

Finding Derivatives

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library.stanford.edu/depts/swain/chem130/chem130.html

Lecture Outline:

- Choosing a derivative
- Synthesizing a derivative
- Finding properties for a derivative

Choosing a Derivative

- See *Guidelines for Recommended Derivatives*
 - Organized by class of parent compound
 - IN Chem 130/132 Course Pack, Lectures, pgs 50-53
 - On the web:
library.stanford.edu/depts/swain/chem130.derivatives.html
- Examples (if you have, then make):
 - Aldehydes and Ketones
 - 2,4-DNP
 - Semicarbazone
 - Oxime
 - Primary and Secondary

Need to Know “Parent” Unknown Before Making a Derivative?

■ Ideal:

- Know exact structure of “parent” unknown compound
- Consult “Guidelines” and choose which derivative to make
- Find a literature reference on the synthesis of a derivative as they include physical property data and a spectral diagram
- Locate additional property data in POC, CCD, or Beilstein

■ Reality:

- Sometimes, don’t know exact structure of “parent” unknown
- Must know compound class of “parent” unknown
- Consult with a TA

Synthesizing a Derivative

- Print and electronic resources are available:
library.stanford.edu/depts/swain/chem130/derivbibl.html
- Print resources:
 - Usually arranged by class of compound.
 - One particularly helpful text is Vogel's Textbook of Practical Organic Chemistry
 - Other helpful texts include Pasto, Harwood, & Shriner
- Electronic Resources:
 - Combined Chemical Dictionary via CHEMnetBASE
 - Beilstein Crossfire

Synthesizing a Derivative: Overview of Search Methods in Electronic Resources

- Use the Combined Chemical Dictionary (CCD) via CHEMnetBASE and Beilstein Crossfire
- Two search methods for finding derivatives:
 - Search by CAS Registry Number (CCD or Beilstein)
 - Search by chemical reaction (Beilstein)

Searching by CAS Registry Number

- **CCD** and **Beilstein** include derivatives in a record for a compound.
- **CCD:**
 - Use CCD **first** because it has a carefully chosen set of derivatives.
 - If your unknown is a “main entry” compound, then look for a recommended derivative.
 - Consult literature references labeled “deriv” or “synth”
 - If your unknown compound is listed as a derivative in CCD, then search Beilstein Crossfire by CAS Registry Number
- **Beilstein:**
 - See Derivative field in record.
 - Note: Beilstein has a narrower definition for derivatives than is used in Chemistry 130/132.

Finding Derivatives: CAS Registry Number Search in CCD and Brief Display Format

THE COMBINED CHEMICAL DICTIONARY

Chemical Databases Online

SEARCH | HELP | TECHNICAL SUPPORT | GET PLUGIN | TOUR | CRCPRESS | CHEMNETBASE

Submit Search
Clear Search

Searching

Enter a query, then press 'Submit Search'. Enter a word(s) into one or more of the boxes below. You may truncate on the left or right hand side of the word with an asterisk(*)

☒ Substructure ☐ Exact Match

Draw Query

Query Not Defined

AND

Chemical Name

Browse Index

AND All Text

Browse Index

AND CAS Registry No.

62-23-7

AND Molecular Formula

THE COMBINED CHEMICAL DICTIONARY

Chemical Databases Online

SEARCH | HELP | TECHNICAL SUPPORT | GET PLUGIN | TOUR | CRCPRESS | CHEMNETBASE

Return to Search

Print Preview

First Entry

Previous Entry

Next Entry

Last Entry

1 of 471504 documents matched query. Hits 1 to 1

Name	CAS Registry Number	Molecular Formula
4-Nitrobenzoic acid	62-23-7	C ₇ H ₅ NO ₄

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Full Display Format in CCD

THE COMBINED CHEMICAL DICTIONARY

Chemical Databases Online

SEARCH | HELP | TECHNICAL SUPPORT | GET PLUGIN | TOUR | CRCPRESS | CHEMNETBASE

Return to Search

Print Preview Text

Print Preview Text & Struct.

List


First Entry

Previous Entry

Next Entry

Last Entry

Hit 1 of 1

 **Entry Name:** 4-Nitrobenzoic acid

Chapman & Hall Number: DTS50-I

CAS Registry Number: 62-23-7

Related CAS Registry Numbers(s): 3847-57-2

Extra CAS Registry Numbers(s): 27178-83-2

Molecular Formula: $C_7H_5NO_4$

Molecular Weight: 167.121

Accurate Mass: 167.021859

Percentage Composition: C 50.31%; H 3.02%; N 8.38%; O 38.29%

Physical Description: Leaflets (H_2O)

Melting Point: Mp 241.5° (236-239°)

pKa Value: pK_a 3.45 (25°, H_2O)

Other Data: Sublimes

Hazard & Toxicity: Eye irritant. LD₅₀ (rat, oral) 1960 mg/kg

RTECS Accession Number: DH5075000

Aldrich: 46109-1

Fluka: 72910

 **Derivative:** Me ester

Chapman & Hall Number: DTS51-J

CAS Registry Number: 619-50-1

 **Derivative:** Amide

Chapman & Hall Number: DTS55-N

CAS Registry Number: 619-80-7

Molecular Formula: $C_7H_6N_2O_3$

Molecular Weight: 166.136

Accurate Mass: 166.037843

Percentage Composition: C 50.61%; H 3.64%; N 16.86%; O 28.89%


Physical Description: Needles (H_2O)

Melting Point: Mp 206°

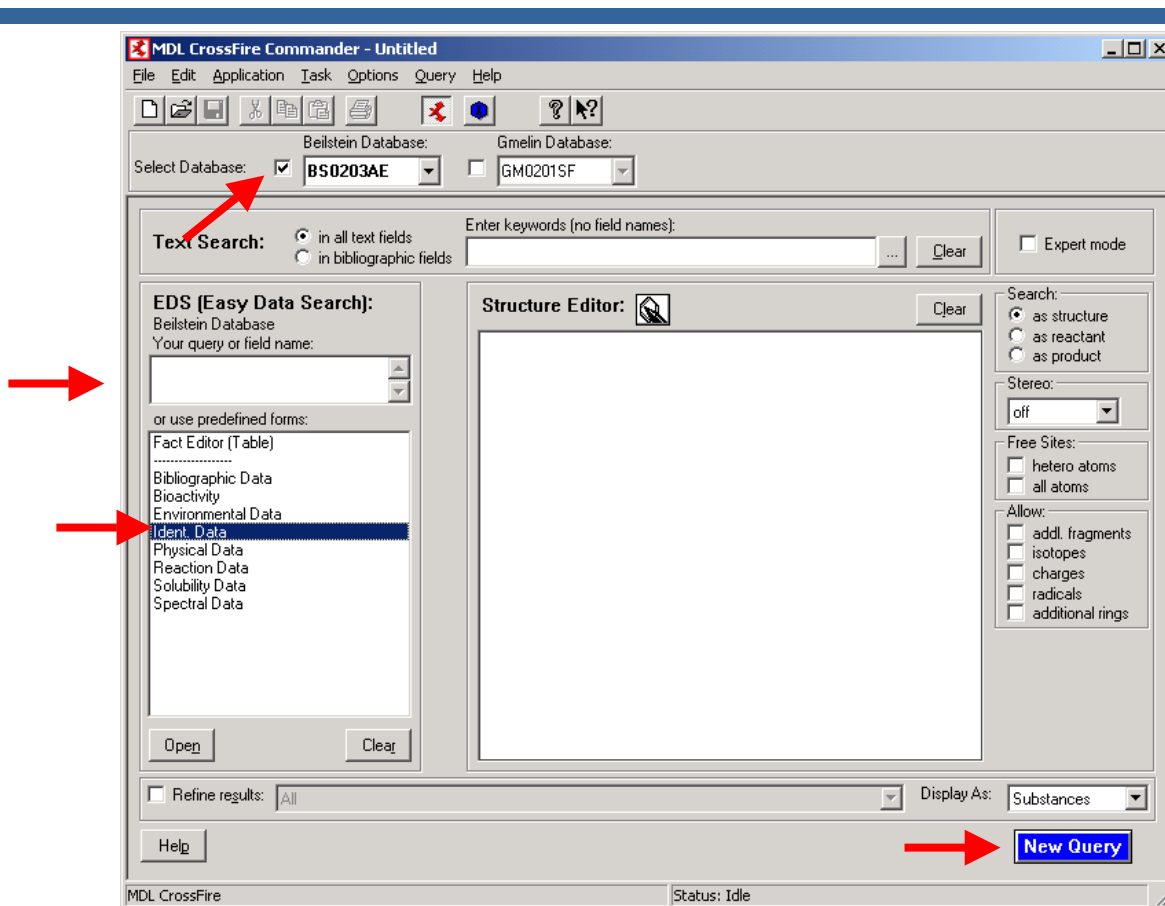
RTECS Accession Number: CV5601000

Aldrich: 18928-6

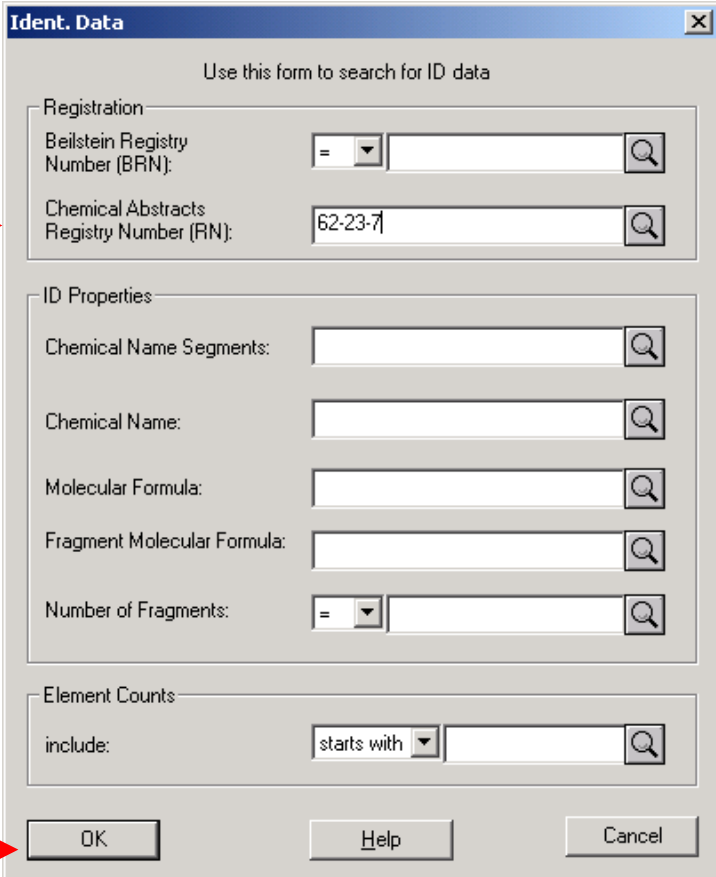
Full Display Format in CCD (Literature References)

Aldrich Library of NMR Spectra, **6**, 152B, (pmr)
 Org. Synth., Coll. Vol., **1**, 1932, 392
 394, (chloride)
 Papariello, G.J. *et al.*, *Anal. Chem.*, 1964, **36**, 1028, (use, hydrazide)
 Litvinenko, L.M., *Zh. Anal. Khim.*, 1966, **21**, 200, (use, chloride)
 Koehergin, P.M. *et al.*, *CA*, 1967, **66**, 10702w, (synth)
 Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 736
 Tavale, S.S. *et al.*, *Acta Cryst. B*, 1971, **27**, 1479, (cryst struct)
 Turner, K.B. *et al.*, *Org. Mass Spectrom.*, 1973, **7**, 383, (ms)
 Kamath, B.V. *et al.*, *J. Appl. Chem. Biotechnol.*, 1975, **25**, 743, (uv)
 Nachtmann, F. *et al.*, *J. Chromatogr.*, 1976, **122**, 293
 1977, **136**, 279, (use, chloride)
 Di Rienzo, F. *et al.*, *Acta Cryst. B*, 1977, **33**, 3854, (cryst struct)
 Dignam, V.J. *et al.*, *J.C.S. Perkin 2*, 1977, 1457-1462, (nitrile N-oxide)
 Kosugi, Y. *et al.*, *Tetrahedron*, 1980, **36**, 2741, (cmr)
 Hammela, P.J. *et al.*, *Aust. J. Chem.*, 1989, **42**, 1257-1262, (nitrile N-oxide)
 Niazi, M.S.K., *Bull. Chem. Soc. Jpn.*, 1989, **62**, 1253, (pKa)
 Murray, R.W. *et al.*, *J.O.C.*, 1989, **54**, 5783, (synth)
 Kocevar, M. *et al.*, *J.O.C.*, 1995, **60**, 1466, (synth, derivs) 
 Sato, K. *et al.*, *Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306, (synth, pmr, cmr)
 Kong, Y.C. *et al.*, *J. Het. Chem.*, 1999, **36**, 515-523, (Me ester)
 Sakamoto, T. *et al.*, *J.C.S. Perkin 1*, 1999, 2323-2326, (nitrile, synth, ir, pmr)
 Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 2529
 Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992,
 904
 Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand
 Reinhold, 1992, CCI250
 ENO000
 MMIO00
 NFHO00
 NFK100

Finding Derivatives: CAS Registry Number Search in Beilstein Crossfire



Finding Derivatives: Using Beilstein Crossfire continued



Ident. Data

Use this form to search for ID data

Registration

Beilstein Registry Number (BRN):

Chemical Abstracts Registry Number (RN):

ID Properties

Chemical Name Segments:

Chemical Name:

Molecular Formula:

Fragment Molecular Formula:

Number of Fragments:

Element Counts

include:

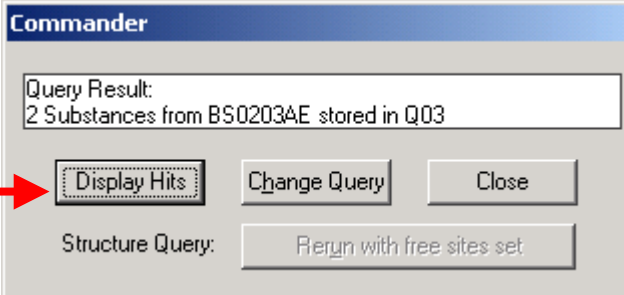
OK Help Cancel

Red arrows point to the Chemical Abstracts Registry Number (RN) field, the OK button, and the Beilstein Registry Number (BRN) field.



Start Search

A red arrow points to the button.



Commander

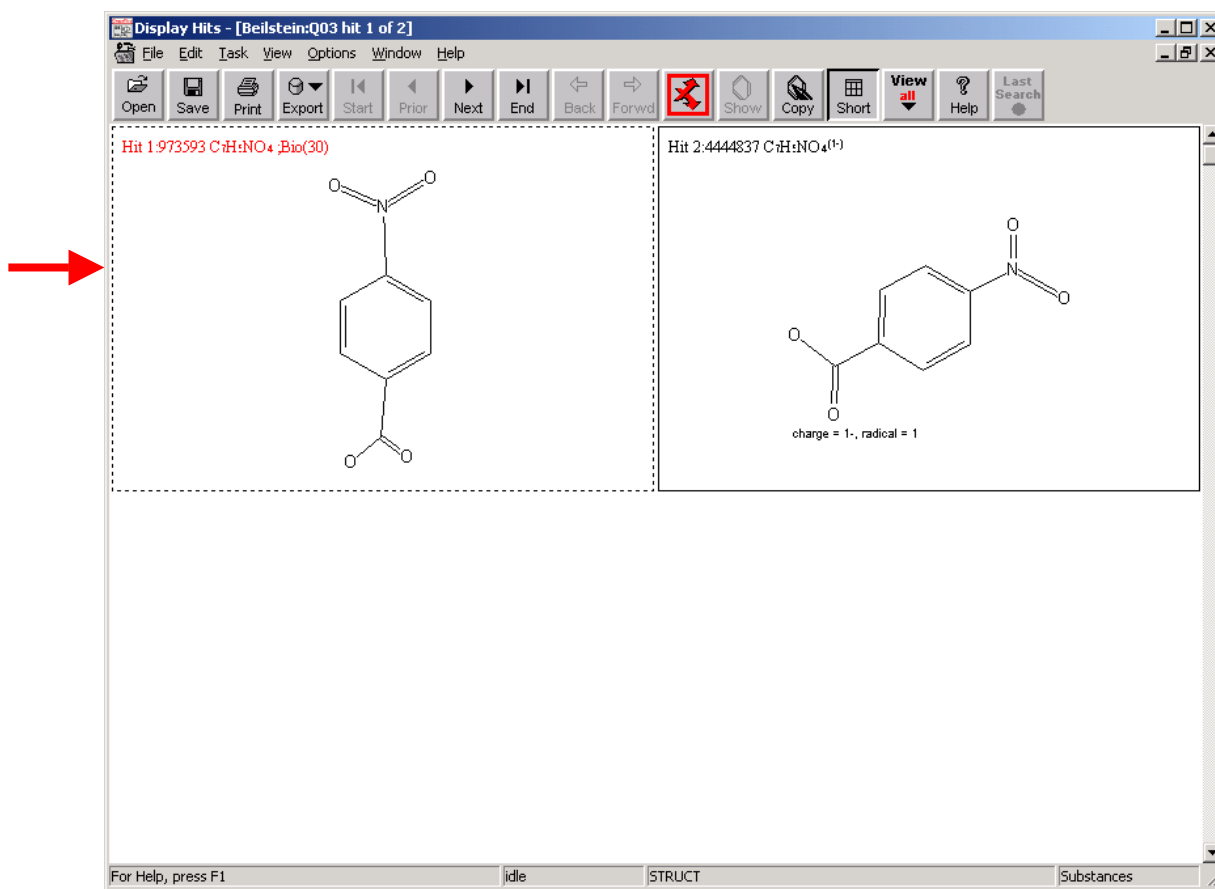
Query Result:
2 Substances from BS02034E stored in Q03

Display Hits Change Query Close

Structure Query:

A red arrow points to the Display Hits button.

Finding Derivatives: Using Beilstein Crossfire continued



Finding Derivatives: Using Beilstein Crossfire continued

Field Availability - Beilstein:Q03 hit 1 of 2

Code	FieldName	Occ.
<input checked="" type="checkbox"/> XREF	Crossfile Reference	10
<input checked="" type="checkbox"/> CRYPH	Crystal Phase	9
<input checked="" type="checkbox"/> CPD	Crystal Property Description	2
<input checked="" type="checkbox"/> CSYS	Crystal System	2
<input checked="" type="checkbox"/> CDEN	Density of the Crystal	3
<input checked="" type="checkbox"/> DEN	Density of the Liquid	3
<input checked="" type="checkbox"/> CDER	Derivative	104
<input checked="" type="checkbox"/> DIC	Dielectric Constant	2
<input checked="" type="checkbox"/> EDIS	Dissociation Energy	1

Occ.: Order:

- ☐ Beilstein/Gmelin
- ☐ Alphabetical by code
- ☒ Alphabetical by name

Buttons: Go to, Close, Help, Put checkmarks on all lines, Remove all checkmarks, Apply selections to User View, Apply to all windows

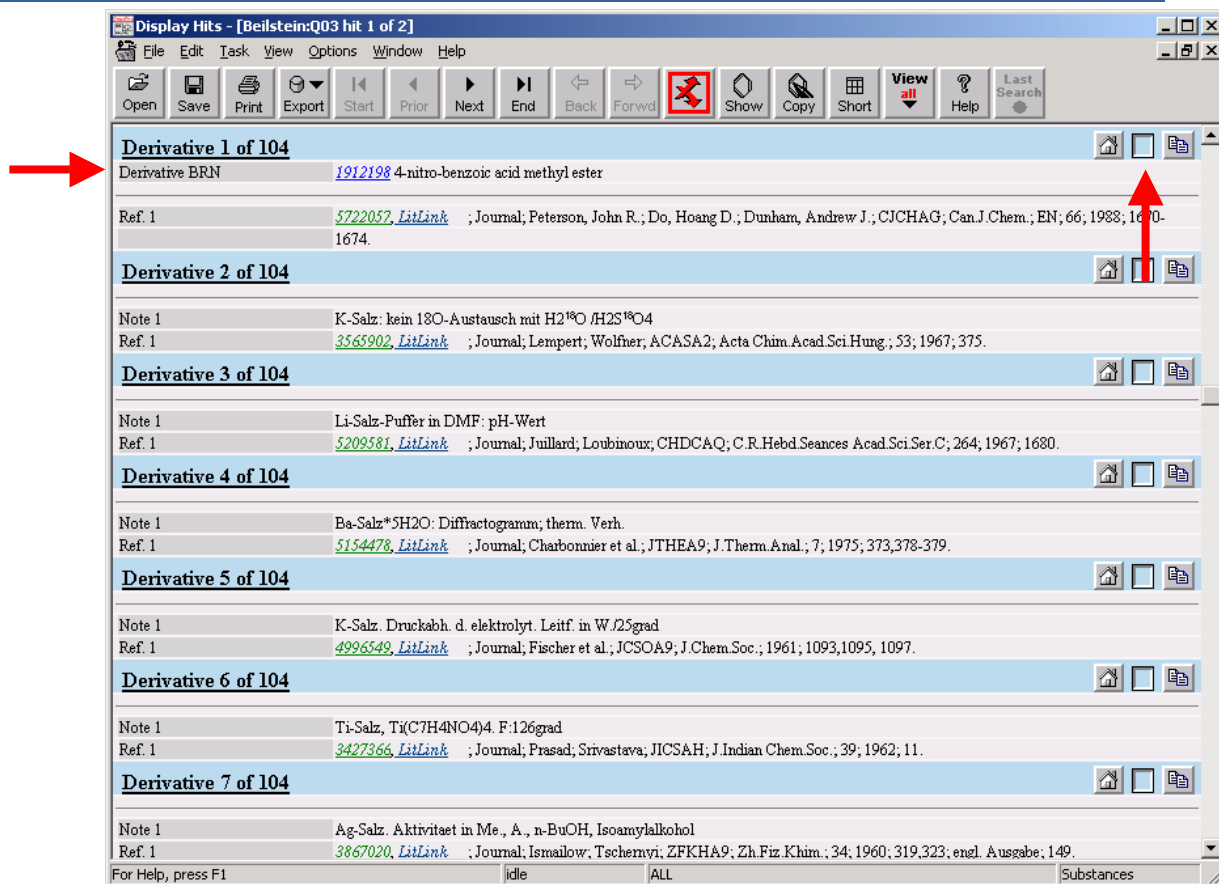
Reaction 1 of 1652

Reaction ID: 4244
 Reactant BRN: 102410 2-ethyl-aziridine
 Product BRN: 973593 4-nitro-benzoic acid
 No. of Reaction Details: 1
 Reaction Classification: Preparation

Reaction 2 of 1652

Reaction ID: 19845
 Reactant BRN: 103233 pyridine
 Product BRN: 1916959 bis-(4-nitro-benzoyl)-peroxide
 Product BRN: 973593 4-nitro-benzoic acid

Finding Derivatives: Using Beilstein Crossfire continued



Display Hits - [Beilstein:Q03 hit 1 of 2]

File Edit Task View Options Window Help

Open Save Print Export Start Prior Next End Back Forwd Show Copy Short View Help Last Search

Derivative 1 of 104

Derivative BRN [1912198](#) 4-nitro-benzoic acid methyl ester

Ref. 1 [5722057](#), [LitLink](#) ; Journal; Peterson, John R.; Do, Hoang D.; Dunham, Andrew J.; CJCHAG; Can.J.Chem.; EN; 66; 1988; 1670-1674.

Derivative 2 of 104

Note 1 K-Salz: kein 18O-Austausch mit H₂¹⁸O /H₂S¹⁸O₄

Ref. 1 [3565902](#), [LitLink](#) ; Journal; Lempert; Wolfner; ACASA2; Acta Chim.Acad.Sci.Hung.; 53; 1967; 375.

Derivative 3 of 104

Note 1 Li-Salz: Puffer in DMF: pH-Wert

Ref. 1 [5209581](#), [LitLink](#) ; Journal; Juillard; Loubinoux; CHDCAQ; C.R.Hebd.Seances Acad.Sci.Ser.C; 264; 1967; 1680.

Derivative 4 of 104

Note 1 Ba-Salz*5H₂O: Diffractogramm; therm. Verh.

Ref. 1 [5154478](#), [LitLink](#) ; Journal; Charbonnier et al.; JTSEA9; J.Therm.Anal.; 7; 1975; 373,378-379.

Derivative 5 of 104

Note 1 K-Salz: Druckabh. d. elektrolyt. Leiff. in W./25grad

Ref. 1 [4996549](#), [LitLink](#) ; Journal; Fischer et al.; JCSOA9; J.Chem.Soc.; 1961; 1093,1095, 1097.

Derivative 6 of 104

Note 1 Ti-Salz, Ti(C₇H₄NO₄)₄. F:126grad

Ref. 1 [3427366](#), [LitLink](#) ; Journal; Prasad; Srivastava; JICSAH; J.Indian.Chem.Soc.; 39; 1962; 11.

Derivative 7 of 104

Note 1 Ag-Salz. Aktivitaet in Me., A., n-BuOH, Isoamylalkohol

Ref. 1 [3867020](#), [LitLink](#) ; Journal; Ismailov; Tschernvi; ZFKHA9; Zh.Fiz.Khim.; 34; 1960; 319,323; engl. Ausgabe; 149.

For Help, press F1 idle ALL Substances

Finding Derivatives: Using Beilstein Crossfire continued

Display Hits - [Beilstein:Q03 hit 1 of 2]

File Edit Task View Options Window Help

Open Save Print Export Start Prior Next End Back Forwd Show Copy Short View all Help Last Search

Derivative 1 of 104

Derivative BRN [1912198](#) 4-nitro-benzoic acid methyl ester

Ref. 1 [5722052](#), [LitLink](#) ; Journal; Peterson, John R.; Do, Hoang D.; Dunham, Andre 1674.

Derivative 2 of 104

Note 1 K-Salz: kein 18O-Austausch mit H₂¹⁸O /H₂S¹⁸O₄

Ref. 1 [3565902](#), [LitLink](#) ; Journal; Lempert; Wolfner; ACASA2; Acta Chim Acad Sci

Derivative 3 of 104

Note 1 Li-Salz-Puffer in DMF: pH-Wert

Ref. 1 [5209581](#), [LitLink](#) ; Journal; Juillard; Loubinoux; CHDCAQ; C.R.Hebd Seances Acad.Sci.Ser.C; 264; 1967; 1680.

Derivative 4 of 104

Note 1 Ba-Salz*5H₂O: Diffractogram, therm. Verh.

Ref. 1 [5154478](#), [LitLink](#) ; Journal; Charbonnier et al.; JTHERA9; J.Therm.Anal.; 7; 1975; 373,378-379.

Derivative 5 of 104

Note 1 K-Salz. Druckabh. d. elektrolyt. Leitf. in W./25grad

Ref. 1 [4996549](#), [LitLink](#) ; Journal; Fischer et al.; JCSOA9; J.Chem.Soc.; 1961; 1093,1095, 1097.

Derivative 6 of 104

Note 1 Ti-Salz, Ti(C₇H₄NO₄)₄. F:126grad

Ref. 1 [3427366](#), [LitLink](#) ; Journal; Prasad; Srivastava; JICSAH; J.Indian.Chem.Soc.; 39; 1962; 11.

Derivative 7 of 104

Note 1 Ag-Salz. Aktivitaet in Me., A., n-BuOH, Isoamylalkohol

Ref. 1 [3867020](#), [LitLink](#) ; Journal; Ismailov; Tschernvi; ZFKHA9; Zh.Fiz.Khim.; 34; 1960; 319,323; engl. Ausgabe; 149.

For Help, press F1 idle ALL Substances

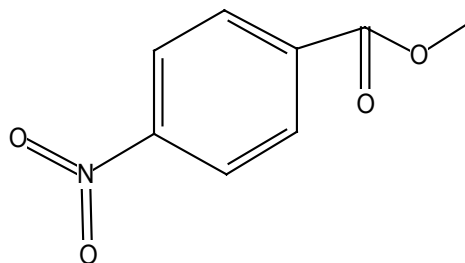


Finding Derivatives: Using Beilstein Crossfire continued

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Derivative 1 of 104 (BS0203AE:Substances:Q03 hit 1, BRN [973593](#))

Derivative BRN	1912198 4-nitro-benzoic acid methyl ester
Ref. 1	5722057 ; LitLink ; Journal; Peterson, John R.; Do, Hoang D.; Dunham, Andrew J.; CJCHAG; Can.J.Chem.; EN; 66; 1988; 1670-1674.



Derivative Entries in Beilstein

- Information varies but commonly includes the name of the derivative, MP/BP, and literature reference where derivative was synthesized.
- For more information about a derivative, try
 - **BRN** link (medium blue) next to name of derivative (if one exists)
 - **Citation** link (green) for literature reference
 - If neither option yields results, then do a **structure search** of the derivative in Beilstein.
- Sometimes, the full-text for a journal article indicates that the derivative you plan to make is an intermediate compound in a multi-step reaction. As long as there is physical property data for the derivative of interest, it is okay to use this reference for your lab report.

Displaying Derivative Entries in Beilstein and Using Hyperlinks Within Entries

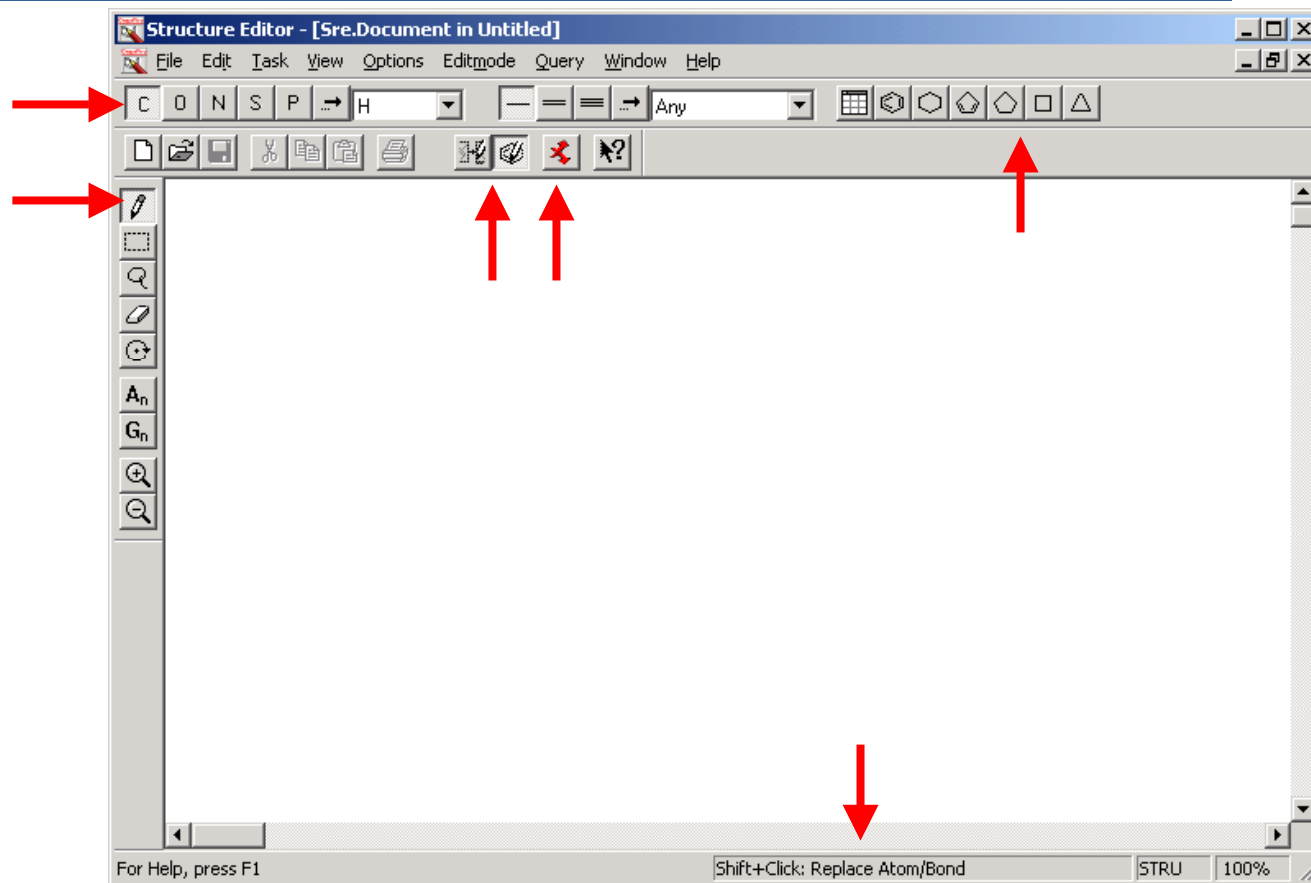
The screenshot shows the 'Display Hits' window for Beilstein:Q01 hit 1 of 2. The menu bar includes File, Edit, Task, View, Options, Window, and Help. The toolbar contains icons for Open, Save, Print, Export, Start, Prior, Next, End, Back, Forward, a red 'X' icon, Show, Copy, Short, View all, Help, and Last Search. The main content area displays 'Derivative 1 of 104'. Below this, the 'Derivative BRN' is listed as [1912198](#) 4-nitro-benzoic acid methyl ester. A red arrow points from the text 'Derivative BRN' to the BRN number. Below this, 'Ref. 1' is listed as [5722057, LitLink](#); Journal; Peterson, John R.; Do, Hoang D.; Dunham, Andrew J.; CJCHAG; Can.J.Chem.; EN; 66; 1988; 1670-1674.

The screenshot shows the 'Display Hits' window for Beilstein:Q01 hit 1 of 2, displaying two derivative entries. The menu bar and toolbar are the same as in the previous screenshot. The main content area displays 'Derivative 93 of 104'. Below this, 'Note 1' is listed as 4-bromo-phenacyl ester (mp: 134 degree) and 'Note 2' is listed as Handbook. 'Ref. 1' is listed as [2101916, LitLink](#); Journal; Kelly; Howard; JACSAT; J.Amer.Chem.Soc.; 54; 1932; 4383. A red arrow points from the 'End' button in the toolbar to the 'Ref. 1' entry. Below this, 'Derivative 94 of 104' is displayed. Below this, 'Note 1' is listed as 4-phenyl-phenacyl ester (mp: 182 degree) and 'Note 2' is listed as Handbook. 'Ref. 1' is listed as [1813579, LitLink](#); Journal; Drake; Sweeney; JACSAT; J.Amer.Chem.Soc.; 54; 1932; 2059. A red arrow points from the 'End' button in the toolbar to the 'Ref. 1' entry. A red arrow points from the 'Ref. 1' entry of 'Derivative 93 of 104' to the 'Ref. 1' entry of 'Derivative 94 of 104'.

Finding Derivatives in Beilstein Crossfire: Doing a Chemical Reaction Search

- After consulting Guidelines to determine what derivative you want to make, you can perform a reaction search two ways:
 - Unknown is a reactant and the derivative is a product
 - Unknown is a reactant and complete structure of derivative is not known
 - For example, product can be as small as a functional group. Define the point of attachment for the structural fragment of the derivative as an open site (see slide 25).

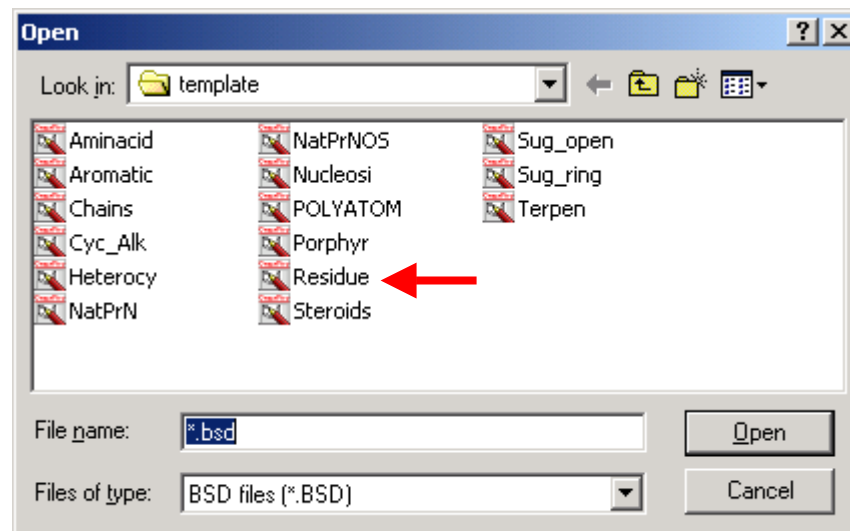
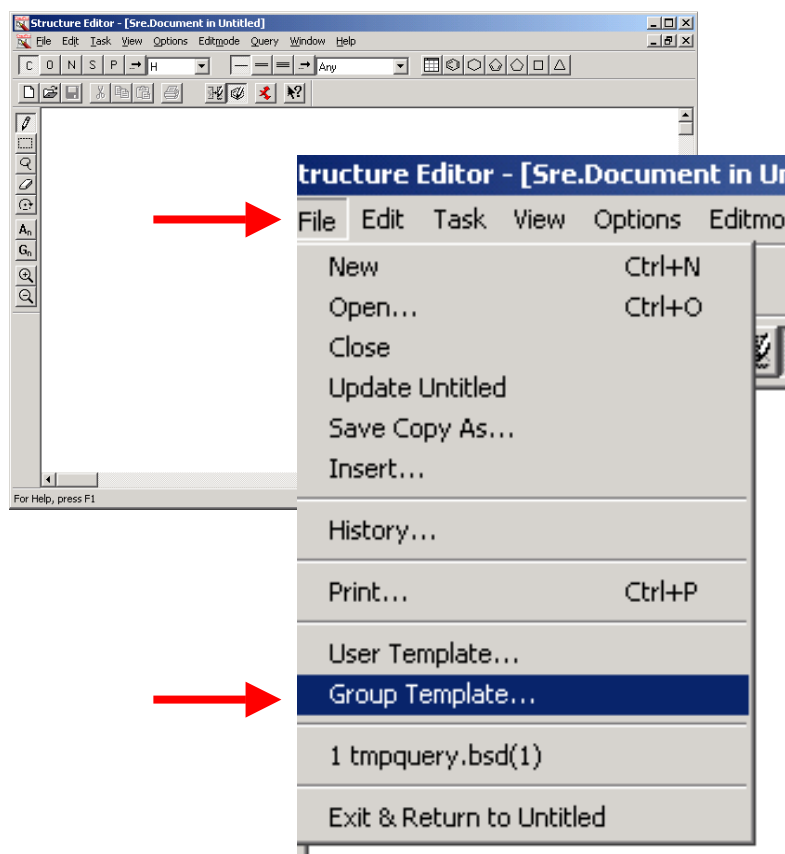
Beilstein Crossfire Structure Editor



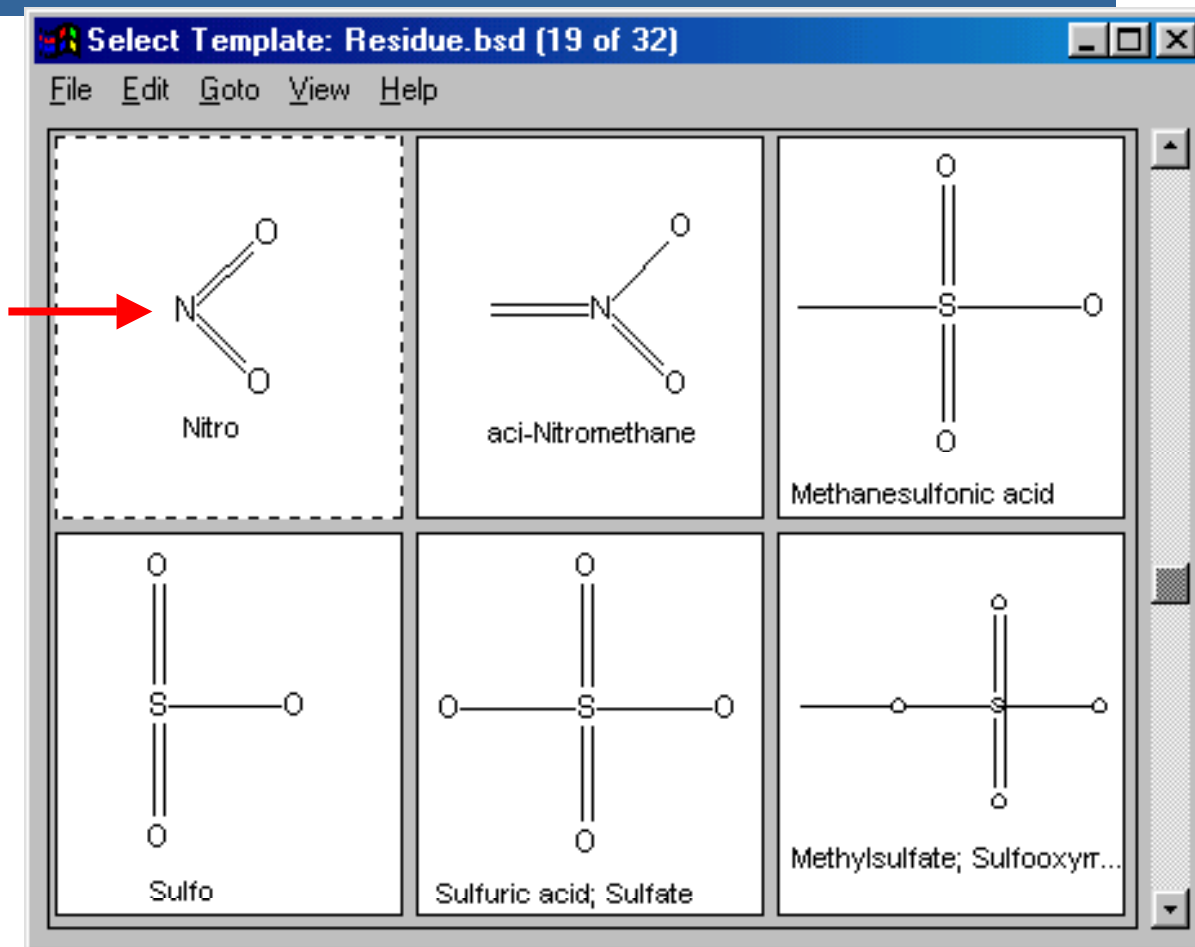
Structure Drawing Tips for Atoms, Bonds, and Functional Groups in Beilstein Crossfire

- Use Pencil and ring icons for drawing.
 - A = cursor positioned on an atom
 - B = cursor positioned on a bond
- Hold down **shift key** to change change **atoms** and **bonds**.
- To draw functional groups:
 - **File** menu bar > **Group Template** > **Residue** > double click to select desired item
 - Note all functional groups are drawn as if they were electrically neutral in Beilstein (e.g. a nitro group has double bonds to both Oxygen atoms)
- Don't need to draw Hydrogen atoms as Hydrogen saturation is assumed when search is run.

Using Group Templates in Beilstein Crossfire

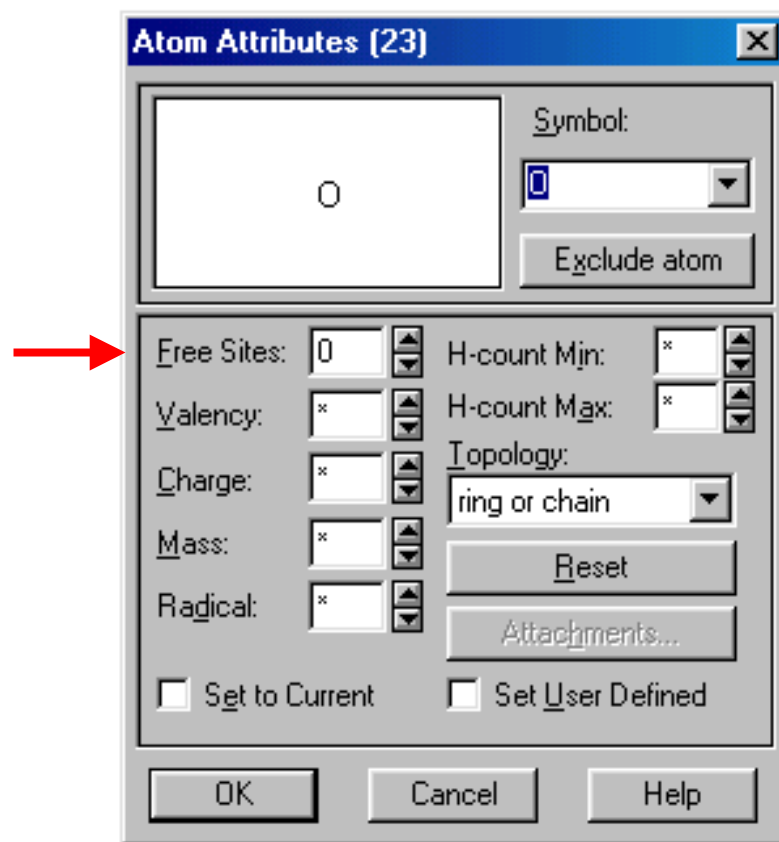


“Residues” or Functional Groups are Drawn Electrically Neutral in Beilstein Crossfire



Drawing Tip on How to Leave a Atom Position Open in Beilstein Crossfire

- If you need to leave a position open in a structure
 - Using Pencil tool, click once on an atom without holding the shift key down
 - A dialog box will open automatically. Set **Free Sites** to **Maximum** by clicking once on **Down Arrow**. Or, click on Up Arrow to indicate a specific number of connections at this position in the structure.



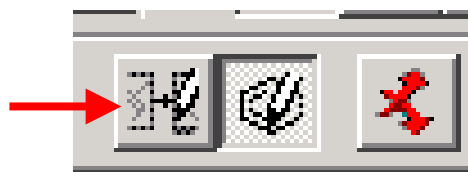
Copying Structures From Records to Structure Editor to Save Time in Beilstein

- Reduce the amount of drawing you need to do by copying the structure of your unknown into Structure Editor.
 - View full record for parent compound. If you do not see structure of compound, press F2. Highlight structure by clicking once on it.
 - Go to **Edit** menu bar and select **Copy Structure to SE** (Structure Editor).
 - Structure will now appear in **Structure Editor** window.

Duplicating Structures Within the Structure Editor in Beilstein Crossfire

- Instead of drawing out the derivative or product you want to search, copy and modify the reactant (your parent unknown).
 - Highlight unknown with **Highlighter** tool (rectangle located directly below pencil tool).
 - Hold down **shift key** and **drag structure** to copy it.
 - Modify copied structure.
 - Make sure both structures are visible in structure drawing workspace on your screen.

Running a Reaction Search in Beilstein - Overview



- After structures are drawn, click on **Reaction Attribute** Icon.
- Highlight each structure and label as reactant or product.
- Press Red Crosses icon to return to the main interface. Run search and view results in short display format.
- Note: if you need to modify a structure, you must do this in the **Structure Editor**.

Copying structure to Structure Editor - Sample Search in Beilstein Crossfire

The screenshot shows the 'Display Hits - [Beilstein:Q01 hit 1 of 2]' window. The 'Edit' menu is open, highlighting 'Copy structure to editor' (Ctrl+Shift+C). A red arrow points to this menu item. Another red arrow points to the chemical structure of 4-nitrobenzoic acid in the 'Q01: Hit 1' window.

Subst:
Beilstein
Beilstein
CAS Registry Number 62-23-7
Chemical Name 4-nitro-benzoic acid
4-Nitro-benzoesaure
Autoname 4-nitro-benzoic acid
Molecular Formula $C_6H_5NO_4$
Molecular Weight 167.12
Lawson Number 10582
Compound Type isocyclic
Constitution ID 855191
Tautomer ID 884333
Beilstein Reference 0-09-00-00389, 1-09-00-00157, 2-09-00-00256, 3-09-00-01537, 4-09-00-01072, 5-09, 6-09
Entry Date 1989/06/29
Update Date 2002/07/19

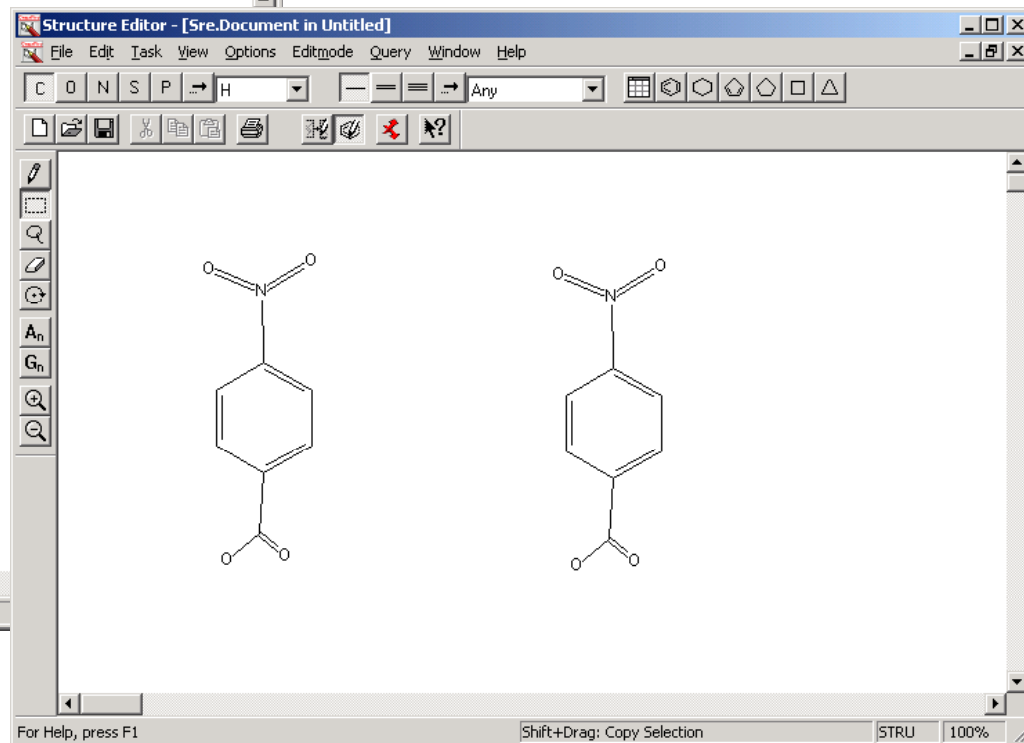
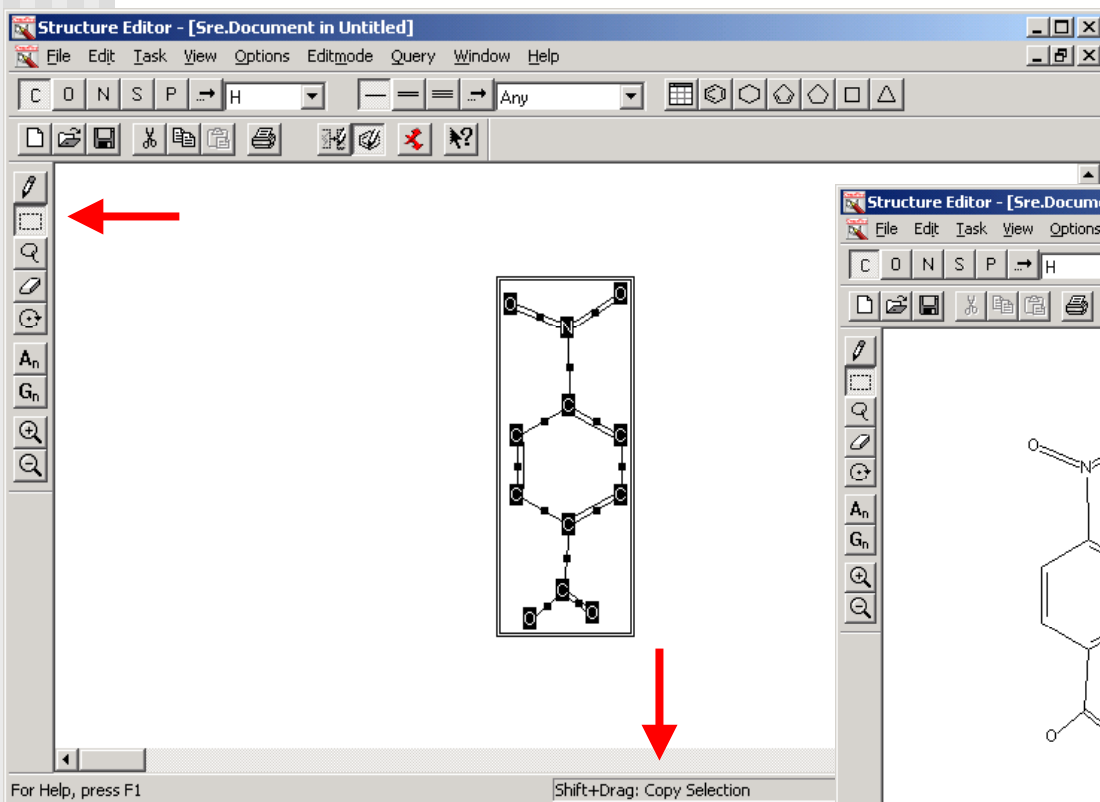
Reaction 1 of 1652
Reaction ID [4244](#)
Reactant BRN [102410](#) 2-ethyl-aziridine
[973593](#) 4-nitro-benzoic acid
Product BRN [2621820](#) 2-(4-nitro-benzoylamino)-butan-1-ol
No. of Reaction Details 1
Reaction Classification Preparation

Note 1 Handbook
Ref. 1 [733946](#) [LitLink](#) ; Journal; Powers et al.; JACSAT; J.Amer.Chem.Soc.; 78; 1956; 907, 910.

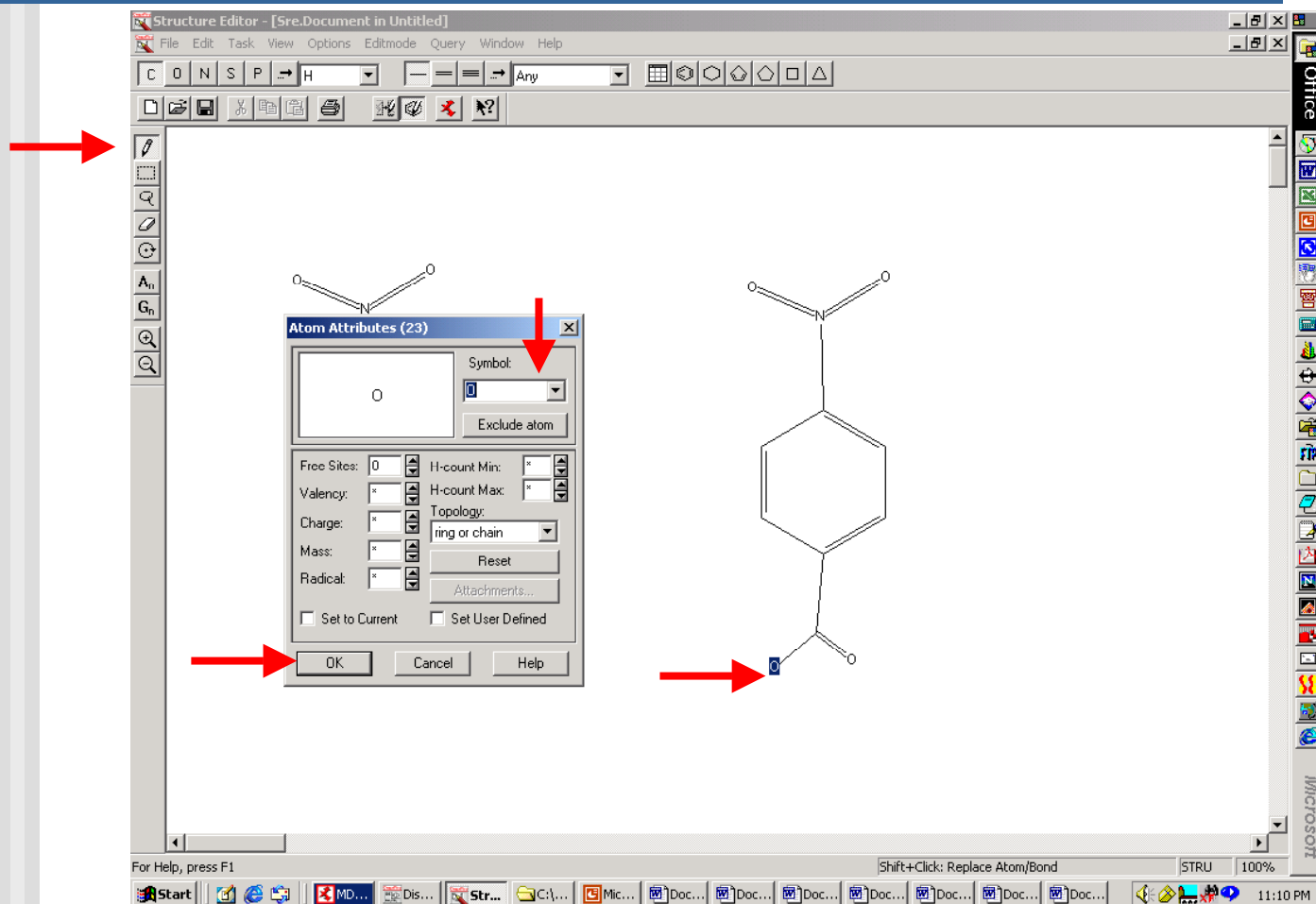
Reaction 2 of 1652
Reaction ID [19845](#)
Reactant BRN [103233](#) pyridine
[1916959](#) bis-(4-nitro-benzoyl)-peroxide
Product BRN [973593](#) 4-nitro-benzoic acid
No. of Reaction Details 1
Reaction Classification Chemical behaviour
Temperature 110 C
Other Conditions anschliessendes Behandeln mit wss. Natronlauge

Copy the structure to the editor idle ALL Substances

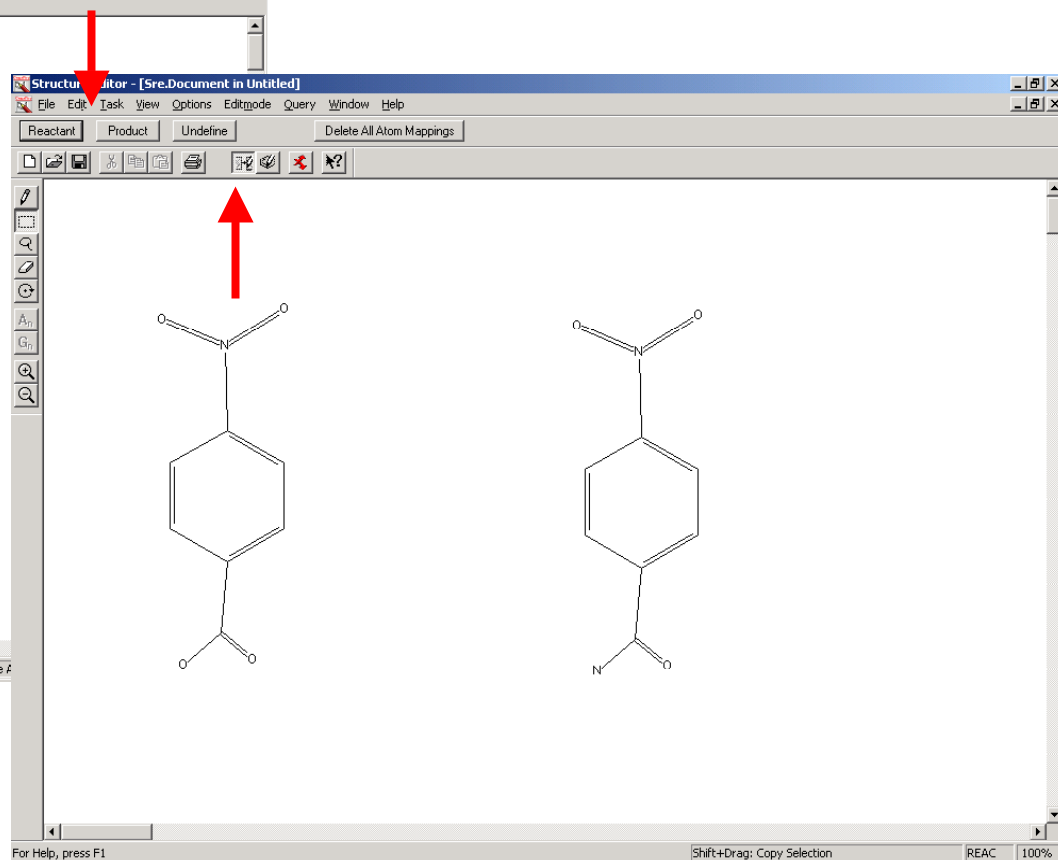
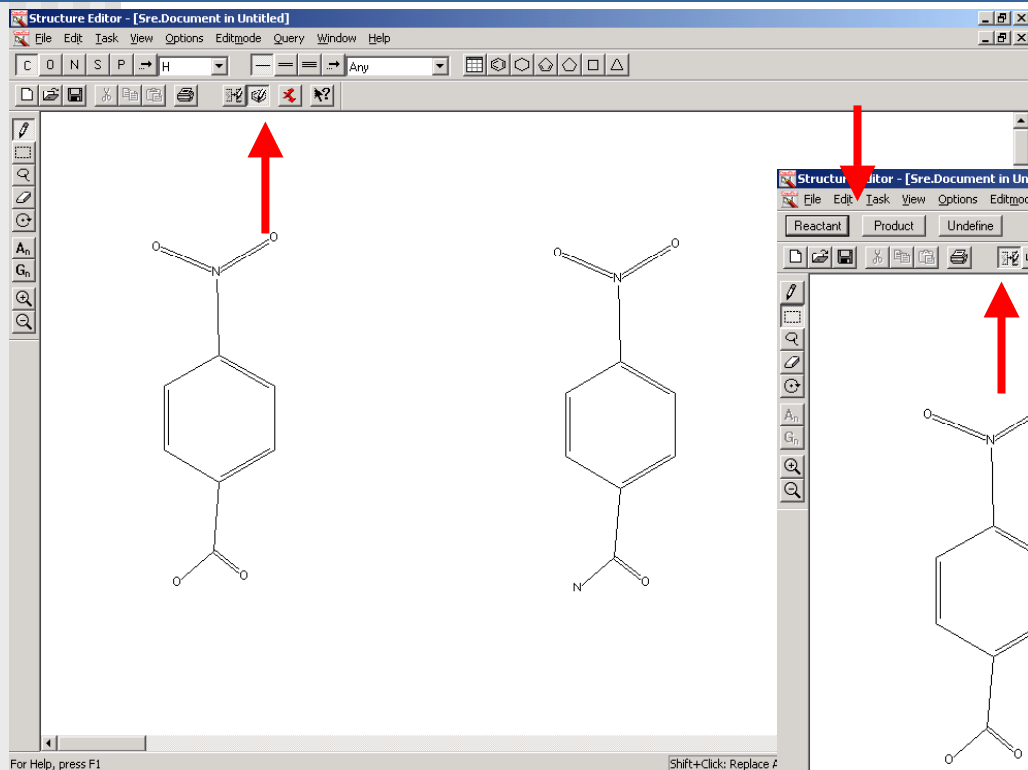
Making 2nd Copy of Structure Within Structure Editor in Beilstein Crossfire



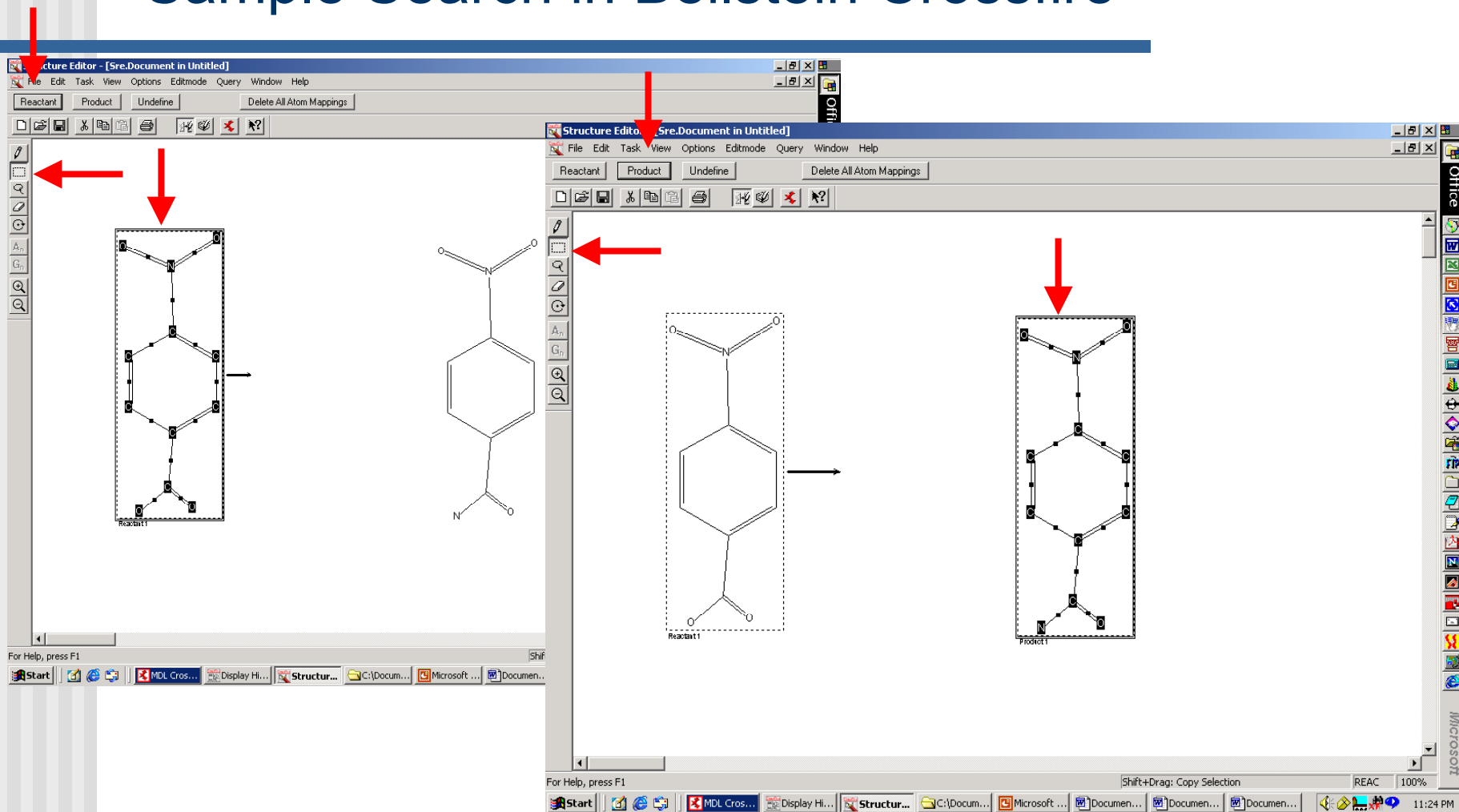
Changing an Atom Value of a Structure in Beilstein Crossfire



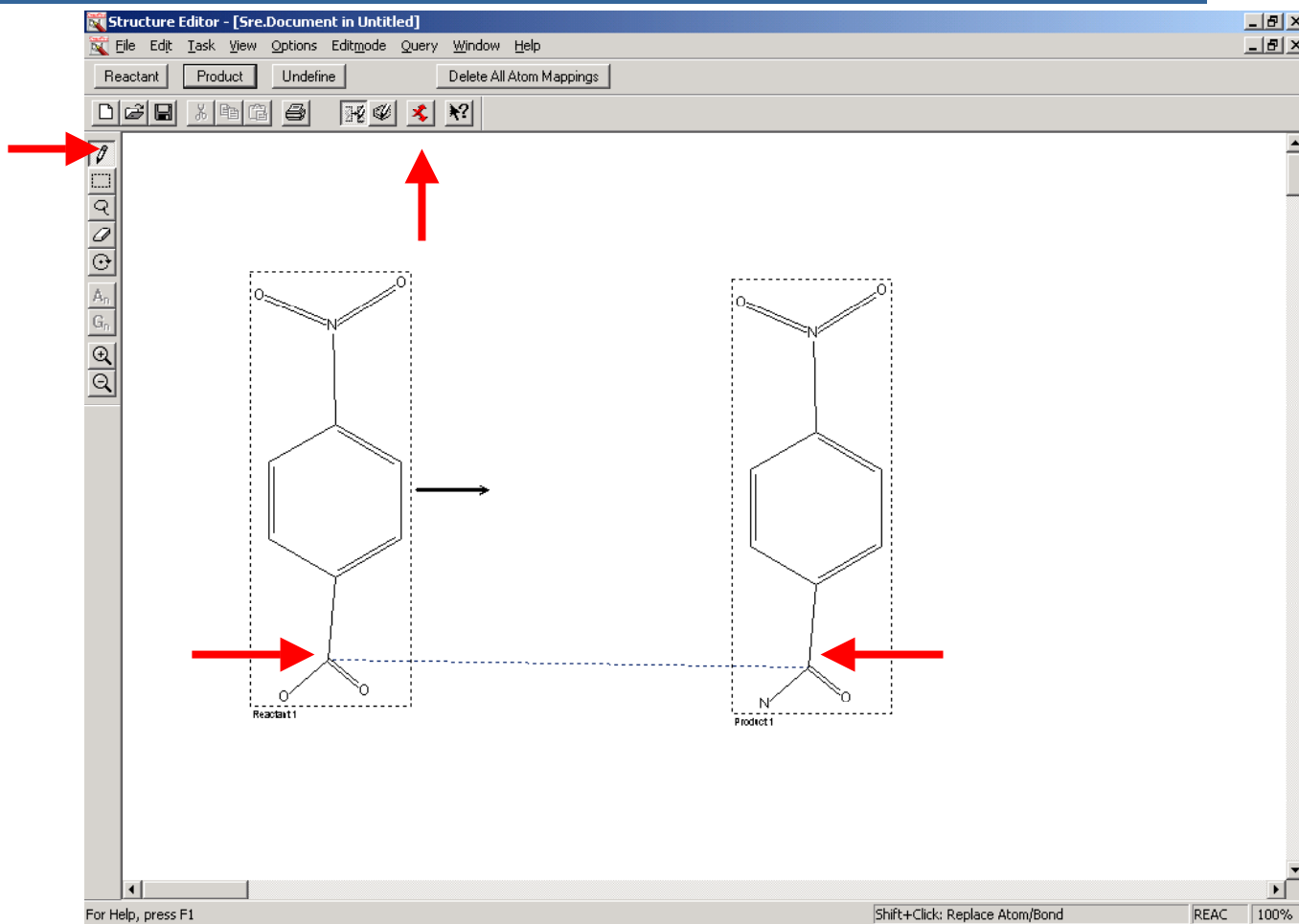
Structure Editor and Reaction Mode in Beilstein Crossfire



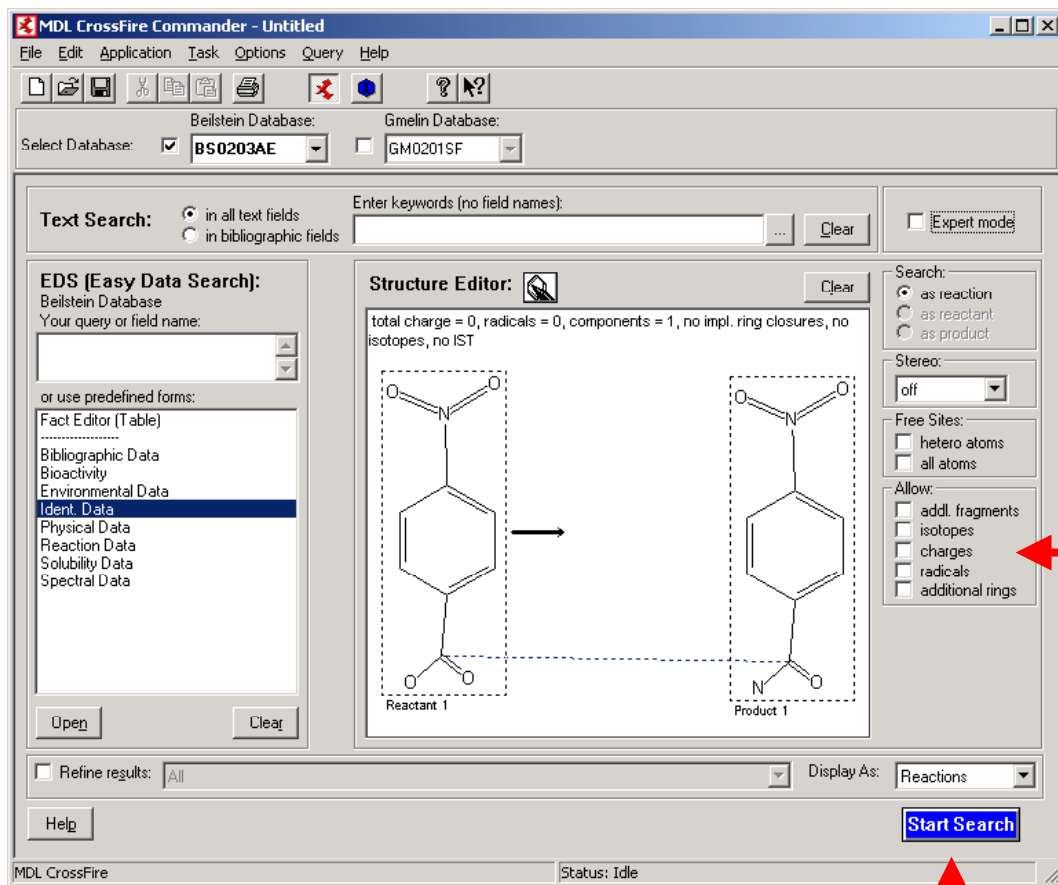
Specifying Reactant and Product of a Reaction - Sample Search in Beilstein Crossfire



Mapping Atoms to Make a Reaction Search More Precise in Beilstein Crossfire



Performing a Reaction Search in Beilstein Crossfire

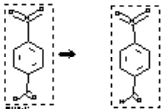


Viewing Results of Reaction Search in the Short Display Format in Beilstein Crossfire

Results of the Structure Queries (1)

Your recent search had the following hits in Reactions:

Select	Hits	Note	Query
01 <input checked="" type="checkbox"/>	3	Original query	total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST



View **Back to Query**

Display Hits - [BeilsteinQ02 hit 1 of 3]

Hit 1:740400

Hit 2:855625

Hit 3:855652

For Help, press F1

Display Hits - [BeilsteinQ02 hit 3 of 3]

Hit 1:740400

Hit 2:855625

Hit 3:855652

For Help, press F1

STRUCT

Reactions

Viewing Reaction Entries and Clicking on Substance Hyperlink in Beilstein Crossfire

Display Hits - [Beilstein:Q02 hit 3 of 3]

File Edit Task View Options Window Help

Open Save Print Export Start Prior Next End Back Forward Show Copy Short View all Help Last Search

Reaction

Reaction ID	855652
Reactant BRN	273593 4-nitro-benzoic acid
Product BRN	639263 4-nitro-benzamide
No. of Reaction Details	4

Reaction Details 1 of 4

Reaction Classification	Preparation
Yield	81 percent (BRN=639263)
Reagent	NH ₄ HCO ₃ HCONH ₂
Time	8 min
Other Conditions	Irradiation

Ref. 1 [6332322, LitLink](#) ; Journal; Peng, Yanqing; Song, Gonghus; OPPIAK; Org.Prep.Proced.Int.;

Reaction Details 2 of 4

Reaction Classification	Preparation
Reagent	NH ₄ (g), ethyl polyphosphate
Solvent	CHCl ₃
Other Conditions	1.) 0 - 5 deg C, 30 min, 2.) room temp., 1.5h

Ref. 1 [5571369, LitLink](#) ; Journal; Imamoto, Tsuneo; Takaoka, Tomoko; Yokoyama, Masataka; SYNTBF; Synthesis; EN; 2; 1983; 142-143.

Reaction Details 3 of 4

Reaction Classification	Preparation
Reagent	PCl ₅
Other Conditions	man behandelt das Chlorid mit konz. Ammoniakloesung

Ref. 1 [2070324, LitLink](#) ; Journal; Reichenbach; Beilstein; JLACBF; Justus Liebigs Ann. Chem.; 132; 1864; 143.

Reaction Details 4 of 4

Reaction Classification	Preparation
Reagent	pyridine sulfamide

Ref. 1 [2104340, LitLink](#) ; Journal; Kirsanow, Solutow; ZOKHA4; Zh.Obshch.Khim.; 19; 1949; 2201, 2205; CHZEA6; Chem.Zentralbl.; GE; 1950 II 2903.

For Help, press F1

idle ALL Reactions

Q02: Hit 3

Finding Physical Properties for a Derivative in Beilstein Crossfire

The screenshot shows the Beilstein Crossfire software interface. The main window displays the 'Display Hits' for Beilstein entry 639263. The 'Field Availability' dialog box is open, showing a list of fields and their occurrence counts. The 'MP' (Melting Point) field is highlighted, and a red arrow points to it. The 'MP' field is checked, and its occurrence count is 26. The 'Field Availability' dialog box also shows options for ordering the fields (Beilstein/Gmelin, Alphabetical by code, Alphabetical by name) and buttons for 'Go to', 'Close', and 'Help'.

Substance

- Beilstein Registry Nu
- Beilstein Preferred Rn
- CAS Registry Number
- Chemical Name
- Autoname
- Molecular Formula
- Molecular Weight
- Lawson Number
- Compound Type
- Constitution ID
- Tautomer ID
- Beilstein Reference
- Entry Date
- Update Date

Field Availability - Beilstein:639263 hit 1 of 1

Code	FieldName	Occ.
<input checked="" type="checkbox"/>	IR	Infrared Spectra 10
<input checked="" type="checkbox"/>	IDA	Interatomic Distances and Angles 2
<input checked="" type="checkbox"/>	IP	Ionization Potential 1
<input checked="" type="checkbox"/>	LLSM	Liquid/Liquid Systems (MCS) 1
<input checked="" type="checkbox"/>	LUM	Luminescence 1
<input checked="" type="checkbox"/>	MS	Mass Spectrum 2
<input checked="" type="checkbox"/>	MP	Melting Point 26
<input checked="" type="checkbox"/>	NMR	Nuclear Magnetic Resonance 10
<input checked="" type="checkbox"/>	OPT	Optical Properties 1

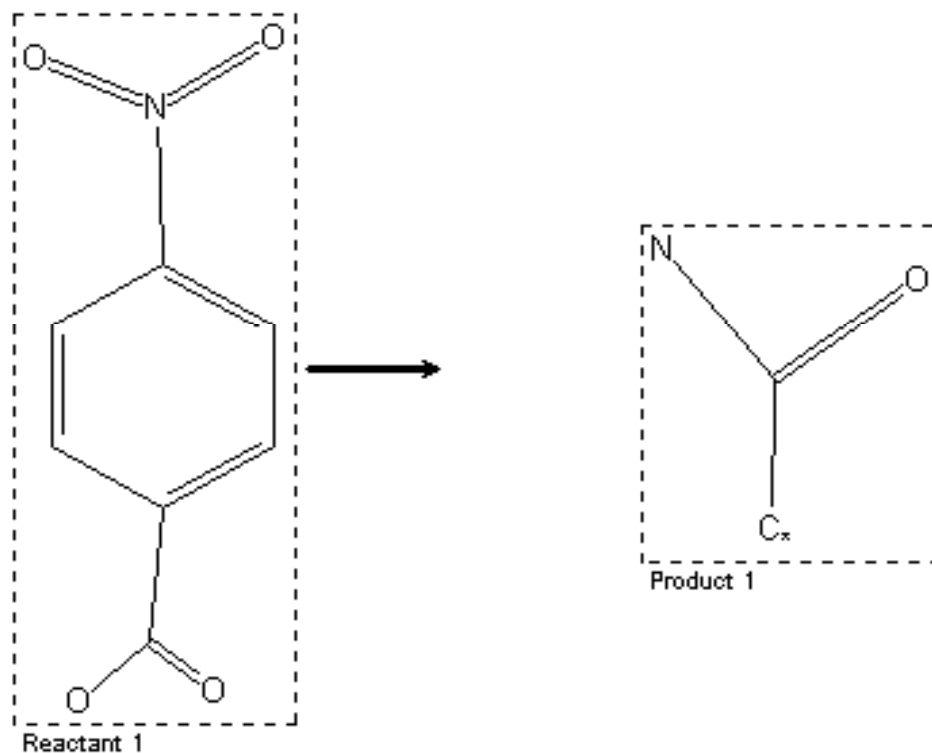
Reaction 1 of 159

Reaction ID: 24315
Reactant BRN: 10395 xanthen-9-ol
Product BRN: 639263 4-nitro-benzamide
No. of Reaction Details: 3
Reaction Classification: Preparation
Reagent: aq.-ethanolic acetic acid

Reaction 2 of 159

Reaction ID: 363947
Reactant BRN: 251122 2,6-diamino-5-benzoylamino-3H-pyrimidin-4-one
Product BRN: 639263 4-nitro-benzamide
No. of Reaction Details: 1
Reaction Classification: Preparation
Temperature: 290 - 300 C

Search Tip: Reaction Search in Beilstein Where Product is a Substructure Because you Don't Know What Complete Structure Looks Like



Finding Physical Properties for a Derivative in Beilstein

- Options for finding physical property data for a derivative:
 - View Derivative field usually includes MP/BP data.
 - View citation link as it may include a Substance link for the derivative.
 - Perform a structure search of the derivative and view compiled data.
 - After doing a reaction search, click on the Beilstein Registry Number (BRN) link of derivative to see data.

Finding Physical Properties for a Derivative in CCD, POC, Merck, & Preparation Papers

- Using a CAS Registry Number, molecular formula, or chemical name, it is also possible to search CCD, POC, or Merck to see what physical property data has been compiled for a derivative.
- Preparation or synthesis papers for substances usually contain complete descriptions, including physical properties, of compounds.

Help

- Please consult a TA if you need help selecting a derivative or interpreting lab data.
- Consult with librarians if you need help with “mechanics” of doing searches.
- Good luck and have fun searching!