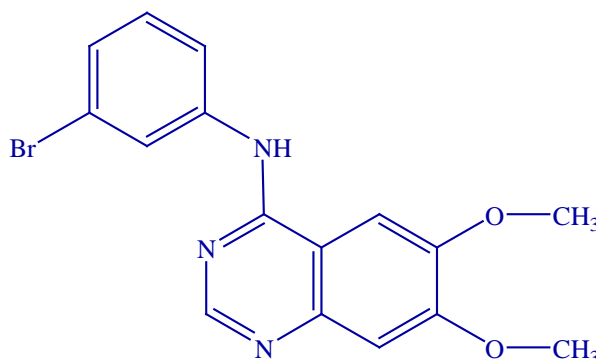


- Query input: Markush TOPFRAG
- Searching
- Accessing structure answers

- **Searching MMS**

- The question



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III - 2

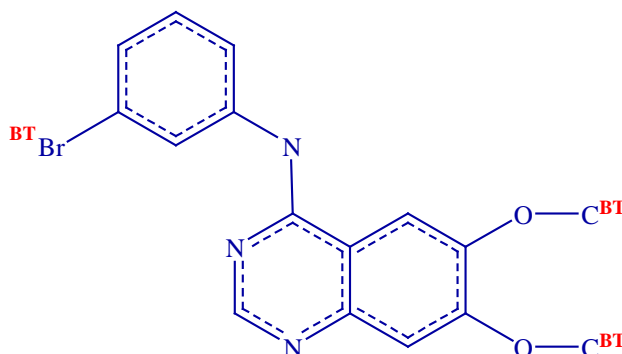
- **Query input: MTF**

- **Query formulation**

A bibliographic reference cites the compound shown on this slide, PD 153035, which specifically inhibits epidermal growth factor (EGF) receptor. This compound has 10,000 to 100,000 times the potency of other tyrosine kinase inhibitors.

This news item might suggest areas of interest for which a search might be performed: a search for patents which cite this specific compound.

- Converting question to query



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- **Query input: MTF**

- **Query formulation**

– **Converting the question to a query**

In order not to miss those documents which also cited only generic representations (HAL instead of Br and alkoxy instead of methoxy), Broad Translation (BT) is used on those atoms.

Query input

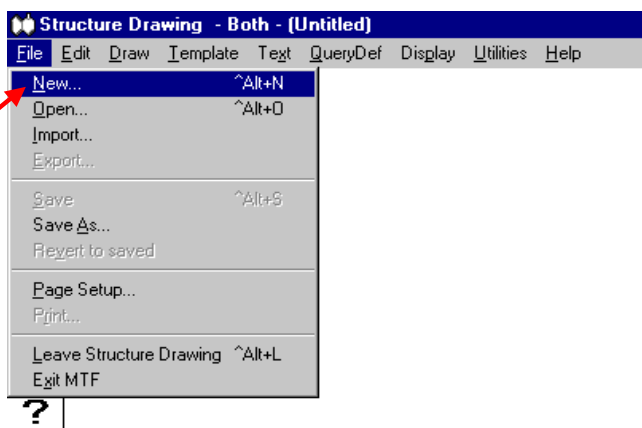


Using Markush TOPFRAG

1- Run *Markush TOPFRAG*

2- Click on the *Structure drawing* window

3- Select *New...* from the *File* menu




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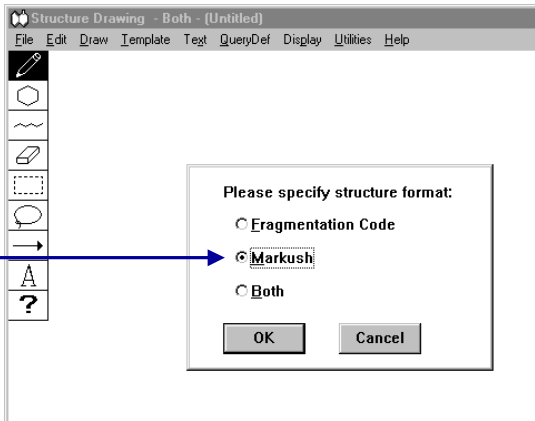
3 - 4

- Query input: MTF
 - Query formulation
 - Using Markush TOPFRAG

Query input



Using Markush TOPFRAG



Choose *Markush* in order to generate a strategy for searching MMS

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- Query input: MTF
 - Query formulation
 - Using Markush TOPFRAG

Structure drawing

The program will ask whether you draw for Markush DARC, the Fragmentation Code or both. Select the *Markush* option and click on the *OK* button.

Query input

Using Markush TOPFRAG

Recall the benzene ring
then the naphthalene ring
from the *Template* menu

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- **Query input: MTf**
 - **Query formulation**
 - **Using Markush TOPFRAG**

Structure drawing

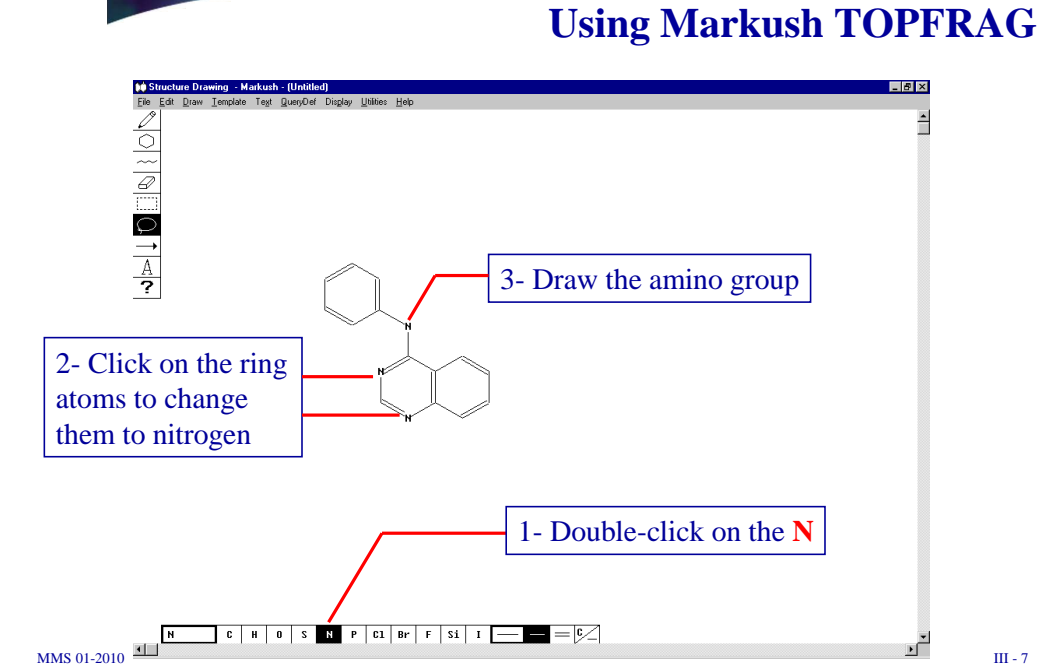
A benzene ring and a naphthalene ring can be recalled from the *Template* menu: click on the *Template* menu heading and click on *Display* to see a list of the available templates. The template required is called *01 aromat*. Double-click on this and a screen with various aromatic rings is displayed. Click on one atom or bond of the benzene ring and the cursor changes to a double arrow. Click somewhere on the screen to place the benzene ring.

A naphthalene ring can be placed close to the benzene ring in the same way.

Query input



Using Markush TOPFRAG



The screenshot shows the Markush TOPFRAG software interface. At the top, there is a menu bar with options: File, Edit, Draw, Template, Text, QueryDef, Display, Utilities, Help. Below the menu is a toolbar with various drawing tools. The main workspace displays a chemical structure consisting of a naphthalene ring system with two nitrogen atoms at the 1 and 8 positions, and an amino group (-NH₂) attached to the 2-position. Three callout boxes with red lines pointing to specific parts of the structure provide instructions:

- 1- Double-click on the **N** (pointing to the nitrogen atom in the naphthalene ring)
- 2- Click on the ring atoms to change them to nitrogen (pointing to the two ring nitrogen atoms)
- 3- Draw the amino group (pointing to the amino group)


 At the bottom of the interface is a 'Common Atoms palette' with buttons for H, C, H, O, S, **N**, P, Cl, Br, F, Si, I, and a bond type selector. The 'N' button is highlighted. The bottom left corner of the window shows 'MMS 01-2010' and the bottom right corner shows 'III - 7'.

- **Query input: MTf**
 - **Query formulation**
 - **Using Markush TOPFRAG**

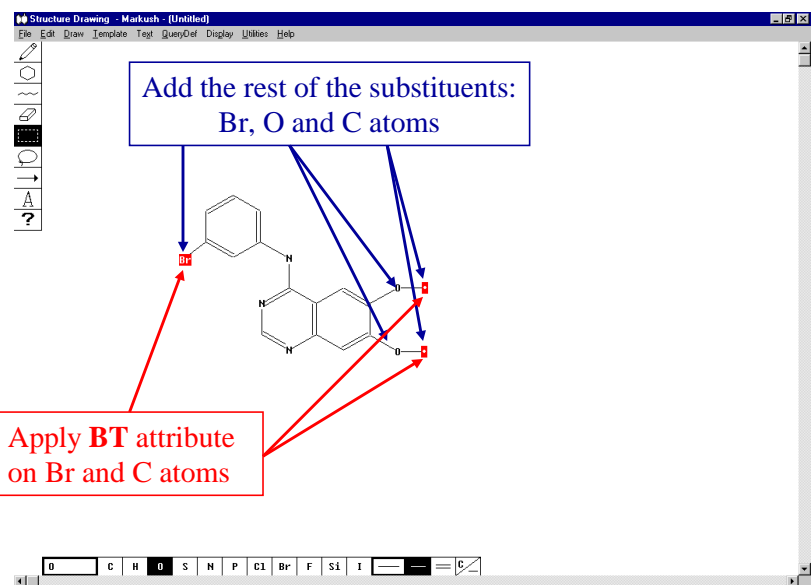
Structure drawing

- 1- Modify two of the naphthalene ring atoms to nitrogen: change the current atom to nitrogen by double-clicking on the **N** in the *Common Atoms palette*.
- 2- Click on the ring atoms to change them to nitrogen.
- 3- Draw the amino group: point to the benzene ring atom using the pencil cursor, and hold down the mouse button. With the mouse still held down, drag the cursor away from the ring atom. When it is positioned where you want the amino group, release the mouse button.

Query input



Using Markush TOPFRAG



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III - 8

- **Query input: MTF**
 - **Query formulation**
 - **Using Markush TOPFRAG**

Structure drawing

Add the rest of the substituents:


Click on the **Br** symbol in the *Common Atoms palette* to change the current atom to Br, point to the meta position of the benzene ring and drag the mouse to attach a bromine atom.

Double-click on the **O** symbol in the *Common Atoms palette* to change the current atom to O, point to the 6- position of the quinazoline ring and drag the mouse to attach an oxygen atom, then point to the 7-position and drag the mouse to attach a second oxygen atom.

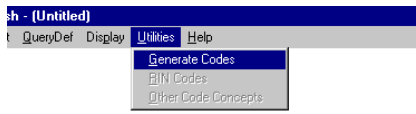
Click on the **C** symbol in the *Common Atoms palette* to change the current atom to C, point to one of the oxygen atom and drag the mouse to attach a carbon atom. Point then to the second oxygen atom and drag the mouse to attach a carbon atom.

Broad Translation attributes are applied on the two methyl groups and on the bromine atom by first selecting the atoms using the box-shaped selection tool and clicking on the required nodes while holding down the *Shift* key, then selecting the BT attribute (choose *Translation Level* from the *QueryDef* menu and select *BT*).


Query input

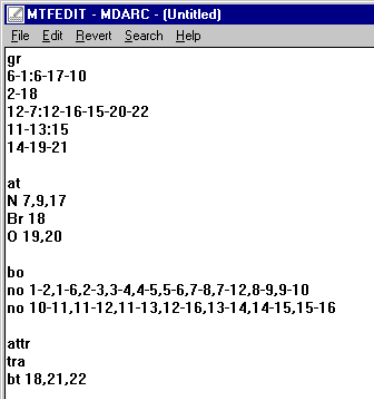


Generate strategy



Select *Generate Codes* under the *Utilities* menu





```

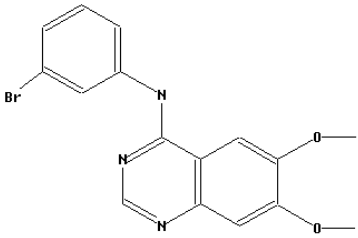
gr
6-1:6-17-10
2-18
12-7:12-16-15-20-22
11-13:15
14-19-21

at
N 7,9,17
Br 18
O 19,20

bo
no 1-2,1-6,2-3,3-4,4-5,5-6,7-8,7-12,8-9,9-10
no 10-11,11-12,11-13,12-16,13-14,14-15,15-16

attr
tra
bt 18,21,22

```



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- **Query input: MTF**

- **Generate strategy**

When the query is complete, select the *Generate Codes* command from the *Utilities* menu. The program will look for tautomeric bonds and make any changes necessary to the structure to comply with the Markush DARC drawing conventions. Alternating single and double bonds in the benzene and quinazoline rings will be normalised.

The strategy is displayed in the *MTFEDIT* window.

The strategy file can be edited, using the *Cut* or *Copy* functions from the *Edit* menu.

The strategy can be saved after editing.

Upload the strategy

- Logon to MMS
- Type QT (Query Text)
 - ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ? **QT**
- Upload strategy: by copy/paste in the Imagination command window
- Verify query
 - QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ? **VE**

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• Query input

• Upload the strategy

– First logon to MMS. You will see the -ST- prompt:

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

– Type **QT** (Query Text) at the ST level:


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

– Upload the strategy generated from Markush TOPFRAG drawing: paste the text file which has been copied in the *MTFEDIT* window.

– Verify the query: type **VE** at the QT level.

- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ? **VE**

Query input



Upload the strategy

MTFEDIT - MDARC - (Untitled)

File Edit Revert Search Help

```

gr
6-1:6-17-10
2-18
12-7:12-16-15-20-22
11-13:15
14-19-21

at
N 7,9,17
Br 18
O 19,20

bo
no 1-2,1-6,2-3,3-4,4-5,5-6,7-8,7-12,8-9,9-10
no 10-11,11-12,11-13,12-16,13-14,14-15,15-16

attr
tra
bt 18,21,22
          
```

COPY

➔

```

*** QT ***
Previous valid input (Answer No to draw a new query) ? ( Y/N )
?
N
- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ?
X - QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ?
          
```

```

attr
tra
bt 18,21,22
          
```

.... PASTE

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- **Query input**

- **Upload the strategy**

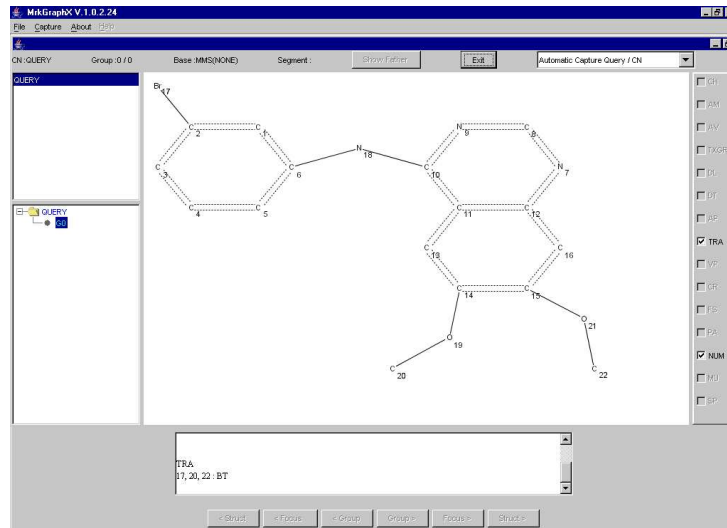
Upload the strategy generated from Markush TOPFRAG drawing: paste the text file which has been copied in the *MTFEDIT* window.

Query input



Query verification

- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ? **VE**



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- Query input

- Verify query

Type **VE** at the QT level.

- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ? **VE**

Query input



Finish 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) ?
```

- **Query input**

- **Finish query**

Type **FI** at the QT level

```
- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ? FI
```

The search can then be launched.

Two steps

Fragment Search

RE - Retrieve candidates (RE is currently defaulting to the SB search)

or

SB - Bit-Screen search

Then

AA - Atom-by-Atom

SEARCH FULL runs the **RE** and **AA** search automatically

• Searching MMS

The search in MMS takes place in two steps:

- The RE or SB
- The AA.

The RE process

```

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

*** RE ***
File Segment restriction :
NONE
RE search started
* SEARCH IN PROGRESS *
*** SB ***

Bitscreen Search started
* SEARCH IN PROGRESS *
Bitscreen Search completed
Result stored in R set : R33
R33 - BS / MMS FRONTF MPHARM WPIM BACKF : 276215 answer(s)
    
```

Automatic answer set numbering:
up to 90 answer sets kept for the current week

Up to 1,000,000 candidates

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• Searching MMS

• The RE process

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

The RE search is fragment (or FREL) based screening step to eliminate those candidates that are not at least similar to the target compound.

Fragments are generated by the system "looking" at an atom and its' neighbors and constructing fragments in this way. So long as an atom is connected by a defined bond to at least one neighbor, fragments can be generated and compared with those stored in the database. The rarest fragments (i.e. those with the least number of "postings") are compared first, to eliminate as many candidates as possible in the first step.

After the RE search is completed, an automatic Bit Screen search is carried out, where bits are set according to type and number of atoms and bonds present.

The process is carried out successively on the four segments of the MMS database.

The results of the RE search are saved automatically in the R33 answer set (in our example), which is numbered automatically. It contains 276215 answers.

Up to 1,000,000 candidates can be processed on the whole MMS file (4 segments).

The AA process

```

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

Atom by Atom Search started on R set R33
  8 answer(s) for 67661 candidates (no rx candidate(s) )
 12 answer(s) for 126821 candidates (no rx candidate(s) )
 19 answer(s) for 187670 candidates (no rx candidate(s) )
 29 answer(s) for 241830 candidates (no rx candidate(s) )

Removing duplicates
Atom by Atom Search completed on R set R33
- 32 answer(s) stored in R set R34
R34 - AA / R33 : 32 answer(s)
    
```

Automatic answer set numbering

```

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

• Searching MMS

• The AA process

```

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

In this second step of the search, an Atom-by-Atom search is performed on the results from the RE search.

The AA search requires that all elements in the query be in the answer and that the elements have the same relationship as defined in the query.

The AA search is carried out successively on lists of candidates and progression can be followed on the screen.

```

  8 answer(s) for 57551 candidates (no rx candidate(s) )
 12 answer(s) for 125821 candidates (no rx candidate(s) )
  ...
    
```

When the search is finished, the answers are automatically saved in the next available answer set: R34 in this case.

A total of 90 answer sets are available. Each of the answer sets remains available for the current week.

For this search, the CPU time limit authorized for processing one compound has not been reached and the RX file is empty.

The AA process

```
- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ? AA
*** AA ***
Atom by Atom Search started on R set R28

    29 answer(s) for 11830 candidates (no rx candidate(s) )
   106 answer(s) for 18900 candidates (no rx candidate(s) )
   191 answer(s) for 27037 candidates (no rx candidate(s) )
   273 answer(s) for 35893 candidates (no rx candidate(s) )
   392 answer(s) for 45623 candidates (no rx candidate(s) )

Removing duplicates
So far,
- 434      answer(s)   are obtained
- 1        candidates  could not be processed (RX candidates)
- 10860    candidates  remain to be processed

Please type :
- A        to carry on the Atom by Atom search on-line
- B        to request a Batch processing of this complete R set R28
- P        to request a Power-Batch processing of this complete R set R28
- C        to cancel the search
? A
```

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• Searching MMS

• The AA process

In most cases, the AA processes until completion without any interruption. When for some reason - higher number of candidates, difficult query - the AA takes longer, it is interrupted after a predefined elapsed time.

At that stage, you can settle one of the following options:

- Cancel the search (type **C**)
- Resume AA and have it go until completion (type **A**)
- Request a delayed AA processing using more CPU resources (the so-called Batch options, type **B** or **P**)

The AA process

```
Atom by Atom search continuing on-line
      503 answer(s) for 62949 candidates (      1 rx candidate(s) )

Atom by Atom Search completed on R set R28
- 509 answers stored in R set R29
- 1 RX candidates stored in RXR29
#. Name Search Database      answer(s)      RX      RX File
29 R29 AA      R28              509      1      RXR29

This AA search let some RX candidates.
Please type :
- B      to request a Batch processing of these RX candidates
- P      to request a Power-Batch processing of these RX candidates
- C      to move to the ST level without requesting any further processing
? C

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

Please note: this step usually requires synchronization. Double click on the red bar.

• Searching MMS

• The AA process

The AA on this slide let some RX candidates. RX candidates are candidates which the system can not process on-line (because they require a processing time higher than the limit allotted for on-line processing).

In such a case, the system offers you the possibility to process RX candidates using the Batch or Power-Batch capability, which have higher limits for the processing time.


Accessing structure answers

- LI
- VI Focus (VI FO)
- VI

- **Accessing structure answers**

3 commands are available to list or display the structure answers.

Listing answers



```
- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ? LI 1-22
1      CN = 93100262-01
2      CN = 92110697-01
3      CN = 94070160-03
4      CN = 95060702-01
5      CN = 96125323-01
6      CN = 97085530-01
7      CN = 97085530-03
8      CN = 8931-64502
9      CN = 9530-90201
10     CN = 9740-27001
11     CN = 0011-05401
12     CN = 0014-51201
13     CN = 0035-61501
14     CN = 0054-43201
15     CN = 0055-44901
16     CN = 0066-57602
17     CN = 0069-32406
18     CN = 0086-05301
19     CN = 0120-07201
20     CN = 0124-20801
21     CN = 0124-36403
22     CN = 0126-55901
?
```

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

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- **Accessing structure answers**

- **Listing answers**

- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ? LI 1-22

The Compound Numbers identifying the structure answers are listed.

The first 7 CN's of the list identify structures of the MPHARM/BackFile segment, produced by INPI, while the following CN's identify structures of the WPIM/FrontFile segment, produced by Thomson Scientific.

Viewing results

VI FO

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

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III - 21

- Accessing structure answers

- Viewing results

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

The **VI FO** command allows automatic display of the portions of the structure which match the query. The groups containing the portions of the structure which caused the retrieval can be displayed one after the other using the **Focus >** button. For each group displayed, the first value of the group which caused the retrieval is highlighted.

Typing VI FO will display the first answer.

Viewing results



VI FO

The screenshot shows the MikGraph V1.0.2.24 software interface. On the left is a tree view of groups (G1 to G26) under the project '9740-27001'. The main window displays a chemical structure of a pyridine ring with several substituents labeled G1 through G8. A callout box with a red arrow points to group G1 in the tree view, containing the text: "Directly click on the G group you want to display...". Another callout box with a red arrow points to the 'Focus' button in the bottom navigation bar, containing the text: "... or use the navigation bar". The bottom navigation bar includes buttons for '< Struct', '< Focus', '< Group', 'Group >', 'Focus >', and 'Struct >'. The top right of the window shows a menu with 'Exit' and 'Automatic Capture Query / CN'.

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- Accessing structure answers
- Viewing results

Viewing results



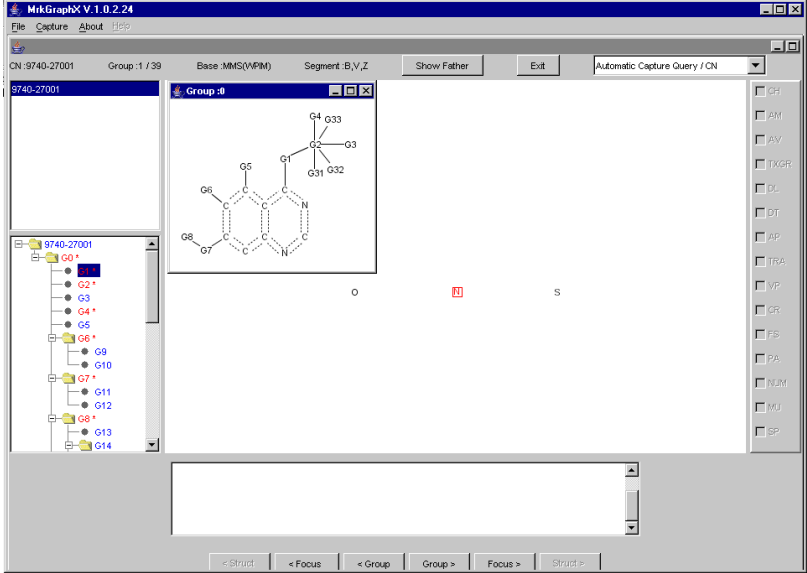
VI FO



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

The next group causing the retrieval is displayed: group G1.




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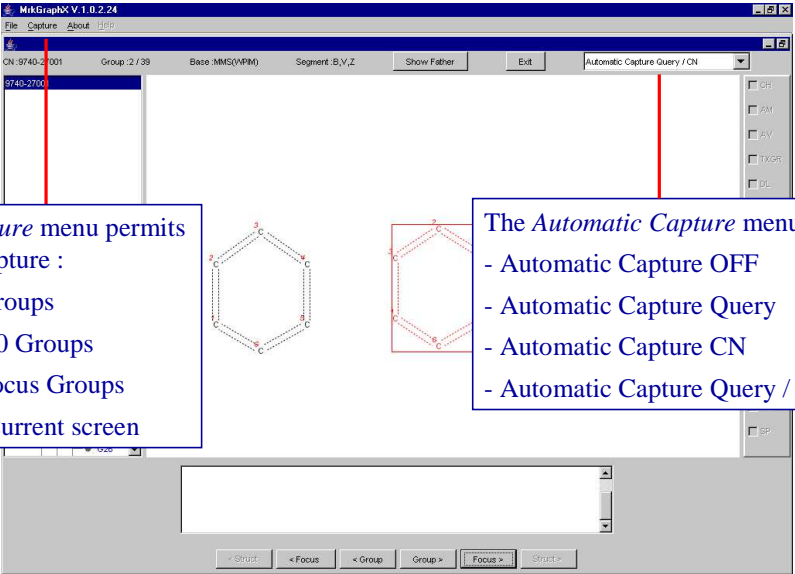
III - 24

- Accessing structure answers
 - Viewing results

Viewing results



VI FO



The *Capture* menu permits you to capture :

- All Groups
- All G0 Groups
- All Focus Groups
- The Current screen

The *Automatic Capture* menu:

- Automatic Capture OFF
- Automatic Capture Query
- Automatic Capture CN
- Automatic Capture Query / CN

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

The next group causing the retrieval is displayed: group G2.

Saving Results



SV CN

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

```
sv cn chap3ex
```

```
Saving in progress
```

```
The following set was saved successfully
```

| #. | Name | CN Search File | Date |
|----|---------|----------------|------------|
| 9 | chap3ex | 32 AA R34 | 2009-01-15 |

To save your answer set, use SV CN and give your set a name. Saved CN lists can be transferred to the bibliographic databases PHARM and DWPI.

Transfer to Questel



..BI

- 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

- ENHANCED PDF EMAIL DELIVERY WITH LINKS TO DOWNLOAD RESULTS
- New Export Feature: improved offline options - INFO EXPORT
- *PatentExaminer portfolio manager available - INFO PATEXAM

↑ ..FILE / ..INFO / ..GUIDE ?

Terminal Services Results

- Services
 - Business
 - Energy
 - Patents
 - News
 - Sciences & Technology
 - Trademarks
 - Designs & Models
 - Domain names
 - Training Databases

Select...

SubAccount :

<< main >>

your postal address

your email address

Help Options...

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Bibliographic processing

- 1- Select the bibliographic file PHARM
FILE PHARM
- 2- Process the Compound Number list in the PHARM file
***MD chap3ex/CN**
- 3- Select the bibliographic file DWPI
FILE DWPI
- 2- Process the Compound Number list in the DWPI file
***MDARCLIST chap3ex/CN**

Recalling saved CN lists in PHARM



***MD**

..FILE / ..INFO / ..GUIDE

file pharm

QUESTEL - Time in minutes : 0,69
The cost estimation below is based on Questel's
standard price list

| | |
|---|----------|
| Estimated cost : | 0.86 USD |
| Cost estimated for the last database search : | 0.86 USD |
| Estimated total session cost : | 0.86 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).

Search statement 1

***md chap3ex/cn**

** SS 1: Results 6

*Use **FILE PHARM**
to enter **PHARM**
database.*

*Use ***MD** in Pharm to recall an
MMS saved CN list. Qualify the
list to the CN field.*

PRT

prt mmsf img 2

2/6 PHARM - (C) INPI- image

CPIM N/A

AN - 96125323

CN - 96125323-01-N; 96125323-01-K; 96125323-01-T

PN - WO9639145 - 19961212 [WO9639145]

AP - WOUS9609606 19960606 [1996WO-US09606]

PR - US46914795 19950606 [1995US-0469147]

PA - RHONE-POULENC RORER PHARMACEUTICALS INC. /P.O. Box 5093 Collegevi

PA 19426-0997 (US)

IN - MYERS, MICHAEL, R. (US)

- SPADA, ALFRED, P. (US)

- MAGUIRE, MARTIN, P. (US)

- PERSONS, PAUL, E. (US)

IC1 - A61K-031/535

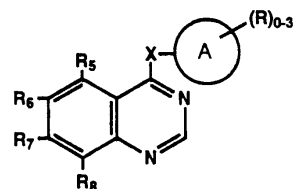
IC2 - A61K-031/495; A61K-031/50; A61K-031/505

ET - Protein tyrosine kinase aryl and heteroaryl quinazoline compounds having selective inhibition of HER-2 autophosphorylation properties

EAB - Use of quinazoline derivatives of formula (1) wherein A is mono- or bi-cyclic aryl, heteroaryl, cycloalkyl or heterocycloalkyl, X is a bond, O, S, SO, SO₂, OCH₂, CR₄=CR₄, C C, NR₄ or NR₄CH₂, R independently includes hydrogen, alkyl, phenyl, halophenyl, aralkyl, hydroxy, alkoxy, aryloxy, acyloxy, halo, haloalkyl, amino, alkylamino, dialkylamino, acylamino, carboxy, amido, alkylamido, dialkylamido, alkylthio, alkylsulfanyl and alkylsulfonyl, R₄ is hydrogen, alkyl or aralkyl, and R₅, R₆, R₇ and R₈ are hydrogen, alkoxy or aralkoxy, as inhibitors of HER2 (human epidermal growth factor receptor type 2) and thus for the selective treatment of cell growth and differentiation.

Some of said compounds are novel. Process of preparation thereof.

FT - Composés de quinazoline aryle et hétéroaryle avec protéine-tyrosine-kinase ayant des capacités d'inhibition sélective des propriétés d'autophosphorylation de HER-2.....



PRT MMSF IMG

will display the full record with the front-page image.

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Viewing DWPI results

Type:

FILE DWPI

then

***MDARCLIST chap3ex/CN**

(*MDARCLIST will list CN numbers in DWPI with 0 postings*)

then

PRT MMSF 1-25

* Occasionally, CNs from the MMS file are not found in DWPI. Please report these CNs to Questel or to Thomson Reuters. *MDARCLIST should only be used in DWPI.

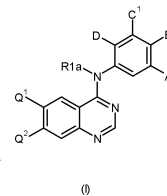
Displaying/Exporting Results



prt mmsf img 1

1/25 DWPI - (C) Thomson Reuters- image
CPIM Thomson Reuters
AN - 2008-K90001 [64]
XR - 2007-457884
XA - C2008-315508
XP - N2008-796964
TI - New quinazoline compounds comprising polyalkylene glycol moiety covalently attached with it, are epidermal growth factor receptor tyrosine kinase inhibitors useful to treat e.g. papilloma, blastoglioma, Kaposi's sarcoma and melanoma
DC - A96 B02 B04 P31
PA - (TKSI-) TK SIGNAL LTD
IN - ABOURBEH G; DISSOKI S; LEVITZKI A; MISHANI E
NP - 1
NC - 1
PN - US20080056990 A1 20080306 DW2008-64 Eng 56p *
AP: 2007US-0714760 20070307, CIP of 2006WO-IL01038 2
PR - 2007US-0714760 20070307; 2006WO-IL01038 20060906
IC - A61K-031/517; A61B-005/055; A61K-051/04; A61P-035/00
C12N-005/00; A61K-051/02; C07D-239/00
ICAA- A61K-031/517 [2006-01 A F I B - -]; A61B-005/055 [2006-01 A L I B - -]; A61K-051/04 [2006-01 A L I B - -]; A61P-035/00 [2006-01 A L I B - -]; C07D-239/72 [2006-01 A L I B - -]; C12N-005/00 [2006-01 A L I B - -]
ICCA- A61B-005/055 [2006 C - I B - -]; A61K-031/517 [2006 C - I B - -]; A61K-051/02 [2006 C - I B - -]; A61P-035/00 [2006 C - I B - -]; C07D-239/00 [2006 C - I B - -]; C12N-005/00 [2006 C - I B - -]
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PRT



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MMS 01-2010

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