MS73.P21

Acta Cryst. (2011) A**67,** C669

Crystal Structure of N-(4-heptylphenyl)acetamide

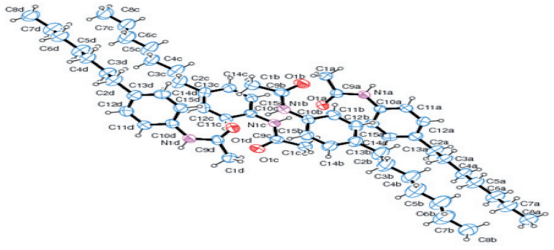
Jeyaseelan, S,[a] Vinduvahini, M,[b] and Devarajegowda, H. C,[a] *[a]Department of Physics, Yuvaraja's College (Constituent College), University of Mysore, Mysore-570005, Karnataka, (India). [b]Department of Physics, Sri D. Devaraja Urs Govt. First Grade College, Hunsur-571105, Mysore District, Karnataka, (India).* E-mail: seelansjey@yahoo.in

The crystal structure of the title compound, N-(4-heptylphenyl)acetamide ($C_{15}H_{23}NO$), is determined by X-ray diffraction method and crystallizes in the Triclinic space group *P-1* with cell parameters a = 9.5432(4)Å, b = 17.3533(7)Å, c = 18.8570(7)Å, V = 2892.6(2)Å^3, Z = 8, D_{calc} = 1.072mg/m^3, μ = 0.066mm^{-1}, F_{000}=1024, λ(Mok$_\alpha$) = 0.71073Å and the structure was refined to R = 0.0684.

The structure contains four independent molecules (A & C and B & D) linked by a strong N---H...O hydrogen bond. The aromatic rings and alkyl chains of each molecule are non coplanar; the dihedral angles between phenyl rings and alkyl chains of molecules A, B, C & D are 64.10(3)Å, 30.5(5)Å, 27.8(4)Å & 73.4(3)Å respectively. The molecular assembly in the structure is established by an intramolecular N---H...O & C---H...O, intermolecular N---H...O hydrogen bonds and as well as C---H....π-electron ring C_g(3) [C10D-C15D] interactions. Intermolecular N---H...O hydrogen bonds involving different types of molecules generate an infinite ACAC...and BDBD ... chain running parallel to the [100] direction and packing of the molecules show the stacking when viewed along *a*.

Small biological molecules like amino acids, DNA bases or drug related molecules have been extensively studied for physisorption on electronically conducting surfaces. 4-acetaminophenol is a common antipyretic and analgesic drug used for the treatment of headaches and fever. In this molecule the 4-acetyl-amine group in *para* position to the phenol functionality owing to such remarkable biological activity.

The dihedral angles between the independent one pair of molecules with another pair molecules are 61.5(2) Å and 64.0(2) Å and heptylphenyl and acetamide groups of the molecules A, B, C and D are 16.32(15)Å, 15.78(15)Å, 15.30(15)Å and 6.14(16)Å respectively.



[1] J.J. Benattar, A.M. Levelut, E.L. Strzelecki, *J. de. Physique*, **1978,** *39*, 1233-1240. [2] Bruker. *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA, **2001**. [3] L.J. Farrugia, *J. Appl. Cryst*. **1997**, *30*, 565. [4] L.Z. Gandel'sman, S.V. Shelyazhenko, L. Nechitailo, [5] G.M. Sheldrick, *Acta Cryst. A.* **2008,** *64,* 112-122.

Keywords: Crystal, Hydrogenbond, diffractometer

MS73.P22

Acta Cryst. (2011) A**67,** C669

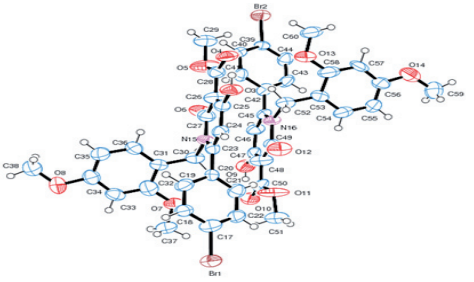
X-ray structure of poly substituted 1,2-dihydropyridine derivative

Vinduvahini, M,[a] Jeyaseelan, S,[b] and Devarajegowda, H. C,[b] *[a]Department of Physics, Sri D D Urs Govt. First Grade College, Hunsur, Mysore, Karnataka, [b]Department of Physics, Yuvaraja's College, University of Mysore, Mysore, Karnataka, (India).* E-mail: vinduvaninim@yahoo.in

The crystal structure of the title derivative, methyl 6-(4-bromophenyl)-1-(2,4-dimethoxybenzyl)-4-hydroxy-2-oxo-1,2-dihydropyridine-3-carboxylate ($C_{22}H_{20}NO_6Br$) is determined by X-ray diffraction method and crystallizes in the Orthorhombic space group *Pca21* with cell parameters a = 16.1028(12) Å, b = 9.7450(7)Å, c = 27.0253(14)Å, V = 4240.9(5)Å^3, Z = 8, D_{calc} = 1.486mg/m^3, μ = 1.977mm^{-1}, F_{000}=1936, λ(Mok$_\alpha$) = 0.71073 Å and the structure was refined to R = 0.0622.

Polysubstituted pyridines represent molecular frameworks that serve as a platform for developing pharmaceutical agents for various applications. They show modulating activity on cardiovascular and neuronal processes and on corticosteroid regulatory circuits and prevent inflammatory and diabetic processes and some show antineoplastic , geroprotective, radioprotective and radiosensitizing effects.

The structure of methyl 6-(4-bromophenyl)-1-(2,4-dimethoxybenzyl)-4-hydroxy-2-oxo-1,2-dihydropyridine-3-carboxylate contains two independent molecules in the asymmetric unit. The aromatic rings and pyridine ring systems are non coplanar with one another. The Pyridine ring makes dihedral angles of 71.3(4)Å and 85.2(4)Å respectively with the two aromatic ring systems. The structure of the molecules is stabilized by intermolecular C--H...O and intramolecular C--H...O & O--H...O hydrogen bonds.



[1] J. Briede, K. Heidemanis, I. Dabina, G. Duburs, *Cell Biochem. Funct.* **2002,** *20*, 177–181. [2] J. Briede, D. Daija, E. Bisenieks, N. Makarova, J. Uldrikis, J. Poikans, G. Duburs, *Cell Biochem. Funct.* **1999,** *17*, 97–105. [3]. L.J. Farrugia, *J. Appl. Cryst*. **1997,** *30*, 565. [4] A. Klegeris, E. Liutkevicius, G. Mikalauskiene, G. Duburs, P.L. McGeer, V. Klusa *Eur. J. Pharmacol.* **2002,** *441*, 203–208. [5] E. Liutkevicius, A. Ulinskaite, R. Meskys, K. Kraujelis, G. Duburs, V. Klusa, *Biomed. Lett.* **1999,** *60*, 39–46. [6] I. Misane, V. Klusa, M. Dambrova, S. Germane, G. Duburs, E. Bisenieks, R. Rimondini, S.O. O¨gren, *Eur. Neuropsychopharmacol*. **1998,** *8*, 329–347. [7]. G.M. Sheldrick, *Acta Cryst. A* **2008,** *64,* 112-122.

Keywords: Crystal, Intermolecular, Diffractometer

MS73.P23

Acta Cryst. (2011) A**67,** C669-C670

Conformational adaptations of a versatile podand

I. Đilović, K. Užarević , M. Cindrić, D. Matković-Čalogović, *Laboratory of General and Inorganic Chemistry, Chemistry Department, Faculty of Science and Mathematics, University of Zagreb, Zagreb, (Croatia).* E-mail: idilovic@chem.pmf.hr

Flexible anion receptors draw significant scientific attention in the last few decades [1]. Even though peak selectivity with flexible podands is not always accomplished, conformational adaptability of the host may be exploited for other purposes, such as sensor design or signal transduction [2]. Studies of spatial rearrangements of a host during interactions with a guest are important in crystal engineering for supramolecular template synthesis [3].