

# Query definition



- Define the question
- Convert the question to a query
- Input the query

# Query definition



## What do you need to use MMS?

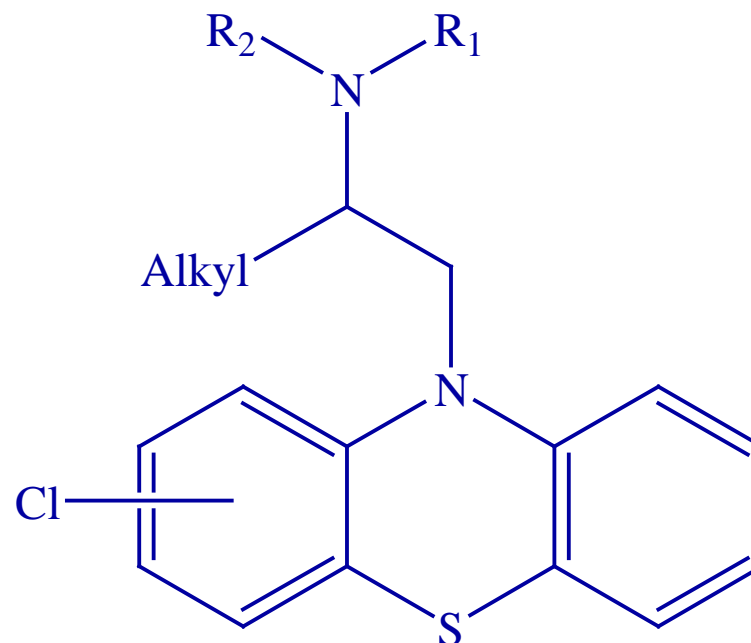
- Login and password from Questel-Orbit
- Imagination, available from Questel-Orbit. (STN Express version 8.01 and later can also be used.)

Markush TOPFRAG, available from Thomson Scientific, can also be used with MMS.

# Query definition



## The question



*R1 and R2 may be anything, including joining together to form a ring*

- **Symbols available for searching:**
  - All the symbols used in the database:
    - Atoms, Shortcuts, Superatoms
    - All bonds: single, double, triple, normalized ...
    - Attributes: chain-ring attributes (LO, BRA ...)...
    - G groups: up to 20

# Search tools



- **Symbols available for searching:**
  - Free Site: optional site of substitution

*By default, the nodes are not substituted. Substitution is opened only when Free Sites are specified.*

# Search tools



- **Symbols available for searching:**
  - **Specific symbols:**
    - **X** atom: any atom except hydrogen
    - **X** bond: any bond
    - **Z** bond: list of bonds
    - **SN/DN** bonds
    - Bond attributes: **CY, AC, CX**

# Search tools

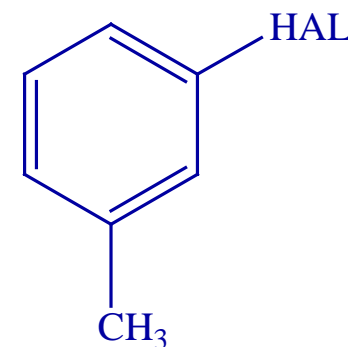
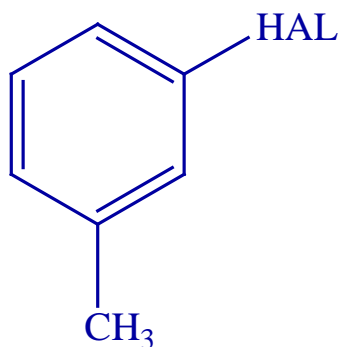


- **Symbols available for searching:**
  - Translation attributes:
    - Equal translation
    - Narrow translation
    - Broad translation

- **Equal translation:**

The default when using the on-line keyboard commands

Query

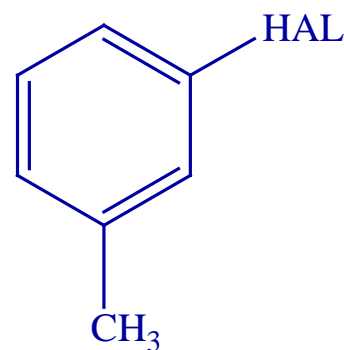
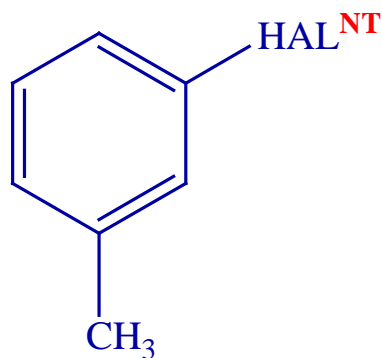


MMS

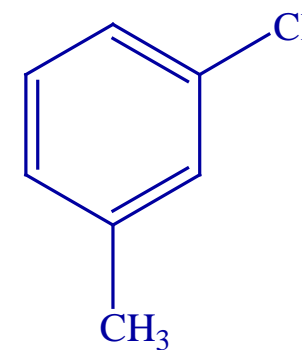
- **Narrow translation:**

To retrieve any specific moiety from a chemical group

Query



*and*



MMS

# Search tools



## Narrow Translation

NT on:	Would retrieve:	
	<i>Term itself</i>	<i>More specific terms</i>
<b>HAL</b>	HAL	Cl, Br, F, I
<b>CHK</b>	CHK	Me, Et, tBu, C <sub>12</sub> H <sub>25</sub>
<b>MX</b>	MX	AMX, A35, TRM, LAN, ACT All specifics (Na, Al, Fe, La, U)
<b>CHK<sup>LO</sup></b>	CHK <sup>LO</sup>	Me, Et, iPr, Bu, iBu, sBu ... C6
<b>ARY<sup>MON</sup></b>	ARY <sup>MON</sup>	Benzene

# Search tools



## Free sites and Narrow Translation

NT on:	Would retrieve:	
	<i>Term itself</i>	<i>Narrower terms</i>
<b>ARY<sup>3*</sup></b>	ARY ARY-Br ARY(Br) <sub>2</sub> ARY(Br) <sub>3</sub>	Benzene Bromobenzene 1,3-dibromobenzene 1,3,5-tribromobenzene 1-(2-pyridyl)-3-chlorobenzene naphthalene 1,4,6-trimethylnaphthalene
<b>ARY<sup>MON, 3*</sup></b>	ARY <sup>MON</sup> ARY <sup>MON</sup> Br ARY <sup>MON</sup> Br <sub>2</sub> ARY <sup>MON</sup> Br <sub>3</sub>	Benzene Bromobenzene 1,3-dibromobenzene 1,3,5-tribromobenzene 1-(2-pyridyl)-3-chlorobenzene

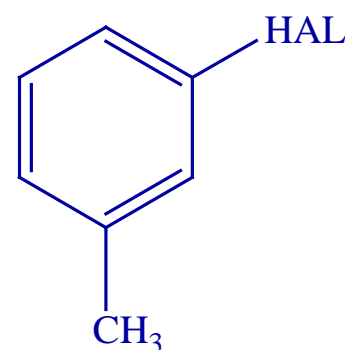
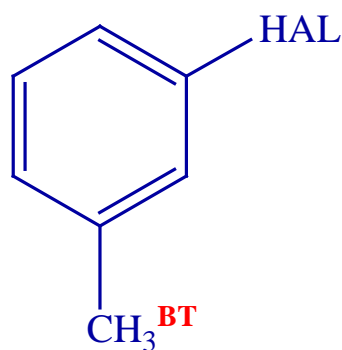
# Search tools



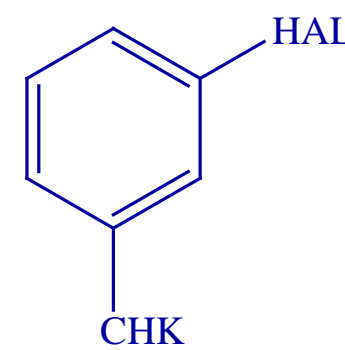
- **Broad translation:**

To broaden the scope of a search which was too specific

Query



*and*



MMS

# Search tools



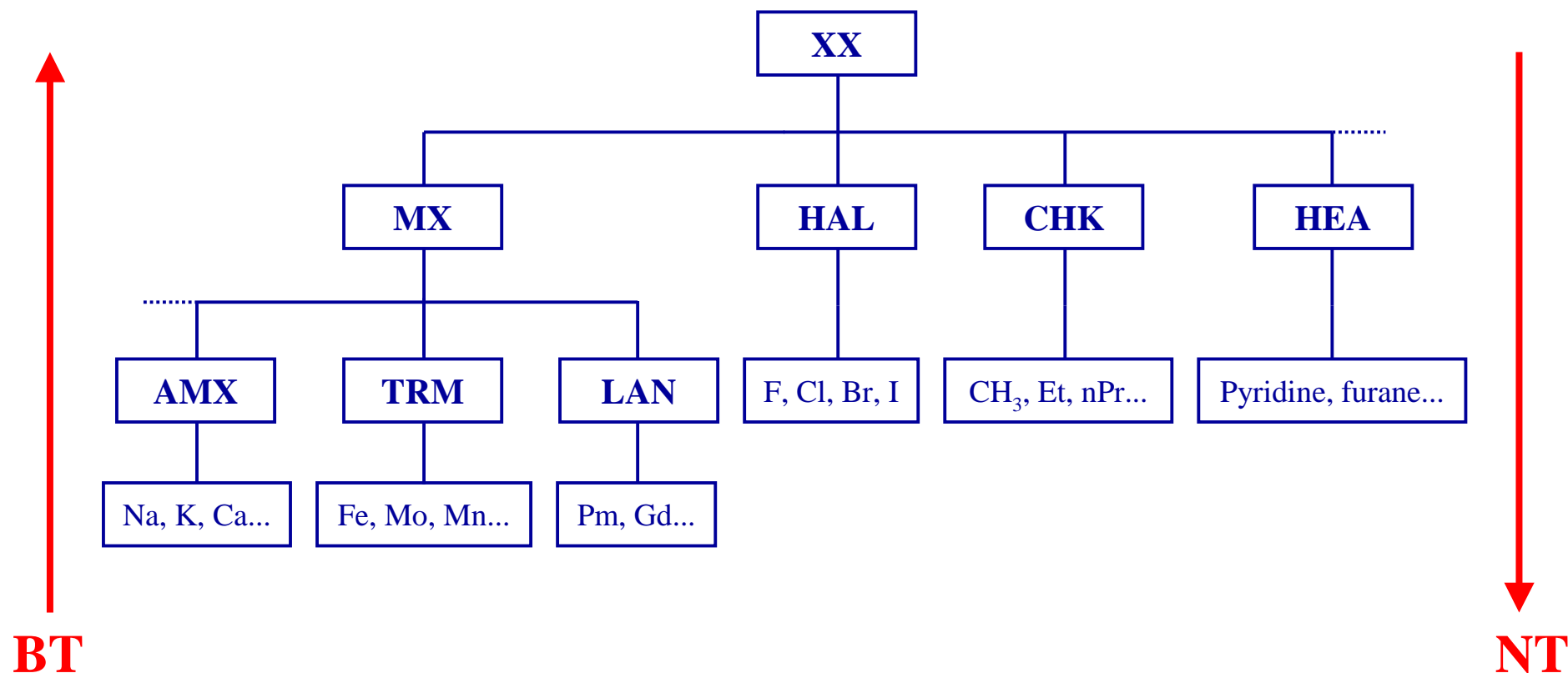
## Broad Translation

<b>BT on:</b>	<b>Would retrieve:</b>	
	<i>Term itself</i>	<i>Broader term</i>
Cl	Cl	HAL, XX
Pyridine	Pyridine	HEA, XX
C	C	CHK <sup>LO</sup> , CHK, CHK(1-4), XX

# Search tools



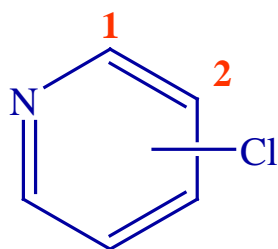
## Element hierarchy and translation



## Variable position of attachment

- Symbols available for searching:
  - Variable attachments:

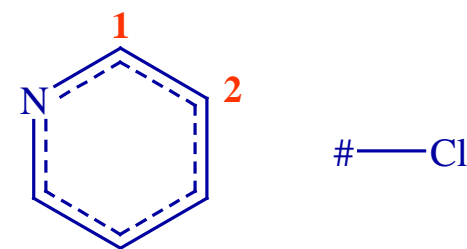
### Question



Chlorine may be connected to positions 1 or 2

*will be input*

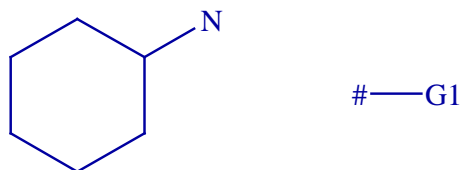
### Query



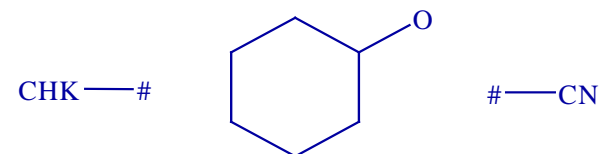
While specifying that the # atom (dummy atom) can be connected to positions 1 or 2

## Variable position of attachment

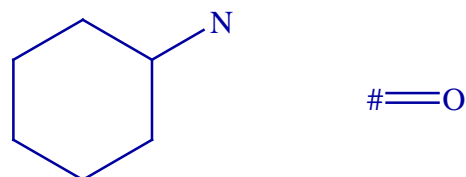
- Single attachment to ring



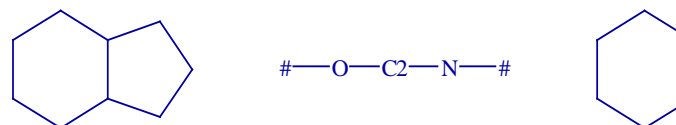
- Several variable attachments to one ring



- Attachment via double bond

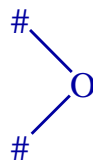
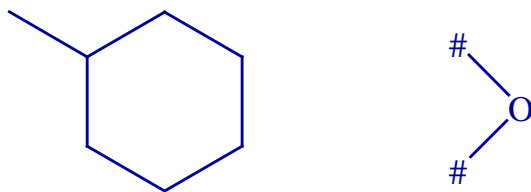


- Single fragment - attachments to different rings

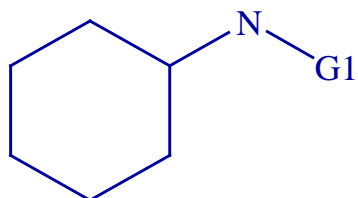


## Variable position of attachment

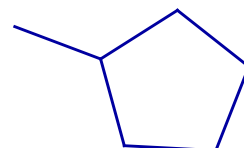
- Single fragment - attachment to same ring



- Attachment within a G group



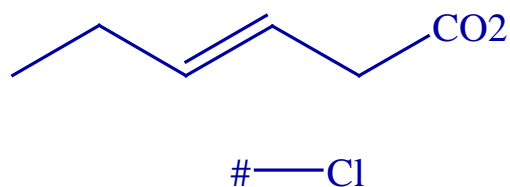
G1 =



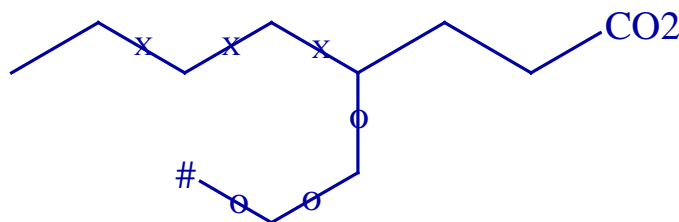
#—G2—G3

## Variable position of attachment

- Attachment to chains



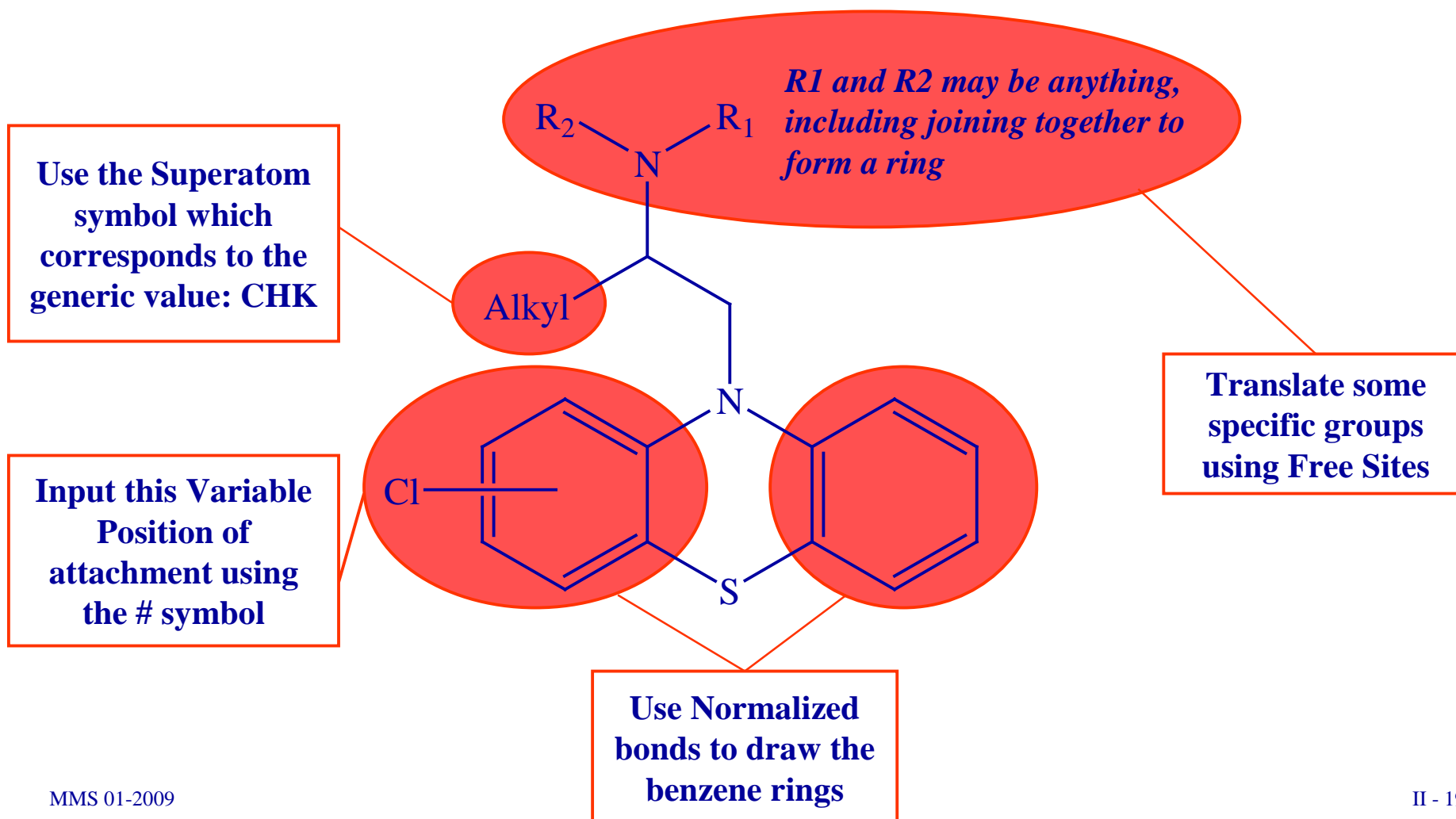
- Chain fragment closing to form ring



# Query definition



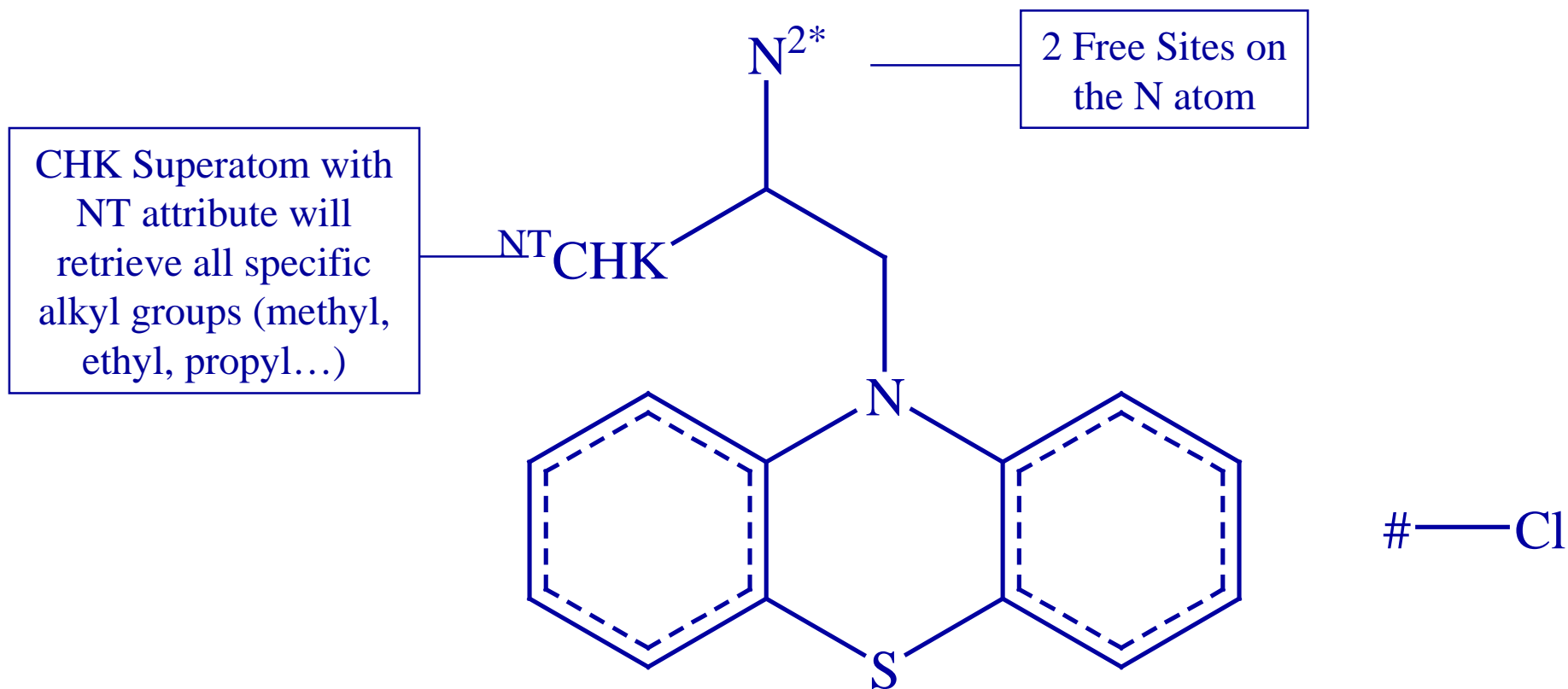
From the question...



# Query definition



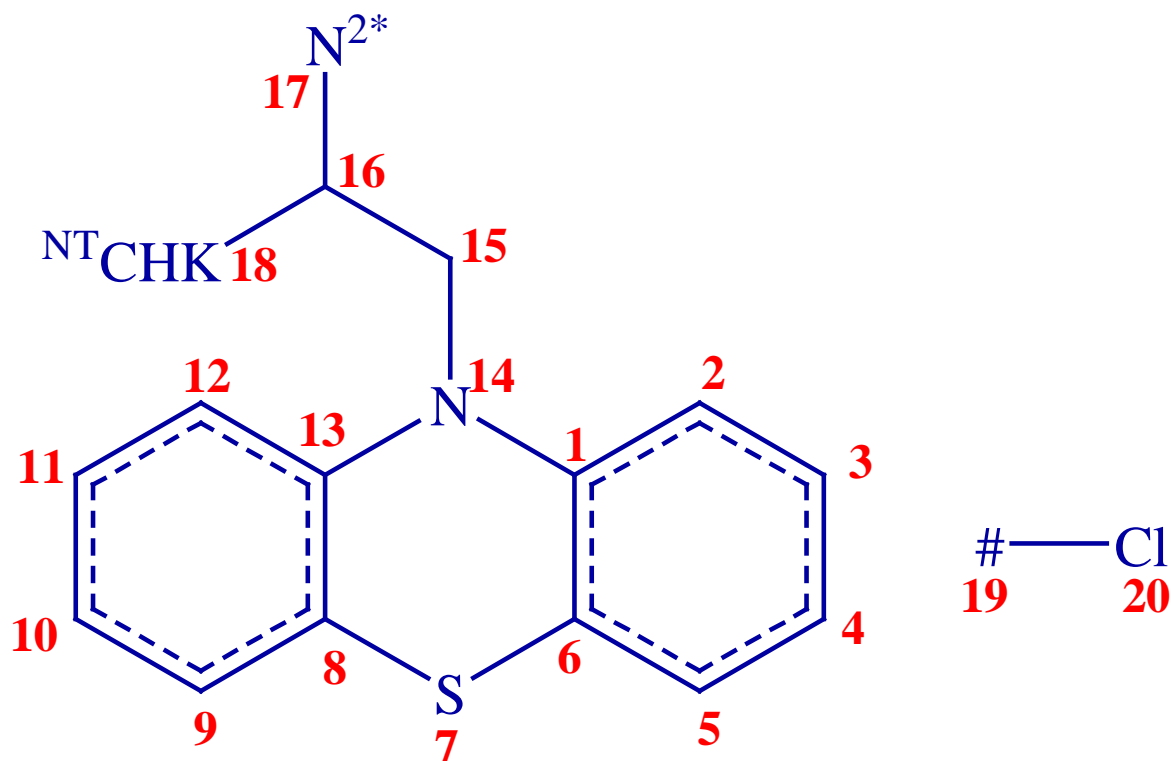
... to the query



# Query input



## Numbering nodes of the query



# Query input



## Connection using Imagination

The screenshot shows the Questel.Orbit Imagination application window. The title bar reads "Questel.Orbit Imagination". The menu bar includes "File", "Edit", "Session", "Export", "Settings", "Window", and "Help". The toolbar contains icons for file operations, a "Break" button, a dropdown menu showing "Markush - Internet", and a help icon. A red circle highlights the "Break" button and the dropdown menu. A red line connects this circle to a text box that says "Select the appropriate service first (if not proposed by default): Markush DARC - Internet". Another red line connects the "Break" button to a text box that says "Then click on the connection tool". At the bottom of the window, there is a status bar with a green arrow icon on the left and a blue vertical bar. A red line connects this blue bar to a text box that says "The connection status bar is blue: you are not yet connected". Below the status bar, the text "Connect/Disconnect to the service" is visible.

Select the appropriate service first (if not proposed by default): Markush DARC - Internet

Then click on the connection tool

The connection status bar is blue: you are not yet connected

Connect/Disconnect to the service

# Query input



## Use of Imagination

The screenshot shows the Questel Imagination software interface. The main window displays the following text:

```
The SDI requests saved on your account are :  
#. Name                Start date  Last Update  Answ.  
  
1 joemonthly           2007-11-14  2008-01-01   0  
2 joeweekly            2007-11-14  2007-12-29   0  
  
****    CURRENT SELECTED DATA BASE :MMS    ****  
  
**** BASE MMS - 12/21/2007 - 2273652 Compounds ****  
****    LAST SELECTED SEGMENT(S) :  
FRONTE  
MPHARM  
WPIM  
BACKF  
  
- ST - (BA, CN, QT, RF, RE, AA, SB, BL, INFO, HELP) ?  
↑ - ST - (BA, CN, QT, RF, RE, AA, SB, BL, INFO, HELP) ?
```

A callout box with a blue border and red text is overlaid on the bottom right of the command window, containing the text: "The Command Window: type your commands here".

# Query input



- Logon to MMS

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

- Type **QT**

- Answer **No** to draw a new query

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

  - \*\*\* QT \*\*\*

  - Previous valid input (Answer No to draw a new query) ? ( Y/N ) ? **N**

- Input the query

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

# Query input



## The way to proceed

- Define the skeleton: graph input (**GR**)
- Define nodes (**AT** for atom)
- Define bonds (**BO**)
- Define substitutable positions: Free Sites (**FS**)
- Define other attributes
  - Variable Positions (**VP**)
  - Translation (**TRA**)
- Define variable groups (if any)

# Query input



## The way to proceed

- Define the skeleton: graph input (**GR**)
- Define nodes (**AT** for atom)
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# Query input



## Graph input

- for connections
- , for new starting points
- : for series of nodes
- / to remove nodes

# Query input



## Graph input

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

Graph specification

Enter the graph definition using the number you assigned to the non-hydrogen nodes in your query.

Separators are ":" (series of consecutive nodes),

"-" (link between two nodes),

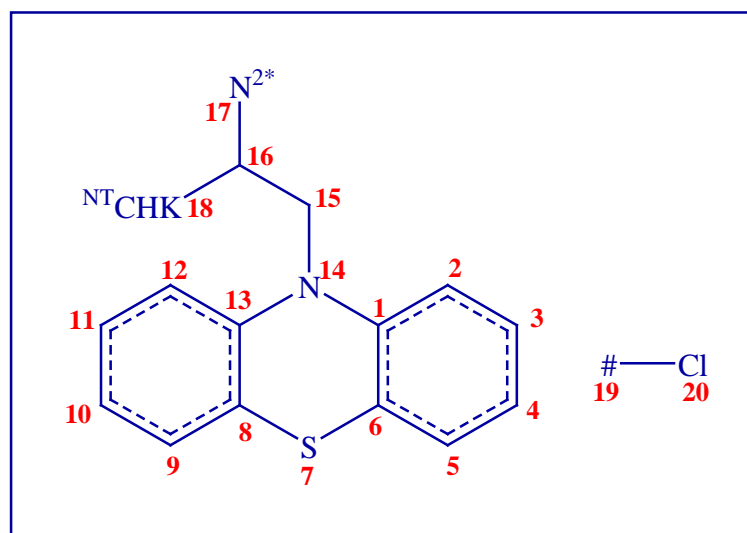
"," (new starting point).

e.g. : "1:6-1, 6-7" input a 6-membered ring substituted with a single carbon.

? **1:17,1-6,1-14,8-13,16-18,19-20**

?

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



# Query input



## Query verification

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

The screenshot shows the MrkGraphX V.1.0.2.24 interface. The main display window shows a chemical structure with atoms labeled C1 through C19. The interface includes a menu bar (File, Capture, About, Help), a toolbar with buttons like Show Father and Exit, and a status bar. On the left, there is a 'QUERY' frame and a 'Group' frame. On the right, there is an 'Attribute bar' with various checkboxes (ICH, AM, AV, TXGR, DL, DT, AP, TRA, VP, CR, FS, PA, NUM, MU, SP). At the bottom, there is a 'Text note frame' and a 'Navigation bar' with buttons for navigation.

CN frame /  
Query

Group frame

Attribute bar

Display window

Text note frame

Navigation bar

# Query verification



## Capturing structure display

To leave the display

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

# Query input



## The way to proceed

- Define the skeleton: graph input (**GR**)
- Define nodes (**AT** for atom)
- Define bonds (**BO**)
- Define substitutable positions: Free Sites (**FS**)
- Define other attributes
  - Variable Positions (**VP**)
  - Translation (**TRA**)
- Define variable groups (if any)

# Query input



## Define atoms

- Elements symbols
- Shortcuts
- Variable groups (G groups)
- Superatoms
- **X** atom (any atom or Superatom except hydrogen)
- # variable attachment node

# Query input



## Define atoms

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

Atom specification

Enter the node value (e.g. N, CHK, G1, NO2), a space then the position(s) where to specify this value using commas to separate positions. e.g. "O 1,3" specifies a O atom at positions 1 and 3.

? **S 7**

? **N 14,17**

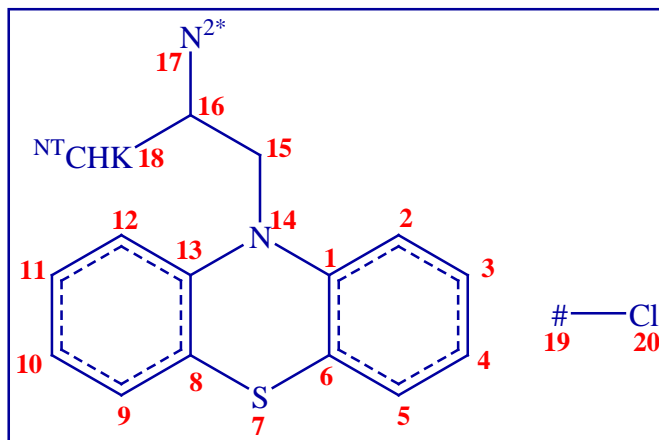
? **CHK 18**

? **# 19**

? **Cl 20**

?

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



**N 14,17**

*Element  
symbol*

*Space*

*Node numbers  
(comma used as a  
separator)*

# Query input



## The way to proceed

- Define the skeleton: graph input (**GR**)
- Define nodes (**AT** for atom)
- Define bonds (**BO**)
- Define substitutable positions: Free Sites (**FS**)
- Define other attributes
  - Variable Positions (**VP**)
  - Translation (**TRA**)
- Define variable groups (if any)

## Define bonds

- **Type**

- **SI** Single
- **DO** Double
- **TR** Triple
- **NO** Normalized
- **SN** Single / Normalized
- **DN** Double / Normalized
- **X** Undefined
- **Z** List of bonds

- **Nature**

- **CY** Cyclic
- **AC** Acyclic
- **CX** Cyclic or Acyclic

# Query input



## Define bonds

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

Bond specification

Enter the bond value (e.g. DO, NO, X), a space then the connections(s).

Separators are ":" (series of consecutive nodes),

"-" (link between two nodes),

"," (new starting point).

e.g. "NO 1:6-1, 8-9" specifies NOrmalized bonds at connections 1-2-3-4-5-6, 6-1 and 8-9.

? **NO 1:6-1, 8:13-8**

?

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

**NO 1:6-1, 8:13-8**

*Bond symbol*

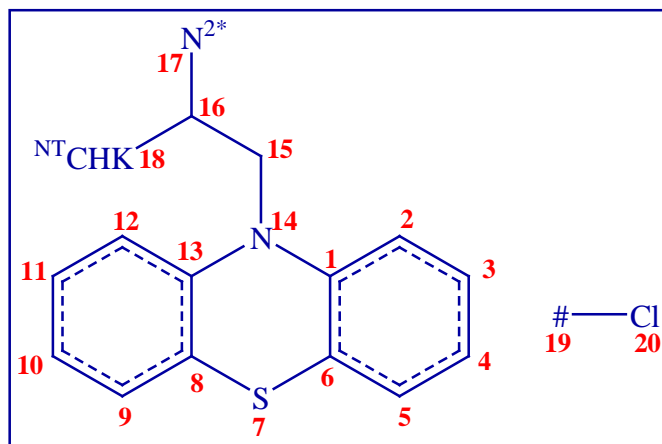
*Space*

*Node numbers:*

*: series of nodes*

*- connections*

*, new starting points*



# Query input



## The way to proceed

- Define the skeleton: graph input (**GR**)
- Define nodes (**AT** for atom)
- Define bonds (**BO**)
- Define substitutable positions: Free Sites (**FS**)
- Define other attributes
  - Variable Positions (**VP**)
  - Translation (**TRA**)
- Define variable groups (if any)

# Query input



## Free Sites

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

Free site (substitution) specification

Enter the number of free sites, a space then the position(s) using commas to separate positions. e.g. "2 1,3" specifies 2 free sites at positions 1 and 3.

? **2 17**

?

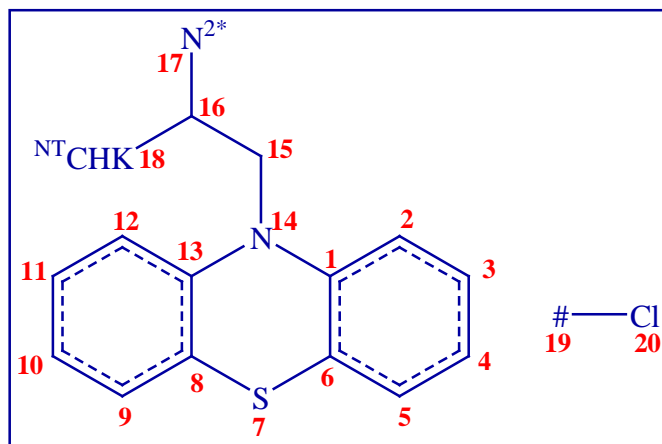
- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ?

2 17

Number of  
Free Sites

Space

Node number  
(comma used as a  
separator)



# Query input



## The way to proceed

- Define the skeleton: graph input (**GR**)
- Define nodes (**AT** for atom)
- Define bonds (**BO**)
- Define substitutable positions: Free Sites (**FS**)
- Define other attributes
  - Variable Positions (**VP**)
  - Translation (**TRA**)
- Define variable groups (if any)

## Define other attributes

- **Translation**

- **NT**          Narrow Translation
- **BT**          Broad Translation
- **EQ**          Equal translation (no translation)
- **ANY**        Both Broad and Narrow Translation

# Query input



## Define other attributes

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

Translation Attribute specification

Enter an attribute value (taken from NT, BT, ANY, EQ), a space then the position(s) using commas to separate positions.

e.g. "NT 1,3" specifies a translation attribute NT at nodes 1 and 3.

? **NT 18**

?

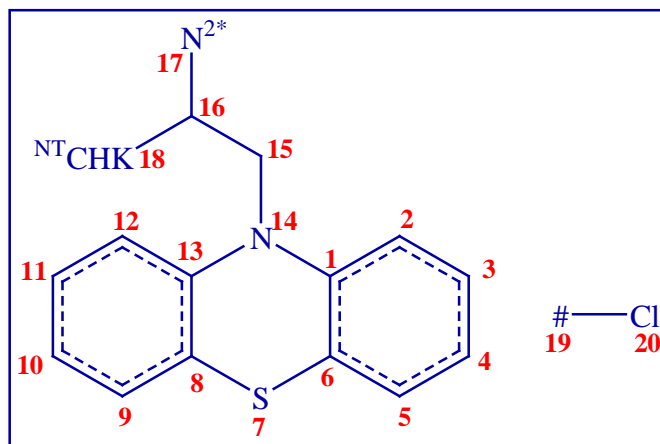
- QT - (CN,CA,GM,GI,GR,BO,AT,FS,AP,VP,ATTR,VE) ?

**NT 18**

Attribute  
symbol

Space

Node number  
(comma used as a  
separator)



# Query input



## Define variable attachments

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

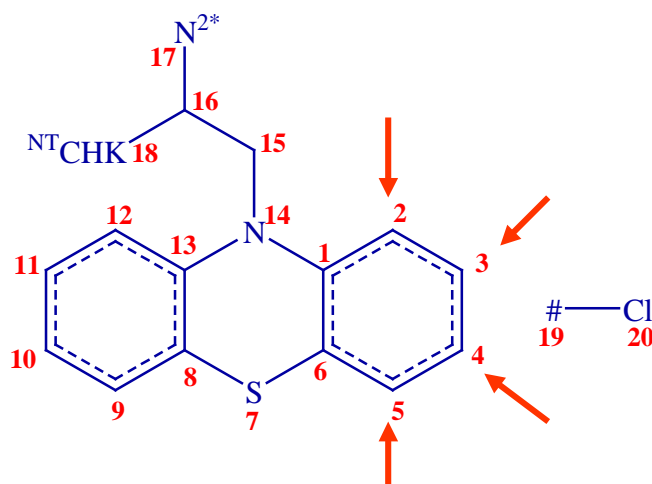
Variable Position specification

Type the numbers of the nodes, separated by commas, to which the designated dummy atom (#) is attached

# Atom 19 of group 0

? **2,3,4,5**

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



# Query input



## Query verification

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

The screenshot shows the MrgGraphX V.1.0.2.24 interface. The main window displays a chemical structure with atoms numbered 1 through 18. A text box in the center of the structure reads: "Attributes specified for the query are ticked off by default". On the right side, there is a vertical list of attributes with checkboxes: GH, AM, AV, TXGR, DL, DT, AP, TRA (checked), VP (checked), CR, FS (checked), PA, NUM (checked), MU, and SP. At the bottom, a text area shows the query results: "TRA: 13 : NT", "VP: 19 : 2, 3, 4, 5".

# 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) ?