Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Supplementary Information

Discovery of Highly Potent Antifungal Triazoles by Structure-based Lead Fusion

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Table 1. Comparison of Physicochemical Properties of Compound 10a and Azole Antifungal Agents[a,b]

compounds	AlogP	MW	HBA	HBD	Num-Rot bond	Molecular-Surface	PSA
10a	2.699	428.48	5	1	8	403.22	63.41
Fluconazole	0.75	306.27	5	1	5	283.02	81.65
Itraconazole	6.057	691.61	9	0	11	629.22	100.79
Posaconazole	5.096	700.78	9	1	12	649.42	111.79
Voriconazole	2.071	349.31	5	1	5	320.89	76.72

[a] The physicochemical properties of the compounds were calculated by Discovery Studio 2.5 software package; [b] Abbreviations: MW = Molecular Weight; HBA = Hydrogen Bond Acceptor; HBD = Hydrogen Bond Donor; Num-Rot bond = Number of Rotatable Bonds; PSA = Polar Surface Area