Supplementary Information

Enantioselective and Protecting Group-Free Synthesis of 1-Deoxythionojirimycin, 1-Deoxythiomannojirimycin and 1-Deoxythiotalonojirimycin

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General Procedures

Melting points were recorded on a BUCHI B540 melting point apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a BRUKER−400 and 100 MHz spectrometer, respectively. Chemical shifts are reported in parts per million downfield from the internal reference, tetramethylsilane. Coupling constants are reported wherever necessary in Hertz (Hz). Column chromatography was performed on silica gel (230−400 mesh). Mass spectra were recorded on a Q-TOF electrospray instrument. Micro analysis were recorded on Thermo Finnigan FLASH EA 1112 CHNS analyser. Optical rotation was recorded on polarimeter model P-1020 (A077860638). X-ray data collection was recorded on a BRUKER-SMART APEX CCD−single crystal diffractometer.

2,6-Dibromo-2,6-dideoxy-D-idono-1,4-lactone (10).[1]

L-gulonic acid-γ-lactone **9** (10g, 0.056 mol) was treated with HBr in glacial acetic acid (33%, 56.2 mL) at 30 °C and stirred for 4.5 h. Methanol (150 mL) was then added and the mixture kept overnight at room temperature. The solution was concentrated to ca. 50 mL, diluted with water (200 mL), and extracted with diethyl ether (4 x 100 mL). The dried ($MgSO_4$) extracts were concentrated *in vacuo* to yield 2,6-dibromo-2,6-dideoxy-D-idono-1,4-lactone **10** (14.6g, 85%) as a pale yellow syrup. The crude product was sufficiently pure for further transformation. IR (neat): 3443, 1779, 1428, 1221, 1183, 1100, 1059, 1014 cm^{-1}; ^{1}H NMR (400 MHz, CD_3COCD_3) δ 3.56 (d, J = 6.4 Hz, 2H), 4.31 (td, J = 9.5, 5.5 Hz, 1H), 4.63 (d, J = 5.0 Hz, 1H), 4.83–4.75 (m, 4H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ 34.1, 44.8, 68.9, 75.5, 82.0, 171.4.

2,6-Dibromo-2,6-dideoxy-D-allono-1,4-lactone (19).

The bromination[1b] procedure was similar as carried out with L-gulonic acid-γ-lactone **9**. $[\alpha]_D$ +5.2 (*c* 1, $CHCl_3$); IR (neat): 3403, 2323, 1770, 1626, 1161, 1012 cm^{-1}; ^{1}H NMR

[1] (a) Vekemans, J. A. J. M.; Dapperens, C. W. M.; Claessen, R.; Koten, A. M. J.; Godefroi, E. F. *J. Org. Chem.* **1990**, *55*, 5336; (b) Bock, K.; Lundt, I.; Pedersen, C.; Refn, S. *Acta Chem. Scand.* **1986**, *B40*, 740.

(400 MHz, D_2O) δ 3.36 (dd, J = 11.1, 7.2 Hz, 1H), 3.49 (dd, J = 4.0, 11.1 Hz, 1H), 4.08 (td, J = 7.2, 7.1Hz, 1H), 4.38 (t, J = 5.9 Hz, 1H), 4.54 (t, J = 7.1 Hz, 1H), 4.69 (d, J = 7.5 Hz, 1H); ^{13}C NMR (100 MHz, D_2O) δ 33.0, 45.0, 69.5, 74.8, 83.8, 172.8.

2,6-Dibromo-2,6-dideoxy-D-glucono-1,4-lactone (15) from D-mannose.[2]

To D-mannose **14** (10g, 0.056 mol) and $BaCO_3$ (20g) in water (200 mL) was added slowly bromine (ca. 4 mL, 0.076 mol) over a period of 10 min. After stirring overnight a yellow colour persists. Filtration through active charcoal and concentration (50° C) followed by coevaporation with AcOH (2 x 10 mL) gave a solid residue to which HBr/AcOH (100 mL) was added. The mixture was stirred for 3−4 h. Then, MeOH (200 mL) was added (caution: addition is exothermic reaction), stirring was continued overnight. The solution was concentrated to a syrupy residue. This was coevaporated with MeOH (ca. 10 mL) and with water (2 x ca. 10 mL). To the syrupy residue was added water (10 mL) and the mixture extracted with Et_2O (ca. 10 mL). It was dried and concentrated and purified by column chromatography (elution with 2:3 EtOAc/hexanes) to yield the dibromo lactone **15** (4.6g, 27%). $[\alpha]_D$ +22.3 (*c* 1, H_2O), lit.[2] $[\alpha]_D$ +29.0 (*c* 2, EtOAc); IR (neat): 3438, 1777, 1424, 1219, 1181, 1073, 1028, 993 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$+CD_3SOCD_3) δ 3.6 (dd, J = 10.9, 5.7 Hz, 1H), 3.76 (dd, J = 10.8, 2.8 Hz, 1H), 4.22–4.17 (m, 1H), 4.23 (s, 1H), 4.57 (d, J = 3.1 Hz, 1H), 4.64 (dd, J = 8.7, 3.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 36.3, 40.9, 67.8, 74.5, 80.7, 171.6.

1-Deoxy-5-thio-D-glucopyrano-3,6-lactone (12).

A solution of dibromolactone **10** (0.320g, 1.05 mmol) in DMSO (2 mL) was added to a solution of benzyltriethylammonium tetrathiomolybdate $[BnEt_3N]_2MoS_4$ **5** (1.411g, 2.3 mmol in DMSO (15 mL) over a period of 15 min. After stirring the reaction mixture for 30 min, DMSO was removed under reduced pressure and the residue was repeatedly extracted with THF (5 × 10 mL) and filtered over Celite pad. The solvent was concentrated to give the crude product which was subjected to column chromatography

[2] Lundt, I.; Pedersen, C. *Synthesis* **1991**, 669.

on silica gel (elution with hexanes:ethyl acetate 1:1) furnishing white solid which was then recrystallized from acetone to afford colorless crystals of lactone **12** (0.104g, 56%). M.p. : 156−157˚ C; $[\alpha]_D$ +13.0 (*c* 1.0, MeOH); IR (neat): 3422, 1430, 1288, 1170, 1116, 1054 cm^{-1}; ^1H NMR (400 MHz, CD_3COCD_3) δ 2.68 (d, J = 15 Hz, 1H), 3.2 (dd, J = 14.5, 3.3 Hz, 1H), 3.41 (d, J = 5.5 Hz, 1H), 4.36 (bs, 1H), 4.55 (t, J = 5.4 Hz, 1H), 4.60 (bs, 1H), 5.43 (d, J = 5.3 Hz, 1H), 5.63 (d, J = 4.5 Hz, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ 31.5, 44.6, 66.7, 69.0, 74.5, 171.8; HRMS for $C_6H_8O_4S$+Na calcd 199.0041; found 199.0043; Anal. calcd for: C,41.01; H,5.08; S,17.98. Found: C,40.90; H,4.58; S,18.2.

Crystal structure data: CCDC 774511: C6 H8 O4 S1, Mwt = 176.18, Crystal dimensions 0.26 × 0.21 × 0.18, T = 293(2)K, Orthorhombic, Space group P 21 21 21, a = 5.7460(18), b = 11.149(4), c = 11.329(4) Å, $\alpha = \beta = \gamma$ = 90.00˚, Z = 4, V = 725.8(4) cm^3, ρ_{calcd} = 1.61 g/cm^3, MoK_α radiation (λ˚ = 0.71073 Å), μ = 4.06 mm^{-1}, 2θ = 2.60-28.0˚; of 3594 reflections collected, 1623 were independent (R (int) = 0.0368); refinement method full matrix least squares on F_2, 102 refined parameters, absorption correction (SADABS, Bruker, 1996 software, T_{min} 0.9019 and T_{max} 0.9306), GooF = 1.221, R_1 = 0.0620, wR_2 = 0.1910 ($\sigma > 2\sigma$(I)), absolute structure parameter 0.00(2), residual electron density 0.553/-0.739 $eÅ^{-3}$. The structure was solved and refined with the programs WinGXv1.64.05, Sir92, and SHELXL-97.

The synthesis of 1-Deoxy-5-thio-D-mannopyrano-3,6-lactone **16** and 1-Deoxy-5-thio-D-talopyrano-3,6-lactone **20** were done in similar manner as described for 1-Deoxy-5-thio-D-glucopyrano-3,6-lactone **12** .

1-Deoxy-5-thio-D-mannopyrano-3,6-lactone (16).

M.p. : 188−189˚ C; $[\alpha]_D$ –39.0 (*c* 1.0, MeOH); IR (neat): 3402, 1772, 1160, 1100, 1050 cm^{-1}; ^1H NMR (400 MHz, CD_3COCD_3) δ 2.67 (dd, J = 10.3, 12.9 Hz, 1H), 2.80 (dd, J = 6.0, 12.9 Hz, 1H), 3.36 (d, J = 5.46 Hz, 1H), 4.29 (td, J = 10.2, 6.2 Hz, 1H), 4.55 (dd, J = 6.5, 22.6 Hz, 1H), 4.75 (dd, J = 6.0, 12.0 Hz, 1H), 4.84 (d, J = 6.1 Hz, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ 28.9, 44.2, 63.9, 69.4, 83.4, 172.3; HRMS for $C_6H_8O_4S$+Na

calcd 199.0041; found 199.0036; Anal. calcd for: C,41.01; H,4.61; S,18.30. Found: C,40.90; H,4.58; S,18.2.

Crystal structure data: CCDC 774514: C6 H8 O4 S1, Mwt = 176.18, Crystal dimensions 0.28 × 0.21 × 0.16, T = 296(2)K, Tetragonal, Space group P 42, a = 9.0100(4), b = 9.0100(4), c = 8.8021(5) Å, $\alpha = \beta = \gamma = 90.00^{\circ}$, Z = 4, V = 725.8(4) cm^3, ρ_{calcd} = 1.64 g/cm^3, MoK_{α} radiation (λ° = 0.71073 Å), μ = 4.12 mm^{-1}, 2θ = 2.30-29.5°; of 2974 reflections collected, 1796 were independent (R (int) = 0.0368); refinement method full matrix least squares on F_2, 102 refined parameters, absorption correction (SADABS, Bruker, 1996 software, T_{min} 0.8934 and T_{max} 0.9370), GooF = 1.045, R_1 = 0.0350, wR_2 = 0.0840 ($\sigma > 2\sigma(I)$), absolute structure parameter 0.03(10), residual electron density 0.187/-0.230 $eÅ^{-3}$.

1-Deoxy-5-thio-D-talopyrano-3,6-lactone (20).

M.p. : 145−146° C; $[\alpha]_D$ +24.5 (c 1.0, MeOH); IR (neat): 3419, 3265, 1421, 1358, 1159, 1037 cm^{-1}; ^{1}H NMR (400 MHz, CD_3COCD_3) δ 2.61 (dd, J = 13.0, 10.2 Hz, 1H), 2.86 (dd, J = 13.1, 5.8 Hz, 1H), 3.26 (s, 1H), 4.08 (td, J = 10.1, 5.9 Hz, 1H), 4.27 (d, J = 2.9 Hz, 1H), 4.59 (s, 1H), 4.78 (d, J = 6.1 Hz, 1H), 5.21 (d, J = 2.9, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ 28.8, 44.7, 70.0, 77.1, 89.2, 173.7; HRMS for $C_6H_8O_4S$+Na calcd 199.0041; found 199.0032; Anal. calcd for: C,40.85; H,5.27; S,17.92. Found: C,40.90; H,4.58; S,18.20.

Crystal structure data: CCDC 774512: C6 H8 O4 S1, Mwt = 176.18, Crystal dimensions 0.26 × 0.21 × 0.18, T = 293(2)K, Tetragonal, Space group P 41, a = 11.1600(3), b = 11.1600(3), c = 5.9040(3) Å, $\alpha = \beta = \gamma = 90.00^{\circ}$, (3), Z = 4, V = 735.3(5) cm^3, ρ_{calcd} = 1.59 g/cm^3, MoK_{α} radiation (λ° = 0.71073 Å), μ = 4.00 mm^{-1}, 2θ = 1.80-26.0°; of 5584 reflections collected, 1438 were independent (R (int) = 0.0368); refinement method full matrix least squares on F_2, 102 refined parameters, absorption correction (SADABS, Bruker, 1996 software, T_{min} 0.9019 and T_{max} 0.9306), GooF = 1.132, R_1 = 0.0290, wR_2 = 0.0720 ($\sigma > 2\sigma(I)$), absolute structure parameter 0.03(8), residual electron density 0.194/-0.116 $eÅ^{-3}$.

Preparation of borohydride exchange resin (BER).[3]

Aqueous sodium borohydride (0.5 M, 100 mL) was stirred with the chloride form resin (Amberlite IRA−400, 10.0g) for 1 h. The resulting borohydride-bound ion exchange resin was washed thoroughly with distilled water until free of excess sodium borohydride and dried *in vacuo* at 60˚ C for 5 h.

1-Deoxythiomannojirimycin (13).

To a stirred solution of thialactone **16** (0.079g, 0.464 mmol) in dry methanol (6 mL) at 0˚ C was added borohydride exchange resin (0.618g, 1.85 mmol) and the solution was stirred for 3 h. The reaction mixture was filtered and methanol (10 mL) was added to the resin and was sonicated for 5 min at room temperature. The sonicated resin was acidified using glacial acetic acid so as to neutralize the pH and filtered. The solution was then concentrated *in vacuo* to afford the crude product which was subjected to column chromatography on silica gel eluting with methanol/chloroform 1.5:8.5 to furnish the 1-deoxythiomannojirimycin as white solid, which was recrystallized from methanol:chloroform to furnish colorless crystals of **13** (0.060g, 74%). Nature of compound : Colorless crystals; M.p. : 128−129 °C; $[\alpha]_D$ –48.1 (*c* 1.0, MeOH), lit.[4] $[\alpha]_D$ – 43.0 (*c* 0.7, MeOH); IR (neat): 3377, 2919, 2887, 1418, 1085, 1051 cm^{-1}; ^1H NMR (400 MHz, CD_3OD) δ 4.13 (quint, J = 2.4 Hz, 1H), 3.94 (dd, J = 11.4, 4.2 Hz, 1H), 3.80 (t, J = 8.6 Hz, 1H), 3.72 (dd, J = 11.4, 7.0 Hz, 1H), 3.35 (dd, J = 8.4, 2.8 Hz, 1H), 2.83 (dd, J = 14.0, 1.5 Hz, 1H), 2.82-2.76 (m, 1H), 2.67 (dd, J = 14.0, 5.2 Hz, 1H); ^{13}C NMR (100 MHz, CD_3OD) δ 33.0, 50.2, 63.3, 70.2, 72.2, 76.7; HRMS for $C_6H_{12}O_4S$+Na calcd 203.0354; found 203.0350; Anal. calcd for: C,40.04; H,6.42; S,17.50. Found: C,39.99; H,6.71; S,17.79.

[3] (a) Bandgar, B. P.; Modhave, R. K.; Wadgaonkar, P. P.; Sande, A. R. *J. Chem. Soc. Perkin Trans. 1* **1996**, 1993; (b) Gibson, H. W.; Bailey, F. C. *J. Chem. Soc. Chem. Commun.* **1977**, 815a.
[4] Cubero, I. I.; López-Espinosa, M. T. P.; Richardson, A. C.; Suarez Ortéga, M. D. *Carbohydr. Res.* **1993**, *242*, 109.

Crystal structure data: CCDC 774513: C6 H8 O4 S1, Mwt = 180.22, Crystal dimensions 0.26 × 0.21 × 0.16, T = 293(2)K, Monoclinic, Space group P 2(1), a = 4.8443(10), b = 8.1458(17), c = 9.6690(2) Å, $\alpha = \gamma = 90.00^{\circ}$, β = 94.020(3), Z = 2, V = 380.59(14) cm^3, ρ_{calcd} = 1.57 g/cm^3, MoK_α radiation (λ° = 0.71073 Å), μ = 3.88 mm^{-1}, 2θ = 2.10-26.0°; of 3799 reflections collected, 1469 were independent (R (int) = 0.0192); refinement method full matrix least squares on F_2, 104 refined parameters, absorption correction (SADABS, Bruker, 1996 software, T_{min} 0.9058 and T_{max} 0.9405), GooF = 1.171, R_1 = 0.0250, wR_2 = 0.0700 ($\sigma > 2\sigma$(I)), absolute structure parameter 0.00(12), residual electron density 0.321/-0.350 $eÅ^{-3}$.

1-Deoxythionojirimycin (**8**) and 1-deoxythiotalonojirimycin (**17**) were prepared by the above procedure as adopted with 1-deoxythiomannojirimycin (**13**).

1-Deoxythionojirimycin (8).

Gummy solid; $[\alpha]_D$ +78.6 (*c* 1.0, MeOH), lit.[5] $[\alpha]_D$ +50.0 (*c* 1.39, H_2O); IR (neat): 3368, 2925, 1430, 1103, 1043 cm^{-1}; ^1H NMR (400 MHz, CD_3OD) δ 4.27 (quint, J = 2.0 Hz, 1H), 4.01 (t, J = 3.2 Hz, 1H), 3.71–3.62 (m, 2H), 3.61–3.53 (m, 1H), 3.31 (quint, J = 1.6 Hz, 1H), 3.19 (dd, J = 11.3, 4.4 Hz, 1H), 2.67 (dd, J = 11.3, 1.2 Hz, 1H), 2.11–2.00 (m, 1H), 1.86–1.75 (m, 1H); ^{13}C NMR (100 MHz, CD_3OD) δ 34.2, 36.7, 47.8, 62.2, 79.4, 80.0; HRMS for $C_6H_{12}O_4S$+1 calcd 181.0535; found 181.0526.

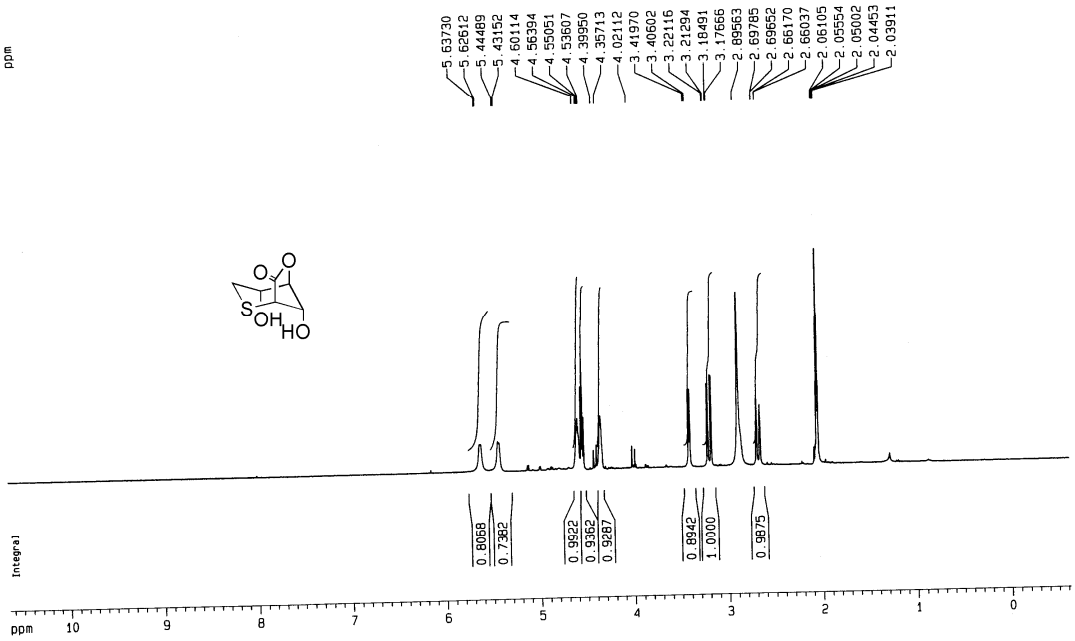
1-Deoxythiotalonojirimycin (17).

Gummy solid; $[\alpha]_D$ +20.6 (*c* 1.0, MeOH), lit.[6] $[\alpha]_D$ +28.0 (*c* 1.1, MeOH); IR (neat): 3369, 2916, 1420, 1073, 1018 cm^{-1}; ^1H NMR (400 MHz, CD_3OD) δ 4.00 (t, J = 3.0 Hz, 1H), 3.89 (dt, J = 7.6, 3.2 Hz, 1H), 3.85-3.74 (m, 2H), 3.59 (s, 1H), 2.87 (td, J = 6.1, 3.5 Hz, 1H), 2.78 (dd, J = 13.5, 7.6 Hz, 1H), 2.57 (bd, J = 13.1 Hz, 1H); ^{13}C NMR (100 MHz,

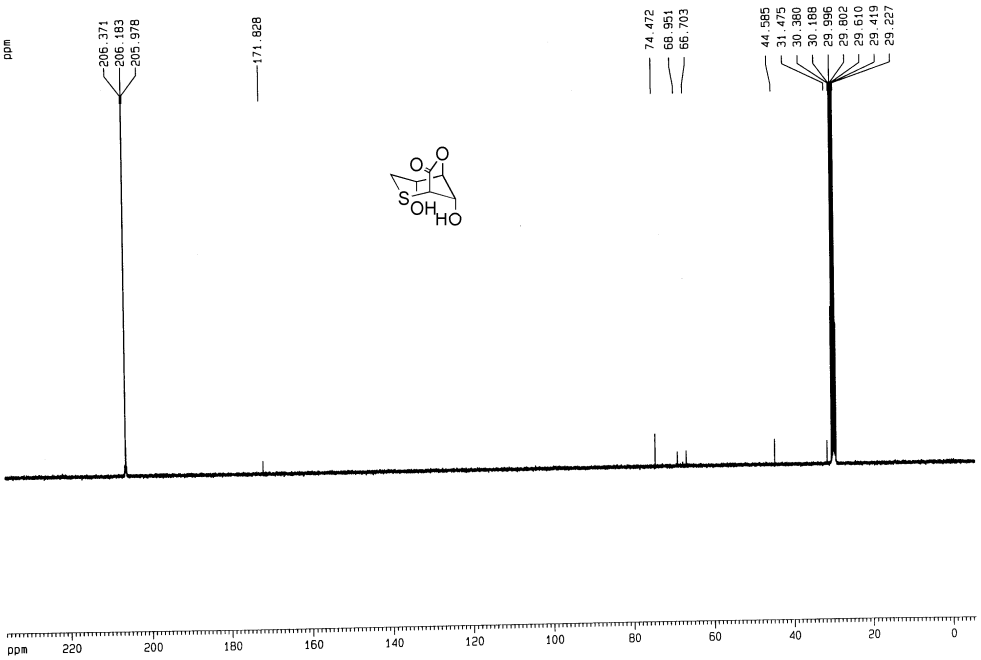
[5] Merrer, Y. L.; Fuzier, M.; Dosbaa, I.; Foglietti, M. J.; Depezay, J. C. *Tetrahedron* **1997**, *53*, 16731 and references cited therein.
[6] Cubero, I. I.; López-Espinosa, M. T. P.; Asenjo, R. A.; Fernández, A. R. *Carbohydr. Lett.* **1999**, *3*, 323.

D_2O) δ 30.1, 47.5, 61.3, 69.5, 70.9, 71.4; HRMS for $C_6H_{12}O_4S$+Na calcd 203.0354; found 203.0356.

The structures were solved and refined with the programs WinGXv1.64.05, Sir92, and SHELXL-97. Crystallographic data for the above compounds **12**, **16**, **13**, and **20** have been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK, +44 1223 336408; email: deposit@ccdc.cam.ac.uk.



^{1}H NMR spectrum of 1-deoxy-5-thio-D-glucopyrano-3,6-lactone **12** (CD_3COCD_3, 400 MHz)



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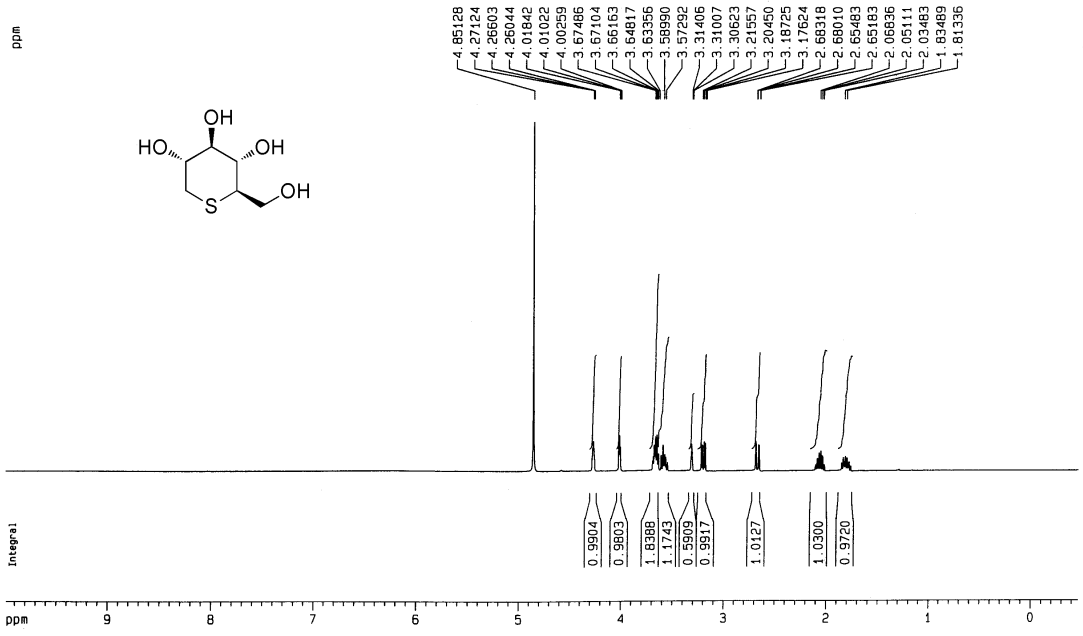
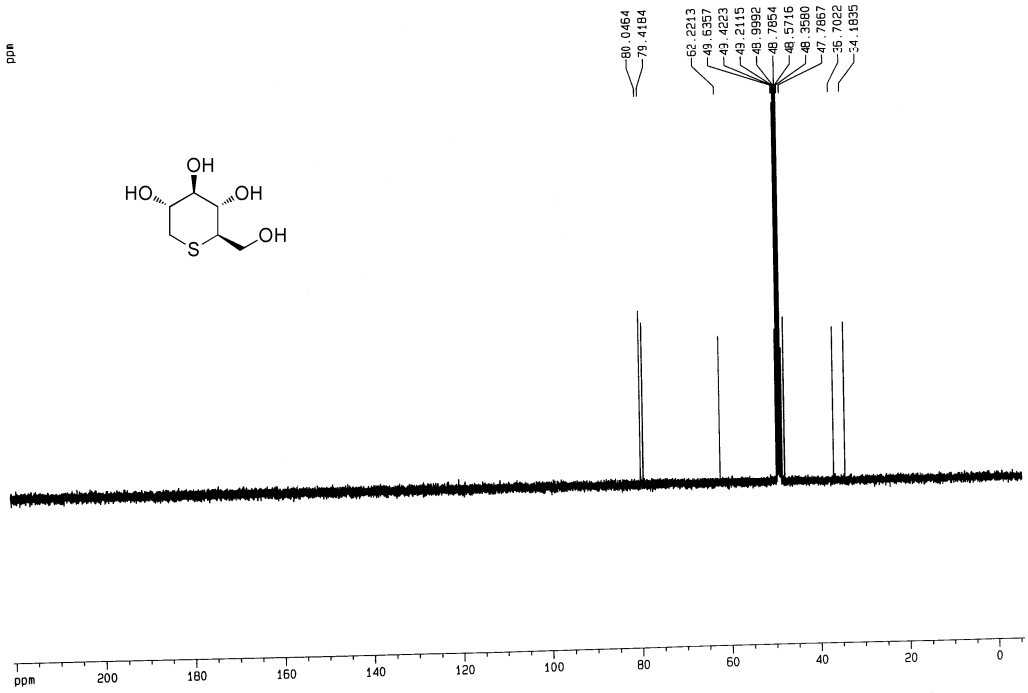
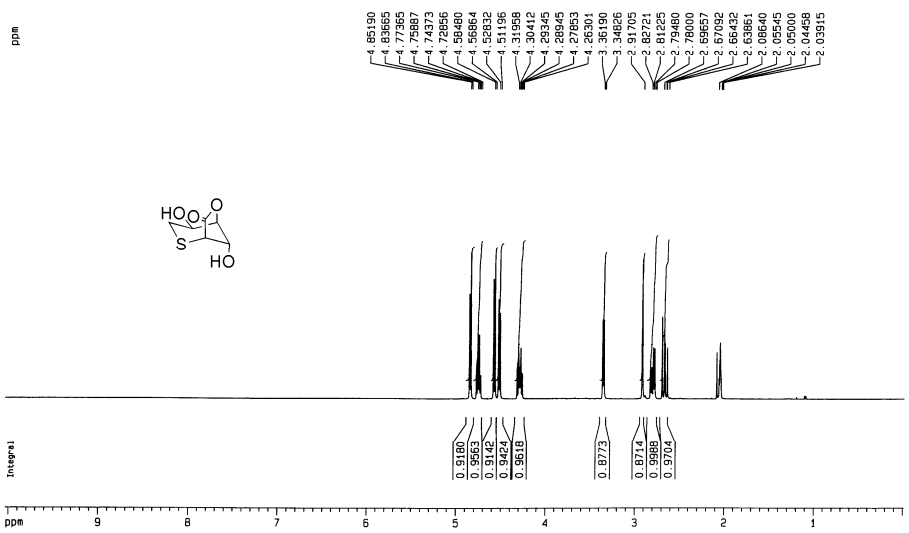


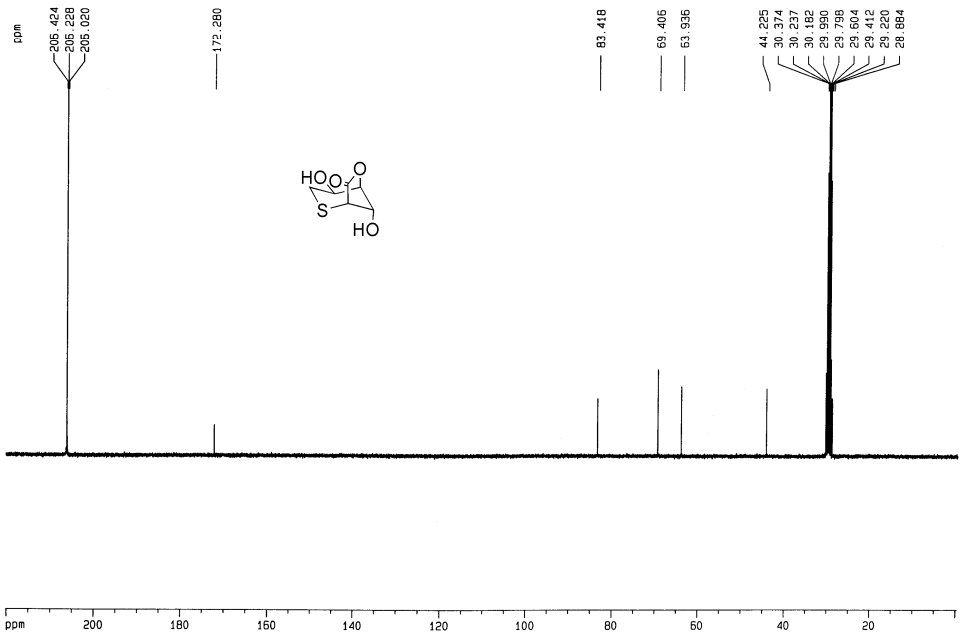
^{1}H NMR spectrum of 1-deoxythionojirimycin **8** (CD_3OD, 400 MHz)



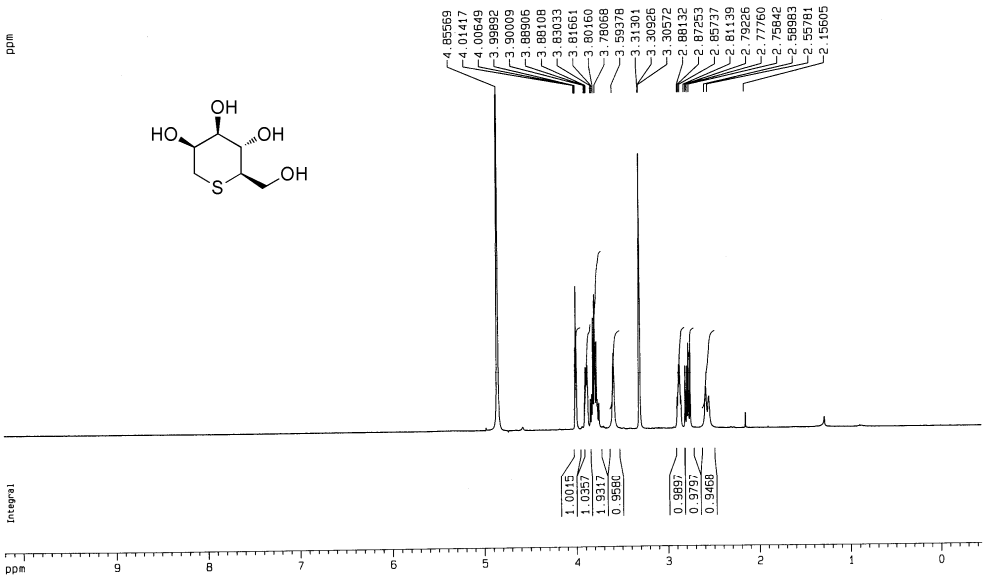
^{13}C NMR spectrum of 1-deoxythionojirimycin **8** (CD_3OD, 100 MHz)



^{1}H NMR spectrum of 1-deoxy-5-thio-D-mannopyrano-3,6-lactone **16** (CD_3COCD_3, 400 MHz)



^{13}C NMR spectrum of 1-deoxy-5-thio-D-mannopyrano-3,6-lactone **16** (CD_3COCD_3, 100 MHz)



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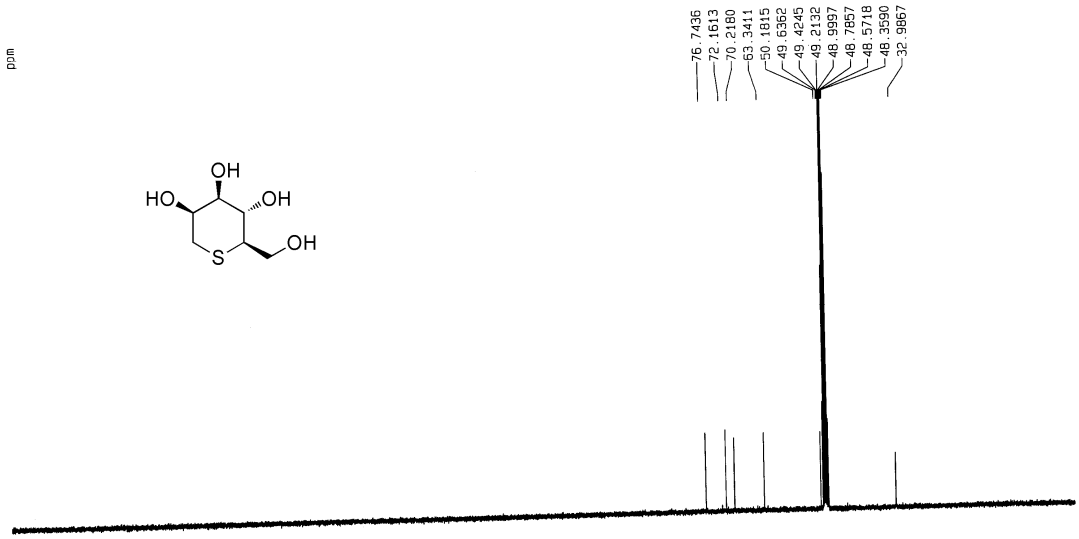

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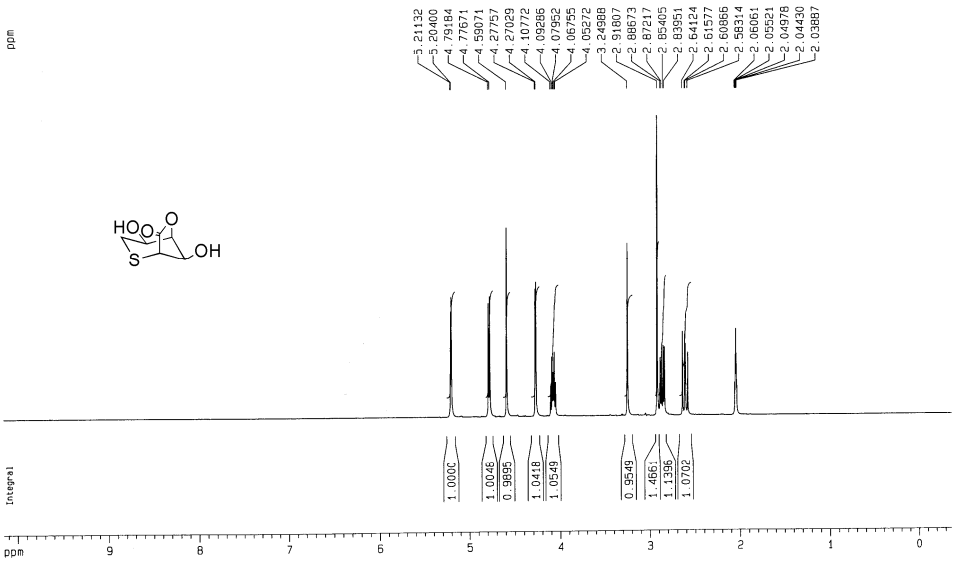

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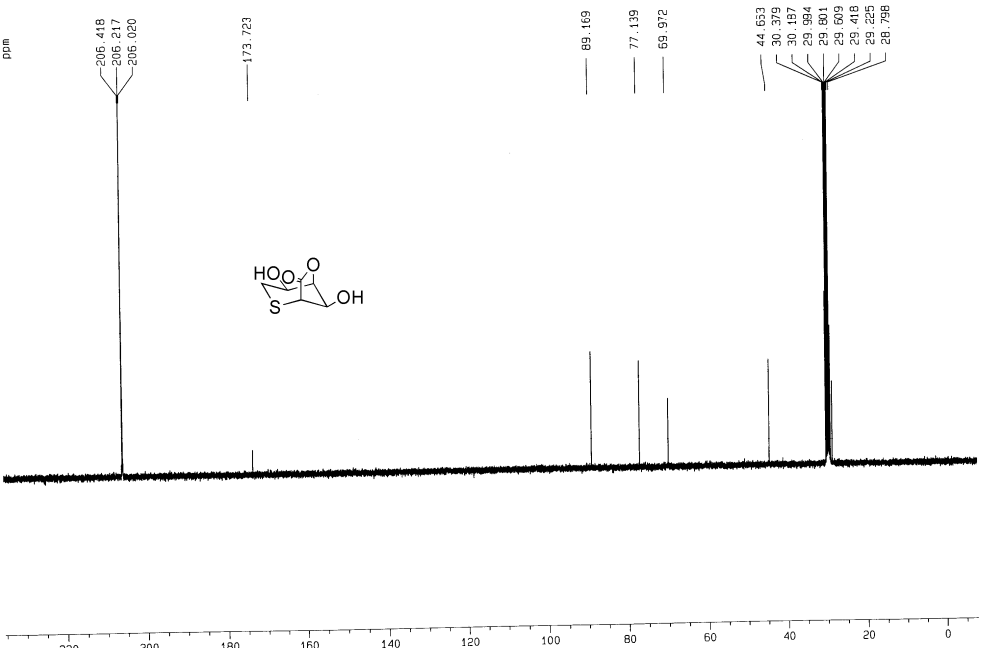
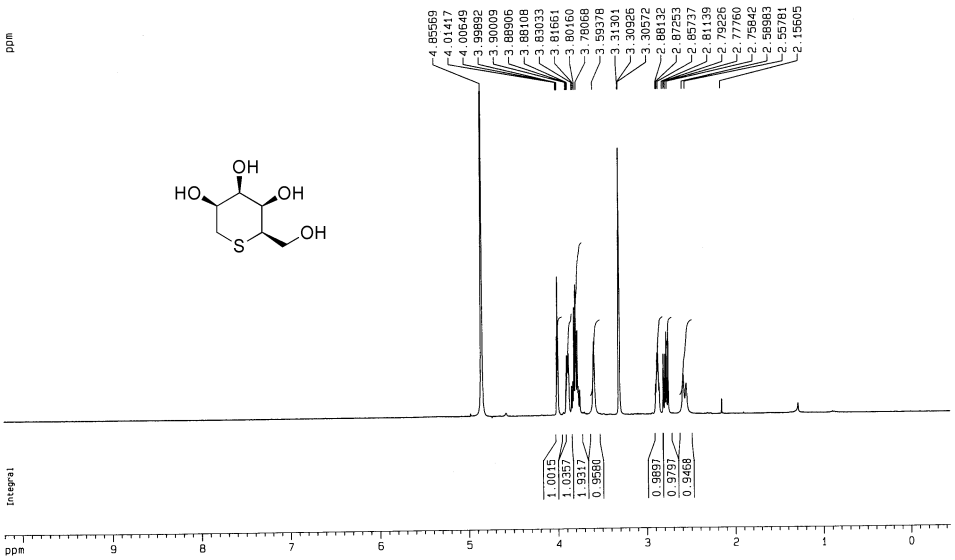
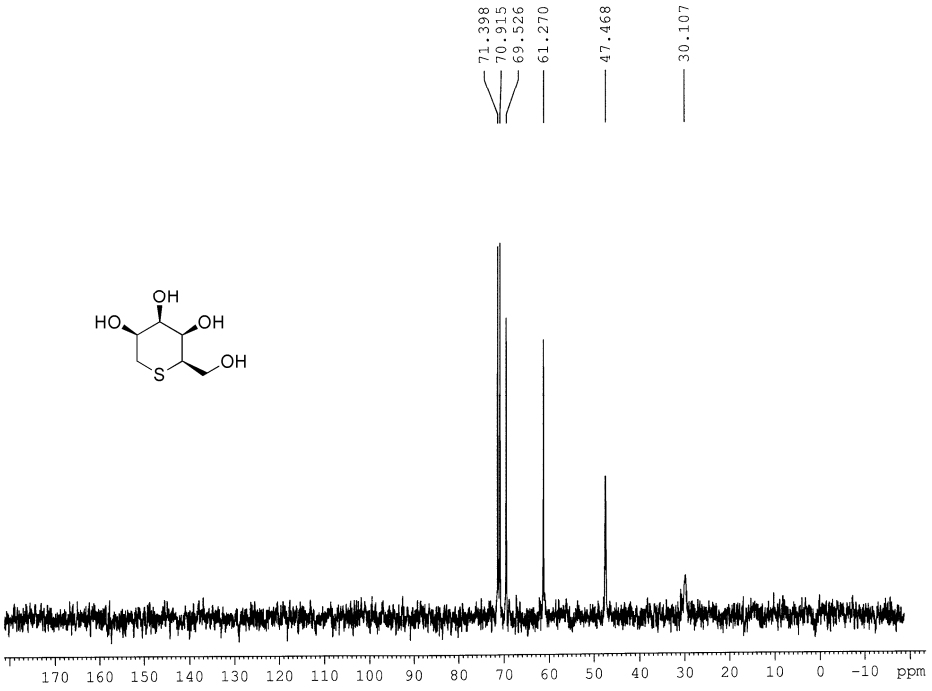


^{13}C NMR spectrum of 1-deoxy-5-thio-D-talopyrano-3,6-lactone **20** (CD_3COCD_3, 100 MHz)

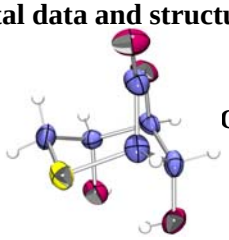


^{1}H NMR spectrum of 1-deoxythiotalonojirimycin **17** (CD_3OD, 400 MHz)

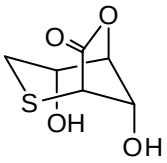


^{13}C NMR spectrum of 1-deoxythiotalonojirimycin **17** (D_2O, 100 MHz)

Crystal data and structure refinement for 1-deoxy-5-thio-D-glucopyrano-3,6-lactone (12)

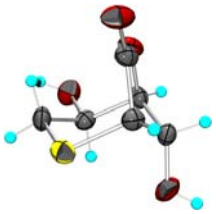


Ortep diagram of Compound 12

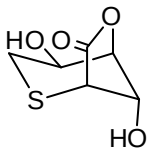


DATA	**Compound 12**
Formula	C6 H8 O4 S1
Formula weight	176.18
Color	Colorless
Crystal morphology	Block
Temperature/K	293(2)
Radiation	Mo Kα
Wavelength/Å	0.71073
Crystal system	Orthorhombic
Space group	*P* 21 21 21
a (Å)	5.7460(18)
b (Å)	11.149(4)
c (Å)	11.329(4)
β (°)	90.000(0)
Volume (Å^3)	725.8(4)
Z	4
Density (g/cm)	1.61
μ (1/mm)	0.406
F (000)	368.0
θ (min, max)	2.6, 28.0
No. of unique refln	1623
No. of parameters	102
*R*_obs, wR_2_obs	0.062, 0.191
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	-0.739, 0.553
GooF	1.221

Crystal data and structure refinement for 1-deoxy-5-thio-D-mannopyrano-3,6-lactone (16)

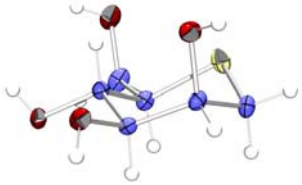


Ortep diagram of Compound 16

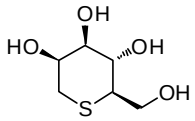


DATA	Compound 16
Formula	C6 H8 O4 S1
Formula weight	176.18
Color	Colorless
Crystal morphology	Block
Temperature/K	296(2)
Radiation	Mo Kα
Wavelength/Å	0.71073
Crystal system	Tetragonal
Space group	*P* 42
a (Å)	9.0100(4)
b (Å)	9.0100(4)
c (Å)	8.8021(5)
β (°)	90.000(0)
Volume (Å^3)	714.56(6)
Z	4
Density (g/cm)	1.64
μ (1/mm)	0.412
F (000)	368.0
θ (min, max)	2.3, 29.5
No. of unique refln	1796
No. of parameters	102
*R*_obs, wR_2_obs	0.035, 0.084
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	-0.230, 0.187
GooF	1.045

Crystal data and structure refinement for 1-deoxythiomannojirimycin (13)

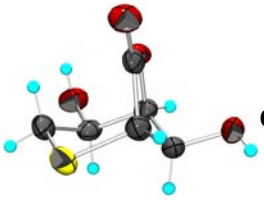


Ortep diagram of Compound 13

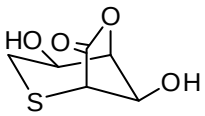


DATA	Compound 13
Formula	C6 H12 O4 S1
Formula weight	180.2
Color	Colorless
Crystal morphology	Block
Temperature/K	273(2)
Radiation	Mo Kα
Wavelength/Å	0.71073
Crystal system	Monoclinic
Space group	*P* 2(1)
a (Å)	4.8443(10)
b (Å)	8.1458(17)
c (Å)	9.669(2)
β (°)	94.020(3)
Volume ($Å^3$)	380.59(14)
Z	2
Density (g/cm)	1.57
μ (1/mm)	0.388
F (000)	192.0
θ (min, max)	2.1, 26.0
No. of unique refln	1469
No. of parameters	104
*R*_obs, wR_2_obs	0.025, 0.070
$\Delta\rho_{min}$, $\Delta\rho_{max}$ ($eÅ^{-3}$)	-0.350, 0.321
GooF	1.171

Crystal data and structure refinement for 1-deoxy-5-thio-D-talopyrano-3,6-lactone (20)



Ortep diagram of Compound 20



DATA	Compound 20
Formula	C6 H8 O4 S1
Formula weight	176.18
Color	Colorless
Crystal morphology	Block
Temperature/K	293(2)
Radiation	Mo Kα
Wavelength/Å	0.71073
Crystal system	Tetragonal
Space group	*P* 41
a (Å)	11.160(3)
b (Å)	11.160(3)
c (Å)	5.904(3)
β (°)	90.000(0)
Volume (Å^3)	735.3(5)
Z	4
Density (g/cm)	1.59
μ (1/mm)	0.400
F (000)	368.0
θ (min, max)	1.8, 26.0
No. of unique refln	1438
No. of parameters	102
*R*_obs, wR_2_obs	0.029, 0.072
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	-0.116, 0.194
GooF	1.132