

Poster Presentations

[MS25-P23] A Systematic Comparison of the Structures of Substituted Mandelic Acids.

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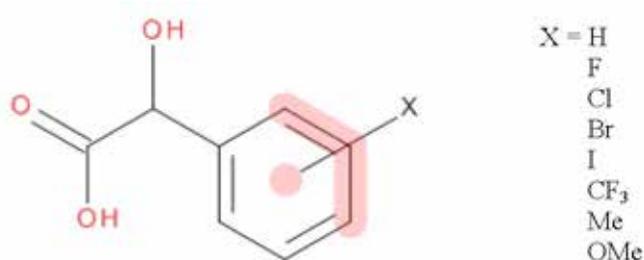
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For several years we have been making detailed comparisons of the crystal structures of large sets of related compounds in an attempt to understand the factors determining the adoption of particular molecular arrangements within crystal structures [1-2]. In all these projects, the XPac program [3] was used to identify similarity between structures in 0-dimensions (0D) (discrete molecular arrangements e.g. dimers, trimers etc), 1D (chains or stacks), 2D (sheets or planes) and 3D (frameworks or full isostructurality) as a preliminary to the detailed comparison of the similarities so identified. As part of a larger crystallographic project to investigate the relationship between structure and chirality, we have synthesized and determined crystal structures of families of monosubstituted racemic mandelic acids with fluoro, chloro, bromo, iodo, trifluoromethyl, methyl and methoxy substituents at the ortho, meta and para positions. Of these 21 permutations only four are described in the literature [5-8].

The substituted mandelic acids are polymorphically prolific and with the inclusion of unsubstituted mandelic acid, 28 structures have been compared. The structures can be based on either traditional carboxylic acid dimers or on side chain hydroxyl to carbonyl dimers or on catemers, or on mixtures. These interrelationships have been established by the XPac program and are displayed using structural similarity diagrams based on Hasse diagrams. Amongst the structures compared we have found four isostructural groups displaying 3D similarity, each containing from two to four structures as well as numerous 1D and 2D relationships.

Of special note amongst the relationships discovered was the isostructurality of one of the polymorphs of 2-fluoromandelic acid and one of the polymorphs of 3-fluoromandelic acid. We wonder, contemplating this pair of structures, why isostructurality between ortho and meta substituted compounds (where the substituents are of a very similar nature) is not commonplace?



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