



## Mini-Guide

November 2010

Merged Markush Service





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# 1 – MARKUSH DARC COMMANDS

## 1-1 ST Level Commands

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

### *ST Level Commands – Input Commands*

**BA** Specify or change structure database  
**CN** Compound Number search  
**QT** Query Text (alphanumeric input of query with Power-Editor)

### *ST Level Commands – Searching Commands*

**RE** Retrieve candidates (perform fragment search)  
**SB** Search Bit Screens (perform bit-screen search)  
**AA** Atom-by-Atom search (perform Atom-by-Atom search on candidates)  
**AA/Ri** Atom-by-Atom search on an Ri subset  
**SEARCH FULL** RE/SB + AA search on the current file  
**BT** Power Batch search on the latest R set  
**BT Ri** Power Batch search on a Ri subset  
**BT RX Ri** Power Batch search on an RX candidates in an Ri subset  
**BT ALL** RE/SB + Power Batch Search  
**SEARCH SAMPLE** Sample search on the current file  
**SEARCH** Same as SEARCH SAMPLE

### *ST Level Commands – Display Commands*

**LI** List Compound Numbers  
**LI RX** List RX Compound Numbers  
**VI** View structure answers  
**VI RX** View structure answers of RX candidates  
**VI FO** View Focus the parts of the answers which match the query structure  
**PARSE** Separate an answer set into different CN file-formatted lists  
**PARSE *name*** Separate a named CN list into different CN file-formatted lists

## ***ST Level Commands (LI,VI,VI FO) –Display Command Parameters***

- n1** To display answer number *n1* of the latest answer set (*VI FO 3* to display answer number 3 in View Focus)
- n1-n2** To display a range (*n1 to n2*) of answers contained in the latest answer set (*LI 1-6* to list from the 1<sup>st</sup> to the 6<sup>th</sup> CN)
- Ri** To display answers contained in the *Ri* answer set (*VI RX R3* to display the RX candidates contained in the R3 answer set)

## ***ST Level Commands – Housekeeping Commands***

- SV** Save query or answer set as a CN list
- RF** Recall File (recall saved batch, query, CN or Questel·Orbit list)
- ER** Erase (erase previously saved batch, query, CN or Questel·Orbit list)

## ***ST Level Commands – Save Commands***

- SV QU** Save a Query
- SV QU *name*** Save the Query with *name*
- SV CN** Save an answer set as a CN list
- SV CN *name*** Save the answer set with *name* as a CN list
- SV CN Ri** Save the answer set *Ri* as a CN list
- SV CN Ri *name*** Save the answer set *Ri* with *name* as a CN list
- SV CN RX** Save the RX candidates of an answer set as a CN list
- SV CN RX *name*** Save the RX candidates of an answer set with *name* as a CN list
- SV CN RX Ri *name*** Save the RX candidates of an answer set Ri with *name* as a CN list

## ***ST Level Commands – Recall File Commands***

- RF QU** Recall a Query
- RF QU *name*** Recall the Query with *name*
- RF CN** Recall a CN list
- RF CN *name*** Recall the CN list saved with *name*
- RF BT** Recall a Batch or Power Batch
- RF BT *name*** Recall a Batch or Power Batch with *name*
- RF QO** Recall a Questel·Orbit list
- RF QO *name*** Recall the Questel·Orbit list saved with *name*

## ***ST Level Commands – Erase Commands***

- ER R** Erase an answer set
- ER R x-y** Erase a range of answer sets (*x to y*)
- ER R x,y** Erase answer sets *x* and *y*
- ER QU** Erase a query
- ER QU *name*** Erase the query saved with *name*

*(Erase Commands cont'd)*

<b>ER CN</b>	Erase a CN list
<b>ER CN name</b>	Erase the CN list saved with <i>name</i>
<b>ER CN x-y</b>	Erase a range of CN lists ( <i>x</i> to <i>y</i> )
<b>ER BT</b>	Erase a Batch or Power Batch
<b>ER BT name</b>	Erase the Batch or Power Batch saved with <i>name</i>
<b>ER QO</b>	Erase a Questel·Orbit list
<b>ER QO name</b>	Erase the Questel·Orbit list saved with <i>name</i>

(Right-hand truncation can be used at erasing; e.g., *ER CN TEST+* for erasing all CN lists saved with a name starting with TEST)

***ST Level Commands – History Commands***

<b>HI R</b>	History of answer sets of the current week
<b>HI QU</b>	History of saved queries
<b>HI CN</b>	History of saved CN lists
<b>HI BT</b>	History of saved Batch or Power-Batch
<b>HI QO</b>	History of saved Questel·Orbit lists

***ST Level Commands – SDI Commands***

<b>SV SDI name</b>	Save an SDI query
<b>RF SDI name</b>	Recall an SDI answer set
<b>RF HISDI</b>	Recall all SDIs saved on an account
<b>HI SDI</b>	Listing of SDIs
<b>ER SDI name</b>	Erase an SDI query

***ST Level Commands – Other Commands***

<b>..BI</b>	Bibliographic system (switch to bibliographic system)
<b>BL</b>	Boolean Logic search
<b>FI</b>	Finish (log off of the MMS system)
<b>SUBACCT</b>	Billing to subaccount
<b>SUBACCT name</b>	Billing to subaccount <i>name</i>
<b>EMAIL</b>	Saves an email address on your account
<b>HELP</b>	Help menu
<b>INFO</b>	Information (display news or information)
<b>OP</b>	Options (change terminal options, cost, etc.)
<b>AC</b>	View cost estimator

## **1-2 QT Level Commands**

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

### ***QT Level Commands – Basic Commands***

**CN** Recall a Compound Number as a query  
**CA** Cancel entire query, a G group or attributes  
**GM** Group Markush: specify variable group being defined  
**GI** Group Identical: create a new group identical to an existing group

### ***QT Level Commands – Query Input Commands***

**GR** Graph: specify the skeleton of the query  
**BO** Bonds: specify the bonds in the query  
**AT** Atoms: specify the atoms in the query  
**FS** Free Sites: specify desired substitution in query  
**AP** Attachment Points: define attachments of G group to its father group  
**VP** Variable points of attachment: define points of variable attachment  
**ATTR** Attributes: define attributes on atoms or Superatoms in the query  
**VE** Verify: graphic verification of the query  
**VE TX** Verify: text verification of the query  
**FI** Finish query input: return to ST level

### ***QT Level Commands – Attributes***

**FS** Free Sites  
**TRA** Translation  
**CR** Chain/Ring  
**CH** Charges  
**AV** Abnormal Valency  
**AM** Abnormal Mass  
**PA** Polymer  
**DT** Deuterium/Tritium

### ***QT Level Commands – Chain/Ring Attributes***

#### **Chain**

**LO** Low (1 to 6 carbons)  
**MID** Middle (7 to 10 carbons)  
**HI** High (11 or more)  
**STR** Straight  
**BRA** Branched

#### **Ring**

<b>MON</b>	Monocyclic
<b>FU</b>	Fused
<b>SAT</b>	Saturated
<b>UNS</b>	Unsaturated

### *QT Level Commands – Translation Attributes*

<b>BT</b>	Broad translation
<b>NT</b>	Narrow translation
<b>ANY</b>	Both broad and narrow translation
<b>EQ</b>	Equal (no translation)

## **2 – MARKUSH DARC QUERY INPUT**

### **2-1 ELEMENT SYMBOLS**

1																	2																																																								
<b>H</b>																	<b>He</b>																																																								
3	4											5	6	7	8	9	10																																																								
<b>Li</b>	<b>Be</b>											<b>B</b>	<b>C</b>	<b>N</b>	<b>O</b>	<b>F</b>	<b>Ne</b>																																																								
11	12											13	14	15	16	17	18																																																								
<b>Na</b>	<b>Mg</b>											<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>Cl</b>	<b>Ar</b>																																																								
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<b>K</b>	<b>Ca</b>	<b>Sc</b>	<b>Ti</b>	<b>V</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>	<b>Co</b>	<b>Ni</b>	<b>Cu</b>	<b>Zn</b>	<b>Ga</b>	<b>Ge</b>	<b>As</b>	<b>Se</b>	<b>Br</b>	<b>Kr</b>																																																								
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### **2-2 Markush Darc Superatoms**

#### **Acyclic Hydrocarbons**

**CHK** Alkyl or alkylene

**CHE** Alkenyl or alkenylene

**CHY** Alkynyl or alkynylene

### Cyclic Systems

**ARY** Carbocyclic system, optionally fused, containing at least one benzene (aryl)

**CYC** Cycloaliphatic carbocyclic, optionally fused

**HEA** Monocyclic, aromatic heterocycle (heteroaryl)

**HET** Non-aromatic monocyclic heterocycle

**HEF** Fused heterocycle

### Metals

**MX** Any metal

**AMX** Alkali or alkaline earth metal

**A35** Group IIIA – VA metal – Al, Ga, In, Ge, Sn, Pb, Sb, Bi

**TRM** Transition metal excluding Lanthanum (La)

**LAN** Lanthanides including Lanthanum (La)

**ACT** Actinides

### Miscellaneous

**HAL** Halogen

**ACY** Acyl, i.e., residue after removing 1 or more OH from an acid

**DYE** Dye group or residue (chromophore, fluorophore)

**POL** Polymer, peptide residue

**PRT** Protecting group

**UNK** Undefined group

**PEG** Polymer end group

**XX** Any atom or group excluding hydrogen (display only)

### 2-3 Markush DARC Shortcuts

Shortcut	Definition	Shortcut	Definition
<b>CO2</b>	-COOH	<b>ET</b>	ethyl
<b>CO1</b>	-C(O)- (divalent)	<b>NPR</b>	n-propyl
<b>SO2</b>	-SO2- (divalent)	<b>IPR</b>	isopropyl
<b>SO3</b>	-S(O)2(OH)	<b>NBU</b>	n-butyl
<b>PO3</b>	-P(O)2(OH)	<b>SBU</b>	s-butyl
<b>PO4</b>	-OP(O)(OH)2	<b>TBU</b>	tert-butyl
<b>CN</b>	-CN	<b>IBU</b>	isobutyl
<b>NO2</b>	-NO2	<b>PH</b>	phenyl
<b>ACE</b>	-C(O)CH3		
<b>Cn</b>	alkylene where n is a user specified integer indicating chain length		
<b>MBE</b>	m-substituted benzene (divalent)		
<b>PBE</b>	p-substituted benzene (divalent)		
<b>OBE</b>	o-substituted benzene (divalent)		

## 2-4 Markush DARC Special Symbols

**X** any atom or superatom, except hydrogen  
**#** to specify variable points of attachment of a node to another part of the structure

## 2-5 Markush DARC Bonds

### **Bond Nature**

**SI** Single  
**DO** Double  
**TR** Triple  
**NO** Normalized  
**SN** Single or Normalized  
**DN** Double or Normalized  
**X** Undefined  
**Z** List

### **Bond Type**

**CY** Cyclic  
**AC** Acyclic  
**CX** Cyclic or acyclic

## **3 – ATTRIBUTES AND SUPERATOMS AVAILABLE IN MMS RECORDS ONLY**

### 3-1 Attributes

**MU** Multiplier  
**SP** Position of substitution on amino acids  
**DL** D, L, DL amino acid configuration

### 3-2 Peptides Superatoms

<b>ABU</b>	Aminobutyric acid	<b>LEU</b>	Leucine
<b>ALA</b>	Alanine	<b>LYS</b>	Lysine
<b>ARG</b>	Arginine	<b>MET</b>	Methionine
<b>ASN</b>	Asparagine	<b>NLE</b>	Norleucine
<b>ASP</b>	Aspartic Acid	<b>NVA</b>	Norvaline
<b>ASU</b>	Aminosuberic acid	<b>ORN</b>	Ornithine
<b>CYS</b>	Cysteine	<b>PHE</b>	Phenylalanine

<b>GLN</b>	Glutamine	<b>PRO</b>	Proline
<b>GLP</b>	Pyroglutamic acid	<b>SAR</b>	Sarcosine
<b>GLU</b>	Glutamic acid	<b>SER</b>	Serine
<b>GLY</b>	Glycine	<b>STA</b>	Statine
<b>HYC</b>	Homocysteine	<b>THR</b>	Threonine
<b>HIS</b>	Histadine	<b>TRP</b>	Tryptophan
<b>HSE</b>	Homoserine	<b>TYR</b>	Tyrosine
<b>ILE</b>	Isoleucine	<b>VAL</b>	Valine

The X (unspecified) bond should be used with the Peptide superatoms.

## 4 - QUESTEL COMMANDS

### 4-1 Basic Commands

<b>BA or FI</b>	Database (File) selection
<b>BA or FI name</b>	Specified database (file) selection
<b>LI or PRT</b>	List (display) answers online
<b>ST</b>	Stop to logoff
<b>..ST MDARC</b>	Stop and switch to Markush DARC
<b>MEM</b>	Memory to extract terms from an answer set ( <i>MEM TEST /XPN</i> to save the patent number in the file <i>TEST</i> )
<b>JOIN</b>	To transfer Compound Numbers from Questel·Orbit to MMS
<b>HI</b>	History

### 4-2 Account Management Commands

<b>OP</b>	Options: to set options for this session only
<b>POP</b>	Permanent Options
<b>SUBACCT</b>	Subaccount
<b>SUBACCT name</b>	Subaccount to <i>name</i>

### 4-3 List Processing Commands

<b>*MD listname /CN</b>	to process a list from Markush DARC
<b>*MDARCLIST listname /CN</b>	to process a list and audit compound numbers with no postings (*MDARCLIST can be used in place of *MD for the following variations)
<b>*MD listname.ROLE /CN</b>	to process a list of compound numbers from Markush DARC, limiting with a ROLE qualifier
<b>*MD listname.R1.R2 /CN</b>	to process a list of compound numbers from Markush DARC, limiting with several role qualifiers (R1, R2,...: up to six roles)
<b>*MD Ri /CN</b>	to process an R answer set from Markush DARC
<b>*MD Ri.ROLE /CN</b>	to process an R answer set from Markush DARC, limiting with a role qualifier

<b>*MD Ri.R1.R2 /CN</b>	to process an R answer set from Markush DARC, limiting with several role qualifiers that are ORed together (R1, R2,...: up to six roles)
<b>*MEM field</b>	to process a memory list in the specified field
<b>*MEMS field</b>	to process a memory sort list in the specified field

#### **4-4 Using the JOIN Command**

<b>JOIN TO filename VIA listname GEN</b>	Only markush CNs are extracted
<b>JOIN TO filename VIA listname SPE</b>	Only specific CNs are extracted
<b>JOIN TO filename VIA listname ROLE N, M,</b>	CNs are extracted with specific role indicators n, m; (up to 10 role indicators)
<b>JOIN SS n TO filename VIA listname</b>	Join on Search Set n
<b>JOIN x-y TO filename VIA listname GEN</b>	Set up of an interval

(filename = WPIM or MPHARM)  
(listname = name up to 8 characters)

#### **4-5 Truncation**

<b>Types</b>	Left-hand Right-hand Embedded
<b>Symbols</b>	+ Open truncation (unlimited) ? Limited truncation (zero or one character per ?) # Mask (exactly one character per #)

#### **4-6 Operators**

##### **Boolean**

<b>AND</b>	Intersection
<b>OR</b>	Union of sets
<b>NOT</b>	Exclusion of sets

##### **Proximity**

<b>W</b>	Adjacent terms in order specified
<b>xW</b>	Adjacency in the order specified within x terms
<b>D</b>	Adjacent terms in any order
<b>xD</b>	Proximity within x terms in any order

##### **Location**

<b>S</b>	In the same sentence
<b>P</b>	In the same paragraph
<b>L</b>	Link
<b>F</b>	In the same field
<b>NOTS</b>	NOT in the same sentence
<b>NOTP</b>	NOT in the same paragraph
<b>NOTF</b>	NOT in the same field

## 5- TRANSFERRING RESULTS FROM MMS TO Q•O

### 5-1 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.
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).

### 5-2 Search and Display Command Summary

#### **FILE PHARM**

**\*MD <NAME1> /CN**

**PRT MAX IMG SET** (optional to see records with images in PHARM)

**MEM <NAME2> /XPN**

#### **FILE DWPI**

**\*MD <name1> /CN**

**\*MEM <NAME2> /XPN**

**1 OR 2**

**PRT MMSF IMG SET**

## 6- MMS FILE SEGMENTS AND ROLES

### 6-1 File Segments

#### **CPI Sections**

**A** Section A

**B** Section B or C

E Section E

**General**

Y Mixture  
Z Salt  
1 Registry

**Polypeptides**

P Polypeptide

**Non-polymeric Compounds**

C Coordination compound/Complex  
L Oligomer  
W Extended structure  
M Metals and alloys  
V Ordinary organic chemicals  
7 Inorganics

**Polymers**

F Any polymer

**Backbone**

H Homopolymer/homocondensate  
S Simple binary condensate  
J Alternating copolymer/condensate  
K Block copolymer/condensate  
R Random copolymer/condensate  
N Natural polymer  
Q No backbone

**Number of components in backbone**

2 2 monomers/condensates  
3 3 monomers/condensates  
4 4 monomers/condensates  
T End-modified polymer  
5 Surface-modified polymer  
U Unmodified polymer

**Modification**

X Crosslinked polymer  
D Derivative polymer  
G Grafted polymer

**6-2 Roles**

A Substance analyzed or detected  
C Catalyst  
D Detecting agent

<b>E</b>	Recipient
<b>K</b>	Known compound
<b>M</b>	Component of mixture
<b>N</b>	New compound
<b>P</b>	Known compound produced
<b>Q</b>	Product defined in terms of starting materials
<b>R</b>	Removing/purifying agent
<b>S</b>	Starting materials or reactant
<b>T</b>	Therapeutically active substance
<b>U</b>	Use of a compound for a new application
<b>V</b>	Reagent
<b>X</b>	Substance removed
<b>Z</b>	Miscellaneous

## 7- MMS SYSTEM LIMITS

### 7-1 Answer Sets

<b>Number of answer sets available:</b>	90
<b>Lifetime of answer sets:</b>	Current week
<b>Number of answers:</b>	1,000,000 per answer set

### 7-2 Batch Search

<b>Number of candidates you can process in batch:</b>	1,000,000 per batch request
<b>Number of Batch or Power Batch requests:</b>	20 per day

### 7-3 Saved Queries and CN Lists

<b>Number of saved CN lists:</b>	90
<b>Number of saved queries:</b>	20

### 7-4 Structural Queries

<b>Number of atoms:</b>	255
<b>Number of G groups:</b>	20
<b>Number of levels of nesting:</b>	3

### 7-5 CN Lists

<b>Number of CNs in QP lists using JOIN to MMS:</b>	50000
<b>Number of CNs in SV lists to Questel:</b>	60000

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