

Using SIMDIS Expert[®] 9 (Separation Systems) with Clarity

SIMDIS Expert® 9 may be used with **Clarity** or **Clarity Lite** software to process the acquired chromatograms according to Simulated Distillation. The acquired chromatograms are exported as **AIA (*.cdf)** files and automatically opened in SIMDIS Expert® for processing.

Settings in Clarity

In the Sequence window, add the necessary columns via **Edit – Setup Columns...** as shown in the figure below:

- Export AIA activate the export of chromatogram in cdf format
- Run Program run the selected program (defined in Program To Run)
- Program To Run define an external program to run (in this case, SIMDIS Expert®)
- Parameters use %e for the exported file name (including path)

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Notes:

- The path for the exported data should not contain spaces. By default, the exported files are saved in the Data subdirectory of your Project location. Export path can be changed in the Options dialog, Directories tab (menu View Options... in the Instrument window).
- In the Program To Run column, chose simdis.exe to open the exported chromatograms in SIMDIS Expert[®] and process them manually, or use autosde9.exe for fully automated processing.

The same settings may be used in the Batch dialog to export chromatograms batch-wise (accessible from the **Analysis** – **Batch** menu in the Instrument window).

Batch		
atch nga - 1_9_2009 5_07_15 PM nga - 1_9_2009 5_42_17 PM	File Type: Chromatograms Select All Unselect All Sort by: Modification Time Order: Ascending Descending	Options Complete Processing Integration Preserve Update Calibration Preserve Update Clone New Reprocess by Method DEMO_NGA Integration Preserve Update Calibration Preserve Update Calibration Preserve Update Post Run Options Open in Chromatogram Window Print Results to PDF Export Data Show Alerts Open in Calibration Unchanged Votematication Unchanged Export Chromatogram in AIA Format
		Export Chromatogram in TXT Format Export Chromatogram in EZChrom Ascii Format Export Chromatogram in Multidetector Format
		Program to Run C:\Program Files (x86)\SeparationSystems\SDE9\SimDis Exp

Caution:

- To enable automatic processing of data, the method name used in Clarity should be the same as the name of the processing method in SIMDIS Expert[®]
- The sample type identifier (\$B Blank, \$T Retention time standard, \$A Analysis) should be included in the Sample (since version 9.09, this can also be set in Sample ID)

Important settings in SIMDIS Expert[®] 9

Channel configuration:

• Click **Configure** and the **Channels** button to display the *Detector & Signal Configuration* dialog.



• Click Manual Configuration.



• In the *Channels* dialog, configure the number of signals and their types. Click **OK** to save your settings.

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FID	•
Channel Type FID 💌 📩 Detector Name	
Channel ID 1 Wave 1	_
V Ok Pelp	Cancel

Processing method:

Using the Editor, prepare the method according to the SIMDIS Expert[®] Installation & User's Manual.

• Click the **Load Signal** button. This will allow you to import the desired samples into SDE90 for analysis and manipulation.



• In the *Process Chromatogram* window, click the button to add a file or data to SIMDIS Expert®

Process Chromatograms
Image: Sample File Sample Id Parameter Mode Channel Baseline IDC Smp Amt Std Amt Smp Dnsty Res Dnsty Image: Sample File Sample Id Parameter Mode Channel Baseline IDC Smp Amt Std Amt Smp Dnsty Res Dnsty Image: Sample File Sample Id Parameter Mode Channel Baseline IDC Smp Amt Std Amt Smp Dnsty Res Dnsty Image: Sample File Sample Id Parameter Mode Channel Baseline IDC Smp Amt Std Amt Smp Dnsty Res Dnsty Image: Sample File Sample Id Parameter Signal cdf Image: Sample Id Parame
 Image: Save process list
Image: Automatic baseline selection Image: Ok Image: Ok Image: Ok

If you receive a "skull" warning sign:

This could be caused by one or more of the following three reasons:

- 1. The Acquisition method name does not match the PDF.
- 2. The sample file lacks the proper flag depending on the method or configuration.
- 3. File format error occurred.

The acquisition mode should automatically default to "A" for Analysis if the sample is injected and acquired correctly.

Clicking on the *button* or double-clicking the line containing the Sample File will display the *Ignore* window. It allows the user to choose the injection type a the Parameter Data.

Process Chromato	Ignore Parameter Data CLARITY Channel FID(1) Injection Type (T] R. Time Calibration (IF) R. Factor Calibration (IS) Standard (D) Detector RF (N) Noack Calibration (DIN 51581-2)	Cancel
Automatic be	? Help	Cancel

When finished, click the **OK** buttons in the *Ignore* and *Process Chromatograms* windows to start the analysis.

Observed troubles

Crash reasons:

- Automated Blank processing should not be used if there is no blank run (corrected after version 9.09).
- The method parameter file must be calibrated before attempting to process unknowns.

Other troubles:

The Inverse Processing option should be unchecked in the processing method, Integration Parameters, Baseline Parameters for automated processing.

Using *Export*, the e-mail parameters must be configured.

- 1. Load a signal
- 2. Click on the **E-Mail** button

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Exit	Help	Configure	Load Signal	Load Report	Editor	Prin	E-Mail	Export

3. In the displayed *RM_Mailer* dialog, click the **Configure** button.

RM_Mailer	×
Message Log	
То:	
Cc:	
Bcc:	
Subject	
C:\Program Files (x86)\SeparationSystems\SDE9\\Mail\SDEReport_20101025_173614.MCR	0

4. Enter the information in the *Connection* tab and click the **Save** button.

Save (Connection	Xancel
SMTP: Port: User ID:	smtp.testdomain.com 25 john.legrace@testdomain.com Send attempts: 5
Name: E-Mail:	John LeGrace John legrace.com

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