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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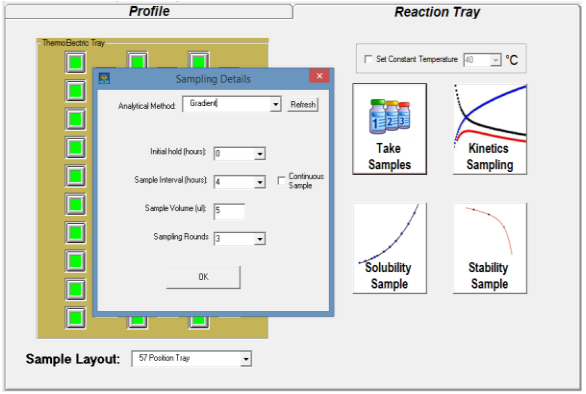
- iChemExplorer Reporter
  - Load HPLC Data
  - Data Analysis
  - Solubility
  - Plot Export
  - Data Export

iChemExplorer Integration with Agilent HPLC

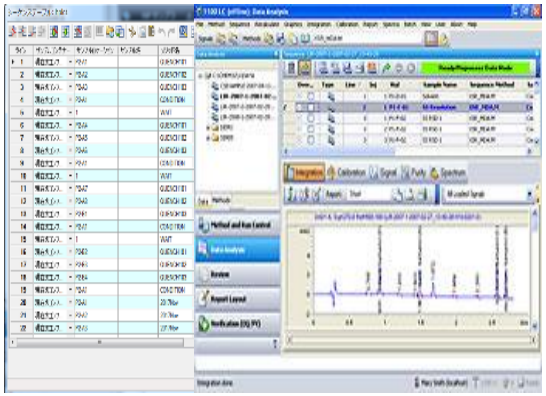
Fully controlled autosampler

Heating/Stirring

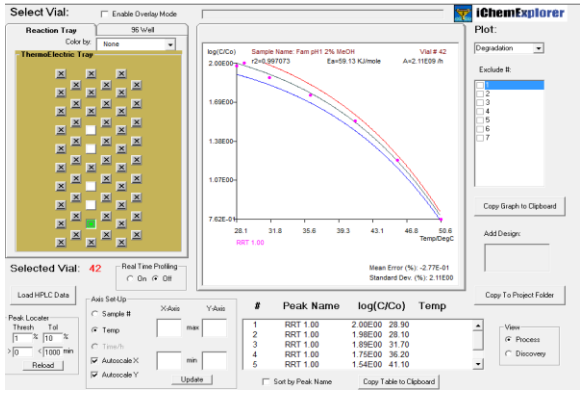
iCE Control Software



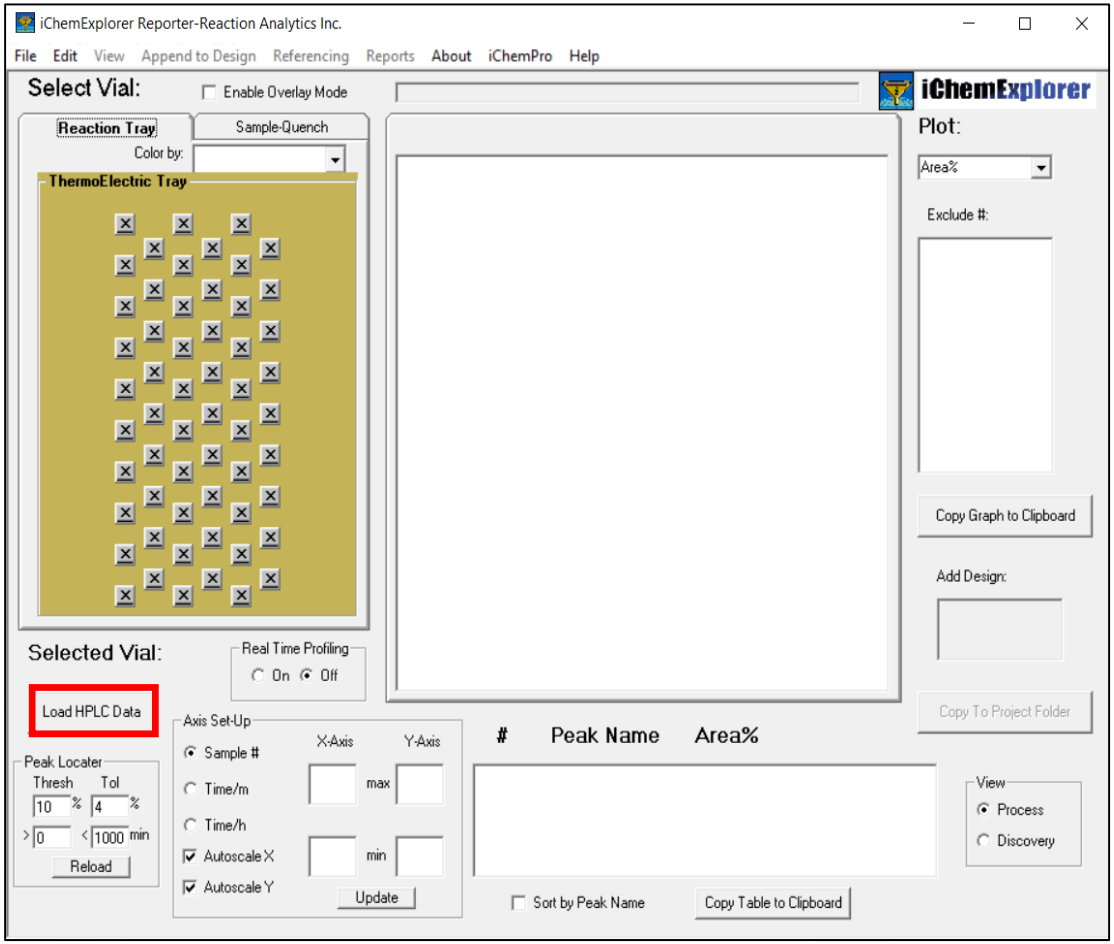
Agilent ChemStation



iCE Reporter Software

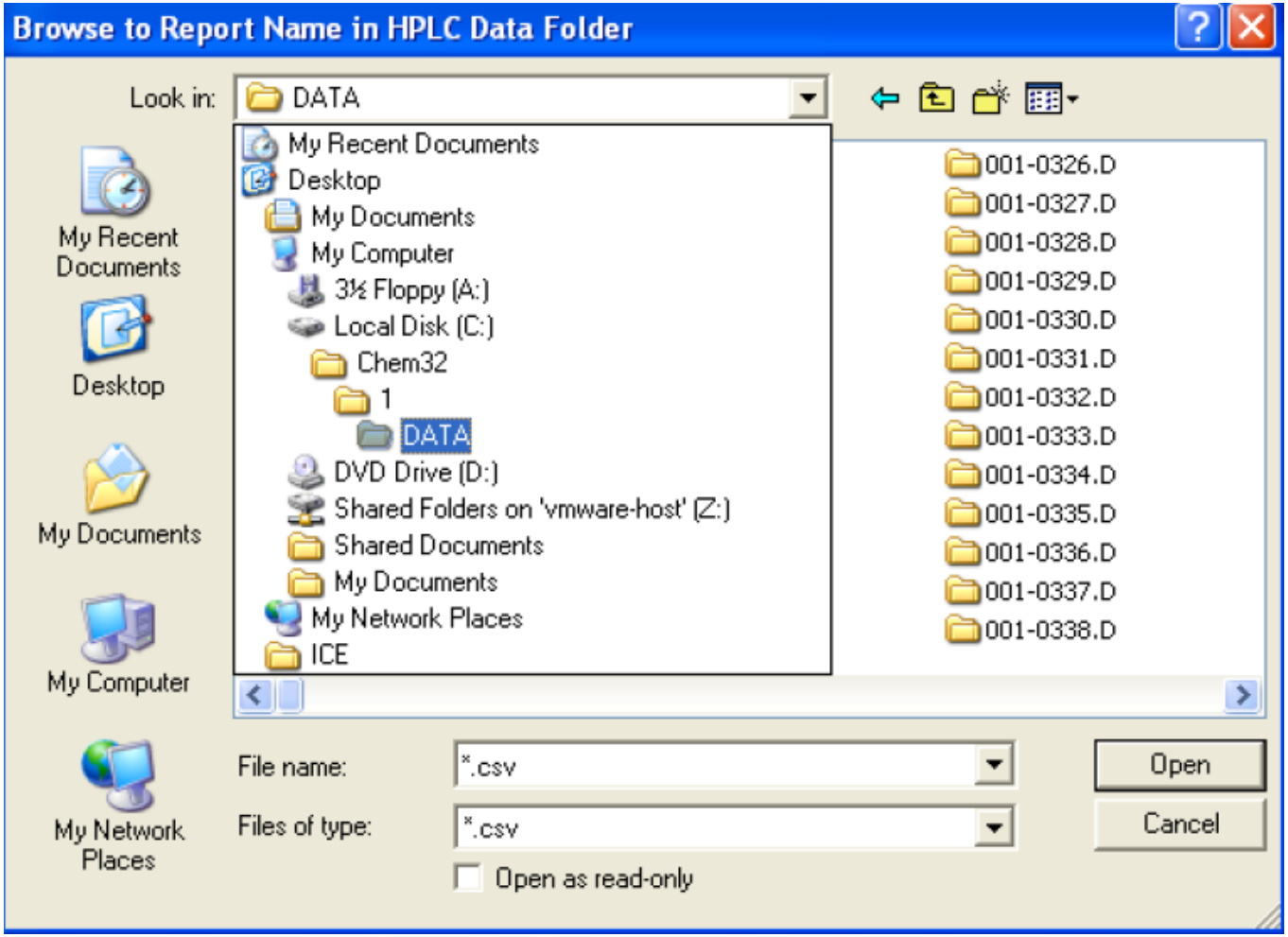


iChemExplorer Reporter: Load HPLC Data



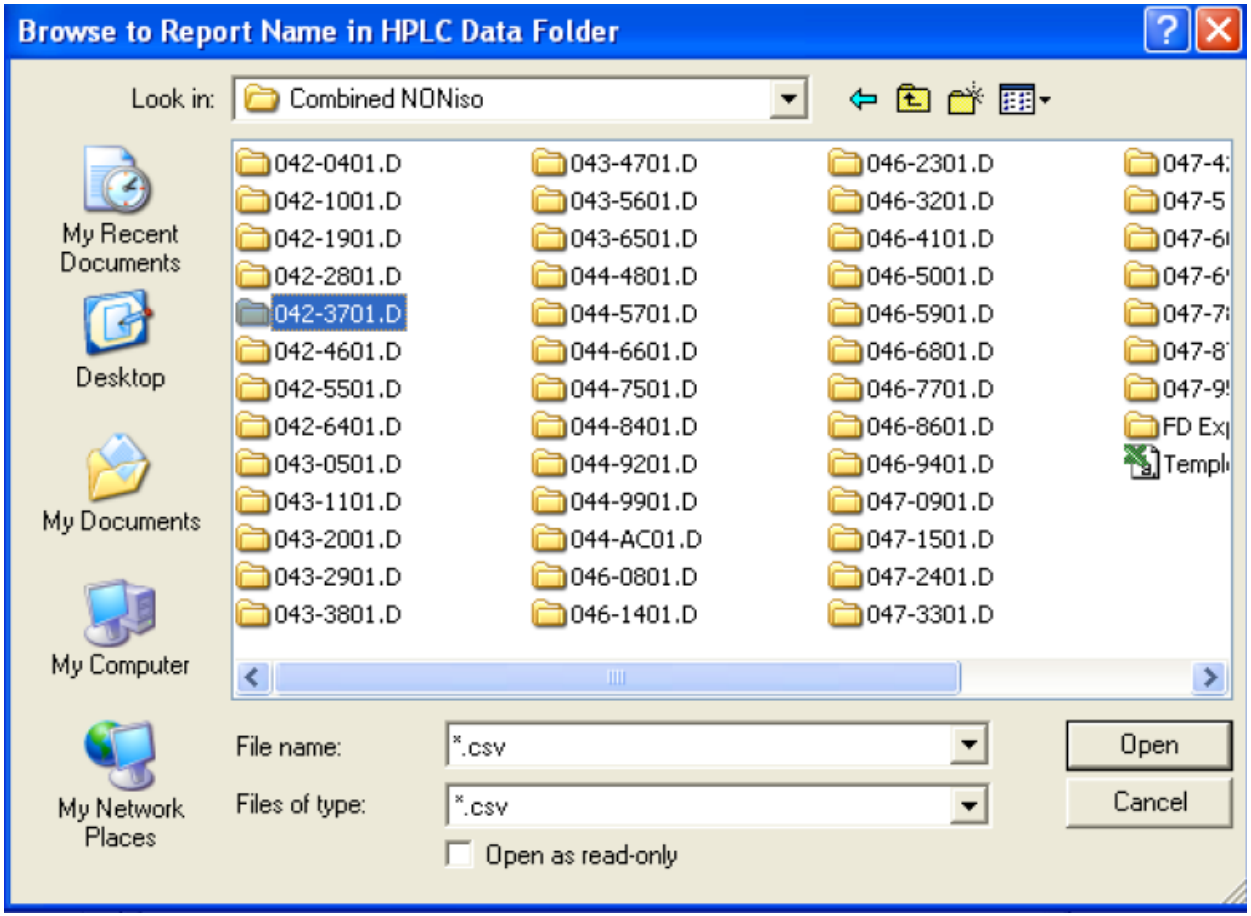
- Open iChemExplorer Reporter
- To load the Agilent HPLC data files collected with iChemExplorer control software, click on Load HPLC Data button

iChemExplorer Reporter: Load HPLC Data



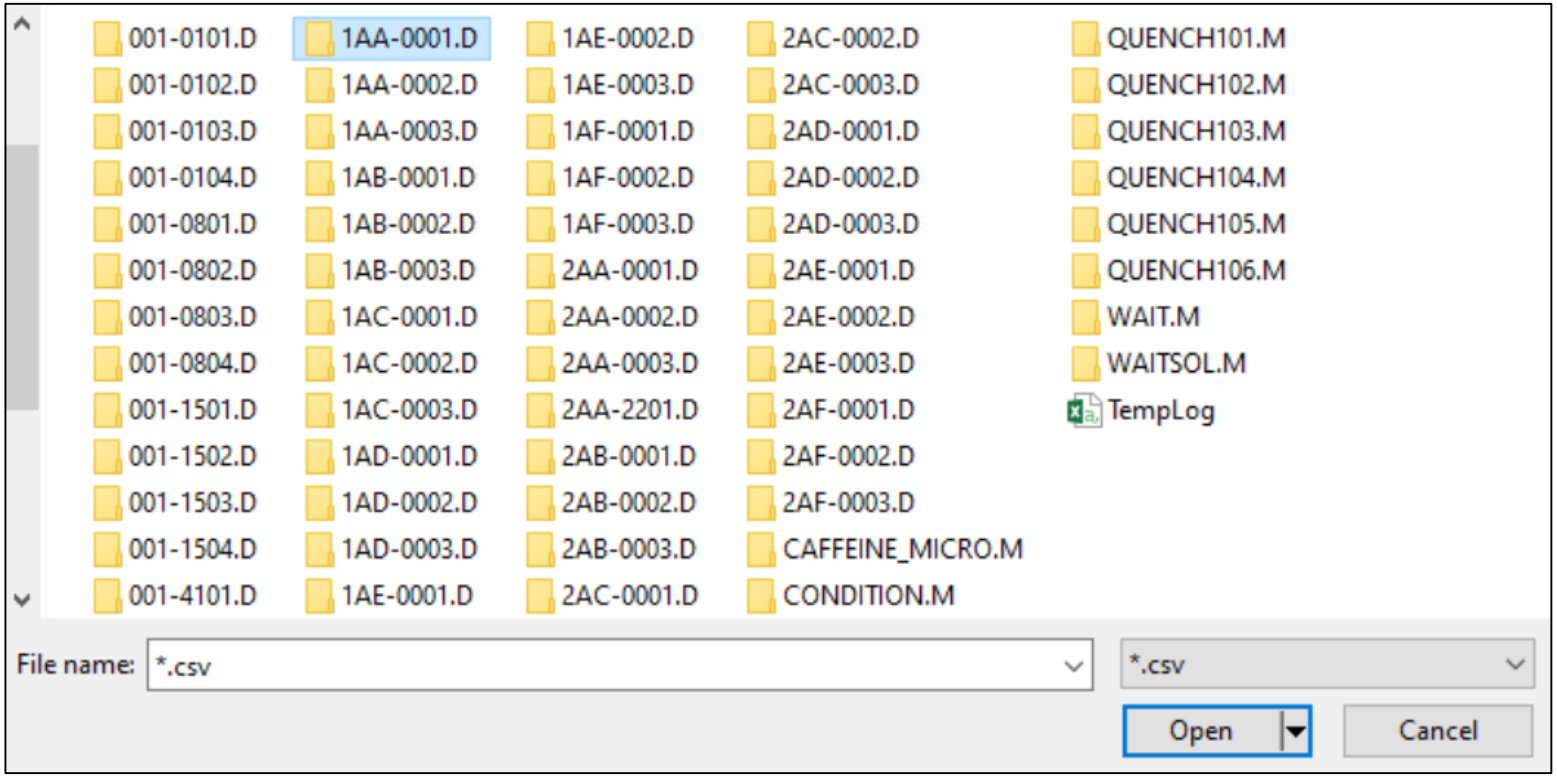
- The File Explorer window appears
- Browse to locate the folder of sample sequence run, typically under C:\Chem32\1\Data

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

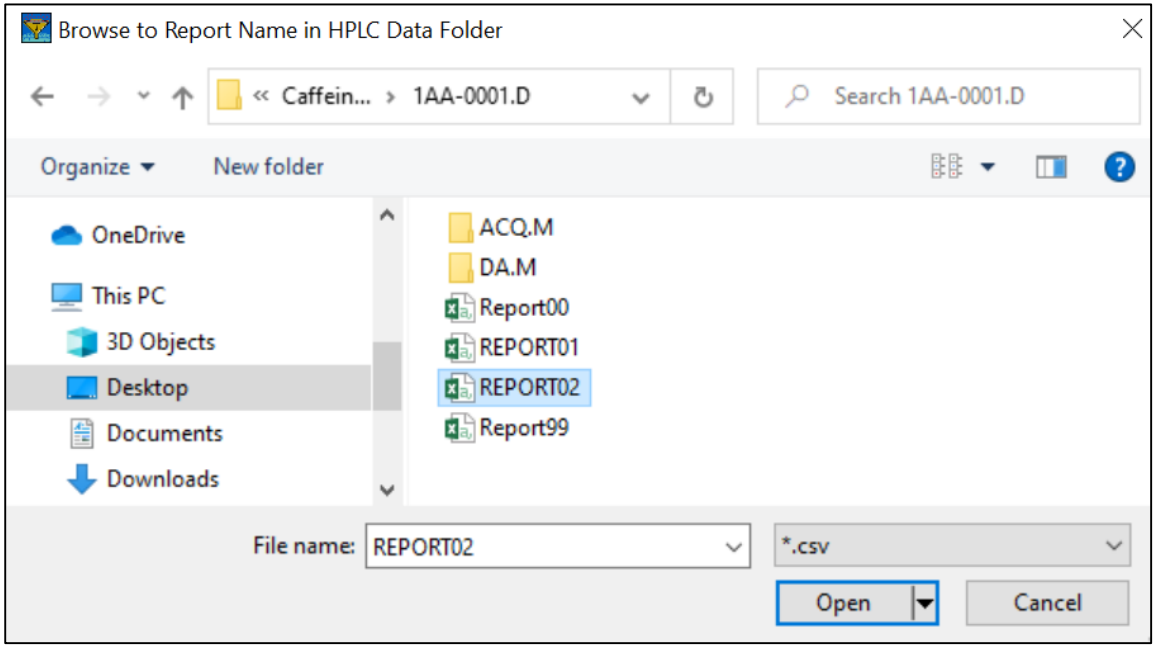
iChemExplorer Reporter: Load HPLC Data



- 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

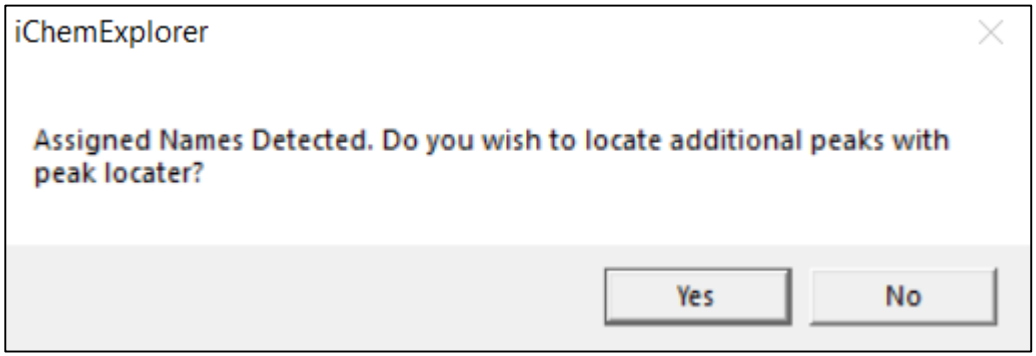


- Report00 records method run details
- Report99 records date time, set point and actual temperature
- Report01 and Report02 record integrated peak areas at selected wavelengths (i.e. 220 nm and 254 nm)

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

iChemExplorer Reporter: Load HPLC Data

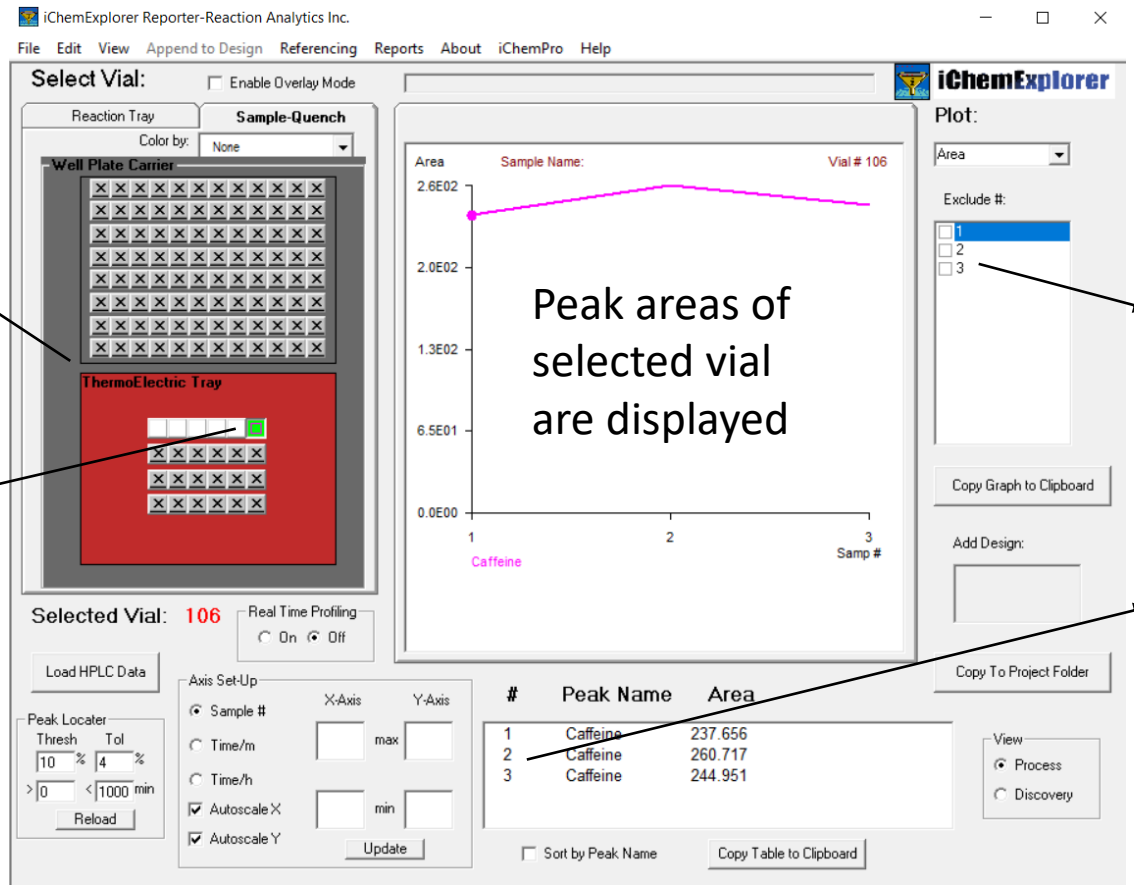
- iChemExplorer loads the integrated peak areas from all the data folders in the sample sequence run
- The following windows pops if the peak name is already assigned in the LC method (typically for solubility assay), select No to load the peak area of the assigned name.



iChemExplorer Reporter: Data Analysis

Sequence run sample layout

Select vial position to display data



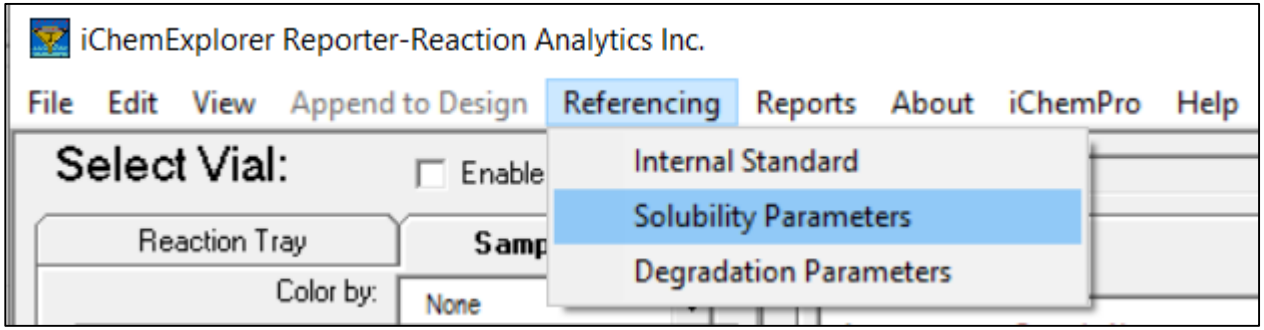
Peak areas of selected vial are displayed

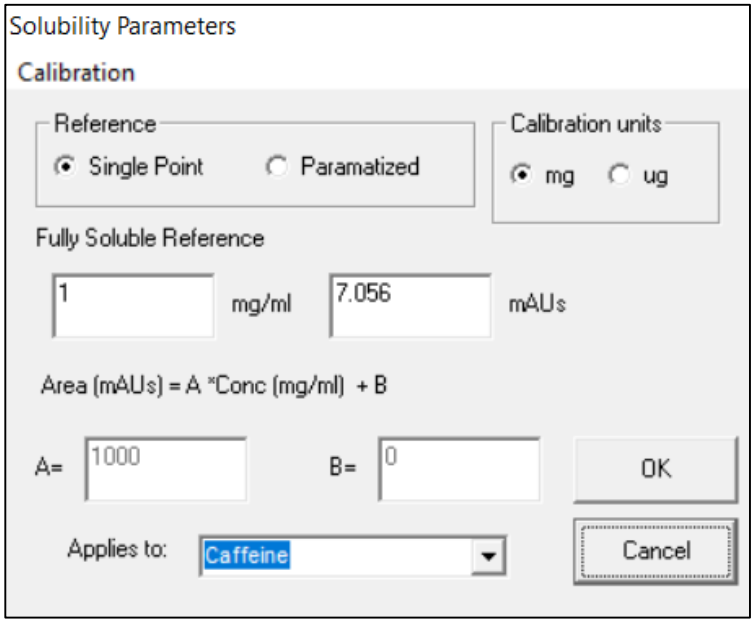
# of injection can be excluded

# of injection from selected vial

iChemExplorer Reporter: Solubility

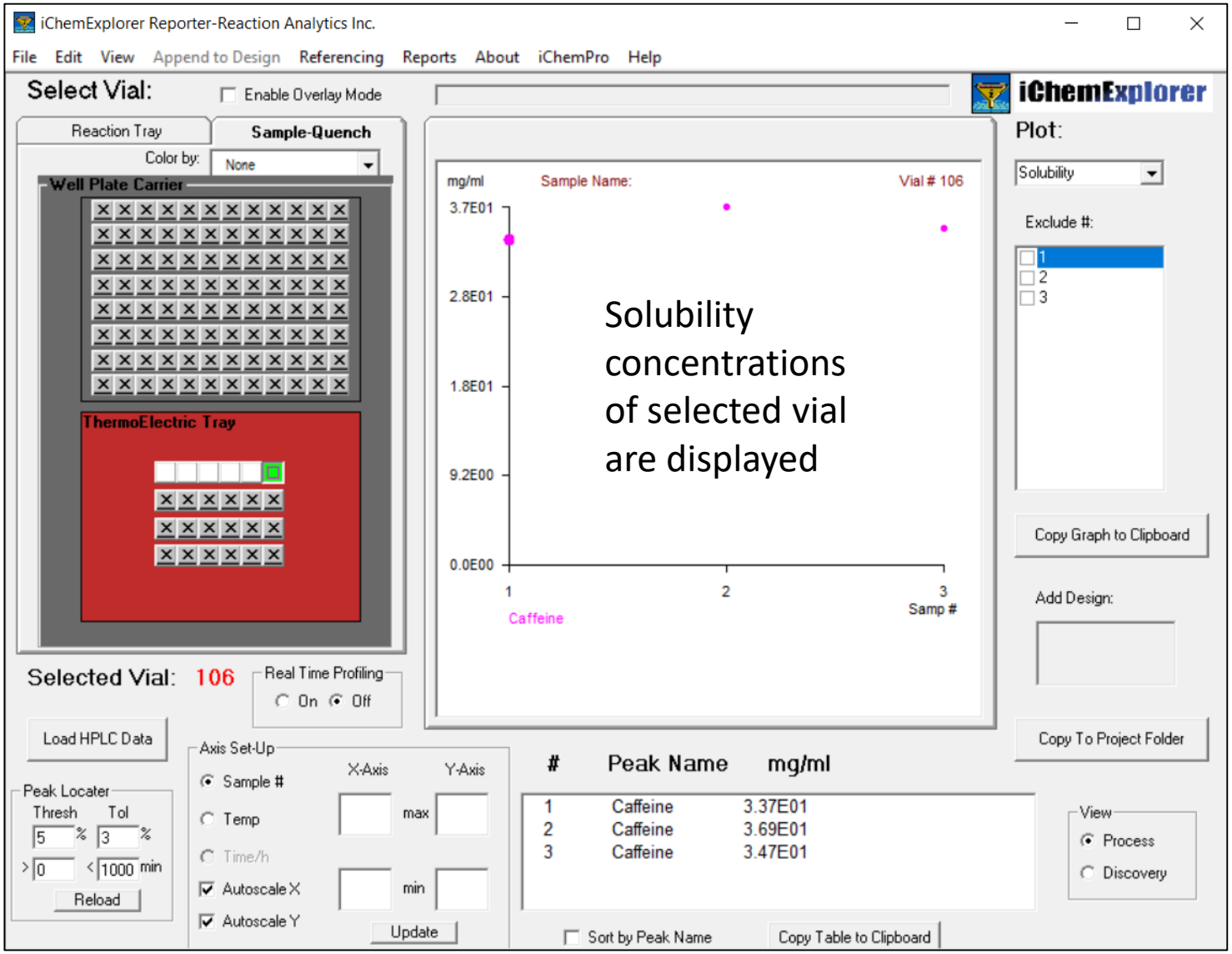
- Select Referencing – Solubility Parameters





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

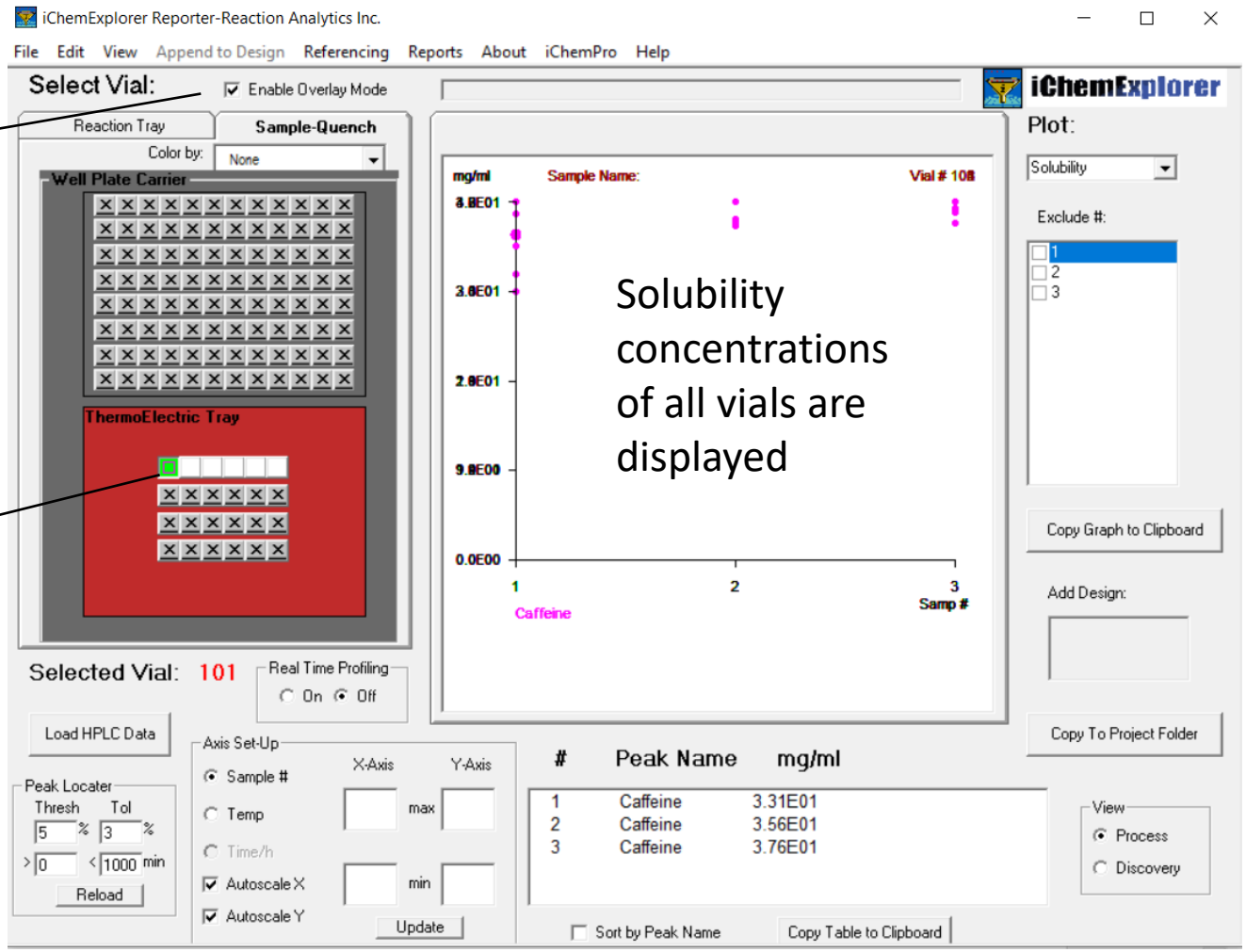
iChemExplorer Reporter: Solubility



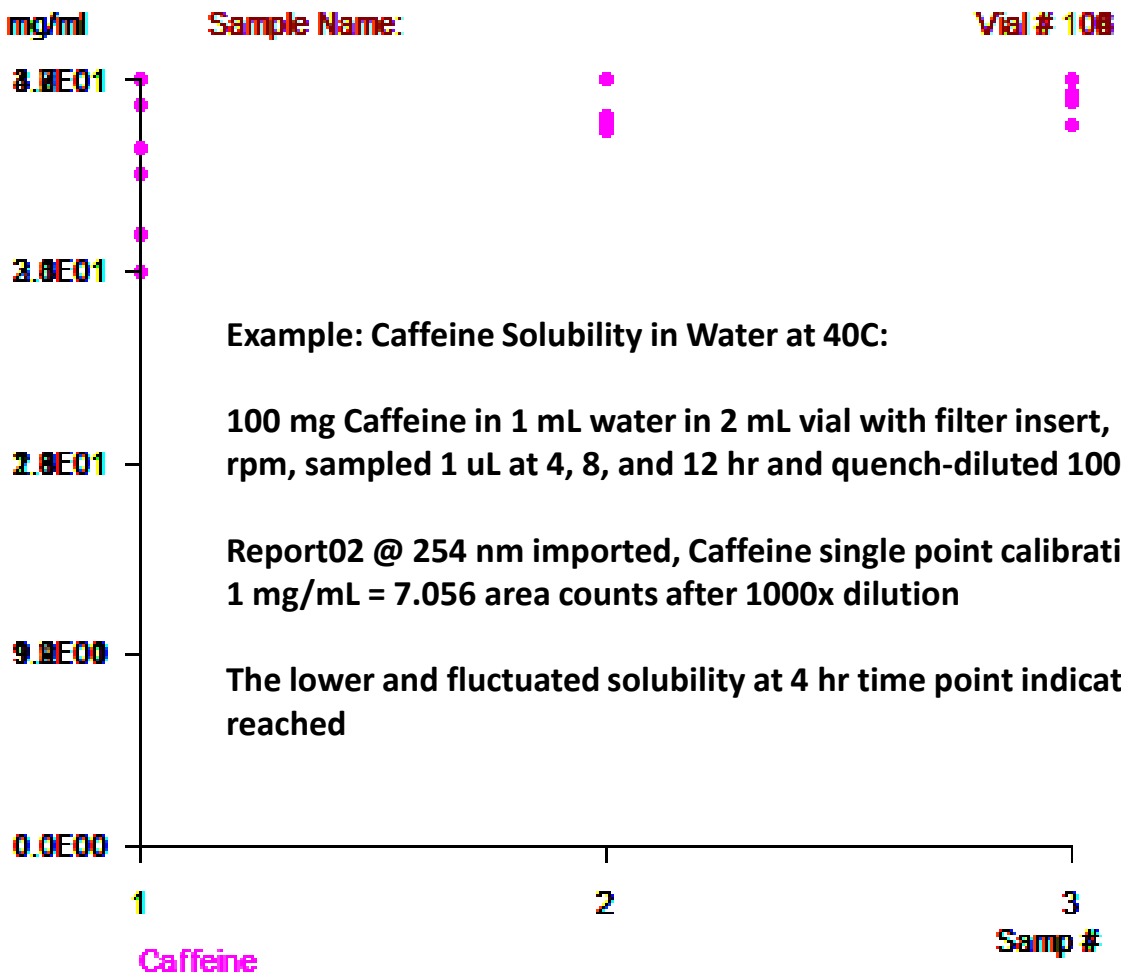
iChemExplorer Reporter: Solubility

Check box to enable data overlay

Select vial position to overlay data



iChemExplorer Reporter: Plot Export



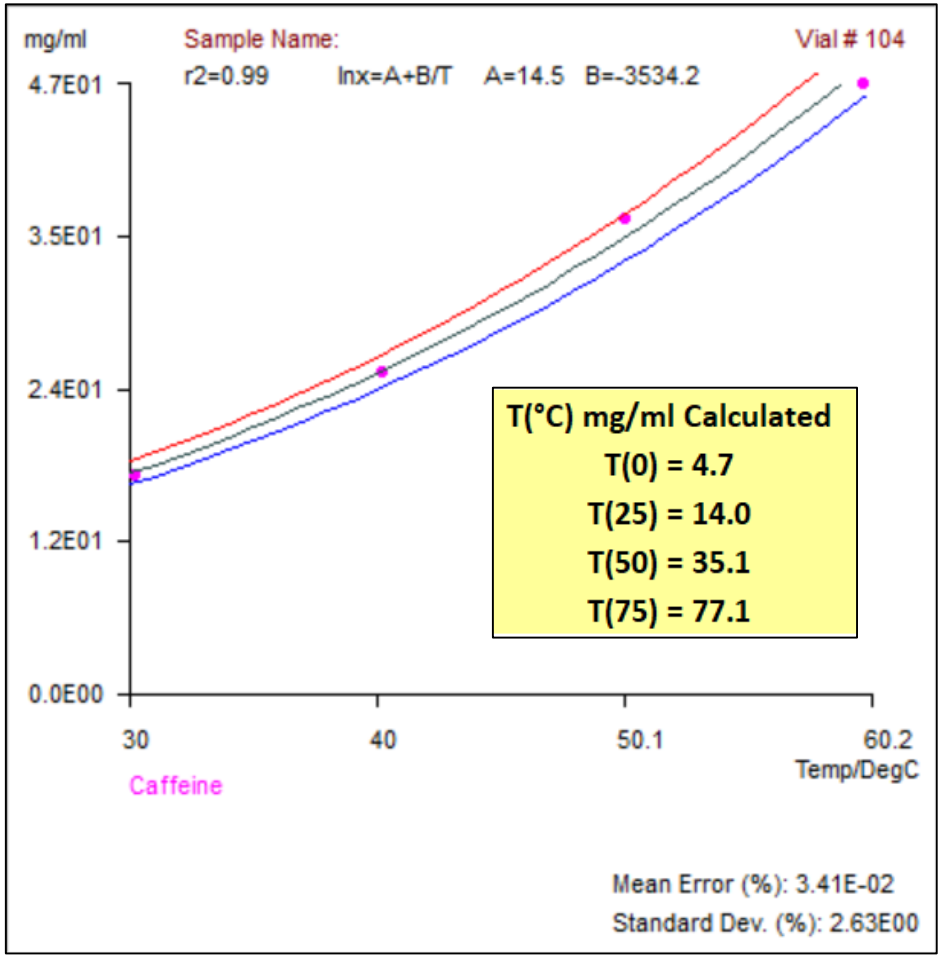
Example: Caffeine Solubility in Water at 40C:

100 mg Caffeine in 1 mL water in 2 mL vial with filter insert, 6 replicate vials at 40C and 200 rpm, sampled 1 uL at 4, 8, and 12 hr and quench-diluted 1000x in water for HPLC analysis

Report02 @ 254 nm imported, Caffeine single point calibration in ICE solubility parameter: 1 mg/mL = 7.056 area counts after 1000x dilution

The lower and fluctuated solubility at 4 hr time point indicated a full equilibrium might not be reached

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