



Краткая инструкция

Поисковый запрос

Home About us Web APIs Help Sign in

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)-C₆H₄-O-C(=O)-CH₃

Buttons: Save, 3D, Search

Aspirin

Molecular Formula	C ₉ H ₈ O ₄
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

Advert: Learn more about mass spectrometry solutions from Agilent Technologies

Spotlight

Books Catalogue 2017

Download your copy now

▼ 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)
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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> COPY
Std. InChi	InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H.1H3.(H,11,12) COPY
Std. InChIKey	BSYNYRMUTXBXSQ-UHFFFAOYSA-N COPY
Cite this record	CSID:2157, http://www.chemspider.com/Chemical-Structure.2157.html (accessed 09:54, May 17, 2017) COPY

[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]	
2-Acetoxybenzenecarboxylic acid	
2-Acetoxybenzoesäure [German] [ACD/IUPAC Name]	
2-Acetoxybenzoic acid [ACD/IUPAC Name]	

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

Chemical structure editor interface showing various drawing tools and a list of elements (A, H, C, N, O, S, F, P, Cl, Br, I) on the right side.

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

Search options

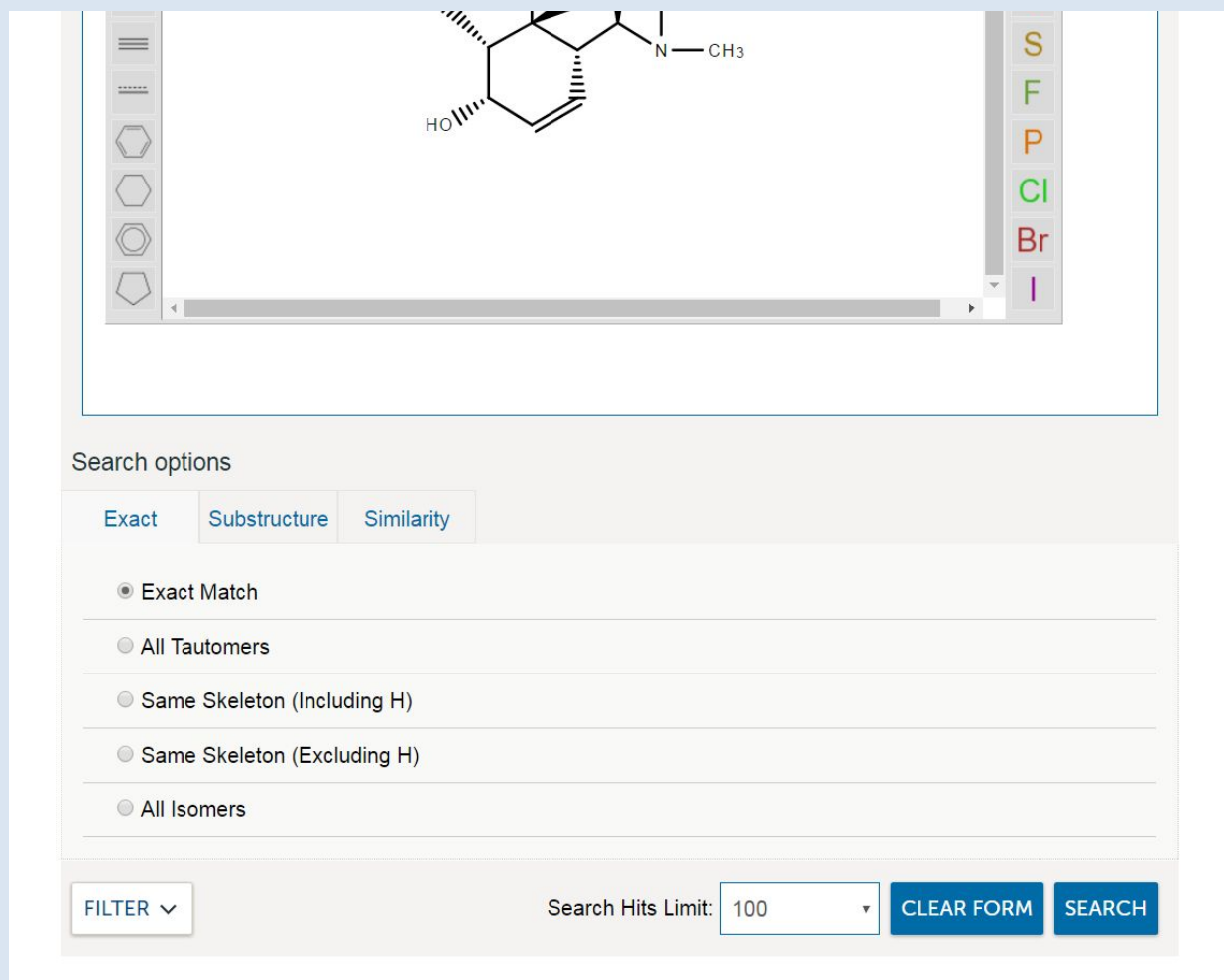
Структуру можно сохранить на свой компьютер в файле формата mol, sdf, cdx or skc. Кроме того, структуру можно редактировать, используя инструменты слева, справа и вверху поля.

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 tabs: 'Draw structure', 'Convert structure', and 'Load structure', with 'Load structure' being the active tab. A text prompt says 'Select a structure file and upload it (MOL, SDF, CDX) or image file (PNG, JPG, GIF)'. Below this is a file selection box with the text 'Выберите файл' and '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



The image shows a chemical search interface. At the top, a 3D molecular structure is displayed, featuring a bicyclic core with a methylamino group (N-CH_3) and a hydroxyl group (HO). Below the structure, there are search options: **Exact**, **Substructure**, and **Similarity**. Under **Exact**, there are five radio button options: Exact Match, 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:** field set to 100, a **CLEAR FORM** button, and a **SEARCH** button.

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 %.)