



An Introduction to PubChem for Life Scientists

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National Library of Medicine
National Center for Biotechnology Information

[Workshop Details](#)

Overview

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



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.

POLL (1/4)

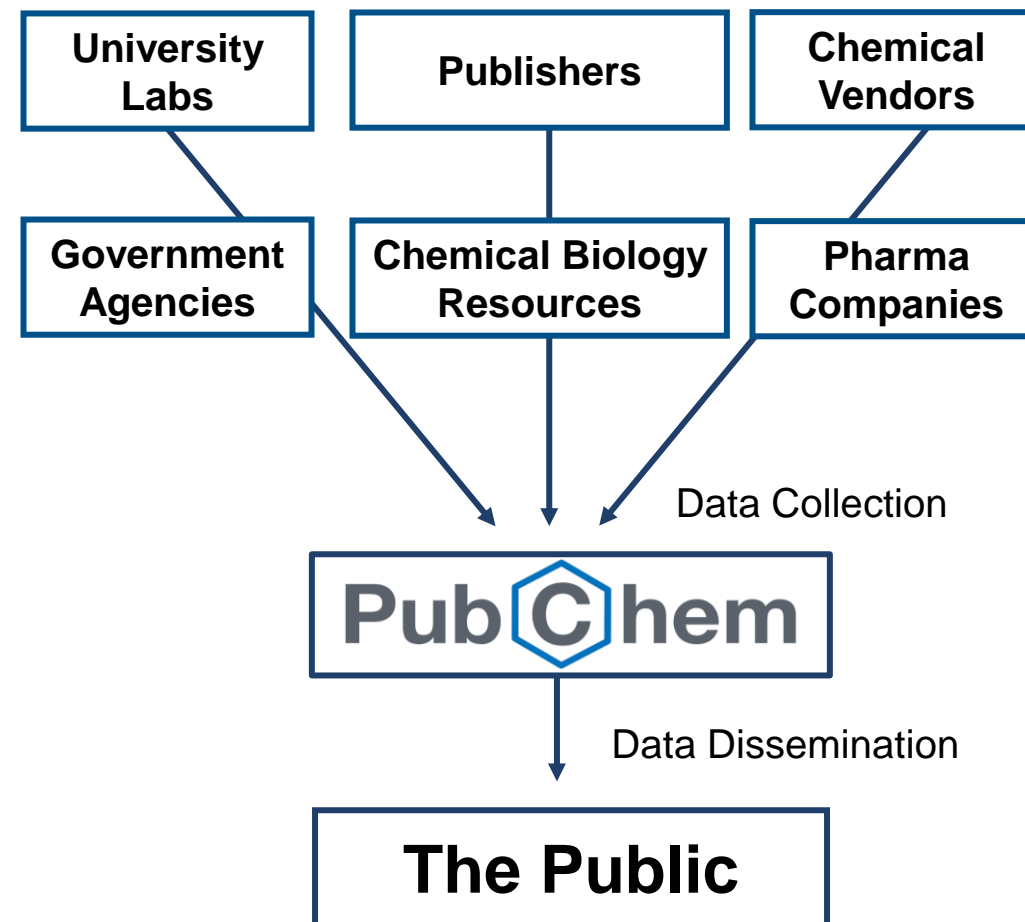
Which best describe your work, research,
or educational background?

POLL (2/4)

Have you attended an NCBI
workshop before?

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>



What's in PubChem?

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



The screenshot shows the top portion of the PubChem website. At the top, the NIH logo and the text "National Library of Medicine National Center for Biotechnology Information" are displayed in white on a dark blue background. Below this is the PubChem logo and a hamburger menu icon. The main content area has a dark blue header with the text "Explore Chemistry" and "Quickly find chemical information from authoritative sources". A search bar is present with a magnifying glass icon. Below the search bar, several search suggestions are listed: "Try covid-19 aspirin EGFR C9H8O4 57-27-2". There is a checkbox labeled "Use Entrez". At the bottom of the main content area, four icons represent different functions: "Draw Structure" (a pencil drawing a chemical structure), "Upload ID List" (an upward arrow), "Browse Data" (a grid of squares), and "Periodic Table" (a grid of dots representing the periodic table). The footer of the page shows "112M Compounds" and "871 Data Sources" in white text on a light gray background.

Common uses for PubChem

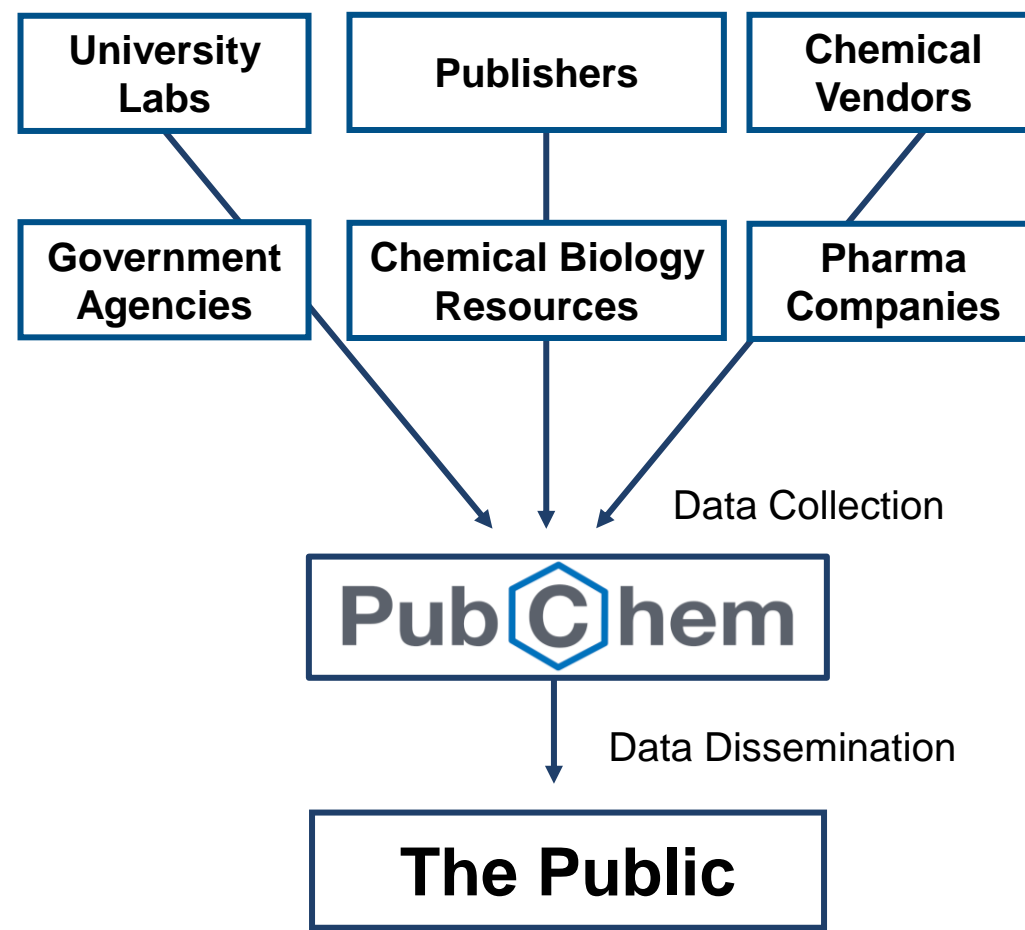
- Learn about a chemical, drug, or medication
- Get biological function, molecular structure, molecular weight, chemical safety, etc. data for fundamental research
- Mine data for biochemical research
 - Drug discovery, drug-gene targeting, toxicology

POLL (3/4)

What do you currently
use PubChem for?

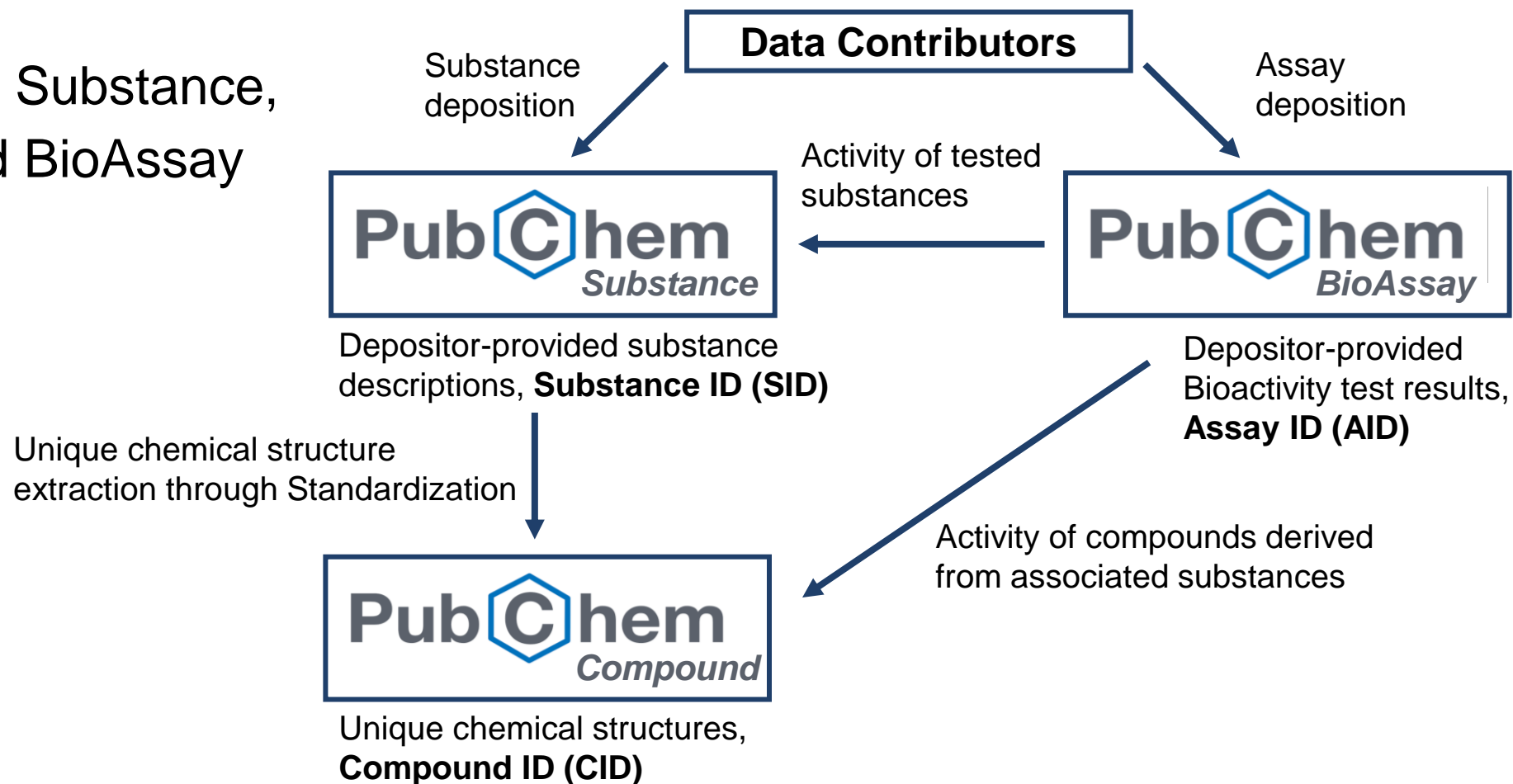
Who provides PubChem Data?

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



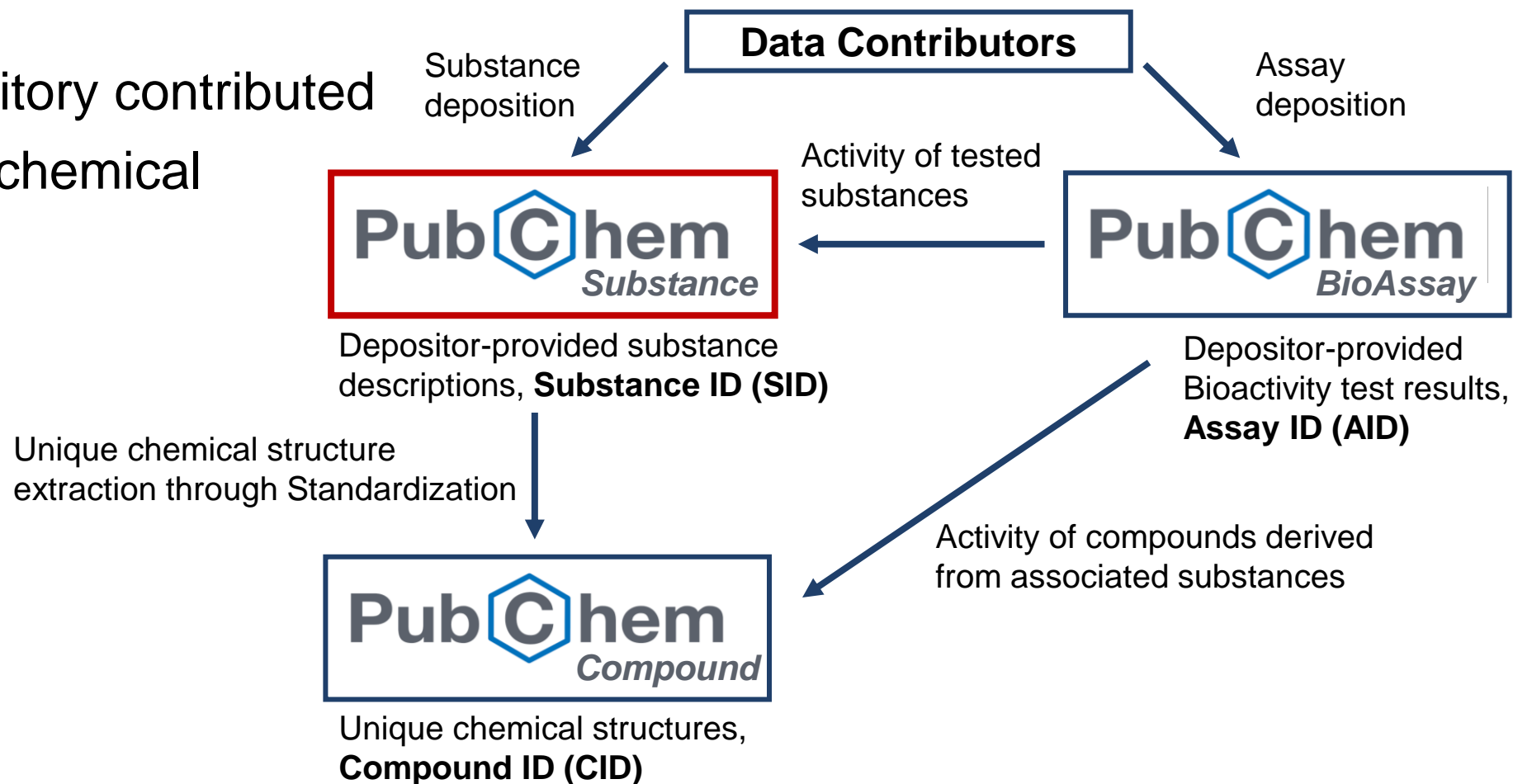
Data Organization

- Three Linked to Substance, Compound, and BioAssay Databases



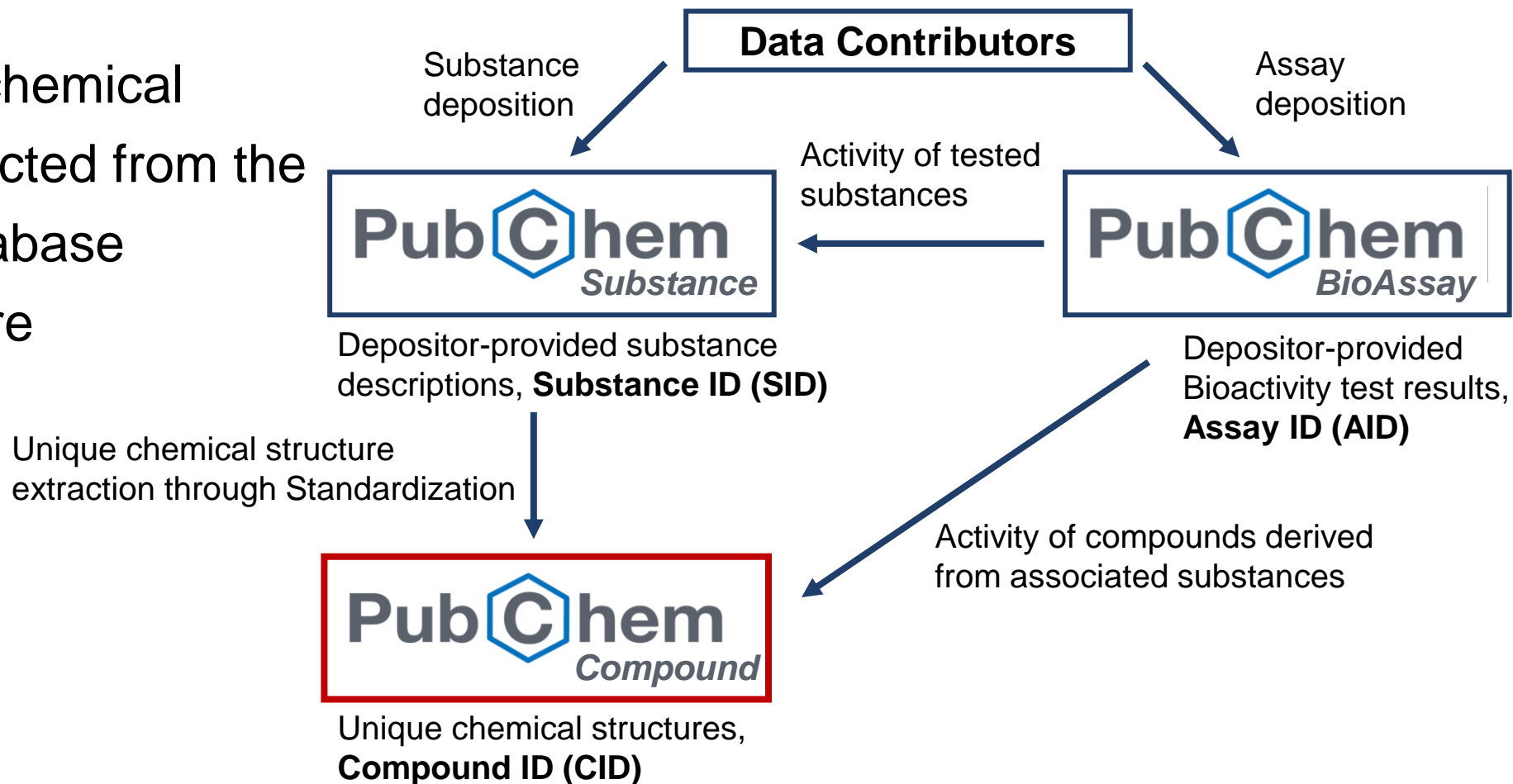
Substance Database

- Archives depository contributed descriptions of chemical substances



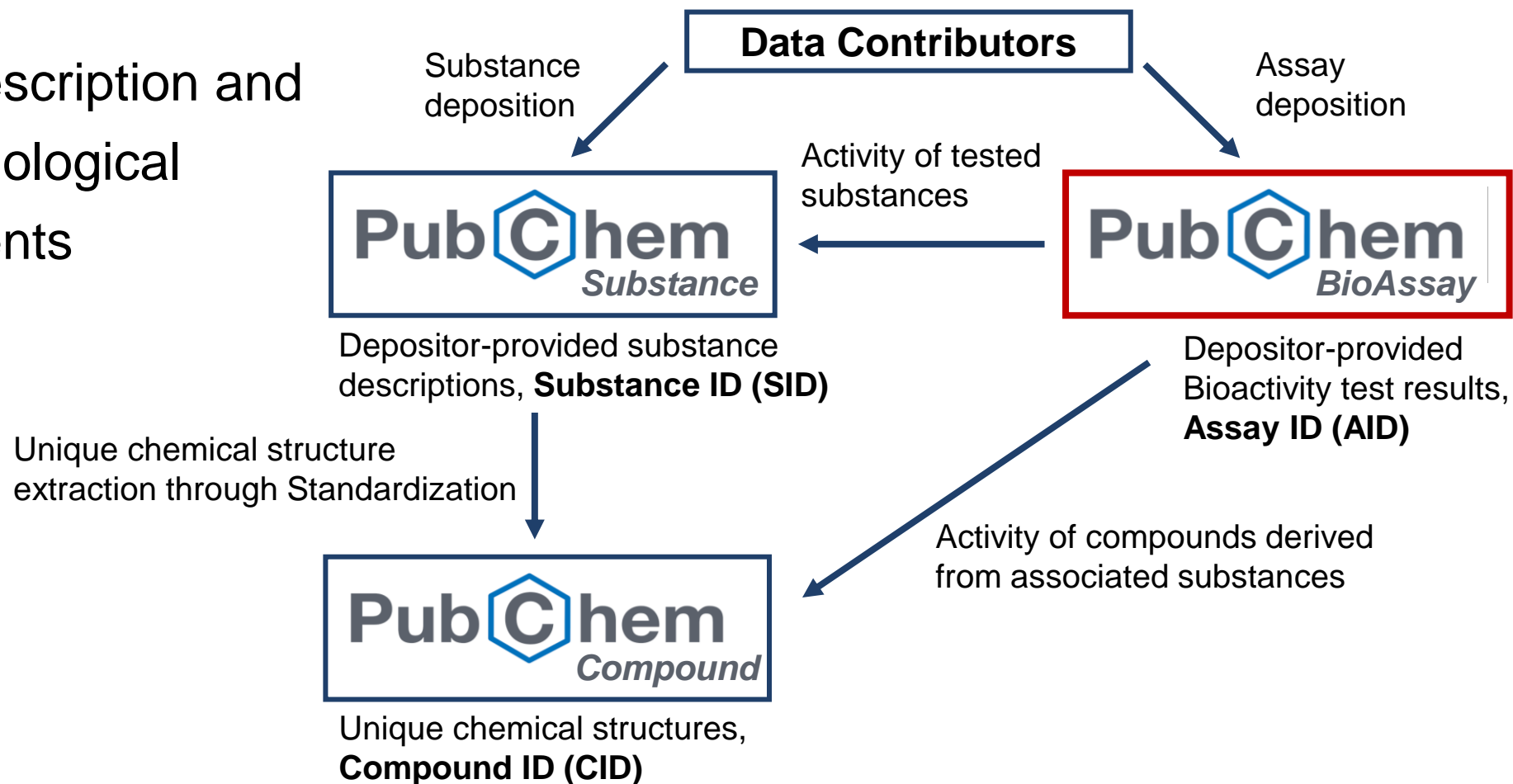
Compound Database

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



BioAssay Database

- Contains the description and test results of biological assay experiments



Searching in [PubChem](#)

The image shows the 'Explore Chemistry' search page on PubChem. At the top, the text 'Explore Chemistry' is displayed in large white font on a dark blue background. Below it, a subtitle reads 'Quickly find chemical information from authoritative sources'. A large white search bar is centered, with a magnifying glass icon on the right. Below the search bar, a row of search suggestions is shown: 'Try covid-19 aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3'. Below the suggestions, there are four radio button options: 'Use Entrez' (unchecked), 'Compounds' (checked), 'Substances' (unchecked), and 'BioAssays' (unchecked). At the bottom, there are four icons with labels: 'Draw Structure' (a chemical structure with a pencil), 'Upload ID List' (an upward arrow), 'Browse Data' (a grid of squares), and 'Periodic Table' (a grid of dots).

Common Search Strategies

Text

covid-19 OR aspirin

Molecular Formula

C9H8O4

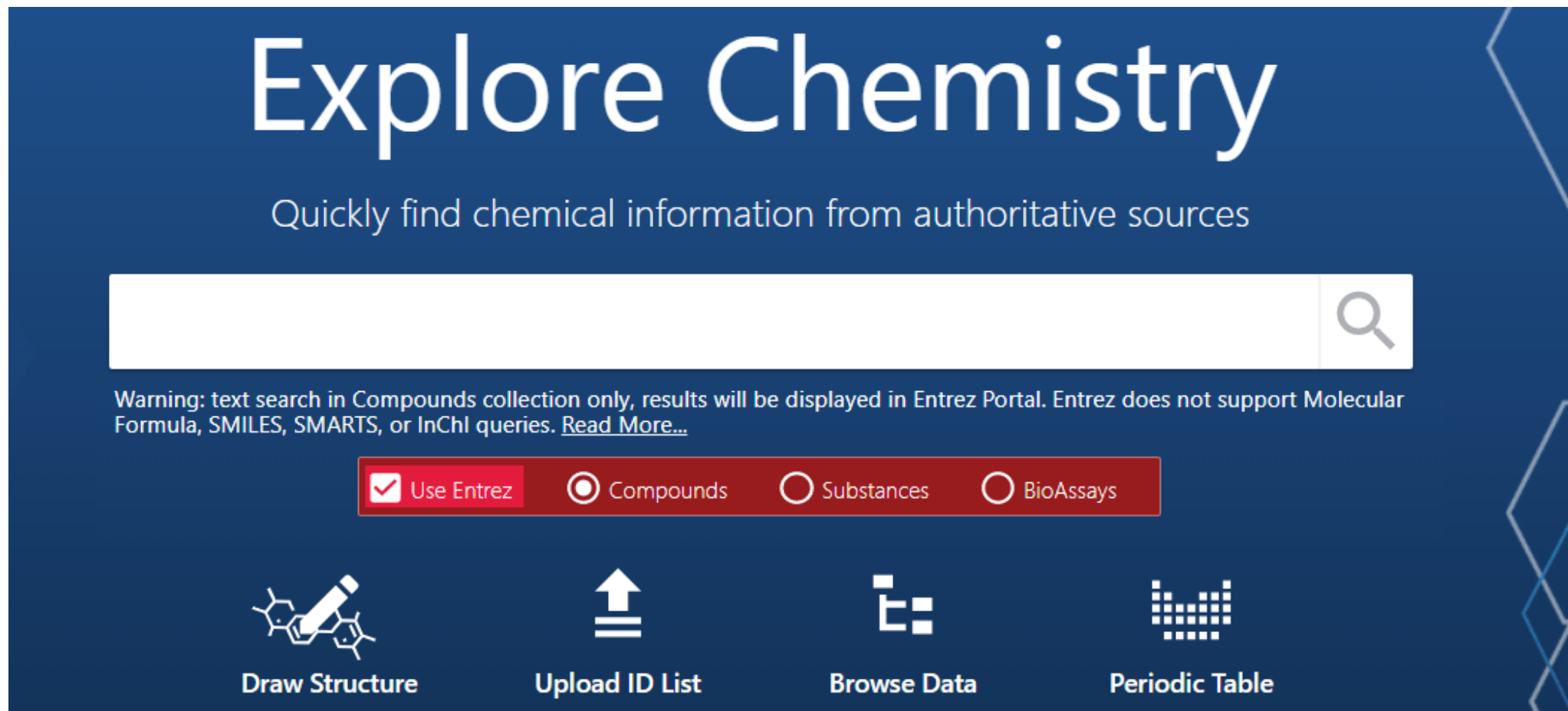
**Simplified Molecular Input
Line Entry System (SMILES)**

C1=CC=C (C=C1) C=O

InChI Identifier

InChI=1S/C3H6O/c1-3 (2) 4/h1-2H3


Searching with Entrez



The screenshot shows the 'Explore Chemistry' search page. At the top, the title 'Explore Chemistry' is displayed in large white font on a dark blue background. Below it, the subtitle 'Quickly find chemical information from authoritative sources' is shown in a smaller white font. A large white search input field with a magnifying glass icon on the right is positioned below the subtitle. Underneath the search field, a warning message reads: 'Warning: text search in Compounds collection only, results will be displayed in Entrez Portal. Entrez does not support Molecular Formula, SMILES, SMARTS, or InChI queries. [Read More...](#)'. Below the warning is a red navigation bar with four options: 'Use Entrez' (checked), 'Compounds', 'Substances', and 'BioAssays'. At the bottom of the interface, there are four icons with corresponding labels: 'Draw Structure' (a chemical structure with a pencil), 'Upload ID List' (an upward arrow), 'Browse Data' (a grid of squares), and 'Periodic Table' (a grid of dots).





Explore Chemistry

Quickly find chemical information from authoritative sources



Warning: text search in Compounds collection only, results will be displayed in Entrez Portal. Entrez does not support Molecular Formula, SMILES, SMARTS, or InChI queries. [Read More...](#)

Use Entrez Compounds Substances BioAssays

 Draw Structure  Upload ID List  Browse Data  Periodic Table

Search Tips

Entrez is a molecular biology database system that provides access to a wealth of NCBI data

- More [Entrez Help](#) is available on the NCBI website

Finding structures with Entrez

```
"anti inflammatory agents, non steroidal"[pharmacation]
```

- Use field limits and Boolean operators
- Put phrases in quotes

Text searching in PubChem (1/8)

Click Use Entrez and Compounds, then use the field PharmAction to limit by Pharmacological action:

"anti inflammatory agents, non steroidal"[PharmAction]



Warning: text search in Compounds collection only, results will be displayed in Entrez Portal. Entrez does not support Molecular Formula, SMILES, SMARTS, or InChI queries. [Read More...](#)



Use Entrez



Compounds



Substances



BioAssays

Text searching in PubChem (2/8)

Narrow your search to single chemical NSAIDS by adding another term, and **1[CovalentUnitCount]**:

...non steroidal"[PharmAction] and 1[CovalentUnitCount]



Warning: text search in Compounds collection only, results will be displayed in Entrez Portal. Entrez does not support Molecular Formula, SMILES, SMARTS, or InChI queries. [Read More...](#)



Use Entrez



Compounds



Substances



BioAssays

Text searching in PubChem (3/8)

Or narrow your search to smaller chemical molecules (<400 g/mol) with, and **0:400[MolecularWeight]**

... agents, non steroidal"[PharmAction] and 0:400[MolecularWeight]



Warning: text search in Compounds collection only, results will be displayed in Entrez Portal. Entrez does not support Molecular Formula, SMILES, SMARTS, or InChI queries. [Read More...](#)



Use Entrez



Compounds



Substances



BioAssays

Text searching in PubChem (4/8)

Or narrow your search by including a simple term, and aspirin:

"anti inflammatory agents, non steroidal"[pharmaction] and aspirin



Warning: text search in Compounds collection only, results will be displayed in Entrez Portal. Entrez does not support Molecular Formula, SMILES, SMARTS, or InChI queries. [Read More...](#)



Use Entrez



Compounds



Substances



BioAssays

Text searching in PubChem (5/8)

Answer the following:

5-minute exercise!

- What are synonyms for aspirin?
- What is the Molecular Formula?
- Molecular weight?
- Are there patents associated with this entry?
- Do you recognize any of the information sources?

Share an information source
you recognize in the chat!

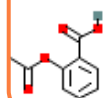
Text searching in PubChem (6/8)

Click on the Best Match result:

aspirin

Treating this as a text search.

BEST MATCH



Aspirin; ACETYLSALICYLIC ACID; 50-78-2; 2-Acetoxybenzoic Acid; 2-(Acetyloxy)Benzoic Acid; O-Acetylsalicylic Acid; O-Acetoxybenzoic Acid; Acylpyrin; ...

Compound CID: 2244

MF: C₉H₈O₄ MW: 180.16g/mol

IUPAC Name: 2-acetoxybenzoic acid

Isomeric SMILES: CC(=O)OC1=CC=CC=C1C(=O)O

InChIKey: BSYNRYMUTXBXSQ-UHFFFAOYSA-N

InChI: InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)

Create Date: 2004-09-16

[Summary](#)

[Similar Structures Search](#)

[Related Records](#)

[PubMed \(MeSH Keyword\)](#)

Text searching in PubChem (7/8)

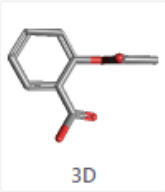
Review the compound summary page:

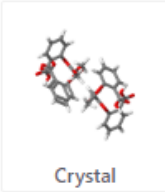
Aspirin

PubChem CID 2244

Structure


 2D

 3D

 Crystal

[Find Similar Structures](#)

Chemical Safety



Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula $C_9H_8O_4$ or $CH_3COOC_6H_4COOH$

CONTENTS

- Title and Summary
- 1 Structures
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Spectral Information
- 5 Related Records
- 6 Chemical Vendors
- 7 Drug and Medication Information
- 8 Pharmacology and Biochemistry
- 9 Use and Manufacturing
- 10 Identification
- 11 Safety and Hazards
- 12 Toxicity
- 13 Associated Disorders and Diseases
- 14 Literature
- 15 Patents

Text searching in PubChem (8/8)

Click on the LCSS Datasheet:

Aspirin


PubChem CID 2244

Structure

2D 3D Crystal

Find Similar Structures

Chemical Safety


Irritant

[Laboratory Chemical Safety Summary \(LCSS\) Datasheet](#)

Molecular Formula $C_9H_8O_4$ or $CH_3COOC_6H_4COOH$

CONTENTS

Title and Summary

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8 Pharmacology and Biochemistry

9 Use and Manufacturing

10 Identification

11 Safety and Hazards

12 Toxicity

13 Associated Disorders and Diseases

14 Literature

15 Patents

Finding safety information

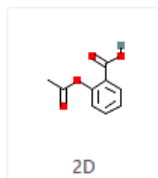
COMPOUND SUMMARY > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS)

Aspirin

PubChem CID

2244

Structure



[Find Similar Structures](#)

Synonyms

aspirin
ACETYLSALICYLIC ACID
50-78-2
2-Acetoxybenzoic acid
2-(Acetyloxy)benzoic acid

[More...](#)

Molecular Formula

$C_9H_8O_4$ or $CH_3COOC_6H_4COOH$

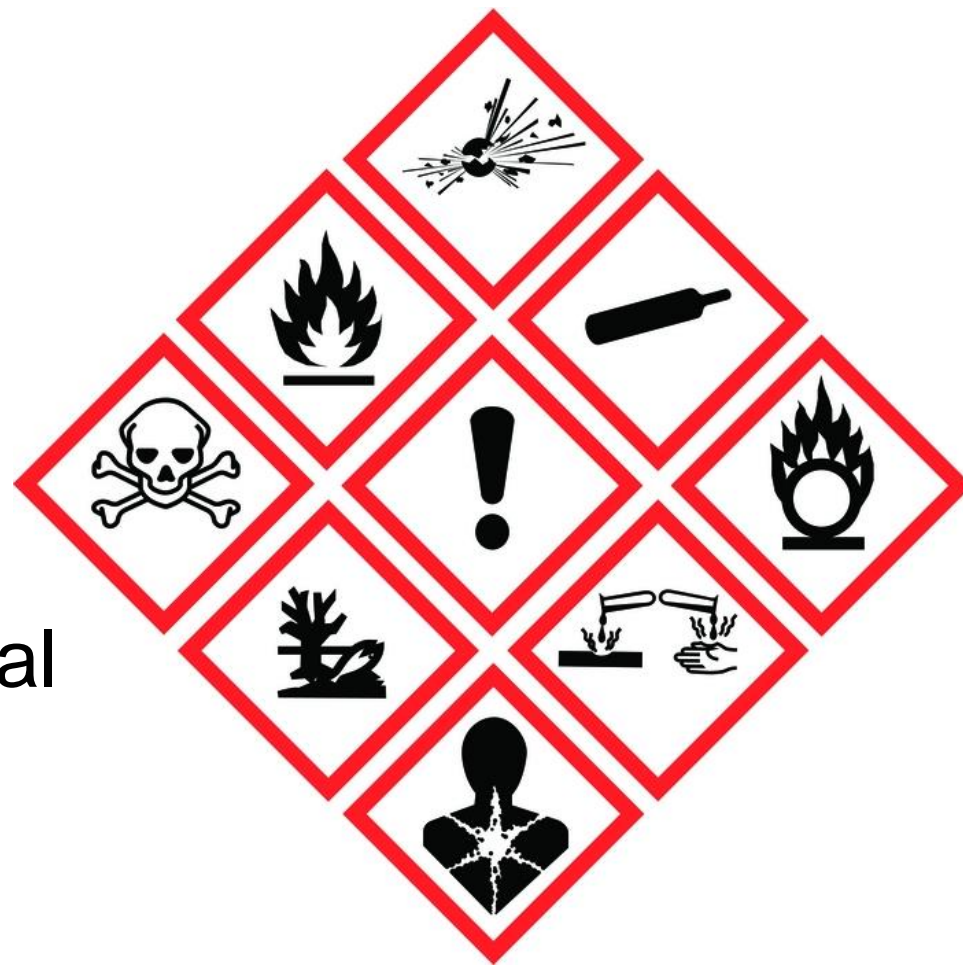
Molecular Weight

180.16

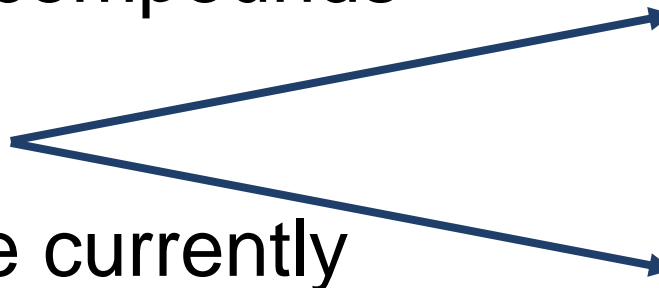
[Learn More About LCSS Project >](#)

Chemical safety information

- Lab safety is an essential topic in all labs
- PubChem's Laboratory Chemical Safety Summary (LCSS) is a thorough online resource for chemical safety information



PubChem LCSS

- You can find LCSS from the summary page of applicable compounds
 - 12 main headings
 - >170,000 LCSS are currently available in PubChem
- 

Contents

1 GHS Classification [Learn more](#)

2 Identifiers

3 Physical Properties

4 Toxicity Information

5 Exposure Limits

6 Health and Symptoms

7 First Aid

8 Flammability and Explosivity

9 Stability and Reactivity

3-minute exercise!

12 Information Sources

Searching with [PubChem Sketcher](#)

- PubChem Sketcher is a web-based chemical structure sketching tool
- Allows users to search a manually drawn or modified structure
- Supports [CID](#), [SMILES](#), [SMARTS](#), [InChI](#), Molecular Formula, and select uploaded file formats
- More information at [PubChem Sketcher Help](#)

Searching with PubChem Sketcher (1/10)

Go to the [PubChem homepage](#). You can search by structure from the start by clicking on Draw Structure:

The screenshot shows the PubChem homepage with the following elements:

- Header:** "Explore Chemistry" in large white font, with the subtitle "Quickly find chemical information from authoritative sources" below it.
- Search Bar:** A large white search bar with a magnifying glass icon on the right.
- Example Searches:** A row of search suggestions: "Try covid-19 aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3".
- Filters:** A row of radio buttons: "Use Entrez" (unchecked), "Compounds" (checked), "Substances" (unchecked), and "BioAssays" (unchecked).
- Navigation Buttons:** Four buttons at the bottom: "Draw Structure" (with a pencil and chemical structure icon, highlighted with a red dashed box), "Upload ID List" (with an upload icon), "Browse Data" (with a grid icon), and "Periodic Table" (with a periodic table icon).

Searching with PubChem Sketcher (2/10)

And manually drawing a structure of interest or inputting SMILES, SMARTS, InChI, and InChiKey information:

SMILES O(C1=CC=CC=C1C(O[H])=O)[H]

InChIKey=YGSDEFSMJLZEOE-UHFFFAOYSA-N

Formula C₇H₆O₃ [138.123 gr/mol]

EDIT STRUCTURE

Broadband ▾ Formula ▾ C₇H₆O₃ [138.123 gr/mol]

New Undo Cln Sty Del Qry

SMILES O(C1=CC=CC=C1C(O[H])=O)[H]

InChIKey=YGSDEFSMJLZEOE-UHFFFAOYSA-N

Formula C₇H₆O₃ [138.123 gr/mol]

Export MDL Molfile ▾ Done

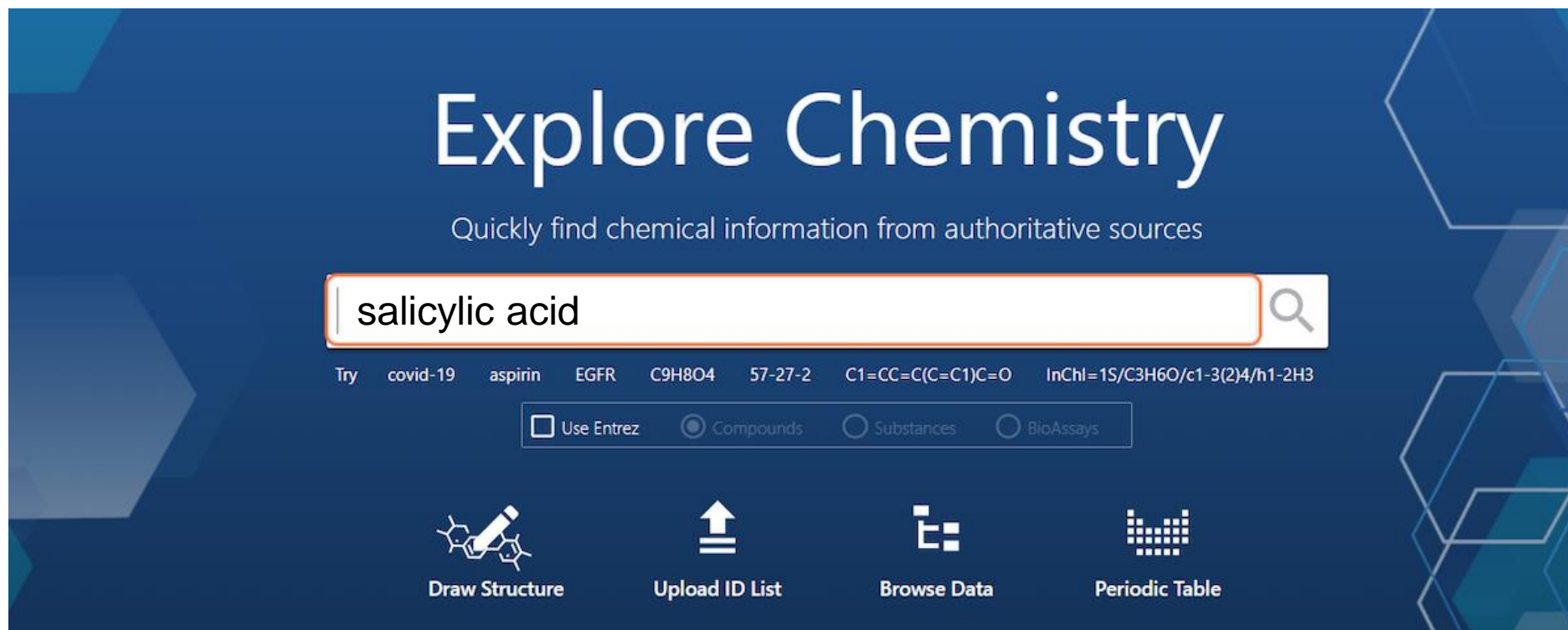
Hydrogen Keep AsIs ▾ Help

Import Choose File No file chosen

Search for This Structure

Searching with PubChem Sketcher (3/10)

Or you can find a similar structure during a text query. Here we will type "salicylic acid" into input:



Explore Chemistry

Quickly find chemical information from authoritative sources

salicylic acid

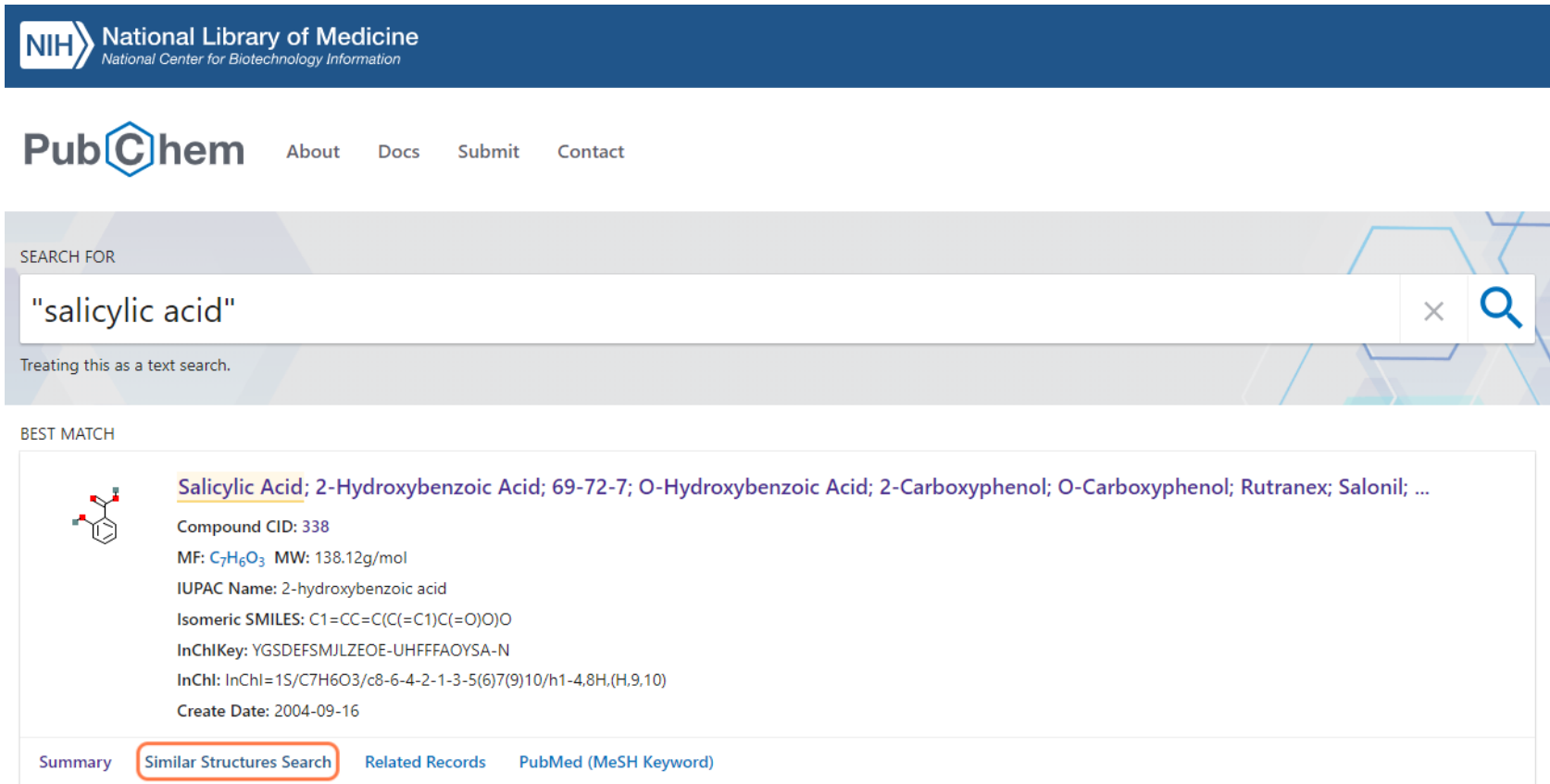
Try covid-19 aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3

Use Entrez Compounds Substances BioAssays

Draw Structure Upload ID List Browse Data Periodic Table

Searching with PubChem Sketcher (4/10)

And click on the Similar Structures Search:



The screenshot shows the PubChem website interface. At the top, there is a blue header with the NIH logo and the text "National Library of Medicine National Center for Biotechnology Information". Below this is the PubChem logo and navigation links: "About", "Docs", "Submit", and "Contact". The main search area has a search bar containing the text "salicylic acid" and a search icon. Below the search bar, it says "Treating this as a text search." The results section is titled "BEST MATCH" and shows a card for Salicylic Acid. The card includes a chemical structure icon, the name "Salicylic Acid; 2-Hydroxybenzoic Acid; 69-72-7; O-Hydroxybenzoic Acid; 2-Carboxyphenol; O-Carboxyphenol; Rutranex; SaloniL; ...", and various identifiers: "Compound CID: 338", "MF: C₇H₆O₃ MW: 138.12g/mol", "IUPAC Name: 2-hydroxybenzoic acid", "Isomeric SMILES: C1=CC=C(C(=C1)C(=O)O)O", "InChIKey: YGSDEFSMJLZEOE-UHFFFAOYSA-N", "InChI: InChI=1S/C7H6O3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H,(H,9,10)", and "Create Date: 2004-09-16". At the bottom of the card, there are four tabs: "Summary", "Similar Structures Search" (which is highlighted with an orange border), "Related Records", and "PubMed (MeSH Keyword)".

NIH National Library of Medicine
National Center for Biotechnology Information


PubChem About Docs Submit Contact

SEARCH FOR

"salicylic acid"

Treating this as a text search.

BEST MATCH

 [Salicylic Acid; 2-Hydroxybenzoic Acid; 69-72-7; O-Hydroxybenzoic Acid; 2-Carboxyphenol; O-Carboxyphenol; Rutranex; SaloniL; ...](#)

Compound CID: 338
MF: C₇H₆O₃ MW: 138.12g/mol
IUPAC Name: 2-hydroxybenzoic acid
Isomeric SMILES: C1=CC=C(C(=C1)C(=O)O)O
InChIKey: YGSDEFSMJLZEOE-UHFFFAOYSA-N
InChI: InChI=1S/C7H6O3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H,(H,9,10)
Create Date: 2004-09-16

Summary **Similar Structures Search** Related Records PubMed (MeSH Keyword)

Searching with PubChem Sketcher (5/10)

Select Edit Structures:

NIH National Library of Medicine
National Center for Biotechnology Information

PubChem About Docs Submit Contact

SEARCH FOR

CID338 structure

Treating this as a structure search for CID 338. [Edit Structure](#) Search for **CID338 structure as text** instead.

Identity (1) **Similarity (>1,000)** Substructure (>1,000) Superstructure (>1,000) 3D Similarity (>794) [Settings](#)

Fingerprint Tanimoto-based 2-dimensional similarity search.

Searching with PubChem Sketcher (6/10)

Then make any changes:

SEARCH FOR

CID338 stru

Treating this as a struct

Identity (1)

Fingerprint Tanimoto-ba

Percentage of the

Search All

1,000 results (incom

SEARCH FOR

EDIT STRUCTURE

Broadband SMILES O(C1=CC=CC=C1C(O[H])=O)[H]

New Undo Clear Style Delete Query Rotate Copy Paste

Single bond Double bond Triple bond Arrow Wedge Dotted line Wavy line X-Ray S/A D/A S/D

Triangle Square Pentagon Hexagon Heptagon Octagon Nonagon Decagon Grid Plus Minus Circle

Alkyl groups: Methyl, Ethyl, Propyl, Isopropyl, Butyl, Pentyl, Hexyl, Heptyl, Octyl, Nonyl, Decyl, Undecyl, Dodecyl, Tridecyl, Tetradecyl, Pentadecyl, Hexadecyl, Heptadecyl, Octadecyl, Nonadecyl, Eicosyl, Heteroalkyl groups: CHO, CO₂H, NO₂, SO₃H

H		?	? ▼							He
Li	Be				B	C	N	O	F	Ne
Na	Mg				Al	Si	P	S	Cl	Ar
K	Ca	Sc	Sc ▼		Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Y ▼		In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Lu ▼		Tl	Pb	Bi	Po	At	Rn

Export MDL Molfile Done

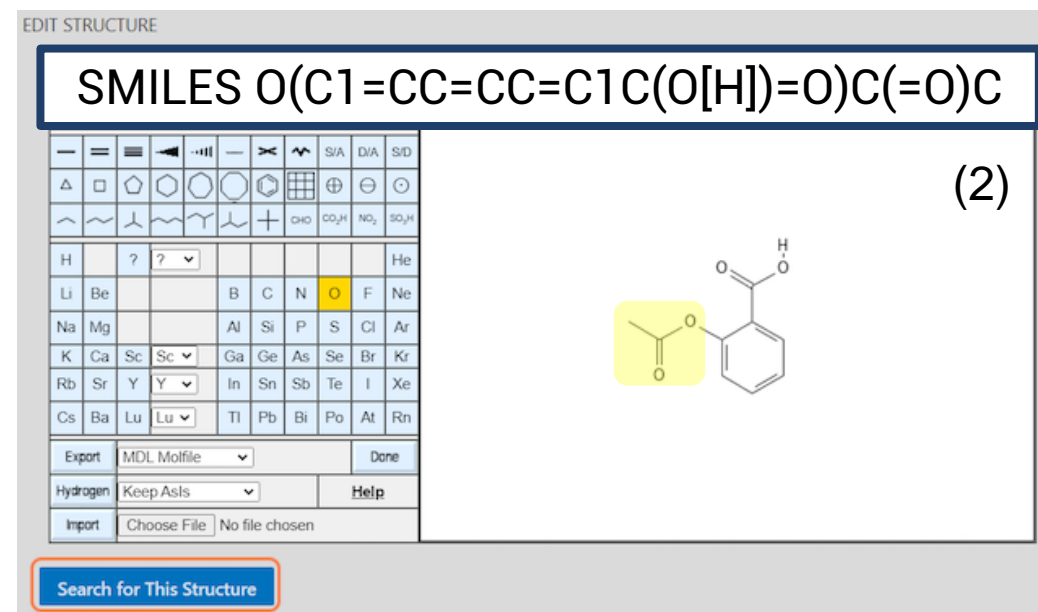
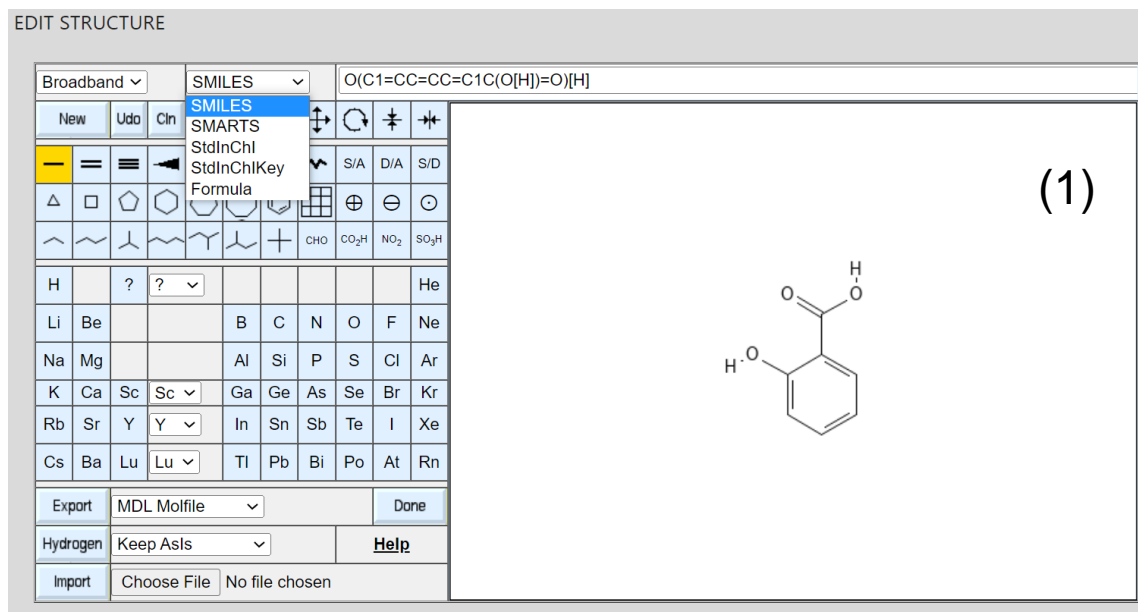
Hydrogen Keep AsIs Help

Import Choose File No file chosen

Search for This Structure

Searching with PubChem Sketcher (7/10)

Here, you can replace the phenol (1) with a carboxyl manually (2) or change the SMILES String to O(C1=CC=CC=C1C(O[H])=O)C(=O)C:



Searching with PubChem Sketcher (8/10)

And click on Search for This Structure to see how this effects the PubChem results:

EDIT STRUCTURE

SMILES O(C1=CC=CC=C1C(O[H])=O)C(=O)C

Periodic Table: O is highlighted.

Chemical Structure: Aspirin (acetylsalicylic acid).


Buttons: Search for This Structure

Searching with PubChem Sketcher (9/10)

You will find a handful of results, one that may be of interest is Aspirin; ACETYLSALICYLIC ACID. You can open this entry to learn more:


PubChem

Summary Similar Structures Search Related Records

 **Aspirin; ACETYLSALICYLIC ACID; 50-78-2; 2-Acetoxybenzoic Acid; 2-(Acetyloxy)Benzoic Acid; ...**

Compound CID: 2244
MF: C₉H₈O₄ MW: 180.16g/mol
IUPAC Name: 2-acetoxybenzoic acid
Isomeric SMILES: CC(=O)OC1=CC=CC=C1C(=O)O
InChIKey: BSYNRYMUTXBXSQ-UHFFFAOYSA-N
InChI: InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)
Create Date: 2004-09-16

Summary Similar Structures Search Related Records PubMed (MeSH Keyword)

 **2-METHOXYBENZOIC ACID; O-Anisic Acid; 579-75-9; O-Methylsalicylic Acid; O-Methoxybenzoic Acid; ...**

Compound CID: 11370
MF: C₈H₈O₃ MW: 152.15g/mol
IUPAC Name: 2-methoxybenzoic acid
Isomeric SMILES: COC1=CC=CC=C1C(=O)O
InChIKey: ILUJQPXNXACGAN-UHFFFAOYSA-N

Searching with PubChem Sketcher (10/10)

More information about the PubChem Sketcher can be found [here](#):

5-minute break!

[PubChem](#) » [PubChem Help](#) » Sketcher Help

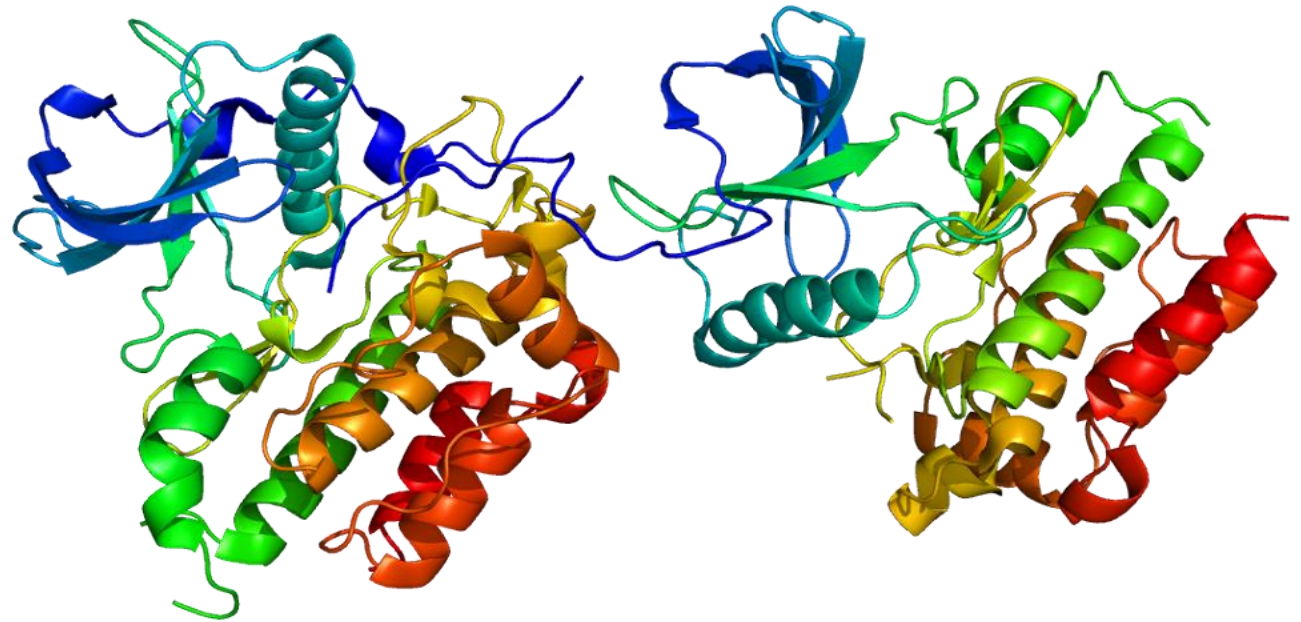
PubChem Sketcher Help

1. [Example](#)
2. [Editor Window Layout](#)
3. [Button Area](#)
4. [Mouse Use](#)
5. [Error Reporting](#)
6. [Bandwidth Control](#)
7. [Element Buttons](#)
8. [Bond Drawing](#)
9. [Special Bond Types](#)
10. [Atomic Charges](#)
11. [Fragments](#)
12. [Templates](#)
13. [Graphical Manipulations](#)
14. [Deleting Objects](#)
15. [Undoing, Redoing, and Starting Fresh](#)
16. [Cleaning up Structures](#)
17. [Setting Query Attributes on Atoms](#)
18. [Display of Atom Query Attributes](#)
19. [Setting Bond Query Attributes](#)
20. [Display of Bond Query Attributes](#)
21. [The Structure Data Line](#)
22. [Structure Input via the Structure Data Line](#)
23. [Structure Import via Keyboard Paste](#)
24. [Structure Import via File Upload](#)
25. [Structure Export](#)
26. [Hydrogen Manipulation](#)
27. [Keyboard Shortcuts](#)
28. [Data Transfer to Caller Forms](#)
29. [Quitting the Sketcher](#)

Finding a potential inhibitor (Background)

- Increased gene expression leads to disease
- Research on KIT inhibitors can help drug discovery

The KIT protooncogene encodes for a receptor tyrosine kinase protein



Finding a potential inhibitor (1/11)

Go to the [PubChem homepage](#) and search for “[kit protooncogene](#)”:

PubChem About Posts Submit Contact

Explore Chemistry

Quickly find chemical information from authoritative sources

kit protooncogene

Compound	Gene
Protoanemonene	Sno oncogene
Delta(6)-protoilludene	Raf oncogene
6-protoilludene	Ret oncogene
Delta6-Protoilludene	Mos oncogene
PROTOXIDE OF NITROGEN	Crk oncogene
Protoapigenone	ect2 oncogene
	MAS1 oncogene
	Pvt1 oncogene

Finding a potential inhibitor (2/11)

Click on the result, which will direct you to the gene summary page:

SEARCH FOR

kit protooncogene

Treating this as a text search.

Substances (1) **Genes (1)** Literature (142) Patents (11)

Searching gene targets tested in PubChem bioassays and those involved in PubChem pathways. [Read More...](#)

1 result

KIT - KIT proto-oncogene, receptor tyrosine kinase (human)

Gene ID: 3815 Gene Symbol: **KIT** Taxonomy: [Homo sapiens \(human\)](#)

Gene Synonyms: **KIT** proto-oncogene, receptor tyrosine kinase; C-**Kit**; CD117; MASTC; ...; c-**Kit** protooncogene; ...

Linked BioAssays Count: **1,731** Linked Pathways Count: **37**

Source: BioAssay; Pathway; Patent

Finding a potential inhibitor (3/11)

Review fundamental information and the Contents table:

GENE SUMMARY

KIT - KIT proto-oncogene, receptor tyrosine kinase (human)

Gene	3
Symbol	K
Taxonomy	H
Dates	C 2016-09-14 2023-06-20
Description	This gene encodes a receptor tyrosine kinase. This gene was initially identified as a homolog of the feline sarcoma viral oncogene v-kit and is often referred to as proto-oncogene c-Kit. The canonical form of this glycosylated transmembrane protein has an N-terminal extracellular region with five immunoglobulin-like domains, a transmembrane region, and an intracellular tyrosine kinase domain at the C-terminus. Upon activation by its cytokine ligand, stem cell factor (SCF), this protein phosphorylates multiple intracellular proteins that play a role in the proliferation, differentiation, migration and apoptosis of many cell types

Where can we find info on potential inhibitors? (Answer in Chat)

Quote Icon	Cite
Download Icon	Download
CONTENTS	
Title and Summary	
Identifiers	▼
	▼
	▼
Bioactivities	▼
	▼
Phenotypes	▼
Pathways	▼
Actions	
9 Expression	
10 Target Development Level	
11 Literature	▼
12 Patents	
13 Classification	▼
14 Information Sources	

Finding a potential inhibitor (4/11)

Click on 4 Chemicals and Bioactivities and 4.1 Tested Compounds:

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)

4.1 Tested Compounds

95,627 items Download

Search SORT BY Activity Value - Increasing

Structure	Activity	Activity Type	Activity Value, μM	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537

Cite Download

CONTENTS

- Title and Summary
- 1 Names and Identifiers
- 2 Related Genes
- 3 Proteins
- 4 Chemicals and Bioactivities
 - 4.1 Tested Compounds
- 5 BioAssays
- 6 Diseases and Phenotypes
- 7 Interactions and Pathways
- 8 Biochemical Reactions
- 9 Expression

Finding a potential inhibitor (5/11)

Click Download to download the bioactivity data in CSV format:

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)



4 Chemicals and Bioactivities






4.1 Tested Compounds



90,525 items [View More Rows & Details](#)

[Download](#)

SORT BY Activity Value

Structure	Activity ?	Activity Type ?	Activity Value, μM	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537
	Active	Kd	0.000024	451705

Cite

Download

CONTENTS

Title and Summary

1 Names and Identifiers

2 Related Genes

3 Proteins

4 Chemicals and Bioactivities

4.1 Tested Compounds

5 BioAssays

6 Diseases and Phenotypes

7 Interactions and Pathways

8 Biochemical Reactions

9 Expression

10 Literature

11 Patents

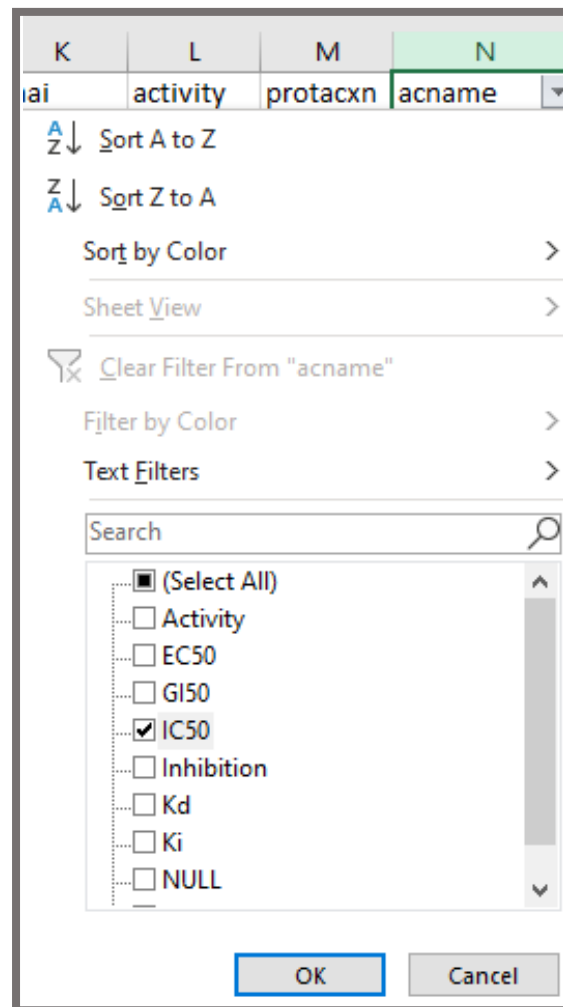
12 Classification

13 Information Sources

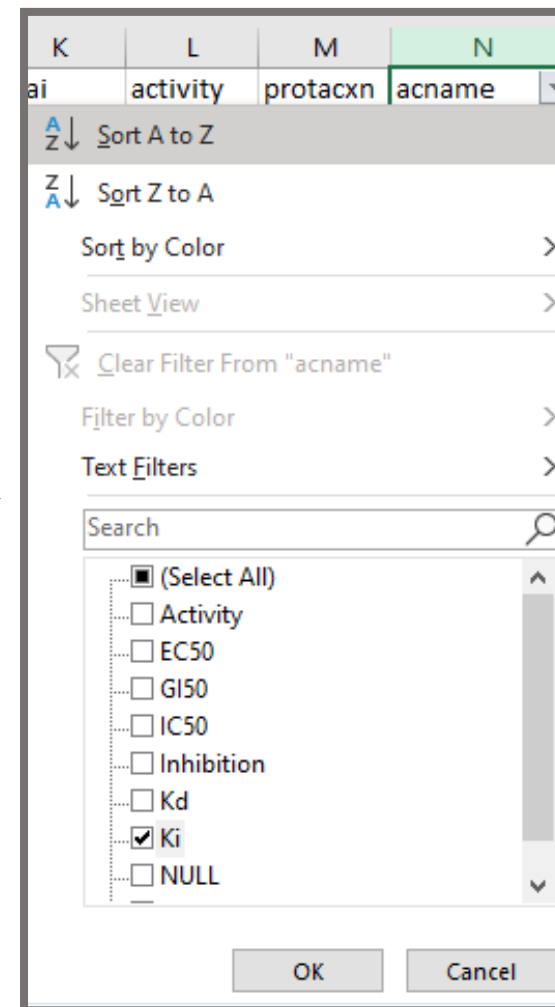
Finding a potential inhibitor (6/11)

Open the CSV file:

- The CSV file contains more detailed information
- You can filter or order the dataset based on measures of inhibition (K_i or IC_{50} values) or substrate binding (K_D)



OR



Finding a potential inhibitor (7/11)

Search or filter the tested compound section:

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)

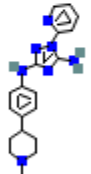
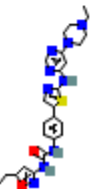
4.1 Tested Compounds

95,627 items

Download

Search

SORT BY Activity Value - Increasing

Structure	Activity	Activity Type	Activity Value, μM	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537

Finding a potential inhibitor

3-minute exercise!

Sort Structures by Activity Value

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)

4.1 Tested Compounds

95,627 items

Download

Search

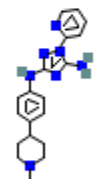
Value - Increasing

Find a compound to learn more about!

Structure

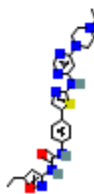
Activity

Compound CID



Active

56593836



Active

IC50

0.00002

130313537

Finding a potential inhibitor (9/11)

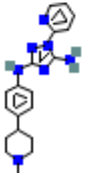
Click on a relevant Compound CID for more information

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)

4.1 Tested Compounds

95,627 items Download

Search SORT BY Activity Value - Increasing

Structure	Activity	Activity Type	Activity Value, μM	Compound CID
	Active	Ki	0.000001	56593836

Finding a potential inhibitor (9/11)


Click on a relevant Compound CID for more information, including how to buy the compound:

PubChem KIT - KIT proto-oncogene, receptor tyrosine kinase (human) (Gene)

4.1 Tested Compounds

95,627 items Download

Search SORT BY Activity Value - Increasing

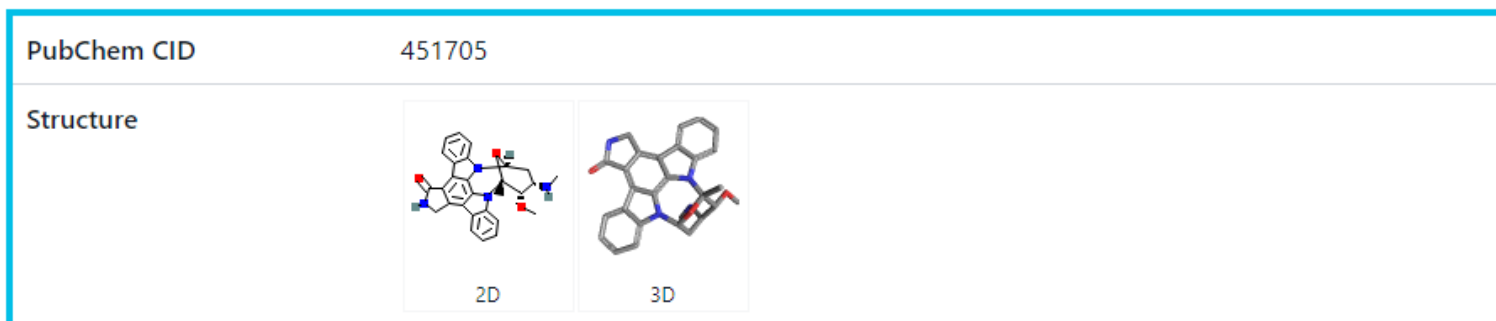
Structure	Activity	Activity Type	Activity Value, μM	Compound CID
	<u>Active</u>	Kd	0.000024	451705

Finding a potential inhibitor (10/11)

Click on 5 Chemical Vendors:

COMPOUND SUMMARY

9,13-Epoxy-1H,9H-diindolo[1,2,3-gh:3',2',1'-lm]pyrrolo[3,4-j][1,7]benzodiazonin-1-one, 2,3,10,11,12,13-hexahydro-10-methoxy-9-methyl-11-(methylamino)-, (9S,10R,11R,13R)-



Quote Icon Cite

Download Icon Download

CONTENTS

Title and Summary

1 Structures

2 Names and Identifiers

3 Chemical and Physical Properties

4 Spectral Information

5 Related Records

6 Chemical Vendors

7 Safety and Hazards

8 Literature

9 Patents




10 Biological Test Results

11 Classification

12 Information Sources

Finding a potential inhibitor (11/11)

Click on Purchasable Chemical ID for more information:

6 Chemical Vendors		 
4 vendors		 Download
MuseChem PubChem SID: 355053279	Purchasable Chemical: M032889	
BenchChem PubChem SID: 445822950	Purchasable Chemical: B060605	
THE BioTek PubChem SID: 446502889	Purchasable Chemical: bt-1180455	
Santa Cruz Biotechnology, Inc. PubChem SID: 473052579	Purchasable Chemical: sc-360258	

► PubChem

Conclusion

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



POLL (4/4)

What aspects of PubChem would you like to learn more about in the future?

Continue learning about PubChem



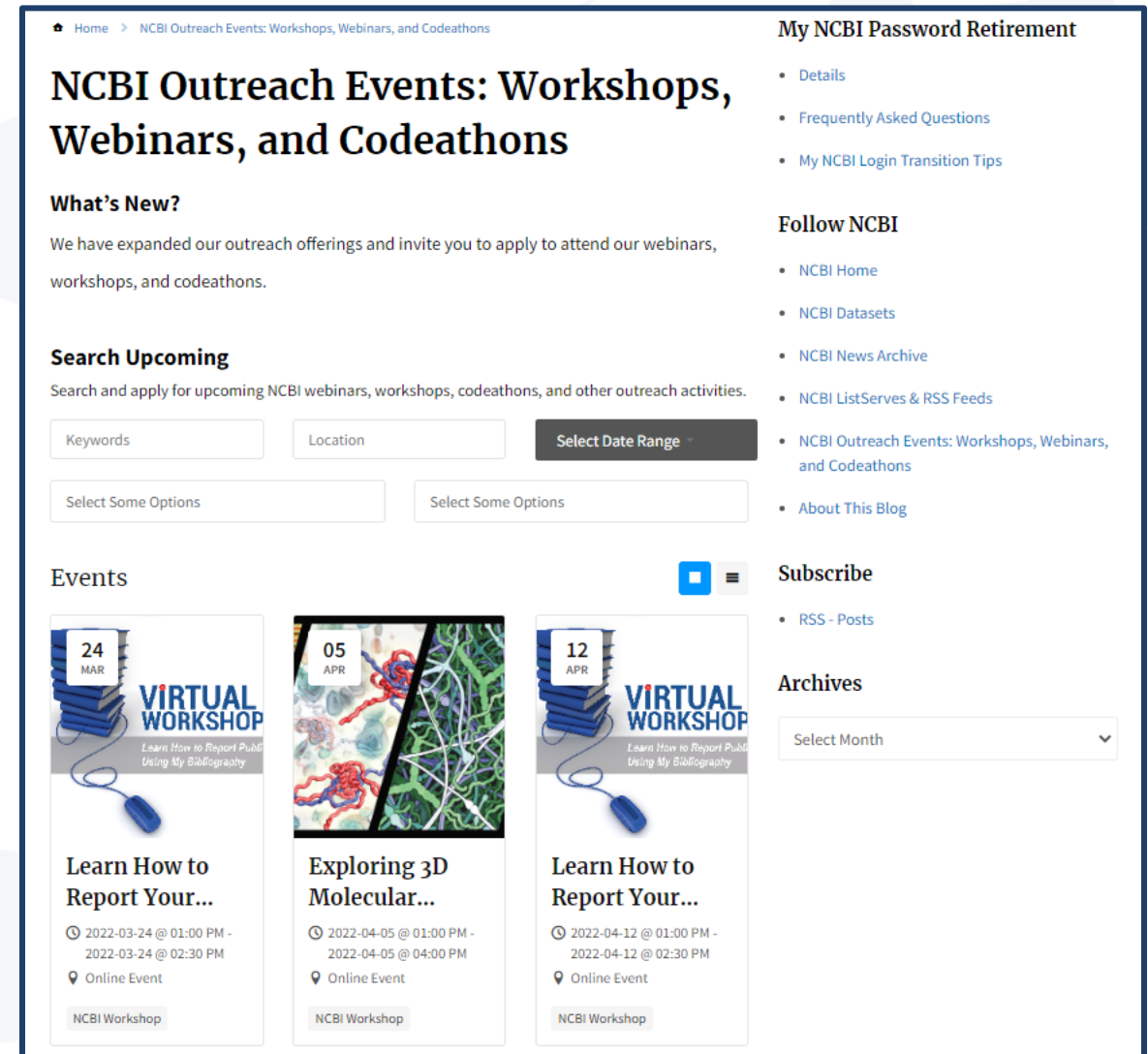
- PubChem [Tutorials](#) and a [training course](#)
- Visit the [PubChem Help Guide](#)
- Use the [Contact PubChem page](#)
- Browse the [PubChem Publications page](#) for journal articles about PubChem

Continue learning about NCBI Resources

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[NCBI Insights Blog](#)

- Follow us on social media:



The screenshot shows the NCBI Outreach Events page. At the top, there is a breadcrumb trail: Home > NCBI Outreach Events: Workshops, Webinars, and Codeathons. The main heading is "NCBI Outreach Events: Workshops, Webinars, and Codeathons". Below this, there is a "What's New?" section with a paragraph: "We have expanded our outreach offerings and invite you to apply to attend our webinars, workshops, and codeathons." There is also a "Search Upcoming" section with a search bar containing "Keywords", "Location", and "Select Date Range". Below the search bar are two "Select Some Options" dropdown menus. The "Events" section features three event cards. The first card is for a "VIRTUAL WORKSHOP" on 24 MAR, titled "Learn How to Report Your..." with a time slot of 2022-03-24 @ 01:00 PM - 2022-03-24 @ 02:30 PM. The second card is for a "VIRTUAL WORKSHOP" on 05 APR, titled "Exploring 3D Molecular..." with a time slot of 2022-04-05 @ 01:00 PM - 2022-04-05 @ 04:00 PM. The third card is for a "VIRTUAL WORKSHOP" on 12 APR, titled "Learn How to Report Your..." with a time slot of 2022-04-12 @ 01:00 PM - 2022-04-12 @ 02:30 PM. On the right side of the page, there are sections for "My NCBI Password Retirement" (with links for Details, Frequently Asked Questions, and My NCBI Login Transition Tips), "Follow NCBI" (with links for NCBI Home, NCBI Datasets, NCBI News Archive, NCBI ListServes & RSS Feeds, NCBI Outreach Events: Workshops, Webinars, and Codeathons, and About This Blog), "Subscribe" (with a link for RSS - Posts), and "Archives" (with a "Select Month" dropdown menu).