



Краткая инструкция

# Поисковый запрос

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ROYAL SOCIETY OF CHEMISTRY

## ChemSpider

Search and share chemistry

Search ChemSpider

Simple Structure Advanced History

### Search ChemSpider

Matches any text strings used to describe a molecule.

Search

Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ?

Systematic names	Synonyms	Trade names	Registry numbers	SMILES	InChI
1,2-dihydroxybenzene	AIBN	Aspirin	7732-18-5	O=C(OCC)C	InChI=1/CH4/h1H4

What is ChemSpider? Search by chemical names Search by chemical structure Find important data

*ChemSpider* is a free chemical structure database providing fast text and structure search access to over 58 million structures from hundreds of data sources.

- Systematic names
- Synonyms
- Trade names
- Database identifiers

- Create structure-based queries
- Draw structures in the web page
- Use structure files from your computer

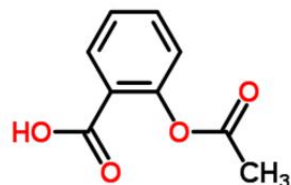
- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers

Поиск может осуществляться по систематическому названию, синониму, торговому названию, регистрационному номеру, химической формуле (SMILES), международному текстовому химическому идентификатору (InChI).

# Результаты поиска

Found 1 result

Search term: **aspirin** (Found by approved synonym)



## Aspirin

Molecular Formula  $C_9H_8O_4$   
Average mass 180.157 Da  
Monoisotopic mass 180.042252 Da  
ChemSpider ID 2157



3D



More details:

analgesic anti-inflammatory drug antipyretic antirheumatic drug

+ TAG

Names and identifiers Properties Searches Spectra Vendors Articles More

Names and Synonyms Database ID(s)

Validated by Experts, Validated by Users, Non-Validated, Removed by Users

EDIT

2-(Acetyloxy)benzoic acid

200-064-1 [EINECS](#)

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Featured data source



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В базе можно найти химические структуры в формате 2D и 3D, основную информацию о веществе.

# Результаты поиска

Подробная информация о веществе, названия и идентификаторы (Names and identifiers), свойства (Properties), ссылки на поисковые запросы (Searches), спектры (Spektra), производители (Vendors), статьи (Articles).

^ More details:

Systematic name	2-Acetoxybenzoic acid
SMILES	<chem>CC(=O)Oc1ccccc1C(=O)O</chem> <a href="#">COPY</a>
Std. InChi	<a href="#">InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H.1H3.(H,11,12)</a> <a href="#">COPY</a>
Std. InChIKey	<a href="#">BSYNYRMUTXBXSQ-UHFFFAOYSA-N</a> <a href="#">COPY</a>
Cite this record	CSID:2157, <a href="http://www.chemspider.com/Chemical-Structure.2157.html">http://www.chemspider.com/Chemical-Structure.2157.html</a> (accessed 09:54, May 17, 2017) <a href="#">COPY</a>

[analgesic](#) [anti-inflammatory drug](#) [antipyretic](#) [antirheumatic drug](#) [+ TAG](#)

**Names and identifiers** [Properties](#) [Searches](#) [Spectra](#) [Vendors](#) [Articles](#) [More](#) ▾

Names and Synonyms	Database ID(s)
Validated by <b>Experts</b> , <a href="#">Validated by Users</a> , <a href="#">Non-Validated</a> , <a href="#">Removed by Users</a>	<a href="#">EDIT</a>
<b>2-(Acetyloxy)benzoic acid</b>	
200-064-1 <a href="#">[EINECS]</a>	
<b>2-Acetoxybenzenecarboxylic acid</b>	
<b>2-Acetoxybenzoesäure</b> <i>[German]</i> <a href="#">[ACD/IUPAC Name]</a>	
<b>2-Acetoxybenzoic acid</b> <a href="#">[ACD/IUPAC Name]</a>	

# Результаты поиска

More details:

analgesic anti-inflammatory drug antipyretic antirheumatic drug + TAG

Names and identifiers Properties Searches Spectra Vendors Articles More

Names and Synonyms Database ID(s) Wikipedia EDIT

Validated by Experts, Validated by Users, Non-Validated, Removed by Users

2-(Acetyloxy)benzoic acid  
200-064-1 [EINECS]  
2-Acetoxybenzenecarboxylic acid  
2-Acetoxybenzoesäure [German] [ACD/IUPAC Name]  
2-Acetoxybenzoic acid [ACD/IUPAC Name]  
2-Acetyloxybenzoic acid  
2-Carboxyphenyl acetate  
50-78-2 [RN]  
A.S.A.  
Acesan [Trade name]  
[More...](#)

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По ссылке “More” открываются дополнительные параметры: патенты, аудиовизуальные материалы и многое другое.

# Поиск по химической структуре

## Structure search

Draw structure

Convert structure

Load structure

Use our editor to draw your structure

CLEAN

Ketcher

Elemental

Accelrys JDraw

The screenshot shows the Ketcher chemical structure editor interface. At the top, there are three tabs: "Draw structure" (selected), "Convert structure", and "Load structure". Below the tabs, there is a text prompt "Use our editor to draw your structure" and a "CLEAN" button. The main workspace is divided into three sections: "Ketcher", "Elemental", and "Accelrys JDraw". The "Ketcher" section contains a toolbar with icons for drawing, editing, and saving. The "Elemental" section contains a vertical toolbar with various chemical symbols and shapes. The "Accelrys JDraw" section contains a vertical toolbar with a list of chemical elements: A, H, C, N, O, S, F, P, Cl, Br, I.

Химическую структуру можно нарисовать, выбрав раздел "Structure search", подраздел "Draw structure". Затем запустить поиск - "Search".

# Поиск химической структуры

The screenshot displays the ChemSpider website's search interface. At the top, the ChemSpider logo is accompanied by the tagline "Search and share chemistry". Below this, navigation tabs for "Simple", "Structure", "Advanced", and "History" are visible, with "Structure" being the active tab. The main heading is "Structure search". Underneath, there are three buttons: "Draw structure", "Convert structure" (which is highlighted), and "Load structure". A search input field contains the text "Aspirin" and has a search icon on the right. Below the input field, a note states: "Matches any text strings used to describe a molecule." and a smaller note lists search criteria: "Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID". The "Search options" section includes three tabs: "Exact", "Substructure", and "Similarity". Under the "Exact" tab, there are five radio button options: "Exact Match" (selected), "All Tautomers", "Same Skeleton (Including H)", "Same Skeleton (Excluding H)", and "All Isomers".

Для поиска химической структуры по названию вещества выберите раздел "Structure", подраздел "Convert structure", введите название вещества и запустите поиск.

# Результат поиска химической структуры

www.chemspider.com/StructureSearch.aspx

Use our editor to draw your structure

CLEAN

Ketcher Elemental Accelrys JDraw

HO-C(=O)-C<sub>6</sub>H<sub>4</sub>-O-C(=O)-CH<sub>3</sub>

Search options

Структуру можно сохранить на свой компьютер в файле формата mol, sdf, cdx or skc. Кроме того, структуру можно редактировать, используя инструменты слева, справа и вверху поля.

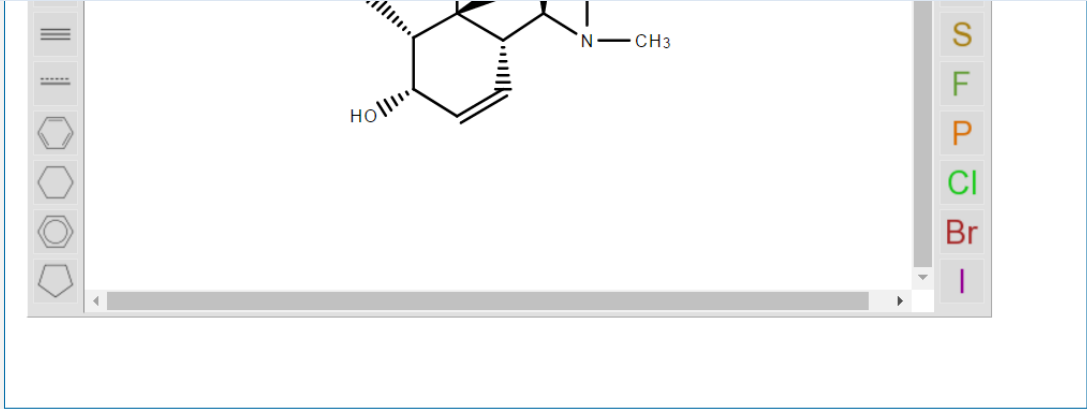


# Поиск по химической структуре

The screenshot shows the ChemSpider website interface. At the top, there is a navigation bar with links for Home, About us, Web APIs, Help, and Sign in. The ChemSpider logo and tagline 'Search and share chemistry' are prominently displayed. Below the logo, there are tabs for 'Simple', 'Structure', 'Advanced', and 'History', with 'Structure' being the active tab. The main heading is 'Structure search'. Underneath, there are three sub-tabs: 'Draw structure', 'Convert structure', and 'Load structure', with 'Load structure' being the active one. A text prompt asks the user to 'Select a structure file and upload it (MOL, SDF, CDX) or image file (PNG, JPG, GIF)'. Below this is a file selection button labeled 'Выберите файл' and a status indicator 'Файл не выбран'. Further down, there are 'Search options' with three tabs: 'Exact', 'Substructure', and 'Similarity'. Under the 'Exact' tab, there are five radio button options: 'Exact Match' (selected), 'All Tautomers', 'Same Skeleton (Including H)', 'Same Skeleton (Excluding H)', and 'All Isomers'.

Для поиска информации по химической формуле выберите раздел “Structure”, подраздел “Load structure”, загрузите структуру в одном из следующих форматов: mol, sdf, cdx or skc, jpeg, gif.

# Настройки поиска по структуре



Search options

Exact  Substructure  Similarity

- Exact Match
- All Tautomers
- Same Skeleton (Including H)
- Same Skeleton (Excluding H)
- All Isomers

Search Hits Limit: 100

Можно выбрать несколько настроек поиска по структуре: Exact – поиск точного совпадения, Substructure – поиск всех структур, включающих данную структуру, Similarity – поиск схожих структур (процент схожести не рекомендуется ставить более 90 %.)