s7.m24.p4 **Hydrophobic vs. hydrophilic: ionic competition in remacemide salt structures.** Gareth R. Lewis,[a] Gerry Steele,[a] Alastair J. Florence[b] and Norman Shankland[bc], [a]*AstraZeneca R&D Charnwood, Bakewell Road, Loughborough, Leicestershire LE11 5RH, UK,* [b]*Department of Pharmaceutical Sciences, University of Strathclyde, 27 Taylor Street, Glasgow G4 0NR, UK, and* [c]*CrystallografX Limited, 38 Queen Street, Glasgow G1 3DX, UK. E-mail: gareth.r.lewis@astrazeneca.com*

Keywords: Salt selection; Hydrogen bonding; π···π interactions

Remacemide [2-Amino-N-(1-methyl-1,12-diphenylethyl)-acetamide] was developed as a potential antagonist for epilepsy, Parkinsonism and Huntingon's disease. This paper reports the crystal structure of remacemide **1** and six of its salts [**2** = chloride; **3** = nitrate; **4** = acetate; **5** = hemi-fumarate ($C_4H_3O_4$-); **6** = naphthalene-2-sulphonate (napsilate, $C_{10}H_7O_3S^-$); **7** = 1-hydroxynaphthalene-2-carboxylate (xinafoate, $C_{11}H_7O_3$-)], and an investigation of which H-bond motifs and hydrophobic interactions recur across the structural series.

The salts **2-7** are polarised into hydrophobic and hydrophilic regions, giving bilayer structures. Within these segregated regions, a range of intermolecular interactions between hydrophilic and hydrophobic components is observed. The molecules occupying the hydrophilic regions of these structures form multiple H-bonds, with the charged NH_3^+ group in **2-7** being very aggressive in forming contacts from each of the three protons. The majority of the H-bonds are discrete interactions, as shown by Graph Set Analysis. As most hydrophilic regions form layers, where the individual H-bonds extend to give more complex patterns, these are shown to be chain and ring motifs. Very few intermolecular interactions between the phenyl interactions are identified between the aromatic rings which constitute the hydrophobic regions of the crystal structures, indicating that the observed crystal structures of **1-7** result from dominating H-bonds.

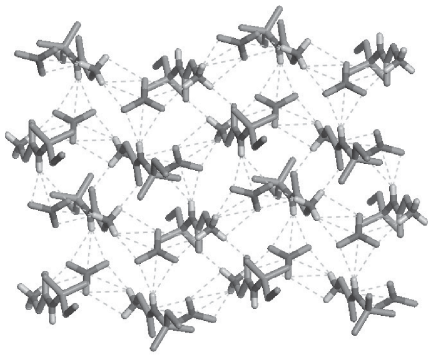

Figure. The network of H-bonds between remacemide cations and nitrate anions in the structure of **3**.

s7.m24.p5 **Structural analysis of a newly identified class of plant protective microbial glycoside hydrolase inhibitors.** S. Sansen[a], C. J. De Ranter[a], K. Gebruers[b], K. Brijs[b], C. M. Courtin[b], J. A. Delcour[b] and A. Rabijns[a], [a]*Laboratory of Analytical Chemistry and Medicinal Physicochemistry, K.U.Leuven, E. Van Evenstraat 4, B-3000 Leuven, Belgium,* [b]*Laboratory of Food Chemistry, K.U.Leuven, Kasteelpark Arenberg 20, B-3001 Leuven, Belgium. E-mail: Stefaan.Sansen@pharm.kuleuven.ac.be*

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Endo-β-1,4-xylanases (endoxylanases or xylanases, E.C. 3.2.1.8) from microbial, fungal or plant origin hydrolyse β-1,4-linkages between the D-xylosyl residues in (arabino)xylan, releasing xylo-oligosaccharides of different lengths [1]. In plants they are a key enzyme in the breakdown of the hemicellulose of the cell walls. Nowadays, microbial xylanases are frequently used to modify the functionality of (arabino)xylan in feed and food applications, such as bread-making [2] and gluten/starch separation [3], and in other applications, such as paper and pulp biobleaching [4]. In this context, an important recent development is the discovery of proteinaceous xylanase inhibitors in different cereals [5]. To date two different types have been identified, i.e. TAXI-type (*T. aestivum* xylanase inhibitor) [6] and XIP-type (xylanase inhibiting protein) [7] inhibitors, with clearly distinct xylanase specificities. The TAXI-type inhibitors have a molecular mass of approx. 40 kDa and a basic pI. Additional purification steps revealed two highly homologous TAXI-I and TAXI-II type inhibitors, with slight differences in pI (8.9 and 9.3, respectively) and xylanase specificity. While TAXI-I inhibition activity seems to be independent of the pH optima of xylanases, TAXI-II inhibition of xylanases with low pH optima is weak or absent [8]. On the other hand, XIP-type inhibitors with molecular masses of 29-32 kDa, inhibit both family 10 as well as family 11 xylanases, as long as they are of fungal origin [9]. Studies on the molecular identification, isolation and characterization of the TAXI-I gene, together with screening of the available wheat EST libraries, showed clear evidence that TAXIs belong to a newly identified class of plant proteins to which a function as plant protective microbial glycoside hydrolase inhibitor can be suggested [10]. In order to study this class of proteins, their inhibition mechanics and specificities, and their influence in the above mentioned industrial processes, a crystallographic study was undertaken. This poster describes the structure determination of TAXI-I, by means of the SAD approach, as well as the crystallographic study of TAXI-I in complex with *A. niger* xylanase.

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