Supporting Information for:

Synthesis, crystallisation and thermodynamics of two polymorphs of a derivative of meglumine: 1-(2,2,3-trimethyl-1,3-oxazolidin-5-yl)-butane-1,2,3,4-tetrol

Michael Svärd,[a,b] Gamidi Rama Krishna,[a] and Åke C. Rasmuson[a,b]

[a] Synthesis and Solid State Pharmaceutical Centre, Department of Chemical and Environmental Science, Bernal Institute, University of Limerick, Castletroy, Ireland

[b] Department of Chemical Engineering, KTH Royal Institute of Technology, Stockholm, Sweden

Table S1. Hydrogen bond geometry of the crystal structures of FI and FII at 100 K.

Polymorph	**D–H···A**	**D···A (Å)**	**H···A (Å)**	**D–H···A (°)**
FI	O1–H1···O3	2.7311(13)	1.91(2)	165(2)
	O2–H2A···O1	2.7481(13)	1.93(2)	166.7(18)
	O3–H3A···O4	2.7041(13)	1.91(2)	167(2)
	O4–H4A···O2	2.7133(13)	1.94(2)	159(2)
	C1–H1B···O5	3.3627(16)	2.434(17)	166.9(15)
	C3–H3···O1	2.9358(15)	2.551(18)	103.4(11)
	C4–H4···O2	2.9574(15)	2.582(17)	103.2(11)
FII	O1–H1···O4	2.7310(17)	1.91(2)	172(2)
	O2–H2···O1	2.9168(17)	2.58(3)	108(2)
	O2–H2···O5	2.8423(17)	2.10(3)	163(2)
	O3–H3···N1	2.8173(19)	2.02(2)	170(2)
	O4–H4···O2	2.6666(17)	1.80(3)	175(2)
	C2–H2A···O4	2.9815(18)	2.55(2)	106.3(14)
	C6–H6B···O1	3.247(2)	2.43	140

Table S2. Torsion angles of the crystal structures of FI and FII at 100 K.

Atoms				**Angle (°)**	
				FI	*FII*
O1	C1	C2	C3	58.1(1)	62.1(2)
O1	C1	C2	O2	-63.0(1)	-61.9(2)
C1	C2	C3	C4	-176.8(1)	157.2(1)
C1	C2	C3	O3	63.4(1)	38.0(2)
O2	C2	C3	C4	-58.2(1)	-77.3(1)
O2	C2	C3	O3	-177.89(9)	163.5(1)
C2	C3	C4	C5	174.4(1)	167.2(1)
C2	C3	C4	O4	-60.9(1)	-72.4(1)
O3	C3	C4	C5	-65.4(1)	-70.6(2)
O3	C3	C4	O4	59.4(1)	49.9(2)
C3	C4	C5	C6	-64.1(1)	-66.4(2)
C3	C4	C5	O5	178.72(9)	176.9(1)
O4	C4	C5	C6	171.8(1)	173.4(1)
O4	C4	C5	O5	54.6(1)	56.7(2)
C4	C5	C6	N1	-143.1(1)	-142.4(1)
O5	C5	C6	N1	-22.6(1)	-22.6(1)
C4	C5	O5	C7	120.8(1)	121.3(1)
C6	C5	O5	C7	-1.2(1)	-0.7(2)
C5	C6	N1	C7	38.1(1)	37.4(1)
C5	C6	N1	C8	166.7(1)	163.3(1)
C9	C7	N1	C6	-154.0(1)	-152.6(1)
C9	C7	N1	C8	78.8(1)	83.4(2)
C10	C7	N1	C6	78.0(1)	80.2(2)
C10	C7	N1	C8	-49.3(2)	-43.8(2)
O5	C7	N1	C6	-39.3(1)	-38.0(1)
O5	C7	N1	C8	-166.6(1)	-162.0(1)
C9	C7	O5	C5	141.0(1)	140.5(1)
C10	C7	O5	C5	-98.0(1)	-98.7(1)
N1	C7	O5	C5	24.4(1)	23.6(1)
O1	C1	C2	C3	58.1(1)	62.1(2)

Table S3. Selected experimental heat capacity data values for FI and FII and the melt at 0.1 MPa. Standard uncertainties: $u(T) = 0.10$ K, $u(C_p^{FI}) = 10$ J K^{-1} mol^{-1}, $u(C_p^{FII,L}) = 8$ J K^{-1} mol^{-1}.

Solid phases			*Melt*	
T / K	C_p^{FI} / J·K^{-1}·mol^{-1}	C_p^{FII} / J·K^{-1}·mol^{-1}	T / K	C_p^{L} / J·K^{-1}·mol^{-1}
275.0		317	365.0	570
280.0	313	322	370.0	571
285.0	318	327	375.0	573
290.0	323	332	380.0	574
295.0	328	337	385.0	576
300.0	334	342	390.0	577
305.0	339	347	395.0	579
310.0	344	352	400.0	582
315.0	349	357	405.0	583
320.0	354	362	410.0	585
325.0	360	367	413.0	585
330.0	365	373		
335.0	370	378		
340.0	375	383		
345.0	381	388		
350.0	386	393		
355.0	391	399		
360.0	397	405		
365.0	402	411		
370.0	407	418		
375.0	413			
379.0	418			

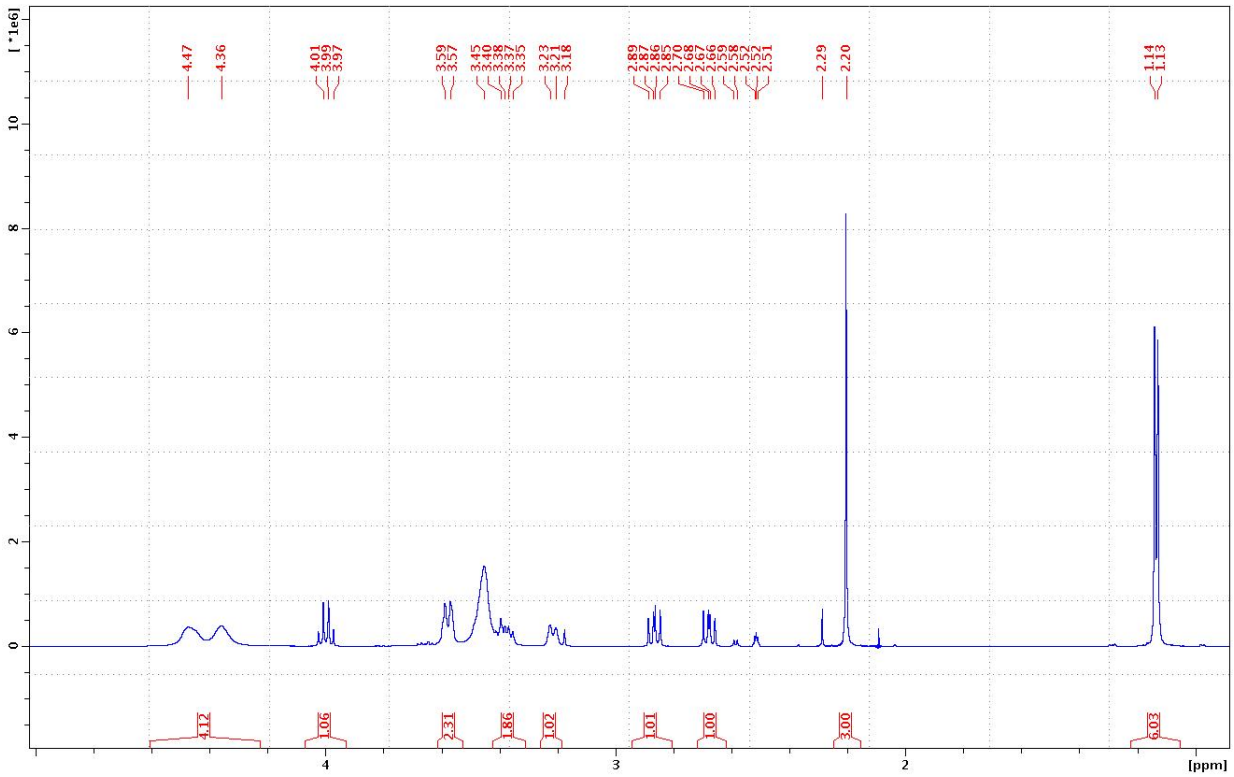

Figure S1. ^{1}H-NMR spectra of the title compound, collected in DMSO-d_6 solvent.

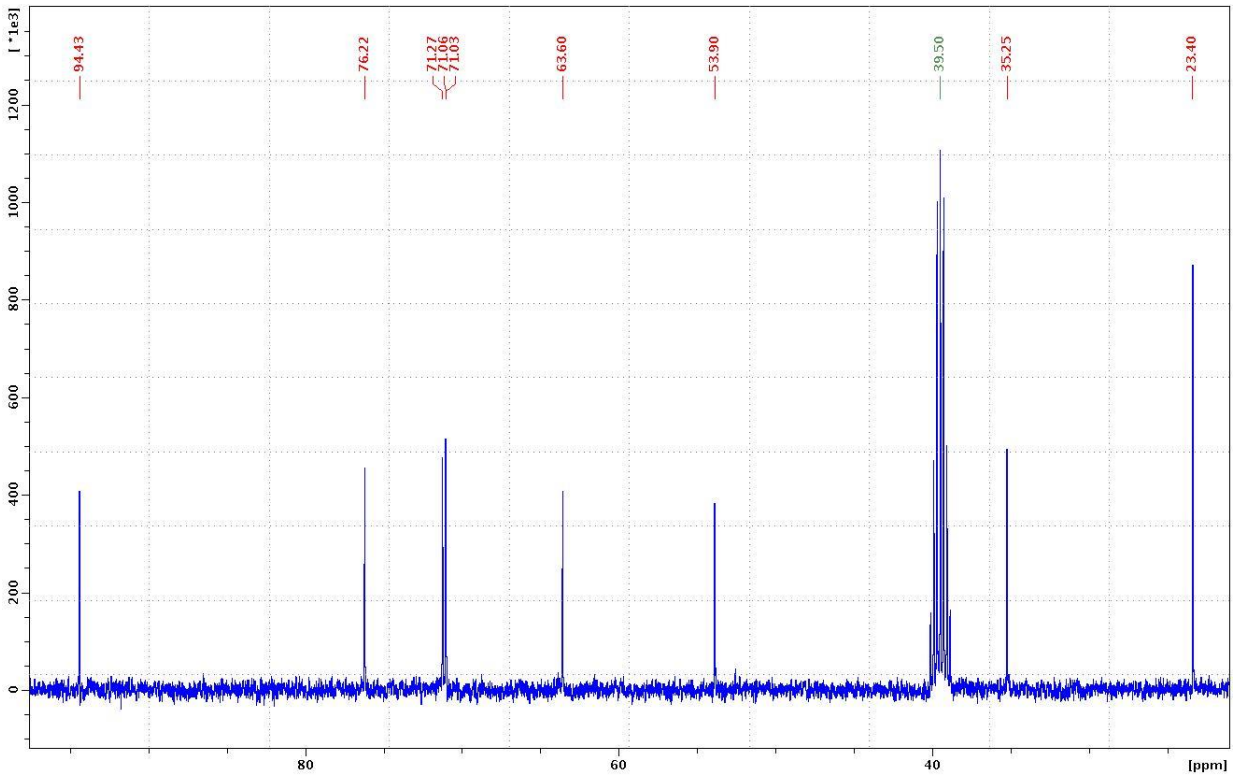

Figure S2. ^{13}C-NMR spectra of the title compound, collected in DMSO-d_6 solvent.

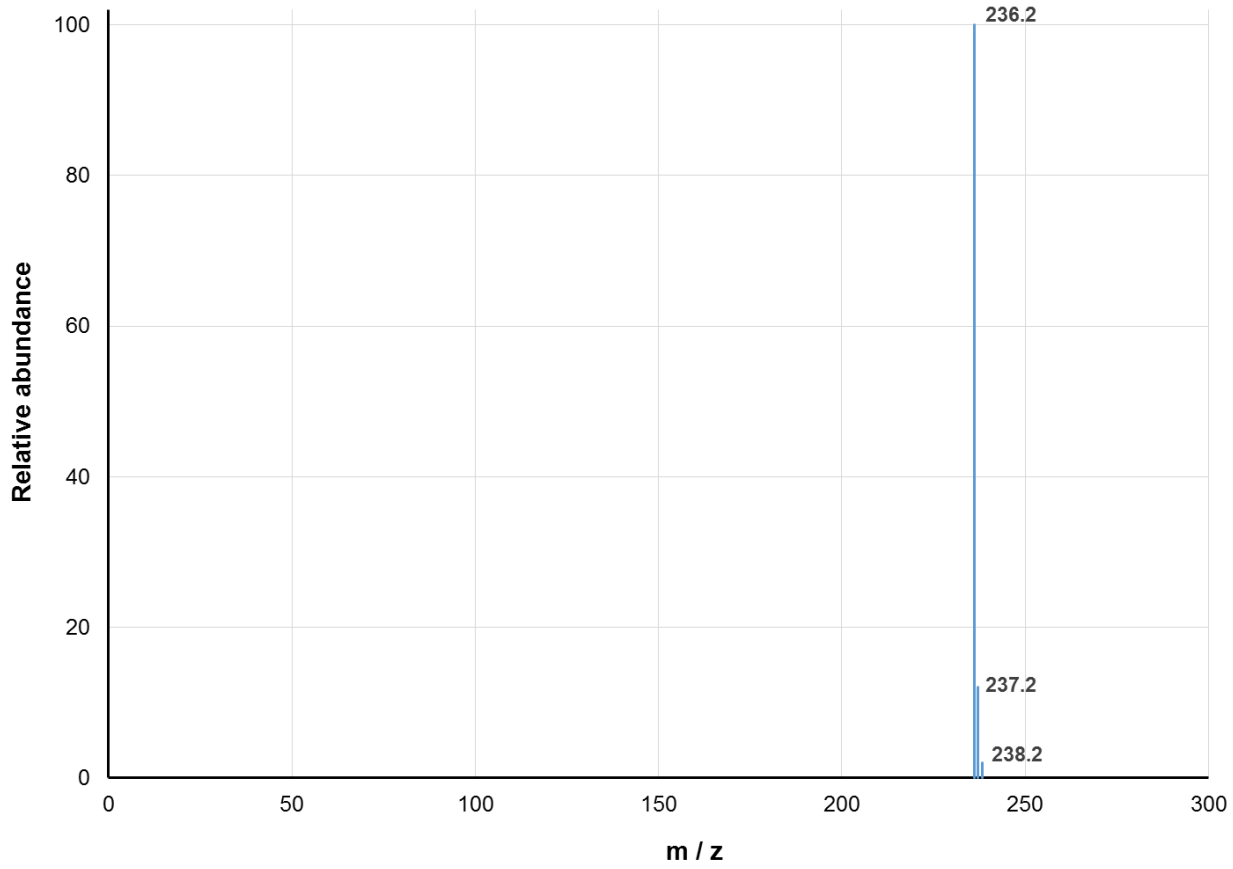

Figure S3. LC-MS of the title compound.