SUPPORTING MATERIAL

Strain-Release Rearrangement of *N*-Vinyl-2-Arylaziridines. Total Synthesis of the Anti-Leukemia Alkaloid (–)-Deoxyharringtonine.

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General Procedures. All reactions were performed in flame-dried modified Schlenk (Kjeldahl shape) flasks fitted with a glass stopper under a positive pressure of argon, unless otherwise noted. Air- and moisture-sensitive liquids and solutions were transferred via syringe. Organic solutions were concentrated by rotary evaporation below 30 °C at ca. 25 Torr. Flash column chromatography was performed employing 230-400 mesh silica gel. Thin-layer chromatography (analytical and preparative) was performed using glass plates pre-coated to a depth of 0.25 mm with 230-400 mesh silica gel impregnated with a fluorescent indicator (254 nm).

Materials. Dichloromethane (DCM), tetrahydrofuran (THF), acetonitrile, diethyl ether, hexane, toluene, and benzene were purified by passage through two packed columns of neutral alumina under an argon atmosphere. Methanol was distilled from magnesium at 760 Torr. Dimethylformamide (DMF), isopropanol (IPA), and ethanol were dried over 4Å molecular sieves. Trifluoromethanesulfonic anhydride (Tf₂O) was distilled from phosphorus pentoxide at 760 Torr.

Instrumentation. Infrared (IR) spectra were obtained using a Perkin Elmer Spectrum BX spectrophotometer referenced to a polystyrene standard. Data are presented as the frequency of absorption (cm⁻¹). Proton and carbon-13 nuclear magnetic resonance (¹H NMR or ¹³C NMR) spectra were recorded on a Varian 400, a Varian 500, or a Varian Inova 500 NMR spectrometer; chemical shifts are expressed in parts per million (δ scale) downfield from tetramethylsilane and are referenced to the residual protium in the NMR solvent (CHCl₃: δ 7.26 for ¹H NMR, δ 77.23 for ¹³C NMR; CD₃OD: δ 3.30 for ¹H NMR, δ 49.00 for ¹³C NMR). Data are presented as follows: chemical shift, multiplicity (s = singlet, bs = broad singlet, d = doublet, bd = broad doublet, t = triplet, m = multiplet and/or multiple resonances), coupling constant in Hertz (Hz), integration, assignment.

1-Benzo[1,3]dioxol-5-yl-ethanone oxime (S1). Powdered sodium hydroxide (6.6 g, 170 mmol, 9.0 equiv) and hydroxylamine hydrochloride (3.8 g, 55 mmol, 3.0 equiv) were sequentially added to a stirred suspension of 3,4-(methylenedioxy)acetophenone (**3**) (3.0 g, 18 mmol, 1.0 equiv) in ethanol (32 mL) and distilled water (13 mL) at 25 °C. The reaction vessel was equipped with a reflux condenser and heated to 80 °C via oil bath for 3 h. The reaction mixture was cooled to 25 °C, diluted with saturated aqueous ammonium chloride (400 mL), and the product was extracted with dichloromethane (5 x 125 mL). The combined organic layers were dried (sodium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by rinsing with cold dichloromethane followed by vacuum filtration to afford **S1** (2.9 g, 87% yield) as an off-white crystalline solid. $R_f = 0.41$ (25% ethyl acetate in hexane); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.77 (s, 1H, *OH*), 7.18 (d, 1H, $J=1.5$ Hz, *ArH*), 7.10 (dd, 1H, $J=6, 1.5$ Hz, *ArH*), 6.81 (d, 1H, $J=6$ Hz, *ArH*), 5.99 (s, 2H, OCH_2O), 2.24 (s, 3H, CH_3); IR (neat film) 3296 (w, br), 3228 (w, br), 2907 (w), 1505 (s), 1266 (s), 1227 (s), 1037 (s) cm^{-1} ; HRMS (EI) m/z : Calcd for $\text{C}_9\text{H}_9\text{NO}_3$ (M^+) 179.0582, observed 179.0584.

2-Benzo[1,3]dioxol-5-yl-aziridine (4). A solution of oxime **S1** (2.7 g, 15 mmol, 1.0 equiv) in tetrahydrofuran (60 mL) at 25 °C was transferred via cannula to a stirred suspension of lithium aluminum hydride (3.5 g, 61 mmol, 4.0 equiv) and di-*iso*-propyl amine (8.5 mL, 61 mmol, 4.0 equiv) in tetrahydrofuran (70 mL) at 25 °C. The emptied reaction vessel was rinsed with tetrahydrofuran (22 mL) and the resulting solution was also transferred via cannula. The reaction vessel was equipped with a reflux condenser under nitrogen atmosphere and heated to 60 °C via oil bath for 4 h. The mixture was cooled to 25 °C, diluted with ice water (400 mL), and the product was extracted with dichloromethane (5 x 200 mL). The combined organic layers were dried (sodium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (5% triethylamine in ethyl acetate) to afford **4** (2.17 g, 88% yield) as a pale yellow oil. $R_f = 0.40$ (5% triethylamine in ethyl acetate); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 6.75 (br s, 2H, *ArH*), 6.70 (br s, 1H, *ArH*), 5.93 (s, 2H, OCH_2O), 2.97 (br s, 1H, *ArCH*), 2.17 (br s, 1H, CH_2), 1.67 (br s, 1H, CH_2).

3-(2-Benzo[1,3]dioxol-5-yl-2-chloro-ethylamino)-cyclopent-2-enone (5). A solution of 3-chloro-2-cyclopentenone (98 mg, 0.84 mmol, 1.2 equiv) in tetrahydrofuran (2.5 mL) at 25 °C was transferred via cannula to a stirred solution of aziridine **4** (110 mg, 0.70 mmol, 1.0 equiv) and triethylamine (0.20 mL, 1.4 mmol, 2.0 equiv) in tetrahydrofuran (2.5 mL) at 25 °C. The

reaction vessel was sealed under argon and heated to 60 °C via oil bath for 24 h. The reaction mixture was cooled to 25 °C and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (7% triethylamine in ethyl acetate) to afford **5** (120 mg, 64% yield) as a yellow film. R_f = 0.13 (5% triethylamine in ethyl acetate); ^1H NMR (500 MHz, C_6D_6) δ 6.64 (d, 1H, J =2 Hz, ArH), 6.47 (d, 1H, J =8 Hz, ArH), 6.31 (dd, 1H, J =8, 2 Hz, ArH), 5.24 (d, 1H, J =1.5 Hz, OCH_2O), 5.22 (d, 1H, J =1.5 Hz, OCH_2O), 4.99 (s, 1H, vinyl H), 4.51 (br s, 1H, CHCl), 3.92 (br s, 1H, NH), 2.93 (m, 2H, CH_2), 2.14 (t, 2H, J =5.5 Hz, CH_2), 1.62 (m, 2H, CH_2); IR (neat film) 3242 (w, br), 3061 (w), 2915 (w), 1565 (s), 1504 (m), 1490 (m), 1445 (m), 1251 (m), 1187 (w), 1038 (m) cm^{-1} ; HRMS (EI) m/z : Calcd for $\text{C}_{14}\text{H}_{15}\text{NO}_3\text{Cl}$ (MH^+) 280.0740, observed 280.0740.

Tetracyclic benzazepine 8. Cesium carbonate (170 mg, 0.50 mmol, 4.0 equiv) was added to a stirred solution of chloride **5** (35 mg, 0.13 mmol, 1.0 equiv) in 1,4-dioxane (18 mL) at 25 °C. The reaction vessel was sealed under argon and heated to 100 °C via oil bath for 4 d. The reaction mixture was cooled to 25 °C, gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (10% methanol in chloroform) to afford **8** (20 mg, 67% yield) as a tan amorphous solid. R_f = 0.43 (10% methanol in chloroform); ^1H NMR (500 MHz, CDCl_3) δ 7.85 (s, 1H, ArH), 6.53 (s, 1H, ArH), 5.91 (s, 2H, OCH_2O), 5.37 (s, 1H, NH), 3.61 (br s, 2H, CH_2), 2.93 (m, 2H, CH_2), 2.56 (m, 4H, CH_2); ^{13}C NMR (125 MHz, CDCl_3) δ 202.06, 169.13, 146.07, 145.29, 132.39, 126.19, 110.34, 108.83, 108.57, 100.79, 48.20, 37.00, 33.77, 27.06; IR (neat film) 3260 (w, br), 3074 (w), 2923 (w), 1557 (s), 1244 (m), 1038 (m) cm^{-1} ; HRMS (EI) m/z : Calcd for $\text{C}_{14}\text{H}_{13}\text{NO}_3$ (M^+) 243.0895, observed 243.0895.

6-Chloro-2,2-dimethyl-5-phenylselenanyl-tetrahydro-cyclopenta[1,3]dioxol-4-ol (S2). To a solution of enone **9** (246 mg, 1.60 mmol, 1.00 equiv) in MeOH (16 mL) was added $\text{CeCl}_3 \cdot 7\text{H}_2\text{O}$ (715 mg, 1.92 mmol, 1.20 equiv). The solids were allowed to dissolve completely and then NaBH_4 (72.6 mg, 1.92 mmol, 1.20 equiv) was added in several small portions. After the vigorous bubbling had subsided, the reaction was quenched with H_2O (15 mL) and poured into CH_2Cl_2 (16 mL). The phases were separated and the aqueous phase was extracted with CH_2Cl_2 (2x 16 mL). The combined organic phases were dried over MgSO_4 and concentrated under a stream of N_2 to a volume of 16 mL. This compound was not isolated to avoid loss due to its volatility. This solution was then cooled to 0 °C and PhSeCl (337 mg, 1.76 mmol, 1.10 equiv) was added and the resulting orange solution was stirred at 0 °C for 1 h. The solvent was then removed by rotary evaporation and the orange residue was purified by silica gel column chromatography (gradient; 4:1-1:1 Hex:EtOAc) to yield selenide **S2** (403 mg, 73% over 2 steps).

$R_f=0.5$ (2:1 hex:EtOAc); ^1H NMR (500 MHz, C_6D_6) δ 7.55 (m, 2H, ArH), 6.94 (m, 3H, ArH), 4.68 (s, 1H, CHCl), 4.42 (pentet, 1H, $J=5.5$ Hz, CHOH), 4.34 (d, 1H, $J=5.8$ Hz, CHClCHO), 4.12 (t, 1H, $J=5.5$, CHOHCHO), 3.70 (d, 1H, $J=6.0$ Hz, CHSe), 3.28 (d, 1H, $J=11.2$ Hz, OH), 1.48 (s, 3H, $\text{C}(\text{CH}_3)_2$), 0.95 (s, 3H, $\text{C}(\text{CH}_3)_2$); ^{13}C NMR (125 MHz, C_6D_6) δ 185.13, 133.74, 133.69, 133.65, 132.93, 129.403, 111.99, 85.82, 78.88, 71.59, 63.76, 57.71, 25.50, 23.45; IR (neat film) 3509 (m), 3057 (w), 2987 (m), 2940 (m), 1579 (m), 1384 (s), 1208 (s), 972 (m); HRMS (EI) m/z calcd for $\text{C}_{14}\text{H}_{17}\text{O}_3\text{ClSe}$ (M^+) 348.0031 observed 348.0027; $[\alpha]_D = +14.1^\circ$ (c 2.19, CHCl_3).

6-Chloro-2,2-dimethyl-4,6a-dihydro-3aH-cyclopenta[1,3]dioxol-4-ol (S3). To a solution of selenide **S2** (402 mg, 1.16 mmol, 1.00 equiv) in CH_2Cl_2 (12 mL) was added washed *m*-CPBA (220 mg, 1.28 mmol, 1.10 equiv). This solution was stirred for 15 min and then triethylamine (323 μL , 2.32 mmol, 2.00 equiv) was added via syringe and the solution was heated to 40 $^\circ\text{C}$ for 17 h. The solution was then allowed to cool and was partitioned between sat'd NaHCO_3 (15 mL) and CH_2Cl_2 (15 mL). The phases were separated and the aqueous phase was extracted with CH_2Cl_2 (2x 15 mL) and the combined organic phases were dried over MgSO_4 . Solvent removal by rotary evaporation yielded a bright orange oil that was purified by silica gel column chromatography (2:1 hex:EtOAc) to yield allylic alcohol **S3** (201 mg, 91%) as a white, crystalline solid. $R_f=0.25$ (2:1 Hex:EtOAc); ^1H NMR (400 MHz, C_6D_6) δ 5.51 (m, 1H, vinyl H), 4.24 (d, 1H, $J=5.3$ Hz, CClCHO), 4.06 (m, 2H, CHOHCHO and CHOHCHO), 2.68 (d, 1H, $J=9.8$ Hz, OH), 1.22 (s, 3H, CH_3), 1.15 (s, 3H, CH_3); ^{13}C NMR (125 MHz, C_6D_6) δ 136.55, 132.08, 113.03, 84.27, 77.76, 71.96, 27.49, 26.85; IR (neat film) 3322 (m), 2989 (m), 2939 (m), 1632 (m), 1380 (m), 1371 (m), 1213 (m), 1125 (s), 1064 (s); HRMS (EI) m/z calcd for $\text{C}_8\text{H}_{12}\text{O}_3\text{Cl}$ ($\text{M}^+ + \text{H}$) 191.0475 observed 191.0471; $[\alpha]_D = -37^\circ$ (c 1.98, CHCl_3).

6-Chloro-2,2-dimethyl-3a,6a-dihydro-cyclopenta[1,3]dioxol-4-one (10). To a solution of alcohol **S3** (30.0 mg, 0.157 mmol, 1.00 equiv) in CH_2Cl_2 (1.6 mL) was added Dess-Martin Periodane (100 mg, 0.236 mmol, 1.50 equiv). The resulting suspension was stirred at 23 $^\circ\text{C}$ for 2 h at which time the suspension was loaded directly onto a plug of silica gel (1 g) and flushed with 15 mL CH_2Cl_2 . Solvent removal by rotary evaporation yielded chloroenone **10** (29 mg, 98%) as a white, crystalline solid. $R_f = 0.35$ (25% ethyl acetate in hexane); ^1H NMR (500 MHz, C_6D_6) δ 5.54 (s, 1H, ClCCH), 4.21 (d, 1H, $J=5.5$ Hz, $\text{CH}(\text{OR})$), 3.94 (d, 1H, $J=5.5$ Hz, $\text{CH}(\text{OR})$), 1.19 (s, 3H, CH_3), 1.10 (d, 3H, $J=0.3$ Hz, CH_3); ^{13}C NMR (125 MHz, C_6D_6) δ 196.82, 145.39, 131.16, 115.65, 81.01, 79.00, 27.30, 26.31; IR (neat film) 2987 (w), 2933 (w), 1722 (s), 1582 (s) cm^{-1} ; HRMS (EI) m/z : Calcd for $\text{C}_8\text{H}_9\text{ClO}_3$ (M^+) 188.0240, observed 188.0242.

6-(2-Benzo[1,3]dioxol-5-yl-aziridin-1-yl)-2,2-Dimethyl-3a,6a-dihydro-cyclopenta[1,3]dioxol-4-one (11). Triethylamine (0.4 mL, 3.0 mmol, 2.0 equiv) and β -chloroenone **10** (280 mg, 1.5 mmol, 1.0 equiv) were sequentially added to a stirred solution of aziridine **4** (360 mg, 2.2 mmol, 1.5 equiv) in tetrahydrofuran (10 mL) at 25 °C. The resulting white mixture was stirred at 25 °C for 3 h. The crude reaction mixture was loaded directly onto a column and purified by silica gel column chromatography (1% triethylamine and 49% benzene in ethyl acetate) to afford **11** (400 mg, 85% yield) as a yellow foam. R_f = 0.68 (1% triethylamine and 49% benzene in ethyl acetate); ^1H NMR (500 MHz, C_6D_6) δ 6.55-6.70 (m, 3H, ArH), 5.24-5.28 (m, 2H, OCH_2O), 5.14-5.18 (m, 1H, NCCH), 4.50-4.56 (m, 1H, CH(OR)), 4.19-4.27 (m, 1H, CH(OR)), 2.46-3.18 (m, 1H, ArCHN), 1.84-2.17 (m, 1H, CH_2N), 1.63-1.78 (m, 1H, CH_2N), 1.28-1.32 (m, 3H, CH_3), 1.10-1.12 (m, 3H, CH_3); IR (neat film) 2989 (w), 1703 (m), 1586 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{18}\text{NO}_5$ (MH^+) 316.1185, observed 316.1186.

[3]Benzazepine 12. Cesium carbonate (3.2 g, 9.8 mmol, 4.0 equiv) was added to a stirred solution of aziridine **11** (770 mg, 2.4 mmol, 1.0 equiv) in 1,4-dioxane (350 mL) at 25 °C. The reaction vessel was sealed under argon and heated to 100 °C via oil bath for 18 h. The reaction mixture was gravity filtered and concentrated by rotary evaporation. The residue was purified by passage through a plug of silica gel (ethyl acetate) to afford **12** (590 mg, 76% yield) as a tan foam. R_f = 0.27 (50% ethyl acetate in benzene); ^1H NMR (500 MHz, CDCl_3) δ 7.82 (br s, 1H, ArH), 6.54 (s, 1H, ArH), 5.93 (d, 1H, J =1.5 Hz, OCH_2O), 5.91 (d, 1H, J =1.5 Hz, OCH_2O), 5.77 (br s, 1H, NH), 4.97 (d, 1H, J =6 Hz, CH(OR)), 4.65 (d, 1H, J =6 Hz, CH(OR)), 3.80-3.85 (m, 1H, $\text{ArCH}_2\text{CH}_2\text{N}$), 3.60-3.65 (m, 1H, $\text{ArCH}_2\text{CH}_2\text{N}$), 2.95 (br t, 2H, J =4 Hz, $\text{ArCH}_2\text{CH}_2\text{N}$), 1.44 (s, 3H, CH_3), 1.43 (s, 3H, CH_3); ^{13}C NMR (125 MHz, C_6D_6) δ 195.02, 165.26, 146.76, 146.28, 133.02, 126.24, 113.71, 109.55, 109.10, 109.00, 100.84, 78.98, 76.30, 47.65, 36.87, 27.89, 26.87; IR (neat film) 3266 (w), 2924 (s), 2855 (m), 1705 (w), 1585 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{18}\text{NO}_5$ (MH^+) 316.1185, observed 316.1189.

N-(trimethylsilyl)methyl vinylogous amide 13. Cesium carbonate (1.1 g, 3.5 mmol, 2.0 equiv) and (iodomethyl)trimethylsilane (1.3 mL, 8.7 mmol, 5.0 equiv) were sequentially added to a stirred solution of [3]benzazepine **12** (540 mg, 1.7 mmol, 1.0 equiv) in acetonitrile (12 mL) at 25 °C. The resulting brown mixture was stirred at 25 °C for 20 h. The reaction mixture was

diluted with a saturated solution of sodium sulfate (50 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic layers were dried (magnesium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (50% benzene in ethyl acetate) to afford **13** (490 mg, 75% yield) as a pale yellow film. $R_f = 0.55$ (50% benzene in ethyl acetate); ^1H NMR (500 MHz, CDCl_3) δ 7.73 (s, 1H, ArH), 6.49 (s, 1H, ArH), 5.92 (d, 1H, $J=1.5$ Hz, OCH_2O), 5.88 (d, 1H, $J=1.5$ Hz, OCH_2O), 5.10 (d, 1H, $J=6$ Hz, $\text{CH}(\text{OR})$), 4.66 (d, 1H, $J=6$ Hz, $\text{CH}(\text{OR})$), 3.55-3.65 (m, 2H, $\text{ArCH}_2\text{CH}_2\text{N}$), 3.20-3.40 (m, 2H, $\text{NCH}_2\text{SiMe}_3$), 2.85-3.00 (m, 2H, $\text{ArCH}_2\text{CH}_2\text{N}$), 1.44 (s, 3H, CH_3), 1.43 (s, 3H, CH_3), 0.14 (s, 9H, $\text{Si}(\text{CH}_3)_3$); ^{13}C NMR (125 MHz, C_6D_6) δ 194.10, 164.04, 146.93, 146.24, 133.16, 127.00, 113.48, 110.62, 109.77, 108.22, 100.95, 78.78, 75.94, 57.48, 46.81, 35.82, 28.15, 26.84, -1.53; IR (neat film) 2924 (w), 1662 (w), 1567 (s) cm^{-1} ; HRMS (ESI) m/z ; Calcd for $\text{C}_{21}\text{H}_{28}\text{NO}_5\text{Si}$ (MH^+) 402.1737, observed 402.1745.

Hexacyclic sulfone 15. Pivaloyl chloride (62 μL , 0.50 mmol, 1.2 equiv) and silver trifluoromethanesulfonate (130 mg, 0.50 mmol, 1.2 equiv) were sequentially added to a stirred solution of vinylogous amide **13** (170 mg, 0.42 mmol, 1.0 equiv) in dichloromethane (5.6 mL) at 25 $^\circ\text{C}$. The resulting yellow mixture was stirred at 25 $^\circ\text{C}$ for 1 h, cooled to $-45\text{ }^\circ\text{C}$, and stirred for 15 min. Phenyl vinyl sulfone (280 mg, 1.7 mmol, 4.0 equiv) and tetrabutylammonium triphenyldifluorosilicate (290 mg, 0.54 mmol, 1.3 equiv) were sequentially added at $-45\text{ }^\circ\text{C}$. The resulting tan mixture was stirred at $-45\text{ }^\circ\text{C}$ for 4 h, warmed to 25 $^\circ\text{C}$, and stirred for 16 h. The crude reaction mixture was loaded directly onto a column and purified by silica gel column chromatography (50% hexane in ethyl acetate) to afford **15** (190 mg, 77% yield) as a tan amorphous solid. $R_f = 0.43$ (50% hexane in ethyl acetate); ^1H NMR (500 MHz, C_6D_6) δ 7.04 (s, 1H, ArH), 6.80-6.85 (m, 3H, SO_2Ph), 6.70-6.75 (m, 2H, SO_2Ph), 6.45 (s, 1H, ArH), 5.71 (d, 1H, $J=5.5$ Hz, $\text{CH}(\text{OR})$), 5.32 (d, 1H, $J=1.4$ Hz, OCH_2O), 5.24 (d, 1H, $J=1.4$ Hz, OCH_2O), 4.20 (d, 1H, $J=5.5$ Hz, $\text{CH}(\text{OR})$), 3.80-3.85 (m, 1H, CH_2), 3.45-3.55 (m, 2H, CH_2), 3.20-3.35 (m, 2H, CH_2), 2.55-2.60 (m, 2H, CH_2), 2.22-2.32 (m, 2H, CH_2), 1.28 (s, 3H, CH_3), 1.20 (s, 3H, CH_3), 1.08 (s, 9H, $\text{C}(\text{CH}_3)_3$); ^{13}C NMR (125 MHz, C_6D_6) δ 175.16, 148.43, 148.00, 146.23, 140.11, 133.69, 133.10, 129.12, 128.43, 123.26, 112.29, 110.61, 110.14, 101.18, 83.80, 80.59, 79.55, 63.46, 51.04, 50.97, 38.89, 32.39, 32.27, 30.96, 28.16, 26.99, 26.97; IR (neat film) 2981 (m), 2934 (m), 1751 (m), 1668 (w), 1568 (m) cm^{-1} ; HRMS (ESI) m/z ; Calcd for $\text{C}_{31}\text{H}_{36}\text{NO}_8\text{S}$ (MH^+) 582.2162, observed 582.2159.

Hexacyclic pyrrolidine S4. *tert*-Butyl alcohol (50 μ L, 0.52 mmol, 10 equiv) was added to hexacyclic sulfone **15** (14 mg, 24 μ mol) at 25 $^{\circ}$ C. The resulting tan mixture was stirred at 25 $^{\circ}$ C for 10 min, cooled to -78° C, and stirred for 10 min. A 0.1 molar solution of samarium diiodide (2.6 mL, 0.26 mmol, 5.0 equiv) was added at -78° C. The resulting dark blue mixture was stirred at -78° C for 10 min. Hexamethyl phosphoric triamide (0.22 mL, 1.3 mmol, 25 equiv) was added at -78° C. The resulting purple mixture was stirred at -78° C for 1 h, warmed to -45° C, and stirred for 2 h. The reaction mixture was warmed to 25 $^{\circ}$ C, diluted with water (60 mL), and extracted with ethyl acetate (4 x 50 mL). The combined organic layers were dried (magnesium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (50% benzene in ethyl acetate) to afford **S4** (17 mg, 74% yield) as an off-white crystalline solid. R_f = 0.39 (50% benzene in ethyl acetate); ^1H NMR (500 MHz, C_6D_6) δ 7.03 (s, 1H, ArH), 6.45 (s, 1H, ArH), 5.72 (d, 1H, $J=6$ Hz, CH(OR)), 5.31 (d, 1H, $J=1.5$ Hz, OCH_2O), 5.26 (d, 1H, $J=1.5$ Hz, OCH_2O), 4.56 (d, 1H, $J=6$ Hz, CH(OR)), 3.70 (ddd, 1H, $J=2, 12, 14$ Hz, CH_2), 3.00 (ddd, 1H, $J=3, 8, 11$ Hz, CH_2), 2.82 (m, 1H, CH_2), 2.60-2.70 (m, 2H, CH_2), 2.50 (ddd, 1H, $J=1.4, 6.6, 12$ Hz, CH_2), 2.24 (ddd, 1H, $J=1.7, 4, 18$ Hz, CH_2), 1.78-1.88 (m, 1H, CH_2), 1.56-1.64 (m, 1H, CH_2), 1.51 (s, 3H, CH_3), 1.40-1.48 (m, 1H, CH_2), 1.30 (s, 3H, CH_3), 1.10 (s, 9H, $\text{C}(\text{CH}_3)_3$); ^{13}C NMR (125 MHz, C_6D_6) δ 175.43, 147.62, 147.18, 145.95, 132.86, 130.44, 124.40, 111.97, 110.44, 110.25, 101.07, 86.00, 80.68, 78.90, 50.38, 48.51, 38.88, 32.07, 30.75, 28.28, 27.04, 26.85, 25.10; IR (neat film) 2930 (m), 1751 (m), 1485 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{25}\text{H}_{32}\text{NO}_6$ (MH^+) 442.2230, observed 442.2231.

Hexacyclic enol/ketone (S5). Schwartz's reagent (140 mg, 0.53 mmol, 3.0 equiv) was added to a stirred solution of enol-pivaloate **S4** (78 mg, 0.18 μ mol, 1.0 equiv) in tetrahydrofuran (0.33 mL) at 25 $^{\circ}$ C. The reaction vessel was sealed under argon and heated to 40 $^{\circ}$ C via oil bath for 16 h. The crude reaction mixture was loaded directly onto a column and purified by silica gel column chromatography (10% methanol in chloroform) to afford **S5** (63 mg, 99% yield) as a tan solid. R_f = 0.34 (10% methanol in chloroform); ^1H NMR (500 MHz, C_6D_6) δ 6.44 (br s, 2H, ArH), 5.32 (d, 2H, $J=1.5$ Hz, OCH_2O), 5.29 (br s, 2H, $\text{C}(\text{O})\text{CH}$), 4.77 (br s, 1H, OH), 2.00-2.50 (m, 10H, CH_2), 1.35 (s, 3H, CH_3), 1.34 (s, 3H, CH_3); IR (neat film) 3417 (w), 2986 (m), 2935 (m), 2590 (w), 1720 (m), 1504 (m), 1485 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{20}\text{H}_{24}\text{NO}_5$ (MH^+) 358.1654, observed 358.1667.

Hexacyclic carbonate 16. Potassium bis (trimethylsilyl)amide (63 mg, 0.30 mmol, 1.2 equiv) was added to a stirred solution of enol **S5** (89 mg, 0.25 mmol, 1.0 equiv) in tetrahydrofuran (2.5 mL) at 0 °C. The resulting orange solution was stirred at 0 °C for 15 min. Benzyl chloroformate (43 μ L, 0.30 mmol, 1.2 equiv) was added at 0 °C. The resulting yellow solution was stirred at 0 °C for 1 h. The reaction mixture was diluted with water (40 mL) and extracted with dichloromethane (2 x 40 mL). The combined organic layers were dried (magnesium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (50% benzene in ethyl acetate) to afford **16** (110 mg, 86% yield) as a tan foam. R_f = 0.34 (10% methanol in chloroform); ^1H NMR (500 MHz, C_6D_6) δ 7.07 (s, 1H, ArH), 6.94-6.97 (m, 3H, Ph), 6.90-6.93 (m, 2H, Ph), 6.41 (s, 1H, ArH), 5.77 (d, 1H, $J=6$ Hz, C(O)CH), 5.24 (d, 1H, $J=1.5$ Hz, OCH₂O), 5.21 (d, 1H, $J=1.5$ Hz, OCH₂O), 4.76 (d, 1H, $J=12$ Hz, OCH₂Ph), 4.68 (d, 1H, $J=12$ Hz, OCH₂Ph), 4.56 (d, 1H, $J=6$ Hz, C(O)CH), 3.64 (m, 1H, CH₂), 2.98 (m, 1H, CH₂), 2.60-2.68 (m, 2H, CH₂), 2.46 (ddd, 1H, $J=12, 6.5, 1.5$ Hz, CH₂), 2.28 (ddd, 1H, $J=17, 4, 1.5$ Hz, CH₂), 1.76-1.84 (m, 1H, CH₂), 1.54-1.60 (m, 1H, CH₂), 1.48 (s, 3H, CH₃), 1.38-1.43 (m, 1H, CH₂), 1.30 (s, 3H, CH₃); ^{13}C NMR (125 MHz, C_6D_6) δ 152.35, 147.79, 146.30, 146.12, 135.05, 132.45, 130.82, 128.40, 128.25, 128.16, 123.69, 112.04, 110.12, 109.95, 100.92, 85.70, 80.29, 78.70, 70.06, 50.21, 48.21, 31.85, 30.44, 28.10, 26.70, 24.88; IR (neat film) 2932 (w), 1762 (m), 1504 (m), 1485 (m), 1379 (m), 1222 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{28}\text{H}_{30}\text{NO}_7$ (MH^+) 492.2022, observed 492.2032.

Pentacyclic diol S6. A 33% solution of methanol in 2 molar hydrochloric acid (5 mL) was added to acetonide **16** (60 mg, 0.12 mmol, 1.0 equiv) at 25 °C. The resulting cloudy white solution was stirred at 25 °C for 16 h. The reaction mixture was diluted with methanol and concentrated by rotary evaporation. This process was repeated four times. The residue was diluted with a 50% solution of methanol in toluene and concentrated by rotary evaporation. This process was repeated four times to afford **S6** (60 mg, 99% yield) as a white film. ^1H NMR (500 MHz, CD_3OD) δ 7.10-7.30 (m, 5H, Ph), 6.73 (s, 1H, ArH), 6.70 (s, 1H, ArH), 5.92 (d, 1H, $J=1$ Hz, OCH₂O), 5.90 (d, 1H, $J=1$ Hz, OCH₂O), 5.10 (d, 1H, $J=12$ Hz, OCH₂Ph), 5.06 (d, 1H, $J=12$ Hz, OCH₂Ph), 4.95 (d, 1H, $J=6$ Hz, CH(OH)), 4.40 (d, 1H, $J=6$ Hz, CH(OH)), 3.64-3.74 (m, 2H, CH₂), 3.10-3.32 (m, 4H, CH₂), 2.45 (m, 1H, CH₂), 2.00-2.10 (m, 2H, CH₂), 1.79 (m, 1H, CH₂); ^{13}C NMR (125 MHz, CD_3OD) δ 152.46, 152.30, 150.03, 148.12, 136.05, 131.33, 129.77, 129.62, 129.44, 126.73, 122.58, 111.40, 110.48, 103.02, 85.29, 73.97, 71.79, 71.01, 53.31, 49.85, 30.55, 29.45, 23.00; IR (neat film) 3294 (s), 2957 (m), 2605 (m), 1766 (s), 1672 (w), 1621 (w), 1504

(s), 1487 (s), 1458 (s), 1380 (s), 1228 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{25}\text{H}_{26}\text{NO}_7$ (MH^+) 452.1709, observed 452.1717.

Pentacyclic mono-carbonate S7. Ytterbium trifluoromethanesulfonate hydrate (87 mg, 0.12 mmol, 1.0 equiv) and di-*tert*-butyldicarbonate (0.11 mL, 0.48 mmol, 4.0 equiv) were sequentially added to a stirred solution of pentacyclic diol **S6** (58 mg, 0.12 mmol, 1.0 equiv) in dichloromethane (3.0 mL) at 0 °C. The resulting cloudy pale yellow solution was stirred at 0 °C for 2 d. The reaction mixture was diluted with water (50 mL) and extracted with ethyl acetate (3 x 40 mL). The combined organic layers were dried (magnesium sulfate), gravity filtered, and concentrated by rotary evaporation to afford the crude monocarbonate (70 mg) as a pale yellow foam. R_f = 0.65 (10% methanol in chloroform). *ortho*-Iodoxy benzoic acid (100 mg, 0.36 mmol, 3.0 equiv) was added to a stirred solution of crude mono-carbonate (66 mg, 0.12 mmol, 1.0 equiv) in dimethylsulfoxide (3.0 mL) at 25 °C. The resulting orange solution was stirred at 25 °C for 20 h. The reaction mixture was diluted with water (200 mL) and extracted with diethyl ether (5 x 40 mL). The combined organic layers were dried (magnesium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (12.5% ethyl acetate in benzene) to afford **S7** (33 mg, 50% yield from **S6**) as a pale yellow film. R_f = 0.45 (12.5% ethyl acetate in benzene); ^1H NMR (500 MHz, C_6D_6) δ 6.95-6.99 (m, 5H, *Ph*), 6.71 (s, 1H, *ArH*), 6.29 (s, 1H, *ArH*), 5.79 (s, 1H, *CH*(OBoc)), 5.17 (d, 1H, J =1.5 Hz, OCH_2O), 5.13 (d, 1H, J =1.5 Hz, OCH_2O), 4.81 (d, 1H, J =12 Hz, OCH_2Ph), 4.73 (d, 1H, J =12 Hz, OCH_2Ph), 3.09 (ddd, 1H, J =14.5, 11.5, 4.5 Hz, CH_2), 2.67 (ddd, 1H, J =17, 11, 6 Hz, CH_2), 2.60 (ddd, 1H, J =14.5, 8, 2 Hz, CH_2), 2.45-2.55 (m, 2H, CH_2), 2.36 (m, 1H, CH_2), 2.15 (dd, 1H, J =13, 7 Hz, CH_2), 1.86 (m, 1H, CH_2), 1.46 (m, 1H, CH_2), 1.32 (s, 9H, $\text{OC}(\text{CH}_3)_3$), 1.30 (m, 1H, CH_2); ^{13}C NMR (125 MHz, C_6D_6) δ 191.35, 158.90, 153.68, 152.04, 149.30, 146.46, 142.65, 134.88, 132.69, 128.64, 128.58, 128.56, 121.72, 110.44, 110.07, 101.37, 82.49, 81.78, 73.31, 71.00, 48.45, 41.84, 34.29, 32.79, 27.62, 24.78; IR (neat film) 2978 (m), 2929 (m), 1753 (s), 1736 (s), 1692 (m), 1505 (m), 1485 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{30}\text{H}_{32}\text{NO}_9$ (MH^+) 550.2077, observed 550.2080.

Pentacyclic enone S8. A stirred solution of α -oxyketone **S7** (30 mg, 55 μmol , 1.0 equiv) in acetone (2.0 mL) was subjected to five freeze-pump-thaw cycles. A solution of water (1.0 mL) was subjected to 5 freeze-pump-thaw cycles, chromium(II) chloride (67 mg, 0.55 mmol, 10 equiv) was added, and the resulting blue/green solution was subjected to another five freeze-pump-thaw cycles. The aqueous chromium solution was transferred via cannula to the reaction

mixture at 25 °C. The resulting green solution was subjected to another 5 freeze-pump-thaw cycles. The green solution was stirred at 25 °C for 1 h. The reaction mixture was diluted with water (50 mL) and extracted with ethyl acetate (4 x 40 mL). The combined organic layers were dried (magnesium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (50% benzene in ethyl acetate) to afford **S8** (10 mg, 42% yield) as a colorless film. R_f = 0.45 (12.5% ethyl acetate in benzene); ^1H NMR (500 MHz, C_6D_6) δ 6.96-7.02 (m, 5H, *Ph*), 6.83 (s, 1H, *ArH*), 6.37 (s, 1H, *ArH*), 5.21 (d, 1H, $J=1.5$ Hz, OCH_2O), 5.16 (d, 1H, $J=1.5$ Hz, OCH_2O), 4.88 (d, 1H, $J=12$ Hz, OCH_2Ph), 4.77 (d, 1H, $J=12$ Hz, OCH_2Ph), 3.14 (ddd, 1H, $J=15.5, 12, 4$ Hz, CH_2), 2.80 (ddd, 1H, $J=16.5, 11.5, 5.5$ Hz, CH_2), 2.54-2.62 (m, 2H, $\text{C}(\text{O})\text{CH}_2$, CH_2), 2.47-2.53 (m, 2H, CH_2), 2.37-2.45 (m, 2H, $\text{C}(\text{O})\text{CH}_2$, CH_2), 1.55 (m, 1H, CH_2), 1.43 (m, 1H, CH_2), 1.23-1.29 (m, 2H, CH_2); ^{13}C NMR (125 MHz, C_6D_6) δ 196.81, 161.39, 152.63, 149.13, 146.48, 145.12, 134.96, 132.54, 128.46, 128.31, 128.25, 122.90, 110.29, 109.39, 101.17, 70.58, 70.17, 51.35, 48.80, 42.97, 38.83, 32.44, 24.37; IR (neat film) 2924 (m), 1767 (s), 1718 (s), 1643 (w), 1504 (m), 1485 (s), 1382 (m), 1227 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{25}\text{H}_{24}\text{NO}_6$ (MH^+) 434.1604, observed 434.1616.

(+)-Demethylcephalotaxinone (17). 10% Palladium on carbon (5 mg, ~33 wt.%) was added to a stirred solution of benzyl carbonate **S8** (14 mg, 32 μmol , 1.0 equiv) in ethyl acetate (5.0 mL) at 25 °C. The resulting black mixture was charged with an atmosphere of hydrogen (balloon) and stirred at 25 °C for 6 h. The crude reaction mixture was eluted through a short plug of celite (ethyl acetate followed by dichloromethane) and the organic layer was concentrated by rotary evaporation to afford (+)-**17** (10 mg, 99% yield) as a colorless film. R_f = 0.30 (10% methanol in chloroform); ^1H NMR (500 MHz, C_6D_6) δ 7.04 (s, 1H, *ArH*), 6.42 (s, 1H, *ArH*), 5.27 (d, 1H, $J=1.5$ Hz, OCH_2O), 5.23 (d, 1H, $J=1.5$ Hz, OCH_2O), 2.83-2.97 (m, 2H, CH_2), 2.52-2.62 (m, 3H, CH_2), 2.43 (d, 1H, $J=18$ Hz, $\text{C}(\text{O})\text{CH}_2$), 2.30-2.36 (m, 2H, $\text{C}(\text{O})\text{CH}_2$, CH_2), 1.58 (m, 1H, CH_2), 1.48 (m, 1H, CH_2), 1.35 (m, 1H, CH_2), 1.19 (dd, 1H, $J=12, 6$ Hz, CH_2); ^{13}C NMR (125 MHz, C_6D_6) δ 218.26, 161.31, 148.42, 148.02, 146.26, 132.65, 124.69, 110.51, 110.12, 101.18, 70.67, 51.28, 49.22, 44.37, 39.15, 32.75, 24.54; IR (neat film) 3386 (w, br) 2922 (m), 1702 (s), 1506 (m), 1484 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{18}\text{NO}_4$ (MH^+) 300.1236, observed 300.1246; $[\alpha]_D^{23}$ 358.8 (c 0.39, CHCl_3).

(-)-Cephalotaxinone (S9). Trimethyl orthoformate (33 μL , 0.30 mmol, 10 equiv) and tosylic acid monohydrate (12 mg, 60 μmol , 2.0 equiv) were sequentially added to a stirred solution of (+)-demethylcephalotaxinone (**17**) (9.0 mg, 30 μmol , 1.0 equiv) in dichloromethane (0.65 mL) at 0 °C. The resulting dark orange solution was stirred at 0 °C for 30 min, warmed to 25 °C, and stirred for 6.5 h. The reaction mixture was diluted with a saturated solution of

sodium bicarbonate (30 mL) and extracted with dichloromethane (4 x 20 mL). The combined organic layers were dried (sodium sulfate), gravity filtered, and concentrated by rotary evaporation. The residue was purified by silica gel column chromatography (10% methanol in chloroform) to afford (-)-**S9** (5.5 mg, 55% yield) as a pale yellow film. $R_f = 0.46$ (10% methanol in chloroform); $^1\text{H NMR}$ (500 MHz, C_6D_6) δ 6.58 (s, 1H, ArH), 6.47 (s, 1H, ArH), 5.76 (s, 1H, vinyl H), 5.34 (d, 1H, $J=1.5$ Hz, OCH_2O), 5.32 (d, 1H, $J=1.5$ Hz, OCH_2O), 3.16 (m, 4H, CH, OCH_3), 2.71 (m, 1H, CH_2), 2.44-2.60 (m, 2H, CH_2), 2.28-2.40 (m, 2H, CH_2), 2.01 (dd, 1H, $J=14$, 7 Hz, CH_2), 1.72 (m, 1H, CH_2), 1.30-1.50 (m, 3H, CH_2); IR (neat film) 2928 (m), 1722 (s), 1624 (m), 1503 (m), 1486 (s), 1229 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{18}\text{H}_{20}\text{NO}_4$ (MH^+) 314.1392, observed 314.1390.

(-)-Cephalotaxine (2). Sodium borohydride (27 mg, 0.70 mmol, 40 equiv) was added to a stirred solution of (-)-cephalotaxinone (**S9**) (5.5 mg, 18 μmol , 1.0 equiv) in methanol (0.65 mL) at -78 $^\circ\text{C}$. The resulting white mixture was stirred at -78 $^\circ\text{C}$ for 10 min, warmed to 25 $^\circ\text{C}$, and stirred for 1 h. The reaction mixture was diluted with water (30 mL) and extracted with dichloromethane (4 x 15 mL). The combined organic layers were dried (sodium sulfate), gravity filtered, and concentrated by rotary evaporation to afford (-)-**2** (5.2 mg, 95% yield) as a pale yellow film. $R_f = 0.08$ (10% methanol in chloroform); $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 6.68 (s, 1H, ArH), 6.65 (s, 1H, ArH), 5.90 (s, 2H, OCH_2O , $J=1.7$ Hz), 4.93 (s, 1H, vinyl H), 4.76 (d, 1H, $J=9$ Hz, $\text{CH}(\text{OH})$), 3.73 (s, 3H, OCH_3), 3.68 (d, 1H, $J=9$ Hz, ArCHCH(OH)), 3.35 (m, 1H, CH_2), 3.08 (m, 1H, CH_2), 2.92 (ddd, 1H, $J=12$, 11, 7 Hz, CH_2), 2.54-2.62 (m, 2H, CH_2), 2.36 (dd, 1H, $J=14$, 7 Hz, CH_2), 2.00 (m, 1H, CH_2), 1.60-1.90 (m, 4H, CH_2); IR (neat film) 3411 (br, w), 2926 (m), 1651 (m), 1503 (m), 1486 (s), 1222 (s) cm^{-1} ; HRMS (ESI) m/z : Calcd for $\text{C}_{18}\text{H}_{22}\text{NO}_4$ (MH^+) 316.1549, observed 316.1559.

Authentic sample of cephalotaxine (Aldrich) $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 6.68 (s, 1H, ArH), 6.65 (s, 1H, ArH), 5.90 (q, 2H, OCH_2O , $J=1.7$ Hz), 4.93 (s, 1H, vinyl H), 4.77 (dd, 1H, $J=9$, 3 Hz, $\text{CH}(\text{OH})$), 3.73 (s, 3H, OCH_3), 3.68 (d, 1H, $J=9$ Hz, ArCHCH(OH)), 3.35 (m, 1H, CH_2), 3.08 (m, 1H, CH_2), 2.92 (ddd, 1H, $J=7$, 11, 12 Hz, CH_2), 2.61-2.55 (m, 2H, CH_2), 2.35 (dd, 1H, $J=7$, 14 Hz, CH_2), 2.01 (m, 1H, CH_2), 1.87 (m, 2H, CH_2), 1.74 (m, 1H, CH_2), 1.61 (d, 1H, $J=3$ Hz, CH_2).

[2-tert-Butyl-4-(3-methyl-but-2-enyl)-5-oxo-[1,3]dioxolan-4-yl]-acetic acid (S10). A solution of LHMDS (413 mg, 2.47 mmol, 1.00 equiv) in THF (5 mL) at -78 $^\circ\text{C}$ was transferred *via* cannula to a stirred solution of acid **19**¹ (500 mg, 2.47 mmol, 1.00 equiv) in THF (25 mL) at -78 $^\circ\text{C}$. The resulting solution was stirred at -78 $^\circ\text{C}$ for 15 minutes. A solution of LHMDS (496 mg, 2.96 mmol, 1.20 equiv) in THF (5 mL) at -78 $^\circ\text{C}$ was then added *via* cannula and the

resulting solution was stirred for 20 min at -78 °C. 3,3 dimethylallyl bromide (316 μ L, 2.72 mmol, 1.10 equiv) was then added via syringe and the resulting solution was stirred at -78 °C for 19 h, at which time the reaction was quenched with 25 mL sat'd NH_4Cl , removed from the cold bath, and allowed to warm to RT. The solution was then poured into 75 mL 1N HCl, extracted with 3x 75 mL CH_2Cl_2 , the combined organic phases were dried over MgSO_4 and concentrated *via* rotary evaporation to yield an oily solid. Purification by silica gel column chromatography (19:1 $\text{MeOH}:\text{CH}_2\text{Cl}_2$) yielded **S10** (438 mg, 66%) as a white powder. R_f = 0.51 (19:1 $\text{CH}_2\text{Cl}_2:\text{MeOH}$); ^1H NMR (400 MHz, CDCl_3) δ 5.16 (m, 2H, $\text{CH}(\text{CH}_3)_3$; vinyl H), 2.83 (m, 2H, CH_2), 2.50 (d, 2H, $J=7.7$ Hz, CH_2), 1.74 (d, 3H, $J=0.8$ Hz, CH_3), 1.64 (d, 3H, $J=0.8$ Hz, CH_3), 0.93 (s, 9H, $\text{CH}(\text{CH}_3)_3$); ^{13}C NMR (100 MHz, CDCl_3) δ 174.91, 173.84, 137.96, 115.55, 108.42, 80.54, 39.44, 34.28, 32.40, 25.97, 23.60, 18.03; IR (neat film) 2973 (m), 2916 (m), 1800 (s), 1710 (s), 1181 (m), 1156 (m) cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{23}\text{O}_5$ (M^+) 271.1545, observed 271.1553; $[\alpha]_D = -266^\circ$ (c 2.98 CHCl_3).

2-Hydroxy-2-(3-methyl-but-2-enyl)-succinic acid 1-benzyl ester (20). A solution of dioxolanone **S10** (120 mg, 0.444 mmol, 1.00 equiv) in THF (4.5 mL) was cooled to 0 °C and benzyl alcohol (69 μ L, 0.67 mmol, 1.5 equiv) was added via syringe followed by a 60% dispersion of NaH in mineral oil (45 mg, 1.1 mmol, 2.5 equiv) which resulted in vigorous evolution of gas. The solution was allowed to stir at 0 °C for 30 min, at which time the reaction was quenched with 4.5 mL NaHCO_3 , removed from the cold bath and allowed to warm to room temperature. The solution was then poured into H_2O (4.5 mL), washed with CH_2Cl_2 (1x 6 mL), acidified to pH <5 with 1N HCl, and then extracted with Et_2O (4x 6 mL). The combined ethereal phases were dried over MgSO_4 and solvent removal by rotary evaporation yielded a white solid which was purified by silica gel column chromatography (70:28:2 hex:EtOAc:HOAc) to yield **20** (114 mg, 88%) as a white solid. R_f = 0.39 (60:38:2 EtOAc:Hex:HOAc); ^1H NMR (500 MHz, CDCl_3) δ 7.35 (m, 5H, ArH), 5.20 (s, 2H, PhCH_2), 5.07 (m, 1H, vinyl H), 3.00 (d, 1H, $J=16.7$ Hz, $\text{C}(\text{O})\text{CH}_2$), 2.76 (d, 1H, $J=16.7$ Hz, $\text{C}(\text{O})\text{CH}_2$), 2.41 (m, 2H, CHCH_2), 1.67 (d, 3H, $J=0.7$ Hz, CH_3), 1.54 (d, 3H, $J=0.7$ Hz, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 176.43, 174.60, 136.79, 135.21, 128.71, 128.64, 128.61, 116.45, 75.41, 67.95, 42.69, 38.14, 26.06, 18.09; IR (neat film) 3483 (br m), 2968 (m), 1736 (s), 1498 (w), 1195 (s) cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{20}\text{O}_5\text{Na}$ ($\text{M}^+ + \text{Na}^+$) 315.1208, observed 315.1214; $[\alpha]_D = -18^\circ$ (c 2.98, CHCl_3).

2-(3-Methyl-but-2-enyl)-4-oxo-oxetane-2-carboxylic acid benzyl ester (S11). A solution of hydroxyester **20** (100 mg, 0.342 mmol, 1.00 equiv) and triethylamine (166 μ L, 1.20 mmol, 3.50 equiv) in CH_2Cl_2 (14 mL) was added via syringe pump over 4 h to a solution of 2,4,6-trichlorobenzoyl chloride (80 μ L, 0.51 mmol, 1.5 equiv) and N,N -dimethylaminopyridine (DMAP) (46 mg, 0.38 mmol, 1.1 equiv) in CH_2Cl_2 (3.4 mL). The solution was then allowed to

stir for 1 h after complete addition after which time it was quenched with H₂O (10 mL). The phases were separated and the aqueous phase was extracted with CH₂Cl₂ (2x 10 mL). The organic phases were combined, dried over Na₂SO₄, and the solvent was removed via rotary evaporation to yield a red solid which was purified by silica gel column chromatography (CH₂Cl₂) to yield **S11** (47 mg, 50%) as a pale yellow oil. *R*_f=0.79 (60:38:2 Hex:EtOAc:HOAc); ¹H NMR (500 MHz, CDCl₃) δ 7.37 (m, 5H, ArH), 5.25 (s, 2H, ArCH₂), 5.09 (m, 1H, vinyl H), 3.61 (d, 1H, *J*=16.4 Hz, C(O)CH₂), 3.36 (d, 1H, *J*=16.4 Hz, C(O)CH₂), 2.79 (m, 2H, CHCH₂), 1.70 (d, 3H, *J*=0.8 Hz, CH₃), 1.60 (d, 3H, *J*=0.8 Hz, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ 169.21, 165.84, 138.67, 134.67, 128.68, 128.38, 114.24, 76.28, 67.84, 45.56, 33.43, 25.87, 17.99; IR (neat film) 2966 (m), 2914 (m), 1842 (s), 1737 (s), 1452 (m) 962 (m) cm⁻¹; HRMS (EI) *m/z* calcd for C₁₆H₁₈O₄ (M⁺) 274.120509, observed 274.120646; [α]_D = +1.2° (c 2.92, CHCl₃).

2-(3-Methyl-butyl)-4-oxo-oxetane-2-carboxylic acid (21). To a solution of benzyl ester **S11** (220 mg, 0.802 mmol, 1.00 equiv) in EtOAc (8 mL) was added Pd/C (10 wt% on C, 44 mg, 20% by weight). The resulting suspension was stirred under H₂ (1 atm) for 23 h, then filtered through a plug of celite. Solvent removal by rotary evaporation yielded an oil which showed alkene peaks by ¹H NMR, so the residue was resubjected to the reaction conditions to yield carboxylic acid **21** (150 mg, >99%) as a clear, colorless oil. *R*_f=0.11 (60:38:2 hex:EtOAc:HOAc); ¹H NMR (400 MHz, CDCl₃) δ 10.30 (br s, 1H, C(O)OH), 3.71 (d, 1H, *J*=16.6 Hz, C(O)CH₂), 3.45 (d, 1H, *J*=16.6 Hz, C(O)CH₂), 2.19 (ddd, 1H, *J*=14.2, 12.3, 4.8 Hz, CCH₂), 2.04 (ddd, 1H, *J*=14.2, 12.3, 4.8 Hz, CCH₂), 1.61 (septet, 1H, *J*=6.6 Hz (CH₃)₂CH), 1.40 (m, 1H, (CH₃)₂CHCH₂), 1.27 (m, 1H, (CH₃)₂CHCH₂), 0.92 (d, 6H, *J*=6.6 Hz (CH₃)₂); ¹³C NMR (400 MHz, CDCl₃) δ 174.96, 165.69, 76.43, 46.78, 33.17, 32.109, 27.89, 22.27, 22.20; IR (neat film) 3514 (br m), 3184 (br s), 2958 (s), 1828 (s), 1729 (s), 1408 (m), 1173 (s) cm⁻¹; [α]_D = 22.1° (c 1.67, CHCl₃).

Deoxyharringtonine, β-lactone (22). To a solution of β-lactone **21** (8.9 mg, 0.048 mmol, 1.5 equiv) and triethylamine (19.9 μL, 0.143 mmol, 4.50 equiv) in CH₂Cl₂ (320 μL) was added 2,4,6-trichlorobenzoyl chloride (8.2 μL, 0.052 mmol, 1.7 equiv) *via* syringe. The resulting dark purple solution was stirred at 23 °C for 1 h. This solution was then transferred *via* syringe to a solution of cephalotaxine (10 mg, 0.032 mmol, 1.0 equiv) and *N,N*-dimethylaminopyridine (DMAP) in CH₂Cl₂ (320 μL). This solution was then stirred for 15 min, concentrated under a stream of N₂, and loaded directly onto a silica gel column that had been packed with 5% triethylamine in hexanes. The column was eluted with 1:1 hex:EtOAc to yield **22** (12.4 mg, 81%) as an oil. *R*_f=0.39 (1:1 hex:EtOAc on plates pretreated with 5% TEA in pentane); ¹H NMR

(500 MHz, CDCl₃) δ 6.60 (app d, 2H, ArH), 5.91 (dd, 1H, J=9.6, 0.7 Hz, ArCHCH), 5.86 (dd, 2H, J=4.1, 1.4 Hz, OCH₂O), 5.08 (s, 1H, vinyl H), 3.81 (d, 1H, J=9.5 Hz, ArCHCH), 3.69 (s, 3H, OCH₃), 3.10 (m, 2H, CH₂), 2.98 (d, 1H, J=16.5 Hz, C(O)CH₂), 2.93 (m, 1H, CH₂), 2.73 (d, 1H, J=16.5 Hz, C(O)CH₂), 2.58 (m, 2H, CH₂), 2.35 (dd, 1H, J=14.3, 6.9, CH₂), 2.04 (m, 1H, CH₂), 1.88 (m, 2H, CH₂), 1.75 (m, 2H, CH₂), 1.62 (m, 1H, CH₂), 1.47 (septet, 1H, J=6.7 Hz, (CH₃)₂CH), 1.15 (m, 1H, CH₂), 1.02 (m, 1H, CH₂), 0.85 (dd, 6H, J=6.7, 1.2 Hz, (CH₃)₂CH); ¹³C (500 MHz, CDCl₃) δ 171.03, 168.57, 166.25, 113.17, 109.96, 109.91, 101.11, 76.53, 75.62, 65.63, 57.36, 54.05, 48.60, 46.31, 41.74, 33.21, 31.97, 27.91, 22.46, 22.14, 20.39; IR (neat film) 2958 (m), 1842 (s), 1750 (s), 1656 (m), 1504 (m), 1488 (s), 1037 (m) cm⁻¹; HRMS (EI) m/z calcd for C₂₇H₃₃NO₇ (M⁺) 483.225703 found 483.224659; [α]_D = -95° (c 2.77, CHCl₃).

Deoxyharringtonine (1). To a solution of β -lactone **22** (18 mg, 0.0372 mmol, 1.00 equiv) in MeOH (370 μ L) was added a freshly prepared solution of 0.5M NaOMe in MeOH (82 μ L, 0.0409 mmol, 1.10 equiv). After 15 min the solution was quenched with half sat'd NH₄Cl solution (300 μ L) and partitioned between H₂O (10 mL) and CH₂Cl₂ (10 mL). The phases were separated and the aqueous phase was extracted with CH₂Cl₂ (2x 10 mL), the combined organic phases were dried over MgSO₄, and concentrated by rotary evaporation to yield a yellow oil that was purified by silica gel column chromatography (70:28:2 benzene:hex:TEA) to yield deoxyharringtonine (**1**) (14.6 mg, 76%) as a clear, colorless oil. R_f=0.24 (9:1 benzene:EtOAc on plates pretreated with 5% TEA in pentane); ¹H NMR (500 MHz, CDCl₃) δ 6.62 (s, 1H, ArH), 6.53 (s, 1H, ArH), 5.99 (dd, 1H, J=9.8, 0.7 Hz ArCHCH), 5.86 (dd, 2H, J=11.8, 1.5 Hz, OCH₂O), 5.04 (d, 1H, J=0.6 Hz, vinyl H), 3.77 (d, 1H, J=9.8 Hz, ArCHCH), 3.67 (s, 3H, OCH₃), 3.57 (s, 3H, OCH₃), 3.48 (s, 1H, OH), 3.12 (m, 2H, CH₂), 2.94 (td, 1H, J=11.1, 7.1 Hz, CH₂), 2.58 (m, 2H, CH₂), 2.37 (dd, 1H, J=14.3, 7 Hz, CH₂), 2.27 (d, 1H, J=16.6 Hz, C(O)CH₂), 2.04 (m, 1H, CH₂), 1.91 (m, 1H, CH₂), 1.88 (d, 1H, J=16.2 Hz, C(O)CH₂), 1.75 (m, 2H, CH₂), 1.42 (m, 3H, CH₂ & (CH₃)₂CH), 1.29 (m, 1H, CH₂), 0.97 (m, 1H, CH₂), 0.84 (d, 3H, J=7.0 Hz, (CH₃)₂CH), 0.83 (d, 3H, J=7.0 Hz, (CH₃)₂CH) ¹³C NMR (400 MHz, CDCl₃) δ 174.19, 170.57, 157.87, 146.75, 145.92, 133.43, 128.55, 128.46 (residual benzene), 112.75, 109.80, 100.94, 100.16, 74.83, 74.69, 70.70, 57.25, 55.98, 54.12, 51.63, 48.82, 43.54, 42.89, 36.87, 31.70, 31.48, 28.13, 22.83, 22.38, 20.42; IR (neat film) 3527 (w), 2955 (m), 1748 (s), 1653 (m), 1504 (m), 1488 (s), 1225 (s), 1036 (m), 754 (m); HRMS (ESI) calcd for C₂₈H₃₈NO₈ (M⁺ + H) 516.2597 observed 516.2581; [α]_D = -110° (c 1.46, CHCl₃).

Lit ¹H NMR of **1**^{*} (100 MHz, CDCl₃) δ 6.59 (s, 1H, ArH), 6.50 (s, 1H, ArH), 5.96 (d, 1H, J=10 Hz ArCHCH), 5.82 (m, 2H, OCH₂O), 5.01 (s, 1H, vinyl H), 3.64 (s, 3H, OCH₃), 3.53 (s, 3H, OCH₃), 2.06 (q, 2H, J=16Hz, CH₂), 0.82 (d, J=6 Hz, (CH₃)₂CH); [α]_D = -119° (c 0.6, CHCl₃).

* Mikolajczak, K. L.; Powell, R. G.; Smith, C. R. Jr. *Tetrahedron*, **1972**, 28, 1995.

Also, T. Ross Kelly and K. L. Mikolajczak compare deoxyharringtonine with its C2'-sidechain epimer: ¹H NMR of C2'-*epi*-**1**[†] Deoxyharringtonine: δ 6.59 (s, 1H, ArH), 6.50 (s, 1H, ArH), 5.97 (d, 1H, ArCHCH), 3.64 (s, 3H, CH₃), 3.53 (s, 3H, CH₃), 2.26 (d, 1H, CH₂), 1.86 (d, 1H, CH₂) Sidechain epimer: 6.56 (s, 2H, ArH), 5.86 (d, 1H, ArCHCH), 3.62 (s, 3H, CH₃) 3.60 (s, 3H, CH₃), 2.66 (d, 1H, CH₂), 2.46 (d, 1H, CH₂) The spectrum of our synthetic **1** clearly matches that of deoxyharringtonine and not its C2'-sidechain epimer.

[†] Mikolajczak, K.L.; Smith, C. R. Jr.; Weisleder, D.; Kelly, T. R.; McKenna, J. C.; Christenson, P.A. *Tet. Lett.* **1974**, 283-286.

Note: this numbering system is for the X-ray crystal structure of **15** only and does not correspond to the numbering system of cephalotaxine (**2**).

Crystal data and structure refinement for **15**:

Identification code	ga61fas	
Empirical formula	C ₆₈ H ₈₄ N ₂ O ₁₆ S ₂	
Formula weight	1249.49	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 10.4431(16) Å	a = 90°.
	b = 16.639(3) Å	b = 90°.
	c = 38.548(6) Å	c = 90°.
Volume	6698.2(18) Å ³	
Z	4	
Density (calculated)	1.239 Mg/m ³	
Absorption coefficient	0.147 mm ⁻¹	
F(000)	2664	

Crystal size	0.40 x 0.08 x 0.06 mm ³
Theta range for data collection	1.33 to 25.70°
Index ranges	-12<=h<=12, -20<=k<=20, -47<=l<=45
Reflections collected	32544
Independent reflections	12606 [R(int) = 0.1206]
Completeness to theta = 25.70°	99.6 %
Absorption correction	Integration
Max. and min. transmission	0.9940 and 0.9617
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	12606 / 220 / 889
Goodness-of-fit on F ²	0.932
Final R indices [I>2sigma(I)]	R1 = 0.0655, wR2 = 0.1174
R indices (all data)	R1 = 0.1715, wR2 = 0.1546
Absolute structure parameter	-0.03(11)
Largest diff. peak and hole	0.233 and -0.275 e.Å ⁻³

Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for 15. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor:

	x	y	z	U(eq)
C(1)	365(5)	17(3)	5873(2)	41(2)
C(2)	1352(5)	511(3)	5675(1)	37(1)
C(3)	2108(5)	1124(3)	5881(1)	33(1)
C(4)	3243(5)	1409(3)	5724(2)	41(1)
C(5)	3942(5)	1958(3)	5904(2)	45(2)
C(6)	3602(5)	2238(3)	6227(2)	43(2)
C(7)	2503(5)	1977(3)	6385(1)	43(2)
C(8)	1728(5)	1409(3)	6205(1)	34(1)
C(9)	490(5)	1196(3)	6368(1)	32(1)
C(10)	259(5)	1009(3)	6699(2)	41(2)
C(11)	-1137(5)	909(3)	6781(2)	44(2)
C(12)	-1799(5)	1165(3)	6445(1)	37(1)
C(13)	-734(5)	1172(3)	6160(1)	33(1)
C(14)	-898(5)	1846(3)	5894(1)	36(1)
C(15)	-1916(4)	1496(3)	5648(1)	32(1)
C(16)	-1751(5)	569(3)	5681(1)	40(1)
C(17)	5346(6)	2915(4)	6062(2)	68(2)
C(18)	1316(6)	301(4)	7134(2)	49(2)
C(19)	2319(5)	347(3)	7412(2)	56(2)
C(20)	2607(10)	-494(5)	7538(3)	89(3)
C(21)	3536(7)	715(7)	7268(3)	87(3)
C(22)	1777(10)	869(6)	7701(2)	96(3)
C(23)	-2497(6)	1968(4)	6885(2)	57(2)

C(24)	-3800(5)	1616(4)	6967(2)	67(2)
C(25)	-2365(8)	2811(4)	7009(2)	97(3)
C(26)	-1762(5)	2855(3)	5233(1)	37(1)
C(27)	-625(5)	3277(4)	5216(1)	47(2)
C(28)	-684(6)	4110(4)	5238(2)	55(2)
C(29)	-1818(6)	4504(4)	5279(2)	59(2)
C(30)	-2948(6)	4084(3)	5294(2)	56(2)
C(31)	-2928(5)	3252(3)	5273(1)	44(2)
N(1)	-853(4)	412(2)	5966(1)	36(1)
O(1)	5105(3)	2306(2)	5808(1)	56(1)
O(2)	4490(4)	2781(2)	6349(1)	57(1)
O(3)	1196(3)	995(2)	6958(1)	45(1)
O(4)	684(5)	-277(3)	7062(1)	91(2)
O(5)	-1528(4)	1484(3)	7036(1)	61(1)
O(6)	-2244(3)	1949(2)	6521(1)	46(1)
O(7)	-492(3)	1555(2)	5088(1)	49(1)
O(8)	-2850(3)	1517(2)	5024(1)	51(1)
S(1)	-1744(1)	1802(1)	5211(1)	41(1)
C(32)	5226(5)	4716(3)	8797(2)	44(2)
C(33)	6511(5)	4299(3)	8732(2)	54(2)
C(34)	6488(5)	3557(3)	8502(1)	41(2)
C(35)	7678(5)	3316(4)	8367(1)	47(2)
C(36)	7723(6)	2654(4)	8160(2)	49(2)
C(37)	6643(6)	2233(4)	8076(2)	49(2)
C(38)	5452(5)	2451(3)	8201(1)	46(2)
C(39)	5395(5)	3142(3)	8415(1)	37(1)
C(40)	4135(5)	3330(3)	8568(1)	31(1)
C(41)	3016(5)	3392(3)	8412(1)	36(1)
C(42)	1916(5)	3604(3)	8644(1)	42(2)
C(43)	2485(5)	3454(3)	9001(1)	36(1)
C(44)	3958(5)	3495(3)	8948(1)	34(1)
C(45)	4713(5)	2953(3)	9199(1)	37(1)
C(46)	4733(5)	3448(3)	9531(1)	39(1)
C(47)	4776(6)	4329(3)	9408(1)	45(2)
C(48)	8329(6)	1559(5)	7871(2)	77(2)
C(49)	2962(6)	3942(4)	7851(2)	50(2)
C(50)	2648(6)	3762(4)	7479(2)	55(2)
C(51)	2596(10)	4558(4)	7285(2)	128(4)
C(52)	1408(6)	3314(5)	7442(2)	85(2)
C(53)	3757(7)	3257(5)	7330(2)	85(2)
C(54)	1023(5)	2432(4)	8854(2)	47(2)
C(55)	-174(5)	2365(4)	9073(2)	69(2)
C(56)	1370(7)	1675(4)	8663(2)	90(3)
C(57)	6109(5)	2178(3)	9827(1)	37(1)
C(58)	7166(5)	1794(4)	9693(1)	48(2)
C(59)	7203(6)	963(4)	9703(2)	57(2)

C(60)	6203(7)	531(4)	9835(2)	64(2)
C(61)	5153(7)	923(4)	9968(2)	61(2)
C(62)	5110(5)	1756(4)	9966(1)	48(2)
N(2)	4332(4)	4337(2)	9042(1)	38(1)
O(9)	8766(4)	2311(3)	7996(1)	68(1)
O(10)	6927(4)	1597(3)	7861(1)	69(1)
O(11)	2802(3)	3284(2)	8054(1)	40(1)
O(12)	3293(5)	4571(3)	7971(1)	67(1)
O(13)	838(3)	3088(2)	8619(1)	51(1)
O(14)	2084(3)	2645(2)	9070(1)	51(1)
O(15)	7209(3)	3515(2)	9649(1)	54(1)
O(16)	5705(4)	3547(2)	10151(1)	54(1)
S(2)	6045(1)	3240(1)	9812(1)	41(1)
C(63)	5084(17)	5485(10)	6208(5)	192(6)
C(64)	3613(16)	5543(8)	6267(4)	174(5)
C(65)	2893(12)	4738(7)	6200(5)	162(5)
C(66)	1434(12)	4838(7)	6274(4)	164(5)
C(67)	687(14)	4031(7)	6215(5)	184(6)
C(68)	-763(16)	4207(9)	6288(5)	228(9)
C(69)	3468(14)	-145(13)	7287(5)	92(4)
C(70)	2750(20)	1202(7)	7484(6)	88(4)
C(71)	1804(19)	-22(14)	7745(3)	91(4)
C(72)	6780(30)	4790(40)	6361(14)	340(50)
C(73)	5380(40)	5070(30)	6443(8)	191(8)
C(74)	4540(30)	5110(20)	6108(8)	182(6)
C(75)	3090(30)	5150(20)	6209(14)	166(6)
C(76)	2310(40)	4439(19)	6047(11)	169(6)
C(77)	870(40)	4580(30)	6140(14)	177(6)

Bond lengths [Å] and angles [°] for 15:

C(1)-N(1)	1.476(6)
C(1)-C(2)	1.523(7)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.515(7)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(8)	1.394(7)
C(3)-C(4)	1.412(7)
C(4)-C(5)	1.360(7)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.374(7)
C(5)-O(1)	1.396(6)
C(6)-C(7)	1.369(7)

C(6)-O(2)	1.378(6)
C(7)-C(8)	1.423(7)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.480(7)
C(9)-C(10)	1.335(7)
C(9)-C(13)	1.509(7)
C(10)-O(3)	1.398(6)
C(10)-C(11)	1.501(7)
C(11)-O(5)	1.431(6)
C(11)-C(12)	1.528(7)
C(11)-H(11A)	1.0000
C(12)-O(6)	1.417(6)
C(12)-C(13)	1.564(7)
C(12)-H(12A)	1.0000
C(13)-N(1)	1.473(6)
C(13)-C(14)	1.527(7)
C(14)-C(15)	1.539(6)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.557(6)
C(15)-S(1)	1.769(5)
C(15)-H(15A)	1.0000
C(16)-N(1)	1.470(6)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-O(1)	1.433(7)
C(17)-O(2)	1.439(7)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-O(4)	1.199(7)
C(18)-O(3)	1.346(6)
C(18)-C(19)	1.500(8)
C(19)-C(20)	1.512(7)
C(19)-C(21)	1.516(7)
C(19)-C(70)	1.517(8)
C(19)-C(71)	1.522(8)
C(19)-C(22)	1.524(7)
C(19)-C(69)	1.529(8)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800

C(22)-H(22C)	0.9800
C(23)-O(5)	1.418(7)
C(23)-O(6)	1.427(6)
C(23)-C(25)	1.489(8)
C(23)-C(24)	1.516(8)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-C(27)	1.381(7)
C(26)-C(31)	1.394(7)
C(26)-S(1)	1.753(5)
C(27)-C(28)	1.390(8)
C(27)-H(27)	0.9500
C(28)-C(29)	1.363(8)
C(28)-H(28)	0.9500
C(29)-C(30)	1.372(8)
C(29)-H(29)	0.9500
C(30)-C(31)	1.388(7)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
O(7)-S(1)	1.451(3)
O(8)-S(1)	1.444(3)
C(32)-N(2)	1.468(6)
C(32)-C(33)	1.532(7)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.520(7)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(39)	1.375(7)
C(34)-C(35)	1.406(7)
C(35)-C(36)	1.361(8)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.367(8)
C(36)-O(9)	1.383(6)
C(37)-O(10)	1.378(6)
C(37)-C(38)	1.382(7)
C(38)-C(39)	1.415(7)
C(38)-H(38A)	0.9500
C(39)-C(40)	1.476(7)
C(40)-C(41)	1.318(7)
C(40)-C(44)	1.502(7)
C(41)-O(11)	1.409(6)

C(41)-C(42)	1.498(7)
C(42)-O(13)	1.419(6)
C(42)-C(43)	1.520(7)
C(42)-H(42A)	1.0000
C(43)-O(14)	1.436(6)
C(43)-C(44)	1.553(7)
C(43)-H(43A)	1.0000
C(44)-N(2)	1.499(6)
C(44)-C(45)	1.540(7)
C(45)-C(46)	1.521(7)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.541(7)
C(46)-S(2)	1.782(5)
C(46)-H(46A)	1.0000
C(47)-N(2)	1.487(6)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-O(9)	1.417(8)
C(48)-O(10)	1.466(7)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-O(12)	1.195(7)
C(49)-O(11)	1.357(7)
C(49)-C(50)	1.501(8)
C(50)-C(52)	1.501(8)
C(50)-C(51)	1.524(8)
C(50)-C(53)	1.542(8)
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-O(13)	1.431(6)
C(54)-O(14)	1.432(6)
C(54)-C(56)	1.504(8)
C(54)-C(55)	1.513(7)
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800

C(56)-H(56C)	0.9800
C(57)-C(62)	1.366(7)
C(57)-C(58)	1.376(7)
C(57)-S(2)	1.769(5)
C(58)-C(59)	1.383(8)
C(58)-H(58)	0.9500
C(59)-C(60)	1.367(8)
C(59)-H(59)	0.9500
C(60)-C(61)	1.375(8)
C(60)-H(60)	0.9500
C(61)-C(62)	1.387(8)
C(61)-H(61)	0.9500
C(62)-H(62)	0.9500
O(15)-S(2)	1.444(4)
O(16)-S(2)	1.447(4)
C(63)-C(64)	1.556(9)
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-C(65)	1.557(9)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(65)-C(66)	1.559(9)
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(66)-C(67)	1.569(9)
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
C(67)-C(68)	1.568(10)
C(67)-H(67A)	0.9900
C(67)-H(67B)	0.9900
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-C(73)	1.566(11)
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800

C(72)-H(72C)	0.9800
C(73)-C(74)	1.564(11)
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(74)-C(75)	1.563(11)
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(75)-C(76)	1.567(11)
C(75)-H(75A)	0.9900
C(75)-H(75B)	0.9900
C(76)-C(77)	1.565(11)
C(76)-H(76A)	0.9900
C(76)-H(76B)	0.9900
C(77)-H(77A)	0.9800
C(77)-H(77B)	0.9800
C(77)-H(77C)	0.9800
N(1)-C(1)-C(2)	117.6(4)
N(1)-C(1)-H(1A)	107.9
C(2)-C(1)-H(1A)	107.9
N(1)-C(1)-H(1B)	107.9
C(2)-C(1)-H(1B)	107.9
H(1A)-C(1)-H(1B)	107.2
C(3)-C(2)-C(1)	117.0(5)
C(3)-C(2)-H(2A)	108.0
C(1)-C(2)-H(2A)	108.0
C(3)-C(2)-H(2B)	108.0
C(1)-C(2)-H(2B)	108.0
H(2A)-C(2)-H(2B)	107.3
C(8)-C(3)-C(4)	120.6(5)
C(8)-C(3)-C(2)	123.4(5)
C(4)-C(3)-C(2)	116.0(5)
C(5)-C(4)-C(3)	117.2(5)
C(5)-C(4)-H(4A)	121.4
C(3)-C(4)-H(4A)	121.4
C(4)-C(5)-C(6)	123.4(5)
C(4)-C(5)-O(1)	127.5(6)
C(6)-C(5)-O(1)	109.0(5)
C(7)-C(6)-C(5)	120.8(5)
C(7)-C(6)-O(2)	128.3(6)
C(5)-C(6)-O(2)	111.0(5)
C(6)-C(7)-C(8)	118.1(5)
C(6)-C(7)-H(7A)	120.9
C(8)-C(7)-H(7A)	120.9
C(3)-C(8)-C(7)	119.9(5)
C(3)-C(8)-C(9)	123.1(5)
C(7)-C(8)-C(9)	116.9(5)

C(10)-C(9)-C(8)	128.1(5)
C(10)-C(9)-C(13)	110.4(5)
C(8)-C(9)-C(13)	121.5(4)
C(9)-C(10)-O(3)	124.1(5)
C(9)-C(10)-C(11)	113.7(5)
O(3)-C(10)-C(11)	121.8(5)
O(5)-C(11)-C(10)	110.4(5)
O(5)-C(11)-C(12)	105.4(4)
C(10)-C(11)-C(12)	103.3(5)
O(5)-C(11)-H(11A)	112.4
C(10)-C(11)-H(11A)	112.4
C(12)-C(11)-H(11A)	112.4
O(6)-C(12)-C(11)	103.3(4)
O(6)-C(12)-C(13)	111.8(4)
C(11)-C(12)-C(13)	106.0(4)
O(6)-C(12)-H(12A)	111.8
C(11)-C(12)-H(12A)	111.8
C(13)-C(12)-H(12A)	111.8
N(1)-C(13)-C(9)	111.3(4)
N(1)-C(13)-C(14)	106.3(4)
C(9)-C(13)-C(14)	115.6(4)
N(1)-C(13)-C(12)	106.8(4)
C(9)-C(13)-C(12)	103.3(4)
C(14)-C(13)-C(12)	113.4(4)
C(13)-C(14)-C(15)	102.3(4)
C(13)-C(14)-H(14A)	111.3
C(15)-C(14)-H(14A)	111.3
C(13)-C(14)-H(14B)	111.3
C(15)-C(14)-H(14B)	111.3
H(14A)-C(14)-H(14B)	109.2
C(14)-C(15)-C(16)	104.4(4)
C(14)-C(15)-S(1)	114.1(3)
C(16)-C(15)-S(1)	110.5(3)
C(14)-C(15)-H(15A)	109.2
C(16)-C(15)-H(15A)	109.2
S(1)-C(15)-H(15A)	109.2
N(1)-C(16)-C(15)	107.8(4)
N(1)-C(16)-H(16A)	110.1
C(15)-C(16)-H(16A)	110.1
N(1)-C(16)-H(16B)	110.1
C(15)-C(16)-H(16B)	110.1
H(16A)-C(16)-H(16B)	108.5
O(1)-C(17)-O(2)	107.9(5)
O(1)-C(17)-H(17A)	110.1
O(2)-C(17)-H(17A)	110.1
O(1)-C(17)-H(17B)	110.1

O(2)-C(17)-H(17B)	110.1
H(17A)-C(17)-H(17B)	108.4
O(4)-C(18)-O(3)	121.4(6)
O(4)-C(18)-C(19)	126.0(6)
O(3)-C(18)-C(19)	112.5(5)
C(18)-C(19)-C(20)	108.8(5)
C(18)-C(19)-C(21)	110.2(5)
C(20)-C(19)-C(21)	109.0(6)
C(18)-C(19)-C(70)	112.5(8)
C(20)-C(19)-C(70)	138.6(9)
C(21)-C(19)-C(70)	56.0(9)
C(18)-C(19)-C(71)	109.7(8)
C(20)-C(19)-C(71)	55.0(9)
C(21)-C(19)-C(71)	140.1(9)
C(70)-C(19)-C(71)	109.1(8)
C(18)-C(19)-C(22)	107.0(5)
C(20)-C(19)-C(22)	111.4(6)
C(21)-C(19)-C(22)	110.4(6)
C(70)-C(19)-C(22)	55.9(9)
C(71)-C(19)-C(22)	58.6(9)
C(18)-C(19)-C(69)	107.3(8)
C(20)-C(19)-C(69)	56.6(8)
C(21)-C(19)-C(69)	56.2(9)
C(70)-C(19)-C(69)	109.2(9)
C(71)-C(19)-C(69)	109.0(8)
C(22)-C(19)-C(69)	145.6(9)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
O(5)-C(23)-O(6)	105.0(5)
O(5)-C(23)-C(25)	109.8(6)
O(6)-C(23)-C(25)	108.6(5)
O(5)-C(23)-C(24)	109.6(5)
O(6)-C(23)-C(24)	111.3(5)
C(25)-C(23)-C(24)	112.3(6)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5

H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(27)-C(26)-C(31)	121.0(5)
C(27)-C(26)-S(1)	119.8(4)
C(31)-C(26)-S(1)	119.2(4)
C(26)-C(27)-C(28)	117.8(5)
C(26)-C(27)-H(27)	121.1
C(28)-C(27)-H(27)	121.1
C(29)-C(28)-C(27)	121.7(6)
C(29)-C(28)-H(28)	119.2
C(27)-C(28)-H(28)	119.2
C(28)-C(29)-C(30)	120.5(6)
C(28)-C(29)-H(29)	119.7
C(30)-C(29)-H(29)	119.7
C(29)-C(30)-C(31)	119.5(6)
C(29)-C(30)-H(30)	120.3
C(31)-C(30)-H(30)	120.3
C(30)-C(31)-C(26)	119.5(5)
C(30)-C(31)-H(31)	120.2
C(26)-C(31)-H(31)	120.2
C(16)-N(1)-C(13)	106.3(4)
C(16)-N(1)-C(1)	116.6(4)
C(13)-N(1)-C(1)	115.6(4)
C(5)-O(1)-C(17)	105.2(4)
C(6)-O(2)-C(17)	104.8(4)
C(18)-O(3)-C(10)	116.1(4)
C(23)-O(5)-C(11)	107.6(4)
C(12)-O(6)-C(23)	106.5(4)
O(8)-S(1)-O(7)	117.7(2)
O(8)-S(1)-C(26)	110.1(2)
O(7)-S(1)-C(26)	108.0(3)
O(8)-S(1)-C(15)	107.5(2)
O(7)-S(1)-C(15)	108.8(2)
C(26)-S(1)-C(15)	104.0(2)
N(2)-C(32)-C(33)	117.9(5)
N(2)-C(32)-H(32A)	107.8
C(33)-C(32)-H(32A)	107.8
N(2)-C(32)-H(32B)	107.8
C(33)-C(32)-H(32B)	107.8
H(32A)-C(32)-H(32B)	107.2
C(34)-C(33)-C(32)	116.7(5)

C(34)-C(33)-H(33A)	108.1
C(32)-C(33)-H(33A)	108.1
C(34)-C(33)-H(33B)	108.1
C(32)-C(33)-H(33B)	108.1
H(33A)-C(33)-H(33B)	107.3
C(39)-C(34)-C(35)	119.9(5)
C(39)-C(34)-C(33)	124.4(5)
C(35)-C(34)-C(33)	115.7(5)
C(36)-C(35)-C(34)	118.6(5)
C(36)-C(35)-H(35A)	120.7
C(34)-C(35)-H(35A)	120.7
C(35)-C(36)-C(37)	121.6(6)
C(35)-C(36)-O(9)	129.0(6)
C(37)-C(36)-O(9)	109.3(5)
C(36)-C(37)-O(10)	111.0(5)
C(36)-C(37)-C(38)	121.7(6)
O(10)-C(37)-C(38)	127.3(6)
C(37)-C(38)-C(39)	117.0(5)
C(37)-C(38)-H(38A)	121.5
C(39)-C(38)-H(38A)	121.5
C(34)-C(39)-C(38)	121.1(5)
C(34)-C(39)-C(40)	122.3(5)
C(38)-C(39)-C(40)	116.2(5)
C(41)-C(40)-C(39)	128.7(5)
C(41)-C(40)-C(44)	108.8(5)
C(39)-C(40)-C(44)	122.6(4)
C(40)-C(41)-O(11)	125.3(5)
C(40)-C(41)-C(42)	115.2(5)
O(11)-C(41)-C(42)	119.5(5)
O(13)-C(42)-C(41)	115.2(4)
O(13)-C(42)-C(43)	105.9(4)
C(41)-C(42)-C(43)	101.7(4)
O(13)-C(42)-H(42A)	111.2
C(41)-C(42)-H(42A)	111.2
C(43)-C(42)-H(42A)	111.2
O(14)-C(43)-C(42)	102.0(4)
O(14)-C(43)-C(44)	110.8(4)
C(42)-C(43)-C(44)	105.1(4)
O(14)-C(43)-H(43A)	112.7
C(42)-C(43)-H(43A)	112.7
C(44)-C(43)-H(43A)	112.7
N(2)-C(44)-C(40)	112.0(4)
N(2)-C(44)-C(45)	105.2(4)
C(40)-C(44)-C(45)	116.4(4)
N(2)-C(44)-C(43)	105.5(4)
C(40)-C(44)-C(43)	104.0(4)

C(45)-C(44)-C(43)	113.5(4)
C(46)-C(45)-C(44)	102.7(4)
C(46)-C(45)-H(45A)	111.2
C(44)-C(45)-H(45A)	111.2
C(46)-C(45)-H(45B)	111.2
C(44)-C(45)-H(45B)	111.2
H(45A)-C(45)-H(45B)	109.1
C(45)-C(46)-C(47)	104.9(4)
C(45)-C(46)-S(2)	114.7(4)
C(47)-C(46)-S(2)	110.4(4)
C(45)-C(46)-H(46A)	108.9
C(47)-C(46)-H(46A)	108.9
S(2)-C(46)-H(46A)	108.9
N(2)-C(47)-C(46)	106.9(4)
N(2)-C(47)-H(47A)	110.3
C(46)-C(47)-H(47A)	110.3
N(2)-C(47)-H(47B)	110.3
C(46)-C(47)-H(47B)	110.3
H(47A)-C(47)-H(47B)	108.6
O(9)-C(48)-O(10)	107.0(5)
O(9)-C(48)-H(48A)	110.3
O(10)-C(48)-H(48A)	110.3
O(9)-C(48)-H(48B)	110.3
O(10)-C(48)-H(48B)	110.3
H(48A)-C(48)-H(48B)	108.6
O(12)-C(49)-O(11)	121.3(6)
O(12)-C(49)-C(50)	127.4(6)
O(11)-C(49)-C(50)	111.3(5)
C(49)-C(50)-C(52)	112.3(5)
C(49)-C(50)-C(51)	107.7(5)
C(52)-C(50)-C(51)	110.7(6)
C(49)-C(50)-C(53)	107.5(5)
C(52)-C(50)-C(53)	110.0(5)
C(51)-C(50)-C(53)	108.6(6)
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5

C(50)-C(53)-H(53A)	109.5
C(50)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(50)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
O(13)-C(54)-O(14)	106.6(4)
O(13)-C(54)-C(56)	111.3(5)
O(14)-C(54)-C(56)	107.8(5)
O(13)-C(54)-C(55)	107.4(5)
O(14)-C(54)-C(55)	109.3(5)
C(56)-C(54)-C(55)	114.2(6)
C(54)-C(55)-H(55A)	109.5
C(54)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(54)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(54)-C(56)-H(56A)	109.5
C(54)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(54)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(62)-C(57)-C(58)	121.4(5)
C(62)-C(57)-S(2)	119.7(4)
C(58)-C(57)-S(2)	118.8(4)
C(57)-C(58)-C(59)	118.4(6)
C(57)-C(58)-H(58)	120.8
C(59)-C(58)-H(58)	120.8
C(60)-C(59)-C(58)	121.0(6)
C(60)-C(59)-H(59)	119.5
C(58)-C(59)-H(59)	119.5
C(59)-C(60)-C(61)	119.8(6)
C(59)-C(60)-H(60)	120.1
C(61)-C(60)-H(60)	120.1
C(60)-C(61)-C(62)	120.0(6)
C(60)-C(61)-H(61)	120.0
C(62)-C(61)-H(61)	120.0
C(57)-C(62)-C(61)	119.3(6)
C(57)-C(62)-H(62)	120.3
C(61)-C(62)-H(62)	120.3
C(32)-N(2)-C(47)	114.5(4)
C(32)-N(2)-C(44)	114.4(4)
C(47)-N(2)-C(44)	107.6(4)
C(36)-O(9)-C(48)	105.5(5)

C(37)-O(10)-C(48)	103.4(5)
C(49)-O(11)-C(41)	116.2(4)
C(42)-O(13)-C(54)	108.1(4)
C(54)-O(14)-C(43)	110.4(4)
O(15)-S(2)-O(16)	119.3(2)
O(15)-S(2)-C(57)	107.4(3)
O(16)-S(2)-C(57)	109.5(2)
O(15)-S(2)-C(46)	108.6(2)
O(16)-S(2)-C(46)	107.0(2)
C(57)-S(2)-C(46)	104.0(3)
C(64)-C(63)-H(63A)	109.5
C(64)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(64)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
C(63)-C(64)-C(65)	113.5(11)
C(63)-C(64)-H(64A)	108.9
C(65)-C(64)-H(64A)	108.9
C(63)-C(64)-H(64B)	108.9
C(65)-C(64)-H(64B)	108.9
H(64A)-C(64)-H(64B)	107.7
C(64)-C(65)-C(66)	110.5(10)
C(64)-C(65)-H(65A)	109.6
C(66)-C(65)-H(65A)	109.6
C(64)-C(65)-H(65B)	109.6
C(66)-C(65)-H(65B)	109.6
H(65A)-C(65)-H(65B)	108.1
C(65)-C(66)-C(67)	111.6(10)
C(65)-C(66)-H(66A)	109.3
C(67)-C(66)-H(66A)	109.3
C(65)-C(66)-H(66B)	109.3
C(67)-C(66)-H(66B)	109.3
H(66A)-C(66)-H(66B)	108.0
C(68)-C(67)-C(66)	107.1(10)
C(68)-C(67)-H(67A)	110.3
C(66)-C(67)-H(67A)	110.3
C(68)-C(67)-H(67B)	110.3
C(66)-C(67)-H(67B)	110.3
H(67A)-C(67)-H(67B)	108.5
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5

C(19)-C(69)-H(69A)	109.5
C(19)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(19)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(19)-C(70)-H(70A)	109.5
C(19)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(19)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(19)-C(71)-H(71A)	109.5
C(19)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(19)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
C(73)-C(72)-H(72A)	109.5
C(73)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(73)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(74)-C(73)-C(72)	111.8(14)
C(74)-C(73)-H(73A)	109.2
C(72)-C(73)-H(73A)	109.2
C(74)-C(73)-H(73B)	109.2
C(72)-C(73)-H(73B)	109.3
H(73A)-C(73)-H(73B)	107.9
C(75)-C(74)-C(73)	110.0(13)
C(75)-C(74)-H(74A)	109.7
C(73)-C(74)-H(74A)	109.7
C(75)-C(74)-H(74B)	109.7
C(73)-C(74)-H(74B)	109.7
H(74A)-C(74)-H(74B)	108.2
C(74)-C(75)-C(76)	111.4(13)
C(74)-C(75)-H(75A)	109.3
C(76)-C(75)-H(75A)	109.4
C(74)-C(75)-H(75B)	109.4
C(76)-C(75)-H(75B)	109.3
H(75A)-C(75)-H(75B)	108.0
C(77)-C(76)-C(75)	107.1(12)
C(77)-C(76)-H(76A)	110.3
C(75)-C(76)-H(76A)	110.3
C(77)-C(76)-H(76B)	110.3

C(75)-C(76)-H(76B)	110.3
H(76A)-C(76)-H(76B)	108.6
C(76)-C(77)-H(77A)	109.5
C(76)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
C(76)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5

Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 15. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$:

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	40(3)	33(3)	51(4)	-3(3)	2(3)	8(3)
C(2)	38(3)	36(3)	38(4)	4(3)	6(3)	0(3)
C(3)	25(3)	42(3)	33(4)	9(3)	-4(3)	4(3)
C(4)	36(3)	45(3)	41(4)	1(3)	4(3)	2(3)
C(5)	34(3)	48(4)	53(4)	16(3)	14(3)	5(3)
C(6)	30(3)	44(4)	55(4)	7(3)	-6(3)	-6(3)
C(7)	38(3)	55(4)	36(4)	6(3)	4(3)	-5(3)
C(8)	28(3)	45(3)	29(3)	11(3)	0(3)	3(3)
C(9)	30(3)	32(3)	33(4)	3(3)	-4(3)	-3(2)
C(10)	45(4)	42(4)	36(4)	10(3)	2(3)	-1(3)
C(11)	39(3)	48(4)	44(4)	4(3)	6(3)	0(3)
C(12)	38(3)	35(3)	38(4)	1(3)	1(3)	1(3)
C(13)	25(3)	39(3)	35(3)	8(3)	4(3)	0(3)
C(14)	31(3)	34(3)	43(3)	-4(3)	0(3)	-3(3)
C(15)	22(3)	36(3)	37(3)	-3(3)	2(3)	-1(2)
C(16)	29(3)	48(4)	43(4)	2(3)	-1(3)	-4(3)
C(17)	34(4)	74(5)	96(6)	-3(5)	13(4)	-12(4)
C(18)	48(4)	40(4)	58(5)	6(4)	2(3)	0(3)
C(19)	49(4)	64(4)	53(4)	16(3)	-12(3)	5(3)
C(20)	92(7)	85(6)	91(7)	34(5)	-26(6)	7(5)
C(21)	53(5)	117(7)	91(7)	30(6)	-21(4)	-16(5)
C(22)	101(7)	122(7)	66(6)	-13(6)	-20(5)	14(6)
C(23)	59(4)	65(5)	47(4)	1(4)	20(4)	8(4)
C(24)	48(4)	89(5)	63(5)	6(4)	22(3)	8(4)
C(25)	127(7)	74(5)	89(6)	-27(5)	34(5)	-14(5)
C(26)	30(3)	49(4)	31(3)	9(3)	-2(3)	-1(3)
C(27)	35(3)	54(4)	52(4)	2(4)	1(3)	-7(3)
C(28)	51(4)	59(4)	56(4)	4(4)	2(4)	-13(4)
C(29)	60(4)	43(4)	75(5)	9(4)	-14(4)	-3(4)
C(30)	52(4)	42(4)	74(5)	14(3)	-11(4)	4(3)
C(31)	34(3)	43(3)	56(4)	10(3)	3(3)	-4(3)

N(1)	39(3)	32(3)	37(3)	0(2)	0(2)	-1(2)
O(1)	36(2)	61(3)	70(3)	1(3)	16(2)	-15(2)
O(2)	37(2)	66(3)	68(3)	-4(2)	1(2)	-15(2)
O(3)	43(2)	52(3)	41(2)	14(2)	-3(2)	-4(2)
O(4)	84(4)	49(3)	140(5)	15(3)	-39(4)	-7(3)
O(5)	47(2)	96(3)	42(3)	-14(3)	2(2)	11(3)
O(6)	48(2)	42(2)	49(3)	-4(2)	12(2)	8(2)
O(7)	36(2)	63(3)	49(3)	10(2)	11(2)	10(2)
O(8)	44(2)	49(2)	59(3)	-4(2)	-26(2)	-1(2)
S(1)	34(1)	45(1)	43(1)	2(1)	-4(1)	2(1)
C(32)	47(4)	35(3)	52(4)	-2(3)	-3(3)	-3(3)
C(33)	45(4)	49(4)	68(5)	-7(4)	8(3)	-15(3)
C(34)	37(3)	50(4)	35(4)	5(3)	-1(3)	-2(3)
C(35)	33(3)	57(4)	50(4)	-3(4)	4(3)	-9(3)
C(36)	37(4)	73(5)	37(4)	-4(4)	5(3)	0(4)
C(37)	54(4)	57(4)	36(4)	-15(3)	1(3)	4(4)
C(38)	31(3)	57(4)	49(4)	0(4)	-6(3)	2(3)
C(39)	38(3)	42(3)	31(3)	-6(3)	-4(3)	3(3)
C(40)	34(3)	30(3)	30(3)	-3(3)	-3(3)	-6(3)
C(41)	38(3)	33(3)	36(4)	2(3)	2(3)	-8(3)
C(42)	31(3)	45(3)	49(4)	5(3)	-3(3)	0(3)
C(43)	42(3)	35(3)	32(3)	0(3)	-5(3)	3(3)
C(44)	32(3)	34(3)	37(4)	-1(3)	-5(3)	1(3)
C(45)	42(3)	37(3)	32(3)	2(3)	-5(3)	-4(3)
C(46)	28(3)	46(4)	43(4)	-1(3)	-4(3)	3(3)
C(47)	51(4)	42(4)	44(4)	-9(3)	-16(3)	7(3)
C(48)	59(5)	105(6)	65(5)	-19(5)	2(4)	39(5)
C(49)	52(4)	59(4)	39(4)	3(4)	6(3)	4(4)
C(50)	73(5)	54(4)	39(4)	9(3)	-6(4)	11(4)
C(51)	242(12)	91(6)	50(5)	29(5)	-13(7)	4(7)
C(52)	70(5)	128(7)	59(5)	-9(5)	-24(4)	3(5)
C(53)	81(5)	123(7)	52(5)	-31(5)	-1(4)	9(5)
C(54)	38(3)	54(4)	48(4)	6(3)	-7(3)	-11(3)
C(55)	43(4)	105(6)	57(5)	19(4)	9(3)	-9(4)
C(56)	108(6)	70(5)	93(6)	-33(5)	-8(5)	3(5)
C(57)	36(3)	44(3)	31(3)	1(3)	-3(3)	2(3)
C(58)	43(4)	47(4)	55(4)	2(3)	-2(3)	-5(3)
C(59)	51(4)	62(5)	57(5)	-2(4)	-3(4)	13(4)
C(60)	88(5)	45(4)	60(5)	8(4)	-3(5)	5(4)
C(61)	80(5)	54(5)	49(5)	19(4)	-1(4)	-19(4)
C(62)	43(3)	57(4)	44(4)	0(4)	6(3)	-3(3)
N(2)	39(3)	36(3)	38(3)	-6(2)	1(2)	0(2)
O(9)	47(3)	89(4)	67(3)	-17(3)	15(2)	10(3)
O(10)	64(3)	84(3)	59(3)	-31(3)	-1(2)	12(3)
O(11)	45(2)	41(2)	34(2)	4(2)	-6(2)	-6(2)
O(12)	110(4)	42(3)	48(3)	0(2)	4(3)	-6(3)

O(13)	35(2)	68(3)	50(3)	14(2)	-13(2)	-14(2)
O(14)	43(2)	64(3)	48(3)	12(2)	-10(2)	-14(2)
O(15)	36(2)	53(3)	73(3)	18(2)	-7(2)	-10(2)
O(16)	78(3)	52(2)	33(2)	-10(2)	-11(2)	-2(2)
S(2)	38(1)	43(1)	41(1)	5(1)	-9(1)	-4(1)
C(63)	268(13)	173(13)	136(11)	-49(10)	-50(13)	45(11)
C(64)	274(13)	143(10)	104(8)	-67(8)	-27(11)	52(10)
C(65)	270(13)	120(9)	96(8)	-50(8)	-55(10)	64(10)
C(66)	267(13)	103(8)	123(9)	-32(8)	-81(11)	59(9)
C(67)	282(14)	107(10)	163(12)	-5(11)	-94(12)	48(10)
C(68)	332(17)	134(14)	220(20)	-2(14)	60(20)	-12(14)
C(69)	68(7)	109(8)	98(9)	14(8)	-16(6)	12(7)
C(70)	79(8)	106(7)	80(9)	2(7)	-26(7)	-13(7)
C(71)	102(8)	106(8)	65(8)	16(7)	-15(6)	1(8)
C(72)	230(30)	330(90)	460(120)	-170(80)	-110(40)	10(50)
C(73)	272(15)	168(16)	134(14)	-39(13)	-52(14)	41(15)
C(74)	270(14)	158(12)	118(11)	-60(10)	-39(12)	49(12)
C(75)	271(13)	131(11)	96(9)	-59(10)	-39(10)	58(11)
C(76)	273(14)	115(10)	120(10)	-30(9)	-67(11)	59(10)
C(77)	272(13)	110(11)	148(12)	-15(11)	-86(12)	62(11)

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 15:

	x	y	z	U(eq)
H(1A)	161	-464	5732	50
H(1B)	771	-175	6090	50
H(2A)	1966	135	5566	45
H(2B)	904	797	5486	45
H(4A)	3506	1225	5502	49
H(7A)	2266	2170	6607	52
H(11A)	-1355	345	6849	53
H(12A)	-2518	795	6383	44
H(14A)	-87	1956	5770	43
H(14B)	-1203	2346	6005	43
H(15A)	-2786	1650	5733	38
H(16A)	-2588	313	5730	48
H(16B)	-1411	344	5461	48
H(17A)	5196	3454	5961	81
H(17B)	6246	2885	6142	81
H(20A)	2903	-824	7343	134
H(20B)	1830	-732	7637	134
H(20C)	3276	-473	7716	134
H(21A)	3797	423	7059	131

H(21B)	4216	680	7442	131
H(21C)	3381	1280	7210	131
H(22A)	2382	882	7896	145
H(22B)	960	645	7780	145
H(22C)	1642	1416	7615	145
H(24A)	-3844	1063	6880	100
H(24B)	-4467	1939	6855	100
H(24C)	-3933	1617	7219	100
H(25A)	-1495	3003	6962	145
H(25B)	-2531	2832	7259	145
H(25C)	-2983	3154	6887	145
H(27)	171	3007	5191	56
H(28)	85	4413	5223	66
H(29)	-1827	5073	5297	71
H(30)	-3738	4362	5318	67
H(31)	-3703	2954	5286	53
H(32A)	5407	5266	8882	53
H(32B)	4783	4771	8572	53
H(33A)	7101	4695	8626	65
H(33B)	6877	4144	8959	65
H(35A)	8434	3609	8419	56
H(38A)	4706	2150	8147	55
H(42A)	1662	4179	8615	50
H(43A)	2172	3845	9179	43
H(45A)	4272	2433	9235	45
H(45B)	5590	2852	9113	45
H(46A)	3916	3356	9660	47
H(47A)	4210	4666	9554	55
H(47B)	5660	4542	9424	55
H(48A)	8613	1120	8026	92
H(48B)	8675	1456	7636	92
H(51A)	1873	4877	7370	192
H(51B)	2486	4456	7036	192
H(51C)	3394	4855	7323	192
H(52A)	703	3649	7526	128
H(52B)	1446	2817	7578	128
H(52C)	1267	3182	7197	128
H(53A)	3799	2740	7452	128
H(53B)	4566	3546	7362	128
H(53C)	3612	3162	7082	128
H(55A)	-339	2881	9188	103
H(55B)	-55	1946	9248	103
H(55C)	-903	2226	8925	103
H(56A)	2182	1753	8540	136
H(56B)	695	1544	8496	136
H(56C)	1460	1233	8829	136

H(58)	7854	2092	9596	58
H(59)	7935	689	9617	68
H(60)	6232	-40	9835	77
H(61)	4459	624	10061	73
H(62)	4392	2031	10060	57
H(63A)	5261	5083	6028	289
H(63B)	5505	5327	6424	289
H(63C)	5411	6009	6132	289
H(64A)	3258	5961	6112	209
H(64B)	3453	5715	6509	209
H(65A)	3248	4313	6353	195
H(65B)	3021	4570	5957	195
H(66A)	1080	5257	6119	197
H(66B)	1311	5018	6516	197
H(67A)	804	3841	5974	221
H(67B)	1007	3611	6375	221
H(68A)	-849	4487	6510	342
H(68B)	-1238	3699	6297	342
H(68C)	-1110	4545	6102	342
H(69A)	4113	-167	7472	138
H(69B)	3839	109	7081	138
H(69C)	3189	-691	7230	138
H(70A)	3421	1198	7660	132
H(70B)	2015	1516	7568	132
H(70C)	3076	1443	7270	132
H(71A)	1311	-506	7690	137
H(71B)	1250	367	7863	137
H(71C)	2521	-164	7897	137
H(72A)	6766	4261	6253	506
H(72B)	7276	4772	6576	506
H(72C)	7177	5180	6201	506
H(73A)	4987	4683	6608	229
H(73B)	5397	5602	6555	229
H(74A)	4772	5591	5971	218
H(74B)	4691	4629	5963	218
H(75A)	2724	5669	6126	199
H(75B)	3003	5138	6464	199
H(76A)	2429	4428	5792	203
H(76B)	2614	3921	6144	203
H(77A)	380	4092	6085	265
H(77B)	538	5031	6005	265
H(77C)	793	4695	6388	265

Torsion angles [°] for 15:

N(1)-C(1)-C(2)-C(3)	76.2(6)
C(1)-C(2)-C(3)-C(8)	-18.0(7)
C(1)-C(2)-C(3)-C(4)	162.6(4)
C(8)-C(3)-C(4)-C(5)	0.8(7)
C(2)-C(3)-C(4)-C(5)	-179.8(5)
C(3)-C(4)-C(5)-C(6)	0.4(8)
C(3)-C(4)-C(5)-O(1)	178.0(5)
C(4)-C(5)-C(6)-C(7)	-0.8(8)
O(1)-C(5)-C(6)-C(7)	-178.8(5)
C(4)-C(5)-C(6)-O(2)	179.3(5)
O(1)-C(5)-C(6)-O(2)	1.3(6)
C(5)-C(6)-C(7)-C(8)	0.0(8)
O(2)-C(6)-C(7)-C(8)	179.9(5)
C(4)-C(3)-C(8)-C(7)	-1.6(7)
C(2)-C(3)-C(8)-C(7)	179.1(5)
C(4)-C(3)-C(8)-C(9)	173.8(5)
C(2)-C(3)-C(8)-C(9)	-5.6(8)
C(6)-C(7)-C(8)-C(3)	1.1(7)
C(6)-C(7)-C(8)-C(9)	-174.5(4)
C(3)-C(8)-C(9)-C(10)	138.3(6)
C(7)-C(8)-C(9)-C(10)	-46.2(8)
C(3)-C(8)-C(9)-C(13)	-42.3(7)
C(7)-C(8)-C(9)-C(13)	133.2(5)
C(8)-C(9)-C(10)-O(3)	0.8(9)
C(13)-C(9)-C(10)-O(3)	-178.7(5)
C(8)-C(9)-C(10)-C(11)	173.9(5)
C(13)-C(9)-C(10)-C(11)	-5.6(7)
C(9)-C(10)-C(11)-O(5)	-118.7(5)
O(3)-C(10)-C(11)-O(5)	54.5(7)
C(9)-C(10)-C(11)-C(12)	-6.5(7)
O(3)-C(10)-C(11)-C(12)	166.8(5)
O(5)-C(11)-C(12)-O(6)	13.2(5)
C(10)-C(11)-C(12)-O(6)	-102.6(5)
O(5)-C(11)-C(12)-C(13)	130.9(4)
C(10)-C(11)-C(12)-C(13)	15.1(6)
C(10)-C(9)-C(13)-N(1)	-99.4(5)
C(8)-C(9)-C(13)-N(1)	81.1(6)
C(10)-C(9)-C(13)-C(14)	139.2(5)
C(8)-C(9)-C(13)-C(14)	-40.3(7)
C(10)-C(9)-C(13)-C(12)	14.8(6)
C(8)-C(9)-C(13)-C(12)	-164.7(5)
O(6)-C(12)-C(13)-N(1)	-148.9(4)
C(11)-C(12)-C(13)-N(1)	99.3(5)
O(6)-C(12)-C(13)-C(9)	93.7(5)
C(11)-C(12)-C(13)-C(9)	-18.1(5)
O(6)-C(12)-C(13)-C(14)	-32.1(6)

C(11)-C(12)-C(13)-C(14)	-144.0(4)
N(1)-C(13)-C(14)-C(15)	36.4(5)
C(9)-C(13)-C(14)-C(15)	160.4(4)
C(12)-C(13)-C(14)-C(15)	-80.7(5)
C(13)-C(14)-C(15)-C(16)	-26.6(5)
C(13)-C(14)-C(15)-S(1)	-147.4(3)
C(14)-C(15)-C(16)-N(1)	8.5(5)
S(1)-C(15)-C(16)-N(1)	131.6(4)
O(4)-C(18)-C(19)-C(20)	11.7(9)
O(3)-C(18)-C(19)-C(20)	-167.0(6)
O(4)-C(18)-C(19)-C(21)	131.1(8)
O(3)-C(18)-C(19)-C(21)	-47.6(7)
O(4)-C(18)-C(19)-C(70)	-168.4(12)
O(3)-C(18)-C(19)-C(70)	13.0(12)
O(4)-C(18)-C(19)-C(71)	-46.8(12)
O(3)-C(18)-C(19)-C(71)	134.5(11)
O(4)-C(18)-C(19)-C(22)	-108.9(8)
O(3)-C(18)-C(19)-C(22)	72.5(7)
O(4)-C(18)-C(19)-C(69)	71.5(12)
O(3)-C(18)-C(19)-C(69)	-107.1(11)
C(31)-C(26)-C(27)-C(28)	-0.6(8)
S(1)-C(26)-C(27)-C(28)	-179.4(4)
C(26)-C(27)-C(28)-C(29)	1.0(9)
C(27)-C(28)-C(29)-C(30)	-1.2(10)
C(28)-C(29)-C(30)-C(31)	1.1(10)
C(29)-C(30)-C(31)-C(26)	-0.7(9)
C(27)-C(26)-C(31)-C(30)	0.5(8)
S(1)-C(26)-C(31)-C(30)	179.3(4)
C(15)-C(16)-N(1)-C(13)	14.1(5)
C(15)-C(16)-N(1)-C(1)	-116.5(4)
C(9)-C(13)-N(1)-C(16)	-158.5(4)
C(14)-C(13)-N(1)-C(16)	-31.8(5)
C(12)-C(13)-N(1)-C(16)	89.5(4)
C(9)-C(13)-N(1)-C(1)	-27.4(6)
C(14)-C(13)-N(1)-C(1)	99.3(5)
C(12)-C(13)-N(1)-C(1)	-139.4(4)
C(2)-C(1)-N(1)-C(16)	71.9(6)
C(2)-C(1)-N(1)-C(13)	-54.2(6)
C(4)-C(5)-O(1)-C(17)	172.6(6)
C(6)-C(5)-O(1)-C(17)	-9.5(6)
O(2)-C(17)-O(1)-C(5)	14.1(6)
C(7)-C(6)-O(2)-C(17)	-172.4(5)
C(5)-C(6)-O(2)-C(17)	7.5(6)
O(1)-C(17)-O(2)-C(6)	-13.3(6)
O(4)-C(18)-O(3)-C(10)	2.6(8)
C(19)-C(18)-O(3)-C(10)	-178.6(4)

C(9)-C(10)-O(3)-C(18)	-124.2(6)
C(11)-C(10)-O(3)-C(18)	63.2(7)
O(6)-C(23)-O(5)-C(11)	-27.0(6)
C(25)-C(23)-O(5)-C(11)	-143.6(5)
C(24)-C(23)-O(5)-C(11)	92.6(6)
C(10)-C(11)-O(5)-C(23)	119.3(5)
C(12)-C(11)-O(5)-C(23)	8.4(6)
C(11)-C(12)-O(6)-C(23)	-30.0(5)
C(13)-C(12)-O(6)-C(23)	-143.6(5)
O(5)-C(23)-O(6)-C(12)	36.3(6)
C(25)-C(23)-O(6)-C(12)	153.7(6)
C(24)-C(23)-O(6)-C(12)	-82.2(6)
C(27)-C(26)-S(1)-O(8)	-144.3(4)
C(31)-C(26)-S(1)-O(8)	36.9(5)
C(27)-C(26)-S(1)-O(7)	-14.6(5)
C(31)-C(26)-S(1)-O(7)	166.6(4)
C(27)-C(26)-S(1)-C(15)	100.8(5)
C(31)-C(26)-S(1)-C(15)	-78.0(5)
C(14)-C(15)-S(1)-O(8)	-172.5(3)
C(16)-C(15)-S(1)-O(8)	70.2(4)
C(14)-C(15)-S(1)-O(7)	59.1(4)
C(16)-C(15)-S(1)-O(7)	-58.2(4)
C(14)-C(15)-S(1)-C(26)	-55.8(4)
C(16)-C(15)-S(1)-C(26)	-173.1(4)
N(2)-C(32)-C(33)-C(34)	75.7(7)
C(32)-C(33)-C(34)-C(39)	-14.9(8)
C(32)-C(33)-C(34)-C(35)	162.9(5)
C(39)-C(34)-C(35)-C(36)	-2.3(8)
C(33)-C(34)-C(35)-C(36)	179.8(5)
C(34)-C(35)-C(36)-C(37)	1.4(9)
C(34)-C(35)-C(36)-O(9)	179.2(6)
C(35)-C(36)-C(37)-O(10)	179.1(5)
O(9)-C(36)-C(37)-O(10)	0.9(7)
C(35)-C(36)-C(37)-C(38)	-1.0(10)
O(9)-C(36)-C(37)-C(38)	-179.2(5)
C(36)-C(37)-C(38)-C(39)	1.4(9)
O(10)-C(37)-C(38)-C(39)	-178.7(5)
C(35)-C(34)-C(39)-C(38)	2.8(8)
C(33)-C(34)-C(39)-C(38)	-179.4(5)
C(35)-C(34)-C(39)-C(40)	175.5(5)
C(33)-C(34)-C(39)-C(40)	-6.7(9)
C(37)-C(38)-C(39)-C(34)	-2.3(8)
C(37)-C(38)-C(39)-C(40)	-175.5(5)
C(34)-C(39)-C(40)-C(41)	135.9(6)
C(38)-C(39)-C(40)-C(41)	-51.0(8)
C(34)-C(39)-C(40)-C(44)	-43.4(8)

C(38)-C(39)-C(40)-C(44)	129.6(5)
C(39)-C(40)-C(41)-O(11)	0.2(9)
C(44)-C(40)-C(41)-O(11)	179.6(4)
C(39)-C(40)-C(41)-C(42)	-179.2(5)
C(44)-C(40)-C(41)-C(42)	0.2(6)
C(40)-C(41)-C(42)-O(13)	-128.2(5)
O(11)-C(41)-C(42)-O(13)	52.4(6)
C(40)-C(41)-C(42)-C(43)	-14.2(6)
O(11)-C(41)-C(42)-C(43)	166.4(4)
O(13)-C(42)-C(43)-O(14)	26.4(5)
C(41)-C(42)-C(43)-O(14)	-94.4(4)
O(13)-C(42)-C(43)-C(44)	142.0(4)
C(41)-C(42)-C(43)-C(44)	21.3(5)
C(41)-C(40)-C(44)-N(2)	-99.7(5)
C(39)-C(40)-C(44)-N(2)	79.8(6)
C(41)-C(40)-C(44)-C(45)	139.3(5)
C(39)-C(40)-C(44)-C(45)	-41.2(7)
C(41)-C(40)-C(44)-C(43)	13.7(6)
C(39)-C(40)-C(44)-C(43)	-166.8(5)
O(14)-C(43)-C(44)-N(2)	-154.5(4)
C(42)-C(43)-C(44)-N(2)	96.1(5)
O(14)-C(43)-C(44)-C(40)	87.5(5)
C(42)-C(43)-C(44)-C(40)	-21.9(5)
O(14)-C(43)-C(44)-C(45)	-39.9(6)
C(42)-C(43)-C(44)-C(45)	-149.3(4)
N(2)-C(44)-C(45)-C(46)	35.1(5)
C(40)-C(44)-C(45)-C(46)	159.7(4)
C(43)-C(44)-C(45)-C(46)	-79.7(5)
C(44)-C(45)-C(46)-C(47)	-32.9(5)
C(44)-C(45)-C(46)-S(2)	-154.3(4)
C(45)-C(46)-C(47)-N(2)	19.2(6)
S(2)-C(46)-C(47)-N(2)	143.3(4)
O(12)-C(49)-C(50)-C(52)	-132.0(7)
O(11)-C(49)-C(50)-C(52)	46.9(7)
O(12)-C(49)-C(50)-C(51)	-9.8(10)
O(11)-C(49)-C(50)-C(51)	169.0(6)
O(12)-C(49)-C(50)-C(53)	107.0(8)
O(11)-C(49)-C(50)-C(53)	-74.2(6)
C(62)-C(57)-C(58)-C(59)	-0.3(9)
S(2)-C(57)-C(58)-C(59)	-179.5(4)
C(57)-C(58)-C(59)-C(60)	1.5(9)
C(58)-C(59)-C(60)-C(61)	-1.5(10)
C(59)-C(60)-C(61)-C(62)	0.4(10)
C(58)-C(57)-C(62)-C(61)	-0.9(9)
S(2)-C(57)-C(62)-C(61)	178.3(4)
C(60)-C(61)-C(62)-C(57)	0.8(9)

C(33)-C(32)-N(2)-C(47)	66.9(6)
C(33)-C(32)-N(2)-C(44)	-57.9(6)
C(46)-C(47)-N(2)-C(32)	-125.3(5)
C(46)-C(47)-N(2)-C(44)	3.0(6)
C(40)-C(44)-N(2)-C(32)	-22.7(6)
C(45)-C(44)-N(2)-C(32)	104.6(5)
C(43)-C(44)-N(2)-C(32)	-135.2(4)
C(40)-C(44)-N(2)-C(47)	-151.1(4)
C(45)-C(44)-N(2)-C(47)	-23.8(5)
C(43)-C(44)-N(2)-C(47)	96.4(5)
C(35)-C(36)-O(9)-C(48)	169.2(6)
C(37)-C(36)-O(9)-C(48)	-12.7(7)
O(10)-C(48)-O(9)-C(36)	19.2(7)
C(36)-C(37)-O(10)-C(48)	10.8(7)
C(38)-C(37)-O(10)-C(48)	-169.0(6)
O(9)-C(48)-O(10)-C(37)	-18.4(7)
O(12)-C(49)-O(11)-C(41)	1.6(8)
C(50)-C(49)-O(11)-C(41)	-177.3(5)
C(40)-C(41)-O(11)-C(49)	-87.1(6)
C(42)-C(41)-O(11)-C(49)	92.3(6)
C(41)-C(42)-O(13)-C(54)	87.5(5)
C(43)-C(42)-O(13)-C(54)	-24.0(5)
O(14)-C(54)-O(13)-C(42)	11.8(6)
C(56)-C(54)-O(13)-C(42)	-105.4(5)
C(55)-C(54)-O(13)-C(42)	128.9(5)
O(13)-C(54)-O(14)-C(43)	6.0(6)
C(56)-C(54)-O(14)-C(43)	125.5(5)
C(55)-C(54)-O(14)-C(43)	-109.8(5)
C(42)-C(43)-O(14)-C(54)	-19.7(5)
C(44)-C(43)-O(14)-C(54)	-131.1(4)
C(62)-C(57)-S(2)-O(15)	-179.0(4)
C(58)-C(57)-S(2)-O(15)	0.2(5)
C(62)-C(57)-S(2)-O(16)	50.0(5)
C(58)-C(57)-S(2)-O(16)	-130.7(4)
C(62)-C(57)-S(2)-C(46)	-64.0(5)
C(58)-C(57)-S(2)-C(46)	115.2(5)
C(45)-C(46)-S(2)-O(15)	68.4(4)
C(47)-C(46)-S(2)-O(15)	-49.9(4)
C(45)-C(46)-S(2)-O(16)	-161.6(4)
C(47)-C(46)-S(2)-O(16)	80.1(4)
C(45)-C(46)-S(2)-C(57)	-45.8(4)
C(47)-C(46)-S(2)-C(57)	-164.1(4)
C(63)-C(64)-C(65)-C(66)	178.7(15)
C(64)-C(65)-C(66)-C(67)	-178.9(13)
C(65)-C(66)-C(67)-C(68)	-178.7(15)
C(72)-C(73)-C(74)-C(75)	165(4)

C(73)-C(74)-C(75)-C(76)	-122(4)
C(74)-C(75)-C(76)-C(77)	-176(3)

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