BRENDA Tutorial

Ligand Search
How to find ligands / metabolites such as substrates, products, inhibitors etc. Substances interacting with enzymes
Enter the ligand name or a part of it and perform the search.
Choose „Ligands“ to display the enzyme-related information on vanillic acid.
The result page shows all enzymes interacting with the ligand, including their derivatives, and their roles.

# Search Ligands

## Search term: vanillic acid

<table>
<thead>
<tr>
<th>Ligand</th>
<th>EC Number</th>
<th>Role</th>
<th>Structure</th>
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<tbody>
<tr>
<td>vanillic acid</td>
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<td>Inhibitor</td>
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<td>1.10.3.2</td>
<td>Substrate; Turnover Number; KM Value</td>
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<td>1.11.1.1</td>
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<td>1.11.1.7</td>
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<td>1.2.1.30</td>
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you can display the molecular structure
Search Ligands

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On the next page you get basic information on the Ligand Summary Page with...
Ligand vanillic acid

Basic Ligand Information

Molecular Structure

![Molecular Structure Diagram]

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

Roles as Enzyme Ligand

In Vivo Substrate in Enzyme-catalyzed Reactions (7 results)

<table>
<thead>
<tr>
<th>EC NUMBER</th>
<th>PROVEN IN VIVO REACTION</th>
<th>REACTION DIAGRAM</th>
<th>LITERATURE</th>
<th>ENZYME 3D STRUCTURE</th>
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In Vivo Product in Enzyme-catalyzed Reactions (7 results)

...more detailed information on the structure, synonyms, and their roles in the enzyme-ligand interaction, enzyme kinetic parameters, and references in BRENDA
you can directly switch to the „Substructure Search“ to find similar ligands interacting with enzymes in BRENDA
On the result page all ligands structurally similar to the searched ligand are displayed.
If you find an appropriate ligand, you can perform a search in BRENDA to get more information.
On the result page you find further details of the searched ligand.
Otherwise you could perform a new Substructure Search by drawing the molecular structure with the editor and choosing appropriate search options.