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### I. Overview

This document explains how to read the CQSAR distribution off of the CD, and how to install and configure it for your system. Installation requires a privileged account (specifically: CMKRNL privilege and the ability to create a top-level directory)

The two most important configuration steps are setting the CQSAR disk device (covered on the top of page 3) and updating the license key (covered on lower half of page 5). Follow these steps carefully—when people have trouble with the CQSAR installation, the problem is usually with one of these two steps.

## II. Reading the CD

In what follows, it is assumed that the CQSAR system will be placed on the `dka0`: disk drive, and that the CD is being read from the `dka400`: CD drive. Throughout, substitute the names appropriate for your disk and CD drive.

### Disk space requirements

The size of the CQSAR system varies considerably, depending on the databases supplied, and so forth. Approximate values are 20,000 blocks for the 'economy' package, 75,000 blocks for the 'regular' and 'super' packages, and 150,000 blocks for the 'qsar' package. Look at the label on the CD to see which version you have received.

If you cannot, in the long term, spare the disk space consumed by the distribution, contact BioByte for details on exactly which files can be removed after the installation is complete. If you do not have the required disk space free now, do not proceed with the installation. Instead, contact Biobyte for further instructions.

### Create a temporary directory

The CQSAR system must be installed at a top-level directory. To create such a directory usually requires an account that has special privileges, such as `SYSTEM`. If need be, login to such an account now. You will then need to create a temporary directory to hold the contents of the CD, which you can delete after the installation is complete:

```
create /directory dka0:[temp]
```

### Copy the CQSAR system from CD

To transfer the contents of the CD to disk, issue the following commands:

```
mount /system dka400: biobyte
set default dka0:[temp]
copy dka400:[alpha]*.* *
```

or, if you are installing on a VAX:

```
copy dka400:[vax]*.* *
```

### Uncompress the QSAR.BKP-GZ file and restore the saveset to disk

The QSAR.BKP saveset is compressed with a program called GZIP, and needs to be uncompressed before you can restore the saveset to disk. If you have GZIP already installed on your system, you can skip the first step:

```
GZIP == "$dka0:[temp]GZIP"
gzip -d QSAR.BKP-GZ
$ @gzfix QSAR.BKP
```

(this last step is to fix the file attributes for the saveset, which are changed by GZIP)

You are now ready to fully expand the QSAR.BKP file:

```
backup QSAR.BKP/SAVE_SET dka0:[*...]
```

### Deleting the previous CQSAR release.

Each new CQSAR release is placed in a separate tree, `[qsar.verxxx]` where the version number is `xxx`, so there are no overlapping files. Thus, you are free to keep running both versions, but can also delete one release without any danger of affecting another. Though you may wish to keep the previous CQSAR release on disk until you are sure that the new system is working, you will eventually want to reclaim the disk space that it occupies.

The following sequence of commands can be used to delete the old release (here called '1.85'; you must substitute the correct name for your site):

```
@dka0:[qsar.ver185]login man
merlin_deinstall
qsar_deinstall
set def dka0:[qsar]
delrecursive ver185.dir
```

### III. Configuring CQSAR

Before you run any CQSAR programs, you need to edit the login command file, [qsar.ver410]login.com. There are five possible changes to make. A description of each change is given below, along with the relevant portion of the login.com.

#### 1. Define the program disk [this change is *mandatory*].

The definition of QSAR\$DISK must be changed to refer to the actual disk upon which the [QSAR] directory resides. Don't forget the colon if you're using a 'raw' device name! If the CQSAR program will be run on a cluster, make sure that the disk name is valid for all nodes of the cluster.

```
$!-* 1 *-----
$! Define program disk.
$!   Enter the name of the disk upon which the QSAR system resides. If
$!   your system is part of a VAXcluster, be sure to give the full
$!   'cluster name' of the disk, so all nodes can run the QSAR program.
$ define /nolog qsar$disk dka0:
```

#### 2. Define the electronic mail address for bug reports [this change is *optional*, but strongly encouraged].

When this is defined, you will be able to submit bug reports, or just ask questions, from within the qsar program, via electronic mail. Although this step is not obligatory, I strongly encourage you to determine the correct procedure for mailing, and to define it here. If you are not sure what to do, ask your local system administrator how an Internet address should be specified.

```
$!-* 2 *-----
$! Define mailing addresses for MedChem accounts (for bug reports, datasets).
$!   DECNET sites vary in the means they use to send mail to Internet
$!   addresses. Locally, we send mail to a gateway node. Ask your system
$!   administrator you address mail for Internet sites.
$ define /nolog mmedlin   "ymir::in%"mmedlin@clogp.pomona.edu" " "
$ define /nolog biobyte  "ymir::in%"clogp@biobyte.com" " " "
```

#### 3. Define the aliases for print command(s) [this change is *optional*].

The CQSAR system has only one program for making hardcopy, but it can also call upon the programs already set up on your machine to do printing for it. One alias must be defined for each print command that you wish to define. Here, the default print command, qsar\$print, calls a program that sends the out put to printers attached directly to terminals. The second command, qsar\$print1, spools jobs to a laserprinter. The third print command sends PostScript to the laserprinter. See the Notes for Managers section for more information.

```
$-----
$! Define the command(s) for printing.
$!   Enter the command you use to print files at your site. It may be
$!   as simple as 'print', or may be fancier than that. Multiple definitions
$!   may be made, for alternate types of printing. (see manual for details)
$!   Individual users are free to override/reassign these definitions.
$ qsar$print   ::= "$qsar$root:[exe]drip"
$ qsar$print1  ::= "@qsar$dka0:[apps.print]laser dummy"
$ qsar$print2  ::= "@qsar$dka0:[apps.print]laser /form=post "
```

#### 4. Define the location of the CQSAR databases [this change is *optional*].

By default this value points to the databases which Pomona distributes, but you may want to change it if you make local copies and/or databases.

```
$!-* 4 *-----
$! Define the location of the QSAR databases.
$! By default this value points to the databases which Pomona distributes,
$! but you may want to change it if you make local copies and/or databases.
$ define /nolog qsar$bigdata qsar$root:[data.bigdata]
```

#### 5. Define local commands [this change is *optional*].

The programs savol and concord are needed for the add savol command to work in qsar; they are *not* provided with CQSAR. Contact Tripos Associates for licensing information.

```
$!-* 5 *-----
$! Local commands
$! You have the option of using the MedChem version (3.55) supplied
$ qsar$savol == "$disk$qsar:[apps.savol]savol2 "
$ qsar$concord == "$day_exe:day_concordusr "
```

## IV. Installing and Managing Shared Memory

The `merlin_install` command is *required* in order to run both the `qsar` and `merlin` programs. If you do not plan on running these programs (e.g. you have only licensed the 'economy' package), then this section *should be* skipped.

In what follows, it is presumed that you have made the necessary changes to the `login.com` described on the previous page. When ready, login to the CQSAR system as a manager with the command:

```
@[qsar.ver410]login manager
```

### Installing shared memory

It is simple to install the CQSAR shared memory. The following command performs all of the necessary actions:

```
merlin_install
```

To undo the installation of shared memory, use the command:

```
merlin_deinstall
```

These procedures must be run by an account with CMKRNL privilege (such as the SYSTEM account).

To verify the installation of the shared memory, you could run the `install` command, and `list` the shared images. You should see four images for the current release (the device name will of course be different):

```
dka0:<QSAR.VER410.MEDCHEM.VER355.MERLIN.MASTER.SHARED>.EXE
  BSHARE_MASTER;1 Open Shar Lnkbl Wrt
  PSHARE_MASTER;1 Open Shar Lnkbl Wrt

dka0:<QSAR.VER410.MEDCHEM.VER355.MERLIN.QSAR.SHARED>.EXE
  BSHARE_QSAR;1 Open Shar Lnkbl Wrt
  PSHARE_QSAR;1 Open Shar Lnkbl Wrt
```

Another (quick-and-dirty) method: just enter `qsar`; if you get the `qsar>` prompt, the installation was successful (enter `quit` to return to VMS).

If the installation should fail (with a verbose set of messages regarding insufficient free global pages or global sections), or if users see the warning `shareable images must be installed when starting qsar or merlin`, then installation was *not* successful. If this happens, it is almost certainly due of a lack of system resources: global pages and/or global sections. The system manager must either 1) remove other images from shared memory or 2) modify certain system parameters and reboot the system. The error messages generated by the `merlin_install` procedure should describe the problem in sufficient detail to diagnose the problem.

This procedure for installing shared memory will need to be repeated after system reboots. It might be a good idea to call the `merlin_install` (and perhaps `merlin_deinstall`) from your local system-startup (shutdown) command files. For example, the following lines might be added to the appropriate `SYSTARTUP.COM` which is run a boot time:

```
@dka0:[qsar.ver410]login manager
merlin_install
```

### Managing shared memory

Both sets of shared images are 'pre-loaded' with the proper data, so no further action is required on your part, in the course of normal operations. Should the shared images ever become corrupted, you can reload them with the following procedure:

1. Start MERLIN with the command `merlin master` command
2. Go to the 'setup' menu, and chose the 'lock/unlock' option.  
You type 8 and then 8 again. Answer *yes* to the prompt.
3. Wait while the pools load, then quit MERLIN.  
Type 0 (zero) twice, and answer *yes* to the prompt.

Repeat the procedure, but in step 1 use the command `merlin qsar`.

How would you know if there is a problem? When you first start `merlin`, at the upper left of the screen is a count of the elements in the pool. For 'master' this should be about 28000, for 'qsar' about 45,000.

## V. Running CQSAR programs

### Logging in to CQSAR

In order to run any CQSAR program, each time you log in you must first run the CQSAR login script:

```
@dka0:[qsar.ver410]login
```

One way of doing this is for users to place this line in their own LOGIN.COM. You can always edit your LOGIN.COM, whatever your current directory, with the command:

```
edit sys$login:login.com
```

The login procedure takes a single argument, either *user* or *manager*; the default is *user*. There is no reason to use the *manager* level access except when installing or deinstalling shared memory. In either case, this *login.com* script must be run to access *any* BioByte programs, even if you do not plan on running the *qsar* program itself.

**Managers:** If all, or most, users of the machine on which the CQSAR system has been installed will be using this software, you might consider running the CQSAR login script from the system-wide login command file.

### Running programs

Executables which you should be able to run now include (depending on the contents of and license on the CD):

Main CQSAR programs	qsar	merlin	udrive	thor	genie	
QSAR utilities	merlin_install		merlin_deinstall			
THOR utilities	thorbuild	thorsize	thorsum	thorlist	thortosmi	thordump
SMILES utilities	usmiles	pssmiles	cct			
Batch utilities	bprep	bdrive				
Terminal utilities	termreset	qtermtype				
Public utilities (non-Biobyte)	perl	most				

Most of these programs will provide a screen of help if you call them with the */help* switch, e.g. *thor /help*. Many of these programs will prompt you to determine your terminal type (see next page for further information).

### License Manager

Access to BioByte programs is controlled by a 'license key' file. The key is designed to ensure that CQSAR programs are run only on one 'licensed' machine. Further, the distributed key may restrict access to certain programs and databases.

The CQSAR CD is distributed with a 'demonstration' key which will allow it to run on any machine, so you are able use the system without requiring immediate contact with BioByte. However, to get the proper key which will allow full access to the software and databases, you *must* edit the license file and generate a 'canonical' version, which you must send to BioByte. From this information, we generate the new key.

To get your full key, first, edit the file *qsar\$license:license.txt* with your favorite text editor (but login to the CQSAR system first, as described above). Fill in the fields as indicated by the comments contained throughout. Before we send the CD to you, we will fill in as many fields as is practical, your name, address, phone, so you do not need to re-enter these (but check them for accuracy). Be sure to remove the word 'demonstration' when selecting the 'package'.

The save your changes, exit editor, then enter the command (at the '\$' prompt):

```
@[qsar.ver410.com]lman
```

This reads the license file you just modified and transforms it, generating a 'canonical' license file, *license.dat*. This newly generated file (*not* *license.txt*) should be sent to BioByte by email (*clogp@biobyte.com*) or FAX (909-624-1398). When we receive this file, we will generate a 'key', a 16 digit code, which we will send to you. When you enter this code on the 'key' line of the *license.dat* file, it will enable access to all the proper programs and databases.

## Terminal Type

In order to use the graphics capabilities of your terminal with the CQSAR programs, you must tell the programs' input/output package (aka PMCIO) what type of terminal you are using. When the program does not know what terminal type to use, it automatically queries you with the following line:

```
(TERMINAL) Enter device type (or ? or "quit"):
```

If you enter a '?', you receive the following table:

Possible device types:

### Standalone ("dumb") terminals

generic non-graphics	GLASS DUMB
VT100 nongraphics	VT100 VT100BIG VT100TALL
VTxxx graphics	VT240GRAPHON VT340 DECTERM VT640
various C.Itoh	CIT201 CIT300 CIT310 CIT414AH CIT467 CIT467H CIT8510
Lear Siegler	710x ENVISION
TEK	TEK4105 TEK4107 TEK4207 T4207
Miscellaneous	GR301 HP150 HP2623A MG200 MIME740G MX4000 RAMTEK SELANAR

### Terminal emulation for Macintosh

Tripos Nitro	NITRO
TEK TGRAFMAC	VERSATERM VERSATERM2

### Terminal emulation for PC

TEK	EMU4105 EMU4107 EMUTEK TGRAF
VT340	ZSTEM

### Printers

BW/color PostScript	PS CPS
HP Laserjet	LASERJET
dumb lineprinter	LP132 LP80

Enter device type (or ? or "quit"):

These are all of the pre-written 'terminal capability files'. You must select one of these to proceed further. If you have a non-graphics terminal, use 'vt100' (or 'dumb'). If your terminal is/emulates a DEC VT240, use 'vt240', and so on. Note that there are several TEK formats to choose from. 'versaterm' and 'tgraf' are for use with the Macintosh and PC terminal-emulator programs of the same names.

If your specific terminal does not appear in this list, experiment with some of the existing capability files; it may be that one of them, if not a perfect match, is good enough to work with. As a last resort, you can write a new capability file. Call the MedChem support number for more information.

If you consistently use a single terminal, and do not wish to be bothered with repeatedly entering the terminal type, you can put a line of the following form in your login.com file:

```
qtermtype vt240
```

where you must replace vt240 with the appropriate terminal designation.

## VI. Notes for Managers

### Useful symbols

Enter `qsarsymbols` to see the symbols and logicals defined when you run the `login.com` procedure. From the second page of that display, here are some of the most useful manager symbols:

<code>QSAR_REQUIRE</code>	Show minimum UAF settings an account needs to run QSAR
<code>QSAR_PROFILE</code>	Edit startup options and aliases
<code>QSAR_GLOBAL</code>	Edit startup global settings
<code>QSAR_HELP</code>	Rebuild system startup file (needed after use of <code>QSAR_PROFILE</code> or <code>QSAR_GLOBAL</code> )

Currently, the output of the `qsar_require` command should be:

At minimum, the following process limits are required to run QSAR:

("--" = don't care)

<code>Maxjobs:</code>	--	<code>Fillm:</code>	20	<code>Byt1m:</code>	--
<code>Maxacctjobs:</code>	--	<code>Shrfillm:</code>	--	<code>Pbyt1m:</code>	--
<code>Maxdetach:</code>	--	<code>BI01m:</code>	--	<code>JTquota:</code>	--
<code>Prclm:</code>	2	<code>DI01m:</code>	--	<code>WSdef:</code>	--
<code>Prio:</code>	--	<code>AST1m:</code>	--	<code>WSquo:</code>	512
<code>Queprio:</code>	--	<code>TQE1m:</code>	--	<code>WSextent:</code>	1024
<code>CPU:</code>	--	<code>Enqlm:</code>	15	<code>Pgflquo:</code>	60000

In general, the larger the `WSextent`, the better, especially for the database.

### Printing

To illustrate the proper use of the QSAR printing system, let me describe how it is set up here at Pomona. We have three methods for printing: sending output from terminals to dot-matrix printers connected directly to those terminals, and spooling jobs to a laserwriter through a print queue (the later may be plain text or PostScript). Users thus have three commands available from DCL: `printlocal`, `printlaser` and `printpost`.

This setup is mirrored exactly from within the QSAR program. First, as explained in the Configuring section, three symbols for printing are set. On our system they have the values:

```
qsar$print ::= "$qsar$root:[exe]drip"
qsar$print1 ::= "@qsar$dka0:[apps.print]laser dummy"
qsar$print2 ::= "@qsar$dka0:[apps.print]laser /form=post dummy"
```

Then, two aliases are set for the QSAR program. From the `qsar_profile.dat` (which can be edited with the command `qsar_profile`):

```
alias printlocal print /style=0
alias printlaser print /style=1
alias printpost print /style=2
```

Note that `/style=0` corresponds with `qsar$print`, and `/style=1` with `qsar$print1`, etc. The result is simple: our users have exactly the same print functions available from DCL and `qsar`. The number of styles available is essentially unlimited. Simply define a DCL symbol `qsar$printn` for the  $n^{\text{th}}$  type of printing, then set a `qsar` alias to match. After making the needed changes, rebuild system startup file with the command `qsar_help`.

### Location of THOR databases

The THOR databases distributed with this release of the `qsar` program reside at:

```
[qsar.ver410.medchem.ver355.bigdata]
```

If you already use a previous release of MedChem software, and wish to place these databases with your existing ones, you will need to move the files from this directory to the directory where the other public THOR databases are kept. One typical place is `[medchem.ver354.bigdata]`, but it varies from site to site. Then re-define the value of the logical `qsar_mc$bigdata` to point to the new location; the logical is defined in the file `qsar$root:[medchem.ver355]login.com`

## VII. Common Questions

Q: I get an error message like the following when I enter the command "qsar":

```
%DCL-W-ACTIMAGE, error activating image BSHARE_QSAR_VER410
-CLI-E-IMGNAME, image file
QSAR$dkka0:[QSAR.VER410.MEDCHEM.VER355.MERLIN.QSAR.SHARED]BSHARE_QSAR.EXE;1
-SYSTEM-F-NOTINSTALL, writable shareable images must be installed
```

A: You need to install shared memory before you can run QSAR. You can do this with the command `merlin_install`, but you must be using a privileged account to do this.

Q: Why can't I save from QSAR?

A: If the program license is still running on the 'demonstration' license, certain functions, such as saving, are disabled. When the demonstration license is in effect, most CQSAR programs bring up a banner which explains this fact. After the demonstration license expires, no programs

Q: How can a get graphical depictions of molecules on my terminal? Can I also print these?

A: CQSAR software can display images on a variety of terminals, but you must first tell the program what hardware you are using--it cannot be determined automatically. Use `qtermtype` to list and set supported terminal types. Available 'terminals' include popular Macintosh and PC terminal emulators. The QSAR program can generate PostScript output (the program must be configured properly—see section VI) with `printpost`; terminal emulators generally have their own system for image capture and printing.