

Here are some links that I promised to send your way:

- Github link-1:  
Classical Machine-Learning to predict drug molecule class  
<https://github.com/ravichas/ML-predict-drugclass>
- Github Link 2:  
Neural network modeling to classify cancer types:  
<https://github.com/ravichas/ML-TC1>

**Drug like data sources:**

- PubChem: <https://pubchem.ncbi.nlm.nih.gov/>
- ChEMBL: <https://www.ebi.ac.uk/chembl/>
- NCATS: <https://opendata.ncats.nih.gov/covid19/>

**Useful Python Libraries:**

rdkit: Chemoinformatics library: <https://www.rdkit.org/docs/GettingStartedInPython.html>

DeepChem: Drug discovery software: <https://github.com/deepchem>

ATOM/AMPL: <https://github.com/ATOMconsortium/AMPL>