Subject: Generating 2D Coords does not work with 3D structures
Posted by richards99 on Mon, 08 Mar 2021 10:56:47 GMT
View Forum Message <> Reply to Message

It seems that when I what to regenerate 2D coordinates for structures from Chemistry/Generate 2D Coordinates, and provide a Substructure to align too, this does not seem to work if the structures already have 3D coordinates.

Workaround currently, is I generated SMILES of these structures, do Name to Structure, and then generate 2D coordinates on these.

Simon.