The intended ring opening of a diketocyclobutane with Snl2 was complicated by an in situ intramolecular Aldol reaction which could not be prevented. The structure of the resulting Aldol product was characterized by X-ray crystallography (see Fig. 1).

The crystal structure exhibits a network of O-H...H hydrogen bonds which form an infinite chain along the [0 1 0] direction in the crystal. There are also a number of close C-H...O contacts in the structure.

Another interesting feature of this structure is the presence of void space in the lattice. The total void volume in the unit cell is 33.4 Å3 distributed over 4 symmetry equivalent sites. The difference Fourier map is featureless in the void region of the cell.

This poster will present the structure of this novel tetracyclic compound, an analysis of the hydrogen bonding, and the geometry around the lattice voids. Crystal Data: C29H25N5O7, orthorhombic, P212121, a = 8.9058(7) Å, b = 15.2549(9) Å, c = 17.455(1) Å; V = 2371.4(3) Å3, Z = 4, R = 0.050, Rw = 0.053.

The effect of substituents in position 1 and 3 in the distribution of single bonds from C5 to C9. The planarity of substituents with respect to the indolizine ring is clear if no steric hindrance is present.

The title compound is an example of the rare 1,2-alternate conformation one of the four basic conformations known in calix-[n]arenes (Groenen et al., 1991). In this compound two phenolic hydroxy groups have been replaced by H atoms. The asymmetric unit contains half a molecule; the other half being generated by an inversion centre. Due to the point symmetry the OH-depleted phenyl rings as well as the methoxy phenyl rings are positioned anti-parallel with respect to each other. One of the two phenyl rings is planar, the other shows a small boat-like deformation (max. deviation 0.011(2)Å), which was also previously found (Ting et al., 1995).

The ethyl groups of the molecule is directed to the aromatic rings and in the units B, C and D it is oriented to the cavity, while in the unit A this orientation is vice versa.