SUPPLEMENTARY MATERIAL

5-Methyl-4-thiazolidinones: Synthesis and evaluation as antitubercular agents

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Table S1. Crystal data and structure refinement for 2a and 2c.

Identification code	2a	2c
Empirical formula	$C_{16}H_{16}N_2OS$	$C_{17}H_{18}N_2OS$
Formula weight	284.37	298.39
Temperature/K	100	100
Crystal system	triclinic	orthorhombic
Space group	*P*-1	*P*ca2$_1$
a/Å	9.0795(3)	13.7180(4)
b/Å	12.5706(4)	15.1096(5)
c/Å	13.6556(4)	7.5723(2)
α/°	99.650(2)	90
β/°	108.571(2)	90
γ/°	101.952(2)	90
Volume/Å^3	1398.79(8)	1569.54(8)
Z	4	4
ρ_{calc}g/cm^3	1.350	1.263
μ/mm^{-1}	2.021	1.825
F(000)	600.0	632.0
Crystal size/mm^3	0.35 × 0.25 × 0.11	0.46 × 0.16 × 0.06
Radiation	CuKα (λ = 1.54186)	CuKα (λ = 1.54186)
2Θ range for data collection/°	7.056 to 143.558	5.85 to 143.66
Index ranges	-11 ≤ h ≤ 7, -11 ≤ k ≤ 15, -16 ≤ l ≤ 16	-15 ≤ h ≤ 16, -18 ≤ k ≤ 17, -5 ≤ l ≤ 9
Reflections collected	24198	29208
Independent reflections	5223 [R_{int} = 0.0151, R_{sigma} = 0.0111]	2380 [R_{int} = 0.0263, R_{sigma} = 0.0133]
Data/restraints/parameters	5223/0/371	2380/1/192
Goodness-of-fit on F^2	1.056	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.1086	R_1 = 0.0317, wR_2 = 0.0865
Final R indexes [all data]	R_1 = 0.0461, wR_2 = 0.1094	R_1 = 0.0323, wR_2 = 0.0868
Largest diff. peak/hole / e Å^{-3}	0.93/-0.37	0.35/-0.33
Flack parameter	-	-0.02(2)

Table S2. Bond lengths for 2a and 2c.

2a						2c		
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
S1	C1	1.824(2)	S2	C17	1.840(2)	S1	C1	1.823(3)
S1	C10	1.829(2)	S2	C26	1.830(2)	S1	C10	1.833(3)
O1	C2	1.213(2)	O2	C18	1.211(3)	O1	C2	1.228(3)
N1	N2	1.393(2)	N3	N4	1.390(2)	N1	N2	1.400(3)
N1	C2	1.352(3)	N3	C18	1.355(3)	N1	C2	1.348(3)
N1	C10	1.466(3)	N3	C26	1.465(2)	N1	C10	1.460(3)
N2	C4	1.409(3)	N4	C20	1.405(3)	N2	C4	1.420(3)
C1	C2	1.514(3)	C17	C18	1.511(3)	C1	C2	1.512(4)
C1	C3	1.512(3)	C17	C19	1.510(3)	C1	C3	1.522(4)
C4	C5	1.393(3)	C20	C21	1.390(3)	C4	C5	1.392(3)
C4	C9	1.389(3)	C20	C25	1.394(3)	C4	C9	1.394(3)
C5	C6	1.381(3)	C21	C22	1.391(3)	C5	C6	1.387(4)
C6	C7	1.385(3)	C22	C23	1.382(3)	C6	C7	1.389(4)
C7	C8	1.385(3)	C23	C24	1.388(3)	C7	C8	1.391(4)
C8	C9	1.389(3)	C24	C25	1.376(3)	C8	C9	1.381(3)
C10	C11	1.517(3)	C26	C27	1.519(3)	C10	C11	1.504(4)
C11	C12	1.386(3)	C27	C28	1.385(3)	C11	C12	1.394(3)
C11	C16	1.390(3)	C27	C32	1.390(3)	C11	C16	1.382(3)
C12	C13	1.382(3)	C28	C29	1.384(3)	C12	C13	1.381(4)
C13	C14	1.379(3)	C29	C30	1.389(3)	C13	C14	1.393(4)
C14	C15	1.382(3)	C30	C31	1.387(3)	C14	C15	1.386(4)
C15	C16	1.398(3)	C31	C32	1.386(3)			

Table S3. Bond angles for 2a and 2c.

2a				2c			
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C1	S1	C10	94.31(9)	C1	S1	C10	94.48(11)
N2	N1	C10	117.87(16)	N2	N1	C10	117.15(19)
C2	N1	N2	119.68(16)	C2	N1	N2	122.08(19)
C2	N1	C10	120.20(16)	C2	N1	C10	120.2(2)
N1	N2	C4	117.55(17)	N1	N2	C4	116.5(2)
C2	C1	S1	106.65(14)	C2	C1	S1	105.33(18)
C3	C1	S1	111.35(15)	C2	C1	C3	112.4(2)
C3	C1	C2	111.47(17)	C3	C1	S1	111.84(18)
O1	C2	N1	124.37(18)	O1	C2	N1	123.0(2)
O1	C2	C1	123.28(18)	O1	C2	C1	123.7(2)
N1	C2	C1	112.31(17)	N1	C2	C1	113.3(2)
C5	C4	N2	117.23(19)	C5	C4	N2	122.4(2)
C9	C4	N2	122.93(18)	C5	C4	C9	119.9(2)
C9	C4	C5	119.71(19)	C9	C4	N2	117.5(2)
C6	C5	C4	120.2(2)	C6	C5	C4	119.7(2)
C5	C6	C7	120.4(2)	C5	C6	C7	120.5(2)
C6	C7	C8	119.4(2)	C6	C7	C8	119.4(2)
C7	C8	C9	120.7(2)	C9	C8	C7	120.5(2)
C4	C9	C8	119.54(19)	C8	C9	C4	119.9(2)
N1	C10	S1	103.58(13)	N1	C10	S1	103.61(17)
N1	C10	C11	113.45(16)	N1	C10	C11	114.4(2)
C11	C10	S1	113.23(14)	C11	C10	S1	110.22(16)
C12	C11	C10	122.78(18)	C12	C11	C10	121.0(2)
C12	C11	C16	119.19(19)	C16	C11	C10	120.1(2)
C16	C11	C10	118.02(19)	C16	C11	C12	118.8(2)
C13	C12	C11	120.5(2)	C13	C12	C11	120.1(2)

C14	C13	C12	120.2(2)	C12	C13	C14	121.7(2)
C13	C14	C15	120.4(2)	C13	C14	C17	121.2(2)
C14	C15	C16	119.4(2)	C15	C14	C13	117.6(2)
C11	C16	C15	120.3(2)	C15	C14	C17	121.2(2)
C26	S2	C17	95.31(9)	C14	C15	C16	121.1(2)
N4	N3	C26	119.10(16)	C11	C16	C15	120.6(2)
C18	N3	N4	119.00(16)				
C18	N3	C26	121.46(16)				
N3	N4	C20	118.91(16)				
C18	C17	S2	106.27(15)				
C19	C17	S2	112.25(16)				
C19	C17	C18	110.97(19)				
O2	C18	N3	124.92(19)				
O2	C18	C17	122.13(19)				
N3	C18	C17	112.95(18)				
C21	C20	N4	123.42(18)				
C21	C20	C25	119.53(18)				
C25	C20	N4	116.98(18)				
C20	C21	C22	119.43(19)				
C23	C22	C21	121.1(2)				
C22	C23	C24	119.0(2)				
C25	C24	C23	120.7(2)				
C24	C25	C20	120.2(2)				
N3	C26	S2	103.99(13)				
N3	C26	C27	111.97(16)				
C27	C26	S2	115.49(14)				
C28	C27	C26	118.40(18)				
C28	C27	C32	119.34(19)				
C32	C27	C26	122.10(18)				
C29	C28	C27	120.7(2)				
C28	C29	C30	119.7(2)				
C31	C30	C29	119.9(2)				
C32	C31	C30	120.1(2)				
C31	C32	C27	120.2(2)				

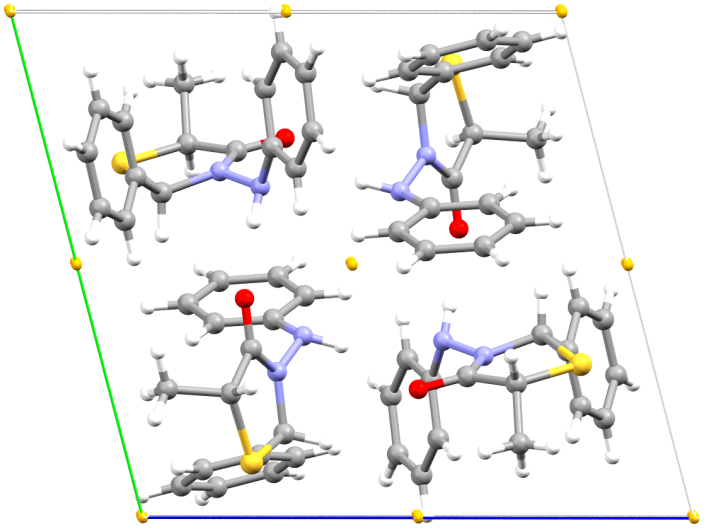

Figure S1. The crystal packing of **2a** with drawing centres of symmetry (yellow points).

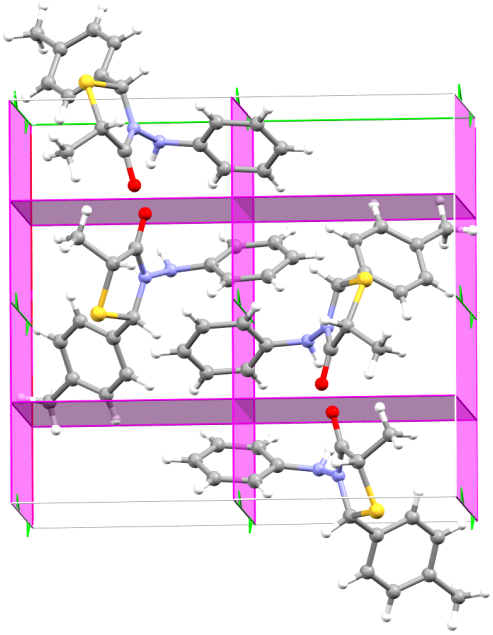

Figure S2. The crystal packing of **2c** with drawing glides plane (violet places) and 2-fold screw axes (green lines).