3D World of ChemAxon

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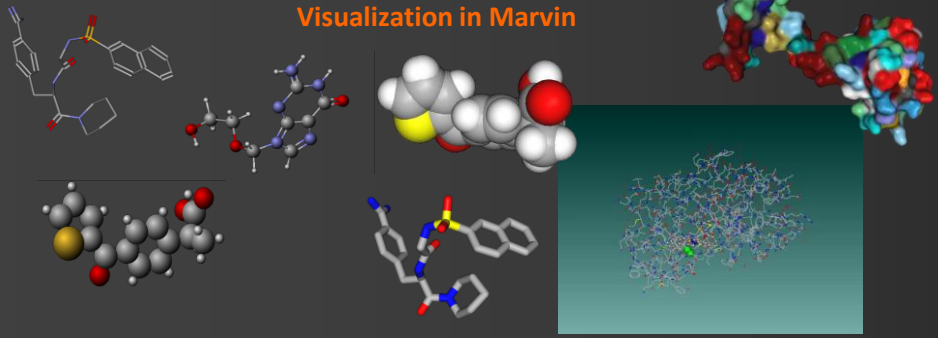
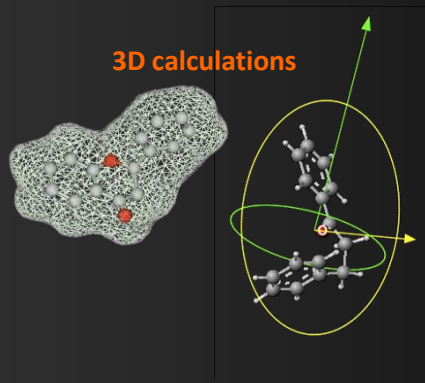
Visualization in Marvin



MarvinView provide lightweight 3D visualisation of small molecules for all platforms and for the web.

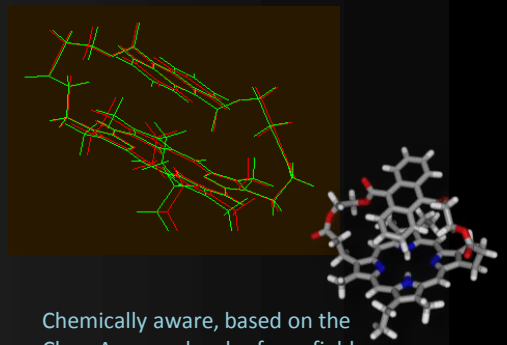
MarvinSpace displays macromolecules, calculates and draws surfaces, secondary structures.

3D calculations



Molecular volume, length, minimal projection area, surface area can be calculated.

3D structure generation

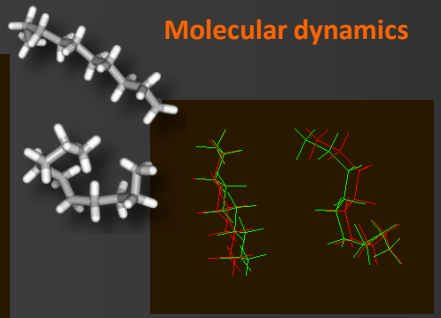


Chemically aware, based on the ChemAxon molecular force field. Reliable and robust (99.5% success ratio).

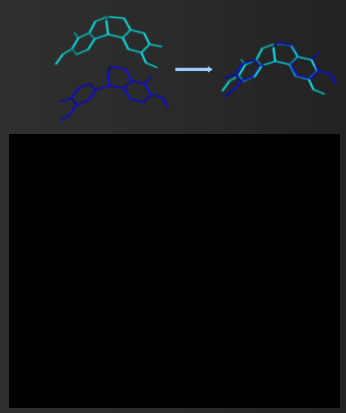
Molecular mechanics

Molecular mechanics based geometry optimization and multi-conformer generation (256 ms/conformer)

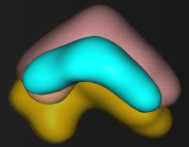
Molecular dynamics



Traditional and projected MD providing fast conformational transitions by the elimination of vibration components.



Flexible alignment



- Rigid and flexible
- multi-molecule
- distance or volumetric
- extended atom types
- Pharmacophores
- Pseudo-docking
- 3D screening