Target Chromatography Software

1. SCOPE AND APPLICATION

1.1. Target is a chromatography software package that is used throughout the Chemistry Section. Target is used for GC chromatographic - data processing, reporting and storage. It runs on the DEP network.

1.2. This SOP will address basic background information necessary for processing samples using Target software.

1.3. This is not a comprehensive document on Target. To master many of the finer points of Target and to get more information on the options discussed below see the REFERENCE in section 8.

2. TARGET ACCESS

2.1. The chromatographic hardware (i.e., GC,) must be connected to EZChrom data acquisition system from Scientific Software Inc., which acquires data from the instrument and transfers the files to the network computer system. Each data file is exported from EZChrom to Target, rawdata - ("Z"- and the Laboratory Information Management System (LIMS) uploadable files for the results are placed on the "Tlhlab1" drive in LIMS_UPLOAD subdirectory for each instrument.

2.2. Target may be accessed from each PC on which the Target software has been installed. To log on click on the "Target Browser" icon and enter your password (case sensitive).

3. TARGET BROWSER

3.1. Target comprises of eight major components: TARGET Browser, Utilities, Data Surveyor, Edit Sample, Edit Method, Process, Target Review, and System Administration. Launching the Target software opens two windows: a main Target Browser window and an Xstatus window that only informs about the operations currently being performed by the program. The Target Browser window resembles and works like Windows Explorer. The screen consists of three major parts: the toolbars at the top, the directories on the left and the subdirectories or the organic groups (eg GC, LC) on the right. Target Menu functions may be accessed from drop-down menus, by clicking on the appropriate icons or by highlighting the file of interest, right-clicking on it, and choosing from the drop-down menu. The method currently in use is always displayed in the tool bar menu.

3.2. The subdirectory for each kind of instrument is further subdivided into instruments. Each instrument in turn has the following directories:

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3.2.1. Detector (two for GC analysis type, called “A” and “B”), here the actual datafiles are found.

3.2.2. LIMS_upload, where LIMS upload files are stored

3.2.3. Remote - for automation purposes.

3.2.4. Sample info.

3.2.5. SRCMETHS (source methods), where copies of Target methods are kept for that instrument.

4. TARGET FILES

4.1. There are two major types of files that are created in Target: Method files and Data files.

4.1.1. The Method File contains the settings with which the sample data is processed, reported and plotted.

4.1.2. The Data File (with an extension .d) contains the raw data file (.cdf) imported from EZChrom (chromatograms, sample information), and integration / quantitation information for the current sample.

4.2. All data files acquired in the same run are placed together in a Batch Folder, which also contains a current method used for processing the data. The raw data can be viewed by utilizing the Target Browser. To view the raw datafile or files of interest, highlight them, right-click and select “open raw data” from the drop-down menu.

5. CREATING A METHOD FILE

5.1. To create an entirely new method, in Target Browser go to “File-New-Target Methods” and select an appropriate kind of method for your applications.

5.2. Alternatively, a new method can be created by modifying an already existing default method provided with the Target software. These default methods can be found at C:/tp/target/methods.

5.3. To edit an entire method go to the drop-down menu list and edit successively from left to right. This description of the method editing process is not meant to be complete. For detailed explanations of many specific features included in the software refer to the Target Software “User’s Guide” and “Administrator’s Reference Guide”.

5.4. Method configuration.

5.4.1. Go to “File-Configuration”. In the upper part of the window select the Integrator Type, Fraction, Maximum Number of Calibration Levels and Signals, and Data Type (GC, HPLC, etc.).

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5.4.2. In the lower part of the window select the desired features for your method.

5.5. Global parameters.

5.5.1. Integration.

5.5.1.1. Select global integration parameters. In order to quickly find a set of reasonable values open a typical chromatogram and go to “Integration Parameters”. Select “Auto Calc” feature. The software will automatically find a set of integration parameters to best integrate the current sample. Save those values to the method. The integration parameters may be further modified to suit specific needs for a particular run or samples.

5.5.2. Compound ID.

5.5.2.1. Select a default RT window for compounds in your method and click “update compounds”. It can be later modified on individual basis for a particular compound if deemed necessary. Other identification parameters entered here are RT units, shifting RTs, and identification mode.

5.5.3. Quantitation.

5.5.3.1. Select quantitation parameters such as internal or external standards methods and “quantitate by area or height”. For dual column application select the reporting mode (“This column” or “Other column”) followed by “update compounds”.

5.5.4. Rounding Rules.

5.5.4.1. Select your rounding rules here. Even though sample results are to be reported in LIMS with 2 significant figures, 5 significant figures are selected here. Rounding to 2 significant figures is performed in the QCM upload.

5.5.5. Calibration parameters.

5.5.5.1. Select the curve type, update types for response factors and RTs and internal standard amount if applicable. Enter concentrations for each calibration level. For compounds with different concentration values the levels can be corrected later, on individual basis.

5.6. Editing compounds.

5.6.1. Compounds can be edited from the main “edit method” window. Click on “edit compound” and edit parameter name and all the other pertinent information required including expected retention time. Under “compound type” internal standards and surrogates are to be declared. Curve fit and identification mode may be changed on individual basis if required. For external calibration methods RT reference compound should be defined. “Calibration” enables editing calibration levels, if different from the global

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settings, and also allows to selectively disable particular levels. It is imperative to disable all the calibration levels for internal standards.

5.6.2. The "Edit Parms" window is used to enter quantitation and detection limits for Target Software. Target "limit of quantitation" is equal to DEP Method Detection Limit. Target "limit of detection" is equal to 0.5 MDL. Under Maximum Compound Amount Limit enter the concentration in the highest calibration level for a given compound. Enter linearity requirements according to the current SOP.

5.7. Sublists.

5.7.1. Sublists are used by Target software to process samples with only limited number of parameters instead of the entire list for a given method. Separate sublists should be created for each calibration standard mix and also for each test/template requested by the customer. The "Edit Sublist Compound Parameter" window should show Maximum Compound Amount and Target Limit of Quantitation (DEP's MDL). For surrogate compounds the "Surrogate Recovery Limits" button allows recovery limits for surrogates and expected surrogate concentrations to be entered.

5.7.2. Spike sublists are used to analyze spike samples and other QC-control samples like continuous calibration checks and second source standards (QCS standards). Spike sublists are created similarly to general sublists and they must contain information about expected compound concentration and recovery limits for precision and accuracy.

5.8. Editing sample information.

5.8.1. Under "Default Sample" select "Sample Matrix". Currently all Target methods are matrix specific.

5.8.2. Edit "Gas Concentration Parameters", or "Liquid Concentration Parameters" or "Solid Concentration Parameters" depending on the matrix for the current method.

5.8.3. In "Surrogate/ISTD params" window enter "1" for "volume of surrogate solution added".

5.8.4. Fill in "Column Parameters" window. Column number "1" should be selected if "This Column" was selected under "Global – Quantitation – Dual Column Quantitation Mode". Column number "2" should be associated with "Other Column".

5.9. Reports.

5.9.1. Target reports format is edited in "reports – tabular" and "reports – graphic" options. Specific descriptions of all the options and report forms are given in the Target software manual. It is noteworthy that "alternate printer" selected in "reports – tabular" will apply to the reports generated in

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Target Review window only; other reports, like recovery reports will be sent to PC's default printer.

5.10. Auto QC options.

5.10.1. In "tabular reports", flagging of several reporting conditions can be activated. Compounds reported below Target Limit of Quantitation (DEP's MDL) will be reported with Target flag "a", whereas compounds exceeding Maximum Compound Amount (the highest level of calibration standard) will receive a Target flag "A".

5.10.2. "Edit std/spike QC parameters" enables flagging QC failures for internal standards and surrogates.

5.10.3. "Calibration" allows flagging failures for linearity requirements.

5.11. The "View" drop-down menu is used only for reviewing purposes, and enables, among other things" to view and print a concise form of the calibration table.

6. PROCESSING DATA

NOTE: It is important that the following events be followed in the sequence given to insure proper calibration and correct quantitation of samples and standards!

6.1. In Target Browser go to your instrument detector (A-front, B-back) and you will find all your EZChrom data files there. Create a batch analysis folder in that detector. All batch analysis folders should have a .B (or .b) extension. Transfer raw data (cdf) files to your folder by using cut or copy-and –paste procedure. Copy the most recent method from the source to your batch folder (copy and paste procedure).

6.2. Before processing samples:

6.2.1. Rename Method

6.2.2. Select Method

6.2.3. Edit Method

6.2.4. Go to "File – zero calibration file"

6.2.5. Create specific sublists if needed. Each sample ought to be processed with exact sublists according to client's request – consult the backlog!

6.2.6. Check the global integration parameters.

6.2.7. Edit "sample – default sample" panel.

6.2.8. Save Method

6.3. Processing raw data.

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6.3.1. Select samples to be processed (the entire run can be selected by right clicking on the batch folder), right click – process raw data.

6.3.2. In "edit sample window" put the correct sublist for each injection and declare the calibrants indicating the appropriate levels. Continuous calibration checks and QCS standards should be declared QC control samples and processed as spikes (spike button on!) using appropriate spike sublists. Similarly edit the QC samples by choosing the sublist, QC control sample type and spike sublist. The rest of the editing is preferably done after matching the samples. Continue processing – the raw data files will become .d files now.

6.3.3. Update retention times. For each type of calibrator go to Target Review and update retention times using the "Assign Peak" feature. Check the correctness of your assignments by using the "Autostep on" feature.

6.3.4. Reprocess your run for each detector (calibrants first!). For internal standard methods the response for the last calibrant in the processing sequence is used to calculate the internal standard recoveries for samples.

6.3.5. For dual column applications decide which column will be designated as "primary". If your default assignment happens to be wrong you need to go to the method in each detector and change under global quantitation "this column" to "other column" (or the other way round) followed by "update compounds" and under sample info- column parameters – column 1 to column 2 or again the other way round. Having made those changes you need to reprocess the results in both detectors.

6.4. Matching dual column samples and requantifying.

6.4.1. Select samples to be matched from detector 1 (primary- designated as "this column" under "Global – Quantitation"). Go to "process- match dual column samples". Select samples from the other column and add to the selection window. Click OK. Check the matches and save them.

6.4.2. Requant the matched samples. Click on "edit sample". In editing window edit your QA/QC samples and internal standards amounts if different from required by the method. Sample dry weights/sample volumes are not currently edited in Target. Instead those calculations, along with dilutions, are now performed in QC Manager. Also make sure that sample numbers appear in the client ID field. It is advisable to indicate the dilution factor next to the sample ID, for instance: 1234567_DF=5. Additionally, for continuous calibration checks the client ID field should read for Water "ECDW-CCV" or "NPDW-CCV" and for Soil will be the same except replace "W" with "S", for the extraction blank "MBLK" and for LFB -LFB. In case when two laboratory fortified blanks are extracted they are to be called LFB_1and LFB_2. When samples are matched edit the primary channel –the second channel will be updated automatically.

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6.4.3. The QA\QC samples have to be edited as qc control samples with appropriate spike sublist and their names have to appear in the Client ID field according to the following convention:

- For 2 LFB and 2 matrix spikes
  - LFB_1
  - LFB_2
  - 411722MS
  - 411722MSD
  - 411722 (the sample spiked has to also appear in the client ID field)

- For 2 LFBs and 1 matrix spike
  - LFB_1
  - LFB_2
  - 411723MS
  - 411723 (the sample spiked has to also appear in the client ID field)

6.5. Target Review.

6.5.1. Select a Group of samples to review (blanks should also be included). Go to Target Review and open the confirmatory column (File- open confirmation Column). Chromatograms for the first sample you selected will be displayed. Subsequent sample chromatograms can be viewed by clicking the next sample located on the left bottom of the top chromatograms screen.

6.5.2. For each sample scroll down the list of parameters for the upper chromatogram (should say “this column” and “column 1”). Those indicated with + are detects. Review the results and dismiss false positives by putting the appropriate review code (Display _review codes). Manual integration can be done at this stage. Save reports for each sample remembering to save results to sample. Note that after manual integration samples can only be requanted and never reprocess, since reprocessing erases all manual changes to the baseline.

6.5.3. When applying the review codes you only have to apply them to parameters coming as hits in the primary channel. Parameters coming with Target qualifier “a” are below MDL (and higher than 0.5 MDL) and are usually not reported.

6.5.4. Target Limit of Detection (LOD) is equal to 0.5 of our MDL, and Target Limit of Quantitation (LOQ) is equal to our MDL. Target qualifier “a” flags hits between Target LOD and LOQ which means between half of our MDL and MDL. Hits below Target LOD (half of our MDL) are ignored by the software, regardless whether they are integrated or not. To view the positives below Target LOD (1/2 of MDL) in Target Rreview go to Process/Identify Sample.

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6.5.5. Another frequently encountered Target qualifier "A" means that parameter is quantitated above the calibration range (L-1 standard). If you did not use level L-1 in your particular curve Target will still flag with "A" only those above L-1 so extreme caution should be exercise here.

6.6. Creating LIMS-uploadable files.

In order to generate LIMS upload files for the samples, QA/QC samples, CCVs and the Extraction Blank, highlight the data files to be uploaded in the primary column batch analysis folder and go to "Custom functions" – "Upload to DEP QCM". Generate the upload file. The upload file will be placed in the LIMS_UPLOAD folder and will be named with complete date and time it was created followed by an ".lmu" extension.

7. TARGET REVIEW CODES

Note: All codes beginning with "X" and act as "nondetects" will upload the default values of MDLs to the LIMS.

Code	Definition/Description
XNPC	*Not positively confirmed by the second column.*
XNPCRT	*Not positively confirmed by the retention time.*
XNPCPS	*Not positively confirmed by peak shape (non Gaussian/poor shape).*
XFP	*False positive confirmed by mass spectrum (not meeting mass spectrum method criteria).*
XNPCPP	*Not positively confirmed by peak pattern (for GC multipeak parameters).*
XNPCF	*Not positively confirmed by preparative fraction.*
NPCQT	*Not positively confirmed by quantity, and is not currently in use.*
MDLADJUST	*Acts as "positive" for "this column" or "other column" followed by LIMS qualifier "U".*
NPCB	*Not positively confirmed by blank; and is not currently in use.* In case of blank contamination positives are reported in LIMS with a "V" qualifier up to ten times the amount found in the blank.
FN	*False negative (compound identified and requantified manually).* It also requires results be edited in the upload program.
NR	*Component not requested.* Used when parameter is not on the requested list. No upload to LIMS.

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NA	*No Upload; nothing goes to LIMS.* Used when parameter is requested but could not be analyzed, for example due to extensive decomposition.
NOUPLOAD	*Nothing goes to LIMS.* Used when parameter will be uploaded from another run or dilution.
PCBM	*Positive detected and confirmed below MDL.* We may use this code when we decide to report a confirmed positive detected below MDL. Those hits are currently flagged with "A" by Target and are supposed to appear as non-detects (report MDLs, with Target qualifier "J") in the upload program in LIMS. When we select "PCBM" review code the actual (below MDL) value is sent to the upload program where it appears with LIMS qualifier "T".
Blank Code (nothing)	Target does not allow undo of a wrong code entered by mistake once a review code was selected. The selection of blank code allows returning the result back to "no code" status.

8. REFERENCES

8.1. Target User's Guide, Copyright 1999, Thru-Put Systems, Inc.

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