SARvision|SM and Matched Molecular Pairs

An Update

The Molecular Pair table has been modified:

1. To be more compact we have reduced the 5 columns to 3: molecule1 + data, molecule2+data and finally ratio of data.
2. Filter by R-group: show only pairs involving selected R-group positions (i.e. R1).
3. Sort by values in a column OR by R-group position, then by complexity of R-group1, then by complexity of R-group2. (i.e. sort pairs by R1, R2, R3 then by Molecule 1 R-groups (phenyl substitutions) then by Molecule2 R-groups (phenyl substitutions).
Core-hopping is similar to before just more compact. R-group sorting is only meaningful if there are more than 3 scaffolds being compared. There are not R-group position to filter by.