

MMS™

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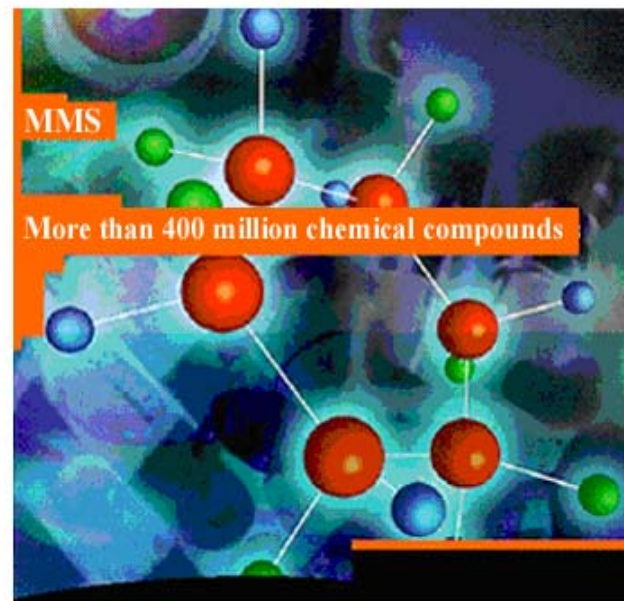
or contact:

MMS HELP DESK
In US and Canada: 800-634-9978
In Europe: 8000-783-7835

Questel·Orbit, S.A. Headquarters
4, Rue des Colonnes
75082 Paris Cedex 02
France

Questel·Orbit, Inc.
1725 Duke St. Suite 625
Alexandria, VA 22314
USA

US Questel Help Desk Telephone: 800-456-7248



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TABLE OF CONTENTS

1 – MARKUSH DARC COMMANDS.....	3
1-1 ST LEVEL COMMANDS	3
1-2 QT LEVEL COMMANDS	6
2 – MARKUSH DARC QUERY INPUT	8
2-1 ELEMENT SYMBOLS	8
2-2 MARKUSH DARC SUPERATOMS	8
2-3 MARKUSH DARC SHORTCUTS	9
2-4 MARKUSH DARC SPECIAL SYMBOLS	10
2-5 MARKUSH DARC BONDS	10
3 – ATTRIBUTES AND SUPERATOMS AVAILABLE IN MMS RECORDS ONLY	11
3-1 ATTRIBUTES	11
3-2 PEPTIDES SUPERATOMS	11
4 - QUESTEL·ORBIT COMMANDS.....	12
4-1 BASIC COMMANDS	12
4-2 ACCOUNT MANAGEMENT COMMANDS	12
4-3 LIST PROCESSING COMMANDS	12
4-4 USING THE JOIN COMMAND	13
4-5 TRUNCATION	13
4-6 OPERATORS	13
5- TRANSFERRING RESULTS FROM MMS TO Q·O.....	14
5-1 PROCEDURE.....	14
5-2 SEARCH AND DISPLAY COMMAND SUMMARY	14
6- MMS FILE SEGMENTS AND ROLES.....	15
6-1 FILE SEGMENTS	15
6-2 ROLES	16
7- MMS SYSTEM LIMITS	17
7-1 ANSWER SETS	17
7-2 BATCH SEARCH	17
7-3 SAVED QUERIES AND CN LISTS	17
7-4 STRUCTURAL QUERIES	17
7-5 CN LISTS.....	17

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
OS File Segments (Other Specifications)

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 1st to the 6th 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)

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

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

ST Level Commands – SDI Commands

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

ST Level Commands – Other Commands

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

MON	Monocyclic
FU	Fused
SAT	Saturated
UNS	Unsaturated

QT Level Commands – Translation Attributes

BT	Broad translation
NT	Narrow translation
ANY	Both broad and narrow translation
EQ	Equal (no translation)

2 – MARKUSH DARC QUERY INPUT

2-1 ELEMENT SYMBOLS

1 H																	2 He														
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne														
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar														
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr														
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe														
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn														
87 Fr	88 Ra	89 Ac	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	110 Uun																						
																		58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
																		90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

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

ABU	Aminobutyric acid	LEU	Leucine
ALA	Alanine	LYS	Lysine
ARG	Arginine	MET	Methionine
ASN	Asparagine	NLE	Norleucine
ASP	Aspartic Acid	NVA	Norvaline
ASU	Aminosuberic acid	ORN	Ornithine
CYS	Cysteine	PHE	Phenylalanine
GLN	Glutamine	PRO	Proline
GLP	Pyroglutamic acid	SAR	Sarcosine
GLU	Glutamic acid	SER	Serine
GLY	Glycine	STA	Statine
HYC	Homocysteine	THR	Threonine
HIS	Histadine	TRP	Tryptophan
HSE	Homoserine	TYR	Tyrosine
ILE	Isoleucine	VAL	Valine

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

4 - QUESTEL·ORBIT COMMANDS

4-1 Basic Commands

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

4-2 Account Management Commands

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

4-3 List Processing Commands

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

4-4 Using the JOIN Command

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

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

4-5 Truncation

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

4-6 Operators

Boolean

AND	Intersection
OR	Union of sets
NOT	Exclusion of sets

Proximity

W	Adjacent terms in order specified
xW	Adjacency in the order specified within x terms
D	Adjacent terms in any order
xD	Proximity within x terms in any order

Location

S	In the same sentence
P	In the same paragraph
L	Link
F	In the same field
NOTS	NOT in the same sentence
NOTP	NOT in the same paragraph
NOTF	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 ***MDARCLIST <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 MAX PLUS CN 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

***MDARCLIST <name1> /CN**

***MEM <NAME2> /XPN**

1 OR 2

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

7- MMS SYSTEM LIMITS

7-1 Answer Sets

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

7-2 Batch Search

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

7-3 Saved Queries and CN Lists

Number of saved CN lists: 40
Number of saved queries: 20

7-4 Structural Queries

Number of atoms: 255
Number of G groups: 20
Number of levels of nesting: 3

7-5 CN Lists

Number of CNs in QP lists using JOIN to MMS: 50000
Number of CNs in SV lists to Questel: 10000

Index

A

A35, 9
AA, 3
Abnormal Mass, 6
Abnormal Valency, 6
ACT, 9
ACY, 9
Acyclic Hydrocarbons, 8
AMX, 9
ANY, 7
Any atom, 9
AP, 6
ARY, 9
AT, 6
Atom-by-Atom search, 3
Attachment Points, 6
ATTR, 6
AV, 6

B

BA, 3
Batch search, 3
BO, 6
Bond Nature, 10
Bond Type, 10
Bonds, 10
Boolean, 13
Broad translation, 7
BT, 3, 7

C

CA, 6
Cancel entire query, 6
CH, 6
Chain/Ring, 6
Chain/Ring Attributes, 7
Charges, 6
CHE, 8
CHK, 8
CHY, 8
CN, 3, 6
CR, 6
CYC, 9
Cyclic Systems, 9

D

Define Attributes, 6
Deuterium/Tritium, 6
Display Commands, 3
DT, 6
DYE, 9

E

Element Symbols, 8
EMAIL, 5

EQ

Equal translation, 7
ER, 4
Erase a Batch or Power Batch, 5
Erase a CN list, 5
Erase a query, 5
Erase a Questel-Orbit list, 5
Erase an answer set, 4
Erase Commands, 4

F

File Segments, 3, 15
Free Sites, 6
FS, 6

G

GI, 6
GM, 6
GR, 6

H

HAL, 9
Halogen, 9
HEA, 9
HEF, 9
HET, 9
HI, 5, 7, 12
History Commands, 5
Housekeeping Commands, 4

I

Input Commands, 3

J

JOIN, 12, 13

L

LAN, 9
LI, 3
List Compound Numbers, 3

M

***MD**, 12
***MDARCLIST**, 12
MEM, 12
Metals, 9
MX, 9

N

Narrow translation, 7
NT, 7

O

Operators, 13

OP, 5, 12
Options, 5, 12
OS, 3
Other Specifications, 3

P

PA, 6
PARSE, 3
PEG, 9
Peptide Superatoms, 11
POL, 9
Polymer, 6
POP, 12
Proximity, 13
PRT, 9

Q

QO lists, recalling, 4
QT, 3, 6
QT Level Commands, 6
Questel-Orbit Commands, 12

R

RE, 3
Recall a Batch or Power Batch, 4
Recall a CN list, 4
Recall a Query, 4
Recall a Questel-Orbit list, 4
Recall File Commands, 4
Retrieve Candidates, 3
RF, 4
Roles, 16

S

Sample Search, 3
Save a Query, 4
Save an Answer Set, 4
Save Commands, 4
Save the RX Candidates, 4
SDI Commands, 5
SEARCH, 3

Search Bit Screens, 3
SEARCH FULL, 3
SEARCH SAMPLE, 3
Searching Commands, 3
Shortcuts, 9
Special Symbols, 10
Specify the atoms, 6
Specify the bonds, 6
Specify the skeleton, 6
ST, 3
ST Level Commands, 3
Subaccount, 5
SUBACCT, 5, 12
Superatoms, 8
SV, 4
System Limits, 17

T

TRA, 6
Transferring results from MMS to QO, 14
Translation, 6
Translation Attributes, 7
TRM, 9
Truncation, 13

U

UNK, 9

V

Variable points of attachment, 6
VE, 6
Verify, 6
VI, 3
VI FO, 3
View Focus, 3
View Structure Answers, 3
VP, 6

X

X atom, 10
XX, 9