



# **Searching for Bioactivity Data using DiscoveryGate**

DiscoveryGate®  
Exercise Guide

# Searching for Bioactivity Data using DiscoveryGate

## DiscoveryGate<sup>®</sup> Exercise Guide

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**Exercise descriptions**

The following descriptions explain the goal of each exercise. If you like to figure things out on your own, use the descriptions to conduct the exercises. If you prefer step-by-step instructions, go to the page listed below the description.

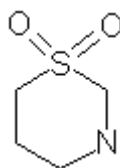
**Exercise 1**

Search for transformations in the Metabolite Database that have chloramphenicol as the parent compound. View the transformation, parent, and metabolite data. View the toxicity data if available.

For a step-by-step solution, see page 1-2.

**Exercise 2**

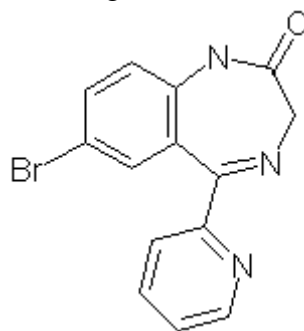
Search the Metabolite Database for transformations in which the following thiazane structure is contained in the substrate. Create a report of the search results.



For a step-by-step solution, see page 1-8.

**Exercise 3**

Search the CrossFire Beilstein database to retrieve pharmacological data for bromazepam.



For a step-by-step solution, see page 1-15.

### Exercise 1

Launch the MDL Database Browser

Choose the MDL Metabolite Database

Add the Chemical Name field to the query form

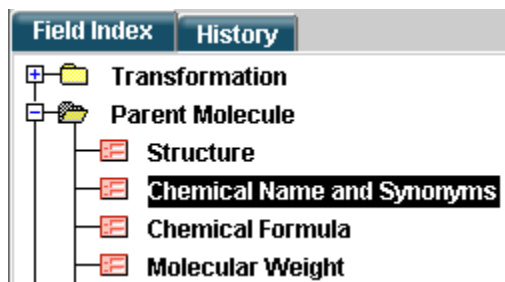
Enter the query

View the details for a transformation

Search for Chloramphenicol as Parent

Search the MDL Metabolite Database for transformations that have chloramphenicol as the parent compound.

1. From the DiscoveryGate home page, click **Search Databases**.
2. Choose **MDL Metabolite Database** from the Database list. If the default query form does not contain the field to search for Chemical Name, you need to add the field to the form.
3. In the Field Index, open the **Parent Molecule** folder. Double-click the **Chemical Name and Synonyms** field.

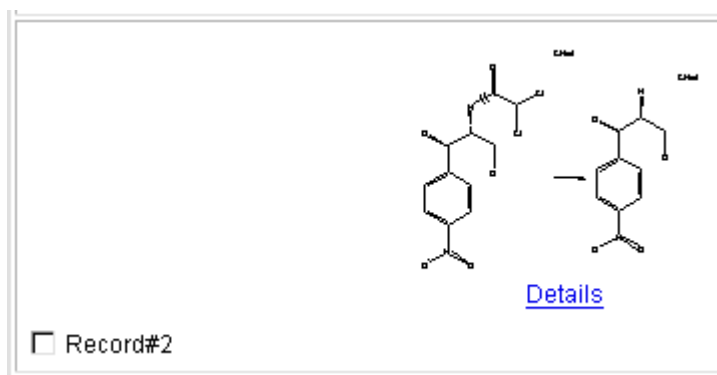


4. Enter **chloramphenicol** into the text box.



The image shows a search form titled 'Parent Molecule'. It has a dropdown menu set to 'AND', a text box containing 'Chemical Name and Synonyms', another dropdown menu set to 'Contains', and a text input field containing 'chloramphenicol'.

5. Click **start search**.
6. Click the **Details** link for one of the transformations retrieved. For example:



The details for the transformation are displayed.

[Return to Search Results](#)

[View selected records in another database](#)

← Record # 2 →

**Total Records:** 64

Also found in: [ACD](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [OHS MSDS](#) [Toxicity](#) [xPharm](#)

### MDL® Metabolite Database

[Use as Query](#)

Select current record

**Available Data**  
Click on a link to add the information to this page

Set current view as default

View results as **transformations:**      View results as **molecules:**

|                                    |                                |
|------------------------------------|--------------------------------|
| <a href="#">Transformation</a> (1) | <a href="#">Parent</a> (1)     |
| <a href="#">Reference</a> (12)     | <a href="#">Species</a> (56)   |
| <a href="#">Species</a> (12)       | <a href="#">Substrate</a> (1)  |
| <a href="#">Enzyme</a> (12)        | <a href="#">Metabolite</a> (1) |

### Transformation Results -- Transformation [\(hide\)](#)

|  |                    |
|--|--------------------|
| <b>MDL number</b>  | RMTB00004053       |
| <b>Path</b>  | MTB697-B, MTB697-C |
| <b>Step</b>  | 1 of 2, 1 of 2     |
| <b>Scheme</b>  | MTB697             |
| <b>Chemical Name and Synonyms :</b>  |                    |
| <ul style="list-style-type: none"> <li>• Chloramphenicol</li> <li>• D-(-)-threo-2-(Dichloroacetamido)-1-(p-nitrophenyl)-1,3-propanediol</li> <li>• (R-(R*,R*))-(2,2-Dichloro-N-(2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl)acetamido)</li> <li>• (1R,2R)-1-(p-Nitrophenyl)-2-(2,2-dichloroacetamido)-1,3-propanediol</li> <li>• D-threo-Chloramphenicol</li> </ul> |                    |
| <b>Reaction Class :</b>  |                    |
| <ul style="list-style-type: none"> <li>• Hydrolysis</li> <li>• N-Deacylation</li> </ul>  |                    |

View the references for the transformation

7. Click the **Reference** link for transformation results. In this example, 12 references are available:

View results as **transformations**:

- [Transformation](#) (1)
- [Reference](#) (12)
- [Species](#) (12)
- [Enzyme](#) (12)

The references are added to the bottom of the page.

Transformation Results -- References [\(hide\)](#)

| Reference Full Citation 1 of 12  |   |
|--|---|
| <a href="#">Cravedi, J. P.; Perdu-Durand, E.; Baradat, M.; Alary, J.; Debrauwer, L.; Bories, G.; Chem Res Toxicol [CRTOEC] 1995, 8 (5), 642.</a> |   |
| <b>Title</b>   | Chloramphenicol Oxamylethanolamine as an End Product of Chloramphenicol Metabolism in Rat and Humans: Evidence for the Formation of a Phospholipid Adduct |
| <b>Analytical Data for Current Reference</b>   | (3)H, HPLC, MS, Scintillation Counter   |
| <b>Reactant Grade</b>  |   |
| <b>Product Grade</b>   |   |
| <b>Comments</b>  |   |

| Reference Full Citation 2 of 12  |  |
|--|--|
| <a href="#">Cravedi, J. P.; Baradat, M.; Debrauwer, L.; Alary, J.; Tulliez, J.; Bories, G.; Drug Metab Dispos [DMDSA] 1994, 22 (4), 578.</a> |  |
| <b>Title</b>   | Evidence For New Metabolic Pathways of Chloramphenicol in The Duck |
| <b>Analytical Data for Current Reference</b>   | HPLC, MS, TLC  |
| <b>Reactant Grade</b>  |  |
| <b>Product Grade</b>   |  |
| <b>Comments</b>  |  |

8. Scroll back to the top of the page, or click **Top of Page**.
9. Click the **Parent** link for molecule results.

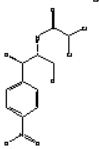
Display the parent molecule data

View results as **molecules**:

- [Parent](#) (1)
- [Species](#) (56)
- [Substrate](#) (1)
- [Metabolite](#) (1)

Molecule data for the Parent is added to the display.

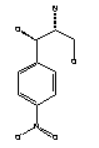
Molecule Results -- Parent [\(hide\)](#)

|  |                          |   |
|--|--------------------------|---|
| <br><a href="#">Use As Query</a>  | <b>CAS Number</b>        |   |
|  |                          | 56-75-7   |
|  | <b>Molecular Formula</b> | C11 H12 Cl2 N2 O5                               |
|  | <b>Molecular Weight</b>  | 323.131   |
|  | <b>Use</b>               | 1. Veterinary Agent<br>2. Veterinary Antibiotic |
|  | <b>Scheme</b>            | MTB697  |
| <b>Chemical Name and Synonyms :</b>  |                          |   |
| <ul style="list-style-type: none"> <li>• Chloramphenicol</li> <li>• D-(-)-threo-2-(Dichloroacetamido)-1-(p-nitrophenyl)-1,3-propanediol</li> <li>• (R-(R*,R*))-2,2-Dichloro-N-(2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl)acetamide</li> <li>• (1R,2R)-1-(p-Nitrophenyl)-2-(2,2-dichloroacetamido)-1,3-propanediol</li> <li>• D-threo-Chloramphenicol</li> </ul> |                          |   |
| <b>Activity :</b>  |                          |   |
| Antibacterial , Antibiotic , Antirickettsial , Toxic   |                          |   |
| <b>Compound Class :</b>  |                          |   |
| Alcohol , Aliphatic alcohol , Aliphatic amide , Aliphatic carboxylic acid amide , Aromatic nitro compound , Carboxamide , Halogen compound   |                          |   |
| <a href="#">Molecule References</a> (56)   |                          |   |

Display the metabolite  
molecule data

10. Return to the top of the page, and then click the Metabolite link for molecule results.

Molecule Results -- Metabolite [\(hide\)](#)

|   |                          |              |
|---|--------------------------|--------------|
| <br><a href="#">Use As Query</a> | <b>CAS Number</b>        |              |
|   |                          |              |
|   | <b>Molecular Formula</b> | C9 H12 N2 O4 |
|   | <b>Molecular Weight</b>  | 212.204      |
|   | <b>Use</b>               |              |
|   | <b>Scheme</b>            | MTB697       |
| <b>Chemical Name and Synonyms :</b>   |                          |              |
| <b>Activity :</b>   |                          |              |
| <b>Compound Class :</b>   |                          |              |

View the toxicity data

11. Return to the top of the page. Click the **Toxicity** link for "Also found in".

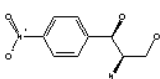
Also found in: [ACD](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [OHS MSDS](#) [Toxicity](#) [xPharm](#)

In this example, two records are retrieved from the MDL Toxicity Database. The first record is for the metabolite.

[Return to MDL® Metabolite Database](#)

Record # 1 ➡ Total Records: 2

## MDL® Toxicity Database

|   |   |
|---|---|
|  | <p><b>Available Data</b></p> <p><i>Click on a link to add the information to this page</i></p> <p><input type="checkbox"/> Set current view as default</p> <p> <a href="#">Chemical</a> (1)      <a href="#">Acute Toxicity</a> (2)<br/> <a href="#">Mutagenicity</a> (1)      <a href="#">Model</a> (1)         </p> |
|---|---|

### Chemical [\(hide\)](#)

|   |              |
|---|--------------|
| <b>Molecular Formula</b>  | C9 H12 N2 O4 |
| <b>Molecular Weight</b>   | 212.2038     |
| <b>MDL Number</b>   | MFCD00078126 |
| <b>CAS Registry Number</b>  | 716-61-0     |
| <b>Beilstein Number</b>   |              |
| <b>Beilstein Handbook</b>   |              |
| <b>RTECS Number</b>   | TY3100000    |
| <b>CCRIS Number</b>   |              |
| <b>GENE-TOX Number</b>  |              |
| <b>GENOTOXICITY Number</b>  |              |
| <b>CARCINO Number</b>   |              |
| <b>HEPATO Number</b>  |              |
| <b>NEPHRO Number</b>  |              |
| <b>Patch Test</b>   |              |
| <b>Compound Descriptor</b>  | Drug         |
| <b>Chemical Name and Synonyms :</b>   |              |
| <ul style="list-style-type: none"> <li>• 1,3-PROPANEDIOL, 2-AMINO-1-(P-NITROPHENYL)-, D-THREO-(-)-</li> <li>• CHLORAMPHENICOL BASE</li> <li>• D-THREO-(-)-2-AMINO-1-(P-NITROPHENYL)-1,3-PROPANEDIOL</li> <li>• LEVOAMINE</li> </ul> |              |

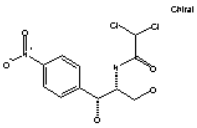
12. Click the right arrow to view the second Toxicity record.  
This data pertains to the parent molecule.



[Return to MDL® Metabolite Database](#)

← Record # 2 Total Records: 2

## MDL® Toxicity Database

|  |  |
|--|--|
|  | <p><b>Available Data</b></p> <p><i>Click on a link to add the information to this page</i></p> <p><input type="checkbox"/> Set current view as default</p> <p><a href="#">Chemical</a> (1)      <a href="#">Acute Toxicity</a> (22)</p> <p><a href="#">Mutagenicity</a> (42)      <a href="#">Skin/Eye Irritation</a> (20)</p> <p><a href="#">Tumorigenicity</a> (5)      <a href="#">Reproductive Effects</a> (18)</p> <p><a href="#">Other Multiple Doses</a> (14)      <a href="#">Review</a> (11)</p> <p><a href="#">Model</a> (1)</p> |
|--|--|

Chemical [\(hide\)](#)

|                            |   |
|----------------------------|---|
| <b>Molecular Formula</b>   | C11 H12 Cl2 N2 O5   |
| <b>Molecular Weight</b>    | 323.1308  |
| <b>MDL Number</b>          | MFCD00078159  |
| <b>CAS Registry Number</b> | 56-75-7   |
| <b>Beilstein Number</b>    | 2225532   |
| <b>Beilstein Handbook</b>  | 4-13-00-02742   |
| <b>RTECS Number</b>        | AB6825000   |
| <b>CCRIS Number</b>        | 3922  |
| <b>GENE-TOX Number</b>     | 139   |
| <b>GENOTOXICITY Number</b> |   |
| <b>CARCINO Number</b>      | 235   |
| <b>HEPATO Number</b>       | 3   |
| <b>NEPHRO Number</b>       | 3   |
| <b>Patch Test</b>          | 264   |
| <b>Compound Descriptor</b> | Agricultural Chemical , Drug , Human Data , Natural Product , Reproductive Effector |

## Chemical Name and Synonyms :

- ACETAMIDE, 2,2-DICHLORO-N-(BETA-HYDROXY-ALPHA-(HYDROXYMETHYL)-P-NITROPHENETHYL)-,D-(-)-THREO-
- ACETAMIDE, 2,2-DICHLORO-N-(2-HYDROXY-1-(4-NITROPHENYL)ETHYL)-, (R-(R\*,R\*))-

Return to the MDL  
Metabolite Database

13. Click **Return to MDL Metabolite Database**.

## Exercise 2

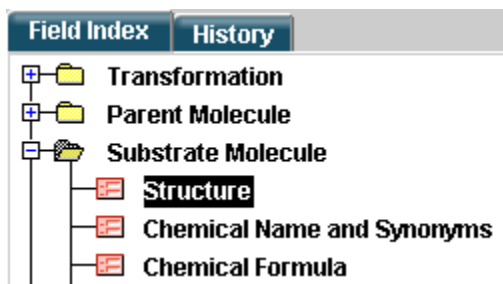
Add the Substrate structure field to the query form

Draw the structure query

### Search for Thiazane substructure as Substrate

Search the MDL Metabolite Database for transformations in which a particular thiazane structure is contained in the substrate. Create a report of the search results.

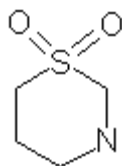
1. Click the **queries** tab.
2. Click **clear form** from the top menu bar. Click **OK** at the confirmation prompt.
3. In the Field Index, open the **Substrate Molecule** folder. Double-click the **Structure** field.



4. Double-click the **Structure** box to launch MDL Draw.




5. Draw the thiazane structure.



6. Click **Done**.
7. Choose **Substructure** as the search type.

**Substrate Molecule**

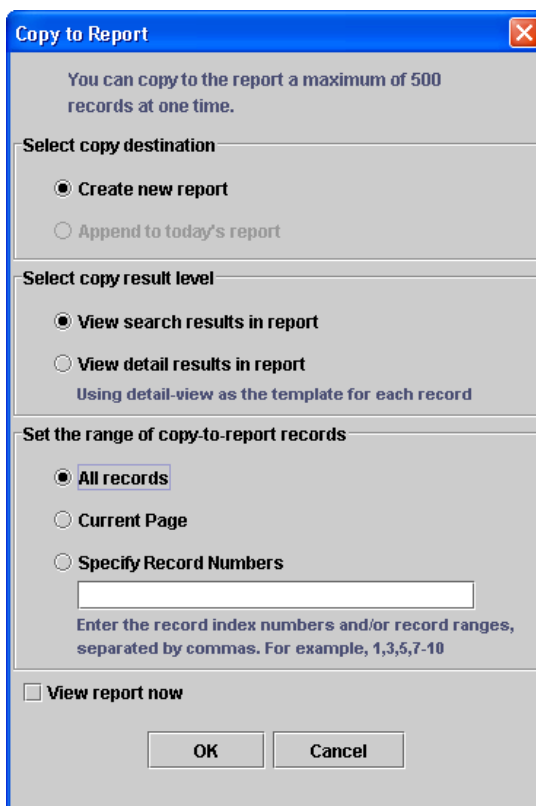
| Structure  | Select Search Type:  |
|--|--|
|  | Substructure ▼<br><small>A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.</small> |

start search

Conduct the search

Create a report

8. Click **start search**.
9. When the search is complete, click **copy to report** on the top menu bar. Select **All records**.



Append details to the report

10. Click **OK**. The table of transformation schemes is copied to Today's Report.
11. Click **Details** for one of the transformations.
12. Click **copy to report**. Select **All records**.

**Copy to Report**

You can copy to the report a maximum of 500 records at one time.

**Select copy destination**

Create new report

Append to Today's Report - Report #1

**Select copy result level**

View search results in report

View detail results in report

Using detail-view as the template for each record

**Set the range of copy-to-report records**

All records

Current Page

Specify Record Numbers

Enter the record index numbers and/or record ranges, separated by commas. For example, 1,3,5,7-10

View report now

OK Cancel

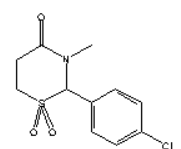
Append toxicity data to the report

13. Click **OK**. The detail pages for all of the transformations will be appended to Today's Report.
14. If present, click the **Toxicity** link for the current transformation. In this example, one record is retrieved from the **MDL Toxicity Database**.

[Return to MDL® Metabolite Database](#)

Record # 1 **Total Records:** 1

## MDL® Toxicity Database

|   |  |
|---|--|
|  | <p><b>Available Data</b></p> <p><i>Click on a link to add the information to this page</i></p> <p><input type="checkbox"/> Set current view as default</p> <p><a href="#">Chemical (1)</a>      <a href="#">Acute Toxicity (11)</a></p> <p><a href="#">Other Multiple Doses (1)</a>      <a href="#">Model (1)</a></p> |
|---|--|

### Chemical [\(hide\)](#)

|  |                   |
|--|-------------------|
| <b>Molecular Formula</b>   | C11 H12 Cl N O3 S |
| <b>Molecular Weight</b>  | 273.7388          |
| <b>MDL Number</b>  | MFCD00143951      |
| <b>CAS Registry Number</b>   | 80-77-3           |
| <b>Beilstein Number</b>  |                   |
| <b>Beilstein Handbook</b>  |                   |
| <b>RTECS Number</b>  | XJ1050000         |
| <b>CCRIS Number</b>  |                   |
| <b>GENE-TOX Number</b>   |                   |
| <b>GENOTOXICITY Number</b>   |                   |
| <b>CARCINO Number</b>  |                   |
| <b>HEPATO Number</b>   |                   |
| <b>NEPHRO Number</b>   |                   |
| <b>Patch Test</b>  |                   |
| <b>Compound Descriptor</b>   | Drug , Human Data |
| <b>Chemical Name and Synonyms :</b>  |                   |
| <ul style="list-style-type: none"> <li>• 4H-1,3-THIAZIN-4-ONE, 2-(P-CHLOROPHENYL)TETRAHYDRO-3-METHYL-, 1,1,-DIOXIDE</li> <li>• 2-(4-CHLOROPHENYL)-3-METHYL-4-METATHIAZANONE-1,1-DIOXIDE</li> <li>• 2-(P-CHLOROPHENYL)-3-METHYL-1,3-PERHYDROTHIAZIN-4-ON-1,1-DIOXIDE</li> <li>• 2-(P-CHLOROPHENYL)TETRAHYDRO-3-METHYL-4H-1,3-THIAZIN-4-ONE 1,1-DIOXIDE</li> <li>• 4H-1,3-THIAZIN-4-ONE, TETRAHYDRO-2-(P-CHLOROPHENYL)-3-METHYL-, 1,1-DIOXIDE</li> </ul> |                   |

15. Click **copy to report**. Check the box for **View report now**.

Copy to Report

Copy current record to the report.

Select copy destination

Create new report

Append to Today's Report - Report #1

Select copy result level

View search results in report

View detail results in report

Set the range of copy-to-report records

All records

Current Page

Specify Record Numbers

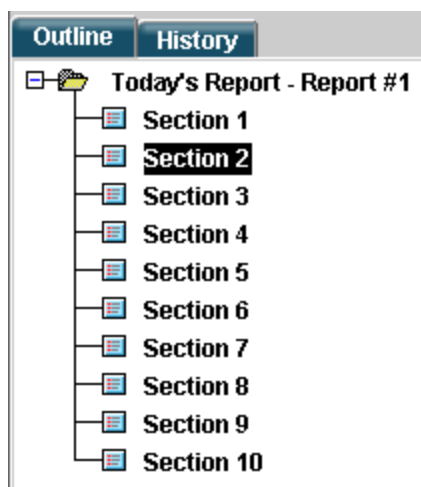
Enter the record index numbers and/or record ranges, separated by commas. For example, 1,3,5,7-10

View report now

OK Cancel

View the report

16. Click **OK**. The toxicity data for the single compound is appended to Today's Report, and you are taken immediately to the Reports page to view it.
17. Scroll the report to view it, or to jump to a specific section, click the section name in the Outline pane.



Return to the MDL  
Metabolite Database

18. Click the **results** tab to return to the Results page.

19. Click **Return to MDL Metabolite Database**.

20. Click **Return to Search Results**.



**Exercise 3**

Open the CrossFire  
Beilstein database

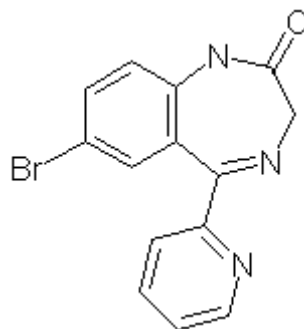
Draw the structure query

Set the structure search  
options

**Retrieve pharmacological data for Bromazepam**

Search the CrossFire Beilstein database using the bromazepam structure.

1. Click the **queries** tab.
2. Choose **CrossFire Beilstein** from the Database list.
3. Click the **Reset** link located to the right of the structure box.
4. Double-click the **Structure** box to launch MDL Draw.
5. Draw bromazepam.



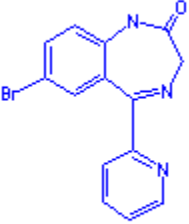
6. Click **Done**.
7. Select **Substitution as drawn, exclude tautomers**.  
Uncheck all of the boxes under Allow.

|  |  |
|--|--|
| Find this compound and its properties ▾                | <input checked="" type="radio"/> Substitution as drawn, exclude tautomers<br><input type="radio"/> Substitution as drawn, include tautomers<br><input type="radio"/> Unlimited substitution on all atoms, exclude tautomers  |
|  | Allow: <input type="checkbox"/> Multi-component substances<br><input type="checkbox"/> Ring closure through substitution<br><input type="checkbox"/> Isotopes <input type="checkbox"/> Charges <input type="checkbox"/> Radicals<br><input type="checkbox"/> Keep fragments separate |
| <input checked="" type="checkbox"/> Query Highlighting | Search Stereoinformation <input type="text" value="As drawn"/> ▾   |

Conduct the search

8. Click **start search**. One compound is retrieved. The green BIO label indicates that biological data is available.

BRN: 618645 BIO



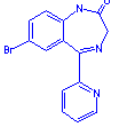
[Details](#)   [Synthesize](#)

Record#1

View the pharmacological data

9. Click **Details**.

#### CrossFire Beilstein Substance 618645



[Use as Query](#)   [Synthesize](#)  
 Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

|  |   |
|--|---|
| <a href="#">Adsorption (MCS)</a> (1)             | <a href="#">Association (MCS)</a> (2)               |
| <a href="#">Dissociation Exponent</a> (1)        | <a href="#">Electrical Moment</a> (1)               |
| <a href="#">Electrochemical Behaviour</a> (1)    | <a href="#">Electrochemical Characteristics</a> (1) |
| <a href="#">Fluorescence Spectroscopy</a> (2)    | <a href="#">Further Information</a> (1)             |
| <a href="#">IR Spectroscopy</a> (4)              | <a href="#">Liquid/Liquid Systems (MCS)</a> (1)     |
| <a href="#">Mass Spectrometry</a> (4)            | <a href="#">Melting Point</a> (12)                  |
| <a href="#">NMR Spectroscopy</a> (13)            | <a href="#">Pharmacological Data</a> (18)           |
| <a href="#">Phosphorescence Spectroscopy</a> (1) | <a href="#">Substance Identification</a> (1)        |
| <a href="#">UVVIS Spectroscopy</a> (7)           |   |

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#### Substance Identification [\(hide\)](#)

| Substance Identification record 1 of 1 |  |                         |        |
|--|--|-------------------------|--------|
| Beilstein Registry Number              | 618645   |                         |        |
| Beilstein Preferred RN                 | 1812-30-2  |                         |        |
| CAS Registry Number                    | 1812-30-2  |                         |        |
| Chemical Name                          | <ul style="list-style-type: none"> <li>• 7-bromo-5-pyridin-2-yl-1,3-dihydro-benzo[e][1,4]diazepin-2-one</li> <li>• bromazepam</li> </ul>                                       |                         |        |
| Autoname                               | 7-bromo-5-pyridin-2-yl-1,3-dihydro-benzo[e][1,4]diazepin-2-one   |                         |        |
| Fragment Molecular Formula             | <table style="width: 100%; border: none;"> <tr> <td style="border: none;"><b>Molecular Weight</b></td> <td style="border: none; text-align: right;">316.16</td> </tr> </table> | <b>Molecular Weight</b> | 316.16 |
| <b>Molecular Weight</b>                | 316.16   |                         |        |
| Molecular Formula                      | C14H10BrN3O  |                         |        |
| Lawson Number                          | 30122  |                         |        |
| Type of Substance                      | heterocyclic   |                         |        |
| Constitution ID                        | 607173   |                         |        |
| Tautomer ID                            | 646319   |                         |        |
| Beilstein Reference                    | 5-26-05-00078, 6-26  |                         |        |
| Entry Date                             | 1988/11/28   |                         |        |
| Update Date                            | 2005/01/21   |                         |        |

10. Click the link for **Pharmacological Data**.

Pharmacological Data [\(hide\)](#)

| Pharmacological Data record 1 of 18 |   |
|-------------------------------------|---|
| Citation Pointer                    | 6431906   |
| Pharmacological Data Citations      | <ul style="list-style-type: none"> <li>Journal; Usami, Noriyuki, Yamamoto, Tomohiro, Shintani, Syunichi, Higaki, Yu, Ishikura, Shuhei, Katagiri, Yoshihiro, Hara, Akira, BPBLEO; Biol. Pharm. Bull., EN, 25; 4; 2002; 441-445;</li> </ul> |
| Effect                              | enzyme; inhib. of   |
| Species or Test-System              | human 3 $\alpha$ -hydroxysteroid dehydrogenase AKR1C3 isoenzyme   |
| Kind of Dosing                      | title comp. was dissolved in methanol and added to reaction mixture (final conc. of methanol was < 2.5 percent)   |
| Method                              | enzyme incubated with title comp. in 0.1 mol/l potassium phosphate buffer (pH 7.4) containing 0.25 mmol/l NADP(1+) and 1.0 mmol/l S-tetralol; dehydrogenase activity determined   |
| Further Details                     | S-tetralol: S-(+)-1,2,3,4-tetrahydronaphth-1-ol   |
| Type                                | IC50  |
| Value of Type                       | 81 $\mu$ mol/l  |
| Entry Date                          | 2004/08/03  |

| Pharmacological Data record 2 of 18 |   |
|-------------------------------------|---|
| Citation Pointer                    | 6431906   |
| Pharmacological Data Citations      | <ul style="list-style-type: none"> <li>Journal; Usami, Noriyuki, Yamamoto, Tomohiro, Shintani, Syunichi, Higaki, Yu, Ishikura, Shuhei, Katagiri, Yoshihiro, Hara, Akira, BPBLEO; Biol. Pharm. Bull., EN, 25; 4; 2002; 441-445;</li> </ul> |
| Effect                              | enzyme; inhib. of   |
| Species or Test-System              | human 3 $\alpha$ -hydroxysteroid dehydrogenase AKR1C4 isoenzyme   |
| Concentration                       | 0.1 mmol/l  |
| Kind of Dosing                      | title comp. was dissolved in methanol and added to reaction mixture (final conc. of methanol was < 2.5 percent)   |
| Method                              | enzyme incubated with title comp. in 0.1 mol/l potassium phosphate buffer (pH 7.4) containing 0.25 mmol/l NADP(1+) and 1.0 mmol/l S-tetralol; dehydrogenase activity determined   |
| Further Details                     | S-tetralol: S-(+)-1,2,3,4-tetrahydronaphth-1-ol   |
| Results                             | title comp. inhibited AKR1C4 isoenzyme by 15 percent  |
| Entry Date                          | 2004/08/03  |

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| Pharmacological Data record 12 of 18 |   |
|--------------------------------------|---|
| Citation Pointer                     | 5833840   |
| Pharmacological Data Citations       | <ul style="list-style-type: none"> <li>Journal; Chambon, J. P.; Perio, A.; Demarne, H.; Hallot, A.; Dantzer, R.; et al.; ARZNAD; Arzneim. Forsch., EN, 35; 10; 1985; 1572-1577;</li> </ul>                    |
| Entry Date                           | 1988/06/27  |
| Comment                              | activity in: antagonizing MES - ED 50: 5.4 mg/kg and PTZ-induced 1)seizures - ED 50: 1.0 and 0.4 mg/kg 2)lethality - ED 50: 0.3 mg/kg; impairment of motor coordination - ED 50: 2.5 mg/kg, p.o., female mice |

[More Pharmacological Data](#)  
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11. The first 12 records are displayed. At the bottom of the Results page, click **More Pharmacological Data** to see the other records.