MolOptimiser utility

OCHEM not only allows to develop QSAR models and to apply them for prediction of properties of new compounds. OCHEM allows to automatically *optimise* the molecular structure in order to improve particular properties using QSAR models. Such optimisation is performed by the MolOptimiser utility.

⚠ The MolOptimiser utility has been introduced in June 2013 (version 1.6.3) and is currently in beta testing.

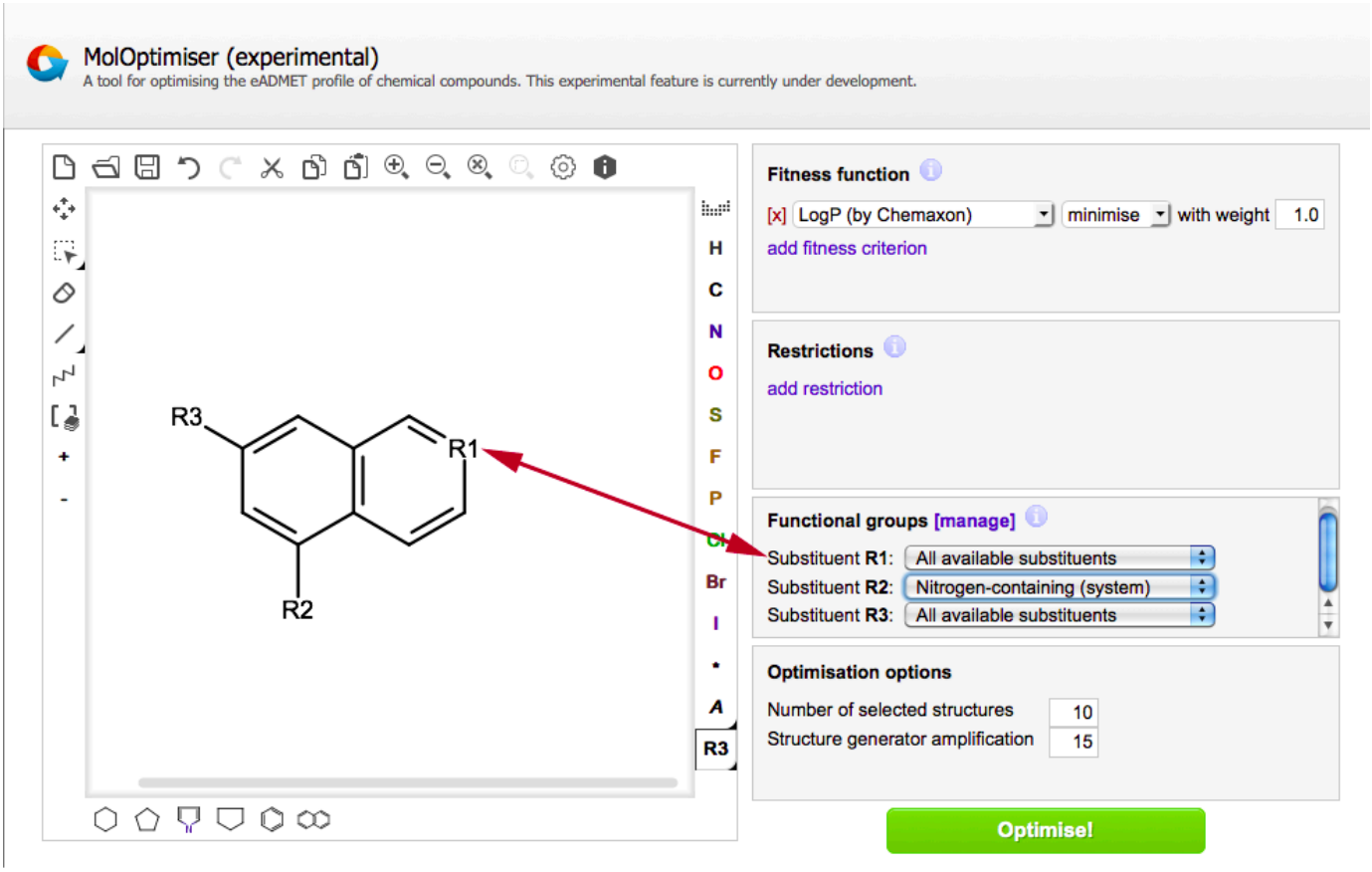
MolOptimiser overview

In short, this is how MolOptimiser works:

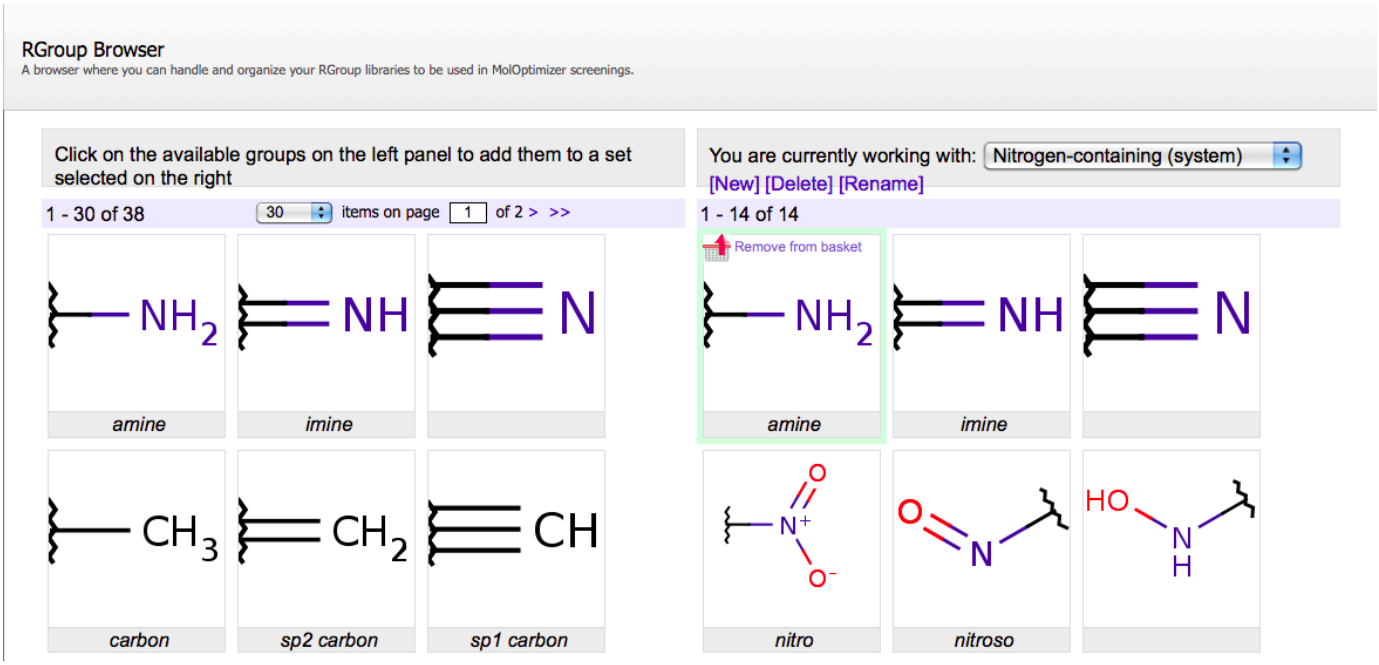
- The user has to:
  - draw the initial structure and defines possible modification points,
  - define the possible substitution groups for the attachment points,
  - define the fitness criteria (e.g., minimise LogP, maximise solubility, reduce toxicity, etc.),
  - (optionally) define a set of restrictions on the structure (e.g., LogP < 5)
- The MolOptimiser will automatically:
  - generate series of chemical structures
  - for these structures, run predictions for the optimised properties
  - select the best structures according to the fitness criteria

Definition of the substitution groups

The user can define the possible substitution groups for each attachment point individually as shown on the screenshot below.



It is possible to manage the functional groups and define custom sets:



The fitness definition

The user defines the fitness function as one or a set of maximisation (or minimisation) criteria: e.g., minimise LogP on the screenshot below:

Fitness function

[x] LogP (by Chemaxon) minimise with weight 1.0

add fitness criterion

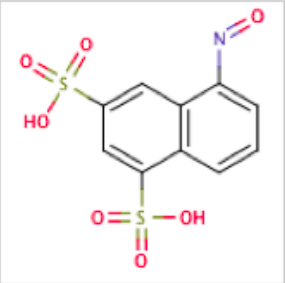
Results

The optimisation procedure take several minutes or longer. If a task is taking too long, it is always possible to fetch the results any time later using the browser of pending tasks.

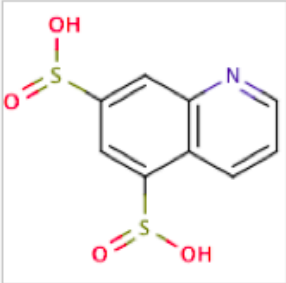
Once the optimisation procedure is completed, a number of the best fitting structures are shown:

Optimised molecules

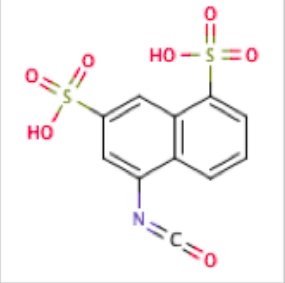
601 unique structures have been scanned, 10 best fitting structures are shown below



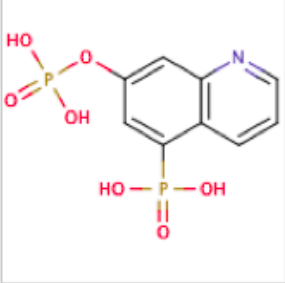
Molecular mass = 317.
Chemaxon LogP = -2.9



Molecular mass = 257.
Chemaxon LogP = -2.5



Molecular mass = 329.
Chemaxon LogP = -2.3



Molecular mass = 305.
Chemaxon LogP = -2.2

How many structures should be shown is determined by the user. The default option is 10 structures.