Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Cyclocondensation reactions of racemic diastereomers of dimethyl-2-oxocyclohexanepropionic acids with (*R*)-phenylglycinol: access to both enantiomers of dimethyl *cis*-decahydroquinolines

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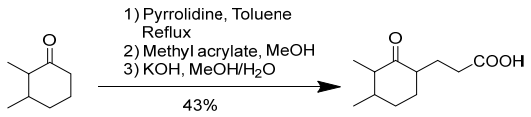
Contents

I) Experimental procedures and spectroscopic data

General Procedures. All air sensitive reactions were performed under a dry argon or nitrogen atmosphere with dry, freshly distilled solvents using standard procedures. For reactions that require heating, a hot plate magnetic stirrer with an aluminium heating block was used. Drying of organic extracts during the work-up of reactions was performed over anhydrous Na_2SO_4 or $MgSO_4$. Evaporation of solvent was accomplished with a rotatory evaporator. Thin-layer chromatography was done on SiO_2 (silica gel 60 F_{254}), and the spots were located by UV and either a 1% $KMnO_4$ solution. Chromatography refers to flash column chromatography and was carried out on SiO_2 (silica gel 60, 230-400 mesh). NMR spectra were recorded at 400 or 500 MHz (1H) and 100.6 or 125 MHz (13C), and chemical shifts are reported in δ values, in parts per million (ppm) relative to Me_4Si (0 ppm) or relative to residual chloroform (7.26 ppm, 77.0 ppm) as an internal standard. Data are reported in the following manner: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constant (*J*) in hertz (Hz), integrated intensity, and assignment (when possible). Assignments and stereochemical determinations are given only when they are derived from definitive two-dimensional NMR experiments (HSQC-COSY). IR spectra were performed in a spectrophotometer Nicolet Avatar 320 FT-IR and only noteworthy IR absorptions (cm^{-1}) are listed. Optical rotation were measured on Perkin-Elmer 241 polarimeter. $[\alpha]_D$ values are given in 10^{-1} deg cm^2 g^{-1}. High resolution mass spectra (HMRS) were performed by *Centres Científics i Tecnològics de la Universitat de Barcelona* using an electrospray (ESI) ionization source and a TOF analyzer.

3,4-Dimethyl-2-oxocyclohexanepropionic acid (4):



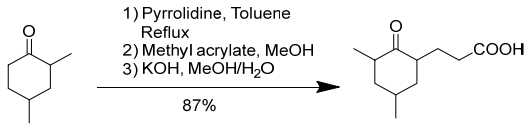
1 **4**

First Step: A solution of 2,3-dimethylcyclohexanone (racemic mixture of diastereomers; 4.44 g, 35.2 mmol) and pyrrolidine (5.11 g, 71.8 mmol) in toluene (10 mL) was heated at reflux temperature under Dean Stark conditions. After 15 h, the mixture was cooled and concentrated. Methyl acrylate (3.46 mL, 38.7 mmol) was added to a solution of the above residue in methanol (11 mL) and the mixture was stirred at reflux temperature for 4 h. Then, a buffer solution (15 mL, HOAc–H_2O–NaOAc 25 mL:25 mL:12.5 g) was added and the reflux was continued for 1 h. After cooling to room temperature, the mixture was diluted with Et_2O, and washed with 2 M aqueous HCl and brine. The organic phase was dried and concentrated.

Second Step: KOH (2.3 g, 34.8 mmol, 85%) was added to a solution of the above crude in MeOH–H_2O (60 mL:30 mL), and the mixture was stirred at room temperature for 6 h. Then, the mixture was

washed with CH_2Cl_2. The combined aqueous extracts were acidified to pH 2-3 by addition of 2 M aqueous HCl and the mixture was extracted with CH_2Cl_2. The combined organic extracts were dried and concentrated to give a diastereomeric mixture of keto-acids **4** (3.01 g, 43% from **1**) as an off-white solid: mp 60-64 ºC (hexane–CH_2Cl_2); IR (NaCl): 1701 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, *g*-HSQC) δ 9.93 (br s, 1H, COOH); 2.43-2.50 (m, 1H); 2.41-2.31 (m, 2H), 2.11- 2.00 (m, 3H), 1.87-1.81 (m, 1H), 1.59-1.48 (m, 2H), 1.47-1.42 (m, 1H), 1.35 (qd, J = 12.8, 3.6 Hz, 1H), 1.05 (d, J = 6.2 Hz, 3H, CH_3), 1.01 (d, J = 6.2 Hz, 3H, CH_3); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 213.5 (CO), 179.8 (CO_2), 51.9 (CH), 49.1 (CH), 42.3 (CH), 34.4 (CH_2), 33.5 (CH_2), 31.6 (CH_2), 24.5 (CH_2), 20.6 (CH_3), 11.6 (CH_3); HRMS calcd for [$C_{11}H_{18}O_3 - H^+$]: 197.1183; found 197.1187.

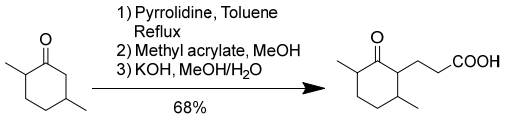
3,5-Dimethyl-2-oxocyclohexanepropionic acid (5):



2 **5**

Operating as described in the preparation of keto-acids **4**, from pyrrolidine (1.7 mL, 21.2 mmol), 2,4-dimethylcyclohexanone (racemic mixture of diastereomers; 1.34 g, 10.6 mmol) in toluene (11 mL), methyl acrylate (0.95 mL, 10.6 mmol) in MeOH (14 mL), and KOH (772 mg, 11.7 mmol, 85%) in MeOH–H_2O (24 mL:12 mL), a diastereomeric mixture of keto-acids **5** (1.83 g, 87%) was obtained as a colorless oil: IR (NaCl):1709 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, *g*-HSQC) δ 7.85 (br s, 1H, COOH); 2.50-2.33 (m, 4H), 2.10-2.01 (m, 4H), 1.55-1.46 (m 1H), 1.16-1.06 (m, 2H), 1.00-0.95 (m, 6H, CH_3); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 214.1 (CO); 179.4 (CO_2), 48.5 (CH), 45.3 (CH_2), 44.5 (CH), 43.2 (CH_2), 31.9 (CH), 31.8 (CH_2), 24.4 (CH_2), 21.1 (CH_3), 14.3 (CH_3); HRMS calcd for [$C_{11}H_{18}O_3 - H^+$]: 197.1183; found 197.1191.

3,6-Dimethyl-2-oxocyclohexanepropionic acid (6):

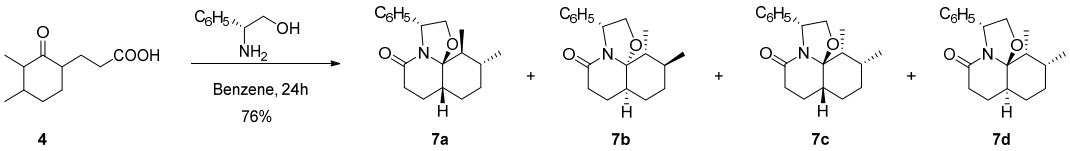


3 **6**

Operating as described in the preparation of keto-acids **4**, from pyrrolidine (3.96 g, 55.6 mmol), 2,5-dimethylcyclohexanone (racemic mixture of diastereomers; 3.51 g, 27.8 mmol) in toluene (25 mL), methyl acrylate (5 mL, 55.6 mmol) in MeOH (25 mL), and KOH (3.67 g, 55.6 mmol) in MeOH–H_2O (72 mL:36 mL), a diastereomeric mixture of keto-acids **6** (3.75 g, 68% from **3**) was obtained as a yellowish oil: IR (NaCl): 1708 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, *g*-HSQC) δ 9.45 (br s, OH)

2.62-2.21 (m, 3H), 2.11-1.81 (m, 4H), 1.69-1.28 (m, 3H), 0.75 and 0.98 and 1.08 [(d, J = 7.2 Hz), (d, J = 6.4 Hz) and (d, J = 4.0 Hz), 6H, $2CH_3$]; ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 213.6 (CO), 179.7 (COO), 56.0 (CH), 45.1 (CH), 39.9 (CH), 37.1 (CH_2), 35.5 (CH_2), 34.5 (CH_2), 20.9 (CH_2), 20.4 (CH_3), 14.3 (CH_3); HRMS calcd for [$C_{11}H_{18}O_3 + H^+$]: 199.1329; found 197.1332.

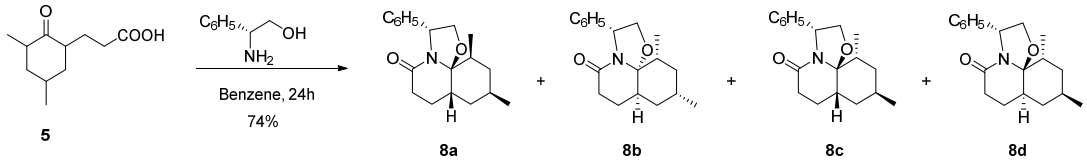
(3*R*,7a*R*,10*R*,11*S*,11a*R*)-10,11-Dimethyl-5-oxo-3-phenyldecahydrooxazolo[2,3-*j*]quinoline (7a) and its (3*R*,7a*S*,10*S*,11*R*,11a*S*), (3*R*,7a*R*,10*R*,11*R*,11a*R*) and (3*R*,7a*S*,10*R*,11*R*,11a*R*) isomers (7b, 7c and 7d, respectively):



(*R*)-phenylglycinol (2.99 g, 21.8 mmol) was added to a solution of a diastereomeric mixture of keto-acids **4** (2.88 g, 14.53 mmol) in benzene (150 mL). The mixture was heated at reflux under Dean Stark conditions for 24 h. After cooling, the solvent was evaporated and the resulting residue was suspended in EtOAc. The organic solution was washed with saturated aqueous $NaHCO_3$, dried and evaporated. Flash chromatography (9:1 to 1:1 hexane–EtOAc) afforded lactams **7a** (1.21 g, 28%), **7b** (1.32 g, 30 %), **7c** (0.41 g, 10 %), and **7d** (0.36 g, 8%) as colorless solids (**7c** as a colorless gum). **7a:** mp: 71-75 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 181.4 (*c* 1.00, $CHCl_3$); IR (NaCl): 1654 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.39-7.36 (m, 2H, ArH), 7.34-7.29 (m, 2H, ArH), 7.25-7.21 (m, 1H, ArH), 5.48 (dd, J = 7.4, 4.2 Hz, 1H, H-3), 4.36 (dd, J = 9.2, 4.2 Hz, 1H, H-2), 4.21 (dd, J = 9.2, 7.4 Hz, 1H, H-2), 2.56-2.52 (m, 2H, H-6), 2.02-1.85 (m, 3H, H-7, H-7a and H-8), 1.82-1.75 (m, 1H, H-7), 1.55-1.39 (m, 4H, H-8, H-9, H-10 and H-11), 1.33-1.22 (m, 1H, H-9), 0.87 (d, J = 6.4 Hz, 3H, CH_3C-11), 0.56 (d, J = 6.8 Hz, 3H, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.4 (CO), 139.2 (C*q*-Ar), 128.2 (CH-Ar), 127.1 (CH-Ar), 127.1 (CH-Ar), 99.3 (C-11a), 68.1 (C-2), 59.2 (C-3), 42.0 (C-11), 38.7 (C-7a), 35.1 (C-10), 29.0 (C-6), 28.9 (C-9), 26.1 (C-8), 20.3 (*C*H_3-C10), 19.3 (C-7), 13.0 (*C*H_3-C11); HRMS calcd for [$C_{19}H_{25}NO_2 + H^+$]: 300.1958; found 300.1960. **7b:** mp: 92-95 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ + 43.2 (*c* 1.02, $CHCl_3$); IR (NaCl): 1654 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.33-7.21 (m, 5H, ArH), 5.07 (dd, J = 7.6, 4.0 Hz, 1H, H-3), 4.55 (dd, J = 8.6, 7.6 Hz, 1H, H-2), 3.91 (dd, J = 8.6, 4.0 Hz, 1H, H-2), 2.44-2.31 (m, 2H, H-6), 2.23-2.16 (m, 1H, H-7a), 2.14-2.04 (m, 1H, H-8), 1.97-1.87 (m, 1H, H-7), 1.83-1.76 (m, 1H, H-7), 1.70-1.46 (m, 4H, H-8, H-9, H-10 and H-11), 1.35-1.24 (m, 1H, H-9), 1.02 (d, J = 6.8 Hz, 3H, CH_3), 0.94 (d, J = 6.8 Hz, 3H, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 168.3 (CO), 141.3 (C*q*-Ar), 127.4 (CH-Ar), 128.5 (CH-Ar), 126.6 (CH-Ar), 97.6 (C-11a), 74.9 (C-2), 62.0 (C-3), 44.9 (C-11), 40.2 (C-7a), 35.0 (C-10), 29.5 (C-6), 29.1 (C-9), 26.5 (C-8), 20.9 (C-7), 20.0 (*C*H_3-C11), 13.1 (*C*H_3-C10); HRMS

calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1950. **7c:** IR (NaCl): 1658 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.36-7.31 (m, 3H, ArH), 7.29-7.27 (m, 1H, ArH), 7.25-7.23 (m, 1H, ArH), 5.39-5.33 (m, 1H, H-3), 4.45-4.41 (m, 1H, H-2), 3.95-3.91 (m, 1H, H-2), 2.70-2.63 (m, 1H, H-6), 2.58-2.47 (m, 1H, H-6), 2.20-1.96 (m, 3H, H-7, H-8 and H-10), 1.90-1.77 (m, 2H, H-7a and H-11), 1.69-1.58 (m, 2H, H-7 and H-8), 1.45-1.35 (m, 1H, H-9), 1.31-1.25 (m, 1H, H-9), 1.01 (d, *J* = 7.6 Hz, 3H, CH_3), 0.86 (d, *J* = 6.8 Hz, 3H, CH_3); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.3 (CO), 140.0 (C*q*-Ar), 126.0 (CH-Ar), 128.5 (CH-Ar), 127.2 (CH-Ar), 97.8 (C-11a), 69.1 (C-2), 60.1 (C-3), 39.2 (C-7a and C-11), 31.6 (C-10), 30.4 (C-6), 27.8 (C-8), 22.8 (C-9), 22.2 (C-7), 19.4 (*C*H_3C-10), 10.4 (*C*H_3C-11); HRMS calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1958. **7d:** mp: 87-92 ºC (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 181.5 (*c* 1.00, $CHCl_3$); IR (NaCl): 1664 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.34-7.30 (m, 2H, ArH), 7.27-7.25 (m, 1H, ArH), 7.23-7.21 (m, 2H, ArH), 5.63 (dd, *J* = 8.8, 6.4 Hz, 1H, H-3), 4.42 (t, *J* = 8.8 Hz, 1H, H-2), 4.08 (dd, *J* = 8, 6.4 Hz, 1H, H-2), 2.64-2.58 (m, 1H, H-6), 2.49- 2.40 (m, 1H, H-6), 2.06-1.98 (m, 2H, H-7a and H-11), 1.74-1.41 (m, 7H, H-7, H-8, H-9 and H-10), 1.22 (qd, *J* = 13.2, 4.8 Hz, 1H, H-9), 0.68 (d, *J* = 7.0 Hz, 3H, CH_3C-10), 0.67 (d, *J* = 7.0 Hz, 3H, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 176.2 (CO), 141.8 (C*q*-Ar), 126.8 (CH-Ar), 125.1 (CH-Ar), 128.3 (CH-Ar), 98.7 (C-11a), 66.6 (C-2), 59.0 (C-3), 36.8 (C-7a), 35.5 (C-11), 35.4 (C-6), 30.3 (C-10), 28.1 (C-9 and C-8), 22.8 (C-7), 19.2 (*C*H_3C-11), 9.0 (*C*H_3C-10); HRMS calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1957.

(3*R*,7a*S*,9*R*,11*S*,11a*S*)-9,11-Dimethyl-5-oxo-3-phenyldecahydrooxazolo[2,3-*j*]quinoline (8a) and its (3*R*,7a*R*,9*S*,11*R*,11a*R*), (3*R*,7a*S*,9*R*,11*R*,11a*S*) and (3*R*,7a*R*,9*R*,11*R*,11a*S*) isomers (8b, 8c and 8d, respectively):



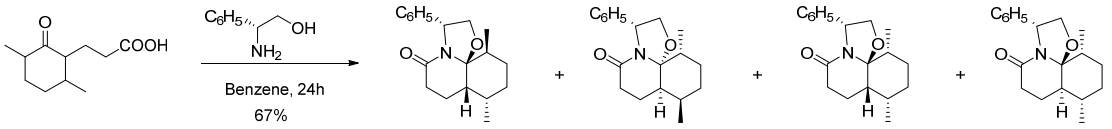
Operating as described in the preparation of lactams **7**, from a diastereomeric mixture of keto-acids **5** (1.07 g, 5.4 mmol) and *(R)*-phenylglycinol (1.13 g, 8.2 mmol) in benzene (55 mL), lactams **8a** (502 mg, 31%), **8b** (543 mg, 34%), **8c** (29 mg, 2 %), and **8d** (59 mg, 4%) were obtained after flash column chromatography (9:1 to 1:1 hexane–EtOAc) as colorless solids (**8c** as a colorless gum).

8a: mp: 82-84 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 153.3 (*c* 1.04, $CHCl_3$); IR (NaCl): 1658 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, *g*-HSQC) δ 7.35-7.20 (m, 5H, ArH), 5.47 (dd, *J* = 7.2, 4.4 Hz, 1H, H-3), 4.32 (dd, *J* = 8.8, 4.4 Hz, 1H, H-2), 4.24 (dd, *J* = 8.8, 7.2 Hz, 1H, H-2), 2.61-2.47 (m, 2H, H-6), 1.98-1.74 (m, 5H, H-7, H-7a, H-9 and H-11), 1.59-1.55 (m, 2H, H-8), 1.51-1.47 (m, 1H, H-10), 1.12 (q, *J* = 12.8 Hz, 1H, H-10), 0.90 (d, *J* = 6.4 Hz, 3H, CH_3C-9), 0.53 (d, *J* = 6.8 Hz, 3H, CH_3C-11); ^{13}C NMR

(100.6 MHz, $CDCl_3$) δ 172.1 (CO), 139.2 (C*q*-Ar), 127.0 (CH-Ar), 128.1 (CH-Ar), 126.7 (CH-Ar), 98.3 (C-11a), 68.4 (C-2), 59.2 (C-3), 40.3 (C-10), 35.6 (C-8), 29.1 (C-6), 39.6 (C-7a), 35.5 (C-11), 25.8 (C-9), 21.8 (*C*H_3C-9), 20.3 (C-7), 16.3 (*C*H_3C-11); HRMS calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1962. **8b:** mp: 66-68 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ + 32.7 (*c* 0.99, $CHCl_3$); IR (NaCl): 1662 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, *g*-HSQC) δ 7.33-7.20 (m, 5H, ArH), 5.07 (dd, *J* = 7.6, 4.0 Hz, 1H, H-3), 4.55 (dd, *J* = 8.8, 7.6 Hz, 1H, H-2), 3.90 (dd, *J* = 8.8, 4.0 Hz, 1H, H-2), 2.46-2.28 (m, 2H, H-6), 2.22-2.15 (m, 1H, H-7a), 1.97-1.87 (m, 2H, H-7 and H-9), 1.87-1.77 (m, 2H, H-7 and H-11), 1.69 (m, 1H, H-8), 1.63 (m, 1H, H-8), 1.58-1.52 (m, 1H, H-10), 1.25 (q, *J* = 12.5 Hz, 1H, H-10), 1.01 (d, *J* = 6.8 Hz, 3H, CH_3C-9), 0.93 (d, *J* = 6.4 Hz, 3H, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 168.1 (CO), 141.3 (C*q*-Ar), 127.3 (CH-Ar), 128.4 (CH-Ar), 126.4 (CH-Ar), 96.8 (C-11a), 74.8 (C-2), 61.7 (C-3), 40.6 (C-7a), 40.0 (C-10), 38.2 (C-9), 35.9 (C-8), 29.7 (C-6), 25.9 (C-11), 21.8 (*C*H_3C-9 and C-7), 16.2 (*C*H_3C-11); HRMS calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1962. **8c:** IR (NaCl): 1656 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, *g*-HSQC) δ 7.34-7.31 (m, 2H, ArH), 7.27-7.22 (m, 3H, ArH), 5.38 (t, *J* = 8.4 Hz, 1H, H-3), 4.43 (t, *J* = 8.8 Hz, 1H, H-2), 3.96 (dd, *J* = 8.8, 8 Hz, 1H, H-2), 2.70-2.63 (m, 1H, H-6), 2.57-2.48 (m, 1H, H-6), 2.21-2.09 (m, 1H, H-7), 2.08-2.01 (m, 1H, H-11), 1.91-1.83 (m, 2H, H-7a and H-9), 1.74-1.50 (m, 4H, H-7, H-8 and H-10), 1.46-1.40 (m, 1H, H-8), 1.16 (d, *J* = 7.6 Hz, 3H, CH_3C-11), 0.93 (d, *J* = 6.4 Hz, 3H, CH_3C-9); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.3 (CO), 139.9 (C*q*-Ar), 127.2 (CH-Ar), 128.5 (CH-Ar), 126.1 (CH-Ar), 96.7 (C-11a), 69.0 (C-2), 60.0 (C-3), 40.3 (C-7a), 37.2 (C-8), 36.9 (C-10), 34.2 (C-11), 30.5 (C-6), 22.8 (C-7), 22.1 (*C*H_3C-9), 20.6 (C-9), 16.5 (*C*H_3C-11); HRMS calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1952. **8d:** mp: 119-121 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 193.3 (*c* 1.01, $CHCl_3$); IR (NaCl): 1668 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, *g*-HSQC) δ 7.34-7.31 (m, 2H, ArH), 7.26-7.22 (m, 3H, ArH), 5.64 (dd, *J* = 8.8, 6.0 Hz, 1H, H-3), 4.42 (dd, *J* = 8.8, 8.0 Hz, 1H, H-2), 4.12 (dd, *J* = 8.0, 6.0 Hz, 1H, H-2), 2.60 (dd, *J* = 16.8, 3.6 Hz, 1H, H-6), 2.45 (dd, *J* = 14.0, 5.2 Hz, 1H, H-6), 2.18 (tt, *J* = 12.4, 2.8 Hz, 1H, H-7a), 1.83-1.68 (m, 3H, H-7, H-9 and H-11) , 1.62-1.57 (m, 1H, H-8), 1.52-1.41 (m, 3H, H-7, H-8 and H-10), 1.23-1.18 (m, 1H, H-10), 0.87 (d, *J* = 6.4 Hz, 3H, CH_3C-9), 0.83 (d, *J* = 6.8 Hz, 3H, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 176.2 (CO), 141.7 (C*q*-Ar), 126.8 (CH-Ar), 128.3 (CH-Ar), 125.2 (CH-Ar), 98.0 (C-11a), 66.6 (C-2), 59.0 (C-3), 37.2 (C-8), 36.4 (C-10), 35.7 (C-7a), 35.4 (C-6), 31.8 (C-11), 26.4 (C-9), 22.9 (C-7), 21.8 (*C*H_3C-9), 14.6 (*C*H_3C-11); HRMS calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1952.

(3*R*,7a*S*,8*S*,11*S*,11a*S*)-8,11-Dimethyl-5-oxo-3-phenyldecahydrooxazolo[2,3-*j*]quinoline (9a) and its (3*R*,7a*R*,8*R*,11*R*,11a*R*) (3*R*,7a*S*,8*S*,11*R*,11a*S*), and (3*R*,7a*R*,8*S*,11*R*,11a*S*) isomers (9b, 9c and

9d, respectively):

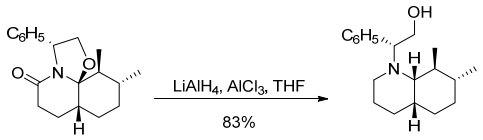


6 9a 9b 9c 9d

Operating as described in the preparation of lactams **7**, from a diastereomeric mixture of keto-acids **6** (4.48 g, 22.58 mmol) and *(R)*-phenylglycinol (4.65 g, 33.86 mmol) in benzene (220 mL), lactams **9a** (2.00 g, 30%), **9b** (1.96 g, 29 %), **9c** (0.34 g, 5 %), and **9d** (0.18 g, 3 %) were obtained after flash column chromatography (9:1 to 1:1 hexane–EtOAc) as colorless solids. **9a:** mp: 123-126 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 173.2 (*c* 1.02, $CHCl_3$); IR (NaCl): 1655 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.35-7.38 (m, 2H, ArH), 7.33-7.29 (m, 2H, ArH), 7.25-7.21 (m, 1H, ArH), 5.47 (dd, *J* = 7.2, 4.4 Hz, 1H, H-3), 4.34 (dd, *J* = 9.2, 4.4 Hz, 1H, H-2), 4.23 (dd, *J* = 9.2, 7.2 Hz, 1H, H-2), 2.54-2.51 (m, 2H, H-6), 2.17-2.10 (m, 1H, H-8), 1.79-1.69 (m, 4H, H-7, H-7a and H-11), 1.55-1.49 (m, 1H, H-9), 1.46-1.18 (m, 3H, H-9 and H-10), 0.91 (d, *J* = 6.8 Hz, 3H, CH_3C-8), 0.55 (d, *J* = 6.8 Hz, 3H, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.2 (CO), 139.2 (C*q*-Ar), 126.9 (CH-Ar), 128.2 (CH-Ar), 127.1 (CH-Ar), 99.1 (C-11a), 68.3 (C-2), 59.2 (C-3), 44.5 (C-7a), 34.9 (C-11), 31.2 (C-9 and C-8), 28.6 (C-6), 27.6 (C-10), 18.6 (CH$_3$C-8), 16.1 (CH$_3$C-11), 14.9 (C-7); HRMS calcd for $[C_{19}H_{25}NO_2 + H^+]$: 300.1958; found 300.1959. **9b:** mp: 174-177 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ + 52.6 (*c* 1.01, $CHCl_3$); IR (NaCl): 1662 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.33-7.21 (m, 5H, ArH), 5.08 (dd, *J* = 8.0, 4.0 Hz, 1H, H-3), 4.55 (dd, *J* = 8.8, 8.0 Hz, 1H, H-2), 3.90 (dd, *J* = 8.8, 4.0 Hz, 1H, H-2), 2.42-2.33 (m, 2H, H-6), 2.28-2.17 (m, 1H, H-11), 2.07-2.01 (m, 1H, H-7a), 1.85-1.68 (m, 3H, H-7 and H-8), 1.60-1.45 (m, 2H, H-9 and H-10), 1.35-1.24 (m, 1H, H-10), 1.01 (d, *J* = 6.8 Hz, 3H, CH_3C-8), 0.96 (d, *J* = 6.8 Hz, 3H, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 168.1 (CO), 141.3 (C*q*-Ar), 127.4 (CH-Ar), 128.5 (CH-Ar), 126.6 (CH-Ar), 97.6 (C-11a), 75.0 (C-2), 61.8 (C-3), 45.7 (C-7a), 37.8 (C-8), 31.4 (C-11), 31.0 (C-9), 29.1 (C-6), 27.7 (C-10), 18.4 (CH$_3$C-11), 16.1 (CH$_3$C-8), 16.0 (C-7); HRMS calcd for $[C_{19}H_{25}NO_2 + H^+]$: 300.1958; found 300.1960. **9c:** mp: 98-102 ºC (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 133.8 (*c* 1.01, $CHCl_3$); IR (NaCl): 1655 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.35-7.30 (m, 2H, ArH), 7.28-7.22 (m, 3H, ArH), 5.37 (t, *J* = 8.0 Hz, 1H, H-3), 4.41 (m, 1H, H-2), 3.95 (dd, *J* = 9.2, 8.0 Hz, 1H, H-2), 2.70-2.63 (m, 1H, H-6), 2.53-2.44 (m, 1H, H-6), 2.20-2.10 (m, 1H, H-8), 2.05-1.96 (m, 1H, H-11), 1.91-1.69 (m, 4H, H-7, H-7a and H-9), 1.48-1.26 (m, 3H, H-9 and H-10), 1.13 (d, *J* = 7.2 Hz, 3H, CH_3C-11), 0.96 (d, *J* = 6.8 Hz, 3H, CH_3C-8); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.1 (CO), 140.0 (C*q*-Ar), 127.2 (CH-Ar), 128.5 (CH-Ar), 126.1 (CH-Ar), 97.7 (C-11a), 69.1 (C-2), 60.1 (C-3), 45.1 (C-7a), 33.4 (C-11), 31.7 (C-8), 30.0 (C-6), 28.3 (C-9), 23.1 (C-10), 18.9 (CH$_3$C-8), 16.1 (C-7), 15.9 (CH$_3$C-11); HRMS calcd for $[C_{19}H_{25}NO_2 + H^+]$: 300.1958; found 300.1958. **9d:** mp: 99-103 ºC (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 194.4

(*c* 1.05, $CHCl_3$); IR (NaCl): 1668 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.34-7.31 (m, 2H, ArH), 7.26-7.21 (m, 3H, ArH), 5.62 (dd, *J* = 8.4, 6.4 Hz, 1H, H-3), 4.42 (t, *J* = 8.4 Hz, 1H, H-2), 4.10 (dd, *J* = 8.4, 6.4 Hz, 1H, H-2), 2.63 (dt, *J* = 16.8, 2.8 Hz, 1H, H-6), 2.38 (ddd, *J* = 16.8, 13.6, 4.4 Hz, 1H, H-6), 1.89-1.70 (m, 5H, H-7, H-7a, H-8, H-9 and H-11), 1.54-1.47 (m, 2H, H-7 and H-10), 1.27-1.16 (m, 2H, H-9 and H-10), 0.94 (d, *J* = 6.8 Hz, CH_3C-8), 0.83 (d, *J* = 6.8 Hz, CH_3C-11); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 175.8 (CO), 141.8 (C*q*-Ar), 126.8 (CH-Ar), 128.3 (CH-Ar), 125.1 (CH-Ar), 98.4 (C-11a), 66.7 (C-2), 58.8 (C-3), 42.4 (C-7a), 35.3 (C-6), 32.6 (C-8), 31.3 (C-11), 29.6 (C-10), 27.0 (C-9), 19.8 (*C*H_3C-8), 19.2 (C-7), 14.0 (*C*H_3C-11); HRMS calcd for [$C_{19}H_{25}NO_2$ + H^+]: 300.1958; found 300.1955.

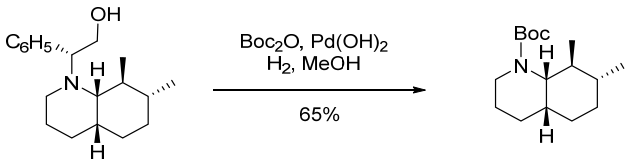
(4a*R*,7*R*,8*S*,8a*S*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-7,8-dimethyldecahydroquinoline (10):



7a **10**

$LiAlH_4$ (13.5 mL of a 1M solution in THF, 13.5 mmol) was slowly added to a stirring suspension of $AlCl_3$ (555 mg, 4.2 mmol) in anhydrous THF (25 mL) at 0 °C. After 1 h, the mixture was cooled at –78 °C, and a solution of the lactam **7a** (623 mg, 2.1 mmol) in anhydrous THF (10 mL) was added dropwise. The stirring was continued at –78 °C for 90 min and at rt for 2 h. Cold water was slowly added until no bubbling is seen and the resulting mixture was filtered over Celite®.The filtrate was dried and concentrated. Flash chromatography (9:1 to 7:3 hexane–EtOAc) afforded decahydroquinoline **10** (498 mg, 83%) as a colorless solid: mp: 94 –97 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 65.8 (*c* 1.0, $CHCl_3$); IR (NaCl): 3420 (OH) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.38- 7.40 (m, 2H, ArH), 7.27-7.34 (m, 3H, ArH), 4.05 (m, 1H, C*H*CH_2O), 3.84 (dd, *J* = 10.8, 5.2 Hz, 1H, CHC*H*$_2$O), 3.74 (dd, *J* = 10.8, 4.4 Hz, 1H, CHC*H*$_2$O), 2.45-2.66 (m, 4H, H-2, H-8a and OH), 2.00-2.05 (m, 1H, H-8), 1.69-1.76 (m, 2H, H-4 and H-4a), 1.54 (dt, *J* = 13.2, 4.4 Hz, 1H, H-6), 1.44-1.48 (m, 1H, H-6), 1.34-1.41 (m, 2H, H-3 and H-5), 1.25-1.30 (m, 1H, H-4), 1.19 (dd, *J* = 13.2, 4.0 Hz, 1H, H-5), 1.08-1.12 (m, 1H, H-3), 1.13-1.15 (m, 1H, H-7), 1.09 (d, *J* = 6.4 Hz, 3H, CH_3C-8), 0.96 (d, *J* = 6.0 Hz, 3H, CH_3C-7); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 142.0 (C*q*-Ar), 127.5 (CH-Ar), 128.6 (CH-Ar), 128.4 (CH-Ar), 65.4 (*C*HCH$_2$O), 63.6 (CH*C*H$_2$O), 63.1 (C-8a), 40.6 (C-2), 39.2 (C-7), 35.9 (C-4a), 31.1 (C-6), 30.0 (C-5), 29.8 (C-8), 25.0 (C-4), 21.1 (C-3), 20.8 (*C*H_3C-8), 15.7 (*C*H_3C-7); HRMS calcd for [$C_{19}H_{29}NO$ + H^+]: 288.2332; found 288.2332.

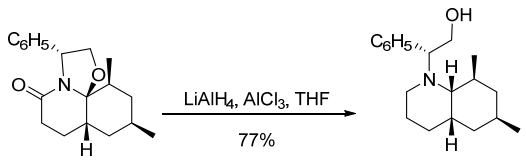
(4a*R*,7*R*,8*S*,8a*S*)-1-(*tert*-Butoxycarbonyl)-7,8-dimethyldecahydroquinoline (11)



10 **11**

A solution of *cis*-decahydroquinoline **10** (160 mg, 0.6 mmol) and Boc_2O (330 mg, 1.5 mmol) in CH_3OH (13 mL) containing 40% $Pd(OH)_2$ (64 mg) was stirred under hydrogen at rt for 8h. The catalyst was removed by filtration over Celite®, and the filtrate was concentrated. Flash chromatography (99:1 to 95:5 hexane–Et_2O) afforded decahydroquinoline **11** (96.4 mg, 65%) as a yellowish oil: $[\alpha]^{23}_D$ – 52.0 (*c* 1.1, $CHCl_3$); IR (NaCl): 1690 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 4.06 and 3.92 [(dd, *J* =11.6, 4.8 Hz) and (dd, *J* = 13.6, 3.6 Hz), 1H, H-2], 3.73 and 3.91-3.86 [(dd, *J* = 11.2, 4.4 Hz) and (m), 1H, H-8a], 2.68 and 2.60 [(td, *J* = 13.6, 2.8 Hz) and (td, *J* = 13.2, 2.4 Hz), 1H, H-2], 1.88-1.77 (m, 1H, H-4a), 1.74-1.70 (m, 1H), 1.67-1.60 (m, 2H), 1.56-1.50 (m, 2H), 1.45 [s, 9H, $(CH_3)_3$], 1.48-1.43 (m, 1H), 1.40-1.34 (m, 2H), 1.19-1.13 (m, 2H), 0.95-0.93 (m, 3H, CH_3C-7), 0.81 (d, *J* = 6.4 Hz, 3H, CH_3C-8); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 155.3 and 155.2 (CO), 78.9 and 78.7 (Cq), 59.1 and 57.6 (C-8a), 38.6 and 38.5 (CH), 38.9 and 37.6 (C-2) 35.6 and 35.3 (CH), 35.3 and 35.1 (C-4a), 30.9 and 30.7 (CH_2), 30.1and 30.0 (CH_2), 28.4 [$(CH_3)_3$], 26.2 and 25.8 (C-3), 24.6 (CH_2), 20.3 (*C*H_3C-7), 14.9 and 14.4 (*C*H_3C-8); HRMS calcd for [$C_{16}H_{29}NO_2$ + Na^+]: 290.2091; found 290.2094.

(4a*S*,6*R*,8*S*,8a*R*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-6,8-dimethyldecahydroquinoline (12):

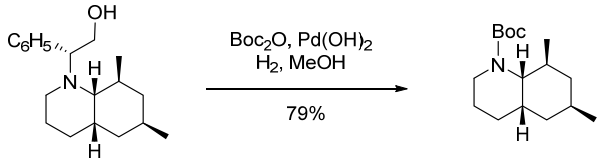


8a **12**

Operating as described in the preparation of decahydroquinoline **10**, from $LiAlH_4$ (5.8 mL of a 1M solution in THF, 5.8 mmol), $AlCl_3$ (240 mg, 1.8 mmol) in anhydrous THF (12 mL), and a solution of lactam **8a** (269 mg, 0.9 mmol) in anhydrous THF (8 mL), decahydroquinoline **12** (200 mg, 77%) was obtained after flash column chromatography (9:1 hexane–EtOAc) as a colorless solid: mp: 38-40 °C (hexane–CH_2Cl_2); $[\alpha]^{23}_D$ – 24.7 (*c* 1.0, $CHCl_3$); IR (NaCl): 3425 (OH) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.25-7.40 (m, 5H, ArH), 4.03 (t, *J* = 5.2 Hz, 1H, C*H*CH_2O), 3.82 (dd, *J* = 10.8, 5.2 Hz, 1H, CHC*H*$_2$O), 3.73 (dd, *J* = 10.8, 4.8 Hz, 1H, CHC*H*$_2$O), 2.61-2.69 (m, 1H, H-2), 2.51-2.55 (m, 1H, H-2), 2.47 (dd, *J* = 10.8, 4.8 Hz, 1H, H-8a), 2.09-2.19 (m, 1H, H-6), 1.96-2.03 (m, 1H, H-4a), 1.63-1.74 (m, 2H, H-5, H-7), 1.59-1.66 (m, 1H, H-8), 1.45-1.50 (m, 1H, H-4), 1.28-1.37 (m,

2H, H-3, H-5), 1.16 (dd, *J* = 12.8, 4.8 Hz, 1H, H-4), 1.06-1.12 (m, 1H, H-3), 1.03 (d, *J* = 6.4 Hz, 3H, CH_3C-6), 0.83 (d, *J* = 6.4 Hz, 3H, CH_3C-8), 0.73 (q, *J* = 12.0 Hz, 1H, H-7); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 141.9 (C*q*-Ar), 128.6 (CH-Ar), 128.4 (CH-Ar), 127.0 (CH-Ar), 65.8 (*C*HCH_2O), 64.3 (C-8a), 63.3 (CH*C*H_2O), 44.6 (C-7), 41.1 (C-4), 40.6 (C-2), 30.6 (C-4a), 28.8 (C-6), 26.7 (C-8), 25.8 (C-5), 22.5 (*C*H_3C-8), 21.6 (C-3), 19.7 (*C*H_3C-6); HRMS calcd for [$C_{19}H_{29}NO$ + H^+]: 288.2322; found 288.2322.

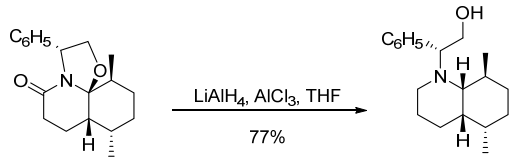
(4a*S*,6*R*,8*S*,8a*R*)-1-(*tert*-Butoxycarbonyl)-6,8-dimethyldecahydroquinoline (13)



12 **13**

Operating as in the preparation of decahydroquinoline **11**, from decahydroquinoline **12** (116 mg, 0.4 mmol), Boc_2O (106 mg, 0.5 mmol) and 40% $Pd(OH)_2$ (46 mg) in CH_3OH (9 mL), decahydroquinoline **13** (88 mg, 79%) was obtained after flash column chromatography (99:1 to 95:5 hexane–Et_2O) as a yellowish oil: $[\alpha]^{23}_D$ – 15.5 (*c* 1.0, $CHCl_3$); IR (NaCl): 1691 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 4.06 and 3.88 [(m) and (dd, *J* = 13.6, 4.0 Hz), 1H, H-2_b], 3.83 and 3.63 [(dd, *J* = 11.6, 4.8 Hz) and (dd, *J* = 16.4, 4.8 Hz), 1H, H-8a], 2.68 and 2.64 [(td, *J* = 13.2, 2.8 Hz) and (td, *J* = 13.2, 2.4 Hz), 1H, H-2_a], 1.99-1.90 (m ,1H, H-8), 1.84-1.77 (m, 1H, H-4a), 1.70-1.58 (m, 4H, H-3, H-6 and H-7_b), 1.53-1.49 (m, 1H, H-5_b), 1.45 [s, 9H, $(CH_3)_3$], 1.40-1.35 (m, 2H, H-4), 1.28-1.21 (m, 1H, H-5_a), 0.85 and 0.83 (d, *J* = 4.2 Hz, 3H, CH_3C-8), 0.79 (d, *J* = 6.4 Hz, 3H, CH_3C-6), 0.72 (q, *J* = 11.6 Hz, 1H, H-7_a); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 155.4 and 155.2 (CO), 78.9 and 78.8 (Cq), 59.4 and 57.9 (C-8a), 43.6 and 43.5 (C-7), 40.6 and 40.5 (C-5), 39.0 and 37.8 (C-2), 36.1 and 35.8 (C-4a), 28.5 [$(CH_3)_3$], 28.4 and 28.2 (C-8), 26.9 and 26.8 (C-6), 26.3 and 25.9 (C-3) 25.5 (C-4), 22.4 (CH_3C-8), 18.6 and 18.0 (CH_3C-6); HRMS calcd for [$C_{16}H_{29}NO_2$ + H^+]: 268.2271; found 268.2268.

(4a*S*,5*S*,8*S*,8a*R*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-5,8-dimethyldecahydroquinoline (14):

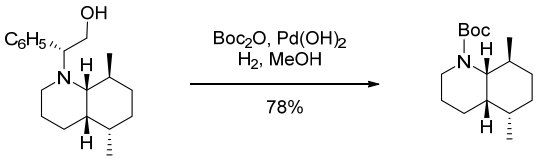


9a **14**

Operating as described in the preparation of decahydroquinoline **10**, from $LiAlH_4$ (13 mL of a 1M solution in THF, 13.0 mmol), $AlCl_3$ (530 mg, 3.97 mmol) in anhydrous THF (25 mL), and a solution

of lactam **9a** (595 mg, 1.99 mmol) in anhydrous THF (15 mL), decahydroquinoline **14** (441 mg, 77%) was obtained after flash column chromatography (95:5 hexane–EtOAc) as a yellowish oil: $[\alpha]^{23}_{D}$ – 33.2 (*c* 1.03, $CHCl_3$); IR (NaCl): 3425 (OH) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.42-7.28 (m, 5H, ArH), 4.11 (t, *J* = 5.2 Hz, 1H, C*H*CH_2O), 3.85 (dd, *J* = 11.0, 5.2 Hz, 1H, CHC*H*$_2$O), 3.78 (dd, *J* = 11.0, 4.8 Hz, 1H, CHC*H*$_2$O), 2.77-2.69 (m, 1H, H-2), 2.58-2.54 (m, 2H, H-2 and H-8a), 2.12-2.04 (m, 1H, H-8), 1.96-1.89 (m, 1H, H-4a), 1.75 (dq, *J* = 9.6, 2.8 Hz, 1H, H-7), 1.63-1.54 (m, 1H, H-5), 1.48-1.42 (m, 2H, H-4), 1.36-1.29 (m, 2H, H-3 and H-6), 1.21-1.09 (m, 3H, H-3, H-6 and H-7), 1.08 (d, *J* = 6.4 Hz, 3H, CH_3C-8), 0.86 (d, *J* = 6.8 Hz, 3H, CH_3C-5); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 141.2 (C*q*-Ar), 128.4 (CH-Ar), 127.6 (CH-Ar), 128.7 (CH-Ar), 65.5 (*C*HCH_2O), 65.4 (C-8a), 63.3 (CH*C*H_2O), 41.3 (C-2), 35.7 (C-5), 35.6 (C-4a), 35.3 (C-7), 28.8 (C-6), 28.5 (C-8), 20.8 (C-3), 19.3 (*C*H_3C-8), 18.9 (C-4 and *C*H_3C-5); HRMS calcd for [$C_{19}H_{29}NO$ + H^+]: 288.2332; found 288.2332.

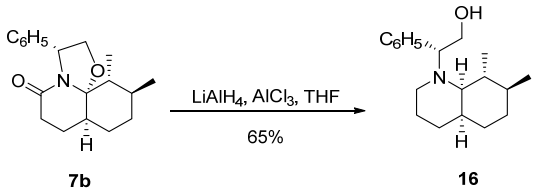
(4a*S*,5*S*,8*S*,8a*R*)-1-(*tert*-Butoxycarbonyl)-5,8-dimethyldecahydroquinoline (15)



14 **15**

Operating as described in the preparation of decahydroquinoline **11**, from decahydroquinoline **14** (439 mg, 1.53 mmol), Boc_2O (900 mg, 4.12 mmol), and 40% $Pd(OH)_2$ (176 mg) in CH_3OH (35 mL), decahydroquinoline **15** (319 mg, 78%) was obtained after flash column chromatography (99:1 to 95:5 hexane–Et_2O) as a colorless liquid: $[\alpha]^{23}_{D}$ – 23.8 (*c* 1.05, $CHCl_3$); IR (NaCl): 1691 (CO) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ4.09-4.05 and 3.92-3.87 [(m) and (m), 1H, H-2], 3.84 and 3.64 [(dd, *J* = 11.2, 4.0 Hz) and (dd, *J* = 11.6, 4.4 Hz), 1H, H-8a], 2.73 and 2.68 [(td, *J* = 12.8, 2.8 Hz) and (td, *J* = 12.8, 2.8 Hz), 1H, H-2], 1.94-1.84 (m, 1H, H-8), 1.75-1.61 (m, 4H, H-3, H-4a, H-5 and H-7), 1.53-1.48 (m, 1H, H-4), 1.46 [s, 9H, $(CH_3)_3$], 1.42-1.33 (m, 3H, H-3, H-4 and H-6), 1.18-1.03 (m, 2H, H-6 and H-7), 0.88 and 0.86 [(d, *J* = 6.8 Hz) and (d, *J* = 6.8 Hz), 3H, CH_3C-5], 0.80 (d, *J* = 6.4 Hz, CH_3C-8); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 155.3 and 155.2 (CO), 78.9 and 78.8 (Cq), 60.4 and 59.0 (C-8a), 41.4 and 41.0 (C-5), 39.4 and 38.1 (C-2), 35.6 and 35.3 (C-4a), 34.4 and 34.2 (C-7), 29.0 and 28.9 (C-6), 28.5 [$(CH_3)_3$], 28.0 and 27.8 (C-8), 26.0 and 25.6 (C-3), 18.9 and 18.8 (CH_3C-5), 18.7 and 18.6 (C-4), 18.3 and 17.8 (CH_3C-8); HRMS calcd for [$C_{16}H_{29}NO_2$ + Na^+]: 290.2091; found 290.2090.

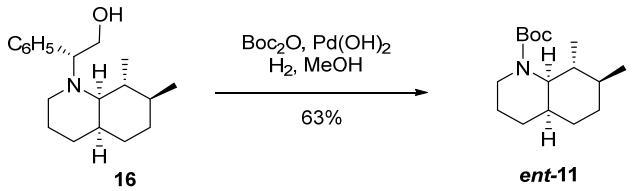
(4a*S*,7*S*,8*R*,8a*R*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-7,8-dimethyldecahydroquinoline (16):



7b **16**

Operating as described in the preparation of decahydroquinoline **10**, from $LiAlH_4$ (14.4 mL of a 1M solution in THF, 14.4 mmol), $AlCl_3$ (590 mg, 4.43 mmol) in anhydrous THF (25 mL), and a solution of lactam **7b** (663 mg, 2.21 mmol) in anhydrous THF (10 mL), decahydroquinoline **16** (412 mg, 65%) was obtained after flash column chromatography (9:1 to 7:3 hexane–EtOAc) as a yellowish oil: $[\alpha]^{23}_D$ – 42.4 (*c* 1.0, $CHCl_3$); IR (NaCl): 3313 (OH) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.39-7.36 (m, 2H, ArH), 7.33-7.24 (m, 3H, ArH), 4.07 (dd, *J* = 5.6, 3.6 Hz, 1H, C*H*CH_2O), 3.87 (dd, *J* = 10.6, 5.6 Hz, 1H, CHC*H*$_2$O), 3.73 (dd, *J* = 10.6, 3.6 Hz, 1H, CHC*H*$_2$O), 2.94-2.83 (m, 2H, H-2), 2.66 (br s, 1H, OH), 2.05 (dd, *J* = 11.2, 3.6 Hz, 1H, H-8a), 1.83-1.67 (m, 3H, H-3, H-4a and H-5), 1.61-1.57 (m, 1H, H-8), 1.38-1.07 (m, 6H, H-3, H-4, H-5 and H-6), 0.91 (d, *J* = 6.4 Hz, 3H, CH_3C-7), 0.86 (d, *J* = 6 Hz, 3H, CH_3C-8), 0.84- 0.78 (m, 1H, H-7); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 141.7 (C*q*-Ar), 127.4 (CH-Ar), 128.3 (CH-Ar), 28.7 (CH-Ar), 64.5 (*C*HCH_2O), 63.8 (CH*C*H$_2$O), 61.1 (C-8a), 42.1 (C-2), 38.9 (C-7), 35.5 (C-8), 30.9 (C-6), 29.9 (C-5), 29.2 (C-4a), 25.2 (C-4), 21.0 (C-3), 20.7 (*C*H_3C-8), 15.5 (*C*H_3C-7); HRMS calcd for [$C_{19}H_{29}NO + H^+$]: 288.2322; found 288.2319.

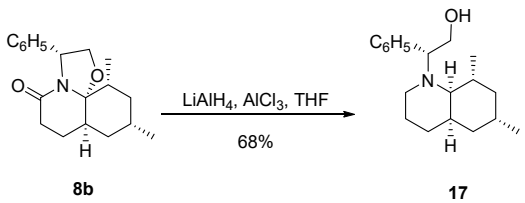
(4a*S*,7*S*,8*R*,8a*R*)-1-(*tert*-Butoxycarbonyl)-7,8-dimethyldecahydroquinoline (*ent*-11)



16 ***ent*-11**

Operating as in the preparation of decahydroquinoline **11**, from decahydroquinoline **16** (156 mg, 0.54 mmol), Boc_2O (319 mg, 1.46 mmol) and 40% $Pd(OH)_2$ (63 mg) in CH_3OH (13 mL), decahydroquinoline ***ent*-11** (91.2 mg, 63%) was obtained after flash column chromatography (99:1 to 95:5 hexane–Et_2O) as a yellowish oil: $[\alpha]^{23}_D$ + 52.5 (*c* 1.2, $CHCl_3$).

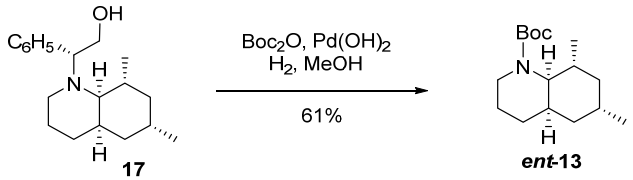
(4a*R*,6*S*,8*R*,8a*S*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-6,8-dimethyldecahydroquinoline (17):



8b **17**

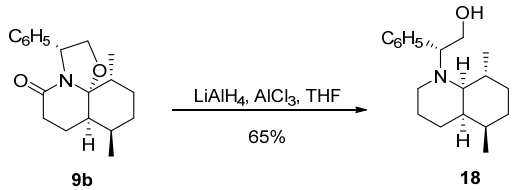
Operating as described in the preparation of decahydroquinoline **10**, from $LiAlH_4$ (7.3 mL of a 1M solution in THF, 7.3 mmol), $AlCl_3$ (300 mg, 2.26 mmol) in anhydrous THF (15 mL), and a solution of lactam **8b** (338.2 mg, 1.13 mmol) in anhydrous THF (10 mL), decahydroquinoline **17** (222 mg, 68%) was obtained after flash column chromatography (9:1 to 7:3 hexane–EtOAc) as a yellowish oil: $[\alpha]^{23}_D$ – 65.2 (*c* 1.1, $CHCl_3$); IR (NaCl): 3395 (OH) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ 7.27-7.40 (m, 5H, ArH), 4.05 (dd, *J* = 5.2 Hz, 4.0 Hz, 1H, C*H*CH_2O), 3.85 (dd, *J* = 10.8, 5.2 Hz, 1H, CHC*H*$_2$O), 3.72 (dd, *J* = 10.8, 4.0 Hz, 1H, CHC*H*$_2$O), 2.91-2.93 (m, 2H, H-2), 1.99-2.07 (m, 2H, H-6, H-8a), 1.69-1.76 (m, 3H, H-3, H-4a, H-5), 1.51-1.59 (m, 2H, H-7, H-8), 1.25-1.36 (m, 3H, H-3, H-5, H-4), 0.87 (d, *J* = 6.4 Hz, 3H, CH_3C-6), 0.76-0.84 (m, 1H, H-4), 0.71 (d, *J* = 6.4 Hz, 3H, CH_3C-8), 0.45 (q, *J* = 12.0 Hz, 1H, H-7); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 141.7 (C*q*-Ar); 127.5 (CH-Ar), 128.3 (CH-Ar), 128.7 (CH-Ar), 64.9 (*C*HCH_2O), 63.6 (CH*C*H_2O), 61.6 (C-8a), 44.4 (C-7), 42.8 (C-2), 40.8 (C-4), 30.2 (C-4a), 28.4 (C-6), 26.6 (C-8), 26.1 (C-5), 22.4 (*C*H_3C-8), 21.4 (C-3), 19.6 (*C*H_3C-6); HRMS calcd for [$C_{19}H_{29}NO$ + H^+]: 288.2322; found 288.2322.

(4a*R*,6*S*,8*R*,8a*S*)-1-(*tert*-Butoxycarbonyl)-6,8-dimethyldecahydroquinoline (*ent*-13)



Operating as described in the preparation of decahydroquinoline **11**, from decahydroquinoline **17** (106 mg, 0.37 mmol), Boc_2O (97 mg, 0.44 mmol), and 40% $Pd(OH)_2$ (43 mg) in CH_3OH (8.5 mL), decahydroquinoline ***ent*-13** (64 mg, 61%) was obtained after flash column chromatography (99:1 to 95:5 hexane–Et_2O) as a yellowish oil: $[\alpha]^{23}_D$ + 15.2 (*c* 1.0, $CHCl_3$).

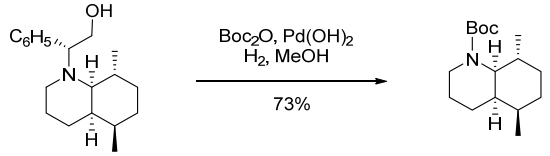
(4aR,5*R*,8*R*,8a*S*)-1-[(1*R*)-2-Hydroxy-1-phenylethyl]-5,8-dimethyldecahydroquinoline (18):



Operating as described in the preparation of decahydroquinoline **10**, from $LiAlH_4$ (11.6 mL of a 1M solution in THF, 11.6 mmol), $AlCl_3$ (477 mg, 3.57 mmol) in anhydrous THF (25 mL), and a solution of lactam **9b** (535 mg, 1.79 mmol) in anhydrous THF (10 mL), decahydroquinoline **18** (412 mg, 65%) was obtained after flash column chromatography (9:1 to 7:3 hexane–EtOAc) as a yellowish oil: $[\alpha]^{23}_D$ – 42.4 (*c* 1.0, $CHCl_3$); IR (NaCl): 3417 (OH) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, COSY, *g*-HSQC) δ

7.40-7.38 (m, 2H, ArH), 7.33-7.26 (m, 3H, ArH), 4.11-4.08 (m, 1H, C*H*CH_2O), 3.87 (dd, *J* = 10.8, 5.6 Hz, 1H, CHC*H*$_2$O), 3.73 (dd, *J* = 10.8, 3.6 Hz, 1H, CHC*H*$_2$O), 2.97-2.94 (m, 2H, H-2), 2.62 (br s, 1H, OH), 2.02-1.94 (m, 2H, H-8 and H-8a), 1.75- 1.68 (m, 1H, H-3), 1.65-1.58 (m, 2H, H-5 and H-7), 1.49-1.45 (m, 2H, H-4), 1.42-1.37 (m, 1H, H-3), 1.21-1.15 (m, 2H, H-4a and H-6), 1.13-1.03 (m, 1H, H-6), 0.88 (d, *J* = 5.6 Hz, 3H, CH_3C-8), 0.75 (d, *J* = 6.4 Hz, 3H, CH_3C-5), 0.79-0.73 (m, 1H, H-7); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 141.4 (C*q*-Ar), 127.5 (CH-Ar), 128.3 (CH-Ar), 128.6 (CH-Ar), 64.5 (*C*HCH_2O), 63.6 (CH*C*H_2O), 63.0 (C-8a), 42.9 (C-2), 35.3 (C-4a), 35.2 (C-5), 35.0 (C-7), 28.7 (C-6), 28.0 (C-8), 20.8 (C-3), 19.3 (*C*H_3C-8), 19.2 (C-4), 18.9 (*C*H_3C-5); HRMS calcd for [$C_{19}H_{29}NO$ + H^+]: 288.2322; found 288.2321.

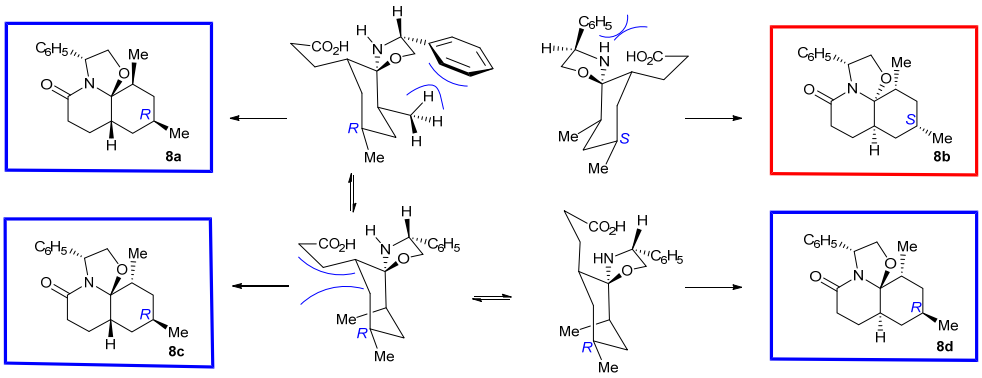
(4a*R*,5*R*,8*R*,8a*S*)-1-(*tert*-Butoxycarbonyl)-5,8-dimethyldecahydroquinoline (*ent*-15)



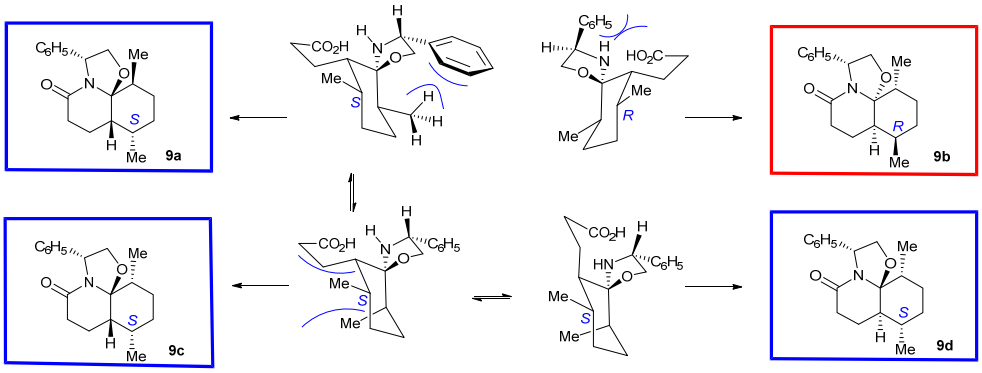
18 ***ent*-15**

Operating as described in the preparation of decahydroquinoline **9**, from decahydroquinoline **18** (439 mg, 1.53 mmol), Boc_2O (900 mg, 4.12 mmol), and 40% $Pd(OH)_2$ (176 mg) in CH_3OH (35 mL), decahydroquinoline ***ent*-15** (300 mg, 73%) was obtained after flash column chromatography (99:1 to 95:5 hexane–Et_2O) as a yellowish oil: $[\alpha]^{23}_D$ + 23.3 (*c* 1.03, $CHCl_3$).

II) Supplementary schemes, figures and tables



Scheme S1. Stereochemical outcome of the cyclocondensation reaction of keto-acid **5**



Scheme S2. Stereochemical outcome of the cyclocondensation reaction of keto-acid **6**

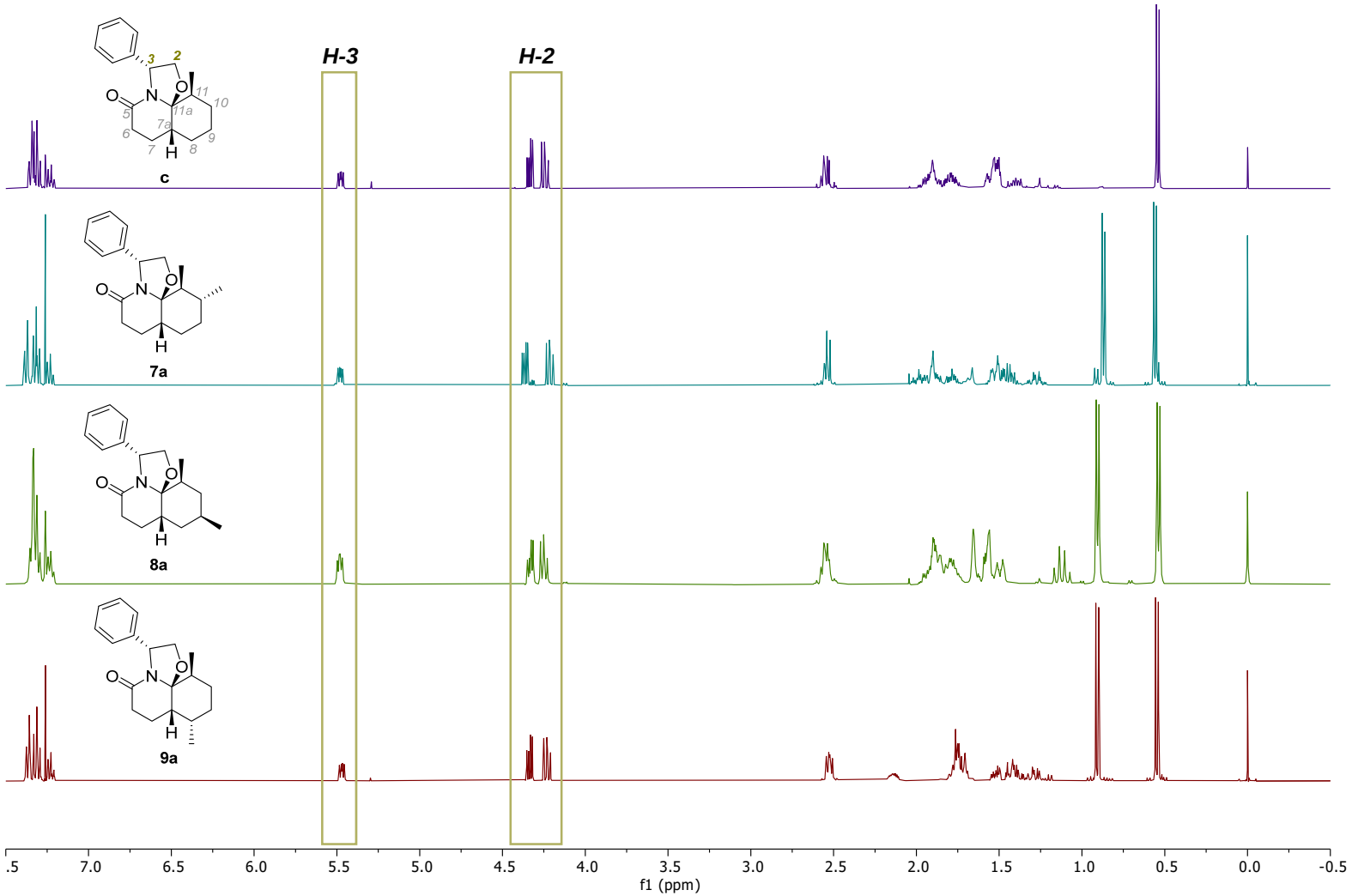


Figure S1. Stacked ^{1}H NMR spectra of **c** and **7a-9a** displaying diagnostic signals

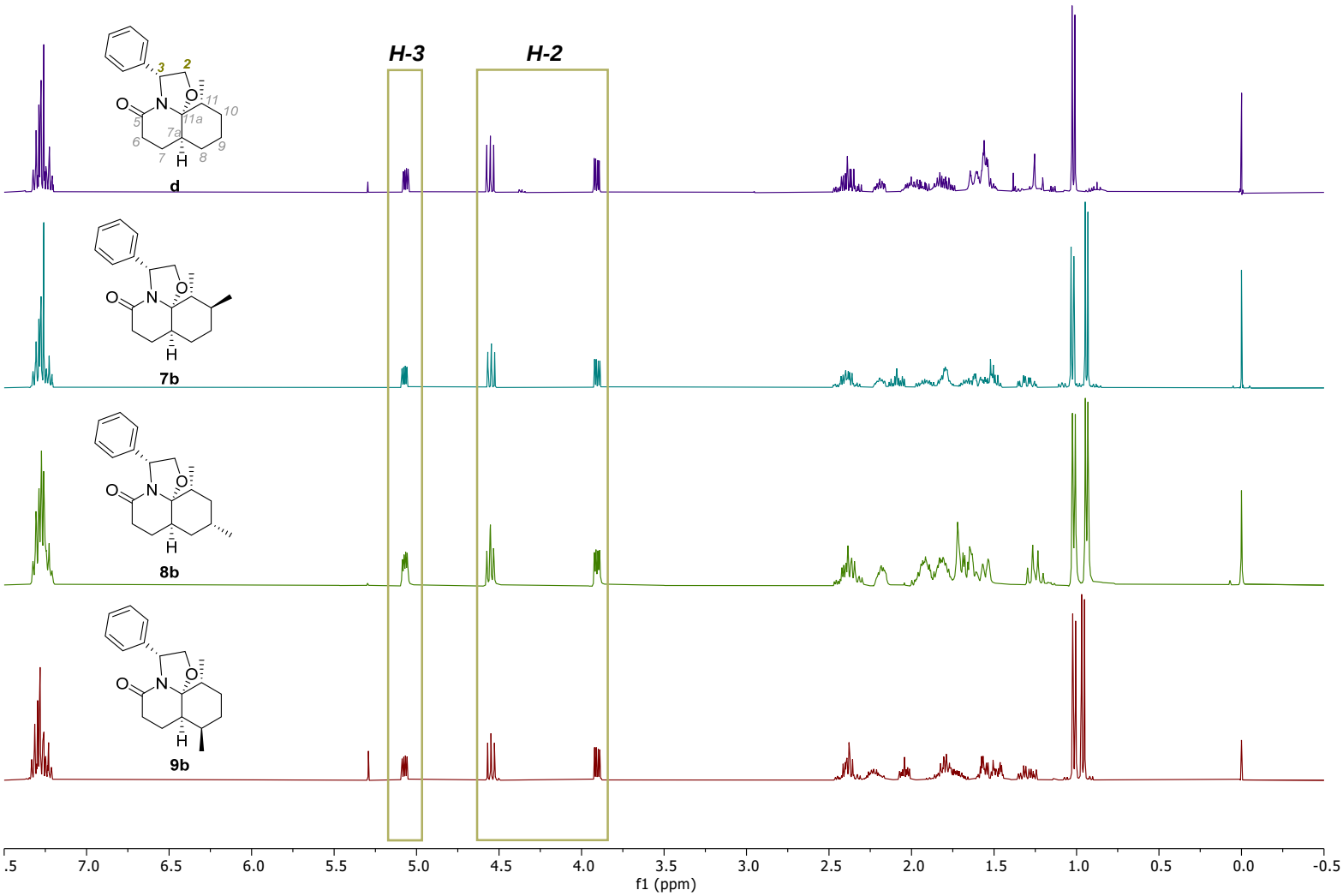


Figure S2. Stacked ^{1}H NMR spectra of **d** and **7b-9b** displaying diagnostic signals

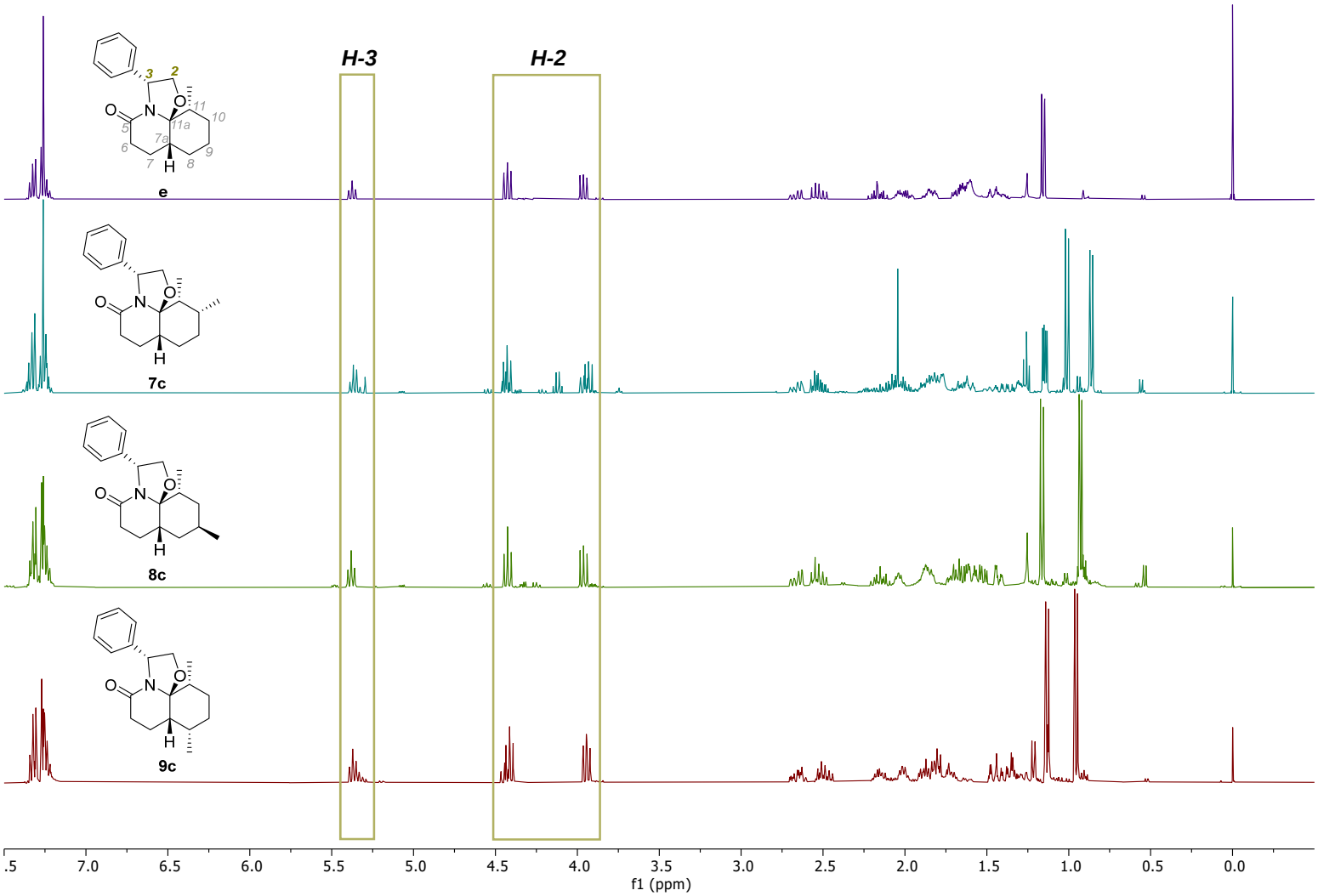


Figure S3. ^{1}H NMR stacked spectra of **e** and **7c-9c** displaying diagnostic signals

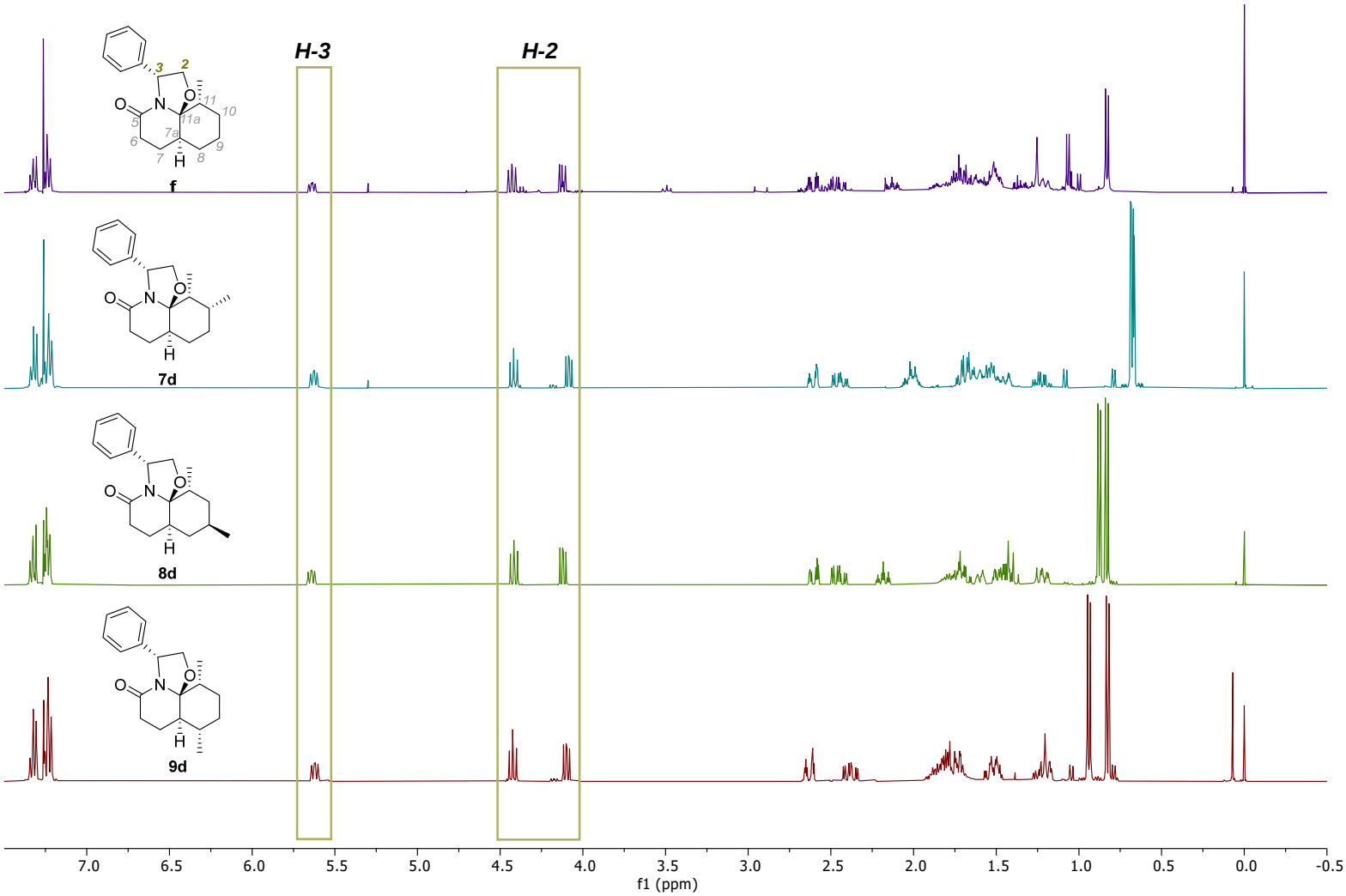


Figure S4. ^{1}H NMR stacked spectra of **f** and **7d-9d** displaying diagnostic signals

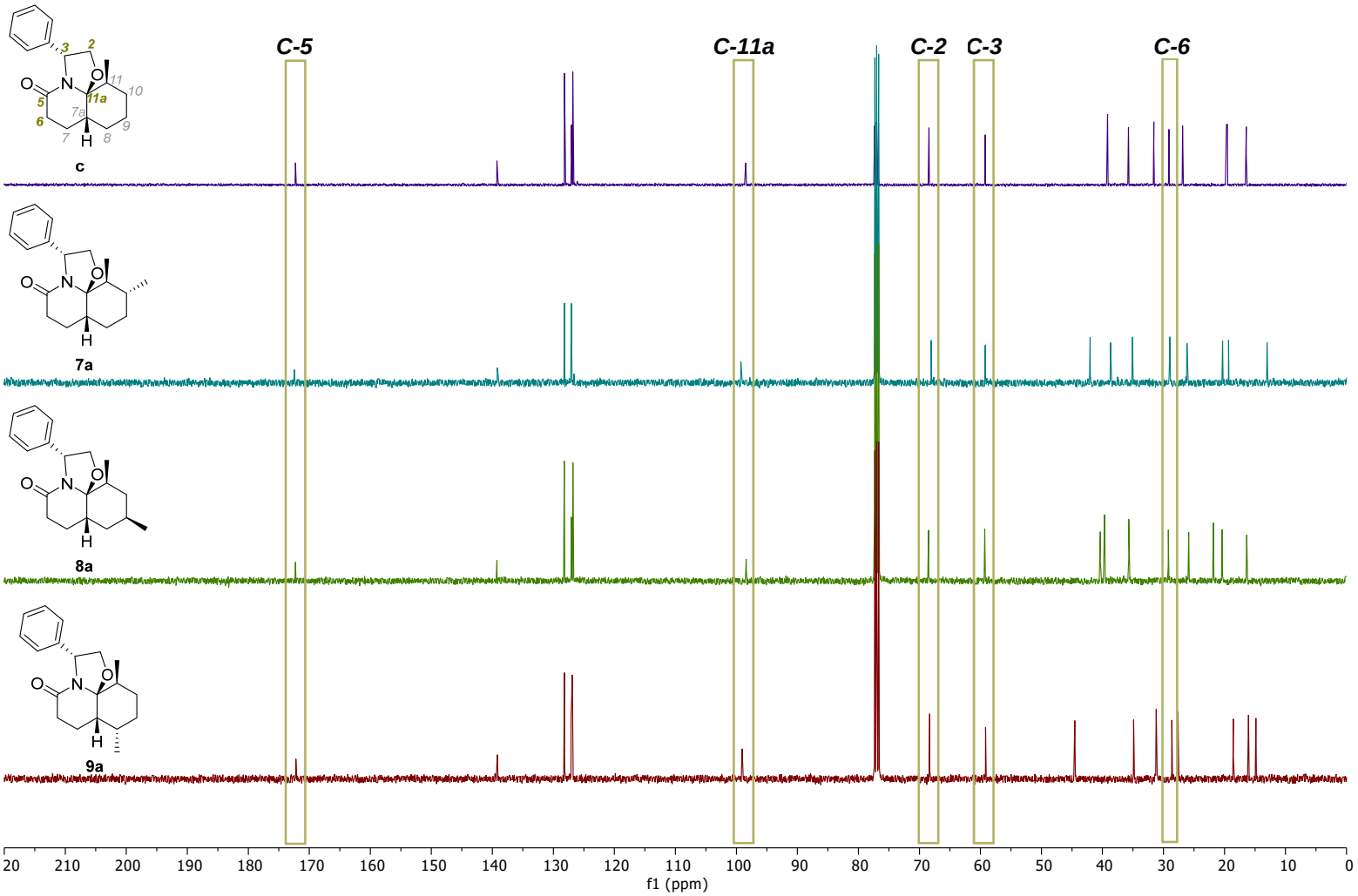


Figure S5. Stacked ^{13}C NMR spectra of **c** and **7a-9a** displaying diagnostic signals

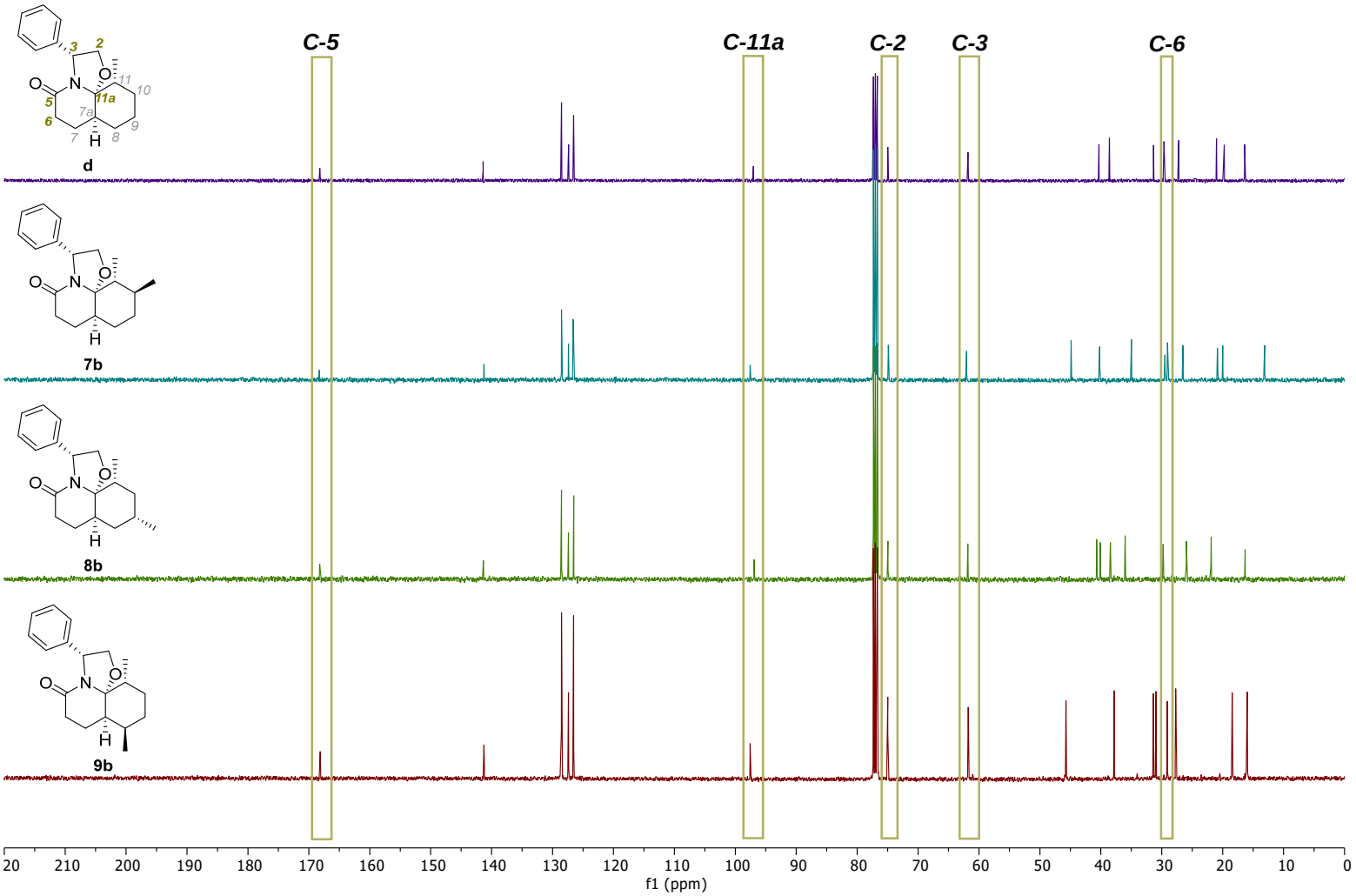


Figure S6. Stacked ^{13}C NMR spectra of **d** and **7b-9b** displaying diagnostic signals

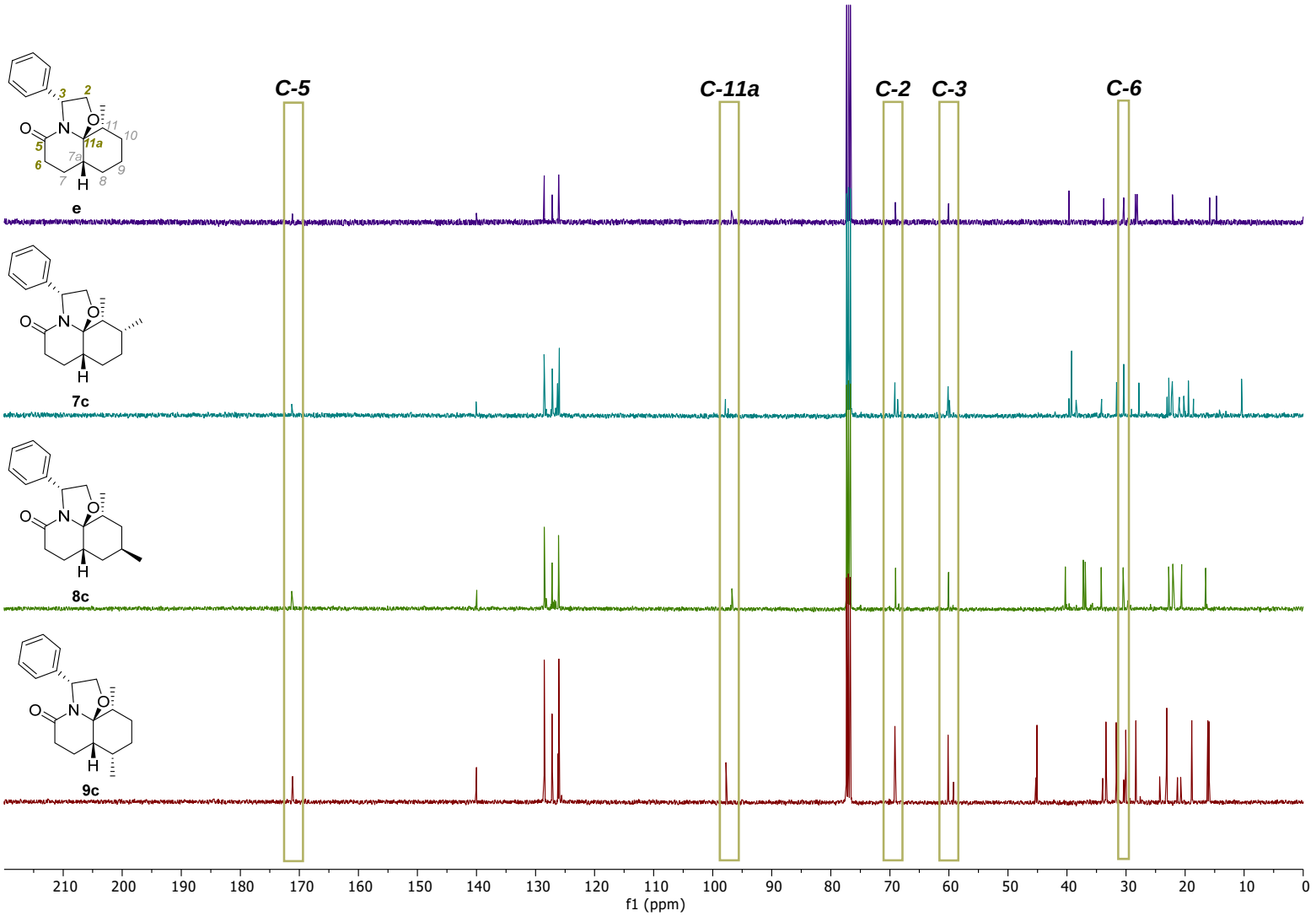


Figure S7. Stacked ^{13}C NMR spectra of **e** and **7c-9c** displaying diagnostic signals

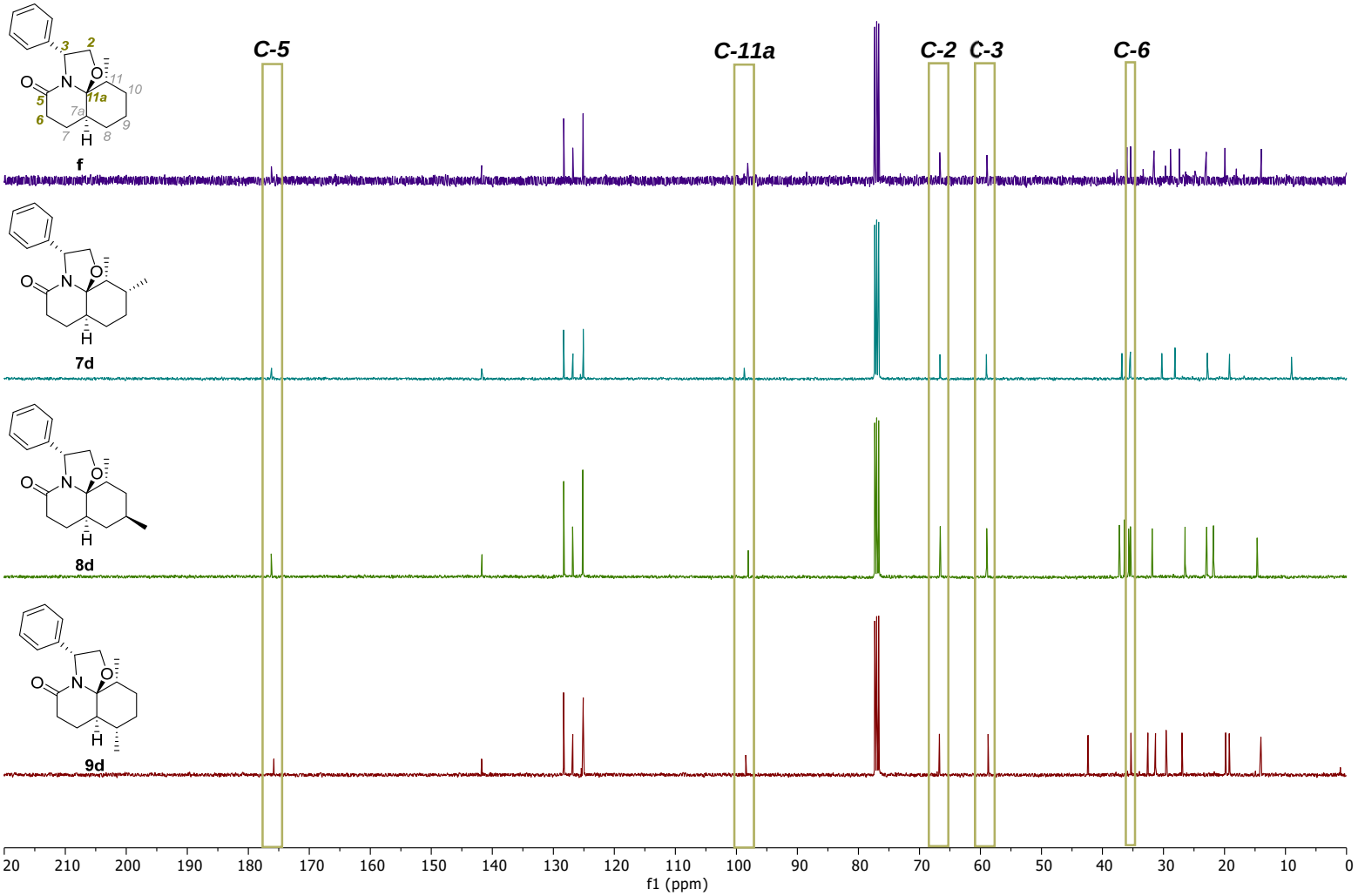


Figure S8. Stacked ^{13}C NMR spectra of **f** and **7d-9d** displaying diagnostic signals

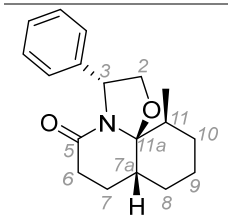
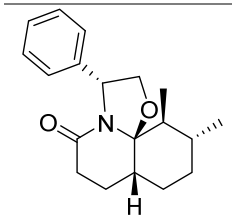
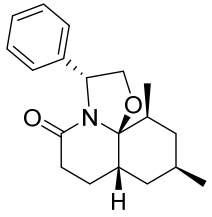
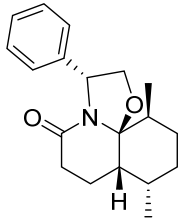
	C-2	C-3	C-5	C-6	C-7	C-7a	C-8	C-9	C-10	C-11	C-11a	CH_3C-11	CH_3C-8/9/10
 **c**	68.4	59.2	172.2	29.1	19.5	39.1	26.8	19.7	31.6	35.7	98.5	16.4	-
 **7a**	68.1	59.2	172.4	29.0	19.3	38.7	26.1	28.9	35.1	42.0	99.3	13.0	20.3
 **8a**	68.4	59.2	172.1	29.1	20.3	39.6	35.6	25.8	40.3	35.5	98.3	16.3	21.8
 **9a**	68.3	59.2	172.2	28.6	14.9	44.5	31.2	31.2	27.6	34.9	99.1	16.1	18.6

Table S1. ^{13}C NMR chemical shift values of **c** and **7a-9a**

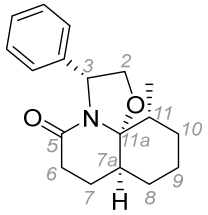
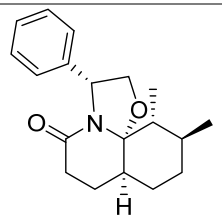
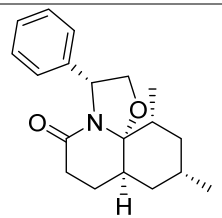
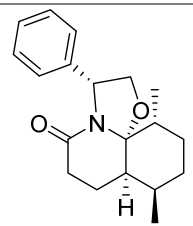
	C-2	C-3	C-5	C-6	C-7	C-7a	C-8	C-9	C-10	C-11	C-11a	CH_3C-11	CH_3C-8/9/10
 **d**	74.9	61.8	168.2	29.6	21.0	40.3	27.2	19.7	31.3	38.6	97.0	16.4	-
 **7b**	74.9	62.0	168.3	29.5	20.9	40.2	26.5	29.1	35.0	44.9	97.6	20.0	13.1
 **8b**	74.8	61.7	168.1	29.7	21.8	40.6	35.9	38.2	40.0	25.9	96.8	16.2	21.8
 **9b**	75.0	61.8	168.1	29.1	16	45.7	37.8	31.0	27.7	31.4	97.6	18.4	16.1

Table S2. ^{13}C NMR chemical shift values of **d** and **7b-9b**

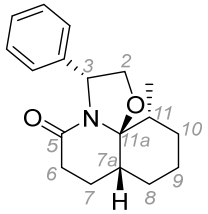
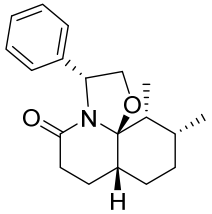
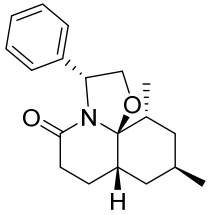
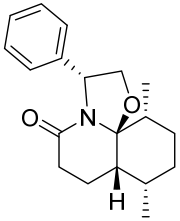
	C-2	C-3	C-5	C-6	C-7	C-7a	C-8	C-9	C-10	C-11	C-11a	CH_3C-11	CH_3C-8/9/10
 **e**	69.1	60.0	171.2	30.4	22.1	39.7	28.1	28.4	14.7	33.8	96.8	15.8	-
 **7c**	69.1	60.1	171.5	30.4	22.7	39.2	27.8	22.8	31.6	39.2	97.8	10.4	19.4
 **8c**	69.0	60.0	171.3	30.5	22.8	40.3	37.2	20.6	36.9	34.2	96.7	16.5	22.1
 **9c**	69.1	60.1	171.1	30.0	16.1	45.1	31.7	28.3	23.1	33.4	97.7	15.9	18.9

Table S3. ^{13}C NMR chemical shift values of **e** and **7c-9c**

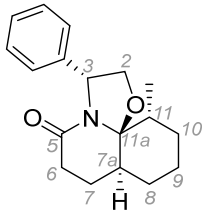
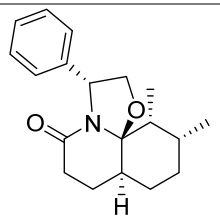
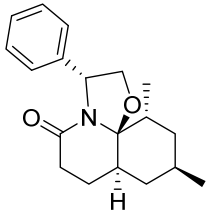
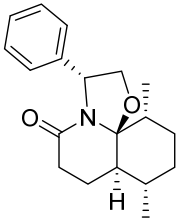
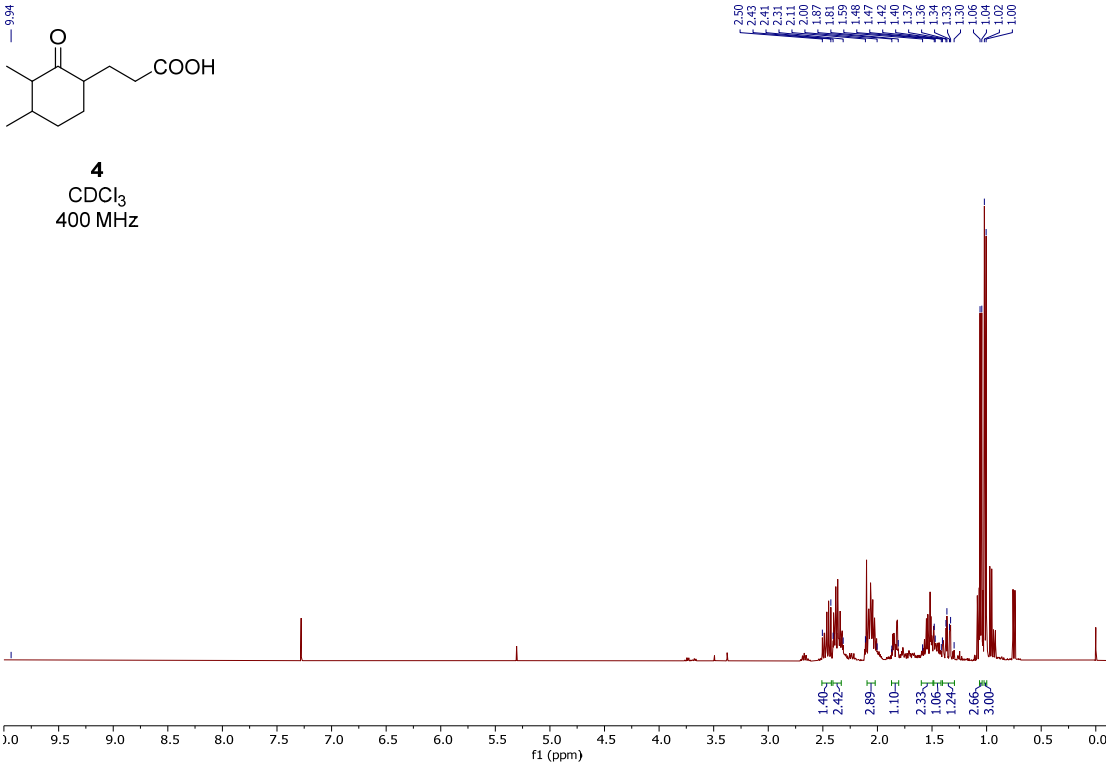
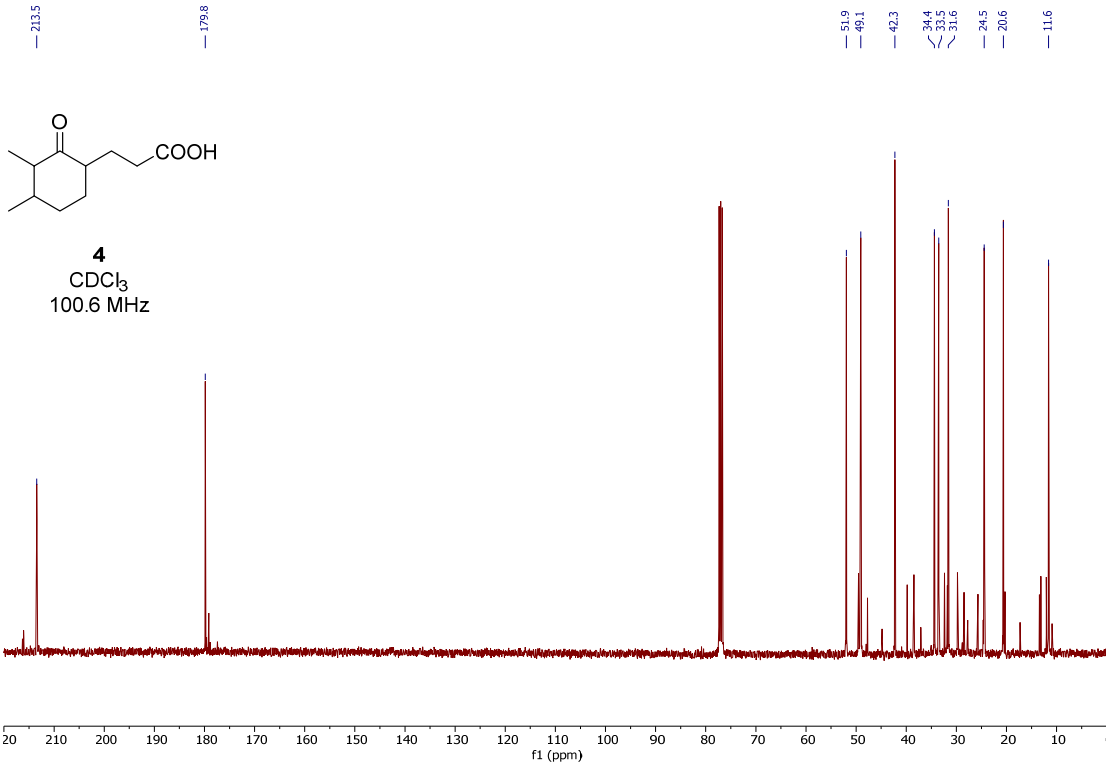
	C-2	C-3	C-5	C-6	C-7	C-7a	C-8	C-9	C-10	C-11	C-11a	CH_3C-11	CH_3C-8/9/10
 **f**	66.7	58.9	176.2	35.4	23.0	36.0	28.8	27.4	19.9	31.5	98.1	14.0	-
 **7d**	66.6	59.0	176.2	35.4	22.8	36.8	28.1	28.1	30.3	35.5	98.7	19.2	9.0
 **8d**	66.6	59.0	176.2	35.4	22.9	35.7	37.2	26.4	36.4	31.8	98.0	14.6	21.8
 **9d**	66.7	58.8	175.8	35.3	19.2	42.4	32.6	27.0	29.6	31.3	98.4	14.0	19.8

Table S4. ^{13}C NMR chemical shift values of **f** and **7d-9d**

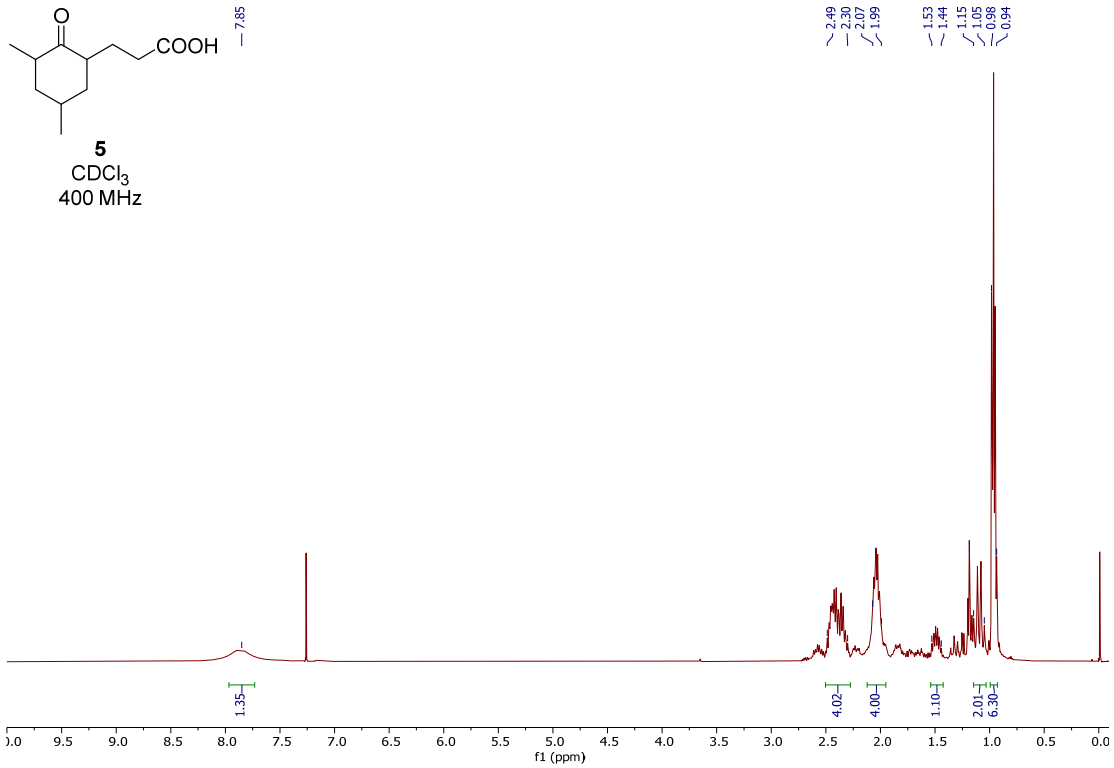
III) Copies of ^{1}H and ^{13}C NMR spectra



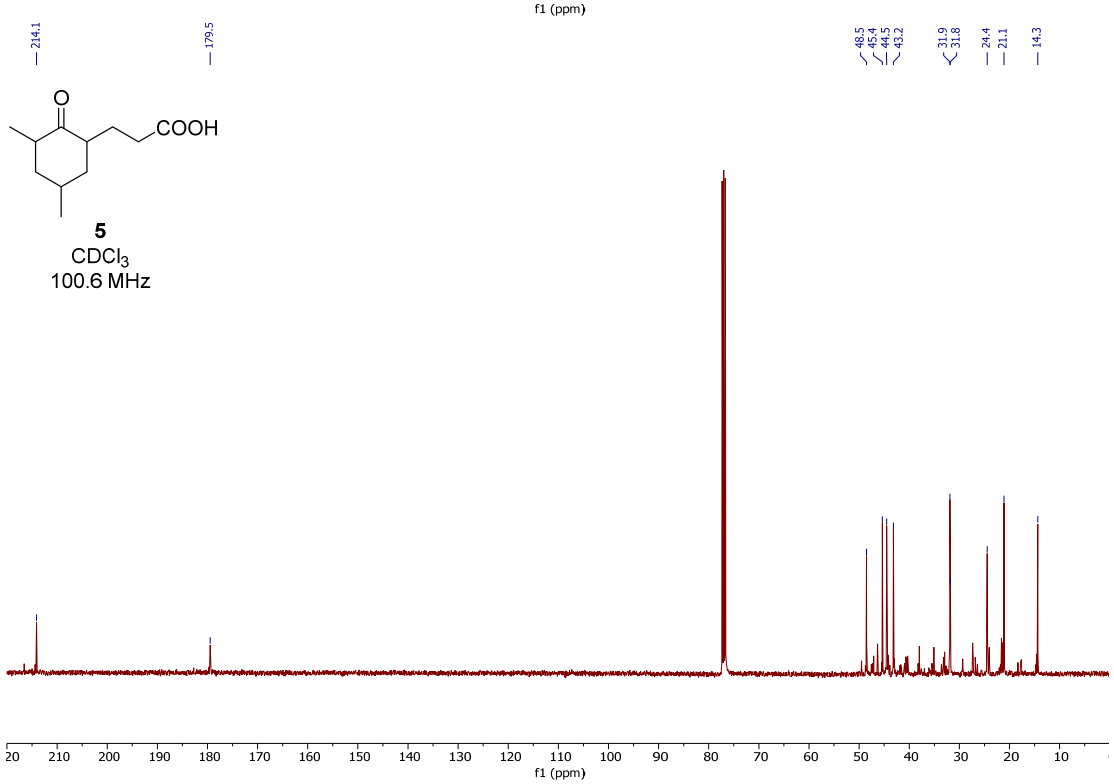
4
$CDCl_3$
400 MHz



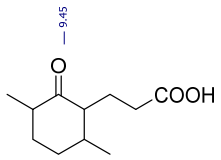
4
$CDCl_3$
100.6 MHz



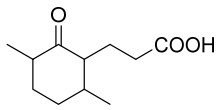
5
$CDCl_3$
400 MHz



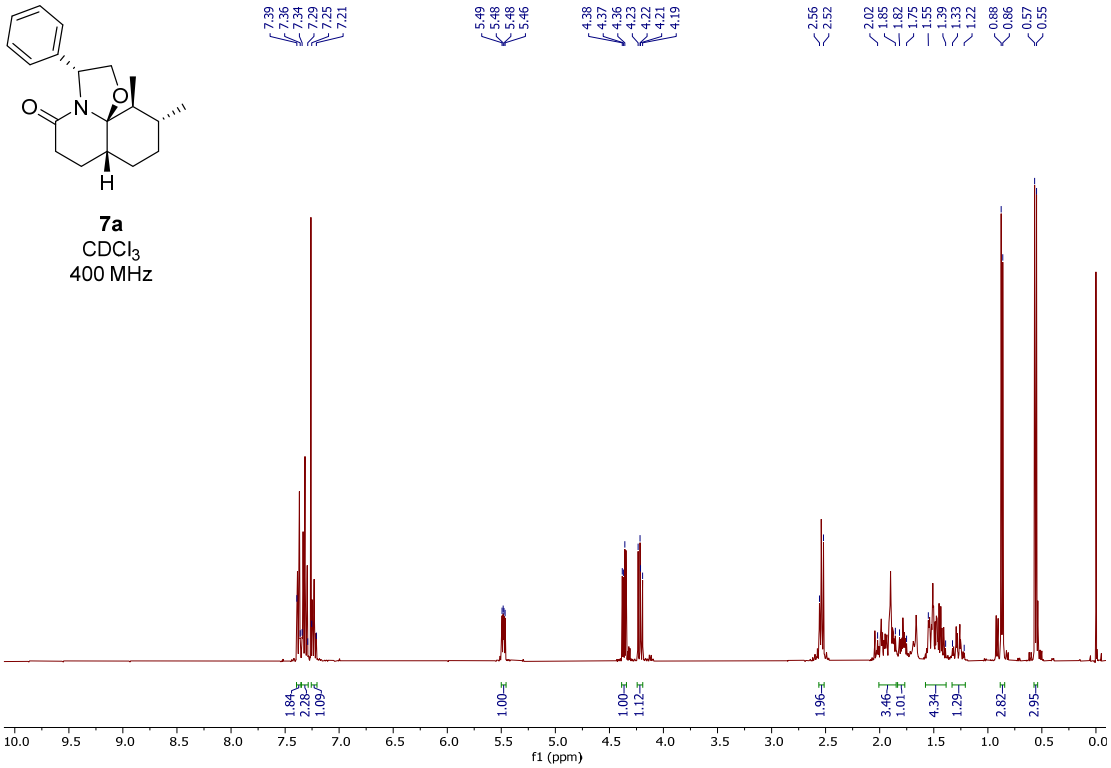
5
$CDCl_3$
100.6 MHz



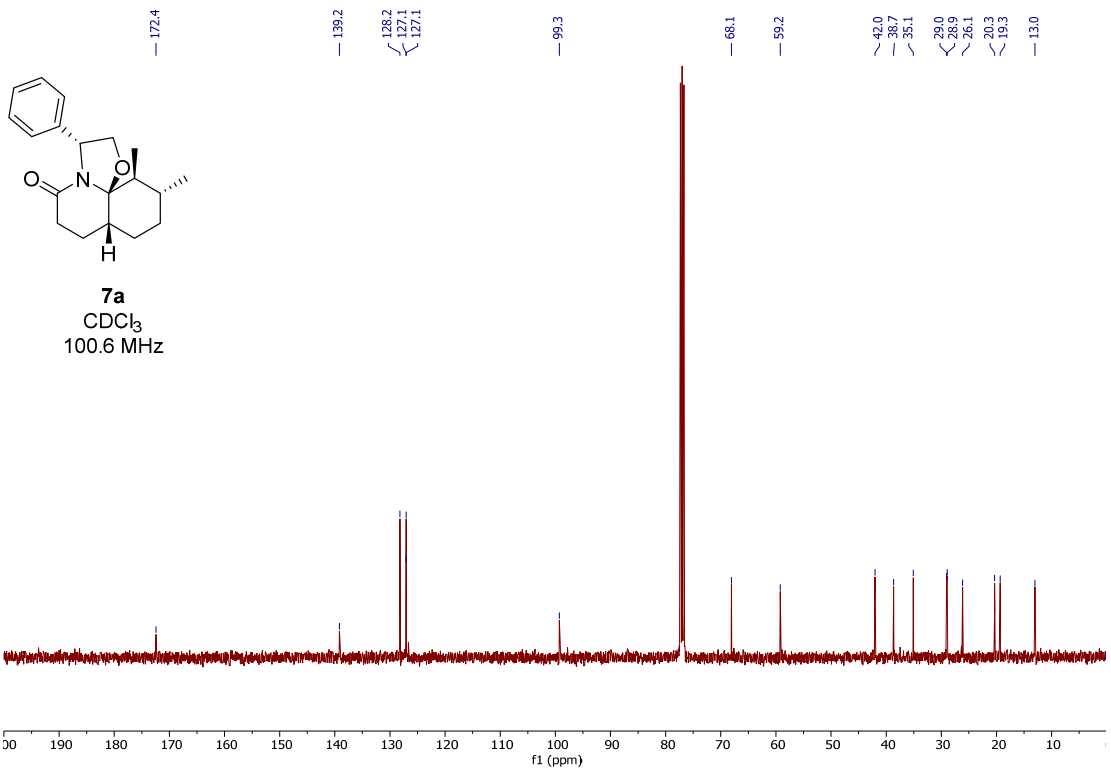
6
$CDCl_3$
400 MHz



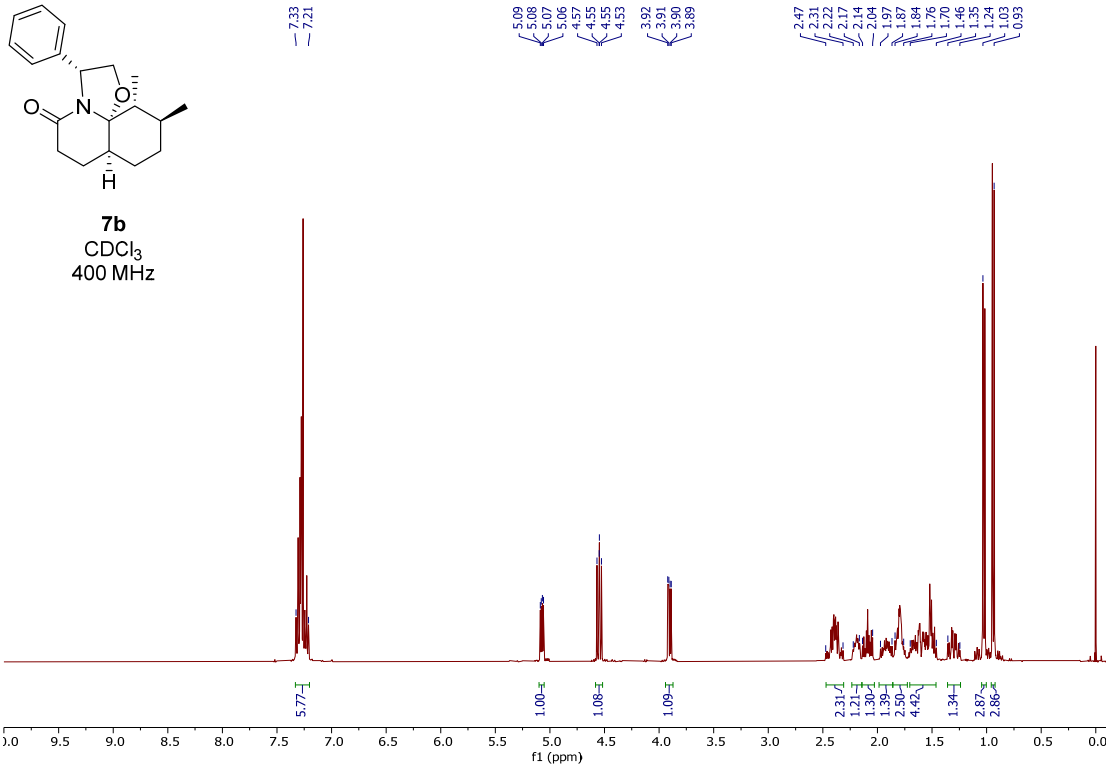
6
$CDCl_3$
100.6 MHz



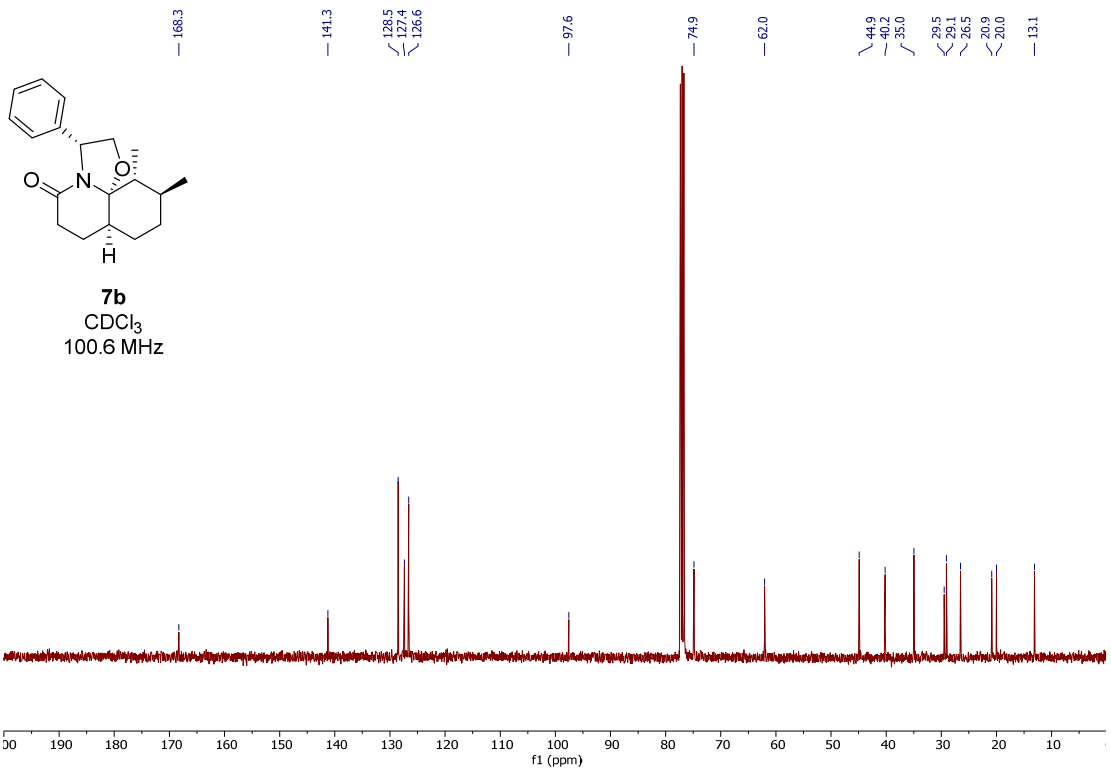
7a
$CDCl_3$
400 MHz



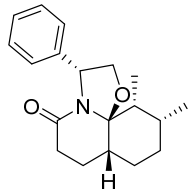
7a
$CDCl_3$
100.6 MHz



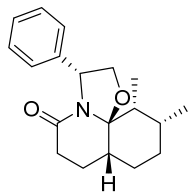
7b
$CDCl_3$
400 MHz



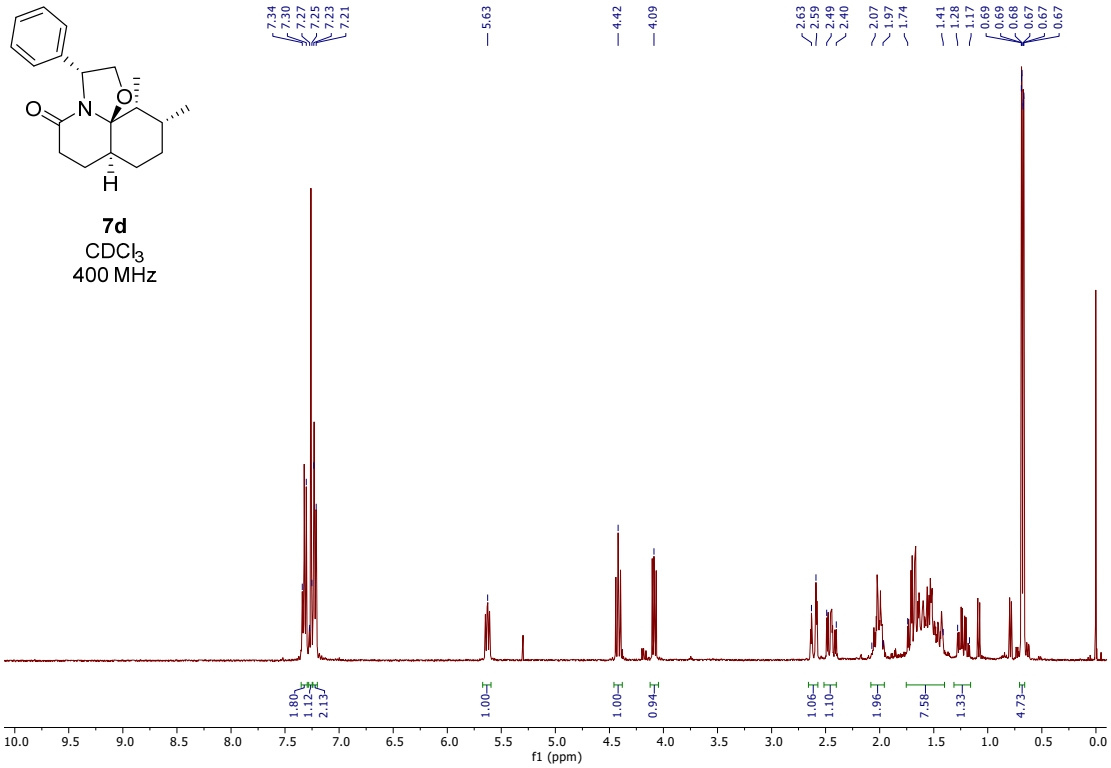
7b
$CDCl_3$
100.6 MHz

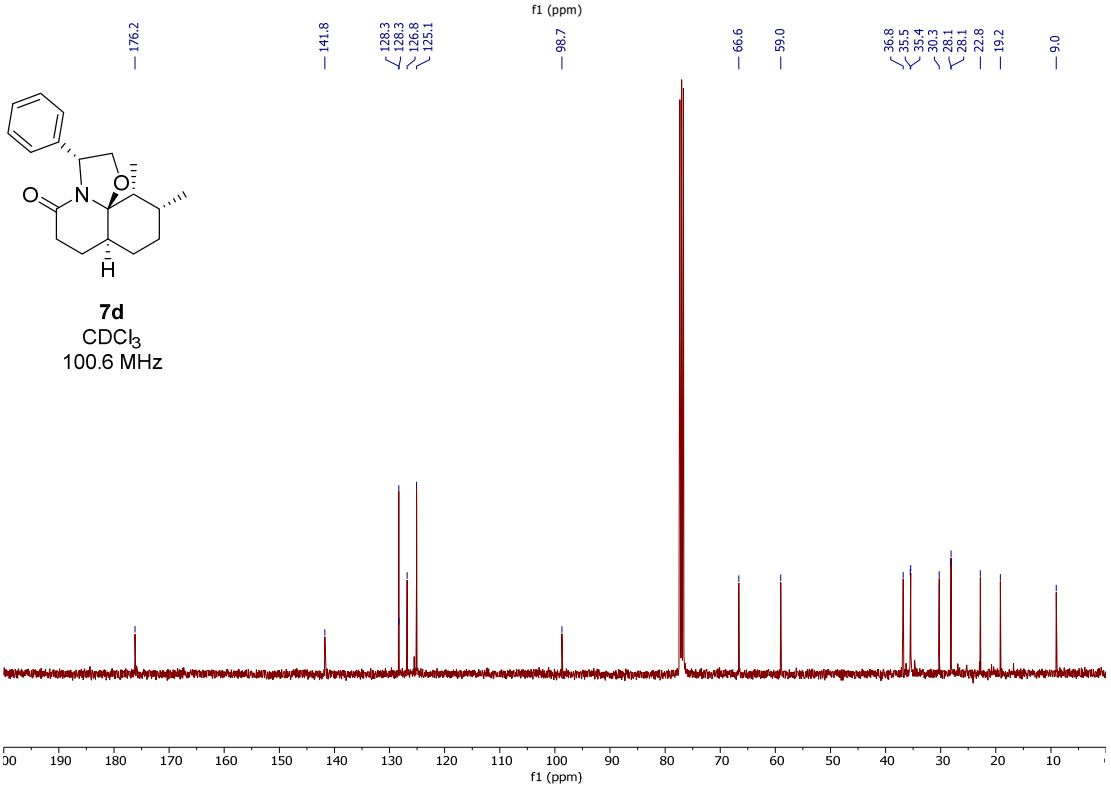


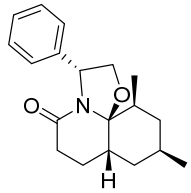
7c
$CDCl_3$
400 MHz



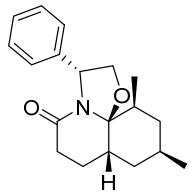
7c
$CDCl_3$
100.6 MHz


7d
CDCl3
400 MHz
f1 (ppm)

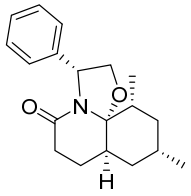

7d
CDCl3
100.6 MHz
f1 (ppm)



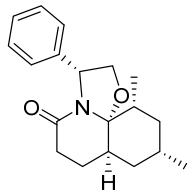
8a
$CDCl_3$
400 MHz



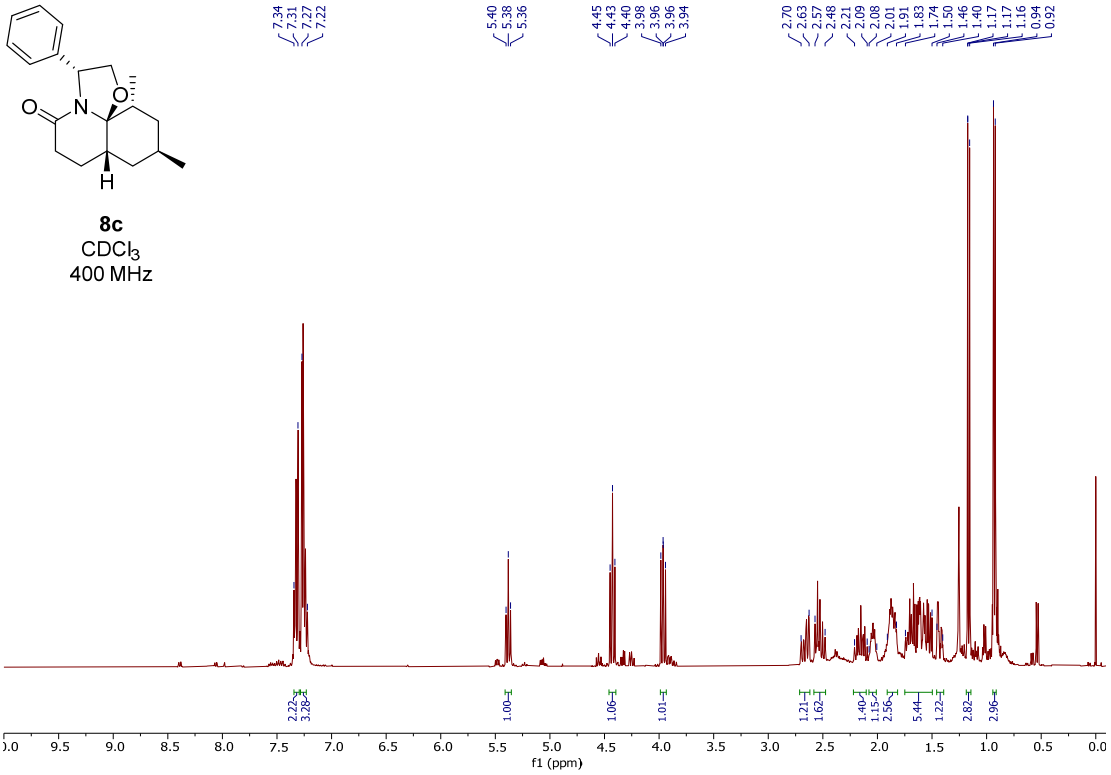
8a
$CDCl_3$
100.6 MHz



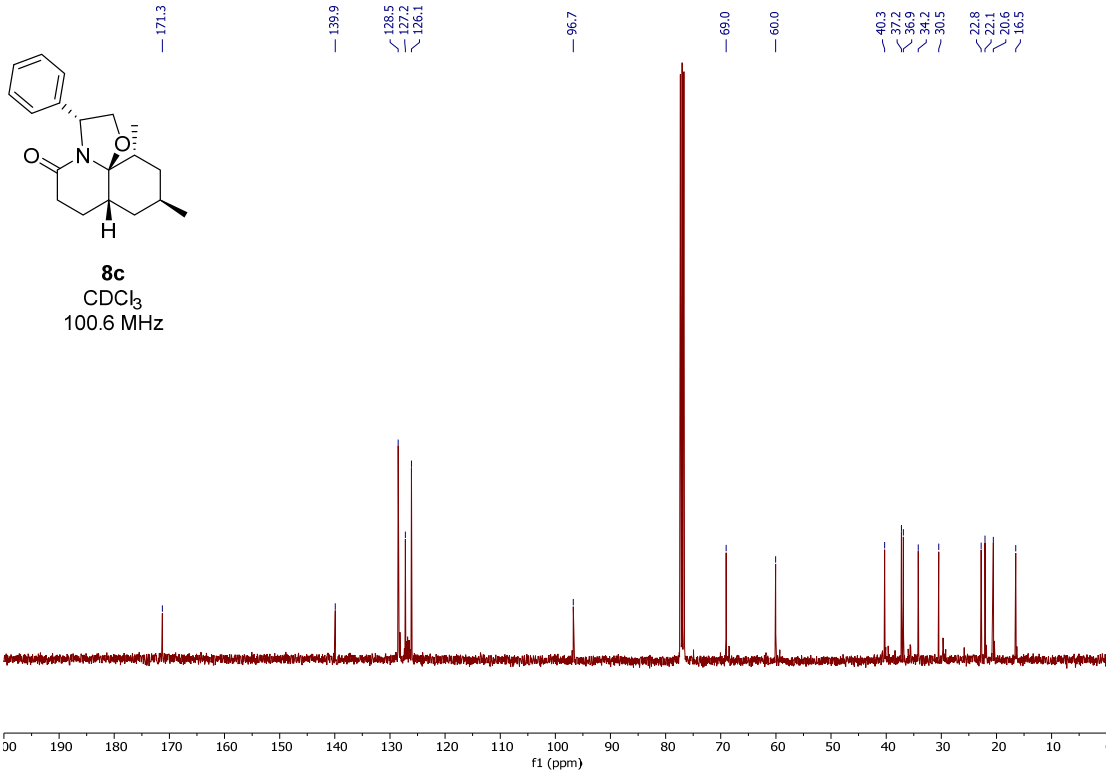
8b
$CDCl_3$
400 MHz



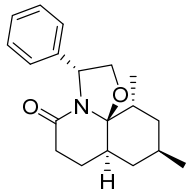
8b
$CDCl_3$
100.6 MHz



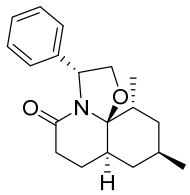
8c
$CDCl_3$
400 MHz



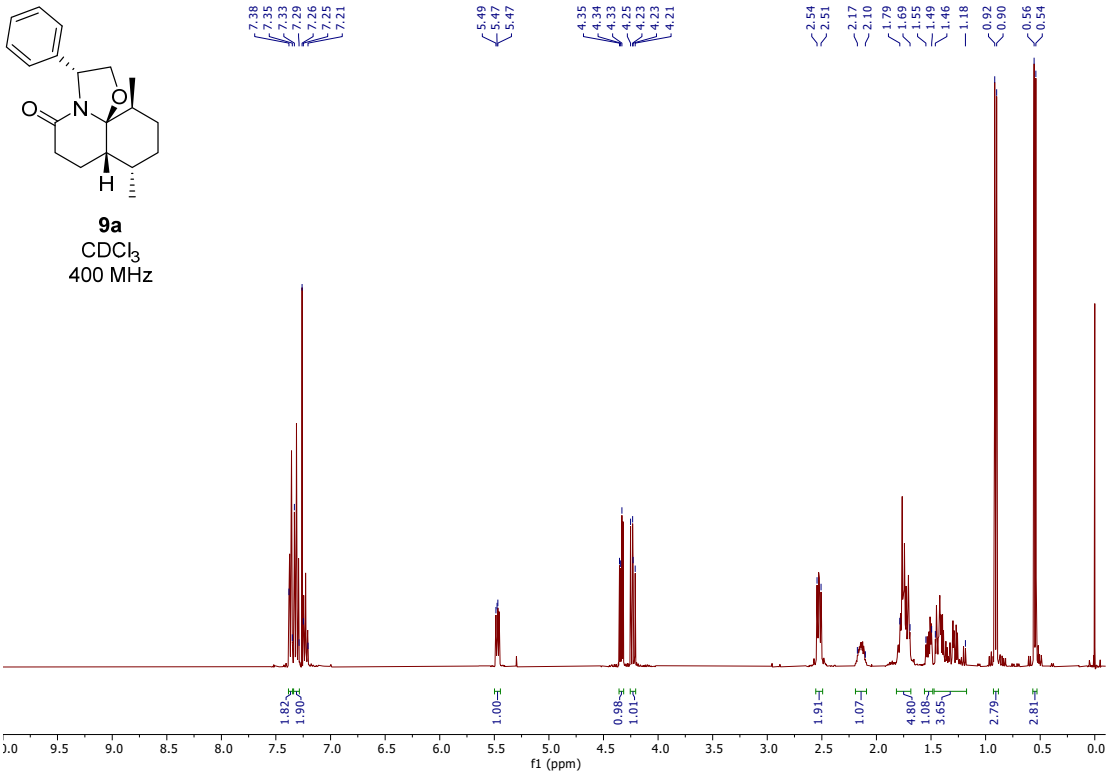
8c
$CDCl_3$
100.6 MHz

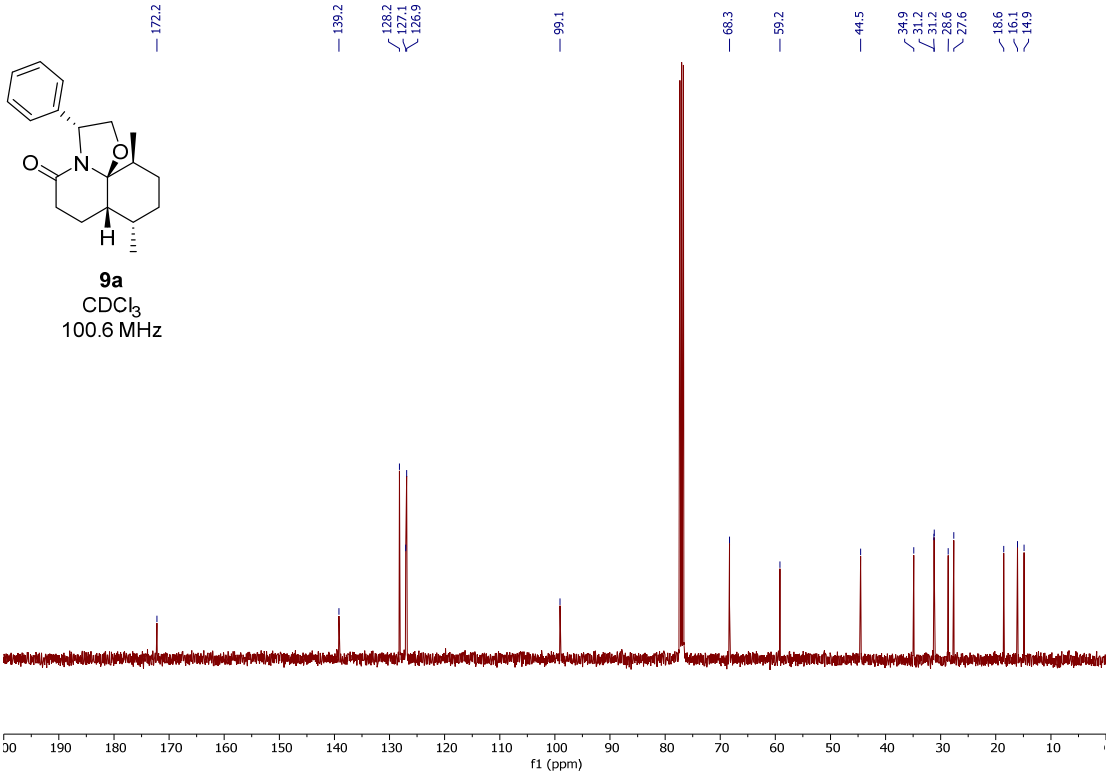


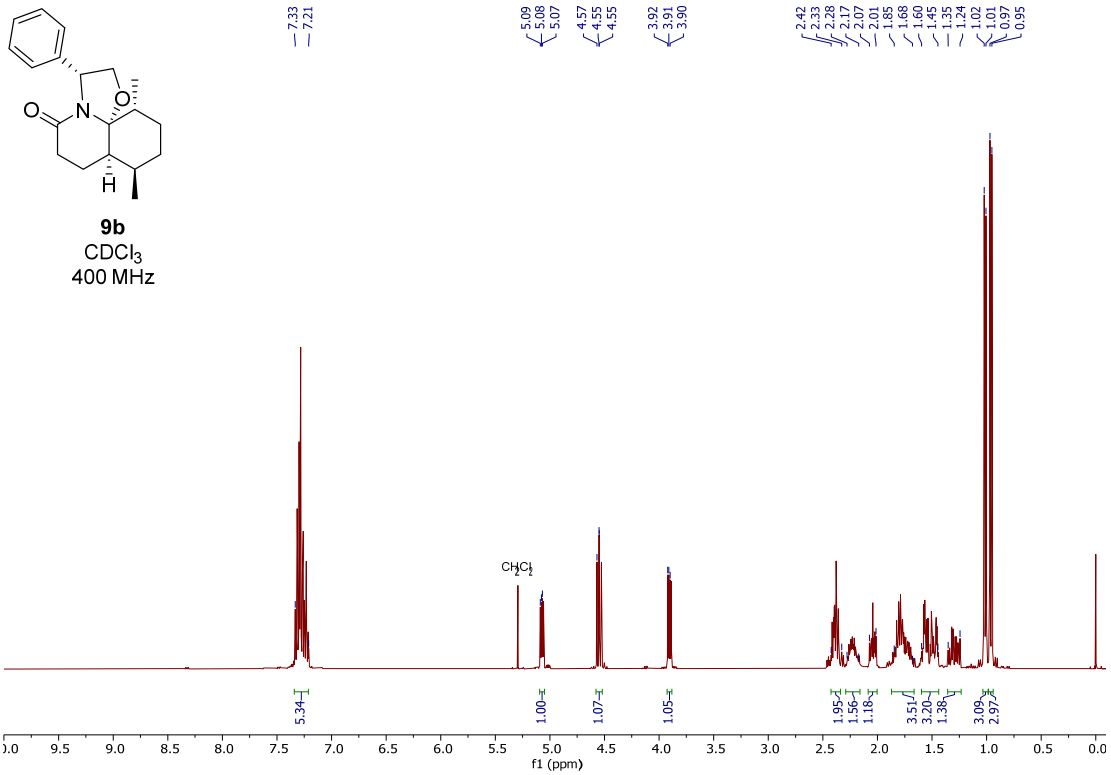
8d
$CDCl_3$
400 MHz



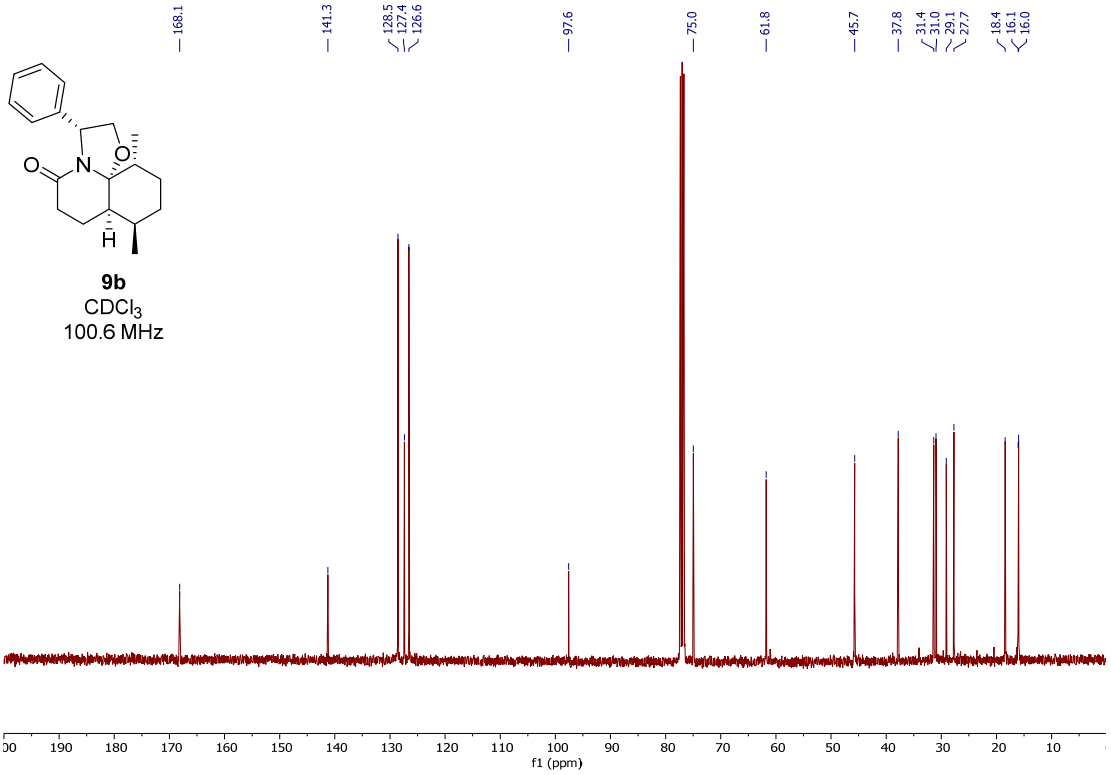
8d
$CDCl_3$
100.6 MHz


9a
CDCl3
400 MHz
f1 (ppm)

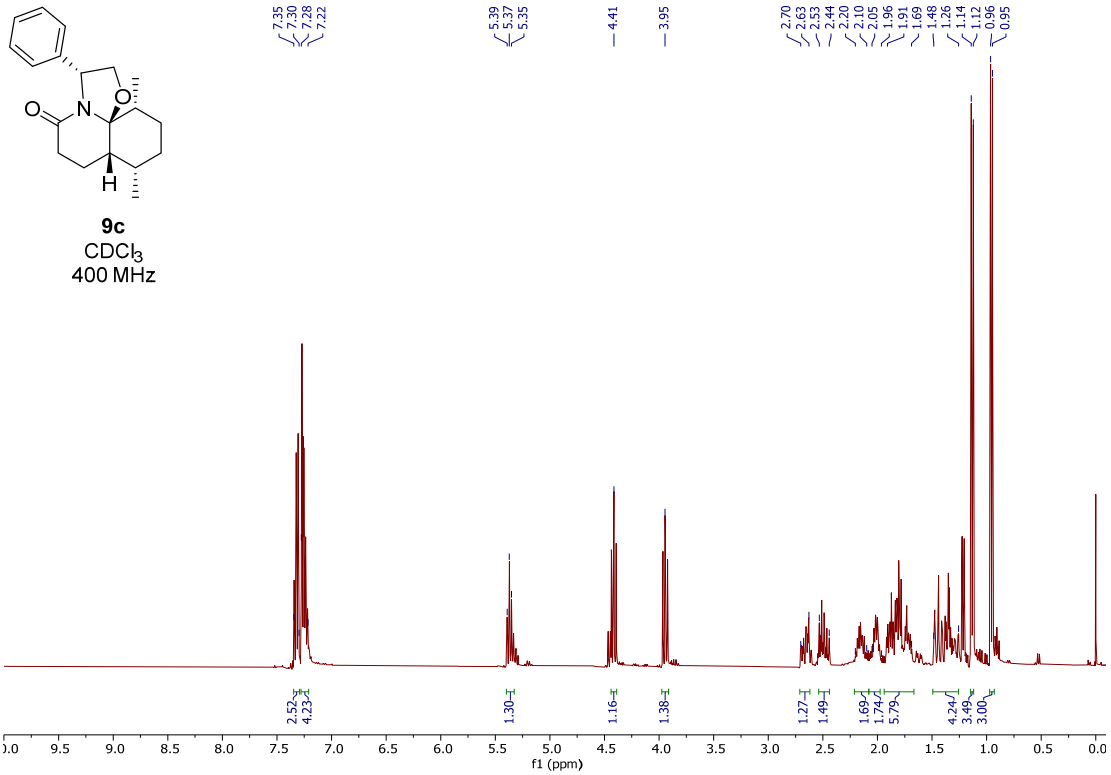

9a
CDCl3
100.6 MHz
f1 (ppm)



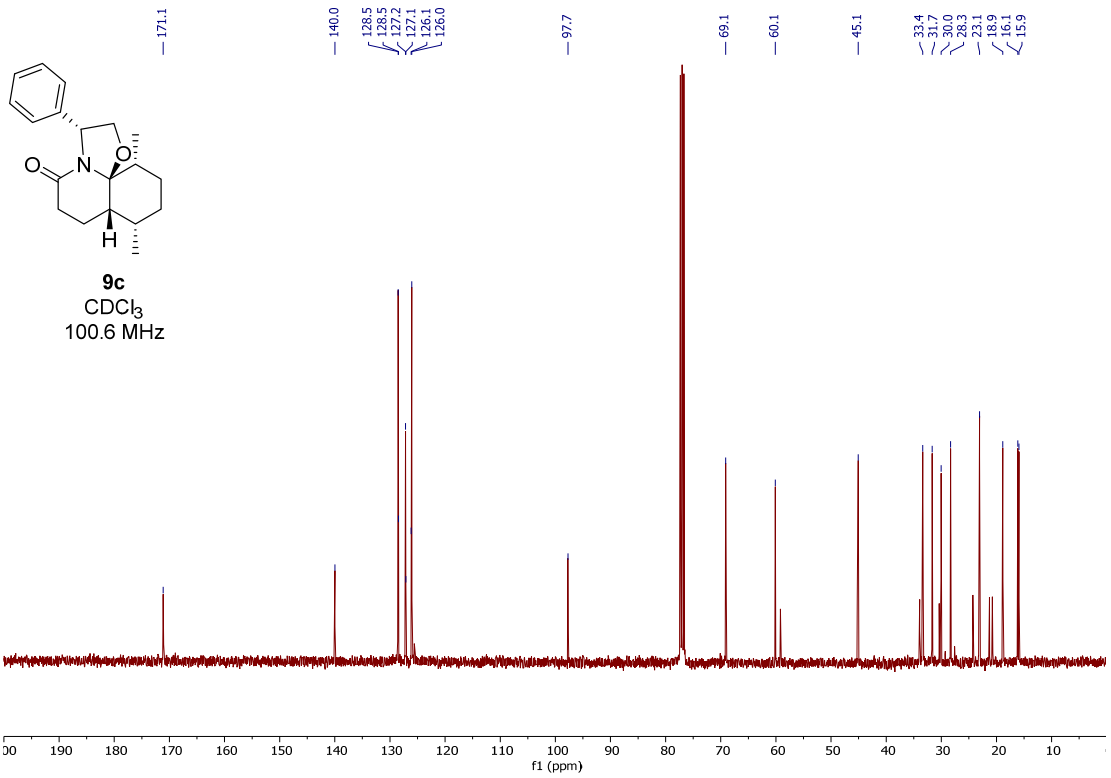
9b
$CDCl_3$
400 MHz



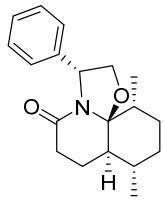
9b
$CDCl_3$
100.6 MHz



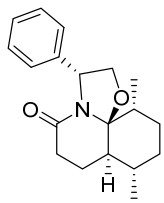
9c
$CDCl_3$
400 MHz



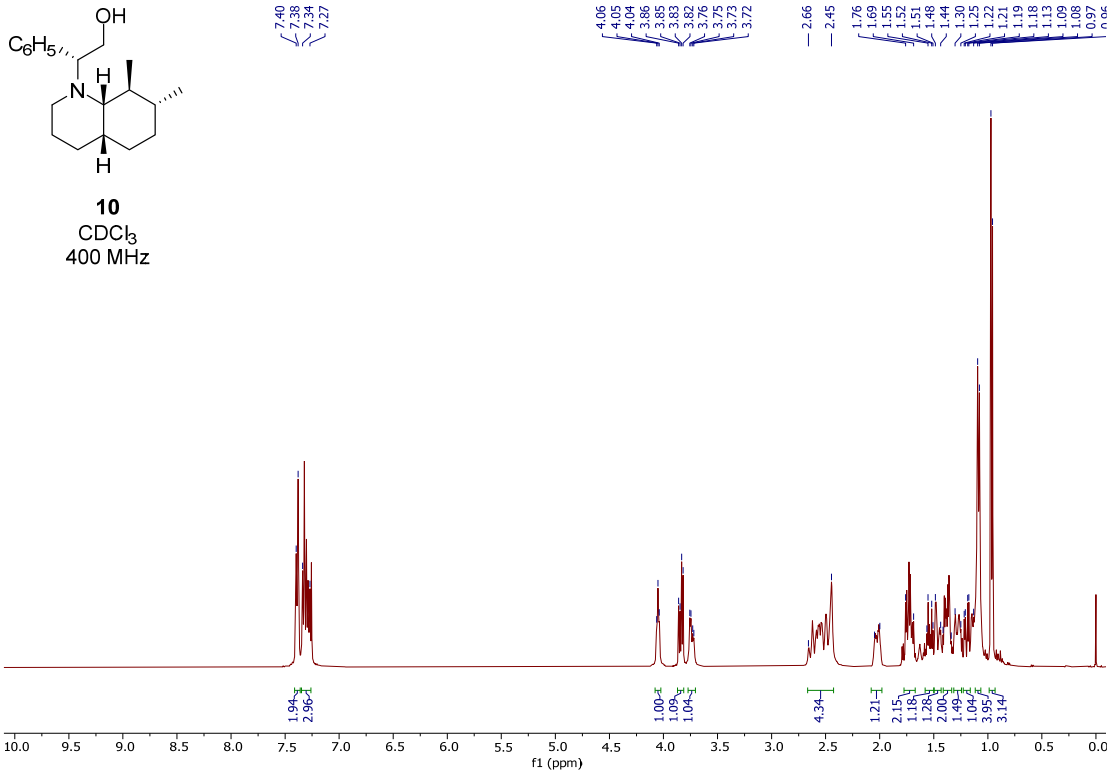
9c
$CDCl_3$
100.6 MHz

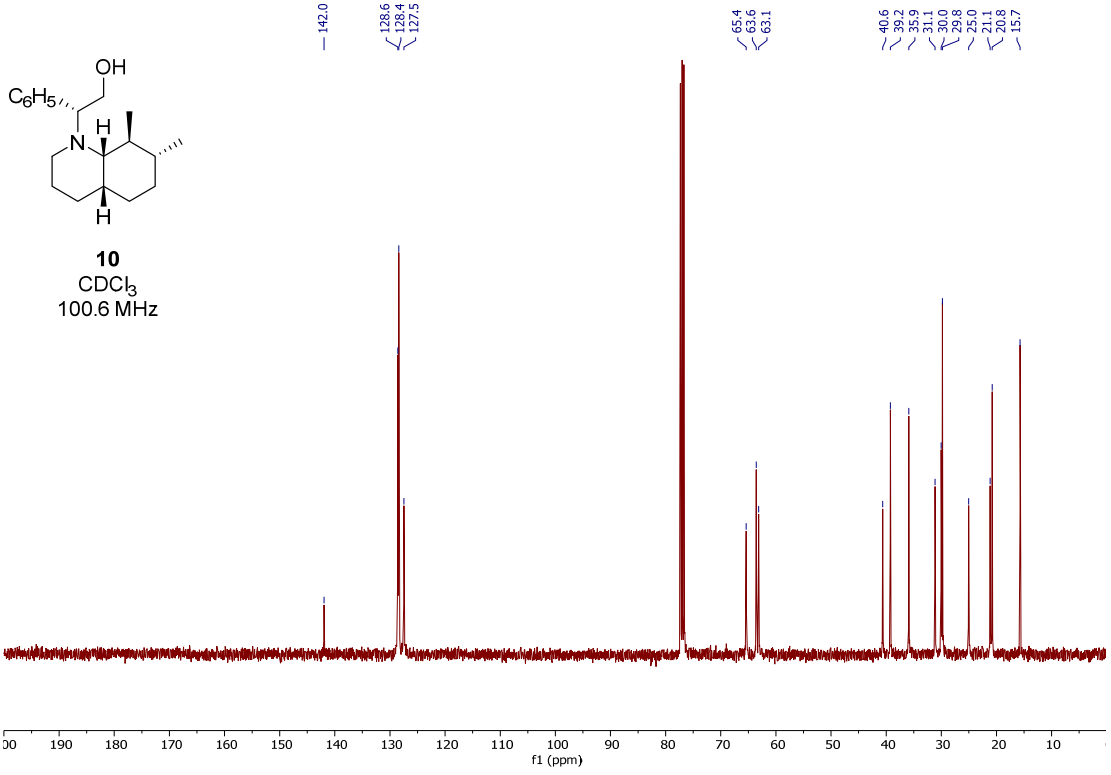


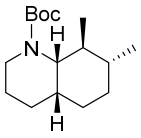
9d
$CDCl_3$
400 MHz



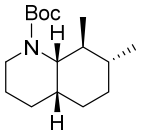
9d
$CDCl_3$
100.6 MHz


OH
C6H5
H
N
H
10
CDCl3
400 MHz
7.40
7.38
7.34
7.27
4.06
4.05
4.04
3.86
3.85
3.83
3.82
3.76
3.75
3.73
3.72
2.66
2.45
1.76
1.69
1.55
1.52
1.51
1.48
1.44
1.30
1.25
1.22
1.21
1.19
1.18
1.13
1.09
1.08
0.97
1.94
2.96
1.00
1.09
1.04
4.34
1.21
2.15
1.18
1.28
2.00
1.49
1.04
3.95
3.14
f1 (ppm)

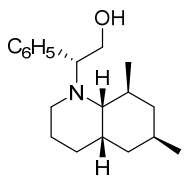

OH
C6H5
H
N
H
10
CDCl3
100.6 MHz
142.0
128.6
128.4
127.5
65.4
63.6
63.1
40.6
39.2
35.9
31.1
30.0
29.8
25.0
21.1
20.8
15.7
f1 (ppm)



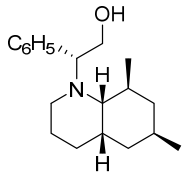
11
$CDCl_3$
400 MHz



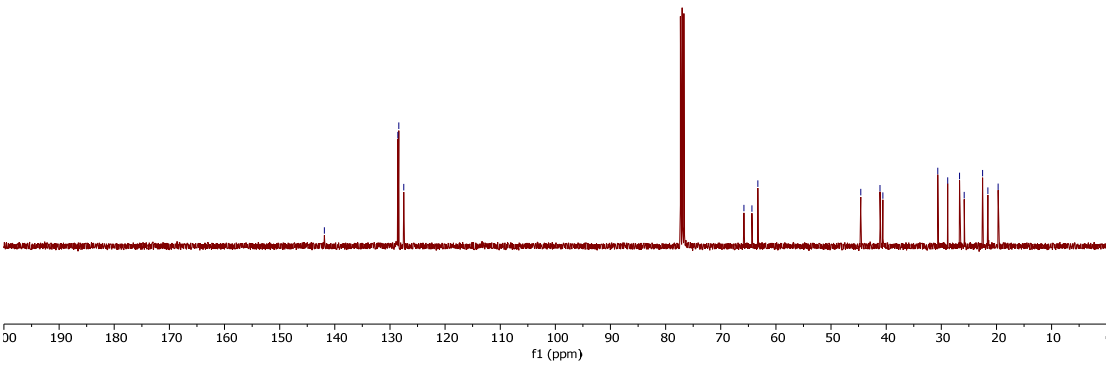
11
$CDCl_3$
100.6 MHz

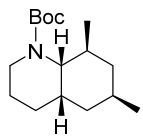


12
$CDCl_3$
400 MHz

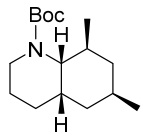


12
$CDCl_3$
100.6 MHz

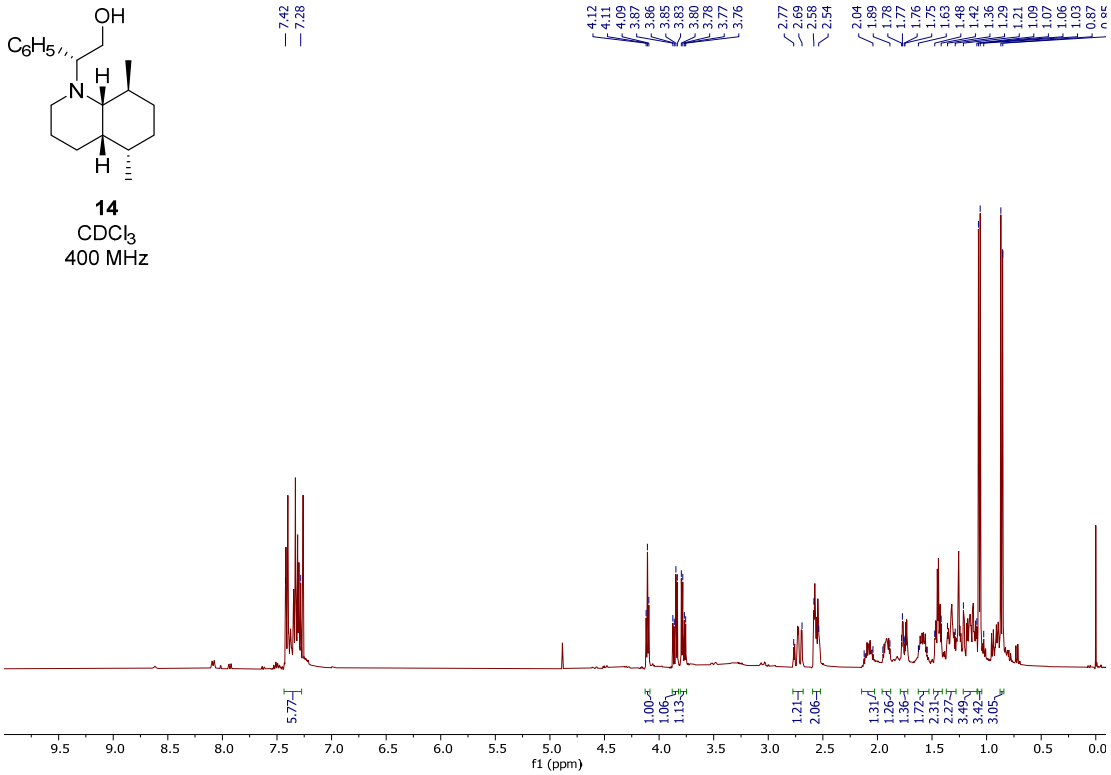


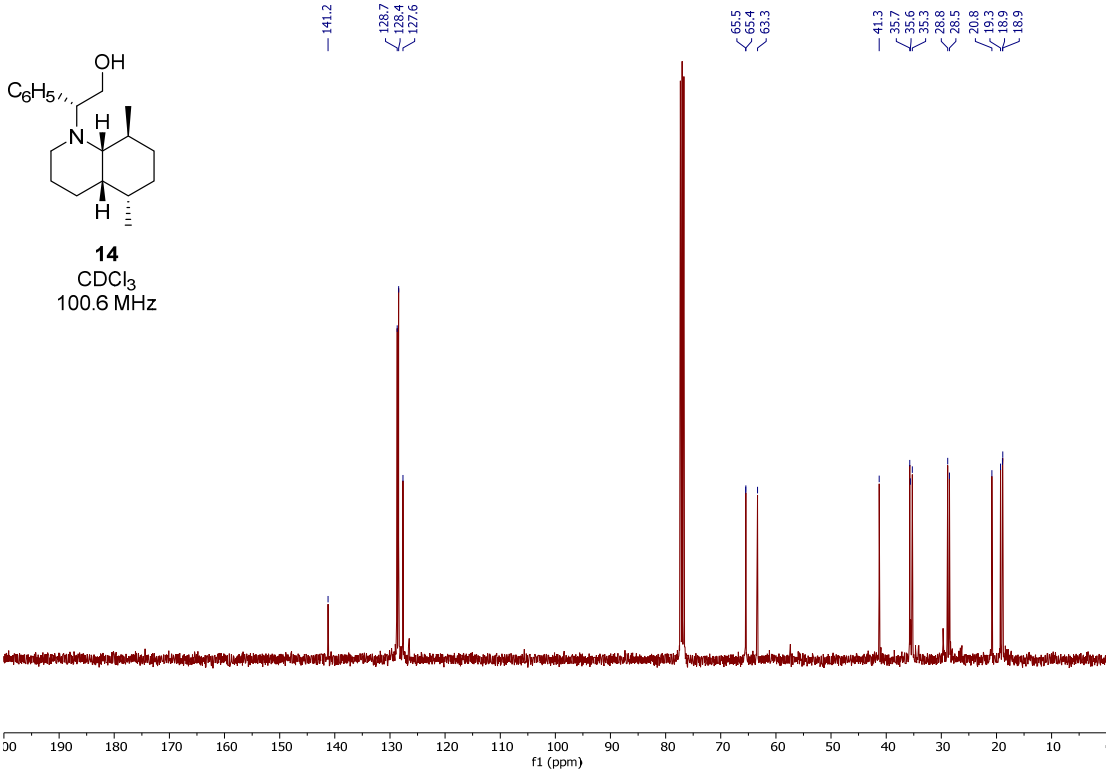


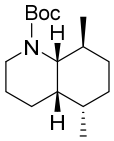
13
$CDCl_3$
400 MHz



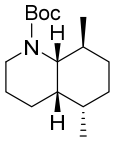
13
$CDCl_3$
100.6 MHz


OH
C6H5
N
H
H
14
CDCl3
400 MHz
f1 (ppm)

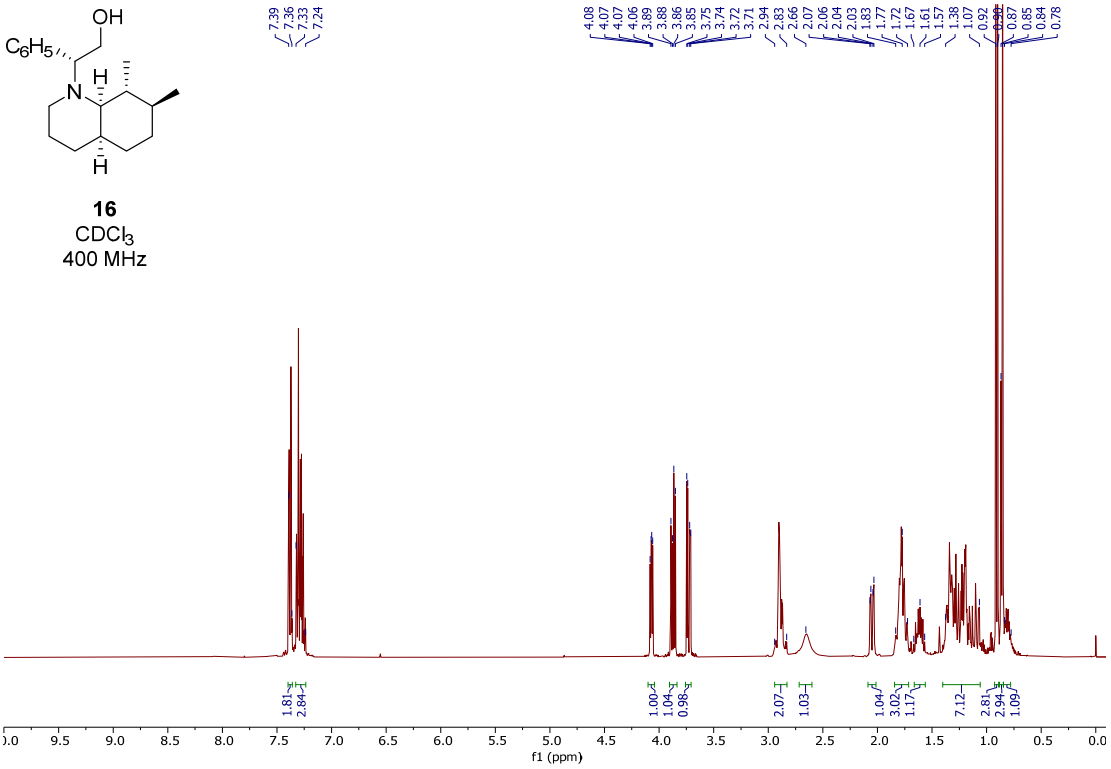

OH
C6H5
N
H
H
14
CDCl3
100.6 MHz
f1 (ppm)

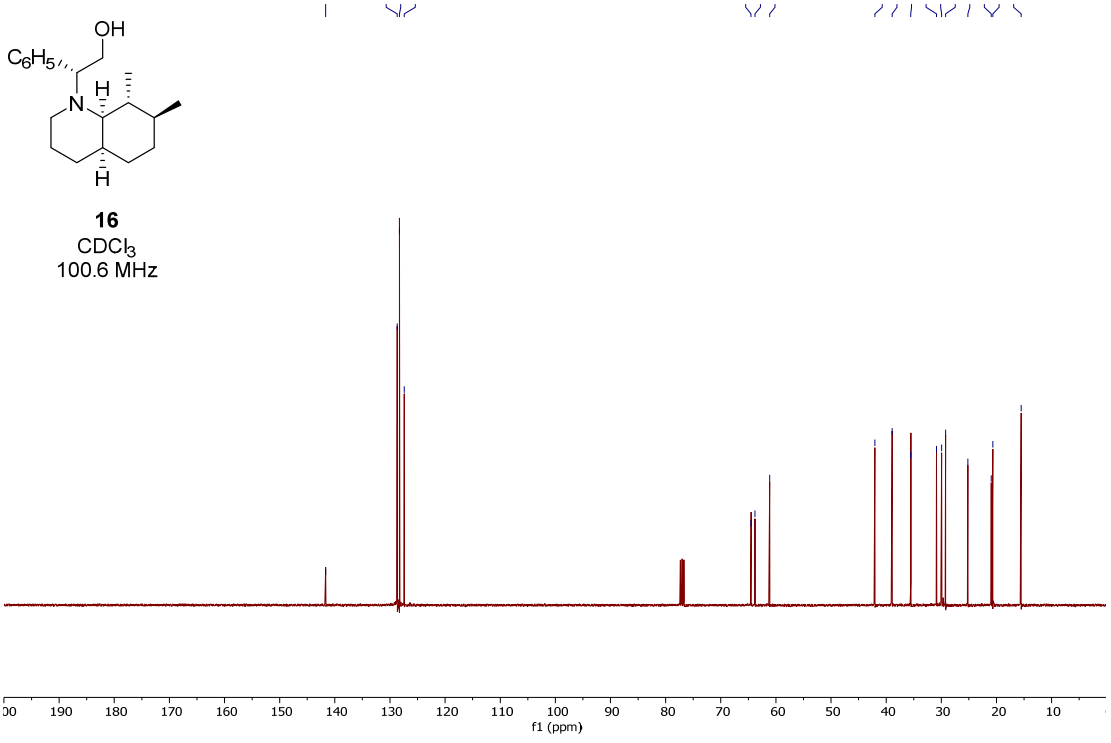


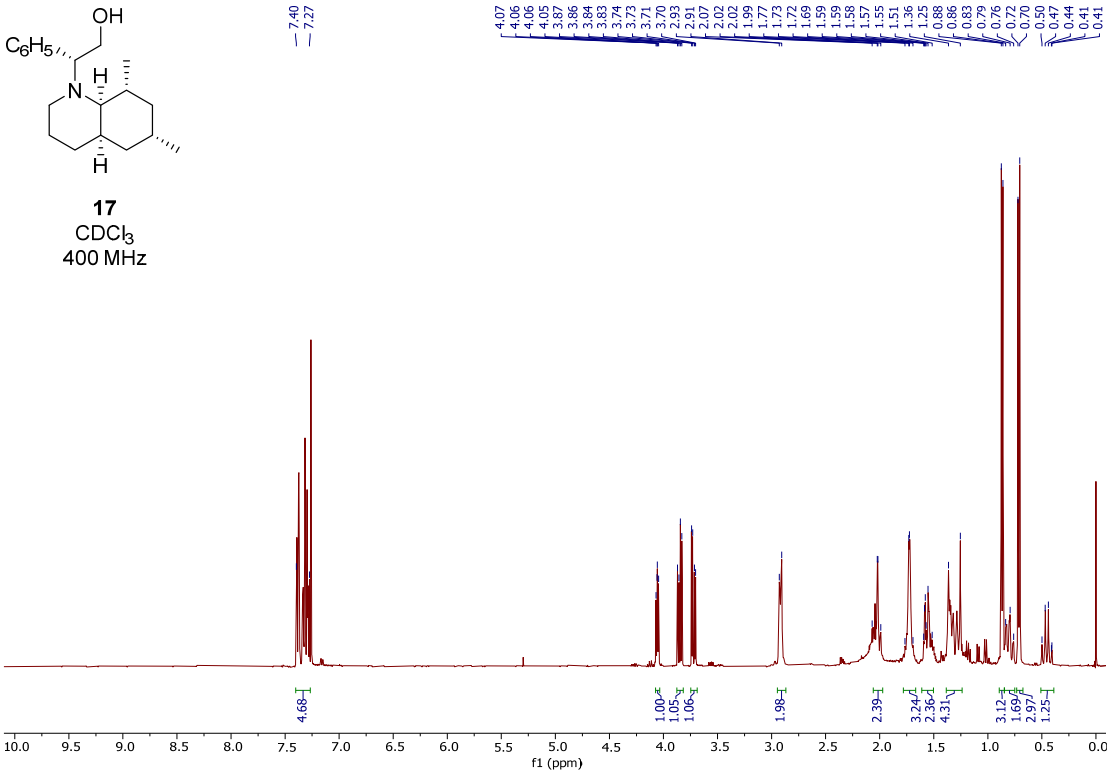
15
$CDCl_3$
400 MHz

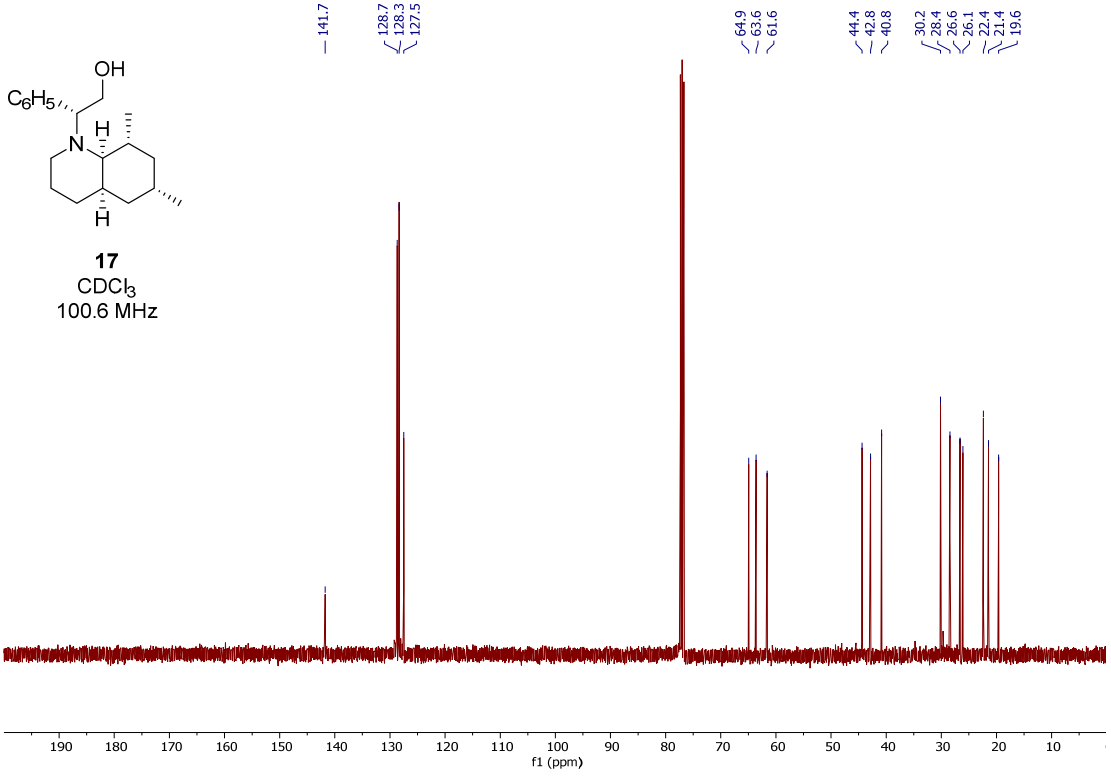


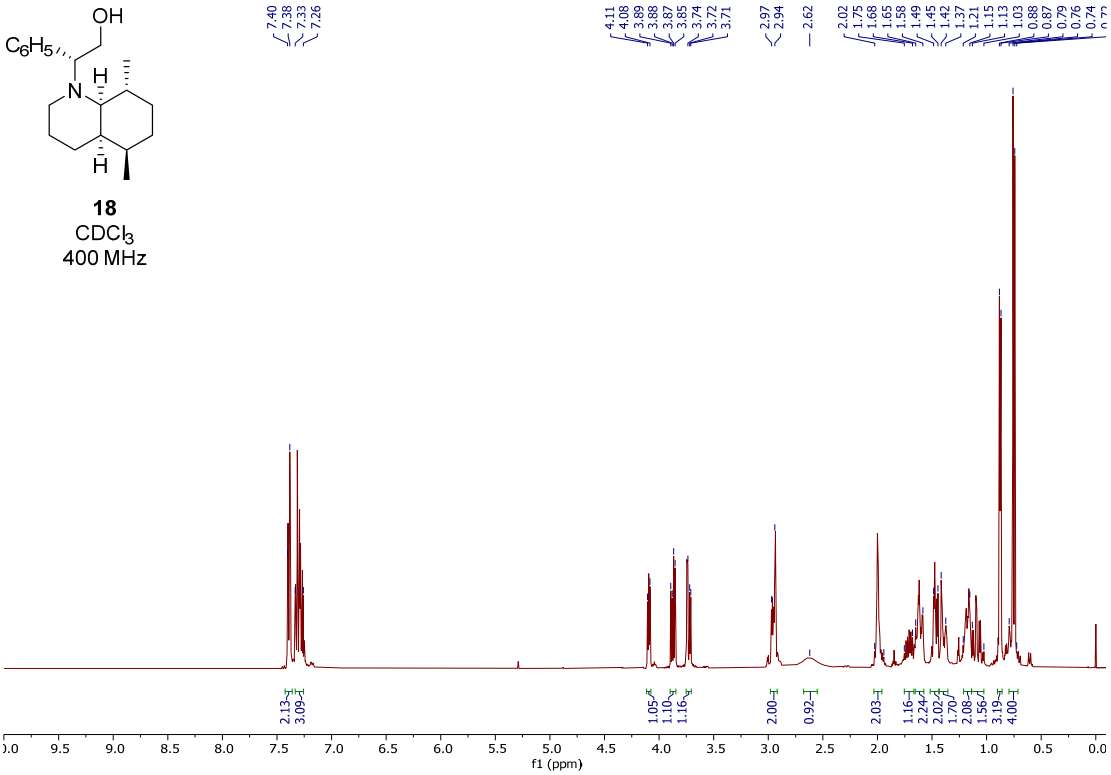
15
$CDCl_3$
100.6 MHz

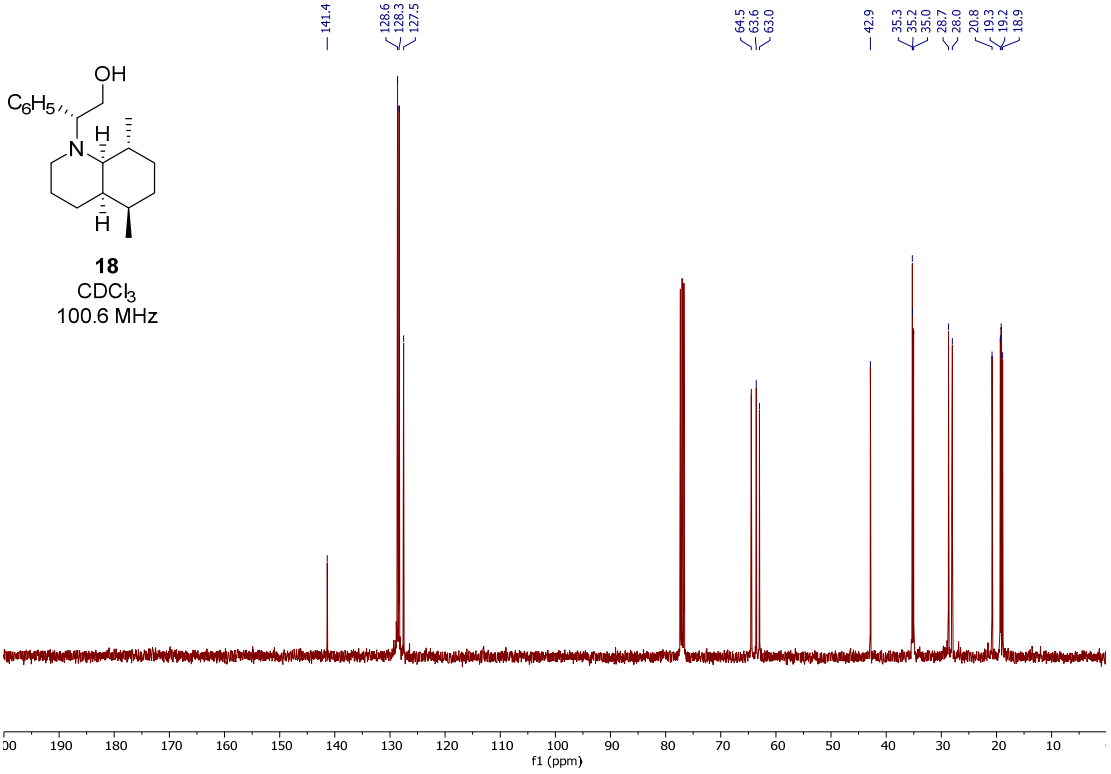

OH
C6H5
H
N
H
16
CDCl3
400 MHz
f1 (ppm)


OH
C6H5
H
N
H
16
CDCl3
100.6 MHz
f1 (ppm)


OH
C6H5
N
H
H
17
CDCl3
400 MHz
7.40
7.27
4.07
4.06
4.06
4.05
3.87
3.86
3.84
3.83
3.74
3.73
3.71
3.70
2.93
2.91
2.07
2.02
2.02
1.99
1.77
1.73
1.72
1.69
1.59
1.59
1.59
1.58
1.57
1.55
1.51
1.36
1.25
0.88
0.86
0.83
0.79
0.76
0.72
0.70
0.50
0.47
0.44
0.41
0.41
4.68
1.00
1.05
1.06
1.98
2.39
3.24
2.36
4.31
3.12
1.69
2.97
1.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

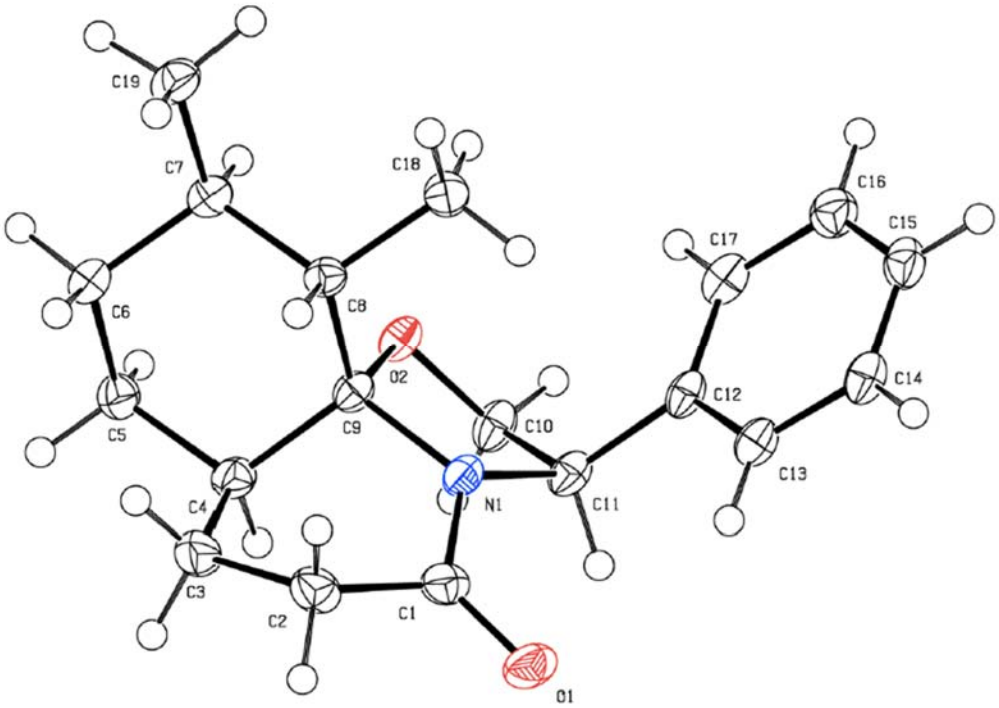

OH
C6H5
N
H
H
17
CDCl3
100.6 MHz
141.7
128.7
128.3
127.5
64.9
63.6
61.6
44.4
42.8
40.8
30.2
28.4
26.6
26.1
22.4
21.4
19.6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

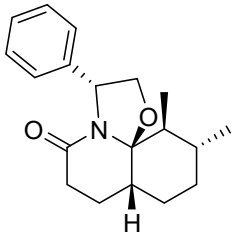

OH
C6H5
N
H
H
18
CDCl3
400 MHz
f1 (ppm)


OH
C6H5
N
H
H
18
CDCl3
100.6 MHz
f1 (ppm)

IV) X- ray crystallographic data for compounds 7a,7b, 7d, 8a, 8b, 8d, 9a, 9b, 9c, and 9d

Crystallographic data for compound **7a**:





7a

Table 1. Crystal data and structure refinement for **7a** (D59ZB41_0m_a).

Identification code	D59ZB41_0m_a	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.1771(3) Å	α= 90°.
	b = 6.3005(2) Å	β= 111.8700(10)°.
	c = 13.2560(3) Å	γ = 90°.
Volume	788.81(4) $Å^3$	
Z	2	
Density (calculated)	1.261 Mg/m^3	
Absorption coefficient	0.635 mm^{-1}	
F(000)	324	
Crystal size	0.200 x 0.020 x 0.020 mm^3	
Theta range for data collection	3.593 to 71.948°.	
Index ranges	-12<=h<=12, -7<=k<=7, -16<=l<=16	
Reflections collected	13380	
Independent reflections	3061 [R(int) = 0.0366]	
Completeness to theta = 67.679°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.5838	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3061 / 1 / 202	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0293, wR2 = 0.0699	
R indices (all data)	R1 = 0.0317, wR2 = 0.0723	
Absolute structure parameter	0.0(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.156 and -0.181 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB41_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4486(2)	5241(3)	-109(1)	29(1)
O(2)	4738(1)	2503(2)	3066(1)	20(1)
N(1)	4754(2)	4527(2)	1638(1)	19(1)
C(1)	5264(2)	4997(3)	846(2)	23(1)
C(2)	6844(2)	5300(4)	1248(2)	27(1)
C(3)	7703(2)	3615(4)	2074(2)	28(1)
C(4)	6851(2)	2371(3)	2614(2)	21(1)
C(5)	7802(2)	1462(3)	3719(2)	22(1)
C(6)	8375(2)	3187(3)	4582(2)	23(1)
C(7)	7194(2)	4553(3)	4691(2)	21(1)
C(8)	6255(2)	5527(3)	3586(1)	18(1)
C(9)	5681(2)	3753(3)	2736(1)	18(1)
C(10)	3615(2)	1784(3)	2108(2)	23(1)
C(11)	3307(2)	3663(3)	1331(2)	22(1)
C(12)	2254(2)	5318(3)	1393(1)	20(1)
C(13)	1941(2)	6984(3)	644(2)	22(1)
C(14)	967(2)	8539(3)	622(2)	24(1)
C(15)	306(2)	8482(3)	1365(2)	25(1)
C(16)	627(2)	6850(4)	2128(2)	27(1)
C(17)	1589(2)	5274(4)	2135(2)	25(1)
C(18)	5065(2)	6898(3)	3675(2)	22(1)
C(19)	7816(2)	6254(4)	5561(2)	28(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB41_0m_a.

O(1)-C(1)	1.227(2)
O(2)-C(10)	1.430(2)
O(2)-C(9)	1.430(2)
N(1)-C(1)	1.366(2)
N(1)-C(11)	1.478(2)
N(1)-C(9)	1.491(2)
C(1)-C(2)	1.506(3)
C(2)-C(3)	1.542(3)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(4)	1.530(3)
C(3)-H(3A)	0.9900
C(3)-H(3AB)	0.9900
C(4)-C(9)	1.532(2)
C(4)-C(5)	1.534(3)
C(4)-H(4)	1.0000
C(5)-C(6)	1.528(3)
C(5)-H(5A)	0.9900
C(5)-H(5AB)	0.9900
C(6)-C(7)	1.528(3)
C(6)-H(6A)	0.9900
C(6)-H(6AB)	0.9900
C(7)-C(19)	1.528(3)
C(7)-C(8)	1.547(2)
C(7)-H(7)	1.0000
C(8)-C(18)	1.527(2)
C(8)-C(9)	1.540(2)
C(8)-H(8)	1.0000
C(10)-C(11)	1.523(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.519(3)
C(11)-H(11)	1.0000
C(12)-C(17)	1.387(3)

C(12)-C(13)	1.397(3)
C(13)-C(14)	1.386(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.385(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.393(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.392(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(10)-O(2)-C(9)	107.89(13)
C(1)-N(1)-C(11)	119.51(15)
C(1)-N(1)-C(9)	122.58(15)
C(11)-N(1)-C(9)	110.58(14)
O(1)-C(1)-N(1)	122.47(18)
O(1)-C(1)-C(2)	122.83(17)
N(1)-C(1)-C(2)	114.63(16)
C(1)-C(2)-C(3)	114.34(18)
C(1)-C(2)-H(2A)	108.7
C(3)-C(2)-H(2A)	108.7
C(1)-C(2)-H(2AB)	108.7
C(3)-C(2)-H(2AB)	108.7
H(2A)-C(2)-H(2AB)	107.6
C(4)-C(3)-C(2)	114.49(16)
C(4)-C(3)-H(3A)	108.6
C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3AB)	108.6
C(2)-C(3)-H(3AB)	108.6
H(3A)-C(3)-H(3AB)	107.6

C(3)-C(4)-C(9)	110.92(16)
C(3)-C(4)-C(5)	111.82(16)
C(9)-C(4)-C(5)	110.47(14)
C(3)-C(4)-H(4)	107.8
C(9)-C(4)-H(4)	107.8
C(5)-C(4)-H(4)	107.8
C(6)-C(5)-C(4)	112.25(16)
C(6)-C(5)-H(5A)	109.2
C(4)-C(5)-H(5A)	109.2
C(6)-C(5)-H(5AB)	109.2
C(4)-C(5)-H(5AB)	109.2
H(5A)-C(5)-H(5AB)	107.9
C(5)-C(6)-C(7)	112.16(15)
C(5)-C(6)-H(6A)	109.2
C(7)-C(6)-H(6A)	109.2
C(5)-C(6)-H(6AB)	109.2
C(7)-C(6)-H(6AB)	109.2
H(6A)-C(6)-H(6AB)	107.9
C(6)-C(7)-C(19)	110.31(15)
C(6)-C(7)-C(8)	111.37(15)
C(19)-C(7)-C(8)	111.87(16)
C(6)-C(7)-H(7)	107.7
C(19)-C(7)-H(7)	107.7
C(8)-C(7)-H(7)	107.7
C(18)-C(8)-C(9)	111.81(14)
C(18)-C(8)-C(7)	112.30(14)
C(9)-C(8)-C(7)	109.69(15)
C(18)-C(8)-H(8)	107.6
C(9)-C(8)-H(8)	107.6
C(7)-C(8)-H(8)	107.6
O(2)-C(9)-N(1)	103.10(13)
O(2)-C(9)-C(4)	110.87(15)
N(1)-C(9)-C(4)	108.44(14)
O(2)-C(9)-C(8)	106.89(13)
N(1)-C(9)-C(8)	113.99(15)
C(4)-C(9)-C(8)	113.10(14)

O(2)-C(10)-C(11)	104.46(15)
O(2)-C(10)-H(10A)	110.9
C(11)-C(10)-H(10A)	110.9
O(2)-C(10)-H(10B)	110.9
C(11)-C(10)-H(10B)	110.9
H(10A)-C(10)-H(10B)	108.9
N(1)-C(11)-C(12)	112.50(16)
N(1)-C(11)-C(10)	99.61(14)
C(12)-C(11)-C(10)	117.97(16)
N(1)-C(11)-H(11)	108.7
C(12)-C(11)-H(11)	108.7
C(10)-C(11)-H(11)	108.7
C(17)-C(12)-C(13)	118.44(18)
C(17)-C(12)-C(11)	124.40(18)
C(13)-C(12)-C(11)	117.16(16)
C(14)-C(13)-C(12)	121.23(17)
C(14)-C(13)-H(13)	119.4
C(12)-C(13)-H(13)	119.4
C(15)-C(14)-C(13)	119.93(19)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	119.43(19)
C(14)-C(15)-H(15)	120.3
C(16)-C(15)-H(15)	120.3
C(17)-C(16)-C(15)	120.36(18)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(12)-C(17)-C(16)	120.59(19)
C(12)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(8)-C(18)-H(18A)	109.5
C(8)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(8)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

C(7)-C(19)-H(19A)	109.5
C(7)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(7)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB41_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

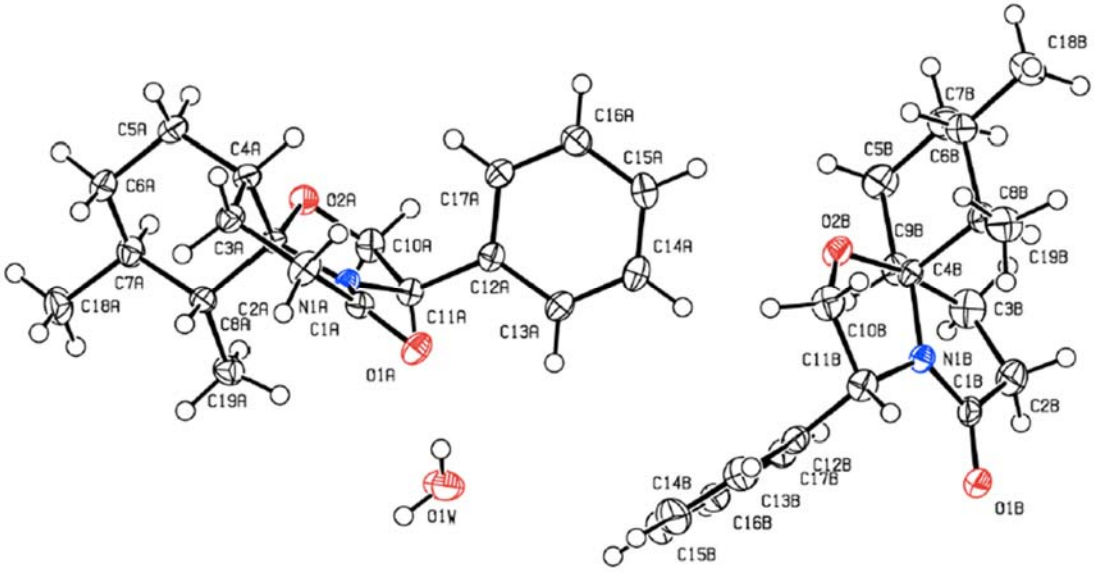
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	40(1)	29(1)	18(1)	4(1)	8(1)	7(1)
O(2)	20(1)	20(1)	17(1)	1(1)	2(1)	-4(1)
N(1)	20(1)	20(1)	15(1)	0(1)	3(1)	1(1)
C(1)	32(1)	19(1)	21(1)	2(1)	11(1)	5(1)
C(2)	31(1)	28(1)	27(1)	5(1)	16(1)	5(1)
C(3)	27(1)	37(1)	22(1)	6(1)	12(1)	9(1)
C(4)	24(1)	19(1)	18(1)	-2(1)	5(1)	3(1)
C(5)	22(1)	21(1)	23(1)	1(1)	7(1)	4(1)
C(6)	21(1)	27(1)	18(1)	0(1)	3(1)	1(1)
C(7)	21(1)	22(1)	18(1)	0(1)	6(1)	-1(1)
C(8)	19(1)	18(1)	18(1)	-2(1)	6(1)	-2(1)
C(9)	20(1)	16(1)	16(1)	2(1)	5(1)	-1(1)
C(10)	22(1)	18(1)	23(1)	1(1)	1(1)	-3(1)
C(11)	22(1)	21(1)	18(1)	-2(1)	2(1)	-3(1)
C(12)	17(1)	18(1)	19(1)	-1(1)	-1(1)	-4(1)
C(13)	20(1)	23(1)	20(1)	0(1)	3(1)	-4(1)
C(14)	20(1)	21(1)	24(1)	2(1)	1(1)	-2(1)
C(15)	19(1)	25(1)	27(1)	-3(1)	3(1)	0(1)
C(16)	23(1)	32(1)	24(1)	0(1)	8(1)	-3(1)
C(17)	24(1)	26(1)	21(1)	3(1)	3(1)	-4(1)
C(18)	22(1)	21(1)	24(1)	-2(1)	7(1)	-1(1)
C(19)	29(1)	31(1)	20(1)	-5(1)	3(1)	1(1)

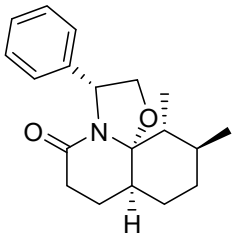
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59ZB41_0m_a.

	x	y	z	U(eq)
H(2A)	7079	6719	1589	32
H(2AB)	7140	5277	616	32
H(3A)	8109	2600	1698	34
H(3AB)	8502	4327	2648	34
H(4)	6388	1152	2128	26
H(5A)	7253	425	3964	27
H(5AB)	8606	699	3635	27
H(6A)	9035	4106	4388	28
H(6AB)	8914	2514	5291	28
H(7)	6581	3609	4937	25
H(8)	6870	6464	3340	22
H(10A)	2769	1406	2268	28
H(10B)	3914	530	1796	28
H(11)	2988	3114	569	26
H(13)	2405	7053	142	27
H(14)	752	9642	96	28
H(15)	-359	9546	1356	30
H(16)	186	6812	2646	32
H(17)	1791	4158	2653	30
H(18A)	4424	7320	2947	33
H(18B)	5470	8168	4106	33
H(18C)	4538	6085	4031	33
H(19A)	8350	7283	5310	43
H(19B)	8450	5586	6234	43
H(19C)	7048	6983	5698	43

- C4 - C3 C5 C9 H4 sp3 R
- C7 - C6 C8 C19 H7 sp3 R
- C8 - C7 C9 C18 H8 sp3 S
- C9 - O2 N1 C4 C8 sp3 R
- C11 - N1 C10 C12 H11 sp3 R

Crystallographic data for compound **7b**:





7b

Table 1. Crystal data and structure refinement for **7b** (D59ZB7_0m_a).

Identification code	D59ZB7_0m_a	
Empirical formula	C76 H102 N4 O9	
Formula weight	1215.61	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2	
Unit cell dimensions	a = 28.4604(11) Å	α= 90°.
	b = 8.5623(3) Å	β= 92.7390(10)°.
	c = 13.3639(5) Å	γ = 90°.
Volume	3252.9(2) $Å^3$	
Z	2	
Density (calculated)	1.241 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	1316	
Crystal size	0.600 x 0.390 x 0.300 mm^3	
Theta range for data collection	2.042 to 30.578°.	
Index ranges	-40<=h<=40, -12<=k<=12, -19<=l<=19	
Reflections collected	27198	
Independent reflections	9714 [R(int) = 0.0333]	
Completeness to theta = 25.242°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6337	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9714 / 3 / 409	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0408, wR2 = 0.0914	
R indices (all data)	R1 = 0.0476, wR2 = 0.0989	
Absolute structure parameter	0.5(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.290 and -0.219 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB7_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	5465(1)	960(2)	6455(1)	25(1)
O(2A)	4365(1)	1777(2)	8710(1)	23(1)
N(1A)	4860(1)	1184(2)	7485(1)	18(1)
C(1A)	5202(1)	363(2)	7052(1)	20(1)
C(2A)	5278(1)	-1310(2)	7389(2)	27(1)
C(3A)	4926(1)	-2028(2)	8084(1)	23(1)
C(4A)	4702(1)	-797(2)	8745(1)	21(1)
C(5A)	4330(1)	-1473(3)	9409(1)	28(1)
C(6A)	3888(1)	-1991(3)	8808(2)	29(1)
C(7A)	3685(1)	-713(2)	8111(1)	25(1)
C(8A)	4064(1)	-84(2)	7426(1)	20(1)
C(9A)	4490(1)	502(2)	8081(1)	18(1)
C(10A)	4446(1)	3218(2)	8199(2)	24(1)
C(11A)	4843(1)	2909(2)	7472(1)	19(1)
C(12A)	5304(1)	3651(2)	7826(1)	20(1)
C(13A)	5536(1)	4649(2)	7190(1)	22(1)
C(14A)	5940(1)	5444(2)	7534(2)	26(1)
C(15A)	6115(1)	5238(2)	8512(2)	27(1)
C(16A)	5894(1)	4212(3)	9143(2)	28(1)
C(17A)	5489(1)	3422(2)	8803(1)	25(1)
C(18A)	3251(1)	-1331(3)	7516(2)	35(1)
C(19A)	3869(1)	1118(2)	6667(1)	26(1)
O(1B)	7105(1)	10468(2)	4854(1)	31(1)
O(2B)	6942(1)	7628(2)	7643(1)	25(1)
N(1B)	7092(1)	9223(2)	6341(1)	19(1)
C(1B)	7060(1)	10522(2)	5761(1)	23(1)
C(2B)	6965(1)	12025(2)	6306(2)	34(1)
C(3B)	6678(1)	11892(3)	7252(2)	34(1)
C(4B)	6621(1)	10230(2)	7672(1)	24(1)
C(5B)	6540(1)	10212(3)	8795(2)	33(1)
C(6B)	6981(1)	10648(3)	9423(2)	36(1)

C(7B)	7406(1)	9657(3)	9170(2)	30(1)
C(8B)	7493(1)	9764(2)	8034(1)	24(1)
C(9B)	7044(1)	9225(2)	7435(1)	19(1)
C(10B)	7130(1)	6674(2)	6877(2)	29(1)
C(11B)	7070(1)	7651(2)	5916(1)	24(1)
C(12B)	6606(1)	7270(2)	5348(1)	24(1)
C(13B)	6582(1)	5834(2)	4847(2)	35(1)
C(14B)	6159(1)	5317(3)	4405(2)	44(1)
C(15B)	5759(1)	6236(3)	4435(2)	40(1)
C(16B)	5783(1)	7687(3)	4895(2)	31(1)
C(17B)	6206(1)	8197(2)	5352(1)	25(1)
C(18B)	7836(1)	10137(3)	9825(2)	41(1)
C(19B)	7939(1)	8894(3)	7761(2)	34(1)
O(1W)	5000	2973(3)	5000	40(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB7_0m_a.

O(1A)-C(1A)	1.231(2)
O(2A)-C(9A)	1.433(2)
O(2A)-C(10A)	1.434(2)
N(1A)-C(1A)	1.352(2)
N(1A)-C(9A)	1.471(2)
N(1A)-C(11A)	1.478(2)
C(1A)-C(2A)	1.515(3)
C(2A)-C(3A)	1.528(3)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
C(3A)-C(4A)	1.534(3)
C(3A)-H(3AA)	0.9900
C(3A)-H(3AB)	0.9900
C(4A)-C(5A)	1.528(3)
C(4A)-C(9A)	1.529(2)
C(4A)-H(4A)	1.0000
C(5A)-C(6A)	1.527(3)
C(5A)-H(5AA)	0.9900
C(5A)-H(5AB)	0.9900
C(6A)-C(7A)	1.531(3)
C(6A)-H(6AA)	0.9900
C(6A)-H(6AB)	0.9900
C(7A)-C(18A)	1.532(3)
C(7A)-C(8A)	1.544(3)
C(7A)-H(7A)	1.0000
C(8A)-C(19A)	1.530(3)
C(8A)-C(9A)	1.546(2)
C(8A)-H(8A)	1.0000
C(10A)-C(11A)	1.549(3)
C(10A)-H(10A)	0.9900
C(10A)-H(10B)	0.9900
C(11A)-C(12A)	1.513(3)
C(11A)-H(11A)	1.0000
C(12A)-C(13A)	1.393(3)

C(12A)-C(17A)	1.398(3)
C(13A)-C(14A)	1.394(3)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.387(3)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.390(3)
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.393(3)
C(16A)-H(16A)	0.9500
C(17A)-H(17A)	0.9500
C(18A)-H(18A)	0.9800
C(18A)-H(18B)	0.9800
C(18A)-H(18C)	0.9800
C(19A)-H(19A)	0.9800
C(19A)-H(19B)	0.9800
C(19A)-H(19C)	0.9800
O(1B)-C(1B)	1.226(2)
O(2B)-C(9B)	1.429(2)
O(2B)-C(10B)	1.433(3)
N(1B)-C(1B)	1.355(2)
N(1B)-C(11B)	1.461(2)
N(1B)-C(9B)	1.475(2)
C(1B)-C(2B)	1.509(3)
C(2B)-C(3B)	1.542(3)
C(2B)-H(2BA)	0.9900
C(2B)-H(2BB)	0.9900
C(3B)-C(4B)	1.542(3)
C(3B)-H(3BA)	0.9900
C(3B)-H(3BB)	0.9900
C(4B)-C(9B)	1.525(2)
C(4B)-C(5B)	1.530(3)
C(4B)-H(4B)	1.0000
C(5B)-C(6B)	1.523(3)
C(5B)-H(5BA)	0.9900
C(5B)-H(5BB)	0.9900
C(6B)-C(7B)	1.528(3)

C(6B)-H(6BA)	0.9900
C(6B)-H(6BB)	0.9900
C(7B)-C(18B)	1.526(3)
C(7B)-C(8B)	1.553(3)
C(7B)-H(7B)	1.0000
C(8B)-C(19B)	1.531(3)
C(8B)-C(9B)	1.547(2)
C(8B)-H(8B)	1.0000
C(10B)-C(11B)	1.535(3)
C(10B)-H(10C)	0.9900
C(10B)-H(10D)	0.9900
C(11B)-C(12B)	1.526(3)
C(11B)-H(11B)	1.0000
C(12B)-C(17B)	1.389(3)
C(12B)-C(13B)	1.400(3)
C(13B)-C(14B)	1.388(4)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.385(4)
C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.386(3)
C(15B)-H(15B)	0.9500
C(16B)-C(17B)	1.394(3)
C(16B)-H(16B)	0.9500
C(17B)-H(17B)	0.9500
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
O(1W)-H(1WA)	0.834(12)
O(1W)-H(1WA)#1	0.834(12)

C(9A)-O(2A)-C(10A)	109.05(13)
C(1A)-N(1A)-C(9A)	124.98(15)
C(1A)-N(1A)-C(11A)	122.56(15)

C(9A)-N(1A)-C(11A)	112.29(14)
O(1A)-C(1A)-N(1A)	122.27(17)
O(1A)-C(1A)-C(2A)	120.14(16)
N(1A)-C(1A)-C(2A)	117.42(16)
C(1A)-C(2A)-C(3A)	118.18(16)
C(1A)-C(2A)-H(2AA)	107.8
C(3A)-C(2A)-H(2AA)	107.8
C(1A)-C(2A)-H(2AB)	107.8
C(3A)-C(2A)-H(2AB)	107.8
H(2AA)-C(2A)-H(2AB)	107.1
C(2A)-C(3A)-C(4A)	112.07(15)
C(2A)-C(3A)-H(3AA)	109.2
C(4A)-C(3A)-H(3AA)	109.2
C(2A)-C(3A)-H(3AB)	109.2
C(4A)-C(3A)-H(3AB)	109.2
H(3AA)-C(3A)-H(3AB)	107.9
C(5A)-C(4A)-C(9A)	110.32(15)
C(5A)-C(4A)-C(3A)	113.08(16)
C(9A)-C(4A)-C(3A)	109.15(13)
C(5A)-C(4A)-H(4A)	108.0
C(9A)-C(4A)-H(4A)	108.0
C(3A)-C(4A)-H(4A)	108.0
C(6A)-C(5A)-C(4A)	112.45(15)
C(6A)-C(5A)-H(5AA)	109.1
C(4A)-C(5A)-H(5AA)	109.1
C(6A)-C(5A)-H(5AB)	109.1
C(4A)-C(5A)-H(5AB)	109.1
H(5AA)-C(5A)-H(5AB)	107.8
C(5A)-C(6A)-C(7A)	112.94(17)
C(5A)-C(6A)-H(6AA)	109.0
C(7A)-C(6A)-H(6AA)	109.0
C(5A)-C(6A)-H(6AB)	109.0
C(7A)-C(6A)-H(6AB)	109.0
H(6AA)-C(6A)-H(6AB)	107.8
C(6A)-C(7A)-C(18A)	109.85(17)
C(6A)-C(7A)-C(8A)	110.91(16)

C(18A)-C(7A)-C(8A)	112.41(16)
C(6A)-C(7A)-H(7A)	107.8
C(18A)-C(7A)-H(7A)	107.8
C(8A)-C(7A)-H(7A)	107.8
C(19A)-C(8A)-C(7A)	112.73(15)
C(19A)-C(8A)-C(9A)	114.01(15)
C(7A)-C(8A)-C(9A)	109.17(14)
C(19A)-C(8A)-H(8A)	106.8
C(7A)-C(8A)-H(8A)	106.8
C(9A)-C(8A)-H(8A)	106.8
O(2A)-C(9A)-N(1A)	102.71(13)
O(2A)-C(9A)-C(4A)	108.39(13)
N(1A)-C(9A)-C(4A)	109.30(14)
O(2A)-C(9A)-C(8A)	111.63(14)
N(1A)-C(9A)-C(8A)	112.64(13)
C(4A)-C(9A)-C(8A)	111.74(15)
O(2A)-C(10A)-C(11A)	106.87(14)
O(2A)-C(10A)-H(10A)	110.3
C(11A)-C(10A)-H(10A)	110.3
O(2A)-C(10A)-H(10B)	110.3
C(11A)-C(10A)-H(10B)	110.3
H(10A)-C(10A)-H(10B)	108.6
N(1A)-C(11A)-C(12A)	112.88(14)
N(1A)-C(11A)-C(10A)	100.82(14)
C(12A)-C(11A)-C(10A)	112.34(14)
N(1A)-C(11A)-H(11A)	110.2
C(12A)-C(11A)-H(11A)	110.2
C(10A)-C(11A)-H(11A)	110.2
C(13A)-C(12A)-C(17A)	119.16(17)
C(13A)-C(12A)-C(11A)	119.74(16)
C(17A)-C(12A)-C(11A)	121.00(16)
C(12A)-C(13A)-C(14A)	120.36(17)
C(12A)-C(13A)-H(13A)	119.8
C(14A)-C(13A)-H(13A)	119.8
C(15A)-C(14A)-C(13A)	120.15(18)
C(15A)-C(14A)-H(14A)	119.9

C(13A)-C(14A)-H(14A)	119.9
C(14A)-C(15A)-C(16A)	119.87(18)
C(14A)-C(15A)-H(15A)	120.1
C(16A)-C(15A)-H(15A)	120.1
C(15A)-C(16A)-C(17A)	120.11(18)
C(15A)-C(16A)-H(16A)	119.9
C(17A)-C(16A)-H(16A)	119.9
C(16A)-C(17A)-C(12A)	120.30(18)
C(16A)-C(17A)-H(17A)	119.9
C(12A)-C(17A)-H(17A)	119.9
C(7A)-C(18A)-H(18A)	109.5
C(7A)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(7A)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
C(8A)-C(19A)-H(19A)	109.5
C(8A)-C(19A)-H(19B)	109.5
H(19A)-C(19A)-H(19B)	109.5
C(8A)-C(19A)-H(19C)	109.5
H(19A)-C(19A)-H(19C)	109.5
H(19B)-C(19A)-H(19C)	109.5
C(9B)-O(2B)-C(10B)	108.67(14)
C(1B)-N(1B)-C(11B)	122.25(15)
C(1B)-N(1B)-C(9B)	123.95(15)
C(11B)-N(1B)-C(9B)	112.43(14)
O(1B)-C(1B)-N(1B)	121.80(19)
O(1B)-C(1B)-C(2B)	122.56(18)
N(1B)-C(1B)-C(2B)	115.64(16)
C(1B)-C(2B)-C(3B)	116.52(17)
C(1B)-C(2B)-H(2BA)	108.2
C(3B)-C(2B)-H(2BA)	108.2
C(1B)-C(2B)-H(2BB)	108.2
C(3B)-C(2B)-H(2BB)	108.2
H(2BA)-C(2B)-H(2BB)	107.3
C(4B)-C(3B)-C(2B)	115.83(17)

C(4B)-C(3B)-H(3BA)	108.3
C(2B)-C(3B)-H(3BA)	108.3
C(4B)-C(3B)-H(3BB)	108.3
C(2B)-C(3B)-H(3BB)	108.3
H(3BA)-C(3B)-H(3BB)	107.4
C(9B)-C(4B)-C(5B)	110.85(16)
C(9B)-C(4B)-C(3B)	110.31(16)
C(5B)-C(4B)-C(3B)	112.97(18)
C(9B)-C(4B)-H(4B)	107.5
C(5B)-C(4B)-H(4B)	107.5
C(3B)-C(4B)-H(4B)	107.5
C(6B)-C(5B)-C(4B)	112.24(17)
C(6B)-C(5B)-H(5BA)	109.2
C(4B)-C(5B)-H(5BA)	109.2
C(6B)-C(5B)-H(5BB)	109.2
C(4B)-C(5B)-H(5BB)	109.2
H(5BA)-C(5B)-H(5BB)	107.9
C(5B)-C(6B)-C(7B)	112.49(18)
C(5B)-C(6B)-H(6BA)	109.1
C(7B)-C(6B)-H(6BA)	109.1
C(5B)-C(6B)-H(6BB)	109.1
C(7B)-C(6B)-H(6BB)	109.1
H(6BA)-C(6B)-H(6BB)	107.8
C(18B)-C(7B)-C(6B)	110.18(19)
C(18B)-C(7B)-C(8B)	112.52(18)
C(6B)-C(7B)-C(8B)	110.37(17)
C(18B)-C(7B)-H(7B)	107.9
C(6B)-C(7B)-H(7B)	107.9
C(8B)-C(7B)-H(7B)	107.9
C(19B)-C(8B)-C(9B)	113.95(16)
C(19B)-C(8B)-C(7B)	112.17(17)
C(9B)-C(8B)-C(7B)	108.74(15)
C(19B)-C(8B)-H(8B)	107.2
C(9B)-C(8B)-H(8B)	107.2
C(7B)-C(8B)-H(8B)	107.2
O(2B)-C(9B)-N(1B)	102.78(14)

O(2B)-C(9B)-C(4B)	109.24(14)
N(1B)-C(9B)-C(4B)	108.56(14)
O(2B)-C(9B)-C(8B)	110.84(14)
N(1B)-C(9B)-C(8B)	113.56(14)
C(4B)-C(9B)-C(8B)	111.45(15)
O(2B)-C(10B)-C(11B)	104.84(15)
O(2B)-C(10B)-H(10C)	110.8
C(11B)-C(10B)-H(10C)	110.8
O(2B)-C(10B)-H(10D)	110.8
C(11B)-C(10B)-H(10D)	110.8
H(10C)-C(10B)-H(10D)	108.9
N(1B)-C(11B)-C(12B)	114.22(15)
N(1B)-C(11B)-C(10B)	100.17(15)
C(12B)-C(11B)-C(10B)	111.06(16)
N(1B)-C(11B)-H(11B)	110.3
C(12B)-C(11B)-H(11B)	110.3
C(10B)-C(11B)-H(11B)	110.3
C(17B)-C(12B)-C(13B)	118.85(19)
C(17B)-C(12B)-C(11B)	124.43(16)
C(13B)-C(12B)-C(11B)	116.58(19)
C(14B)-C(13B)-C(12B)	120.4(2)
C(14B)-C(13B)-H(13B)	119.8
C(12B)-C(13B)-H(13B)	119.8
C(15B)-C(14B)-C(13B)	120.2(2)
C(15B)-C(14B)-H(14B)	119.9
C(13B)-C(14B)-H(14B)	119.9
C(14B)-C(15B)-C(16B)	120.0(2)
C(14B)-C(15B)-H(15B)	120.0
C(16B)-C(15B)-H(15B)	120.0
C(15B)-C(16B)-C(17B)	119.9(2)
C(15B)-C(16B)-H(16B)	120.1
C(17B)-C(16B)-H(16B)	120.1
C(12B)-C(17B)-C(16B)	120.68(19)
C(12B)-C(17B)-H(17B)	119.7
C(16B)-C(17B)-H(17B)	119.7
C(7B)-C(18B)-H(18D)	109.5

C(7B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(7B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
C(8B)-C(19B)-H(19D)	109.5
C(8B)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19E)	109.5
C(8B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
H(1WA)-O(1W)-H(1WA)#1	107(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB7_0m_a. 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}
O(1A)	24(1)	24(1)	26(1)	3(1)	11(1)	2(1)
O(2A)	26(1)	23(1)	21(1)	-6(1)	7(1)	-2(1)
N(1A)	17(1)	18(1)	18(1)	0(1)	5(1)	0(1)
C(1A)	18(1)	23(1)	19(1)	0(1)	2(1)	2(1)
C(2A)	28(1)	22(1)	32(1)	4(1)	10(1)	5(1)
C(3A)	24(1)	21(1)	23(1)	4(1)	1(1)	0(1)
C(4A)	21(1)	25(1)	17(1)	2(1)	1(1)	-2(1)
C(5A)	28(1)	35(1)	21(1)	6(1)	2(1)	-6(1)
C(6A)	26(1)	34(1)	27(1)	5(1)	4(1)	-9(1)
C(7A)	20(1)	29(1)	26(1)	0(1)	4(1)	-4(1)
C(8A)	20(1)	22(1)	19(1)	-1(1)	1(1)	-1(1)
C(9A)	18(1)	20(1)	16(1)	-2(1)	3(1)	-1(1)
C(10A)	22(1)	22(1)	30(1)	-4(1)	8(1)	1(1)
C(11A)	18(1)	18(1)	21(1)	-1(1)	4(1)	2(1)
C(12A)	21(1)	18(1)	22(1)	-1(1)	6(1)	1(1)
C(13A)	23(1)	20(1)	25(1)	4(1)	5(1)	3(1)
C(14A)	23(1)	19(1)	35(1)	3(1)	7(1)	1(1)
C(15A)	21(1)	24(1)	36(1)	-4(1)	2(1)	-3(1)
C(16A)	26(1)	34(1)	25(1)	-2(1)	1(1)	-4(1)
C(17A)	25(1)	28(1)	22(1)	1(1)	5(1)	-3(1)
C(18A)	22(1)	38(1)	43(1)	2(1)	-3(1)	-9(1)
C(19A)	24(1)	27(1)	26(1)	1(1)	-3(1)	1(1)
O(1B)	29(1)	39(1)	25(1)	7(1)	-1(1)	-12(1)
O(2B)	30(1)	21(1)	25(1)	5(1)	4(1)	-1(1)
N(1B)	18(1)	20(1)	21(1)	1(1)	4(1)	0(1)
C(1B)	18(1)	24(1)	27(1)	6(1)	-2(1)	-5(1)
C(2B)	42(1)	20(1)	39(1)	5(1)	-1(1)	-3(1)
C(3B)	34(1)	24(1)	43(1)	-2(1)	4(1)	8(1)
C(4B)	17(1)	27(1)	28(1)	-2(1)	4(1)	2(1)
C(5B)	25(1)	45(1)	30(1)	-4(1)	12(1)	2(1)
C(6B)	34(1)	48(1)	27(1)	-8(1)	7(1)	-3(1)

C(7B)	30(1)	35(1)	24(1)	2(1)	-1(1)	-5(1)
C(8B)	18(1)	28(1)	25(1)	2(1)	2(1)	-1(1)
C(9B)	16(1)	19(1)	21(1)	2(1)	4(1)	0(1)
C(10B)	32(1)	19(1)	36(1)	1(1)	1(1)	6(1)
C(11B)	23(1)	22(1)	27(1)	-3(1)	8(1)	4(1)
C(12B)	32(1)	21(1)	19(1)	0(1)	6(1)	-5(1)
C(13B)	50(1)	23(1)	31(1)	-3(1)	4(1)	-1(1)
C(14B)	68(2)	27(1)	36(1)	-6(1)	-4(1)	-14(1)
C(15B)	49(1)	41(1)	31(1)	2(1)	-6(1)	-24(1)
C(16B)	31(1)	40(1)	23(1)	3(1)	2(1)	-9(1)
C(17B)	28(1)	26(1)	20(1)	-2(1)	4(1)	-5(1)
C(18B)	40(1)	50(1)	32(1)	0(1)	-7(1)	-9(1)
C(19B)	18(1)	49(1)	36(1)	2(1)	1(1)	6(1)
O(1W)	61(2)	30(1)	27(1)	0	-8(1)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59ZB7_0m_a.

	x	y	z	U(eq)
H(2AA)	5594	-1376	7730	33
H(2AB)	5284	-1971	6782	33
H(3AA)	5088	-2820	8516	27
H(3AB)	4675	-2565	7676	27
H(4A)	4957	-329	9191	25
H(5AA)	4465	-2380	9782	33
H(5AB)	4244	-676	9904	33
H(6AA)	3646	-2303	9277	35
H(6AB)	3963	-2918	8403	35
H(7A)	3582	171	8538	30
H(8A)	4176	-994	7032	24
H(10A)	4542	4044	8686	29
H(10B)	4156	3561	7823	29
H(11A)	4747	3291	6785	23
H(13A)	5419	4788	6519	27
H(14A)	6095	6129	7099	31
H(15A)	6387	5796	8749	32
H(16A)	6018	4050	9807	34
H(17A)	5338	2725	9238	30
H(18A)	3017	-1686	7982	52
H(18B)	3342	-2207	7095	52
H(18C)	3115	-496	7092	52
H(19A)	3708	1950	7020	38
H(19B)	3645	607	6191	38
H(19C)	4128	1565	6304	38
H(2BA)	6797	12741	5830	40
H(2BB)	7271	12515	6499	40
H(3BA)	6831	12550	7783	40
H(3BB)	6361	12330	7097	40
H(4B)	6337	9756	7320	29

H(5BA)	6285	10956	8938	40
H(5BB)	6436	9156	8990	40
H(6BA)	6920	10515	10141	44
H(6BB)	7054	11763	9311	44
H(7B)	7332	8544	9327	36
H(8B)	7541	10893	7874	28
H(10C)	6955	5678	6807	35
H(10D)	7466	6440	7034	35
H(11B)	7340	7472	5479	29
H(13B)	6857	5210	4810	42
H(14B)	6144	4329	4081	53
H(15B)	5469	5873	4140	49
H(16B)	5512	8332	4899	37
H(17B)	6221	9190	5670	29
H(18D)	7757	10120	10531	62
H(18E)	7933	11193	9642	62
H(18F)	8094	9405	9722	62
H(19D)	7938	7843	8051	51
H(19E)	8216	9465	8026	51
H(19F)	7949	8817	7030	51
H(1WA)	5170(9)	2400(30)	5368(19)	48

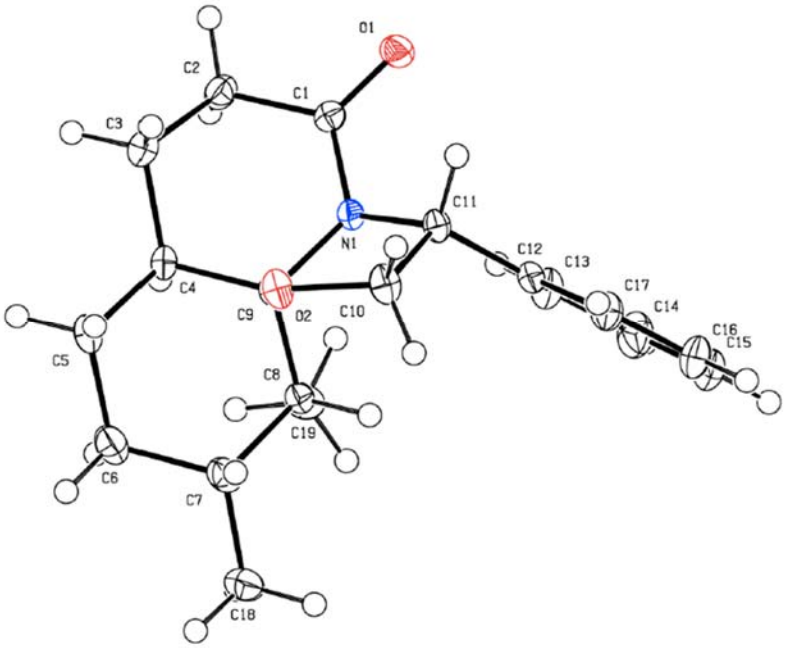
Table 6. Hydrogen bonds for D59ZB7_0m_a.

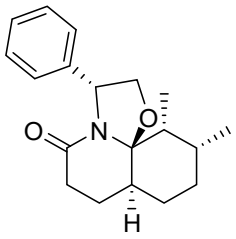
Donor --- H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
O1W --H1WA ..O1A	[ ]	0.83(3)	2.05(3)	2.874(2)	168(2)

C4A - C3A C5A C9A H4A sp3 S
C7A - C6A C8A C18A H7A sp3 S
C8A - C7A C9A C19A H8A sp3 R
C9A - O2A N1A C4A C8A sp3 S
C11A - N1A C10A C12A H11A sp3 R

C4B - C3B C5B C9B H4B sp3 S
C7B - C6B C8B C18B H7B sp3 S
C8B - C7B C9B C19B H8B sp3 R
C9B - O2B N1B C4B C8B sp3 S
C11B - N1B C10B C12B H11B sp3 R

Crystallographic data for compound **7d**:





7d

Table 1. Crystal data and structure refinement for **7d** (D59ZB2_0m_a).

Identification code	D59ZB2_0m_a	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.0138(5) Å	α= 90°.
	b = 6.3391(3) Å	β= 93.122(2)°.
	c = 16.0011(9) Å	γ = 90°.
Volume	811.65(8) $Å^3$	
Z	2	
Density (calculated)	1.225 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	324	
Crystal size	0.250 x 0.150 x 0.139 mm^3	
Theta range for data collection	3.701 to 30.636°.	
Index ranges	-11<=h<=11, -8<=k<=9, -22<=l<=22	
Reflections collected	17964	
Independent reflections	4884 [R(int) = 0.0236]	
Completeness to theta = 25.242°	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6752	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4884 / 1 / 201	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2sigma(I)]	R1 = 0.0343, wR2 = 0.0915	
R indices (all data)	R1 = 0.0356, wR2 = 0.0931	
Absolute structure parameter	-0.2(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.365 and -0.164 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB2_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	11072(1)	2202(2)	2632(1)	21(1)
O(2)	8374(1)	7664(2)	2064(1)	19(1)
N(1)	8781(1)	4278(2)	2462(1)	15(1)
C(1)	9979(2)	2969(2)	2162(1)	16(1)
C(2)	9909(2)	2531(2)	1232(1)	22(1)
C(3)	9324(2)	4459(3)	722(1)	22(1)
C(4)	7608(2)	5068(2)	1002(1)	17(1)
C(5)	6713(2)	6845(2)	515(1)	22(1)
C(6)	4914(2)	7028(3)	797(1)	26(1)
C(7)	4835(2)	7297(2)	1745(1)	23(1)
C(8)	5845(2)	5580(2)	2234(1)	16(1)
C(9)	7651(2)	5609(2)	1933(1)	14(1)
C(10)	8838(2)	7784(2)	2944(1)	20(1)
C(11)	9261(2)	5491(2)	3226(1)	16(1)
C(12)	8434(2)	4806(2)	4009(1)	18(1)
C(13)	7647(2)	2859(3)	4062(1)	24(1)
C(14)	6911(2)	2252(3)	4794(1)	33(1)
C(15)	6980(2)	3587(4)	5480(1)	35(1)
C(16)	7788(2)	5511(4)	5443(1)	33(1)
C(17)	8516(2)	6121(3)	4710(1)	26(1)
C(18)	3034(2)	7415(3)	1995(1)	28(1)
C(19)	5064(2)	3382(2)	2184(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB2_0m_a.

O(1)-C(1)	1.2233(16)
O(2)-C(9)	1.4363(15)
O(2)-C(10)	1.4379(16)
N(1)-C(1)	1.3747(17)
N(1)-C(9)	1.4714(16)
N(1)-C(11)	1.4773(16)
C(1)-C(2)	1.5125(18)
C(2)-C(3)	1.529(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5185(19)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.5262(19)
C(4)-C(9)	1.5285(17)
C(4)-H(4A)	1.0000
C(5)-C(6)	1.537(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.532(2)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(18)	1.521(2)
C(7)-C(8)	1.5435(19)
C(7)-H(7A)	1.0000
C(8)-C(19)	1.5281(19)
C(8)-C(9)	1.5497(18)
C(8)-H(8A)	1.0000
C(10)-C(11)	1.554(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.5127(18)
C(11)-H(11A)	1.0000
C(12)-C(13)	1.390(2)

C(12)-C(17)	1.3953(19)
C(13)-C(14)	1.393(2)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.385(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.384(3)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.393(2)
C(16)-H(16A)	0.9500
C(17)-H(17A)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(9)-O(2)-C(10)	105.74(9)
C(1)-N(1)-C(9)	124.38(10)
C(1)-N(1)-C(11)	116.60(10)
C(9)-N(1)-C(11)	107.56(10)
O(1)-C(1)-N(1)	121.07(12)
O(1)-C(1)-C(2)	121.20(12)
N(1)-C(1)-C(2)	117.73(11)
C(1)-C(2)-C(3)	111.87(12)
C(1)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2B)	109.2
C(3)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(4)-C(3)-C(2)	107.61(11)
C(4)-C(3)-H(3A)	110.2
C(2)-C(3)-H(3A)	110.2
C(4)-C(3)-H(3B)	110.2
C(2)-C(3)-H(3B)	110.2
H(3A)-C(3)-H(3B)	108.5

C(3)-C(4)-C(5)	116.48(11)
C(3)-C(4)-C(9)	111.81(11)
C(5)-C(4)-C(9)	108.47(11)
C(3)-C(4)-H(4A)	106.5
C(5)-C(4)-H(4A)	106.5
C(9)-C(4)-H(4A)	106.5
C(4)-C(5)-C(6)	109.19(11)
C(4)-C(5)-H(5A)	109.8
C(6)-C(5)-H(5A)	109.8
C(4)-C(5)-H(5B)	109.8
C(6)-C(5)-H(5B)	109.8
H(5A)-C(5)-H(5B)	108.3
C(7)-C(6)-C(5)	112.86(12)
C(7)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6A)	109.0
C(7)-C(6)-H(6B)	109.0
C(5)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(18)-C(7)-C(6)	110.90(12)
C(18)-C(7)-C(8)	112.38(12)
C(6)-C(7)-C(8)	112.00(12)
C(18)-C(7)-H(7A)	107.1
C(6)-C(7)-H(7A)	107.1
C(8)-C(7)-H(7A)	107.1
C(19)-C(8)-C(7)	114.47(11)
C(19)-C(8)-C(9)	112.42(11)
C(7)-C(8)-C(9)	107.90(11)
C(19)-C(8)-H(8A)	107.2
C(7)-C(8)-H(8A)	107.2
C(9)-C(8)-H(8A)	107.2
O(2)-C(9)-N(1)	101.86(9)
O(2)-C(9)-C(4)	109.45(10)
N(1)-C(9)-C(4)	114.40(11)
O(2)-C(9)-C(8)	109.94(10)
N(1)-C(9)-C(8)	111.76(10)
C(4)-C(9)-C(8)	109.18(10)

O(2)-C(10)-C(11)	106.02(10)
O(2)-C(10)-H(10A)	110.5
C(11)-C(10)-H(10A)	110.5
O(2)-C(10)-H(10B)	110.5
C(11)-C(10)-H(10B)	110.5
H(10A)-C(10)-H(10B)	108.7
N(1)-C(11)-C(12)	115.47(11)
N(1)-C(11)-C(10)	101.73(10)
C(12)-C(11)-C(10)	114.27(11)
N(1)-C(11)-H(11A)	108.3
C(12)-C(11)-H(11A)	108.3
C(10)-C(11)-H(11A)	108.3
C(13)-C(12)-C(17)	118.89(13)
C(13)-C(12)-C(11)	121.72(12)
C(17)-C(12)-C(11)	119.34(13)
C(12)-C(13)-C(14)	120.72(15)
C(12)-C(13)-H(13A)	119.6
C(14)-C(13)-H(13A)	119.6
C(15)-C(14)-C(13)	119.76(17)
C(15)-C(14)-H(14A)	120.1
C(13)-C(14)-H(14A)	120.1
C(16)-C(15)-C(14)	120.22(15)
C(16)-C(15)-H(15A)	119.9
C(14)-C(15)-H(15A)	119.9
C(15)-C(16)-C(17)	119.95(16)
C(15)-C(16)-H(16A)	120.0
C(17)-C(16)-H(16A)	120.0
C(16)-C(17)-C(12)	120.44(17)
C(16)-C(17)-H(17A)	119.8
C(12)-C(17)-H(17A)	119.8
C(7)-C(18)-H(18A)	109.5
C(7)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(7)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

C(8)-C(19)-H(19A)	109.5
C(8)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(8)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB2_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

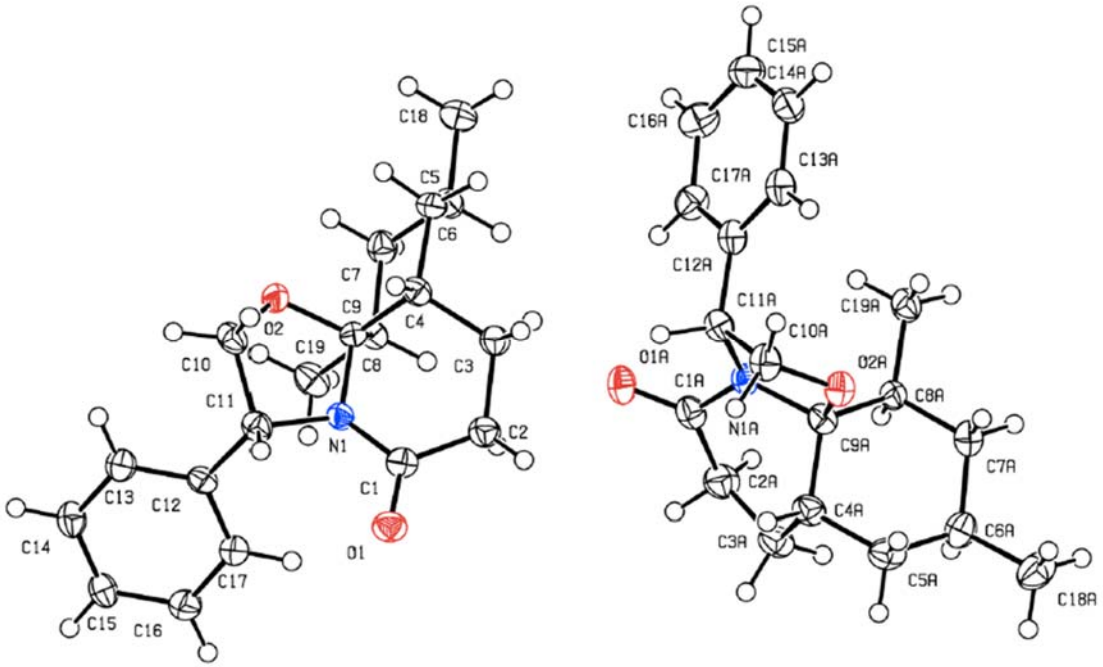
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	20(1)	21(1)	22(1)	4(1)	1(1)	3(1)
O(2)	24(1)	14(1)	18(1)	2(1)	-4(1)	-5(1)
N(1)	16(1)	15(1)	13(1)	0(1)	-1(1)	0(1)
C(1)	17(1)	14(1)	18(1)	2(1)	3(1)	-2(1)
C(2)	26(1)	22(1)	18(1)	-1(1)	4(1)	3(1)
C(3)	23(1)	26(1)	16(1)	2(1)	4(1)	0(1)
C(4)	20(1)	19(1)	12(1)	1(1)	0(1)	-2(1)
C(5)	27(1)	24(1)	16(1)	5(1)	-2(1)	0(1)
C(6)	28(1)	26(1)	22(1)	3(1)	-5(1)	4(1)
C(7)	24(1)	21(1)	23(1)	2(1)	-2(1)	4(1)
C(8)	17(1)	15(1)	16(1)	0(1)	-1(1)	0(1)
C(9)	17(1)	12(1)	14(1)	0(1)	-1(1)	-2(1)
C(10)	27(1)	15(1)	18(1)	-2(1)	-4(1)	-4(1)
C(11)	18(1)	15(1)	14(1)	-1(1)	-2(1)	-2(1)
C(12)	17(1)	21(1)	14(1)	0(1)	-2(1)	2(1)
C(13)	30(1)	23(1)	18(1)	1(1)	2(1)	-2(1)
C(14)	34(1)	39(1)	25(1)	10(1)	4(1)	-7(1)
C(15)	30(1)	58(1)	18(1)	8(1)	5(1)	3(1)
C(16)	36(1)	49(1)	15(1)	-6(1)	0(1)	7(1)
C(17)	28(1)	30(1)	18(1)	-6(1)	-3(1)	1(1)
C(18)	23(1)	33(1)	28(1)	-2(1)	-1(1)	9(1)
C(19)	19(1)	18(1)	29(1)	1(1)	1(1)	-3(1)

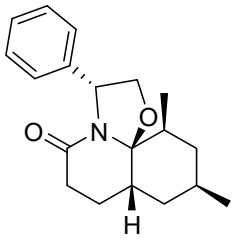
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59ZB2_0m_a.

	x	y	z	U(eq)
H(2A)	9136	1342	1106	26
H(2B)	11033	2109	1065	26
H(3A)	10118	5641	820	26
H(3B)	9262	4119	117	26
H(4A)	6887	3788	925	20
H(5A)	6696	6545	-92	27
H(5B)	7313	8193	620	27
H(6A)	4364	8252	513	31
H(6B)	4285	5745	620	31
H(7A)	5368	8683	1894	27
H(8A)	5910	6007	2837	19
H(10A)	7903	8349	3256	24
H(10B)	9821	8713	3044	24
H(11A)	10499	5379	3332	19
H(13A)	7611	1934	3595	28
H(14A)	6364	926	4821	39
H(15A)	6470	3181	5977	42
H(16A)	7847	6415	5917	40
H(17A)	9071	7442	4686	31
H(18A)	2449	8540	1677	42
H(18B)	3014	7718	2595	42
H(18C)	2477	6065	1874	42
H(19A)	4627	3111	1610	33
H(19B)	4149	3302	2565	33
H(19C)	5913	2324	2345	33

- C(4) - C(3) C(5) C(9) H(4A) sp3 S
- C(7) - C(6) C(8) C(18) H(7A) sp3 R
- C(8) - C(7) C(9) C(19) H(8A) sp3 R
- C(9) - O(2) N(1) C(4) C(8) sp3 R
- C(11) - N(1) C(10) C(12) H(11A) sp3 R

Crystallographic data for compound **8a**:





8a

Table 1. Crystal data and structure refinement for **8a** (D59YB89_0m_a).

Identification code	D59YB89_0m_a	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 13.0323(13) Å	α= 90°.
	b = 7.7488(6) Å	β= 95.606(4)°.
	c = 16.1799(16) Å	γ = 90°.
Volume	1626.1(3) $Å^3$	
Z	4	
Density (calculated)	1.223 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	648	
Crystal size	0.09 x 0.06 x 0.03 mm^3	
Theta range for data collection	2.110 to 30.609°.	
Index ranges	-18<=h<=18, -11<=k<=11, -23<=l<=23	
Reflections collected	37613	
Independent reflections	9872 [R(int) = 0.1209]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6649	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9872 / 1 / 402	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.0967	
R indices (all data)	R1 = 0.1655, wR2 = 0.1403	
Absolute structure parameter	-2.0(9)	
Extinction coefficient	0.0196(17)	
Largest diff. peak and hole	0.358 and -0.345 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59YB89_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4086(2)	4409(4)	5417(2)	30(1)
O(2)	860(2)	3586(3)	4232(2)	24(1)
N(1)	2580(2)	3767(4)	4663(2)	22(1)
C(1)	3509(3)	4570(5)	4769(2)	26(1)
C(2)	3787(3)	5584(6)	4040(2)	29(1)
C(3)	2897(3)	6669(5)	3610(3)	27(1)
C(4)	1809(3)	6042(5)	3746(2)	24(1)
C(5)	1021(3)	6470(5)	3004(2)	25(1)
C(6)	1135(3)	5357(5)	2242(2)	26(1)
C(7)	1118(3)	3456(5)	2485(2)	28(1)
C(8)	1973(3)	3023(5)	3174(2)	24(1)
C(9)	1813(3)	4120(5)	3940(2)	22(1)
C(10)	971(3)	3675(6)	5123(2)	28(1)
C(11)	2081(3)	3094(5)	5374(2)	25(1)
C(12)	2260(3)	1178(5)	5550(2)	23(1)
C(13)	1511(3)	128(5)	5835(2)	28(1)
C(14)	1727(3)	-1558(5)	6072(3)	29(1)
C(15)	2703(3)	-2227(5)	6027(2)	28(1)
C(16)	3450(3)	-1206(5)	5723(3)	31(1)
C(17)	3229(3)	488(6)	5487(2)	29(1)
C(18)	292(3)	5762(6)	1538(3)	37(1)
C(19)	2011(4)	1089(5)	3353(3)	32(1)
O(1A)	4312(2)	5645(4)	2072(2)	32(1)
O(2A)	5916(2)	10764(4)	2099(2)	27(1)
N(1A)	5139(3)	8155(4)	1823(2)	24(1)
C(1A)	5102(3)	6401(5)	1900(2)	27(1)
C(2A)	6056(3)	5445(6)	1713(3)	35(1)
C(3A)	7075(3)	6295(5)	2041(3)	32(1)
C(4A)	6976(3)	8179(5)	2301(2)	28(1)
C(5A)	7994(3)	9184(6)	2293(3)	33(1)
C(6A)	8287(3)	9555(6)	1419(3)	33(1)

C(7A)	7385(3)	10403(6)	903(3)	31(1)
C(8A)	6386(3)	9377(6)	873(2)	24(1)
C(9A)	6116(3)	9098(5)	1765(2)	23(1)
C(10A)	5090(3)	10590(6)	2620(2)	30(1)
C(11A)	4371(3)	9273(5)	2174(2)	26(1)
C(12A)	3542(3)	9937(5)	1535(2)	26(1)
C(13A)	3361(4)	11672(5)	1373(3)	30(1)
C(14A)	2559(3)	12195(6)	797(3)	34(1)
C(15A)	1914(4)	11004(6)	382(3)	36(1)
C(16A)	2084(4)	9264(6)	528(3)	38(1)
C(17A)	2888(3)	8742(6)	1100(3)	32(1)
C(18A)	9260(3)	10634(6)	1444(3)	43(1)
C(19A)	5530(3)	10217(6)	305(2)	31(1)

Table 3. Bond lengths [Å] and angles [°] for D59YB89_0m_a.

O(1)-C(1)	1.235(5)
O(2)-C(9)	1.432(4)
O(2)-C(10)	1.436(4)
N(1)-C(1)	1.358(5)
N(1)-C(11)	1.472(5)
N(1)-C(9)	1.487(5)
C(1)-C(2)	1.491(5)
C(2)-C(3)	1.542(6)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(4)	1.535(5)
C(3)-H(3A)	0.9900
C(3)-H(3AB)	0.9900
C(4)-C(9)	1.522(5)
C(4)-C(5)	1.538(5)
C(4)-H(4)	1.0000
C(5)-C(6)	1.524(5)
C(5)-H(5A)	0.9900
C(5)-H(5AB)	0.9900
C(6)-C(7)	1.526(5)
C(6)-C(18)	1.536(5)
C(6)-H(6)	1.0000
C(7)-C(8)	1.534(5)
C(7)-H(7A)	0.9900
C(7)-H(7AB)	0.9900
C(8)-C(19)	1.526(5)
C(8)-C(9)	1.533(5)
C(8)-H(8)	1.0000
C(10)-C(11)	1.531(5)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.525(5)
C(11)-H(11)	1.0000
C(12)-C(13)	1.384(5)

C(12)-C(17)	1.385(5)
C(13)-C(14)	1.382(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.382(6)
C(14)-H(14)	0.9500
C(15)-C(16)	1.381(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.389(6)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
O(1A)-C(1A)	1.241(5)
O(2A)-C(9A)	1.433(5)
O(2A)-C(10A)	1.436(4)
N(1A)-C(1A)	1.366(5)
N(1A)-C(11A)	1.478(5)
N(1A)-C(9A)	1.478(5)
C(1A)-C(2A)	1.502(6)
C(2A)-C(3A)	1.530(6)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AC)	0.9900
C(3A)-C(4A)	1.528(6)
C(3A)-H(3AA)	0.9900
C(3A)-H(3AC)	0.9900
C(4A)-C(9A)	1.526(5)
C(4A)-C(5A)	1.539(6)
C(4A)-H(4A)	1.0000
C(5A)-C(6A)	1.528(6)
C(5A)-H(5AA)	0.9900
C(5A)-H(5AC)	0.9900
C(6A)-C(18A)	1.516(6)

C(6A)-C(7A)	1.523(6)
C(6A)-H(6A)	1.0000
C(7A)-C(8A)	1.522(5)
C(7A)-H(7AA)	0.9900
C(7A)-H(7AC)	0.9900
C(8A)-C(19A)	1.521(6)
C(8A)-C(9A)	1.534(5)
C(8A)-H(8A)	1.0000
C(10A)-C(11A)	1.520(6)
C(10A)-H(10C)	0.9900
C(10A)-H(10D)	0.9900
C(11A)-C(12A)	1.510(6)
C(11A)-H(11A)	1.0000
C(12A)-C(13A)	1.386(6)
C(12A)-C(17A)	1.401(6)
C(13A)-C(14A)	1.390(6)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.378(6)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.383(6)
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.389(6)
C(16A)-H(16A)	0.9500
C(17A)-H(17A)	0.9500
C(18A)-H(18D)	0.9800
C(18A)-H(18E)	0.9800
C(18A)-H(18F)	0.9800
C(19A)-H(19D)	0.9800
C(19A)-H(19E)	0.9800
C(19A)-H(19F)	0.9800

C(9)-O(2)-C(10)	108.2(3)
C(1)-N(1)-C(11)	121.3(3)
C(1)-N(1)-C(9)	122.5(3)
C(11)-N(1)-C(9)	111.5(3)
O(1)-C(1)-N(1)	121.5(4)

O(1)-C(1)-C(2)	123.4(4)
N(1)-C(1)-C(2)	115.0(3)
C(1)-C(2)-C(3)	114.5(3)
C(1)-C(2)-H(2A)	108.6
C(3)-C(2)-H(2A)	108.6
C(1)-C(2)-H(2AB)	108.6
C(3)-C(2)-H(2AB)	108.6
H(2A)-C(2)-H(2AB)	107.6
C(4)-C(3)-C(2)	115.3(3)
C(4)-C(3)-H(3A)	108.5
C(2)-C(3)-H(3A)	108.5
C(4)-C(3)-H(3AB)	108.5
C(2)-C(3)-H(3AB)	108.5
H(3A)-C(3)-H(3AB)	107.5
C(9)-C(4)-C(3)	110.8(3)
C(9)-C(4)-C(5)	111.1(3)
C(3)-C(4)-C(5)	112.0(3)
C(9)-C(4)-H(4)	107.6
C(3)-C(4)-H(4)	107.6
C(5)-C(4)-H(4)	107.6
C(6)-C(5)-C(4)	113.5(3)
C(6)-C(5)-H(5A)	108.9
C(4)-C(5)-H(5A)	108.9
C(6)-C(5)-H(5AB)	108.9
C(4)-C(5)-H(5AB)	108.9
H(5A)-C(5)-H(5AB)	107.7
C(5)-C(6)-C(7)	109.4(3)
C(5)-C(6)-C(18)	111.4(3)
C(7)-C(6)-C(18)	111.2(3)
C(5)-C(6)-H(6)	108.2
C(7)-C(6)-H(6)	108.2
C(18)-C(6)-H(6)	108.2
C(6)-C(7)-C(8)	111.8(3)
C(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7AB)	109.3

C(8)-C(7)-H(7AB)	109.3
H(7A)-C(7)-H(7AB)	107.9
C(19)-C(8)-C(9)	113.3(3)
C(19)-C(8)-C(7)	111.1(3)
C(9)-C(8)-C(7)	108.6(3)
C(19)-C(8)-H(8)	107.9
C(9)-C(8)-H(8)	107.9
C(7)-C(8)-H(8)	107.9
O(2)-C(9)-N(1)	103.0(3)
O(2)-C(9)-C(4)	111.4(3)
N(1)-C(9)-C(4)	109.3(3)
O(2)-C(9)-C(8)	107.3(3)
N(1)-C(9)-C(8)	113.5(3)
C(4)-C(9)-C(8)	112.0(3)
O(2)-C(10)-C(11)	104.6(3)
O(2)-C(10)-H(10A)	110.8
C(11)-C(10)-H(10A)	110.8
O(2)-C(10)-H(10B)	110.8
C(11)-C(10)-H(10B)	110.8
H(10A)-C(10)-H(10B)	108.9
N(1)-C(11)-C(12)	114.8(3)
N(1)-C(11)-C(10)	99.6(3)
C(12)-C(11)-C(10)	117.4(4)
N(1)-C(11)-H(11)	108.2
C(12)-C(11)-H(11)	108.2
C(10)-C(11)-H(11)	108.2
C(13)-C(12)-C(17)	118.4(4)
C(13)-C(12)-C(11)	122.3(4)
C(17)-C(12)-C(11)	119.1(4)
C(14)-C(13)-C(12)	121.1(4)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(13)-C(14)-C(15)	120.3(4)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	119.2(4)

C(16)-C(15)-H(15)	120.4
C(14)-C(15)-H(15)	120.4
C(15)-C(16)-C(17)	120.3(4)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-H(16)	119.9
C(12)-C(17)-C(16)	120.7(4)
C(12)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(6)-C(18)-H(18A)	109.5
C(6)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(6)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(8)-C(19)-H(19A)	109.5
C(8)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(8)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(9A)-O(2A)-C(10A)	108.1(3)
C(1A)-N(1A)-C(11A)	121.1(3)
C(1A)-N(1A)-C(9A)	122.4(4)
C(11A)-N(1A)-C(9A)	110.7(3)
O(1A)-C(1A)-N(1A)	121.9(4)
O(1A)-C(1A)-C(2A)	122.2(4)
N(1A)-C(1A)-C(2A)	115.8(4)
C(1A)-C(2A)-C(3A)	115.2(4)
C(1A)-C(2A)-H(2AA)	108.5
C(3A)-C(2A)-H(2AA)	108.5
C(1A)-C(2A)-H(2AC)	108.5
C(3A)-C(2A)-H(2AC)	108.5
H(2AA)-C(2A)-H(2AC)	107.5
C(4A)-C(3A)-C(2A)	114.4(4)
C(4A)-C(3A)-H(3AA)	108.7
C(2A)-C(3A)-H(3AA)	108.7

C(4A)-C(3A)-H(3AC)	108.7
C(2A)-C(3A)-H(3AC)	108.7
H(3AA)-C(3A)-H(3AC)	107.6
C(9A)-C(4A)-C(3A)	111.5(3)
C(9A)-C(4A)-C(5A)	110.2(3)
C(3A)-C(4A)-C(5A)	112.6(4)
C(9A)-C(4A)-H(4A)	107.4
C(3A)-C(4A)-H(4A)	107.4
C(5A)-C(4A)-H(4A)	107.4
C(6A)-C(5A)-C(4A)	113.4(3)
C(6A)-C(5A)-H(5AA)	108.9
C(4A)-C(5A)-H(5AA)	108.9
C(6A)-C(5A)-H(5AC)	108.9
C(4A)-C(5A)-H(5AC)	108.9
H(5AA)-C(5A)-H(5AC)	107.7
C(18A)-C(6A)-C(7A)	112.0(4)
C(18A)-C(6A)-C(5A)	111.3(4)
C(7A)-C(6A)-C(5A)	109.9(3)
C(18A)-C(6A)-H(6A)	107.8
C(7A)-C(6A)-H(6A)	107.8
C(5A)-C(6A)-H(6A)	107.8
C(8A)-C(7A)-C(6A)	113.8(4)
C(8A)-C(7A)-H(7AA)	108.8
C(6A)-C(7A)-H(7AA)	108.8
C(8A)-C(7A)-H(7AC)	108.8
C(6A)-C(7A)-H(7AC)	108.8
H(7AA)-C(7A)-H(7AC)	107.7
C(19A)-C(8A)-C(7A)	111.7(3)
C(19A)-C(8A)-C(9A)	114.0(3)
C(7A)-C(8A)-C(9A)	108.6(3)
C(19A)-C(8A)-H(8A)	107.4
C(7A)-C(8A)-H(8A)	107.4
C(9A)-C(8A)-H(8A)	107.4
O(2A)-C(9A)-N(1A)	103.4(3)
O(2A)-C(9A)-C(4A)	110.9(3)
N(1A)-C(9A)-C(4A)	108.8(3)

O(2A)-C(9A)-C(8A)	107.2(3)
N(1A)-C(9A)-C(8A)	114.0(3)
C(4A)-C(9A)-C(8A)	112.2(3)
O(2A)-C(10A)-C(11A)	104.3(3)
O(2A)-C(10A)-H(10C)	110.9
C(11A)-C(10A)-H(10C)	110.9
O(2A)-C(10A)-H(10D)	110.9
C(11A)-C(10A)-H(10D)	110.9
H(10C)-C(10A)-H(10D)	108.9
N(1A)-C(11A)-C(12A)	113.8(3)
N(1A)-C(11A)-C(10A)	99.6(3)
C(12A)-C(11A)-C(10A)	117.5(4)
N(1A)-C(11A)-H(11A)	108.5
C(12A)-C(11A)-H(11A)	108.5
C(10A)-C(11A)-H(11A)	108.5
C(13A)-C(12A)-C(17A)	117.5(4)
C(13A)-C(12A)-C(11A)	123.9(4)
C(17A)-C(12A)-C(11A)	118.5(4)
C(12A)-C(13A)-C(14A)	120.8(4)
C(12A)-C(13A)-H(13A)	119.6
C(14A)-C(13A)-H(13A)	119.6
C(15A)-C(14A)-C(13A)	121.0(4)
C(15A)-C(14A)-H(14A)	119.5
C(13A)-C(14A)-H(14A)	119.5
C(14A)-C(15A)-C(16A)	119.3(4)
C(14A)-C(15A)-H(15A)	120.4
C(16A)-C(15A)-H(15A)	120.4
C(15A)-C(16A)-C(17A)	119.7(5)
C(15A)-C(16A)-H(16A)	120.2
C(17A)-C(16A)-H(16A)	120.2
C(16A)-C(17A)-C(12A)	121.7(4)
C(16A)-C(17A)-H(17A)	119.2
C(12A)-C(17A)-H(17A)	119.2
C(6A)-C(18A)-H(18D)	109.5
C(6A)-C(18A)-H(18E)	109.5
H(18D)-C(18A)-H(18E)	109.5

C(6A)-C(18A)-H(18F)	109.5
H(18D)-C(18A)-H(18F)	109.5
H(18E)-C(18A)-H(18F)	109.5
C(8A)-C(19A)-H(19D)	109.5
C(8A)-C(19A)-H(19E)	109.5
H(19D)-C(19A)-H(19E)	109.5
C(8A)-C(19A)-H(19F)	109.5
H(19D)-C(19A)-H(19F)	109.5
H(19E)-C(19A)-H(19F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59YB89_0m_a. 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}
O(1)	29(2)	32(2)	29(2)	0(1)	-5(1)	-1(1)
O(2)	22(2)	29(2)	22(1)	3(1)	2(1)	-2(1)
N(1)	22(2)	23(2)	20(2)	2(1)	-1(1)	-2(1)
C(1)	27(2)	23(2)	26(2)	-3(2)	0(2)	0(2)
C(2)	28(2)	28(2)	30(2)	2(2)	-1(2)	-2(2)
C(3)	27(2)	21(2)	31(2)	1(2)	0(2)	-2(2)
C(4)	27(2)	22(2)	21(2)	0(2)	0(2)	0(2)
C(5)	23(2)	25(2)	26(2)	3(2)	-1(2)	3(2)
C(6)	28(2)	26(2)	25(2)	4(2)	0(2)	-2(2)
C(7)	31(2)	29(2)	24(2)	0(2)	3(2)	-3(2)
C(8)	28(2)	21(2)	22(2)	1(2)	2(2)	1(2)
C(9)	19(2)	25(2)	22(2)	3(2)	0(2)	-1(2)
C(10)	35(3)	30(2)	21(2)	5(2)	6(2)	3(2)
C(11)	29(2)	28(2)	19(2)	1(2)	5(2)	1(2)
C(12)	26(2)	24(2)	19(2)	1(2)	-1(2)	1(2)
C(13)	28(2)	27(2)	28(2)	-1(2)	4(2)	-2(2)
C(14)	33(3)	23(2)	31(2)	0(2)	8(2)	-3(2)
C(15)	36(3)	19(2)	29(2)	1(2)	5(2)	-2(2)
C(16)	28(2)	28(2)	37(2)	4(2)	2(2)	2(2)
C(17)	25(2)	29(2)	34(2)	6(2)	1(2)	-2(2)
C(18)	36(3)	43(3)	30(2)	6(2)	-5(2)	2(2)
C(19)	43(3)	23(2)	29(2)	-1(2)	0(2)	1(2)
O(1A)	38(2)	25(2)	32(2)	0(1)	7(1)	-9(1)
O(2A)	31(2)	26(2)	26(1)	-4(1)	5(1)	-5(1)
N(1A)	27(2)	22(2)	23(2)	0(1)	3(2)	-4(1)
C(1A)	34(3)	26(2)	21(2)	0(2)	0(2)	-5(2)
C(2A)	36(3)	26(3)	43(3)	0(2)	-1(2)	0(2)
C(3A)	36(3)	29(2)	30(2)	0(2)	-6(2)	-1(2)
C(4A)	31(3)	32(2)	21(2)	0(2)	-4(2)	-1(2)
C(5A)	33(3)	32(3)	31(2)	-4(2)	-7(2)	-1(2)
C(6A)	30(3)	32(3)	36(2)	-3(2)	3(2)	-6(2)

C(7A)	33(3)	31(2)	29(2)	1(2)	7(2)	-5(2)
C(8A)	24(2)	28(2)	21(2)	4(2)	2(2)	-2(2)
C(9A)	29(2)	16(2)	24(2)	-3(2)	1(2)	-2(2)
C(10A)	37(3)	33(2)	21(2)	-5(2)	6(2)	-4(2)
C(11A)	31(2)	25(2)	21(2)	-1(2)	5(2)	0(2)
C(12A)	31(3)	25(2)	24(2)	-3(2)	7(2)	-3(2)
C(13A)	35(3)	27(2)	28(2)	-3(2)	9(2)	-3(2)
C(14A)	37(3)	33(3)	35(3)	7(2)	10(2)	5(2)
C(15A)	32(3)	45(3)	31(2)	2(2)	3(2)	5(2)
C(16A)	35(3)	43(3)	35(3)	-9(2)	-1(2)	0(2)
C(17A)	32(3)	28(2)	36(2)	-4(2)	3(2)	-3(2)
C(18A)	31(3)	41(3)	57(3)	-5(3)	2(2)	-5(2)
C(19A)	33(3)	37(3)	23(2)	4(2)	3(2)	-4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59YB89_0m_a.

	x	y	z	U(eq)
H(2A)	4033	4778	3628	34
H(2AB)	4365	6366	4225	34
H(3A)	2974	7873	3813	32
H(3AB)	2963	6683	3006	32
H(4)	1590	6663	4242	28
H(5A)	317	6317	3174	30
H(5AB)	1098	7698	2853	30
H(6)	1820	5615	2040	32
H(7A)	1207	2737	1992	33
H(7AB)	440	3174	2678	33
H(8)	2647	3364	2976	29
H(10A)	474	2898	5361	34
H(10B)	860	4868	5315	34
H(11)	2349	3756	5880	30
H(13)	837	573	5869	33
H(14)	1203	-2259	6265	35
H(15)	2858	-3375	6202	34
H(16)	4118	-1664	5677	37
H(17)	3749	1179	5279	35
H(18A)	333	6982	1384	55
H(18B)	-386	5525	1726	55
H(18C)	392	5039	1055	55
H(19A)	1352	717	3536	48
H(19B)	2567	847	3790	48
H(19C)	2140	463	2847	48
H(2AA)	6044	5316	1104	42
H(2AC)	6033	4272	1954	42
H(3AA)	7383	5627	2524	39
H(3AC)	7556	6232	1604	39
H(4A)	6786	8183	2885	34

H(5AA)	7932	10292	2589	39
H(5AC)	8554	8512	2600	39
H(6A)	8428	8425	1153	39
H(7AA)	7268	11560	1135	37
H(7AC)	7570	10562	329	37
H(8A)	6521	8216	636	29
H(10C)	4734	11705	2676	36
H(10D)	5352	10173	3179	36
H(11A)	4034	8597	2599	31
H(13A)	3790	12516	1658	36
H(14A)	2454	13390	689	41
H(15A)	1358	11375	-1	43
H(16A)	1653	8429	238	45
H(17A)	2997	7545	1200	38
H(18D)	9460	10772	879	65
H(18E)	9816	10057	1790	65
H(18F)	9132	11772	1678	65
H(19D)	5746	10312	-257	46
H(19E)	5388	11371	514	46
H(19F)	4905	9510	291	46

C4 - C3 C5 C9 H4 sp3 S

C6 - C5 C7 C18 H6 sp3 S

C8 - C7 C9 C19 H8 sp3 S

C9 - O2 N1 C4 C8 sp3 R

C11 - N1 C10 C12 H11 sp3 R

C4A - C3A C5A C9A H4A sp3 S

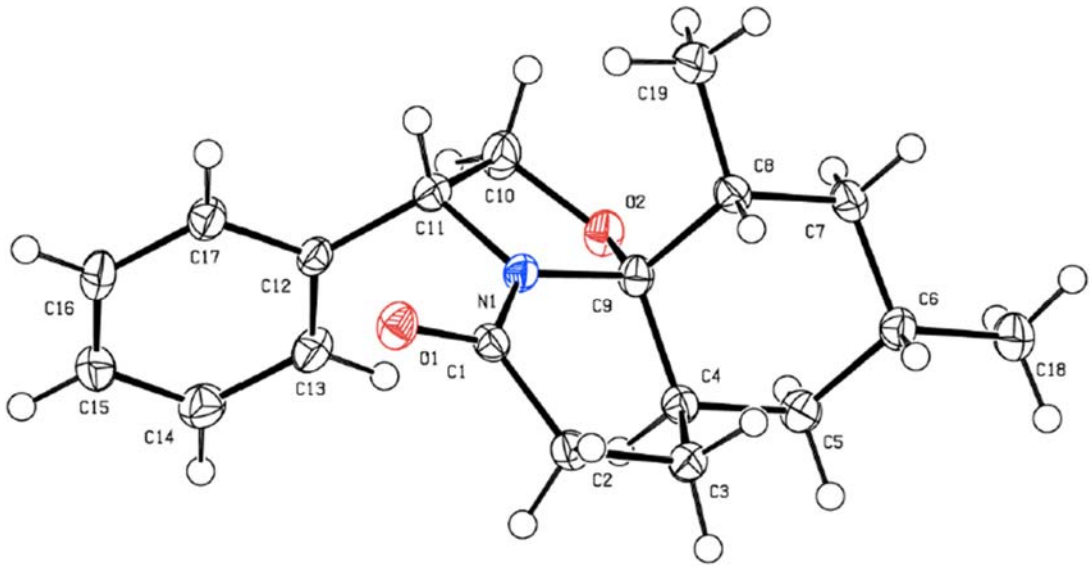
C6A - C5A C7A C18A H6A sp3 S

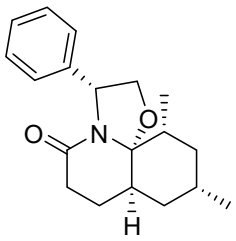
C8A - C7A C9A C19A H8A sp3 S

C9A - O2A N1A C4A C8A sp3 R

C11A - N1A C10A C12A H11A sp3 R

Crystallographic data for compound **8b**:





8b

Table 1. Crystal data and structure refinement for **8b** (D59ZB1A_0m_a).

Identification code	D59ZB1A_0m_a	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.8915(3) Å	α= 90°.
	b = 10.8740(7) Å	β= 90°.
	c = 25.1352(17) Å	γ = 90°.
Volume	1610.27(17) $Å^3$	
Z	4	
Density (calculated)	1.235 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	648	
Crystal size	0.150 x 0.100 x 0.090 mm^3	
Theta range for data collection	2.041 to 30.514°.	
Index ranges	-8<=h<=7, -15<=k<=15, -35<=l<=35	
Reflections collected	34286	
Independent reflections	4900 [R(int) = 0.0799]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6792	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4900 / 0 / 201	
Goodness-of-fit on F^2	1.116	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.0896	
R indices (all data)	R1 = 0.0812, wR2 = 0.1098	
Absolute structure parameter	0.1(6)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.245 and -0.279 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB1A_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7481(3)	6571(2)	5674(1)	24(1)
O(2)	1504(3)	7478(2)	6700(1)	22(1)
N(1)	4731(3)	7246(2)	6221(1)	18(1)
C(1)	6051(4)	7356(2)	5786(1)	18(1)
C(2)	5596(4)	8417(2)	5412(1)	19(1)
C(3)	3876(4)	9381(2)	5590(1)	21(1)
C(4)	2058(4)	8856(2)	5962(1)	18(1)
C(5)	427(4)	9851(2)	6160(1)	22(1)
C(6)	1509(4)	10753(2)	6552(1)	22(1)
C(7)	2591(4)	10036(2)	7008(1)	22(1)
C(8)	4344(4)	9098(2)	6807(1)	20(1)
C(9)	3177(4)	8185(2)	6425(1)	18(1)
C(10)	2525(5)	6357(2)	6880(1)	28(1)
C(11)	4527(4)	6073(2)	6509(1)	22(1)
C(12)	4056(4)	5000(2)	6141(1)	19(1)
C(13)	2062(4)	4953(2)	5851(1)	25(1)
C(14)	1613(5)	3952(2)	5524(1)	29(1)
C(15)	3154(5)	2994(2)	5485(1)	28(1)
C(16)	5147(4)	3038(2)	5773(1)	26(1)
C(17)	5598(4)	4039(2)	6101(1)	23(1)
C(18)	-215(5)	11693(2)	6745(1)	30(1)
C(19)	5645(5)	8514(2)	7268(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB1A_0m_a.

O(1)-C(1)	1.233(3)
O(2)-C(9)	1.427(3)
O(2)-C(10)	1.433(3)
N(1)-C(1)	1.348(3)
N(1)-C(9)	1.465(3)
N(1)-C(11)	1.471(3)
C(1)-C(2)	1.512(3)
C(2)-C(3)	1.525(3)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(4)	1.532(3)
C(3)-H(3A)	0.9900
C(3)-H(3AB)	0.9900
C(4)-C(9)	1.524(3)
C(4)-C(5)	1.529(3)
C(4)-H(4)	1.0000
C(5)-C(6)	1.530(3)
C(5)-H(5A)	0.9900
C(5)-H(5AB)	0.9900
C(6)-C(18)	1.520(3)
C(6)-C(7)	1.525(3)
C(6)-H(6)	1.0000
C(7)-C(8)	1.537(3)
C(7)-H(7A)	0.9900
C(7)-H(7AB)	0.9900
C(8)-C(19)	1.528(4)
C(8)-C(9)	1.542(3)
C(8)-H(8)	1.0000
C(10)-C(11)	1.535(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.515(3)
C(11)-H(11)	1.0000
C(12)-C(13)	1.383(3)

C(12)-C(17)	1.388(3)
C(13)-C(14)	1.390(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.385(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.380(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.392(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(9)-O(2)-C(10)	108.72(18)
C(1)-N(1)-C(9)	125.66(19)
C(1)-N(1)-C(11)	121.53(19)
C(9)-N(1)-C(11)	112.45(18)
O(1)-C(1)-N(1)	121.2(2)
O(1)-C(1)-C(2)	120.5(2)
N(1)-C(1)-C(2)	118.06(19)
C(1)-C(2)-C(3)	117.34(19)
C(1)-C(2)-H(2A)	108.0
C(3)-C(2)-H(2A)	108.0
C(1)-C(2)-H(2AB)	108.0
C(3)-C(2)-H(2AB)	108.0
H(2A)-C(2)-H(2AB)	107.2
C(2)-C(3)-C(4)	112.84(19)
C(2)-C(3)-H(3A)	109.0
C(4)-C(3)-H(3A)	109.0
C(2)-C(3)-H(3AB)	109.0
C(4)-C(3)-H(3AB)	109.0
H(3A)-C(3)-H(3AB)	107.8

C(9)-C(4)-C(5)	111.22(19)
C(9)-C(4)-C(3)	110.01(19)
C(5)-C(4)-C(3)	111.96(19)
C(9)-C(4)-H(4)	107.8
C(5)-C(4)-H(4)	107.8
C(3)-C(4)-H(4)	107.8
C(4)-C(5)-C(6)	113.6(2)
C(4)-C(5)-H(5A)	108.8
C(6)-C(5)-H(5A)	108.8
C(4)-C(5)-H(5AB)	108.8
C(6)-C(5)-H(5AB)	108.8
H(5A)-C(5)-H(5AB)	107.7
C(18)-C(6)-C(7)	112.6(2)
C(18)-C(6)-C(5)	111.0(2)
C(7)-C(6)-C(5)	109.3(2)
C(18)-C(6)-H(6)	107.9
C(7)-C(6)-H(6)	107.9
C(5)-C(6)-H(6)	107.9
C(6)-C(7)-C(8)	111.94(19)
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7AB)	109.2
C(8)-C(7)-H(7AB)	109.2
H(7A)-C(7)-H(7AB)	107.9
C(19)-C(8)-C(7)	111.3(2)
C(19)-C(8)-C(9)	115.4(2)
C(7)-C(8)-C(9)	109.4(2)
C(19)-C(8)-H(8)	106.8
C(7)-C(8)-H(8)	106.8
C(9)-C(8)-H(8)	106.8
O(2)-C(9)-N(1)	103.00(17)
O(2)-C(9)-C(4)	109.17(18)
N(1)-C(9)-C(4)	109.68(19)
O(2)-C(9)-C(8)	110.74(19)
N(1)-C(9)-C(8)	112.82(19)
C(4)-C(9)-C(8)	111.10(18)

O(2)-C(10)-C(11)	107.60(19)
O(2)-C(10)-H(10A)	110.2
C(11)-C(10)-H(10A)	110.2
O(2)-C(10)-H(10B)	110.2
C(11)-C(10)-H(10B)	110.2
H(10A)-C(10)-H(10B)	108.5
N(1)-C(11)-C(12)	112.50(19)
N(1)-C(11)-C(10)	100.75(18)
C(12)-C(11)-C(10)	112.6(2)
N(1)-C(11)-H(11)	110.2
C(12)-C(11)-H(11)	110.2
C(10)-C(11)-H(11)	110.2
C(13)-C(12)-C(17)	119.4(2)
C(13)-C(12)-C(11)	120.4(2)
C(17)-C(12)-C(11)	120.2(2)
C(12)-C(13)-C(14)	120.1(2)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(15)-C(14)-C(13)	120.4(2)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(16)-C(15)-C(14)	119.7(2)
C(16)-C(15)-H(15)	120.2
C(14)-C(15)-H(15)	120.2
C(15)-C(16)-C(17)	120.0(2)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(12)-C(17)-C(16)	120.4(2)
C(12)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(6)-C(18)-H(18A)	109.5
C(6)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(6)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

C(8)-C(19)-H(19A)	109.5
C(8)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(8)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB1A_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

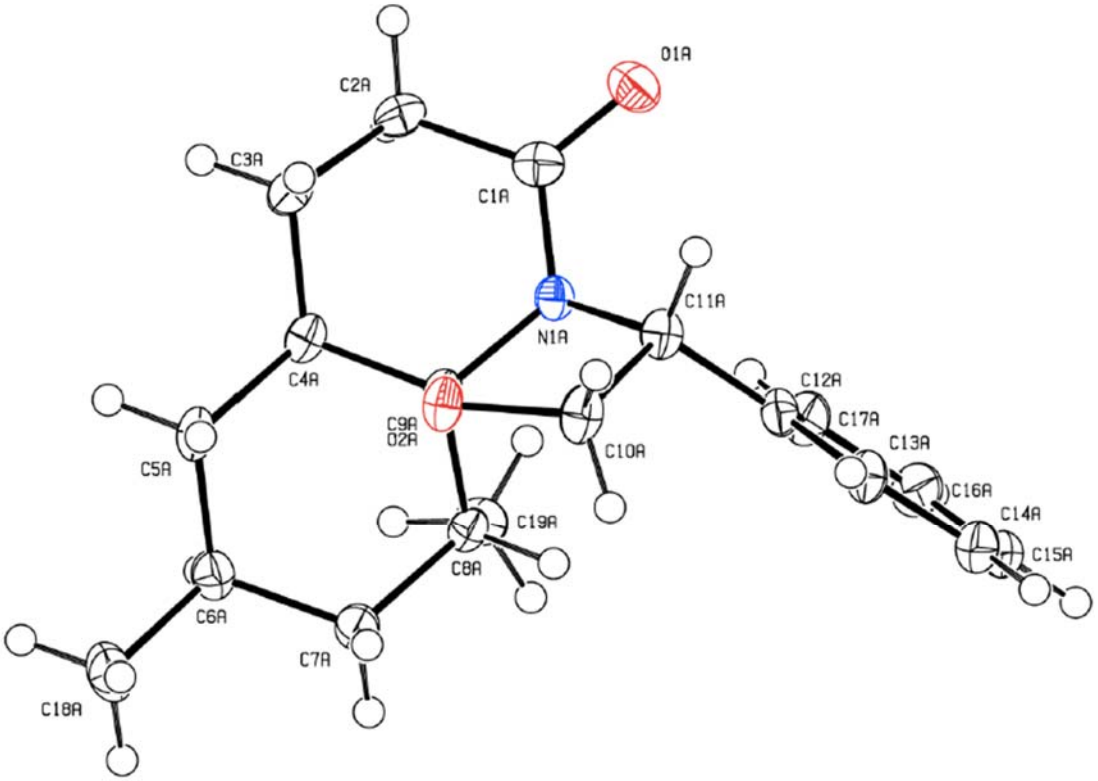
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	21(1)	24(1)	28(1)	-1(1)	4(1)	6(1)
O(2)	24(1)	19(1)	23(1)	2(1)	7(1)	0(1)
N(1)	22(1)	16(1)	17(1)	1(1)	3(1)	3(1)
C(1)	18(1)	19(1)	17(1)	-3(1)	0(1)	1(1)
C(2)	20(1)	20(1)	18(1)	0(1)	2(1)	-1(1)
C(3)	25(1)	19(1)	19(1)	1(1)	1(1)	2(1)
C(4)	18(1)	19(1)	19(1)	-2(1)	0(1)	1(1)
C(5)	18(1)	24(1)	23(1)	-1(1)	0(1)	3(1)
C(6)	24(1)	19(1)	23(1)	-1(1)	2(1)	3(1)
C(7)	24(1)	21(1)	20(1)	-5(1)	1(1)	3(1)
C(8)	22(1)	21(1)	17(1)	-2(1)	0(1)	2(1)
C(9)	17(1)	17(1)	21(1)	-1(1)	3(1)	1(1)
C(10)	39(2)	19(1)	25(1)	2(1)	9(1)	3(1)
C(11)	28(1)	19(1)	18(1)	2(1)	1(1)	4(1)
C(12)	22(1)	15(1)	19(1)	3(1)	3(1)	2(1)
C(13)	25(1)	20(1)	30(1)	3(1)	-2(1)	5(1)
C(14)	31(1)	25(1)	31(1)	2(1)	-9(1)	-1(1)
C(15)	39(2)	20(1)	26(1)	-2(1)	-2(1)	-1(1)
C(16)	29(1)	17(1)	32(1)	-1(1)	3(1)	5(1)
C(17)	23(1)	19(1)	26(1)	0(1)	-1(1)	3(1)
C(18)	34(1)	27(1)	29(1)	-5(1)	-1(1)	9(1)
C(19)	35(1)	29(1)	25(1)	-4(1)	-7(1)	7(1)

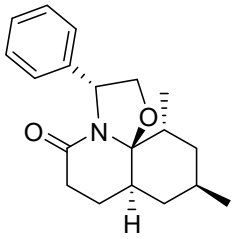
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59ZB1A_0m_a.

	x	y	z	U(eq)
H(2A)	5071	8073	5069	23
H(2AB)	7055	8840	5344	23
H(3A)	3128	9735	5272	25
H(3AB)	4686	10054	5775	25
H(4)	1153	8241	5756	22
H(5A)	-886	9450	6334	26
H(5AB)	-151	10317	5850	26
H(6)	2742	11204	6361	26
H(7A)	1390	9599	7208	26
H(7AB)	3342	10618	7254	26
H(8)	5477	9567	6591	24
H(10A)	1405	5679	6868	33
H(10B)	3065	6450	7250	33
H(11)	5931	5914	6722	26
H(13)	998	5607	5876	30
H(14)	241	3924	5325	35
H(15)	2840	2310	5262	34
H(16)	6213	2386	5746	31
H(17)	6968	4065	6300	28
H(18A)	-709	12202	6445	45
H(18B)	481	12217	7017	45
H(18C)	-1529	11266	6897	45
H(19A)	6671	7881	7130	44
H(19B)	4569	8140	7517	44
H(19C)	6528	9148	7452	44

C4 - C3 C5 C9 H4 sp3 R
C6 - C5 C7 C18 H6 sp3 R
C8 - C7 C9 C19 H8 sp3 R
C9 - O2 N1 C4 C8 sp3 S
C11 - N1 C10 C12 H11 sp3 R

Crystallographic data for compound **8d**:





8d

Table 1. Crystal data and structure refinement for **8d** (D59ZB10_0ma_a1).

Identification code	D59ZB10_0ma_a1	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.1740(7) Å	α= 90°.
	b = 8.1207(9) Å	β= 90°.
	c = 32.235(3) Å	γ = 90°.
Volume	1616.2(3) $Å^3$	
Z	4	
Density (calculated)	1.230 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	648	
Crystal size	0.210 x 0.090 x 0.06 mm^3	
Theta range for data collection	2.527 to 31.697°.	
Index ranges	-8<=h<=8, -11<=k<=11, -47<=l<=46	
Reflections collected	52659	
Independent reflections	5291 [R(int) = 0.1293]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6273	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5291 / 0 / 202	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0675, wR2 = 0.1230	
R indices (all data)	R1 = 0.1220, wR2 = 0.1532	
Absolute structure parameter	0(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.399 and -0.482 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB10_0ma_a1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1A)	723(5)	10085(3)	3695(1)	28(1)
O(2A)	5751(4)	6826(3)	3916(1)	20(1)
N(1A)	2449(4)	7623(3)	3690(1)	18(1)
C(1A)	1261(5)	8839(4)	3883(1)	22(1)
C(2A)	646(6)	8581(5)	4331(1)	26(1)
C(3A)	2397(6)	7667(5)	4572(1)	25(1)
C(4A)	2770(6)	6030(4)	4359(1)	21(1)
C(5A)	4318(6)	4821(4)	4571(1)	23(1)
C(6A)	4321(6)	3151(4)	4356(1)	23(1)
C(7A)	4786(5)	3345(4)	3890(1)	21(1)
C(8A)	3361(5)	4634(4)	3674(1)	19(1)
C(9A)	3536(5)	6273(4)	3911(1)	17(1)
C(10A)	6141(5)	7497(5)	3512(1)	24(1)
C(11A)	3918(5)	8160(4)	3355(1)	20(1)
C(12A)	3339(6)	7580(4)	2919(1)	21(1)
C(13A)	4908(6)	7702(4)	2610(1)	23(1)
C(14A)	4447(7)	7212(4)	2207(1)	27(1)
C(15A)	2413(6)	6593(4)	2107(1)	27(1)
C(16A)	847(6)	6488(5)	2413(1)	28(1)
C(17A)	1312(6)	6987(5)	2817(1)	26(1)
C(18A)	5937(7)	1972(5)	4554(1)	33(1)
C(19A)	1012(6)	4046(4)	3624(1)	25(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB10_0ma_a1.

O(1A)-C(1A)	1.226(4)
O(2A)-C(10A)	1.435(4)
O(2A)-C(9A)	1.439(4)
N(1A)-C(1A)	1.378(4)
N(1A)-C(9A)	1.469(4)
N(1A)-C(11A)	1.476(4)
C(1A)-C(2A)	1.509(5)
C(2A)-C(3A)	1.524(5)
C(2A)-H(1)	0.9700
C(2A)-H(2)	0.9700
C(3A)-C(4A)	1.514(5)
C(3A)-H(3)	0.9700
C(3A)-H(4)	0.9700
C(4A)-C(5A)	1.532(5)
C(4A)-C(9A)	1.533(4)
C(4A)-H(4A)	0.9800
C(5A)-C(6A)	1.523(5)
C(5A)-H(5)	0.9700
C(5A)-H(6)	0.9700
C(6A)-C(18A)	1.523(5)
C(6A)-C(7A)	1.535(4)
C(6A)-H(6A)	0.9800
C(7A)-C(8A)	1.535(5)
C(7A)-H(7)	0.9700
C(7A)-H(8)	0.9700
C(8A)-C(19A)	1.535(5)
C(8A)-C(9A)	1.538(4)
C(8A)-H(8A)	0.9800
C(10A)-C(11A)	1.559(5)
C(10A)-H(10A)	0.9700
C(10A)-H(10B)	0.9700
C(11A)-C(12A)	1.524(5)
C(11A)-H(11A)	0.9800
C(12A)-C(17A)	1.381(5)

C(12A)-C(13A)	1.393(5)
C(13A)-C(14A)	1.390(5)
C(13A)-H(13A)	0.9300
C(14A)-C(15A)	1.390(5)
C(14A)-H(14A)	0.9300
C(15A)-C(16A)	1.384(5)
C(15A)-H(15A)	0.9300
C(16A)-C(17A)	1.395(5)
C(16A)-H(16A)	0.9300
C(17A)-H(17A)	0.9300
C(18A)-H(18A)	0.9600
C(18A)-H(18B)	0.9600
C(18A)-H(18C)	0.9600
C(19A)-H(19A)	0.9600
C(19A)-H(19B)	0.9600
C(19A)-H(19C)	0.9600

C(10A)-O(2A)-C(9A)	105.4(2)
C(1A)-N(1A)-C(9A)	124.0(3)
C(1A)-N(1A)-C(11A)	116.4(3)
C(9A)-N(1A)-C(11A)	107.1(2)
O(1A)-C(1A)-N(1A)	120.9(3)
O(1A)-C(1A)-C(2A)	121.3(3)
N(1A)-C(1A)-C(2A)	117.8(3)
C(1A)-C(2A)-C(3A)	112.2(3)
C(1A)-C(2A)-H(1)	109.2
C(3A)-C(2A)-H(1)	109.2
C(1A)-C(2A)-H(2)	109.2
C(3A)-C(2A)-H(2)	109.2
H(1)-C(2A)-H(2)	107.9
C(4A)-C(3A)-C(2A)	107.7(3)
C(4A)-C(3A)-H(3)	110.2
C(2A)-C(3A)-H(3)	110.2
C(4A)-C(3A)-H(4)	110.2
C(2A)-C(3A)-H(4)	110.2
H(3)-C(3A)-H(4)	108.5

C(3A)-C(4A)-C(5A)	117.0(3)
C(3A)-C(4A)-C(9A)	111.2(3)
C(5A)-C(4A)-C(9A)	108.2(3)
C(3A)-C(4A)-H(4A)	106.6
C(5A)-C(4A)-H(4A)	106.6
C(9A)-C(4A)-H(4A)	106.6
C(6A)-C(5A)-C(4A)	111.5(3)
C(6A)-C(5A)-H(5)	109.3
C(4A)-C(5A)-H(5)	109.3
C(6A)-C(5A)-H(6)	109.3
C(4A)-C(5A)-H(6)	109.3
H(5)-C(5A)-H(6)	108.0
C(18A)-C(6A)-C(5A)	111.6(3)
C(18A)-C(6A)-C(7A)	110.6(3)
C(5A)-C(6A)-C(7A)	110.8(3)
C(18A)-C(6A)-H(6A)	107.9
C(5A)-C(6A)-H(6A)	107.9
C(7A)-C(6A)-H(6A)	107.9
C(6A)-C(7A)-C(8A)	114.0(3)
C(6A)-C(7A)-H(7)	108.7
C(8A)-C(7A)-H(7)	108.7
C(6A)-C(7A)-H(8)	108.7
C(8A)-C(7A)-H(8)	108.7
H(7)-C(7A)-H(8)	107.6
C(19A)-C(8A)-C(7A)	112.2(3)
C(19A)-C(8A)-C(9A)	112.8(3)
C(7A)-C(8A)-C(9A)	108.9(3)
C(19A)-C(8A)-H(8A)	107.6
C(7A)-C(8A)-H(8A)	107.6
C(9A)-C(8A)-H(8A)	107.6
O(2A)-C(9A)-N(1A)	102.0(2)
O(2A)-C(9A)-C(4A)	108.7(2)
N(1A)-C(9A)-C(4A)	114.3(3)
O(2A)-C(9A)-C(8A)	110.1(2)
N(1A)-C(9A)-C(8A)	111.9(2)
C(4A)-C(9A)-C(8A)	109.5(3)

O(2A)-C(10A)-C(11A)	106.1(2)
O(2A)-C(10A)-H(10A)	110.5
C(11A)-C(10A)-H(10A)	110.5
O(2A)-C(10A)-H(10B)	110.5
C(11A)-C(10A)-H(10B)	110.5
H(10A)-C(10A)-H(10B)	108.7
N(1A)-C(11A)-C(12A)	116.0(3)
N(1A)-C(11A)-C(10A)	101.7(2)
C(12A)-C(11A)-C(10A)	113.4(3)
N(1A)-C(11A)-H(11A)	108.5
C(12A)-C(11A)-H(11A)	108.5
C(10A)-C(11A)-H(11A)	108.5
C(17A)-C(12A)-C(13A)	119.0(3)
C(17A)-C(12A)-C(11A)	122.7(3)
C(13A)-C(12A)-C(11A)	118.3(3)
C(14A)-C(13A)-C(12A)	120.5(3)
C(14A)-C(13A)-H(13A)	119.8
C(12A)-C(13A)-H(13A)	119.8
C(13A)-C(14A)-C(15A)	120.3(3)
C(13A)-C(14A)-H(14A)	119.8
C(15A)-C(14A)-H(14A)	119.8
C(16A)-C(15A)-C(14A)	119.3(3)
C(16A)-C(15A)-H(15A)	120.4
C(14A)-C(15A)-H(15A)	120.4
C(15A)-C(16A)-C(17A)	120.3(3)
C(15A)-C(16A)-H(16A)	119.9
C(17A)-C(16A)-H(16A)	119.9
C(12A)-C(17A)-C(16A)	120.7(3)
C(12A)-C(17A)-H(17A)	119.6
C(16A)-C(17A)-H(17A)	119.6
C(6A)-C(18A)-H(18A)	109.5
C(6A)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(6A)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5

C(8A)-C(19A)-H(19A)	109.5
C(8A)-C(19A)-H(19B)	109.5
H(19A)-C(19A)-H(19B)	109.5
C(8A)-C(19A)-H(19C)	109.5
H(19A)-C(19A)-H(19C)	109.5
H(19B)-C(19A)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB10_0ma_a1. 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}
O(1A)	30(1)	24(1)	32(1)	2(1)	-4(1)	3(1)
O(2A)	15(1)	29(1)	16(1)	3(1)	-2(1)	-4(1)
N(1A)	17(1)	20(1)	16(1)	1(1)	-1(1)	-1(1)
C(1A)	17(2)	21(2)	26(2)	-4(1)	-3(1)	-2(1)
C(2A)	27(2)	27(2)	24(2)	-4(1)	6(2)	6(2)
C(3A)	29(2)	29(2)	18(2)	-3(1)	2(1)	3(2)
C(4A)	21(2)	27(2)	16(1)	-1(1)	-1(1)	-2(1)
C(5A)	25(2)	29(2)	15(2)	3(1)	-2(1)	-3(2)
C(6A)	22(2)	26(2)	21(2)	3(1)	-1(1)	1(1)
C(7A)	19(2)	25(2)	20(2)	0(1)	0(1)	2(1)
C(8A)	18(2)	24(2)	15(1)	-1(1)	0(1)	0(1)
C(9A)	14(1)	22(2)	15(1)	-1(1)	-2(1)	-2(1)
C(10A)	18(2)	36(2)	19(2)	4(2)	0(1)	-4(2)
C(11A)	18(2)	23(2)	20(2)	2(1)	1(1)	-5(1)
C(12A)	24(2)	22(2)	16(1)	4(1)	0(1)	1(1)
C(13A)	24(2)	26(2)	19(2)	4(1)	1(1)	-4(1)
C(14A)	33(2)	27(2)	20(2)	3(1)	3(2)	0(2)
C(15A)	34(2)	28(2)	18(2)	-1(1)	-6(1)	8(2)
C(16A)	22(2)	37(2)	25(2)	-4(2)	-8(1)	5(2)
C(17A)	18(2)	36(2)	22(2)	0(2)	-2(1)	4(2)
C(18A)	35(2)	34(2)	29(2)	9(2)	-3(2)	5(2)
C(19A)	22(2)	24(2)	30(2)	-3(1)	-6(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for D59ZB10_0ma_a1.

	x	y	z	U(eq)
H(1)	-693	7957	4344	31
H(2)	391	9642	4460	31
H(3)	3725	8305	4575	30
H(4)	1936	7492	4856	30
H(4A)	1358	5482	4344	25
H(5)	5773	5272	4568	28
H(6)	3887	4680	4859	28
H(6A)	2872	2673	4386	27
H(7)	4574	2289	3756	26
H(8)	6294	3651	3855	26
H(8A)	3953	4810	3395	23
H(10A)	6686	6652	3326	29
H(10B)	7195	8381	3526	29
H(11A)	3970	9367	3355	24
H(13A)	6272	8115	2674	28
H(14A)	5505	7298	2002	32
H(15A)	2108	6254	1838	32
H(16A)	-522	6084	2348	34
H(17A)	245	6919	3020	31
H(18A)	5580	1823	4841	49
H(18B)	7371	2421	4531	49
H(18C)	5880	929	4414	49
H(19A)	915	3312	3391	38
H(19B)	86	4979	3578	38
H(19C)	565	3481	3871	38

Table 6. Torsion angles [°] for D59ZB10_0ma_a1.

C(9A)-N(1A)-C(1A)-O(1A)	166.7(3)
C(11A)-N(1A)-C(1A)-O(1A)	29.7(4)
C(9A)-N(1A)-C(1A)-C(2A)	-13.4(5)
C(11A)-N(1A)-C(1A)-C(2A)	-150.4(3)
O(1A)-C(1A)-C(2A)-C(3A)	-145.3(3)
N(1A)-C(1A)-C(2A)-C(3A)	34.8(4)
C(1A)-C(2A)-C(3A)-C(4A)	-58.1(4)
C(2A)-C(3A)-C(4A)-C(5A)	-174.3(3)
C(2A)-C(3A)-C(4A)-C(9A)	60.8(4)
C(3A)-C(4A)-C(5A)-C(6A)	172.6(3)
C(9A)-C(4A)-C(5A)-C(6A)	-60.9(4)
C(4A)-C(5A)-C(6A)-C(18A)	177.3(3)
C(4A)-C(5A)-C(6A)-C(7A)	53.6(4)
C(18A)-C(6A)-C(7A)-C(8A)	-174.8(3)
C(5A)-C(6A)-C(7A)-C(8A)	-50.4(4)
C(6A)-C(7A)-C(8A)-C(19A)	-72.1(4)
C(6A)-C(7A)-C(8A)-C(9A)	53.4(4)
C(10A)-O(2A)-C(9A)-N(1A)	-41.8(3)
C(10A)-O(2A)-C(9A)-C(4A)	-162.9(3)
C(10A)-O(2A)-C(9A)-C(8A)	77.1(3)
C(1A)-N(1A)-C(9A)-O(2A)	-101.4(3)
C(11A)-N(1A)-C(9A)-O(2A)	38.9(3)
C(1A)-N(1A)-C(9A)-C(4A)	15.8(4)
C(11A)-N(1A)-C(9A)-C(4A)	156.0(3)
C(1A)-N(1A)-C(9A)-C(8A)	141.0(3)
C(11A)-N(1A)-C(9A)-C(8A)	-78.7(3)
C(3A)-C(4A)-C(9A)-O(2A)	73.5(3)
C(5A)-C(4A)-C(9A)-O(2A)	-56.3(3)
C(3A)-C(4A)-C(9A)-N(1A)	-39.7(4)
C(5A)-C(4A)-C(9A)-N(1A)	-169.5(3)
C(3A)-C(4A)-C(9A)-C(8A)	-166.2(3)
C(5A)-C(4A)-C(9A)-C(8A)	64.0(3)
C(19A)-C(8A)-C(9A)-O(2A)	-175.2(3)
C(7A)-C(8A)-C(9A)-O(2A)	59.7(3)

C(19A)-C(8A)-C(9A)-N(1A)	-62.5(4)
C(7A)-C(8A)-C(9A)-N(1A)	172.3(3)
C(19A)-C(8A)-C(9A)-C(4A)	65.3(3)
C(7A)-C(8A)-C(9A)-C(4A)	-59.8(3)
C(9A)-O(2A)-C(10A)-C(11A)	29.4(3)
C(1A)-N(1A)-C(11A)-C(12A)	-113.2(3)
C(9A)-N(1A)-C(11A)-C(12A)	103.0(3)
C(1A)-N(1A)-C(11A)-C(10A)	123.2(3)
C(9A)-N(1A)-C(11A)-C(10A)	-20.5(3)
O(2A)-C(10A)-C(11A)-N(1A)	-5.1(3)
O(2A)-C(10A)-C(11A)-C(12A)	-130.4(3)
N(1A)-C(11A)-C(12A)-C(17A)	17.2(5)
C(10A)-C(11A)-C(12A)-C(17A)	134.4(4)
N(1A)-C(11A)-C(12A)-C(13A)	-164.8(3)
C(10A)-C(11A)-C(12A)-C(13A)	-47.6(4)
C(17A)-C(12A)-C(13A)-C(14A)	-0.9(5)
C(11A)-C(12A)-C(13A)-C(14A)	-179.0(3)
C(12A)-C(13A)-C(14A)-C(15A)	0.0(5)
C(13A)-C(14A)-C(15A)-C(16A)	0.7(5)
C(14A)-C(15A)-C(16A)-C(17A)	-0.5(6)
C(13A)-C(12A)-C(17A)-C(16A)	1.2(6)
C(11A)-C(12A)-C(17A)-C(16A)	179.2(3)
C(15A)-C(16A)-C(17A)-C(12A)	-0.5(6)

Symmetry transformations used to generate equivalent atoms:

C4A - C3A C5A C9A H4A sp3 R

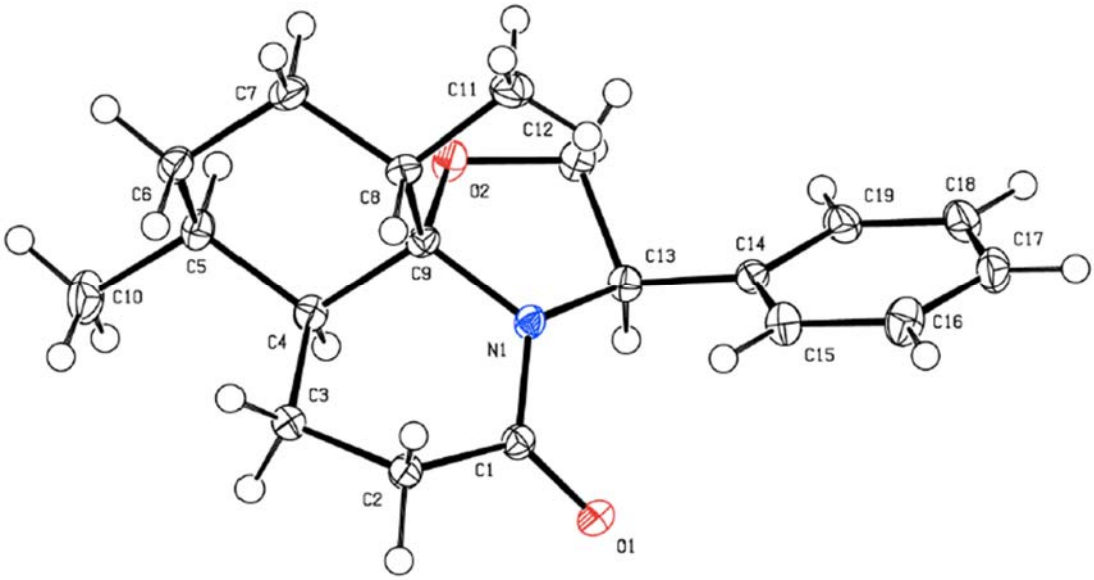
C6A - C5A C7A C18A H6A sp3 S

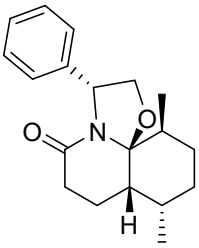
C8A - C7A C9A C19A H8A sp3 R

C9A - O2A N1A C4A C8A sp3 R

C11A - N1A C10A C12A H11A sp3 R

Crystallographic data for compound **9a**:





9a

Table 1. Crystal data and structure refinement for **9a** (D59ZB54_0m_a).

Identification code	D59ZB54_0m_a	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.4807(5) Å	α= 90°.
	b = 10.7621(5) Å	β= 97.909(2)°.
	c = 8.7322(4) Å	γ = 90°.
Volume	789.41(7) $Å^3$	
Z	2	
Density (calculated)	1.260 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	324	
Crystal size	0.350 x 0.200 x 0.120 mm^3	
Theta range for data collection	2.425 to 30.524°.	
Index ranges	-11<=h<=12, -15<=k<=15, -12<=l<=12	
Reflections collected	12791	
Independent reflections	4701 [R(int) = 0.0480]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6549	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4701 / 1 / 201	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0431, wR2 = 0.0983	
R indices (all data)	R1 = 0.0470, wR2 = 0.1010	
Absolute structure parameter	0.0(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.294 and -0.218 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB54_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	146(2)	6086(1)	3421(2)	20(1)
O(2)	3801(2)	3255(1)	4945(2)	17(1)
N(1)	2355(2)	5055(1)	4524(2)	14(1)
C(1)	1570(2)	5847(2)	3459(2)	15(1)
C(2)	2611(2)	6441(2)	2396(2)	18(1)
C(3)	3603(2)	5489(2)	1618(2)	19(1)
C(4)	3898(2)	4271(2)	2534(2)	15(1)
C(5)	5453(2)	3618(2)	2255(2)	17(1)
C(6)	6900(2)	4376(2)	2940(2)	18(1)
C(7)	6889(2)	4588(2)	4665(2)	18(1)
C(8)	5345(2)	5186(2)	5041(2)	14(1)
C(9)	3882(2)	4466(2)	4273(2)	13(1)
C(10)	5464(3)	3326(2)	542(3)	29(1)
C(11)	5410(2)	5303(2)	6793(2)	21(1)
C(12)	2677(2)	3252(2)	6025(2)	20(1)
C(13)	1460(2)	4279(2)	5485(2)	15(1)
C(14)	838(2)	4933(2)	6820(2)	15(1)
C(15)	829(2)	6219(2)	6988(2)	18(1)
C(16)	139(3)	6758(2)	8187(2)	23(1)
C(17)	-522(2)	6026(2)	9239(2)	24(1)
C(18)	-495(3)	4743(2)	9089(2)	24(1)
C(19)	181(2)	4199(2)	7893(2)	19(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB54_0m_a.

O(1)-C(1)	1.231(2)
O(2)-C(12)	1.430(2)
O(2)-C(9)	1.435(2)
N(1)-C(1)	1.365(2)
N(1)-C(13)	1.468(2)
N(1)-C(9)	1.485(2)
C(1)-C(2)	1.508(3)
C(2)-C(3)	1.542(3)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(4)	1.538(3)
C(3)-H(3A)	0.9900
C(3)-H(3AB)	0.9900
C(4)-C(9)	1.535(2)
C(4)-C(5)	1.544(3)
C(4)-H(4)	1.0000
C(5)-C(6)	1.526(3)
C(5)-C(10)	1.530(3)
C(5)-H(5)	1.0000
C(6)-C(7)	1.525(3)
C(6)-H(6A)	0.9900
C(6)-H(6AB)	0.9900
C(7)-C(8)	1.534(3)
C(7)-H(7A)	0.9900
C(7)-H(7AB)	0.9900
C(8)-C(11)	1.529(3)
C(8)-C(9)	1.536(2)
C(8)-H(8)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800

C(12)-C(13)	1.540(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.517(3)
C(13)-H(13)	1.0000
C(14)-C(15)	1.391(3)
C(14)-C(19)	1.399(3)
C(15)-C(16)	1.395(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.386(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.387(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.388(3)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500

C(12)-O(2)-C(9)	110.21(14)
C(1)-N(1)-C(13)	120.20(15)
C(1)-N(1)-C(9)	121.32(15)
C(13)-N(1)-C(9)	111.81(14)
O(1)-C(1)-N(1)	122.25(18)
O(1)-C(1)-C(2)	123.36(17)
N(1)-C(1)-C(2)	114.33(16)
C(1)-C(2)-C(3)	112.98(16)
C(1)-C(2)-H(2A)	109.0
C(3)-C(2)-H(2A)	109.0
C(1)-C(2)-H(2AB)	109.0
C(3)-C(2)-H(2AB)	109.0
H(2A)-C(2)-H(2AB)	107.8
C(4)-C(3)-C(2)	113.36(15)
C(4)-C(3)-H(3A)	108.9
C(2)-C(3)-H(3A)	108.9
C(4)-C(3)-H(3AB)	108.9
C(2)-C(3)-H(3AB)	108.9
H(3A)-C(3)-H(3AB)	107.7

C(9)-C(4)-C(3)	112.09(15)
C(9)-C(4)-C(5)	110.02(15)
C(3)-C(4)-C(5)	112.78(15)
C(9)-C(4)-H(4)	107.2
C(3)-C(4)-H(4)	107.2
C(5)-C(4)-H(4)	107.2
C(6)-C(5)-C(10)	112.37(17)
C(6)-C(5)-C(4)	110.68(15)
C(10)-C(5)-C(4)	111.62(17)
C(6)-C(5)-H(5)	107.3
C(10)-C(5)-H(5)	107.3
C(4)-C(5)-H(5)	107.3
C(7)-C(6)-C(5)	110.68(15)
C(7)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6A)	109.5
C(7)-C(6)-H(6AB)	109.5
C(5)-C(6)-H(6AB)	109.5
H(6A)-C(6)-H(6AB)	108.1
C(6)-C(7)-C(8)	113.30(15)
C(6)-C(7)-H(7A)	108.9
C(8)-C(7)-H(7A)	108.9
C(6)-C(7)-H(7AB)	108.9
C(8)-C(7)-H(7AB)	108.9
H(7A)-C(7)-H(7AB)	107.7
C(11)-C(8)-C(7)	109.52(15)
C(11)-C(8)-C(9)	113.19(15)
C(7)-C(8)-C(9)	110.89(15)
C(11)-C(8)-H(8)	107.7
C(7)-C(8)-H(8)	107.7
C(9)-C(8)-H(8)	107.7
O(2)-C(9)-N(1)	103.62(14)
O(2)-C(9)-C(4)	106.77(14)
N(1)-C(9)-C(4)	109.28(14)
O(2)-C(9)-C(8)	111.17(14)
N(1)-C(9)-C(8)	112.88(14)
C(4)-C(9)-C(8)	112.59(15)

C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(2)-C(12)-C(13)	106.02(15)
O(2)-C(12)-H(12A)	110.5
C(13)-C(12)-H(12A)	110.5
O(2)-C(12)-H(12B)	110.5
C(13)-C(12)-H(12B)	110.5
H(12A)-C(12)-H(12B)	108.7
N(1)-C(13)-C(14)	115.94(15)
N(1)-C(13)-C(12)	101.89(14)
C(14)-C(13)-C(12)	112.77(15)
N(1)-C(13)-H(13)	108.6
C(14)-C(13)-H(13)	108.6
C(12)-C(13)-H(13)	108.6
C(15)-C(14)-C(19)	118.86(18)
C(15)-C(14)-C(13)	123.38(17)
C(19)-C(14)-C(13)	117.71(16)
C(14)-C(15)-C(16)	120.14(19)
C(14)-C(15)-H(15)	119.9
C(16)-C(15)-H(15)	119.9
C(17)-C(16)-C(15)	120.7(2)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(16)-C(17)-C(18)	119.3(2)
C(16)-C(17)-H(17)	120.3
C(18)-C(17)-H(17)	120.3

C(17)-C(18)-C(19)	120.3(2)
C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(18)-C(19)-C(14)	120.63(19)
C(18)-C(19)-H(19)	119.7
C(14)-C(19)-H(19)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB54_0m_a. 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}
O(1)	16(1)	26(1)	21(1)	3(1)	4(1)	6(1)
O(2)	20(1)	10(1)	24(1)	4(1)	10(1)	2(1)
N(1)	12(1)	13(1)	16(1)	2(1)	5(1)	0(1)
C(1)	16(1)	14(1)	15(1)	-1(1)	3(1)	1(1)
C(2)	17(1)	19(1)	18(1)	6(1)	6(1)	4(1)
C(3)	18(1)	24(1)	16(1)	4(1)	5(1)	5(1)
C(4)	14(1)	16(1)	16(1)	-2(1)	2(1)	-1(1)
C(5)	18(1)	16(1)	20(1)	-2(1)	6(1)	1(1)
C(6)	15(1)	18(1)	22(1)	3(1)	5(1)	2(1)
C(7)	13(1)	19(1)	21(1)	3(1)	1(1)	1(1)
C(8)	13(1)	12(1)	16(1)	1(1)	0(1)	0(1)
C(9)	12(1)	11(1)	16(1)	1(1)	2(1)	1(1)
C(10)	29(1)	34(1)	26(1)	-10(1)	10(1)	2(1)
C(11)	22(1)	21(1)	18(1)	-2(1)	-2(1)	2(1)
C(12)	22(1)	14(1)	26(1)	5(1)	10(1)	3(1)
C(13)	16(1)	13(1)	17(1)	1(1)	4(1)	-2(1)
C(14)	12(1)	18(1)	14(1)	0(1)	2(1)	-1(1)
C(15)	20(1)	17(1)	19(1)	-2(1)	5(1)	-4(1)
C(16)	22(1)	22(1)	25(1)	-8(1)	6(1)	-2(1)
C(17)	19(1)	35(1)	17(1)	-6(1)	5(1)	-1(1)
C(18)	22(1)	33(1)	17(1)	4(1)	6(1)	-1(1)
C(19)	19(1)	21(1)	18(1)	4(1)	4(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59ZB54_0m_a.

	x	y	z	U(eq)
H(2A)	3340	7038	2996	21
H(2AB)	1931	6913	1585	21
H(3A)	3044	5296	574	23
H(3AB)	4642	5866	1492	23
H(4)	3000	3696	2162	18
H(5)	5501	2807	2819	21
H(6A)	7885	3931	2777	21
H(6AB)	6893	5188	2405	21
H(7A)	7798	5129	5063	22
H(7AB)	7040	3780	5208	22
H(8)	5286	6045	4599	17
H(10A)	4504	2856	147	43
H(10B)	6409	2831	419	43
H(10C)	5486	4104	-39	43
H(11A)	6229	5908	7188	31
H(11B)	5669	4493	7276	31
H(11C)	4373	5582	7037	31
H(12A)	3215	3429	7082	24
H(12B)	2142	2435	6029	24
H(13)	541	3895	4810	18
H(15)	1294	6730	6284	22
H(16)	121	7637	8284	28
H(17)	-988	6398	10055	28
H(18)	-942	4234	9807	29
H(19)	198	3319	7802	23

C4 - C3 C5 C9 H4 sp3 S

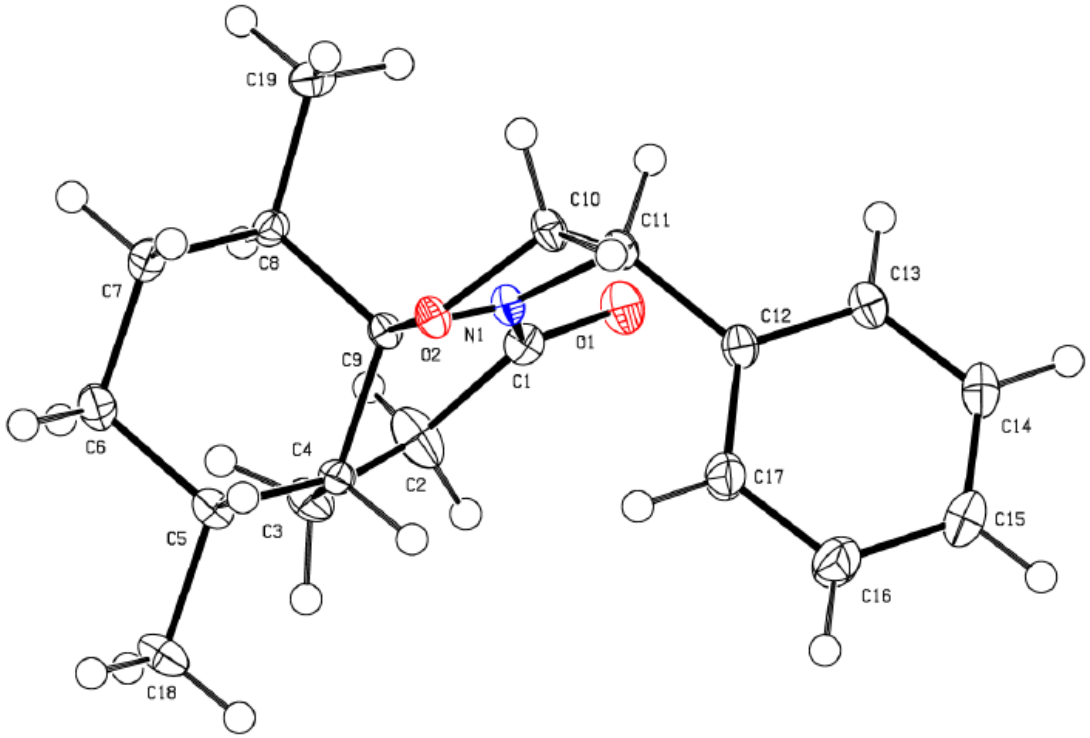
C5 - C4 C6 C10 H5 sp3 S

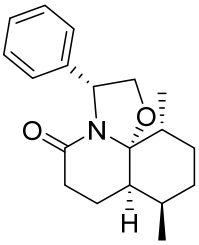
C8 - C7 C9 C11 H8 sp3 S

C9 - O2 N1 C4 C8 sp3 S

C13 - N1 C12 C14 H13 sp3 R

Crystallographic data for compound **9b**:





9b

Table 1. Crystal data and structure refinement for **9b** (D59ZB89_0m).

Identification code	d59zb89_0m	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.2337(3) Å	α= 90°.
	b = 12.0198(3) Å	β= 90°.
	c = 15.9765(5) Å	γ = 90°.
Volume	1581.15(9) $Å^3$	
Z	4	
Density (calculated)	1.258 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	648	
Crystal size	0.300 x 0.260 x 0.150 mm^3	
Theta range for data collection	4.185 to 30.522°.	
Index ranges	-11<=h<=10, -12<=k<=17, -22<=l<=17	
Reflections collected	15601	
Independent reflections	4717 [R(int) = 0.0285]	
Completeness to theta = 25.242°	97.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6604	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4717 / 0 / 201	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0918	
R indices (all data)	R1 = 0.0375, wR2 = 0.0943	
Absolute structure parameter	0.0(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.352 and -0.196 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB89_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3782(1)	6671(1)	4561(1)	21(1)
O(2)	5037(1)	5387(1)	7129(1)	14(1)
N(1)	4219(1)	6144(1)	5899(1)	14(1)
C(1)	3247(2)	6308(1)	5225(1)	16(1)
C(2)	1483(2)	5989(2)	5319(1)	27(1)
C(3)	936(2)	5357(1)	6102(1)	20(1)
C(4)	2326(2)	4941(1)	6667(1)	14(1)
C(5)	1766(2)	4566(1)	7543(1)	17(1)
C(6)	1154(2)	5549(1)	8063(1)	19(1)
C(7)	2420(2)	6485(1)	8101(1)	18(1)
C(8)	2984(2)	6859(1)	7225(1)	14(1)
C(9)	3628(2)	5844(1)	6737(1)	12(1)
C(10)	6461(2)	5846(1)	6745(1)	16(1)
C(11)	5998(2)	6094(1)	5831(1)	14(1)
C(12)	6560(2)	5194(1)	5233(1)	16(1)
C(13)	7538(2)	5460(1)	4553(1)	18(1)
C(14)	8144(2)	4630(1)	4029(1)	22(1)
C(15)	7756(2)	3525(1)	4179(1)	26(1)
C(16)	6755(2)	3250(1)	4850(1)	29(1)
C(17)	6165(2)	4077(1)	5373(1)	24(1)
C(18)	503(2)	3637(1)	7505(1)	23(1)
C(19)	4179(2)	7824(1)	7291(1)	19(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB89_0m.

O(1)-C(1)	1.2291(18)
O(2)-C(9)	1.4281(15)
O(2)-C(10)	1.4341(16)
N(1)-C(1)	1.3556(18)
N(1)-C(11)	1.4699(17)
N(1)-C(9)	1.4703(17)
C(1)-C(2)	1.509(2)
C(2)-C(3)	1.532(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.541(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.5294(18)
C(4)-C(5)	1.542(2)
C(4)-H(4)	1.0000
C(5)-C(18)	1.526(2)
C(5)-C(6)	1.529(2)
C(5)-H(5)	1.0000
C(6)-C(7)	1.535(2)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.541(2)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(19)	1.5246(19)
C(8)-C(9)	1.5413(18)
C(8)-H(8)	1.0000
C(10)-C(11)	1.5389(19)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.5162(19)
C(11)-H(11)	1.0000
C(12)-C(13)	1.3899(19)

C(12)-C(17)	1.399(2)
C(13)-C(14)	1.394(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.386(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.393(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.386(2)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(9)-O(2)-C(10)	109.18(9)
C(1)-N(1)-C(11)	122.39(12)
C(1)-N(1)-C(9)	124.29(11)
C(11)-N(1)-C(9)	112.78(11)
O(1)-C(1)-N(1)	121.70(13)
O(1)-C(1)-C(2)	121.36(13)
N(1)-C(1)-C(2)	116.91(12)
C(1)-C(2)-C(3)	119.35(13)
C(1)-C(2)-H(2A)	107.5
C(3)-C(2)-H(2A)	107.5
C(1)-C(2)-H(2B)	107.5
C(3)-C(2)-H(2B)	107.5
H(2A)-C(2)-H(2B)	107.0
C(2)-C(3)-C(4)	114.87(12)
C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3A)	108.6
C(2)-C(3)-H(3B)	108.6
C(4)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.5

C(9)-C(4)-C(3)	109.47(11)
C(9)-C(4)-C(5)	110.50(11)
C(3)-C(4)-C(5)	113.83(11)
C(9)-C(4)-H(4)	107.6
C(3)-C(4)-H(4)	107.6
C(5)-C(4)-H(4)	107.6
C(18)-C(5)-C(6)	111.25(12)
C(18)-C(5)-C(4)	112.42(12)
C(6)-C(5)-C(4)	111.43(11)
C(18)-C(5)-H(5)	107.1
C(6)-C(5)-H(5)	107.1
C(4)-C(5)-H(5)	107.1
C(5)-C(6)-C(7)	111.34(11)
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6B)	109.4
C(7)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(6)-C(7)-C(8)	112.48(11)
C(6)-C(7)-H(7A)	109.1
C(8)-C(7)-H(7A)	109.1
C(6)-C(7)-H(7B)	109.1
C(8)-C(7)-H(7B)	109.1
H(7A)-C(7)-H(7B)	107.8
C(19)-C(8)-C(9)	114.55(11)
C(19)-C(8)-C(7)	110.72(12)
C(9)-C(8)-C(7)	109.38(11)
C(19)-C(8)-H(8)	107.3
C(9)-C(8)-H(8)	107.3
C(7)-C(8)-H(8)	107.3
O(2)-C(9)-N(1)	103.01(10)
O(2)-C(9)-C(4)	109.17(10)
N(1)-C(9)-C(4)	109.83(11)
O(2)-C(9)-C(8)	111.22(10)
N(1)-C(9)-C(8)	112.32(10)
C(4)-C(9)-C(8)	110.99(10)

O(2)-C(10)-C(11)	106.15(10)
O(2)-C(10)-H(10A)	110.5
C(11)-C(10)-H(10A)	110.5
O(2)-C(10)-H(10B)	110.5
C(11)-C(10)-H(10B)	110.5
H(10A)-C(10)-H(10B)	108.7
N(1)-C(11)-C(12)	112.34(11)
N(1)-C(11)-C(10)	100.64(11)
C(12)-C(11)-C(10)	112.62(11)
N(1)-C(11)-H(11)	110.3
C(12)-C(11)-H(11)	110.3
C(10)-C(11)-H(11)	110.3
C(13)-C(12)-C(17)	118.76(13)
C(13)-C(12)-C(11)	120.33(13)
C(17)-C(12)-C(11)	120.86(13)
C(12)-C(13)-C(14)	120.70(14)
C(12)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6
C(15)-C(14)-C(13)	120.03(14)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	119.75(15)
C(14)-C(15)-H(15)	120.1
C(16)-C(15)-H(15)	120.1
C(17)-C(16)-C(15)	120.07(15)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(12)	120.68(15)
C(16)-C(17)-H(17)	119.7
C(12)-C(17)-H(17)	119.7
C(5)-C(18)-H(18A)	109.5
C(5)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(5)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

C(8)-C(19)-H(19A)	109.5
C(8)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(8)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB89_0m. 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}
O(1)	21(1)	26(1)	15(1)	5(1)	0(1)	2(1)
O(2)	9(1)	17(1)	14(1)	3(1)	-1(1)	1(1)
N(1)	11(1)	16(1)	13(1)	1(1)	1(1)	1(1)
C(1)	16(1)	16(1)	15(1)	1(1)	-1(1)	2(1)
C(2)	15(1)	42(1)	24(1)	12(1)	-5(1)	-3(1)
C(3)	14(1)	24(1)	21(1)	2(1)	-3(1)	-3(1)
C(4)	12(1)	13(1)	15(1)	0(1)	0(1)	-1(1)
C(5)	14(1)	17(1)	19(1)	2(1)	1(1)	-2(1)
C(6)	17(1)	22(1)	20(1)	1(1)	4(1)	0(1)
C(7)	19(1)	18(1)	16(1)	-2(1)	2(1)	2(1)
C(8)	14(1)	12(1)	15(1)	-1(1)	0(1)	1(1)
C(9)	10(1)	13(1)	12(1)	1(1)	0(1)	1(1)
C(10)	10(1)	21(1)	16(1)	1(1)	0(1)	-1(1)
C(11)	12(1)	16(1)	15(1)	2(1)	1(1)	0(1)
C(12)	13(1)	18(1)	16(1)	1(1)	1(1)	2(1)
C(13)	14(1)	22(1)	18(1)	2(1)	1(1)	0(1)
C(14)	18(1)	31(1)	17(1)	-1(1)	3(1)	3(1)
C(15)	27(1)	28(1)	22(1)	-5(1)	3(1)	7(1)
C(16)	37(1)	19(1)	30(1)	-2(1)	9(1)	3(1)
C(17)	28(1)	19(1)	23(1)	1(1)	10(1)	1(1)
C(18)	20(1)	23(1)	26(1)	5(1)	0(1)	-9(1)
C(19)	20(1)	14(1)	22(1)	-2(1)	-2(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59ZB89_0m.

	x	y	z	U(eq)
H(2A)	1186	5532	4827	32
H(2B)	834	6681	5287	32
H(3A)	278	4709	5925	24
H(3B)	224	5850	6436	24
H(4)	2832	4284	6385	16
H(5)	2739	4258	7837	20
H(6A)	904	5293	8637	23
H(6B)	138	5839	7812	23
H(7A)	3373	6224	8424	21
H(7B)	1949	7130	8400	21
H(8)	2006	7139	6920	16
H(10A)	7370	5308	6769	19
H(10B)	6795	6537	7035	19
H(11)	6440	6833	5656	17
H(13)	7797	6217	4443	22
H(14)	8822	4821	3570	26
H(15)	8171	2958	3824	31
H(16)	6476	2494	4950	34
H(17)	5486	3884	5831	28
H(18A)	272	3372	8073	35
H(18B)	925	3021	7167	35
H(18C)	-497	3922	7251	35
H(19A)	5061	7623	7673	28
H(19B)	3614	8483	7505	28
H(19C)	4628	7987	6736	28

Table 6. Torsion angles [°] for D59ZB89_0m.

C(11)-N(1)-C(1)-O(1)	-16.8(2)
C(9)-N(1)-C(1)-O(1)	172.30(12)
C(11)-N(1)-C(1)-C(2)	161.24(14)
C(9)-N(1)-C(1)-C(2)	-9.7(2)
O(1)-C(1)-C(2)-C(3)	169.44(14)
N(1)-C(1)-C(2)-C(3)	-8.6(2)
C(1)-C(2)-C(3)-C(4)	-9.3(2)
C(2)-C(3)-C(4)-C(9)	41.75(17)
C(2)-C(3)-C(4)-C(5)	165.97(13)
C(9)-C(4)-C(5)-C(18)	-178.17(12)
C(3)-C(4)-C(5)-C(18)	58.16(16)
C(9)-C(4)-C(5)-C(6)	56.16(14)
C(3)-C(4)-C(5)-C(6)	-67.50(15)
C(18)-C(5)-C(6)-C(7)	-179.91(12)
C(4)-C(5)-C(6)-C(7)	-53.61(16)
C(5)-C(6)-C(7)-C(8)	54.03(16)
C(6)-C(7)-C(8)-C(19)	177.31(11)
C(6)-C(7)-C(8)-C(9)	-55.53(14)
C(10)-O(2)-C(9)-N(1)	25.72(12)
C(10)-O(2)-C(9)-C(4)	142.40(11)
C(10)-O(2)-C(9)-C(8)	-94.80(12)
C(1)-N(1)-C(9)-O(2)	160.07(11)
C(11)-N(1)-C(9)-O(2)	-11.63(14)
C(1)-N(1)-C(9)-C(4)	43.87(16)
C(11)-N(1)-C(9)-C(4)	-127.84(12)
C(1)-N(1)-C(9)-C(8)	-80.16(15)
C(11)-N(1)-C(9)-C(8)	108.13(12)
C(3)-C(4)-C(9)-O(2)	-169.48(11)
C(5)-C(4)-C(9)-O(2)	64.38(13)
C(3)-C(4)-C(9)-N(1)	-57.22(14)
C(5)-C(4)-C(9)-N(1)	176.63(10)
C(3)-C(4)-C(9)-C(8)	67.58(14)
C(5)-C(4)-C(9)-C(8)	-58.56(14)
C(19)-C(8)-C(9)-O(2)	60.96(15)

C(7)-C(8)-C(9)-O(2)	-64.00(13)
C(19)-C(8)-C(9)-N(1)	-53.90(15)
C(7)-C(8)-C(9)-N(1)	-178.86(11)
C(19)-C(8)-C(9)-C(4)	-177.29(12)
C(7)-C(8)-C(9)-C(4)	57.75(14)
C(9)-O(2)-C(10)-C(11)	-30.31(13)
C(1)-N(1)-C(11)-C(12)	-57.46(17)
C(9)-N(1)-C(11)-C(12)	114.43(12)
C(1)-N(1)-C(11)-C(10)	-177.48(11)
C(9)-N(1)-C(11)-C(10)	-5.59(14)
O(2)-C(10)-C(11)-N(1)	20.90(13)
O(2)-C(10)-C(11)-C(12)	-98.91(12)
N(1)-C(11)-C(12)-C(13)	122.92(14)
C(10)-C(11)-C(12)-C(13)	-124.29(14)
N(1)-C(11)-C(12)-C(17)	-59.87(18)
C(10)-C(11)-C(12)-C(17)	52.93(18)
C(17)-C(12)-C(13)-C(14)	-1.3(2)
C(11)-C(12)-C(13)-C(14)	175.98(13)
C(12)-C(13)-C(14)-C(15)	0.8(2)
C(13)-C(14)-C(15)-C(16)	0.3(2)
C(14)-C(15)-C(16)-C(17)	-0.8(3)
C(15)-C(16)-C(17)-C(12)	0.2(3)
C(13)-C(12)-C(17)-C(16)	0.8(2)
C(11)-C(12)-C(17)-C(16)	-176.46(15)

Symmetry transformations used to generate equivalent atoms:

C(4) - C(3) C(5) C(9) H(4) sp3 R

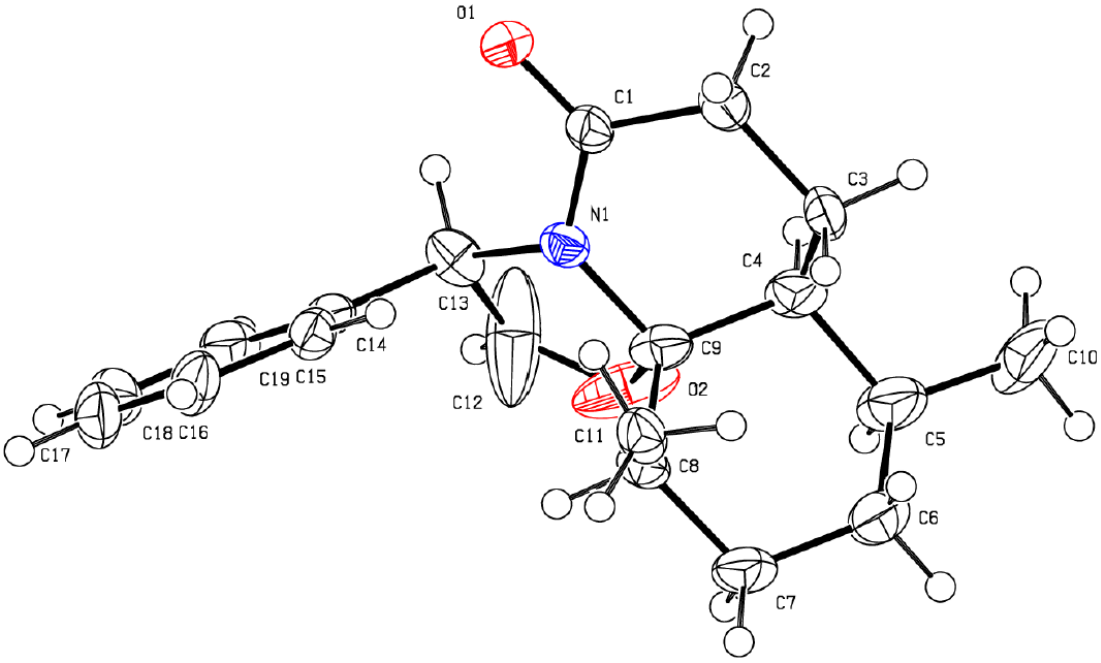
C(5) - C(4) C(6) C(18) H(5) sp3 R

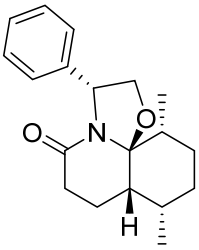
C(8) - C(7) C(9) C(19) H(8) sp3 R

C(9) - O(2) N(1) C(4) C(8) sp3 R

C(11) - N(1) C(10) C(12) H(11) sp3 R

Crystallographic data for compound **9c**:





9c

Table 1. Crystal data and structure refinement for **9c** (D59ZB65_0m_a).

Identification code	D59ZB65_0m_a	
Empirical formula	C19 H24 N O2	
Formula weight	298.39	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2	
Unit cell dimensions	a = 23.3675(16) Å	α= 90°.
	b = 6.3104(4) Å	β= 113.927(2)°.
	c = 11.8556(8) Å	γ = 90°.
Volume	1597.97(19) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	644	
Crystal size	0.350 x 0.200 x 0.150 mm^3	
Theta range for data collection	3.458 to 26.398°.	
Index ranges	-29<=h<=29, -7<=k<=7, -14<=l<=14	
Reflections collected	10863	
Independent reflections	3131 [R(int) = 0.0240]	
Completeness to theta = 25.242°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6953	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3131 / 1 / 201	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0641, wR2 = 0.1406	
R indices (all data)	R1 = 0.0683, wR2 = 0.1441	
Absolute structure parameter	0.0(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.689 and -0.507 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for D59ZB65_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7498(1)	7842(5)	8310(2)	33(1)
O(2)	6360(2)	2084(6)	7154(4)	66(1)
N(1)	6714(1)	5483(5)	7516(3)	26(1)
C(1)	7055(2)	6912(7)	8382(3)	26(1)
C(2)	6890(2)	7283(8)	9476(3)	36(1)
C(3)	6357(2)	5910(9)	9541(4)	45(1)
C(4)	6305(2)	3784(8)	8907(4)	42(1)
C(5)	5798(2)	2217(10)	8933(5)	57(2)
C(6)	5137(2)	2998(11)	8082(4)	54(1)
C(7)	5072(2)	3225(9)	6784(4)	41(1)
C(8)	5561(2)	4768(7)	6682(3)	30(1)
C(9)	6226(2)	4071(7)	7592(4)	33(1)
C(10)	5871(2)	1730(11)	10196(5)	71(2)
C(11)	5388(2)	7080(8)	6776(3)	33(1)
C(12)	6793(5)	2270(10)	6692(7)	97(3)
C(13)	6978(2)	4523(7)	6708(4)	33(1)
C(14)	6771(2)	5498(7)	5425(3)	26(1)
C(15)	6437(2)	7378(7)	5101(3)	29(1)
C(16)	6274(2)	8227(8)	3921(4)	38(1)
C(17)	6432(2)	7162(10)	3071(4)	47(1)
C(18)	6761(2)	5293(9)	3383(4)	42(1)
C(19)	6936(2)	4465(7)	4555(4)	35(1)

Table 3. Bond lengths [Å] and angles [°] for D59ZB65_0m_a.

O(1)-C(1)	1.223(5)
O(2)-C(12)	1.337(7)
O(2)-C(9)	1.439(5)
N(1)-C(1)	1.356(5)
N(1)-C(13)	1.464(5)
N(1)-C(9)	1.478(5)
C(1)-C(2)	1.513(5)
C(2)-C(3)	1.545(6)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(4)	1.518(8)
C(3)-H(3A)	0.9900
C(3)-H(3AB)	0.9900
C(4)-C(9)	1.505(6)
C(4)-C(5)	1.553(6)
C(4)-H(4)	1.0000
C(5)-C(10)	1.468(7)
C(5)-C(6)	1.543(6)
C(5)-H(5)	1.0000
C(6)-C(7)	1.491(6)
C(6)-H(6A)	0.9900
C(6)-H(6AB)	0.9900
C(7)-C(8)	1.542(6)
C(7)-H(7A)	0.9900
C(7)-H(7AB)	0.9900
C(8)-C(11)	1.530(6)
C(8)-C(9)	1.554(5)
C(8)-H(8)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800

C(12)-C(13)	1.483(8)
C(12)-H(12)	0.9500
C(13)-C(14)	1.526(5)
C(13)-H(13)	1.0000
C(14)-C(15)	1.385(5)
C(14)-C(19)	1.400(5)
C(15)-C(16)	1.398(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.379(7)
C(16)-H(16)	0.9500
C(17)-C(18)	1.375(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.382(6)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500

C(12)-O(2)-C(9)	112.5(4)
C(1)-N(1)-C(13)	119.8(3)
C(1)-N(1)-C(9)	125.8(3)
C(13)-N(1)-C(9)	109.3(3)
O(1)-C(1)-N(1)	121.3(3)
O(1)-C(1)-C(2)	120.2(4)
N(1)-C(1)-C(2)	118.5(3)
C(1)-C(2)-C(3)	116.5(4)
C(1)-C(2)-H(2A)	108.2
C(3)-C(2)-H(2A)	108.2
C(1)-C(2)-H(2AB)	108.2
C(3)-C(2)-H(2AB)	108.2
H(2A)-C(2)-H(2AB)	107.3
C(4)-C(3)-C(2)	112.1(4)
C(4)-C(3)-H(3A)	109.2
C(2)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3AB)	109.2
C(2)-C(3)-H(3AB)	109.2
H(3A)-C(3)-H(3AB)	107.9
C(9)-C(4)-C(3)	111.0(4)

C(9)-C(4)-C(5)	108.9(4)
C(3)-C(4)-C(5)	117.5(4)
C(9)-C(4)-H(4)	106.3
C(3)-C(4)-H(4)	106.3
C(5)-C(4)-H(4)	106.3
C(10)-C(5)-C(6)	113.9(4)
C(10)-C(5)-C(4)	112.3(4)
C(6)-C(5)-C(4)	110.6(4)
C(10)-C(5)-H(5)	106.5
C(6)-C(5)-H(5)	106.5
C(4)-C(5)-H(5)	106.5
C(7)-C(6)-C(5)	111.2(4)
C(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6AB)	109.4
C(5)-C(6)-H(6AB)	109.4
H(6A)-C(6)-H(6AB)	108.0
C(6)-C(7)-C(8)	111.9(4)
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7AB)	109.2
C(8)-C(7)-H(7AB)	109.2
H(7A)-C(7)-H(7AB)	107.9
C(11)-C(8)-C(7)	111.8(3)
C(11)-C(8)-C(9)	116.0(3)
C(7)-C(8)-C(9)	109.3(3)
C(11)-C(8)-H(8)	106.4
C(7)-C(8)-H(8)	106.4
C(9)-C(8)-H(8)	106.4
O(2)-C(9)-N(1)	102.5(3)
O(2)-C(9)-C(4)	108.4(4)
N(1)-C(9)-C(4)	111.3(3)
O(2)-C(9)-C(8)	107.4(3)
N(1)-C(9)-C(8)	111.5(3)
C(4)-C(9)-C(8)	114.9(3)
C(5)-C(10)-H(10A)	109.5

C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(2)-C(12)-C(13)	110.1(5)
O(2)-C(12)-H(12)	125.0
C(13)-C(12)-H(12)	125.0
N(1)-C(13)-C(12)	102.0(4)
N(1)-C(13)-C(14)	115.9(3)
C(12)-C(13)-C(14)	113.6(4)
N(1)-C(13)-H(13)	108.3
C(12)-C(13)-H(13)	108.3
C(14)-C(13)-H(13)	108.3
C(15)-C(14)-C(19)	119.1(4)
C(15)-C(14)-C(13)	122.5(3)
C(19)-C(14)-C(13)	118.4(4)
C(14)-C(15)-C(16)	120.0(4)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(17)-C(16)-C(15)	119.9(4)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(18)-C(17)-C(16)	120.5(4)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	120.0(4)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-C(14)	120.5(4)

C(18)-C(19)-H(19)	119.7
C(14)-C(19)-H(19)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for D59ZB65_0m_a. 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}
O(1)	26(1)	41(2)	29(1)	2(1)	9(1)	-8(1)
O(2)	32(2)	32(2)	122(3)	-21(2)	18(2)	-5(2)
N(1)	22(1)	30(2)	22(1)	0(1)	6(1)	1(1)
C(1)	22(2)	33(2)	21(2)	5(2)	6(1)	4(2)
C(2)	30(2)	52(3)	25(2)	-3(2)	11(2)	0(2)
C(3)	25(2)	92(4)	18(2)	6(2)	9(2)	-3(2)
C(4)	25(2)	54(3)	36(2)	17(2)	-1(2)	-4(2)
C(5)	35(2)	70(4)	51(3)	25(3)	0(2)	-15(3)
C(6)	34(2)	76(4)	45(3)	16(3)	8(2)	-16(2)
C(7)	24(2)	51(3)	39(2)	2(2)	3(2)	-5(2)
C(8)	23(2)	40(2)	22(2)	-1(2)	4(1)	2(2)
C(9)	23(2)	30(2)	38(2)	2(2)	4(2)	-2(2)
C(10)	38(3)	93(5)	78(4)	50(4)	19(3)	-9(3)
C(11)	28(2)	45(2)	25(2)	6(2)	10(1)	8(2)
C(12)	206(9)	34(3)	119(6)	19(3)	136(6)	25(4)
C(13)	35(2)	31(2)	28(2)	2(2)	8(2)	12(2)
C(14)	20(2)	31(2)	27(2)	-4(2)	8(1)	-4(2)
C(15)	27(2)	32(2)	30(2)	2(2)	14(2)	0(2)
C(16)	33(2)	45(3)	40(2)	17(2)	19(2)	7(2)
C(17)	36(2)	76(4)	32(2)	18(2)	17(2)	4(3)
C(18)	34(2)	63(3)	32(2)	-8(2)	17(2)	-1(2)
C(19)	27(2)	39(2)	36(2)	-5(2)	10(2)	-2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for D59ZB65_0m_a.

	x	y	z	U(eq)
H(2A)	6773	8792	9473	43
H(2AB)	7271	7039	10239	43
H(3A)	6434	5673	10416	54
H(3AB)	5956	6681	9144	54
H(4)	6717	3059	9345	51
H(5)	5865	857	8572	69
H(6A)	4821	1978	8110	65
H(6AB)	5057	4383	8383	65
H(7A)	4647	3748	6266	49
H(7AB)	5123	1818	6466	49
H(8)	5546	4584	5833	36
H(10A)	5594	555	10178	106
H(10B)	5763	2982	10557	106
H(10C)	6306	1329	10695	106
H(11A)	5752	7986	6921	50
H(11B)	5260	7233	7462	50
H(11C)	5042	7503	6005	50
H(12)	6958	1127	6396	116
H(13)	7445	4614	7129	40
H(15)	6319	8090	5679	35
H(16)	6056	9536	3706	46
H(17)	6311	7724	2264	56
H(18)	6869	4571	2794	50
H(19)	7169	3185	4772	42

C4 - C3 C5 C9 H4 sp3 S

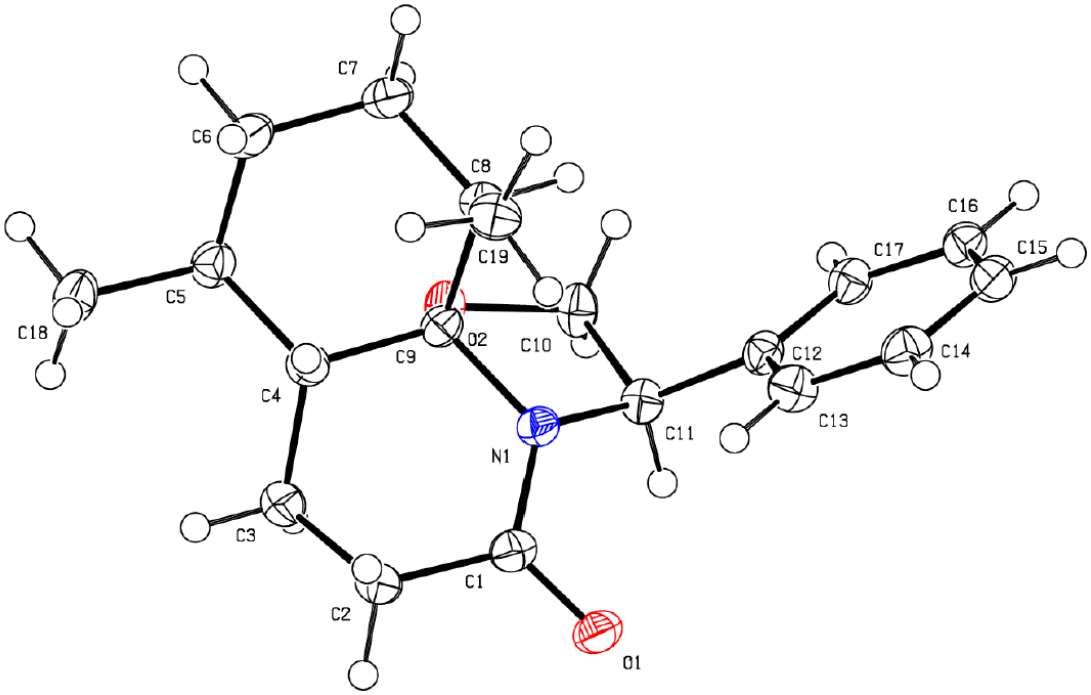
C5 - C4 C6 C10 H5 sp3 S

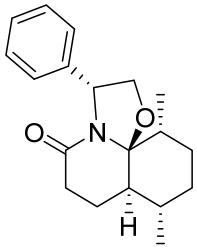
C8 - C7 C9 C11 H8 sp3 R

C9 - O2 N1 C4 C8 sp3 S

C13 - N1 C12 C14 H13 sp3 R

Crystallographic data for compound **9d**:





9d

Table 1. Crystal data and structure refinement for **9d** (I59ZB79_0m_a).

Identification code	I59ZB79_0m_a	
Empirical formula	C19 H25 N O2	
Formula weight	299.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.0011(14) Å	α= 90°.
	b = 11.0886(15) Å	β= 105.404(7)°.
	c = 9.5396(17) Å	γ = 90°.
Volume	816.0(2) $Å^3$	
Z	2	
Density (calculated)	1.219 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	324	
Crystal size	0.200 x 0.080 x 0.040 mm^3	
Theta range for data collection	2.214 to 30.538°.	
Index ranges	-11<=h<=11, -15<=k<=15, -13<=l<=13	
Reflections collected	16724	
Independent reflections	4969 [R(int) = 0.0605]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6879	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4969 / 1 / 201	
Goodness-of-fit on F^2	1.112	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.0907	
R indices (all data)	R1 = 0.0929, wR2 = 0.1228	
Absolute structure parameter	-0.1(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.261 and -0.305 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for I59ZB79_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1415(3)	3048(2)	5026(2)	26(1)
O(2)	3243(3)	6077(2)	7645(2)	22(1)
N(1)	3115(3)	4644(2)	5950(3)	20(1)
C(1)	2638(4)	3457(3)	5978(3)	22(1)
C(2)	3613(4)	2703(3)	7237(3)	25(1)
C(3)	4158(4)	3449(3)	8627(3)	25(1)
C(4)	5329(4)	4459(2)	8371(3)	22(1)
C(5)	6262(4)	5248(3)	9669(3)	24(1)
C(6)	7530(4)	6070(3)	9177(3)	28(1)
C(7)	6711(4)	6805(3)	7810(3)	27(1)
C(8)	5655(4)	6029(3)	6545(3)	22(1)
C(9)	4362(4)	5274(2)	7129(3)	20(1)
C(10)	2002(4)	6533(3)	6380(3)	25(1)
C(11)	1782(4)	5515(3)	5218(3)	21(1)
C(12)	1912(4)	5904(3)	3731(3)	21(1)
C(13)	2604(4)	5111(3)	2893(3)	26(1)
C(14)	2639(4)	5422(3)	1495(3)	28(1)
C(15)	1977(4)	6522(3)	903(3)	27(1)
C(16)	1274(4)	7306(3)	1726(3)	24(1)
C(17)	1242(4)	7000(3)	3133(3)	22(1)
C(18)	7218(5)	4505(3)	10989(3)	31(1)
C(19)	6797(4)	5269(3)	5833(3)	27(1)

Table 3. Bond lengths [Å] and angles [°] for I59ZB79_0m_a.

O(1)-C(1)	1.231(3)
O(2)-C(10)	1.436(3)
O(2)-C(9)	1.439(3)
N(1)-C(1)	1.373(4)
N(1)-C(9)	1.467(4)
N(1)-C(11)	1.470(4)
C(1)-C(2)	1.501(4)
C(2)-C(3)	1.524(4)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(4)	1.521(4)
C(3)-H(3A)	0.9900
C(3)-H(3AB)	0.9900
C(4)-C(9)	1.528(4)
C(4)-C(5)	1.538(4)
C(4)-H(4)	1.0000
C(5)-C(6)	1.528(4)
C(5)-C(18)	1.529(4)
C(5)-H(5)	1.0000
C(6)-C(7)	1.530(4)
C(6)-H(6A)	0.9900
C(6)-H(6AB)	0.9900
C(7)-C(8)	1.539(4)
C(7)-H(7A)	0.9900
C(7)-H(7AB)	0.9900
C(8)-C(19)	1.528(4)
C(8)-C(9)	1.545(4)
C(8)-H(8)	1.0000
C(10)-C(11)	1.559(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.512(4)
C(11)-H(11)	1.0000
C(12)-C(17)	1.388(4)

C(12)-C(13)	1.398(4)
C(13)-C(14)	1.384(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.389(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.387(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.391(4)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(10)-O(2)-C(9)	106.5(2)
C(1)-N(1)-C(9)	125.3(2)
C(1)-N(1)-C(11)	118.0(2)
C(9)-N(1)-C(11)	108.1(2)
O(1)-C(1)-N(1)	120.6(3)
O(1)-C(1)-C(2)	121.9(3)
N(1)-C(1)-C(2)	117.5(2)
C(1)-C(2)-C(3)	111.2(2)
C(1)-C(2)-H(2A)	109.4
C(3)-C(2)-H(2A)	109.4
C(1)-C(2)-H(2AB)	109.4
C(3)-C(2)-H(2AB)	109.4
H(2A)-C(2)-H(2AB)	108.0
C(4)-C(3)-C(2)	107.8(2)
C(4)-C(3)-H(3A)	110.1
C(2)-C(3)-H(3A)	110.1
C(4)-C(3)-H(3AB)	110.1
C(2)-C(3)-H(3AB)	110.1
H(3A)-C(3)-H(3AB)	108.5

C(3)-C(4)-C(9)	110.7(2)
C(3)-C(4)-C(5)	118.6(2)
C(9)-C(4)-C(5)	109.0(2)
C(3)-C(4)-H(4)	105.9
C(9)-C(4)-H(4)	105.9
C(5)-C(4)-H(4)	105.9
C(6)-C(5)-C(18)	110.3(3)
C(6)-C(5)-C(4)	108.2(2)
C(18)-C(5)-C(4)	112.7(2)
C(6)-C(5)-H(5)	108.5
C(18)-C(5)-H(5)	108.5
C(4)-C(5)-H(5)	108.5
C(5)-C(6)-C(7)	114.3(2)
C(5)-C(6)-H(6A)	108.7
C(7)-C(6)-H(6A)	108.7
C(5)-C(6)-H(6AB)	108.7
C(7)-C(6)-H(6AB)	108.7
H(6A)-C(6)-H(6AB)	107.6
C(6)-C(7)-C(8)	113.1(2)
C(6)-C(7)-H(7A)	109.0
C(8)-C(7)-H(7A)	109.0
C(6)-C(7)-H(7AB)	109.0
C(8)-C(7)-H(7AB)	109.0
H(7A)-C(7)-H(7AB)	107.8
C(19)-C(8)-C(7)	112.8(3)
C(19)-C(8)-C(9)	113.4(2)
C(7)-C(8)-C(9)	107.5(2)
C(19)-C(8)-H(8)	107.6
C(7)-C(8)-H(8)	107.6
C(9)-C(8)-H(8)	107.6
O(2)-C(9)-N(1)	101.5(2)
O(2)-C(9)-C(4)	109.5(2)
N(1)-C(9)-C(4)	114.5(2)
O(2)-C(9)-C(8)	109.0(2)
N(1)-C(9)-C(8)	111.5(2)
C(4)-C(9)-C(8)	110.5(2)

O(2)-C(10)-C(11)	105.4(2)
O(2)-C(10)-H(10A)	110.7
C(11)-C(10)-H(10A)	110.7
O(2)-C(10)-H(10B)	110.7
C(11)-C(10)-H(10B)	110.7
H(10A)-C(10)-H(10B)	108.8
N(1)-C(11)-C(12)	114.2(2)
N(1)-C(11)-C(10)	102.0(2)
C(12)-C(11)-C(10)	116.0(2)
N(1)-C(11)-H(11)	108.1
C(12)-C(11)-H(11)	108.1
C(10)-C(11)-H(11)	108.1
C(17)-C(12)-C(13)	118.9(3)
C(17)-C(12)-C(11)	121.3(3)
C(13)-C(12)-C(11)	119.6(3)
C(14)-C(13)-C(12)	120.5(3)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(13)-C(14)-C(15)	120.4(3)
C(13)-C(14)-H(14)	119.8
C(15)-C(14)-H(14)	119.8
C(16)-C(15)-C(14)	119.3(3)
C(16)-C(15)-H(15)	120.3
C(14)-C(15)-H(15)	120.3
C(15)-C(16)-C(17)	120.4(3)
C(15)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(12)-C(17)-C(16)	120.4(3)
C(12)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(5)-C(18)-H(18A)	109.5
C(5)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(5)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

C(8)-C(19)-H(19A)	109.5
C(8)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(8)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for I59ZB79_0m_a. 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}
O(1)	25(1)	29(1)	25(1)	-4(1)	6(1)	-8(1)
O(2)	23(1)	25(1)	18(1)	-1(1)	5(1)	5(1)
N(1)	18(1)	21(1)	20(1)	0(1)	5(1)	-2(1)
C(1)	22(1)	24(1)	21(1)	-4(1)	9(1)	-3(1)
C(2)	28(2)	21(1)	25(2)	1(1)	7(1)	-4(1)
C(3)	28(2)	25(1)	23(2)	2(1)	7(1)	-2(1)
C(4)	22(1)	21(1)	22(1)	0(1)	6(1)	1(1)
C(5)	26(2)	22(1)	23(1)	-2(1)	4(1)	2(1)
C(6)	24(2)	25(2)	31(2)	-4(1)	1(1)	-2(1)
C(7)	24(2)	24(2)	31(2)	-2(1)	5(1)	-5(1)
C(8)	21(1)	20(1)	25(1)	0(1)	6(1)	-2(1)
C(9)	20(1)	20(1)	19(1)	-2(1)	5(1)	0(1)
C(10)	27(2)	28(2)	19(1)	-1(1)	4(1)	6(1)
C(11)	19(1)	24(1)	21(1)	0(1)	6(1)	2(1)
C(12)	18(1)	27(1)	19(1)	0(1)	4(1)	-2(1)
C(13)	29(2)	24(1)	26(2)	-3(1)	11(1)	0(1)
C(14)	30(2)	32(2)	25(2)	-6(1)	10(1)	-4(1)
C(15)	26(2)	35(2)	21(1)	0(1)	7(1)	-8(1)
C(16)	20(1)	28(2)	24(2)	2(1)	4(1)	-2(1)
C(17)	19(1)	26(1)	22(1)	-1(1)	5(1)	1(1)
C(18)	35(2)	30(2)	24(2)	-5(1)	-1(1)	3(1)
C(19)	25(2)	27(2)	32(2)	0(1)	12(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for I59ZB79_0m_a.

	x	y	z	U(eq)
H(2A)	4656	2359	7016	29
H(2AB)	2871	2026	7384	29
H(3A)	3124	3789	8867	30
H(3AB)	4787	2936	9448	30
H(4)	6264	4058	8023	26
H(5)	5381	5763	9956	29
H(6A)	8473	5569	8991	34
H(6AB)	8058	6632	9978	34
H(7A)	7640	7227	7494	32
H(7AB)	5942	7426	8050	32
H(8)	4965	6589	5788	26
H(10A)	2433	7282	6032	30
H(10B)	884	6707	6599	30
H(11)	620	5134	5103	25
H(13)	3054	4354	3285	31
H(14)	3119	4878	937	34
H(15)	2004	6734	-55	33
H(16)	811	8058	1326	29
H(17)	759	7544	3688	27
H(18A)	8007	3938	10701	47
H(18B)	6376	4055	11365	47
H(18C)	7885	5044	11747	47
H(19A)	6068	4715	5129	40
H(19B)	7623	4804	6581	40
H(19C)	7432	5799	5333	40

C4 - C3 C5 C9 H4 sp3 R

C5 - C4 C6 C18 H5 sp3 S

C8 - C7 C9 C19 H8 sp3 R

C9 - O2 N1 C4 C8 sp3 S

C11 - N1 C10 C12 H11 sp3 R