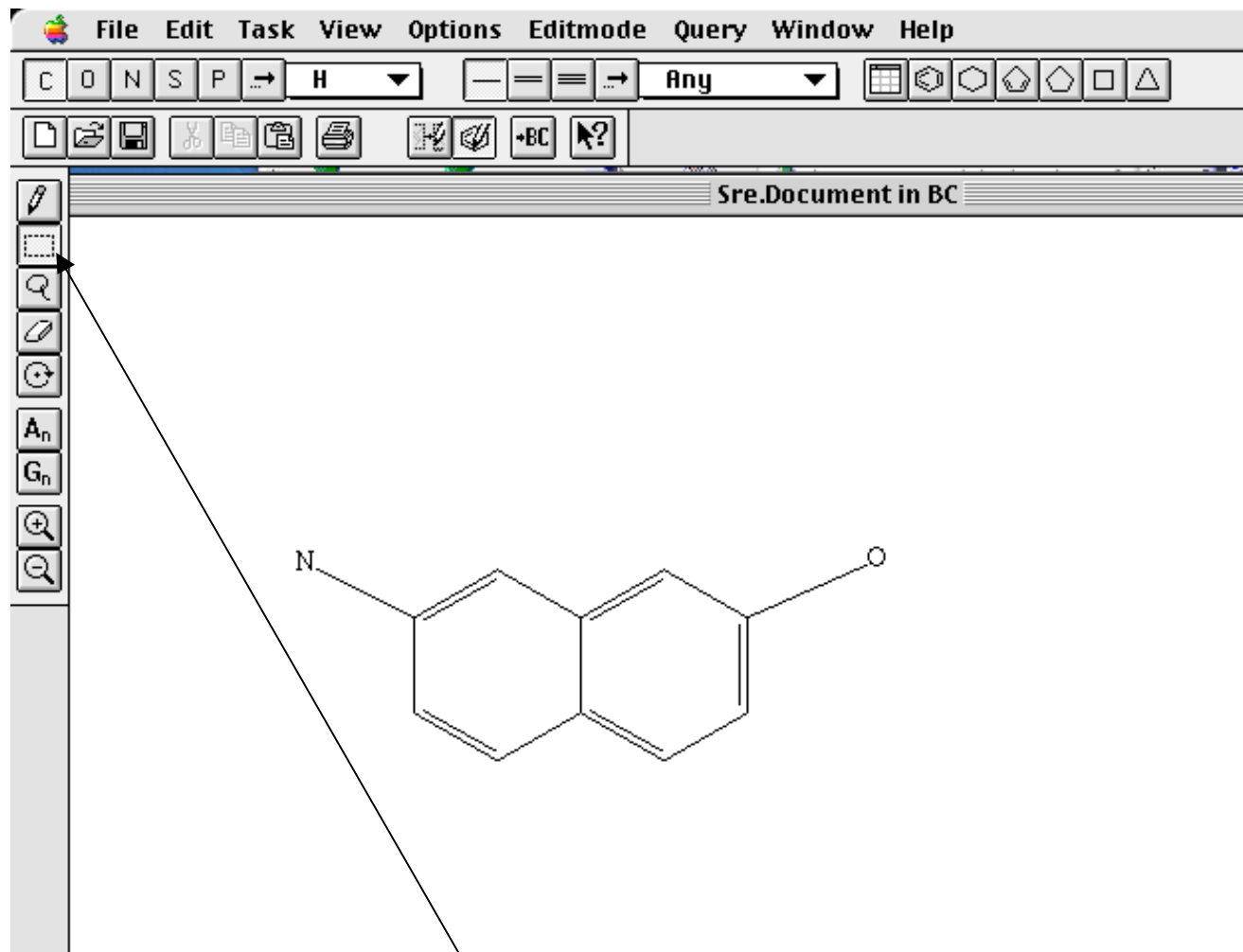


Chem 634, Advanced Organic Chemistry- Synthesis and Reactivity  
Prof. Joseph Fox

**Chemical Database Searching- Handout 3**  
Substructure Searching using Beilstein

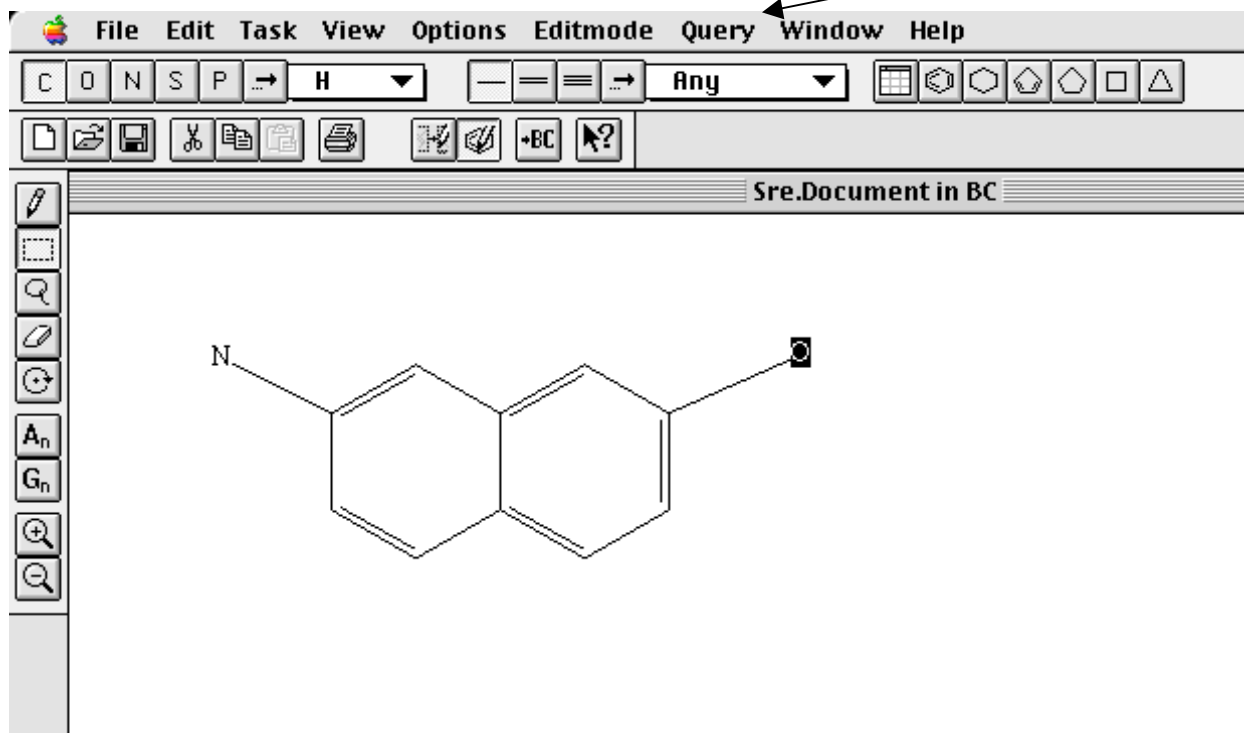
The purpose of this tutorial is to do a  
Substructure search on Beilstein

1. Following the steps from the last tutorial, construct the following structure within the Structure Editor

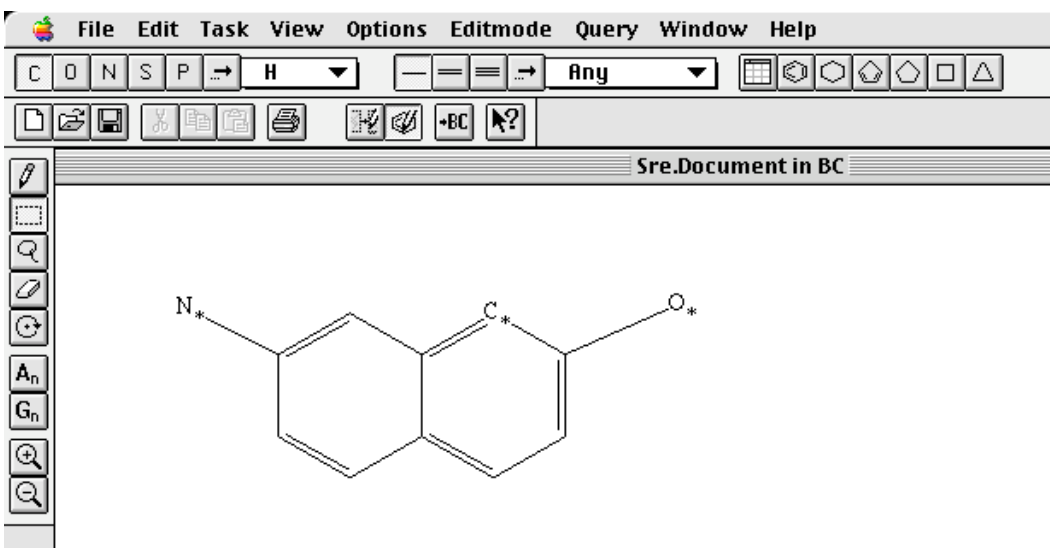


2. Highlight the oxygen atom using the “rectangle” tool

3. When the atom is highlighted, pull down “Set Free Sites” from the Query pull down menu.



4. This will put an asterisk next to the oxygen atom. Repeat this for the nitrogen atom and for one of the ring carbons as shown below.



5. A “Free Site” means that anything can be attached to that atom. For other atoms, it is implied that there is a hydrogen attached

7. Now, return to the Commander window and start the search

Beilstein Commander - BC

Switch Database:  BS0304AE

Subset: All Display Substances **Start Search**

EDS (Easy Data Search):

- Fact Editor (Table)
- 
- Bibliographic Data
- Bioactivity
- Environmental Data
- Ident. Data
- Physical Data
- Reaction Data
- Solubility Data

Query:

Structure:

C1=CC=C2C(=C1)C(=O)N2

8. This produces 115 hits (as of Feb 27, 2004). Hit "Display Hits"

Commander

Query Result:  
115 Substances from BS0304AE stored in Q01

Server Messages:  
CPU 0.70 sec  
ELA 2.00 sec

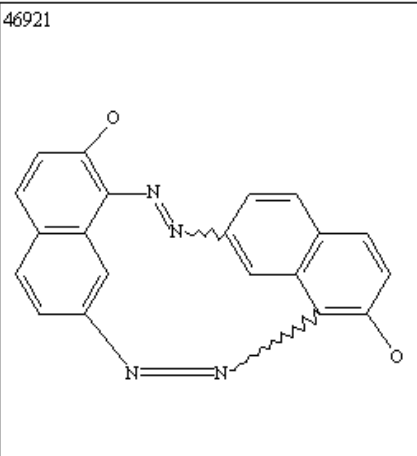
8. This brings you to the first of 115 hits. This number is too large to scroll through manually, so pull down the "View" menu and select "Short Display"

Q01:BS0304AE hit 1 of 115

**Substance**

Beilstein Registry Number **46921**  
 Chemical Name 2,3,5,6-tetraaza-1,4-di-(1,7)naphthalena-cyclohexaphane-2,5-diene-1<sup>2</sup>,4<sup>2</sup>-diol  
 Molecular Formula C<sub>20</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>  
 Molecular Weight 340.34  
 Lawson Number 30470  
 Compound Type heterocyclic  
 Constitution ID 59312  
 Tautomer ID 81010  
 Beilstein Reference 0-26-00-00402  
 Entry Date 1988/06/27  
 Update Date 1988/06/30

46921



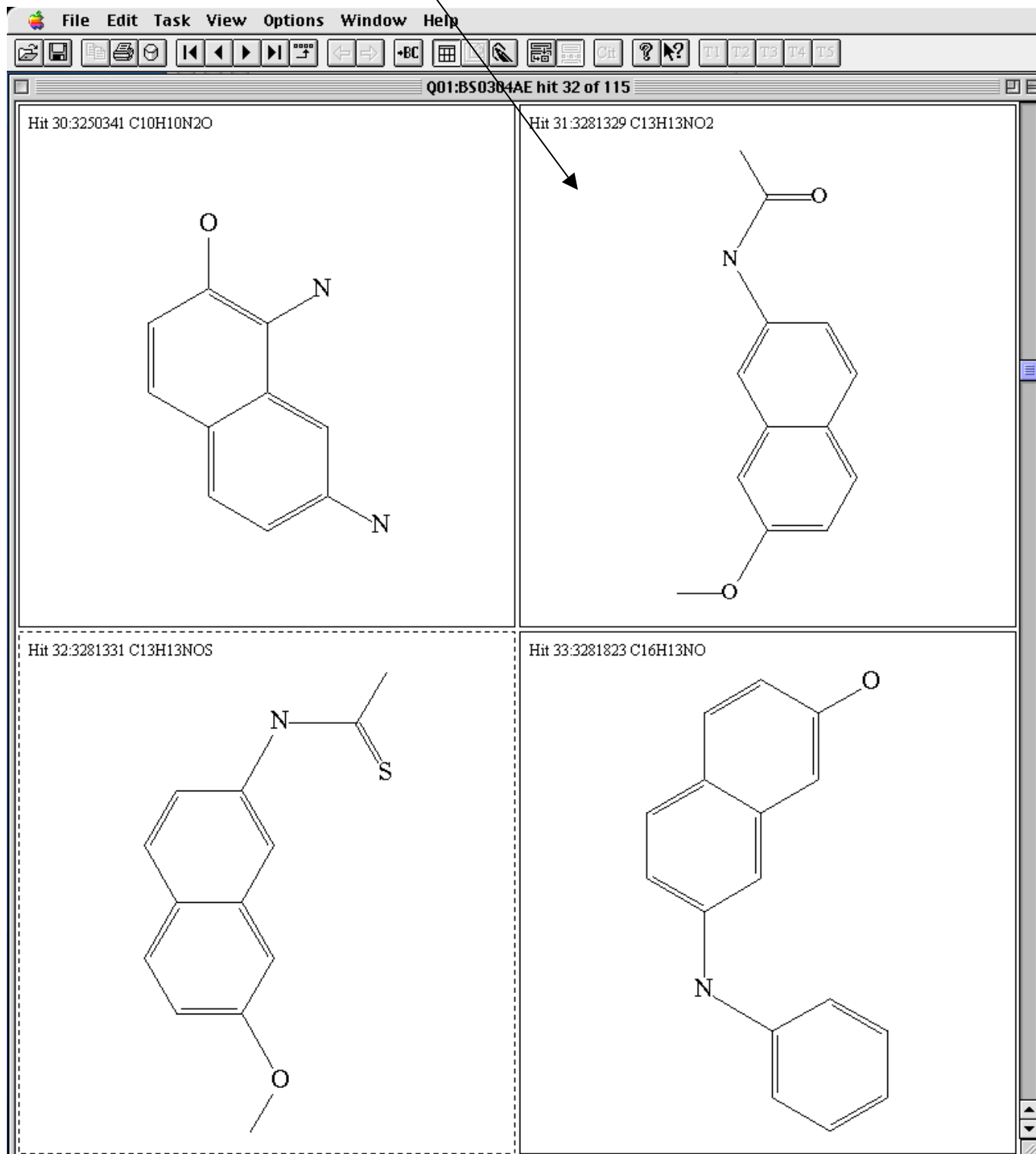
**Field Availability List 1-3 of 3** [Home](#)

Code	Field Name	Occ.
<a href="#">RX</a>	Reaction	1
<a href="#">CPD</a>	Crystal Property Description	1
<a href="#">MP</a>	Melting Point	1

**Reaction** [Home](#)

Reaction ID **393634**  
 Reactant BRN **2802482** 7-Amino-[2]naphthol  
 Product BRN **46921** 2,3,5,6-tetraaza-1,4-di-(1,7)naphthalena-cyclohexaphane-2,5-diene-1<sup>2</sup>,4<sup>2</sup>-diol  
 No. of Reaction Details 1  
 Reaction Classification Preparation  
 Other Conditions Diazotization.durch Eintragen in verd. Soda-Loesung

9. From here, we get a pictorial view of the 115 hits — four at a time. Scroll down to hit number 31, and double click in the box.



10. As in the last tutorial, we can now get data for this compound- in this case there is reaction data, crystal data and mp data. We can also link to papers and information about other reactants and products, etc.

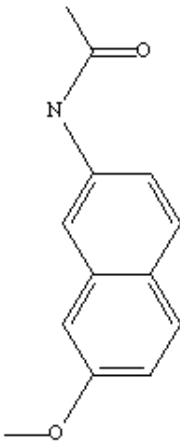
File Edit Task View Options Window Help

Q01:BS0304AE hit 31 of 11

### Substance

Beilstein Registry Number **3281329**  
 Beilstein Preferred RN 102871-76-1  
 CAS Registry Number 102871-76-1  
 Chemical Name *N*-(7-methoxy-[2]naphthyl)-acetamide  
 Autname *N*-(7-methoxy-naphthalen-2-yl)-acetamide  
 Molecular Formula C<sub>13</sub>H<sub>13</sub>NO<sub>2</sub>  
 Molecular Weight 215.25  
 Lawson Number 15022, 1155, 289  
 Compound Type isocyclic  
 Constitution ID 2926241  
 Tautomer ID 3132861  
 Beilstein Reference 2-13-00-00417  
 Entry Date 1990/02/15  
 Update Date 1992/06/02

3281329



**Field Availability List 1-3 of 3** [Home](#)

Code	Field Name	Occ.
<a href="#">RX</a>	Reaction	1
<a href="#">CPD</a>	Crystal Property Description	1
<a href="#">MP</a>	Melting Point	1

**Reaction** [Home](#)

Reaction ID **571676**  
 Reactant BRN [637610](#) 7-methoxy-[2]naphthylamine  
[385737](#) acetic acid anhydride  
 Product BRN **3281329** *N*-(7-methoxy-[2]naphthyl)-acetamide  
 No. of Reaction Details 1  
 Reaction Classification Preparation