



# 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)

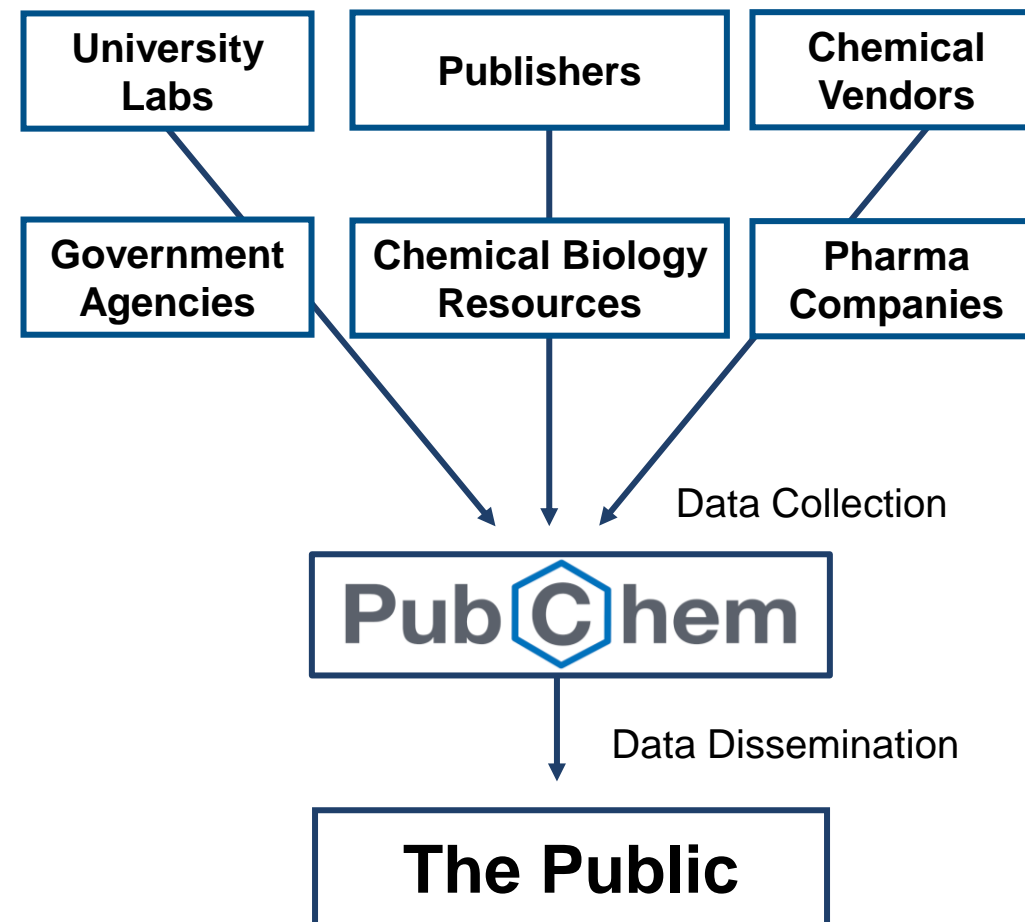
Which best describe your work, research,  
or educational background?

# 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 PubChem website homepage. At the top, there is a dark 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 a hamburger menu icon. The main content area has a dark blue background with the heading "Explore Chemistry" and the subtext "Quickly find chemical information from authoritative sources". A search bar is present with a magnifying glass icon. Below the search bar, there are several search suggestions: "Try covid-19 aspirin EGFR C9H8O4 57-27-2". There is a checkbox labeled "Use Entrez". At the bottom of the main content area, there are four icons with labels: "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 is light gray and contains the text "112M Compounds" and "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

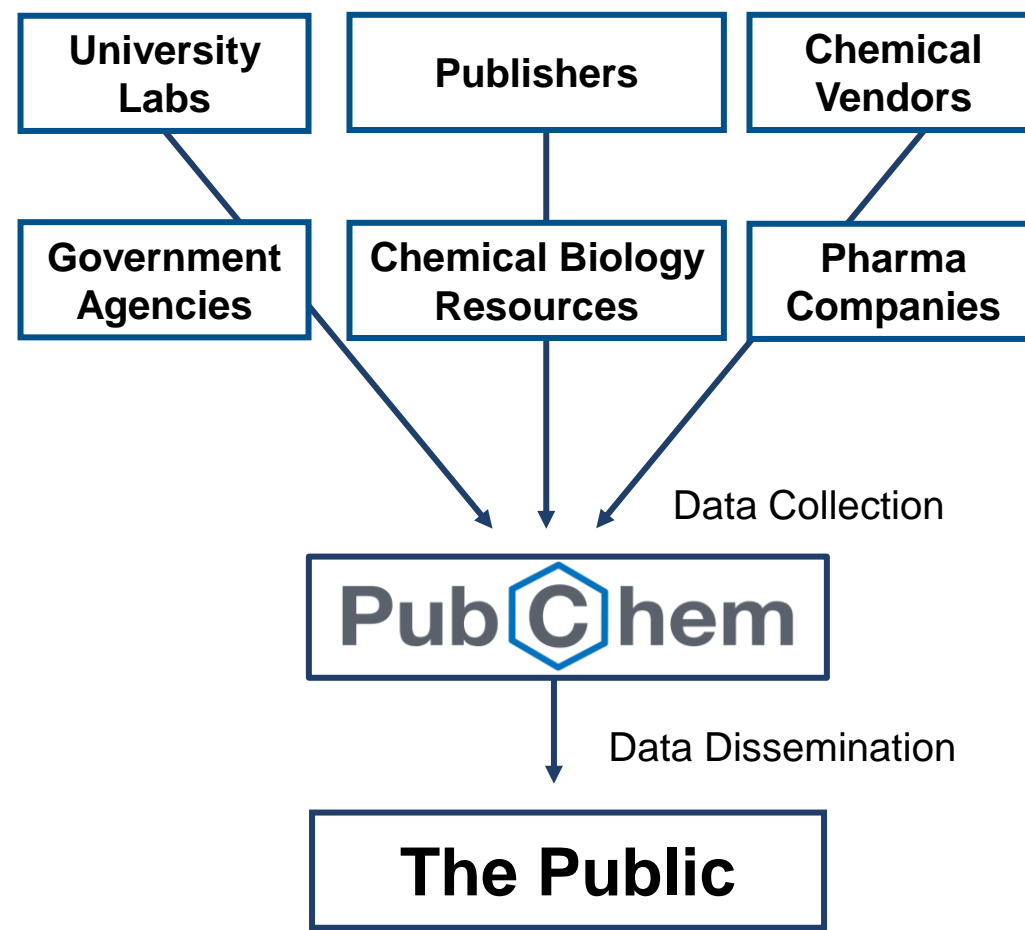
# POLL (3/4)

What do you currently  
use PubChem for?



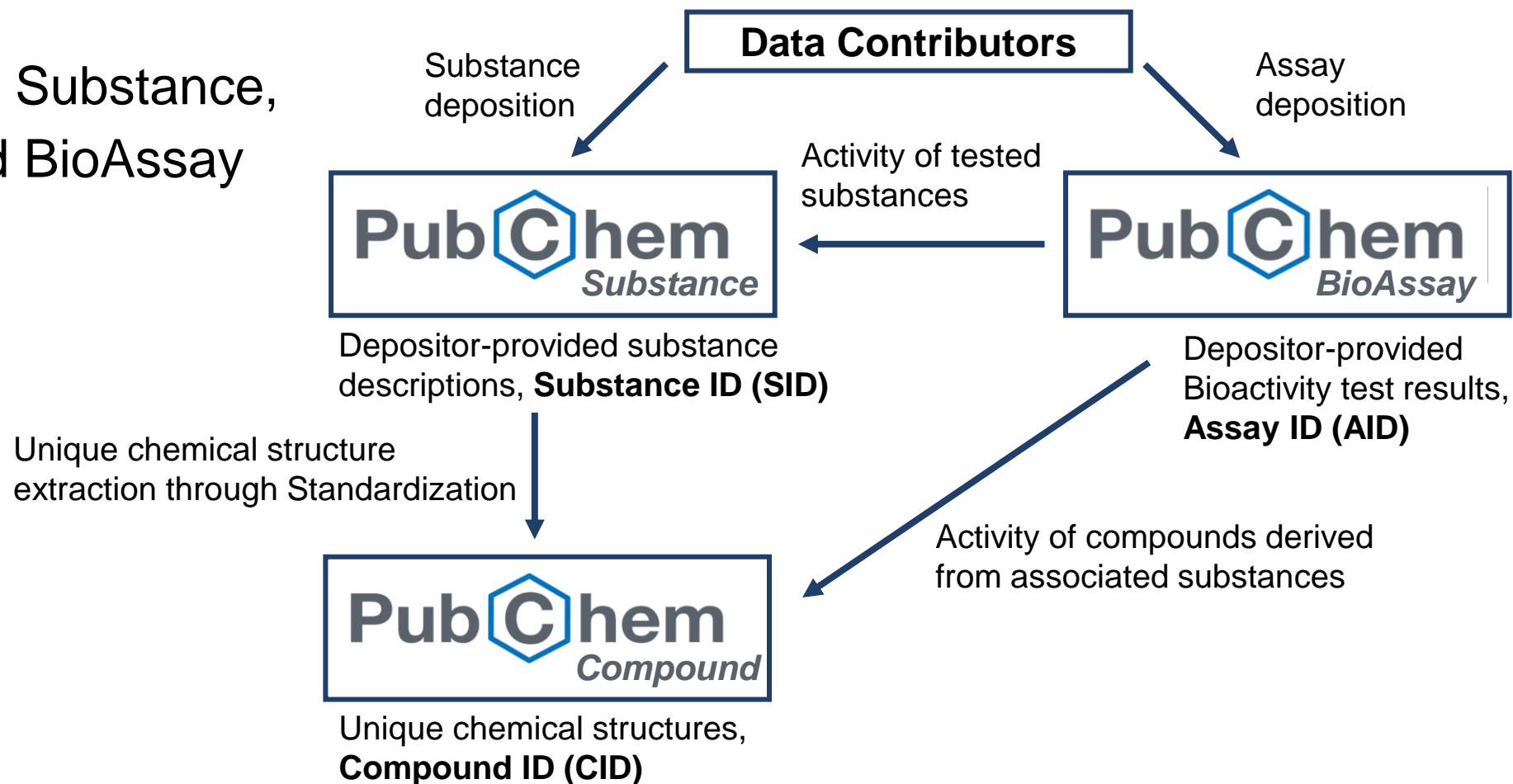
# Who provides PubChem Data?

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



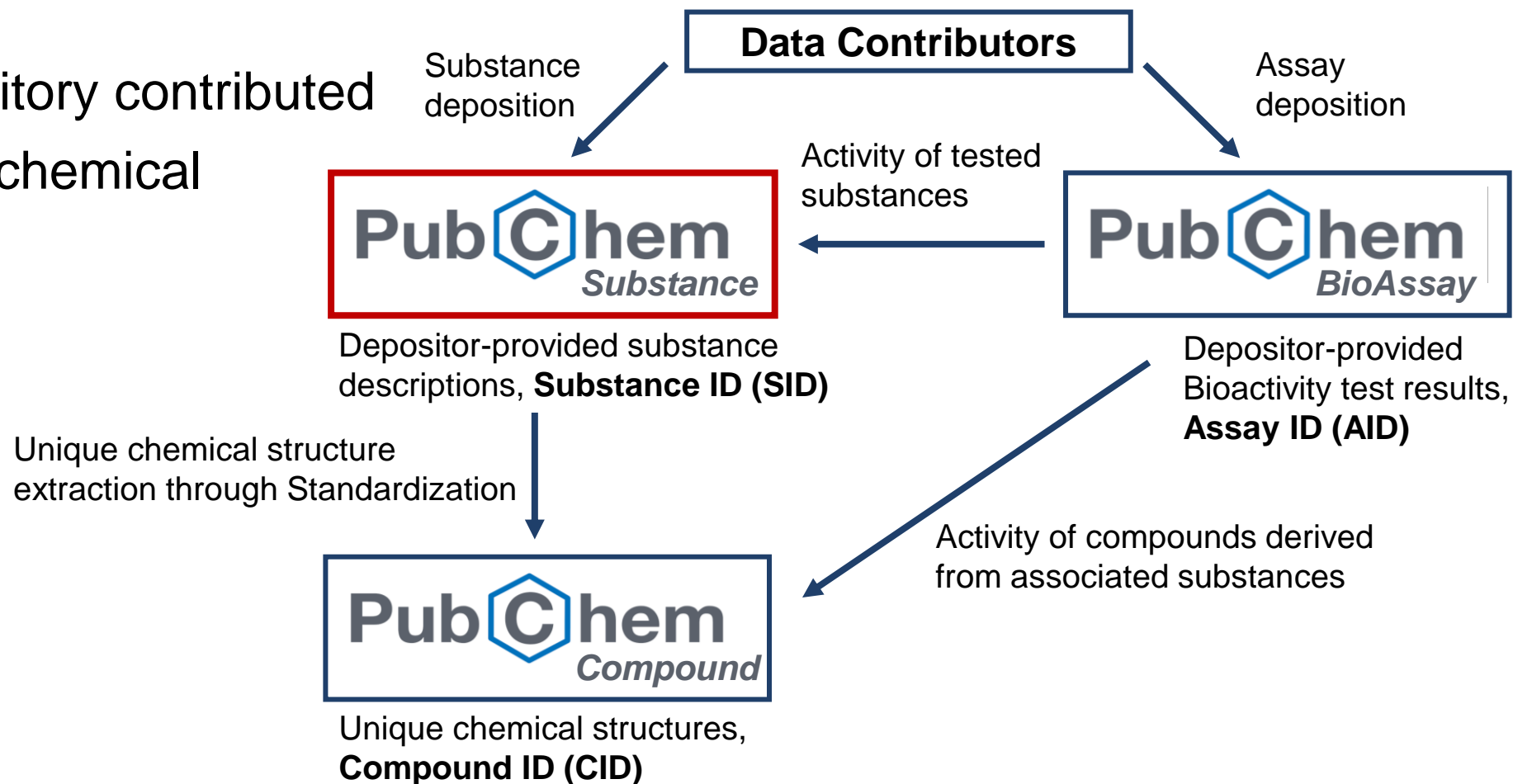
# Data Organization

- Three Linked to Substance, Compound, and BioAssay Databases



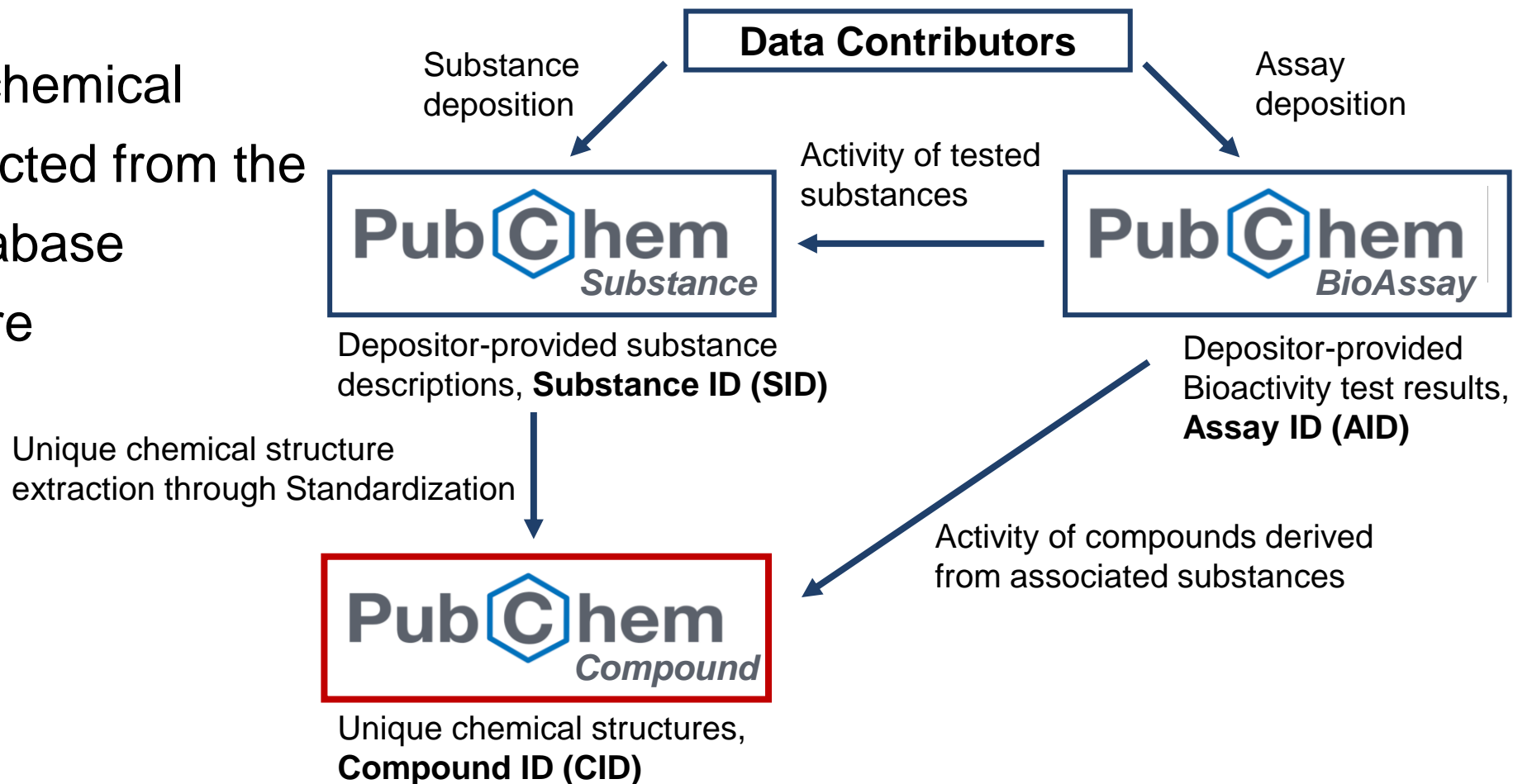
# Substance Database

- Archives depository contributed descriptions of chemical substances



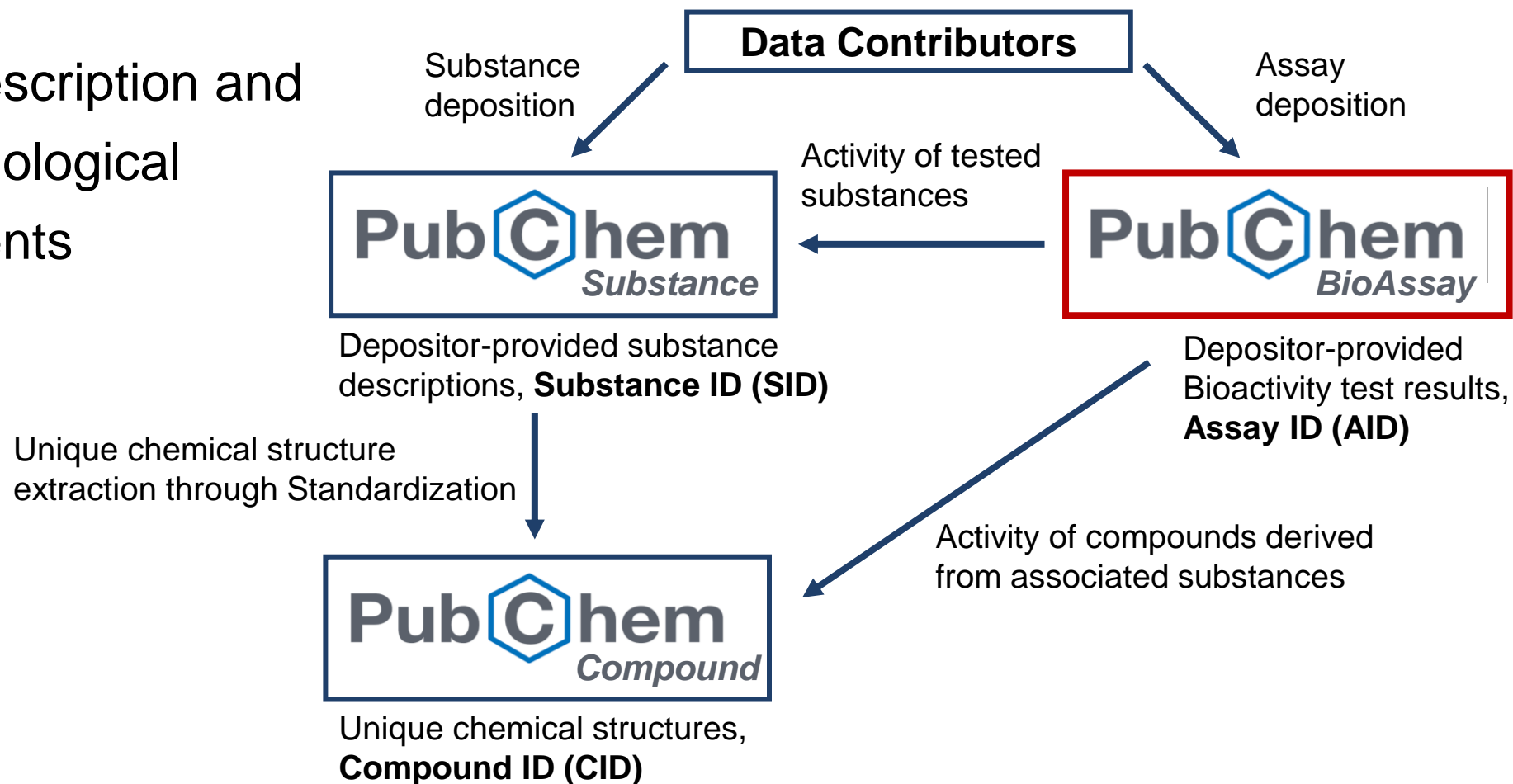
# Compound Database

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

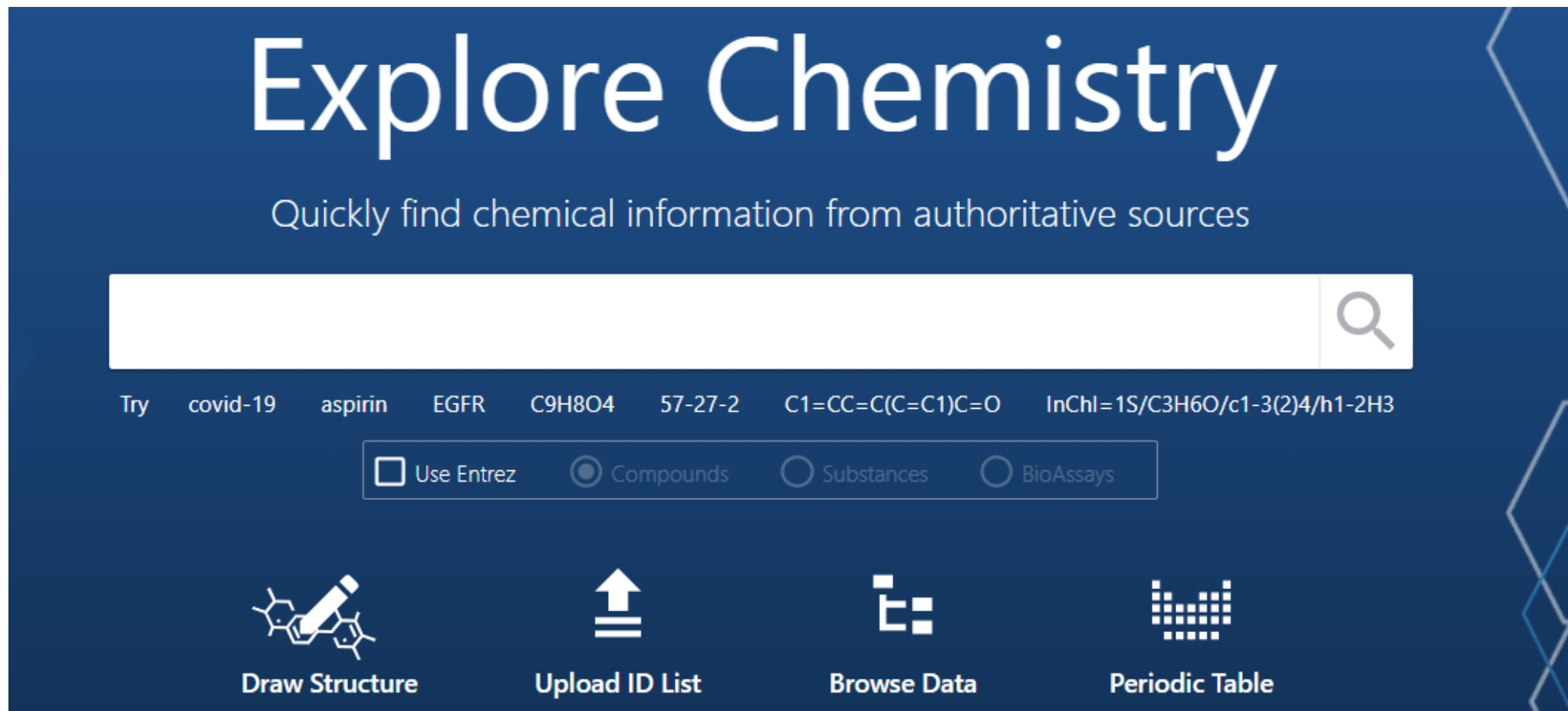


# BioAssay Database

- Contains the description and test results of biological assay experiments



# Searching in [PubChem](#)



The image shows the 'Explore Chemistry' search interface on a dark blue background. At the top, the text 'Explore Chemistry' is written in large white font, followed by the subtitle 'Quickly find chemical information from authoritative sources'. Below this is a large white search bar with a magnifying glass icon on the right. Underneath the search bar, there are several 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'. Below the suggestions is a row of radio buttons for search filters: 'Use Entrez' (unchecked), 'Compounds' (checked), 'Substances' (unchecked), and 'BioAssays' (unchecked). 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).

# Common Search Strategies

**Text**

covid-19 OR aspirin

**Molecular Formula**

C9H8O4

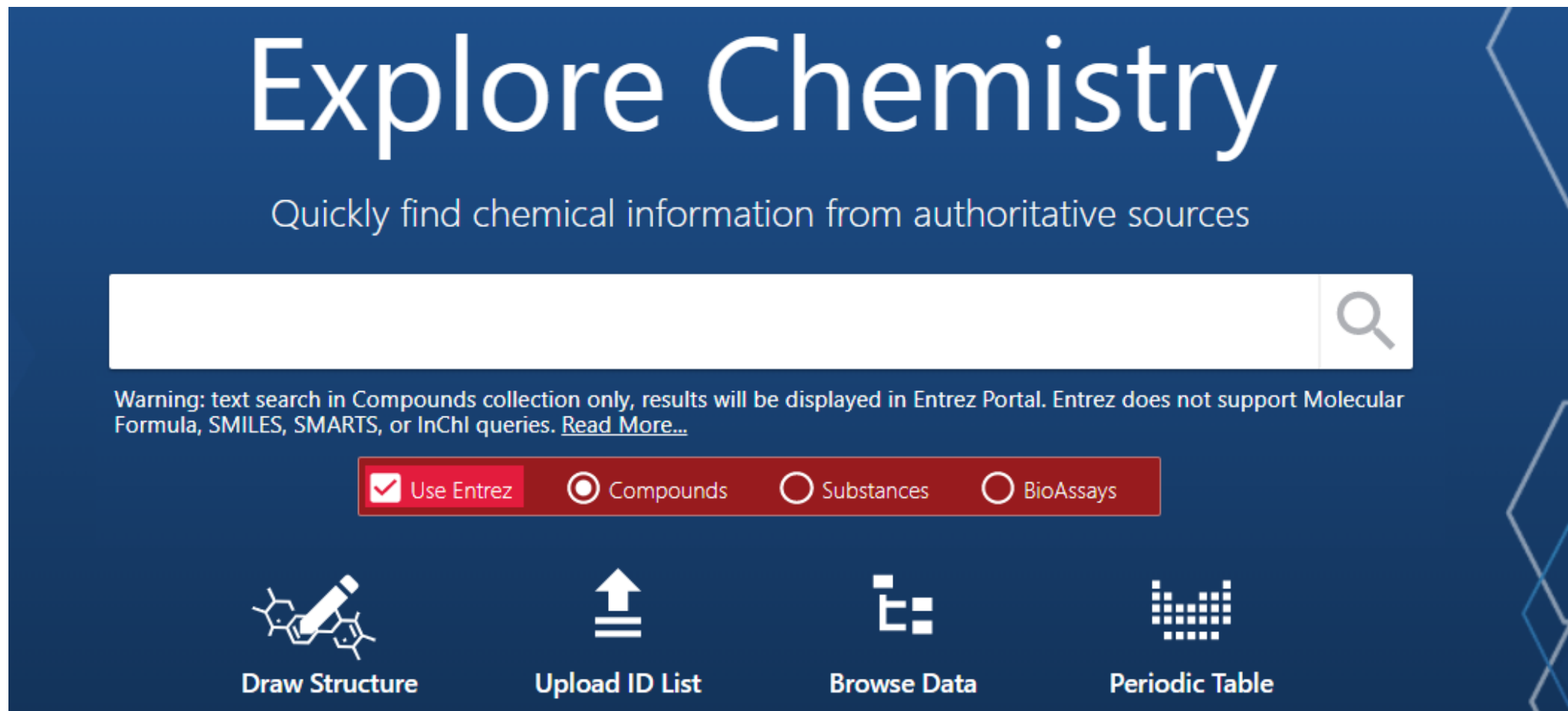
**Simplified Molecular Input  
Line Entry System (SMILES)**

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, a subtitle reads 'Quickly find chemical information from authoritative sources'. 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 states: '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).

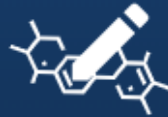



## Explore Chemistry

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!

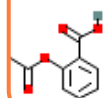
# Text searching in PubChem (6/8)

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: C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 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 \(MeSH Keyword\)](#)

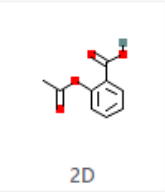
# Text searching in PubChem (7/8)

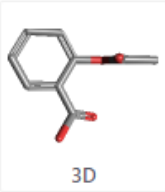
Review the compound summary page:

## 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

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

# Finding safety information

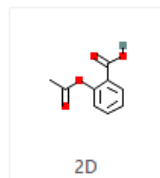
COMPOUND SUMMARY > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS)

## Aspirin

PubChem CID

2244

Structure



[Find Similar Structures](#)

Synonyms

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

[More...](#)

Molecular Formula

$C_9H_8O_4$  or  $CH_3COOC_6H_4COOH$

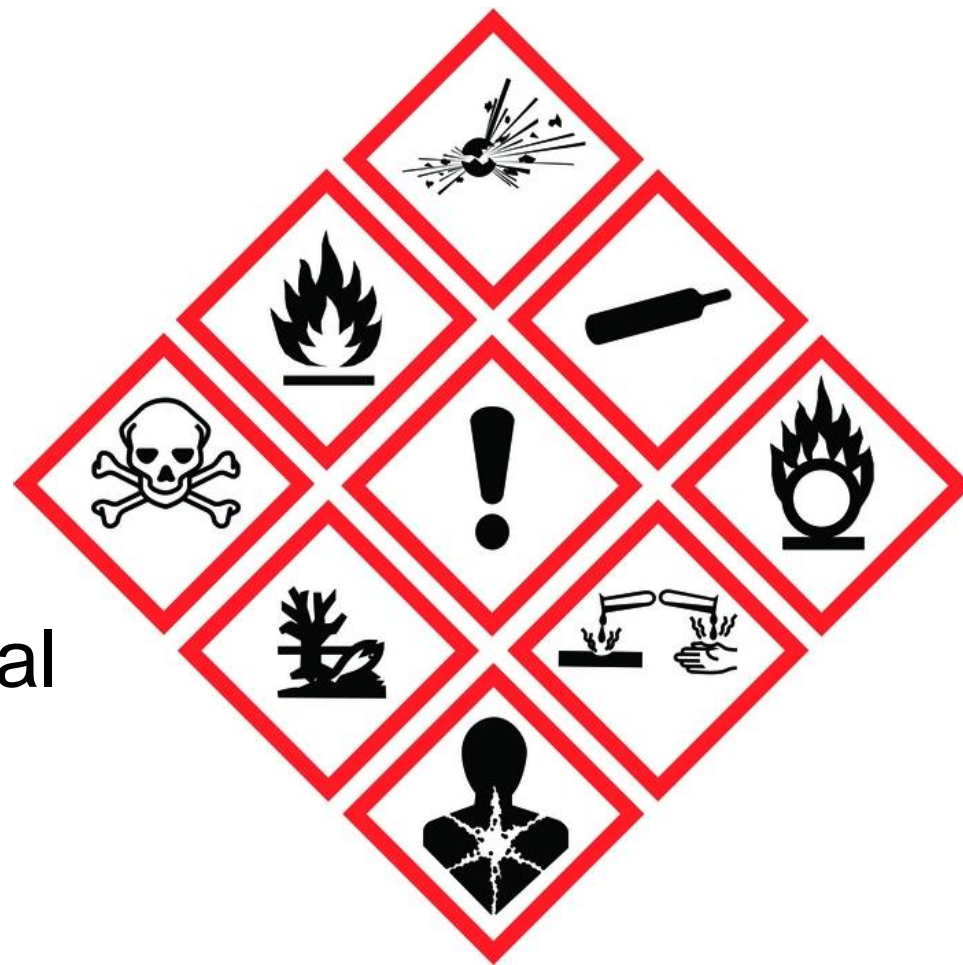
Molecular Weight

180.16

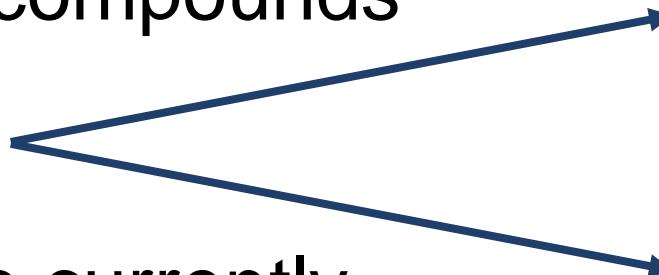
[Learn More About LCSS Project >](#)

# 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

10 Storage and Handling

11 Cleanup and Disposal

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.
- Search Suggestions:** Below the search bar, a row of 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

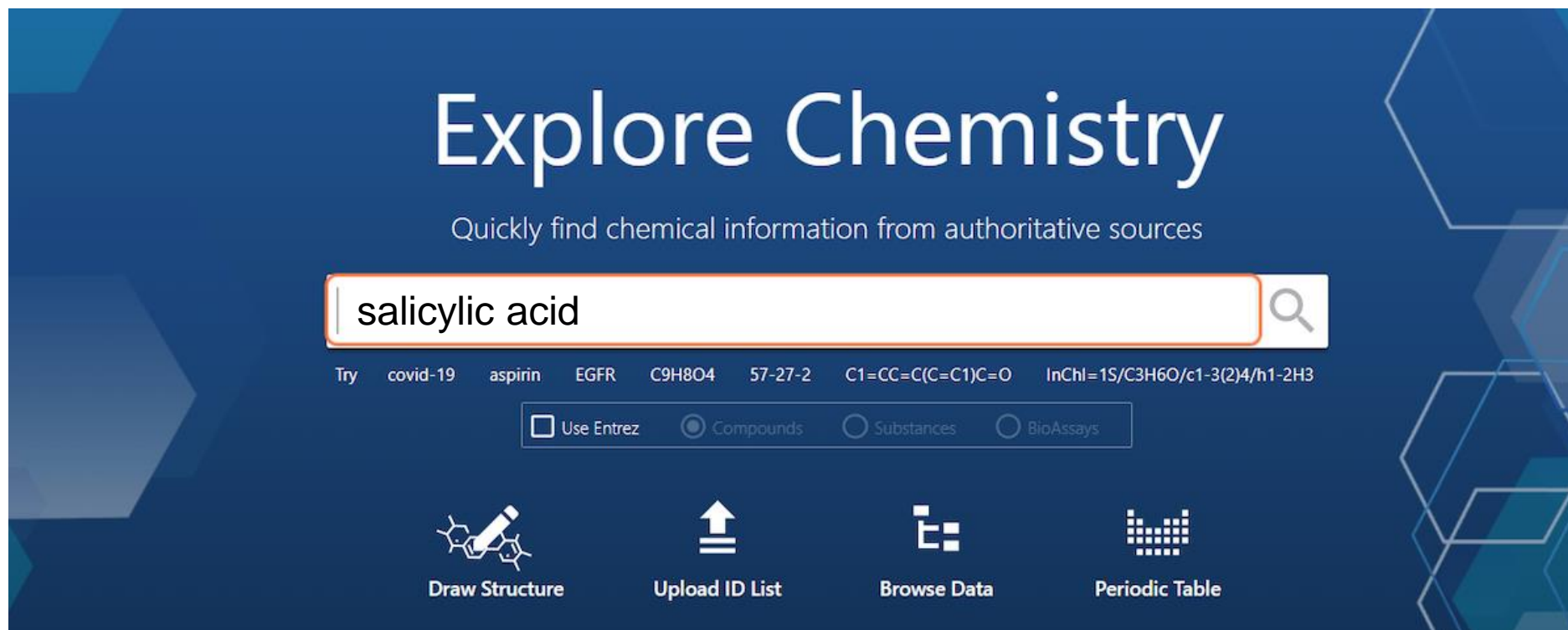
Formula C7H6O3 [138.123 gr/mol]

Search for This Structure

NIH National Library of Medicine  
National Center for Biotechnology Information

# 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 Structure image:

NIH National Library of Medicine  
National Center for Biotechnology Information

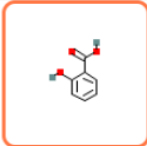
PubChem About Posts Submit Contact

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:  $C_7H_6O_3$  MW: 138.12g/mol  
IUPAC Name: 2-hydroxybenzoic acid  
Isomeric SMILES: C1=CC=C(C(=C1)C(=O)O)O  
InChIKey: YGSDEFMSJLZEOE-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 \(MeSH Keyword\)](#)

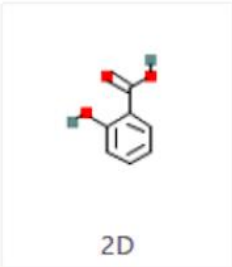
# Searching with PubChem Sketcher (5/10)

Select Find Similar Structures:

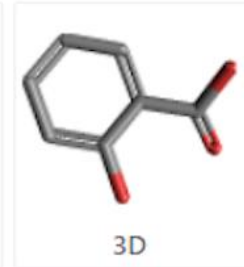
PubChem CID 338

---


Structure



2D



3D






Crystal

[Find Similar Structures](#)

---

Chemical Safety



# Searching with PubChem Sketcher (6/10)

And select Edit Structure to make any changes:

PubChem About Posts Submit Contact

SEARCH FOR

CID338 structure

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

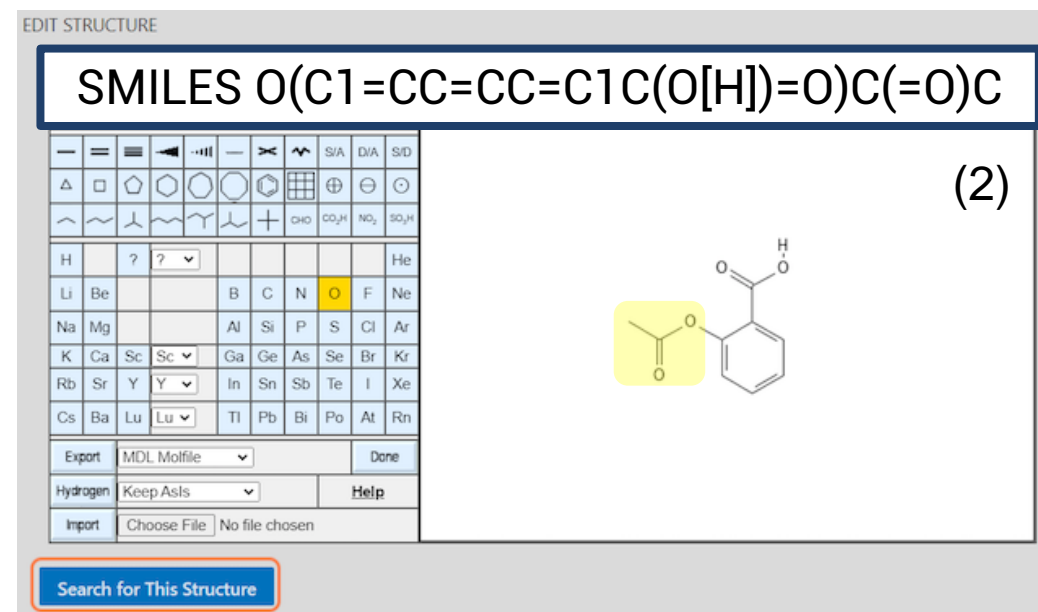
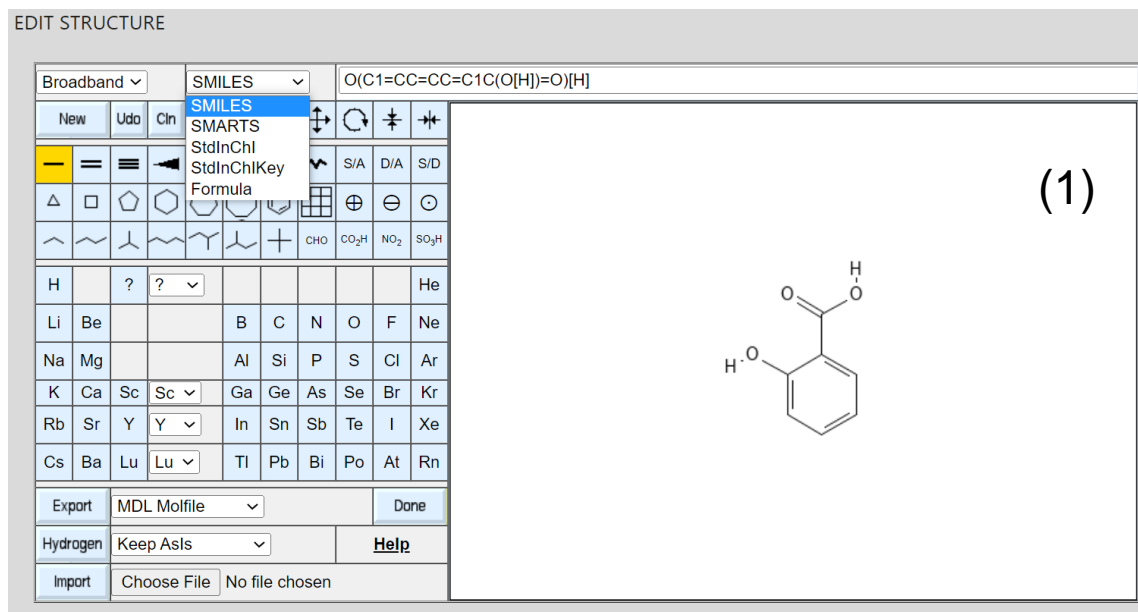
Identity (1) **Similarity (>1,000)** Substructure (>1,000) Superstructure (>1,000) 3D Similarity (>802)

Fingerprint Tanimoto-based 2-dimensional similarity search.

Percentage of the database searched: 42%.  Search All

# 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


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: C<sub>9</sub>H<sub>8</sub>O<sub>4</sub> 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: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub> 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

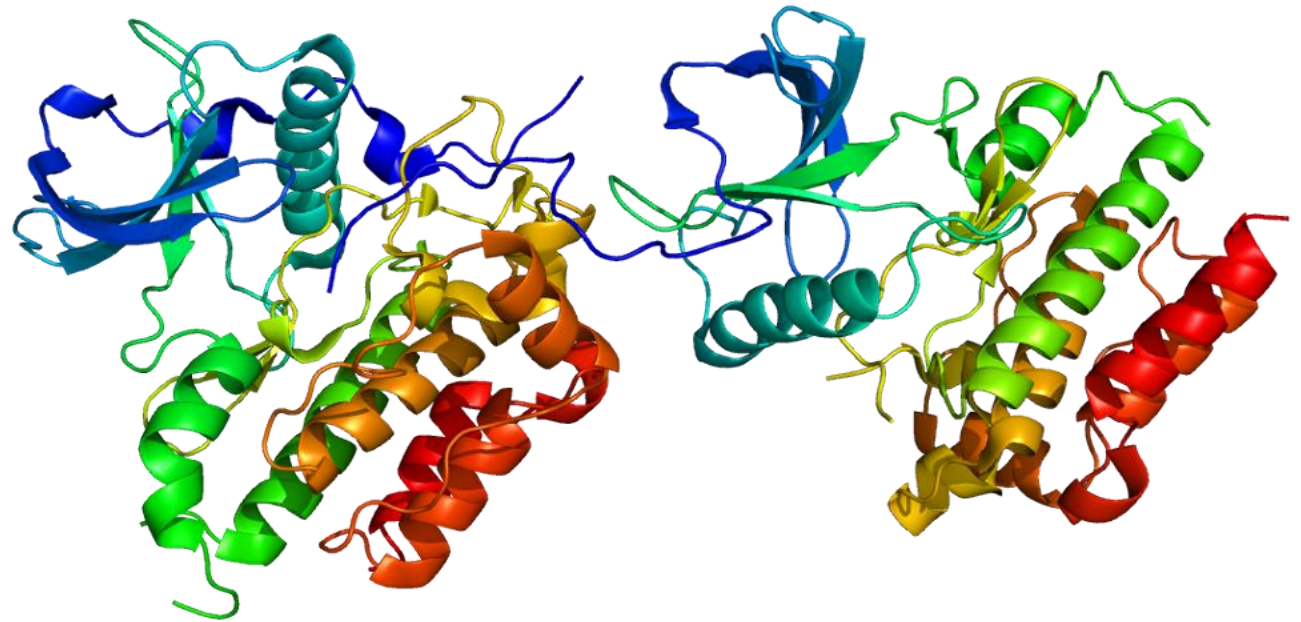
## PubChem Sketcher Help

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.

**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: **1,058** Linked Pathways Count: **34**

Source: Pathway; Patent

# Finding a potential inhibitor (3/11)

Review fundamental information about the KIT protooncogene and navigate to the Contents table:

GENE SUMMARY

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

Gene	3
Symbol	K
Taxonomy	H
Dates	M 2

This gene encodes a receptor tyrosine kinase (KIT) 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 and thereby plays an important role in hematopoiesis, stem cell maintenance, gametogenesis, melanogenesis, and in mast cell development, migration and function. This protein can be a membrane-bound or soluble protein. Mutations in this gene are associated with gastrointestinal stromal tumors, mast cell disease, acute myelogenous leukemia, and piebaldism. Multiple transcript variants encoding different isoforms have been found for this gene. [provided by RefSeq, May 2020]

▶ [NCBI Gene](#)

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

Cite	Download
CONTENTS	
Title and Summary	
Names and Identifiers	
2 Related Genes	
3 Proteins	
4 Chemicals and Bioactivities	
5 BioAssays	
6 Diseases and Phenotypes	
7 Interactions and Pathways	
8 Biochemical Reactions	
9 Expression	
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# 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 Chemicals and Bioactivities

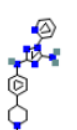
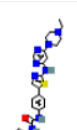
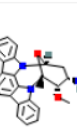


### 4.1 Tested Compounds



90,525 items View More Rows & Details

Download

Structure	Activity	Activity Type	Activity Value, $\mu\text{M}$	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537
	Active	Kd	0.000024	451705

Cite

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# 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, $\mu\text{M}$	Compound CID
	Active	Ki	0.000001	56593836
	Active	IC50	0.00002	130313537
	Active	Kd	0.000024	451705

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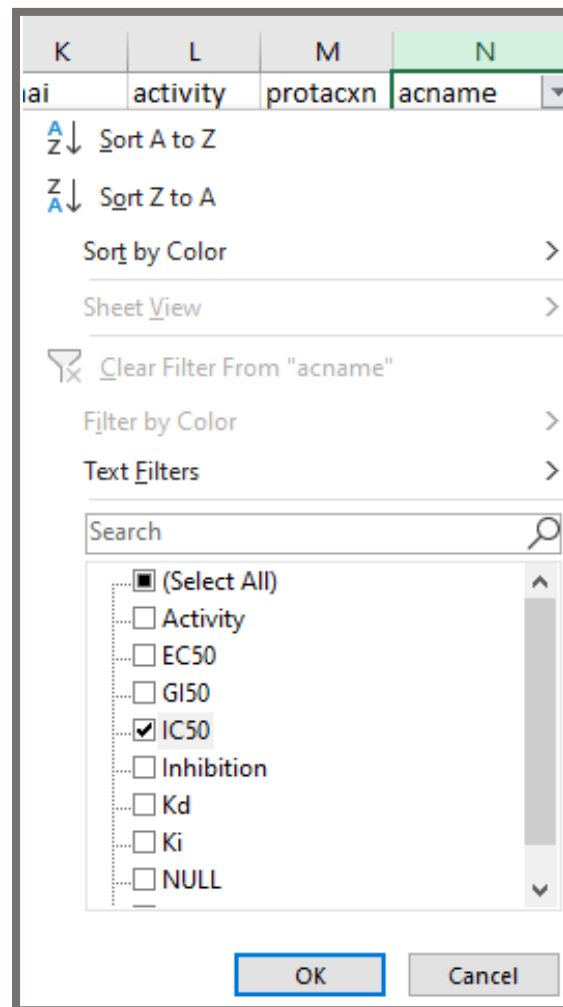
12 Classification

13 Information Sources

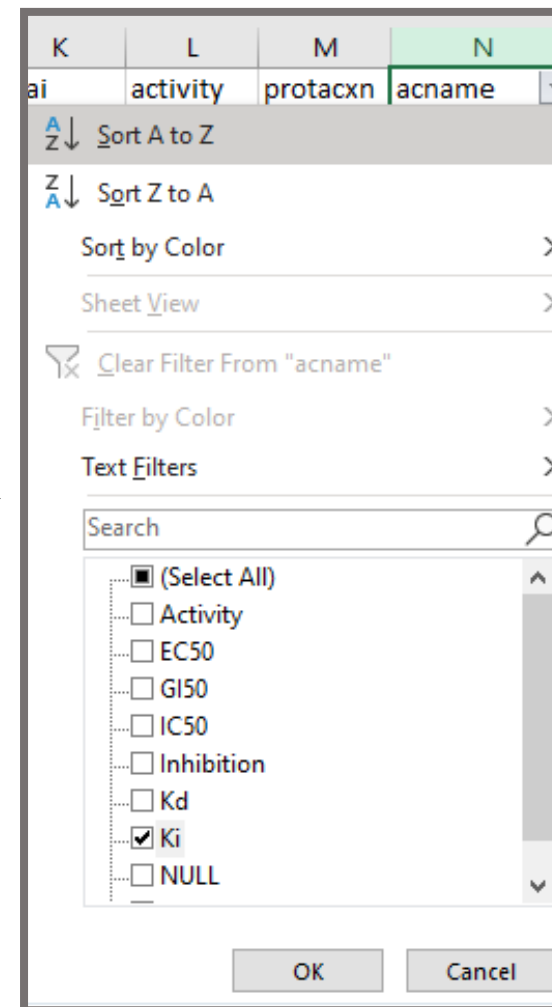
# Finding a potential inhibitor (6/11)

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)

Click View More Rows & Details for more information without downloading a file:


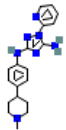
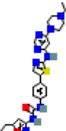
## 4 Chemicals and Bioactivities ?

### 4.1 Tested Compounds ?

90,525 items




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 Download

SORT BY <span>Activity Value</span> 				
Structure	Activity <span>?</span>	Activity Type <span>?</span>	Activity Value, $\mu\text{M}$	Compound CID
	<a href="#">Active</a>	Ki	0.000001	56593836
	<a href="#">Active</a>	IC50	0.00002	130313537

# Finding a potential inhibitor (8/11)

## Sort Structures by Activity Value

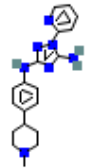
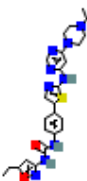
#	Structure	Activity ?	Activity Type ?	Activity Value, $\mu\text{M}$	Compound CID	Substance SID	BioAssay AID	BioAssay Name
1		Active	Ki				46	Displacement of [33P]ATP from human recombinant c-KIT domain after 20 mins by scintillation counting
2		Active	IC				63	Inhibition of human c-KIT A loop exon 17 D820Y single mutant using poly (Glu,Tyr) 4:1 as substrate in presence of 33P-gamma-ATP by hotspot kinase assay
3		Active	Kd	0.000024	451705	5010019	1433	Kinase Inhibitor Selectivity Profiling Assay

Find a compound to learn more about!



# Finding a potential inhibitor (9/11)

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

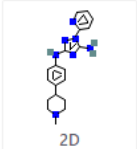
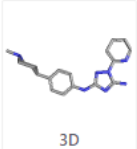
SORT BY <span>Activity Value</span>								
#	Structure	Activity ?	Activity Type ?	Activity Value, $\mu\text{M}$	Compound CID	Substance SID	BioAssay AID	BioAssay Name
1		Active	Ki	0.000001	56593836	134461981	623446	Displacement of [33P]ATP from human recombinant c-KIT domain after 20 mins by scintillation counting
2		Active	IC50	0.00002	130313537	440123730	1587963	Inhibition of human c-KIT A loop exon 17 D820Y single mutant using poly (Glu,Tyr) 4:1 as substrate in presence of 33P-gamma-ATP by hotspot kinase assay

# Finding a potential inhibitor (10/11)

Click on 5 Chemical Vendors:

COMPOUND SUMMARY

## 3-N-[4-(1-methylpiperidin-4-yl)phenyl]-1-pyridin-2-yl-1,2,4-triazole-3,5-diamine

PubChem CID	56593836
Structure	 2D  3D <a href="#">Find Similar Structures</a>
Molecular Formula	C <sub>19</sub> H <sub>23</sub> N <sub>7</sub>
Synonyms	CHEMBL1835867 SCHEMBL4038099 BDBM50355489 ZINC72127621
Molecular Weight	349.4
Dates	Modify 2022-11-05    Create 2012-02-06

Cite

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# Finding a potential inhibitor (11/11)

Click on Purchasable Chemical ID for more information:

## 5 Chemical Vendors



Showing 1 Substance per Vendor [View All](#)

[View in Entrez](#) [Download](#)

ZINC

PubChem SID: [330462129](#) **Purchasable Chemical: [ZINC72127621](#)**

[PubChem](#)

## 6 Patents



### 6.1 Depositor-Supplied Patent Identifiers



7 items [View More Rows & Details](#)

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SORT BY <a href="#">Priority Date</a>			
Publication Number	Title	Priority Date	Grant Date
<a href="#">EP-1562589-A2</a>	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	
<a href="#">EP-1562589-B1</a>	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	2009-01-07
<a href="#">KR-20060013480-A</a>	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	
<a href="#">US-2004214817-A1</a>	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	
<a href="#">US-2008014189-A1</a>	Diaminotriazoles useful as inhibitors of protein kinases	2002-11-15	

1 2 [Next >](#)

# 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

A decorative graphic of a molecular structure, consisting of several light blue circles (atoms) connected by thin lines (bonds). The structure is spread across the right and bottom portions of the slide.

- PubChem [Tutorials](#) and a [training course](#)
- Visit the [PubChem Help Guide](#)
- Use the [Contact PubChem page](#)
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# Continue learning about NCBI Resources

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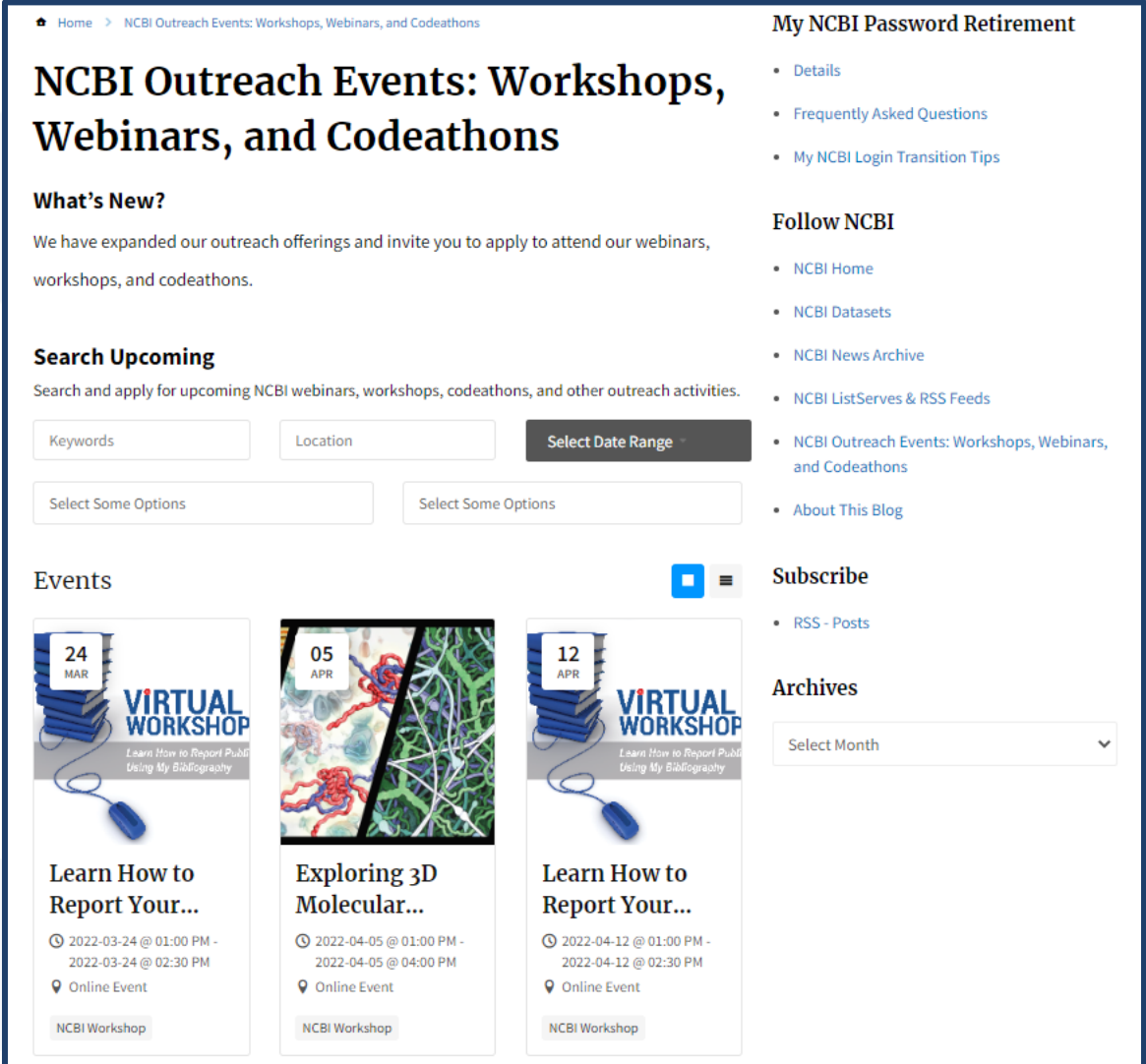
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The screenshot shows the NCBI Outreach Events page. At the top, there is a breadcrumb trail: Home > NCBI Outreach Events: Workshops, Webinars, and Codeathons. The main heading is "NCBI Outreach Events: Workshops, Webinars, and Codeathons". Below this, 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" buttons. 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).