



PDA – PHOTO DIODE ARRAY

CLARITY EXTENSION

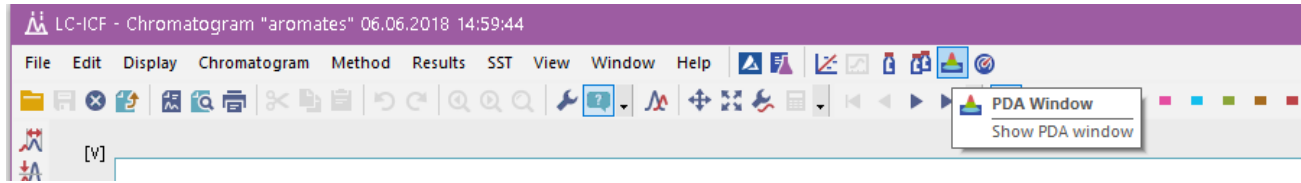
P01/80A 3/2/2020



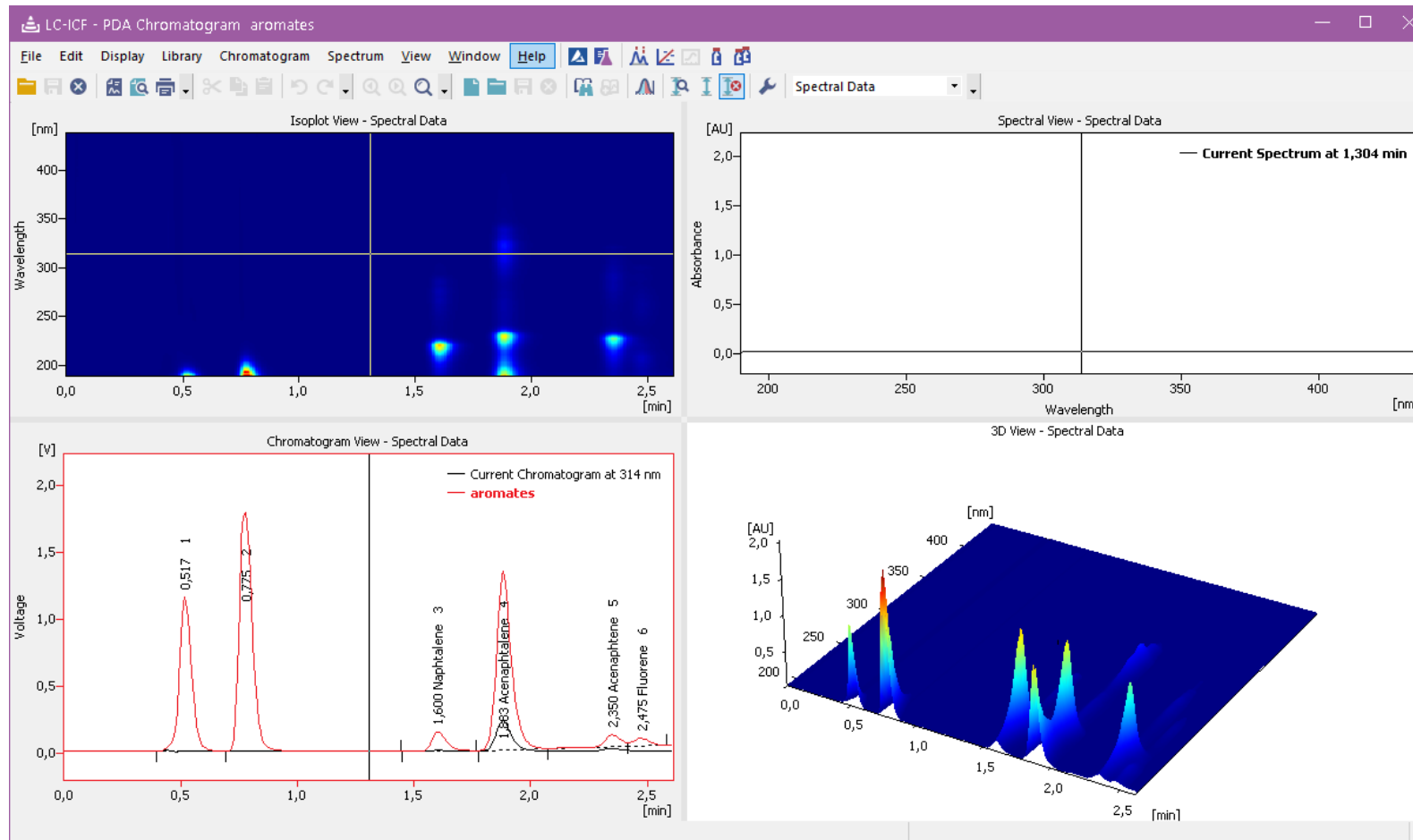
PDA Extension

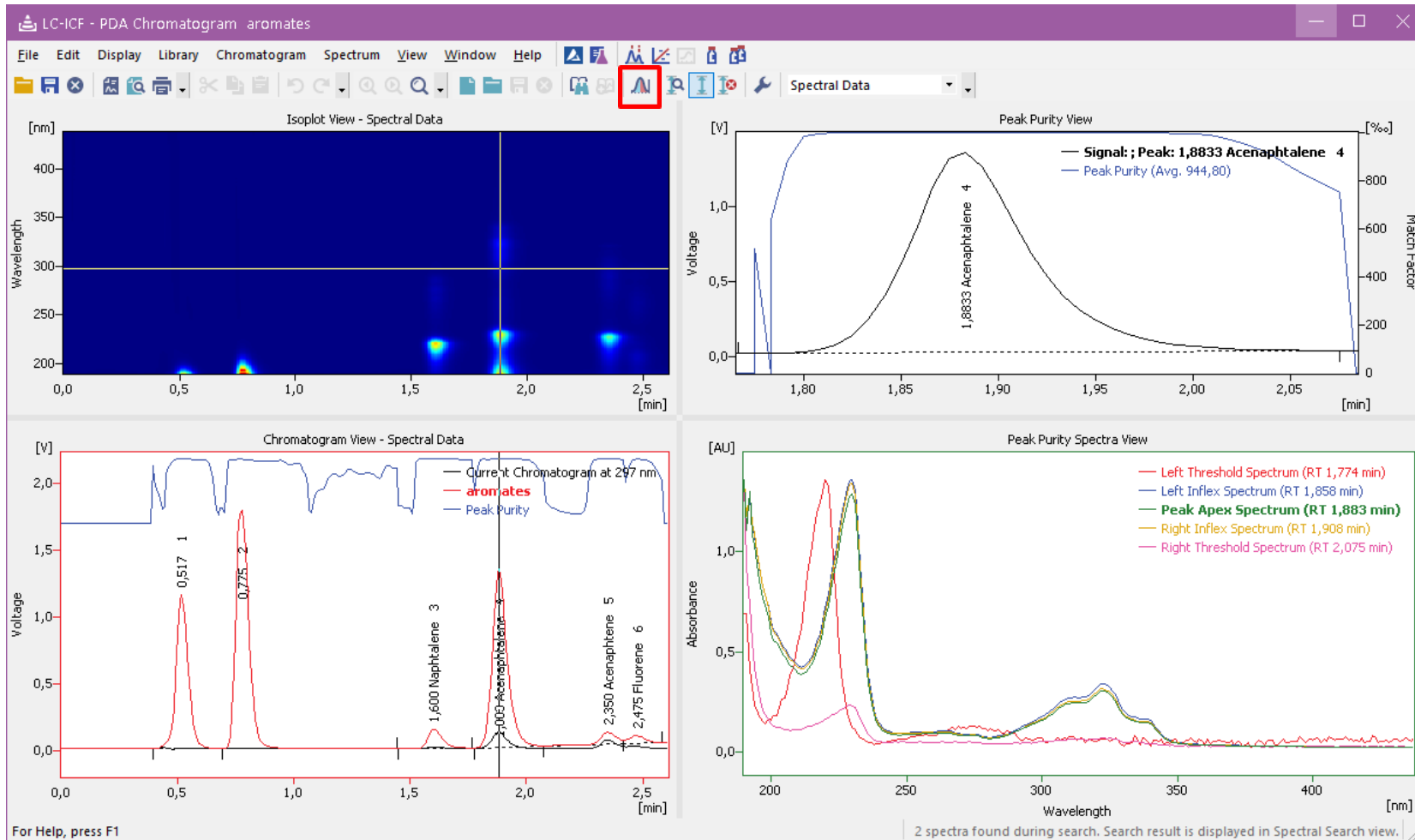
- Spectral data acquisition from selected detectors
- Import and export of spectral data in text format
- Isoplot and 3D plot for spectral data evaluation
- Peak purity evaluation
- Spectral library and spectral library search

PPT PDA Extension → PDA Window



→ PDA window is accessible from the Chromatogram window





- View peak purity for entire chromatogram or a single peak
- Spectra for peak start, end, inflexion and apex are compared in the Peak Purity Spectra View



The screenshot displays the LC-ICF software interface for PDA Chromatogram analysis. The main window is titled "LC-ICF - PDA Chromatogram aromates". The interface is divided into several panels:

- Isoplot View - Spectral Data:** A 2D heatmap showing intensity as a function of Wavelength [nm] (y-axis, 200-400) and Time [min] (x-axis, 0,0-2,5). A red box highlights the "Library Search" icon in the toolbar.
- Spectral View - Spectral Data:** A line graph of Absorbance [AU] vs Wavelength [nm] (200-400). It compares the "Current Spectrum at 1,884 min" (black line) with library matches for "Acenaphthalene (PAH)" (red line) and "Acenaphthene (PAH)" (blue line).
- Chromatogram View - Spectral Data:** A chromatogram showing Voltage [V] vs Time [min] (0,0-2,5). It displays the "Current Chromatogram at 297 nm" (black line) and "aromates" (red line). Peaks are labeled with retention times: 0,517 (1), 0,775 (2), 1,600 (Naphthalene 3), 1,884 (Acenaphthalene), 2,350 (Acenaphthene 5), and 2,475 (Fluorene 6).
- Library Search Result: Acenaphthalene - 1,884 [min]:** A table showing search results for Acenaphthalene and Acenaphthene.

Show	Spectrum Name	Reten. Time	From	To	Step	Match
<input checked="" type="checkbox"/>	Acenaphthalene	6,244	200	447	1	987,7
<input checked="" type="checkbox"/>	Acenaphthene	8,250	200	447	1	883,2

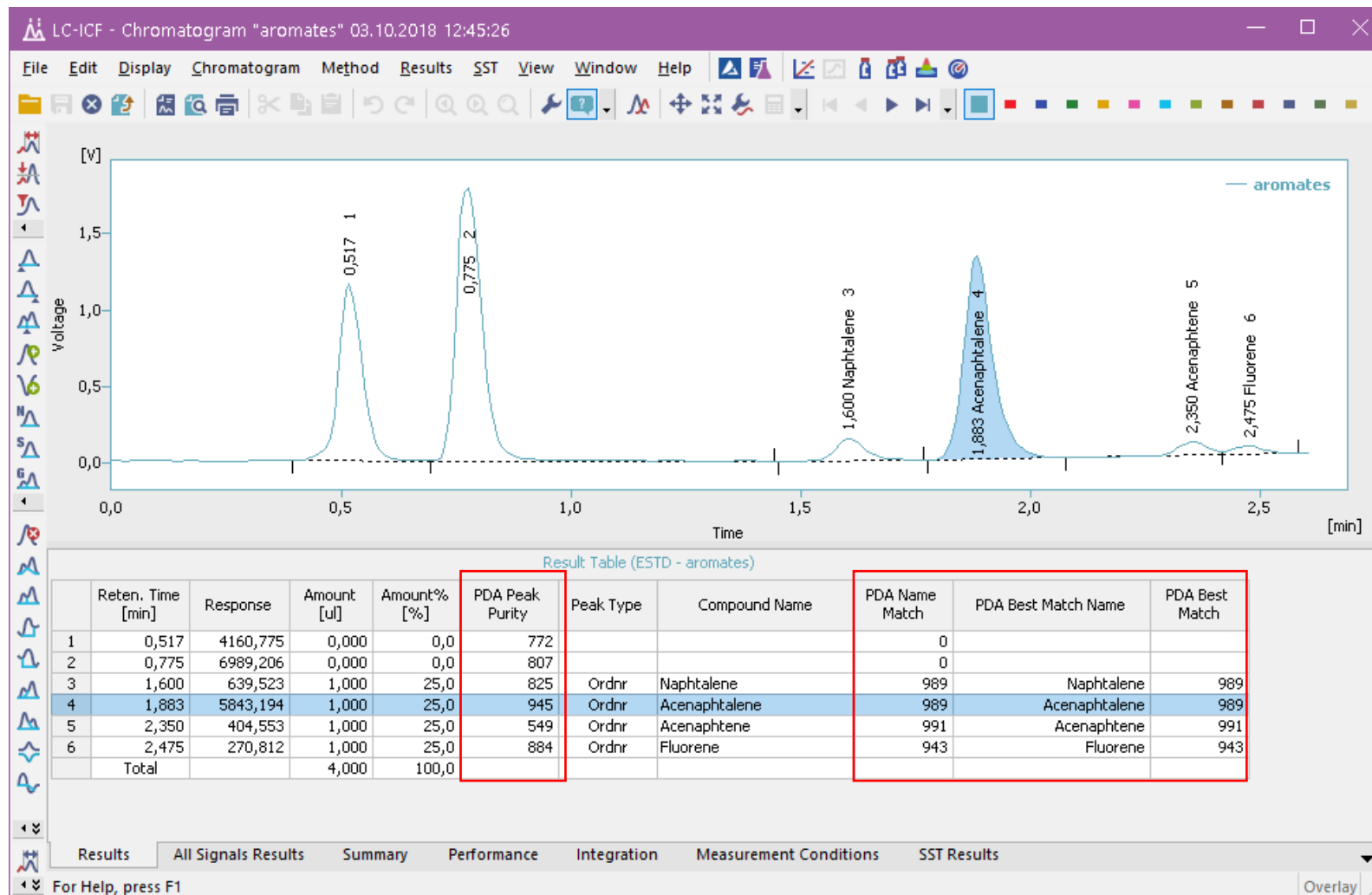
For Help, press F1

2 spectra found during search. Search result is displayed in Spectral Search view.

→ Library search results are displayed as overlay in Spectral View or as a table in Library Search Result

→ Peak Purity and Library Search Options are set on the PDA Method

The screenshot shows the 'PDA Method' configuration window in the LC-ICF software. The window title is 'LC-ICF - Chromatogram "aromates" 03.10.2018 12:45:26'. The 'PDA Spectrum' is set to 'Spectral Data'. Under 'Peak Purity Options', the 'Restrict Wavelength Range' is checked with 'From: 190' and 'To: 900 nm'. The 'Absorbance Threshold' is set to '10 %'. Under 'Used Points', 'All' is selected. 'Use Background Correction' is unchecked. Under 'Library Search Options', 'Match Criteria' is 'Least Square', 'Match Factor Threshold' is '900 (0 .. 1000)', and 'Max. Number of Hits' is '3'. 'Restrict Wavelength Range' is checked with 'From: 190' and 'To: 900 nm'. 'Restrict Retention Time' is unchecked with 'Relative: 1 %'. 'Use Background Correction' and 'For All Detected Peaks' are unchecked. A list of search results shows 'PAH' checked. The bottom of the window has tabs for 'Instrument', 'Event Table', 'GLP Info', 'PDA Method', 'Results', 'All Signals Results', 'Summary', 'Performance', 'Integration', 'Measurement Conditions', and 'SST Results'. The 'PDA Method' tab is active. A status bar at the bottom left says 'For Help, press F1' and a button labeled 'Overlay' is at the bottom right.



→ Library search results are displayed as overlay in Spectral View or as a table in Library Search Result

Report Setup Chromatogram

Page Setup

- Lab. Header
- Report Header
- Method
- Calibration
- Chromatogram
- Results
- Sequence
- SST
- PDA
- Audit & Signatures

Print

On New Page

Signals

All

Active Chromatogram

Only Active Signal

Height of Graphs

Fixed Height: [mm]

PDA Data Plots

Isoplot

3D plot

Graph

Spectra

Peak Purity

Graph

Spectra

All Peaks

Identified Peaks

Library Search Results

Table

Spectra

OK

Cancel

Help

8.1.2013 10:03 PDA Report 0:\Data_40\40913\DEMO_PDA\Default.mxd.PRM Page 1 of 3

Clarity PDA View

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Library Search Results: Acenaphthalene - 1.891 (min)

Show	Spectrum Name	Retain. Time	Match
<input checked="" type="checkbox"/>	Acenaphthalene	6.244	99.7
<input checked="" type="checkbox"/>	Acenaphthalene	6.250	99.3

Search Results - Chromatogram aromates - 1.891 min.

8.1.2013 10:54 Chromatogram 0:\Data_40\40913\DEMO_PDA\Default.mxd.PRM

3D View

8.1.2013 10:03 PDA Report 0:\Data_40\40913\DEMO_PDA\Default.mxd.PRM Page 3 of 4

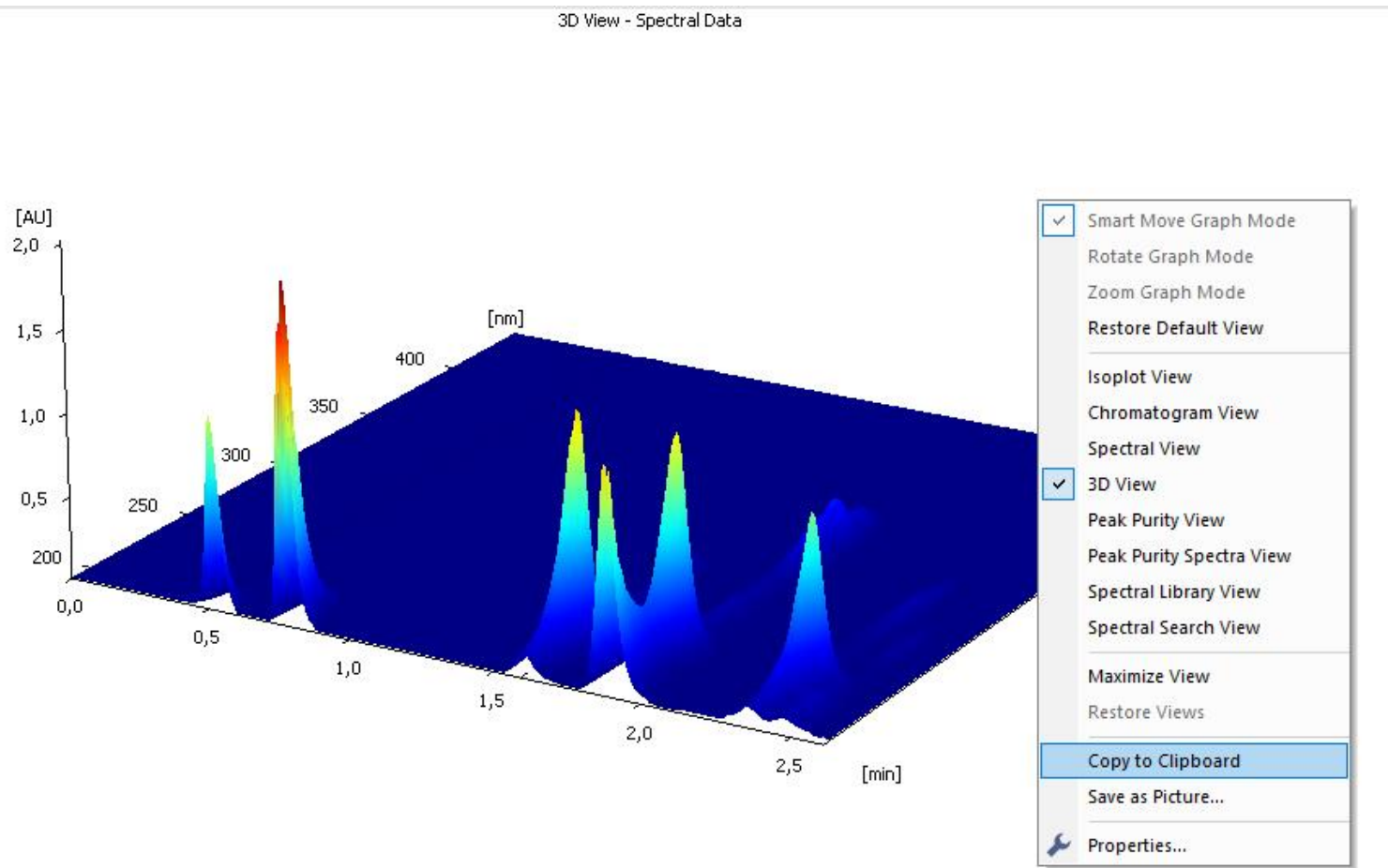
Clarity PDA View

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Peak Purity View

Peak Purity Spectra View

➔ Customize PDA Report to display desired results



→ Export graphs into clipboard or save them as a picture (*.emf)



...THANK YOU FOR YOUR TIME



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