

<PDA spectrum Save and Search>

1. Before you confirm the PDA spectrum result, the calibration data should be prepared.

Prepare STD sample and analyze it, then make a calibration curve.

Without this data, you cannot use PDA library function.

2. The result table of analysis using PDA is as below.

	Reten. Time [min]	Compound Name	Area [mV.s]	Peak Purity [-]	Best match name [-]	Best Match [-]
1	0.517		4144.887	602		-
2	0.775		6949.486	363		-
3	1.600	Naphtalene	639.523	727	Naphtalene1	989
4	1.883	Acenaphtalene	5843.195	896	Acenaphtalene1	990
5	2.350	Acenaphtene	404.552	529	Acenaphtene1	992
6	2.475	Fluorene	270.811	876	Fluorene1	944
	Total		18252.454			

Compound Name : this name come from *.cal file


If there is no calibration file, the results on other columns(Peak Purity, Best match name, Best Match) are not displayed.

Best Match Name : the best matched compound name(comparing with *. lib file)

Best Match : the level of matching with Library(the highest value is 1000)

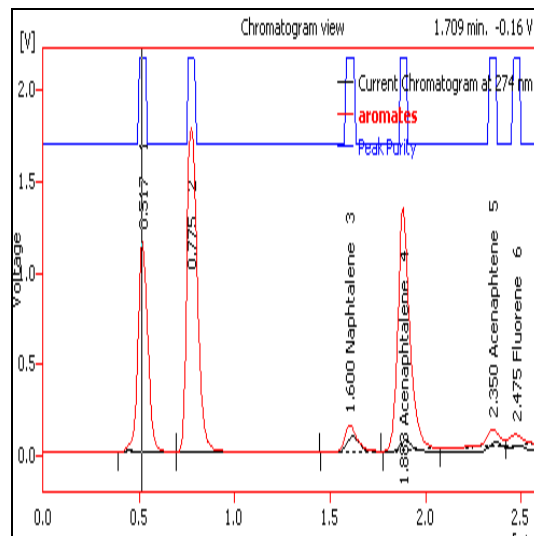
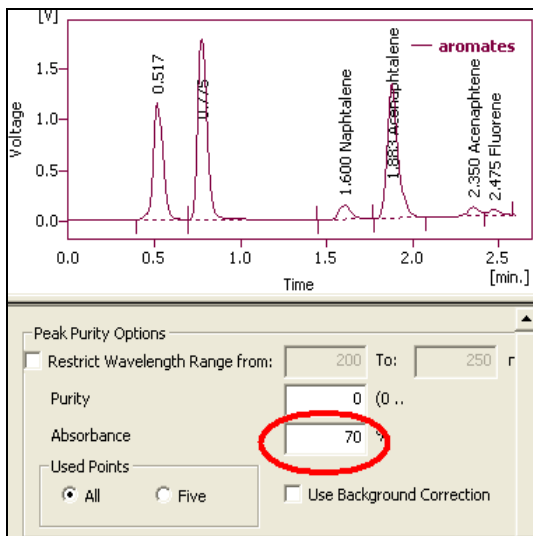
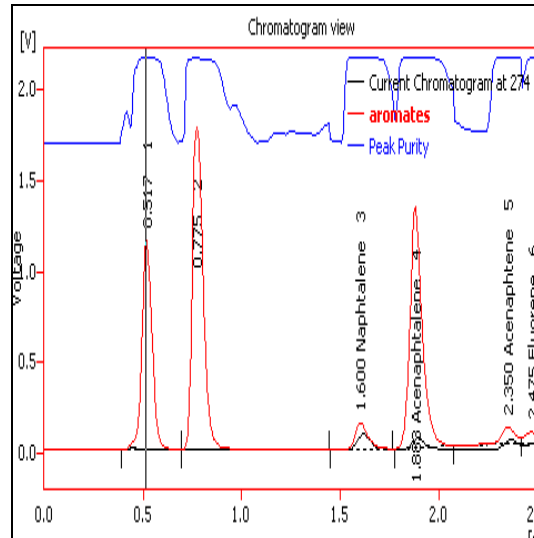
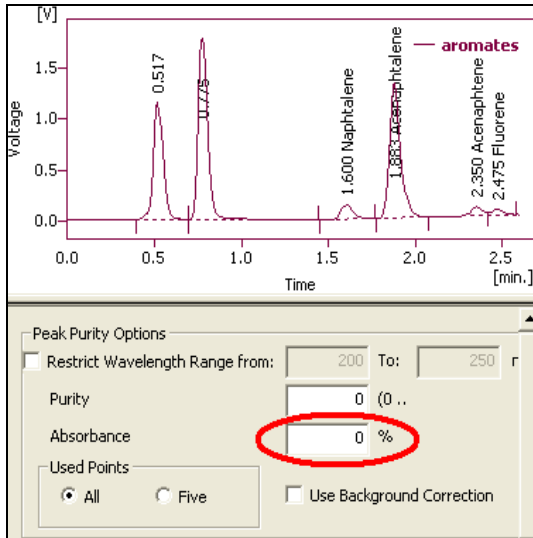
Peak Purity : the purity level, it can be changed according to Purity Option

3. PDA Method : Peak Purity Option and Library Search Option

Peak Purity Options	
<input type="checkbox"/> Restrict Wavelength Range from:	<input type="text" value="190"/> To: <input type="text" value="900"/> nm
Purity	<input type="text" value="900"/> (0 ..
Absorbance	<input type="text" value="2"/> %
Used Points	
<input checked="" type="radio"/> All	<input type="radio"/> Five
<input type="checkbox"/> Use Background Correction	
Library Search Options	
Match	<input type="text" value="Least Square"/>
Match Factor	<input type="text" value="800"/> (0 ..
Max. Number of Hits:	<input type="text" value="3"/>
<input type="checkbox"/> Restrict Wavelength Range From:	<input type="text" value="200"/> To: <input type="text" value="360"/> nm
<input type="checkbox"/> Restrict Retention Time Relative:	<input type="text" value="20"/> %
<input type="checkbox"/> Use Background Correction	
<input type="checkbox"/> For All Detected Peaks	
	
<input checked="" type="checkbox"/> 1	

4. Peak Purity Option : the level for classifying of compound

- Restrict Wavelength range : set the wavelength range for comparison
- Purity Threshold : restrict spectra with match factor below this value from the peak purity
- Absorbance Threshold : defines start and end spectrum for peak purity evaluation in % of detected peak height



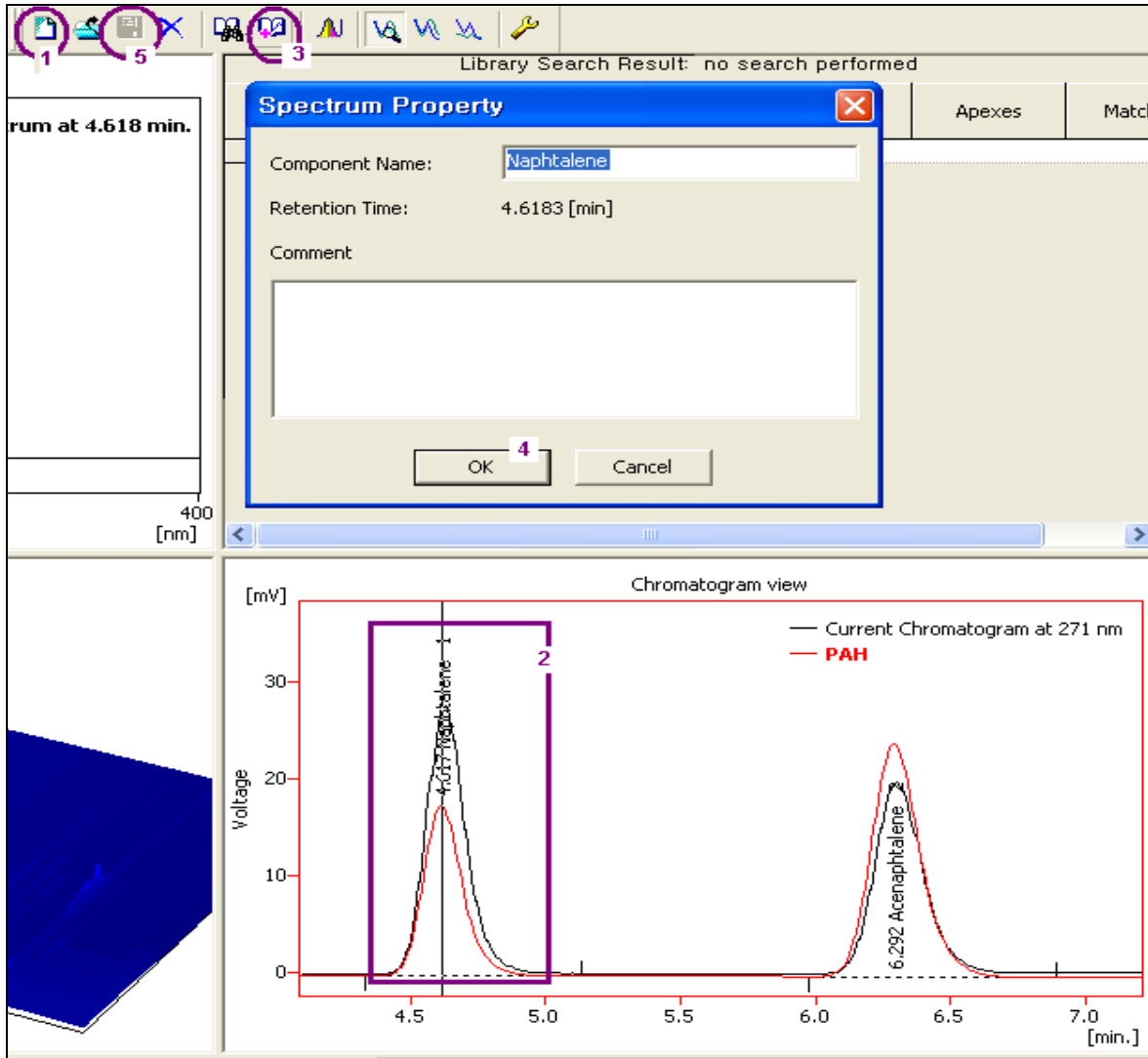
- Used Points : all spectra or only the five significant points(start, inflexes, apex, end).

The Absorbance and Purity Threshold are not used in five points calculation.

- Use Background Correction : the baseline for individual wavelength is interpolated between peak start and peak end points.

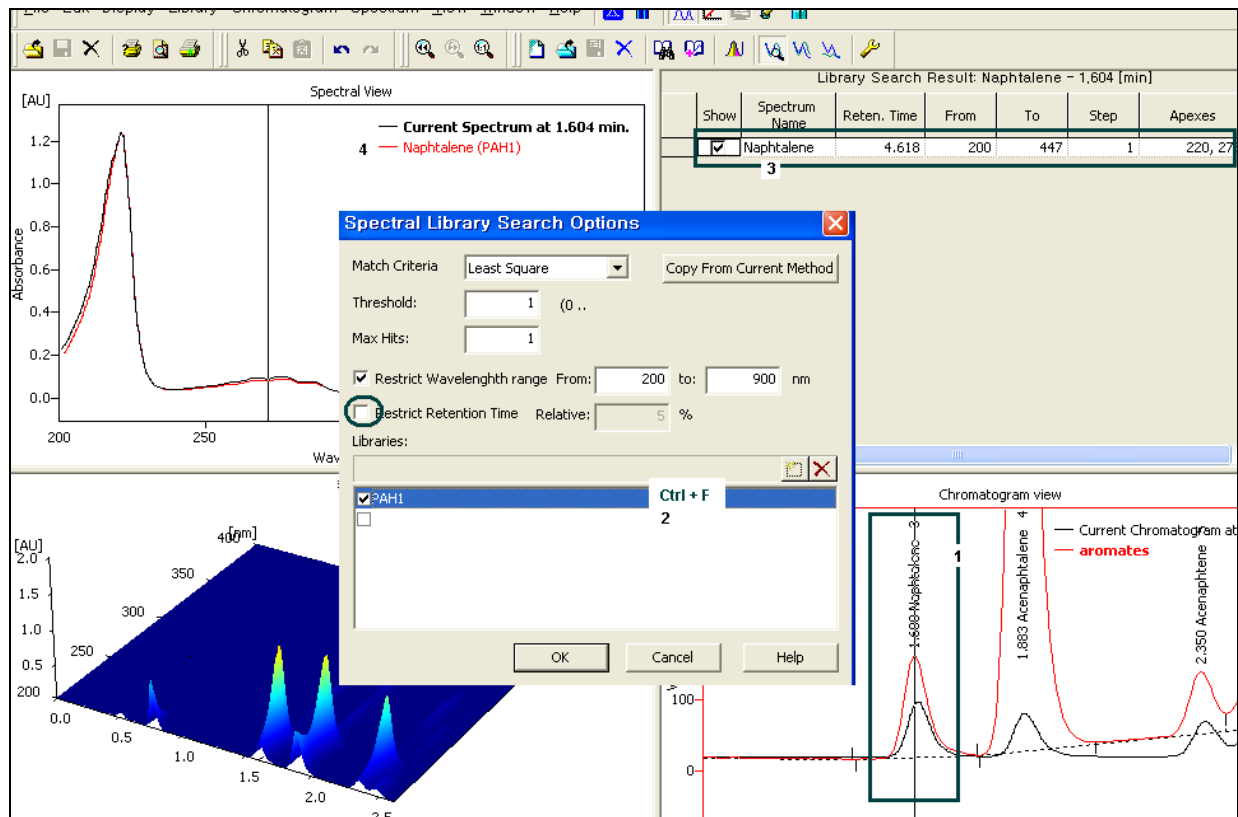
5. Library Search Option

- Save spectrum : Open STD data(calibrated) on the chromatogram window => move to PDA window => New library(1) => Mark Here(2) on the apex of peak => Add spectrum(3) => input component name(4)
=> Save Library(5)



- Spectrum Library Search

Open sample Data => PDA window => Using Ctrl + F, select library(do not check RT)
=> Searched spectrum is displayed

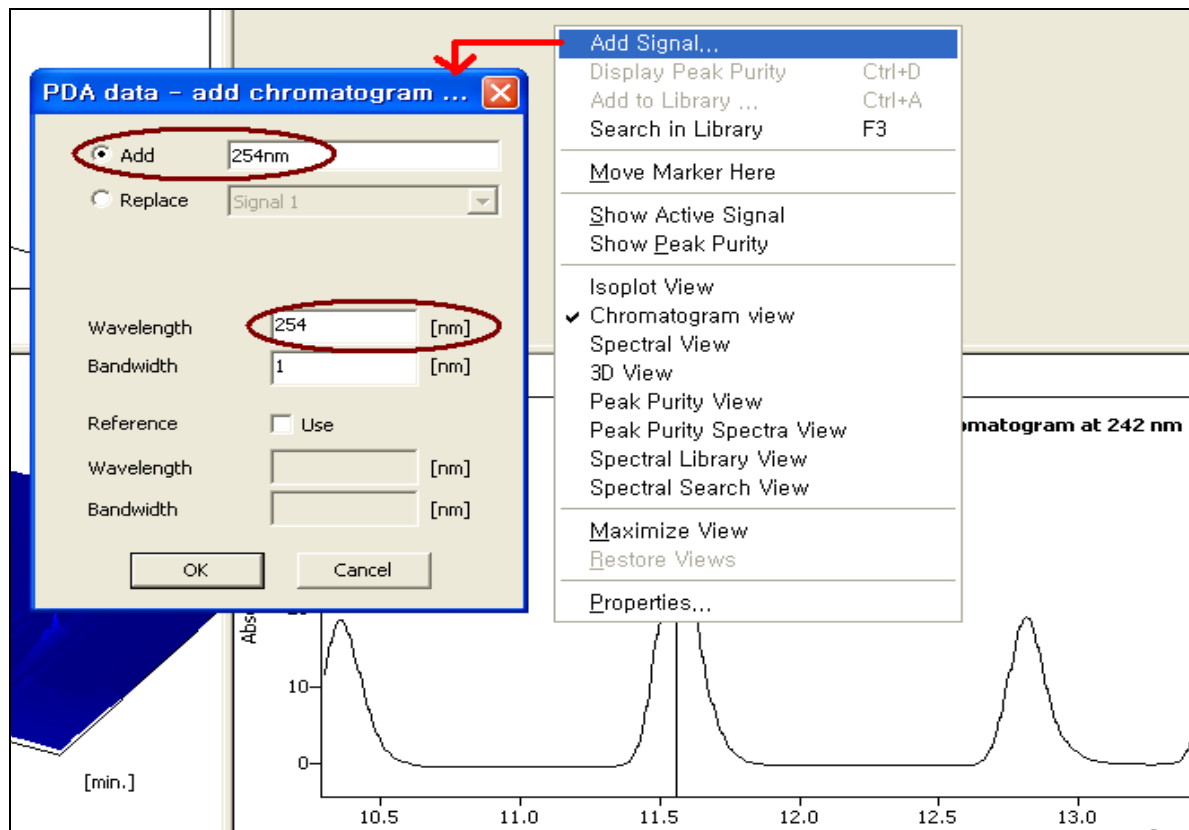


Option

- Match Criteria : select one method for library search
choose Least square or Correlation
(do not recommend to use Weighted Least Square)
- Match Factor Threshold : Only hits with match factor above this value will be displayed.
- Max. Number of Hits : Limits the number of displayed spectra found.
- Restrict Wavelength Range : The spectra comparison will be limited to the specified range.
It is better to compare the spectrum without this function.
- Restrict Wavelength Range : Limits the found spectra only to those RT within specified range.
- Use Background Correction : the baseline for individual wavelength is interpolated between peak start and peak end points.
- For All Detected Peaks : Perform the library search for all detected peak.

6. ADD Signal function

Click right mouse button => ADD SIGNAL => Input the name of this chromatogram and select the wavelength to add



7. Print the Report

