

Standardizer: Molecular cosmetics for cheminformatics

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A chemical compound can be represented in various ways. Therefore the canonicalization of the original structures is usually unavoidable before storing the library in a database or using in cheminformatics applications. To automate this process, ChemAxon has developed a software tool for the batch standardization of molecules according to a user defined configuration. Apart from the visualization issues (cleaning the layout, reorientation of wedges, changing the display mode of hydrogens and aromaticity, etc.), Standardizer helps in the canonicalization of mesomers and tautomers, and allows the removal of counterions or solvents, manipulation of the stereo information, sgroups, attached data, and the custom transformation of functional groups. Standardizer is integrated with the JChem database systems including the JChem Cartridge eliminating many common traps of chemical database administration.