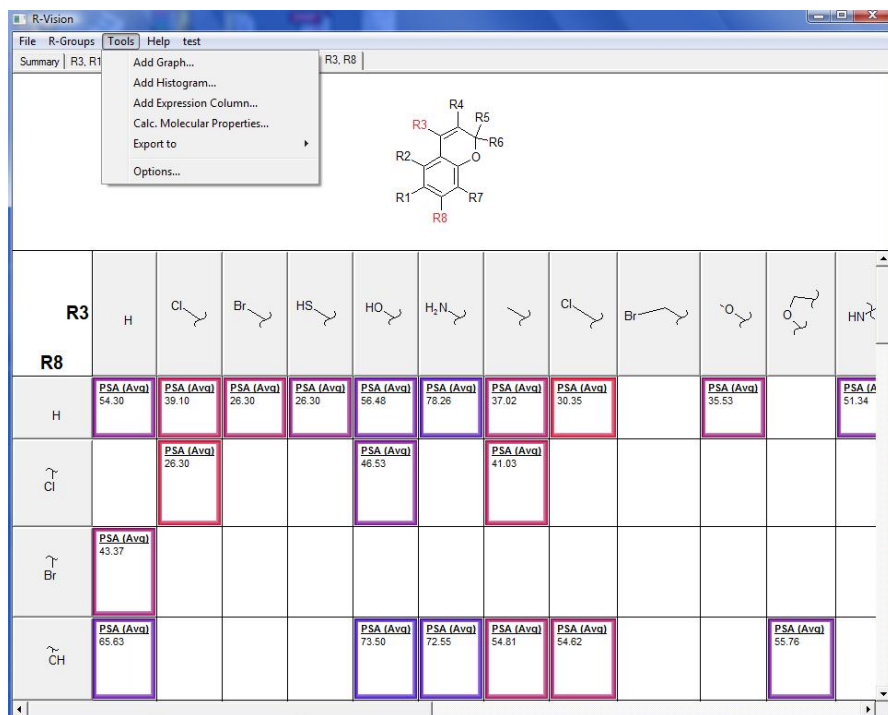


# CHEMSABRE



## SUBSTITUENT ANALYSIS BIOISOSTERIC REPLACEMENT ENUMERATION

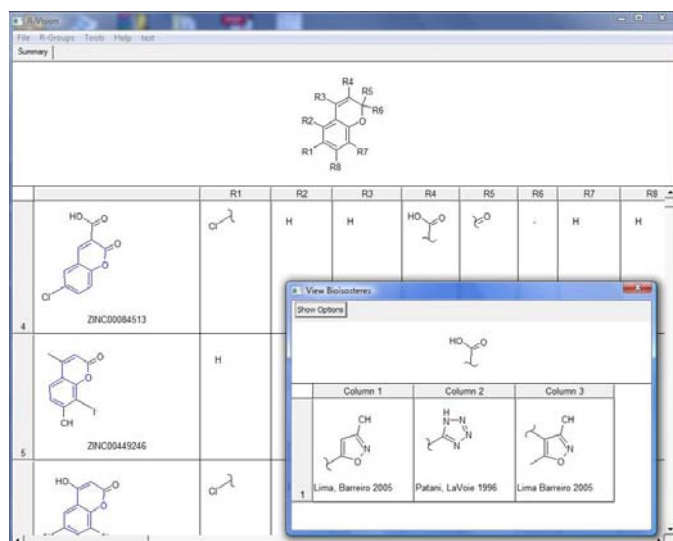
- Build R-group vs R-group tables with heatmaps and other analytical tools
- Plot R-group vs R-group properties
- Enumerate missing combinations of substituents based on the existing ones
- Visualize bioisosteres based on steric, entropic or electronic criteria

**CHEMSABRE** is a desktop application to help in the analysis of substitution patterns in SAR work.

The program creates two way tables for substituents. The cells can be colored by a selected property (Heatmaps) or selected data can be graphed.

From the table, the program can enumerate all possible combinations that are missing in the dataset (Hole enumeration).

**CHEMSABRE** comes with a database of fragment pairs that have been reported in the literature to be bioisosteric replacements. In addition, computed bioisosteric pairs that can be selected based on weighing the contribution of steric electronic or entropic properties.



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