**Installation:**

If using Google Colab use `!pip install polymerization-planner`, else use `pip install polymerization-planner`

For ATRP (Three optimizable reagents, metal, ligand, photocatalyst (PC)

**Example usages of `polymerization_planner` with ATRP.**

These equally can be applied to PET-RAFT (For reaction only requiring two additional optimizable components E.g., photocatalyst (PC) and chain-transfer agent (CTA).

Here we are making different reagent molar ratios,which might require need to reduce either metal, ligand, PC volumes in order to allocate space for a reagent needing a higher ratio.

*** All concentration are in mM !!

--Jump to end to see output (an excel sheet with volumes)

**Input to the function is a path to a single excel workbook having 3 sheets.**

1. The first (Must be named: Sheet1)sheet defines the Reagent ratios for the Monomer, Initiator, Metal, Ligand and Photocatalyst [M] = Stock monomer concentration, The [I], [Metal],[L], [PC] are the stock concentrations of Initiator, Metal and Ligand respectively, an input is necessary but if the script determines using another concentration is more efficient to minimize reagent preparation this will be overwritten. Can always just put the highest concentration available. The columns must match the naming shown below

| Polymer ID | Monomer | Initiator | Metal | Ligand | Photo catalyst | [M] | [I] | [Metal] | [L] | [PC] | Mf | Volume |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 200 | 1 | 0.05 | 0.4 | 0.02 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 1 | 200 | 1 | 0.2 | 2 | 0.4 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 2 | 200 | 1 | 0.1 | 0.04 | 0.1 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 3 | 200 | 1 | 0.4 | 0.1 | 0.2 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 4 | 200 | 1 | 0.05 | 1 | 0.04 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 5 | 200 | 1 | 0.2 | 0.4 | 0.004 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 6 | 200 | 1 | 0.05 | 0.2 | 0.04 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 7 | 200 | 1 | 0.05 | 0.1 | 0.004 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 8 | 200 | 1 | 0.2 | 0.2 | 0.4 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 9 | 200 | 1 | 0.025 | 0.1 | 0.01 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 10 | 200 | 1 | 0.4 | 2 | 0.001 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 11 | 200 | 1 | 0.4 | 2 | 0.004 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 12 | 200 | 1 | 0.05 | 0.04 | 0.001 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 13 | 200 | 1 | 0.2 | 0.4 | 0.002 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 14 | 200 | 1 | 0.05 | 0.1 | 0.2 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |
| 15 | 200 | 1 | 0.1 | 1 | 0.004 | 2000 | 55 | 22.5 | 100 | 4 | 1000 | 200 |

2. The next sheet has information on the monomer name. However if making copolymers these must all have the same concentration for example if making a 50% MA and 50% HEA both HEA and MA must have the same concentration as this will determine their volume based on percent. If making Homopolymers of different monomers at varying concentrations that is ok. However, if going to the same well / same polymer these must be equal stocks. ***The order must be the same as in the previous sheet (same polymer IDs in that order)

| Polymer ID | Mon 1 | Mon 1% | Mon 2 | Mon 2% | Mon 3 | Mon 3% | Mon 4 | Mon 4% |
|---|---|---|---|---|---|---|---|---|
| 0 | HEA | 100 | | | | | | |
| 1 | HEA | 25 | MA | 25 | HPA | 25 | BA | 25 |
| 2 | HEA | 75 | MA | 25 | | | | |
| 3 | HEA | 10 | MA | 50 | HPA | 40 | | |
| 4 | HEA | 100 | | | | | | |
| 5 | HEA | 100 | | | | | | |
| 6 | HEA | 100 | | | | | | |
| 7 | HEA | 100 | | | | | | |
| 8 | HEA | 100 | | | | | | |
| 9 | HEA | 100 | | | | | | |
| 10 | HEA | 100 | | | | | | |
| 11 | HEA | 100 | | | | | | |
| 12 | HEA | 100 | | | | | | |
| 13 | HEA | 100 | | | | | | |
| 14 | HEA | 100 | | | | | | |
| 15 | HEA | 100 | | | | | | |
| 16 | HEA | 100 | | | | | | |
| 17 | HEA | 100 | | | | | | |
| 18 | HEA | 100 | | | | | | |

Sheet1 Sheet2 Sheet3 +

3. **The third sheet (Sheet3) has the possible reagent concentrations the script can consider when making ratios. The most straightforward approach is to just make a high concentration of each reagent, then pass dilutions that can be made by serial dilution to save time for the experimenter.**

| Ligand | Metal | PC |
|---|---|---|
| 200 | 22.5 | 4 |
| 100 | 11.25 | 2 |
| 50 | 5.625 | 1 |
| 25 | 2.8125 | 0.5 |
| 12.5 | | 0.25 |
| 6.25 | | 0.125 |
| 3.125 | | 0.0625 |

Sheet1 Sheet2 Sheet3 +

Accessibility: Investigate

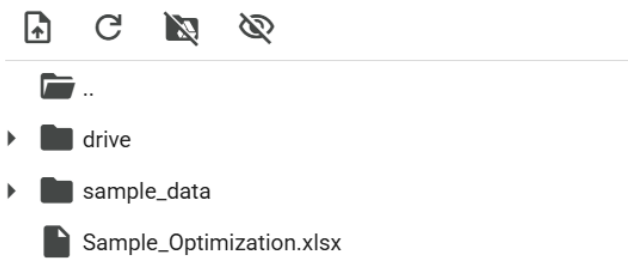
****** All sheet column names must match the examples shown and include all sheets, as a single file.**

**Now can import the module, by calling**

If using Google Colab use `!pip install polymerization-planner`, else use `pip install polymerization-planner`

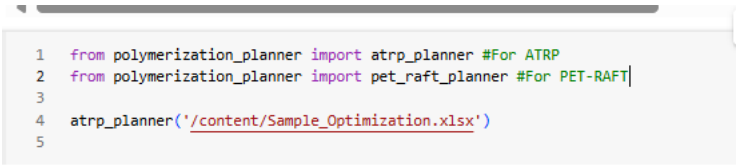
Might need to restart session if in Colab if after installation you get a message saying the modules isn't available, means need to "refresh" so the function can be used.

Once this is installed can now import the function




Can upload the excel sheet to the colab directory or to a folder in your drive, the script will save to the parent folder from where the file was read. Here I just uploaded to the colab notebook directory

Then run this (if PET-RAFT do



```
1  from polymerization_planner import atrp_planner #For ATRP
2  from polymerization_planner import pet_raft_planner #For PET-RAFT
3
4  atrp_planner('/content/Sample_Optimization.xlsx')
5
```

If you ever forget or need a reminder and need to see this again, just pip install as usual then do

```
from polymerization_planner import show_tutorial
show_tutorial()
```

```
Tutorial PDF: https://github.com/C3344/polymerization_planner/blob/main/polymerization_planner/docs/tutorial.pdf
```

Below are sample PET-RAFT sheets same concept just the column names change.

PET-RAFT Sheet1

| Polymer ID | Monomer | CTA | photo catalyst | [M] | [CTA] | [PC] | Mf | Volume |
|---|---|---|---|---|---|---|---|---|
| 0 | 30 | 1 | 0.01 | 2000 | 200 | 2 | 1000 | 200 |
| 1 | 50 | 1 | 0.01 | 2000 | 100 | 1 | 1000 | 200 |
| 2 | 75 | 1 | 0.01 | 2000 | 100 | 1 | 1000 | 200 |
| 3 | 100 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 4 | 125 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 5 | 150 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 6 | 175 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 7 | 200 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 8 | 225 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 9 | 250 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 10 | 275 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 11 | 300 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 12 | 325 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 13 | 350 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 14 | 375 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 15 | 400 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 16 | 425 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 17 | 450 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 18 | 475 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |
| 19 | 500 | 1 | 0.01 | 2000 | 50 | 0.5 | 1000 | 200 |

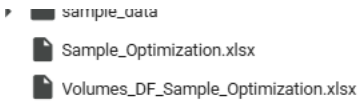
PET-RAFT Sheet2

| Polymer ID | Mon 1 | Mon 1% | Mon 2 | Mon 2% | Mon 3 | Mon 3% | Mon 4 | Mon 4% |
|---|---|---|---|---|---|---|---|---|
| 0 | HEA | 100 | | | | | | |
| 1 | HEA | 100 | | | | | | |
| 2 | HEA | 100 | | | | | | |
| 3 | HEA | 100 | | | | | | |
| 4 | HEA | 100 | | | | | | |
| 5 | HEA | 100 | | | | | | |
| 6 | HEA | 100 | | | | | | |
| 7 | HEA | 100 | | | | | | |
| 8 | HEA | 100 | | | | | | |
| 9 | HEA | 100 | | | | | | |
| 10 | HEA | 100 | | | | | | |
| 11 | HEA | 100 | | | | | | |
| 12 | HEA | 100 | | | | | | |
| 13 | HEA | 100 | | | | | | |
| 14 | HEA | 100 | | | | | | |
| 15 | HEA | 100 | | | | | | |
| 16 | HEA | 100 | | | | | | |
| 17 | HEA | 100 | | | | | | |
| 18 | HEA | 100 | | | | | | |
| 19 | HEA | 100 | | | | | | |
| 20 | HEA | 100 | | | | | | |

PET-RAFT Sheet3

| CTA | PC |
|---|---|
| 200 | 4 |
| 100 | 2 |
| 50 | 1 |
| 25 | 0.5 |
| 12.5 | 0.25 |
| 6.25 | 0.125 |
| 3.125 | 0.0625 |

In this tutorial we just uploaded to the colab directory so our file was saved there, which when we end the session will get deleted, if want to save it can download or first upload your input to your drive and give that path to the functions.




At the end you get a sheet like this that looks like the input but now says volumes and the concentrations to use for each reagent. Hope this was helpful ! Have a nice day 😊

| | [I] | [Metal] | [L] | [PC] | Mf | Volume | Monomer Volume | Initiator Volume | Metal Volume | Ligand Volume | PC Volume | Solvent Volume | Metal Cf |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 00 | 55 | 2.8125 | 12.5 | 4 | 1000 | 200 | 100 | 18.18 | 17.78 | 32 | 5 | 27.04 | 0.250031 |
| 00 | 55 | 2.8125 | 6.25 | 4 | 1000 | 200 | 100 | 18.18 | 35.56 | 6.4 | 25 | 14.86 | 0.500063 |
| 00 | 55 | 22.5 | 12.5 | 4 | 1000 | 200 | 100 | 18.18 | 17.78 | 8 | 50 | 6.04 | 2.00025 |
| 00 | 55 | 5.625 | 200 | 4 | 1000 | 200 | 100 | 18.18 | 8.89 | 5 | 10 | 57.93 | 0.250031 |
| 00 | 55 | 22.5 | 50 | 0.25 | 1000 | 200 | 100 | 18.18 | 8.89 | 8 | 16 | 48.93 | 1.000125 |
| 00 | 55 | 2.8125 | 12.5 | 4 | 1000 | 200 | 100 | 18.18 | 17.78 | 16 | 10 | 38.04 | 0.250031 |
| 00 | 55 | 5.625 | 12.5 | 0.5 | 1000 | 200 | 100 | 18.18 | 8.89 | 8 | 8 | 56.93 | 0.250031 |
| 00 | 55 | 2.8125 | 12.5 | 2 | 1000 | 200 | 100 | 18.18 | 8.89 | 8 | 5 | 59.93 | 0.125016 |
| 00 | 55 | 11.25 | 200 | 0.125 | 1000 | 200 | 100 | 18.18 | 35.56 | 10 | 8 | 28.26 | 2.00025 |
| 00 | 55 | 22.5 | 50 | 0.25 | 1000 | 200 | 100 | 18.18 | 17.78 | 40 | 16 | 8.04 | 2.00025 |
| 00 | 55 | 5.625 | 6.25 | 0.125 | 1000 | 200 | 100 | 18.18 | 8.89 | 6.4 | 8 | 58.53 | 0.250031 |
| 00 | 55 | 22.5 | 50 | 0.25 | 1000 | 200 | 100 | 18.18 | 8.89 | 8 | 8 | 56.93 | 1.000125 |
| 00 | 55 | 2.8125 | 12.5 | 4 | 1000 | 200 | 100 | 18.18 | 17.78 | 8 | 50 | 6.04 | 0.250031 |
| 00 | 55 | 11.25 | 200 | 0.125 | 1000 | 200 | 100 | 18.18 | 8.89 | 5 | 32 | 35.93 | 0.500063 |
| 00 | 55 | 11.25 | 200 | 0.125 | 1000 | 200 | 100 | 18.18 | 17.78 | 5 | 32 | 27.04 | 1.000125 |