

# Searching MMS



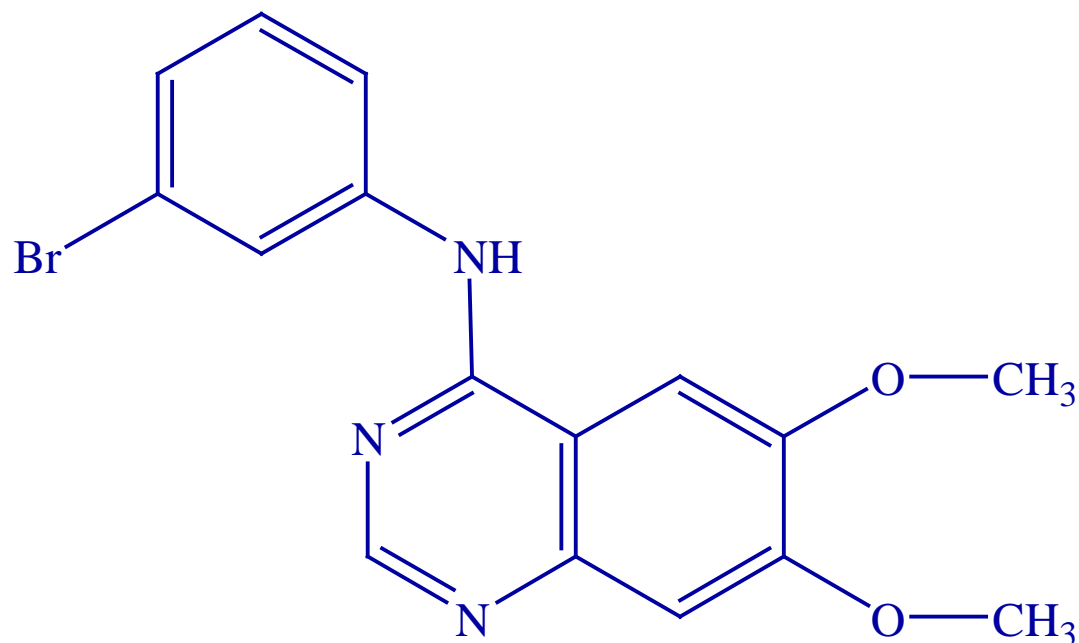
- Query input: Markush TOPFRAG
- Searching
- Accessing structure answers

# Query input



## Query formulation

- The question

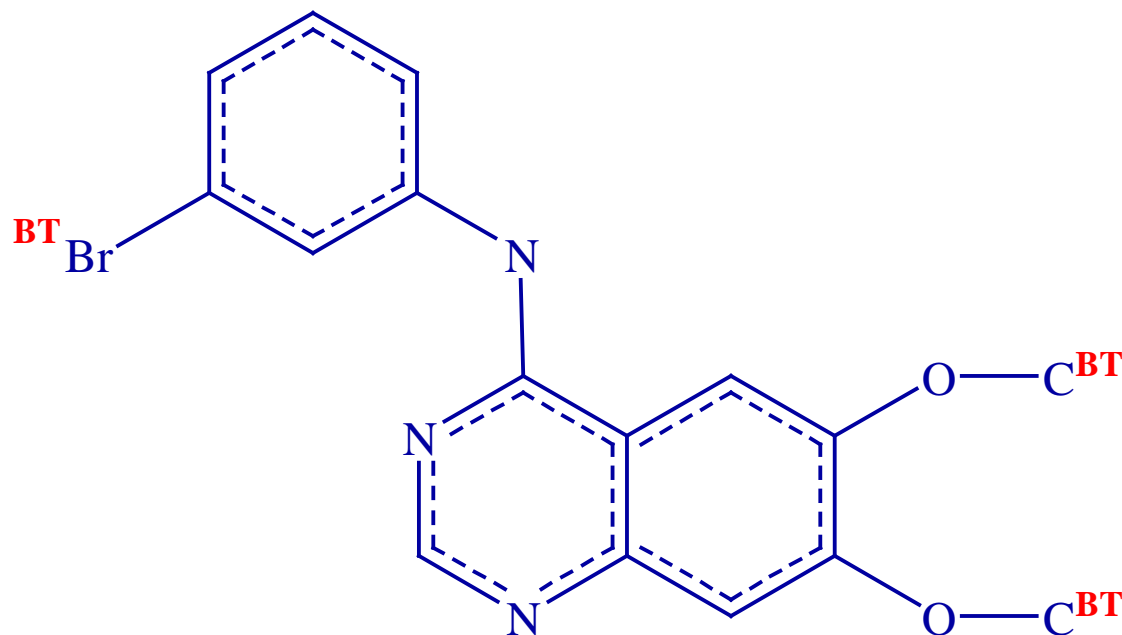


# Query input



## Query formulation

- Converting question to query



# Query input

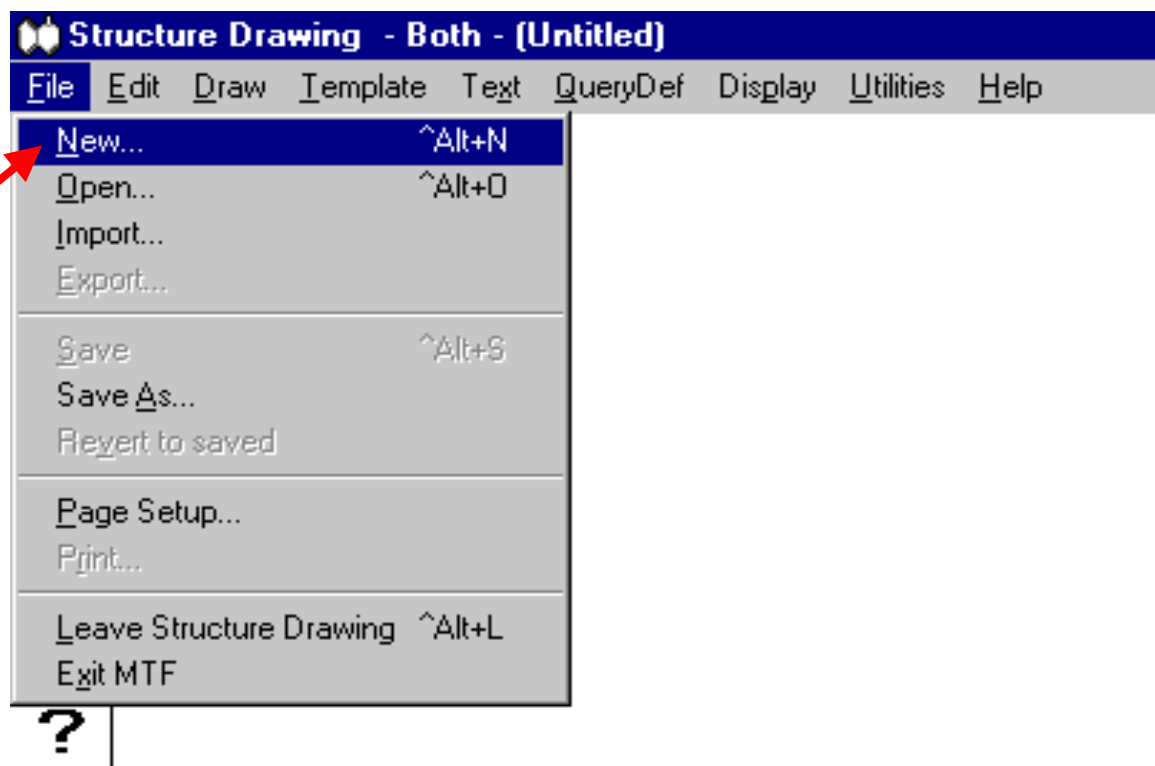


## Using Markush TOPFRAG

1- Run *Markush TOPFRAG*

2- Click on the *Structure drawing* window

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

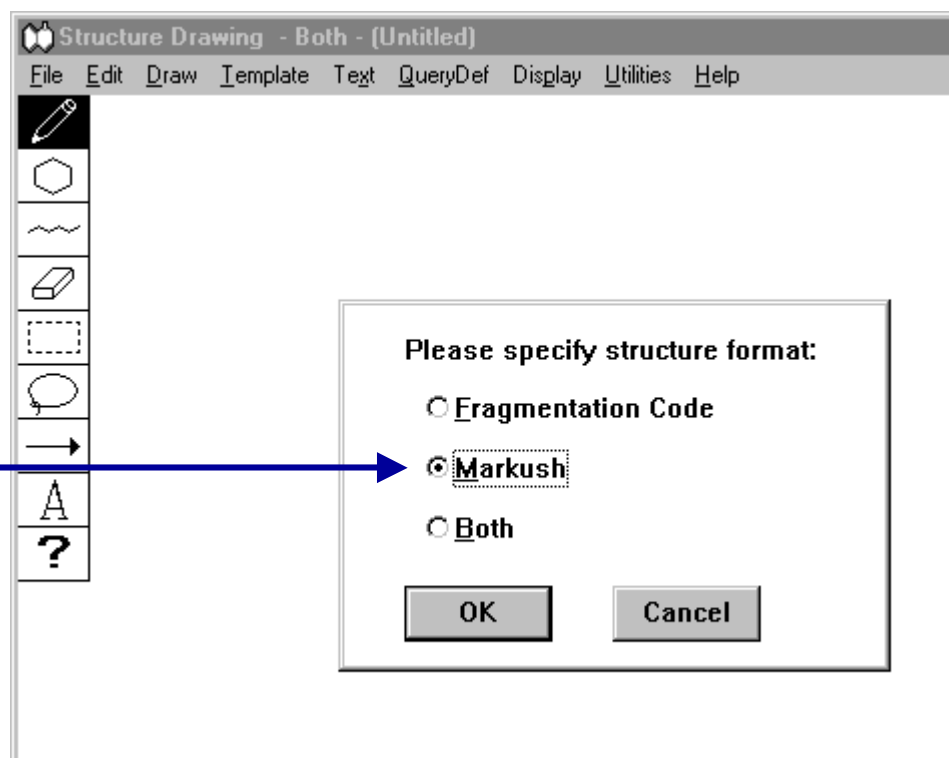


# Query input



## Using Markush TOPFRAG

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



# Query input



## Using Markush TOPFRAG

Structure Drawing - Markush - (Untitled)

File Edit Draw **Template** Text QueryDef Display Utilities Help

Display...

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

C C H O S N P Cl Br F Si I — — = C

# Query input



## Using Markush TOPFRAG

The screenshot shows the Markush software interface with a chemical structure being built. The structure consists of a benzene ring connected to a nitrogen atom, which is in turn connected to a pyridine ring fused to a benzene ring. Three callout boxes provide instructions:

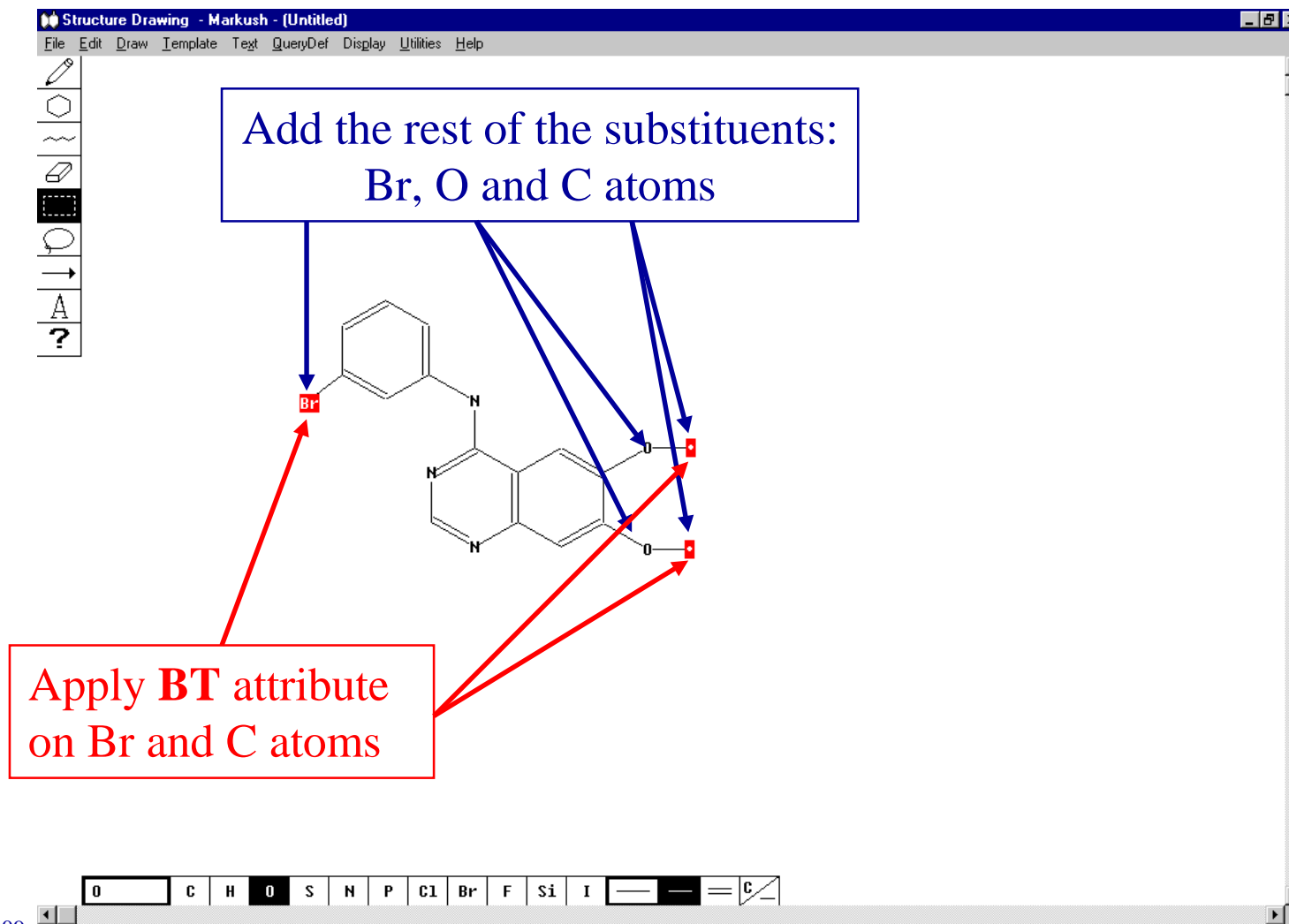
- 1- Double-click on the N**: Points to the nitrogen atom in the pyridine ring.
- 2- Click on the ring atoms to change them to nitrogen**: Points to the two nitrogen atoms in the pyridine ring.
- 3- Draw the amino group**: Points to the bond connecting the benzene ring to the nitrogen atom.

The software interface includes a menu bar (File, Edit, Draw, Template, Text, QueryDef, Display, Utilities, Help), a toolbar with drawing tools, and a bottom toolbar with element selection buttons (N, C, H, O, S, N, P, Cl, Br, F, Si, I, bond types, C).

# Query input



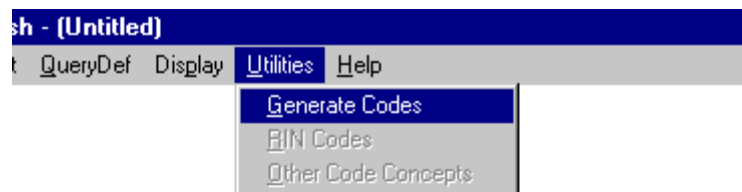
## Using Markush TOPFRAG



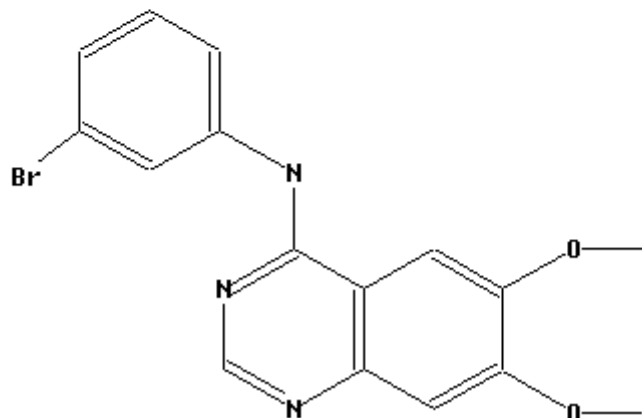
# Query input



## Generate strategy



Select *Generate Codes*  
under the *Utilities* menu



```
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
```

# Query input



## 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**

# Query input



## Upload the strategy

```
MTFEDIT - MDARC - (Untitled)
File Edit Revert Search Help

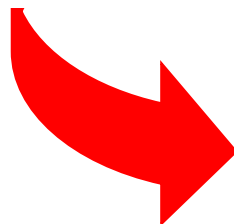
gr
6-1:6-17-10
2-18
12-7:12-16-15-20-22
11-13:15
14-19-21

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 ....*



- Upload strategy:
  - Copy/paste in the Imagination command window
  - Click on the red cross (X)

```
*** 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
```

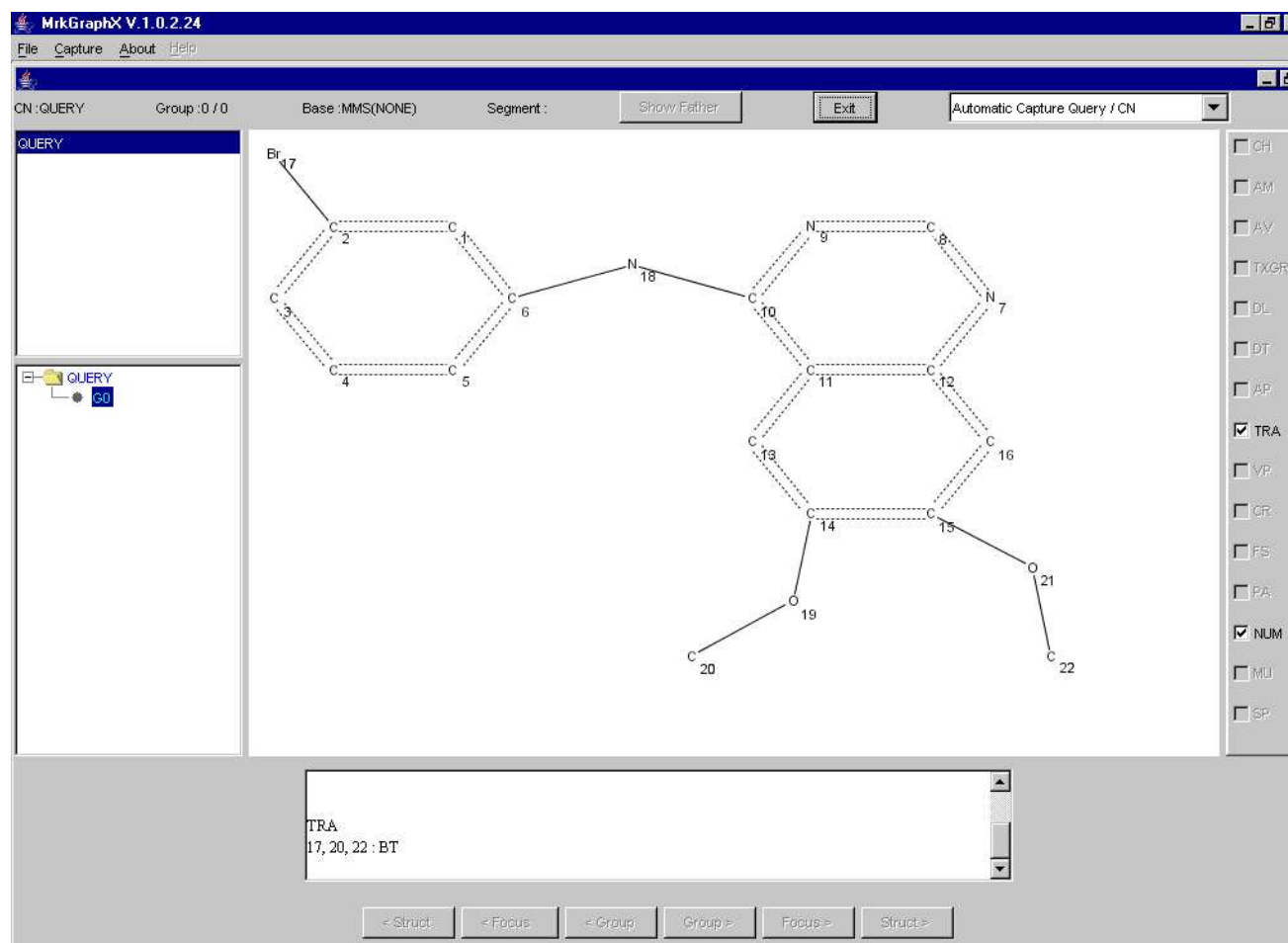
*.... PASTE*

# Query input



## Query verification

- 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) ?

# Searching MMS



**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

# Searching MMS



## 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*

# Searching MMS



## 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 answers(s) for 67661 candidates (no rx candidate(s) )
```

```
12 answers(s) for 126821 candidates (no rx candidate(s) )
```

```
19 answers(s) for 187670 candidates (no rx candidate(s) )
```

```
29 answers(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**

\*\*\* 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**

# Searching MMS



## 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



## Accessing structure answers

- LI
- VI Focus (VI FO)
- VI

# 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

?

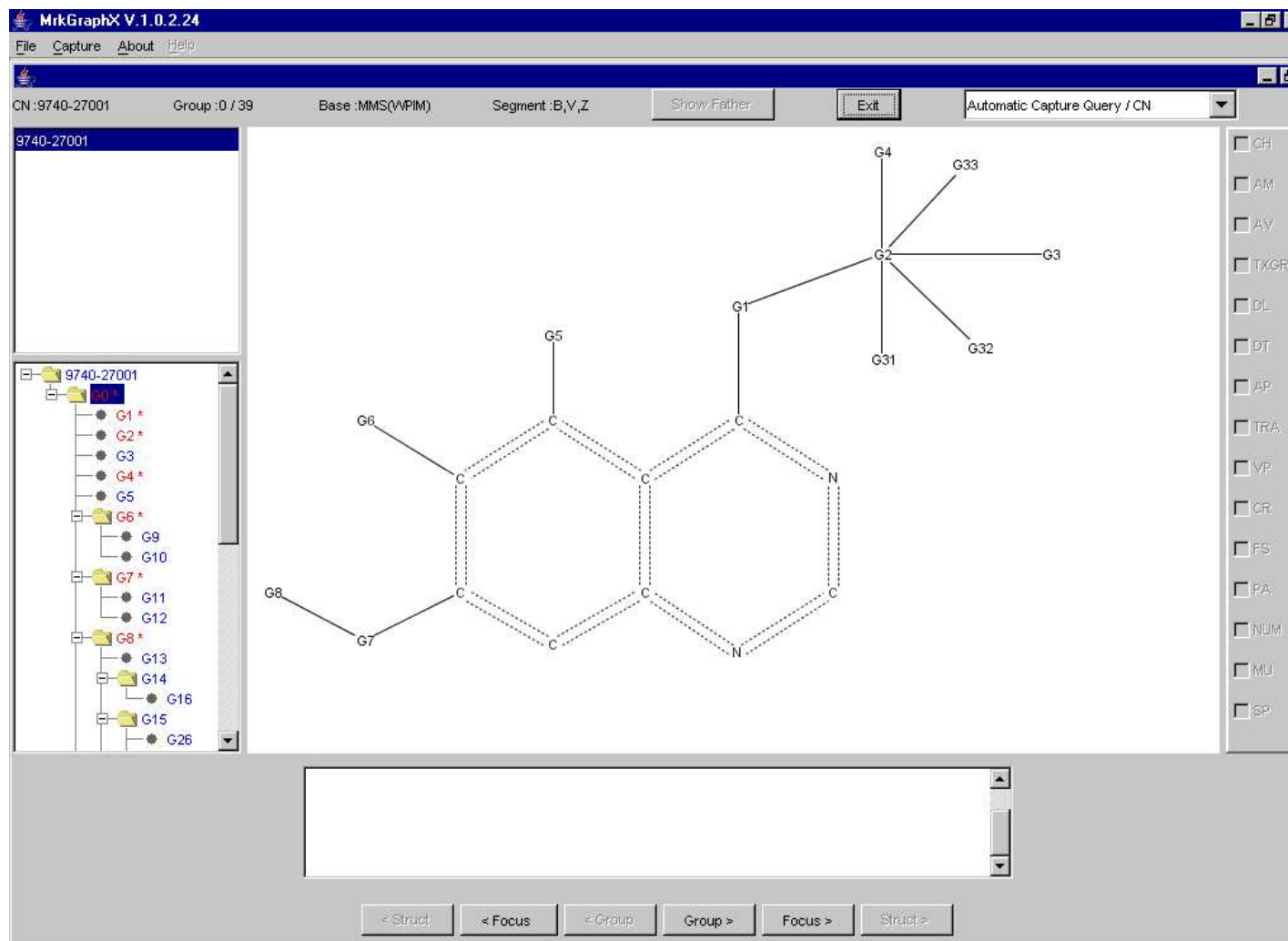
- ST - (BA,CN,QT,RF,RE,AA,SB,BL,INFO,HELP) ?

# Viewing results



VI FO

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



# Viewing results



VI FO

The screenshot shows the MrkGraphX V.1.0.2.24 software interface. The main window displays a chemical structure with atoms labeled G1 through G8. A tree view on the left shows a hierarchy of groups (G1 through G26) under the project name 9740-27001. A navigation bar at the bottom contains buttons: < Struct., < Focus, < Group, Group >, Focus >, and Struct >. A text box on the left says "Directly click on the G group you want to display..." with a red arrow pointing to group G6 in the tree. A text box on the right says "... or use the navigation bar" with a red arrow pointing to the "Focus >" button.

# Viewing results



VI FO

MrkGraphX V.1.0.2.24

File Capture About Help

CN : 9740-27001 Group : 1 / 39 Base : MMS(WPIM) Segment : B,V,Z Show Father Exit Automatic Capture Query / CN

9740-27001

9740-27001

- G0 \*
- G1 \*
- G2 \*
- G3
- G4 \*
- G5
- G6 \*
- G9
- G10
- G7 \*
- G11
- G12
- G8 \*
- G13
- G14
- G16
- G15
- G26

o N s

Click on the *Show Father* icon to display the Father Group

< Struct < Focus < Group Group > Focus > Struct >

# Viewing results



VI FO

The screenshot displays the MrkGraphX V.1.0.2.24 software interface. The main window shows a chemical structure of a nucleotide base, specifically a pyrimidine ring system, with atoms labeled G1 through G8. The structure is rendered in a 3D perspective view. The interface includes a menu bar (File, Capture, About, Help) and a toolbar with buttons for 'Show Father' and 'Exit'. A status bar at the top indicates 'CN : 9740-27001', 'Group : 1 / 39', 'Base : MMS(WPIM)', and 'Segment : B,V,Z'. A dropdown menu is set to 'Automatic Capture Query / CN'. On the left, a tree view shows the hierarchy of groups, with '9740-27001' expanded to show sub-groups G0 through G14. The 'Group : 0' window is active, showing the chemical structure. A vertical toolbar on the right contains checkboxes for various capture queries: CH, AM, AV, TXGR, DL, DT, AP, TRA, VP, CR, FS, PA, NUM, MU, and SP. At the bottom, a navigation bar includes buttons for '< Struct', '< Focus', '< Group', 'Group >', 'Focus >', and 'Struct >'.

# Viewing results



VI FO

The screenshot shows the MrkGraphX V.1.0.2.24 software interface. The main window displays a chemical structure (a hexagon with vertices labeled 1 through 6) and a list of capture options on the right. The 'Automatic Capture Query / CN' menu is selected. The interface includes a menu bar (File, Capture, About, Help), a toolbar (Show Father, Exit), and a status bar (CN: 9740-27001, Group: 2 / 39, Base: MMS(WPIM), Segment: B,V,Z). The 'Capture' menu is open, showing options: CH, AM, AV, TXGR, DL, and SP. The 'Automatic Capture Query / CN' menu is also open, showing options: Automatic Capture OFF, Automatic Capture Query, Automatic Capture CN, and Automatic Capture Query / CN. The 'Focus' button is highlighted in the bottom toolbar.

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

# 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...

## 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.*

# Displaying/Exporting Results



## PRT

**prt max 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 - WO9639145 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)

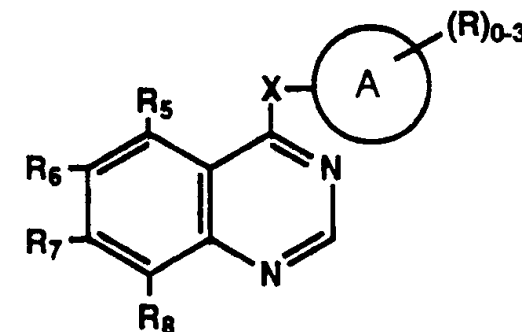
IC1 - A61K-031/535

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, SO<sub>2</sub>, OCH<sub>2</sub>, CR<sub>4</sub>=CR<sub>4</sub>, C C, NR<sub>4</sub> or NR<sub>4</sub>CH<sub>2</sub>, R  
independently includes hydrogen, alkyl, phenyl, haloalkyl, aralkyl,  
hydroxy, alkoxy, aryloxy, acyloxy, halo, haloalkyl, amino, alkylamino,  
dialkylamino, acylamino, carboxy, amido, alkylamido, dialkylamido,  
alkylthio, alkylsulfinyl and alkylsulfonyl, R<sub>4</sub> is hydrogen, alkyl or  
aralkyl, and R<sub>5</sub>, R<sub>6</sub>, R<sub>7</sub> and R<sub>8</sub> 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 MAX IMG**  
*will display the  
full record with  
the front-page  
image.*

# Recalling saved CN lists in DWPI

## 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 ThomsonReuters. \*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

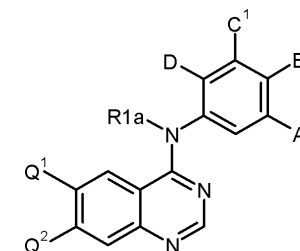
IC - A61K-031/517; A61B-005/055; A61K-051/04; A61P-035/00  
C12N-005/00; A61K-051/02; C07D-239/00

ICAA- A61K-031/517 [2006-01 A F I B - -]; A61B-005/055 [2006-01 A F 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 - -]

PCL - 424001890 424001850 435375000 514266400 544283000

## PRT



(1)

***PRT MMSF IMG***  
*will display the full record with the CN field and the front-page image.*