

Synthesis, single crystal X-ray analysis and antifungal profiling of certain new oximino ethers bearing imidazole nuclei

Reem I. Al-Wabli^{1*}, Alwah R. Al-Ghamdi¹, Hazem A. Ghabbour^{1,2}, Mohamed H. Al-Agamy^{3,4} and Mohamed I. Attia^{1,5*}

¹Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, P.O. Box 2457, Riyadh 11451, Saudi Arabia

²Department of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt

³Department of Pharmaceutics, College of Pharmacy, King Saud University, P.O. Box 2457, Riyadh 11451,

Saudi Arabia; malagamy@ksu.edu.sa

⁴Microbiology and Immunology Department, Faculty of Pharmacy, Al-Azhar University, Cairo 11884, Egypt

⁵Medicinal and Pharmaceutical Chemistry Department, Pharmaceutical and Drug Industries Research Division, National Research Centre (ID: 60014618), El Bohooth Street, Dokki, Giza 12622, Egypt

Table S1. The X-ray experimental details of compound **Vi**.

Crystal data	
Chemical formula	C ₂₀ H ₁₈ BrN ₃ O ₃
Mr	428.28
Crystal system, space group	Monoclinic, P2 ₁ /c
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	18.7879 (14), 5.8944 (4), 16.7621 (12)
β (°)	91.632 (2)
V (Å ³)	1855.5 (2)
Z	4
Radiation type	Mo Kα
μ (mm ⁻¹)	2.24
Crystal size (mm)	0.33 × 0.28 × 0.08
Data collection	
Diffractometer	Bruker APEX-II D8 venture diffractometer
Absorption correction	Multi-scan,SADABS Bruker 2014
Tmin, Tmax	0.528, 0.846
No. of measured, independent and observed [$\text{I} \geq 2\sigma(\text{I})$] reflections	35254, 3848, 2376
R _{int}	0.136
Refinement	
R[F ² > 2σ(F ²)], wR(F ²), S	0.048, 0.111, 1.02
No. of reflections	3848
No. of parameters	244
No. of restraints	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
ΔQ _{max} , ΔQ _{min} (e Å ⁻³)	0.37, -0.43