

iChemExplorer™ Reporter User Guide for Solubility

For iChemExplorer™ Reporter v.10

To Analyze HPLC Data from Agilent Chemstation
Collected with iChemExplorer Control Software
and Publish Excel Reports

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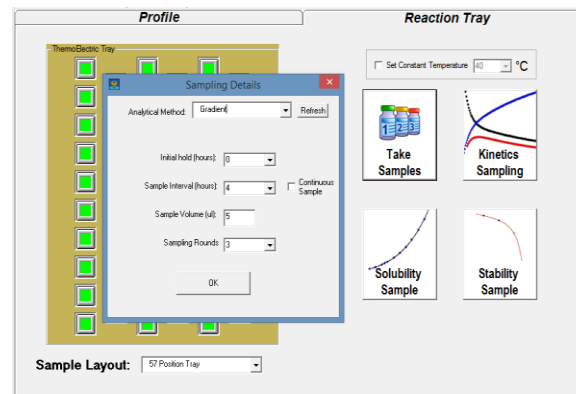
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iChemExplorer Integration with Agilent HPLC

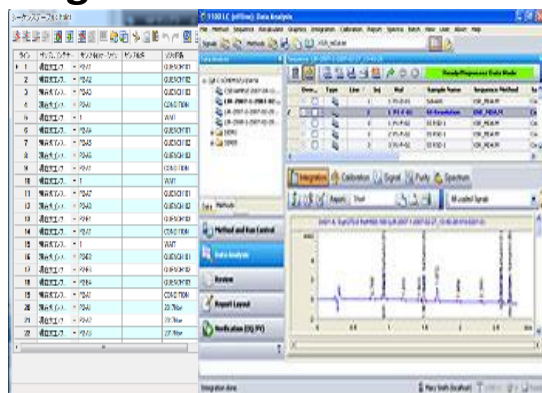


Fully controlled
autosampler
↔
Heating/Stirring

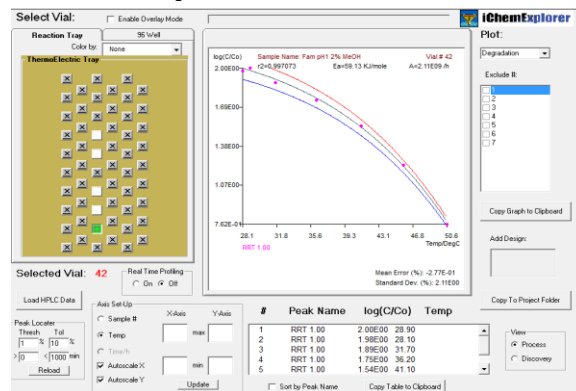
iCE Control Software



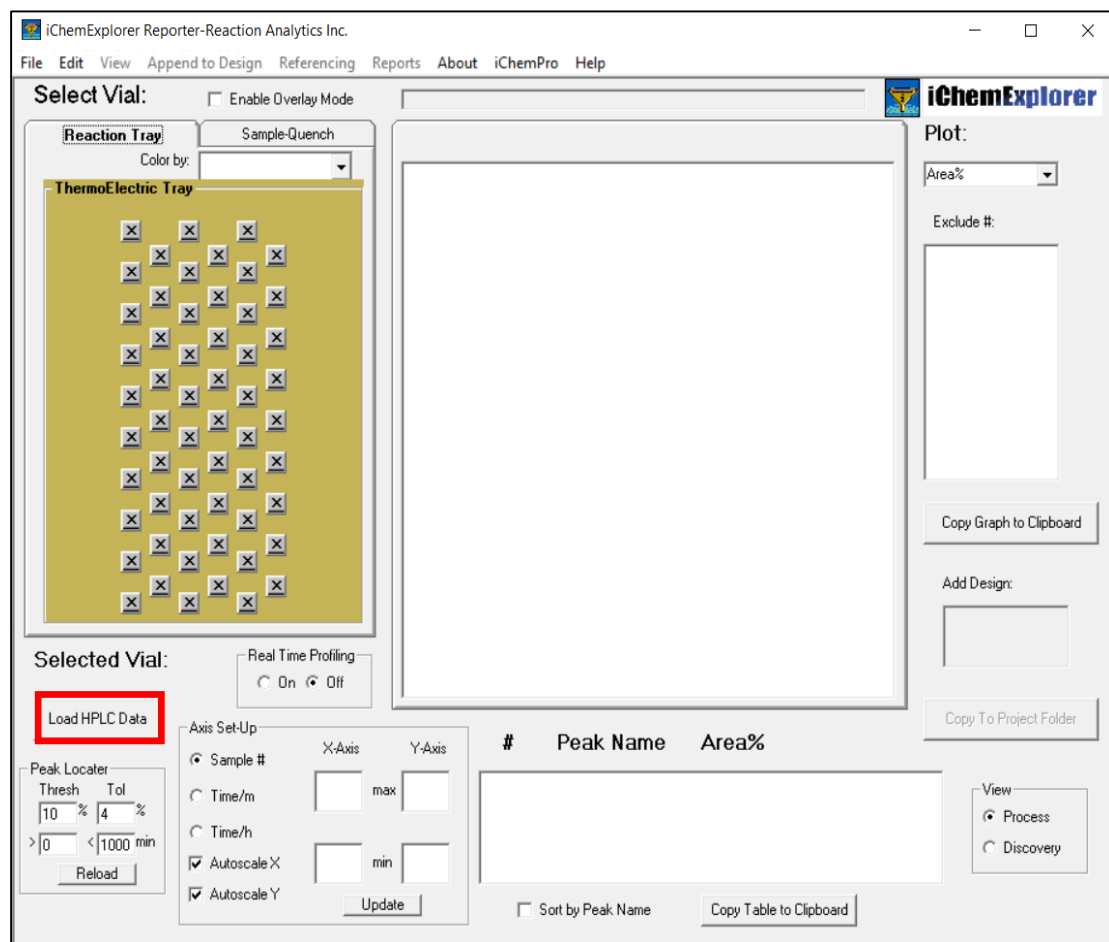
Agilent ChemStation



iCE Reporter Software

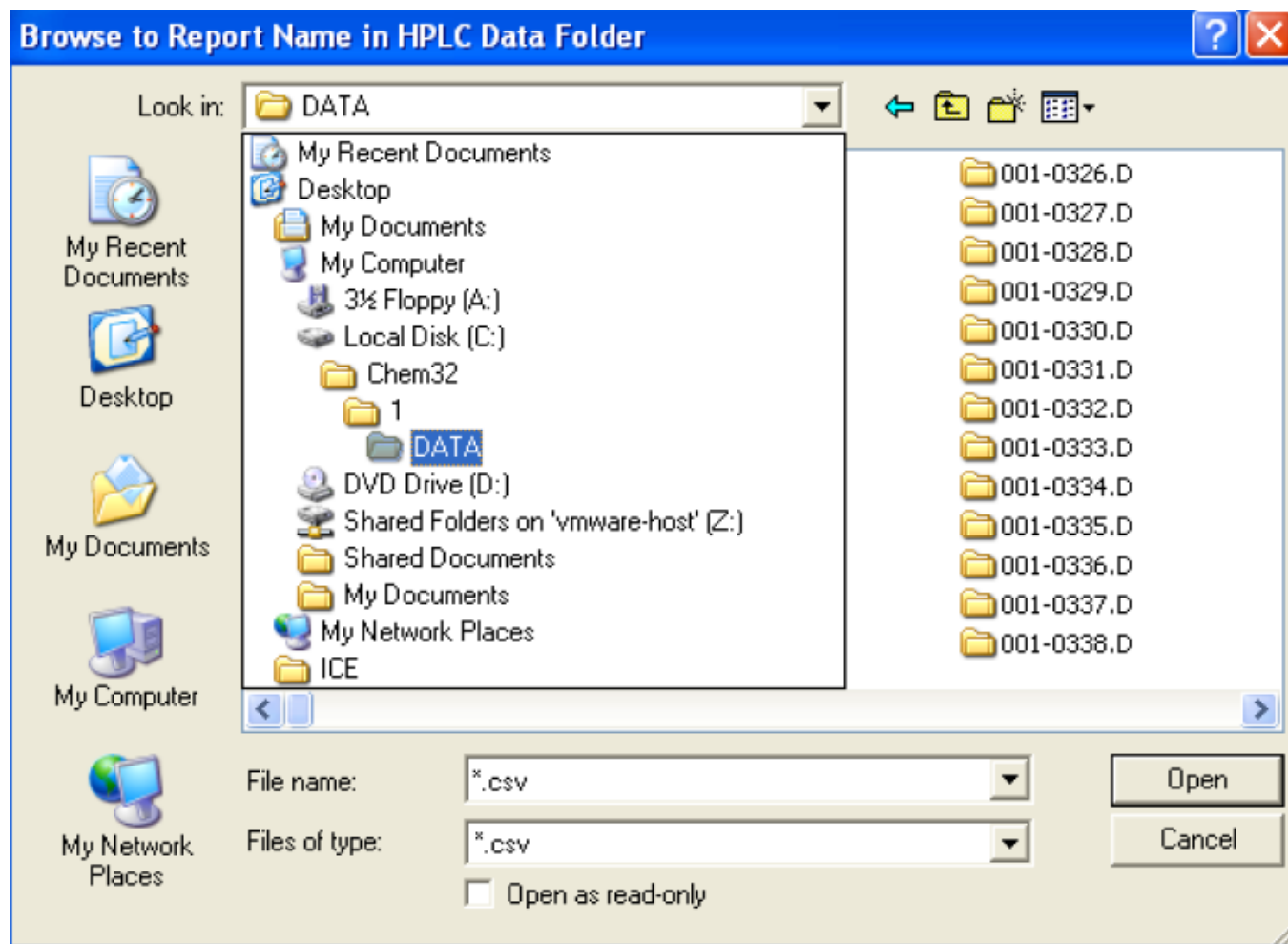


iChemExplorer Reporter: Load HPLC Data



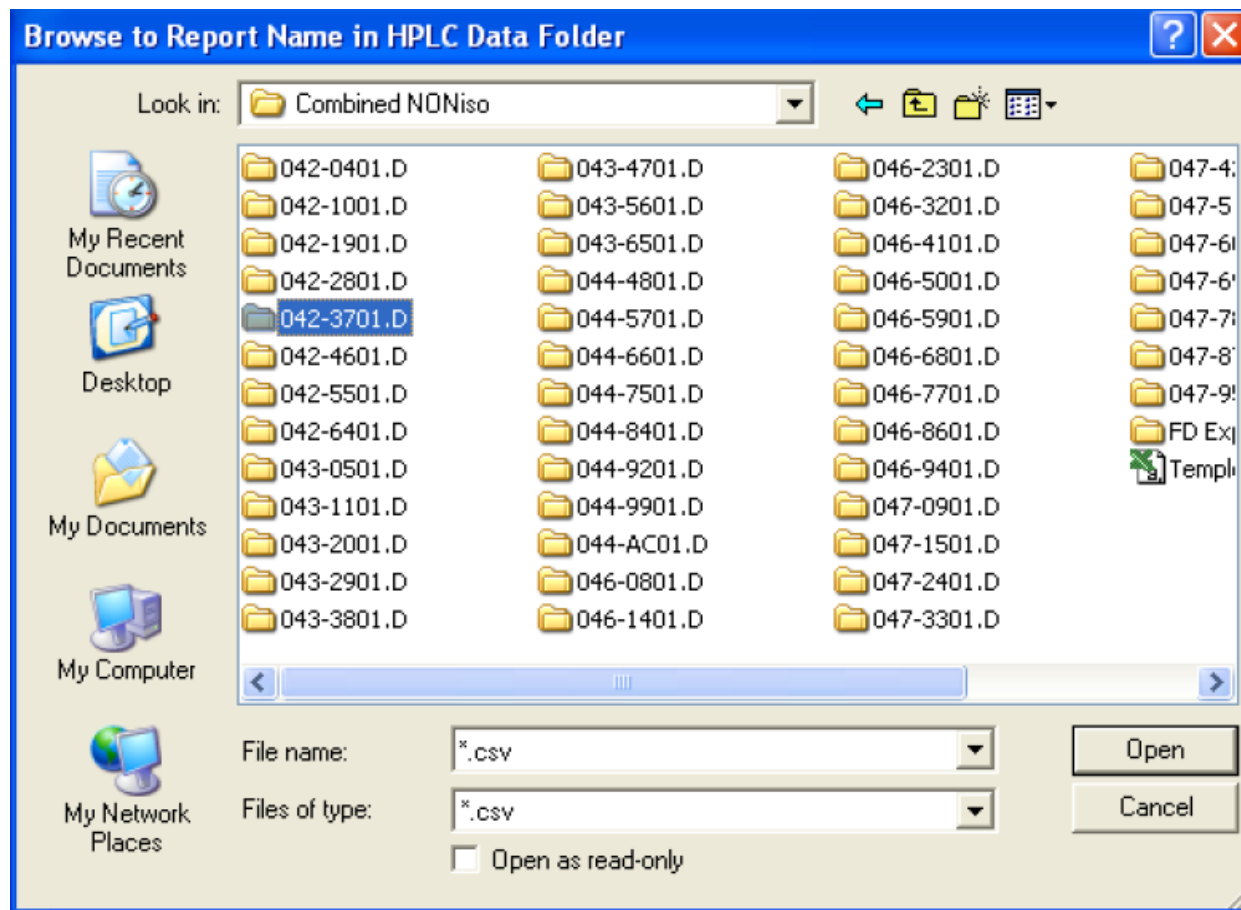
- Open iChemExplorer Reporter
- To load the Agilent HPLC data files collected with iChemExplorer control software, click on Load HPLC Data button

iChemExplorer Reporter: Load HPLC Data



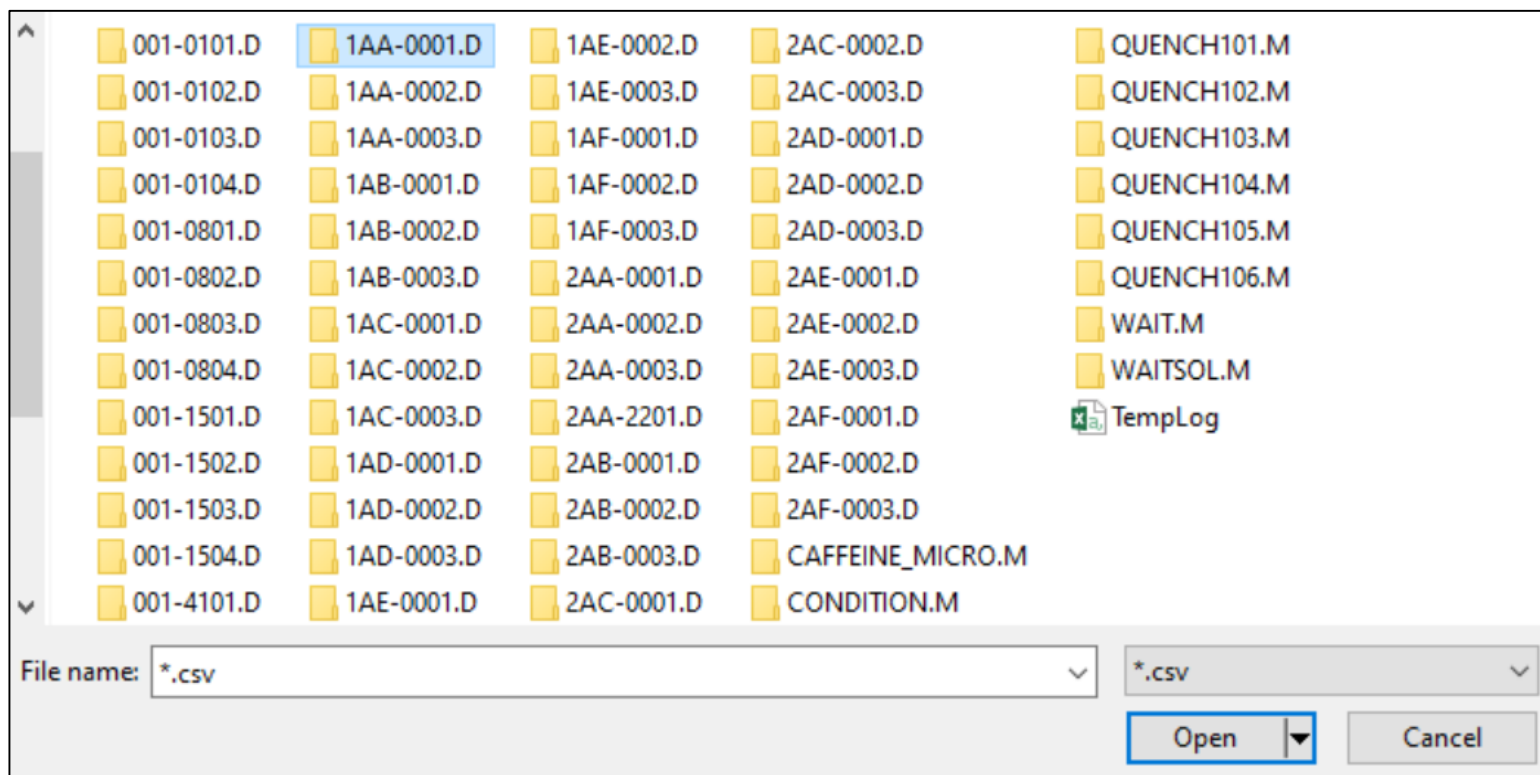
- The File Explorer window appears
- Browse to locate the folder of sample sequence run, typically under C:\Chem32\1\Data

iChemExplorer Reporter: Load HPLC Data



- If the samples were directly injected from tray or plate, each auto-named .D data subfolder shows vial location, sample order and injection number
- A TempLog.CSV file in the same folder records date time, set point and actual temperature created by iChemExplorer

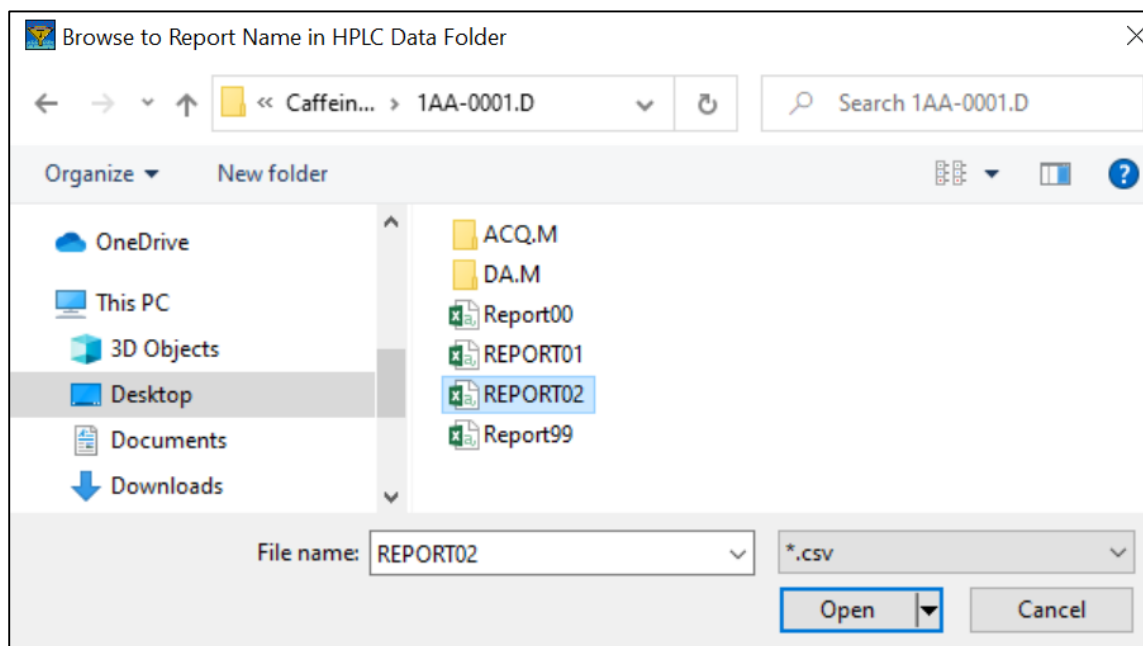
iChemExplorer Reporter: Load HPLC Data



- If quench-sampled from Plate 1 and transferred to Plate 2 then injected to LC, auto-named data subfolder shows plate vial location and injection number (i.e. 1AA-0001.D to 1AF-0003.D) as correlated to source vials
- There are other auto-named subfolders which don't contain LC sample run data, i.e. virtual injections during wait (i.e. 001-0101.D) and quench sampling (i.e. 2AA-0001.D)

iChemExplorer Reporter: Load HPLC Data

- Open a data subfolder of LC sample run, i.e. 1AA-0001.D
- Each data subfolder contains the same filenames

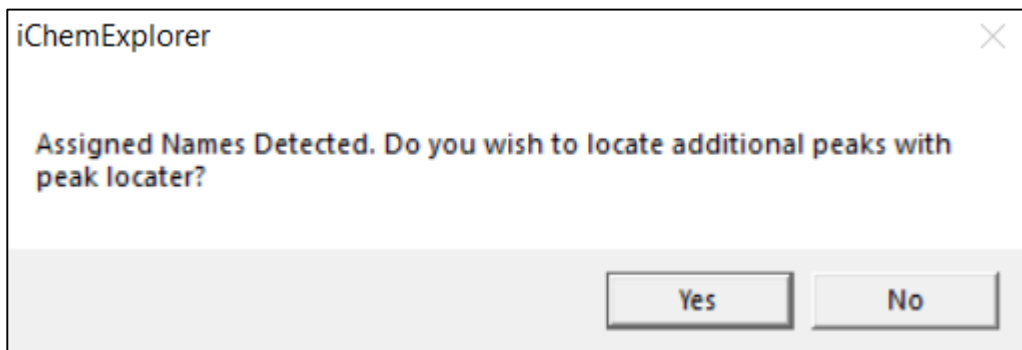


- Report00 records method run details
- Report99 records date time, set point and actual temperature
- Report01 and Report02 record integrated peak areas at selected wavelengths (i.e. 220 nm and 254 nm)

- Select Report file at wavelength (i.e. Report02 at 254 nm) to load HPLC data

iChemExplorer Reporter: Load HPLC Data

- iChemExplorer loads the integrated peak areas from all the data folders in the sample sequence run
- The following window pops if the peak name is already assigned in the LC method (typically for solubility assay), select No to load the peak area of the assigned name.



iChemExplorer Reporter: Data Analysis

Sequence run sample layout

Select vial position to display data

Peak areas of selected vial are displayed

of injection can be excluded

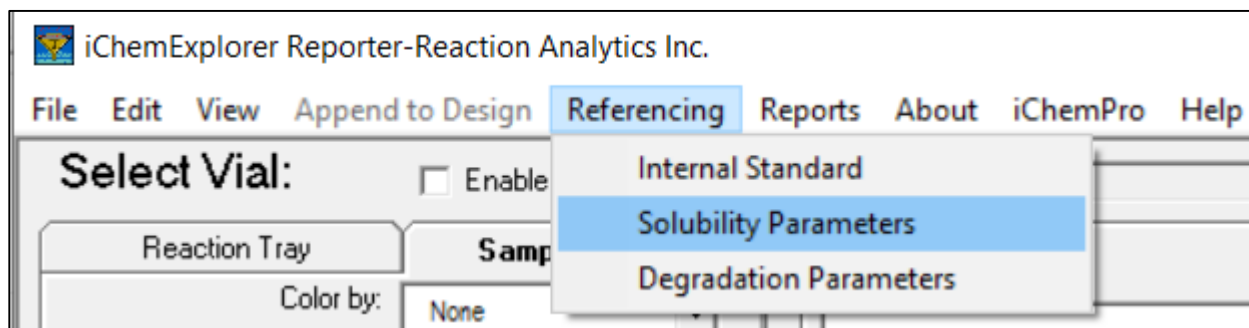
of injection from selected vial

The screenshot displays the iChemExplorer Reporter software interface. The 'Select Vial' section on the left shows a 'Well Plate Carrier' and a 'ThermoElectric Tray' with a grid of vial positions. A vial is selected, and the 'Selected Vial' is 106. The 'Plot' section on the right shows a graph of 'Area' vs 'Samp #' for 'Caffeine'. The graph shows a peak at approximately 2.0 minutes. The 'Exclude #' section on the right shows a list of injections (1, 2, 3) with checkboxes. The 'Add Design' section shows a list of injections (1, 2, 3) with checkboxes. The 'View' section shows 'Process' and 'Discovery' options. The 'Table' section at the bottom shows a list of peaks with columns for '#', 'Peak Name', and 'Area'.

#	Peak Name	Area
1	Caffeine	237.656
2	Caffeine	260.717
3	Caffeine	244.951

iChemExplorer Reporter: Solubility

- Select Referencing – Solubility Parameters



Solubility Parameters

Calibration

Reference: ☒ Single Point ☐ Paramatized

Calibration units: ☒ mg ☐ ug

Fully Soluble Reference

1 mg/ml 7.056 mAU_s

Area (mAU_s) = A * Conc (mg/ml) + B

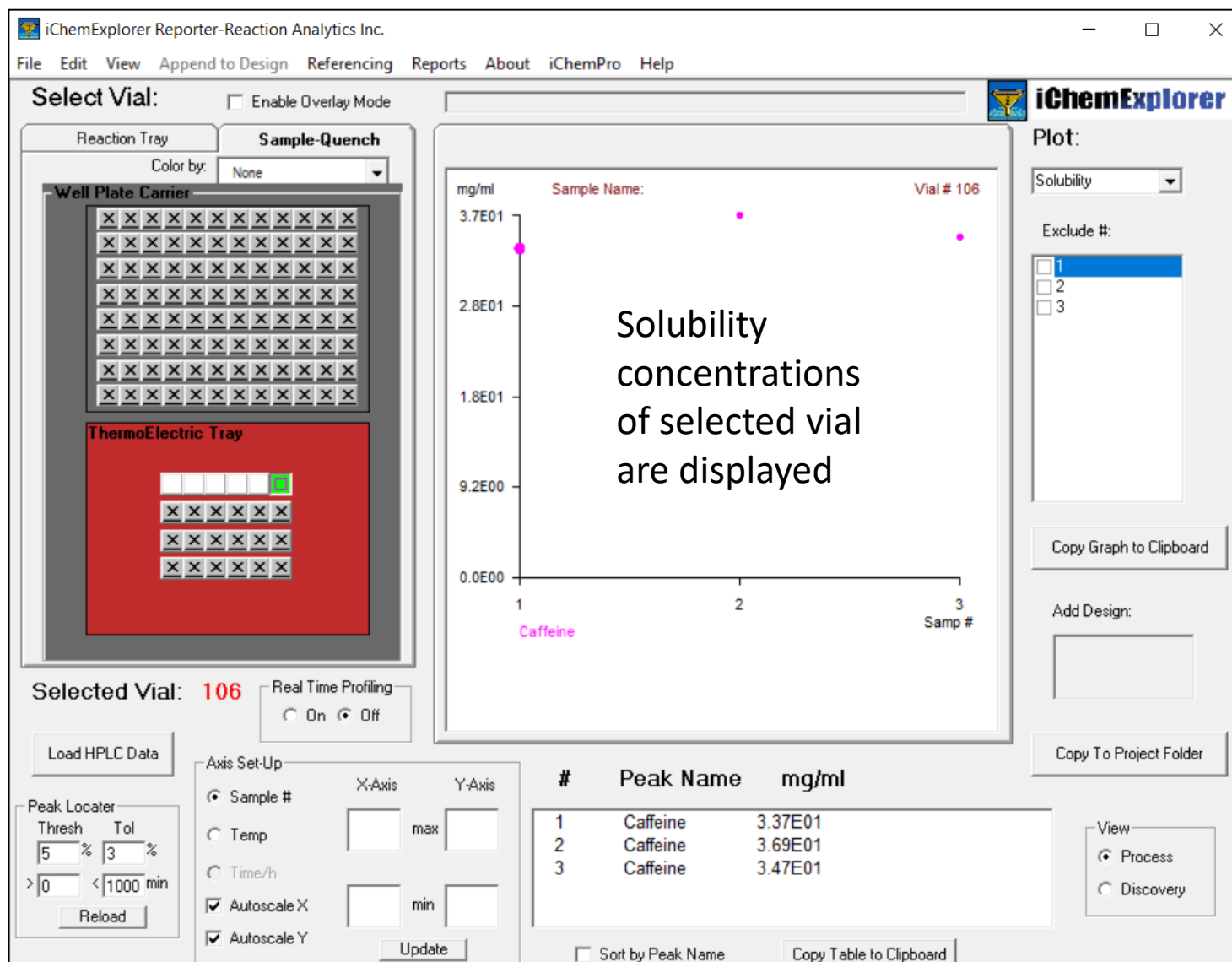
A = 1000 B = 0

Applies to: Caffeine

OK Cancel

- Enter appropriate calibration parameters for the assigned name peak, then OK

iChemExplorer Reporter: Solubility



iChemExplorer Reporter: Solubility

Check box to enable data overlay

Select vial position to overlay data

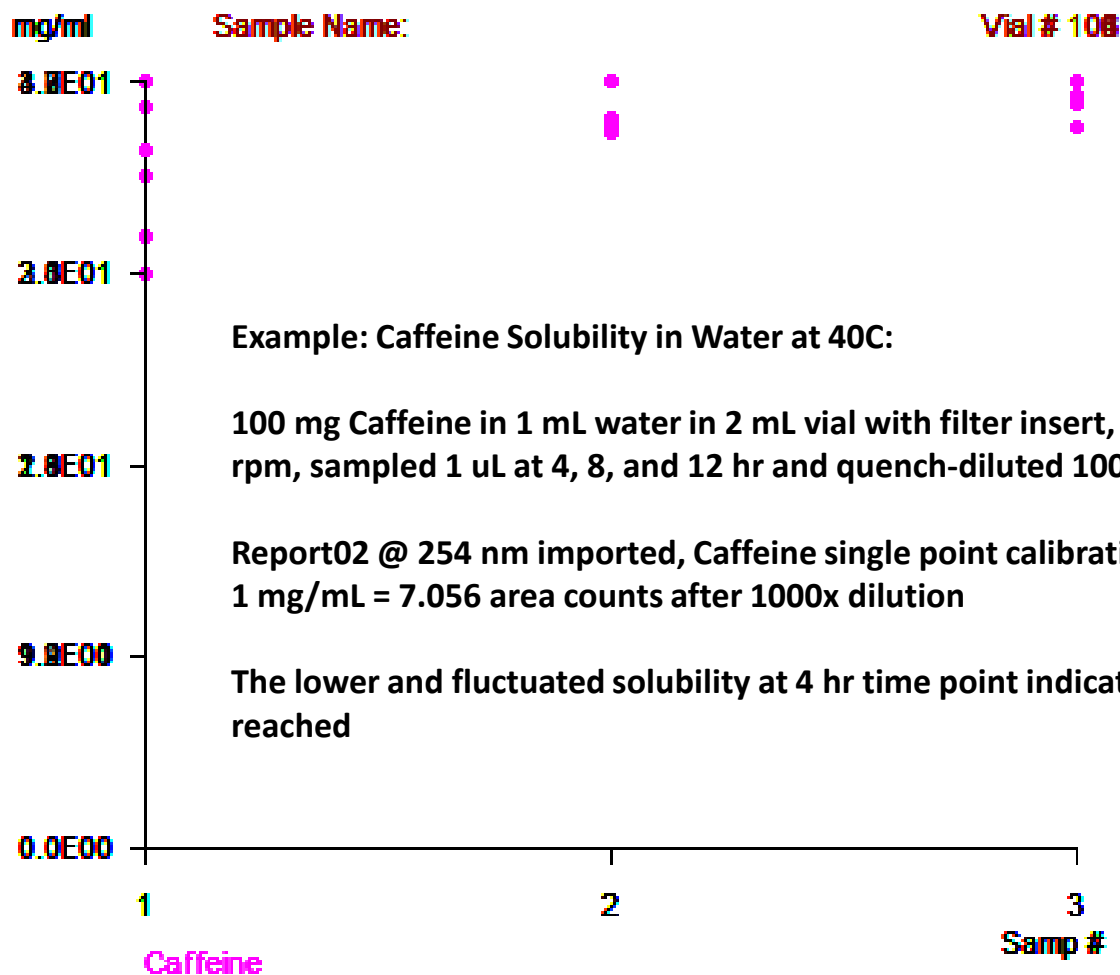
Solubility concentrations of all vials are displayed

The software interface displays the following components:

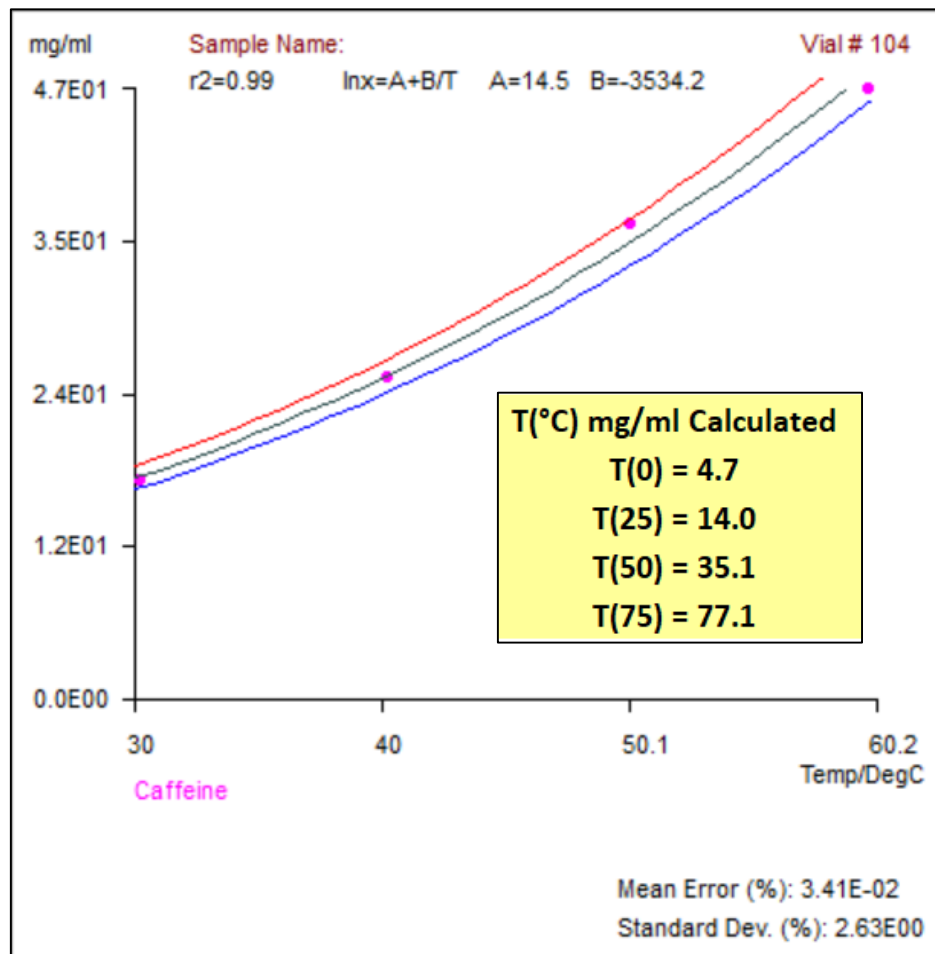
- Select Vial:** Includes a 'Well Plate Carrier' and a 'ThermoElectric Tray'. A checkbox 'Enable Overlay Mode' is checked.
- Plot:** A graph showing 'mg/ml' vs 'Samp #'. The y-axis ranges from 0.0E00 to 3.8E01. The x-axis shows sample numbers 1, 2, and 3. Data points are plotted for each sample, with 'Caffeine' labeled for sample 1.
- Table:** A table listing peak data for three samples.

#	Peak Name	mg/ml
1	Caffeine	3.31E01
2	Caffeine	3.56E01
3	Caffeine	3.76E01

iChemExplorer Reporter: Plot Export



iChemExplorer Reporter: Plot Export



Example: Caffeine Solubility in Ethanol vs. Temperature:

- 60 mg Caffeine in 1 mL ethanol in 2 mL vial with filter insert, 6 replicate vials, equilibrated at 30/40/50/60C for 6 hr, sampled 2 uL and quench-diluted 500x in water for HPLC analysis
- Report01 @ 220 nm imported, Caffeine linear calibration in ICE solubility parameter: $A = 5.3664$, $B = 3.8917$
- Solubility-temperature curve fitted to Van Hoff's equation

iChemExplorer Reporter: Data Export

- Select Reports – Solubility Report to export an Excel file containing HPLC chromatograms, temperatures and solubility data/curves of all sample vials with selected injections
- Select Reports – Collated Report to export an Excel file containing HPLC chromatograms, peak areas, and profile plots of peak area vs. time for all sample vials with selected injections

