

arrangement.

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Keywords: cocrystal, incommensurate modulated structure

FA4-MS26-P20

Fluconazole and its cocrystals with maleic and glutaric acids. Ivan Leban^a, Nina Lah^a, Žiga Hodnik^b, Danijel Kikelj^b, Jože Kastelic^c, ^a*Faculty of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5, SI-1000 Ljubljana, Slovenia*, ^b*Faculty of Pharmacy, University of Ljubljana, Aškerčeva 7, SI-1000 Ljubljana, Slovenia*, ^c*Krka, d. d., Novo mesto, Šmarješka c. 6, SI-8501 Novo mesto, Slovenia*.
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Fluconazole (2-(2,4-difluorophenyl)-1,3-bis(1H-1,2,4-triazol-1-yl)propan-2-ol), is a bis-triazole antifungal drug used to treat invasive infections caused by *Candida*. The drug is available in both oral and intravenous formulations. The crystal structures of three unsolvated forms, designated as polymorph I, II and III, as well as the structures of a monohydrate and the solvates containing ethyl acetate, acetone and benzene have already been reported [1],[2]. Here, the single-crystal X-ray structures of fluconazole (form III) and its cocrystals containing maleic and glutaric acids will be presented.

Fluconazole (III): triclinic, P-1, a=7.4907(10), b=7.7640(10), c=11.9547(10) Å, α=85.012(8), β=84.507(8), γ=75.553(8)°.

Fluconazole with maleic acid: [(FluH₂)(Hmal)₂(H₂mal)], triclinic, P-1, a=5.4983(5), b=13.8723(16), c=18.433(3) Å, α=98.062(8), β=91.748(8), γ=95.479(8)°.

Fluconazole with glutaric acid: [(Flu)(H₂glu)], triclinic, P -1, a=5.6897(10), b=10.6593(15), c=17.063(3) Å, α=72.909(8), β=84.453 (8), γ=80.863(8)°.

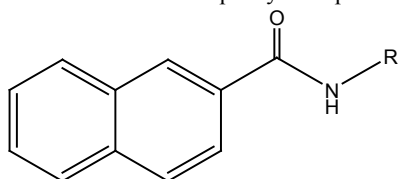
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Keywords: fluconazole, maleic acid, glutaric acid

FA4-MS26-P21

Crystal packing in a series of N-phenyl-2-naphthamide derivatives. Jim Simpson^a, Aamer Saeed^b, Rasheed Ahmad Khera^b, ^a*Department of Chemistry, University of Otago, P.O. Box 56, Dunedin, 9054, New Zealand*, ^b*Department of Chemistry, Quaid-I-Azam University, Islamabad 45320, Pakistan*

Structures of seven N-phenyl-2-naphthamide derivatives



R = C₆H₅—, *p*-Cl—C₆H₄, *p*-CH₃—C₆H₄, *m* and *p*-CH₃O—C₆H₄, *o*-NO₂—C₆H₄ and C₆H₁₀ have been determined and their crystal packing investigated. The pervasive intramolecular contact in all but one of the compounds involves classical N—H...O hydrogen bonding leading to the formation of C(4) chains [1]. The exception is the nitro derivative where a strong intramolecular N—H...O contact to an O atom of the *o*-NO₂ substituent takes precedence. Additional C_{aromatic}—H...O contacts support the formation of chains in some molecules with additional C_{methyl}—H...O interactions in the methoxy derivatives. C—H...π interactions occur in the majority of compounds but surprisingly, despite the presence of the planar naphthyl synthon, significant π...π stacking interactions are observed only for the nitro-derivative.

[1] Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. *Angew. Chem.Int. Ed. Engl.* 1995, 34, 1555--1573.

Keywords: N-phenyl-naphthamides, structure, packing

FA4-MS26-P22

Highly Interpenetrated Organic Networks formed by Halogen Bonding Giancarlo Terraneo^{a,b}, Gabriella Cavallo^a, Pierangelo Metrangolo^{a,b}, Tullio Pilati^c, Giuseppe Resnati^{a,b,c}, ^a*NFMLab - D.C.M.I.C. "Giulio Natta", Politecnico di Milano, Via L. Mancinelli 7, 20131 Milan, Italy*, ^b*CNST - IIT@POLIMI, Politecnico di Milano, Via G. Pascoli 70/3, 20133 Milan, Italy*, ^c*C.N.R. - I.S.T.M., University of Milan, Via C. Golgi 19, 20133 Milan, Italy*

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Halogen bonding (XB) [1], namely the noncovalent interactions wherein halogen atoms function as electrophilic species, can be described by the general scheme D...X-Y where X is the electrophilic halogen atom (Lewis acid, XB-donor), D is a neutral or anionic donor of electron density (Lewis base, XB-acceptor), and Y is carbon, nitrogen, halogen, etc. Recently, XB has proven its efficiency and reliability in the design and construction of self-assembled systems with quite different architectures and properties [2]. New aggregation processes can be realised, the novelty coming from either the molecular identity of assembled modules or from the way the modules are arranged in the supramolecular architecture. In this communication we describe the deliberate construction of highly interpenetrated organic networks. The focus will be on tetradentate tectons. In particular, we will show that DAB-*dendr*-(NHC₆F₄I)₂ self-assembles with (*E*)-1,2-bis-(4-pyridyl)-ethylene thanks to multiple N...I interactions that drive the formation of a supramolecular architecture composed of 2D square networks with a mode of interpenetration of class Ia. We will show that not only tetradentate XB-donor tectons, but also tetradentate XB-acceptors (*e.g.* tetrapyridyl pentaerythritol or cyclobutane derivatives) give rise to highly interpenetrated organic networks (Figure) [3].