

Supporting Information

Diastereoisomerically pure, (*S*)-*O*-1,2-*O*-isopropylidene-(5-*O*- α -D-glucofuranosyl) *t*-butanesulfinate: Synthesis, crystal structure, absolute configuration and reactivity

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Table S1. Crystal data and experimental details for (*S*)-1,2-*O*-isopropylidene-(5-*O*- α -D-glucofuranosyl) *t*-butanesulfinate **10**.

Molecular formula	C ₁₃ H ₂₄ O ₇ S
Formula weight	324.4
Crystallographic system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a [Å]	7.097(3)
b [Å]	9.594(3)
c [Å]	23.832(5)
V [Å ³]	1622.7(9)
Z	4
D _{calcd} [g/cm ³]	1.328
Data collection temperature [K]	100(2)
Crystal dimensions [mm]	0.3, 0.2, 0.1
F(000)	696
Radiation, λ [Å]	MoK α , 0.71073
Scan mode	ω
2 Θ _{max} [°]	72.28
hkl ranges	h (-11,11), k (-15,9), l (-31,37)
Absorption coefficient μ [mm ⁻¹]	0.228
Reflections measured	17405
Reflections unique	6250
Reflections observed, I > 2 σ (I)	5270
R _{int}	0.0375
Parameters refined	263
Flack x parameter	-0.11(9)
wR ² (obs)	0.1440
R ₁ (obs)	0.0633
S (goodness-of-fit)	1.067
Residual density max [eÅ ⁻³]	0.381
Residual density min [eÅ ⁻³]	-0.537
Resolution max [Å]	0.6026

Table S2. Asymmetry parameters for the two five-membered rings in the crystal structure of (*S*)-1,2-*O*-isopropylidene-(5-*O*- α -D-glucofuranose) *t*-butanesulfinate **10**.

Ring C1,C2,C3,C4,O4				Ring C1,C2,O2,C7,O1			
ΔC_s^C	47.5(4)	ΔC_2^{C1-C2}	59.1(4)	ΔC_s^{C1}	36.0(5)	ΔC_2^{C1-C2}	40.9(6)
ΔC_s^C	39.2(4)	ΔC_2^{C2-C3}	38.9(4)	ΔC_s^{C2}	24.1(5)	ΔC_2^{C2-O2}	17.5(6)
ΔC_s^C	17.4(4)	ΔC_2^{C3-C4}	4.1(4)	ΔC_s^{O2}	2.2(6)	ΔC_2^{O2-C7}	12.6(6)
ΔC_s^C	11.0(4)	ΔC_2^{C4-O4}	32.7(4)	ΔC_s^{C7}	20.8(5)	ΔC_2^{C7-O1}	37.9(6)
ΔC_s^O	37.0(4)	ΔC_2^{O4-C1}	56.8(4)	ΔC_s^{O1}	35.4(5)	ΔC_2^{O1-C1}	48.7(6)

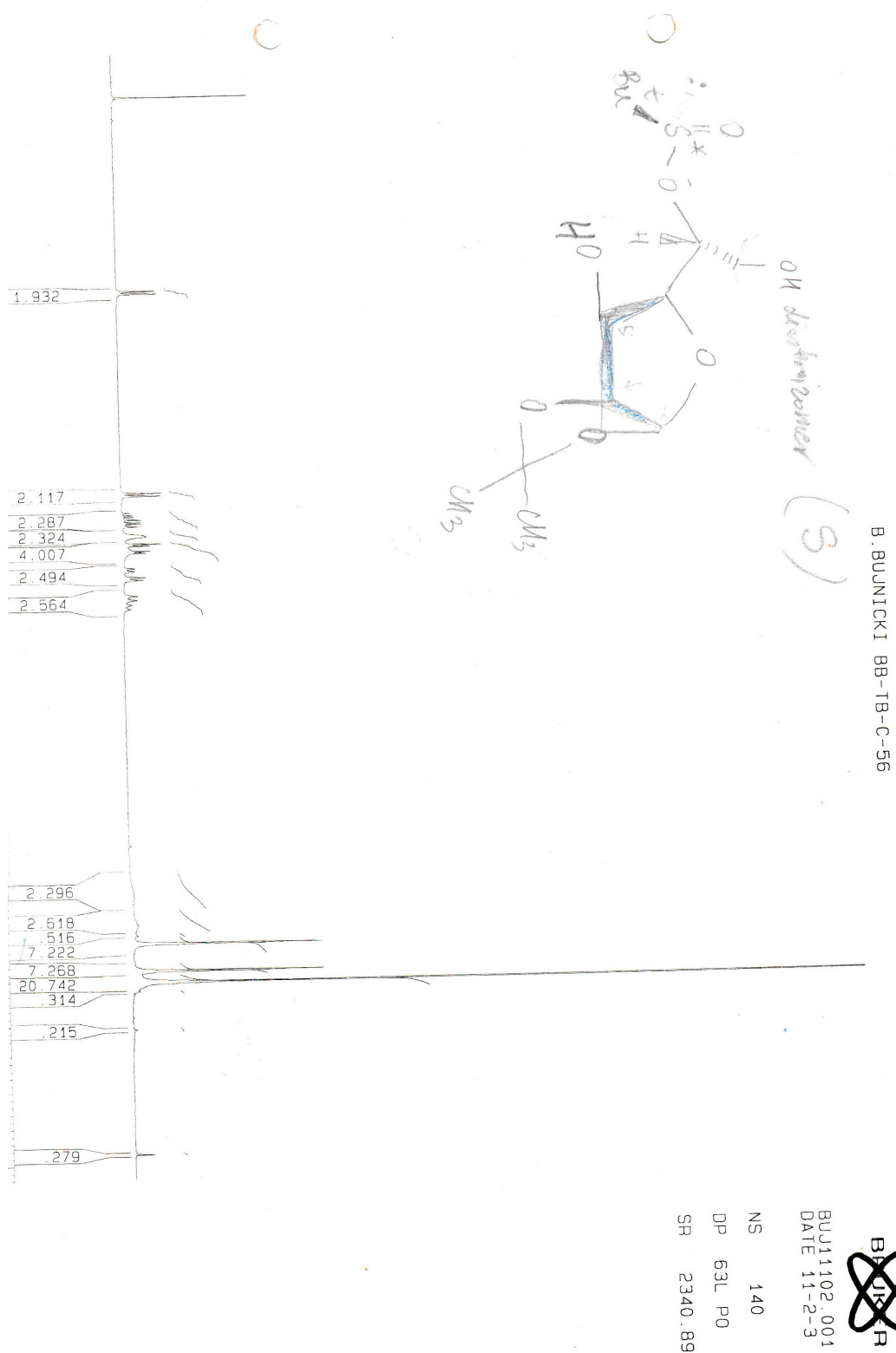


Figure 2S. ^1H NMR Spectrum of (S)-1,2-O-isopropylidene-(5-O- α -D-glucofuranosyl) *t*-butanesulfinate (S)-10

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DATE 11-2-3

NS 140
DP 63L P0
SR 2340.89

B. BUJNICKI BB-TB-C-56

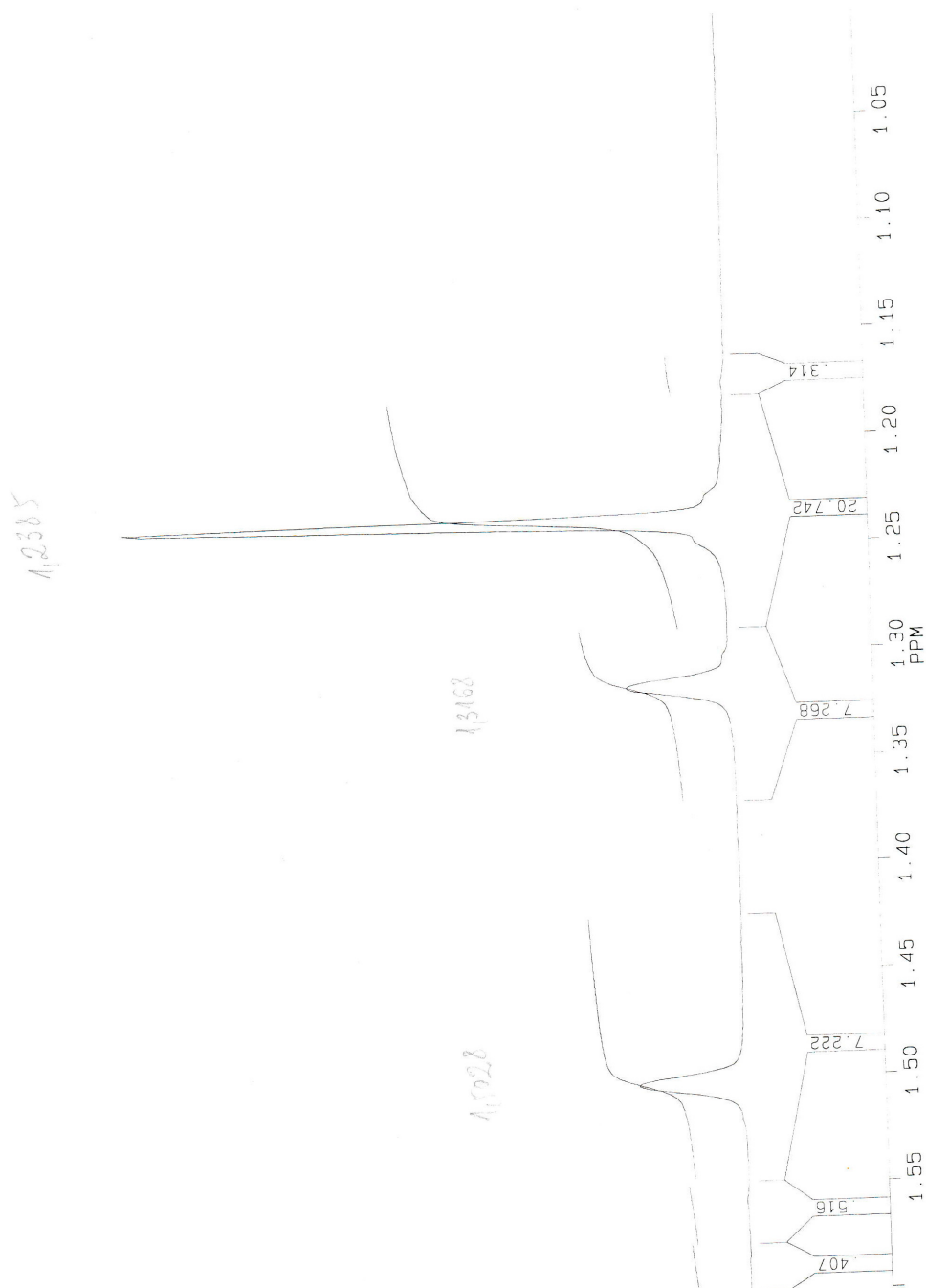


Figure 3S. ^1H NMR Spectrum of (*S*)-1,2-*O*-isopropylidene-(5-*O*- α -D-glucofuranosyl) *t*-butanesulfonate (*S*)-**10** (Range extension 1.0-1.6 ppm)

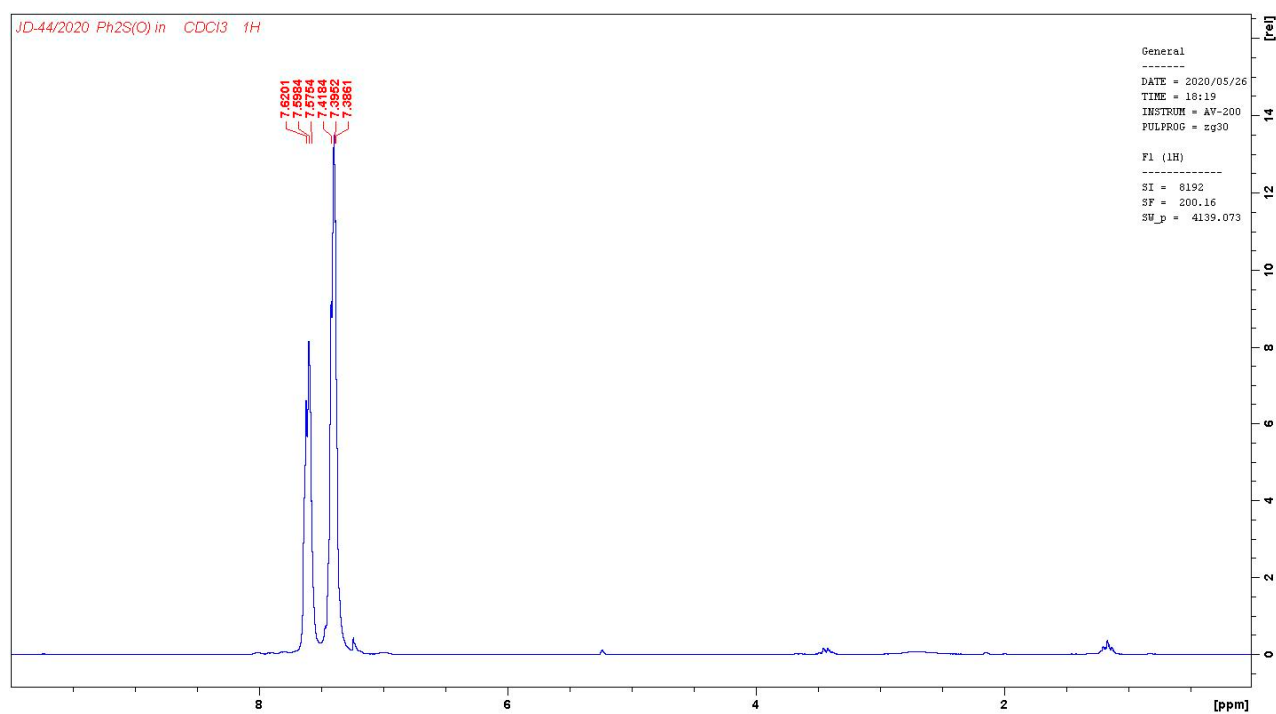


Figure 4S. ^1H NMR Spectrum of diphenyl sulfoxide

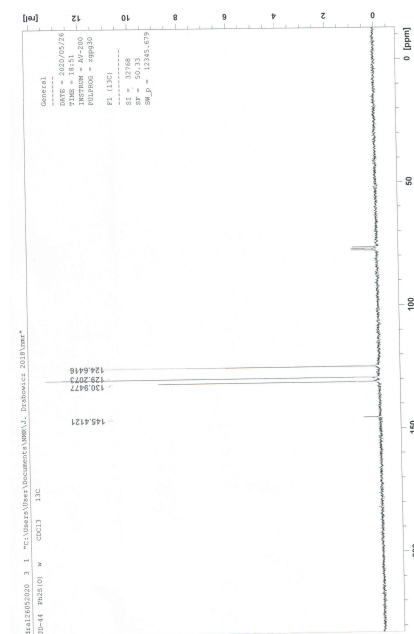


Figure 5S. ^{13}C NMR Spectrum of diphenyl sulfoxide

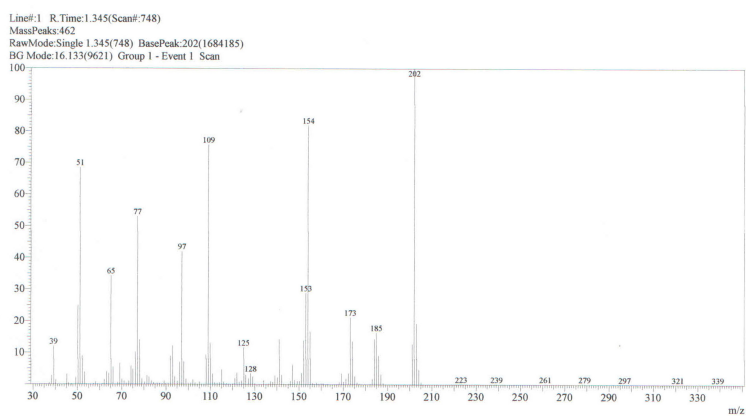


Figure 6. Mass Spectrum of diphenyl sulfoxide

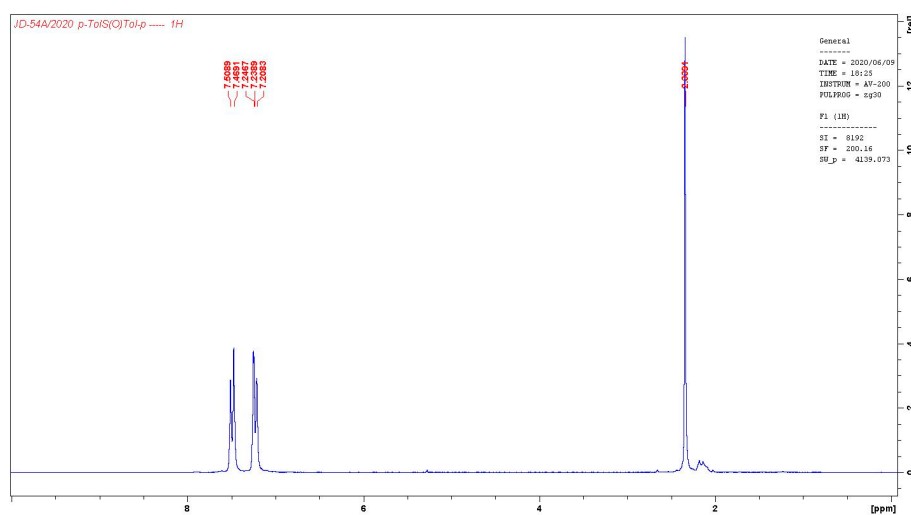


Figure 7S. ¹H NMR Spectrum of di-p-tolylsulfoxide

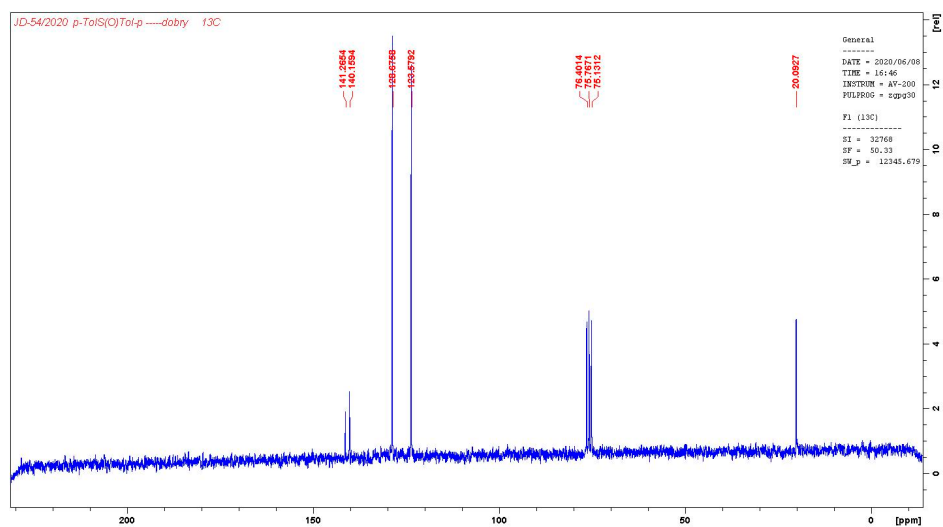


Figure 8S. ¹³C NMR Spectrum of di-p-tolylsulfoxide

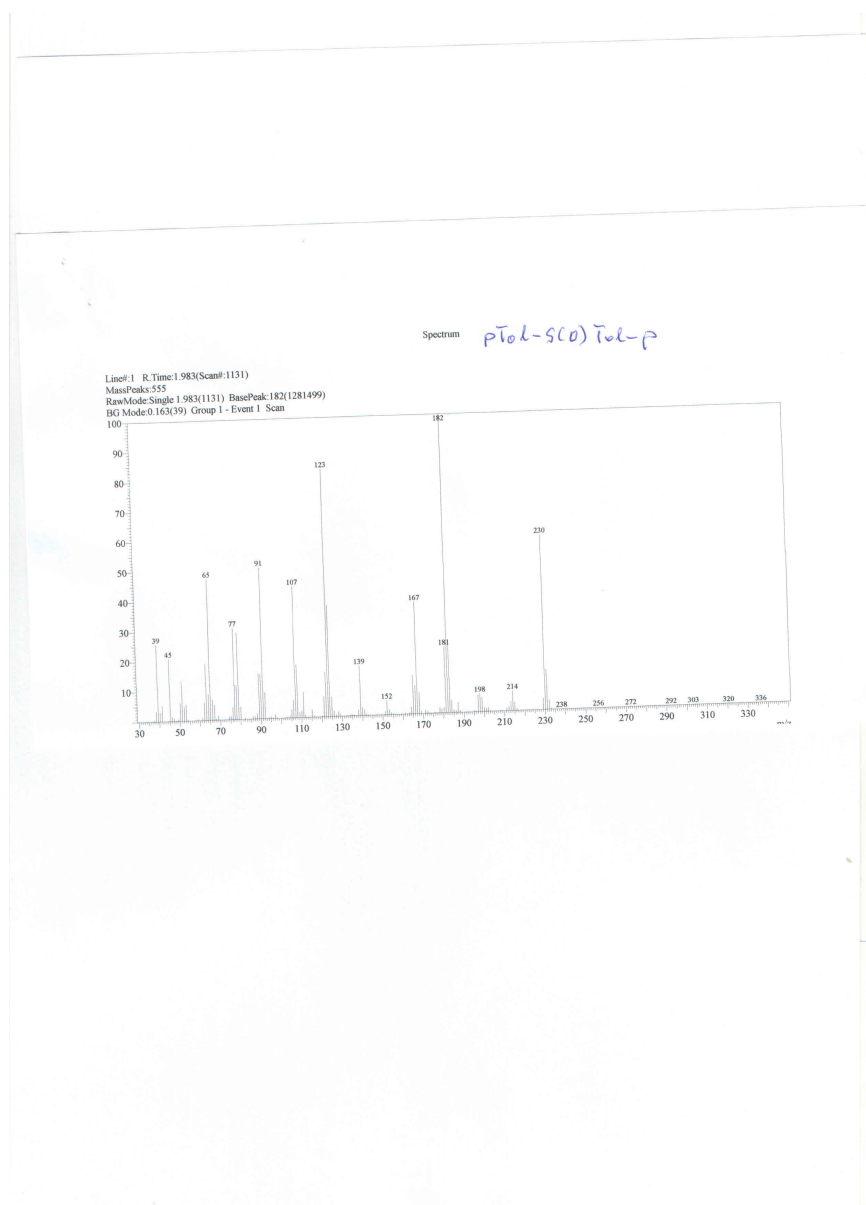


Figure 9S. Mass Spectrum of di-p-tolylsulfoxide