UnknownProcessor

By Leoson

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1. Batch creation

2. Windows and tables overview

3. Alkanes processing

4. Data Reviewing

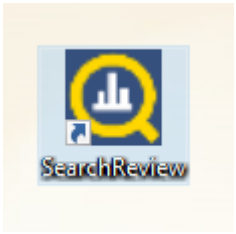
5. Quantitation

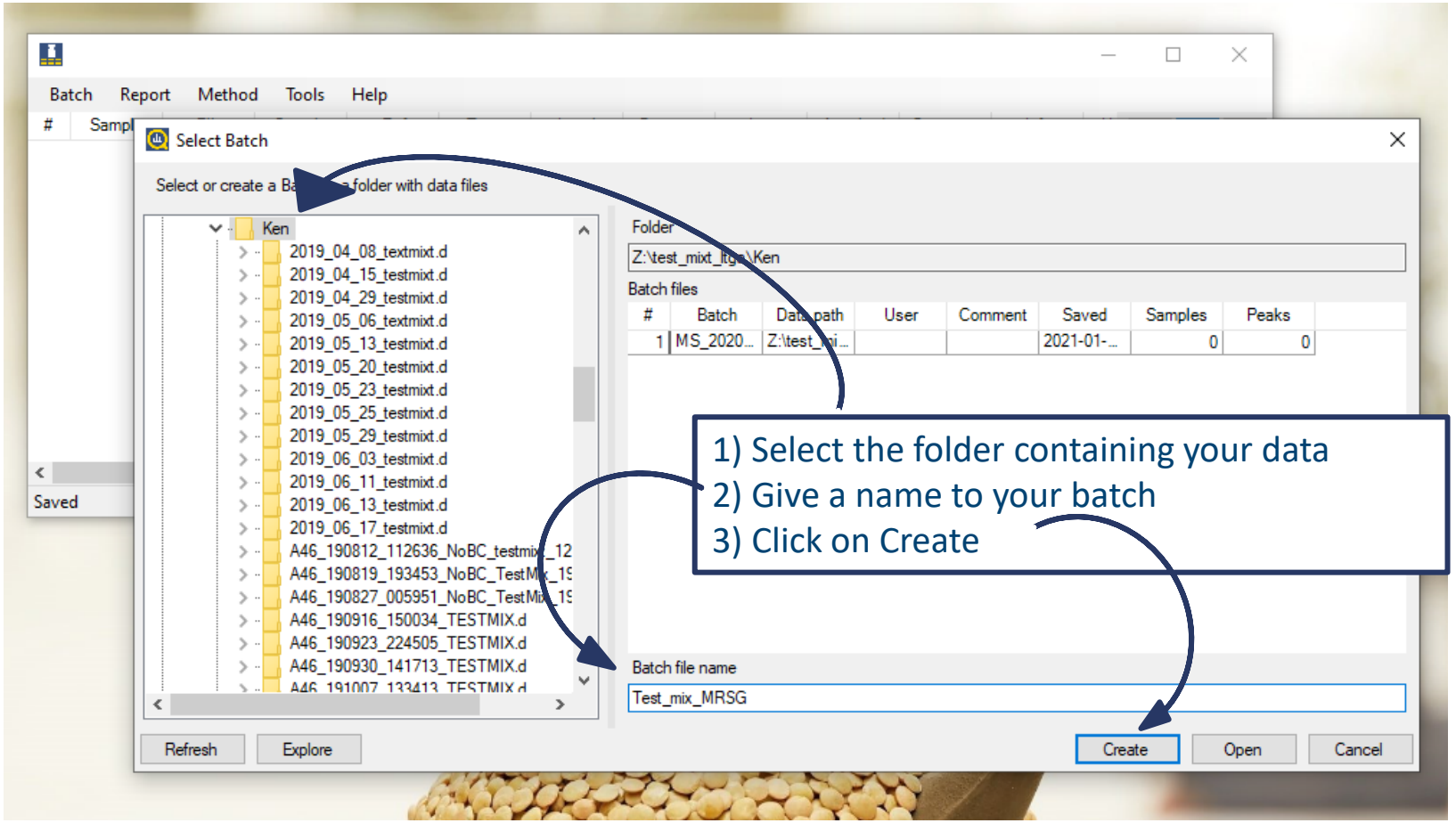
6. Report

01 Batch creation

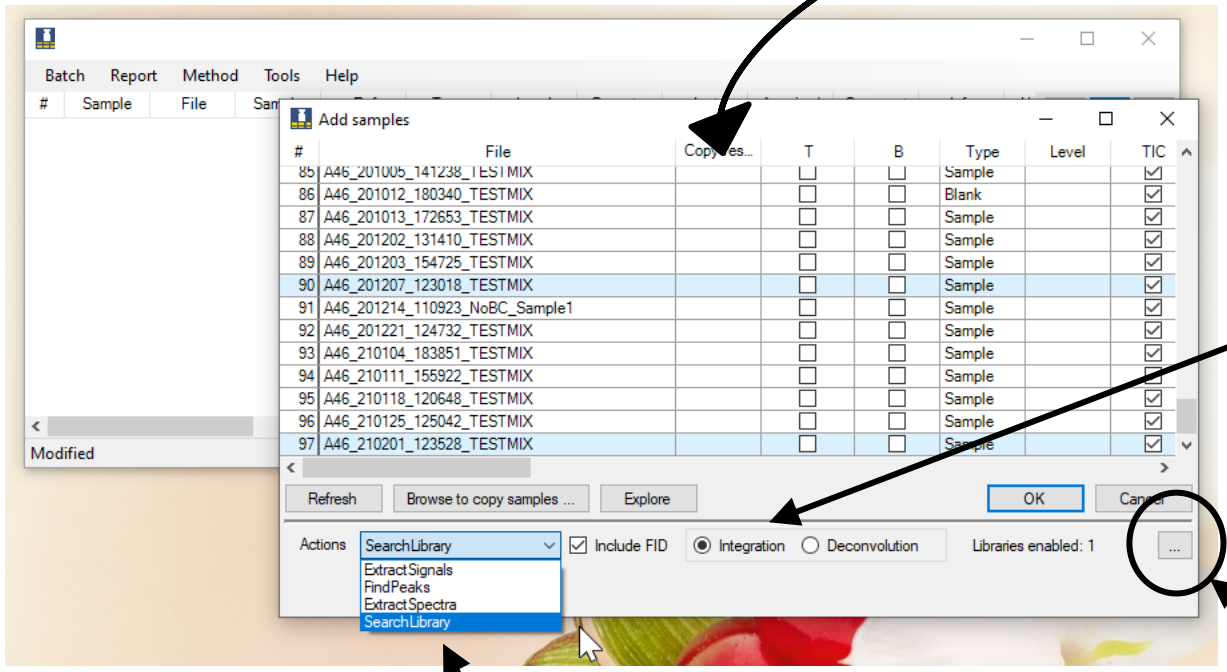
Batch creation

- Open UnknownProcessor: the Select Batch window automatically opens





Batch creation



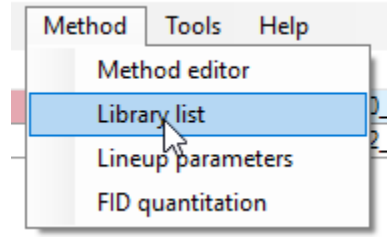
1) Select the files you want to add in your batch

3) Choose to include or not FID
and choose the type of peak extraction

4) Libraries selection and creation

2) Select actions to process the data (all the actions above the selected one will be executed)

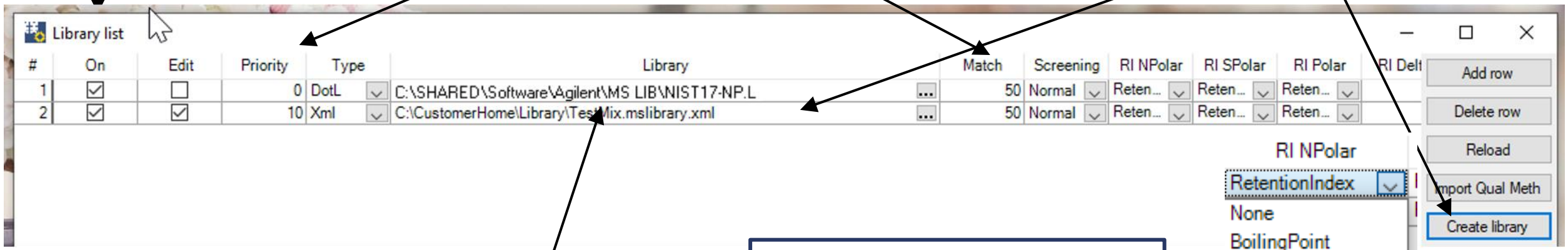
Batch creation – Libraries selection/creation



Choose 1 or more libraries you want to search

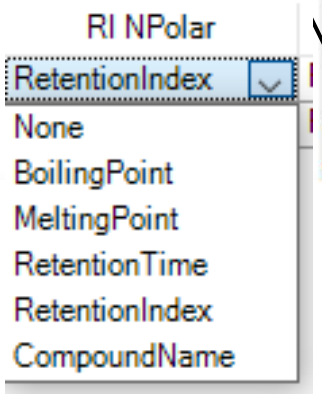
Set the priority and match levels for each library

Create a library if you want to edit it afterwards

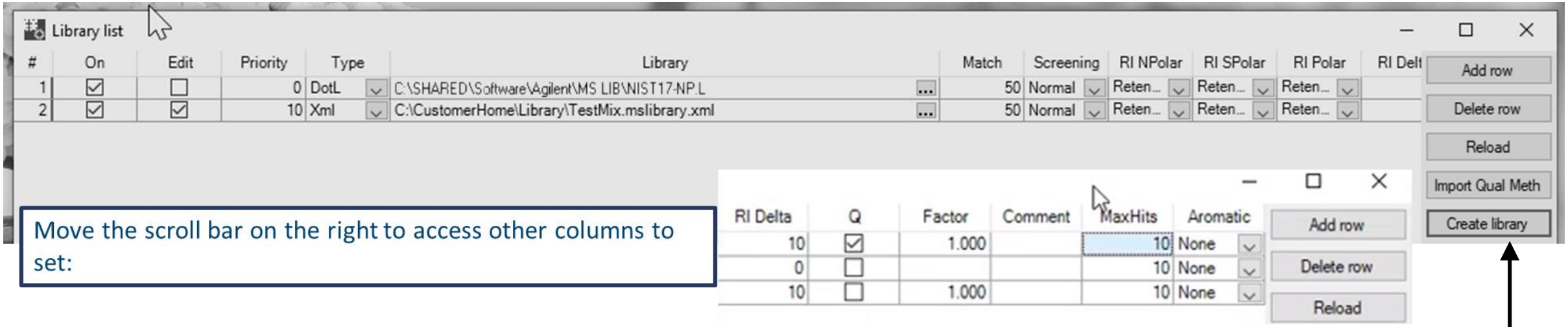


No need to use Library picker, just type the library path and name with the extension (.l; .xml …)

For each library, select for each polarity the field in which Retention Index Data are stored



Batch creation - Libraries selection/creation



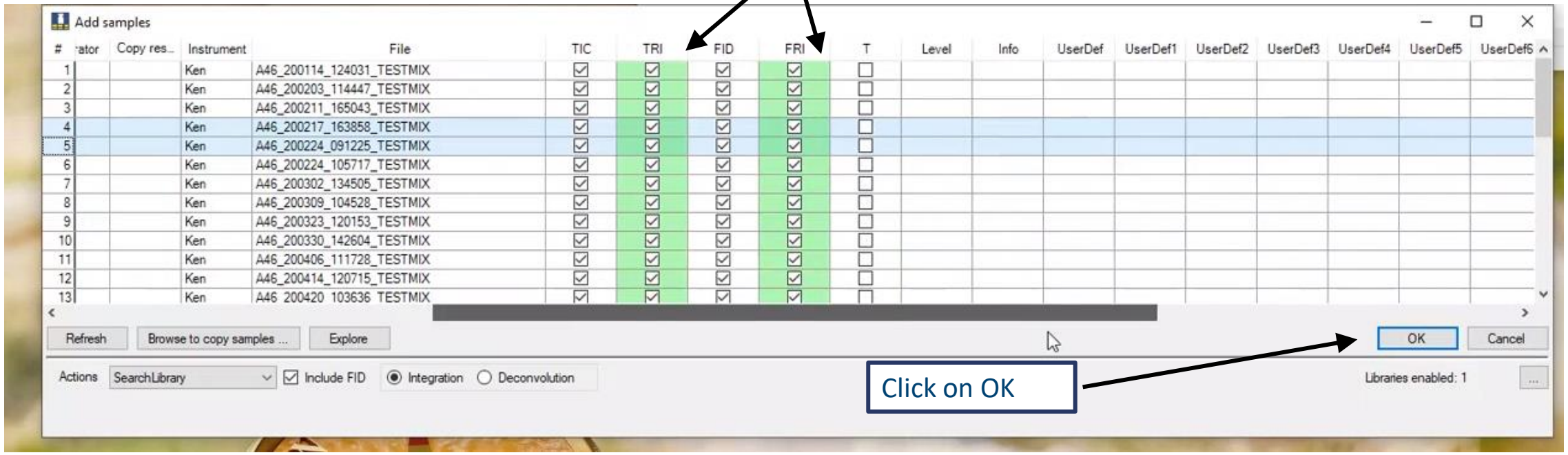
Move the scroll bar on the right to access other columns to set:

- Set the RI Delta you allow for your compounds
- By ticking Q you take into account the priority levels stored in the RI decimal
- Set the maximum number of hits you allow per
- Select the library field in which the Aromatic data and the RI are stored

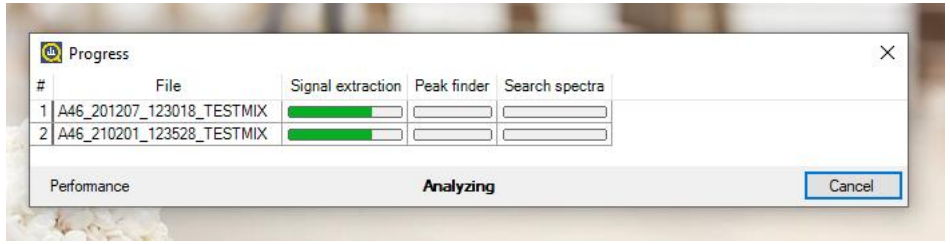
Then click on Create Library

Batch creation

The soft checks if there is a RI calibration for TIC and for FID



Click on OK



Data loading …

02 Windows and tables

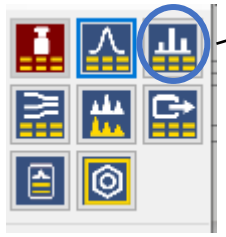
General view after Batch creation

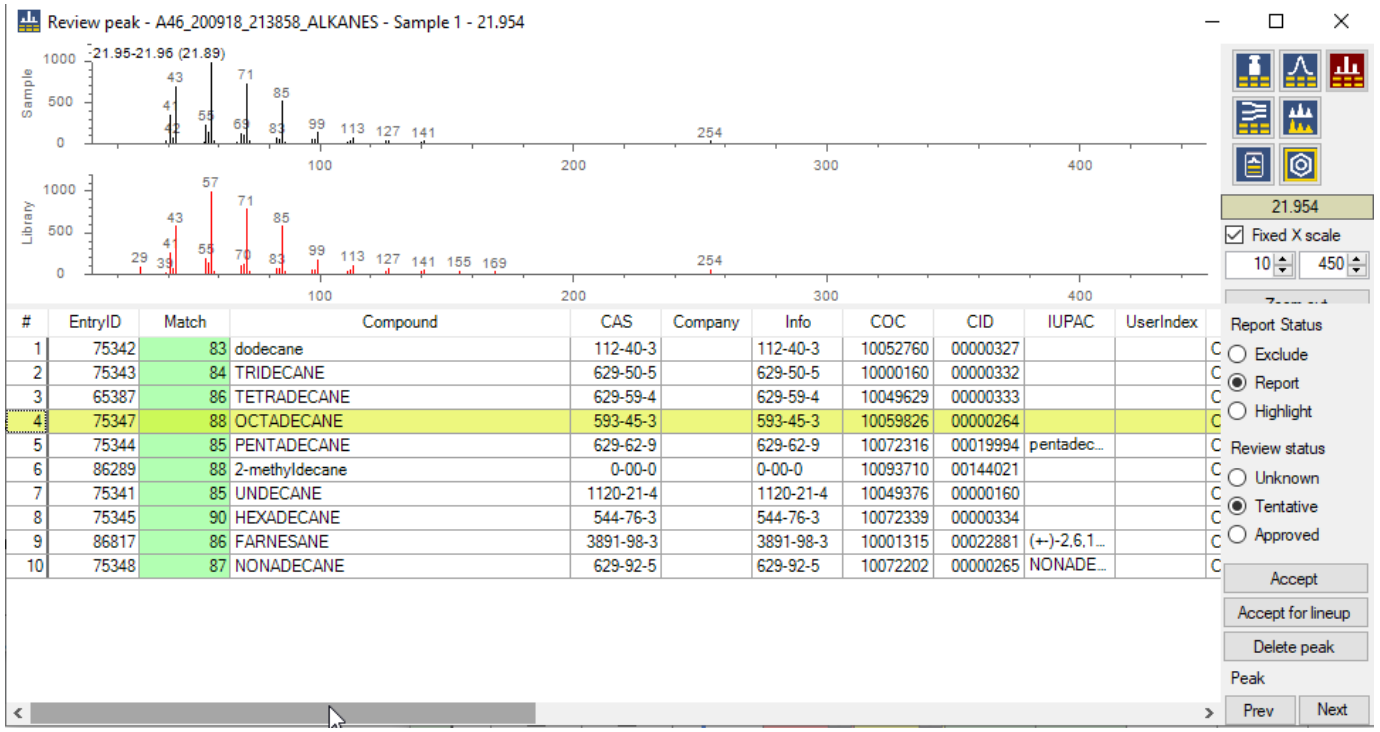
00_alkanes\DEMO BATCH

Batch Report Method Tools Help

#	Sample	Ref	D	File	Inst	Sample	Operator	Acquired	Type	Amount	Dilution	Comment	Volume	IS1 Amo...	IS1 Area	IS1 RT	Int Key	FID	TIC	FRI	TRI	Phase	Int FArea	Int FAmo...	Int FAmo...	Int F
1	0	☐	☑	A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	☑	☑	NonP...	686600			2
2	1	☐	☑	A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	☑	☑	NonP...	766885			2
3	2	☐	☑	A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	☑	☑	NonP...	561428			2

Modified





#	EntryID	Match	Compound	CAS	Company	Info	COC	CID	IUPAC	UserIndex
1	75342	83	dodecane	112-40-3		112-40-3	10052760	00000327		
2	75343	84	TRIDECANE	629-50-5		629-50-5	10000160	00000332		
3	65387	86	TETRADECANE	629-59-4		629-59-4	10049629	00000333		
4	75347	88	OCTADECANE	593-45-3		593-45-3	10059826	00000264		
5	75344	85	PENTADECANE	629-62-9		629-62-9	10072316	00019994	pentadec...	
6	86289	88	2-methyldecane	0-00-0		0-00-0	10093710	00144021		
7	75341	85	UNDECANE	1120-21-4		1120-21-4	10049376	00000160		
8	75345	90	HEXADECANE	544-76-3		544-76-3	10072339	00000334		
9	86817	86	FARNESANE	3891-98-3		3891-98-3	10001315	00022881	(+-)-2,6,1...	
10	75348	87	NONADECANE	629-92-5		629-92-5	10072202	00000265	NONADE...	

MS spectra

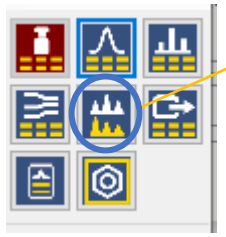
General view after Batch creation

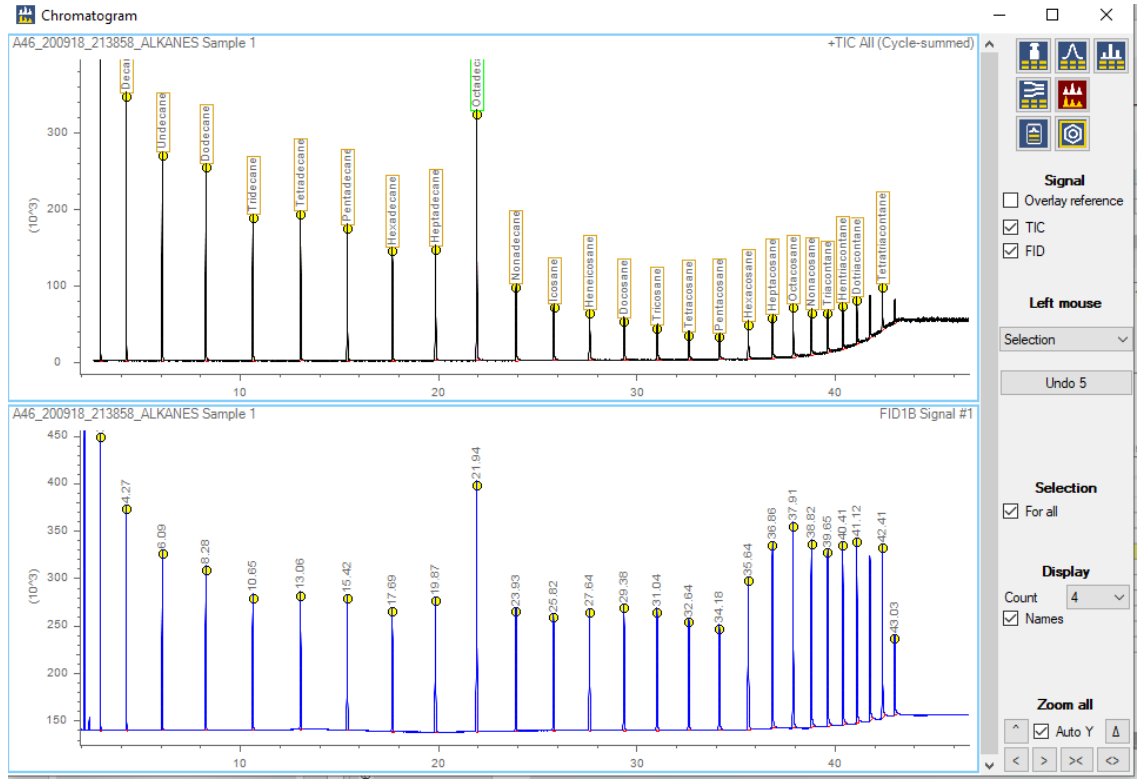
00_alkanes\DEMO BATCH - SearchReview - 2.67 -

Batch Report Method Tools Help

#	Sample	Ref	D	File	Inst	Sample	Operator	Acquired	Type	Amount	Dilution	Comment	Volume	IS1 Amo...	IS1 Area	IS1 RT	Int Key	FID	TIC	FRI	TRI	Phase	Int FArea	Int FAmo...	Int FAmo...	Int F
1	0	☐	☑	A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	☑	☑	NonP...	686600			2
2	1	☐	☑	A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	☑	☑	NonP...	766885			2
3	2	☐	☑	A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	☑	☑	NonP...	561428			2

Modified





Chromatograms

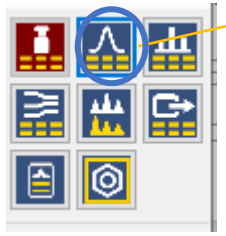
General view after Batch creation

00_alkanes\DEMO BATCH

Batch Report Method Tools Help

#	Sample	Ref	D	File	Inst	Sample	Operator	Acquired	Type	Amount	Dilution	Comment	Volume	IS1 Amo...	IS1 Area	IS1 RT	Int Key	FID	TIC	FRI	TRI	Phase	Int FArea	Int FAmo...	Int FAmo...	Int F
1	0	☐	☑	A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	☑	☑	NonP...	686600			2
2	1	☐	☑	A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	☑	☑	NonP...	766885			2
3	2	☐	☑	A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	☑	☑	NonP...	561428			2

Modified



Peaks - A46_200918_213858_ALKANES - Sample 1

#	Rel	Report	C...	Review	RT	RI	Area	Width	Height	MHit	Compound	COC	CID	CAS	Formula	MW	Match	LRI	FEMA	DRI	ARI	MRI	QRI	Comment	FAmount	FAmount...	DOU	mARC
1		Exclu...	FID	Tentat...	2.968		333941	0.017	313183	☐																	1	
2		Report	TIC	Tentat...	2.966		507120	0.016	482505	☐	Nonane	10000171	00000324	111-84-2	C9H20	128.3	99	900					0				0	
3		Exclu...	FID	Tentat...	4.275		330553	0.022	236933	☐																	1	
4		Report	TIC	Tentat...	4.271		478987	0.021	350968	☐	Decane	10001748	00000326	124-18-5	C10H22	142.3	98	1000					0				0	
5		Exclu...	FID	Tentat...	6.092		329496	0.027	190084	☐																	1	
6		Report	TIC	Tentat...	6.087		476200	0.027	272880	☐	Undecane	10049376	00000160	1120-21-4	C11H24	156.3	97	1100					0				0	
7		Exclu...	FID	Tentat...	8.285		350271	0.032	172664	☐																	1	
8		Report	TIC	Tentat...	8.283		496923	0.029	256797	☐	Dodecane	10052760	00000327	112-40-3	C12H26	170.3	96	1200					0				0	
9		Exclu...	FID	Tentat...	10.655		320088	0.035	143366	☐																	1	
10		Report	TIC	Tentat...	10.654		415808	0.033	191095	☐	Tridecane	10000160	00000332	629-50-5	C13H28	184.4	93	1300					0				0	
11		Exclu...	FID	Tentat...	13.062		345894	0.037	144813	☐																	1	
12		Report	TIC	Tentat...	13.064		421506	0.033	195670	☐	Tetradecane	10049629	00000333	629-59-4	C14H30	198.4	93	1400					0				0	
13		Exclu...	FID	Tentat...	15.418		355174	0.039	142935	☐																	1	
14		Report	TIC	Tentat...	15.420		411435	0.035	177964	☐	Pentadecane	10072316	00919994	629-62-9	C15H32	212.4	91	1500					0				0	
15		Exclu...	FID	Tentat...	17.692		338586	0.041	130942	☐																	1	
16		Report	TIC	Tentat...	17.694		355635	0.036	148406	☐	Hexadecane	10072339	00000334	544-76-3	C16H34	226.4	90	1600					0				0	
17		Exclu...	FID	Tentat...	19.868		382668	0.042	142400	☐																	1	
18		Report	TIC	Tentat...	19.870		370568	0.038	150254	☐	Heptadecane	10052760	00000327	629-78-7	C12H26	170.3	90	1200					0				0	
19		Exclu...	FID	Tentat...	21.945		686600	0.040	264020	☐																	1	
20		Report	TIC	Tentat...	21.954		805562	0.037	326849	☐	Octadecane	10059826	00000264	593-45-3	C18H38	254.5	88	1800					0				0	
21		Exclu...	FID	Tentat...	23.928		349478	0.042	129755	☐																	1	
22		Report	TIC	Tentat...	23.936		272844	0.040	100505	☐	Nonadecane	10072202	00000265	629-92-5	C19H40	268.5	87	1900					0				0	
23		Exclu...	FID	Tentat...	25.825		344783	0.043	123466	☐																	1	
24		Report	TIC	Tentat...	25.834		222960	0.044	74080	☐	Icosane	10024872	00076397	112-95-8	C11H23I	282.2	90	1338					0				0	
25		Exclu...	FID	Tentat...	27.638		361566	0.044	128548	☐																	1	
26		Report	TIC	Tentat...	27.650		205067	0.045	65742	☐	Heneicosane	10049629	00000333	629-94-7	C14H30	198.4	90	1400					0				0	
27		Exclu...	FID	Tentat...	29.378		378923	0.045	133010	☐																	1	
28		Report	TIC	Tentat...	29.379		192403	0.048	56484	☐	Docosane	10049629	00000333	629-97-0	C14H30	198.4	90	1400					0				0	
29		Exclu...	FID	Tentat...	31.045		372773	0.045	128774	☐																	1	
30		Report	TIC	Tentat...	31.049		164445	0.049	46285	☐	Tricosane	10024872	00076397	638-67-5	C11H23I	282.2	89	1338					0				0	
31		Exclu...	FID	Tentat...	32.645		358817	0.047	117641	☐																	1	
32		Report	TIC	Tentat...	32.646		127268	0.050	37079	☐	Tetracosane	10024872	00076397	646-31-1	C11H23I	282.2	89	1338					0				0	
33		Exclu...	FID	Tentat...	34.185		353580	0.048	111110	☐																	1	
34		Report	TIC	Tentat...	34.194		109776	0.047	32960	☐	Pentacosane	10024872	00076397	629-99-2	C11H23I	282.2	89	1338					0				0	
35		Exclu...	FID	Tentat...	35.645		476725	0.045	160692	☐																	1	
36		Report	TIC	Tentat...	35.650		144757	0.044	49196	☐	Hexacosane	10049629	00000333	630-01-3	C14H30	198.4	88	1400					0				0	
37		Exclu...	FID	Tentat...	36.862		499663	0.039	196223	☐																	1	
38		Report	TIC	Tentat...	36.862		172061	0.042	57655	☐	Heptacosane	10049629	00000333	593-49-7	C14H30	198.4	90	1400					0				0	
39		Exclu...	FID	Tentat...	37.908		523971	0.036	216093	☐																	1	
40		Report	TIC	Tentat...	37.909		194118	0.038	70412	☐	Octacosane	10049629	00000333	630-02-4	C14H30	198.4	87	1400					0				0	
41		Exclu...	FID	Tentat...	38.825		455611	0.034	197137	☐																	1	
42		Report	TIC	Tentat...	38.829		151719	0.035	59764	☐	Nonacosane	10024872	00076397	630-03-5	C11H23I	282.2	83	1338					0				0	
43		Exclu...	FID	Tentat...	39.652		420078	0.033	186607	☐																	1	
44		Report	TIC	Tentat...	39.652		131002	0.033	56042	☐	Triacontane	10024872	00076397	638-68-6	C11H23I	282.2	85	1338					0				0	
45		Exclu...	FID	Tentat...	40.412		409972	0.031	193237	☐																	1	
46		Report	TIC	Tentat...	40.411		130211	0.030	60095	☐	Hentriacontane	10024872	00076397	630-04-6	C11H23I	282.2	85	1338					0				0	
47		Exclu...	FID	Tentat...	41.122		430265	0.032	194800	☐																	1	
48		Report	TIC	Tentat...	41.122		138850	0.032	61129	☐	Dotriacontane	10024872	00076397	544-85-4	C11H23I	282.2	80	1338					0				0	
49		Exclu...	FID	Tentat...	41.782		380467	0.032	172736	☐																	1	
50		Report	TIC	Tentat...	41.779		121878	0.032	54324	☐	Tritriacontane	10024872	00076397	630-05-7	C11H23I	282.2	82	1338					0				0	
51		Exclu...	FID	Tentat...	42.408		397238	0.032	182239	☐																	1	
52		Report	TIC	Tentat...	42.407		138347	0.032	60075	☐	Tetratriacontane	10024872	00076397	14167-59...	C11H23I	282.2	77	1338					0				0	
53		Exclu...	FID	Tentat...	43.032		208643	0.036	84262	☐																	1	
54		Report	TIC	Tentat...	43.030		75729	0.034	30170	☐	Pentatriacontane	10075052	00007572	630-07-9	C12H26O2	202.3	60	1515					0				0	

Compound list of selected sample

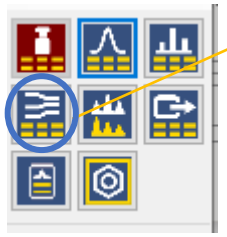
General view after Batch creation

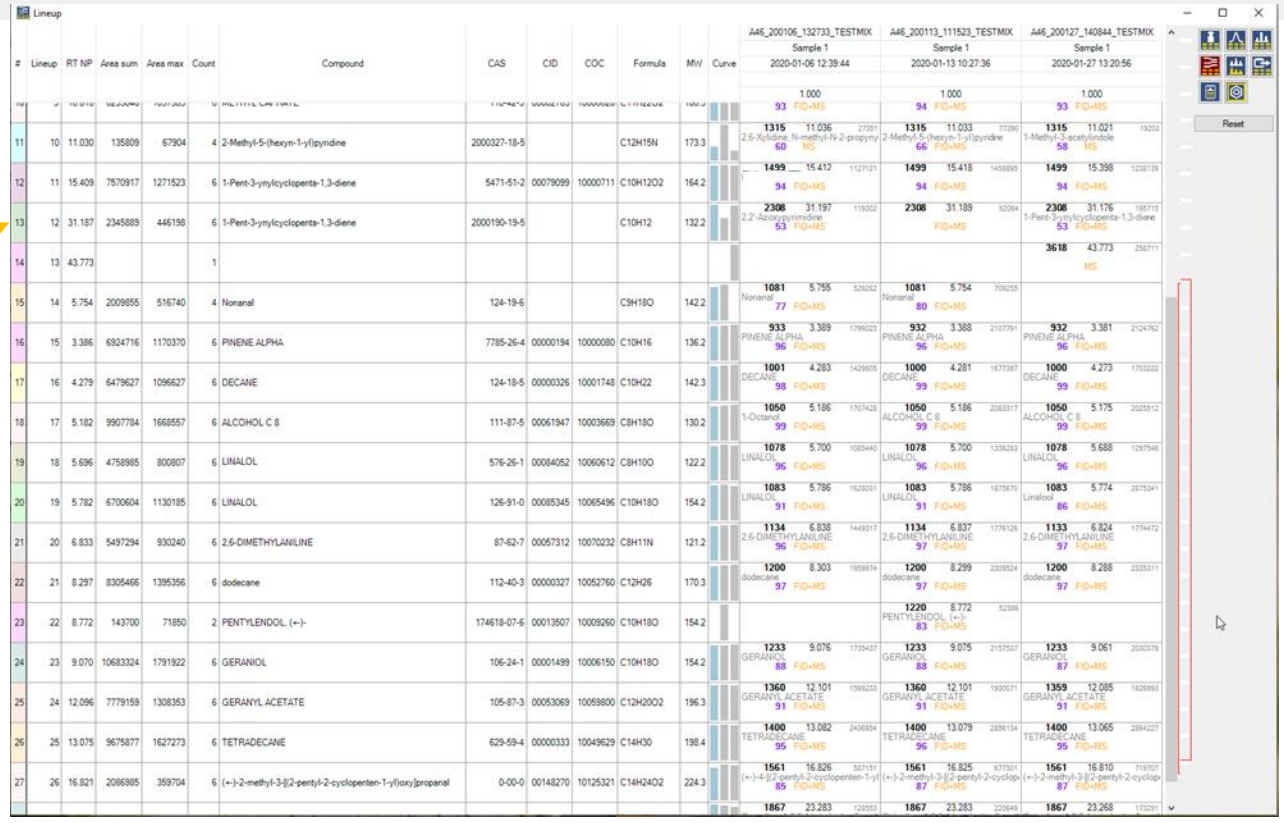
00_alkanes\DEMO BATCH

Batch Report Method Tools Help

#	Sample	Ref	D	File	Inst	Sample	Operator	Acquired	Type	Amount	Dilution	Comment	Volume	IS1 Amo...	IS1 Area	IS1 RT	Int Key	FID	TIC	FRI	TRI	Phase	Int FArea	Int FAmo...	Int FAmo...	Int F
1	0	☐	☑	A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	☑	☑	NonP...	686600			2
2	1	☐	☑	A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	☑	☑	NonP...	766885			2
3	2	☐	☑	A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	☑	☑	NonP...	561428			2

Modified





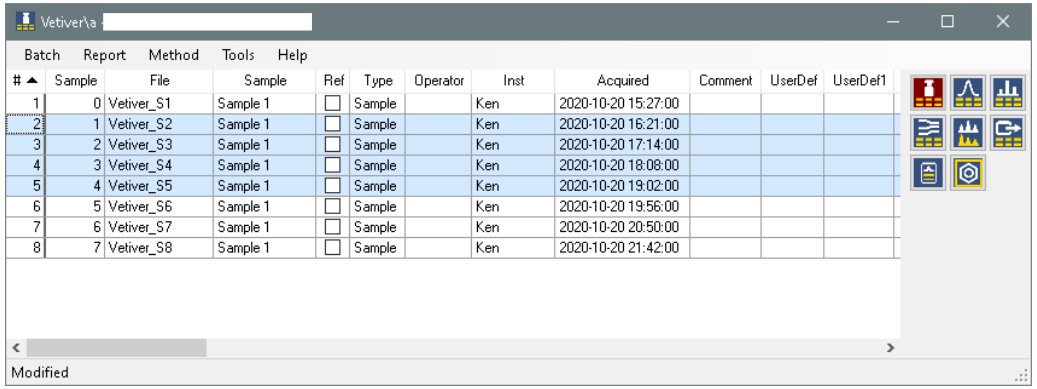
Lineup

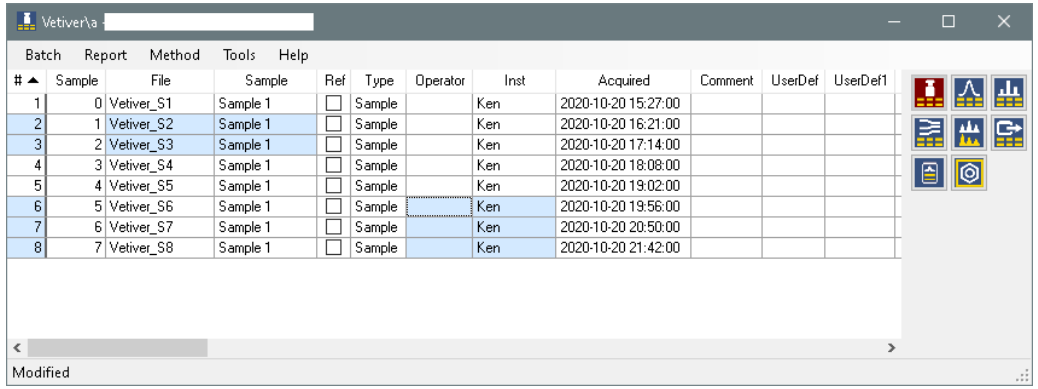
User Interface, tables: selecting and moving rows

The tables have common feature, the sample table is used as example:

- First column cell **turn blue** if any cell in the row is selected
- Click on first column cell to **select all row cells**
- Drag mouse down to **select multiple rows**
- Click on a blue first column cell and drag up or down to **move rows**

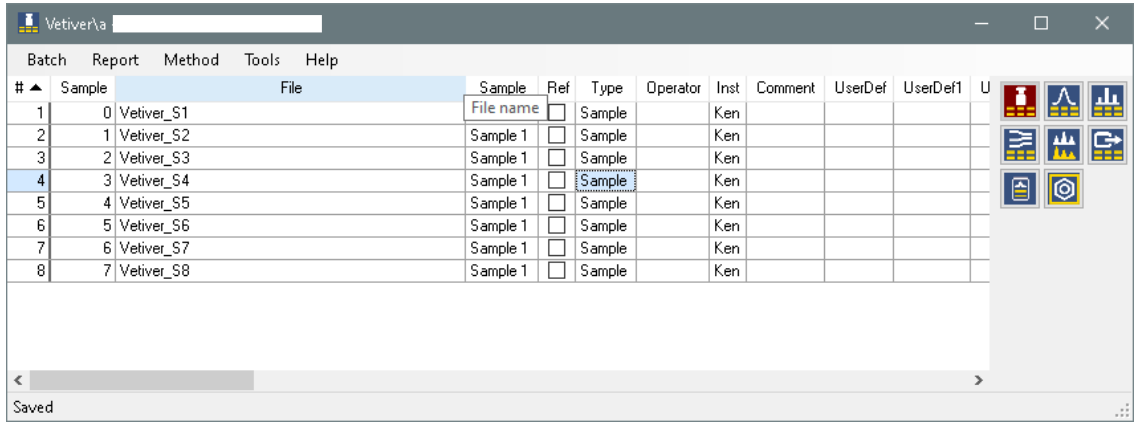
- Use shift and ctrl keys with **mouse click** to select multiple cells
- Use shift and ctrl keys with **cursus keys** (up, down, left, right)
- Click top left cell **'#'** to select all cells
- Click top cell **'column header'** to select all cells in the column

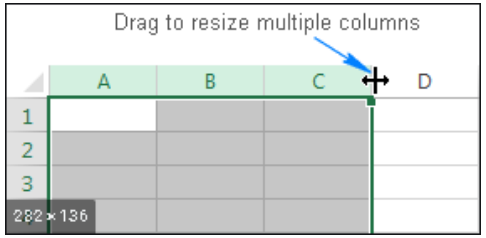




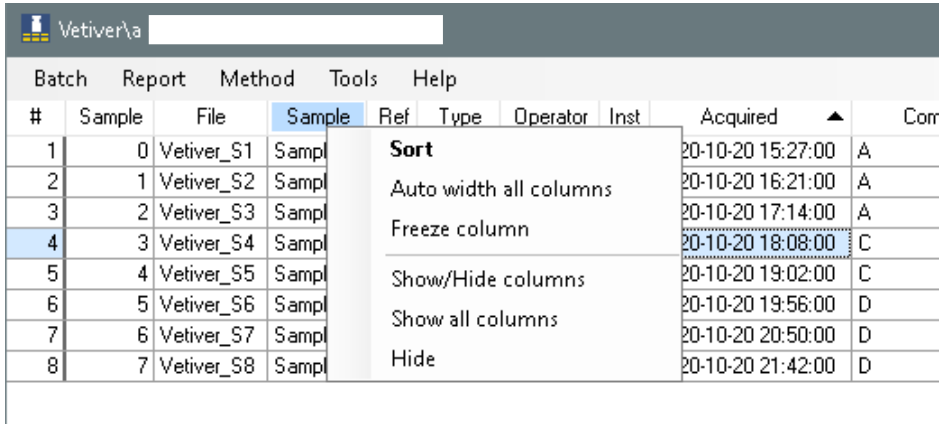
Tables, columns moving and width

- Click and drag column header to **move columns**
- Click and drag between column headers to **adjust the width**
- Double click between column headers to **auto width**
- Ctrl and double click between columns headers to **auto width all**



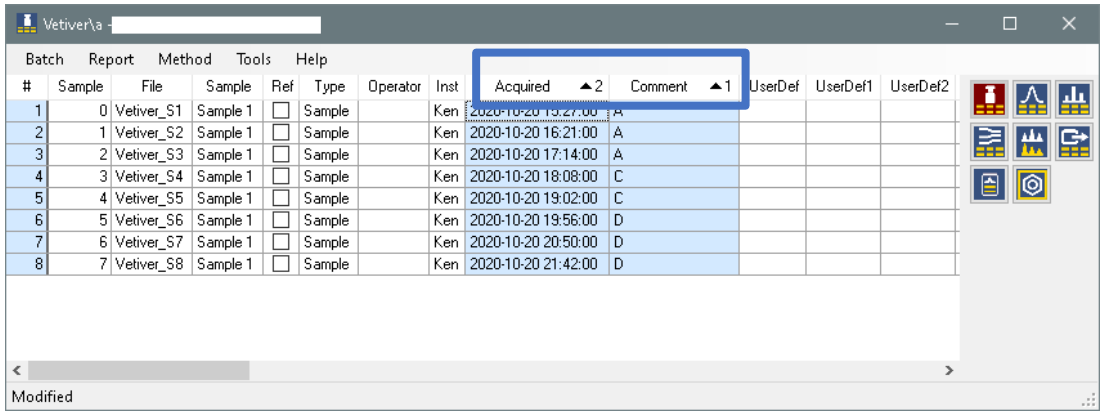


- Double click on a column header to **sort**
- Ctrl double click another column to add an **additional sort**
- Column width and sorting is stored in the **user profile**



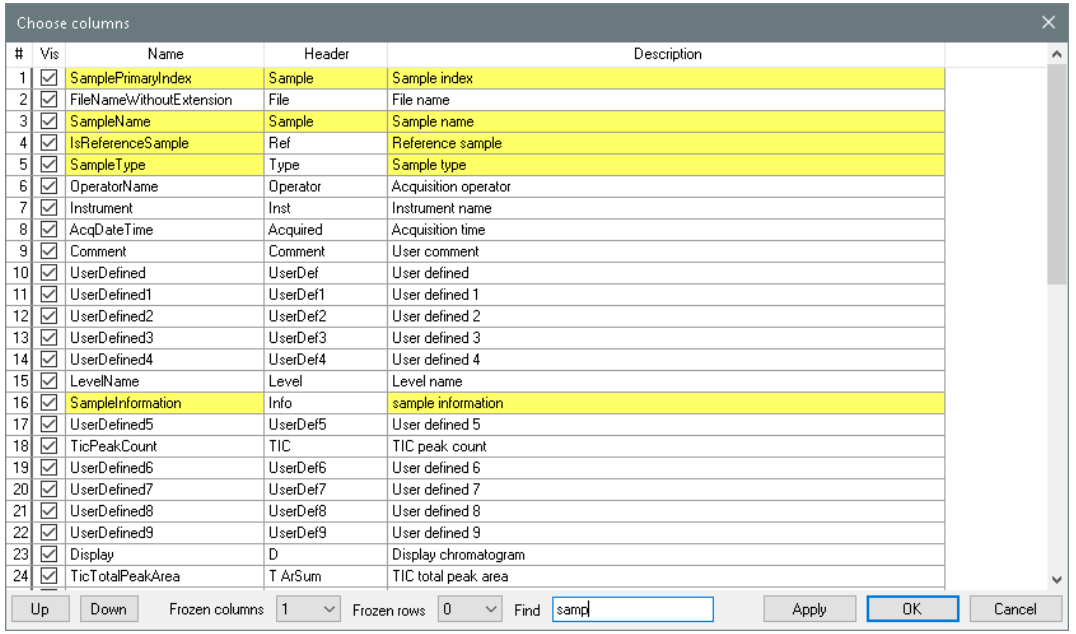
Tables, sorting rows, column header menu

- Double click on a column header to **sort**
- Ctrl double click another column to add an **additional sort**
- Column width and sorting is stored in the **user profile**



#	Sample	File	Sample	Ref	Type	Operator	Inst	Acquired ▲2	Comment ▲1	UserDef	UserDef1	UserDef2
1	0	Vetiver_S1	Sample 1	☐	Sample		Ken	2020-10-20 15:27:00	A			
2	1	Vetiver_S2	Sample 1	☐	Sample		Ken	2020-10-20 16:21:00	A			
3	2	Vetiver_S3	Sample 1	☐	Sample		Ken	2020-10-20 17:14:00	A			
4	3	Vetiver_S4	Sample 1	☐	Sample		Ken	2020-10-20 18:08:00	C			
5	4	Vetiver_S5	Sample 1	☐	Sample		Ken	2020-10-20 19:02:00	C			
6	5	Vetiver_S6	Sample 1	☐	Sample		Ken	2020-10-20 19:56:00	D			
7	6	Vetiver_S7	Sample 1	☐	Sample		Ken	2020-10-20 20:50:00	D			
8	7	Vetiver_S8	Sample 1	☐	Sample		Ken	2020-10-20 21:42:00	D			

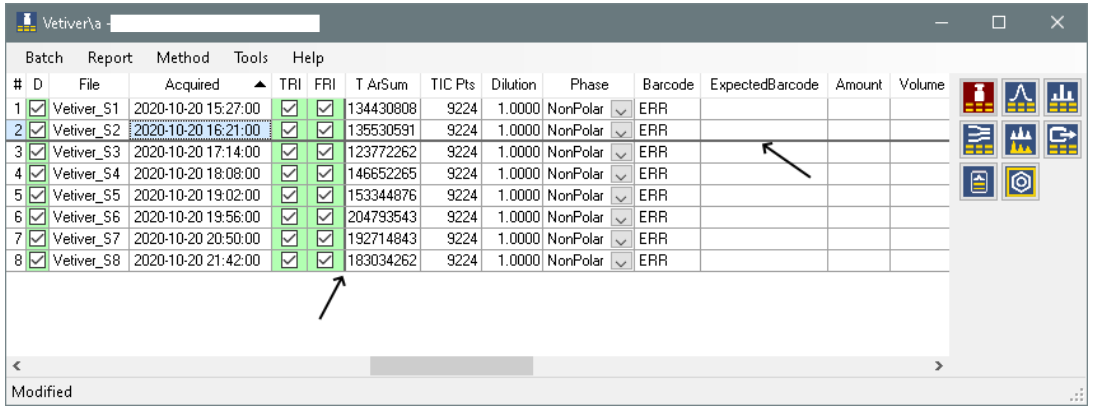
- Right click on a column header to show the column menu
- Show/Hide columns to open a column editor
- Show/Hide columns dialog
- Use the Find text box to search
- Move multiple rows up and down



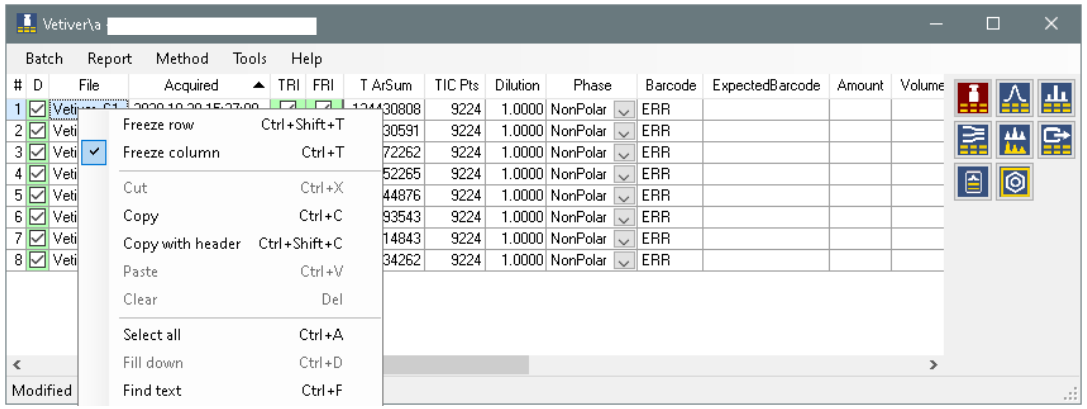
#	Vis	Name	Header	Description
1	☑	SamplePrimaryIndex	Sample	Sample index
2	☑	FileNameWithoutExtension	File	File name
3	☑	SampleName	Sample	Sample name
4	☑	IsReferenceSample	Ref	Reference sample
5	☑	SampleType	Type	Sample type
6	☑	OperatorName	Operator	Acquisition operator
7	☑	Instrument	Inst	Instrument name
8	☑	AcqDateTime	Acquired	Acquisition time
9	☑	Comment	Comment	User comment
10	☑	UserDefined	UserDef	User defined
11	☑	UserDefined1	UserDef1	User defined 1
12	☑	UserDefined2	UserDef2	User defined 2
13	☑	UserDefined3	UserDef3	User defined 3
14	☑	UserDefined4	UserDef4	User defined 4
15	☑	LevelName	Level	Level name
16	☑	SampleInformation	Info	sample information
17	☑	UserDefined5	UserDef5	User defined 5
18	☑	TicPeakCount	TIC	TIC peak count
19	☑	UserDefined6	UserDef6	User defined 6
20	☑	UserDefined7	UserDef7	User defined 7
21	☑	UserDefined8	UserDef8	User defined 8
22	☑	UserDefined9	UserDef9	User defined 9
23	☑	Display	D	Display chromatogram
24	☑	TicTotalPeakArea	T ArSum	TIC total peak area

Tables, freeze columns, rows and body menu

- Right click column and toggle **Freeze**
- Here 5 important columns are frozen add the left side of the table
- And 2 important rows are frozen ad the top of the table
- Frozen column and row count are stored in the user profile



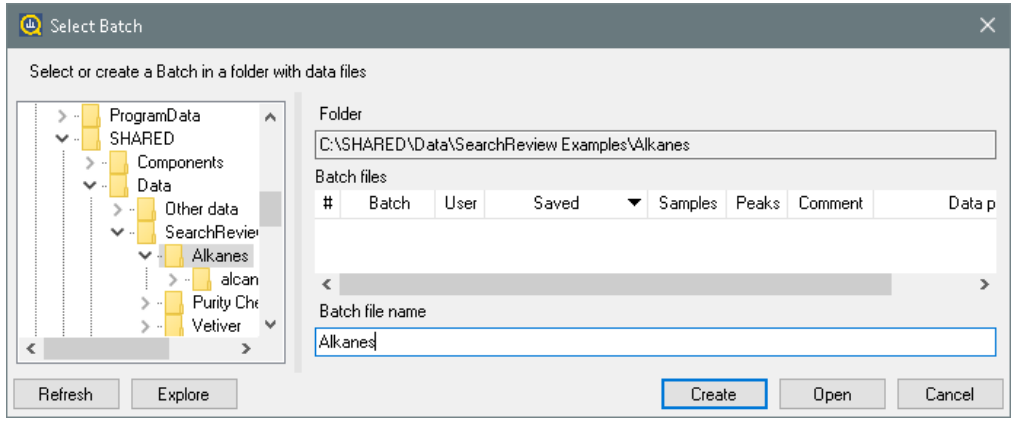
- Right click on a cell: table body menu (combined with context menu)
- Note: Keyboard shortcuts, Copy with header, Fill down, Find text

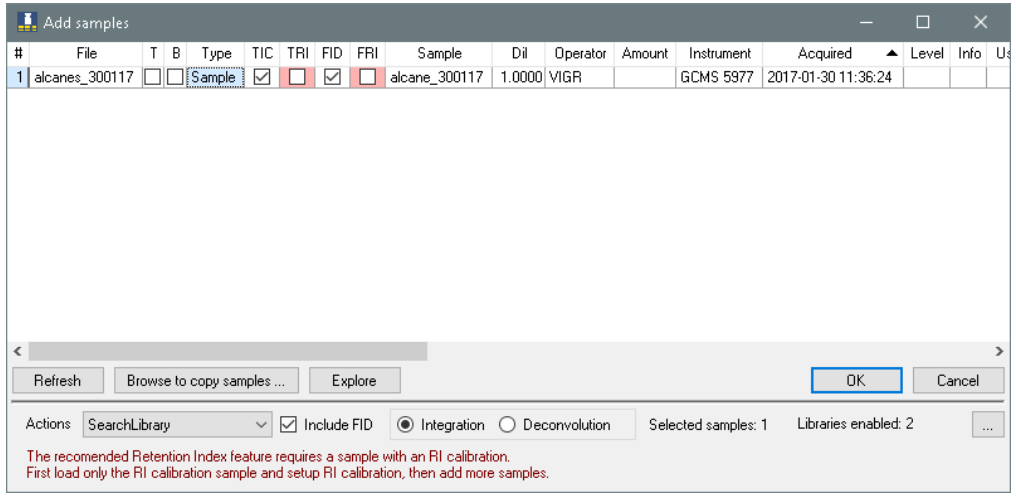


03 Alkanes processing

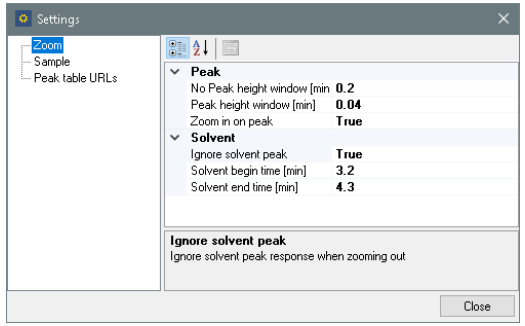
RI calibration setup

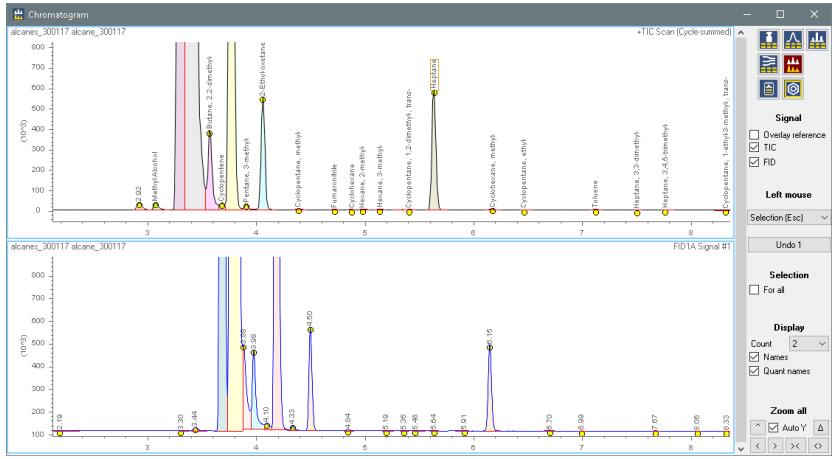
- Create batch in the folder with data files
- Add n-Alkane series sample
- TRI and FRI show invalid RI calibration files





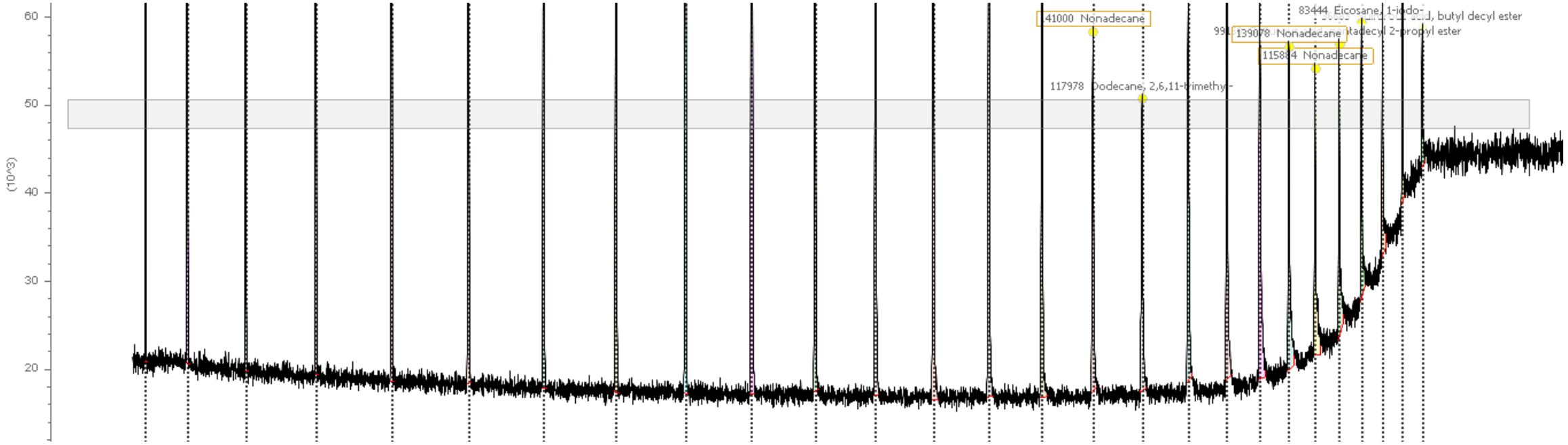
- Tools – Settings
- Zoom, ignore solvent
- In the chromatogram window, Zoom FID and TIC to show n-Hexane





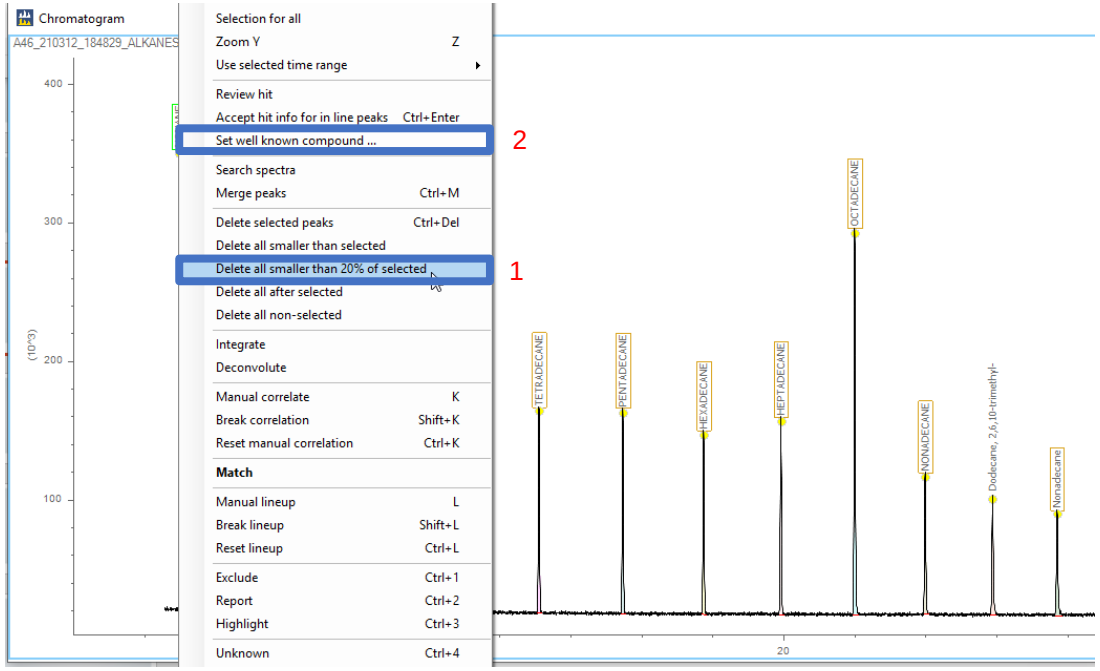
RI calibration setup

The Shift + Left Drag combination is kind of magic.
It selects peaks that are **intersected** (see screenshot) and also peaks that are **fully contained** in the selection.
Now you can select large peaks (or small peaks). This is useful for n-Alkanes. Right click and ‘Delete all non-selected’



RI calibration setup

- Click on the n-Hexane peak, right click: Delete all smaller than 20%
- Select and delete all non n-Alkane peaks



- Click on the n-Hexane peak, **right click** Set well known compound
- Select n-Hexane and click **Set series**, for both FID and TIC signals

#	On	Name	CAS	RI	Formula	MW	Comment
1	☑	Methane	74-82-8	100	CH4	16.0	
2	☑	Ethane	74-84-0	200	C2H6	30.1	
3	☑	Propane	74-98-6	300	C3H8	44.1	
4	☑	Butane	106-97-8	400	C4H10	58.1	
5	☑	Pentane	109-66-0	500	C5H12	72.2	
6	☑	Hexane	110-54-3	600	C6H14	86.2	
7	☑	Heptane	142-82-5	700	C7H16	100.2	
8	☑	Octane	111-65-9	800	C8H18	114.2	
9	☑	Nonane	111-84-2	900	C9H20	128.3	
10	☑	Decane	124-18-5	1000	C10H22	142.3	
11	☑	Undecane	1120-21-4	1100	C11H24	156.3	
12	☑	Dodecane	112-40-3	1200	C12H26	170.3	
13	☑	Tridecane	629-50-5	1300	C13H28	184.4	
14	☑	Tetradeca...	629-59-4	1400	C14H30	198.4	
15	☑	Pentadec...	629-62-9	1500	C15H32	212.4	
16	☑	Hexadeca...	544-76-3	1600	C16H34	226.5	

Successive threshold % 20

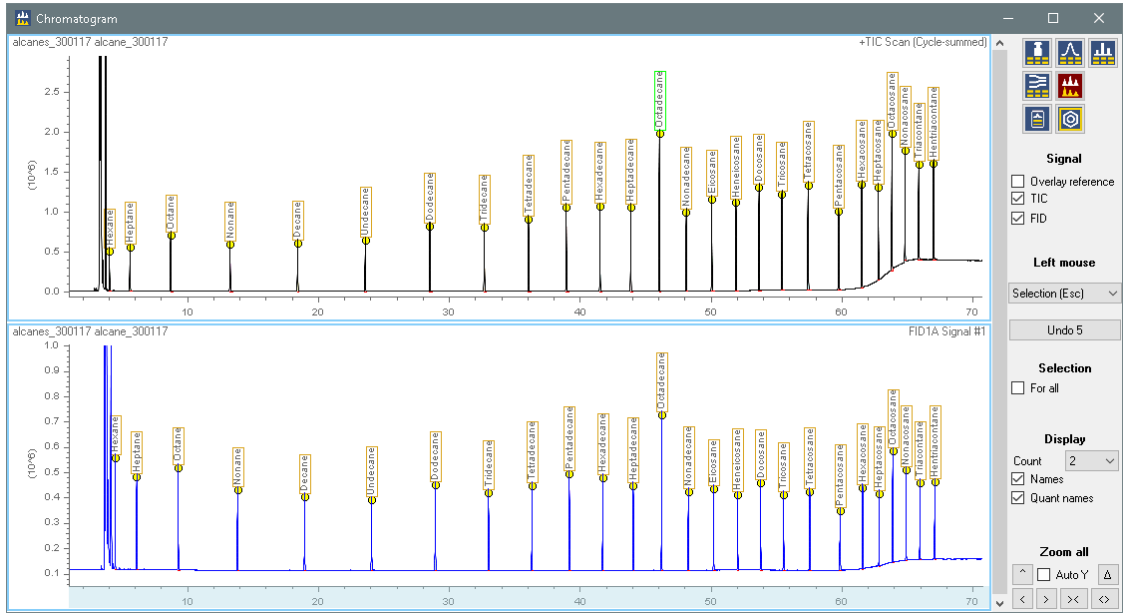
Set series 3

Set current

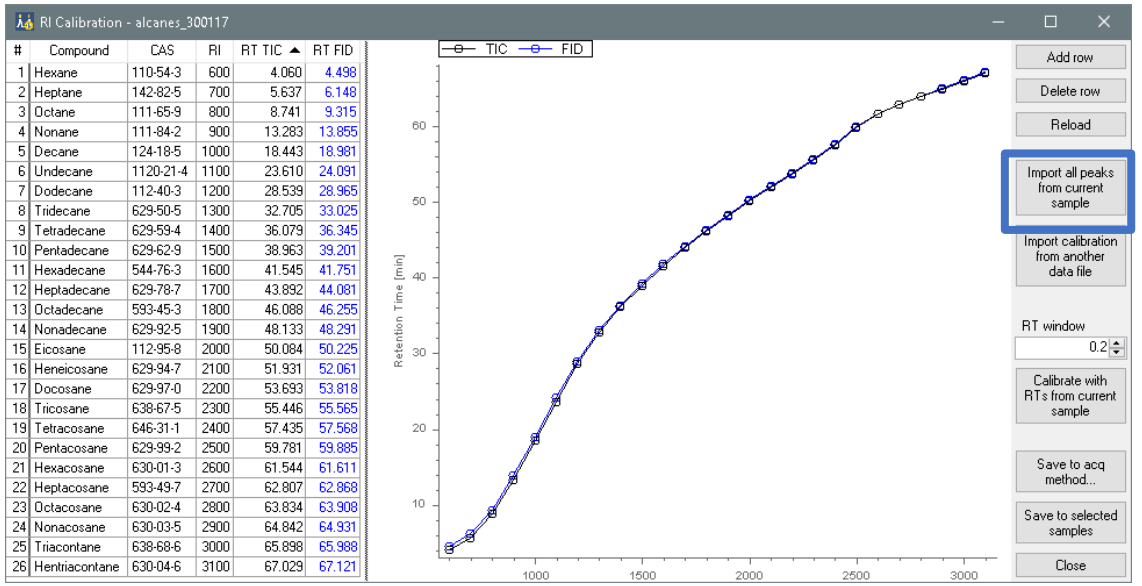
Cancel

RI calibration setup

- All n-Alkanes are labeled



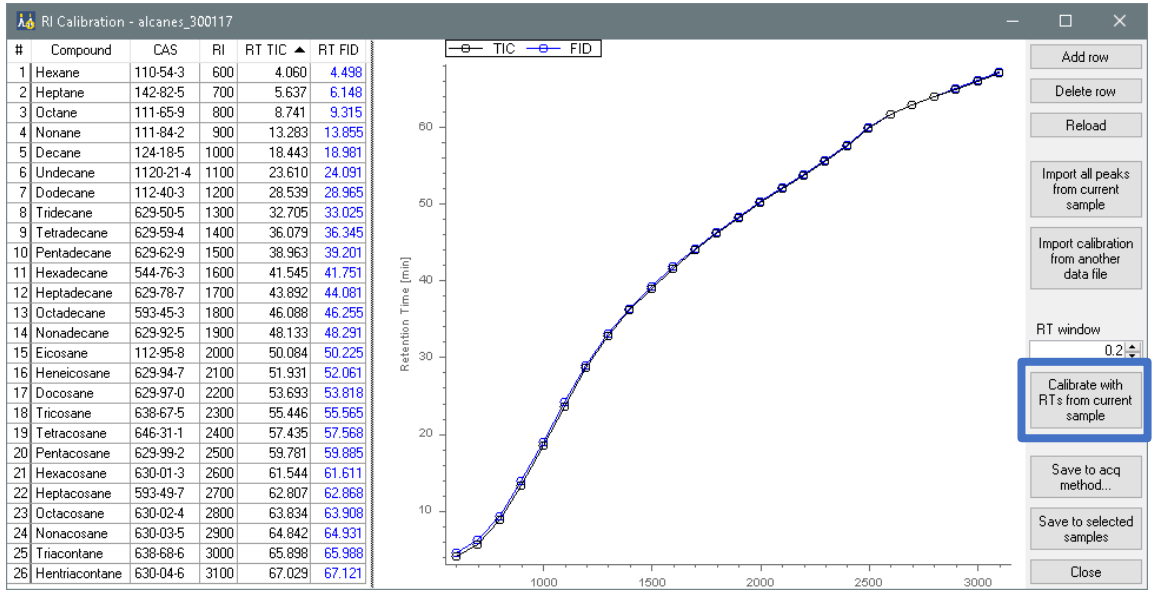
- Tools – RI Calibration
- Select all rows and press Delete row button
- Import All peaks from current sample, and Save to selected samples



#	Compound	CAS	RI	RT TIC	RT FID
1	Hexane	110-54-3	600	4.060	4.498
2	Heptane	142-82-5	700	5.637	6.148
3	Octane	111-65-9	800	8.741	9.315
4	Nonane	111-84-2	900	13.283	13.855
5	Decane	124-18-5	1000	18.443	18.981
6	Undecane	1120-21-4	1100	23.610	24.091
7	Dodecane	112-40-3	1200	28.539	28.965
8	Tridecane	629-50-5	1300	32.705	33.025
9	Tetradecane	629-59-4	1400	36.079	36.345
10	Pentadecane	629-62-9	1500	38.963	39.201
11	Hexadecane	544-76-3	1600	41.545	41.751
12	Heptadecane	629-78-7	1700	43.892	44.081
13	Octadecane	593-45-3	1800	46.088	46.255
14	Nonadecane	629-92-5	1900	48.133	48.291
15	Eicosane	112-95-8	2000	50.084	50.225
16	Heneicosane	629-94-7	2100	51.931	52.061
17	Docosane	629-97-0	2200	53.693	53.818
18	Tricosane	638-67-5	2300	55.446	55.565
19	Tetracosane	646-31-1	2400	57.435	57.568
20	Pentacosane	629-99-2	2500	59.781	59.885
21	Hexacosane	630-01-3	2600	61.544	61.611
22	Heptacosane	593-49-7	2700	62.807	62.868
23	Octacosane	630-02-4	2800	63.834	63.908
24	Nonacosane	630-03-5	2900	64.842	64.931
25	Triacontane	638-68-6	3000	65.898	65.988
26	Hentriacontane	630-04-6	3100	67.029	67.121

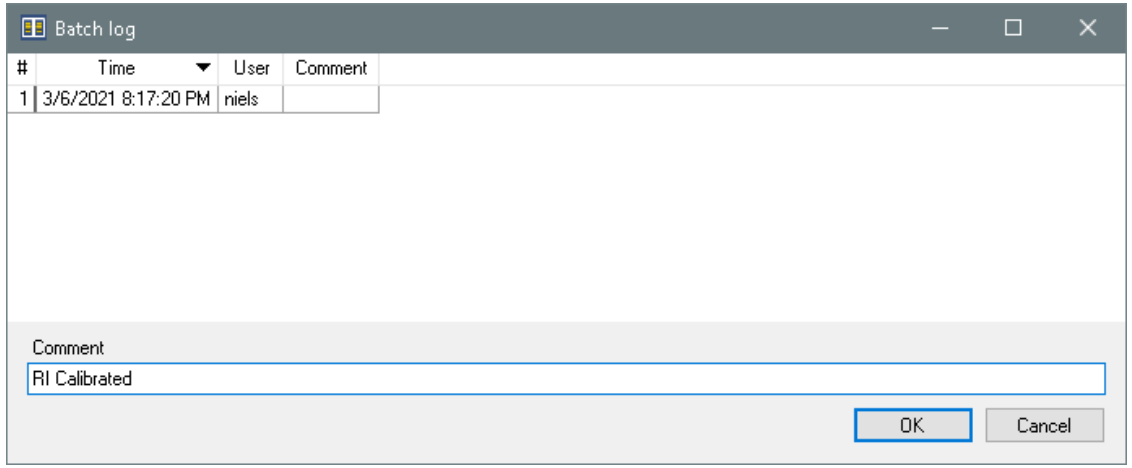
RI calibration setup

- Next RI re-calibration is just one click
- Calibrate with **RTs from current sample**
- The RT of largest peak within the RT window will be used



#	Compound	CAS	RI	RT TIC	RT FID
1	Hexane	110-54-3	600	4.060	4.498
2	Heptane	142-82-5	700	5.637	6.148
3	Octane	111-65-9	800	8.741	9.315
4	Nonane	111-84-2	900	13.283	13.855
5	Decane	124-18-5	1000	18.443	18.981
6	Undecane	1120-21-4	1100	23.610	24.091
7	Dodecane	112-40-3	1200	28.539	28.965
8	Tridecane	629-50-5	1300	32.705	33.025
9	Tetradecane	629-59-4	1400	36.079	36.345
10	Pentadecane	629-62-9	1500	38.963	39.201
11	Hexadecane	544-76-3	1600	41.545	41.751
12	Heptadecane	629-78-7	1700	43.892	44.081
13	Octadecane	593-45-3	1800	46.088	46.255
14	Nonadecane	629-92-5	1900	48.133	48.291
15	Eicosane	112-95-8	2000	50.084	50.225
16	Heneicosane	629-94-7	2100	51.931	52.061
17	Docosane	629-97-0	2200	53.693	53.818
18	Tricosane	638-67-5	2300	55.446	55.565
19	Tetracosane	646-31-1	2400	57.435	57.568
20	Pentacosane	629-99-2	2500	59.781	59.885
21	Hexacosane	630-01-3	2600	61.544	61.611
22	Heptacosane	593-49-7	2700	62.807	62.868
23	Octacosane	630-02-4	2800	63.834	63.908
24	Nonacosane	630-03-5	2900	64.842	64.931
25	Triacontane	638-68-6	3000	65.898	65.988
26	Hentriacontane	630-04-6	3100	67.029	67.121

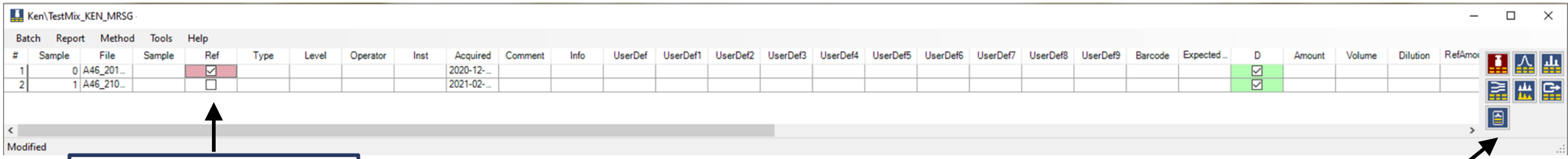
- Save batch
- Enter meaningful text to the logbook



04 Data Reviewing

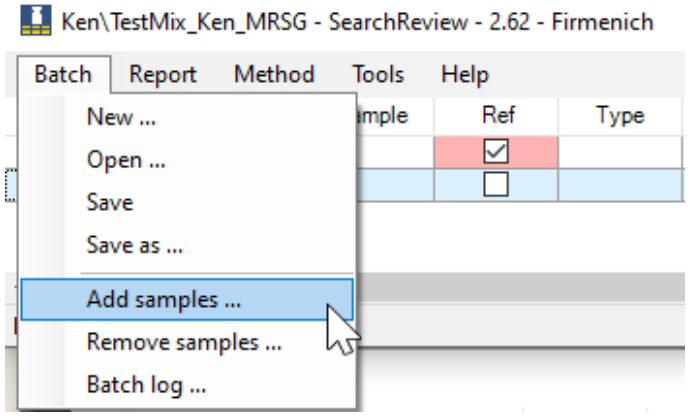
Data Reviewing – Main Window (samples)

This module allows you to navigate between the samples

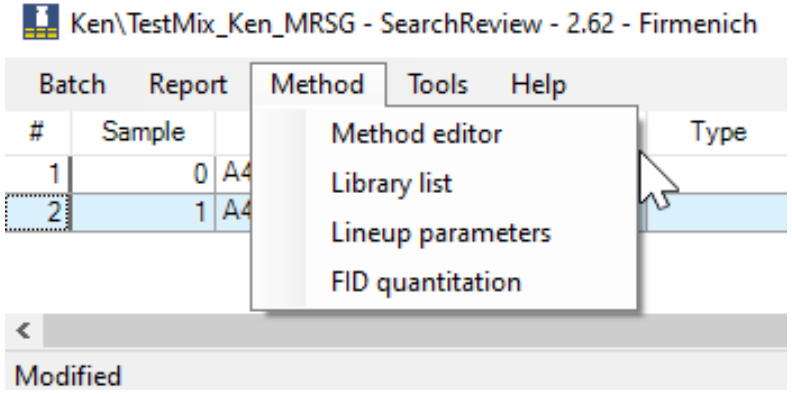


Select the reference sample if needed

Go from a module to another



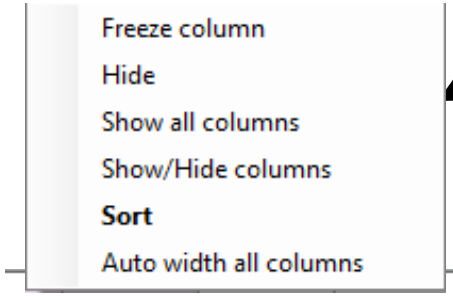
Add or remove samples from the batch



Edit Method, Library and Lineup parameters

Data Reviewing – Peaks Window

Right click on a column to access these actions



Left click on a column and move it to right or left

Selected sample

Peaks - A46_201207_123018_TESTMIX -

#	Rel	Chrom	RT	RI	Compou...	Formula	MW	CAS	FEMA	COC	CID	Area	Height	Width	Dec	Report	MReport	Review
8		TIC	3.405	932	PINENE...	C10H16	136.2	7785-26-4	2902	10000080	00000194	3165606	0.019	2563888		Report		Tentat...
9		FID	3.412	932								2621251	0.019	2130076		Exclu...		Tentat...
10		TIC	3.580	945	CAMPHE...	C10H16	136.2	79-92-5	2229	10000223	00000461	37018	0.020	27442		Report		Tentat...
11		FID	3.585	945								30464	0.020	23853		Exclu...		Unkno...
12		TIC	4.306	1000	DECANE	C10H22	142.3	124-18-5		10001748	00000326	3118323	0.023	2128648		Report		Tentat...
13		FID	4.308	1000								2762747	0.023	1894686		Exclu...		Tentat...
14		TIC	5.216	1050	ALCOHO...	C8H18O	130.2	111-87-5	2800	10003669	00061947	4223225	0.028	2345405		Report		Tentat...
15		FID	5.218	1050								3824302	0.028	2130573		Exclu...		Tentat...
16		TIC	5.328	1056	CIS-LINA...	C10H18O2	170.2	5989-33-3	3746	10063894	00069640	102311	0.025	57983		Report		Appro...
17		FID	5.332	1056								69653	0.024	44523		Exclu...		Unknown
18		TIC	5.586	1070	CIS-LINA...	C10H18O2	170.2	5989-33-3	3746	10063894	00069640	68236	0.028	38155		Report		Tentative
19		FID	5.592	1070								59473	0.027	34301		Exclu...		Approved
20		TIC	5.727	1078	CIS-LINA...	C8H10O	122.2	576-26-1	3249	10060612	00084052	2323865	0.028	1321236		Report		Tentat...
21		FID	5.728	1078								1998719	0.028	1123396		Exclu...		Tentat...

Visual correlation between TIC and FID

Compound status

Data Reviewing – Peaks Window

Peaks - A46_201207_123018_TESTMIX -

#	DOU	mARC	cRRF	mRRF
11	1			
12	0		0.72584	
13	1			
14	0		0.87093	
15	1			
16	2		0.99507	
17	1			
18	2		0.99507	
19	1			
20	4		0.97100	
21	1			
22	1			
23	2		0.86838	
24	1			
25	1		1.05217	

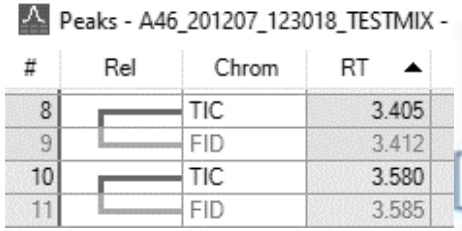
The library can contain the RRF
If you work with another library without RRF data, it can be adjusted by filling in the mARC: manual Aromatic Ring Count, with help of DOU: Degree Of Unsaturation

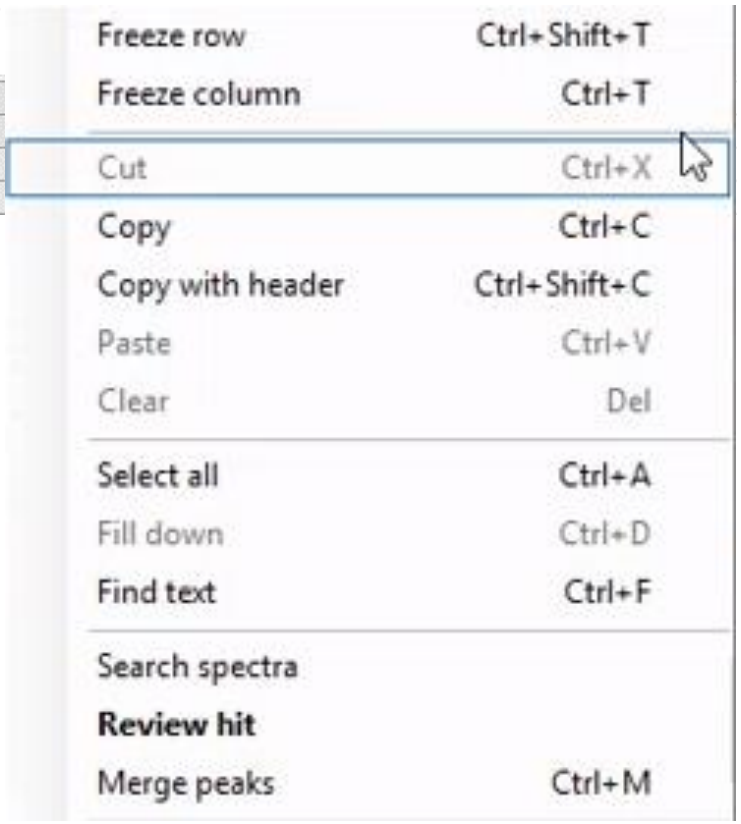
Fields related to internal standard: possibility to quantitate

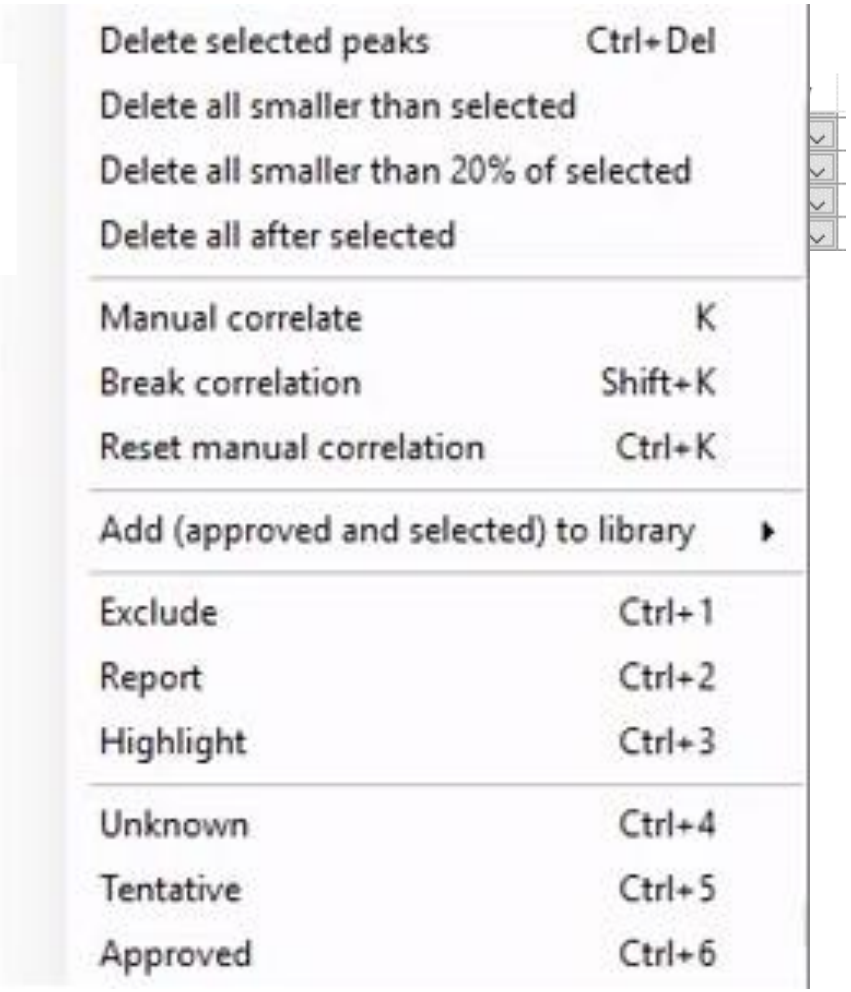
Peaks - A46_201207_123018_TESTMIX -

#	IRRF	IConc	mIConc	ISTD	IsI
1					☐
2					☐
3					☐
4					☐
5					☐
6					☐
7					☐
8					☐
9					☐
10					☐

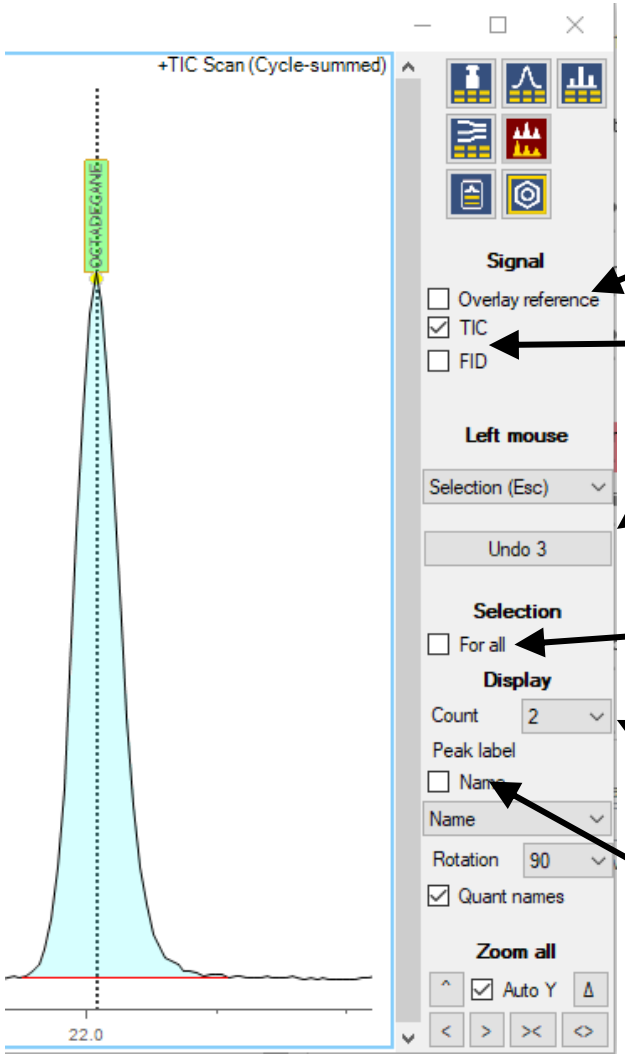
Data Reviewing – Peaks Window







Data Reviewing - Chromatogram



Add ref spectrum in dotted lines on other samples

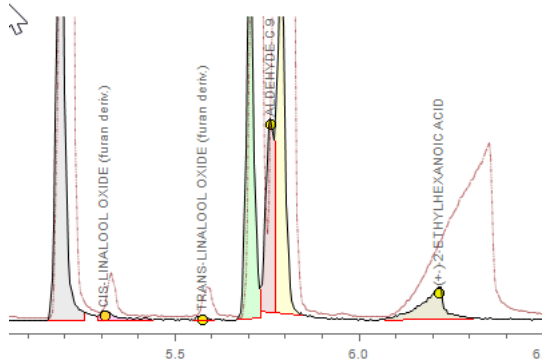
Select TIC and/or FID

Undo until 5 last actions

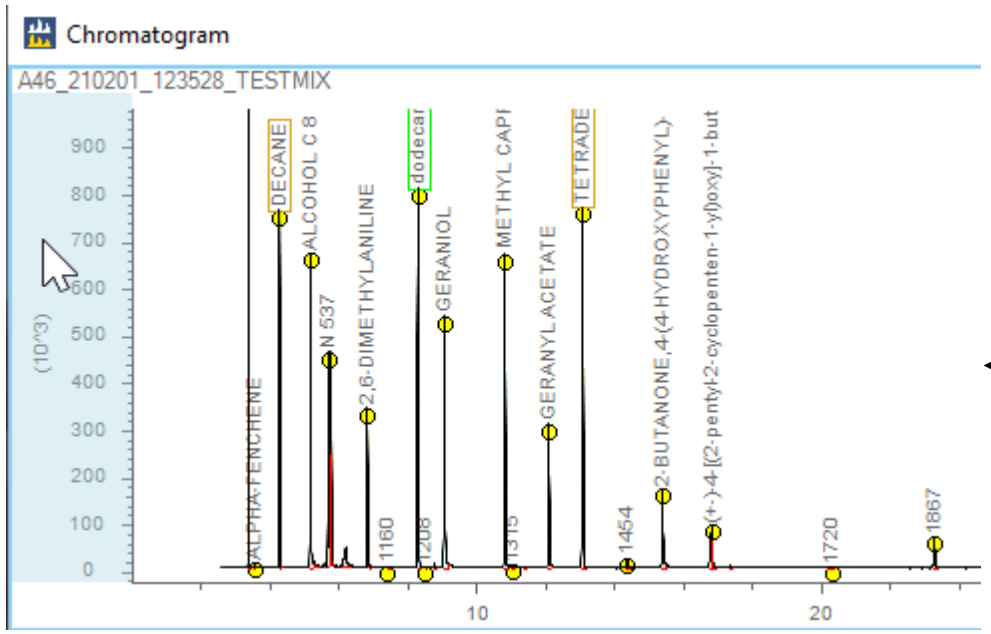
Apply the selected action on all spectra

Select the number of chromatograms you want to see in the window

Add compound names above peaks

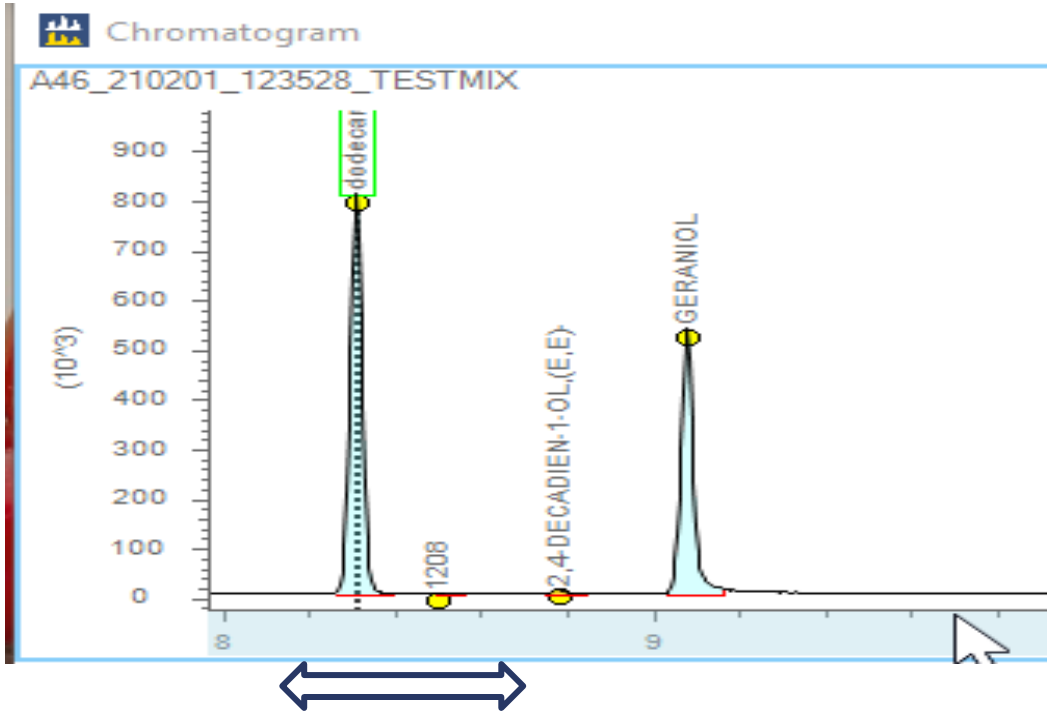


Data Reviewing - Chromatogram



Zoom in by right click-and-drag

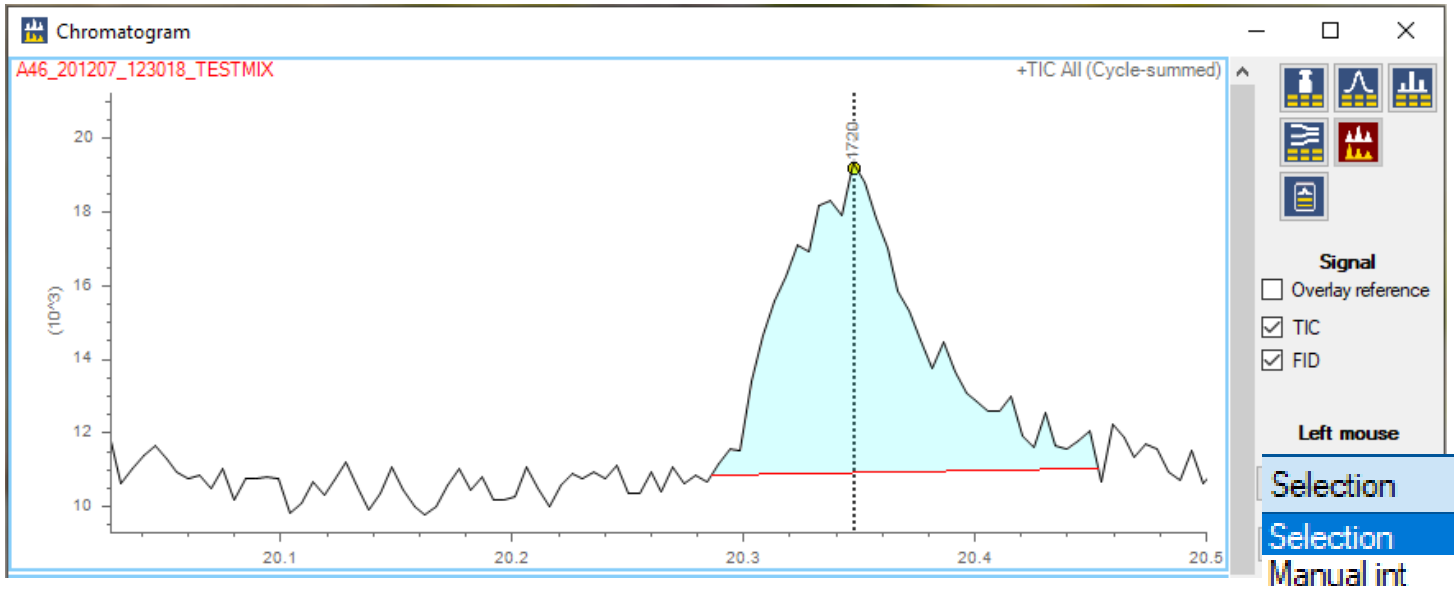
Zoom out by right double click

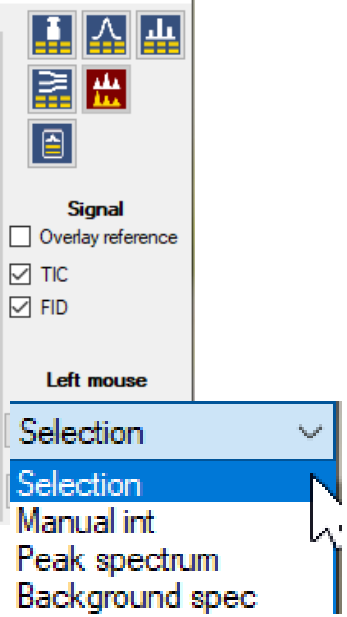


Other zoom and navigation panel

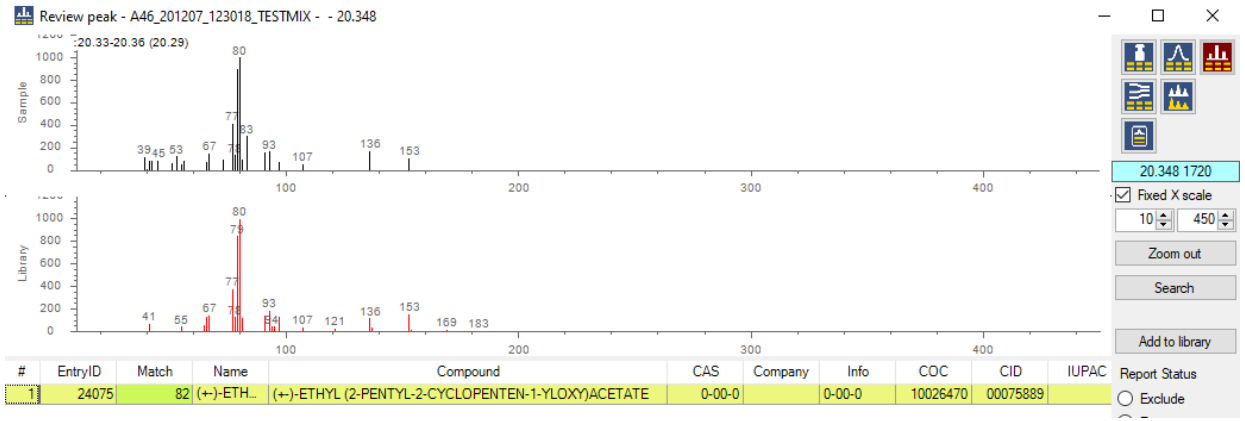
- Left click on x/y axis and move from left to right / up to down by dragging the mouse or with keyboard arrows
- Double click to zoom out
- Right click and move to zoom in / out on the selected axis

Data Reviewing - Chromatogram

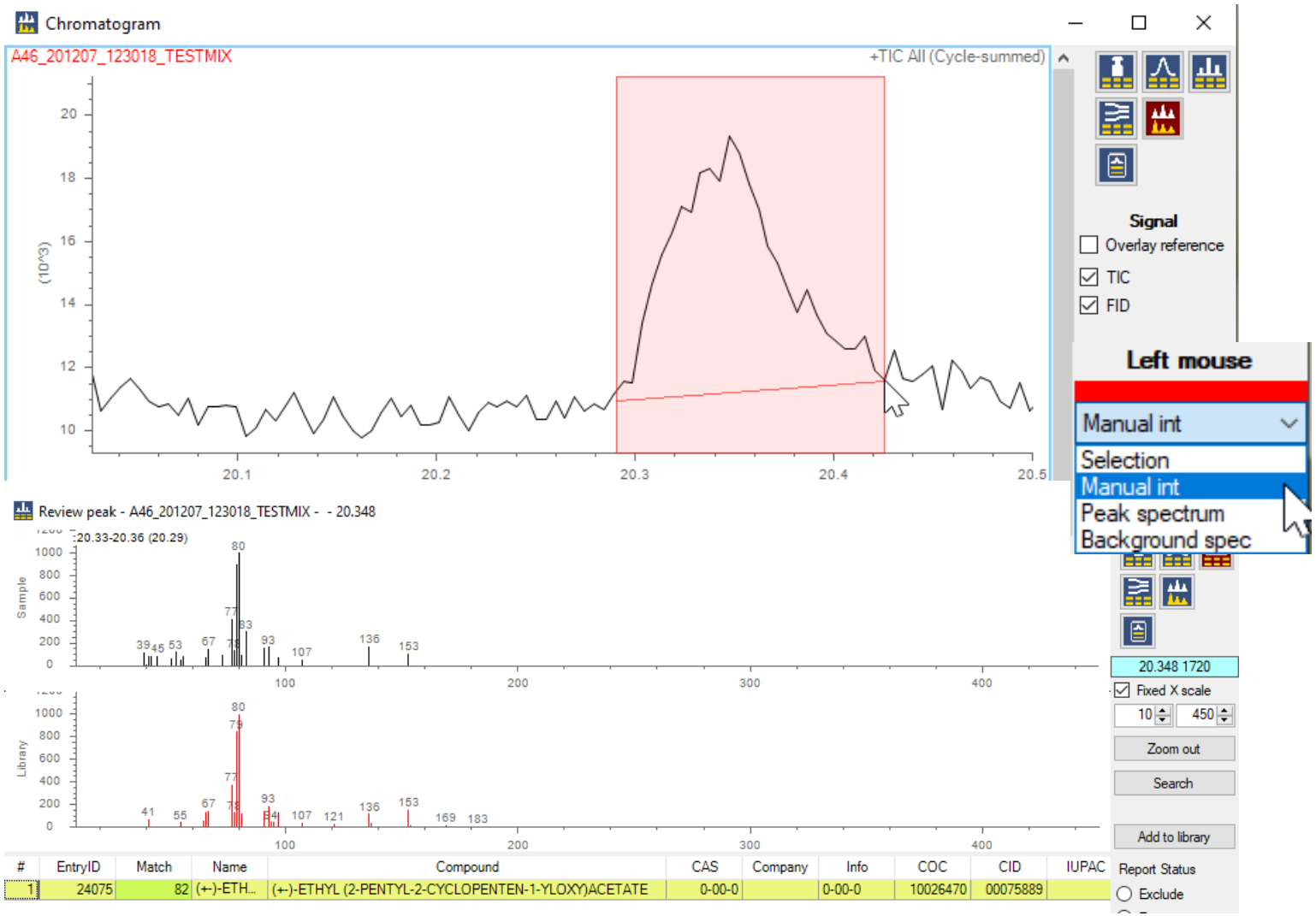




Left mouse in Selection Mode (Keyboard shortcut: Esc.): select a peak and display its spectrum in Review peak module

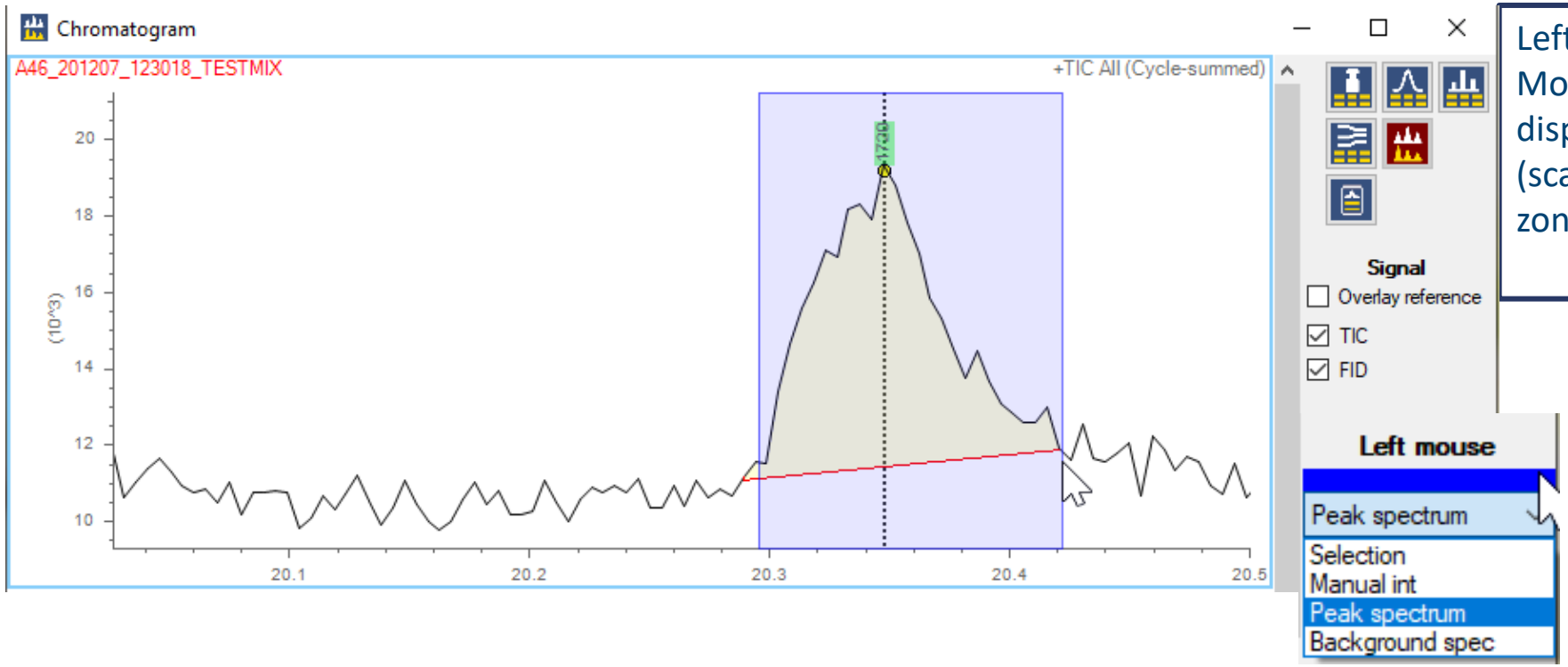


Data Reviewing - Chromatogram



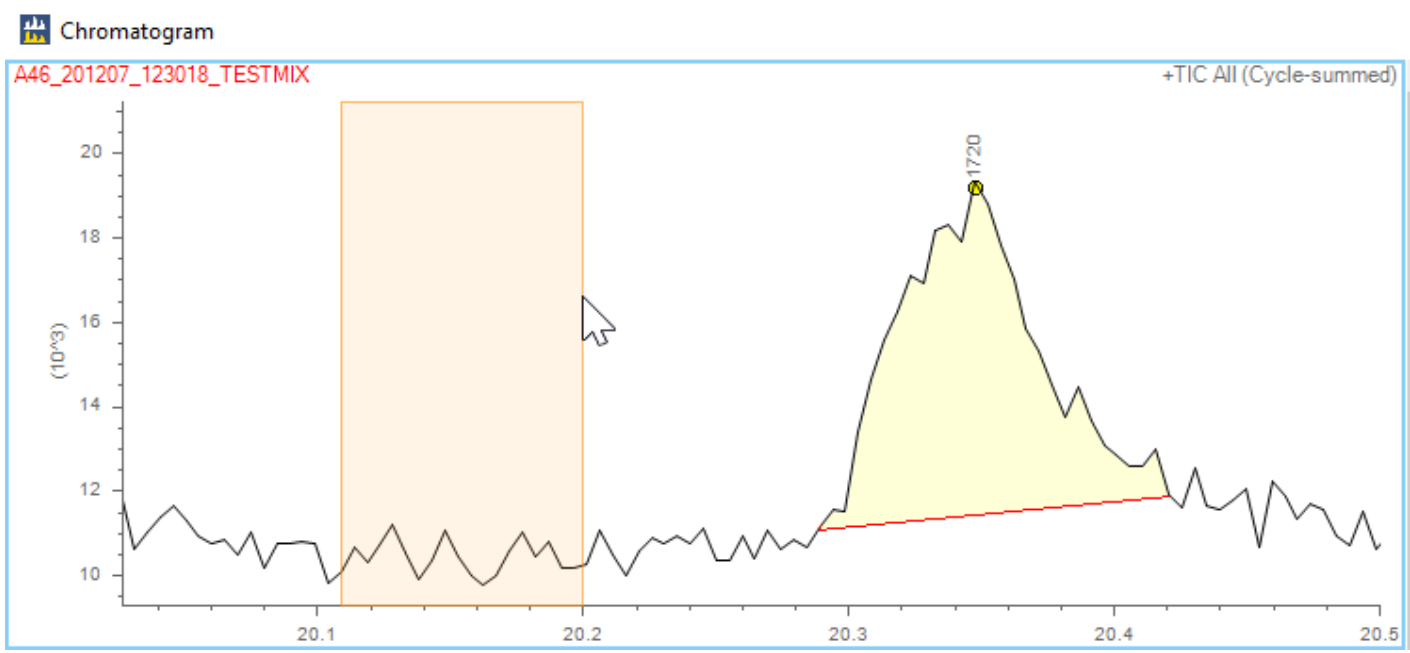
Left mouse in Manual int Mode (Keyboard shortcut: m): integrate a peak and display its spectrum in Review peak module

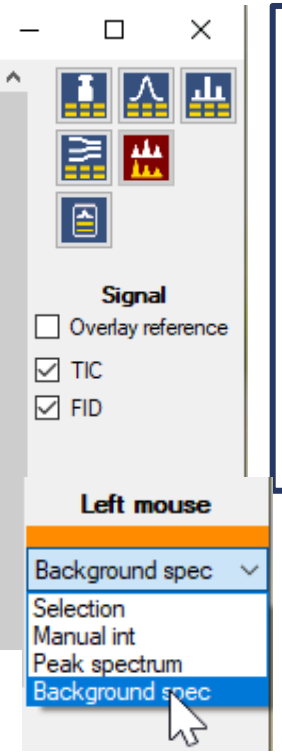
Data Reviewing - Chromatogram

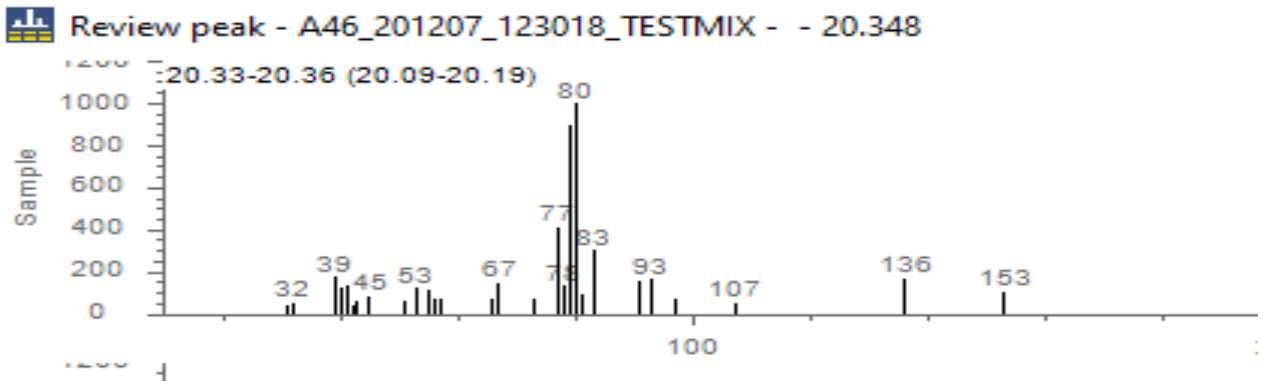


Left mouse in Peak spectrum Mode (Keyboard shortcut: s): display the selected spectrum (scan by scan or average of peak zone)

Data Reviewing - Chromatogram







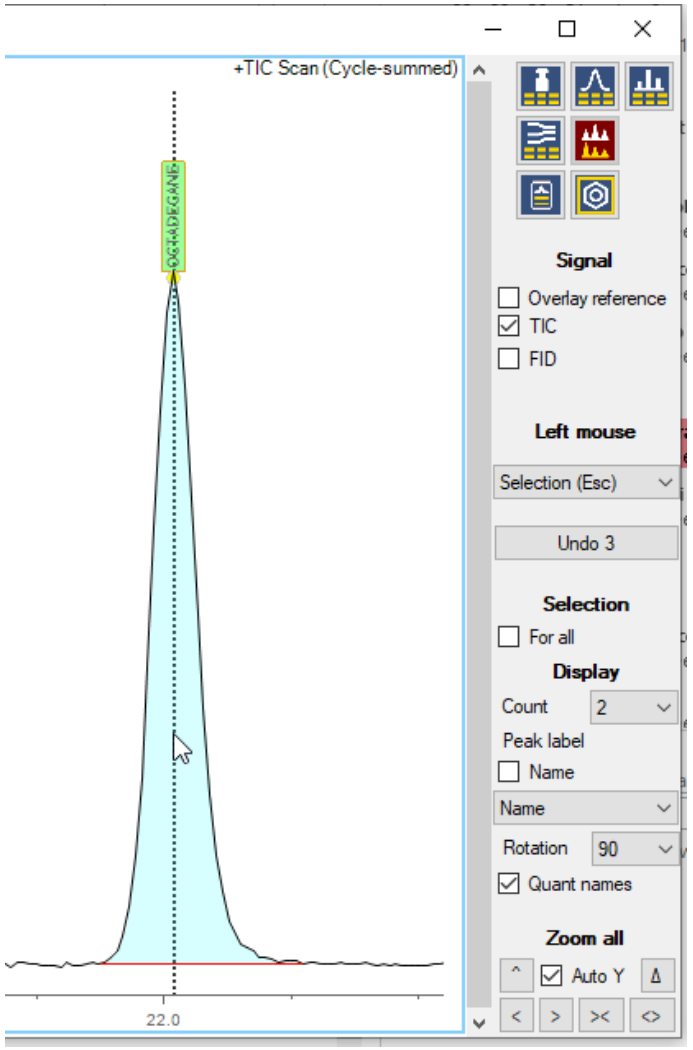
Left mouse in Background spec Mode (Keyboard shortcut: b): select a background zone, and subtract it to the selected peak spectrum in Review peak module

Data Reviewing - Chromatogram

Right-clicking on a peak allows a lot of actions

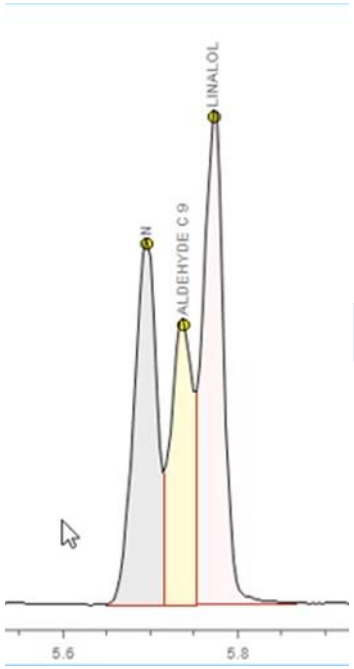
Hide selected sample	Shift+Ctrl+H
Show all samples	Shift+Ctrl+G
Hide non-selected samples	Ctrl+G
Same Y scale for all	Y
Selection for all	
Zoom Y	Z
Review hit	
Accept hit info for in line peaks	Ctrl+Enter
Search spectra	
Merge peaks	Ctrl+M
Delete selected peaks	Ctrl+Del
Delete all smaller than selected	
Delete all smaller than 20% of selected	
Delete all after selected	

Integrate	
Deconvolute	
Manual correlate	K
Break correlation	Shift+K
Reset manual correlation	Ctrl+K
Match	
Manual lineup	L
Break lineup	Shift+L
Reset lineup	Ctrl+L
Exclude	Ctrl+1
Report	Ctrl+2
Highlight	Ctrl+3
Unknown	Ctrl+4
Tentative	Ctrl+5
Approved	Ctrl+6
Append approved to library	▸

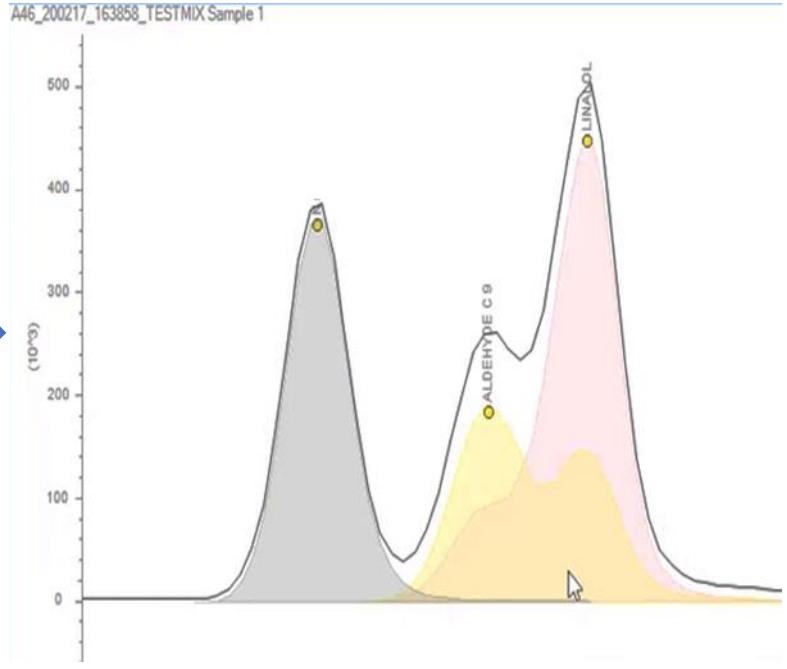


Data Reviewing – Chromatogram

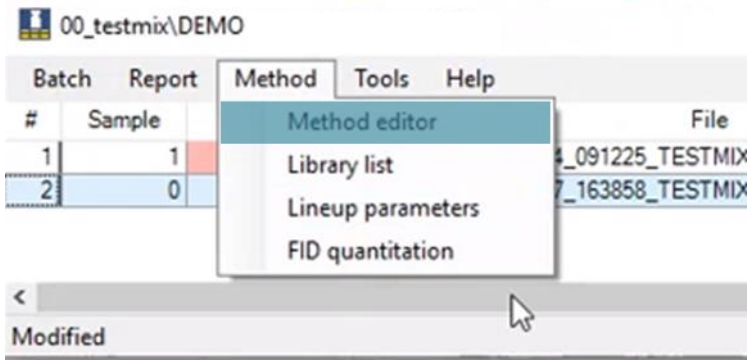
Local deconvolution: right click → deconvolute

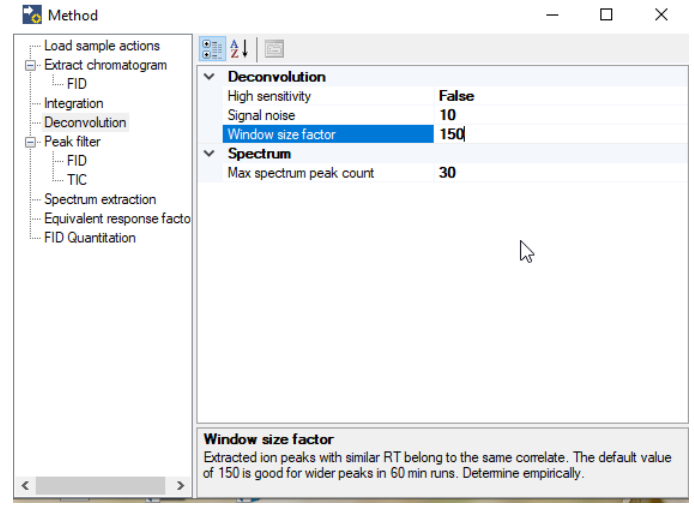


Integration



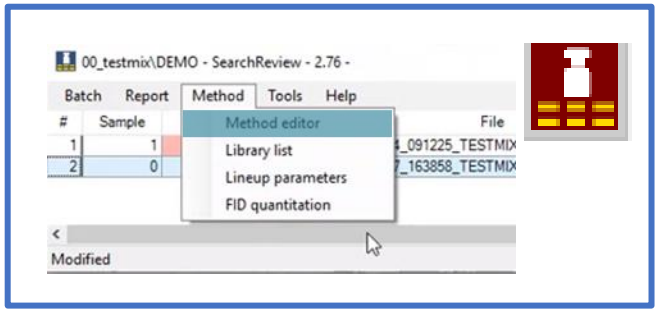
Deconvolution



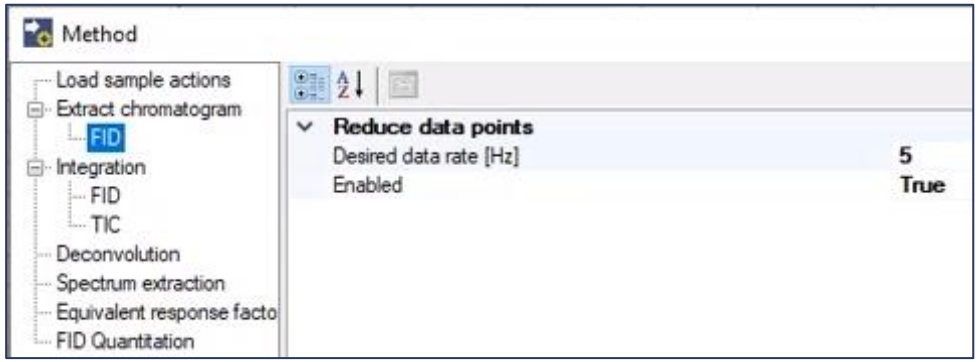


Adjust deconvolution parameters: in the main window, click on Method → Method editor → Deconvolution Tab

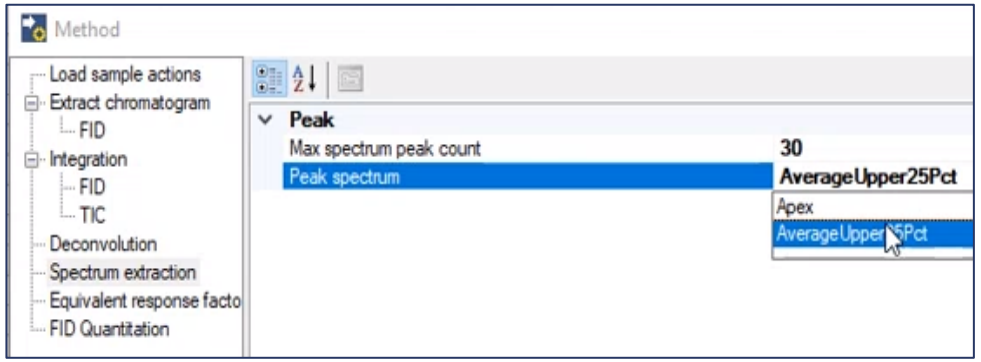
Data Reviewing – Chromatogram



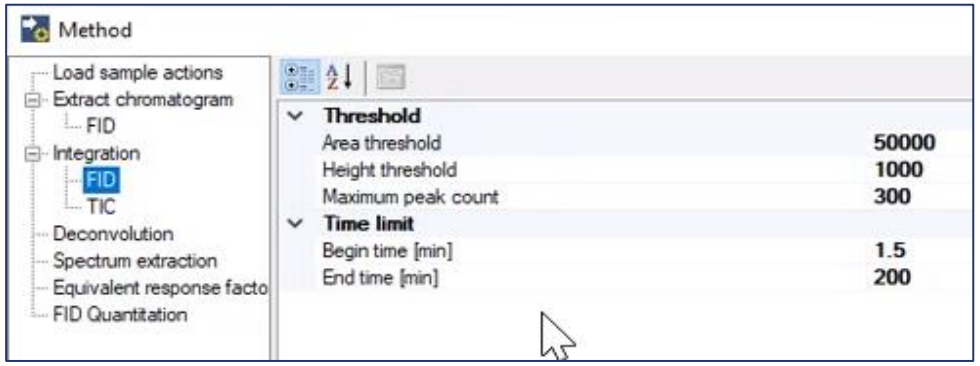
Several other parameters can be adjusted through the Main window:



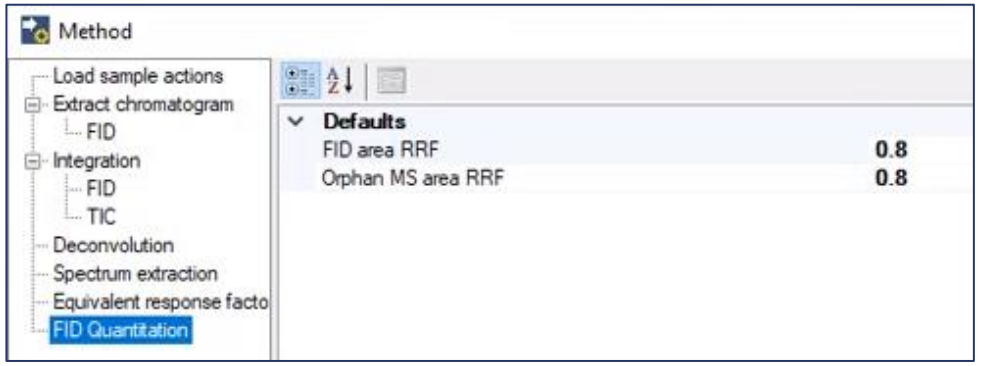
FID: desired data rate for extraction and do we went to extract FID or not



Spectrum extraction type: 1 scan from the apex or average scan for scan upper of 25% peak hight



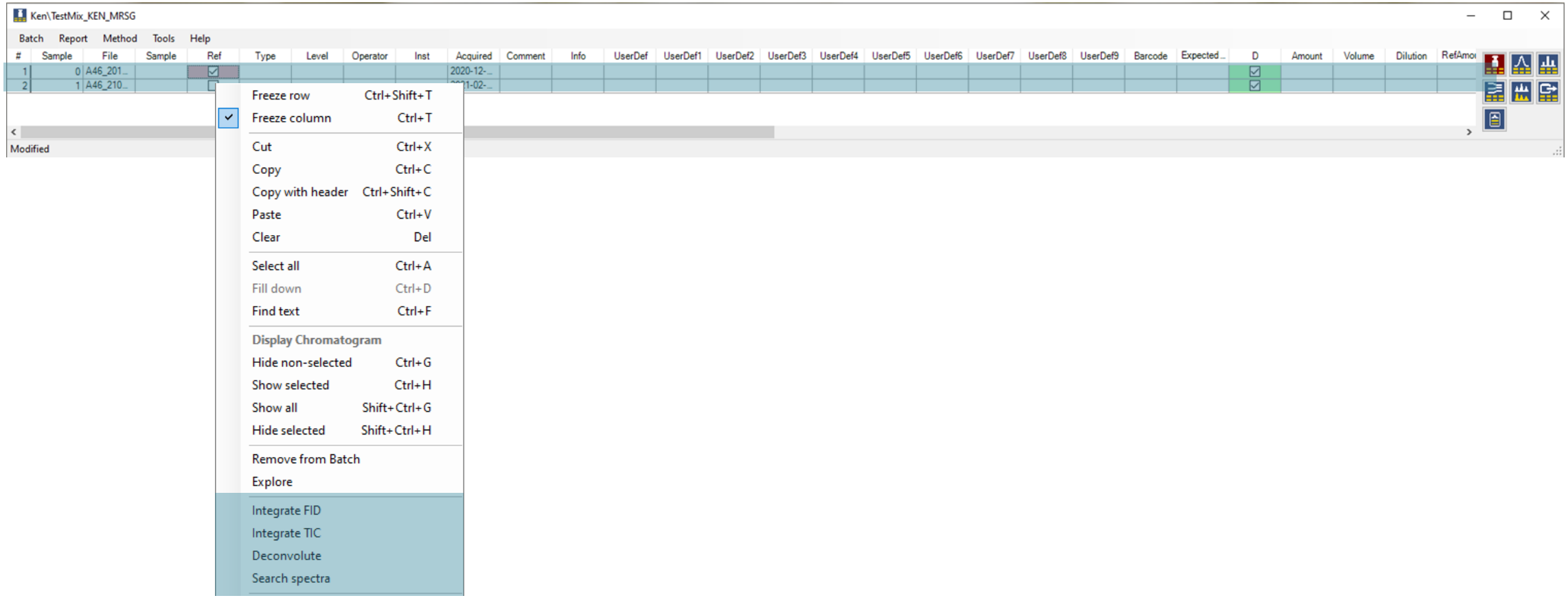
Integration parameters :Area threshold and height threshold for peak exclusion and time range for integration to be on or off



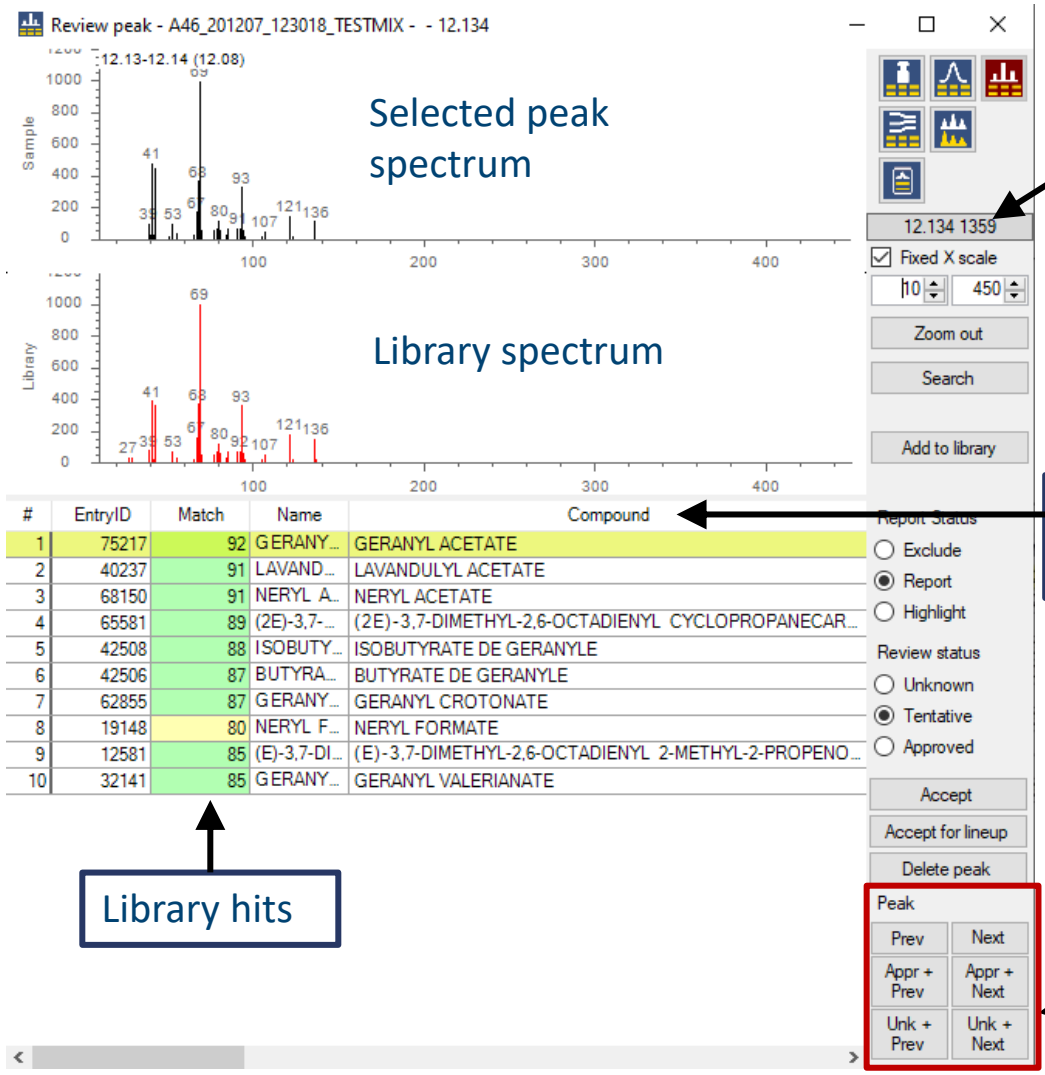
FID quantification: Default RRF used if no rrf could be caculated or extract from Librarie

Data Reviewing – Chromatogram

When you modify any method or library parameter, right click on the samples and select «Integrate», «Deconvolute» or «Search spectra» according to the modification you made to reintegrate data.



Data Reviewing – Review Peak



RT and LRI

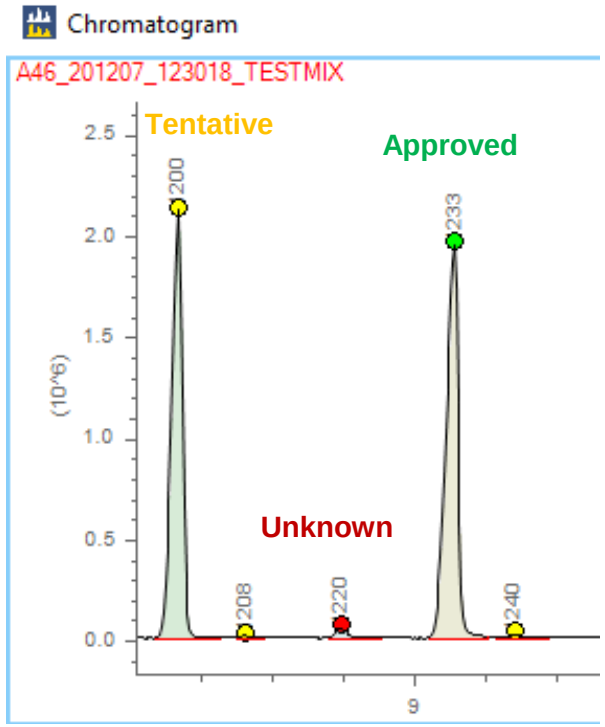
Right click on the first row
→ Show/Hide columns

Library hits

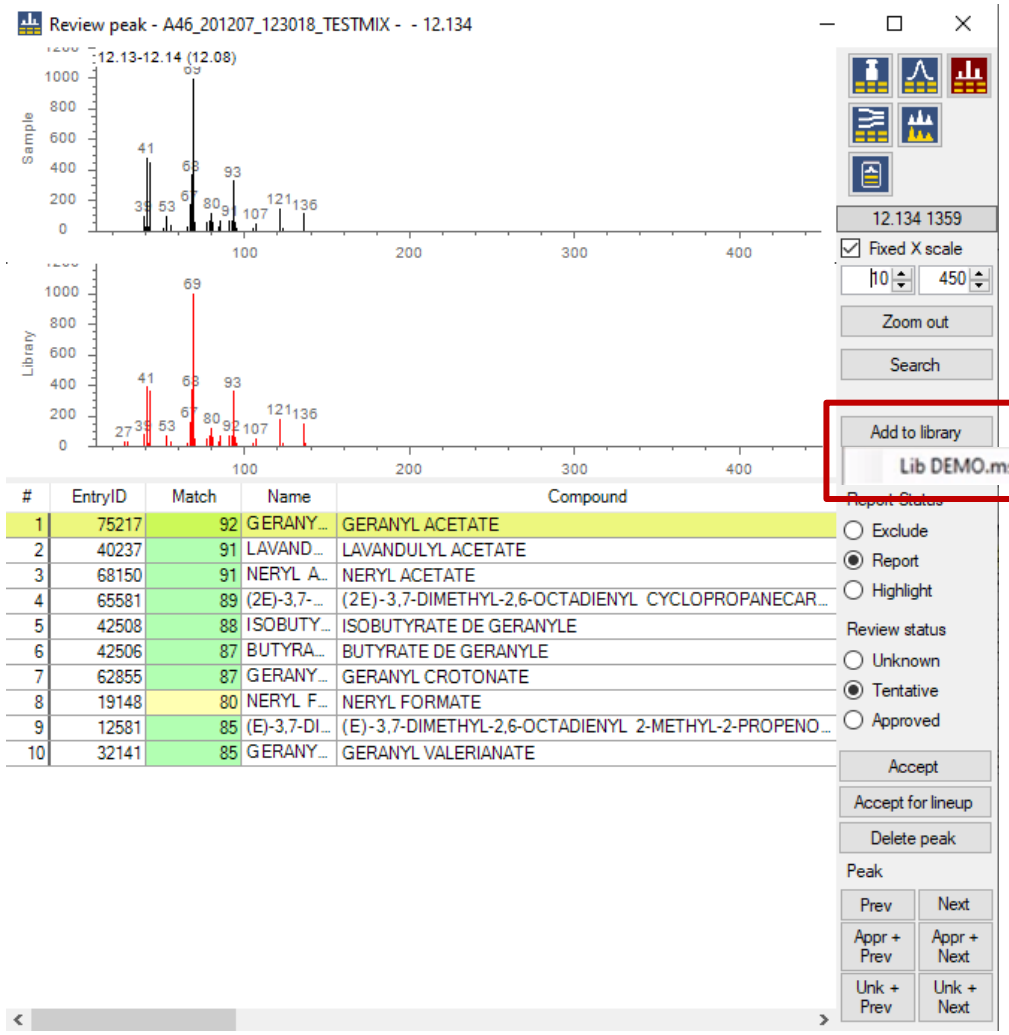
Switch from a peak to another

1) Select the best hit, if available
2) Select the status
3) Click on accept

It updates the chromatogram colors

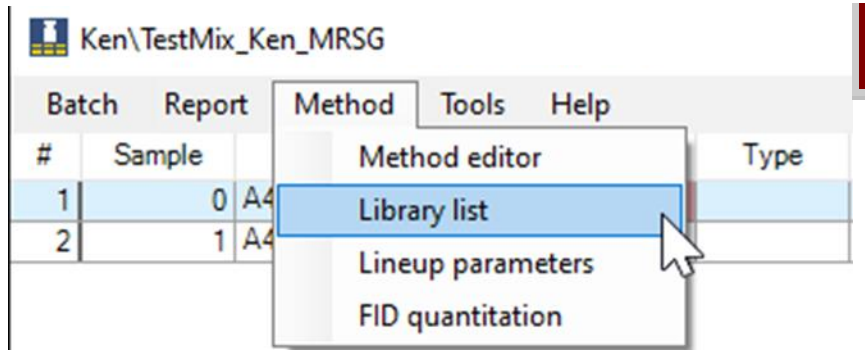


Data Reviewing – Review Peak



#	EntryID	Match	Name	Compound
1	75217	92	GERANY...	GERANYL ACETATE
2	40237	91	LAVAND...	LAVANDULYL ACETATE
3	68150	91	NERYL A...	NERYL ACETATE
4	65581	89	(2E)-3,7-...	(2E)-3,7-DIMETHYL-2,6-OCTADIENYL CYCLOPROPANECAR...
5	42508	88	ISOBUTY...	ISOBUTYRATE DE GERANYLE
6	42506	87	BUTYRA...	BUTYRATE DE GERANYLE
7	62855	87	GERANY...	GERANYL CROTONATE
8	19148	80	NERYL F...	NERYL FORMATE
9	12581	85	(E)-3,7-DI...	(E)-3,7-DIMETHYL-2,6-OCTADIENYL 2-METHYL-2-PROPENO...
10	32141	85	GERANY...	GERANYL VALERIANATE

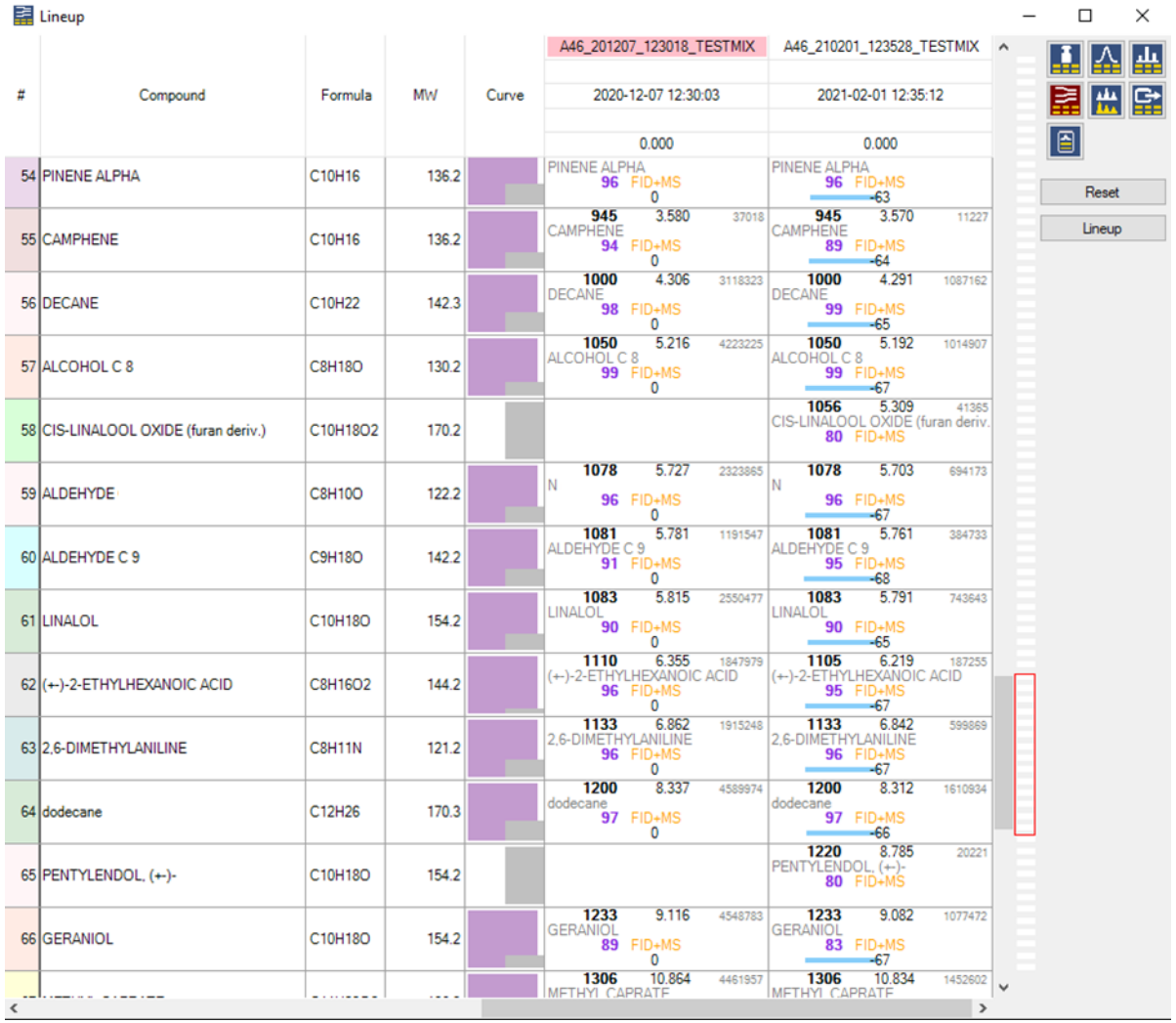
Add a peak to your own editable library



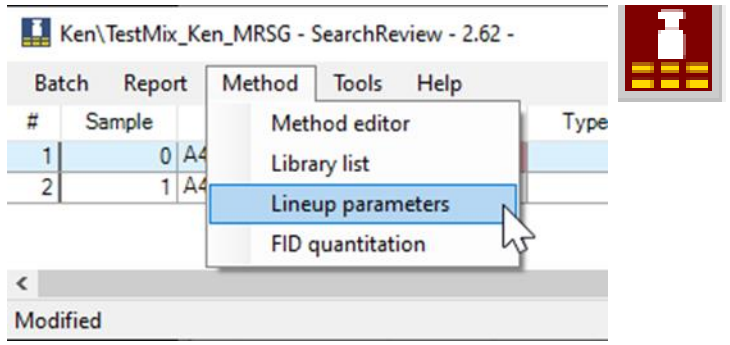
Access libraries parameters at any time via the Main Window

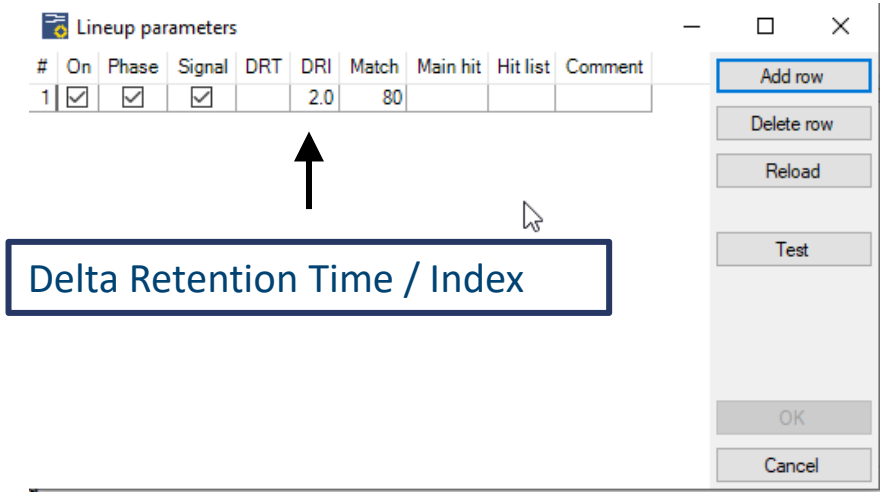
Data Reviewing – Lineup

Peaks lineup/comparison between chromatograms



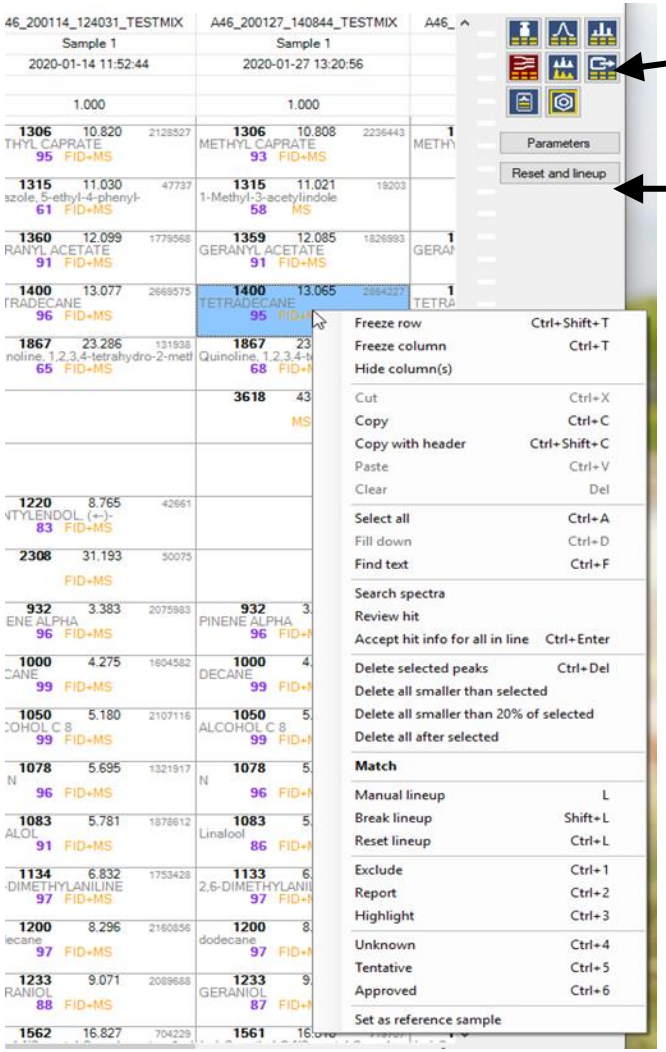
Parameters can be adjusted by clicking on Method -> Lineup parameters in the main window





Delta Retention Time / Index

Data Reviewing – Lineup



Export: Export lineup window to excel file

Reset and Lineup: remove all the lineups and "refresh" with latest parameters

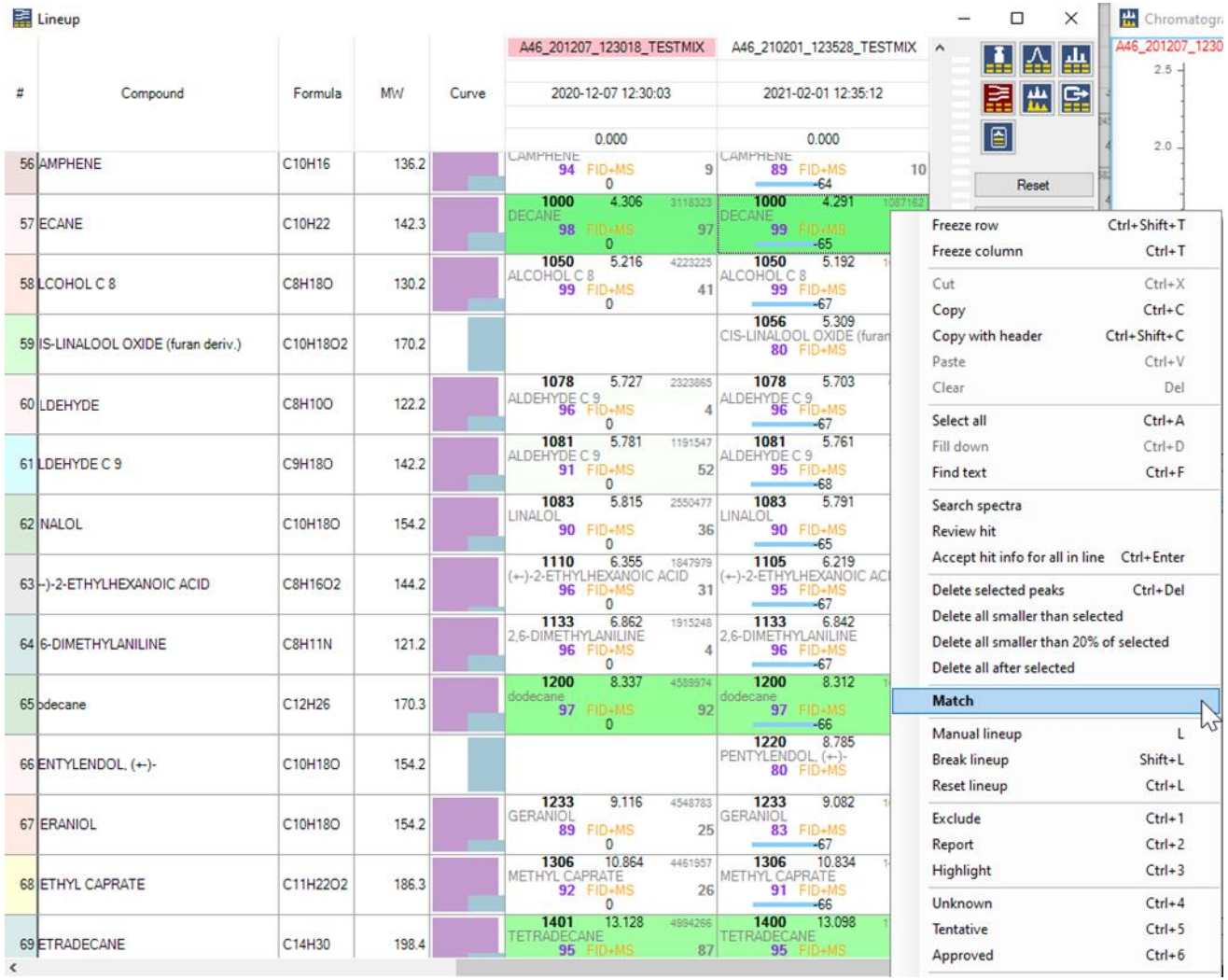
Manual lineup or break lineup:

Select the compounds you want to lineup or reset lineup (Ctrl + left click)

Press "L"→ Manual Lineup

Press shift +"L" → Break Lineup

Data Reviewing – Lineup

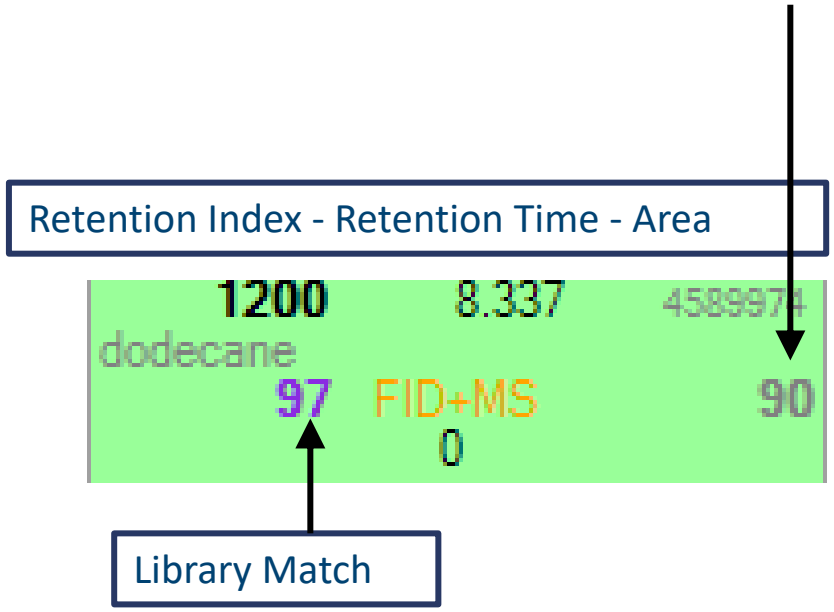


Spectrum Match:

Select a compound Left double click:

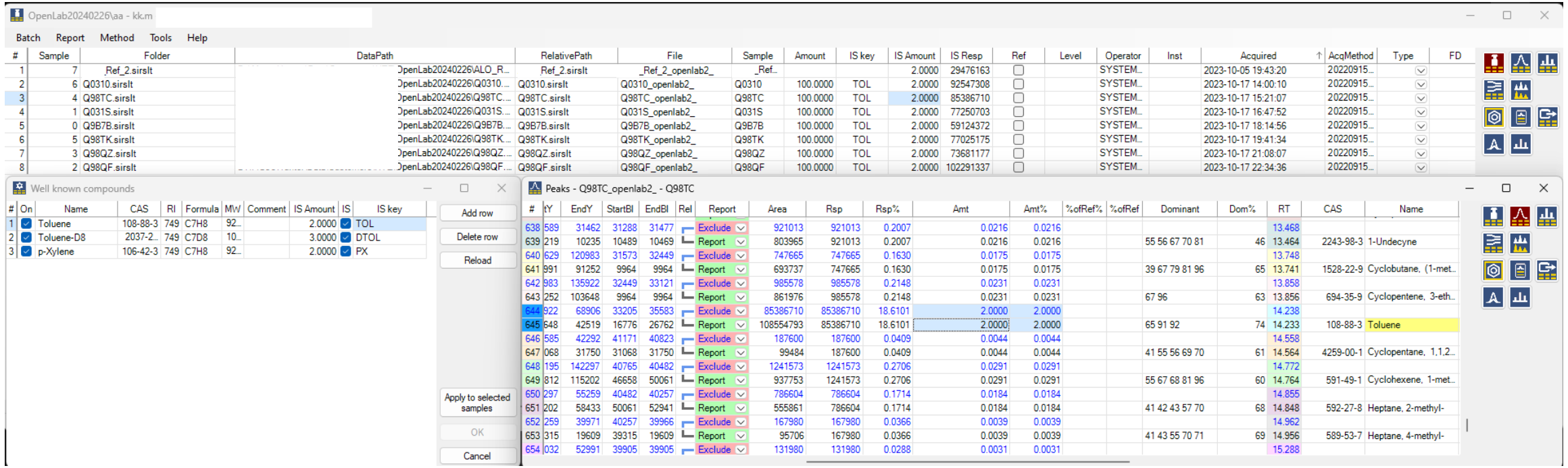
All the compounds with a close spectrum highlight in green.

ie: If DECANE is selected, DODECANE has a match of 90



05 Quantitation

Quantitation



Quantitation:

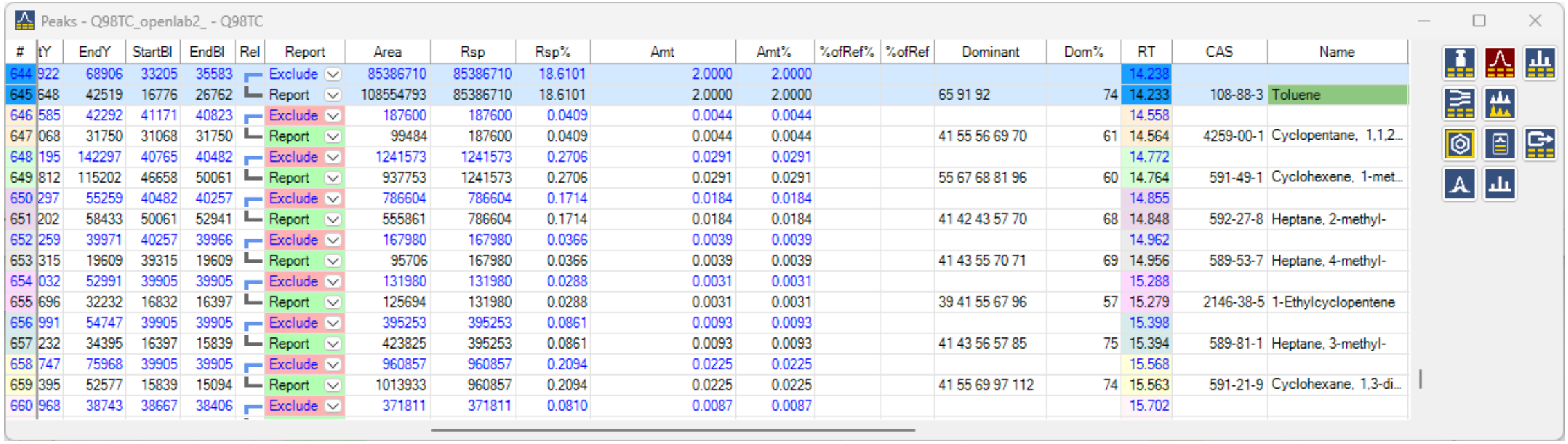
Example: Toluene equivalent base on FID response

Add rows to the Well known compound table

The default IS Amount can be overridden per sample

The sample IS key should correspond with the Well known compound

Quantitation



#	tY	EndY	StartBl	EndBl	Rel	Report	Area	Rsp	Rsp%	Amt	Amt%	%ofRef%	%ofRef	Dominant	Dom%	RT	CAS	Name
644	922	68906	33205	35583		Exclude	85386710	85386710	18.6101	2.0000	2.0000					14.238		
645	648	42519	16776	26762		Report	108554793	85386710	18.6101	2.0000	2.0000			65 91 92	74	14.233	108-88-3	Toluene
646	585	42292	41171	40823		Exclude	187600	187600	0.0409	0.0044	0.0044					14.558		
647	068	31750	31068	31750		Report	99484	187600	0.0409	0.0044	0.0044			41 55 56 69 70	61	14.564	4259-00-1	Cyclopentane, 1,1,2...
648	195	142297	40765	40482		Exclude	1241573	1241573	0.2706	0.0291	0.0291					14.772		
649	812	115202	46658	50061		Report	937753	1241573	0.2706	0.0291	0.0291			55 67 68 81 96	60	14.764	591-49-1	Cyclohexene, 1-met...
650	297	55259	40482	40257		Exclude	786604	786604	0.1714	0.0184	0.0184					14.855		
651	202	58433	50061	52941		Report	555861	786604	0.1714	0.0184	0.0184			41 42 43 57 70	68	14.848	592-27-8	Heptane, 2-methyl-
652	259	39971	40257	39966		Exclude	167980	167980	0.0366	0.0039	0.0039					14.962		
653	315	19609	39315	19609		Report	95706	167980	0.0366	0.0039	0.0039			41 43 55 70 71	69	14.956	589-53-7	Heptane, 4-methyl-
654	032	52991	39905	39905		Exclude	131980	131980	0.0288	0.0031	0.0031					15.288		
655	696	32232	16832	16397		Report	125694	131980	0.0288	0.0031	0.0031			39 41 55 67 96	57	15.279	2146-38-5	1-Ethylcyclopentene
656	991	54747	39905	39905		Exclude	395253	395253	0.0861	0.0093	0.0093					15.398		
657	232	34395	16397	15839		Report	423825	395253	0.0861	0.0093	0.0093			41 43 56 57 85	75	15.394	589-81-1	Heptane, 3-methyl-
658	747	75968	39905	39905		Exclude	960857	960857	0.2094	0.0225	0.0225					15.568		
659	395	52577	15839	15094		Report	1013933	960857	0.2094	0.0225	0.0225			41 55 69 97 112	74	15.563	591-21-9	Cyclohexane, 1,3-di...
660	968	38743	38667	38406		Exclude	371811	371811	0.0810	0.0087	0.0087					15.702		

Quantitation:

Area is the integrated peak area

Response (Rsp) is the area of the correlated FID peak. If 2 MS peaks are correlated with 1 FID, the FID area is divided per MS area.

If there is no correlated FID peak, the response is just the MS area.

Rsp% is the normalized Response

Amt is calculated with the Well known response factor

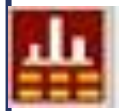
Amt% is (peak Amount / sample Amount) * 100%

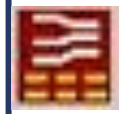
06 Report

Export Data

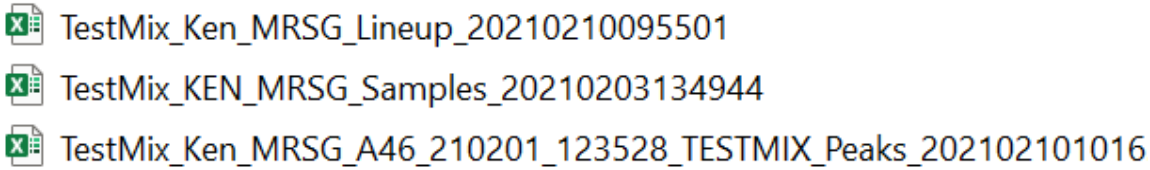
Available for:

Samples (Main Window)

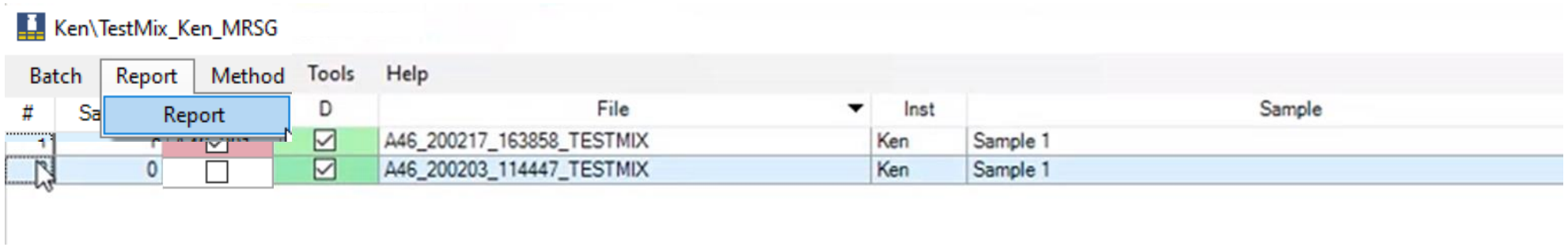
 Peaks

 Lineup

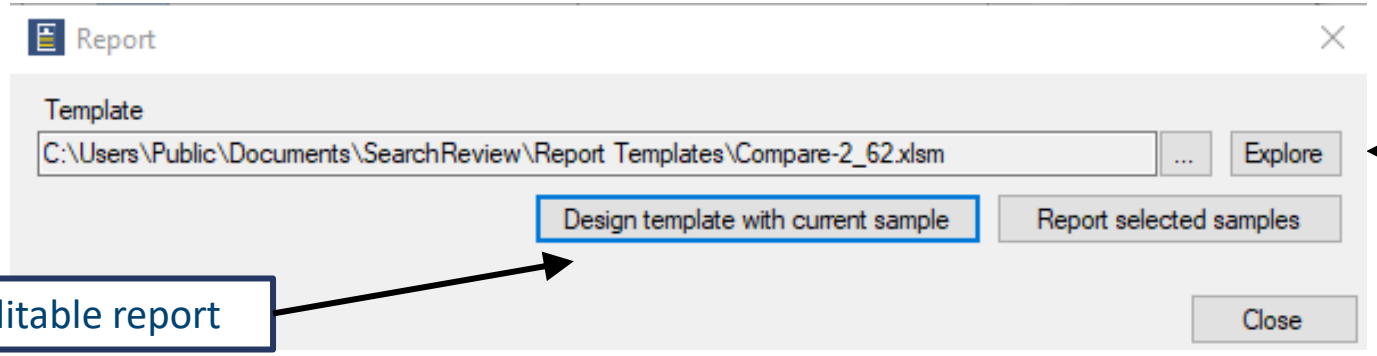
Exports Data to an Excel File in the batch folder



Report from the Samples window



Mind to tick the reference and to select the sample to compare (highlighted line)



Select a template

Editable report

Report

Sample and ref data

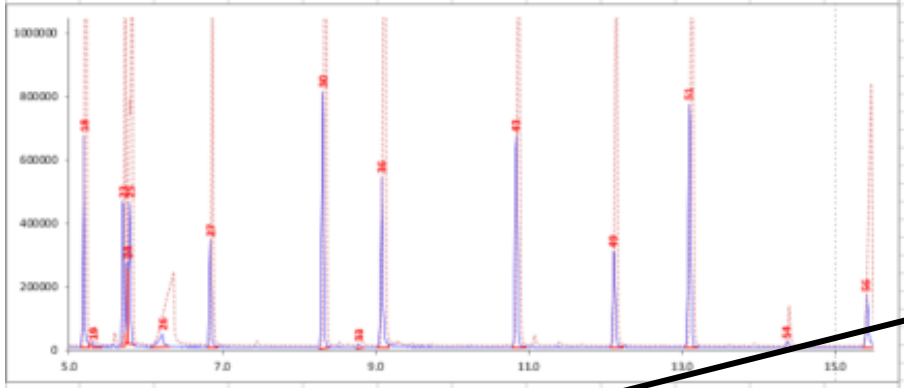
Chromatogram

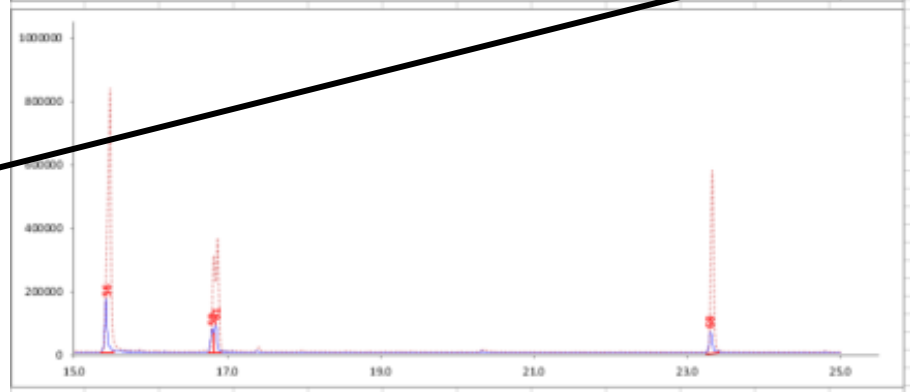
Template settings

Compound data

Reported	2021-02-10 09:58
Comparison mode	Perfume
Sample	Z:\test_mix_ltgal\KenA46_210201_123528_TESTMIX.D
Item	
LotNr	
LIMS_ID	
Runtime	01.02.2021 12:35
Channel	
Timebase	HPTPE_B
Reference	Z:\test_mix_ltgal\KenA46_201207_123018_TESTMIX.D
Item	
LotNr	
LIMS_ID	
Runtime	07.12.2020 12:30
Channel	
Timebase	HPTPE_B

Reformat | Create PDF | Names | Save as template ...





Signal selection	MS
MS	n/a
FID	n/a

Time selection	BothLimit
LowerLimit	5
UpperLimit	25
BothLimit	n/a
Full	n/a
SetInChartAxisScale	n/a
Overlap	0.5

Label selection	ReportIndex
Any	n/a
Comment	format
Name	format
CAS	format
ReportIndex	format
RetentionIndex	format
RetentionTime	format

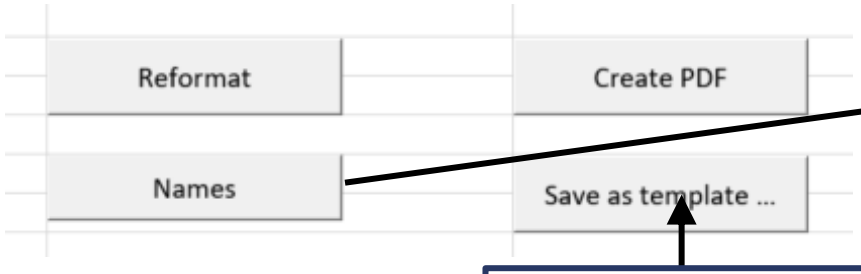
Response Max selection	HighestPointAfter
HighestPointAfter	0
Fixed	800000
ChartNumber	2
ChartsIndividual	n/a
SetInChartAxisScale	n/a

Response Min selection	Fixed
LowestPointAfter	0
Fixed	0
ChartNumber	2
ChartsIndividual	n/a
SetInChartAxisScale	n/a

Index	RT	RT r	RI	RI r	A%	A% r	Dev	Dev%
1	1.315		773		0.028		Extra peak	NaN
2		1.318		773		0.005	Peak missing	
3	1.362		777		0.009		Extra peak	NaN
4		1.392		778		0.005	Peak missing	
5	1.392		779		0.002		Extra peak	NaN
6		1.435		782		99.893	Peak missing	
7	1.435		782		99.923		Extra peak	NaN
8		1.908		818		0.012	Peak missing	
9	1.908		818		0.004		Extra peak	NaN
10	1.948		822		0.021		Extra peak	NaN
11		1.952		821		0.059	Peak missing	
12		2.182		838		0.000	Peak missing	
13	2.465		861		0.000		Extra peak	NaN

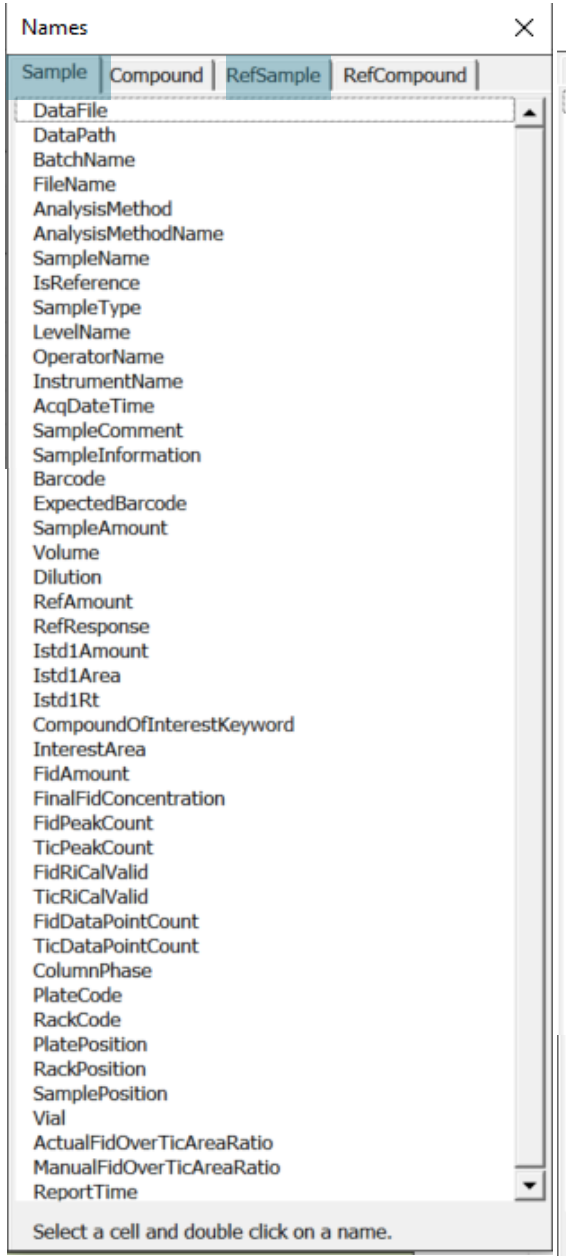
Report

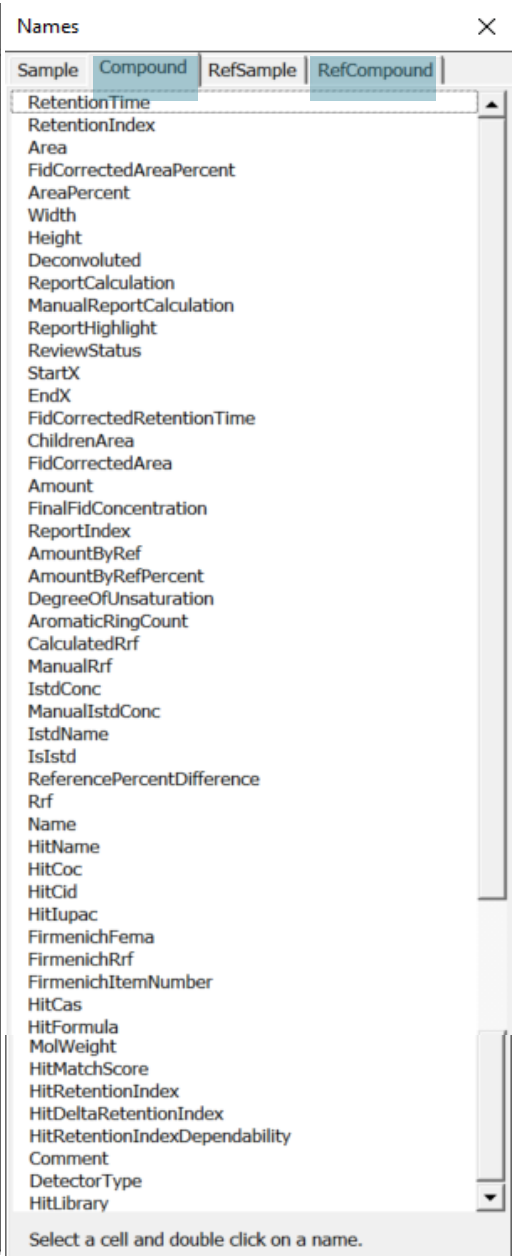
Top right corner of the report



Save new settings in a template

1) Select a cell in the report where you want to add a new field
2) Click on Name: a table with fields concerning the **sample**, the **reference sample** or **compounds found in the sample or in the reference** opens
3) Select the desired field by double clicking
4) Click on «Save as template» and give it a name
5) Re open the report by selecting the new Template





Report

Signal selection	MS
MS	n/a
FID	n/a

MS
FID

Select the signal you want to display

Time selection	BothLimit
LowerLimit	5
UpperLimit	25
BothLimit	n/a
Full	n/a
SetInChartAxisScale	n/a
Overlap	0.5

LowerLimit
UpperLimit
BothLimit
Full
SetInChartAxisScale

Scaling options for x axis

Label selection	ReportIndex
Any	n/a
Comment	format
Name	format
CAS	format
ReportIndex	format
RetentionIndex	format
RetentionTime	format

Any
Comment
Name
CAS
ReportIndex
RetentionIndex
RetentionTime

Chromatogram labelling options

Response Max selection	HighestPointAfter
HighestPointAfter	0
Fixed	800000
ChartNumber	2
ChartsIndividual	n/a
SetInChartAxisScale	n/a

HighestPointAfter
Fixed
ChartNumber
ChartsIndividual
SetInChartAxisScale

Response Min selection	SetInChartAxisScale
LowestPointAfter	0
Fixed	0
ChartNumber	2
ChartsIndividual	n/a
SetInChartAxisScale	n/a

LowestPointAfter
Fixed
ChartNumber
ChartsIndividual
SetInChartAxisScale

Scaling options for y axis

Reformat

Click on reformat to apply the new settings