



Please enter a search term

Enzyme, Ligand ▾

contains ▾

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[Text-based queries](#)

- Full-text Search
- Advanced Search
- Enzyme & Disease

[Structure-based queries](#)

- Ligand Substructure

[Explorer](#)

- Enzyme Classification
- TaxTree
- Protein folding: SCOPe

[Visualization](#)

- Word Maps
- Genomes
- Functional Parameters Statistics
- Metabolic Pathways

BRENDA Tutorial

Ligand Search

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Please enter a search term

Enzyme, Ligand ▾

contains ▾

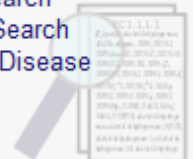
[add search field](#)

[delete search field](#)

[start search](#)

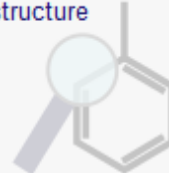
Text-based queries

- Full-text Search
- Advanced Search
- Enzyme & Disease



Structure-based queries

- Ligand Substructure



Explorer

- Enzyme Classification
- TaxTree
- Protein folding: CATH / SCOPe
- Ontologies



Visualization

- Word Maps
- Genomes
- Functional Parameters Statistics
- Metabolic Pathways



Prediction



Supporting

BRENDA
Tissue Ontology
Biochemical Reactions



How to find ligands / metabolites such as substrates, products, inhibitors etc. Substances interacting with enzymes




vanillic aci

- vanillic acid (Ligand)
- vanillic acid 4-O-beta-D-glucoside (Ligand)
- vanillic acid beta-D-glucoside (Ligand)
- vanillic acid O-demethylase (1.14.13.82)
- vanillic acid-4-O-beta-D-glucopyranoside (Ligand)

Enter the ligand name or a part of it and perform the search.

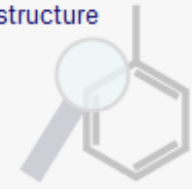
Text-based queries

- Full-text Search
- Advanced Search
- Enzyme & Disease



Structure-based queries

- Ligand Substructure




Explorer

- Enzyme Classification
- TaxTree
- Protein folding: CATH / SCOPe
- Ontologies



Visualization

- Word Maps
- Genomes
- Functional Parameter Statistics
- Metabolic Pathways



Prediction

- Membrane Helices
- EnzymeDetector



Supporting

- BRENDA Tissue Ontology
- Biochemical Reactions



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Advanced Search

| Field | Hits found |
|---|--------------------|
| Enzyme Names (Synonyms) | 1 |
| Ligands | 36 |

Choose „Ligands“ to display the enzyme-related information on vanillic acid.

Advanced Search

The result page shows all enzymes interacting with the ligand, including their derivatives, and their roles.

Search Ligands

Search term: vanillic acid

Results 1 - 10 of 36

download as CSV

download all results as CSV

| Ligand ▼▲ | EC Number ▼▲ | Role ▼▲ | Structure ▼▲ |
|---------------------------|--------------|--|--------------|
| 4-O-glucosylvanillic acid | 2.4.1.104 | Product | |
| dehydrodivanillic acid | 1.2.3.9 | Product | |
| homovanillic acid | 1.10.3.2 | Substrate; Turnover Number | |
| homovanillic acid | 1.14.13.5 | Inhibitor | |
| homovanillic acid | 2.6.1.5 | Inhibitor | |
| homovanillic acid | 2.8.2.1 | KM Value; Substrate | |
| isovanillic acid | 1.14.13.82 | Natural_Product; Natural_Substrate; Product; Substrate | |
| isovanillic acid | 2.1.1.291 | KM Value; Substrate; Turnover Number | |
| vanillic acid | 1.1.1.21 | Inhibitor | |
| vanillic acid | 1.1.99.20 | Product | |

Results 1 - 10 of 36

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download all results as CSV

Advanced Search

Search Ligands

Search term: vanillic acid

Results 1 - 10 of 36

download as CSV
download all results as CSV

| Ligand ▼▲ | EC Number ▼▲ | Role ▼▲ | Structure ▼▲ |
|---------------------------|--------------|--|--------------|
| 4-O-glucosylvanillic acid | 2.4.1.104 | Product | |
| dehydrodivanillic acid | 1.2.3.9 | Product | |
| homovanillic acid | 1.10.3.2 | Substrate; Turnover Number | |
| homovanillic acid | 1.14.13.5 | Inhibitor | |
| homovanillic acid | 2.6.1.5 | Inhibitor | |
| homovanillic acid | 2.8.2.1 | KM Value; Substrate | |
| isovanillic acid | 1.14.13.82 | Natural_Product; Natural_Substrate; Pr | |
| isovanillic acid | 2.1.1.291 | KM Value; Substrate; Turnover Number | |
| vanillic acid | 1.1.1.21 | Inhibitor | |
| vanillic acid | 1.1.99.20 | Product | |

You can display the molecular structure...

Results 1 - 10 of 36

download as CSV
download all results as CSV

Advanced Search

Search Ligands

Search term: va

BRENDA - Chemical structure of vanillic a...

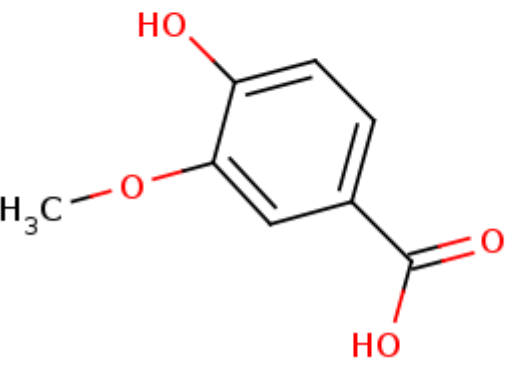
www.brenda-enzymes.org/structure.php?n=18;

BRENDA

vanillic acid = Search

Search again for: [vanillic](#), [acid](#)

Chemical structure of vanillic acid



- Ligand
- 4-O-glucosyl
 - dehydrodivan
 - homovanillic a
 - homovanillic a
 - homovanillic a
 - homovanillic a
 - homovanillic a
 - isovanillic aci
 - isovanillic aci
 - vanillic acid
 - vanillic acid

| Structure | |
|---------------|--|
| | |
| | |
| | |
| | |
| strate; Produ | |
| r Number | |
| | |
| | |

...and see the diagram with more search options

Results 1 - 10 of 36

download as CSV

download all results as CSV




Advanced Search







































































Search Ligands

Search term: vanillic acid

« « Results 1 - 10 of 36 » »


 download as CSV


 download all results as CSV

| Ligand ▼▲ | EC Number ▼▲ | Role ▼▲ | Structure ▼▲ |
|---------------------------|---|--------------------------------------|---|
| 4-O-glucosylvanillic acid |    2.4.1.104 | Product |     |
| dehydrodivanillic acid |    1.2.3.9 | Product |     |
| homovanillic acid |    1.10.3.2 | Substrate; Turnover Number |     |
| homovanillic acid |    1.14.13.5 | Inhibitor |     |
| homovanillic acid |    2.6.1.5 | Inhibitor |     |
| homovanillic acid |    2.8.2.1 | KM Value; Substrate |     |
| isovanillic acid |    1.14.13.82 | Natural_Product; Natural |     |
| isovanillic acid |    2.1.1.291 | KM Value; Substrate; Turnover Number |     |
| vanillic acid |    1.1.1.21 | Inhibitor |     |
| vanillic acid |    1.1.99.20 | Product |     |

This button leads to the detailed information on the ligand...

« « Results 1 - 10 of 36 » »

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 download all results as CSV

Basic Ligand Information

Roles as Enzyme Ligand

- Substrate
- In Vivo* Substrate
- Product
- In Vivo* Product
- Cofactor
- Activator
- Inhibitor
- Metals and Ions

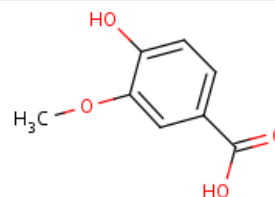
Enzyme Kinetic Parameters

References & Links

Ligand vanillic acid

Basic Ligand Information

Molecular Structure



...on the structure, synonyms, and its roles in the enzyme-ligand interaction in BRENDA, plus its kinetic values and literature references.

| Molecular Formula | BRENDA Name | InChIKey |
|--|---------------|----------------------------|
| C ₈ H ₈ O ₄ | vanillic acid | WKOLLVMJNQZCI-UHFFFAOYSA-N |

Synonyms:

3-methoxy-4-hydroxybenzoate, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 4-hydroxy-3-methoxybenzoic acid, vanillate, vanillinic acid

Roles as Enzyme Ligand

Substrate in Enzyme-catalyzed Reactions (28 results)

| EC_NUMBER | REACTION_PARTNERS | LITERATURE |
|------------|--|--|
| 1.10.3.2 | vanillic acid + O ₂ = 4-carboxy-2-methoxycyclohexa-2,4-dienone + H ₂ O | 396343, 396396, 396399, 396402 |
| 1.10.3.2 | vanillic acid + O ₂ = ? | 671404, 696857, 675042, 701029 |
| 1.10.3.2 | vanillate + O ₂ = ? + H ₂ O | 687338 |
| 1.11.1.7 | vanillic acid + H ₂ O ₂ = ? | 439746 |
| 1.14.13.64 | 4-Hydroxy-3-methoxybenzoate + NADH + O ₂ = ? | 7428 |
| 1.14.13.64 | 4-Hydroxy-3-methoxybenzoate + NADPH + O ₂ = ? | 7428 |
| 1.14.13.82 | vanillate + O ₂ + NADH = 3,4-dihydroxybenzoate + NAD ⁺ + H ₂ O + formaldehyde | 207983, 639292, 658498, 639290, 639289 |
| 1.14.13.82 | vanillate + O ₂ + electron donor + tetrahydrofolate = 3,4-dihydroxybenzoate + oxidized electron donor + H ₂ O + methyltetrahydrofolate | 659009 |
| 1.14.13.82 | vanillic acid + NAD(P)H + O ₂ = protocatechuic acid + NAD(P) ⁺ + H ₂ O + formaldehyde | 673722, 674280 |

Advanced Search

Search Ligands

Search term: vanillic acid

Results 1 - 10 of 36

download as CSV

download all results as CSV

| Ligand | EC Number | Role | Structure |
|---------------------------|------------|--------------------------------------|-----------|
| 4-O-glucosylvanillic acid | 2.4.1.104 | Product | |
| dehydrodivanillic acid | 1.2.3.9 | Product | |
| homovanillic acid | 1.10.3.2 | Substrate; Turnover Number | |
| homovanillic acid | 1.14.13.5 | Inhibitor | |
| homovanillic acid | 2.6.1.5 | Inhibitor | |
| homovanillic acid | 2.8.2.1 | KM Value; Substrate | |
| isovanillic acid | 1.14.13.82 | Natural_Product; Natur | |
| isovanillic acid | 2.1.1.291 | KM Value; Substrate; Turnover Number | |
| vanillic acid | 1.1.1.21 | Inhibitor | |
| vanillic acid | 1.1.99.20 | Product | |

You can directly switch to the „Substructure Search“ to find similar ligands interacting with enzymes in BRENDA.

Results 1 - 10 of 36

download as CSV

download all results as CSV

Substructure search

Sketch molecular structures:

JSME Molecular Editor by Peter Ertl and Bruno Bienfait

Restrict the substructure search to:

- Substrates (S)
- Products (P)
- Cofactors (C)
- Activating Compounds (A)
- Inhibitors (I)

Select maximal time for the search: 5 s

Start substructure search

JSME Editor courtesy of P. Ertl, Novartis

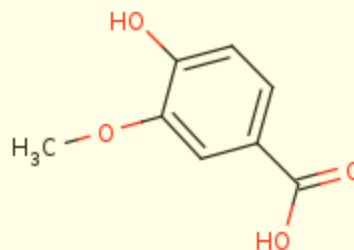
JSME help

Number of hits: 42



- vanillic acid, vanillate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 3-methoxy-4-hydroxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, vanillinic acid

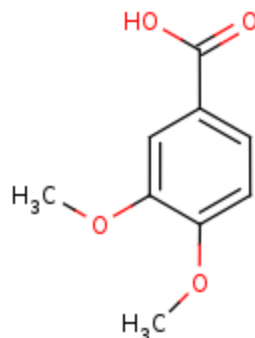
Role : S / P / I / A



start BRENDA search

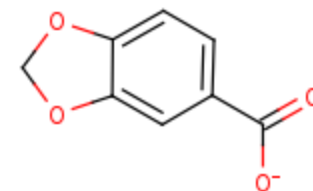
- veratric acid, 3,4-dimethoxybenzoic acid, 3,4-dimethoxybenzoate, veratrate, 3,4-dimethoxy benzoic acid, veratranoate, 4,5-dimethoxybenzoic acid

Role : S / P / I



- (3,4-Methylenedioxy)benzoic acid

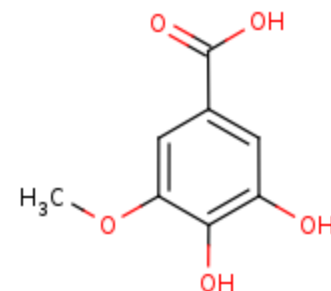
Role : S / P



On the result page which are structural the searched ligands displayed

- 5-methoxygallic acid, 3-Methoxygallic acid

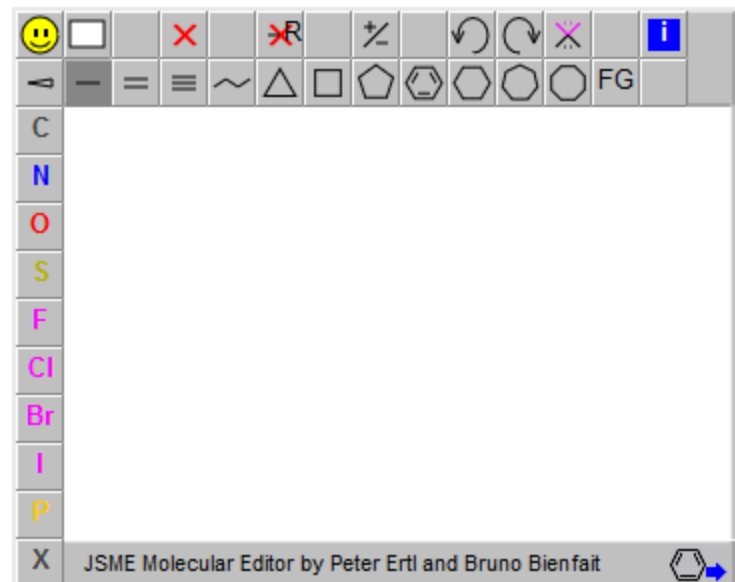
Role : S



start BRENDA search

Substructure search

Sketch molecular structures:



Restrict the substructure search to:

- Substrates (S)
- Products (P)
- Cofactors (C)
- Activating Compounds (A)
- Inhibitors (I)

Select maximal time for the search:

[Start substructure search](#)

JSME Editor courtesy of P. Ertl, Novartis

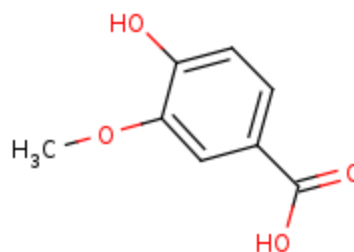
[JSME help](#)

Number of hits: 42



- vanillic acid, vanillate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 3-methoxy-4-hydroxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, vanillinic acid**

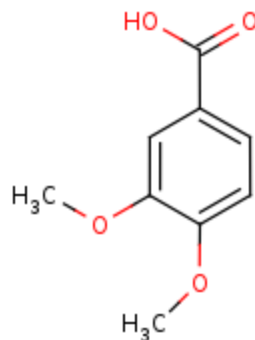
Role : S / P / I / A



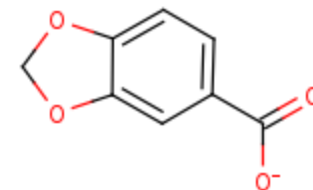
[start BRENDA search](#)

- veratric acid, 3,4-dimethoxybenzoic acid, 3,4-dimethoxybenzoate, veratrate, 3,4-dimethoxy benzoic acid, veratranoate, 4,5-dimethoxybenzoic acid**

Role : S / P / I



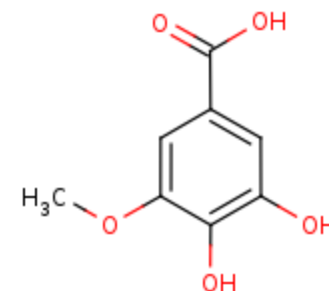
2. **(3,4-Methylenedioxy)benzoic acid**
Role : S / P



[start BRENDA search](#)

If you find an a
ligand, you can
search in BREN
more inform

4. **Methoxygallic acid**
Role : S



[start BRENDA search](#)

Substructure search

Number of hits: 43



Sketch molecular structures:

JME Molecular Editor@, Novartis Pharma AG

Buttons: CLR, DEL, D-R, +/-, UDO

Toolbox: [Icons for drawing rings and bonds]

Element palette: C, N, O, S, F, Cl, Br, I, P, X

Restrict the substructure search to:

- Substrates (S)
- Products (P)
- Cofactors (C)
- Activating Compounds (A)
- Inhibitors (I)

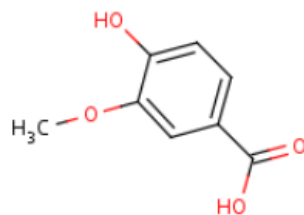
Select maximal time for the search: 5 s

Start substructure search

JME Editor courtesy of P. Ertl, Novartis JME

[vanillic acid, vanillate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 3-methoxy-4-hydroxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, vanillic acid](#)

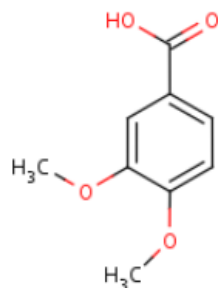
Role : [S / P / I / A](#)



start BRENDA search

3. [veratric acid, 3,4-dimethoxybenzoic acid, 3,4-dimethoxybenzoate, veratrate, 3,4-dimethoxybenzoic acid, veratrate](#)

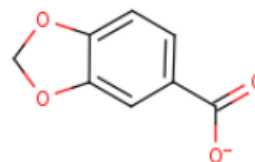
Role : [S / P / I](#)



start BRENDA search

2. [\(3,4-Methylenedioxy\)benzoate, 3,4-Methylenedioxybenzoate](#)

Role : [S / P](#)

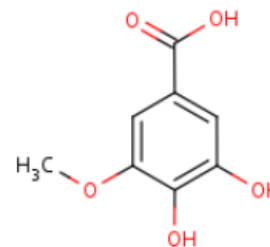


start BRENDA search

If you find an appropriate ligand, you can perform a search in BRENDA to get more information...

4. [5-methoxybenzoic acid, 5-methoxybenzoate](#)

Role : [S](#)



start BRENDA search

Advanced Search

Search Ligands

Ligands: show results

- [Don't show organism specific information \(fast!\)](#)
- Search organism in taxonomic tree (slow, e.g. "mammalia" for rat,human,monkey,...)
(Not possible to combine with the first option)

Refine your search

EC Number: contains

Role: contains

Organism: contains

Reference: contains

Image of 2D Structure
 Search for synonyms (with exact matching searchword)

...which can be seen on this page

The synonyms for (3,4-Methylenedioxy)benzoate are:

(3,4-Methylenedioxy)benzoate, 3,4-Methylenedioxybenzoate
[Ligand Summary Page](#)

Search term: (3,4-Methylenedioxy)benzoate

<< Results 1 - 2 of 2 >>

| Source | Ligand ▼▲ | EC Number ▼▲ | Role ▼▲ | Structure ▼▲ |
|--------|------------------------------|--------------|-----------|--------------|
| BRENDA | (3,4-methylenedioxy)benzoate | 3.5.5.7 | Product | |
| BRENDA | 3,4-methylenedioxybenzoate | 1.14.99.15 | Substrate | |

<< Results 1 - 2 of 2 >>

Substructure search

Number of hits: 43



Sketch molecular structures:

The JME Editor interface includes a toolbar with icons for smile, CLR, DEL, D-R, +/-, and UDO. The canvas shows a chemical structure of benzoic acid (O=C(O)c1ccccc1).

Restrict the substructure search to:

- Substrates (S)
- Products (P)
- Cofactors (C)
- Activating Compounds (A)
- Inhibitors (I)

Select maximal time for the search: 5 s

Start substructure search

[JME Editor](#) courtesy of P. Ertl, Novartis [JME](#)

[vanillic acid, vanillate, 4-hydroxy-3-methoxybenzoate, 4-hydroxy-3-methoxybenzoic acid, 3-methoxy-4-hydroxybenzoate, 4-hydroxy-3-methoxy benzoic acid, 3-methoxy-4-hydroxybenzoic acid, 4-hydroxy-3-methoxy-benzoate, vanillic acid](#)

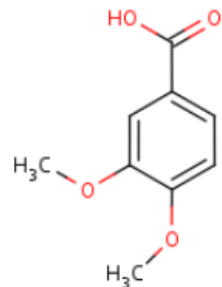
Role : [S / P / I / A](#)



Otherwise you could perform a new Substructure Search by drawing the molecular structure with the editor...

3. [5-methoxybenzoate, veratrate, 3,4-dimethoxybenzoic acid, veratrate](#)

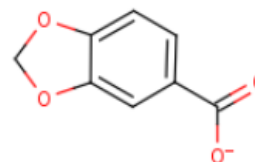
Role : [S / P / I](#)



start BRENDA search

2. [\(3,4-Methylenedioxy\)benzoate, 3,4-Methylenedioxybenzoate](#)

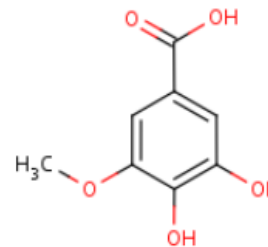
Role : [S / P](#)



start BRENDA search

4. [5-methoxygallic acid, 3-O-Methylgallate, 3-Methoxygallic acid](#)

Role : [S](#)



start BRENDA search

Substructure search

Query was stopped when the max-searchtime (5s) ran out.

Number of hits: 2904



Sketch molecular structures:

JME Molecular Editor

JME Molecular Editor©, Novartis Pharma AG

1. [Benzoate, Benzoic acid, aromatic acid, benzoate/in, benzoate/out, Substituted benzoates, Substituted benzoic acids](#)
Role : [S / P / I / A](#)

start BRENDA search

2. [4-hydroxybenzoate, 4-hydroxybenzoic acid, p-hydroxybenzoic acid, p-hydroxybenzoate, 4-hydroxybenzoic acid, p-hydroxy benzoic acid](#)
Role : [S / P / I / A](#)

...and again, if you find the appropriate ligand, you can perform a search in BRENDA to get more details.

3. [anthranilate, anthranilic Aminobenzoate, 2-aminobenzoic acid, o-aminobenzoate, 2-amino benzoate, 2-Carboxy-1-phenylamine](#)
Role : [S / P / I / A](#)

start BRENDA search

[benzoate, 2-carboxyphenol, 2-Carboxyphenol, o-hydroxy-benzoic acid](#)
Role : [S / P / I / A](#)

start BRENDA search

Restrict the substructure search to:

- Substrates (S)
- Products (P)
- Cofactors (C)
- Activating Compounds (A)
- Inhibitors (I)

Select maximal time for the search: 5 s

Start substructure search