Stereostructure of a Novel Cytotoxic 18-Membered Macrolactone Antibiotic FD-891

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Experimental

General. ^1H and ^{13}C NMR chemical shifts were reported in δ value based on internal TMS ($\delta_{\text{H}} = 0$) or solvent signal (CDCl_3 $\delta_{\text{C}} = 77.0$) as reference. Column chromatography was carried out with a Kieselgel 60 (70-230 mesh, Merck).

FD-891 Tetrabenzoate. To an ice-cooled solution of FD-891 (50 mg, 0.087 mmol) and 4-(dimethylamino)pyridine (21 mg, 0.17 mmol) in pyridine. (2 mL) was added benzoyl chloride (244 μL , 1.74 mmol), and the mixture was stirred for 6.5 h at room temperature. Water was added and the mixture was extracted three times with EtOAc. The combined organic layer was washed with 0.1 N NaOH. and brine, dried over MgSO_4 , filtered, and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (benzene-EtOAc; 10 :1) to give FD-891 tetrabenzoate as an amorphous solid (80 mg, 92% yield); ^1H -NMR (500 MHz) δ 0.81 (d, $J = 6.2$ Hz, 3H), 1.02 (d, $J = 6.9$ Hz, 3H), 1.15 (d, $J = 7.2$ Hz, 3H), 1.16 (d, $J = 6.1$ Hz, 3H), 1.29 (d, $J = 7.1$ Hz, 3H), 1.81 (m, 2H), 1.88 (d, $J = 0.85$ Hz, 1H), 2.02 (m, 1H), 2.07 (d, $J = 0.75$ Hz, 3H), 2.20 (m, 2H), 2.27-2.38 (m, 4H), 2.55 (dt, $J = 6.8, 13.7$ Hz, 1H), 2.69 (m, 1H), 2.95 (dq, $J = 7.2, 7.5$ Hz, 1H), 3.19 (s, 3H), 3.24 (m, 3H), 3.44 (dd, $J = 2.1, 7.4$ Hz, 1H), 4.78 (dt, $J = 3.7, 7.9$ Hz, 1H), 4.84 (dt, $J = 2.1, 8.0$ Hz, 1H), 5.31-5.35 (m, 2H), 5.39-5.52 (m, 4H), 5.59 (dd, $J = 1.4, 4.0$ Hz, 1H), 5.63 (m, 2H), 5.71 (d, $J = 11.0$ Hz, 2H), 7.22-7.61 (m, 12H), 7.84-8.04 (m, 8H); ^{13}C -NMR (126 MHz) δ 9.6,

11.0, 13.5, 15.6, 15.9, 16.2, 16.8, 29.2, 34.2, 34.5, 34.7, 35.0, 35.8, 37.3, 40.2, 53.1, 54.4, 56.3, 71.9, 72.4, 74.9, 76.2, 76.7, 78.7, 125.2, 127.5, 127.6, 128.0, 128.0, 128.3, 128.5, 128.8, 129.5, 129.5, 129.7, 129.8, 130.4, 130.7, 130.8, 132.4, 132.5, 135.8, 140.1, 143.7, 165.2, 165.7, 165.7, 166.0, 169.0.

Ozonolysis of FD-891 Tetrabenzoate. Ozone gas was bubbled into a solution of FD-891 tetrabenzoate (92 mg, 0.093 mmol) in MeOH (8 mL) at -78°C for 15 min. Argon gas was introduced to purge the remaining ozone, and sodium borohydride (105 mg, 2.78 mmol) was added at -78°C. The mixture was stirred at the same temperature for 1 h and then warmed to room temperature. After 12 h, sat. NH₄Cl aq., was added and the mixture was extracted three times with CH₂Cl₂. The combined organic layer was washed with sat. NH₄Cl aq. and brine, dried over Na₂SO₄, filtered, and evaporated under reduced pressure. The residue was purified by preparative TLC (toluene-EtOAc; 1:1) to give **2** (6.4 mg, 17% yield) and **3** (28 mg, 71% yield) as a colorless oil. **2**, ¹H-NMR (500 MHz) δ 1.07 (d, *J*=7.3 Hz, 3H), 1.98-2.12 (m, 2H), 2.21-2.26 (m, 1H), 3.14 (dd, *J*=2.3, 3.2 Hz, 1H), 3.23 (dd, *J*=2.3, 4.2 Hz, 1H), 3.81 (m, 1H), 3.98 (m, 1H), 4.26 (dd, *J*=5.9, 11.1 Hz, 1H), 4.44 (dd, *J*=8.0, 11.0 Hz, 1H), 4.51 (dt, *J*=11.3, 5.7 Hz, 1H), 4.56 (ddd, *J*=5.3, 8.4, 11.2 Hz, 1H), 7.42 (m, 4H), 7.56 (m, 2H), 8.02 (m, 4H); ¹³C-NMR (126 MHz, CDCl₃) δ 10.9, 33.8, 35.9, 57.1, 58.0, 61.3, 66.4, 67.2, 68.3, 128.4, 128.4, 128.5, 129.6, 129.6, 130.0, 133.1, 133.1, 166.7, 166.7. **3**, ¹H-NMR (500 MHz) δ 1.04 (d, *J*=7.0 Hz, 3H), 1.15 (d, *J*=6.2 Hz, 3H), 1.19 (d, *J*=7.1 Hz, 3H), 1.80-

1.81 (m, 1H), 1.93-2.00 (m, 1H), 2.01-2.04 (m, 1H), 2.26 (double quintet, $J=2.0$, 7.1 Hz, 1H), 3.19 (s, 3H), 3.24 (dq, $J=6.1$, 6.2 Hz, 1H), 3.49 (m, 1H), 3.65 (m, 1H), 5.33 (dd, $J=4.1$, 7.6 Hz, 1H), 5.52 (dt, $J=9.7$, 2.3 Hz, 1H), 7.26 (dd, $J=7.7$, 7.8 Hz, 2H), 7.36 (t, $J=7.7$ Hz, 2H), 7.44 (t, $J=7.3$ Hz, 1H), 7.51 (dd, $J=8.3$, 1.2 Hz, 1H), 7.86 (dd, $J=8.3$, 1.2 Hz, 2H), 7.94 (d, $J=8.2$ Hz, 2H); ^{13}C -NMR (126 MHz, CDCl_3): δ 9.7, 11.4, 16.2, 36.0, 39.0, 40.2, 56.4, 58.4, 69.9, 76.1, 79.0, 128.1, 128.3, 129.5, 129.6, 130.2, 130.3, 132.6, 132.9, 166.1, 167.3. Anal. Calcd for $\text{C}_{25}\text{H}_{32}\text{O}_6$: C, 70.07; H, 7.53. Found: C, 69.89; H, 7.61.

(-)-Camphanic Ester (4). To an ice-cooled solution of **2** (7.9 mg, 0.019 mmol) and 4-(dimethylamino)pyridine (2.3 mg, 0.019 mmol) in pyridine (0.5 mL) was added (-)-camphanic chloride (41 mg, 0.19 mmol), and the mixture was stirred for 16 h overnight. The reaction was quenched by addition of water, and the mixture was extracted three times with CH_2Cl_2 . The combined organic layer was washed with sat. NaHCO_3 aq. and brine, dried over MgSO_4 , filtered, and evaporated under reduced pressure. The residue was purified by preparative TLC (toluene-EtOAc; 3:1) to give **4** as a white solid (10 mg, 70% yield); mp 149.3-150.5°C; IR (neat) 1722, 1790, 2854, 2925, 2966 cm^{-1} ; ^1H -NMR (400 MHz) δ 0.95 (s, 3H), 0.99 (s, 3H), 1.03 (s, 3H), 1.05 (s, 3H), 1.11 (s, 3H), 1.15 (d, $J=7.2$ Hz, 3H), 1.26 (s, 3H), 1.68 (m, 4H), 1.92 (m, 2H), 2.04 (m, 2H), 2.19 (m, 1H), 2.40 (m, 2H), 3.10 (dd, $J=5.6$, 2.2 Hz), 3.34 (dd, $J=5.6$, 2.1 Hz, 1H), 4.19 (d, $J=8.4$, 10.0 Hz, 1H), 4.30 (dd, $J=5.6$, 10.2 Hz, 1H), 4.40 (m, 2H) 5.07 (dd, $J=4.0$, 4.6 Hz,

1H), 5.15 (m, 1H), 7.44 (m, 4H), 7.55-7.58 (m, 2H), 8.01-8.03 (m, 4H).

(-)-Camphanic Ester (5). To an ice-cooled solution of **3** (49 mg, 0.11 mmol) in dry MeOH (1 mL) was added potassium *tert*-butoxide (3.8 mg, 0.034 mmol), and the mixture was stirred for 18 h overnight. The reaction was evaporated under reduced pressure to give crude triol (34 mg), which was used for the next reaction without purification. To an ice-cooled solution of the triol (34 mg) and 4-(dimethylamino)pyridine (21 mg, 0.17 mmol) in pyridine (1.5 mL) was added (-)-camphanic chloride (370 mg, 1.71 mmol), and the mixture was stirred at room temperature overnight. The reaction was quenched by addition of water, and the mixture was extracted three times with CH₂Cl₂. The combined organic layer was washed with sat. NaHCO₃ aq. and brine, dried over MgSO₄, filtered, and evaporated under reduced pressure. The residue was purified by silica gel column chromatography (toluene-EtOAc; 3:1) to give **5** as a white solid (45 mg, 68% yield, 2 steps); mp 137.5-139.5°C; IR (neat): 1751, 1790, 2883, 2937, 2972 cm⁻¹; ¹H-NMR (300 MHz) δ 0.87-0.90 (m, 6H), 0.98-1.00 (m, 6H), 1.07-1.12 (m, 12H), 1.16 (d, *J* = 6.4 Hz, 3H), 1.58-1.77 (m, 3H), 1.87-2.20 (m, 7H), 2.40-2.51 (m, 2H), 3.31 (s, 3H), 3.53-3.46 (m, 2H), 4.24-4.29 (m, 2H), 5.64 (ddd, *J* = 1.7, 4.9, 10.0 Hz, 1H); ¹³C-NMR (75 MHz) δ 5.1, 9.6, 16.4, 16.7, 28.9, 30.7, 30.8, 31.7, 39.1, 39.8, 54.1, 54.1, 54.8, 56.1, 62.1, 71.6, 75.4, 82.2, 91.1, 91.3, 167.3, 167.6, 178.1, 178.4. Anal. Calcd for C₃₁H₄₈O₁₀: C, 64.12; H, 8.33. Found: C, 63.84; H, 8.63.

DIBAH Reduction of FD-891. To a solution of FD-891 (23 mg, 0.040 mmol) in dry CH_2Cl_2 (0.4 mL) was added dropwise DIBAH (0.3 mL, 1.0 M solution in toluene, 0.3 mmol) at -78°C under Ar, and the mixture was stirred for 25 min at the same temperature. The reaction was warmed to 0°C , and Rochelle salt (80 mL) was added. After 30 min, the mixture was filtered through a pad of Celite and the filtrate was evaporated under reduced pressure give a crude product (23 mg). To an ice-cooled solution of the crude product (23 mg) and 4-dimethylaminopyridine (2 mg) in pyridine (0.5 mL) was added benzoyl chloride (100 μL , 0.84 mmol), and the mixture was stirred for 5 h at room temperature. The reaction was quenched by addition of water, and the mixture was extracted three times with EtOAc. The combined organic layer was washed with 1 N NaOH aq. and brine, dried over MgSO_4 , filtered, and evaporated under reduced pressure. The residue was purified by preparative TLC (toluene- EtOAc; 4:1) to give **6** (4.9 mg, 19% yield) and hexabenzooate (34.4 mg, 72%) as an amorphous solid.

6: ^1H -NMR (500 MHz) δ 0.74 (d, $J = 6.8$ Hz, 3H), 0.90 (d, $J = 7.1$ Hz, 3H), 0.91 (d, $J = 7.0$ Hz, 3H), 1.11 (d, $J = 6.2$ Hz, 3H), 1.16 (d, $J = 6.8$ Hz, 3H), 1.57 (m, 2H), 1.67 (m, 1H), 1.76 (d, $J = 1.2$ Hz, 3H), 1.78 (d, $J = 1.3$ Hz, 3H), 1.80 (m, 1H), 1.97 (m, 1H), 2.10 (dt, $J = 6.0, 13.2$ Hz, 1H), 2.16-2.29 (m, 2H), 2.40 (m, 2H), 2.52 (m, 1H), 3.00 (m, 1H), 3.11 (dd, $J = 2.1, 5.9$ Hz, 1H), 3.27 (s, 3H), 3.33 (dd, $J = 2.0, 5.7$ Hz, 1H), 3.41-3.47 (m, 2H), 3.76 (d, $J = 2.0$ Hz, 1H), 4.69 (s, 2H), 4.89 (m, 2H), 4.96 (dt, $J = 5.9, 6.4$ Hz, 1H), 5.28-5.41 (m, 5H), 5.60 (ddd, $J = 1.5, 6.5, 6.8$ Hz, 1H), 5.92 (s, 1H), 7.38-7.46 (m, 10H),

7.50-7.58 (m, 5H), 7.93-7.99 (m, 4H), 8.02-8.06 (m, 6H); ^{13}C -NMR (126 MHz) δ 5.8, 9.4, 13.7, 15.5, 16.2, 16.4, 17.1, 29.3, 34.7, 34.8, 35.3, 35.9, 36.1, 36.4, 39.4, 39.6, 54.9, 56.1, 57.2, 70.7, 72.8, 73.2, 74.7, 75.8, 76.1, 81.8, 126.8, 127.6, 128.3, 128.3, 128.5, 129.5, 129.6, 129.6, 129.6, 130.6, 131.0, 131.8, 132.7, 132.8, 132.9, 133.3, 165.5, 165.5, 165.9, 166.3, 166.4. Hexabenzoate: ^1H -NMR (400 MHz) δ 0.75 (d, J = 6.4 Hz, 3H), 1.02 (d, J = 6.8 Hz, 3H), 1.14 (d, J = 6.8 Hz, 3H), 1.15 (d, J = 6.8 Hz, 3H), 1.16 (d, J = 7.2 Hz, 3H), 1.50-1.75 (m, 4H), 1.76 (s, 3H), 1.79 (s, 3H), 2.04-2.13 (m, 2H), 2.20-2.29 (m, 5H), 2.41 (m, 2H), 2.52 (m, 1H), 3.00 (m, 1H), 3.11 (dd, J = 1.6, 5.6 Hz, 1H), 3.16 (s, 3H), 3.24 (m, 1H), 3.34 (dd, J = 2.0, 5.6 Hz, 1H), 4.69 (s, 2H), 4.88-4.93 (m, 2H), 4.98 (q, J = 6.4 Hz, 1H), 5.27-5.36 (m, 6H), 5.41 (m, 2H), 5.93 (s, 1H), 7.20-7.57 (m, 16H), 7.85-8.06 (m, 14H); ^{13}C -NMR (100 MHz) δ 9.5, 11.0, 13.7, 14.2, 15.5, 16.21, 16.24, 17.1, 21.0, 34.6, 34.8, 35.3, 35.8, 36.4, 37.2, 40.2, 54.9, 56.2, 57.1, 60.2, 70.6, 72.3, 72.7, 75.7, 76.0, 76.1, 78.6, 126.7, 127.0, 127.9, 128.0, 128.1, 128.3, 129.3, 129.4, 129.6, 130.1, 130.4, 131.3, 131.6, 132.3, 132.6, 133.0, 133.2, 165.29, 165.34, 165.5, 165.6, 165.8, 166.1, 170.8.

Ozonolysis of Pentabenzoate (6). Ozone gas was bubbled into a solution of **6** (31 mg, 0.028 mmol) in MeOH (10 mL) at -78°C for 15 min. Argon gas was introduced to purge the remaining ozone, and sodium borohydride (42 mg, 1.1 mmol) was added at -78°C . The mixture was stirred at the same temperature for 1 h and then warmed to room temperature. After 12 h, sat. NH_4Cl aq., was added and the mixture was

extracted three times with CH_2Cl_2 . The combined organic layer was washed with sat. NH_4Cl aq. and brine, dried over Na_2SO_4 , filtered, and evaporated under reduced pressure. The residue was purified by preparative TLC (toluene-EtOAc; 1:1) to give **7** (3.8 mg, 54% yield) as a colorless oil. ^1H -NMR (500 MHz) δ 0.95 (d, $J=6.9$ Hz, 3H), 1.55 (ddt, $J=4.7, 14.3, 6.4$, Hz, 1H), 1.74 (ddt, $J=6.2, 14.5, 7.2$ Hz, 1H), 1.84 (double sextet, $J=3.2, 6.8$ Hz, 1H), 1.90 (m, 2H), 3.67 (ddd, $J=4.6, 7.6, 10.9$ Hz, 1H), 3.76 (m, 2H), 4.44 (ddd, $J=5.6, 5.6, 11.2$ Hz, 1H), 4.61 (dt, $J=11.3, 6.8$ Hz, 1H), 7.45 (t, $J=7.8$ Hz, 2H), 7.57 (m, 1H), 8.04 (m, 2H); ^{13}C -NMR (126 MHz) δ 14.4, 32.8, 36.0, 36.4, 60.7, 62.7, 71.4, 128.4, 129.6, 133.0, 167.1.

(3R,4R)-5-Benzyloxy-1,3-*tert*-butyldimethylsilyloxy-4-methylpentane (9). To an ice-cooled solution of alcohol **8**⁷ (1.1 g, 4.9 mmol) and imidazole (2.0 g, 29 mmol) in DMF (5 mL) was added *tert*-butyldimethylsilyl chloride (2.2 g, 14 mmol), and the mixture was stirred for 19 h at room temperature. The reaction was quenched with water, and the mixture was extracted three times with EtOAc. The combined organic layer was washed with brine, dried over MgSO_4 , filtered, and evaporated to dryness. The residue was purified by silica gel column chromatography (hexane-EtOAc; 50:1-10:1) to give di-TBS ether as a colorless oil (2.0 g). To a solution of the obtained di-TBS ether (2.0 g, 4.4 mmol) in EtOH (10 mL) was added 10% Pd-C (390 mg). The mixture was stirred for 1.5 h at room temperature under H_2 atmosphere. The reaction mixture was filtered, and the filtrate was evaporated to dryness. The residue was

purified by silica gel column chromatography (hexane-EtOAc; 15:1) to give **9** as a colorless oil (1.6 g, 89 %); $[\alpha]_D^{23}$ 14.2 ($c = 1.04$, CHCl_3); IR (neat): 1255, 1362, 1389, 1471, 2858, 2884, 2929, 2956, 3356 cm^{-1} ; $^1\text{H-NMR}$ (300 MHz) δ -0.01-0.06 (m, 12H), 0.81-0.85 (m, 21H), 1.58-1.68 (m, 2H), 1.93-2.01 (m, 1H), 3.43 (m, 1H), 3.57-3.70 (m, 3H), 3.89 (m, 1H); $^{13}\text{C-NMR}$ (75 MHz) δ -5.3, -4.6, -4.4, 12.6, 18.0, 18.3, 25.9, 26.0, 35.1, 39.8, 59.8, 65.9, 72.8. Anal. Calcd for $\text{C}_{18}\text{H}_{42}\text{O}_3\text{Si}_2$: C, 59.61; H, 11.67. Found: C, 59.71; H, 11.97.

(2*R*,3*R*)-3,5-*tert*-Butyldimethylsilyloxy-2-methylhexanenitrile (10). To an ice-cooled solution of **9** (1.6 g, 4.4 mmol) and Et_3N (3.0 mL, 2.2 mmol) in CH_2Cl_2 (10 mL) was added methanesulfonyl chloride (674 μL , 8.81 mmol), and the mixture was stirred for 19 h at room temperature. The reaction was quenched with water, and the mixture was extracted three times with EtOAc. The combined organic layer was washed with brine, dried over MgSO_4 , filtered, and evaporated. The residue was purified by silica gel column chromatography (hexane-EtOAc; 10:1) to give mesylate as a colorless oil (1.7 g). To a solution of the mesylate (1.7 g, 3.93 mmol) in DMSO (5 mL) was added sodium cyanide (424 mg, 8.65 mmol), and the mixture was heated at 80°C for 12 h. Water was added and the mixture was extracted three times with EtOAc. The combined organic layer was washed with brine, dried over MgSO_4 , filtered, and evaporated. The residue was purified by silica gel column chromatography (hexane-EtOAc; 30:1) to give **10** as a colorless oil (1.9 g, 69% yield); $[\alpha]_D^{26}$ 10.8 ($c = 0.94$,

CHCl₃); IR (neat); 2247, 2858, 2885, 2929, 2956 cm⁻¹; ¹H-NMR (300 MHz) δ 0.00 (s, 6H), 0.03 (s, 6H), 0.84 (s, 18H), 0.98 (d, *J* = 6.8 Hz, 3H), 1.44-1.66 (m, 2H), 1.95-2.05 (m, 1H), 2.15 (dd, *J* = 8.8, 16.6 Hz, 1H), 2.44 (dd, *J* = 5.4, 16.6 Hz, 1H), 3.52-3.65 (m, 2H), 3.81 (m, 1H); ¹³C-NMR (75 MHz) δ -5.4, -4.7, -4.5, 14.2, 18.0, 19.1, 20.2, 25.78, 25.82, 35.7, 36.0, 59.4, 70.9, 119.6. Anal. Calcd for C₁₉H₄₁NO₂Si₂: C, 61.39; H, 11.12; N, 3.77. Found: C, 61.28; H, 11.17; N, 3.48.

(2*R*,3*R*)-3,5-*tert*-Butyldimethylsilyloxy-2-methylhexan-1-ol (11). To a solution of **10** (1.0 g, 2.7 mmol) in toluene (70 mL) was added dropwise DIBAL (6.2 mL, 1.0 M solution in toluene, 3.2 mmol) at -78°C, and the mixture was stirred for 3 h under Ar at the same temperature. The reaction was warmed to 0°C, and NH₄Cl aq. (80 mL) was added dropwise. After stirring for 30 min, the mixture was filtered through a pad of Celite. The aqueous layer was extracted three times with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄, filtered, and evaporated to give a crude aldehyde as a colorless oil. This was used for next reaction without further purification. To an ice-cooled solution of the aldehyde in MeOH (5 mL) was added sodium borohydride (204 mg, 5.39 mmol), and the mixture was stirred for 3 h at room temperature. The reaction was quenched with sat. NH₄Cl aq., and the mixture was extracted three times with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄, filtered, and evaporated. The residue was purified by silica gel column chromatography (hexane-EtOAc; 20:1) to give **11** as a colorless oil (655 mg,

65% yield, 2 steps); $[\alpha]_{\text{D}}^{28}$ 26.4 ($c = 0.94$, CHCl_3); IR (neat): 2858, 2884, 2929, 2956, 3440 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz) δ 0.00 (s, 6H), 0.09 (s, 6H), 0.88-0.91 (m, 21H), 1.39 (m, 1H), 1.60-1.82 (m, 4H), 3.58-3.72 (m, 4H), 3.84 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz) δ -5.2, -4.6, 17.4, 18.1, 18.3, 25.9, 26.0, 35.1, 35.4, 37.6, 59.9, 62.1, 73.0. Anal. Calcd for $\text{C}_{19}\text{H}_{44}\text{O}_3\text{Si}_2$: C, 60.58; H, 11.77. Found: C, 60.34; H, 12.06.

(3*R*,4*R*)-4-Methylhexane-1,3,6-triol (12). To an ice-cooled solution of **11** (420 mg, 1.12 mmol) in THF (2 mL) was added 2N HCl (20 mL), and the mixture was stirred for 16 h at room temperature. The reaction was evaporated under reduced pressure to give **12** as a colourless oil; $^1\text{H-NMR}$ (400 MHz, D_2O) δ 0.70 (d, $J = 6.8$ Hz, 1H), 1.23 (m, 1H), 1.49-1.56 (m, 4H), 3.45-3.54 (m, 5H); $^{13}\text{C-NMR}$ (100 MHz) δ 13.7, 35.2, 35.6, 36.2, 59.8, 60.6, 72.5. Anal. Calcd for $\text{C}_7\text{H}_{16}\text{O}_3$: C, 56.73; H, 10.88. Found: C, 56.34; H, 11.06.

Table 1. Crystal data and structure refinement for compound 5.

Identification code	compound 5
Empirical formula	C31 H47 O10
Formula weight	579.69
Temperature	173(2) K
Wavelength	1.54178 Å
Crystal system, space group	Monoclinic, P212121
Unit cell dimensions	a = 11.1519(8) Å alpha = 90 deg. b = 39.360(3) Å beta = 90 deg. c = 7.0353(6) Å gamma = 90 deg.
Volume	3088.0(4) Å ³
Z, Calculated density	4, 1.247 Mg/m ³
Absorption coefficient	0.759 mm ⁻¹
F(000)	1252
Crystal size	0.40 x 0.15 x 0.15 mm
Theta range for data collection	2.24 to 68.22 deg.
Limiting indices	-13<=h<=13, -47<=k<=46, -8<=l<=8
Reflections collected / unique	32278 / 5615 [R(int) = 0.0594]
Completeness to theta = 68.22	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8947 and 0.7512
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5615 / 0 / 381
Goodness-of-fit on F ²	1.125
Final R indices [I>2sigma(I)]	R1 = 0.0538, wR2 = 0.1232 [5150refs.]
R indices (all data)	R1 = 0.0601, wR2 = 0.1285
Absolute structure parameter	0.0(2)
Extinction coefficient	0.0066(3)
Largest diff. peak and hole	0.260 and -0.218 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for compound 5.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	7184(2)	1907(1)	3842(3)	59(1)
O(2)	5436(2)	1716(1)	4965(3)	55(1)
O(3)	7852(2)	2842(1)	8162(3)	72(1)
O(4)	7396(2)	2352(1)	6738(3)	50(1)
O(5)	5516(2)	733(1)	10018(2)	49(1)

O(6)	6231(2)	360(1)	12134(3)	69(1)
O(7)	4000(2)	1004(1)	5822(2)	40(1)
O(8)	4145(2)	1230(1)	8753(2)	52(1)
O(9)	1740(2)	1477(1)	8100(3)	56(1)
O(10)	-1590(2)	1107(1)	8970(3)	57(1)
C(1)	7127(3)	2623(1)	7851(4)	51(1)
C(2)	5854(2)	2579(1)	8531(4)	46(1)
C(3)	5957(3)	2278(1)	9945(4)	52(1)
C(4)	6271(3)	1972(1)	8661(4)	51(1)
C(5)	6327(2)	2142(1)	6709(3)	39(1)
C(6)	5307(2)	2409(1)	6758(3)	38(1)
C(7)	4048(2)	2268(1)	7069(4)	47(1)
C(8)	5295(3)	2636(1)	5006(4)	49(1)
C(9)	5274(3)	2896(1)	9320(5)	67(1)
C(10)	6401(2)	1914(1)	5016(4)	42(1)
C(11)	5310(3)	1474(1)	3427(4)	54(1)
C(12)	4001(3)	1395(1)	3219(4)	49(1)
C(13)	3392(2)	1310(1)	5080(3)	41(1)
C(14)	2045(2)	1248(1)	4925(4)	44(1)
C(15)	1738(3)	957(1)	3564(4)	60(1)
C(16)	1477(2)	1197(1)	6885(4)	40(1)
C(17)	104(2)	1155(1)	6885(4)	43(1)
C(18)	-321(2)	1068(1)	8885(4)	44(1)
C(19)	-4(3)	708(1)	9480(4)	58(1)
C(20)	-530(3)	1467(1)	6100(5)	64(1)
C(21)	-2022(3)	1192(1)	10794(5)	70(1)
C(22)	5844(3)	414(1)	10575(4)	49(1)
C(23)	5639(2)	182(1)	8913(4)	44(1)
C(24)	6623(2)	289(1)	7499(4)	52(1)
C(25)	6251(2)	648(1)	6883(4)	47(1)
C(26)	5115(2)	703(1)	8051(3)	38(1)
C(27)	4503(2)	351(1)	8053(4)	43(1)
C(28)	3421(3)	333(1)	9351(5)	70(1)
C(29)	4171(3)	217(1)	6091(5)	60(1)
C(30)	5599(3)	-193(1)	9428(5)	65(1)
C(31)	4374(2)	1010(1)	7625(3)	40(1)

Table 3. Bond lengths [Å] and angles [deg] for compound 5.

O(1)-C(10)	1.202(3)
O(2)-C(10)	1.330(3)
O(2)-C(11)	1.446(3)
O(3)-C(1)	1.202(3)
O(4)-C(1)	1.359(3)
O(4)-C(5)	1.449(3)
O(5)-C(22)	1.366(3)
O(5)-C(26)	1.459(3)
O(6)-C(22)	1.197(3)
O(7)-C(31)	1.335(3)
O(7)-C(13)	1.478(3)
O(8)-C(31)	1.203(3)
O(9)-C(16)	1.426(3)
O(10)-C(21)	1.411(4)
O(10)-C(18)	1.425(3)
C(1)-C(2)	1.508(4)
C(2)-C(9)	1.511(4)
C(2)-C(6)	1.542(3)
C(2)-C(3)	1.551(4)
C(3)-C(4)	1.547(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.530(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(10)	1.495(4)
C(5)-C(6)	1.547(3)
C(6)-C(8)	1.523(3)
C(6)-C(7)	1.525(3)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800

C(7) -H(7C)	0.9800
C(8) -H(8A)	0.9800
C(8) -H(8B)	0.9800
C(8) -H(8C)	0.9800
C(9) -H(9A)	0.9800
C(9) -H(9B)	0.9800
C(9) -H(9C)	0.9800
C(11) -C(12)	1.500(4)
C(11) -H(11A)	0.9900
C(11) -H(11B)	0.9900
C(12) -C(13)	1.513(3)
C(12) -H(12A)	0.9900
C(12) -H(12B)	0.9900
C(13) -C(14)	1.526(4)
C(13) -H(13)	1.0000
C(14) -C(16)	1.530(3)
C(14) -C(15)	1.530(4)
C(14) -H(14)	1.0000
C(15) -H(15A)	0.9800
C(15) -H(15B)	0.9800
C(15) -H(15C)	0.9800
C(16) -C(17)	1.540(4)
C(16) -H(16)	1.0000
C(17) -C(20)	1.521(4)
C(17) -C(18)	1.523(4)
C(17) -H(17)	1.0000
C(18) -C(19)	1.517(4)
C(18) -H(18)	1.0000
C(19) -H(19A)	0.9800
C(19) -H(19B)	0.9800
C(19) -H(19C)	0.9800
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) -C(23)	1.501(4)
C(23) -C(30)	1.520(4)
C(23) -C(24)	1.540(4)
C(23) -C(27)	1.554(3)
C(24) -C(25)	1.534(4)
C(24) -H(24A)	0.9900
C(24) -H(24B)	0.9900
C(25) -C(26)	1.526(3)
C(25) -H(25A)	0.9900
C(25) -H(25B)	0.9900
C(26) -C(31)	1.494(3)
C(26) -C(27)	1.541(3)
C(27) -C(28)	1.515(4)
C(27) -C(29)	1.524(4)
C(28) -H(28A)	0.9800
C(28) -H(28B)	0.9800
C(28) -H(28C)	0.9800
C(29) -H(29A)	0.9800
C(29) -H(29B)	0.9800
C(29) -H(29C)	0.9800
C(30) -H(30A)	0.9800
C(30) -H(30B)	0.9800
C(30) -H(30C)	0.9800
C(10) -O(2) -C(11)	118.9(2)
C(1) -O(4) -C(5)	105.90(19)
C(22) -O(5) -C(26)	106.19(19)
C(31) -O(7) -C(13)	117.77(18)
C(21) -O(10) -C(18)	113.7(2)
O(3) -C(1) -O(4)	121.3(3)
O(3) -C(1) -C(2)	131.2(3)
O(4) -C(1) -C(2)	107.4(2)
C(1) -C(2) -C(9)	115.0(2)
C(1) -C(2) -C(6)	99.6(2)
C(9) -C(2) -C(6)	119.2(2)
C(1) -C(2) -C(3)	102.8(2)

C(9)-C(2)-C(3)	115.3(2)
C(6)-C(2)-C(3)	102.5(2)
C(4)-C(3)-C(2)	103.8(2)
C(4)-C(3)-H(3A)	111.0
C(2)-C(3)-H(3A)	111.0
C(4)-C(3)-H(3B)	111.0
C(2)-C(3)-H(3B)	111.0
H(3A)-C(3)-H(3B)	109.0
C(5)-C(4)-C(3)	101.0(2)
C(5)-C(4)-H(4A)	111.6
C(3)-C(4)-H(4A)	111.6
C(5)-C(4)-H(4B)	111.6
C(3)-C(4)-H(4B)	111.6
H(4A)-C(4)-H(4B)	109.4
O(4)-C(5)-C(10)	107.97(19)
O(4)-C(5)-C(4)	105.7(2)
C(10)-C(5)-C(4)	116.9(2)
O(4)-C(5)-C(6)	102.67(19)
C(10)-C(5)-C(6)	117.8(2)
C(4)-C(5)-C(6)	104.3(2)
C(8)-C(6)-C(7)	108.7(2)
C(8)-C(6)-C(2)	113.8(2)
C(7)-C(6)-C(2)	113.9(2)
C(8)-C(6)-C(5)	112.7(2)
C(7)-C(6)-C(5)	115.8(2)
C(2)-C(6)-C(5)	91.26(19)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(2)-C(9)-H(9A)	109.5
C(2)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(2)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(1)-C(10)-O(2)	123.8(3)
O(1)-C(10)-C(5)	126.9(2)
O(2)-C(10)-C(5)	109.27(19)
O(2)-C(11)-C(12)	107.7(2)
O(2)-C(11)-H(11A)	110.2
C(12)-C(11)-H(11A)	110.2
O(2)-C(11)-H(11B)	110.2
C(12)-C(11)-H(11B)	110.2
H(11A)-C(11)-H(11B)	108.5
C(11)-C(12)-C(13)	113.5(2)
C(11)-C(12)-H(12A)	108.9
C(13)-C(12)-H(12A)	108.9
C(11)-C(12)-H(12B)	108.9
C(13)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
O(7)-C(13)-C(12)	106.20(19)
O(7)-C(13)-C(14)	110.24(19)
C(12)-C(13)-C(14)	114.6(2)
O(7)-C(13)-H(13)	108.6
C(12)-C(13)-H(13)	108.6
C(14)-C(13)-H(13)	108.6
C(13)-C(14)-C(16)	111.3(2)
C(13)-C(14)-C(15)	112.6(2)
C(16)-C(14)-C(15)	111.9(2)
C(13)-C(14)-H(14)	106.8
C(16)-C(14)-H(14)	106.8
C(15)-C(14)-H(14)	106.8
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5

H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(9)-C(16)-C(14)	110.73(19)
O(9)-C(16)-C(17)	106.7(2)
C(14)-C(16)-C(17)	115.2(2)
O(9)-C(16)-H(16)	108.0
C(14)-C(16)-H(16)	108.0
C(17)-C(16)-H(16)	108.0
C(20)-C(17)-C(18)	111.8(2)
C(20)-C(17)-C(16)	112.0(2)
C(18)-C(17)-C(16)	109.5(2)
C(20)-C(17)-H(17)	107.8
C(18)-C(17)-H(17)	107.8
C(16)-C(17)-H(17)	107.8
O(10)-C(18)-C(19)	108.7(2)
O(10)-C(18)-C(17)	108.9(2)
C(19)-C(18)-C(17)	113.1(2)
O(10)-C(18)-H(18)	108.7
C(19)-C(18)-H(18)	108.7
C(17)-C(18)-H(18)	108.7
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(10)-C(21)-H(21A)	109.5
O(10)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(10)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(6)-C(22)-O(5)	121.6(3)
O(6)-C(22)-C(23)	131.3(3)
O(5)-C(22)-C(23)	107.1(2)
C(22)-C(23)-C(30)	114.1(2)
C(22)-C(23)-C(24)	103.2(2)
C(30)-C(23)-C(24)	116.1(2)
C(22)-C(23)-C(27)	99.6(2)
C(30)-C(23)-C(27)	119.0(2)
C(24)-C(23)-C(27)	102.3(2)
C(25)-C(24)-C(23)	104.0(2)
C(25)-C(24)-H(24A)	111.0
C(23)-C(24)-H(24A)	111.0
C(25)-C(24)-H(24B)	111.0
C(23)-C(24)-H(24B)	111.0
H(24A)-C(24)-H(24B)	109.0
C(26)-C(25)-C(24)	101.7(2)
C(26)-C(25)-H(25A)	111.4
C(24)-C(25)-H(25A)	111.4
C(26)-C(25)-H(25B)	111.4
C(24)-C(25)-H(25B)	111.4
H(25A)-C(25)-H(25B)	109.3
O(5)-C(26)-C(31)	107.04(18)
O(5)-C(26)-C(25)	105.5(2)
C(31)-C(26)-C(25)	117.7(2)
O(5)-C(26)-C(27)	102.04(19)
C(31)-C(26)-C(27)	118.7(2)
C(25)-C(26)-C(27)	104.0(2)
C(28)-C(27)-C(29)	109.6(2)
C(28)-C(27)-C(26)	113.3(2)
C(29)-C(27)-C(26)	114.8(2)
C(28)-C(27)-C(23)	113.2(2)
C(29)-C(27)-C(23)	113.7(2)
C(26)-C(27)-C(23)	91.34(19)

C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(23)-C(30)-H(30A)	109.5
C(23)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(23)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
O(8)-C(31)-O(7)	124.9(2)
O(8)-C(31)-C(26)	124.6(2)
O(7)-C(31)-C(26)	110.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 5.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	47(1)	76(1)	55(1)	2(1)	18(1)	5(1)
O(2)	60(1)	58(1)	48(1)	-14(1)	24(1)	-14(1)
O(3)	66(1)	84(2)	64(1)	6(1)	-6(1)	-37(1)
O(4)	34(1)	66(1)	50(1)	10(1)	1(1)	-6(1)
O(5)	64(1)	53(1)	31(1)	-6(1)	-7(1)	3(1)
O(6)	94(2)	77(1)	37(1)	0(1)	-11(1)	23(1)
O(7)	51(1)	39(1)	30(1)	-3(1)	3(1)	0(1)
O(8)	73(1)	51(1)	32(1)	-9(1)	3(1)	6(1)
O(9)	54(1)	63(1)	49(1)	-23(1)	10(1)	-12(1)
O(10)	35(1)	78(1)	58(1)	-17(1)	0(1)	-2(1)
C(1)	50(2)	65(2)	38(1)	7(1)	-6(1)	-16(1)
C(2)	46(1)	54(2)	37(1)	-2(1)	-3(1)	-9(1)
C(3)	53(2)	69(2)	35(1)	6(1)	-3(1)	-15(1)
C(4)	48(2)	61(2)	42(1)	14(1)	-3(1)	0(1)
C(5)	33(1)	49(1)	36(1)	6(1)	3(1)	-3(1)
C(6)	35(1)	45(1)	33(1)	0(1)	-2(1)	1(1)
C(7)	36(1)	56(2)	48(1)	-6(1)	2(1)	0(1)
C(8)	56(2)	50(2)	41(1)	4(1)	-4(1)	6(1)
C(9)	80(2)	63(2)	58(2)	-14(2)	1(2)	-10(2)
C(10)	37(1)	48(1)	41(1)	12(1)	11(1)	9(1)
C(11)	72(2)	49(2)	40(1)	-4(1)	21(1)	-4(1)
C(12)	71(2)	44(1)	33(1)	1(1)	13(1)	2(1)
C(13)	52(1)	36(1)	34(1)	2(1)	5(1)	3(1)
C(14)	54(2)	44(1)	36(1)	-1(1)	0(1)	2(1)
C(15)	63(2)	76(2)	41(2)	-19(1)	-3(1)	-6(2)
C(16)	45(1)	42(1)	35(1)	-6(1)	-1(1)	-3(1)
C(17)	39(1)	46(1)	44(1)	-4(1)	-8(1)	2(1)
C(18)	33(1)	54(1)	46(1)	-7(1)	-3(1)	-3(1)
C(19)	56(2)	61(2)	55(2)	7(1)	6(1)	-1(1)
C(20)	62(2)	63(2)	68(2)	6(2)	-6(2)	16(2)
C(21)	48(2)	86(2)	75(2)	-22(2)	16(2)	-3(2)
C(22)	53(2)	56(2)	38(1)	-1(1)	0(1)	8(1)
C(23)	37(1)	48(1)	46(1)	-3(1)	-3(1)	4(1)
C(24)	40(1)	74(2)	42(1)	-9(1)	1(1)	11(1)
C(25)	35(1)	69(2)	37(1)	-3(1)	6(1)	-6(1)
C(26)	40(1)	47(1)	26(1)	-6(1)	1(1)	-4(1)
C(27)	33(1)	44(1)	51(1)	4(1)	-1(1)	-2(1)

C(28)	39(2)	73(2)	99(3)	35(2)	18(2)	6(1)
C(29)	58(2)	49(2)	72(2)	-6(1)	-28(2)	-3(1)
C(30)	69(2)	53(2)	73(2)	4(2)	-18(2)	6(1)
C(31)	46(1)	46(1)	27(1)	-2(1)	3(1)	-5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 5.

	x	y	z	U(eq)
H(3A)	6598	2320	10891	63
H(3B)	5190	2240	10620	63
H(4A)	7052	1870	9015	61
H(4B)	5640	1795	8707	61
H(7A)	3495	2456	7336	70
H(7B)	4054	2111	8148	70
H(7C)	3784	2148	5924	70
H(8A)	5083	2500	3887	73
H(8B)	6091	2736	4825	73
H(8C)	4702	2817	5177	73
H(9A)	5733	2976	10420	100
H(9B)	4451	2844	9712	100
H(9C)	5263	3073	8339	100
H(11A)	5765	1265	3715	64
H(11B)	5626	1572	2232	64
H(12A)	3909	1200	2341	59
H(12B)	3593	1593	2639	59
H(13)	3529	1502	5989	49
H(14)	1684	1459	4377	53
H(15A)	2135	996	2340	90
H(15B)	868	948	3375	90
H(15C)	2016	742	4105	90
H(16)	1836	988	7463	49
H(17)	-96	958	6041	52
H(18)	55	1230	9800	53
H(19A)	-362	660	10723	86
H(19B)	869	686	9565	86
H(19C)	-314	547	8538	86
H(20A)	-1399	1430	6123	97
H(20B)	-269	1507	4789	97
H(20C)	-331	1665	6883	97
H(21A)	-1846	1006	11680	104
H(21B)	-2890	1228	10736	104
H(21C)	-1628	1400	11234	104
H(24A)	7420	292	8119	63
H(24B)	6650	133	6396	63
H(25A)	6875	817	7205	56
H(25B)	6084	658	5503	56
H(28A)	2756	461	8786	105
H(28B)	3624	431	10590	105
H(28C)	3183	95	9518	105
H(29A)	3940	-23	6192	89
H(29B)	4861	238	5239	89
H(29C)	3497	348	5582	89
H(30A)	6395	-266	9855	97
H(30B)	5362	-325	8311	97
H(30C)	5016	-228	10451	97

Table 1. Crystal data and structure refinement for compound 4.

Identification code	compound 4
Empirical formula	C43 H51 O14
Formula weight	791.84
Temperature	173(2) K
Wavelength	0.71069 Å
Crystal system, space group	Monoclinic, P21
Unit cell dimensions	a = 17.5866(15) Å alpha = 90 deg. b = 6.9086(3) Å beta = 118.114(2) deg. c = 18.5825(8) Å gamma = 90 deg.
Volume	1991.4(2) Å ³
Z, Calculated density	2, 1.321 Mg/m ³
Absorption coefficient	0.099 mm ⁻¹
F(000)	842
Crystal size	0.40 x 0.20 x 0.10 mm
Theta range for data collection	1.24 to 27.48 deg.
Limiting indices	-22<=h<=22, -8<=k<=8, -24<=l<=24
Reflections collected / unique	18145 / 8044 [R(int) = 0.0247]
Completeness to theta = 27.48	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9902 and 0.9616
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8044 / 1 / 514
Goodness-of-fit on F ²	1.115
Final R indices [I>2sigma(I)]	R1 = 0.0437, wR2 = 0.1092 [7438refs.]
R indices (all data)	R1 = 0.0488, wR2 = 0.1137
Absolute structure parameter	-0.4(6)
Largest diff. peak and hole	0.328 and -0.405 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for compound 4.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	10245(1)	-321(2)	2926(1)	31(1)
O(2)	6890(1)	-856(3)	899(1)	40(1)
O(3)	6701(1)	1922(3)	1421(1)	48(1)
O(4)	12627(1)	4961(3)	3747(1)	37(1)
O(5)	13563(1)	4853(3)	3244(1)	52(1)
O(6)	8672(1)	1213(2)	2920(1)	24(1)
O(7)	8580(1)	4399(2)	2618(1)	36(1)

O(8)	8788(1)	5323(2)	4126(1)	30(1)
O(9)	8564(1)	7153(2)	5007(1)	40(1)
O(10)	11067(1)	1886(2)	2169(1)	25(1)
O(11)	12353(1)	376(2)	2800(1)	36(1)
O(12)	11283(1)	2349(2)	868(1)	29(1)
O(13)	11239(1)	3380(3)	-292(1)	40(1)
O(14)	15035(6)	3381(18)	3197(7)	176(4)
C(1)	9603(1)	859(3)	2286(1)	23(1)
C(2)	8696(1)	732(3)	2171(1)	24(1)
C(3)	8376(1)	-1337(3)	1961(1)	29(1)
C(4)	7431(1)	-1638(3)	1706(1)	34(1)
C(5)	6559(1)	903(4)	845(1)	39(1)
C(6)	5985(1)	1486(4)	-23(1)	43(1)
C(7)	5784(2)	215(6)	-664(1)	57(1)
C(8)	5239(2)	824(8)	-1453(2)	80(1)
C(9)	4914(2)	2668(8)	-1592(2)	84(2)
C(10)	5115(2)	3965(7)	-964(2)	72(1)
C(11)	5657(2)	3354(5)	-163(2)	56(1)
C(12)	10335(1)	1749(3)	2978(1)	23(1)
C(13)	11101(1)	2560(3)	2925(1)	23(1)
C(14)	11102(1)	4762(3)	2909(1)	27(1)
C(15)	10333(1)	5575(3)	2148(1)	32(1)
C(16)	11934(1)	5514(4)	2960(1)	34(1)
C(17)	13415(1)	4717(3)	3808(1)	36(1)
C(18)	14065(1)	4341(3)	4668(1)	40(1)
C(19)	13822(2)	3858(4)	5252(1)	51(1)
C(20)	14451(2)	3587(6)	6055(2)	82(1)
C(21)	15312(2)	3822(6)	6263(2)	86(1)
C(22)	15553(2)	4286(5)	5681(3)	81(1)
C(23)	14937(2)	4515(4)	4877(2)	59(1)
C(24)	8606(1)	3102(3)	3057(1)	24(1)
C(25)	8562(1)	3327(3)	3843(1)	24(1)
C(26)	9158(1)	2038(4)	4560(1)	35(1)
C(27)	8787(2)	2362(4)	5158(1)	42(1)
C(28)	8031(1)	3783(3)	4699(1)	32(1)
C(29)	7412(2)	4022(4)	5049(2)	50(1)
C(30)	7662(1)	3120(3)	3794(1)	27(1)
C(31)	6993(1)	4508(4)	3185(1)	39(1)
C(32)	7301(2)	1062(4)	3629(1)	42(1)
C(33)	8468(1)	5634(3)	4656(1)	30(1)
C(34)	11738(1)	919(3)	2196(1)	23(1)
C(35)	11581(1)	531(3)	1335(1)	22(1)
C(36)	10879(1)	-963(4)	860(1)	32(1)
C(37)	10996(1)	-1253(4)	92(1)	34(1)
C(38)	11766(1)	107(3)	246(1)	27(1)
C(39)	12170(1)	-234(4)	-302(1)	37(1)
C(40)	12346(1)	-54(3)	1191(1)	25(1)
C(41)	12693(1)	-2094(3)	1479(1)	35(1)
C(42)	13085(1)	1411(4)	1530(1)	35(1)
C(43)	11411(1)	2122(3)	203(1)	28(1)

Table 3. Bond lengths [Å] and angles [deg] for compound 4.

O(1)-C(12)	1.437(2)
O(1)-C(1)	1.445(2)
O(2)-C(5)	1.330(3)
O(2)-C(4)	1.450(3)
O(3)-C(5)	1.205(3)
O(4)-C(17)	1.346(3)
O(4)-C(16)	1.446(2)
O(5)-C(17)	1.198(3)
O(6)-C(24)	1.345(2)
O(6)-C(2)	1.452(2)
O(7)-C(24)	1.197(2)
O(8)-C(33)	1.363(2)
O(8)-C(25)	1.463(2)
O(9)-C(33)	1.205(3)
O(10)-C(34)	1.335(2)
O(10)-C(13)	1.455(2)
O(11)-C(34)	1.194(2)

O(12)-C(43)	1.365(2)
O(12)-C(35)	1.476(2)
O(13)-C(43)	1.195(3)
C(1)-C(12)	1.458(2)
C(1)-C(2)	1.508(2)
C(1)-H(1)	1.0000
C(2)-C(3)	1.519(3)
C(2)-H(2)	1.0000
C(3)-C(4)	1.513(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.499(3)
C(6)-C(7)	1.384(4)
C(6)-C(11)	1.387(4)
C(7)-C(8)	1.387(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.370(7)
C(8)-H(8)	0.9500
C(9)-C(10)	1.379(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.402(4)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(13)	1.505(2)
C(12)-H(12)	1.0000
C(13)-C(14)	1.522(3)
C(13)-H(13)	1.0000
C(14)-C(16)	1.513(3)
C(14)-C(15)	1.530(3)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.486(3)
C(18)-C(19)	1.380(4)
C(18)-C(23)	1.398(4)
C(19)-C(20)	1.390(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.385(6)
C(20)-H(20)	0.9500
C(21)-C(22)	1.372(6)
C(21)-H(21)	0.9500
C(22)-C(23)	1.381(5)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-C(25)	1.508(2)
C(25)-C(26)	1.533(3)
C(25)-C(30)	1.548(2)
C(26)-C(27)	1.546(3)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.546(3)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(33)	1.513(3)
C(28)-C(29)	1.517(3)
C(28)-C(30)	1.560(2)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.526(3)
C(30)-C(32)	1.528(3)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(34)-C(35)	1.514(2)

C(35)-C(36)	1.531(3)
C(35)-C(40)	1.544(2)
C(36)-C(37)	1.549(3)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.560(3)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.510(2)
C(38)-C(43)	1.512(3)
C(38)-C(40)	1.565(2)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(41)	1.529(3)
C(40)-C(42)	1.530(3)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800

C(12)-O(1)-C(1)	60.80(12)
C(5)-O(2)-C(4)	117.92(17)
C(17)-O(4)-C(16)	117.49(16)
C(24)-O(6)-C(2)	116.58(14)
C(33)-O(8)-C(25)	105.83(15)
C(34)-O(10)-C(13)	119.32(13)
C(43)-O(12)-C(35)	105.71(14)
O(1)-C(1)-C(12)	59.33(11)
O(1)-C(1)-C(2)	116.62(15)
C(12)-C(1)-C(2)	125.76(15)
O(1)-C(1)-H(1)	114.4
C(12)-C(1)-H(1)	114.4
C(2)-C(1)-H(1)	114.4
O(6)-C(2)-C(1)	110.96(14)
O(6)-C(2)-C(3)	106.64(14)
C(1)-C(2)-C(3)	109.35(16)
O(6)-C(2)-H(2)	109.9
C(1)-C(2)-H(2)	109.9
C(3)-C(2)-H(2)	109.9
C(4)-C(3)-C(2)	115.47(17)
C(4)-C(3)-H(3A)	108.4
C(2)-C(3)-H(3A)	108.4
C(4)-C(3)-H(3B)	108.4
C(2)-C(3)-H(3B)	108.4
H(3A)-C(3)-H(3B)	107.5
O(2)-C(4)-C(3)	111.12(16)
O(2)-C(4)-H(4A)	109.4
C(3)-C(4)-H(4A)	109.4
O(2)-C(4)-H(4B)	109.4
C(3)-C(4)-H(4B)	109.4
H(4A)-C(4)-H(4B)	108.0
O(3)-C(5)-O(2)	124.6(2)
O(3)-C(5)-C(6)	123.4(2)
O(2)-C(5)-C(6)	112.0(2)
C(7)-C(6)-C(11)	120.9(3)
C(7)-C(6)-C(5)	121.6(3)
C(11)-C(6)-C(5)	117.5(2)
C(6)-C(7)-C(8)	119.2(4)
C(6)-C(7)-H(7)	120.4
C(8)-C(7)-H(7)	120.4
C(9)-C(8)-C(7)	120.0(4)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	121.8(3)
C(8)-C(9)-H(9)	119.1
C(10)-C(9)-H(9)	119.1
C(9)-C(10)-C(11)	118.6(4)
C(9)-C(10)-H(10)	120.7
C(11)-C(10)-H(10)	120.7
C(6)-C(11)-C(10)	119.6(3)

C(6)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2
O(1)-C(12)-C(1)	59.87(12)
O(1)-C(12)-C(13)	116.07(16)
C(1)-C(12)-C(13)	123.01(15)
O(1)-C(12)-H(12)	115.4
C(1)-C(12)-H(12)	115.4
C(13)-C(12)-H(12)	115.4
O(10)-C(13)-C(12)	108.26(14)
O(10)-C(13)-C(14)	107.52(15)
C(12)-C(13)-C(14)	112.51(15)
O(10)-C(13)-H(13)	109.5
C(12)-C(13)-H(13)	109.5
C(14)-C(13)-H(13)	109.5
C(16)-C(14)-C(13)	110.61(17)
C(16)-C(14)-C(15)	109.79(16)
C(13)-C(14)-C(15)	112.10(16)
C(16)-C(14)-H(14)	108.1
C(13)-C(14)-H(14)	108.1
C(15)-C(14)-H(14)	108.1
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(4)-C(16)-C(14)	107.53(15)
O(4)-C(16)-H(16A)	110.2
C(14)-C(16)-H(16A)	110.2
O(4)-C(16)-H(16B)	110.2
C(14)-C(16)-H(16B)	110.2
H(16A)-C(16)-H(16B)	108.5
O(5)-C(17)-O(4)	123.8(2)
O(5)-C(17)-C(18)	125.5(2)
O(4)-C(17)-C(18)	110.62(19)
C(19)-C(18)-C(23)	120.5(2)
C(19)-C(18)-C(17)	121.4(2)
C(23)-C(18)-C(17)	118.1(2)
C(18)-C(19)-C(20)	119.5(3)
C(18)-C(19)-H(19)	120.3
C(20)-C(19)-H(19)	120.3
C(21)-C(20)-C(19)	119.7(4)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(22)-C(21)-C(20)	120.7(3)
C(22)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(21)-C(22)-C(23)	120.3(3)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(22)-C(23)-C(18)	119.3(3)
C(22)-C(23)-H(23)	120.4
C(18)-C(23)-H(23)	120.4
O(7)-C(24)-O(6)	125.17(17)
O(7)-C(24)-C(25)	125.46(18)
O(6)-C(24)-C(25)	109.37(15)
O(8)-C(25)-C(24)	108.39(15)
O(8)-C(25)-C(26)	106.07(15)
C(24)-C(25)-C(26)	117.17(16)
O(8)-C(25)-C(30)	101.89(14)
C(24)-C(25)-C(30)	116.80(14)
C(26)-C(25)-C(30)	105.01(16)
C(25)-C(26)-C(27)	101.16(17)
C(25)-C(26)-H(26A)	111.5
C(27)-C(26)-H(26A)	111.5
C(25)-C(26)-H(26B)	111.5
C(27)-C(26)-H(26B)	111.5
H(26A)-C(26)-H(26B)	109.4
C(28)-C(27)-C(26)	103.90(16)
C(28)-C(27)-H(27A)	111.0
C(26)-C(27)-H(27A)	111.0
C(28)-C(27)-H(27B)	111.0
C(26)-C(27)-H(27B)	111.0

H(27A)-C(27)-H(27B)	109.0
C(33)-C(28)-C(29)	114.55(19)
C(33)-C(28)-C(27)	103.87(18)
C(29)-C(28)-C(27)	115.94(19)
C(33)-C(28)-C(30)	98.87(15)
C(29)-C(28)-C(30)	118.44(19)
C(27)-C(28)-C(30)	102.76(16)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-C(32)	109.50(18)
C(31)-C(30)-C(25)	113.27(16)
C(32)-C(30)-C(25)	114.46(17)
C(31)-C(30)-C(28)	113.53(17)
C(32)-C(30)-C(28)	114.33(17)
C(25)-C(30)-C(28)	90.84(14)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(9)-C(33)-O(8)	121.9(2)
O(9)-C(33)-C(28)	130.75(19)
O(8)-C(33)-C(28)	107.36(16)
O(11)-C(34)-O(10)	125.92(16)
O(11)-C(34)-C(35)	124.71(16)
O(10)-C(34)-C(35)	109.32(14)
O(12)-C(35)-C(34)	107.99(15)
O(12)-C(35)-C(36)	105.52(14)
C(34)-C(35)-C(36)	115.07(15)
O(12)-C(35)-C(40)	102.58(13)
C(34)-C(35)-C(40)	119.39(14)
C(36)-C(35)-C(40)	104.81(15)
C(35)-C(36)-C(37)	101.37(15)
C(35)-C(36)-H(36A)	111.5
C(37)-C(36)-H(36A)	111.5
C(35)-C(36)-H(36B)	111.5
C(37)-C(36)-H(36B)	111.5
H(36A)-C(36)-H(36B)	109.3
C(36)-C(37)-C(38)	103.51(16)
C(36)-C(37)-H(37A)	111.1
C(38)-C(37)-H(37A)	111.1
C(36)-C(37)-H(37B)	111.1
C(38)-C(37)-H(37B)	111.1
H(37A)-C(37)-H(37B)	109.0
C(39)-C(38)-C(43)	114.92(17)
C(39)-C(38)-C(37)	115.22(18)
C(43)-C(38)-C(37)	104.11(15)
C(39)-C(38)-C(40)	118.70(15)
C(43)-C(38)-C(40)	99.21(15)
C(37)-C(38)-C(40)	102.36(15)
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(41)-C(40)-C(42)	110.15(16)
C(41)-C(40)-C(35)	114.64(16)
C(42)-C(40)-C(35)	113.32(16)
C(41)-C(40)-C(38)	113.60(16)
C(42)-C(40)-C(38)	113.16(16)
C(35)-C(40)-C(38)	90.89(13)

C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
O(13)-C(43)-O(12)	121.5(2)
O(13)-C(43)-C(38)	131.20(18)
O(12)-C(43)-C(38)	107.29(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 4. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	29(1)	25(1)	34(1)	5(1)	12(1)	3(1)
O(2)	33(1)	52(1)	32(1)	-8(1)	15(1)	-6(1)
O(3)	44(1)	57(1)	37(1)	-10(1)	15(1)	5(1)
O(4)	26(1)	50(1)	26(1)	2(1)	5(1)	-7(1)
O(5)	40(1)	68(1)	50(1)	11(1)	23(1)	-2(1)
O(6)	29(1)	23(1)	24(1)	0(1)	17(1)	-1(1)
O(7)	53(1)	25(1)	41(1)	6(1)	32(1)	2(1)
O(8)	33(1)	25(1)	36(1)	-6(1)	19(1)	-5(1)
O(9)	54(1)	28(1)	38(1)	-9(1)	21(1)	0(1)
O(10)	22(1)	36(1)	19(1)	0(1)	11(1)	4(1)
O(11)	32(1)	51(1)	24(1)	8(1)	11(1)	16(1)
O(12)	33(1)	34(1)	27(1)	10(1)	19(1)	13(1)
O(13)	48(1)	46(1)	36(1)	20(1)	27(1)	19(1)
O(14)	159(8)	157(9)	247(11)	18(9)	126(8)	9(7)
C(1)	26(1)	25(1)	23(1)	2(1)	14(1)	1(1)
C(2)	26(1)	27(1)	21(1)	2(1)	13(1)	1(1)
C(3)	34(1)	28(1)	30(1)	-3(1)	18(1)	-3(1)
C(4)	34(1)	38(1)	32(1)	-4(1)	19(1)	-10(1)
C(5)	27(1)	57(2)	36(1)	-8(1)	17(1)	-10(1)
C(6)	23(1)	71(2)	38(1)	1(1)	16(1)	-5(1)
C(7)	43(1)	92(2)	36(1)	-10(1)	17(1)	-17(1)
C(8)	52(2)	145(4)	38(1)	-9(2)	17(1)	-17(2)
C(9)	36(1)	169(5)	41(2)	30(2)	14(1)	8(2)
C(10)	38(1)	122(3)	64(2)	36(2)	30(1)	22(2)
C(11)	32(1)	88(2)	54(1)	13(2)	26(1)	10(1)
C(12)	27(1)	25(1)	19(1)	3(1)	12(1)	2(1)
C(13)	22(1)	31(1)	16(1)	0(1)	9(1)	2(1)
C(14)	26(1)	31(1)	20(1)	-3(1)	9(1)	-3(1)
C(15)	30(1)	30(1)	30(1)	2(1)	10(1)	3(1)
C(16)	28(1)	41(1)	25(1)	3(1)	6(1)	-9(1)
C(17)	31(1)	30(1)	40(1)	1(1)	11(1)	-7(1)
C(18)	34(1)	28(1)	42(1)	-4(1)	5(1)	-2(1)
C(19)	50(1)	58(2)	32(1)	-4(1)	9(1)	22(1)
C(20)	83(2)	109(3)	30(1)	-5(2)	7(1)	60(2)
C(21)	70(2)	74(3)	51(2)	-25(2)	-23(2)	40(2)
C(22)	39(1)	40(2)	98(3)	-4(2)	-22(2)	2(1)
C(23)	34(1)	37(1)	81(2)	11(2)	6(1)	-5(1)
C(24)	22(1)	24(1)	28(1)	1(1)	14(1)	-1(1)
C(25)	25(1)	21(1)	25(1)	-2(1)	12(1)	-1(1)
C(26)	40(1)	32(1)	25(1)	1(1)	8(1)	9(1)
C(27)	67(2)	33(1)	22(1)	1(1)	18(1)	4(1)
C(28)	45(1)	30(1)	24(1)	-6(1)	20(1)	-5(1)
C(29)	76(2)	50(2)	48(1)	-18(1)	48(1)	-16(1)

C(30)	28(1)	34(1)	24(1)	-6(1)	17(1)	-5(1)
C(31)	25(1)	54(2)	36(1)	-5(1)	13(1)	7(1)
C(32)	52(1)	44(1)	44(1)	-17(1)	35(1)	-25(1)
C(33)	32(1)	30(1)	24(1)	-1(1)	10(1)	4(1)
C(34)	23(1)	25(1)	24(1)	2(1)	14(1)	0(1)
C(35)	21(1)	26(1)	21(1)	5(1)	11(1)	5(1)
C(36)	27(1)	43(1)	27(1)	0(1)	13(1)	-6(1)
C(37)	33(1)	41(1)	24(1)	-3(1)	10(1)	-2(1)
C(38)	25(1)	35(1)	21(1)	3(1)	12(1)	6(1)
C(39)	39(1)	50(1)	30(1)	5(1)	22(1)	14(1)
C(40)	21(1)	34(1)	21(1)	3(1)	11(1)	7(1)
C(41)	38(1)	36(1)	31(1)	6(1)	17(1)	13(1)
C(42)	23(1)	47(1)	36(1)	2(1)	16(1)	-1(1)
C(43)	24(1)	39(1)	25(1)	5(1)	14(1)	6(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 4.

	x	y	z	U(eq)
H(1)	9643	868	1767	28
H(2)	8310	1623	1723	29
H(3A)	8486	-1788	1512	35
H(3B)	8719	-2163	2441	35
H(4A)	7314	-3039	1708	40
H(4B)	7288	-996	2104	40
H(7)	6015	-1057	-563	69
H(8)	5091	-38	-1898	96
H(9)	4539	3063	-2136	100
H(10)	4892	5245	-1072	86
H(11)	5799	4214	282	67
H(12)	10200	2381	3388	28
H(13)	11644	2088	3399	27
H(14)	11063	5238	3399	32
H(15A)	9796	5085	2119	47
H(15B)	10372	5170	1661	47
H(15C)	10340	6992	2178	47
H(16A)	12027	4949	2518	41
H(16B)	11911	6941	2902	41
H(19)	13230	3711	5105	61
H(20)	14291	3242	6460	98
H(21)	15741	3661	6814	103
H(22)	16145	4451	5832	97
H(23)	15103	4787	4470	71
H(26A)	9765	2466	4799	42
H(26B)	9116	664	4395	42
H(27A)	8580	1130	5276	50
H(27B)	9226	2932	5677	50
H(29A)	7159	2764	5058	75
H(29B)	6953	4926	4709	75
H(29C)	7724	4530	5606	75
H(31A)	7224	5828	3291	59
H(31B)	6468	4458	3242	59
H(31C)	6858	4130	2629	59
H(32A)	6733	1052	3607	63
H(32B)	7692	204	4067	63
H(32C)	7246	610	3106	63
H(36A)	10298	-456	717	39
H(36B)	10976	-2183	1171	39
H(37A)	10469	-871	-408	41
H(37B)	11134	-2618	40	41
H(39A)	12382	-1569	-235	56
H(39B)	12653	664	-154	56
H(39C)	11739	-19	-871	56
H(41A)	12214	-3019	1262	52
H(41B)	12982	-2137	2077	52
H(41C)	13105	-2434	1284	52
H(42A)	12856	2713	1344	52

H (42B)	13500	1087	1336	52
H (42C)	13373	1371	2128	52