Subject: Re: superpose conformers of different molecules in conformer explorer
Posted by thomas on Thu, 10 Oct 2019 14:17:18 GMT
View Forum Message <> Reply to Message

This is a very good question. Something like this is on my mind since quite some time. The problem is the combinatorial explosion. I am still not sure how to do it that it is useful.

The questions to solve are:
- when superposing different molecules, we must decide, which atoms of both molecules to consider equivalent or similar enough to be superposed. Potentially we have a decent number of atom mappings to consider
- when having x atom mappings and m and n conformers of molecules A and B, respectively, then we have x*n*m possible superpositions. Showing them all would not be very practical. Thus, the UI would need to score the superpositioning.
- a flexible superpositioning after determining the mapping could be a solution, but is algorithmically demanding
- a completely different alternative without atom mapping would be a shape based superpositioning that considers the pharmacophoric interaction similarity of superposed atoms when scoring

A comprehensive solution will take some time, but a simple first step I may provide soon, where one may choose to show the conformer of the reference row (the red marked one) in any other row in addition to the conformer from that row. And there may be a modus to automatically make a shape superpositioning. I need to experiment and have some time...