



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)

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

Buttons: Save, 3D, Search

## Aspirin

Molecular Formula	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>
Average mass Da	180.157
Monoisotopic mass	180.042252 Da
ChemSpider ID	2157

COMMENT ON THIS RECORD

Featured data source

The Merck Index Online has more data on this compound

Advertisement

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▼ 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

2-(Acetyloxy)benzoic acid  
200-064-1 [EINECS]

EDIT

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 (Spectra), 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>
2-(Acetyloxy)benzoic acid	
200-064-1 <a href="#">[EINECS]</a>	
2-Acetoxybenzenecarboxylic acid	
2-Acetoxybenzoesäure <a href="#">[German]</a> <a href="#">[ACD/IUPAC Name]</a>	
2-Acetoxybenzoic acid <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) 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...](#)

Advertisement

CHROMATOGRAPHY SOFTWARE THAT

По ссылке  
“More”  
открываются  
дополнительны  
е параметры:  
патенты,  
аудиовизуальны  
е 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 software interface. At the top, there are three tabs: 'Draw structure' (selected), 'Convert structure', and 'Load structure'. Below the tabs, there is 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 chemical symbols: A, H, C, N, O, S, F, P, Cl, Br, I. The 'Accelrys JDraw' section is currently empty.

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

# Поиск химической структуры

**ChemSpider**  
Search and share chemistry

Simple **Structure** Advanced History

## Structure search

Draw structure **Convert structure** Load structure

Matches any text strings used to describe a molecule.

Aspirin

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

Search options

Exact **Substructure** Similarity

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

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## ChemSpider

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### Structure search

Draw structure Convert structure **Load structure**

Select a structure file and upload it (MOL, SDF, CDX) or image file (PNG, JPG, GIF)

Выберите файл | Файл не выбран

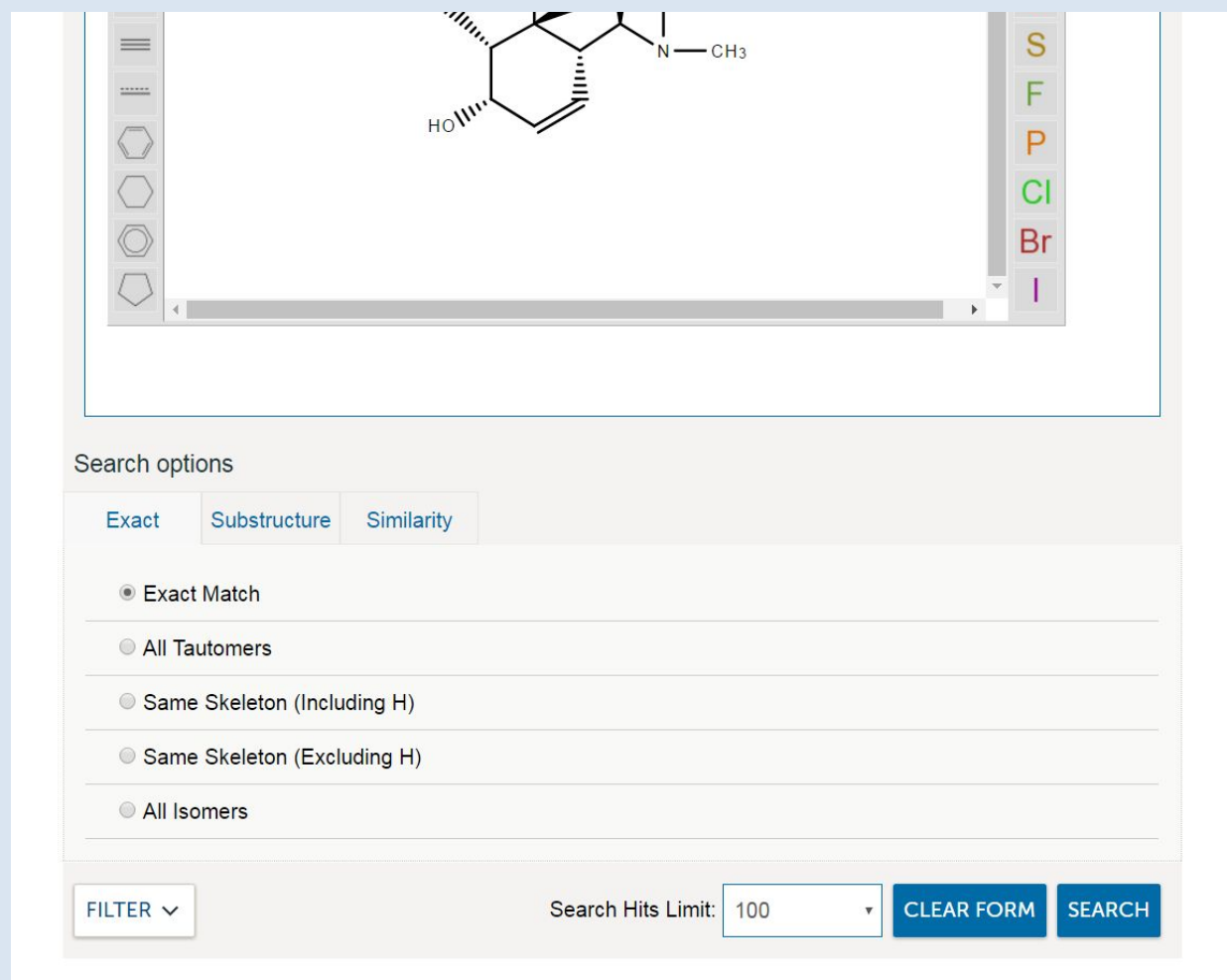
Search options

Exact Substructure Similarity

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



The screenshot displays a chemical search interface. At the top, a 3D ball-and-stick model of a bicyclic molecule is shown, featuring a methylamino group (-N-CH<sub>3</sub>) and a hydroxyl group (-OH). Below the structure, the search options are set to "Exact". The "Exact Match" option is selected, with other options including "All Tautomers", "Same Skeleton (Including H)", "Same Skeleton (Excluding H)", and "All Isomers". At the bottom, there is a "FILTER" dropdown, a "Search Hits Limit" set to 100, and "CLEAR FORM" and "SEARCH" buttons.

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 %.)