

SATELLITES - Wiki page

- Installation -

Requirements:

- Python3.10 or older
- RDKit 2022.03.5 or older
- Pandas
- Numpy
- PyQt5 (pyqt in conda)
- pyreadline3 (cmd line only) - Needs to be fixed

-> Example using Windows 10/11 with python3.10 installed from Windows store:

In powershell terminal (shift + right clic, then "Open PowerShell here"):

Then to launch the software:

-> Classical local installation:

Launch:

-> Virtual environment:

(for my windows version, it's `python3.10 -m venv env`)

Launch:

-> Conda environment:

Launch:

- Explanation of each field -

SMARTS chemical reaction:

- Put here your chemical reaction in a form of a SMARTS string
- 2-reagents reaction = A.B>>P
- 3-reagents reaction = A.B.C>>P

Output directory:

- Select path for the output
- By default, the name of the created directory is "SATELLITES_results"

Logical processors to allocate:

- SATELLITES splits automatically the enumeration of the libraries into multiple CPUs, by batches of 400 cpds.
- Minimum value = 1
- Maximum value = The maximum that you can allocate on your machine
- Default value = Half of your maximum

Choice between 2- or 3-reagents reaction:

- Select your tab associated to your chemical reaction
- Will be automatic in the future

Paths of reagents A/B/C:

- Browse to select your reagents
- Only tab-separated smiles files for now
- Minimum fields: Smi | es Compound | D

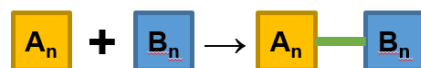
Steps - 2-reagents reaction:

- Step #1 = Minimum Enumeration Library/Basis Products Library (Ab and aB)
 - Enumerate the reagents A/B with the representatives A/B
 - You have to choose between 3 options to set your representatives
 - Smallest = SATELLITES will take your smallest reagent in your subset, based on molecular weight
 - Chosen ID = SATELLITES will find the specific compound in your subset, and set it as the representative
 - Custom SMILES = Set a compatible SMILES as your representative. SATELLITES will show you the 2D depiction and the molecular weight of your SMILES
 - All your generated libraries are inside output_libraries
- Step #2 = Focused Enumeration Library (AB)
 - Select a SMILES file with your selected compounds from the previous step
 - It must be the lines from the output libraries files, with SATELLITES ID

Steps - 3-reagents reaction:

- Step #1 = Minimum Enumeration Library/Basis Products Library #1 (Abc, aBc, abC)
 - Same as the step #1 of 2-reagents reaction
- Step #2 = Intermediate Enumeration Library/Basis Products Library #2 (ABc, AbC, aBC)
 - Mix of the steps #1 and #2 of 2-reagents reaction
- Step #3 = Focused Enumeration Library (ABC)
 - Same as the step #2 of 2-reagents reaction

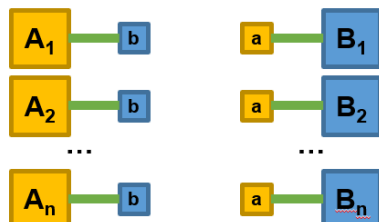
2-reagents reaction - Algorithm



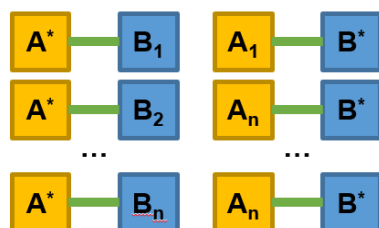
1) Identify representatives A and B



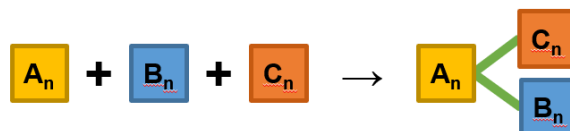
2) Combinations with representatives



3) Combinations using the best hits



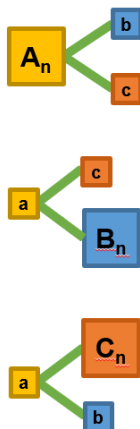
3-reagents reaction - Algorithm



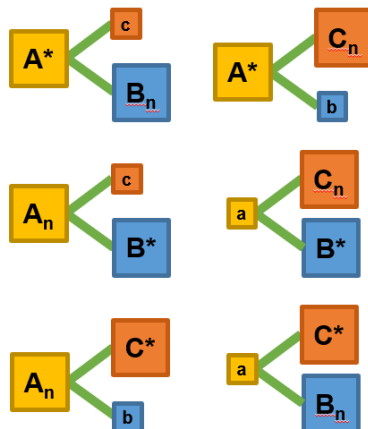
1) Identify representatives A, B and C



2) Combinations with representatives
First iteration



3) Combinations with representatives
Second iteration



4) Final combinations using the
best AB, AC & BC combos

