Subject: Feature Request: Matched Pair Analyis
Posted by richards99 on Sun, 31 May 2020 10:36:50 GMT
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Hi,
It is incredibly useful to use Matched Pair analysis for interpreting SAR.
Please could you consider adding Matched Pair Analysis to Data Warrior using the algorithm by Hussain and Rea. Reference below.
The output ideally should have 5 structure columns (as canonicalised smiles):
Molecule_Left, Molecule_Right, Fragment_Left, Fragment_Right, and Context.

This then becomes a very powerful tool to analyse the dataset.

* Jameed Hussain, Ceara Rea, J. Chem. Inf. Model., 2010, 50, 339348

Thanks,

Simon.