# 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

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

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

```
pip install rdkit pandas numpy pyqt5
```

Then to launch the software:

```
python3.10 .\Run_SATELLiTES_Alpha2_WIP.py
```

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**-> Classical local installation:**

```
pip install rdkit pandas numpy pyqt5
```

**Launch:**

```
python3 .\Run_SATELLiTES_Alpha2_WIP.py
```

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**-> Virtual environment:**

`python3 -m venv /location/of/the/env` (for my windows version, it’s python3.10 -m venv env)

```
source /location/of/the/env/bin/activate

pip install rdkit pandas numpy pyqt5
```

**Launch:**

```
source /location/of/the/env/bin/activate
python3 .\Run_SATELLiTES_Alpha2_WIP.py
```

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**-> Conda environment:**

```
conda create -n satellites python=3.10
source activate satellites
pip install rdkit pandas numpy pyqt5
```

**Launch:**

```
source activate satellites
python3 .\Run_SATELLiTES_Alpha2_WIP.py
```

## - 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: `Smiles  CompoundID`

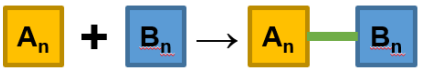
**Steps - 2-reagents reaction:**

- 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:**

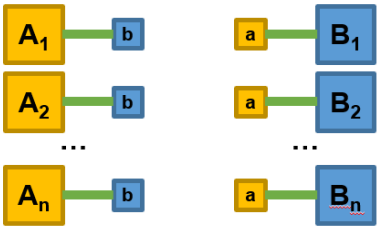
- Step #1 = Minimum Enumeration Library/Basis Products Library #1 (Abc, aBc, abC)
    - Same as the step #1 of 2-reagents reaction
- Step #2 = Intermediate Enumeration Library/Basis Products Library #2 (ABc, AbC, aBC)
    - Mix of the steps #1 and #2 of 2-reagents reaction
- Step #3 = Focused Enumeration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

# 2-reagents reaction - Algorithm

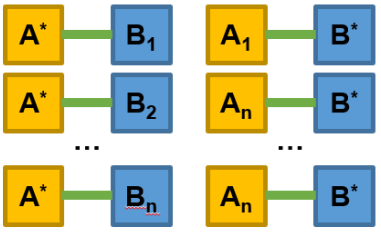



1) Identify representatives A and B

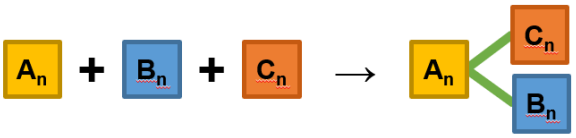

2) Combinations with representatives




3) Combinations using the best hits

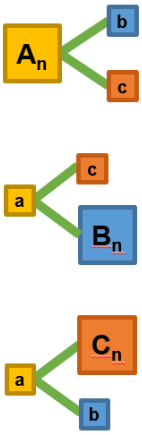



# 3-reagents reaction - Algorithm

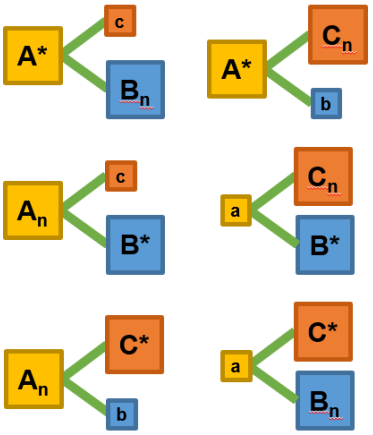



1) Identify representatives A, B and C


2) Combinations with representatives
First iteration




3) Combinations with representatives
Second iteration




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