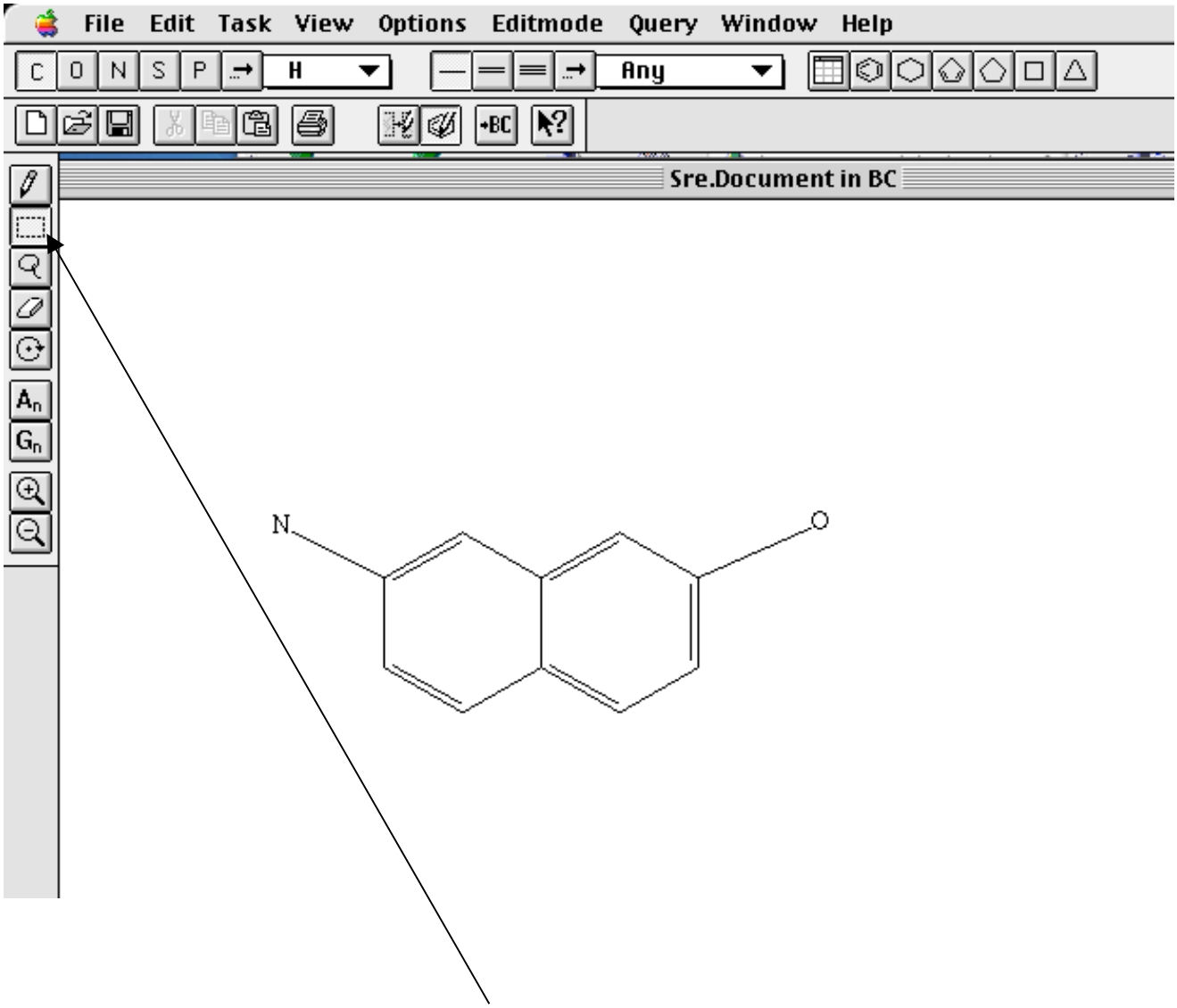
Chem 634, Advanced Organic Chemistry- Synthesis and Reactivity
Prof. Joseph Fox

Chemical Database Searching- Handout 3

Substructure Searching using Beilstein

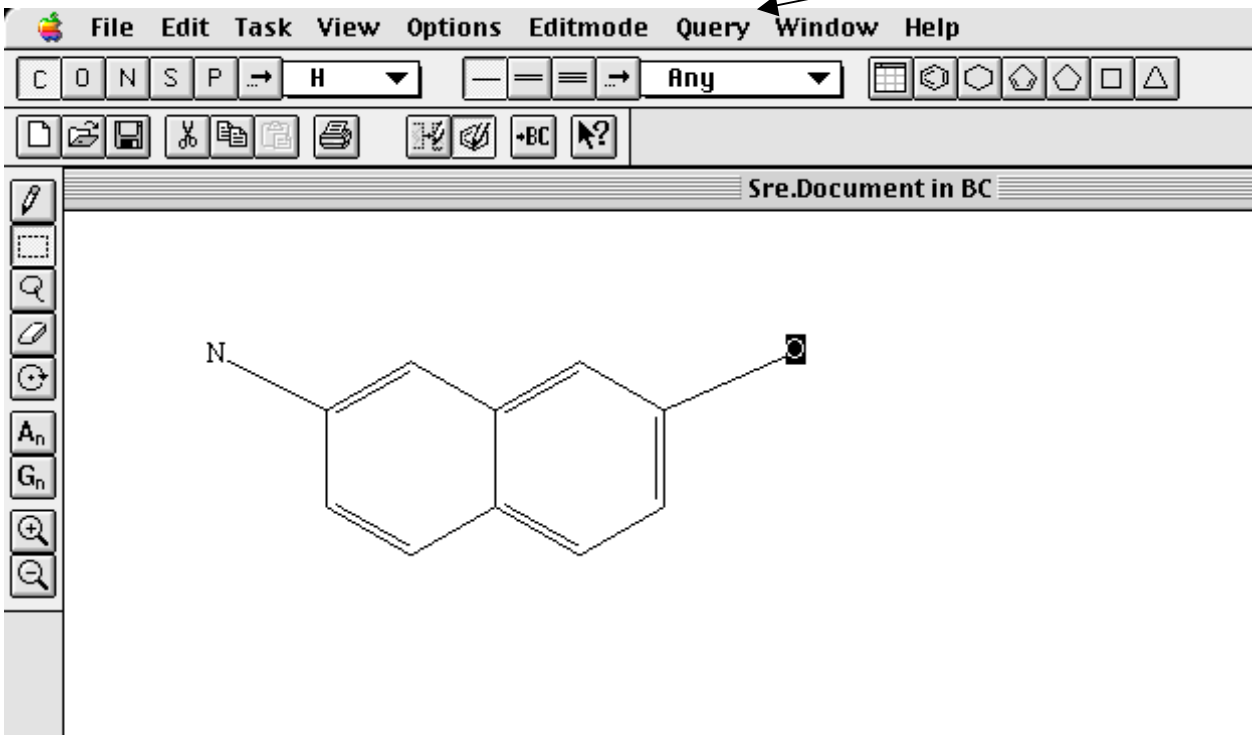
The purpose of this tutorial is to do a Substructure search on Beilstein

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

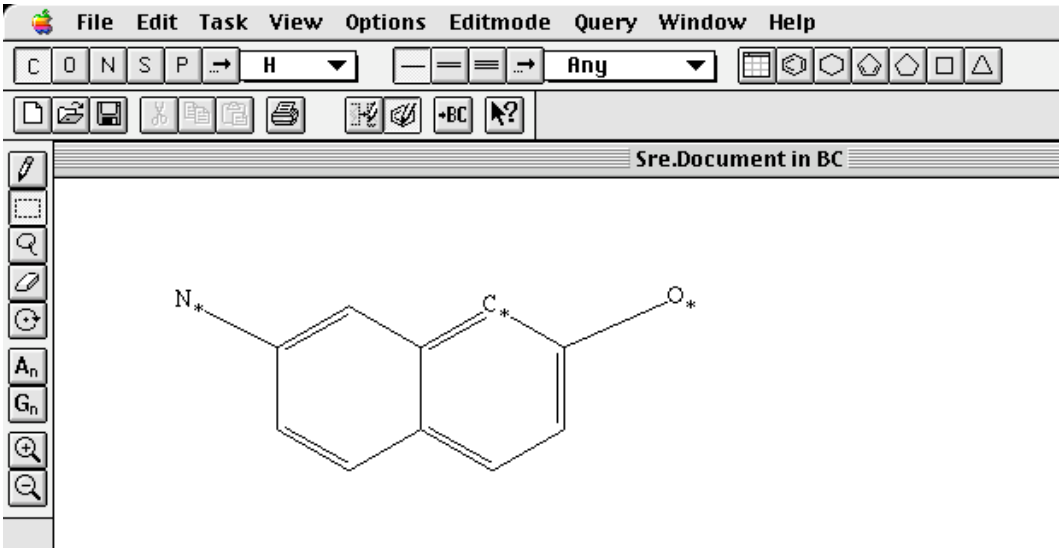


2. Highlight the oxygen atom using the “rectangle” tool

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

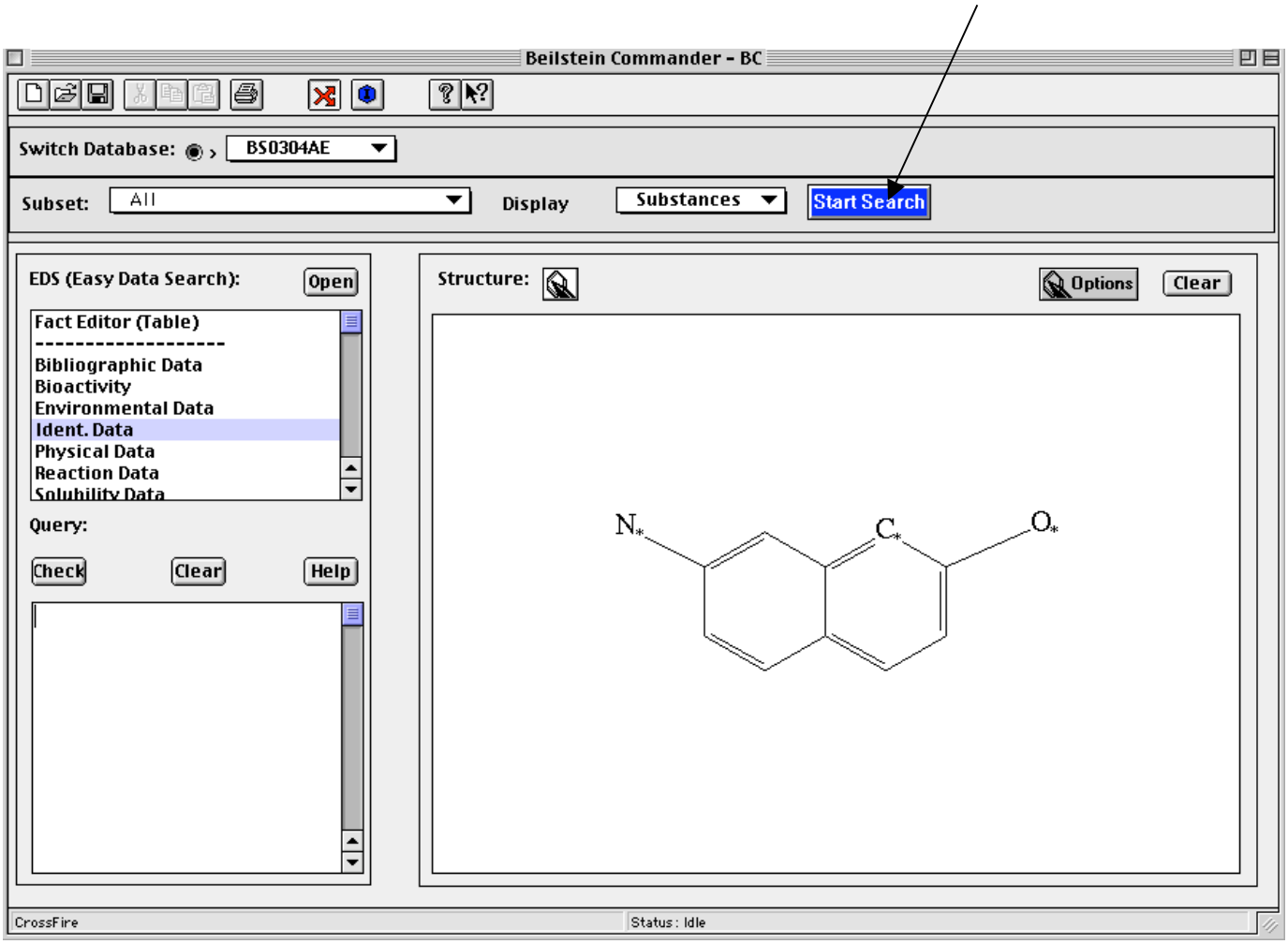


4. This will put an asterisk next to the oxygen atom. Repeat this for the nitrogen atom and for one of the ring carbons as shown below.

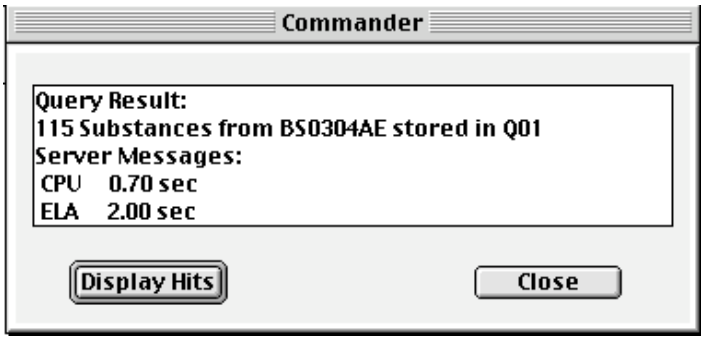


5. A “Free Site” means that anything can be attached to that atom. For other atoms, it is implied that there is a hydrogen attached

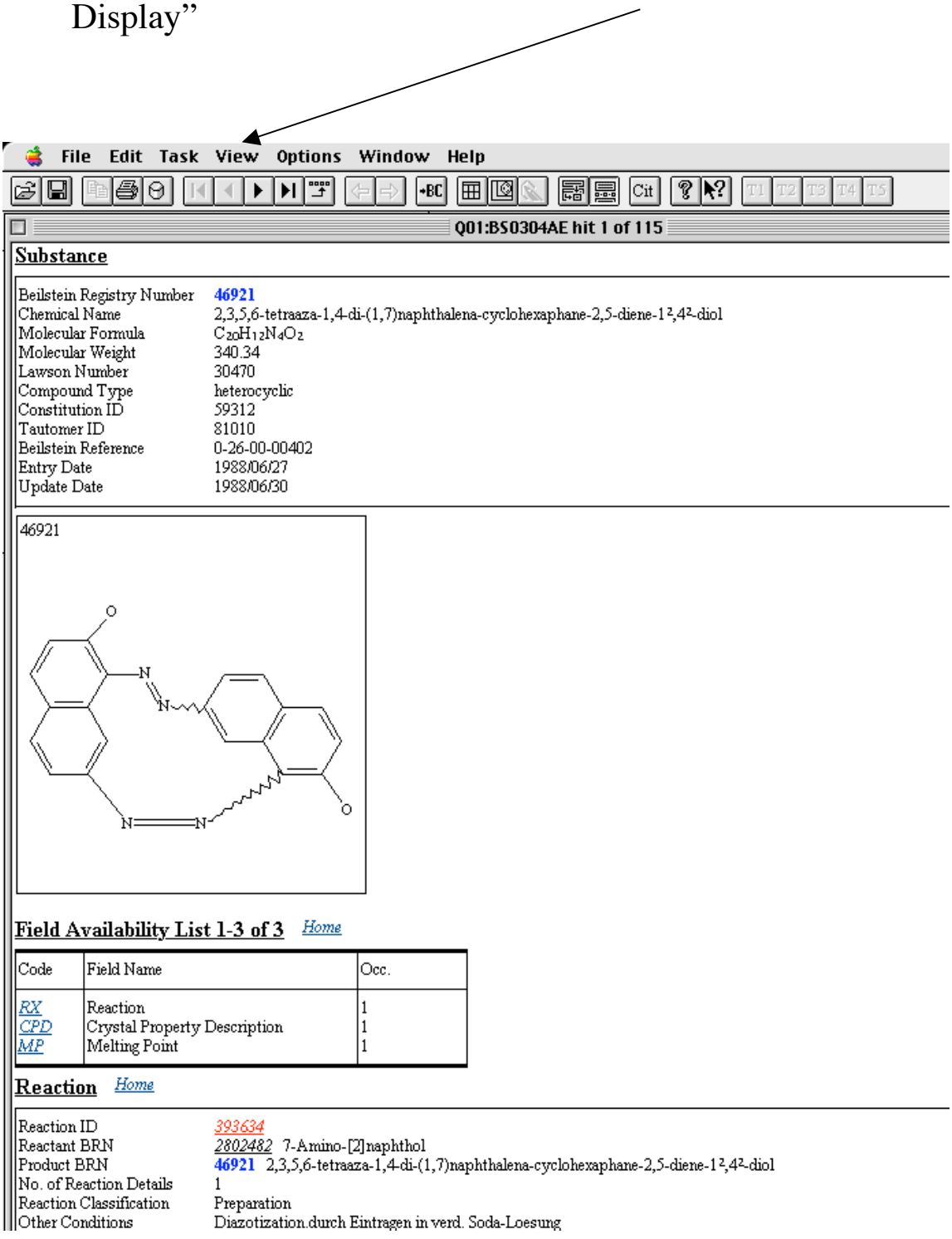
7. Now, return to the Commander window and start the search



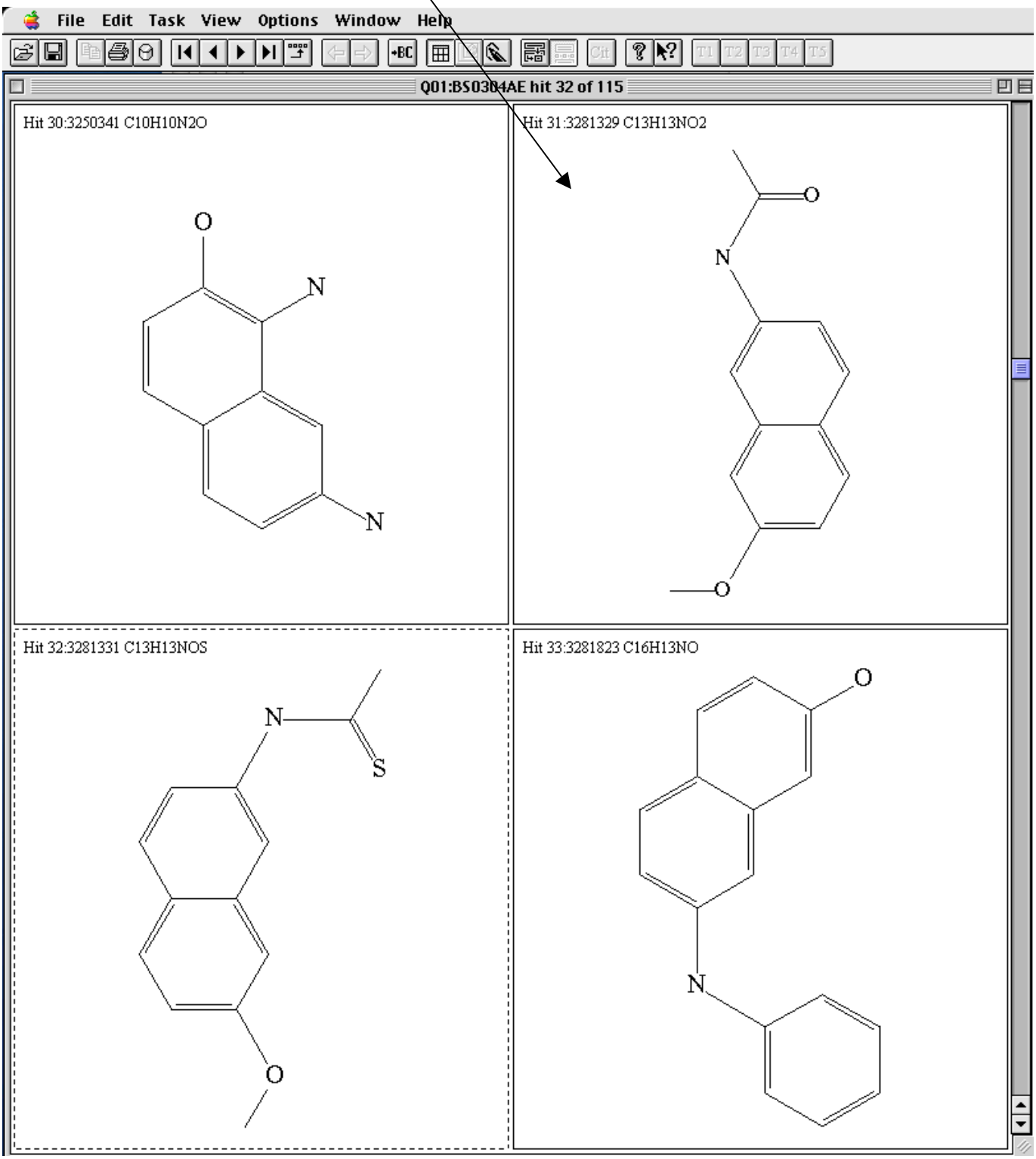
8. This produces 115 hits (as of Feb 27, 2004). Hit "Display Hits"



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"



9. From here, we get a pictoral 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.

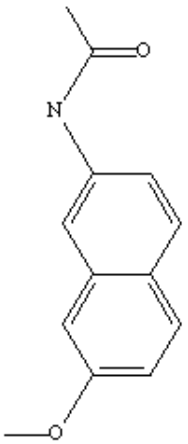
File Edit Task View Options Window Help

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
Autoname	*N* -(7-methoxy-naphthalen-2-yl)-acetamide
Molecular Formula	$C_{13}H_{13}NO_2$
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.
RX	Reaction	1
CPD	Crystal Property Description	1
MP	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