.569834	-3.630579	0.873297
67	1	7.016578	-3.053456	0.000475

Cyclopiamine A (**4**) neutral form, conformer 3

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1550.551423 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.006003	-0.213607	0.012384
2	6	0.389747	1.283372	-0.145693
3	7	1.763397	1.407329	-0.011614
4	6	2.578932	2.639118	-0.222188
5	6	3.964055	2.360202	0.401181
6	6	4.636480	1.052339	0.001918
7	6	3.735385	-0.113765	-0.044231
8	6	4.128584	-1.486667	-0.118049
9	6	3.156374	-2.495477	-0.153166
10	6	1.788672	-2.180154	-0.105840
11	6	1.372517	-0.860486	-0.012654
12	6	2.354235	0.138483	0.000429
13	6	-0.854946	-0.423463	1.360796
14	6	-2.271899	-0.120392	0.802396
15	6	-3.547581	-0.213659	1.639845
16	6	-4.764391	0.230380	0.797132
17	6	-4.984620	1.762876	0.660616
18	6	-5.794627	1.916942	-0.653702
19	6	-5.881709	0.467491	-1.217651
20	7	-4.779751	-0.296386	-0.601045
21	6	-3.519097	-0.106456	-1.343922
22	6	-2.371513	-0.777000	-0.578123
23	6	-0.945955	-0.640648	-1.159626
24	6	1.961552	3.846569	0.498080
25	6	2.698213	2.908308	-1.733380
26	6	-0.681134	-1.845201	1.925777
27	6	-0.481445	0.560344	2.483541
28	6	5.898964	-3.104038	-0.215870
29	8	-0.384931	2.207163	-0.370835
30	8	5.849518	1.016039	-0.199252
31	8	5.455190	-1.742300	-0.144559
32	7	-2.748136	-2.290998	-0.589954
33	8	-3.123486	-2.857357	0.431720
34	8	-2.677123	-2.852244	-1.686439
35	1	3.860997	2.333686	1.495610
36	1	4.638102	3.183046	0.152972
37	1	3.448604	-3.535308	-0.221006
38	1	1.067893	-2.989837	-0.158129
39	1	-2.197359	0.936161	0.514420
40	1	-3.706898	-1.224108	2.017611
41	1	-3.471676	0.454094	2.505739
42	1	-5.664328	-0.186440	1.266836
43	1	-5.515872	2.155494	1.533713
44	1	-4.027792	2.292601	0.597870
45	1	-6.793791	2.329948	-0.483054
46	1	-5.284265	2.583443	-1.356302
47	1	-6.828417	0.005224	-0.913705
48	1	-5.819271	0.417184	-2.308483
49	1	-3.636553	-0.541199	-2.340173
50	1	-3.231709	0.948816	-1.471593
51	1	-0.610074	-1.576773	-1.605388
52	1	-0.941732	0.110230	-1.953948
53	1	1.022291	4.153909	0.037779
54	1	2.667803	4.681483	0.444864
55	1	1.778725	3.621251	1.553795
56	1	3.313028	3.798307	-1.902857
57	1	1.711697	3.082843	-2.172754
58	1	3.165570	2.066337	-2.255324

59	1	-0.775143	-2.632921	1.177560
60	1	-1.436835	-2.029138	2.696290
61	1	0.302391	-1.947978	2.394536
62	1	-0.694374	1.600667	2.220593
63	1	0.580820	0.477866	2.739664
64	1	-1.053168	0.325085	3.387870
65	1	5.548373	-3.587234	-1.134369
66	1	5.567633	-3.676689	0.657447
67	1	6.988630	-3.052534	-0.224884

Cyclopiamine A (**4**) neutral form, conformer 4

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1550.549383 H (rel E = 1.28 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.007505	-0.219904	-0.037970
2	6	0.381936	1.279784	-0.202795
3	7	1.761510	1.396751	-0.241868
4	6	2.573418	2.648685	-0.199283
5	6	3.962738	2.309540	-0.785772
6	6	4.633745	1.042319	-0.274262
7	6	3.734866	-0.120660	-0.158814
8	6	4.132424	-1.492465	-0.112010
9	6	3.162414	-2.503591	-0.095621
10	6	1.794084	-2.188240	-0.080277
11	6	1.374058	-0.866106	-0.078862
12	6	2.353658	0.132428	-0.156746
13	6	-0.833775	-0.428157	1.323146
14	6	-2.259395	-0.124180	0.787238
15	6	-3.521555	-0.217119	1.644676
16	6	-4.750326	0.230456	0.821384
17	6	-4.970207	1.763710	0.691652
18	6	-5.798244	1.922467	-0.610745
19	6	-5.897278	0.474376	-1.175914
20	7	-4.787930	-0.293226	-0.577600
21	6	-3.538240	-0.106140	-1.339653
22	6	-2.380822	-0.780675	-0.591584
23	6	-0.963641	-0.649688	-1.195763
24	6	2.690582	3.102823	1.266995
25	6	1.958266	3.758811	-1.064575
26	6	-0.661601	-1.849395	1.890494
27	6	-0.437787	0.552821	2.441931
28	6	5.907365	-3.107114	-0.155874
29	8	-0.410500	2.212187	-0.290739
30	8	5.842673	1.025179	-0.049278
31	8	5.460299	-1.744955	-0.122604
32	7	-2.763688	-2.293501	-0.599928
33	8	-3.128628	-2.859333	0.425774
34	8	-2.709999	-2.853736	-1.697955
35	1	4.635593	3.151739	-0.610207
36	1	3.864923	2.184385	-1.873951
37	1	3.456283	-3.545175	-0.092585
38	1	1.076884	-3.001990	-0.070385
39	1	-2.187723	0.931944	0.498890
40	1	-3.676835	-1.227549	2.024297
41	1	-3.430809	0.449966	2.509749
42	1	-5.643888	-0.185945	1.303540
43	1	-5.488590	2.154845	1.573122
44	1	-4.013657	2.292353	0.616934
45	1	-6.793691	2.338121	-0.425373
46	1	-5.295776	2.588657	-1.319317
47	1	-6.840353	0.013791	-0.858369
48	1	-5.851721	0.425919	-2.267676
49	1	-3.672453	-0.539548	-2.334385
50	1	-3.249832	0.948514	-1.470654
51	1	-0.635949	-1.588753	-1.641679
52	1	-0.969658	0.096591	-1.994757
53	1	1.703194	3.326579	1.681489
54	1	3.300838	4.010196	1.326825
55	1	3.160665	2.332665	1.887851
56	1	2.679259	4.580174	-1.131480
57	1	1.030298	4.141803	-0.640504
58	1	1.757546	3.398933	-2.078841

59	1	-0.781282	-2.640955	1.150245
60	1	-1.403890	-2.018878	2.677249
61	1	0.329057	-1.961426	2.341461
62	1	-0.672743	1.591211	2.194355
63	1	0.633467	0.482475	2.662977
64	1	-0.975966	0.301353	3.362304
65	1	5.550449	-3.619384	-1.056073
66	1	5.584446	-3.652932	0.737411
67	1	6.996785	-3.053315	-0.174242

Cyclopiamine A (**4**) neutral form, conformer 5

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1550.546837 H (rel E = 2.88 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.025510	-0.221523	-0.110338
2	6	0.356095	1.275296	-0.270881
3	7	1.717957	1.413476	-0.054327
4	6	2.534163	2.650402	-0.225737
5	6	3.880750	2.390404	0.484953
6	6	4.586815	1.084378	0.141558
7	6	3.700128	-0.090079	0.053802
8	6	4.108309	-1.460253	0.027616
9	6	3.148188	-2.478042	-0.050005
10	6	1.777733	-2.174070	-0.092790
11	6	1.345235	-0.857282	-0.047084
12	6	2.316800	0.150249	0.010522
13	6	-0.953709	-0.415440	1.192118
14	6	-2.349929	-0.167815	0.560275
15	6	-3.636144	-0.256248	1.389907
16	6	-4.888514	-0.219117	0.449556
17	6	-5.968548	0.764285	0.918052
18	6	-5.486362	2.121770	0.357775
19	6	-4.675105	1.762659	-0.910528
20	7	-4.601534	0.286231	-0.904331
21	6	-3.549970	-0.362766	-1.671800
22	6	-2.351836	-0.893202	-0.791737
23	6	-0.918547	-0.669838	-1.321318
24	6	1.860112	3.856826	0.444551
25	6	2.745876	2.908509	-1.728704
26	6	-0.791412	-1.824039	1.794409
27	6	-0.659227	0.596096	2.313151
28	6	5.892702	-3.062661	0.124958
29	8	-0.410580	2.187307	-0.560989
30	8	5.810135	1.056962	0.014499
31	8	5.436153	-1.703926	0.088370
32	7	-2.613674	-2.418339	-0.703015
33	8	-3.357073	-2.847770	0.179610
34	8	-2.154563	-3.133236	-1.598424
35	1	3.711165	2.375378	1.571268
36	1	4.562373	3.216037	0.268698
37	1	3.451568	-3.516417	-0.081721
38	1	1.068220	-2.991067	-0.174475
39	1	-2.299946	0.875293	0.223506
40	1	-3.672567	-1.158555	2.005019
41	1	-3.657849	0.601818	2.071536
42	1	-5.282075	-1.237827	0.362808
43	1	-6.932141	0.487501	0.475623
44	1	-6.085634	0.771743	2.006412
45	1	-6.320069	2.795334	0.138798
46	1	-4.843219	2.627166	1.085407
47	1	-5.170925	2.100643	-1.829624
48	1	-3.681471	2.233861	-0.887834
49	1	-3.959283	-1.198523	-2.254653
50	1	-3.145523	0.354512	-2.390837
51	1	-0.521072	-1.569962	-1.787393
52	1	-0.934044	0.110346	-2.085348
53	1	0.945907	4.147855	-0.073336
54	1	2.557439	4.700653	0.426154
55	1	1.617369	3.637678	1.489438
56	1	3.361810	3.803251	-1.866442
57	1	1.787808	3.070186	-2.231235
58	1	3.252894	2.067173	-2.213216

59	1	-0.836981	-2.630178	1.059831
60	1	-1.578256	-2.002722	2.534047
61	1	0.170534	-1.908582	2.308433
62	1	-0.870446	1.627290	2.015674
63	1	0.387282	0.534099	2.632041
64	1	-1.279009	0.371082	3.187860
65	1	5.622471	-3.598793	-0.791422
66	1	5.494147	-3.591227	0.997862
67	1	6.979146	-3.000319	0.200627

Cyclopiamine B (**6**) neutral form, conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.520687 H (rel E = 4.15 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0619299 H (rel E = 5.11 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.082434	-0.023445	0.076277
2	6	-0.630098	-1.398920	0.129211
3	7	-1.998093	-1.188107	0.252351
4	6	-3.067036	-2.224790	0.187863
5	6	-4.356496	-1.563165	0.724334
6	6	-4.718692	-0.202367	0.128805
7	6	-3.569760	0.716730	-0.027115
8	6	-3.646966	2.119163	-0.277966
9	6	-2.474294	2.875030	-0.411158
10	6	-1.211706	2.270619	-0.293402
11	6	-1.100102	0.914721	-0.025514
12	6	-2.284504	0.171242	0.086099
13	6	1.062271	0.137988	1.324246
14	6	2.324637	-0.684355	0.865246
15	6	3.700572	-0.309058	1.453184
16	6	4.350456	0.957598	0.866704
17	6	5.887945	0.981360	0.853108
18	6	6.172379	2.124249	-0.132423
19	6	5.045847	1.980922	-1.187823
20	7	3.950419	1.203000	-0.547441
21	6	3.625991	-0.017089	-1.274542
22	6	2.344531	-0.663614	-0.687568
23	6	1.052332	0.035816	-1.127808
24	6	-2.722642	-3.426796	1.082209
25	6	-3.239392	-2.668090	-1.278258
26	6	1.351139	1.629358	1.580160
27	6	0.480762	-0.446661	2.625538
28	6	-5.032511	4.044588	-0.604359
29	8	-0.083535	-2.490084	0.070885
30	8	-5.881013	0.072707	-0.133303
31	8	-4.886283	2.648235	-0.366329
32	7	2.413589	-2.106711	-1.255396
33	8	1.973189	-2.290862	-2.387069
34	8	3.010916	-2.949732	-0.594205
35	1	-4.252991	-1.414290	1.808929
36	1	-5.204825	-2.232761	0.565122
37	1	-2.527443	3.936692	-0.613795
38	1	-0.327454	2.885802	-0.427147
39	1	2.137122	-1.719705	1.155841
40	1	3.631376	-0.208532	2.542519
41	1	4.361295	-1.165041	1.272730
42	1	4.019485	1.831314	1.441512
43	1	6.321644	1.146954	1.844971
44	1	6.278508	0.028833	0.471254
45	1	6.095303	3.089462	0.381218
46	1	7.167440	2.072459	-0.583985
47	1	4.678220	2.956683	-1.526216
48	1	5.414075	1.446486	-2.072967
49	1	3.439899	0.235391	-2.322914
50	1	4.445359	-0.758318	-1.258005
51	1	1.292670	1.083268	-1.332492
52	1	0.641093	-0.400405	-2.039512
53	1	-1.852440	-3.967262	0.710588
54	1	-3.581732	-4.105103	1.104105

55	1	-2.519131	-3.101727	2.107584
56	1	-4.036224	-3.415030	-1.352022
57	1	-3.507269	-1.823820	-1.921795
58	1	-2.313157	-3.113572	-1.651164
59	1	1.794619	2.129160	0.715354
60	1	2.044240	1.733361	2.419994
61	1	0.431988	2.150712	1.859854
62	1	-0.443323	0.071016	2.907018
63	1	1.191591	-0.312404	3.448595
64	1	0.270327	-1.516347	2.542414
65	1	-4.577887	4.636348	0.199469
66	1	-6.107787	4.222688	-0.625930
67	1	-4.594771	4.332091	-1.567854

Cyclopiamine B (**6**) neutral form, conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.527302 H (rel E = "0" kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0700688 H (rel E = 0.00 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.039007	0.045882	-0.048821
2	6	-0.673439	-1.368001	0.050775
3	7	-2.042648	-1.226872	0.245486
4	6	-3.056438	-2.319520	0.244924
5	6	-4.349817	-1.718777	0.839777
6	6	-4.816300	-0.391222	0.240926
7	6	-3.728375	0.582659	-0.000007
8	6	-3.895001	1.971215	-0.282970
9	6	-2.773845	2.784486	-0.498696
10	6	-1.475933	2.251750	-0.431753
11	6	-1.276883	0.911513	-0.138170
12	6	-2.411228	0.109688	0.057730
13	6	0.935039	0.306177	1.187867
14	6	2.215876	-0.472896	0.739588
15	6	3.531297	-0.246121	1.525225
16	6	4.459499	0.814929	0.931422
17	6	5.913701	0.807542	1.439485
18	6	6.755759	1.275407	0.215406
19	6	5.724326	1.459517	-0.918839
20	7	4.615550	0.599351	-0.511264
21	6	3.374601	0.786808	-1.225397
22	6	2.324797	-0.262430	-0.790397
23	6	0.903334	0.108428	-1.281219
24	6	-2.602173	-3.490265	1.132048
25	6	-3.280423	-2.790597	-1.205546
26	6	1.168237	1.815915	1.390167
27	6	0.382056	-0.255793	2.510384
28	6	-5.398647	3.811440	-0.578378
29	8	-0.077456	-2.429499	-0.047422
30	8	-6.004294	-0.181994	0.041393
31	8	-5.163706	2.430687	-0.319045
32	7	2.785658	-1.578402	-1.478174
33	8	2.680278	-1.615671	-2.704527
34	8	3.263431	-2.471636	-0.793487
35	1	-4.197163	-1.544227	1.914624
36	1	-5.167740	-2.435639	0.737479
37	1	-2.895991	3.835322	-0.726043
38	1	-0.634920	2.910116	-0.625850
39	1	1.961133	-1.527476	0.862093
40	1	3.307577	-0.004074	2.571200
41	1	4.078796	-1.194182	1.529843
42	1	4.034504	1.826217	1.103375
43	1	6.037764	1.458310	2.310320
44	1	6.200007	-0.205510	1.740133
45	1	7.300171	2.203526	0.411555
46	1	7.491950	0.514346	-0.056988
47	1	5.404941	2.519988	-0.979512
48	1	6.100799	1.166663	-1.904246
49	1	2.947905	1.792382	-1.038416
50	1	3.537082	0.699219	-2.304064
51	1	0.909075	1.124794	-1.685461
52	1	0.573713	-0.547490	-2.088049
53	1	-1.721424	-3.985104	0.723203
54	1	-3.418893	-4.215934	1.201425

55	1	-2.368175	-3.143214	2.143681
56	1	-4.042342	-3.576194	-1.229625
57	1	-3.622191	-1.969723	-1.844328
58	1	-2.354003	-3.196575	-1.620572
59	1	1.498658	2.329534	0.483583
60	1	1.934524	1.975127	2.154544
61	1	0.252952	2.302887	1.737714
62	1	-0.585977	0.198064	2.750657
63	1	1.062225	-0.024198	3.336959
64	1	0.258976	-1.341988	2.478128
65	1	-6.481824	3.930264	-0.548306
66	1	-5.026368	4.099447	-1.568769
67	1	-4.937751	4.445295	0.188897

Cyclopiamine B (**6**) neutral form, conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.525245 H (rel E = 1.29 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0681277 H (rel E = 1.22 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.040844	0.046864	-0.049496
2	6	-0.670249	-1.370117	0.085025
3	7	-2.052535	-1.252280	0.022519
4	6	-3.059891	-2.328851	0.249343
5	6	-4.384494	-1.852285	-0.391421
6	6	-4.823829	-0.425593	-0.066504
7	6	-3.732377	0.570623	-0.140427
8	6	-3.896951	1.977272	-0.303276
9	6	-2.772996	2.802182	-0.445526
10	6	-1.476205	2.265735	-0.387049
11	6	-1.279383	0.908243	-0.179464
12	6	-2.417395	0.091638	-0.099725
13	6	0.934360	0.348041	1.175150
14	6	2.217107	-0.444657	0.753429
15	6	3.532881	-0.189550	1.529582
16	6	4.464640	0.845679	0.896855
17	6	5.919331	0.852181	1.403584
18	6	6.761743	1.271736	0.162364
19	6	5.729498	1.418915	-0.976463
20	7	4.618575	0.577248	-0.537226
21	6	3.377470	0.743574	-1.255907
22	6	2.324311	-0.286285	-0.783150
23	6	0.904355	0.074746	-1.285611
24	6	-3.225965	-2.530171	1.768208
25	6	-2.639345	-3.643042	-0.430217
26	6	1.177761	1.862000	1.332035
27	6	0.381938	-0.165488	2.517973
28	6	-5.400505	3.824882	-0.548368
29	8	-0.056916	-2.418632	0.216170
30	8	-5.994731	-0.169776	0.173968
31	8	-5.166693	2.434567	-0.345586
32	7	2.779260	-1.626468	-1.427252
33	8	2.660918	-1.709631	-2.650619
34	8	3.265035	-2.493433	-0.715152
35	1	-5.192294	-2.527117	-0.099403
36	1	-4.287811	-1.907796	-1.485297
37	1	-2.890907	3.866524	-0.601234
38	1	-0.634617	2.939858	-0.505586
39	1	1.961222	-1.493147	0.913399
40	1	3.309097	0.093255	2.565268
41	1	4.078279	-1.137941	1.571743
42	1	4.043302	1.864247	1.031478
43	1	6.202689	-0.149925	1.741384
44	1	6.046346	1.534294	2.249658
45	1	7.310381	2.204025	0.323916
46	1	7.494274	0.498086	-0.083158
47	1	5.413235	2.477597	-1.073891
48	1	6.103783	1.090525	-1.951463
49	1	2.954012	1.756304	-1.102869
50	1	3.538464	0.618574	-2.331145
51	1	0.912138	1.081750	-1.712727
52	1	0.574314	-0.597292	-2.079342
53	1	-2.279768	-2.847160	2.215468
54	1	-3.974635	-3.304517	1.963744

55	1	-3.555439	-1.609200	2.260048
56	1	-3.471541	-4.351246	-0.360855
57	1	-2.417633	-3.480099	-1.489484
58	1	-1.758936	-4.080914	0.038462
59	1	1.499427	2.350463	0.408279
60	1	1.956174	2.034573	2.080969
61	1	0.272495	2.364128	1.683376
62	1	-0.582474	0.303429	2.744944
63	1	1.065168	0.092601	3.334179
64	1	0.254165	-1.250718	2.522976
65	1	-6.484613	3.938879	-0.543528
66	1	-5.000326	4.160734	-1.512680
67	1	-4.965764	4.423339	0.261190

Cyclopiamine B (**6**) neutral form, conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.527299 H (rel E = 0.002 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0700692 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.039026	0.045898	-0.048828
2	6	-0.673417	-1.367978	0.050842
3	7	-2.042633	-1.226882	0.245520
4	6	-3.056409	-2.319550	0.244894
5	6	-4.349801	-1.718838	0.839739
6	6	-4.816301	-0.391255	0.240961
7	6	-3.728387	0.582618	-0.000036
8	6	-3.895018	1.971171	-0.283027
9	6	-2.773878	2.784461	-0.498741
10	6	-1.475960	2.251748	-0.431762
11	6	-1.276903	0.911512	-0.138190
12	6	-2.411234	0.109664	0.057704
13	6	0.935019	0.306290	1.187835
14	6	2.215842	-0.472813	0.739597
15	6	3.531245	-0.246021	1.525239
16	6	4.459474	0.814986	0.931393
17	6	5.913664	0.807636	1.439493
18	6	6.755784	1.275226	0.215347
19	6	5.724367	1.459430	-0.918881
20	7	4.615537	0.599336	-0.511284
21	6	3.374592	0.786789	-1.225433
22	6	2.324789	-0.262438	-0.790387
23	6	0.903322	0.108421	-1.281224
24	6	-2.602175	-3.490326	1.131993
25	6	-3.280355	-2.790580	-1.205600
26	6	1.168190	1.816049	1.390020
27	6	0.382058	-0.255605	2.510402
28	6	-5.398582	3.811433	-0.578375
29	8	-0.077395	-2.429454	-0.047295
30	8	-6.004312	-0.182016	0.041531
31	8	-5.163711	2.430652	-0.319137
32	7	2.785653	-1.578457	-1.478079
33	8	3.263440	-2.471660	-0.793296
34	8	2.680314	-1.615806	-2.704432
35	1	-4.197169	-1.544331	1.914595
36	1	-5.167718	-2.435706	0.737405
37	1	-2.896048	3.835291	-0.726115
38	1	-0.634952	2.910123	-0.625860
39	1	1.961067	-1.527386	0.862145
40	1	3.307505	-0.003888	2.571191
41	1	4.078721	-1.194096	1.529940
42	1	4.034472	1.826285	1.103268
43	1	6.037715	1.458582	2.310196
44	1	6.199926	-0.205360	1.740369
45	1	7.300408	2.203242	0.411394
46	1	7.491794	0.513977	-0.057013
47	1	5.405058	2.519923	-0.979532
48	1	6.100806	1.166558	-1.904296
49	1	2.947914	1.792374	-1.038471
50	1	3.537085	0.699199	-2.304098
51	1	0.909053	1.124793	-1.685475
52	1	0.573704	-0.547479	-2.088068
53	1	-1.721416	-3.985155	0.723162
54	1	-3.418910	-4.215984	1.201324

55	1	-2.368206	-3.143307	2.143643
56	1	-4.042255	-3.576194	-1.229721
57	1	-3.622131	-1.969692	-1.844360
58	1	-2.353918	-3.196524	-1.620620
59	1	1.498768	2.329587	0.483449
60	1	1.934348	1.975330	2.154514
61	1	0.252844	2.303054	1.737359
62	1	-0.585989	0.198234	2.750651
63	1	1.062214	-0.023940	3.336970
64	1	0.259017	-1.341806	2.478220
65	1	-4.937632	4.445206	0.188935
66	1	-6.481752	3.930319	-0.548279
67	1	-5.026293	4.099486	-1.568749

Cyclopiamine B (**6**) neutral form, conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.525244 H (rel E = 1.29 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0681271 H (rel E = 1.22 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.040865	0.046831	-0.049530
2	6	-0.670267	-1.370132	0.084966
3	7	-2.052541	-1.252295	0.022456
4	6	-3.059891	-2.328857	0.249314
5	6	-4.384494	-1.852293	-0.391449
6	6	-4.823836	-0.425606	-0.066523
7	6	-3.732382	0.570614	-0.140422
8	6	-3.896959	1.977269	-0.303222
9	6	-2.773006	2.802181	-0.445460
10	6	-1.476212	2.265735	-0.387019
11	6	-1.279389	0.908236	-0.179492
12	6	-2.417401	0.091626	-0.099767
13	6	0.934333	0.347996	1.175143
14	6	2.217079	-0.444684	0.753384
15	6	3.532846	-0.189643	1.529570
16	6	4.464637	0.845617	0.896925
17	6	5.919330	0.852039	1.403633
18	6	6.761734	1.271709	0.162443
19	6	5.729482	1.419028	-0.976358
20	7	4.618547	0.577337	-0.537191
21	6	3.377423	0.743718	-1.255838
22	6	2.324336	-0.286248	-0.783163
23	6	0.904354	0.074723	-1.285647
24	6	-3.225949	-2.530151	1.768185
25	6	-2.639349	-3.643059	-0.430230
26	6	1.177668	1.861954	1.332092
27	6	0.381919	-0.165604	2.517947
28	6	-5.400486	3.824880	-0.548365
29	8	-0.056934	-2.418636	0.216200
30	8	-5.994747	-0.169788	0.173901
31	8	-5.166694	2.434579	-0.345468
32	7	2.779380	-1.626359	-1.427347
33	8	3.264914	-2.493486	-0.715228
34	8	2.661312	-1.709350	-2.650739
35	1	-5.192287	-2.527137	-0.099439
36	1	-4.287808	-1.907795	-1.485325
37	1	-2.890919	3.866533	-0.601112
38	1	-0.634632	2.939871	-0.505525
39	1	1.961159	-1.493178	0.913292
40	1	3.309057	0.093106	2.565273
41	1	4.078226	-1.138045	1.571682
42	1	4.043321	1.864180	1.031652
43	1	6.046368	1.534059	2.249780
44	1	6.202667	-0.150108	1.741326
45	1	7.310393	2.203970	0.324086
46	1	7.494251	0.498076	-0.083173
47	1	5.413241	2.477724	-1.073684
48	1	6.103746	1.090719	-1.951394
49	1	2.953951	1.756422	-1.102686
50	1	3.538413	0.618847	-2.331089
51	1	0.912078	1.081709	-1.712814
52	1	0.574335	-0.597352	-2.079356
53	1	-2.279744	-2.847120	2.215444
54	1	-3.974609	-3.304501	1.963739

55	1	-3.555432	-1.609175	2.260012
56	1	-3.471538	-4.351270	-0.360832
57	1	-2.417674	-3.480134	-1.489508
58	1	-1.758921	-4.080910	0.038434
59	1	1.499449	2.350460	0.408402
60	1	1.955972	2.034525	2.081140
61	1	0.272336	2.364043	1.683317
62	1	-0.582544	0.303223	2.744893
63	1	1.065093	0.092539	3.334184
64	1	0.254250	-1.250844	2.522930
65	1	-4.965768	4.423395	0.261162
66	1	-6.484595	3.938893	-0.543575
67	1	-5.000265	4.160649	-1.512687

Cyclopiamine B (**6**) neutral form, conformer 6

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.506538 H (rel E = 13.03 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0504817 H (rel E = 12.29 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.083970	-0.340299	0.116845
2	6	-0.779696	-1.620071	-0.081429
3	7	-2.116703	-1.247959	-0.197782
4	6	-3.306909	-2.144906	-0.229421
5	6	-4.459019	-1.349402	-0.886688
6	6	-4.685309	0.073626	-0.377910
7	6	-3.441267	0.853422	-0.200675
8	6	-3.348584	2.275375	-0.158624
9	6	-2.093329	2.893277	-0.084208
10	6	-0.920304	2.124513	-0.003709
11	6	-0.976725	0.740050	0.010656
12	6	-2.237269	0.141258	-0.128376
13	6	0.928444	-0.385340	1.512019
14	6	2.416007	-0.112877	1.056260
15	6	2.798312	1.385054	1.111359
16	6	4.029654	1.796806	0.308608
17	6	5.439269	1.378592	0.804322
18	6	6.303727	1.463326	-0.484444
19	6	5.267459	1.705015	-1.631879
20	7	3.943052	1.337548	-1.092387
21	6	3.749622	-0.112523	-1.181387
22	6	2.512714	-0.614800	-0.397233
23	6	1.160657	-0.257616	-1.013212
24	6	-3.661873	-2.530065	1.220431
25	6	-3.046879	-3.403501	-1.074447
26	6	0.413195	0.636872	2.547138
27	6	0.850886	-1.753757	2.235799
28	6	-4.485571	4.381159	-0.248403
29	8	-0.359974	-2.762129	-0.151018
30	8	-5.816818	0.502448	-0.202194
31	8	-4.512205	2.957583	-0.231840
32	7	2.748815	-2.157158	-0.470494
33	8	3.308271	-2.708969	0.474381
34	8	2.466541	-2.705533	-1.529208
35	1	-5.394767	-1.900649	-0.769079
36	1	-4.259224	-1.265860	-1.964744
37	1	-2.011942	3.972331	-0.085242
38	1	0.031675	2.644323	0.050430
39	1	3.104452	-0.679275	1.688189
40	1	1.968704	1.987217	0.730125
41	1	2.935875	1.680506	2.156606
42	1	4.021320	2.895098	0.260721
43	1	5.795868	2.042243	1.598117
44	1	5.435914	0.362311	1.212685
45	1	7.028816	2.281480	-0.439225
46	1	6.873271	0.542770	-0.643077
47	1	5.240035	2.766373	-1.903201
48	1	5.484132	1.137763	-2.541515
49	1	3.622509	-0.377905	-2.235289
50	1	4.621797	-0.673911	-0.806752
51	1	1.233802	0.770540	-1.378148
52	1	0.928330	-0.895893	-1.867589
53	1	-2.834378	-3.078450	1.679854
54	1	-4.548095	-3.172663	1.233006

55	1	-3.876784	-1.644970	1.828133
56	1	-3.991894	-3.945036	-1.188360
57	1	-2.683353	-3.136020	-2.071292
58	1	-2.312566	-4.061047	-0.611194
59	1	0.414013	1.670989	2.205060
60	1	1.027129	0.582260	3.452939
61	1	-0.614432	0.392898	2.834125
62	1	-0.172637	-1.959292	2.566007
63	1	1.480769	-1.706815	3.130623
64	1	1.180389	-2.595845	1.634399
65	1	-5.529354	4.688646	-0.315042
66	1	-3.934852	4.760210	-1.117909
67	1	-4.044286	4.782332	0.671984

Cyclopiamine B (**6**) neutral form, conformer 7

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.515688 H (rel E = 7.29 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.058343 H (rel E = 7.36 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.056693	-0.398626	0.078869
2	6	0.423699	1.106141	0.159561
3	7	1.803068	1.223759	0.283292
4	6	2.591220	2.488204	0.241054
5	6	4.006753	2.142204	0.755887
6	6	4.677956	0.923271	0.122858
7	6	3.781119	-0.240113	-0.054710
8	6	4.190205	-1.575129	-0.347628
9	6	3.231233	-2.585542	-0.502410
10	6	1.862043	-2.304466	-0.363207
11	6	1.430090	-1.023938	-0.051925
12	6	2.404000	-0.022296	0.078796
13	6	-0.843455	-0.816443	1.328300
14	6	-2.295124	-0.364749	0.889301
15	6	-3.438701	-1.228795	1.465933
16	6	-4.812296	-1.071247	0.788870
17	6	-5.615040	0.212406	1.064376
18	6	-6.556342	0.273257	-0.151088
19	6	-5.677345	-0.220391	-1.316948
20	7	-4.711661	-1.144749	-0.688426
21	6	-3.391937	-1.277647	-1.256542
22	6	-2.304624	-0.324549	-0.663420
23	6	-0.879364	-0.667002	-1.124980
24	6	1.976224	3.549520	1.168247
25	6	2.637559	2.996198	-1.213235
26	6	-0.723423	-2.336205	1.565939
27	6	-0.425517	-0.114436	2.634122
28	6	5.995067	-3.102183	-0.730317
29	8	-0.364498	2.037306	0.119561
30	8	5.869631	0.940705	-0.150453
31	8	5.518782	-1.788791	-0.453479
32	7	-2.677773	1.084721	-1.196121
33	8	-2.403134	1.314768	-2.374161
34	8	-3.303929	1.850047	-0.473052
35	1	3.951691	1.946574	1.836547
36	1	4.668630	2.999141	0.611414
37	1	3.534959	-3.597015	-0.738147
38	1	1.151718	-3.111105	-0.515193
39	1	-2.430789	0.663897	1.228373
40	1	-3.176955	-2.287207	1.384692
41	1	-3.551534	-1.026771	2.537635
42	1	-5.421368	-1.921122	1.141250
43	1	-6.152072	0.163484	2.017808
44	1	-4.957083	1.085224	1.077631
45	1	-7.405180	-0.405380	-0.004255
46	1	-6.957160	1.273802	-0.336342
47	1	-6.269321	-0.741435	-2.080743
48	1	-5.181295	0.626220	-1.807490
49	1	-3.009942	-2.294772	-1.086440
50	1	-3.445482	-1.140516	-2.340591
51	1	-0.836886	-1.734400	-1.367392
52	1	-0.594019	-0.121301	-2.025136
53	1	0.999113	3.876256	0.813242
54	1	2.648195	4.412934	1.207566

55	1	1.864189	3.158595	2.184748
56	1	3.228436	3.916044	-1.268957
57	1	3.096979	2.259017	-1.879711
58	1	1.627705	3.212640	-1.571837
59	1	-1.027078	-2.936361	0.701279
60	1	-1.343254	-2.642201	2.412640
61	1	0.308226	-2.597836	1.812809
62	1	0.606244	-0.367734	2.903969
63	1	-1.067462	-0.441497	3.459534
64	1	-0.510110	0.972918	2.559830
65	1	7.081287	-3.014862	-0.758978
66	1	5.631499	-3.461431	-1.700524
67	1	5.703690	-3.806861	0.058023

Cyclopiamine B (**6**) neutral form, conformer 8

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.514427 H (rel E = 8.08 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0566711 H (rel E = 8.41 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.055639	-0.422528	0.086120
2	6	0.405844	1.083725	0.227971
3	7	1.777287	1.241803	0.083190
4	6	2.564728	2.493611	0.276915
5	6	3.913309	2.293068	-0.452126
6	6	4.645787	0.981479	-0.174547
7	6	3.770852	-0.212110	-0.188488
8	6	4.201732	-1.558490	-0.371620
9	6	3.257183	-2.590317	-0.454824
10	6	1.885225	-2.321886	-0.318620
11	6	1.434047	-1.030645	-0.083415
12	6	2.391573	-0.004377	-0.066142
13	6	-0.858114	-0.903107	1.300745
14	6	-2.309090	-0.439278	0.865139
15	6	-3.454079	-1.351745	1.356006
16	6	-4.822228	-1.130413	0.685981
17	6	-5.617614	0.133054	1.059579
18	6	-6.547220	0.303770	-0.154698
19	6	-5.665421	-0.105808	-1.351117
20	7	-4.709870	-1.082125	-0.790729
21	6	-3.388544	-1.183391	-1.358781
22	6	-2.292176	-0.296267	-0.682405
23	6	-0.868348	-0.639944	-1.141421
24	6	2.782619	2.705974	1.787689
25	6	1.850589	3.705177	-0.345465
26	6	-0.740265	-2.432194	1.472022
27	6	-0.462458	-0.269983	2.648772
28	6	6.024453	-3.069437	-0.732459
29	8	-0.390954	1.983378	0.444779
30	8	5.857560	0.962488	-0.014175
31	8	5.532209	-1.754806	-0.491922
32	7	-2.626245	1.153857	-1.122168
33	8	-2.283274	1.477880	-2.260171
34	8	-3.290901	1.862844	-0.376256
35	1	4.588581	3.114268	-0.201252
36	1	3.736761	2.330233	-1.536694
37	1	3.574302	-3.610695	-0.625899
38	1	1.190304	-3.150840	-0.399052
39	1	-2.464255	0.562134	1.270080
40	1	-3.193017	-2.399436	1.182380
41	1	-3.573650	-1.245548	2.440727
42	1	-5.439730	-2.001885	0.962997
43	1	-6.164295	0.009664	2.000711
44	1	-4.953586	0.996545	1.152325
45	1	-7.406172	-0.372717	-0.069334
46	1	-6.933884	1.321202	-0.261387
47	1	-6.257717	-0.562557	-2.154877
48	1	-5.159706	0.771511	-1.772695
49	1	-3.019227	-2.215594	-1.271601
50	1	-3.432006	-0.957686	-2.428476
51	1	-0.834603	-1.700240	-1.414585
52	1	-0.564127	-0.069708	-2.020028
53	1	1.822464	2.830120	2.295988
54	1	3.380410	3.607401	1.956376

55	1	3.311901	1.859935	2.238006
56	1	2.527214	4.565117	-0.305447
57	1	1.601546	3.514376	-1.393920
58	1	0.930460	3.950787	0.183368
59	1	-1.014753	-2.995414	0.573580
60	1	-1.386485	-2.775124	2.284069
61	1	0.282557	-2.702276	1.744078
62	1	0.566689	-0.534914	2.918951
63	1	-1.113670	-0.648128	3.444681
64	1	-0.552301	0.818055	2.632686
65	1	7.107712	-2.964834	-0.795422
66	1	5.639236	-3.473424	-1.676567
67	1	5.769592	-3.746983	0.091273

Cyclopiamine B (**6**) neutral form, conformer 9

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.519407 H (rel E = 4.95 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0612838 H (rel E = 5.51 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.044911	-0.129488	-0.069214
2	6	0.599847	1.313052	0.109136
3	7	1.986823	1.266807	0.062376
4	6	2.936080	2.384475	0.335809
5	6	4.289298	1.996629	-0.304707
6	6	4.797502	0.583724	-0.021948
7	6	3.758317	-0.463318	-0.138163
8	6	3.995064	-1.853996	-0.344220
9	6	2.915633	-2.729988	-0.521993
10	6	1.592789	-2.261849	-0.458376
11	6	1.326079	-0.922982	-0.211351
12	6	2.420529	-0.052862	-0.095696
13	6	-0.924640	-0.510296	1.136838
14	6	-2.238157	0.238294	0.729384
15	6	-3.545737	-0.107650	1.477525
16	6	-4.416127	-1.228382	0.863295
17	6	-5.877880	-1.190365	1.388286
18	6	-6.747700	-0.772404	0.169501
19	6	-5.734924	-0.228047	-0.849132
20	7	-4.571681	-1.083300	-0.590349
21	6	-3.345303	-0.939480	-1.326803
22	6	-2.322063	0.135356	-0.814933
23	6	-0.888949	-0.171604	-1.312247
24	6	3.076371	2.543541	1.862364
25	6	2.457106	3.698188	-0.304580
26	6	-1.103678	-2.037462	1.245588
27	6	-0.402200	-0.015603	2.498715
28	6	5.593757	-3.611845	-0.643985
29	8	-0.068118	2.325451	0.258897
30	8	5.977948	0.379442	0.221095
31	8	5.286812	-2.244147	-0.391066
32	7	-2.795906	1.475296	-1.417309
33	8	-2.598454	1.643557	-2.621169
34	8	-3.401165	2.265222	-0.698971
35	1	5.059139	2.701083	0.018299
36	1	4.200578	2.083306	-1.397242
37	1	3.088915	-3.781397	-0.710297
38	1	0.786931	-2.973283	-0.604865
39	1	-2.033111	1.290337	0.935132
40	1	-3.321654	-0.356628	2.522577
41	1	-4.147121	0.807490	1.507666
42	1	-3.954425	-2.204607	1.059011
43	1	-6.186959	-2.163963	1.779267
44	1	-5.969037	-0.471506	2.209421
45	1	-7.255198	-1.646525	-0.249952
46	1	-7.511179	-0.034082	0.431225
47	1	-6.063241	-0.347547	-1.887573
48	1	-5.546418	0.842136	-0.674363
49	1	-2.812205	-1.897716	-1.276064
50	1	-3.558818	-0.750749	-2.383889
51	1	-0.858085	-1.173497	-1.751300
52	1	-0.575464	0.520519	-2.094793
53	1	2.111155	2.800135	2.307872
54	1	3.784388	3.346375	2.091466

55	1	3.444888	1.624116	2.328698
56	1	3.251802	4.444214	-0.200769
57	1	2.255288	3.560792	-1.371391
58	1	1.550732	4.074527	0.167922
59	1	-1.417203	-2.508846	0.309862
60	1	-1.862757	-2.266548	1.999070
61	1	-0.174495	-2.513333	1.569966
62	1	0.578520	-0.452895	2.718857
63	1	-1.080045	-0.323568	3.301953
64	1	-0.316975	1.073241	2.535923
65	1	5.188939	-4.262300	0.140602
66	1	6.682340	-3.669049	-0.638170
67	1	5.214393	-3.931885	-1.622000

Cyclopiamine B (**6**) neutral form, conformer 10

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.512411 H (rel E = 9.34 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.053653 H (rel E = 10.30 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.038397	-0.846394	-0.078160
2	6	-1.189768	-1.884646	-0.179995
3	7	-2.392753	-1.234137	0.079273
4	6	-3.752909	-1.833301	-0.025208
5	6	-4.724341	-0.823249	0.624301
6	6	-4.613604	0.621458	0.136489
7	6	-3.224707	1.102226	-0.037539
8	6	-2.831089	2.458584	-0.240146
9	6	-1.478237	2.775116	-0.417037
10	6	-0.493660	1.773401	-0.374982
11	6	-0.833176	0.449616	-0.144962
12	6	-2.198088	0.149205	-0.005715
13	6	0.819465	-1.059915	1.266932
14	6	2.241522	-0.496416	0.891217
15	6	2.516172	0.964347	1.343181
16	6	3.701458	1.654329	0.628443
17	6	5.001663	1.923275	1.400376
18	6	6.065827	2.052587	0.267360
19	6	5.328692	1.602669	-1.024133
20	7	4.189233	0.863590	-0.496673
21	6	3.122755	0.422510	-1.359188
22	6	2.392558	-0.732248	-0.636926
23	6	0.993305	-1.067798	-1.209502
24	6	-3.821313	-3.158042	0.751593
25	6	-4.096685	-2.053520	-1.511847
26	6	0.179225	-0.393376	2.495916
27	6	0.975447	-2.564725	1.596929
28	6	-3.488386	4.752851	-0.433734
29	8	-1.073152	-3.065747	-0.458953
30	8	-5.617944	1.297091	-0.036907
31	8	-3.817743	3.379736	-0.247982
32	7	3.316211	-1.973006	-0.909865
33	8	3.386747	-2.327544	-2.086129
34	8	3.920867	-2.510718	0.008855
35	1	-4.546957	-0.806821	1.709368
36	1	-5.754770	-1.149564	0.465900
37	1	-1.173571	3.798036	-0.595227
38	1	0.536943	2.065276	-0.544923
39	1	2.994029	-1.115551	1.380207
40	1	1.625286	1.577621	1.202895
41	1	2.696084	0.951610	2.423249
42	1	3.335006	2.633300	0.244139
43	1	4.934156	2.819725	2.024489
44	1	5.229619	1.073229	2.052081
45	1	6.437866	3.076357	0.168655
46	1	6.926544	1.409069	0.467219
47	1	5.007502	2.485808	-1.611081
48	1	5.938353	0.967877	-1.674450
49	1	2.391268	1.225472	-1.578869
50	1	3.508056	0.067970	-2.317914
51	1	0.768213	-0.458650	-2.089210
52	1	0.949784	-2.111380	-1.527763
53	1	-3.186974	-3.920538	0.299334
54	1	-4.856589	-3.513868	0.754535

55	1	-3.507818	-3.014291	1.790745
56	1	-5.104987	-2.469642	-1.603402
57	1	-4.068322	-1.113194	-2.071762
58	1	-3.391264	-2.754343	-1.965568
59	1	0.025050	0.680390	2.378823
60	1	0.806257	-0.553746	3.379680
61	1	-0.796110	-0.845832	2.704885
62	1	0.026306	-3.007893	1.907999
63	1	1.685956	-2.671919	2.422906
64	1	1.347782	-3.156260	0.759360
65	1	-4.438413	5.285699	-0.390692
66	1	-3.018678	4.921382	-1.410256
67	1	-2.827001	5.115722	0.362448

Cyclopiamine B (**6**) neutral form, conformer 11

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.513717 H (rel E = 8.52 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.05575 H (rel E = 8.99 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.011802	-0.720782	-0.077091
2	6	-1.076195	-1.850409	-0.172467
3	7	-2.327362	-1.300985	0.086605
4	6	-3.634111	-2.009318	-0.019357
5	6	-4.683745	-1.085354	0.635871
6	6	-4.693035	0.365070	0.153446
7	6	-3.348771	0.958714	-0.023807
8	6	-3.070180	2.343965	-0.220735
9	6	-1.748229	2.772732	-0.394216
10	6	-0.684275	1.855941	-0.358530
11	6	-0.911129	0.506060	-0.141846
12	6	-2.246557	0.093834	0.000756
13	6	0.864396	-0.859371	1.265699
14	6	2.261990	-0.251337	0.872144
15	6	2.521473	1.211924	1.284051
16	6	3.853748	1.774421	0.755051
17	6	5.135078	1.240289	1.423616
18	6	6.193708	1.437306	0.326631
19	6	5.433411	1.061689	-0.954913
20	7	4.047590	1.496942	-0.690198
21	6	2.967265	0.825518	-1.365885
22	6	2.406867	-0.450864	-0.658870
23	6	1.025110	-0.876608	-1.215384
24	6	-3.593671	-3.338972	0.750945
25	6	-3.960313	-2.250014	-1.506690
26	6	0.207748	-0.178414	2.476961
27	6	1.091911	-2.345028	1.637529
28	6	-3.915670	4.576416	-0.404209
29	8	-0.863079	-3.018406	-0.450275
30	8	-5.749858	0.957080	-0.013351
31	8	-4.129893	3.179637	-0.225175
32	7	3.406351	-1.589962	-0.992632
33	8	3.444207	-1.940513	-2.171285
34	8	4.122771	-2.060774	-0.111208
35	1	-4.506112	-1.058373	1.720675
36	1	-5.684269	-1.494415	0.478020
37	1	-1.528686	3.818609	-0.564132
38	1	0.317813	2.236528	-0.521131
39	1	3.032821	-0.851363	1.358043
40	1	1.708978	1.864023	0.951586
41	1	2.530581	1.283544	2.376741
42	1	3.823645	2.866076	0.906476
43	1	5.368392	1.771820	2.351984
44	1	5.036657	0.174034	1.658870
45	1	6.507897	2.487178	0.288532
46	1	7.087476	0.824039	0.471639
47	1	5.833365	1.569806	-1.841138
48	1	5.508559	-0.019775	-1.133048
49	1	2.112267	1.506383	-1.463950
50	1	3.268527	0.565241	-2.384234
51	1	0.753113	-0.287782	-2.096216
52	1	1.046227	-1.922275	-1.528698
53	1	-2.903679	-4.047112	0.292057
54	1	-4.597884	-3.774661	0.756560

55	1	-3.287490	-3.176106	1.789423
56	1	-4.930882	-2.747720	-1.599165
57	1	-4.010215	-1.308051	-2.062300
58	1	-3.199985	-2.888294	-1.964155
59	1	0.031822	0.888300	2.328019
60	1	0.837928	-0.300253	3.364710
61	1	-0.757466	-0.646466	2.698568
62	1	0.166621	-2.828618	1.960737
63	1	1.804075	-2.394477	2.467756
64	1	1.495678	-2.937526	0.814324
65	1	-3.287672	4.989289	0.394557
66	1	-4.906807	5.028092	-0.360077
67	1	-3.460668	4.787697	-1.379317

Cyclopiamine B (**6**) neutral form, conformer 12

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.510576 H (rel E = 10.50 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0528636 H (rel E = 10.80 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.024240	-0.745179	-0.030596
2	6	-1.091974	-1.875959	-0.131581
3	7	-2.356968	-1.302699	-0.158395
4	6	-3.670748	-2.002603	-0.062294
5	6	-4.732097	-1.065134	-0.681915
6	6	-4.699173	0.390850	-0.223122
7	6	-3.340739	0.974885	-0.170641
8	6	-3.037905	2.366871	-0.199858
9	6	-1.702984	2.787803	-0.238621
10	6	-0.655165	1.853578	-0.203993
11	6	-0.907978	0.491899	-0.129518
12	6	-2.253759	0.090624	-0.150548
13	6	0.860500	-0.857931	1.309135
14	6	2.266856	-0.273753	0.895576
15	6	2.578515	1.174180	1.326864
16	6	3.890598	1.730130	0.745552
17	6	5.198410	1.155905	1.322438
18	6	6.200457	1.406893	0.184275
19	6	5.374880	1.101353	-1.076247
20	7	3.999349	1.504059	-0.717333
21	6	2.895636	0.828376	-1.352020
22	6	2.386669	-0.464500	-0.638849
23	6	1.010109	-0.931951	-1.171118
24	6	-3.971621	-2.263633	1.426800
25	6	-3.674189	-3.322205	-0.852774
26	6	0.211886	-0.142627	2.506137
27	6	1.094467	-2.329389	1.731837
28	6	-3.849900	4.616640	-0.304629
29	8	-0.857717	-3.070938	-0.202686
30	8	-5.734311	0.995405	0.016429
31	8	-4.088377	3.214592	-0.224362
32	7	3.411310	-1.573249	-0.997736
33	8	3.427020	-1.925516	-2.176690
34	8	4.166435	-2.019339	-0.136292
35	1	-5.729959	-1.459306	-0.476868
36	1	-4.599342	-1.053186	-1.773313
37	1	-1.460483	3.840974	-0.292416
38	1	0.358678	2.234067	-0.231615
39	1	3.028991	-0.899678	1.361424
40	1	1.765661	1.851806	1.054488
41	1	2.643908	1.218210	2.419254
42	1	3.888633	2.815978	0.936874
43	1	5.481476	1.639094	2.263358
44	1	5.104309	0.079529	1.505844
45	1	6.518499	2.456359	0.185406
46	1	7.097206	0.784522	0.250968
47	1	5.725785	1.665473	-1.949393
48	1	5.446529	0.033926	-1.324702
49	1	2.026182	1.496161	-1.403923
50	1	3.155139	0.585516	-2.386077
51	1	0.724258	-0.386272	-2.074961
52	1	1.050232	-1.990368	-1.436739
53	1	-3.205335	-2.912637	1.860592
54	1	-4.941147	-2.760817	1.532501

55	1	-4.005580	-1.330093	1.997692
56	1	-4.699437	-3.706088	-0.875808
57	1	-3.345866	-3.161551	-1.884036
58	1	-3.023851	-4.070706	-0.402377
59	1	0.047132	0.922825	2.338958
60	1	0.839178	-0.254871	3.397019
61	1	-0.759027	-0.595087	2.736263
62	1	0.173965	-2.813650	2.064068
63	1	1.801101	-2.337158	2.568657
64	1	1.513008	-2.944656	0.933276
65	1	-3.286896	4.974809	0.565586
66	1	-4.837839	5.077322	-0.313437
67	1	-3.314383	4.878421	-1.225251

Cyclopiamine B (**6**) neutral form, conformer 13

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1550.509243 H (rel E = 11.33 kcal/mol)

B3LYP DMF solvent phase single point calculation
HF = -1551.0507585 H (rel E = 12.12 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.056027	-0.923975	-0.020295
2	6	-1.239847	-1.928193	-0.132583
3	7	-2.432964	-1.216401	-0.175320
4	6	-3.817516	-1.766292	-0.102628
5	6	-4.760515	-0.709351	-0.722336
6	6	-4.569772	0.730277	-0.250323
7	6	-3.155038	1.157774	-0.180887
8	6	-2.696185	2.506605	-0.198906
9	6	-1.321789	2.774371	-0.225561
10	6	-0.385863	1.727697	-0.187095
11	6	-0.793374	0.404220	-0.117540
12	6	-2.175168	0.156527	-0.155858
13	6	0.807359	-1.135169	1.317514
14	6	2.240192	-0.594442	0.925718
15	6	2.599112	0.833683	1.442266
16	6	3.642722	1.608899	0.604166
17	6	4.958288	2.035113	1.274109
18	6	5.934983	2.213037	0.072687
19	6	5.156008	1.666134	-1.151936
20	7	4.122949	0.836954	-0.539095
21	6	3.033044	0.355920	-1.353152
22	6	2.364589	-0.814850	-0.607169
23	6	0.966561	-1.201712	-1.150538
24	6	-4.164886	-2.009925	1.379324
25	6	-3.956480	-3.067300	-0.911405
26	6	0.175174	-0.455589	2.544544
27	6	0.967508	-2.634371	1.673635
28	6	-3.248255	4.834205	-0.294692
29	8	-1.141024	-3.142384	-0.195723
30	8	-5.533083	1.445396	-0.015721
31	8	-3.644166	3.467878	-0.226061
32	7	3.317894	-2.031775	-0.906498
33	8	3.387116	-2.364220	-2.089115
34	8	3.932932	-2.578904	-0.000715
35	1	-5.798449	-0.991069	-0.530933
36	1	-4.615848	-0.702906	-1.812275
37	1	-0.961569	3.793735	-0.273855
38	1	0.665320	1.987954	-0.211112
39	1	2.974083	-1.259061	1.380183
40	1	1.703047	1.448989	1.525300
41	1	2.968857	0.721244	2.467113
42	1	3.150992	2.531407	0.219398
43	1	4.841747	2.947321	1.867285
44	1	5.306210	1.240979	1.943039
45	1	6.217771	3.258702	-0.078108
46	1	6.855128	1.645188	0.233758
47	1	4.713546	2.502253	-1.728961
48	1	5.774291	1.075353	-1.834714
49	1	2.273533	1.138608	-1.548136
50	1	3.391289	0.008007	-2.324685
51	1	0.725830	-0.653468	-2.065381
52	1	0.935790	-2.264879	-1.397810
53	1	-3.482632	-2.746535	1.813399
54	1	-5.185796	-2.395047	1.467309

55	1	-4.100365	-1.085568	1.962387
56	1	-5.016622	-3.339276	-0.946626
57	1	-3.605100	-2.928261	-1.938358
58	1	-3.392748	-3.886606	-0.467541
59	1	-0.006372	0.611897	2.412626
60	1	0.818045	-0.586393	3.421590
61	1	-0.786899	-0.925419	2.777095
62	1	0.020485	-3.084243	1.976488
63	1	1.667961	-2.714721	2.511791
64	1	1.361876	-3.235741	0.853363
65	1	-4.177555	5.403920	-0.307255
66	1	-2.679222	5.039410	-1.209586
67	1	-2.654914	5.120886	0.581914

Cyclopiamine B (**6**) neutral form, conformer 4

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1550.566706 H (rel E = "0" kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.036672	0.048432	-0.071449
2	6	-0.665424	-1.364333	0.043373
3	7	-2.032615	-1.228603	0.229421
4	6	-3.048191	-2.320471	0.266840
5	6	-4.331155	-1.704972	0.867797
6	6	-4.802810	-0.393108	0.252255
7	6	-3.727632	0.578507	-0.019775
8	6	-3.893721	1.967920	-0.314593
9	6	-2.773515	2.775492	-0.553260
10	6	-1.475103	2.243054	-0.492066
11	6	-1.276849	0.905881	-0.182939
12	6	-2.406523	0.105008	0.029675
13	6	0.924426	0.347133	1.168306
14	6	2.212190	-0.441915	0.756555
15	6	3.516920	-0.174465	1.548071
16	6	4.455721	0.847201	0.907262
17	6	5.897913	0.883496	1.442114
18	6	6.754159	1.312422	0.214001
19	6	5.745220	1.408044	-0.950741
20	7	4.642750	0.540512	-0.521493
21	6	3.406399	0.715101	-1.257173
22	6	2.327298	-0.289063	-0.782282
23	6	0.917915	0.103012	-1.291136
24	6	-2.592284	-3.470816	1.176639
25	6	-3.299073	-2.823958	-1.166370
26	6	1.154963	1.861684	1.325132
27	6	0.364520	-0.177739	2.501485
28	6	-5.372161	3.841641	-0.560625
29	8	-0.062665	-2.428556	-0.043905
30	8	-6.001796	-0.189747	0.067577
31	8	-5.159433	2.441230	-0.337174
32	7	2.750545	-1.642474	-1.416898
33	8	3.254513	-2.509457	-0.709805
34	8	2.609809	-1.757431	-2.637403
35	1	-4.160875	-1.504041	1.935328
36	1	-5.143119	-2.431633	0.793332
37	1	-2.895785	3.824137	-0.790881
38	1	-0.634424	2.896214	-0.702209
39	1	1.958273	-1.489828	0.922848
40	1	3.272362	0.136537	2.570072
41	1	4.063129	-1.121130	1.629067
42	1	4.020981	1.861540	0.998239
43	1	5.995029	1.573585	2.285589
44	1	6.194106	-0.111459	1.792811
45	1	7.262502	2.267901	0.372747
46	1	7.523166	0.564027	-0.000504
47	1	5.397196	2.451683	-1.072244
48	1	6.150766	1.075715	-1.911955
49	1	2.994830	1.729047	-1.109550
50	1	3.577267	0.586121	-2.330288
51	1	0.950382	1.125070	-1.675743
52	1	0.580906	-0.535311	-2.108623
53	1	-1.736352	-4.000494	0.757480
54	1	-3.421826	-4.176522	1.288121
55	1	-2.323199	-3.100096	2.171151
56	1	-4.064353	-3.607018	-1.153404
57	1	-3.647354	-2.016631	-1.819636
58	1	-2.384249	-3.244592	-1.593778

59	1	1.471007	2.350127	0.400068
60	1	1.926606	2.041997	2.079861
61	1	0.241604	2.354020	1.671420
62	1	-0.607800	0.277666	2.720942
63	1	1.039321	0.082570	3.324210
64	1	0.244844	-1.265680	2.505864
65	1	-4.887770	4.444526	0.215375
66	1	-6.452807	3.981899	-0.510657
67	1	-5.011733	4.146557	-1.549155

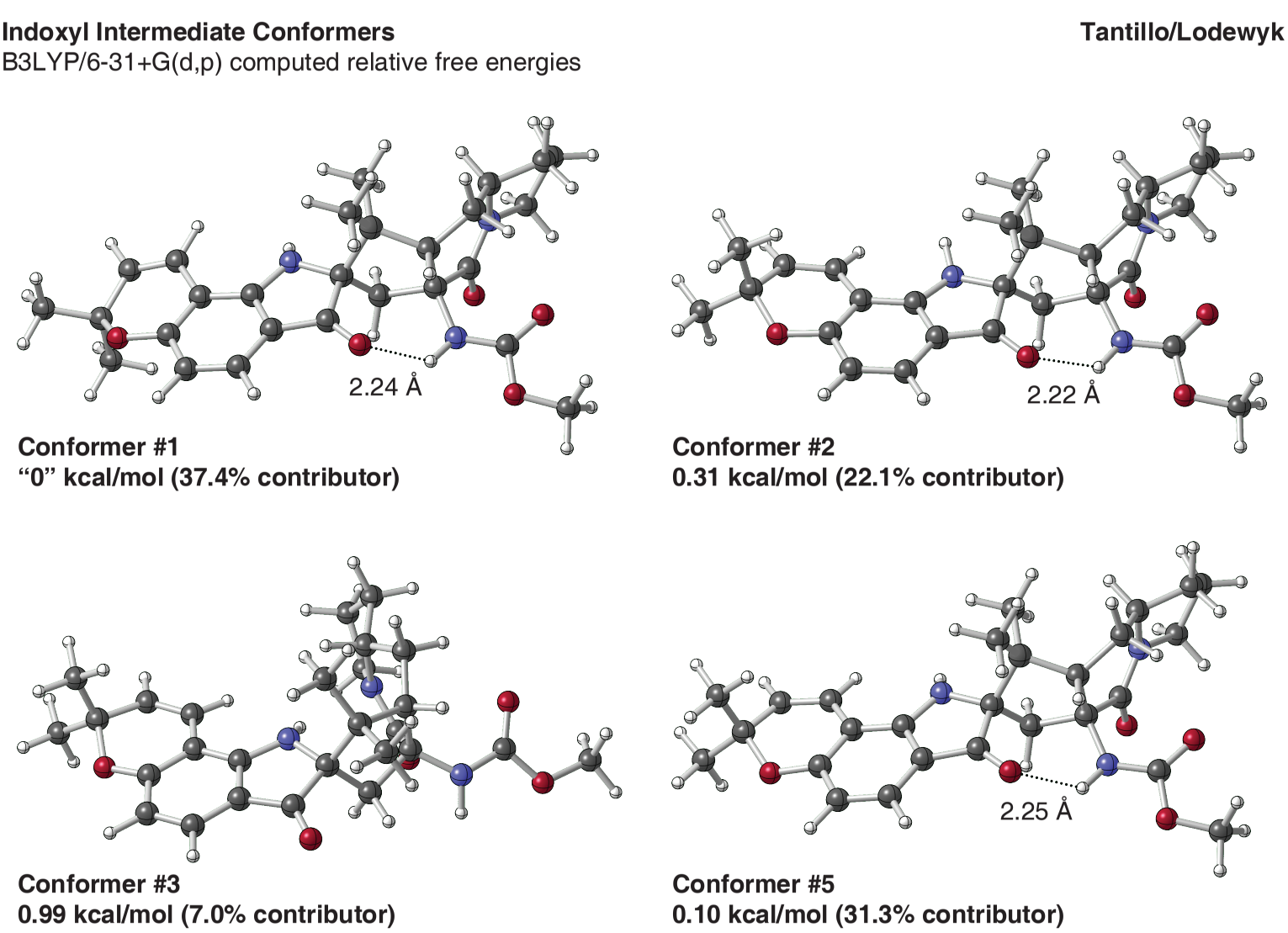
Cyclopiamine B (**6**) neutral form, conformer 5

B3LYP DMF solvent phase calculation
Sum of electronic and thermal free energies = -1550.563649 H (rel E = 1.92 kcal/mol)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.038805	0.047341	-0.078552
2	6	-0.663140	-1.369324	0.047458
3	7	-2.043963	-1.254120	0.028987
4	6	-3.052609	-2.326298	0.280411
5	6	-4.383071	-1.854250	-0.348595
6	6	-4.814235	-0.427025	-0.041946
7	6	-3.731244	0.569279	-0.137980
8	6	-3.892934	1.977520	-0.318711
9	6	-2.768583	2.796485	-0.488376
10	6	-1.472086	2.258380	-0.438814
11	6	-1.278390	0.903159	-0.213525
12	6	-2.412907	0.087751	-0.107270
13	6	0.921750	0.360388	1.157469
14	6	2.212031	-0.431599	0.756282
15	6	3.516532	-0.154211	1.544455
16	6	4.457369	0.857716	0.891505
17	6	5.899231	0.898408	1.426865
18	6	6.756987	1.310349	0.194046
19	6	5.748947	1.392584	-0.972513
20	7	4.644866	0.532268	-0.532960
21	6	3.409309	0.699043	-1.271690
22	6	2.327833	-0.297016	-0.784295
23	6	0.919888	0.092393	-1.298869
24	6	-3.200565	-2.512107	1.801508
25	6	-2.656239	-3.649189	-0.392978
26	6	1.159226	1.875229	1.302814
27	6	0.361578	-0.147501	2.497427
28	6	-5.372279	3.853482	-0.541333
29	8	-0.041288	-2.423175	0.132373
30	8	-5.991885	-0.169308	0.200461
31	8	-5.159607	2.448321	-0.352009
32	7	2.748868	-1.658945	-1.402648
33	8	3.256934	-2.515518	-0.685946
34	8	2.601091	-1.791795	-2.620727
35	1	-5.181112	-2.531330	-0.036262
36	1	-4.299890	-1.920445	-1.443047
37	1	-2.885268	3.858657	-0.659994
38	1	-0.629286	2.926403	-0.579206
39	1	1.957234	-1.476644	0.934213
40	1	3.272290	0.169674	2.562529
41	1	4.061811	-1.100369	1.637367
42	1	4.024372	1.873970	0.968815
43	1	5.996861	1.598970	2.261615
44	1	6.193582	-0.092494	1.790363
45	1	7.266604	2.267035	0.341012
46	1	7.525111	0.558183	-0.010290
47	1	5.402576	2.435141	-1.107375
48	1	6.154707	1.047653	-1.929193
49	1	2.998967	1.715348	-1.137362
50	1	3.580733	0.555816	-2.342931
51	1	0.953469	1.113201	-1.686827
52	1	0.583830	-0.547790	-2.115775
53	1	-2.252815	-2.831604	2.244935
54	1	-3.952638	-3.280298	2.010101
55	1	-3.516122	-1.583829	2.289946
56	1	-3.507338	-4.335516	-0.331554
57	1	-2.419610	-3.495073	-1.450653
58	1	-1.797751	-4.113529	0.091904

59	1	1.474639	2.357417	0.374107
60	1	1.935544	2.054618	2.052942
61	1	0.251646	2.374827	1.653145
62	1	-0.604795	0.320469	2.717191
63	1	1.042284	0.114086	3.314985
64	1	0.231263	-1.233410	2.511075
65	1	-4.915005	4.434786	0.266720
66	1	-6.454566	3.988242	-0.519241
67	1	-4.983241	4.189292	-1.508866

Figure S48. Computer generated images for the lowest energy conformers of pseudoindoxyl (**33**) as determined by computations



Pseudoindoxyl Intermediate (**33**), conformer 1

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1588.755967 H

Relative Energy = “0” kcal/mol

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.666076	-0.571783	-0.773864
2	6	4.877294	0.716128	0.285480
3	6	3.951112	-0.323361	0.057109
4	6	4.469488	-1.634530	-0.306302
5	6	5.757710	-1.776441	-0.655658
6	1	5.265331	2.730521	0.933641
7	6	4.493918	1.988067	0.763176
8	6	2.597812	-0.017956	0.285892
9	1	3.814329	-2.499274	-0.239493
10	1	6.180977	-2.749098	-0.890011
11	6	2.202241	1.258544	0.732912
12	6	3.151868	2.260279	0.982513
13	1	2.826447	3.237333	1.326222
14	8	6.204882	0.503394	0.115390
15	6	8.084246	-0.883401	-0.293896
16	1	8.537194	-1.648061	-0.933016
17	1	8.704192	0.016644	-0.336793
18	1	8.070882	-1.250396	0.736065
19	6	6.669353	-0.022504	-2.209584
20	1	7.318513	0.856564	-2.278257
21	1	7.036637	-0.785402	-2.904048
22	1	5.658444	0.259290	-2.517942
23	7	1.508764	-0.857838	0.157352
24	6	0.752734	1.284540	0.798788
25	8	0.018790	2.230942	1.079146
26	6	0.248790	-0.128131	0.372333
27	1	1.528801	-1.588213	-0.540973
28	6	-0.709785	-0.822202	1.420862
29	6	-0.627512	-0.014585	-0.897061
30	6	-2.086855	0.242554	-0.411925
31	6	-2.071600	-0.117917	1.115705
32	6	-0.714294	-2.345439	1.170059
33	1	0.288498	-2.753251	1.326063
34	1	-1.378712	-2.842165	1.882474
35	1	-1.043538	-2.616478	0.161721
36	6	-0.264669	-0.586331	2.874509
37	1	-0.942517	-1.093983	3.569965
38	1	0.739727	-0.991588	3.042162
39	1	-0.256525	0.476459	3.131576
40	1	-0.293683	0.762795	-1.588151
41	1	-0.586900	-0.958953	-1.448037
42	1	-2.008329	0.845362	1.628862
43	6	-3.383003	-0.774286	1.583563
44	1	-4.149530	0.006681	1.599976
45	1	-3.280046	-1.149255	2.609476
46	6	-3.030442	-0.595933	-1.314785
47	8	-3.057144	-0.380992	-2.527452
48	6	-3.884659	-1.904316	0.688546
49	1	-3.312971	-2.820534	0.890321
50	7	-3.749890	-1.593908	-0.747122
51	6	-4.783915	-2.274923	-1.549184
52	6	-5.647454	-3.011381	-0.505013
53	6	-5.375866	-2.253285	0.807251
54	1	-5.963742	-1.328925	0.848730
55	1	-5.596037	-2.845992	1.700906
56	1	-6.704808	-3.016745	-0.783402
57	1	-5.326829	-4.055413	-0.408558

58	1	-5.344647	-1.516639	-2.104853
59	1	-4.329849	-2.948791	-2.283173
60	7	-2.413956	1.658020	-0.620651
61	1	-1.675076	2.313368	-0.390469
62	6	-3.682067	2.144585	-0.545024
63	8	-4.708972	1.483485	-0.457883
64	8	-3.664607	3.505343	-0.596714
65	6	-4.951942	4.138350	-0.561034
66	1	-4.746621	5.208231	-0.603928
67	1	-5.556655	3.830417	-1.417760
68	1	-5.482445	3.888141	0.361554

Pseudoindoxyl Intermediate (**33**), conformer 2

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1588.755471 H

Relative Energy = 0.31 kcal/mol

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.757073	-0.671464	-0.284085
2	6	4.880135	0.878644	-0.023287
3	6	3.958970	-0.122750	-0.395733
4	6	4.477092	-1.330075	-1.022763
5	6	5.795555	-1.581295	-1.017195
6	1	5.246696	2.865861	0.715614
7	6	4.480240	2.139226	0.471105
8	6	2.597311	0.177103	-0.206711
9	1	3.790808	-1.996264	-1.539375
10	1	6.211382	-2.453269	-1.514048
11	6	2.189143	1.422844	0.315753
12	6	3.130394	2.411503	0.636647
13	1	2.794729	3.369145	1.022569
14	8	6.210601	0.689510	-0.199207
15	6	7.000444	-1.166990	1.150755
16	1	7.434243	-2.172428	1.133468
17	1	7.690606	-0.495749	1.672280
18	1	6.060465	-1.210992	1.708464
19	6	8.072653	-0.509223	-1.047004
20	1	8.727224	0.195477	-0.526165
21	1	8.586525	-1.473151	-1.118984
22	1	7.887887	-0.134221	-2.057305
23	7	1.505984	-0.599658	-0.519548
24	6	0.740788	1.426545	0.387766
25	8	-0.008887	2.353282	0.692976
26	6	0.253470	0.014666	-0.061553
27	1	1.584749	-1.600564	-0.606123
28	6	-0.494061	-0.782660	1.089033
29	6	-0.810598	0.127143	-1.174234
30	6	-2.192991	0.260769	-0.468213
31	6	-1.920853	-0.145571	1.022232
32	6	-0.472193	-2.294776	0.776983
33	1	0.549963	-2.688025	0.814848
34	1	-1.031885	-2.841352	1.540291
35	1	-0.903776	-2.543251	-0.197613
36	6	0.146599	-0.579038	2.473569
37	1	-0.391911	-1.156791	3.233211
38	1	1.187189	-0.922966	2.480083
39	1	0.131578	0.470550	2.779766
40	1	-0.626695	0.959209	-1.857007
41	1	-0.788401	-0.780515	-1.782400
42	1	-1.824433	0.804782	1.554847
43	6	-3.109279	-0.883416	1.663872
44	1	-3.896571	-0.142558	1.833748
45	1	-2.829271	-1.285347	2.645663
46	6	-3.206553	-0.614996	-1.250265
47	8	-3.423017	-0.375455	-2.438523
48	6	-3.698446	-2.009594	0.816456
49	1	-3.075296	-2.910240	0.909959
50	7	-3.781179	-1.666715	-0.615433
51	6	-4.893256	-2.375920	-1.277135
52	6	-5.573446	-3.161281	-0.136882
53	6	-5.144768	-2.413668	1.138805
54	1	-5.749933	-1.510598	1.279006
55	1	-5.216775	-3.026615	2.043043

56	1	-6.658744	-3.201774	-0.263220
57	1	-5.206215	-4.194067	-0.108008
58	1	-5.554504	-1.631320	-1.731164
59	1	-4.524864	-3.020754	-2.081796
60	7	-2.644733	1.653624	-0.563701
61	1	-1.922449	2.354358	-0.436420
62	6	-3.917971	2.047717	-0.298494
63	8	-4.876786	1.315109	-0.087265
64	8	-3.999556	3.407443	-0.312098
65	6	-5.309315	3.946560	-0.082690
66	1	-5.184630	5.028995	-0.120899
67	1	-6.003960	3.614317	-0.858343
68	1	-5.689891	3.640209	0.895318

Pseudoindoxyl Intermediate (**33**), conformer 3

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1588.754387 H

Relative Energy = 0.99 kcal/mol

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-5.692546	1.198821	-0.303170
2	6	-4.339074	-0.823220	-0.564237
3	6	-3.148689	-0.101385	-0.338145
4	6	-3.212546	1.352301	-0.386479
5	6	-4.399920	1.977603	-0.414144
6	1	-5.327163	-2.715503	-0.825869
7	6	-4.375560	-2.231504	-0.637064
8	6	-1.978448	-0.861886	-0.150081
9	1	-2.290089	1.925088	-0.432504
10	1	-4.472157	3.059707	-0.478802
11	6	-2.006607	-2.268192	-0.224516
12	6	-3.203073	-2.954597	-0.472537
13	1	-3.197955	-4.038474	-0.535996
14	8	-5.508349	-0.172147	-0.791096
15	6	-6.158369	1.117134	1.160075
16	1	-6.335496	2.122486	1.556691
17	1	-7.087978	0.542880	1.230362
18	1	-5.396896	0.635430	1.780353
19	6	-6.783950	1.782683	-1.201929
20	1	-7.688492	1.170443	-1.143421
21	1	-7.031268	2.799702	-0.881078
22	1	-6.449731	1.814713	-2.242525
23	7	-0.707594	-0.399855	0.132373
24	6	-0.641437	-2.756849	-0.105587
25	8	-0.229404	-3.904239	-0.224834
26	6	0.265900	-1.514485	0.149969
27	1	-0.410171	0.491662	-0.243778
28	6	1.117715	-1.548788	1.485670
29	6	1.337271	-1.371629	-0.936916
30	6	2.423170	-0.411648	-0.368073
31	6	2.321103	-0.554790	1.193535
32	6	0.270618	-1.209711	2.722813
33	1	-0.524312	-1.953708	2.845829
34	1	0.885812	-1.243250	3.628294
35	1	-0.205260	-0.230042	2.662251
36	6	1.737785	-2.947162	1.727985
37	1	2.381822	-2.889291	2.612811
38	1	0.977325	-3.709348	1.906366
39	1	2.353622	-3.287618	0.892274
40	1	1.781383	-2.359417	-1.095201
41	1	0.934461	-1.027093	-1.893601
42	1	3.233563	-1.062456	1.514288
43	6	2.338970	0.805969	1.914083
44	1	3.355749	1.199908	1.827423
45	1	2.125366	0.672327	2.979517
46	6	2.149438	1.017012	-0.929959
47	8	2.438272	1.272074	-2.099950
48	6	1.378382	1.835835	1.339107
49	1	0.343048	1.556282	1.577353
50	7	1.514773	1.923165	-0.136438
51	6	1.348338	3.309973	-0.623918
52	6	0.965875	4.101548	0.637884
53	6	1.599203	3.290329	1.781407
54	1	2.674868	3.494657	1.846458
55	1	1.152079	3.497268	2.758294
56	1	1.322815	5.134057	0.594659

57	1	-0.123778	4.133881	0.757587
58	1	2.295415	3.646999	-1.058800
59	1	0.594483	3.356380	-1.415780
60	7	3.717701	-0.861924	-0.892907
61	1	3.690682	-1.317822	-1.796048
62	6	4.869580	-0.159260	-0.665964
63	8	5.023358	0.701867	0.187810
64	8	5.850488	-0.584084	-1.501268
65	6	7.124299	0.061248	-1.337452
66	1	7.776303	-0.399794	-2.079166
67	1	7.035649	1.134939	-1.519345
68	1	7.512660	-0.104574	-0.329545

Pseudoindoxyl Intermediate (**33**), conformer 4

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1588.753289 H

Relative Energy = 1.68 kcal/mol

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-5.790763	0.452580	-0.428963
2	6	-4.114482	-1.331169	-0.451512
3	6	-3.063926	-0.399219	-0.320108
4	6	-3.369385	1.007452	-0.536683
5	6	-4.643638	1.418664	-0.631331
6	1	-4.770080	-3.378934	-0.477791
7	6	-3.915446	-2.723401	-0.353873
8	6	-1.785441	-0.925886	-0.051347
9	1	-2.554812	1.717754	-0.652049
10	1	-4.893895	2.458968	-0.819936
11	6	-1.578755	-2.315316	0.045261
12	6	-2.640555	-3.215485	-0.110156
13	1	-2.454014	-4.282986	-0.042515
14	8	-5.372669	-0.915398	-0.750313
15	6	-6.267063	0.467155	1.033221
16	1	-6.616582	1.468421	1.306844
17	1	-7.090091	-0.241780	1.170863
18	1	-5.449640	0.195379	1.707436
19	6	-6.944874	0.736992	-1.391958
20	1	-7.736491	-0.006745	-1.262443
21	1	-7.364140	1.729036	-1.195378
22	1	-6.598294	0.701822	-2.428399
23	7	-0.612333	-0.230677	0.162662
24	6	-0.152008	-2.552950	0.219341
25	8	0.440451	-3.623471	0.242654
26	6	0.535879	-1.155668	0.308709
27	1	-0.472453	0.661057	-0.292897
28	6	1.363936	-0.875403	1.634967
29	6	1.583321	-0.977633	-0.799340
30	6	2.450703	0.244719	-0.377850
31	6	2.434116	0.217178	1.190868
32	6	0.454375	-0.478524	2.811804
33	1	-0.212146	-1.312874	3.055959
34	1	1.054065	-0.277416	3.706002
35	1	-0.177561	0.387066	2.612198
36	6	2.148500	-2.128828	2.094215
37	1	2.778695	-1.845632	2.945607
38	1	1.477212	-2.926737	2.417657
39	1	2.805850	-2.526064	1.321961
40	1	2.217689	-1.867868	-0.807969
41	1	1.146656	-0.856802	-1.794558
42	1	3.407038	-0.165944	1.500505
43	6	2.323851	1.634175	1.779916
44	1	3.258781	2.165544	1.555007
45	1	2.242585	1.589459	2.870793
46	6	1.858822	1.533211	-1.026296
47	8	2.011917	1.719320	-2.238517
48	6	1.167714	2.451001	1.221636
49	1	0.214888	2.040528	1.576930
50	7	1.167427	2.411005	-0.259794
51	6	0.716995	3.691867	-0.847918
52	6	0.326532	4.540791	0.374156
53	6	1.183089	3.958949	1.512476
54	1	2.211257	4.337500	1.451831
55	1	0.793839	4.190657	2.508079
56	1	0.505137	5.605632	0.203404

57	1	-0.738088	4.417427	0.604529
58	1	1.543718	4.129175	-1.417825
59	1	-0.106658	3.529531	-1.549755
60	7	3.799105	0.217651	-0.964913
61	1	3.867933	0.708112	-1.850578
62	6	4.745581	-0.737955	-0.743252
63	8	4.738326	-1.588409	0.134685
64	8	5.757810	-0.595108	-1.644218
65	6	6.848436	-1.518793	-1.494704
66	1	7.548775	-1.265367	-2.290604
67	1	7.321671	-1.401621	-0.516521
68	1	6.500004	-2.548651	-1.604080

Pseudoindoxyl Intermediate (**33**), conformer 5

B3LYP gas phase calculation
Sum of electronic and thermal free energies = -1588.755800 H

Relative Energy = 0.10 kcal/mol

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.753803	-0.640566	-0.469315
2	6	4.849947	0.851827	-0.068027
3	6	3.930922	-0.193935	-0.294781
4	6	4.429995	-1.427120	-0.886612
5	6	5.750003	-1.633517	-1.011504
6	1	5.225395	2.875166	0.558149
7	6	4.461795	2.117934	0.420959
8	6	2.586069	0.075330	0.018994
9	1	3.724294	-2.169324	-1.250419
10	1	6.142578	-2.536432	-1.470694
11	6	2.189161	1.336963	0.509153
12	6	3.126902	2.360654	0.707078
13	1	2.798569	3.327331	1.076409
14	8	6.160371	0.699351	-0.379148
15	6	7.212071	-1.042131	0.942331
16	1	7.688799	-2.027819	0.919116
17	1	7.931835	-0.313307	1.328992
18	1	6.358311	-1.093083	1.624348
19	6	7.944765	-0.469414	-1.414203
20	1	8.627754	0.292105	-1.026775
21	1	8.492008	-1.413218	-1.504982
22	1	7.606597	-0.163538	-2.408001
23	7	1.506085	-0.777762	-0.068682
24	6	0.745174	1.333507	0.650208
25	8	0.008237	2.261178	0.981233
26	6	0.245873	-0.081353	0.226598
27	1	1.506640	-1.530445	-0.742148
28	6	-0.637132	-0.812667	1.316245
29	6	-0.702909	0.034729	-0.989268
30	6	-2.138054	0.249022	-0.420130
31	6	-2.030776	-0.139399	1.097283
32	6	-0.616825	-2.332510	1.044938
33	1	0.402986	-2.715957	1.141494
34	1	-1.228491	-2.856100	1.784855
35	1	-0.992877	-2.599690	0.051941
36	6	-0.119633	-0.583760	2.746897
37	1	-0.747795	-1.115185	3.470688
38	1	0.901362	-0.967079	2.856007
39	1	-0.122407	0.475979	3.016216
40	1	-0.424477	0.831413	-1.682795
41	1	-0.672720	-0.898260	-1.559861
42	1	-1.964748	0.815897	1.625060
43	6	-3.296001	-0.841426	1.623701
44	1	-4.081238	-0.083305	1.704730
45	1	-3.123743	-1.236732	2.632678
46	6	-3.111176	-0.593613	-1.286654
47	8	-3.210660	-0.355434	-2.491158
48	6	-3.818006	-1.964921	0.731883
49	1	-3.209313	-2.867849	0.877682
50	7	-3.776877	-1.618042	-0.701039
51	6	-4.840077	-2.305365	-1.457878
52	6	-5.617965	-3.093351	-0.384483
53	6	-5.289044	-2.360542	0.929142
54	1	-5.899314	-1.455444	1.030096
55	1	-5.438568	-2.981514	1.818215
56	1	-6.689628	-3.123163	-0.599371

57	1	-5.262790	-4.129496	-0.335326
58	1	-5.454342	-1.548232	-1.955547
59	1	-4.415119	-2.945854	-2.237683
60	7	-2.508393	1.659919	-0.582392
61	1	-1.772625	2.329043	-0.384084
62	6	-3.781032	2.114046	-0.426453
63	8	-4.785547	1.426565	-0.293716
64	8	-3.798593	3.475466	-0.453861
65	6	-5.096811	4.075567	-0.335675
66	1	-4.919659	5.150835	-0.368351
67	1	-5.739934	3.768652	-1.164329
68	1	-5.569749	3.794869	0.609115

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