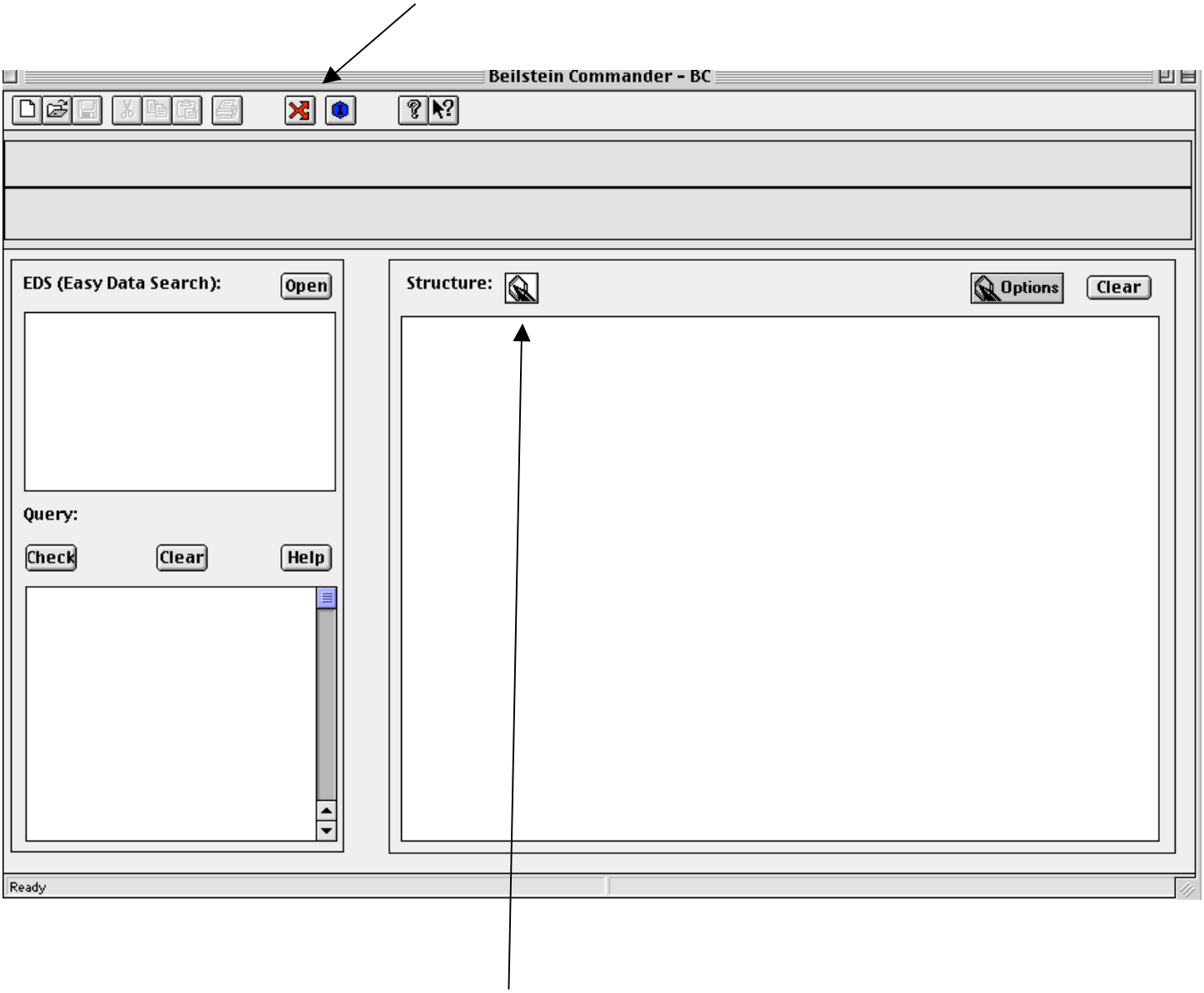
Chem 634, Advanced Organic Chemistry- Synthesis and Reactivity
Prof. Joseph Fox

Chemical Database Searching- Handout 2

Introduction to Beilstein Commander

The purpose of this tutorial is to do a specific structure and
a
Substructure search on Beilstein

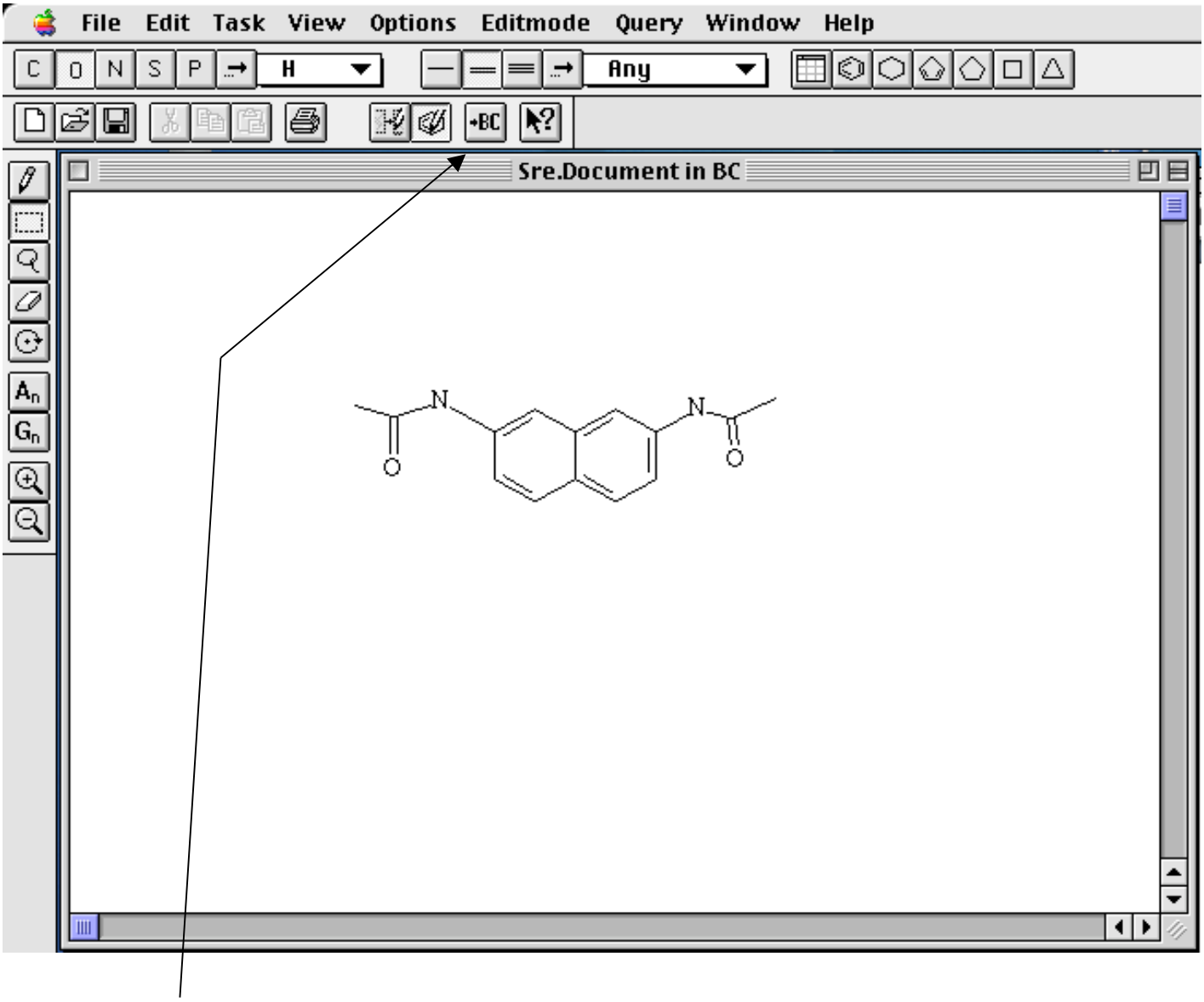
1. Open the Beilstein commander application, and click on the red crossfire button,.



2. Click on the Structure icon

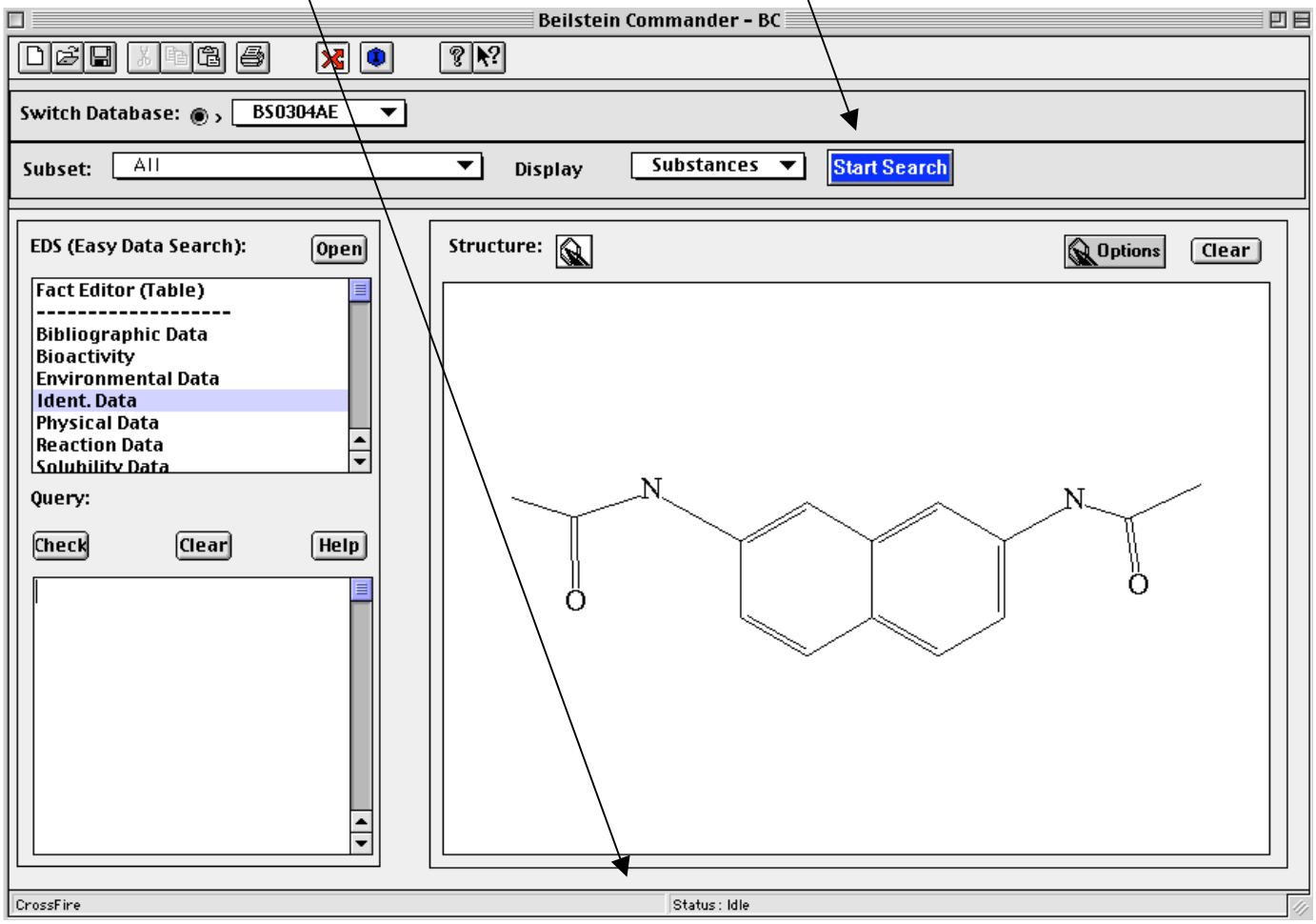
3. This brings us to the structure editor window. We will begin by doing a specific structure search. Construct the structure below.

Note: In Beilstein, hydrogens are implied unless we include a "Free Site"- to be described soon.

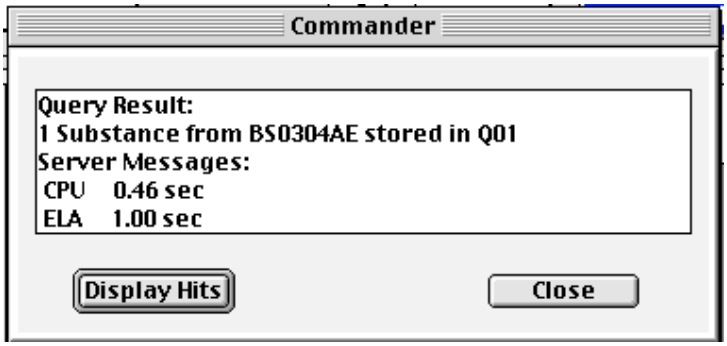


4. Return to the B commander window by pressing the BC icon

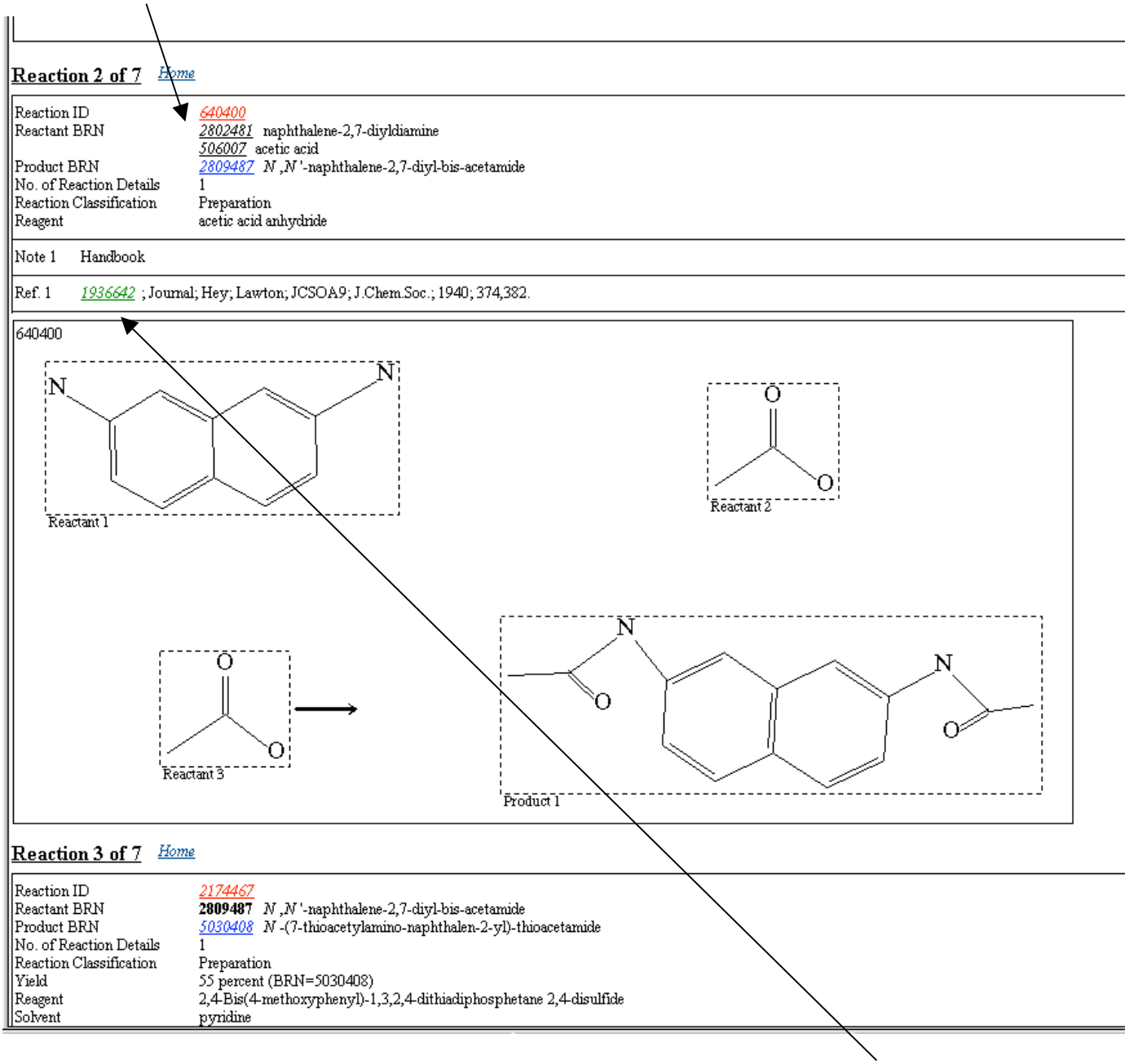
3. In the commander window, wait until the blue “Start Search” appears, and status is “idle”



4. Press Start Search. In a moment, the following pop up appears. Click display hits



5. This brings up the display hits window. Under the "VIEW" pull down, make sure that "Include Structures" and "Include Field Availability" are selected.
6. Now, look at your hit set. Notice that Beilstein directly gives both reactions that produce your structure, and reactions of your structure. Go down to reaction #2 (which prepared your structure). Notice that we get links to all of the compounds referenced in the reaction. For example, you can link to all of the information for reactant 1 by clicking on "BRN2802481".



Reaction 2 of 7 Home

Reaction ID	640400
Reactant BRN	2802481 naphthalene-2,7-diyldiamine
	506007 acetic acid
Product BRN	2809487 *N*,*N*'-naphthalene-2,7-diyl-bis-acetamide
No. of Reaction Details	1
Reaction Classification	Preparation
Reagent	acetic acid anhydride

Note 1 Handbook

Ref. 1 1936642 ; Journal; Hey; Lawton; JCSOA9; J.Chem.Soc.; 1940; 374,382.

Reaction 3 of 7 Home

Reaction ID	2174467
Reactant BRN	**2809487** *N*,*N*'-naphthalene-2,7-diyl-bis-acetamide
Product BRN	5030408 *N*-(7-thioacetylamino-naphthalen-2-yl)-thioacetamide
No. of Reaction Details	1
Reaction Classification	Preparation
Yield	55 percent (BRN=5030408)
Reagent	2,4-Bis(4-methoxyphenyl)-1,3,2,4-dithiadiphosphetane 2,4-disulfide
Solvent	pyridine

7. You can also link directly to the cited paper. For example, click on the link for Ref 1 in reaction 2:

8 . This links us to a 1940 paper in J. Chem. Soc. by Hey and Lawton. By scrolling down, we Can get information and links to every substance in the paper. We can also get details of every Reaction in the paper.

Citation Number

Citation Number 1936642

Field Availability List 1-3 of 3 *Home*

Code	Field Name	Occ.
CIT	Citation	1
IDE	Substance	81
RX	Reaction	86

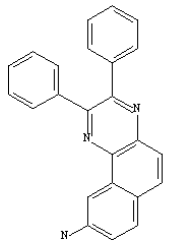
Citation *Home*

Document Type	Journal
Authors	Hey; Lawton
CODEN	JCSOA9
Journal Title	J.Chem.Soc.
Publication Year	1940
Page	374,382

Substance 1 of 81 *Home*

Beilstein Registry Number	*300183*
Chemical Name	2,3-diphenyl-benzo[f]quinoxalin-9-ylamine
Autoname	2,3-diphenyl-benzo[f]quinoxalin-9-ylamine
Molecular Formula	$C_{24}H_{17}N_3$
Molecular Weight	347.42
Lawson Number	29621
Compound Type	heterocyclic
Constitution ID	326179
Tautomer ID	375961
Beilstein Reference	4-25-00-02768
Entry Date	1988/06/27
Update Date	1992/05/13

300183



Substance 2 of 81 *Home*

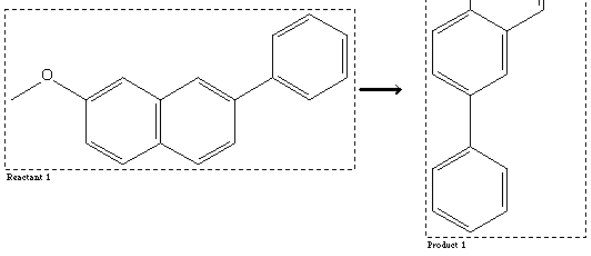
1936642:BS0304AE hit 1 of 1

Reaction 4 of 86 *Home*

Reaction ID	*293799*
Reactant BRN	*1963132* methyl-(7-phenyl-[2]naphthyl)-ether
Product BRN	*3265450* 7-Phenyl-[2]naphthol
No. of Reaction Details	1
Reaction Classification	Preparation
Reagent	aqueous HI glacial acetic acid

Note 1 Handbook

293799

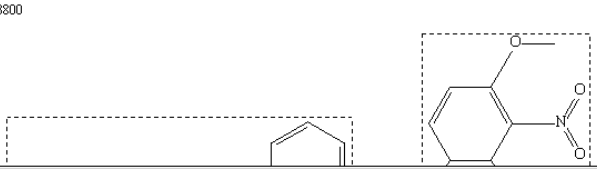


Reaction 5 of 86 *Home*

Reaction ID	*293800*
Reactant BRN	*1963132* methyl-(7-phenyl-[2]naphthyl)-ether
Product BRN	*3379339* methyl-(1-nitro-7-phenyl-[2]naphthyl)-ether
No. of Reaction Details	1
Reaction Classification	Preparation
Reagent	glacial acetic acid aqueous HNO3

Note 1 Handbook

293800

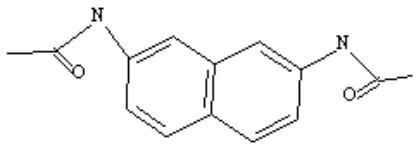


9 . Now, returning to the original search, we should look at the field availability list. In addition to Reaction information, we can find out the melting point and crystal structure data for this substance. For Many substances, even more fields are available, such as NMR data, IR, solubility, etc. This is extremely Useful if you need to find (for e.g.) the 13C NMR data for a specific compound.

Substance

Beilstein Registry Number	2809487
Beilstein Preferred RN	81955-88-6
CAS Registry Number	81955-88-6
Chemical Name	*N*,*N*'-naphthalene-2,7-diyl-bis-acetamide
Autoname	*N*-(7-acetylamino-naphthalen-2-yl)-acetamide
Molecular Formula	$C_{14}H_{14}N_2O_2$
Molecular Weight	242.28
Lawson Number	14582, 1155
Compound Type	isocyclic
Constitution ID	2577180
Tautomer ID	2754414
Beilstein Reference	2-13-00-00086, 3-13-00-00404, 5-13, 6-13
Entry Date	1989/07/11
Update Date	1997/02/03

2809487



Field Availability List 1-3 of 3 Home

Code	Field Name	Occ.
RX	Reaction	7
CPD	Crystal Property Description	1
MP	Melting Point	2

10. Try it: Link to the MP data above

You should see the following;

Melting Point 1-2 of 2 Home

VALUE (MP) C	Solvent (.SOL)	Note	Ref.
264 - 265	H2O	1	1
261	aq. acetic acid	2	2

Note 1	Handbook
Note 2	Handbook

Ref. 1	815817 ; Journal; Leonard; Hyson; JACSAT; J.Amer.Chem.Soc.; 71; 1949; 1961,1962.
Ref. 2	1546308 ; Journal; Windaus; CHBEAM; Chem.Ber.; 57; 1924; 1738.