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.

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
1	200	1	0.05	0.4	0.02	2000	55	22.5	100	4	1000	200
2	200	1	0.2	2	0.4	2000	55	22.5	100	4	1000	200
3	200	1	0.1	0.04	0.1	2000	55	22.5	100	4	1000	200
4	200	1	0.4	0.1	0.2	2000	55	22.5	100	4	1000	200
5	200	1	0.05	1	0.04	2000	55	22.5	100	4	1000	200
6	200	1	0.2	0.4	0.004	2000	55	22.5	100	4	1000	200
7	200	1	0.05	0.2	0.04	2000	55	22.5	100	4	1000	200
8	200	1	0.05	0.1	0.004	2000	55	22.5	100	4	1000	200
9	200	1	0.2	0.2	0.4	2000	55	22.5	100	4	1000	200
10	200	1	0.025	0.1	0.01	2000	55	22.5	100	4	1000	200
11	200	1	0.4	2	0.001	2000	55	22.5	100	4	1000	200
12	200	1	0.4	2	0.004	2000	55	22.5	100	4	1000	200
13	200	1	0.05	0.04	0.001	2000	55	22.5	100	4	1000	200
14	200	1	0.2	0.4	0.002	2000	55	22.5	100	4	1000	200
15	200	1	0.05	0.1	0.2	2000	55	22.5	100	4	1000	200
16	200	1	0.1	1	0.004	2000	55	22.5	100	4	1000	200
17	200	1	0.2	1	0.004	2000	55	22.5	100	4	1000	200
18	200	1	0.1	2	0.001	2000	55	22.5	100	4	1000	200
19	200	1	0.2	0.04	0.001	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.

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

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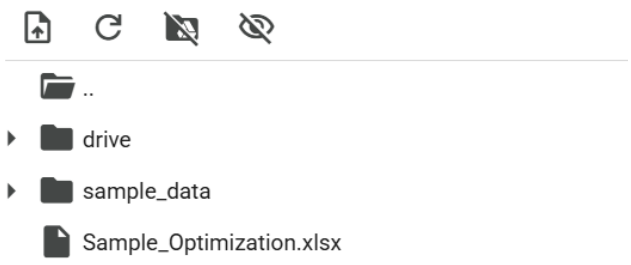
Might need to restart session if in Colab if after installation you get a message saying the modules isn't available, means need to "refresh" so the function can be used.

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