Collated Report and Degradation Report for

iChemExplorer with Agilent Chemstation Data

Introduction:

The iChemExplorer software is used to view and export analytical results from a Sample Sequence. Point to the file location and iChemExplorer automatically acquires all the data for the sequence leaving the source information intact. iChemExplorer presents data in the iGraph window as Peak Profiles – lines that follow peak area from sample to sample. In this way chemical changes are immediately apparent. Export peak profiles for each sample vial with a temperature log for the sample sequence with Collated Report. Apply a calibration standard to convert to concentration (mg/ml) and graph by temperature to display a best-fit solubility curve to the analytical data. Export the solubility curve with the Solubility Report. iChemExplorer makes the acquisition of data easy even for large data sets. The Peak Profiles in the iGraph provide an immediate glimpse into the chemistry happening in the vial. The Solubility and Collated Reports provide the data in a format that is convenient to share and store. The instructions below guide the user to get these results.

Contents:

Acquire the data for presentation in iChemExplorer:

- Open the iChemExplorer application by double clicking the iChem logo on the PC Desktop. The iChemExplorer Main Page should open. See the iGraph window on the right and the tray graphic on the left. Along the top bar are items to select for drop down menus.

- On the iChemExplorer Main Page, Select Load HPLC Data Button. This button is below the tray graphic.

- Windows Explorer window opens to navigate to the data to be loaded for presentation. These are the data files created as each method was run in the Sequence Table.
    - See that the default filetype for the Explorer window is .CSV – comma separated variable. Only .CSV files are viewable in the window.
    - To determine the default data location go to Chemstation. Select View from the top bar and select Preferences near the bottom of the menu. This opens a window with three tabs. The first tab in the window shows the default paths to store Methods and Data. The usual default for Chemstation data is C:/Chem32/1/DATA/<data subdirectory>. This location is also specified in Chemstation from the top bar in Sequence>Sequence Parameters window.
    - Agilent Chemstation follows a standard template for recording analytical results upon execution of a Sequence Table. At the start of the sequence a unique subdirectory is created to store the results. Then as each method in the Sequence Table starts, a folder is created in the subdirectory to hold the data for that sample. The naming of the data folder should be set to Auto in the Sequence Parameters window. The Auto selection folder name follows a standard convention. XXX-XXXX with the first three digits for the vial location of the sample; the next two after the dash as the order of the sample in the sequence and the last two digits as the number of injections from that sample.

- Open any data folder. Find the following files in the Windows Explorer window:

    - [file prefix]00.CSV text file; no good to load
    - [file prefix]01.CSV integrated peak data; GOOD TO LOAD
    - [file prefix]02.CSV integrated peak data; GOOD TO LOAD
    - [file prefix]XX.CSV Increments for wavelengths selected
    - [file prefix]99.CSV temperature record at time of sample

    Note: To set the file prefix, go to Edit Entire Method in Chemstation. Go to the Specify Report window. Enter the file prefix to the File Prefix: field. This name will be applied the next time the method is run.

- Select a file with integrated peak data such as [file prefix]01.CSV. Select Open to close Windows Explorer window and load the data for that wavelength to iChemExplorer.

It doesn't matter which data folder is first selected to acquire data as all data is acquired at once. iChemExplorer automatically acquires the same file name from all the data folders in the subdirectory.

Prepare the Data for Presentation in iGraph

- See the iGraph window. The default axes for the window are Area % by Sample. When data is first acquired, the window shows the Peak Profile for the lowest vial position in the sample sequence. The data is displayed as Peak Profiles – lines that follow peak area from sample to sample. Single samples show peaks as columns. A second sample is needed to draw lines from one sample to the next.

- See the Tray Graphic for vial locations in white. These are the locations for which data has been loaded into iChemExplorer. Click on each location to see Peak Profiles in the iGraph window.

- See the Overlay selection above the Tray Graphic. Select to lay a peak profile for each selected position over the other. Unselect the Overlay button and select a new vial location to clear the iGraph window.

- See the Plot drop down menu. The default graph is in Peak Area % by Sample. An alternate view is Peak Area by Sample. The lines follow peak area from one sample to the next by run-time.

- Open the Chromatograph Viewer by left click on mouse with pointer in iGraph window. A window opens to display a chromatograph for the vial position on display in the iGraph window. All the wavelengths collected in the method are viewed together. See the vial position in the upper left corner. See the buttons on the bottom of the window. Select Scroll Through to view the graphs one after the other as a tool to see trends.

- See the Peak Table for peak data by sample listed with Area % or Area as selected from the PLOT: menu.

- The Peak Profiles may be refined with tools iChemExplorer
    - Threshold sets the minimum peak height to display relative to main peak. Set high for solubility as only main peak is important.
    - Tolerance sets the shift in peak-time acceptable to overlap peaks from one chromatograph to another as in a sample sequence. A low value increases differentiation while a larger value puts peaks together.
    - Range sets the start and stop time to view peaks in iGraph. Peaks before or after the range settings are ignored. This range can be set to a close tolerance with solubility data with only one peak of interest.
    - The Exclusion List below provides selection for each data point at that vial location. Select to exclude and deselect to include the data point. iChemExplorer makes a straight-line approximation between the remaining data points.

- Use Edit>Peak Names to label, hid and color Peak Profiles
    - Go to Edit in the top bar on the iChemExplorer main page. From the menu select Peak Names. A window opens with entries for each peak profile displayed in iGraph assigned by peak run time.
    - Select/Deselect Hide to cloak/display the peak profile line in iGraph
    - Enter a name to display in iGraph in the Re-name to: field
    - Select/Deselect Color and select Color from drop down to change the automatic selections by iChemExplorer
    - Select Close to set selections and close window. Select Apply to view changes with window open.

Publication of Collated Report

- Go to Report in the top bar on the iChemExplorer main page and select Collated Report. The Collated Report includes
    - Peak Profile Charts for each vial position
    - First, mid and last chromatographs for each vial position
    - Templog graph – chart of temperature over time
    - Tables with all data in numerical format by Peak Area and Peak Area %

- Windows Explorer opens to select a location and enter a file name for the report. Select Save to Close. A window opens to show progress to publication. Once complete the window will close. Go to the file location and open the file. See the worksheet tabs with the information as described above.

Publication of Solubility Report

- From the Plot drop down menu below the iGraph window. Select Degradation. A window opens from Referencing on the top bar of the iChemExplorer Main Page. Here select the peak for the Starting Material. Enter the fields for calibration data as this is available. Select OK to close.

- In the iGraph window see that the y-axis is revised to milligrams per milliliter.

- Now in the Axis Locator section find a button for Temperature. Select this button. The graph changes to a curve fit to the data points and the variables that satisfy the Arrhenius Equation for change in solubility by temperature.

- Go to Report in the top bar on the iChemExplorer main page and select Solubility. The Solubility Report includes
    - Chart with best-fit curve to actual data points for each vial position
    - First, mid and last chromatographs for each vial position

    - Tables with all data in numerical format by Peak Area and Peak Area %

- Windows Explorer opens to select a location and enter a file name for the report. Select Save to Close. A window opens to show progress to publication. Once complete the window will close. Go to the file location and open the file. See the worksheet tabs with the information as described above.

Save Analysis and Load Analysis to view data and work from previous sessions.

- Go to File on the top bar of the iChemExplorer main page. Select Save Analysis.

- Windows Explorer opens to select a file location and enter a file name. See the file type is .ICE. This file type is unique to the iChemExplorer application.

- To load the work from a previous session as saved with Save Analytics. Open the iChemExplorer software. Go to File on the top bar of the iChemExplorer main page. Select Load Analysis.

- Windows Explorer opens to navigate to the data location. Select the .ICE file and select Load.

- iChemExplorer is populated with the source data the settings from the previous session.