Supplementary Materials: Synthesis, Biological Evaluation and Molecular Docking of Certain Sulfones as Potential Nonazole Antifungal Agents

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X-ray crystallographic analysis: Crystal of compound **3** was obtained by slow evaporation from solution of ethanol/DMF. The measurements of the crystal were performed on a Bruker SMART APEX II D8 Venture diffractometer with graphite-monochromated Cu *Kα* radiation (*λ* = 1.54178 Å) at 293 K. The structure was solved by direct method and refined with SHELXTL. E-maps provided the positions of all the non-H-atoms. The full-matrix least-squares refinement was carried out on $F^{2\prime}$s using anisotropic temperature factors for all non-*H*-atoms. Crystallographic data for the structure reported in this paper have been deposited at the Cambridge Crystallographic Data Center and allocated with the deposition number: CCDC 1430111.

Table S1. Crystallographic data and refinements for compound **3**.

Crystal data	
$C_{14}H_{11}ClO_3S$	V = 1292.27 (8) Å^3
M_r = 294.74	Z = 4
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation
a = 5.7258 (2) Å	μ = 4.14 mm^{-1}
b = 9.1203 (4) Å	T = 293 K
c = 25.0426 (8) Å	0.50 × 0.11 × 0.07 mm
β = 98.824 (3)°	F(000) = 608
Data collection	
CCD area detector diffractometer	R_{int} = 0.104
7841 measured reflections	θ_{max} = 62.5°
2021 independent reflections	775 reflections with $I > 2\sigma(I)$
Refinement	
$R[F^2 > 2\sigma(F^2)]$ = 0.103	0 restraints
$wR(F^2)$ = 0.311	H atoms treated by a mixture of independent and constrained refinement
S = 0.92	$w = 1/[\sigma^2(F_o^2) + (0.1895P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2021 reflections	$\Delta\rho_{max}$ = 0.49 e·Å^{-3}
173 parameters	$\Delta\rho_{min}$ = −0.58 e·Å^{-3}

The crystallographic structure of **3** is represented in Figure 2. The single crystal X-ray study on this derivative unambiguously defines the exact structure. Crystal packing of **3** which showed the intermolecular hydrogen bond C10—H10A···O_2 is presented in Figure 3. The crystallographic data and refinement for the crystal was presented in Table S1. Selected geometric parameters of compound **3** presented in Table S2 (Supplementary Materials). Hydrogen-bond geometry of **3** is illustrated in Table S3.

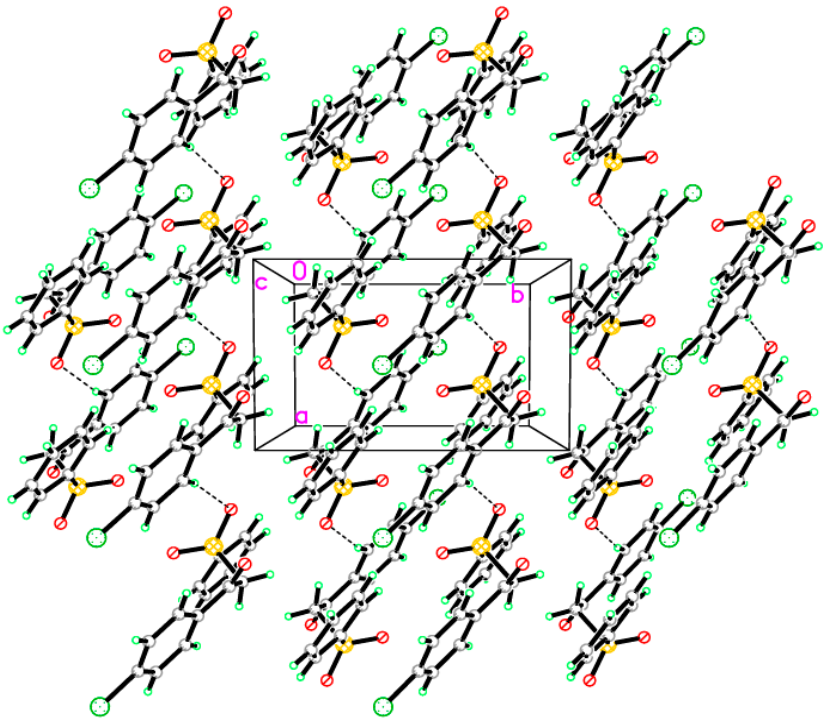

Figure S1. Crystal packing of **3** showing intermolecular hydrogen bonds as dashed lines.

Table S2. Selected geometric parameters (Å, °) for compound **3**.

Bond distance			
Cl1—C12	1.738 (9)	S1—C6	1.753 (8)
S1—O1	1.416 (5)	S1—C7	1.767 (8)
S1—O2	1.446 (7)	O3—C8	1.218 (11)
Bond angle			
O1—S1—O2	118.7 (3)	S1—C6—C5	120.5 (7)
O1—S1—C6	109.5 (3)	S1—C7—C8	110.3 (6)
O1—S1—C7	107.3 (3)	O3—C8—C7	117.4 (7)
O2—S1—C6	108.7 (4)	O3—C8—C9	122.7 (7)
O2—S1—C7	107.7 (3)	Cl1—C12—C11	119.9 (7)
C6—S1—C7	103.9 (4)	Cl1—C12—C13	118.6 (7)
S1—C6—C1	118.9 (6)		

Table S3. Hydrogen-bond geometry (Å, °) of **3**.

D—H···*A*	*D*—H	*H*···*A*	*D*···*A*	*D*—H···*A*
C10—H10A···O2 ^{i}	0.9300	2.5000	3.403 (10)	163.00

Symmetry codes: (i) $x + 1, y, z$.