

Query definition



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

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- **Query definition**

From the question to the query.

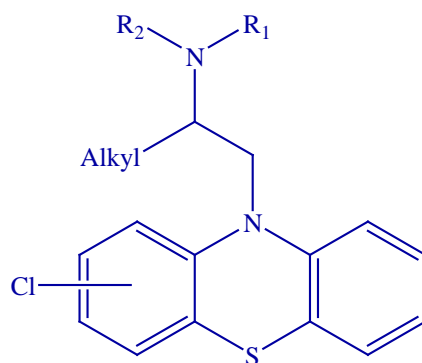
What do you need to use MMS?

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

Markush TOPFRAG can also be used with MMS.

- **Query definition**

The question



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

- Query definition
 - The question

From the question to the query: the question.

- **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

- **Query definition**

- **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.

- **Query definition**

- **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**

- **Query definition**
 - **Search tools**

- **Symbols available for searching:**

- Translation attributes:
 - Equal translation
 - Narrow translation
 - Broad translation

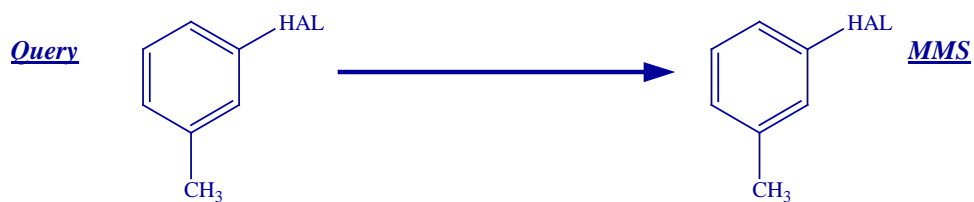
- **Query definition**

- **Search tools**

- **Translation**

- **Equal translation:**

The default when using the on-line keyboard commands



- **Query definition**

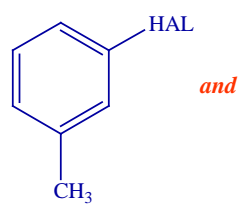
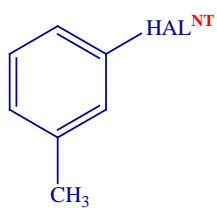
- **Search tools**

- **Translation**

- **Narrow translation:**

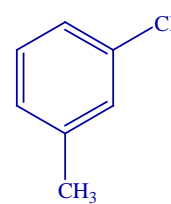
To retrieve any specific moiety from a chemical group

Query



and

MMS



- **Query definition**

- **Search tools**

- **Translation**

Narrow Translation

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

- Query definition
 - Search tools
 - Translation

Free sites and Narrow Translation

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

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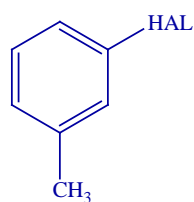
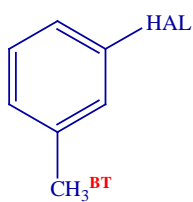
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- Query definition
 - Search tools
 - Translation

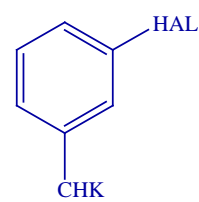
- **Broad translation:**

To broaden the scope of a search which was too specific

Query



and



MMS

- **Query definition**

- **Search tools**

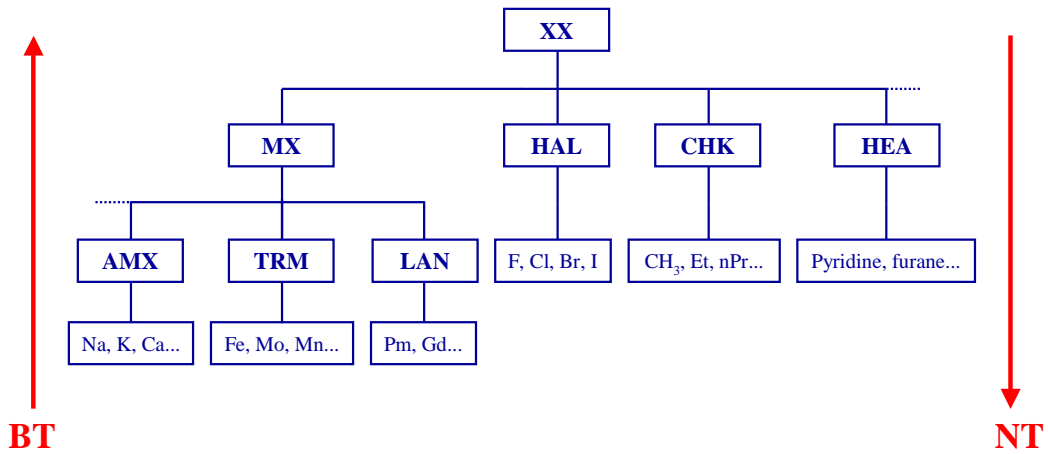
- **Translation**

Broad Translation

BT on:	Would retrieve:	
	<i>Term itself</i>	<i>Broader term</i>
Cl	Cl	HAL, XX
Pyridine	Pyridine	HEA, XX
C	C	CHK ^{LO} , CHK, XX

- Query definition
 - Search tools
 - Translation

Element hierarchy and translation



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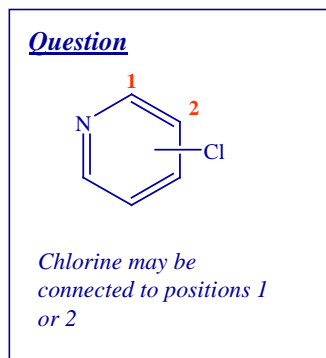
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- Query definition
 - Search tools
 - Translation

Variable position of attachment

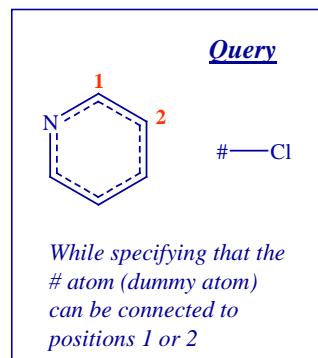
- **Symbols available for searching:**

- Variable attachments:



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will be input



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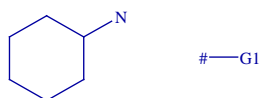
- **Query definition**

- Search tools

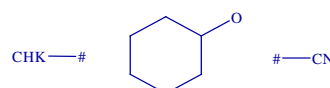
- Variable position of attachment

Variable position of attachment

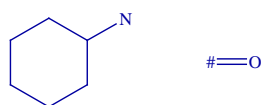
- Single attachment to ring



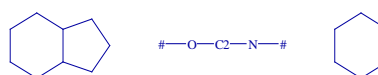
- Several variable attachments to one ring



- Attachment via double bond



- Single fragment - attachments to different rings



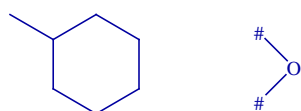
- Query definition

- Search tools

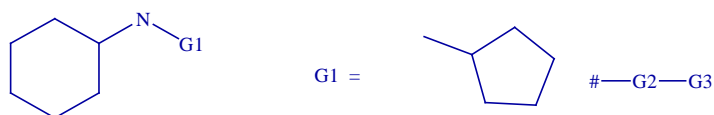
- Variable position of attachment

Variable position of attachment

- Single fragment - attachment to same ring



- Attachment within a G group



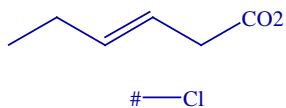
- Query definition

- Search tools

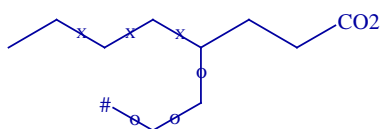
- Variable position of attachment

Variable position of attachment

- Attachment to chains



- Chain fragment closing to form ring

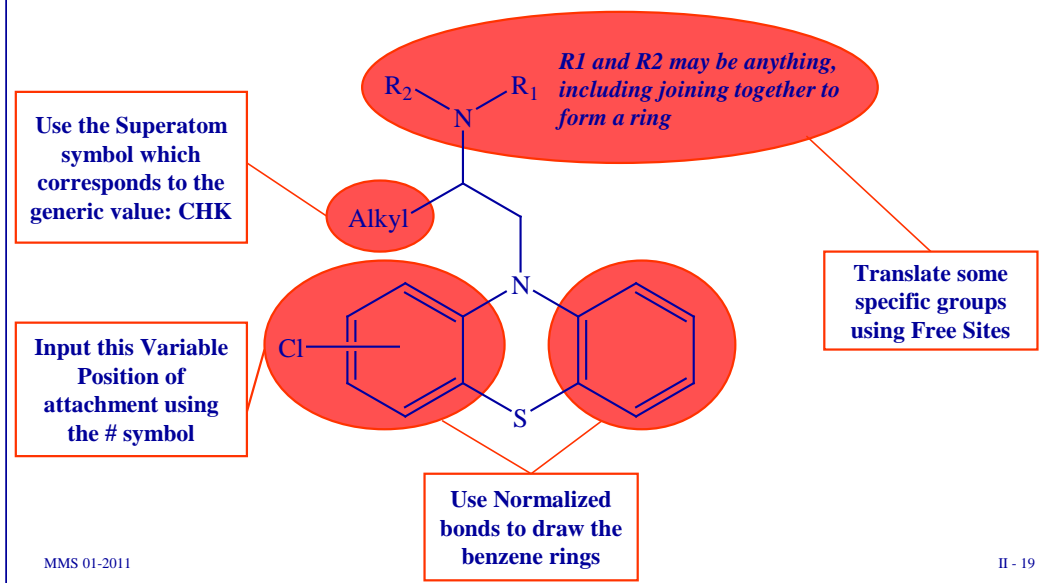


- **Query definition**

- **Search tools**

- **Variable position of attachment**

From the question...



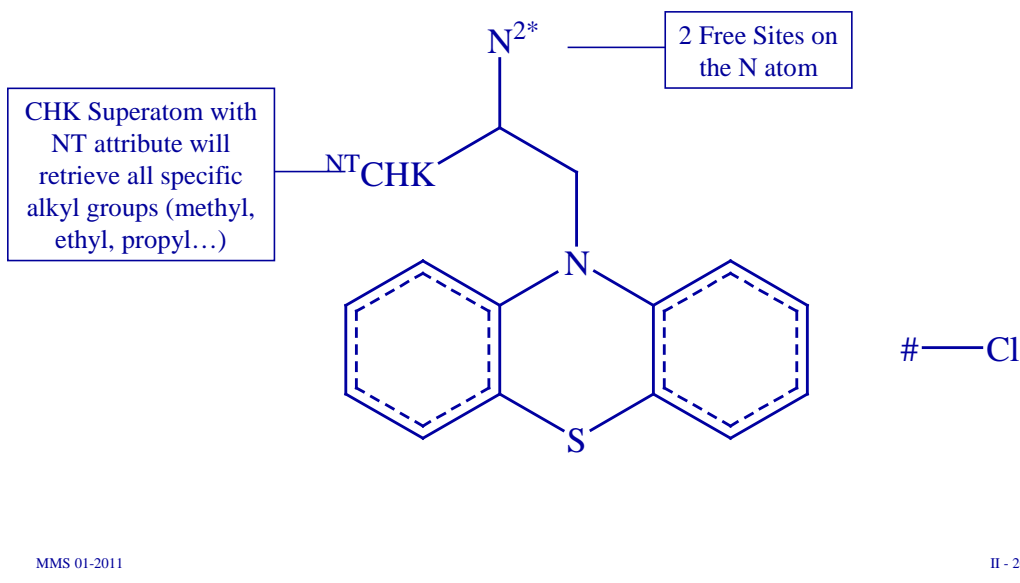
- Query definition

- From the question...

Query definition



... to the query

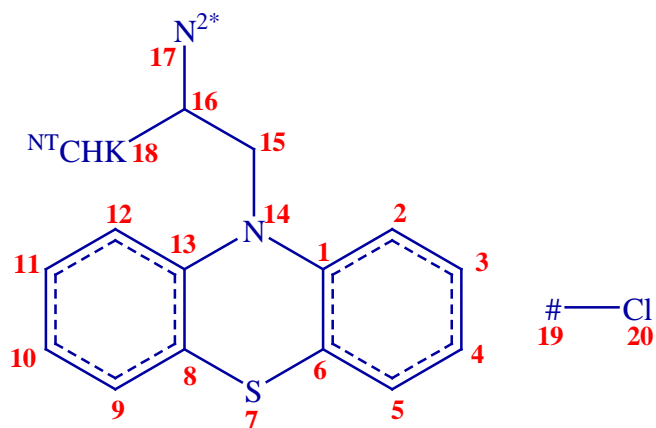


- Query definition
 - ... To the query

Query input



Numbering nodes of the query



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- Query input
 - Numbering nodes of the query

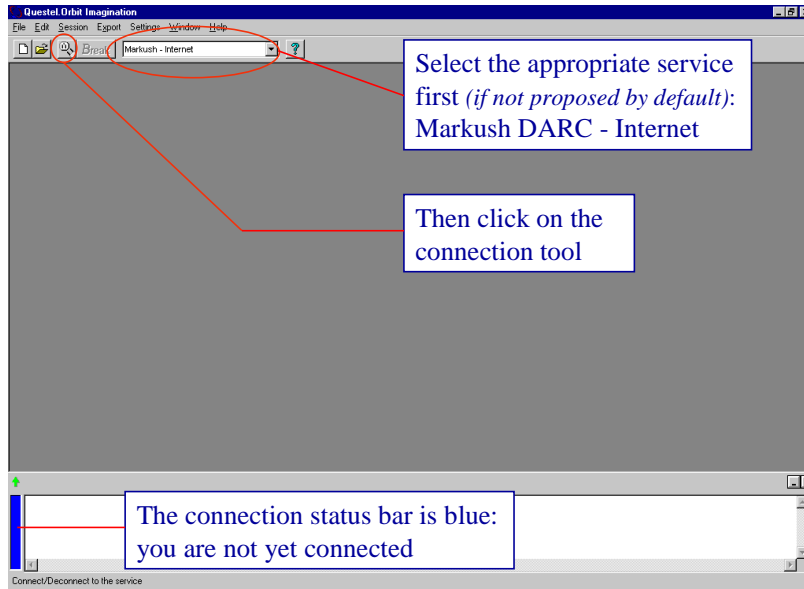
Query definition

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Query input



Connection using Imagination



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- **Query input**

- **Connection**

Once you have numbered the nodes of the query, you can access MMS.

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) :  
FRONTF  
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 points to the command input area at the bottom of the window, containing the text: "The Command Window: type your commands here".

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- Query input
- Connection

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) ?

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- **Query input**

When at ST, type **QT** in order to move to the on-line query editor:

```
**** CURRENT SELECTED DATA BASE :MMS ****
```

```
**** BASE MMS - 01/02/07 - 2101776 Compounds ****
```

```
**** LAST SELECTED SEGMENT(S) :
```

```
FRONTF
```

```
MPHARM
```

```
WPIM
```

```
BACKF
```

```
- 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
```

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

The main menu of this editor (or QT menu) offers various commands which permit to input your query step by step.

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**

The way to proceed

- Define the skeleton: graph input (**GR**)
- Define nodes (**AT** for atom)
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 - Translation (**TRA**)
- Define variable groups (if any)

- **Query input**
 - **The way to proceed**

Query input



Graph input

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

- Query input
 - Graph input

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),

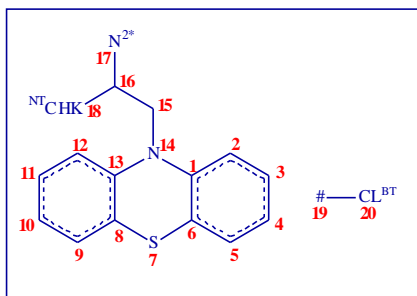
"," (new starting point).

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) ?



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- Query input

- Graph input

Query input



Query verification

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

The screenshot shows the MIMGraph V.1.0.2.24 software interface. The main window displays a chemical structure with atoms labeled C1 through C20. The interface is divided into several frames:

- CN frame / Query:** Located at the top left, it contains a list of query terms.
- Group frame:** Located below the CN frame, it shows the selected group.
- Display window:** The central area showing the chemical structure.
- Text note frame:** Located at the bottom center, it contains a text input field.
- Attribute bar:** Located on the right side, it contains a vertical list of attributes with checkboxes.
- Navigation bar:** Located at the bottom, it contains buttons for navigating between different views.

• Query input

• Query verification

CN frame: CN list of an answer set or Query

Group frame: groups in the query / CN selected in the *CN frame*

Display window: structure display of the group selected in the *Group frame*

Attribute bar: tick-boxes (only those related to attributes present in the group being displayed are active)

Navigation bar: buttons to navigate between CN or groups

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

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- Query input
 - Query verification

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 atoms

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

- **Query input**

- **Define atoms**

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**

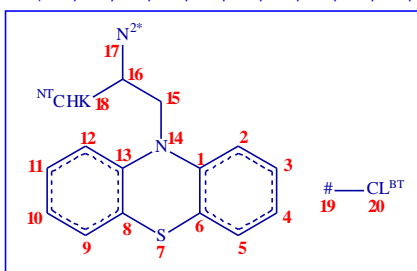
? **CHK 18**

? **# 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

- Define atoms

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 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**

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

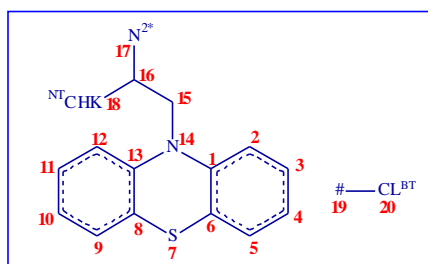
Space

Node numbers:

: series of nodes

- connections

, new starting points



- Query input

- Define bonds

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**

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 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**

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.

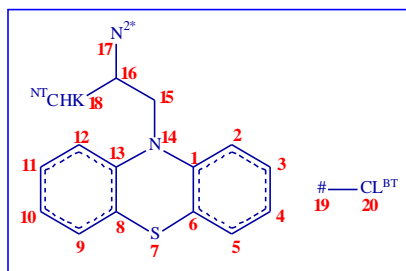
e.g. "NT 1,3" specifies a translation attribute NT at nodes 1 and 3.

? **NT 18**

? **BT 20**

?

- 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 other attributes

Define variable attachments

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

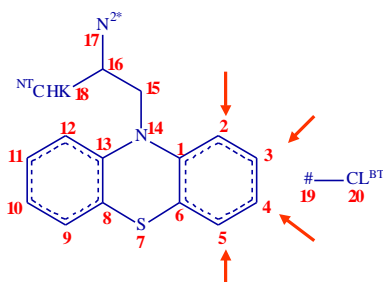
Variable Position specification

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) ?



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- Query input

- Define other attributes

Query input



Query verification

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

Attributes specified for the query are ticked off by default

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- Query input
- Query verification

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