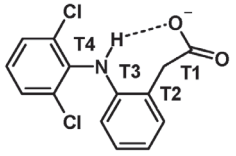
MS7-P7 **Conformation and hydrogen bonding in amine salts of diclofenac.** Carl H Schwalbe,[ab] Miren Ramirez,[a] Barbara R Conway,[c] Peter Timmins,[d] [a]*Aston University, Birmingham B4 7ET, UK,* [b]*Cambridge Crystallographic Data Centre, Cambridge CB2 1EZ, UK,* [c]*University of Huddersfield, Huddersfield HD1 3DH, UK,* [d]*Bristol-Myers Squibb, Moreton CH46 1QW, UK*
E-mail: carlschwalbe@hotmail.com



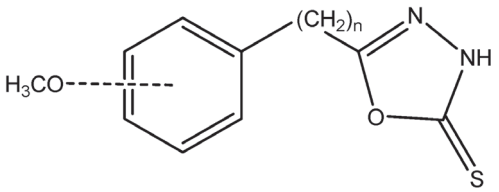
We have augmented the 15 structures in the CSD of amine salts of the anti-inflammatory drug diclofenac with 7 more [1]. Diclofenac is nonplanar, the conflict between steric hindrance and conjugation keeping torsion angle T4 46-69° from planarity. With a minimum magnitude of 154°, T3 shows less twisting between the NH bridge and the other aromatic ring. Both T2 and T1 prefer to be *gauche*, but T1 shows greater variation. Although the bridging NH does not benefit from charge assistance and torsion angles T1, T2, T3 vary, they attain values that enable an intramolecular N-H...$^{-}$OCO hydrogen bond (HB) to form in nearly every case. In addition, RNH_3^+ salts provide the $^{-}$OCO group with 3 $^{+}$NH protons as HB donors. The counterions in most secondary and all tertiary amine salts that have been studied feature OH groups on side chains, or the salts exist as hydrates that provide more donors. Each carboxylate O atom accepts at least one HB, usually 2 and sometimes 3. The O atom that accepts the NH...O HB always accepts at least one more HB, and in 5 cases 2 more. H...O distances almost always increase as the donor changes from (R or H)OH to $^{+}$NH to NH. Many of the primary ammonium salts form the commonly observed [2] ladders built from $R_4^3(10)$ HB rings or alternating $R_4^4(12)$ and $R_4^2(8)$ rings. Sometimes a hydrate uses 2 $^{-}$OCO and 2 HOH to form $R_4^4(12)$ rings. Where the cation has a donor group beta to $^{+}$NH, ion pairs via $R_2^2(9)$ rings may occur.

[1] Schwalbe, C. H., Ramirez, M., Conway, B. R. & Timmins, P. (2011). *Acta Cryst.,* **A67**, C661-662.
[2] Lemmerer, A., Bourne, S. A. & Fernandes, M. A. (2008). *CrystEngComm*, **10**, 1605-1612.

Keywords: conformation; hydrogen bonds in organic crystals; diclofenac

MS7-P8 **Crystal packing in methoxybenzyl and methoxyphenethyl-1,3,4-oxadiazole-2(3H)-thiones.** Jim Simpson,[a] Imtiaz Khan[b], Aliya Ibrar.[b] [a]*Department of Chemistry, University of Otago, P.O. Box 56, Dunedin, New Zealand.* [b] *Department of Chemistry, Quaid-i-Azam University-45320, Islamabad, Pakistan.*
E-mail: jsimpson@alkali.otago.ac.nz

The structures of several methoxybenzyl and methoxyphenylethyl-oxadiazolethiones will be reported and the effect on the crystal packing of varying the position of the methoxy-substituent and the link between the benzene and oxadiazolethione rings examined. The structures are novel with no previous reports of benzyl or phenylethyl-oxadiazolethiones in the Cambridge database [1,2]. A common feature of the packing for the ortho- and meta-substituted derivatives is the formation of inversion dimers through N—H···S hydrogen bonds between the oxadiazolethione rings, regardless of the linker. In contrast, the para-methoxybenzyl compound forms strong N—H…O hydrogen bonds generating infinite chains of molecules. Additional intermolecular C—H···O and C—H···S contacts, together with π···π stacking interactions, augment these contacts in the crystal structure.



2,3 and 4-methoxy derivatives; n = 1, 2

[1] Allen, F. H. (2002). *Acta Cryst.* B**58**, 380—388.
[2] Version 5.33 (November 2011) plus two updates

Keywords: 1,3,4-oxadiazole-2(3H)-thiones, inversion dimers, packing