

Searching CrossFire Databases-

based on CrossFire Beilstein

Chapter 6 Stereochemistry

Training Guide



CrossFire[®] Commander
Version 7.1

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Training Guide: May 2008, for Elsevier CrossFire Commander Version 7.1

Stereochemistry



In this section, you will learn how to:

- Draw structures specifying the stereochemistry
- Conduct a structure search specifying stereochemistry
- Retrieve a list of citations for the current record and a list of records

Key points

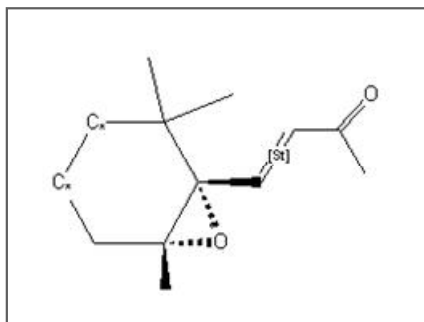
- In this section, you will draw and conduct a search for structures and reactions that have stereochemistry specified.
- You will also retrieve citations for the current record and a list of records.

Notes

Scenario #15 – Stereochemical search



- Retrieve compounds having the same relative stereochemistry as the following compound.
- Retrieve compounds with the absolute stereochemistry of the following compound.



- Convert the hitset to a list of citations.

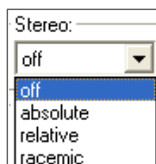
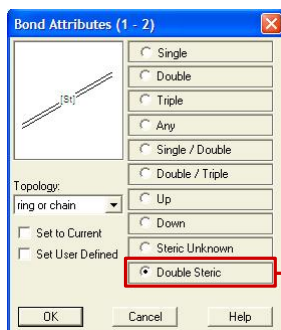
Key points

- You will conduct a search to retrieve compounds that have relative and absolute stereochemistry of the structure drawn.
- Before we begin, let's take a closer look at stereochemical features for double and single bonds.

Notes



(E or Z) Stereochemical settings

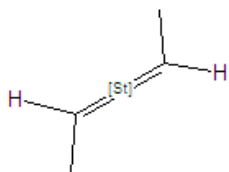


Choose **absolute** or **relative** in the structure Query Builder

Click **Double Steric** in the CrossFire Structure Editor

Defines a double bond where the configuration (E or Z) is considered.

Search for Trans-2-butene



Stereo Off =

<input type="checkbox"/> Hit 1 BRN=1361341 C4H.	<input type="checkbox"/> Hit 2 BRN=1718755 C4H.	<input type="checkbox"/> Hit 3 BRN=1718756 C4H.
(Z)	unspecified	(E)
<input type="checkbox"/> Hit 3 BRN=1718756 C4H.		
(E)		

Absolute =
Relative =

Key points

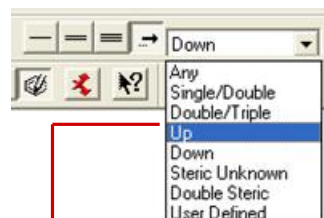
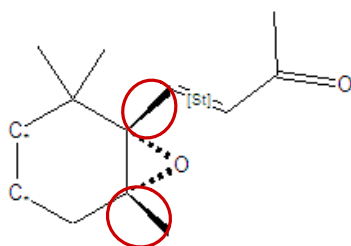
- You can specify stereochemical settings in the Bond Attributes dialog box in the Structure Editor.
- If you select Double Steric, a double bond with either an E or Z configuration is considered.
- To retrieve the Absolute or Relative configuration, set the drop-down menu in the Query Builder to either Absolute or Relative.

Notes



Stereochemical bonds

Apply Up and Down stereo bonds



Defines a stereochemical bond in the up direction

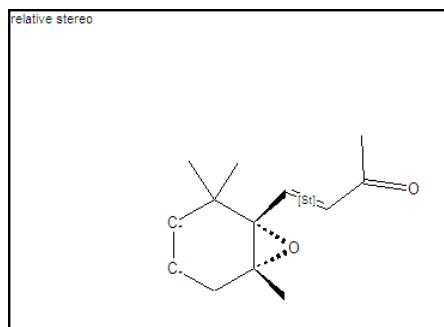
Key points

- You can specify stereochemical settings in the Structure Editor using either the drop-down menu or the Bond Attributes box.
- The Up bond defines a stereochemically directed bond in the up direction. The Down bond defines a stereochemically directed bond in the down direction. The Steric Unknown bond defines any stereo configuration at the site where it is placed.
- Create a query using the structure above, including appropriate stereochemical settings.

Notes



Stereochemical search options



Off – retrieves all configurations of the compound.

Absolute – retrieves compounds which have the identical, absolute configuration as the query structure.

Free Sites: hetero atoms all atoms

Stereo: **relative**

Search: as structure as reactant as product as reagent/
as catalyst/
as solvent

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markush

Clear Structure More...

Relative – retrieves compounds with the absolute configuration, the mirror image, and the racemate of the query.

Racemic – retrieves only the racemate of the query.

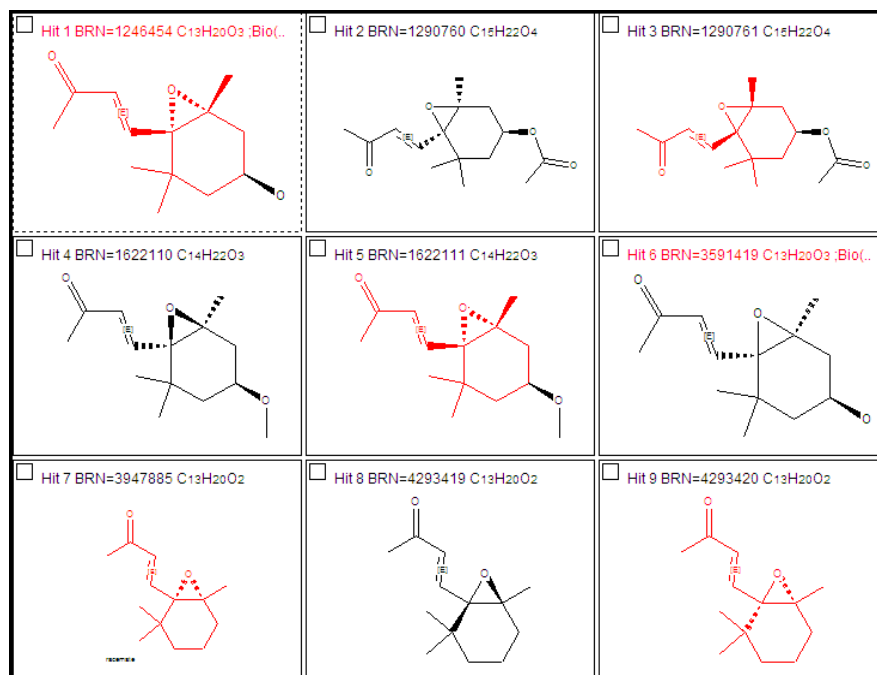
Key points

- Stereochemistry is considered only if the proper Stereo option has been selected.
- To perform a stereo search, activate the appropriate selection. The choices are:
 - **Off**, the stereo search option is not in use
 - **Absolute**, retrieves compounds having the identical absolute configuration as the query structure
 - **Relative**, retrieves compounds and their enantiomers
 - **Racemic**, retrieves only the racemate of the query structure
- Conduct a structure search using your structure query and the settings above.

Notes



Relative search results



Key points

- The search results include the exact stereoconfiguration we drew as well as the enantiomers.

Notes



Retrieve a list of citations for a hitset

Use a structure query to retrieve a list of citations

Results

Document	Author(s)/Assignee	Year	Source Title/Patent Number
1. <input type="checkbox"/> View Details Full Text	Frei,B. et al.	1977	Helv. Chim. Acta 60, pp. 2968-3006
2. <input type="checkbox"/> View Details Full Text	Frei,B. et al.	1979	Helv. Chim. Acta 62, pp. 553-576
3. <input type="checkbox"/> View Details Full Text	Mori,K.	1974	Tetrahedron 30, pp. 1065-1070

Key points

- Let's retrieve the list of citations from the previous search.
- Use the previous query, but change the context to Citations using the drop-down menu next to to "As result I want to get".
- CrossFire Commander 7.1 defines the recommended search context as the one that matches the context of the query.
- Since our search context differs from the recommended search context, the Select Search Context dialog box appears.
- Choose Citations as the Search Context.

Notes



Absolute stereochemical search

CrossFire Commander

Query Results Reports Alerts

Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | Create Alert | Start Search

Find Field or Form Find Next ?

Query Builder ? Search in: Beilstein(2008/01)

absolute stereo

Free Sites: hetero atoms all atoms

Stereo: stereo: absolute

Search: as structure as reactant as product as reagent/
 as catalyst/
 as solvent

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markush

Clear Structure More...

and Search Text/Field Contents ? Advanced Mode Clear Table

	Operator	(Field name	List	Relation	Field content	List)	
3	and				is				
4	and				is				
5	and				is				
6	and				is				
7	and				is				
8	and				is				
9	and				is				
10	and				is				

As result I want to get Substances Start Search

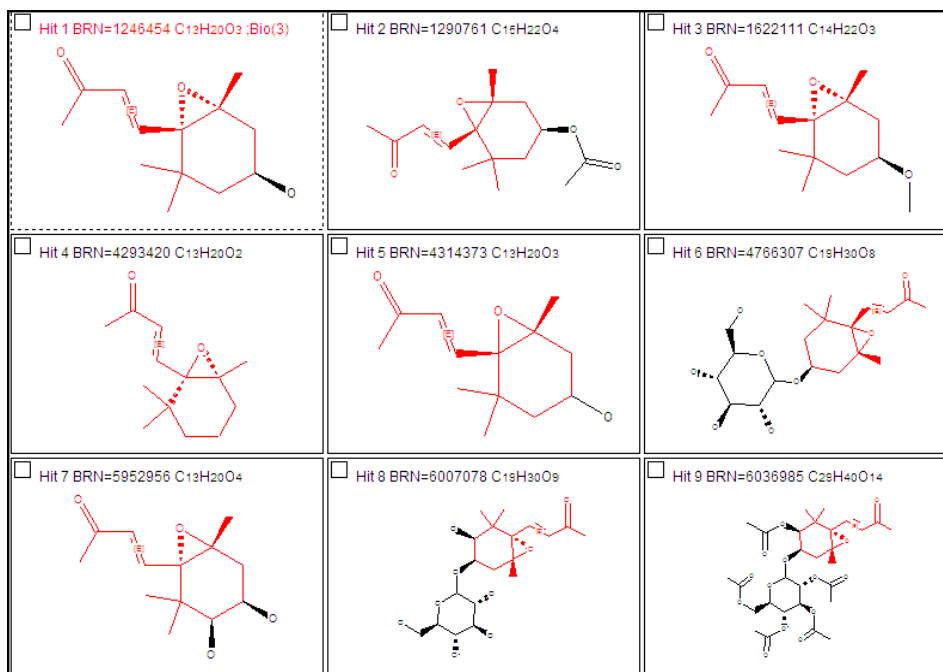
Key points

- Now we will retrieve compounds with the same Absolute stereochemistry shown.

Notes



Absolute search results



Key points

- Fewer compounds are retrieved for this search than with the relative stereochemical search.

Notes



Convert a hit to a list of citations

Choose:
Get > Get All Related Citations

OR
Right-click
the hitset

Key points

- When you have retrieved a list of results, you can convert them from one context to another.
- Click the Get button and choose Substances, Reactions, or Citations to perform the operation.
- You can also right-click on a Hitset in the Tree to perform the same operation.
- The same can be applied to a single hit.
- When converting from Substances to Reactions context, you can choose whether the substance occurs as a reactant, product, or either.

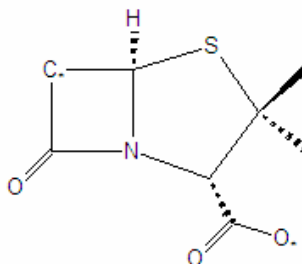
Notes

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 using the **CrossFire Structure Editor**, go to the page listed below the description.

Exercise 1 Retrieve penicillanic acid and esters.

- Search with absolute stereo enabled.



- Repeat the search for reactions where penicillanic acid is a reactant.

For a step-by-step solution, see page 6-2.

Search for penicillanic acid

Exercise 1 Retrieve penicillanic acid and esters. Search with absolute stereo enabled. Repeat the search for reactions where penicillanic acid is a reactant. If you are using the CrossFire Structure Editor, you can use a template to draw it. Be sure to set two explicit Free Sites.

Prepare for a new query



1. Click the **To Commander** button to return to the CrossFire Commander.

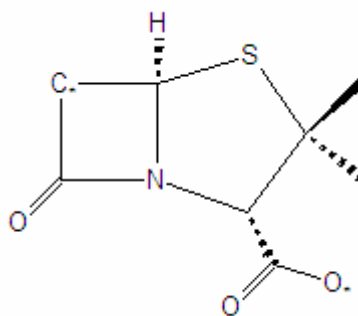
2. Clear the previous query.

Structure Editor

3. Double-click the **Structure/Reaction Search** box.

4. Draw the query structure.

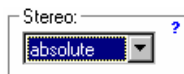
CrossFire Structure Editor instructions



5. Click the **To Commander** icon.

Enable absolute stereo

6. Under stereo, choose **Absolute**.



Conduct the search

7. Click the **Start Search** button.

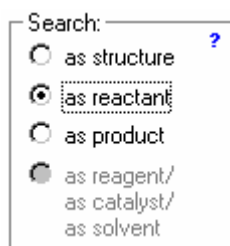
8. Click **View**. Beilstein (2008/01) = 17

9. Click the **Details** button. Browse the hitset.

10. Click the **Query** tab.

Define as a reactant

11. Under Search, in the Structure Query Options area, select **as reactant**.



Search: ?

- as structure
- as reactant
- as product
- as reagent/
as catalyst/
as solvent

Conduct the search

12. Click the **Start Search** button.

13. Click **View**. Beilstein (2008/01) = 11.

14. Hyperlink to a citation.