Subject: Re: Enumerating Combinatorial Libraries
Posted by nbehrnd on Thu, 28 Oct 2021 18:27:48 GMT
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Reformulated as a feature suggest: At present, we define and map a typical reaction (.rdf file) and reagents (.sdf file(s)) accordingly to generate a library saved as .dwar file. For a) a subsequent revision how this library was built, or b) a later correction, or extension of the set of reagents submitted to build the library, one has to retain all of these files.

However, it would be an advantage if the .dwar file were a container of all of these files' content, beyond of storing only the library generated. Then, while reading a .dwar file, Chemistry -> Enumerate Combinational Library would display promptly the generic reaction used earlier (ready to be exported as an .rdf), and offer export of reagent .sdf, too. Conceptually, this were in line with access/subsequent edit of the formulae of Data -> Add Calculated Values already provided.

Norwid