Cocktail Shaker

Suliman Sharif | RDKit UGM 2019

Agenda

1. Introduction & Motivation

Who I am and my motivation behind the building of cocktail shaker.

2. Introduction to Cocktail Shaker

How does Cocktail Shaker work?

3. Future Releases of Cocktail Shaker

What I plan for cocktail shakers future use and where I see this project headed.

4. Conclusion

Interesting thoughts, acknowledgements, and Q & A.

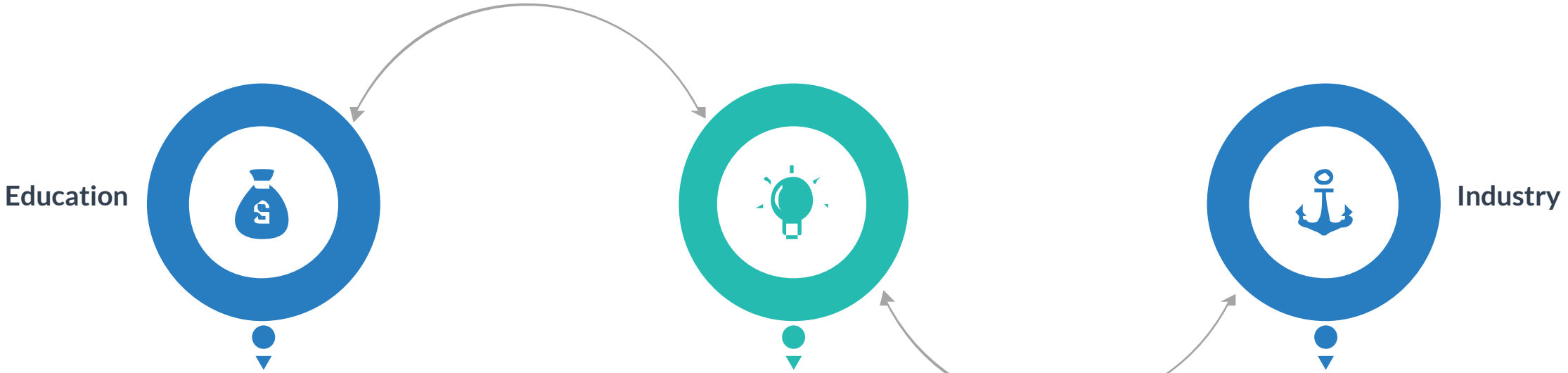
sharifsuliman1@gmail.com

Meet **Suliman Sharif**

British Native turned Austinite. Young Scientist, Entrepreneur, and Rock Climbing Enthusiast.

sharifsuliman1@gmail.com

Software Engineer & Chemist



B.Sc. Biochemistry/Minor in CS | **University of Texas at Austin**

M.Sc. Organic Chemistry | **U.C Riverside School of Medicine**

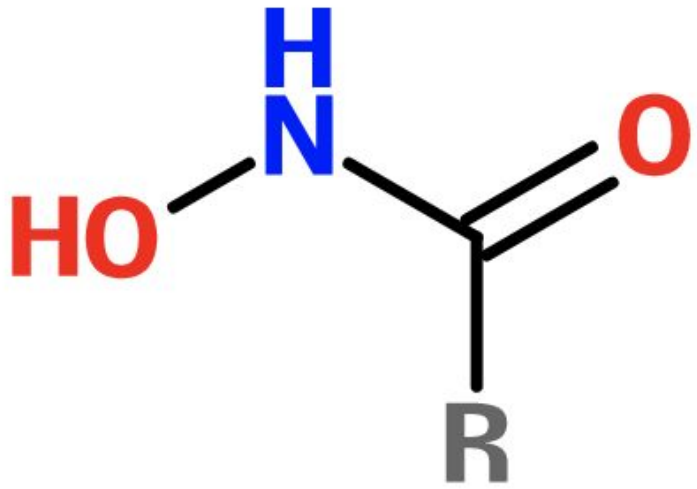
Bioinformatics Scientist | **L7 Informatics**

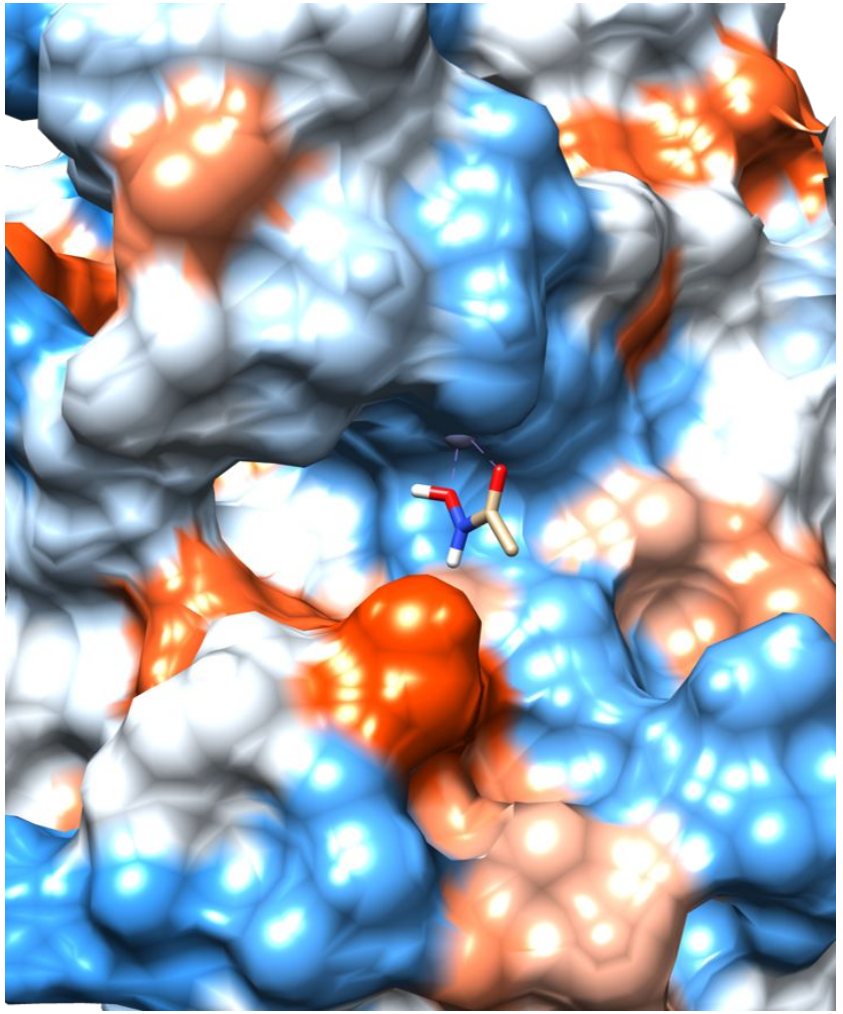
Associate Editor | **Journal of Open Research Software**

Co-Founder | **LifeSciHack**

sharifsuliman1@gmail.com

The Problem





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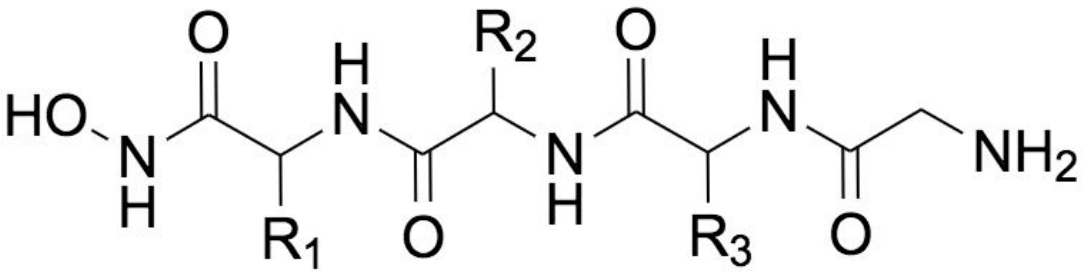
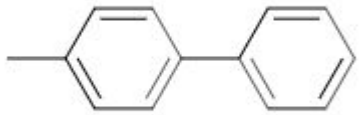
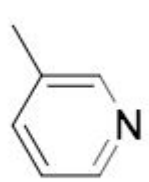
Natural & Non-natural Amino Acids Combinations

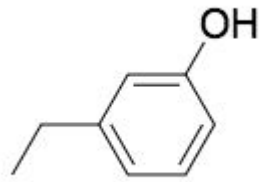


$R_{1\text{-}3}$

Cys	Asp	Ala	Asn	Arg
Ile	His	Glu	Gly	Gln
Pro	Phe	Leu	Met	Lys
Val	Tyr	Ser	Trp	Thr

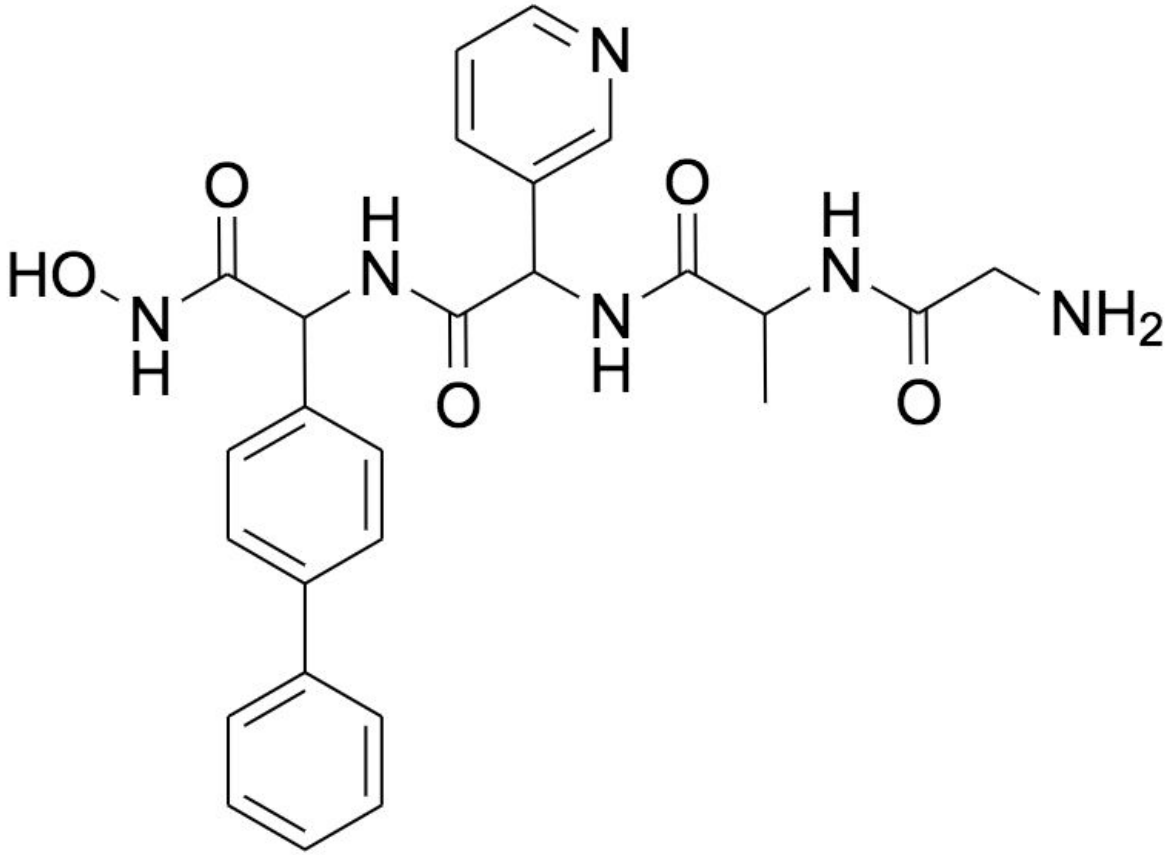






sharifsuliman1@gmail.com

Example Combination



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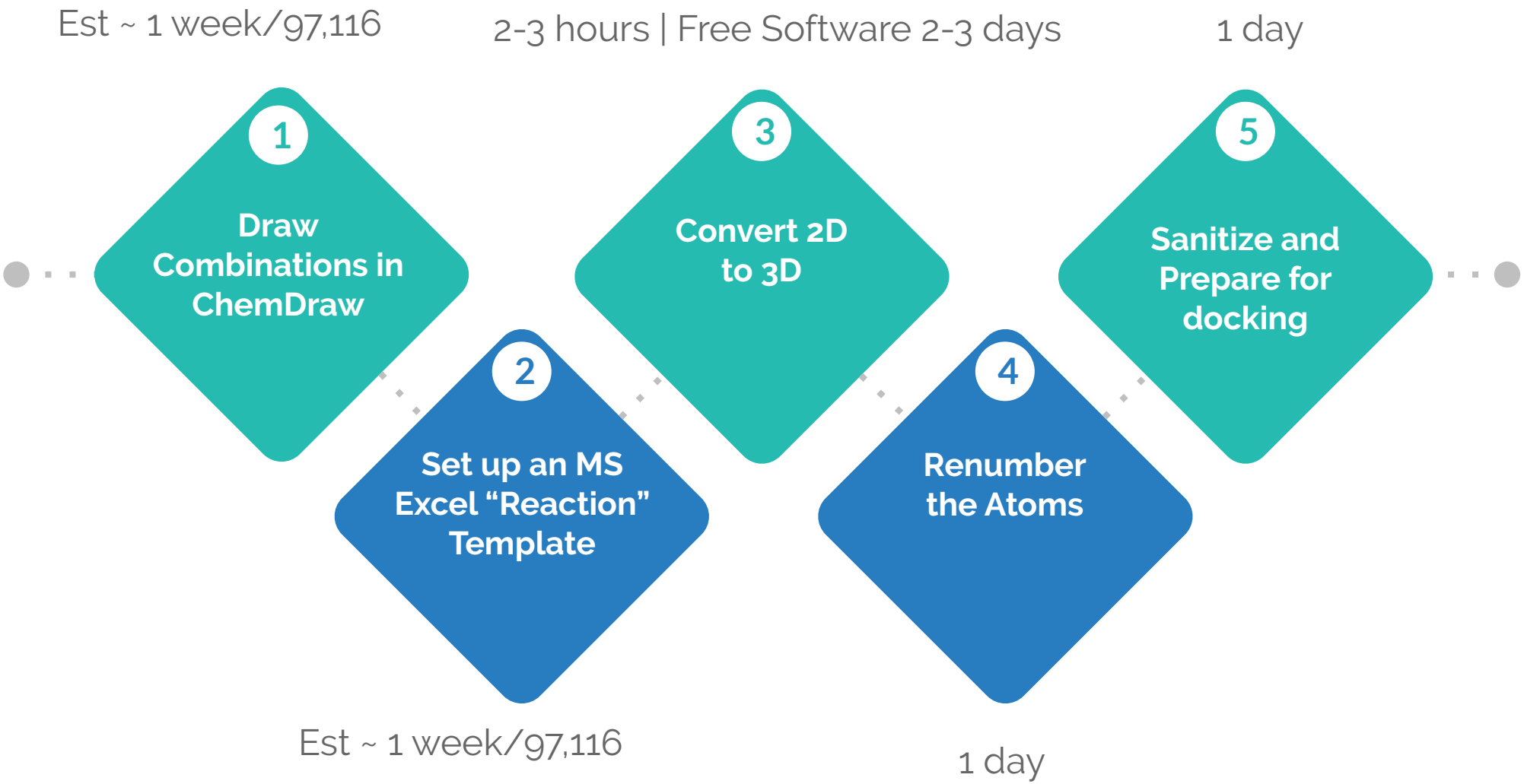
What did it take? Budget: $0



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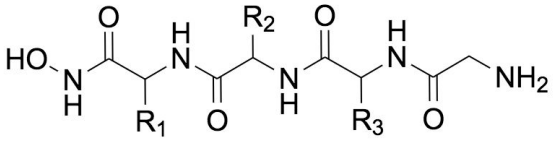
2 Years Later.....

Natural And Non-Natural Amino Acids



Functional Groups

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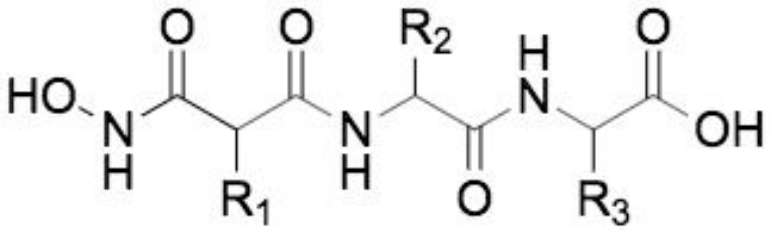
Introducing Cocktail Shaker Package!

Let's Convert the Peptide to SMILES Representation



O=C(NO)C(R1)NC(=O)C(R2)NC(=O)C(R3)C(=O)NO

sharifsuliman1@gmail.com

Expansion Example

Cocktail Shaker reads SMILES

Peptide Molecule = ‘O=C(O)C(R1)NC(=O)C(R2)NC(=O)C(R3)C(=O)NO’

Wrap it in the Cocktail Object

Cocktail = Cocktail(Peptide Molecule)

Shake the Cocktail (Create the combinations)

Combinations = Cocktail.Shake()

Write the combinations to a file

FileWriter(Combinations)

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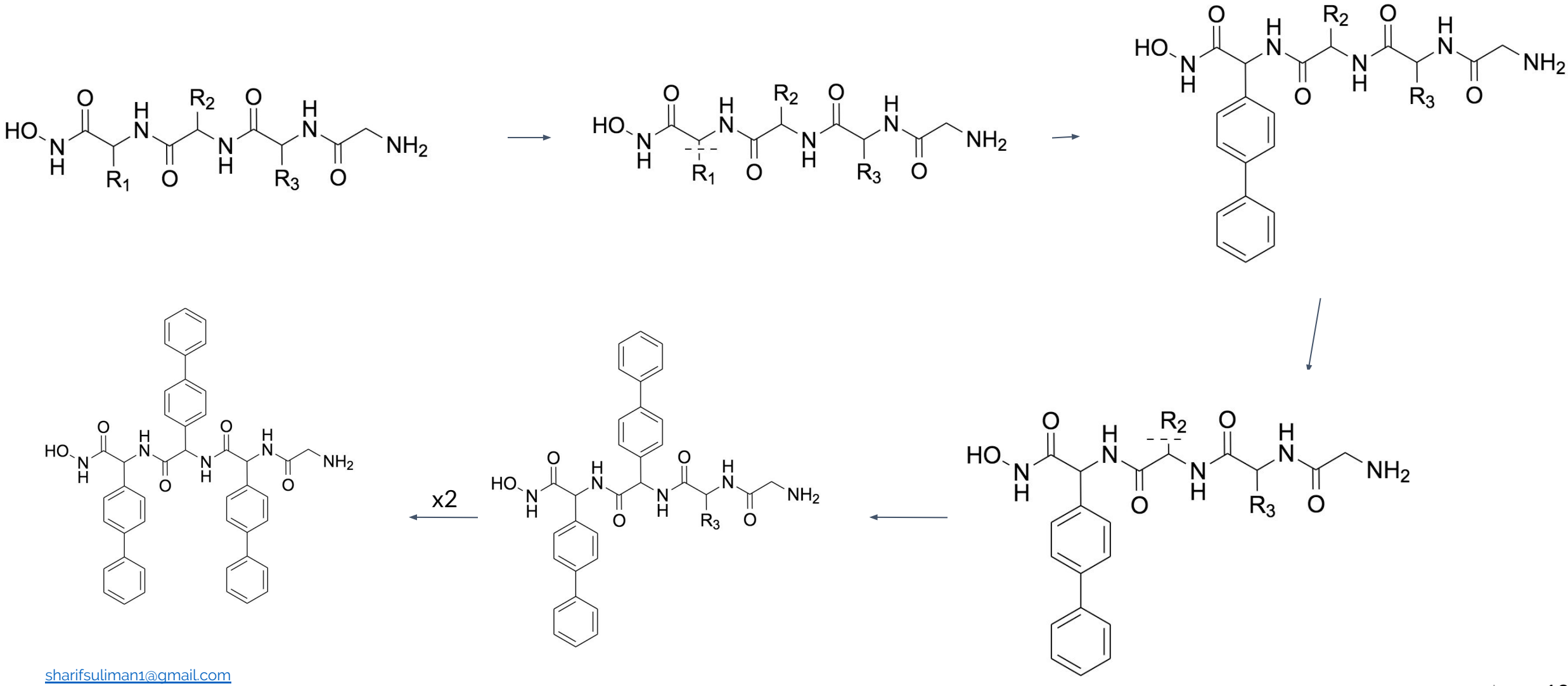
But how does it work? (RDKit's replace substructure functionality)



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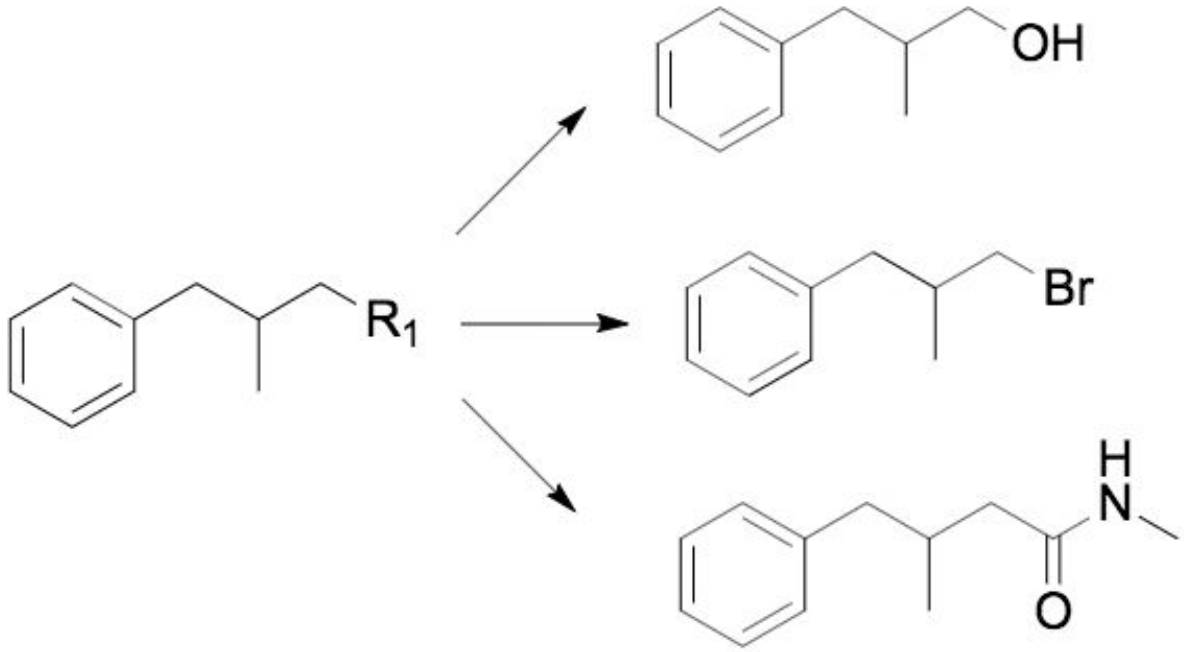
More practical uses.

Take any compound you would like to expand on and pass it through the cocktail to generate a library of compounds with different functional groups.



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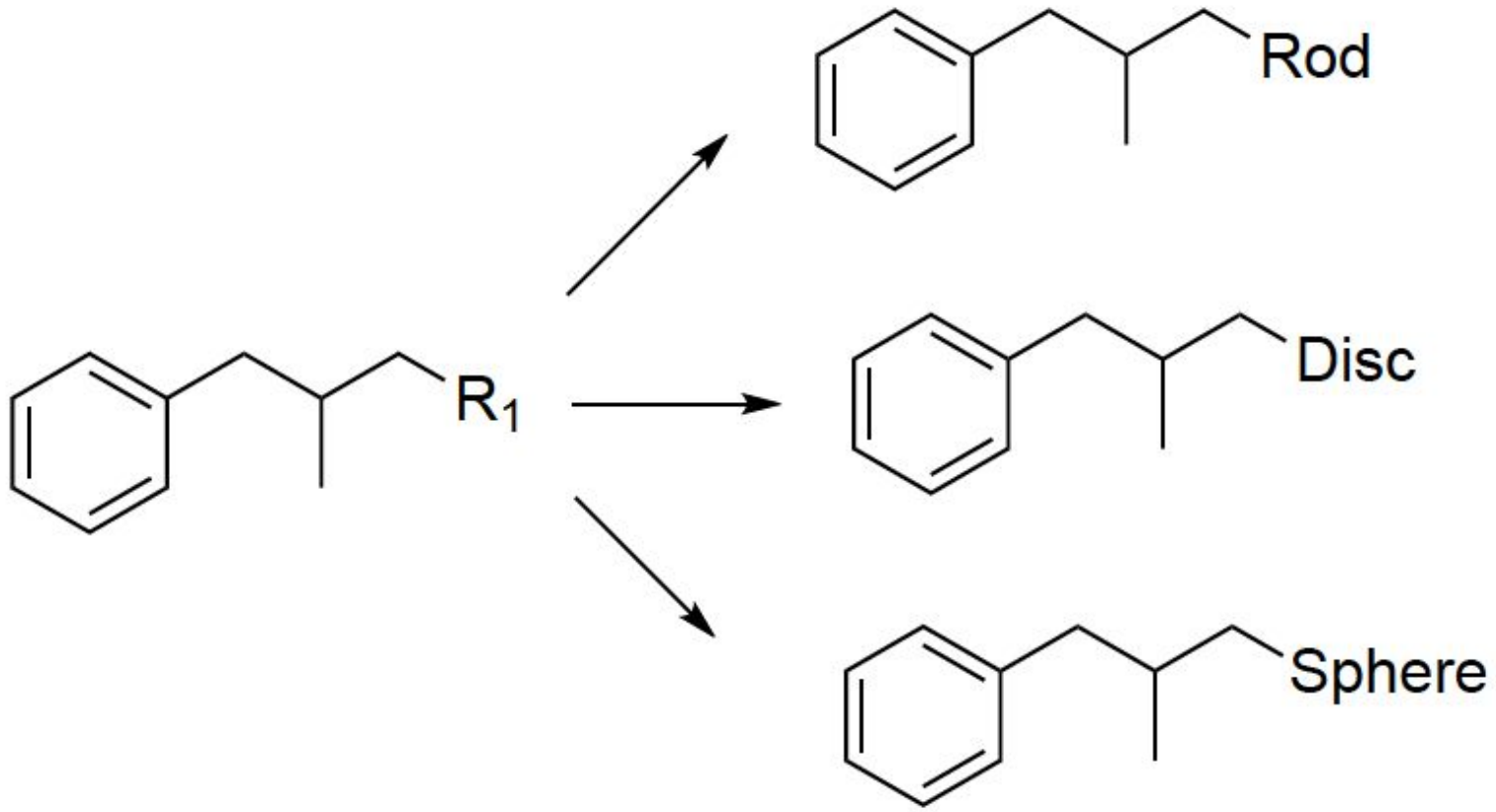
Can we include Shapes? **(Roadmap)**

Take any compound you would like to expand on and pass it through the cocktail to generate a library of compounds with different shapes.



sharifsuliman1@gmail.com

Enumeration Example

Cocktail Shaker reads Smiles

Peptide Molecule = ‘O=C(O)C(R1)NC(=O)C(R2)NC(=O)C(R3)C(=O)NO’

Wrap it in the Cocktail Object

Cocktail = Cocktail(Peptide Molecule)

Shake the Cocktail (Create the combinations)

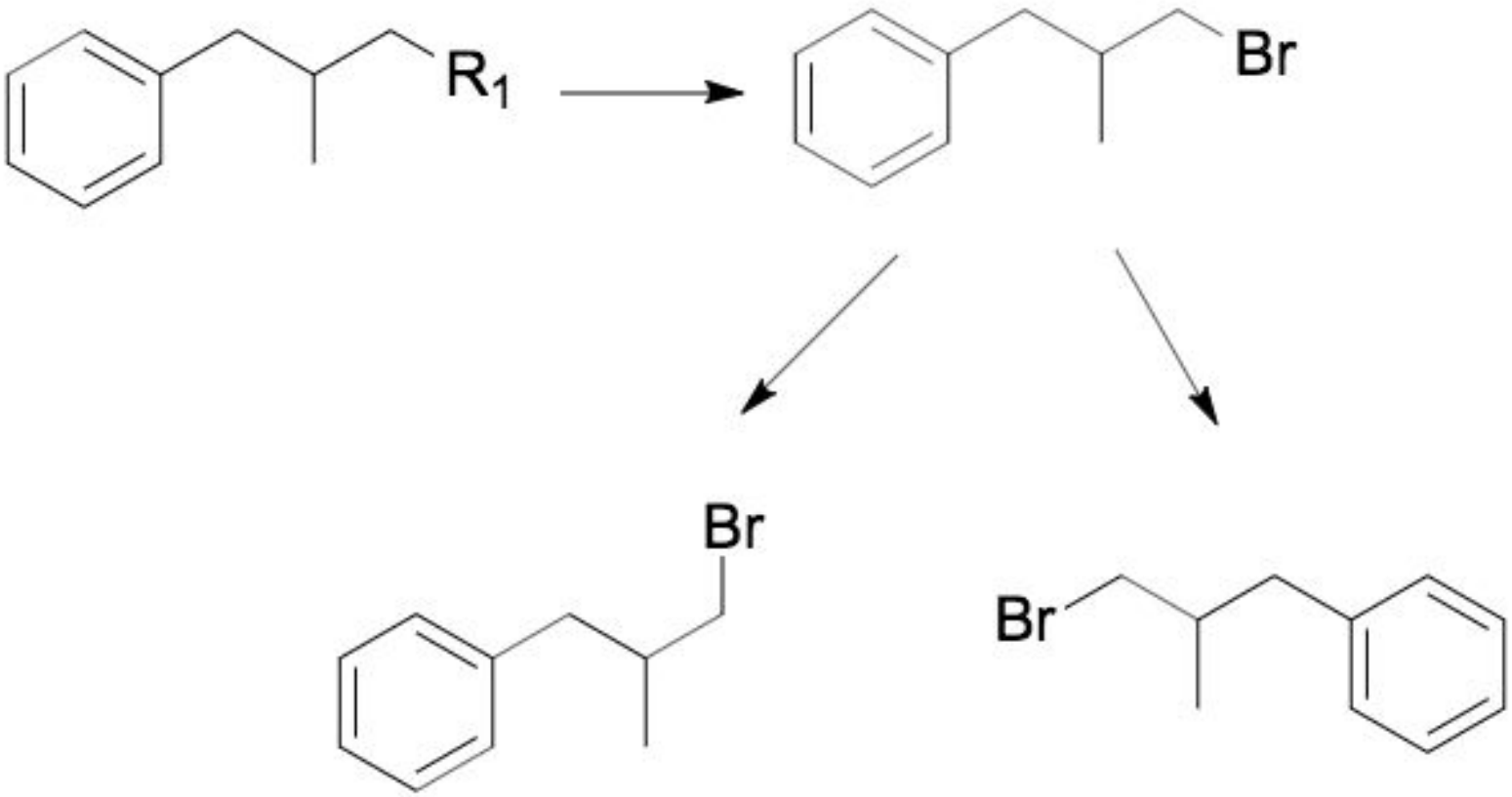
Combinations = Cocktail.Shake()

Enumerate the Combinations

Cocktail.enumerate(‘1D/2D/3D **(TBD)**’, Complexity=’Low/Med/High’)

sharifsuliman1@gmail.com

Enumeration Example (2D)



sharifsuliman1@gmail.com

Features

01 File Writing

File Writing for a lot of different types of chemical formats. As well as the ability to write to one file or many.

02 File Parsing (More coming soon)

Cocktail Shaker is capable of parsing in text, smiles, sdf, mol2

03 Spectral Data (Roadmap)

NMR, IR, HPLC, MS Data for your combination molecules

```
alc         # Alchemy format
cdxml       # CambridgeSoft ChemDraw XML format
cerius      # MSI Cerius II format
charmm      # Chemistry at Harvard Macromolecular Mechanics file format
cif         # Crystallographic Information File
cml         # Chemical Markup Language
gjf         # Gaussian input data file
gromacs     # GROMACS file format
hyperchem   # HyperChem file format
jme         # Java Molecule Editor format
maestro     # Schroedinger MacroModel structure file format
mol         # Symyx molecule file
mol2        # Tripos Sybyl MOL2 format
pdb         # Protein Data Bank
sdf         # 2D formatted structure data files
sdf3000     # Symyx Structure Data Format 3000
sln         # SYBYL Line Notation
xyz         # xyz file format
```

sharifsuliman1@gmail.com

Conclusion

- **Motivation** - simple to use python library to expand compound libraries and write them to chemical files.
- **Implementation** - how cocktail shaker works and utilizes RDKit to construct the molecules.
- **Use Cases/Feature Roadmap** - What is next for Cocktail Shaker?

sharifsuliman1@gmail.com

Cocktail Shaker

TravisCI

For allowing me to have my build system on their platform.

Github

Hosting my repository

ReadTheDocs

For hosting my documentation.

Gitter

Community chat for Cocktail Shaker

Bio-Rad

Access into the Spectral Database

sharifsuliman1@gmail.com

Awesome Team

Rose Gierth

Technical Writer

Marvin Corro

QA Tester

Elena Chow

Graphic Designer

sharifsuliman1@gmail.com

Acknowledgements

User Names:
baoilleach
mcs07
lwatobipen
hsiaoyi0504

Companies:

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Q & A