SetCompare

The analysis like "What is a difference between two sets?" is one of the most frequent and important in data analysis.

Using SetCompare the user can easily compare two sets of molecules. It is possible to select ToxAlerts or Chemical Scaffolds, which will display over- and under- represented groups for visual inspections.

The results of SetCompare can be also published. For example, the analysis of over-represented scaffolds or functional groups in compounds which are not soluble in DMSO are available. The analysis of groups overrepresented in sets of biodegradable and non biodegradable compounds also provides nice illustration of differences in data.

For more information, see the SetCompare tutorial.