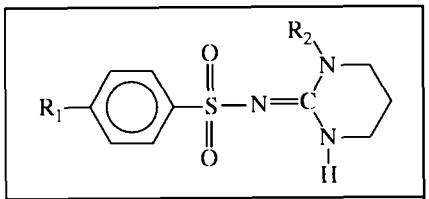
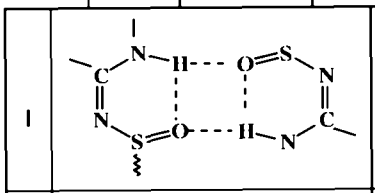
**s9.m1.p7** **The role of intra- and intermolecular hydrogen bonding in the crystal structure of arylsulfonyl- guanidine derivatives.** I. Dybala[1], A.E. Koziol[1], E. Szacoń[2], D. Matosiuk[2]. [1]*Dept. of Chemistry, Maria Curie-Sklodowska Univ., Lublin, Poland,* [2] *Dept. of Medicines Technology, Faculty of Pharmacy, Medical Univ., Lublin, Poland.*
Keywords: arylsulfonylguanidine, hydrogen bond, guanidine derivative.

Three structures of arylsulfonylguanidine derivatives (**I** *N*-aryl-; **II** and **III** *N*-alkyl-) have been determined by X-ray crystal structure analysis. The intramolecular N-H···O hydrogen bonding is observed in all molecules, while various substituents present in analysed compounds determine different types of intermolecular hydrogen bonds.



| | | |
|---|---|---|
| **I** | **-$CH_3$** | **-Ph** |
| ***II*** | **-Cl** | **-$CH_2CH_3$** |
| III | **-Cl** | **-$CH_2$Ph** |



| | | |
|---|---|---|
| I | | intramolecular N···O 2.836 Å ∠125° |
| II | | intramolecular N···O 2.766 Å ∠136° |
| III | | intramolecular N···O 2.799 Å ∠139° |

**I:** Molecules linked by the intermolecular N-H···O hydrogen bonds form dimers (N···O distance 2.942 Å).
**II:** The intramolecular N-H···O hydrogen bond closes a six-membered ring.
**III:** Molecules form chains by weak bifurcated N-H···O and N-H···N intermolecular hydrogen bonds (N···O and N···N distances are 3.282 and 3.408 Å, respectively).

Intermolecular interactions influence a conformation of the O2-S-N2-C2-N3 fragment and orientation of substituents at the N and S atoms.

**s9.m1.p8** **Inclusion crystals of finasteride.** I. Wawrzycka[a], A.E. Koziol[a], E. Cendrowska[b], [a]*Department of Chemistry, M. Curie-Sklodowska Univ. Lublin, Poland,* [b]*Department of Chemistry, A. Mickiewicz Univ. Poznan, Poland.*
Keywords: finasteride, steroids, inclusion crystals.

Finasteride [17β-(*N-tert*-butylcarbamoyl)-4-aza-5a-androst-1-en-3-one] is a modified steroid derivative. The ring A contains lactam group and the C17 atom is substituted with the *tert*-butylamide residue.

Finasteride crystallizes from ethanol[1] and DMSO solutions as the homomolecular crystal. It seems that the size of a solvent molecule has influence on form of inclusion crystals. The crystallization from other organic solvents gives isostructural clathrates (in the orthorhombic space group $P2_12_12_1$) with the bis-finasteride monohydrate unit as a host.

| | ***Solvent*** | **Unit cell dimensions [Å]** |
|---|---|---|
| 1 | ***ethyl acetate***[1] | ***a* = 8.173(3)** |
| | | *b* = 18.364(6) |
| | | *c* = 35.65(2) |
| 2 | ***toluene*** | ***a* = 8.138(2)** |
| | | *b* = 18.526(4) |
| | | *c* = 34.770(7) |
| 3 | ***2-butanol*** | ***a* = 8.113(2)** |
| | | *b* = 17.979(4) |
| | | *c* = 35.802(7) |
| 4 | ***2-propanol*** | ***a* = 8.162(5)** |
| | | *b* = 18.29(2) |
| | | *c* = 35.92(3) |
| 5 | ***butyl acetate*** | ***a* = 8.185(7)** |
| | | *b* = 18.33(3) |
| | | *c* = 35.82(3) |
| 6 | ***chloroform*** | ***a* = 8.167(2)** |
| | | *b* = 17.897(6) |
| | | *c* = 36.24(1) |

Structures of **2** and **3** have been determined by X-ray crystallography using data collected on a KM4CCD diffractometer at 130K. Unit cell dimensions for crystals of **3**, **4** and **5** were determined on a KM4 diffractometer.

In the crystal lattice, two symetrically independent finasteride molecules are linked by N–H···O hydrogen bonds between the lactam groups of the ring A. The water molecule is a double H-bond donor to the lactam O-atoms and an acceptor from the amide N-atom, which gives three-dimensional net with channels. The size of these channels is suitable for enclathration of solvent molecules, both polar and nonpolar.

[1] Wawrzycka I. *et al.* "Structural characterization of polymorphs and molecular complexes of finasteride." J. Mol. Struct. (1999) 474: 157 - 166.