

Materials List for

Curation of Computational Chemical Libraries Demonstrated with Alpha-Amino Acids

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cmayerb1@umbc.edu**Citation**Mayer-Bacon, C., Yirik, M.A. Curation of Computational Chemical Libraries Demonstrated with Alpha-Amino Acids. *J. Vis. Exp.* (182), e63632, doi:10.3791/63632 (2022).**Date Published**

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URL

jove.com/video/63632

Materials

Name	Company	Catalog Number	Comments
conda v. 4.10.3			https://www.anaconda.com/products/individual
Java 17			https://java.com/en/download/help/download_options.html
MAYGEN v. 1.8			https://github.com/MehmetAzizYirik/MAYGEN/releases
PaDEL-Descriptor v. 2.21			http://www.yapcwsoft.com/dd/padeldescriptor/
python v. 3.7.11			included in Anaconda environment
RDKit v. 2020.09.1.0			https://www.rdkit.org/docs/Install.html , or installed via conda: https://anaconda.org/rdkit/rdkit
*These specific versions were used for this manuscript; user can obtain more recent versions if available.			