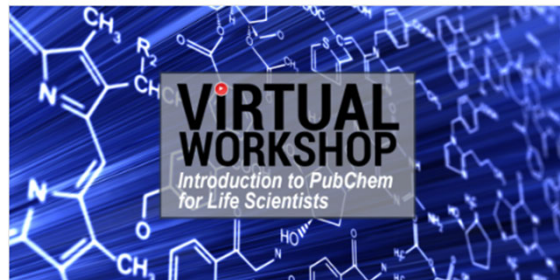


Overview

- Background
- Searching in PubChem
- Finding molecular & chemical safety information
- Using PubChem Sketcher
- Finding a potential inhibitor

NIH National Library of Medicine
National Center for Biotechnology Information



An Introduction to PubChem for Life Scientists

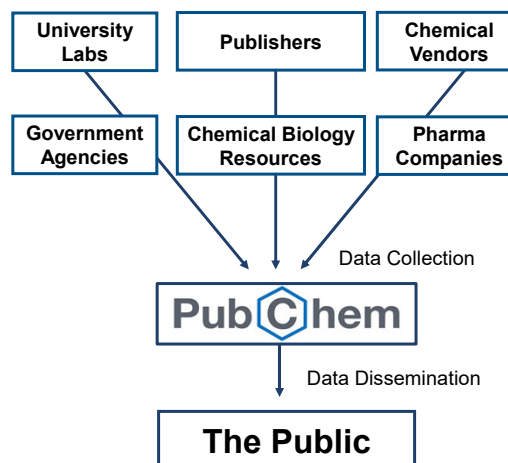
Scientists and educators from many different fields need to find and understand chemical data to perform their work. As such, understanding PubChem, the world's largest collection of freely accessible chemical information, is a powerful skill for researchers, educators, clinicians, and more. In this workshop, participants will have access to NCBI experts and be introduced to the functionality of the PubChem Database.

[Introduction](#)

What is PubChem?

- Created in 2004
- World's largest collection of freely accessible chemical information
 - Key chemical information resource for scientists, students, and the public
- Learn more:
 - <https://pubchem.ncbi.nlm.nih.gov>

NIH National Library of Medicine
National Center for Biotechnology Information



What's in PubChem?

- Small molecules
- Larger molecules
 - Nucleotides
 - Carbohydrates
 - Lipids
 - Peptides
 - Chemically-modified macromolecules
- And more



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PubChem

Explore Chemistry

Quickly find chemical information from authoritative sources

Try covid-19 aspirin EGFR C9H8O4 57-27-2

 Use Entrez

Draw Structure Upload ID List Browse Data Periodic Table

112M Compounds 871 Data Sources

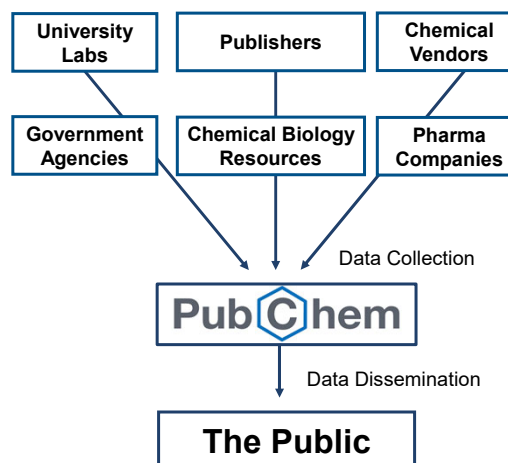
Common uses for PubChem

- Learn about a chemical, drug, or medication
- Get biological function, molecular structure, molecular weight, chemical safety, etc. data for fundamental research
- Mine data for biochemical research
 - Drug discovery, drug-gene targeting, toxicology



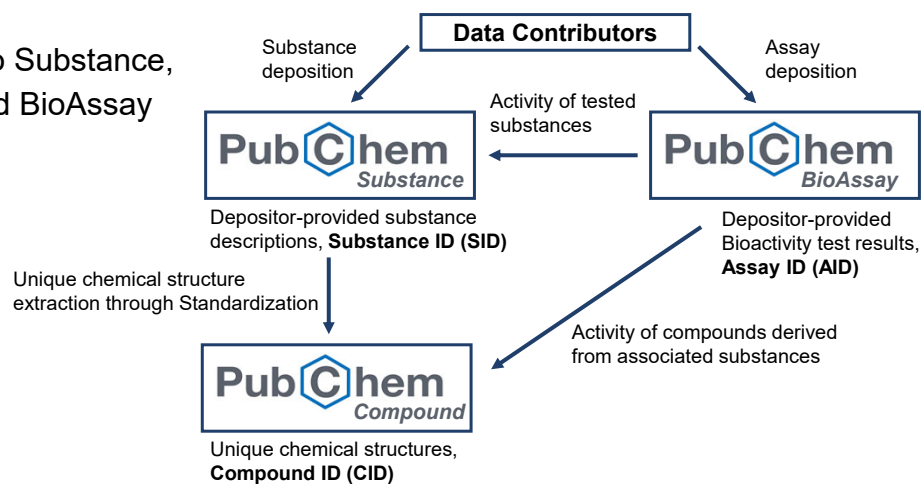
Who provides PubChem Data?

- Submitters and contributors are vetted
 - Algorithmically
 - Manually
 - Post-production



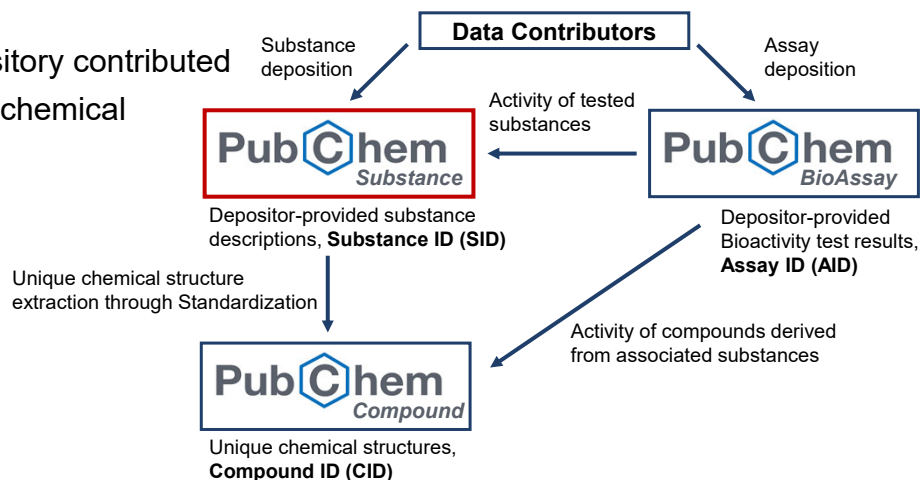
Data Organization

- Three Linked to Substance, Compound, and BioAssay Databases



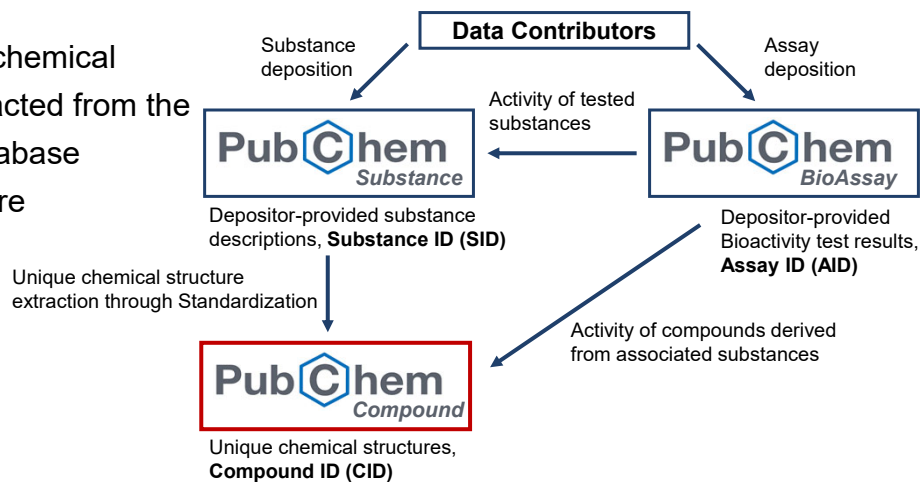
Substance Database

- Archives depository contributed descriptions of chemical substances



Compound Database

- Stores unique chemical structures extracted from the Substance Database through structure standardization



BioAssay Database

- Contains the description and test results of biological assay experiments

