Familial Relationships in Molecular Crystal Structures

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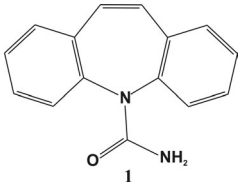
XPac is a computer program for the identification of similar "supramolecular constructs" (sub-components of complete crystal structures) of 0-, 1- or 2-dimensionality in different crystal structures of specific molecules (polymorphs) or crystal structures of similar molecules (families) and of 3-dimensionality in isostructural assemblies.

The *XPac* approach is demonstrated using a family of 20 crystal structures of the carbamazepine molecule (**1**) from the CSD, which includes four polymorphic forms, 13 solvates and salt structures. The structural relationships are visualised in a structure family diagram



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