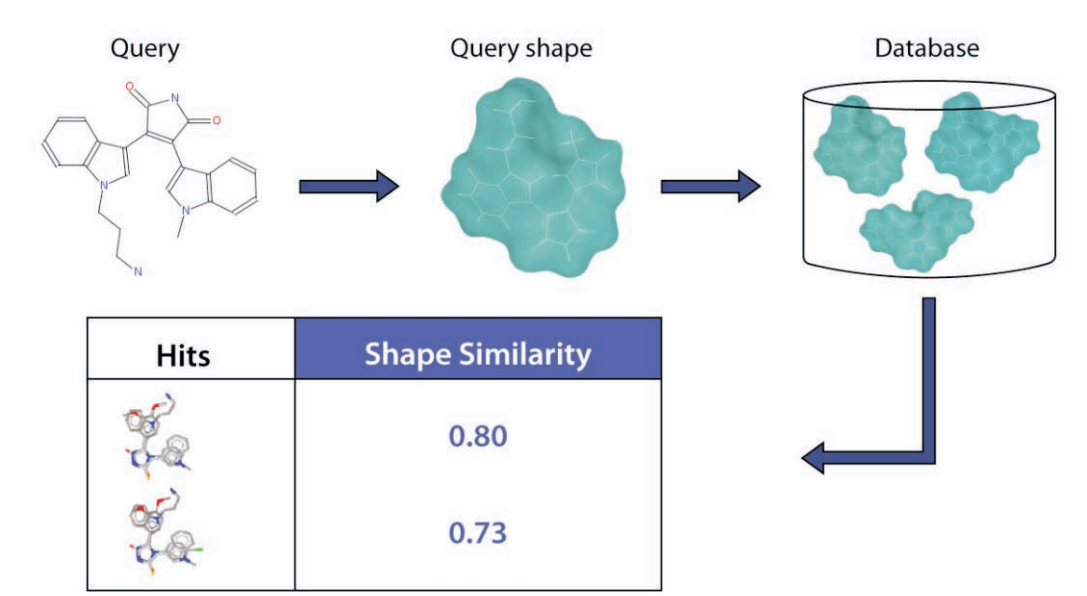
Aakar

The ability to quickly and accurately identify similar molecular structures from a large database of molecules, equips a medicinal chemist with the right tool to realize a number of applications such as scaffold hopping, bioisostere replacement, virtual library design, and flexible ligand superimposition. Aakar provides a powerful and fast alignment independent shape search method with or without taking into consideration the chemical pharmacophoric features.



- Alignment independent shape descriptors
- Multiple shape descriptors:
    - Topological arrangement of atoms
    - Topological & Pharmacophoric feature based
    - Characteristic vector based on spectral distance matrix
    - Characteristic vector & Atomic charge based
- Fast scanning, less than a minute for a database of typically one lakh molecules
- Shape similarity scores are normalized to allow easy comparison
- Standard and user defined multiple databases with shape descriptors can be saved and used as needed
- Results of shape hits may lead to:
    - Scaffold Hopping
    - Bioisosteric Replacement
- Pre-build shape database from publicly available repositories such as FDA approved drugs.
- Provides a user with simplified interface to create or use existing databases with search results presented in worksheets.

vLife
adding value to life

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