Quiral: a Computer Program
for the Synthesis of Chiral Molecules from Sugars
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The Quiral computer program that we have recently developed analyzes the 3D structure of a target organic molecule to find which sugar(s) can be used as a starting material for its synthesis. The program also proposes schemes for the preparation of rare or unavailable sugars whose chiral centres fit with those of the target molecule.

Among naturally chiral compounds, carbohydrates are of particular importance because they generally present adjacent asymmetric centres that may be “recycled” in target molecules that also contain adjacent asymmetric centres. This approach minimizes the waste of high value carbon atoms. We wrote the Quiral program with the same goal in mind, but so that a chemist may more quickly identify to which sugar(s) a synthetic target is structurally related. We chose to focus on sugars as starting materials and gave ways to identify inversion of configurations (inter-relations between sugar families), keeping in mind the practical feasability.

Myoinositol is particularly challenging from a stereochemical point of view. It is achiral in its unprotected form as well as when the hydroxy groups in positions 2 and 5 are protected. Chirality results when any one of the hydroxy groups in positions 1, 3, 4, or 6 are modified. The structural complexity of myoinositol makes it a good candidate to demonstrate how Quiral helps chemists to identify the most adequate starting material in a sugar-based synthetic approach. It does not propose a fully detailed synthetic scheme yet but provides a quick and easy way to define a global strategy.