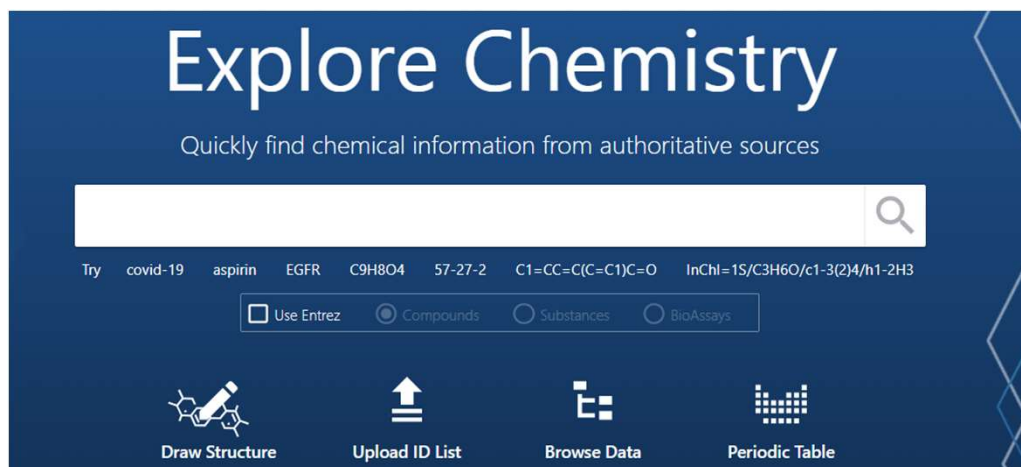


Searching in [PubChem](#)



Explore Chemistry

Quickly find chemical information from authoritative sources

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

NIH National Library of Medicine
National Center for Biotechnology Information

[Beginning of Exercise 1](#)

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](#)

NIH National Library of Medicine
National Center for Biotechnology Information

Searching with Entrez

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

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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"[pharmacion]`

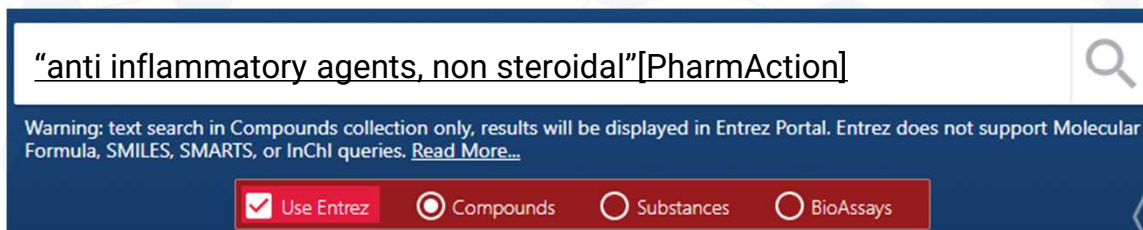
- Use field limits and Boolean operators
- Put phrases in quotes

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[More on Entrez Indices and Filters](#)

Text searching in [PubChem](#) (1/8)

Click Use Entrez and Compounds, then use the field PharmAction to limit by [Pharmacological action](#):



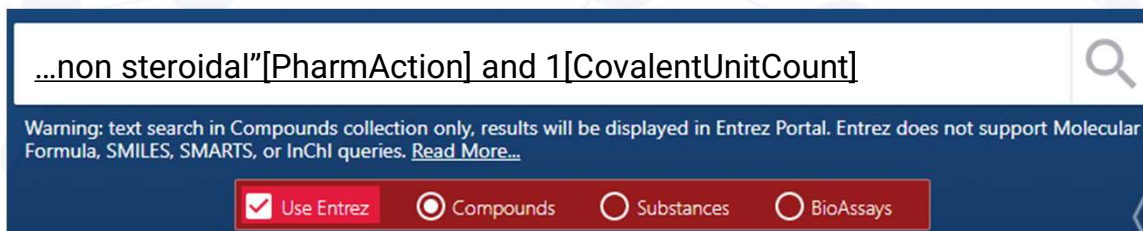
“anti inflammatory agents, non steroidal”[PharmAction]

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:

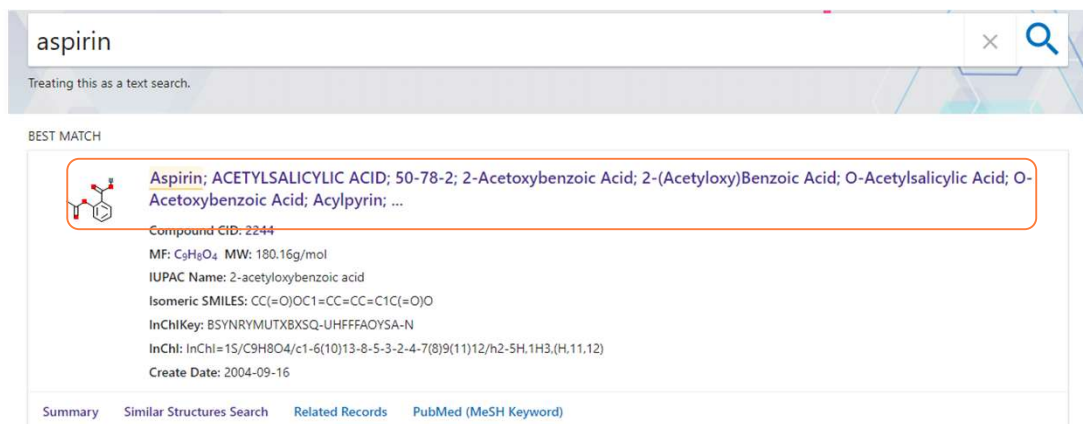
5-minute exercise!

- 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-acetyloxybenzoic 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 $CH_3COOC_6H_4COOH$

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- 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 $CH_3COOC_6H_4COOH$

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
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- 12 Toxicity
- 13 Associated Disorders and Diseases
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- 15 Patents

Finding safety information

COMPOUND SUMMARY > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS)

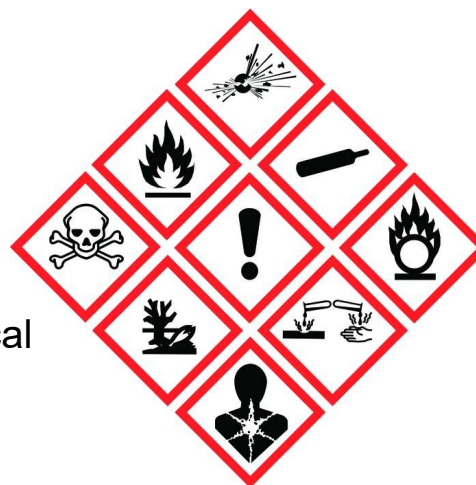
Aspirin

PubChem CID	2244
Structure	 2D 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](#)
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- 4 Toxicity Information
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