Meteor Nexus

The SOM tailoring is done by:

1) Generating the structure fingerprint of the site of metabolism of the query compound (the structure fingerprint is generated to a depth of 8 bonds) (Figure 3)

2) Identifying the examples in the metabolism database that match the same biotransformation as the query compound

3) Eliminating the examples that do not have a molecular weight within a particular percentage of the query compound (user configurable, default is 70%) (Figure 4)

4) Generating the structure fingerprint of the site of metabolism of each example compound (Figure 3)

5) Ordering the examples in terms of the similarities of their SOM structural fingerprints to the query compound using the Tanimoto coefficient (Figure 3)

6) The most similar example compounds (user configurable, default is 8) are then used to modify the Static Score, either upwards or downwards depending on whether or not the biotrasformation has been seen experimentally for them, to generate the SOM score