

Searching MMS...



... and accessing patent references

- Query modification
- Searching
- Accessing structure answers
- Accessing bibliographic answers

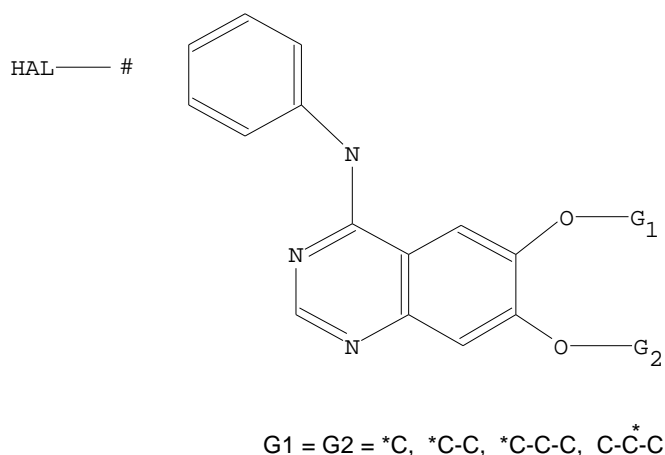
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- **Searching MMS and accessing patent references**

Query modification

Use of Superatoms, G Groups, Attachment Points and Variable Points of Attachment



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• Query modification

A somewhat more general query might be considered where different alkoxy groups are acceptable in place of the methoxy groups and any halogen is acceptable in place of the bromine, in any position on the benzene ring.

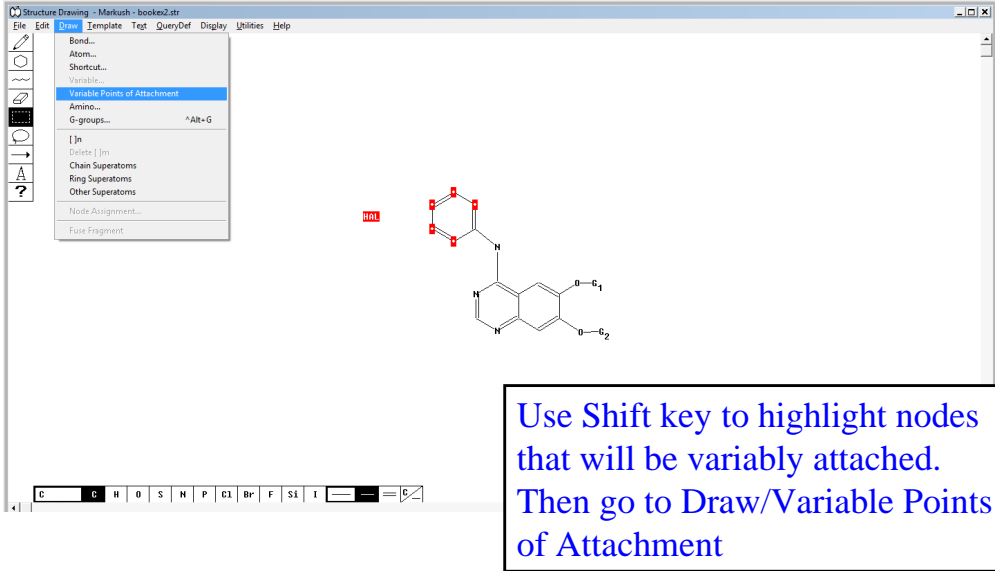
This query will have the following features:

- G groups are used to cover the variable values methyl, ethyl, propyl, isopropyl attached to the oxygen atoms.
- An HAL Superatom is used to express the "halogen" generic term and a NT attribute is applied on this Superatom to retrieve structures where specific values of halogen (e.g. chlorine, bromine, fluorine) have been indexed, and those where only the generic term halogen has been indexed.
- Variable points of attachment should be specified for the halogen Superatom.

Searching MMS



Revising Topfrag Query



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- Topfrag is opened and first query is recalled.
- Bromine is erased. A HAL superatom is drawn outside the ring.
- The Shift key is used to highlight the nodes that will be variably attached. Then go to the Draw drop down menu and Variable Points of Attachment.

Revising Topfrag Query

The screenshot shows the 'G-Group Definitions' dialog box with 'point of attachment' selected. The 'Multiple Use' button is highlighted. A chemical structure is shown with fragments labeled 'c', 'c', and 'c'. A callout box points to the fragment palette, which contains '* C', '* /', '* \', and '* /'.

Add fragments and points of attachment by going to Draw/G groups and highlighting "point of attachment", then clicking Multiple Use.

Add the points of attachment to the fragments

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- Add fragments to the palette. Add Broad Translation to the methyl fragment.
- Add points of attachment by going to Draw and G groups and highlighting "point of attachment", then clicking Multiple Use.
- Add the "point of attachment" to a node on each of the fragments.

Revising Topfrag Query

Go to Draw/G Groups, “New”, then click “Fragments” and select the fragments to be included. Be sure to check “Include Fragment” box.

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- After adding “points of attachment” to fragments, go back to Draw and G groups, click “New”, then click “Fragments”, and select the fragments to be included in that G group.
- Be sure to check the “Include Fragment” box.

Revising Topfrag Query

Go to “Save”, then “New” again, then “Copy G grps.” Select the G group to be copied, then click “OK” and “Save”.

New G-Group Definition

G1: [1]
[2]
[3]
[4]

Atoms Copy G-grps
Shortcuts Fragments
Variables Clear
Cancel Save

Select G-group(s) to be copied

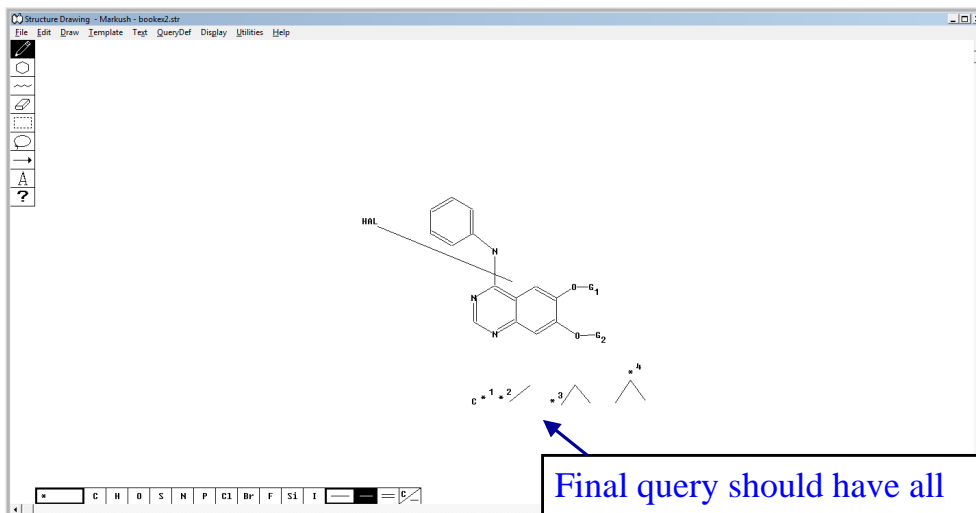
G1 G6 G11 G16
 G2 G7 G12 G17
 G3 G8 G13 G18
 G4 G9 G14 G19
 G5 G10 G15 G20

New Group Cancel OK

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- Save the G1 group.
- To copy G1 to G2, click “New”, then “Copy G Grps.”. Select the G group to be copied, then click OK and SAVE.

Revising Topfrag Query



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- Final query should have all fragments numbered.


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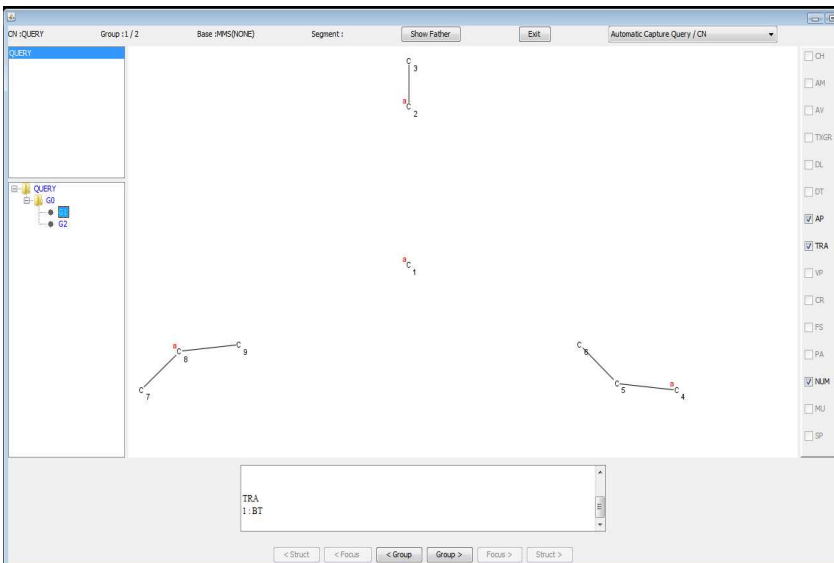
- **Query verification**

Use the **VE** command in MMS to view the query derived from Topfrag.

Query modification



Query verification



The screenshot shows a software window titled 'CN:QUERY' with a 'Group 1: / 2' indicator. The main area displays a chemical structure with atoms labeled C1 through C9. A list of chemical groups is visible on the right side, including CH, AM, AV, TGR, DL, DT, AP, TRA, VP, CR, FS, PA, NUM, MU, and SP. The 'AP' and 'TRA' groups are checked. At the bottom, there is a text box containing 'TRA 1:BT' and navigation buttons: '< Struct', '< Focus', '< Group', 'Group >', 'Focus >', and 'Struct >'.

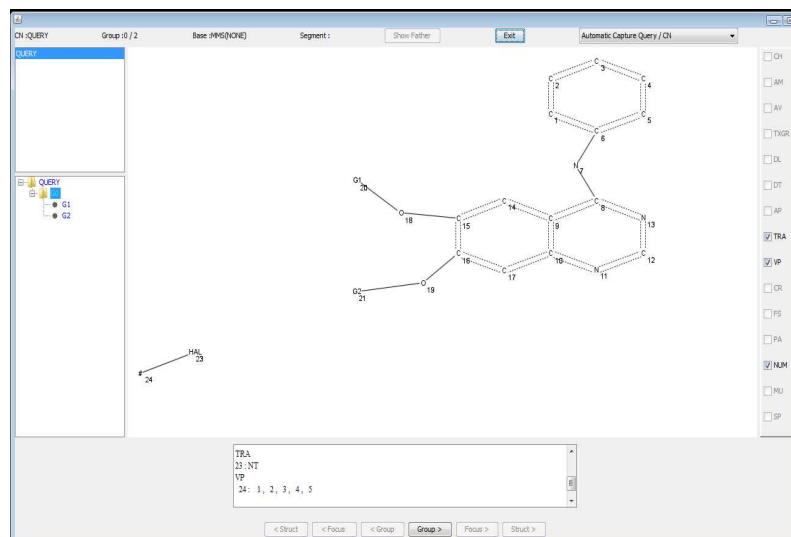
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- Query modification
 - Query verification

Query modification



Query verification



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- Query modification
- Query verification

Searching the modified query

```
- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ? FI  
Query validation in progress  
Query validated  
  
- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ? SEARCH FULL  
  
*** SB ***  
Bitscreen Search started  
  
* SEARCH IN PROGRESS *  
  
Bitscreen Search completed  
Result stored in R set : R03  
  
R03 - BS / MMS FRONTF MPHARM WPIM BACKF : 359030 answer(s)
```

- **Searching the modified query**

- **SEARCH FULL** will run the RE, then the complete AA search.

Searching the modified query

*** AA ***

```
Atom by Atom Search started on R set  R03
 16 answers(s) for  53509 candidates (no rx candidate(s) )
 17 answers(s) for  85659 candidates (no rx candidate(s) )
 26 answers(s) for 112995 candidates (no rx candidate(s) )
 37 answers(s) for 148791 candidates (no rx candidate(s) )
 45 answers(s) for 190040 candidates (no rx candidate(s) )
 55 answers(s) for 225589 candidates (no rx candidate(s) )
 62 answers(s) for 256228 candidates (no rx candidate(s) )
 68 answers(s) for 315587 candidates (no rx candidate(s) )
```

```
Removing duplicates
Atom by Atom Search completed on R set  R03
74 answer(s) stored in R set  R04
```

```
R04 - AA / R03      : 74 answer(s)
```

- **Searching the modified query**

- **AA search**

Answer sets are numbered automatically.

AA answers are stored in the **R04** answer set.

Searching the modified query

| First search | Second search |
|--------------|---------------|
| 34 answers | 74 answers |
| | |

- **Searching the modified query**

The first search contains the answers from Chapter 3. The second search contains the answers from the modified query.

Listing additional results

1) Direct Boolean operation

- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ?

4 not 2

*** BL ***

Boolean Search started : R04 not R02
 Boolean Search completed
 Result stored in R set : R05

| #. | Name | Search Database | answer(s) | RX | RX File |
|----|------|-----------------|-----------|----|---------|
| 5 | R05 | BOOL MMS | 40 | | |

R05 - BOOL / MMS : 40 answer(s)

R04: answer set / second query: 74 answers

R02: answer set / first query: 34 answers

R05: answers not in R02

All answers in R05 are the new answers, not retrieved in R02

- Accessing structure answers

- Listing additional results

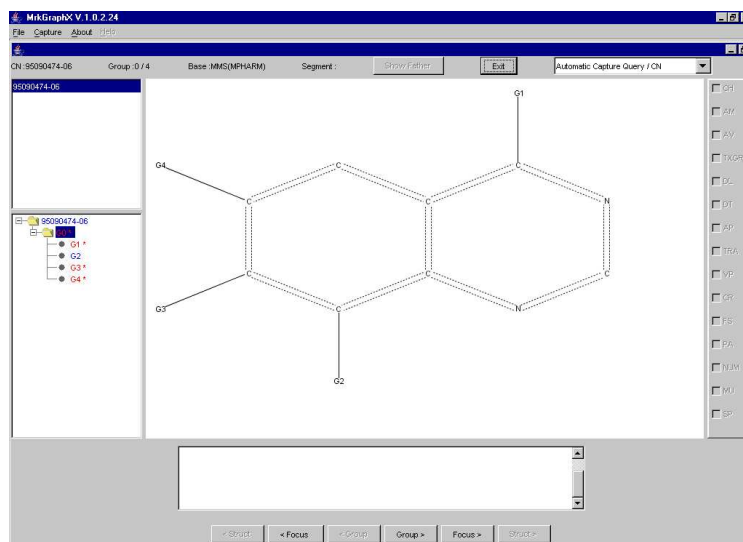
1) A Boolean operation can be performed directly at the ST level by using the answer set numbers in the logical operation. The 74 AA answers of the second search have been saved automatically in R04 and the 34 answers of the first search have been saved in R02. To obtain an answer set containing only the additional answers, we can exclude (NOT Boolean operator) the 34 answers obtained with the first query from the 74 answers obtained with the second query:
R36 NOT R34

The result - 40 answers - is placed in the next available answer set: R05.

2) The 40 additional answers of the second search can then be listed using the LI command: **LI 1-40**

Viewing additional results

-ST- (BA, CN, QT, QG, RF, RE, AA, SB, BL, BI, INFO)? VI FO R05 2



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- Accessing structure answers
 - Viewing additional results

The 40 answers can be displayed in View Focus using the VI FO command (the corresponding query is still active). The viewer is limited to ten structures answers at one time, so the command is VI FO 1-10.

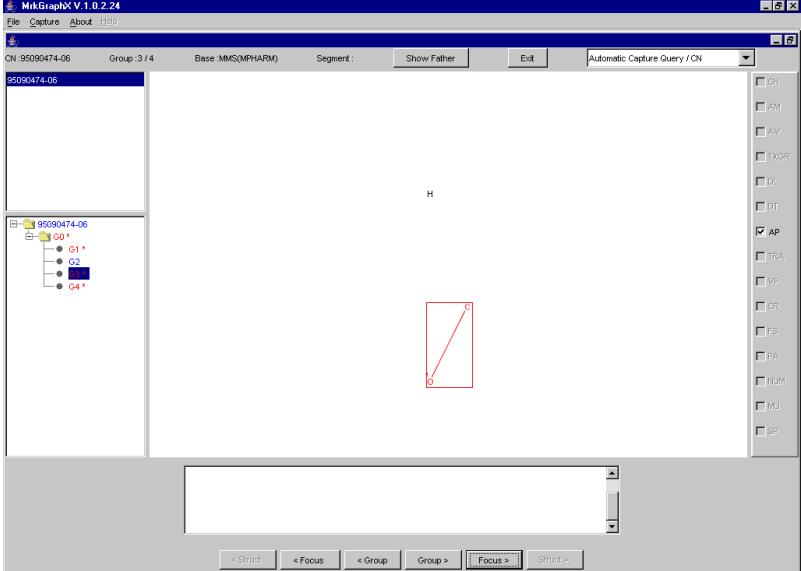
VI FO will display only the first CN. VI FO 2 will display the second answer, focusing on the parts of the molecule which allow the retrieval.

The main group (G0) is displayed first.

Searching MMS



Viewing additional results




The screenshot shows the MikGraph V.1.0.2.24 software interface. The window title is "MikGraph V.1.0.2.24". The menu bar includes "File", "Capture", "About", and "Help". The status bar shows "CN: 95090474-06", "Group: 3 / 4", "Base: MMS(MPHARM)", "Segment:", "Show Father", "Exit", and "Automatic Capture Query / CN". The main display area shows a chemical structure graph with a highlighted path (G0, G1, G2, G3, G4) and a red box highlighting a specific part of the structure. The left sidebar shows a tree view of the graph. The right sidebar shows a list of checkboxes for various categories: G1, AM, AY, FVGT, DL, DT, AP (checked), FRA, VP, GR, FS, PA, HUM, HU, and SP. The bottom of the window has navigation buttons: "< Struct", "< Focus", "< Group", "Group >", "Focus >", and "Struct >".

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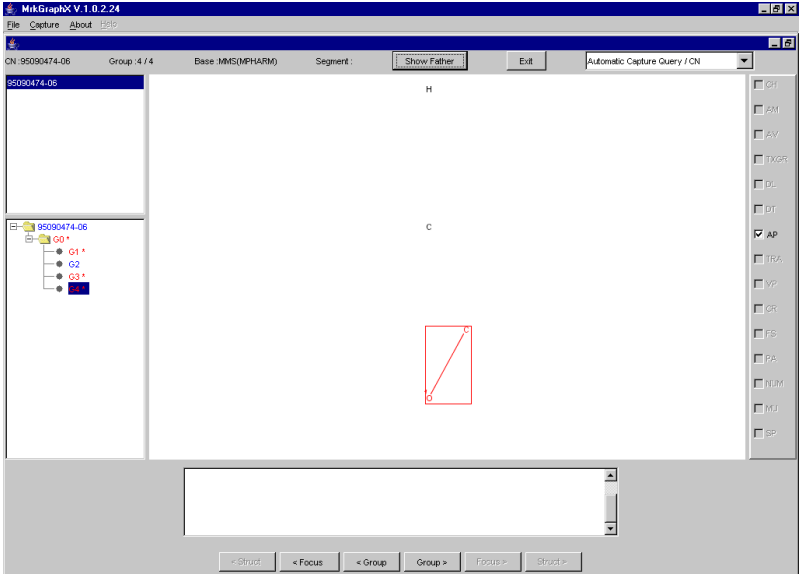
- **Accessing structure answers**
 - **Viewing additional results**

A click on the *Focus>* button displays the next group, G3, with focus on the methoxy group.

Searching MMS



Viewing additional results



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- **Accessing structure answers**
 - **Viewing additional results**

A click on the *Focus*> button displays the next group, G4, with focus on the methoxy group.

Saving answer sets

- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ? **SV CN R05**

Please, enter the name you want to assign to the saved set
(you can use a maximum of 15 characters) ?

bookex4

Saving in progress

.

The following set was saved successfully

| #. | Name | CN | Search | File | Date |
|----|---------|----|--------|------|------------|
| 13 | bookex4 | 74 | BOOL | MMS | 2011-01-19 |

- **Accessing patent references**

Step 1: Saving MMS answer set as a CN list.

Searching MMS



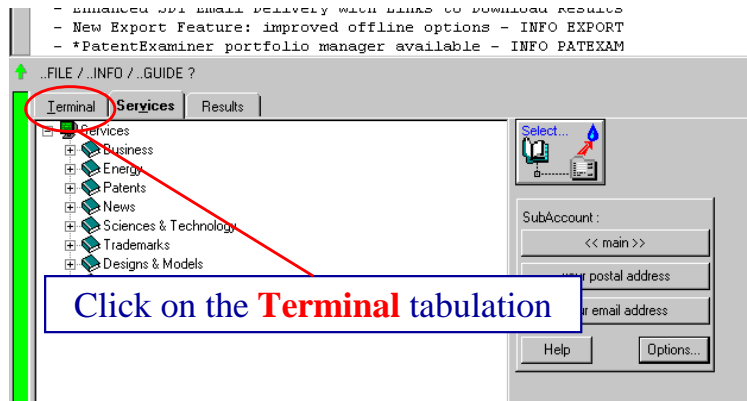
Switching to Questel

- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ? **..BI**

(C) QUESTEL 1994

QUESTEL.ORBIT (TM) 1998

02/01/07 17*34*51



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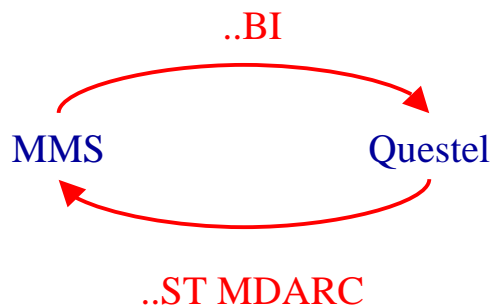
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• Accessing patent references

Step 2: Switch to the bibliographic files

Type **..BI** at the ST level to switch from MMS to the bibliographic files.

To move back to MMS, type **..ST MDARC**.



Note: In order not to be taken by default to the Result tab when running a search, click on **Settings** the **Questel.Orbit Parameters...** then untick *Show results panel when submitting search*.

Bibliographic processing

- 1- Select the bibliographic file PHARM
FILE PHARM
- 2- Process the Compound Number list in the PHARM file
***MD search1/CN**
- 3- Select the bibliographic file DWPI
FILE DWPI
- 2- Process the Compound Number list in the DWPI file
***MD search1/CN**

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- Accessing patent references
 - Bibliographic processing

Step 3: Selecting a bibliographic file: PHARM or DWPI: Type **FILE PHARM** or **FILE DWPI** after the question mark.

Step 4: Processing the Compound Number lists: Processing of CN's lists is performed with the ***MD** command. It is applied directly to the saved answer set. The 8 answers of the Boolean search have been saved using the file *search1*. To process this list of CN's in the bibliographic files, we type: ***MDARC search1/CN**

Viewing PHARM results

PHARM

```
QUESTEL      - Time in minutes :    0,60
The cost estimation below is based on Questel's
standard price list
Estimated cost :    0.82 USD
Cost estimated for the last database search :    0.82 USD
Estimated total session cost :    0.82 USD
```

Selected file: PHARM

Coverage: EP, US & FR patents and PCT applications from 1978 to 1999;
GB and DE patents from 1980 to 1999 and BSM full collection from 1961.
No further updates are planned for the PHARM database. This database
is useful in coordination with the Merged Markush Service (MMS).

1 - *MD BOOKE4/CN - 5

** SS 1: Results 5

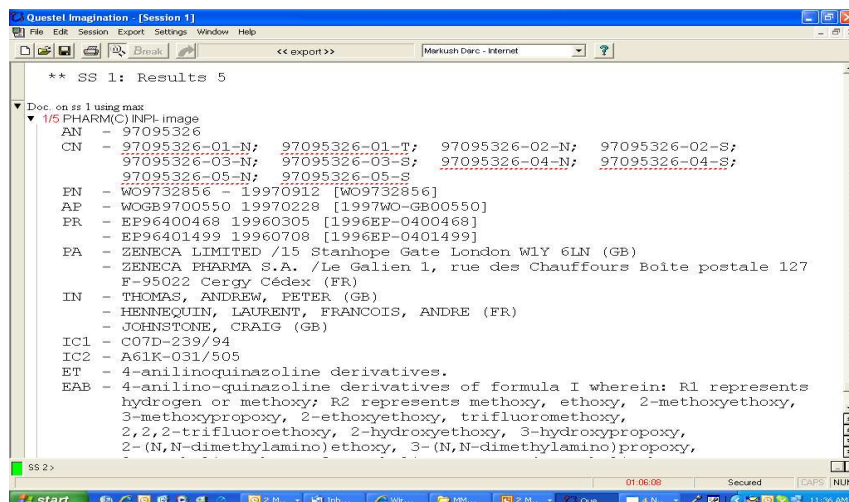
- Accessing patent references
 - Viewing the results in PHARM

The processing of the *search1* list in PHARM gives 5 results.

Keep in mind that in PHARM there are not only pharmaceutical patents but also general chemistry patents.

Viewing PHARM results

Type **PRT MAX 1-5**



```

Questel Imagination - [Session 1]
File Edit Session Export Settings Window Help
<< export >> Markush Desc - Internet

** SS 1: Results 5

Doc. on ss 1 using max
▼ 1/5 (PHARMC) INPL-image
AN - 97095326
CN - 97095326-01-N; 97095326-01-T; 97095326-02-N; 97095326-02-S;
97095326-03-N; 97095326-03-S; 97095326-04-N; 97095326-04-S;
97095326-05-N; 97095326-05-S
EN - WO9732856 - 19970912 [WO9732856]
AP - WOG9700550 19970228 [1997WO-GB00550]
PR - EP96400468 19960305 [1996EP-0400468]
EP - EP96401499 19960708 [1996EP-0401499]
PA - ZENECA LIMITED /15 Stanhope Gate London W1Y 6LN (GB)
- ZENECA PHARMA S.A. /Le Galien 1, rue des Chauffours Boite postale 127
F-95022 Cergy Cédex (FR)
IN - THOMAS, ANDREW, PETER (GB)
- HENNEQUIN, LAURENT, FRANCOIS, ANDRE (FR)
- JOHNSTONE, CRAIG (GB)
IC1 - C07D-239/94
IC2 - A61K-031/505
ET - 4-anilinoquinazoline derivatives.
EAB - 4-anilinoquinazoline derivatives of formula I wherein: R1 represents
hydrogen or methoxy; R2 represents methoxy, ethoxy, 2-methoxyethoxy,
3-methoxypropoxy, 2-ethoxyethoxy, trifluoromethoxy,
2,2,2-trifluoroethoxy, 2-hydroxyethoxy, 3-hydroxypropoxy,
2-(N,N-dimethylamino)ethoxy, 3-(N,N-dimethylamino)propoxy,

```

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- Accessing patent references
 - Viewing the results in PHARM

The MAX format can be used with the PRT or LI command in PHARM. This slide shows part of the MAX record for the first answer. The HIT CN terms are underlined in red.

Viewing DWPI results

Type:

FILE DWPI

then

***MD search1/CN**

then

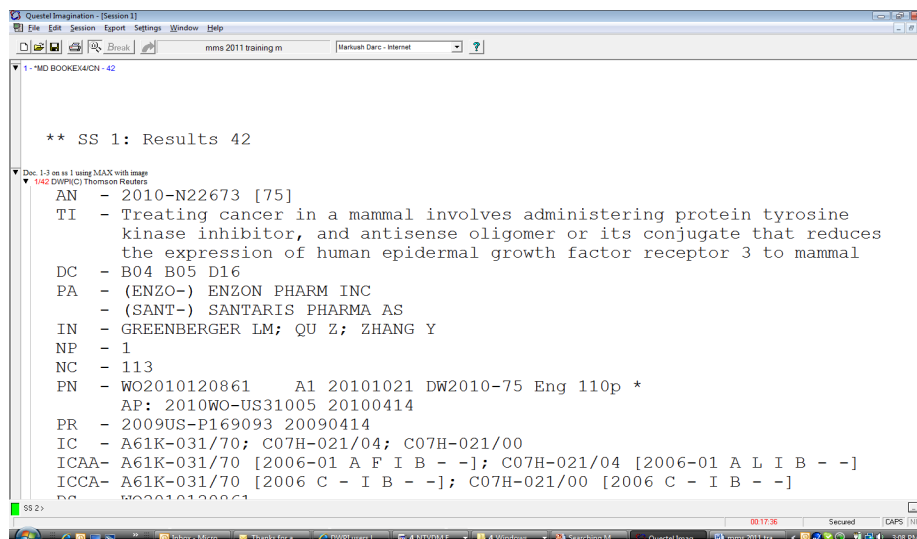
PRT MMSF IMG SET

- **Accessing patent references**
 - **Viewing the results in DWPI**

The MMSF IMG display will display the full bibliographic record with abstract, front page image, and CN field. This differs from the “Full Document with Image” – that format displays all of the DWPI chemical codes (manual, polymer, etc.)

SET will display the entire set of records.

Viewing DWPI results



```
Questel Imagination - [Session 1]
File Edit Session Export Settings Window Help
mms 2011 training m Markush Darc - Internet

1--MO BOOKE4/CN - 42

** SS 1: Results 42

Doc: 1.3 on as 1 using MAX with image
1442 DWPI(C) Thomson Reuters
AN - 2010-N22673 [75]
TI - Treating cancer in a mammal involves administering protein tyrosine
kinase inhibitor, and antisense oligomer or its conjugate that reduces
the expression of human epidermal growth factor receptor 3 to mammal
DC - B04 B05 D16
PA - (ENZO-) ENZO PHARM INC
(SANT-) SANTARIS PHARMA AS
IN - GREENBERGER LM; QU Z; ZHANG Y
NP - 1
NC - 113
PN - WO2010120861 A1 20101021 DW2010-75 Eng 110p *
AP: 2010WO-US31005 20100414
PR - 2009US-P169093 20090414
IC - A61K-031/70; C07H-021/04; C07H-021/00
ICAA- A61K-031/70 [2006-01 A F I B - -]; C07H-021/04 [2006-01 A L I B - -]
ICCA- A61K-031/70 [2006 C - I B - -]; C07H-021/00 [2006 C - I B - -]
PC - WO2010120861
```

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- Accessing patent references
 - Viewing results in DWPI

This slide shows part of the first answer in the MAX format. There is no front-page image in this record.

SUMMARY STEPS FOR TRANSFERRING RESULTS FROM MMS TO Questel

Procedure

1. Type **..BI** to enter Questel Orbit bibliographic files or **FI** to end MMS session and log onto QWEB.
2. Type **FILE PHARM** to enter PHARM database.
3. Type ***MD <name1> /CN** to search your MMS compound numbers saved set (name1) in PHARM
4. Type **PRT MAX IMG SET** to view records with images.
5. Type **MEM <name2> /XPN** to extract standard publication numbers to a named MEM list.

SUMMARY STEPS FOR TRANSFERRING RESULTS FROM MMS TO Questel

Procedure

6. Type **FILE DWPI** to enter Derwent World Patent Index
7. Type ***MD <name1> /CN** to search your MMS compound numbers saved set in the DWPI.
8. Type ***MEM <name2> /XPN** to transfer and search the standard publication numbers retrieved from the PHARM database
9. Combine search sets numbers from the *MD and *MEM sets; e.g.,
1 OR 2
10. Type **PRT MMSF IMG SET** to combine and display all records in DWPI format (back to 1963).