# News And Updates

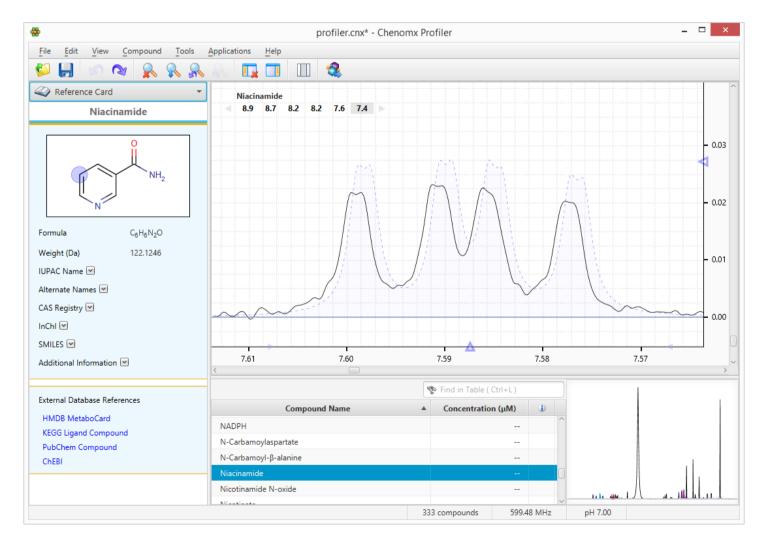
## Chenomx Core Functions - The Profiler

2 DECEMBER 2015 ADMIN COMMENTS OFF BLOG (HTTPS://WWW.CHENOMX.COM/CATEGORY/BLOG/), FEATURES AND FUNCTIONS (HTTPS://WWW.CHENOMX.COM/CATEGORY/FEATURES-AND-FUNCTIONS/)

In this series, we explore some of the core functions of Chenomx Suite. In this edition, we're looking at the "Profiler" module. The Chenomx Profiler is used to identify compounds and quantify their concentrations based on data in an NMR spectrum. Key features include:

- Comprehensive pH sensitive reference compounds
- Computer assisted metabolite assignment and fitting
- Spectral binning
- Spectral overlays
- Multiple file concentration exports
- Detailed reference resources for library compounds

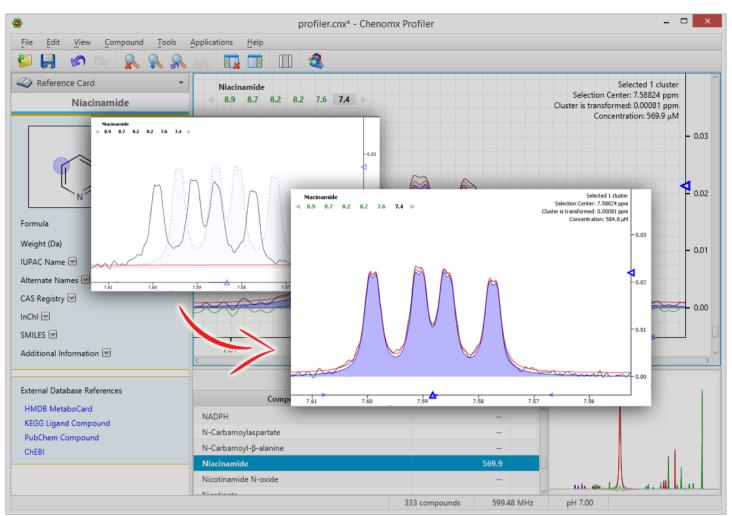
The 'Profiler' module lets you identify and quantify the contents of your mixture spectrum by comparing it to a compound library with hundreds of reference signatures.



(https://www.chenomx.com/wp-content/uploads/2015/11/profiler\_1.png)

### Analysis Tools

You can obtain the concentration of compounds in your mixture by matching Chenomx's compound signatures to the peak shapes in your spectrum.



(https://www.chenomx.com/wp-content/uploads/2015/11/profiler\_2.png) Search Tools

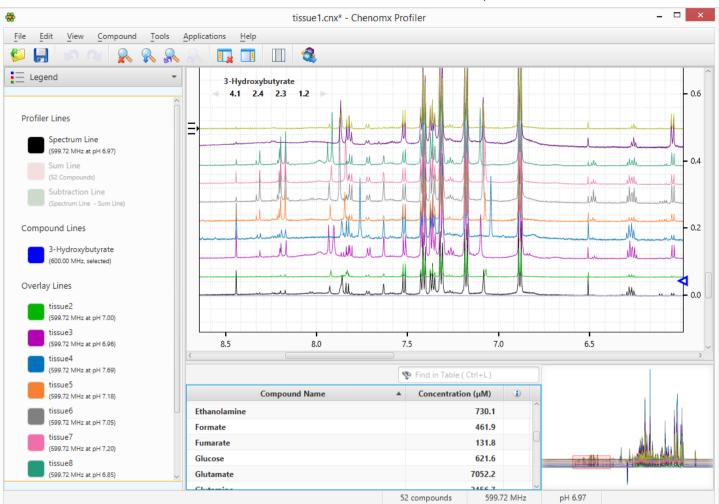
Profiler contains a variety of tools to help you search through all available reference signatures and identify the components in your mixture.

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🗳 🔒 😒 💊	🙊 🙊 🔍 🗖 🗖 🗶 🦧					
Reference Card	<ul> <li>Niacinamide</li> </ul>					
Niacinamid						0.05
	Search for Compounds					
						- 0.04
	Find compounds that have one (or more) clusters located:					
						- 0.03
N	between and	ppm				
Formula	near 7.6 ppm					- 0.02
Weight (Da)						
IUPAC Name 💌	You can use this dialog to filter your displayed compounds bas	ed on				- 0.01
Alternate Names 💌	cluster locations. You can cancel that search at any time by clear Quick Search field or pressing the ESC key.					
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	Acetamide N,N-Dimethylformamide					
	Niacinamide					
	Nicotinamide N-oxide				/	
		5		500 40 MU		
		5 compounds (328	hidden)	599.48 MHz	рН 7.00	

(https://www.chenomx.com/wp-content/uploads/2015/11/profiler\_3.png)

#### Spectral Overlays

You can use 'Overlay Lines' to compare your own spectra with each other. You can also give these overlaid lines an offset with the stacking feature.



(https://www.chenomx.com/wp-content/uploads/2015/11/profiler\_4.png)

#### Data Export

Once you're finished profiling, it's easy to export your quantitative data for further analysis.

*	tissue1.cnx* - Chenomx Profiler – 🗖 🗙				
File Edit View	Compound Tools Applications Help				
🖗 📙 🔊					
Files	Batch Export: Step 1     - 0       Select profiled data to export, and where to save the results.     - 0	.6			
<ul> <li>tissue1.cnx</li> <li>tissue2.cnx</li> <li>tissue3.cnx</li> </ul>	Export Compound Concentrations (μM) - 0	).4			
<ul> <li>tissue4.cnx</li> <li>tissue5.cnx</li> </ul>	Export from these Files and Folders:				
<ul> <li>tissue6.cnx</li> <li>tissue7.cnx</li> </ul>	☐ 10 files selected.           Add Files         Add Folder         Clear	1.2			
<ul> <li>tissue8.cnx</li> <li>tissue9.cnx</li> </ul>					
<ul> <li>tissue9.cnx</li> <li>tissue10.cnx</li> </ul>	Save Exported Data to:	Π			
	⊘ Data from 10 files will be exported.  Next ► Finish Cancel	.0			
	Compound Name Concentration (μΜ	>			
	Ethanolamine 730.1 Formate 461.9				
	Fumarate     131.8       Glucose     621.6				
Previous	Next Glutamate 7052.2				
	52 compounds 599.72 MHz pH 6.97				

(https://www.chenomx.com/wp-content/uploads/2015/11/profiler\_5.png)

#### **Spectral Binning**

Profiler offers a number of binning options, including spectral binning (standard), targeted binning (based on a compound library), or residual binning (based on unmatched regions.)

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File Edit View Compound Tools Applications Help					
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🧔 Overlay Spectra	Choose how the bins will be define	ned.			
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💩 tissue7.cnx					
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💩 tissue9.cnx					
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	Compound Name			ration (µM	
	Ethanolamine			730.1	
Formate				461.9	
		Fumarate		131.8	
Glucose				621.6	
Previous Next Glutamate			7052.2		
Previous	Glutana			7052.2	L. A. HALL & A. LANDANA MANA
			52 compounds		pH 6.97

(https://www.chenomx.com/wp-content/uploads/2015/11/profiler\_6.png)

#### **Batch Fit**

Once you've assigned metabolites to one spectrum, you can use the batch fit tool to autofit multiple spectra with multiple metabolites.

*	Batch Refere	nce.cnx - Chenomx Profiler		_ 🗆	×
File Edit View Compound	Tools Applications Help				
🖉 🗐 🔊 രു 🔒	Add Spectrum Overlays Ctrl+Shift+O		1 1 1 1		
Files	Remove Spectrum Overlays				
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Batch Reference.cnx	Search for Compounds				
Sample 1.cnx	Spectral Binning				- 0.8
Sample 2.cnx	📶 Batch Fit				
Sample 3.cnx					- 0.6
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Sample 5.cnx	Batch Export	My m		Mphin Jefimin	
	- m mm	My moun	mm	Mul Mum	- 0.4
		Fitting 4 of 5 spectra	Stop	Mui fuina Mui fuina Mui fuina	- 0.2
	3.2 3.1	3.0 2.9	2.8	2.7 2.6 2.5	- 0.0
	<	😨 Find in Table	( Ctrl+L )		>
	Compound Name	▲ Concentrat			
	1,3-Diaminopropane	- Concention		<b>^</b>	
	1,3-Dihydroxyacetone				
	1,3-Dimethylurate				
	1,6-Anhydro-β-D-glucose				
Previous Next	1,7-Dimethylxanthine			1	
TREVIOUS	1-Methylnicotinamide				
		333 compounds	599.73 MHz	pH 7.00	

(https://www.chenomx.com/wp-content/uploads/2015/11/profiler\_7.png)

Thanks for reading and learning more about Chenomx. Check out our free demo (https://www.chenomx.com/our-software/our-free-demo/) and learn more about all the features included in our software.