

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:

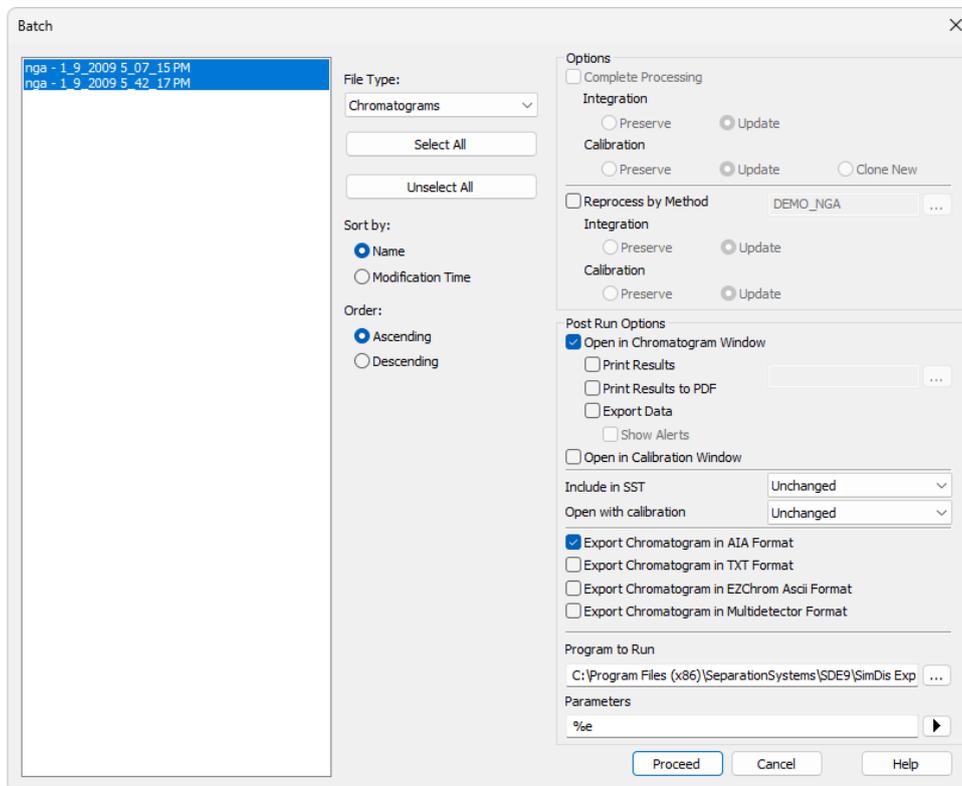
- **Export AIA** activate the export of chromatogram in cdf format
- **Run Program** run the selected program (defined in Program To Run)
- **Program To Run** define an external program to run (in this case, SIMDIS Expert®)
- **Parameters** use %e for the exported file name (including path)

| Status | Run | SV | EV | I/V | Sample ID | Sample | Sample Amount | ISTD1 Amount | Sample Dilut. | Inj. Vol. [µL] | File Name | Sample Type | Lvl | Method Name | Report Style | Open | Open Calib. | Print | Export AIA | Run Program | Program To Run | Parameters |
|--------|-------------------------------------|----|----|-----|-----------|------------|---------------|--------------|---------------|----------------|-----------|-------------|-----|-------------|--------------|-------------------------------------|--------------------------|--------------------------|-------------------------------------|-------------------------------------|----------------|------------|
| 1 | <input checked="" type="checkbox"/> | 1 | 1 | 1 | %s%v | Sample ... | 0.000 | 0.000 | 1.000 | 0.000 | %q_%R... | Unkn | | DEMO_NGA | | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | C:\Prog... | %e |
| 2 | <input checked="" type="checkbox"/> | 2 | 2 | 1 | %s%v | Sample ... | 0.000 | 0.000 | 1.000 | 0.000 | %q_%R... | Unkn | | DEMO_NGA | | <input checked="" type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | C:\Prog... | %e |
| 3 | <input type="checkbox"/> | | | | | | | | | | | | | | | <input type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | <input type="checkbox"/> | | |

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).



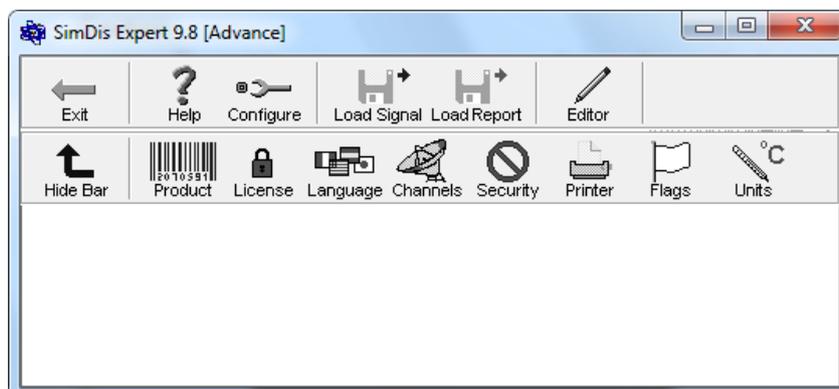
Caution:

- 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)

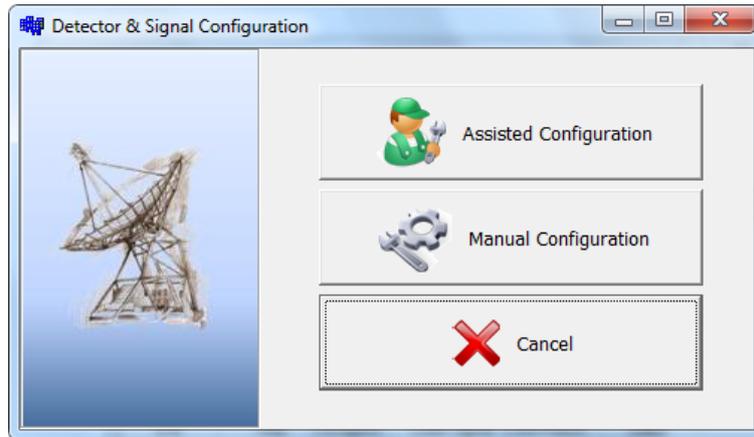
Important settings in SIMDIS Expert® 9

Channel configuration:

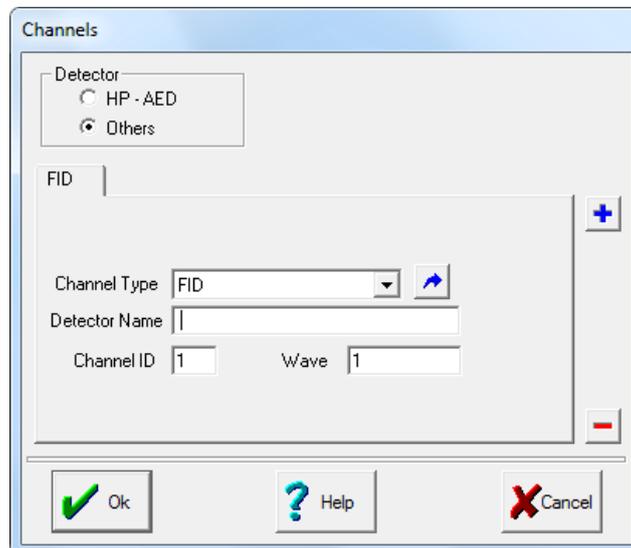
- Click **Configure** and the **Channels** button to display the *Detector & Signal Configuration* dialog.



- Click Manual Configuration.



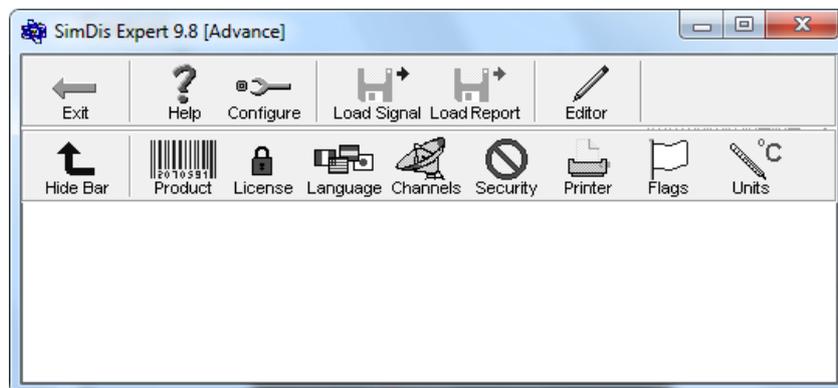
- In the *Channels* dialog, configure the number of signals and their types. Click **OK** to save your settings.



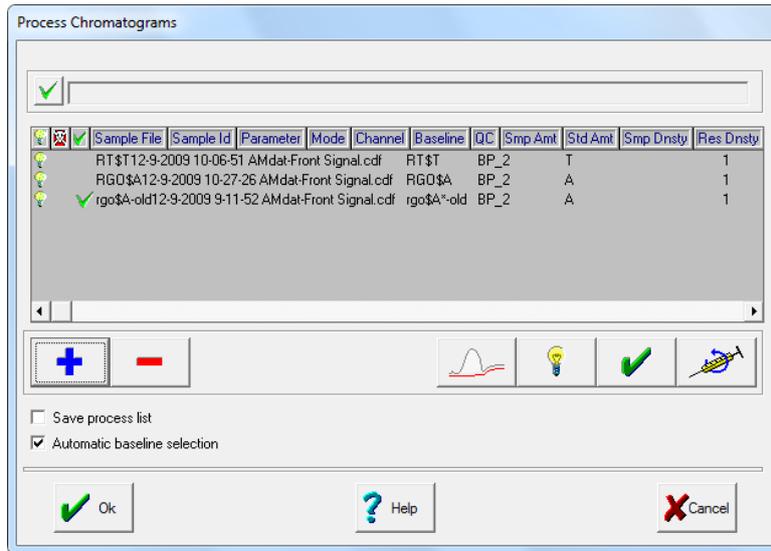
Processing method:

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®



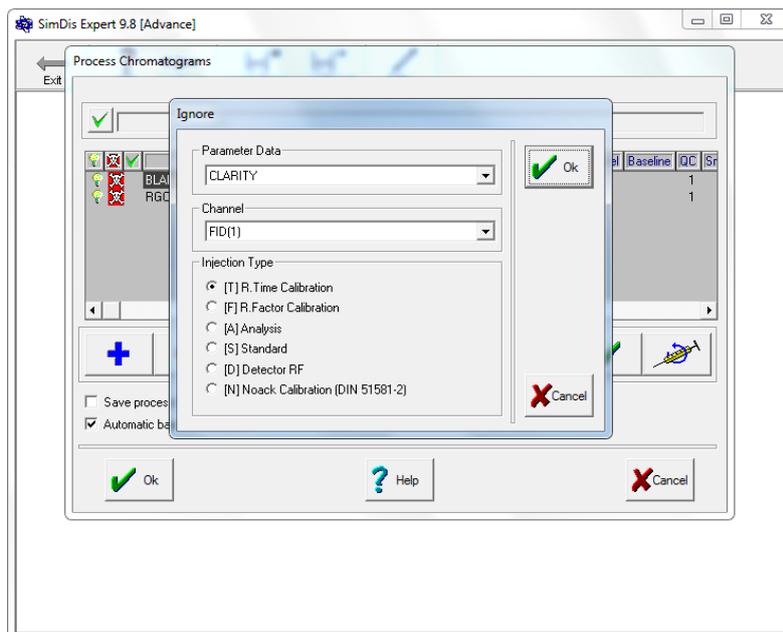
If you receive a "skull" warning sign:

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.



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:

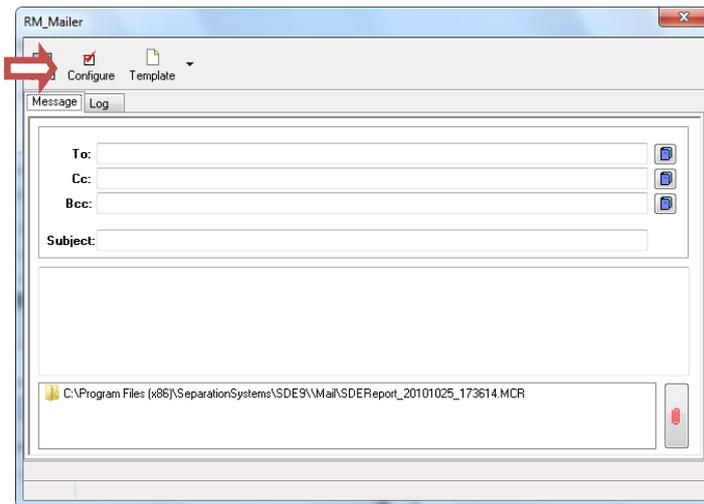
The Inverse Processing option should be unchecked in the processing method, Integration Parameters, Baseline Parameters for automated processing.

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

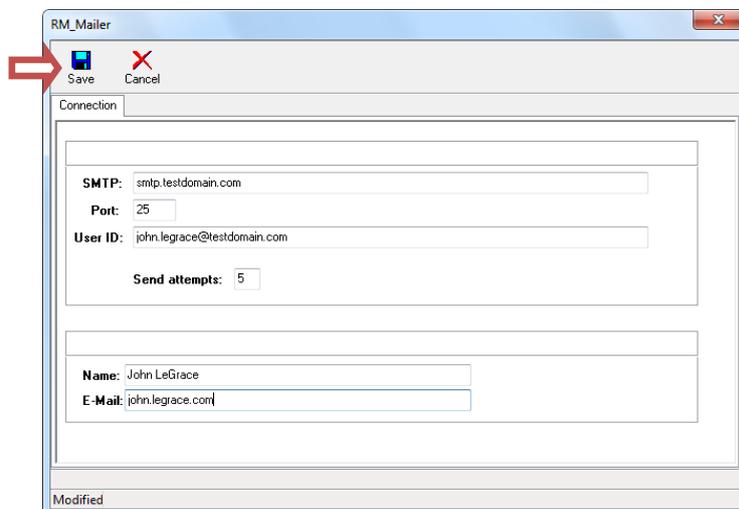
1. Load a signal
2. Click on the **E-Mail** button



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



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



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