

UnknownProcessor

By Leoson

niels@waleson.eu

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4. Data Reviewing

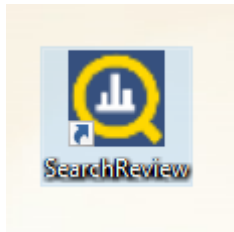
5. Quantitation

6. Report

01 Batch creation

Batch creation

- Open UnknownProcessor: the Select Batch window automatically opens



The screenshot shows the "Select Batch" dialog box in the UnknownProcessor software. The dialog has a menu bar with "Batch", "Report", "Method", "Tools", and "Help". The main area is titled "Select or create a Batch folder with data files". On the left, a file tree shows a folder named "Ken" containing numerous ".d" files, including "2019_04_08_testmixt.d" through "2019_06_17_testmixt.d" and "A46_190812_112636_NoBC_testmix_12.d" through "A46_191007_133413_TESTMIX.d". On the right, the "Folder" field is set to "Z:\test_mix_itg\Ken". Below that, a "Batch files" table is visible:

#	Batch	Data path	User	Comment	Saved	Samples	Peaks
1	MS_2020...	Z:\test_mi...			2021-01-...	0	0

At the bottom, the "Batch file name" field contains "Test_mix_MRSG". The "Create" button is highlighted in blue. A text box with three numbered steps is overlaid on the right side of the dialog:

- 1) Select the folder containing your data
- 2) Give a name to your batch
- 3) Click on Create

Arrows point from the text box to the "Ken" folder in the file tree, the "Batch file name" field, and the "Create" button.

Batch creation

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

#	File	Copy	T	B	Type	Level	TIC
85	A46_201005_141238_1_ESI MIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
86	A46_201012_180340_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Blank		<input checked="" type="checkbox"/>
87	A46_201013_172653_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
88	A46_201202_131410_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
89	A46_201203_154725_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
90	A46_201207_123018_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
91	A46_201214_110923_NoBC_Sample1		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
92	A46_201221_124732_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
93	A46_210104_183851_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
94	A46_210111_155922_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
95	A46_210118_120648_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
96	A46_210125_125042_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>
97	A46_210201_123528_TESTMIX		<input type="checkbox"/>	<input type="checkbox"/>	Sample		<input checked="" type="checkbox"/>

Actions: SearchLibrary (selected), ExtractSignals, FindPeaks, ExtractSpectra, SearchLibrary

Include FID: Integration: Deconvolution: Libraries enabled: 1

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

4) Libraries selection and creation

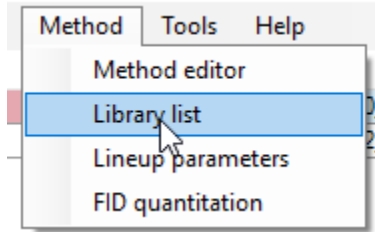
2) Select actions to process the data (all the actions above the selected one will be executed)

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



The screenshot shows the 'Library list' window with a table of libraries and a dropdown menu for 'RI NPolar'. The table has columns for '#', 'On', 'Edit', 'Priority', 'Type', 'Library', 'Match', 'Screening', 'RI NPolar', 'RI SPolar', 'RI Polar', and 'RI Delt'. Two rows are visible. The 'RI NPolar' dropdown menu is open, showing options: 'RetentionIndex', 'None', 'BoilingPoint', 'MeltingPoint', 'RetentionTime', 'RetentionIndex', and 'CompoundName'. The 'RetentionIndex' option is selected.

#	On	Edit	Priority	Type	Library	Match	Screening	RI NPolar	RI SPolar	RI Polar	RI Delt
1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0	DotL	C:\SHARED\Software\Agilent\MS LIB\NIST17-NP.L	50	Normal	Reten...	Reten...	Reten...	
2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	10	Xml	C:\CustomerHome\Library\Test\Mix.mslibrary.xml	50	Normal	Reten...	Reten...	Reten...	

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

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

Batch creation - Libraries selection/creation

The screenshot shows the 'Library list' window with two rows of library data. Below it, a configuration dialog is open, showing settings for a library. A text box on the left explains that the scrollbar on the right of the dialog is used to access other columns. An arrow points from a text box on the right to the 'Create library' button in the dialog.

#	On	Edit	Priority	Type	Library	Match	Screening	RI NPolar	RI SPolar	RI Polar	RI Delt
1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0	DotL	C:\SHARED\Software\Agilent\MS LIB\NIST17-NP.L	50	Normal	Reten...	Reten...	Reten...	
2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	10	Xml	C:\CustomerHome\Library\TestMix.mslibrary.xml	50	Normal	Reten...	Reten...	Reten...	

RI Delta	Q	Factor	Comment	MaxHits	Aromatic
10	<input checked="" type="checkbox"/>	1.000		10	None
0	<input type="checkbox"/>			10	None
10	<input type="checkbox"/>	1.000		10	None

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

Then click on Create Library

- 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

Batch creation

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

#	ator	Copy res...	Instrument	File	TIC	TRI	FID	FRI	T	Level	Info	UserDef	UserDef1	UserDef2	UserDef3	UserDef4	UserDef5	UserDef6
1			Ken	A46_200114_124031_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
2			Ken	A46_200203_114447_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
3			Ken	A46_200211_165043_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
4			Ken	A46_200217_163858_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
5			Ken	A46_200224_091225_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
6			Ken	A46_200224_105717_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
7			Ken	A46_200302_134505_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
8			Ken	A46_200309_104528_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
9			Ken	A46_200323_120153_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
10			Ken	A46_200330_142604_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
11			Ken	A46_200406_111728_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
12			Ken	A46_200414_120715_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									
13			Ken	A46_200420_103636_TESTMIX	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>									

Refresh Browse to copy samples ... Explore

Actions SearchLibrary Include FID Integration Deconvolution

OK Cancel Libraries enabled: 1

#	File	Signal extraction	Peak finder	Search spectra
1	A46_201207_123018_TESTMIX	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
2	A46_210201_123528_TESTMIX	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Performance Analyzing Cancel

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
			<input checked="" type="checkbox"/>		1	0	<input type="checkbox"/>	<input checked="" type="checkbox"/>	A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	686600			2
			<input checked="" type="checkbox"/>		2	1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	766885			2
			<input checked="" type="checkbox"/>		3	2	<input type="checkbox"/>	<input checked="" type="checkbox"/>	A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	561428			2



Review peak - A46_200918_213858_ALKANES - Sample 1 - 21.954

#	EntryID	Match	Compound	CAS	Company	Info	COC	CID	IUPAC	UserIndex	Report Status
1	75342	83	dodecane	112-40-3		112-40-3	10052760	00000327			<input type="radio"/> Exclude
2	75343	84	TRIDECAENE	629-50-5		629-50-5	10000160	00000332			<input type="radio"/> Report
3	65387	86	TETRADECAENE	629-59-4		629-59-4	10049629	00000333			<input type="radio"/> Highlight
4	75347	88	OCTADECANE	593-45-3		593-45-3	10059826	00000264			<input checked="" type="radio"/> Review status
5	75344	85	PENTADECANE	629-62-9		629-62-9	10072316	00019994	pentadec...		<input type="radio"/> Unknown
6	86289	88	2-methyldecane	0-00-0		0-00-0	10093710	00144021			<input type="radio"/> Tentative
7	75341	85	UNDECANE	1120-21-4		1120-21-4	10049376	00000160			<input type="radio"/> Approved
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...		

21.954
Fixed X scale
10 450

Accept
Accept for lineup
Delete peak

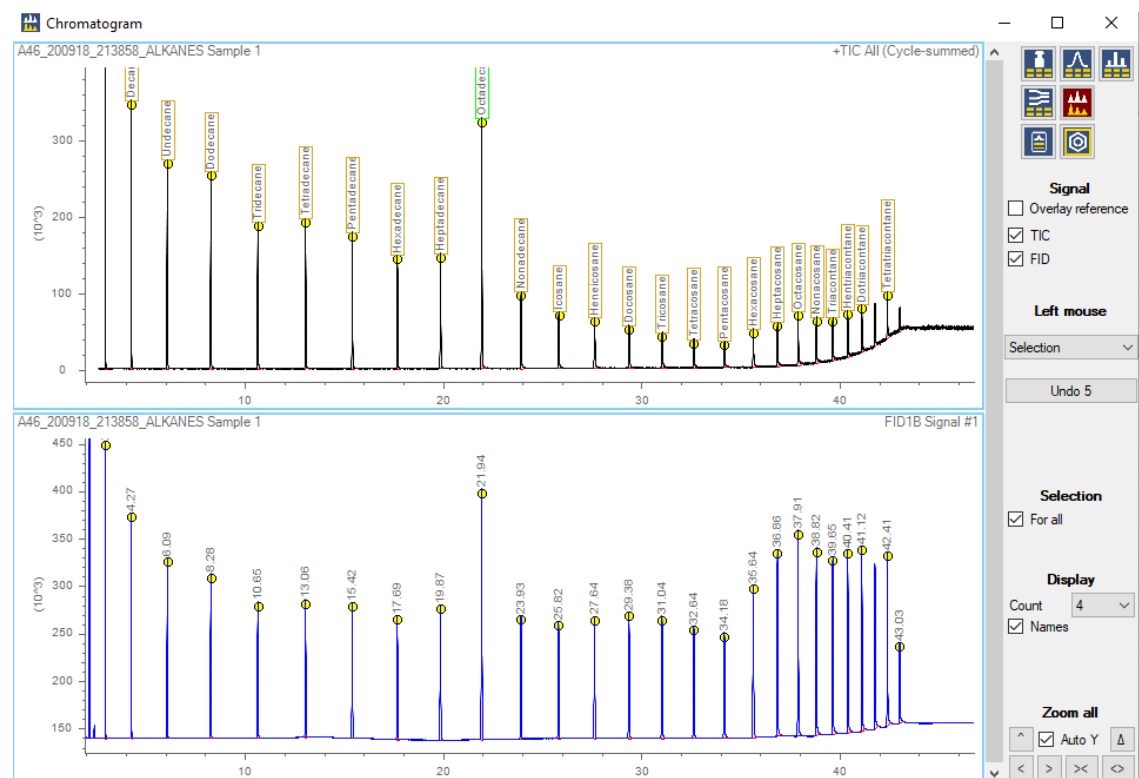
Peak
Prev Next

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		<input checked="" type="checkbox"/>		1	0		<input checked="" type="checkbox"/>	A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	686600			2
2	1		<input checked="" type="checkbox"/>		2	1		<input checked="" type="checkbox"/>	A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	766885			2
3	2		<input checked="" type="checkbox"/>		3	2		<input checked="" type="checkbox"/>	A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	561428			2



Chromatograms

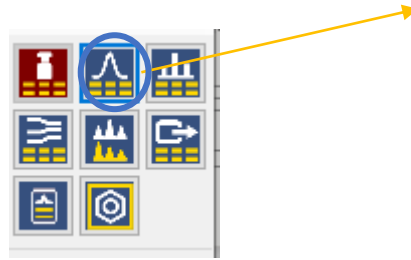
General view after Batch creation

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
			<input checked="" type="checkbox"/>		1	0		<input checked="" type="checkbox"/>	A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	686600			2
			<input checked="" type="checkbox"/>		2	1		<input checked="" type="checkbox"/>	A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	766885			2
			<input checked="" type="checkbox"/>		3	2		<input checked="" type="checkbox"/>	A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	561428			2

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			Nonane	10000171	00000324	111-84-2	C9H20	128.3	99	900							0		1	
2		Report	TIC	Tentat...	2.966	507120	0.016	482506																		0		1
3		Exclu...	FID	Tentat...	4.275	330553	0.022	236933																		0		1
4		Report	TIC	Tentat...	4.271	478987	0.021	350982			Decane	10001748	00000326	124-18-5	C10H22	142.3	98	1000							0		1	
5		Exclu...	FID	Tentat...	6.062	329496	0.027	180994																		0		1
6		Report	TIC	Tentat...	6.087	476200	0.027	272880			Undecane	10049376	00000160	1120-21-4	C11H24	156.3	97	1100							0		1	
7		Exclu...	FID	Tentat...	8.285	350271	0.032	172664																		0		1
8		Report	TIC	Tentat...	8.283	495923	0.029	256797			Dodecane	10052760	00000327	112-40-3	C12H26	170.3	96	1200							0		1	
9		Exclu...	FID	Tentat...	10.655	320369	0.035	143361																		0		1
10		Report	TIC	Tentat...	10.654	415808	0.033	191096			Tridecane	10000160	00000332	629-50-5	C13H28	184.4	93	1300							0		1	
11		Exclu...	FID	Tentat...	13.062	345894	0.037	144813																		0		1
12		Report	TIC	Tentat...	13.064	421506	0.033	195670			Tetradecane	10049629	00000333	629-59-4	C14H30	198.4	93	1400							0		1	
13		Exclu...	FID	Tentat...	15.418	385174	0.039	142935																		0		1
14		Report	TIC	Tentat...	15.420	411455	0.035	173954			Pentadecane	10072316	00019954	629-62-9	C15H32	212.4	91	1500							0		1	
15		Exclu...	FID	Tentat...	17.692	338596	0.041	130942																		0		1
16		Report	TIC	Tentat...	17.694	356635	0.036	148406			Hexadecane	10072339	00000334	544-76-3	C16H34	226.4	90	1600							0		1	
17		Exclu...	FID	Tentat...	19.868	382668	0.042	142400																		0		1
18		Report	TIC	Tentat...	19.870	370568	0.038	150254			Heptadecane	10052760	00000327	629-78-7	C17H36	170.3	90	1200							0		1	
19		Exclu...	FID	Tentat...	21.945	686600	0.040	264020																		0		1
20		Report	TIC	Tentat...	21.954	805562	0.037	326849			Octadecane	10059826	00000264	593-45-3	C18H38	254.5	88	1800							0		1	
21		Exclu...	FID	Tentat...	23.928	349478	0.042	129755																		0		1
22		Report	TIC	Tentat...	23.936	272844	0.040	100505			Nonadecane	10072202	00000265	629-92-5	C19H40	268.5	87	1900							0		1	
23		Exclu...	FID	Tentat...	25.625	344703	0.043	123465																		0		1
24		Report	TIC	Tentat...	25.634	222960	0.044	74090			Icosane	10024872	00076397	112-95-8	C19H40	282.2	90	1338							0		1	
25		Exclu...	FID	Tentat...	27.638	361566	0.044	128548																		0		1
26		Report	TIC	Tentat...	27.650	205067	0.045	65742			Heneicosane	10049629	00000333	629-94-7	C14H30	198.4	90	1400							0		1	
27		Exclu...	FID	Tentat...	29.378	378923	0.045	133010																		0		1
28		Report	TIC	Tentat...	29.379	192403	0.048	56484			Docosane	10049629	00000333	629-97-0	C14H30	198.4	90	1400							0		1	
29		Exclu...	FID	Tentat...	31.045	372773	0.045	128774																		0		1
30		Report	TIC	Tentat...	31.049	164445	0.049	46285			Tricosane	10024872	00076397	638-67-5	C11H23i	282.2	89	1338							0		1	
31		Exclu...	FID	Tentat...	32.645	358817	0.047	117641																		0		1
32		Report	TIC	Tentat...	32.646	127268	0.050	37079			Tetracosane	10024872	00076397	646-31-1	C11H23i	282.2	89	1338							0		1	
33		Exclu...	FID	Tentat...	34.185	353590	0.048	111310																		0		1
34		Report	TIC	Tentat...	34.194	109776	0.047	32960			Pentacosane	10024872	00076397	629-99-2	C11H23i	282.2	89	1338							0		1	
35		Exclu...	FID	Tentat...	35.645	476725	0.045	160692																		0		1
36		Report	TIC	Tentat...	35.650	144757	0.044	49196			Hexacosane	10049629	00000333	630-01-3	C14H30	198.4	88	1400							0		1	
37		Exclu...	FID	Tentat...	36.862	498463	0.039	196223																		0		1
38		Report	TIC	Tentat...	36.862	172961	0.042	57956			Heptacosane	10049629	00000333	693-49-7	C14H30	198.4	90	1400							0		1	
39		Exclu...	FID	Tentat...	37.908	523971	0.036	216093																		0		1
40		Report	TIC	Tentat...	37.909	194118	0.038	70412			Octacosane	10049629	00000333	630-02-4	C14H30	198.4	87	1400							0		1	
41		Exclu...	FID	Tentat...	38.825	456611	0.034	197137																		0		1
42		Report	TIC	Tentat...	38.826	151719	0.035	59764			Nonacosane	10024872	00076397	630-03-5	C11H23i	282.2	89	1338							0		1	
43		Exclu...	FID	Tentat...	39.652	420078	0.033	186607																		0		1
44		Report	TIC	Tentat...	39.652	131002	0.033	56042			triacontane	10024872	00076397	638-68-6	C11H23i	282.2	85	1338							0		1	
45		Exclu...	FID	Tentat...	40.412	409972	0.031	193237																		0		1
46		Report	TIC	Tentat...	40.411	130211	0.030	60095			hentriacontane	10024872	00076397	630-04-6	C11H23i	282.2	85	1338							0		1	
47		Exclu...	FID	Tentat...	41.122	430265	0.032	194000																		0		1
48		Report	TIC	Tentat...	41.122	138850	0.032	61129			dotriacontane	10024872	00076397	544-85-4	C11H23i	282.2	80	1338							0		1	
49		Exclu...	FID	Tentat...	41.782	380467	0.032	172736																		0		1
50		Report	TIC	Tentat...	41.779	121878	0.032	54324			tritriacontane	10024872	00076397	630-05-7	C11H23i	282.2	82	1338							0		1	
51		Exclu...	FID	Tentat...	42.408	397238	0.032	182239																		0		1
52		Report	TIC	Tentat...	42.407	138947	0.032	60076			tetracontane	10024872	00076397	14167-59	C11H23i	282.2	77	1338							0		1	
53		Exclu...	FID	Tentat...	43.032	208643	0.036	84362																		0		1
54		Report	TIC	Tentat...	43.030	75729	0.034	30170			pentatriacontane	10075052	00007572	630-07-9	C12H26O2	202.3	60	1515							0		1	



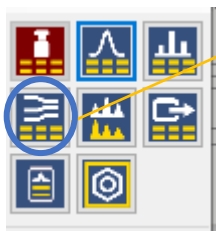
Compound list of selected sample

General view after Batch creation

Batch	Report	Method	Tools	Help	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	<input type="checkbox"/>	<input checked="" type="checkbox"/>		A46_200918_213858_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							32	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	686600			2
2	1	<input type="checkbox"/>	<input checked="" type="checkbox"/>		A46_200912_002505_ALKANES	Ken	Sample 1		2020-09-...	Sample		1.0000							34	27	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	766885			2
3	2	<input type="checkbox"/>	<input checked="" type="checkbox"/>		A46_210105_123640_NoBC_Sample1	Ken	Sample 1		2021-01-...	Blank		1.0000							30	26	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	NonP...	561428			2

#	Lineup	RT	NP	Area sum	Area max	Count	Compound	CAS	CID	COC	Formula	MW	Curve	A46_200106_132733_TESTMX	A46_200113_111523_TESTMX	A46_200127_140844_TESTMX
11	10	11.030	135809	67904	4	2-Methyl-5-(hexyn-1-yl)pyridine	200327-18-5				C12H15N	173.3		1.000 93 FID-MS	1.000 94 FID-MS	1.000 93 FID-MS
12	11	15.409	7570917	1271523	6	1-Pent-3-ynylcyclopenta-1,3-diene	5471-51-2	00079099	10000711		C10H12O2	164.2		1499 15.412 1127121 94 FID-MS	1499 15.418 1408895 94 FID-MS	1499 15.398 1238138 94 FID-MS
13	12	31.187	2345889	446198	6	1-Pent-3-ynylcyclopenta-1,3-diene	2000190-19-5				C10H12	132.2		2308 31.197 119302 53 FID-MS	2308 31.189 82094 FID-MS	2308 31.176 189718 53 FID-MS
14	13	43.773			1											3618 43.773 258711 MS
15	14	5.754	2009555	516740	4	Nonanal	124-19-6				C9H18O	142.2		1081 5.755 526202 77 FID-MS	1081 5.754 309255 80 FID-MS	1081 5.754 309255 80 FID-MS
16	15	3.386	6924716	1170370	6	PINENE ALPHA	7785-26-4	00000194	10000080		C10H16	136.2		933 3.389 1796023 96 FID-MS	932 3.388 2107391 96 FID-MS	932 3.381 2124762 96 FID-MS
17	16	4.279	6479627	1096627	6	DECANE	124-18-5	00000326	10001748		C10H22	142.3		1001 4.283 1429605 98 FID-MS	1000 4.281 1877987 99 FID-MS	1000 4.273 1503022 99 FID-MS
18	17	5.182	9907784	1668857	6	ALCOHOL C 8	111-87-5	00061947	10003689		C8H18O	130.2		1050 5.186 1707428 99 FID-MS	1050 5.186 2083317 99 FID-MS	1050 5.175 2025912 99 FID-MS
19	18	5.696	4758985	800807	6	LINALOL	576-26-1	00084052	10006912		C8H10O	122.2		1078 5.700 1035440 96 FID-MS	1078 5.700 1336263 96 FID-MS	1078 5.688 1297548 96 FID-MS
20	19	5.782	6700604	1130185	6	LINALOL	126-91-0	00085345	10065496		C10H18O	154.2		1083 5.786 1628021 91 FID-MS	1083 5.786 1879670 91 FID-MS	1083 5.774 2815341 86 FID-MS
21	20	6.833	5497294	930240	6	2,6-DIMETHYLANILINE	87-62-7	00057312	10070232		C8H11N	121.2		1134 6.838 1449313 96 FID-MS	1134 6.837 1776138 97 FID-MS	1133 6.824 1774472 97 FID-MS
22	21	8.297	8305466	1395356	6	dodecane	112-40-3	00000327	10052760		C12H26	170.3		1200 8.303 1898874 97 FID-MS	1200 8.299 2309524 97 FID-MS	1200 8.288 2335311 97 FID-MS
23	22	8.772	143700	71850	2	PENTYLENDOL (+)-	174618-07-6	00013507	10009260		C10H18O	154.2				1220 8.772 82388 83 FID-MS
24	23	9.070	10683324	1791922	6	GERANIOL	106-24-1	00001499	10006150		C10H18O	154.2		1233 9.076 1728437 88 FID-MS	1233 9.075 2103537 88 FID-MS	1233 9.061 2020378 87 FID-MS
25	24	12.096	7779159	1308353	6	GERANYL ACETATE	105-87-3	00053069	10059800		C12H20O2	196.3		1360 12.101 1586233 91 FID-MS	1360 12.101 1820071 91 FID-MS	1359 12.085 1628983 91 FID-MS
26	25	13.075	9675877	1627273	6	TETRADECANE	629-59-4	00000333	10049629		C14H30	198.4		1400 13.082 2406894 95 FID-MS	1400 13.079 2886138 96 FID-MS	1400 13.065 2884227 95 FID-MS
27	26	16.821	2086985	359704	6	(-)-2-methyl-3-[(2-pentyl-2-cyclopenten-1-yl)oxy]propanal	0-00-0	00148270	10125321		C14H24O2	224.3		1561 16.826 361135 85 FID-MS	1561 16.825 873501 87 FID-MS	1561 16.810 319107 87 FID-MS
														1867 23.283 125505 FID-MS	1867 23.283 125549 FID-MS	1867 23.268 173291 FID-MS

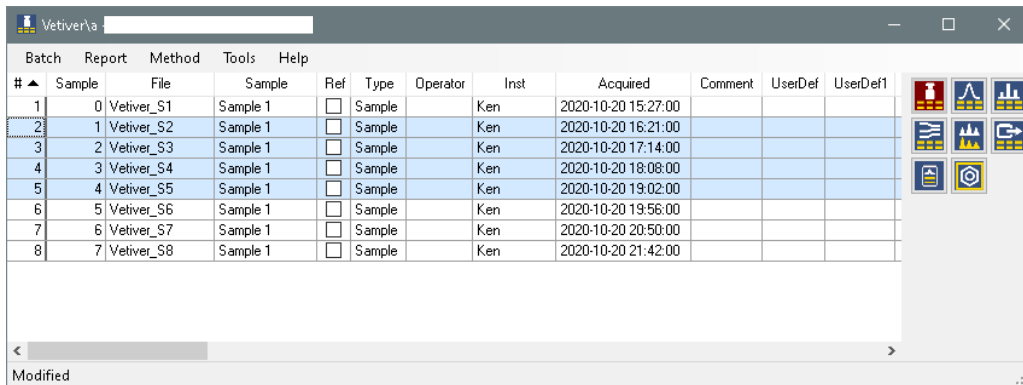
Lineup



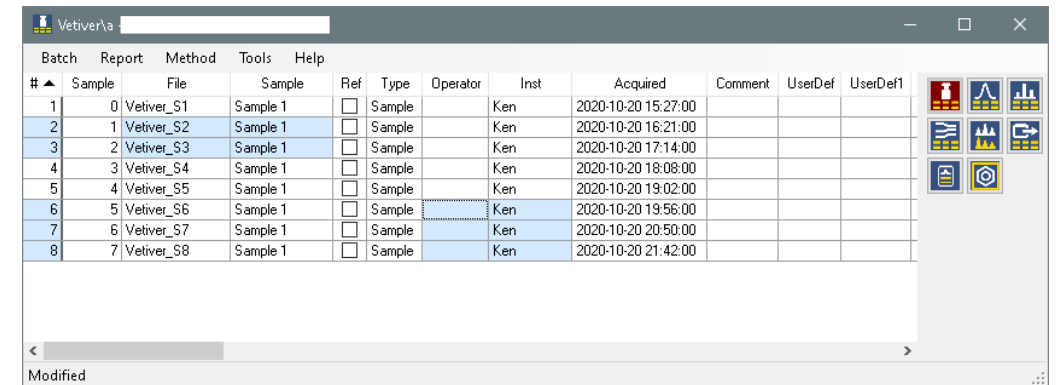
User Interface, tables: selecting and moving rows

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 **cursor 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



#	Sample	File	Sample	Ref	Type	Operator	Inst	Acquired	Comment	UserDef	UserDef1
1	0	Vetiver_S1	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 15:27:00			
2	1	Vetiver_S2	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 16:21:00			
3	2	Vetiver_S3	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 17:14:00			
4	3	Vetiver_S4	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 18:08:00			
5	4	Vetiver_S5	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 19:02:00			
6	5	Vetiver_S6	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 19:56:00			
7	6	Vetiver_S7	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 20:50:00			
8	7	Vetiver_S8	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 21:42:00			

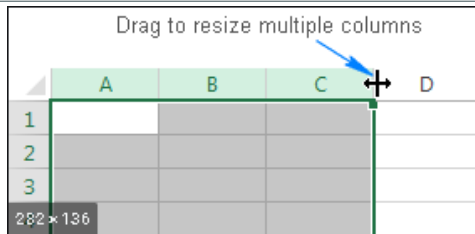


#	Sample	File	Sample	Ref	Type	Operator	Inst	Acquired	Comment	UserDef	UserDef1
1	0	Vetiver_S1	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 15:27:00			
2	1	Vetiver_S2	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 16:21:00			
3	2	Vetiver_S3	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 17:14:00			
4	3	Vetiver_S4	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 18:08:00			
5	4	Vetiver_S5	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 19:02:00			
6	5	Vetiver_S6	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 19:56:00			
7	6	Vetiver_S7	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 20:50:00			
8	7	Vetiver_S8	Sample 1	<input type="checkbox"/>	Sample		Ken	2020-10-20 21:42:00			

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**

#	Sample	File	Sample	Ref	Type	Operator	Inst	Comment	UserDef	UserDef1	U
1	0	Vetiver_S1	File name	<input type="checkbox"/>	Sample		Ken				
2	1	Vetiver_S2	Sample 1	<input type="checkbox"/>	Sample		Ken				
3	2	Vetiver_S3	Sample 1	<input type="checkbox"/>	Sample		Ken				
4	3	Vetiver_S4	Sample 1	<input type="checkbox"/>	Sample		Ken				
5	4	Vetiver_S5	Sample 1	<input type="checkbox"/>	Sample		Ken				
6	5	Vetiver_S6	Sample 1	<input type="checkbox"/>	Sample		Ken				
7	6	Vetiver_S7	Sample 1	<input type="checkbox"/>	Sample		Ken				
8	7	Vetiver_S8	Sample 1	<input type="checkbox"/>	Sample		Ken				



- 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	Corr
1	0	Vetiver_S1	Sampl					20-10-20 15:27:00	A
2	1	Vetiver_S2	Sampl					20-10-20 16:21:00	A
3	2	Vetiver_S3	Sampl					20-10-20 17:14:00	A
4	3	Vetiver_S4	Sampl					20-10-20 18:08:00	C
5	4	Vetiver_S5	Sampl					20-10-20 19:02:00	C
6	5	Vetiver_S6	Sampl					20-10-20 19:56:00	D
7	6	Vetiver_S7	Sampl					20-10-20 20:50:00	D
8	7	Vetiver_S8	Sampl					20-10-20 21:42:00	D

Sort
Auto width all columns
Freeze column
Show/Hide columns
Show all columns
Hide

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**

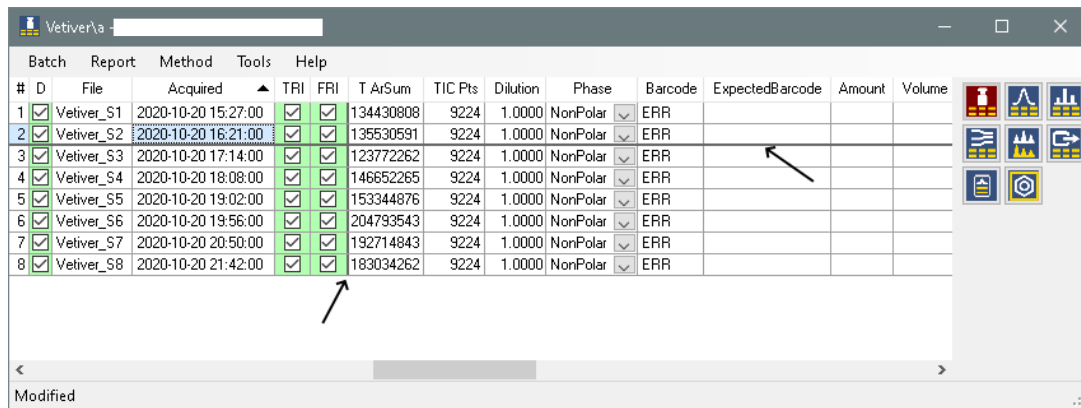
- Right click on a column header to show the column menu
- Show/Hide columns to open a column editor
- Show/Hide columns dialog
- Use the Find text box to search
- Move multiple rows up and down

#	Sample	File	Sample	Ref	Type	Operator	Inst	Acquired	Comment	UserDef	UserDef1	UserDef2
1	0	Vetiver_S1	Sample 1	<input type="checkbox"/>	Sample			2020-10-20 13:27:00	A			
2	1	Vetiver_S2	Sample 1	<input type="checkbox"/>	Sample	Ken		2020-10-20 16:21:00	A			
3	2	Vetiver_S3	Sample 1	<input type="checkbox"/>	Sample	Ken		2020-10-20 17:14:00	A			
4	3	Vetiver_S4	Sample 1	<input type="checkbox"/>	Sample	Ken		2020-10-20 18:08:00	C			
5	4	Vetiver_S5	Sample 1	<input type="checkbox"/>	Sample	Ken		2020-10-20 19:02:00	C			
6	5	Vetiver_S6	Sample 1	<input type="checkbox"/>	Sample	Ken		2020-10-20 19:56:00	D			
7	6	Vetiver_S7	Sample 1	<input type="checkbox"/>	Sample	Ken		2020-10-20 20:50:00	D			
8	7	Vetiver_S8	Sample 1	<input type="checkbox"/>	Sample	Ken		2020-10-20 21:42:00	D			

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

Tables, freeze columns, rows and body menu

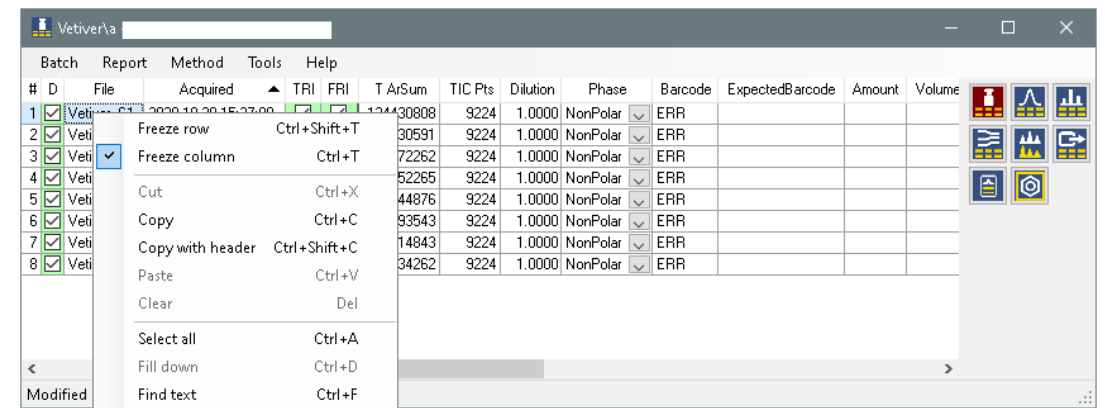
- Right click column and toggle **Freeze**
- Here 5 important columns are frozen add the left side of the table
- And 2 important rows are frozen ad the top of the table
- Frozen column and row count are stored in the user profile



The screenshot shows a data table with 15 columns. The first five columns (D, File, Acquired, TRI, FRI) are frozen, indicated by a vertical line and a grey background. The first two rows (1 and 2) are also frozen, indicated by a horizontal line and a grey background. Arrows point to the frozen columns and rows.

#	D	File	Acquired	TRI	FRI	T ArSum	TIC Pts	Dilution	Phase	Barcode	ExpectedBarcode	Amount	Volume
1	✓	Vetiver_S1	2020-10-20 15:27:00	✓	✓	134430808	9224	1.0000	NonPolar	ERR			
2	✓	Vetiver_S2	2020-10-20 16:21:00	✓	✓	135530591	9224	1.0000	NonPolar	ERR			
3	✓	Vetiver_S3	2020-10-20 17:14:00	✓	✓	123772262	9224	1.0000	NonPolar	ERR			
4	✓	Vetiver_S4	2020-10-20 18:08:00	✓	✓	146652265	9224	1.0000	NonPolar	ERR			
5	✓	Vetiver_S5	2020-10-20 19:02:00	✓	✓	153344876	9224	1.0000	NonPolar	ERR			
6	✓	Vetiver_S6	2020-10-20 19:56:00	✓	✓	204793543	9224	1.0000	NonPolar	ERR			
7	✓	Vetiver_S7	2020-10-20 20:50:00	✓	✓	192714843	9224	1.0000	NonPolar	ERR			
8	✓	Vetiver_S8	2020-10-20 21:42:00	✓	✓	183034262	9224	1.0000	NonPolar	ERR			

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



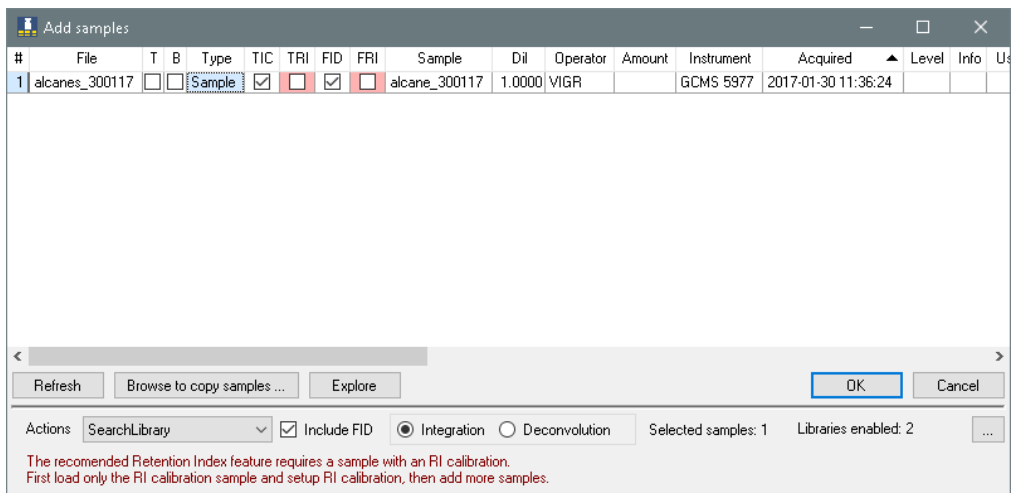
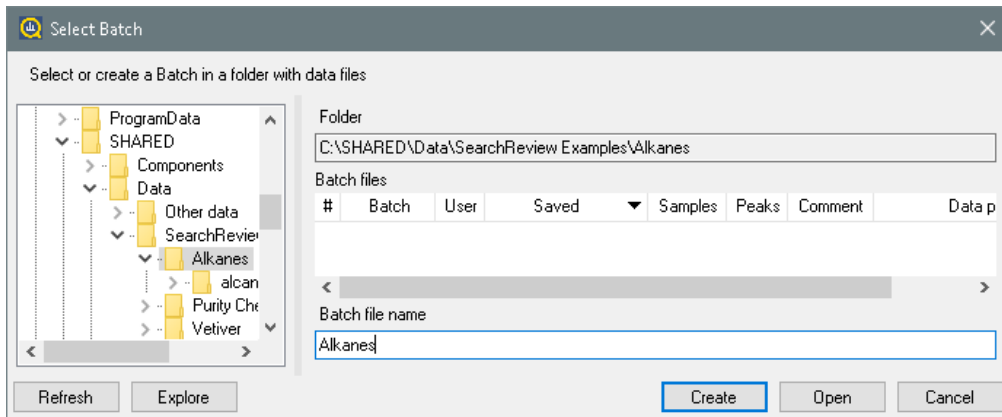
The screenshot shows the same data table with a context menu open over a cell. The menu includes options like 'Freeze row', 'Freeze column', 'Copy with header', 'Fill down', and 'Find text'. Keyboard shortcuts are listed next to each option.

#	D	File	Acquired	TRI	FRI	T ArSum	TIC Pts	Dilution	Phase	Barcode	ExpectedBarcode	Amount	Volume
1	✓	Vetiver_S1	2020-10-20 15:27:00	✓	✓	134430808	9224	1.0000	NonPolar	ERR			
2	✓	Vetiver_S2	2020-10-20 16:21:00	✓	✓	135530591	9224	1.0000	NonPolar	ERR			
3	✓	Vetiver_S3	2020-10-20 17:14:00	✓	✓	123772262	9224	1.0000	NonPolar	ERR			
4	✓	Vetiver_S4	2020-10-20 18:08:00	✓	✓	146652265	9224	1.0000	NonPolar	ERR			
5	✓	Vetiver_S5	2020-10-20 19:02:00	✓	✓	153344876	9224	1.0000	NonPolar	ERR			
6	✓	Vetiver_S6	2020-10-20 19:56:00	✓	✓	204793543	9224	1.0000	NonPolar	ERR			
7	✓	Vetiver_S7	2020-10-20 20:50:00	✓	✓	192714843	9224	1.0000	NonPolar	ERR			
8	✓	Vetiver_S8	2020-10-20 21:42:00	✓	✓	183034262	9224	1.0000	NonPolar	ERR			

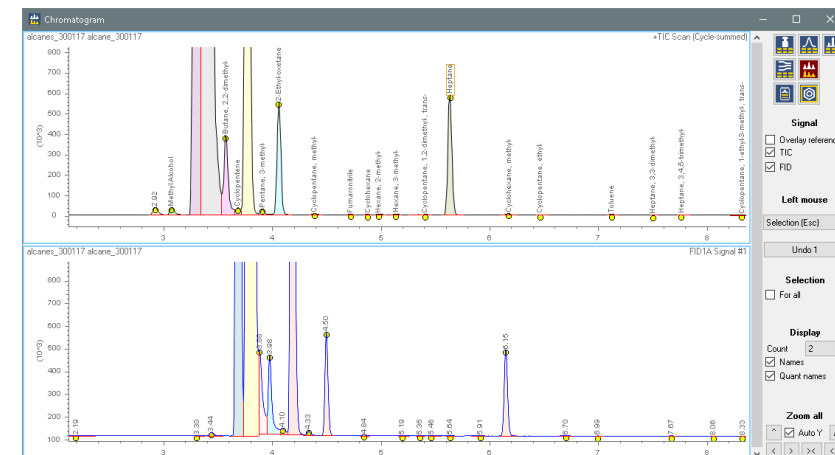
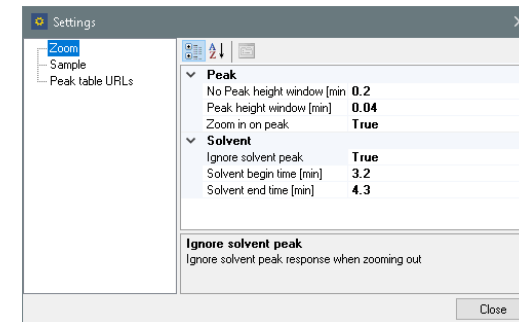
03 Alkanes processing

RI calibration setup

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

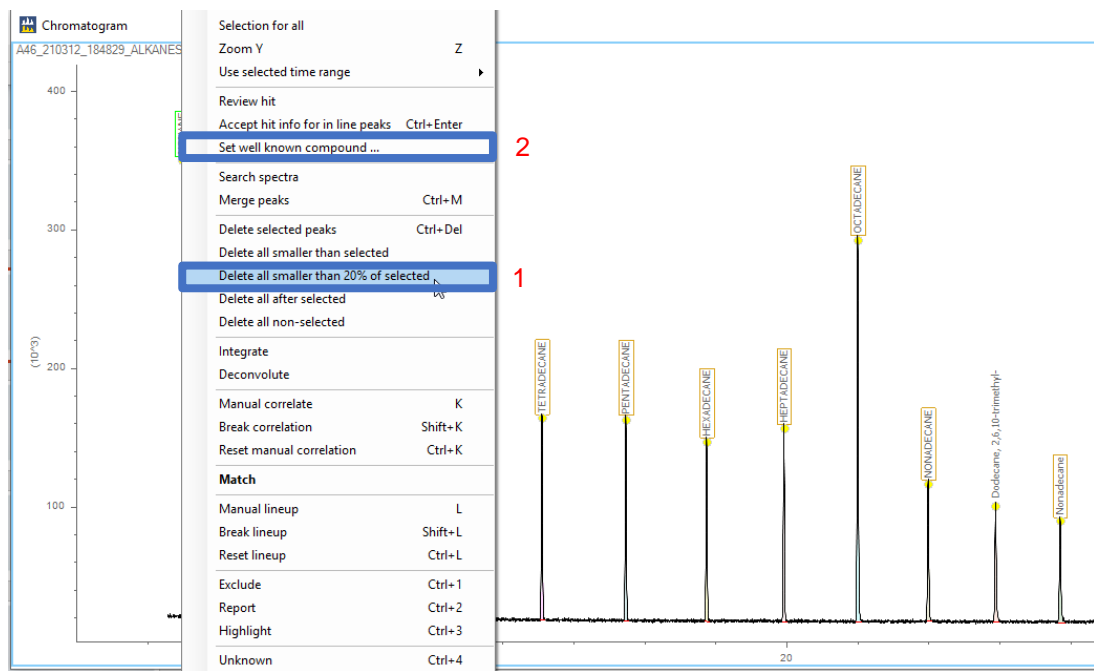


- Tools – Settings
- Zoom, ignore solvent
- In the chromatogram window, Zoom FID and TIC to show n-Hexane



RI calibration setup

- 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

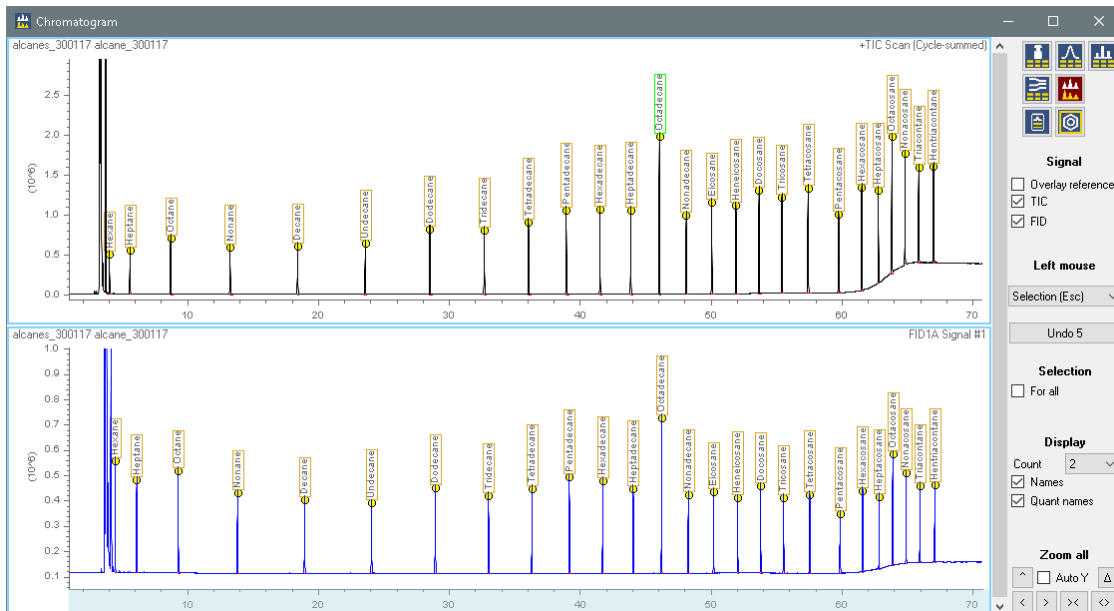
#	On	Name	CAS	RI	Formula	MW	Comment
1	<input checked="" type="checkbox"/>	Methane	74-82-8	100	CH4	16.0	
2	<input checked="" type="checkbox"/>	Ethane	74-84-0	200	C2H6	30.1	
3	<input checked="" type="checkbox"/>	Propane	74-98-6	300	C3H8	44.1	
4	<input checked="" type="checkbox"/>	Butane	106-97-8	400	C4H10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

Successive threshold %: 20

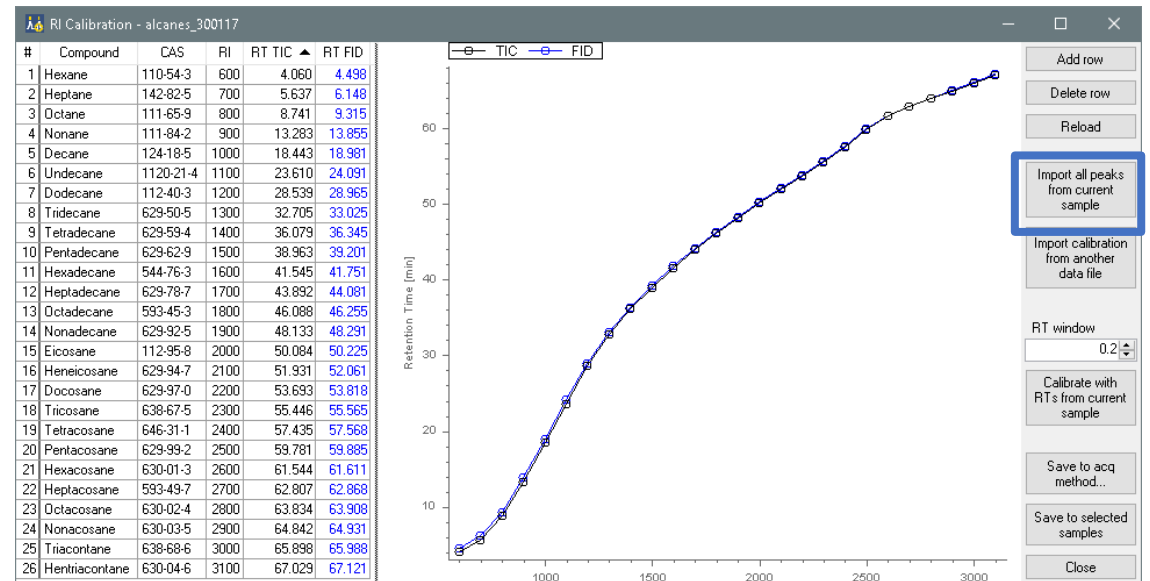
Buttons: Set series, Set current, Cancel

RI calibration setup

- All n-Alkanes are labeled

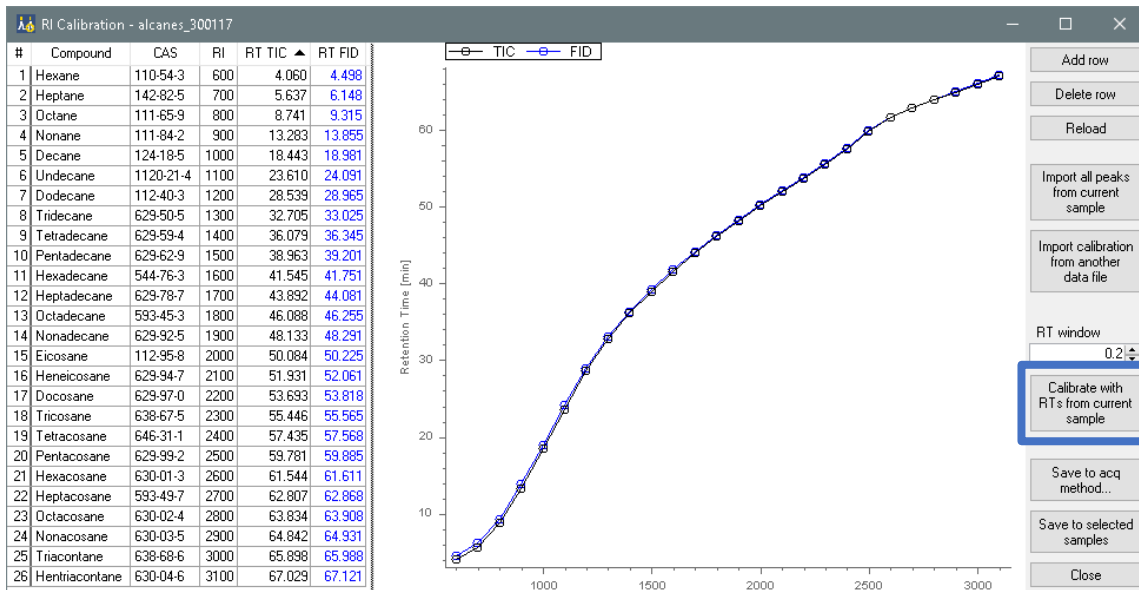


- Tools – RI Calibration
- Select all rows and press Delete row button
- Import All peaks from current sample, and Save to selected samples

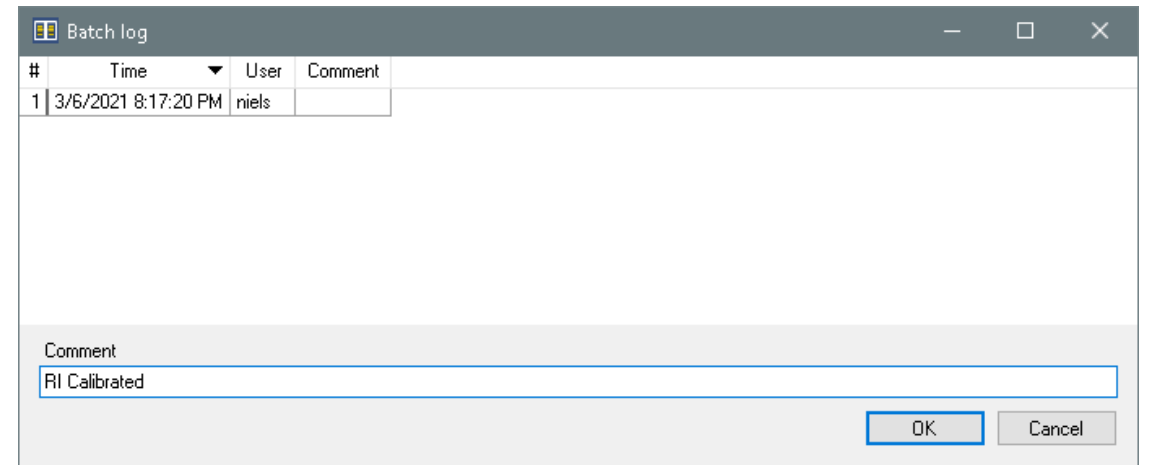


RI calibration setup

- 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



- Save batch
- Enter meaningful text to the logbook



04 Data Reviewing

Data Reviewing – Main Window (samples)

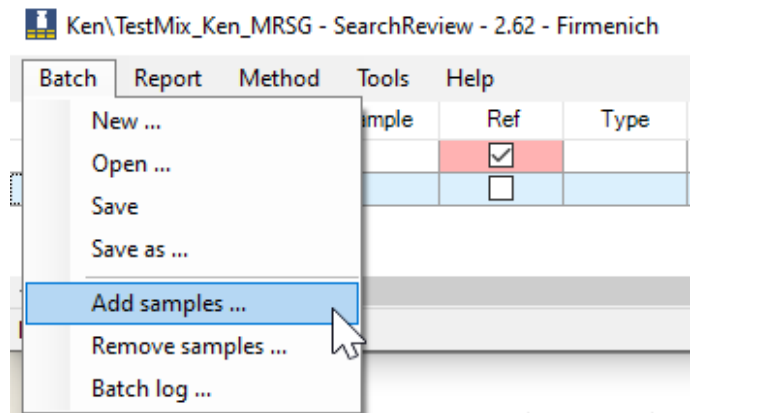


This module allows you to navigate between the samples

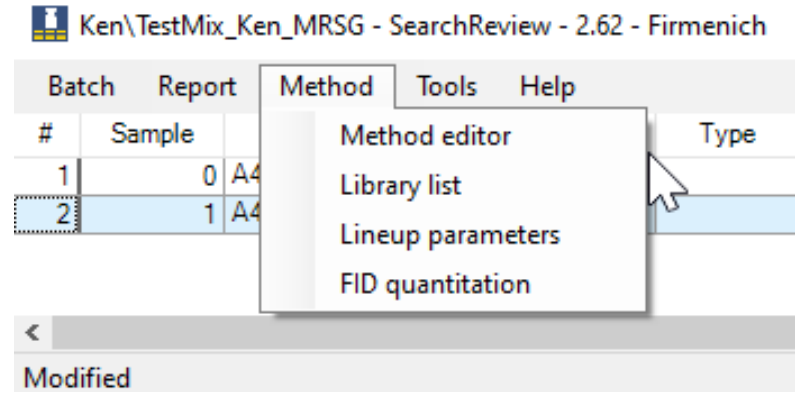
Batch	Report	Method	Tools	Help	#	Sample	File	Sample	Ref	Type	Level	Operator	Inst	Acquired	Comment	Info	UserDef	UserDef1	UserDef2	UserDef3	UserDef4	UserDef5	UserDef6	UserDef7	UserDef8	UserDef9	Barcode	Expected...	D	Amount	Volume	Dilution	RefAmor	
1		0	A46_201...						<input checked="" type="checkbox"/>					2020-12-...																<input checked="" type="checkbox"/>				
2		1	A46_210...						<input type="checkbox"/>					2021-02-...																<input checked="" type="checkbox"/>				

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

- Freeze column
- Hide
- Show all columns
- Show/Hide columns
- Sort**
- Auto width all columns

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	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	

Fields related to internal standard: possibility to quantitate

Peaks - A46_201207_123018_TESTMIX -

#	IRRF	IConc	mIConc	ISTD	IsI
1					<input type="checkbox"/>
2					<input type="checkbox"/>
3					<input type="checkbox"/>
4					<input type="checkbox"/>
5					<input type="checkbox"/>
6					<input type="checkbox"/>
7					<input type="checkbox"/>
8					<input type="checkbox"/>
9					<input type="checkbox"/>
10					<input type="checkbox"/>
11					<input type="checkbox"/>

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

Data Reviewing – Peaks Window



Peaks - A46_201207_123018_TESTMIX -

#	Rel	Chrom	RT
8		TIC	3.405
9		FID	3.412
10		TIC	3.580
11		FID	3.585

Freeze row Ctrl+Shift+T

Freeze column Ctrl+T

Cut Ctrl+X

Copy Ctrl+C

Copy with header Ctrl+Shift+C

Paste Ctrl+V

Clear Del

Select all Ctrl+A

Fill down Ctrl+D

Find text Ctrl+F

Search spectra

Review hit

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

Manual correlate K

Break correlation Shift+K

Reset manual correlation Ctrl+K

Add (approved and selected) to library ▶

Exclude Ctrl+1

Report Ctrl+2

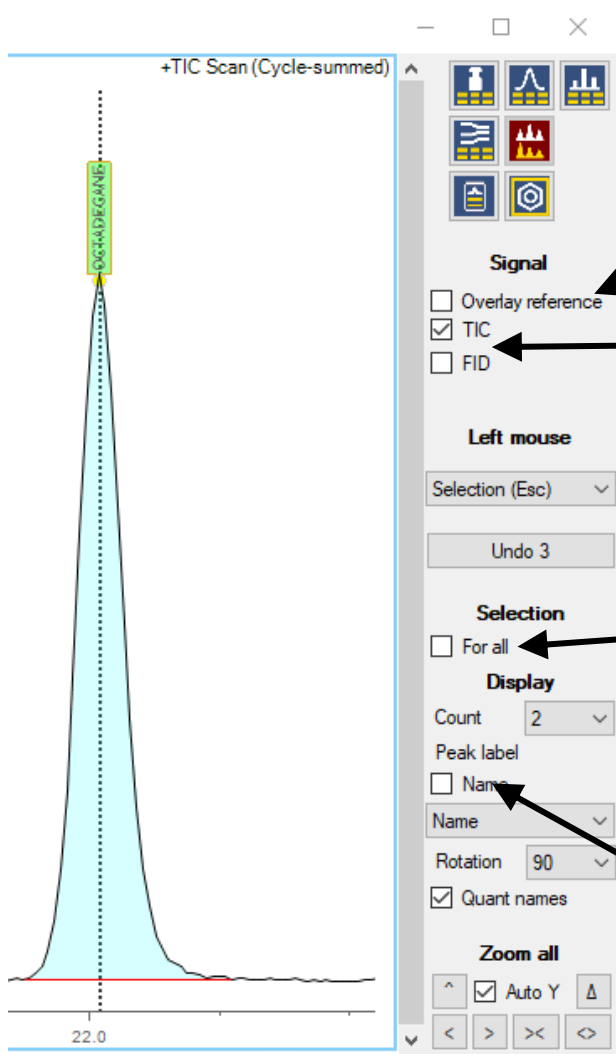
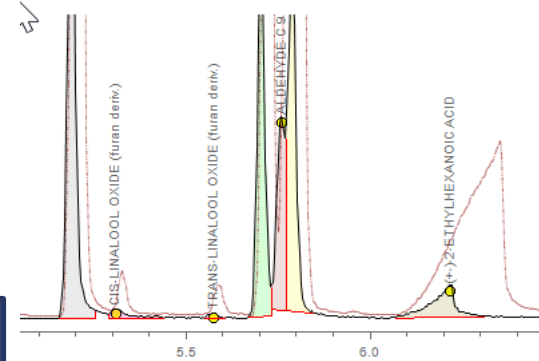
Highlight Ctrl+3

Unknown Ctrl+4

Tentative Ctrl+5

Approved Ctrl+6

Data Reviewing - Chromatogram



Signal

Overlay reference

TIC

FID

Left mouse

Selection (Esc) ▾

Undo 3

Selection

For all

Display

Count 2 ▾

Peak label

Name

Name ▾

Rotation 90 ▾

Quant names

Zoom all

Auto Y

⏪ ⏩ ⏴ ⏵

Add ref spectrum in dotted lines on other samples

Select TIC and/or FID

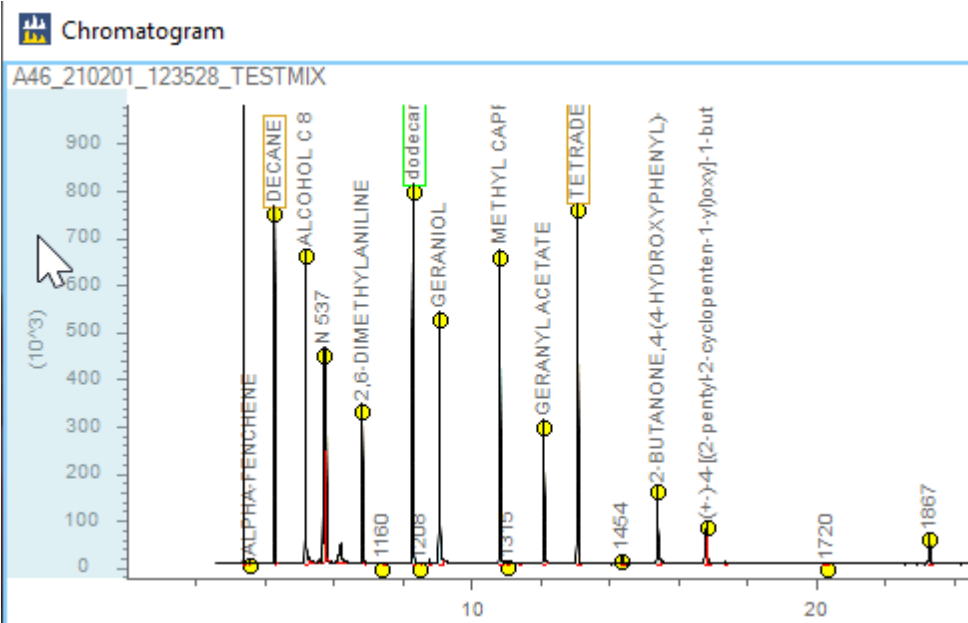
Undo until 5 last actions

Apply the selected action on all spectra

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

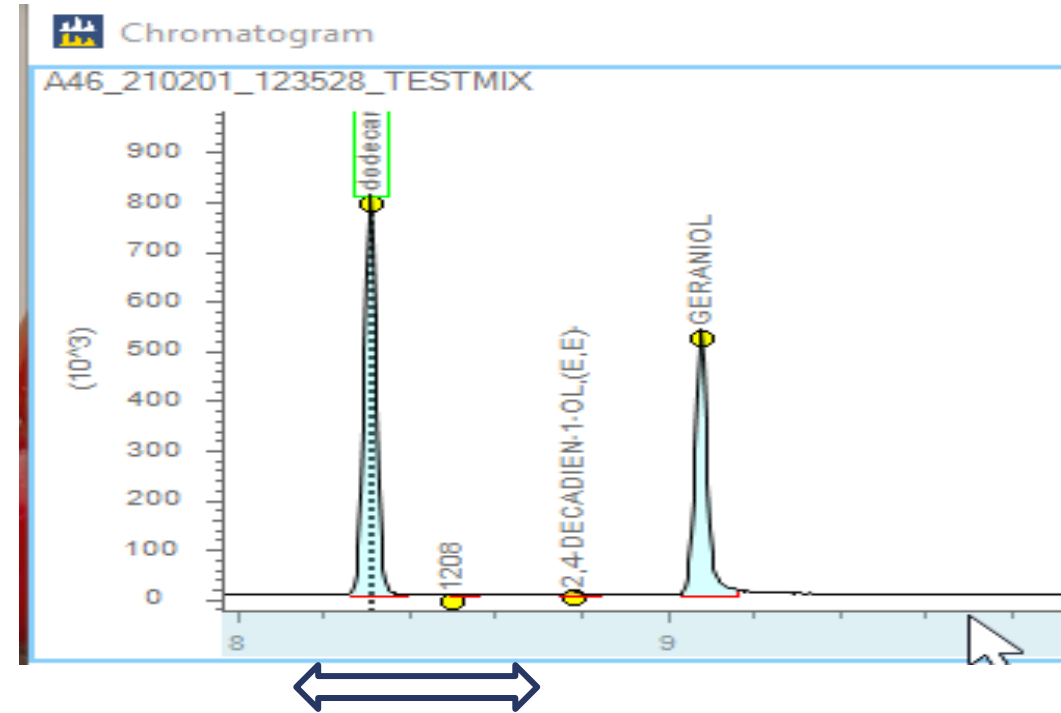
Add compound names above peaks

Data Reviewing - Chromatogram



Zoom in by right click-and-drag

Zoom out by right double click



Zoom all

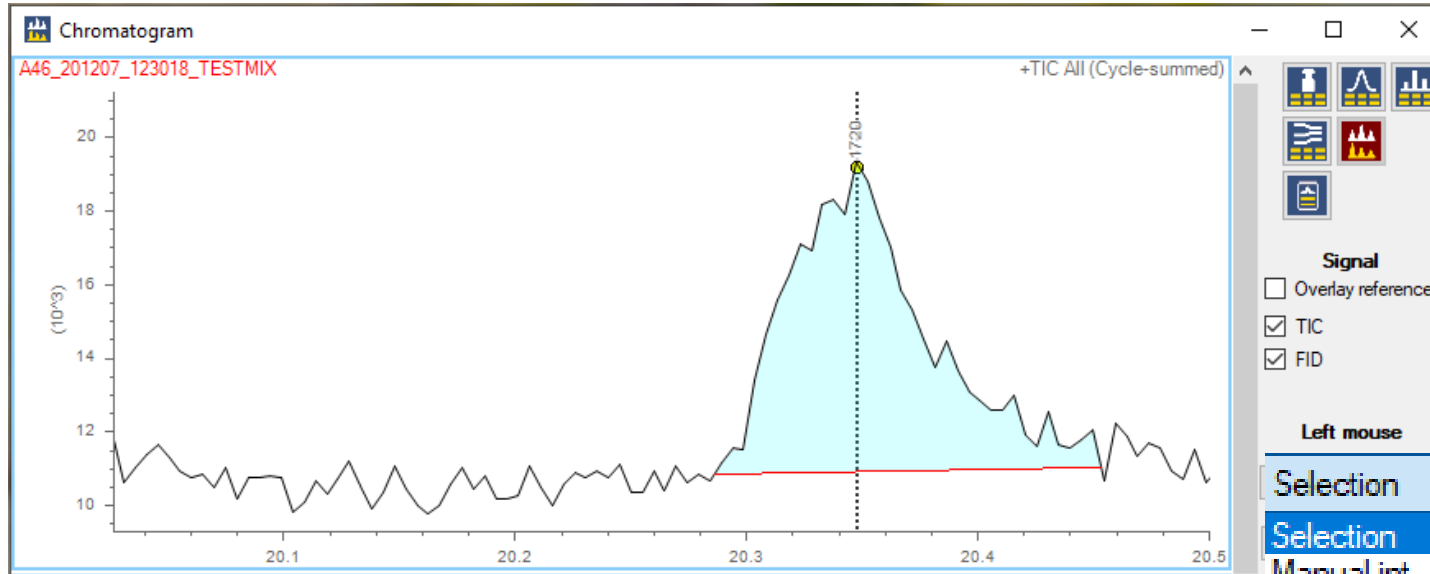
Auto Y

< > >> <<

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

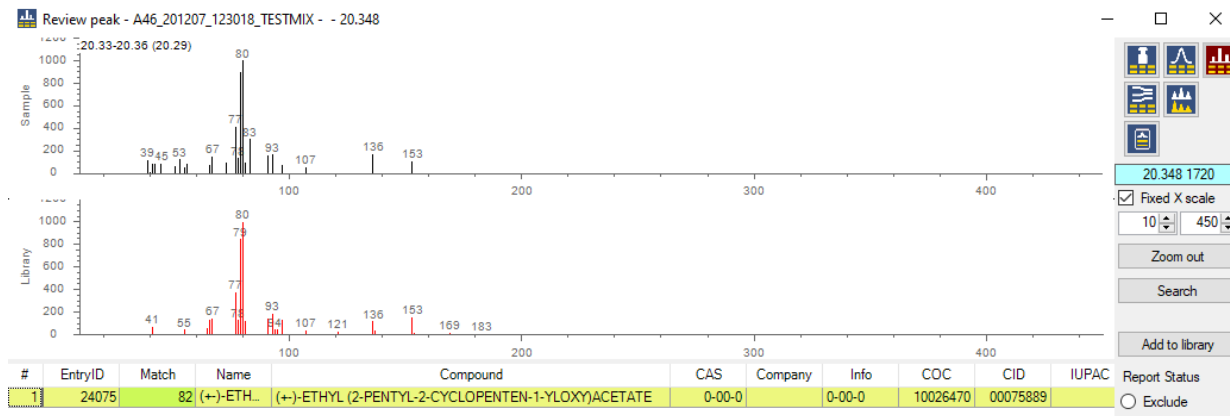


Overlay reference
 TIC
 FID

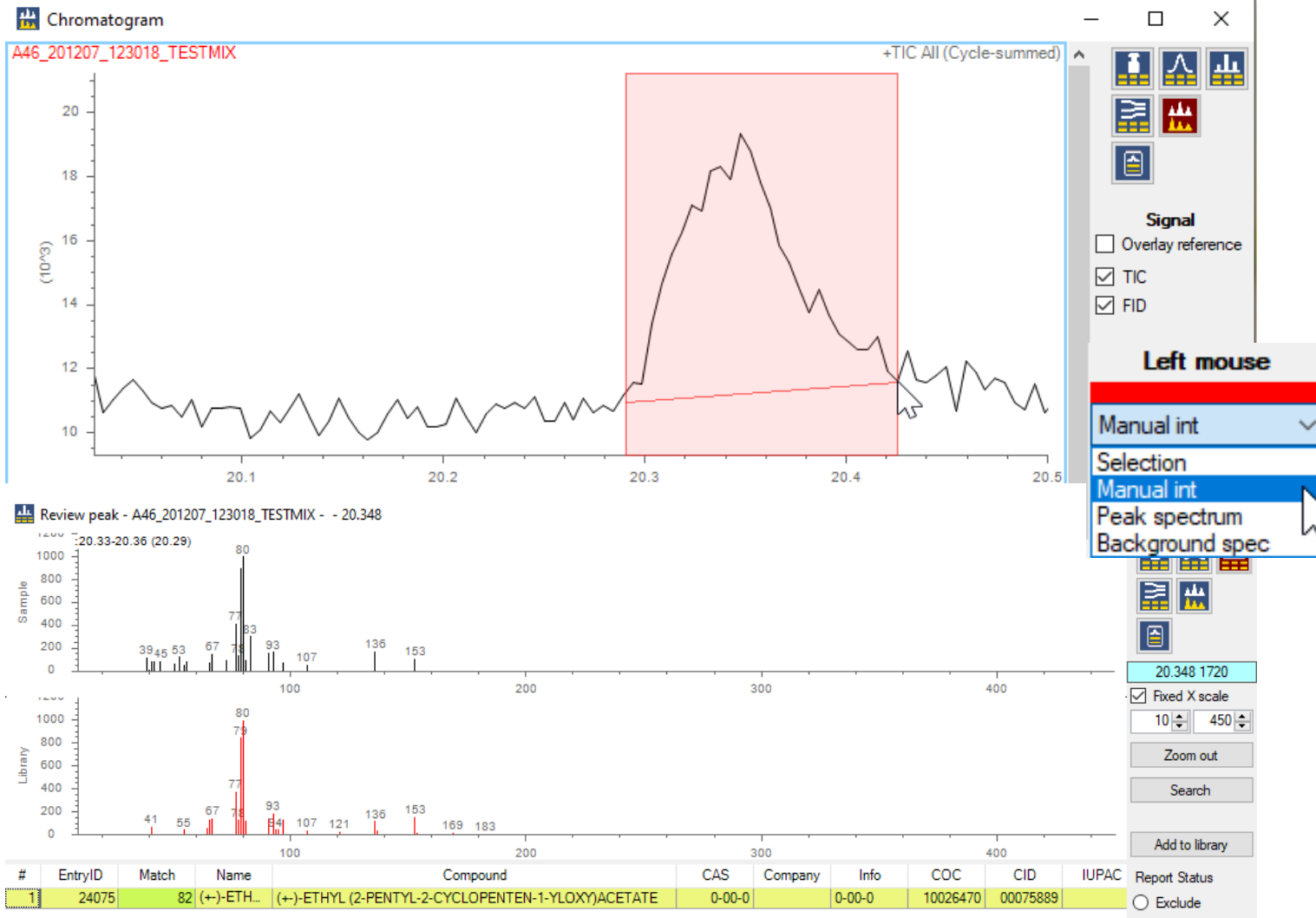
Left mouse

- Selection
- Selection
- Manual int
- Peak spectrum
- Background spec

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



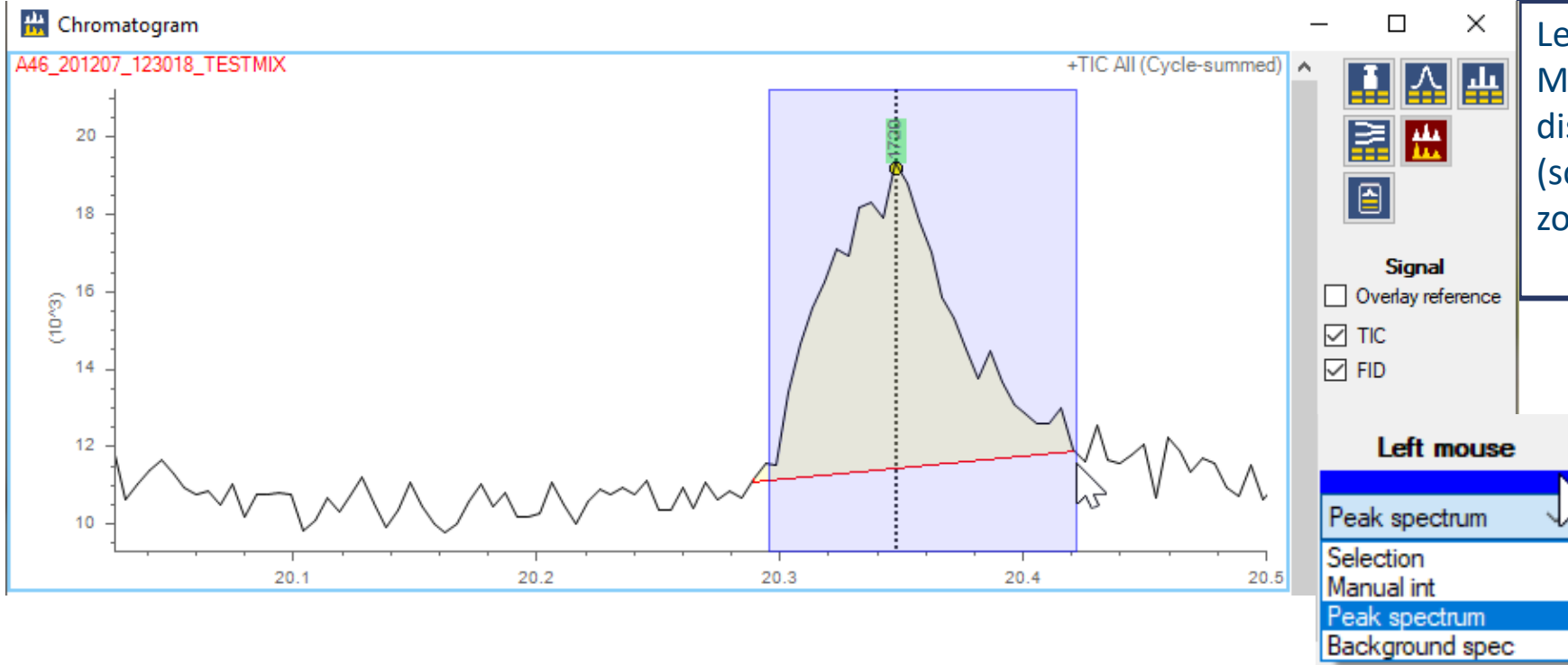
Data Reviewing - Chromatogram



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



Data Reviewing - Chromatogram



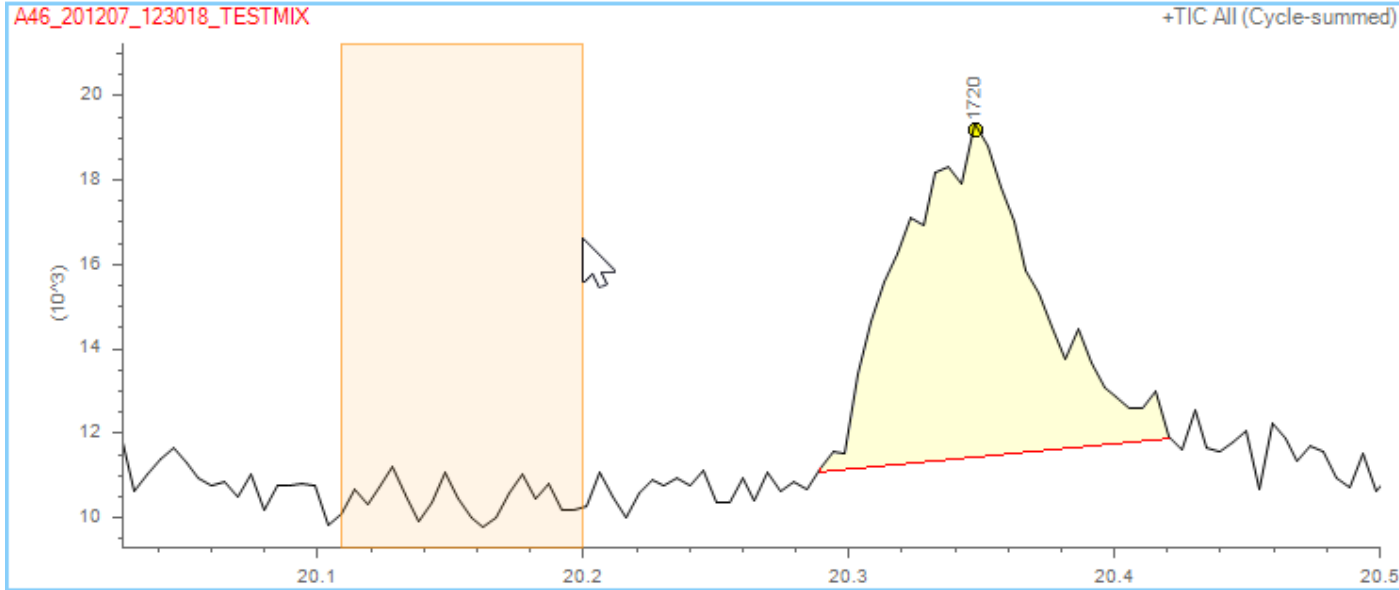
Left mouse in Peak spectrum Mode (Keyboard shortcut: s): display the selected spectrum (scan by scan or average of peak zone)



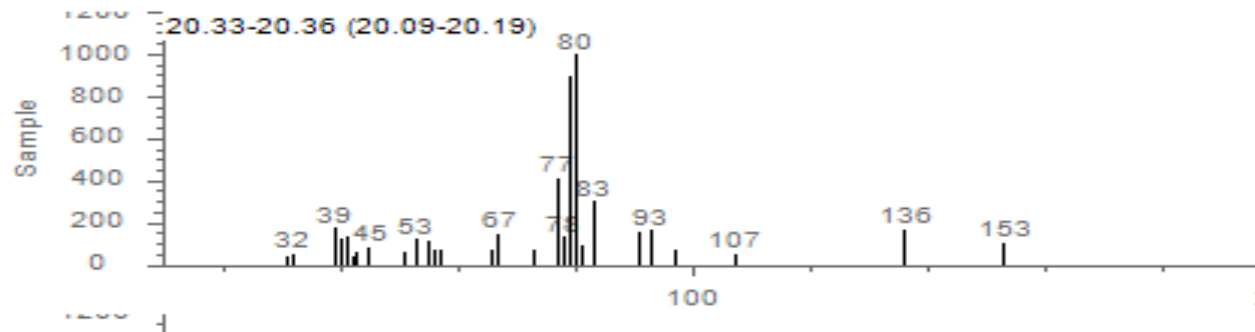
Data Reviewing - Chromatogram



Chromatogram



Review peak - A46_201207_123018_TESTMIX - - 20.348



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

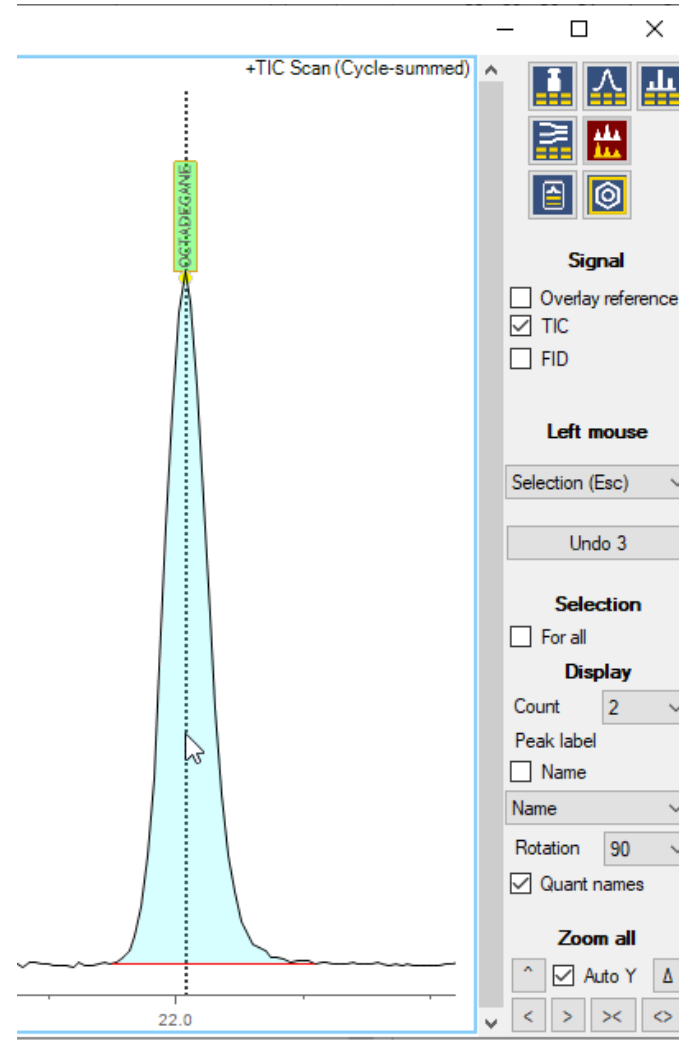


Data Reviewing - Chromatogram

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
<hr/>	
Review hit	
Accept hit info for in line peaks	Ctrl+Enter
<hr/>	
Search spectra	
Merge peaks	Ctrl+M
<hr/>	
Delete selected peaks	Ctrl+Del
Delete all smaller than selected	
Delete all smaller than 20% of selected	
Delete all after selected	

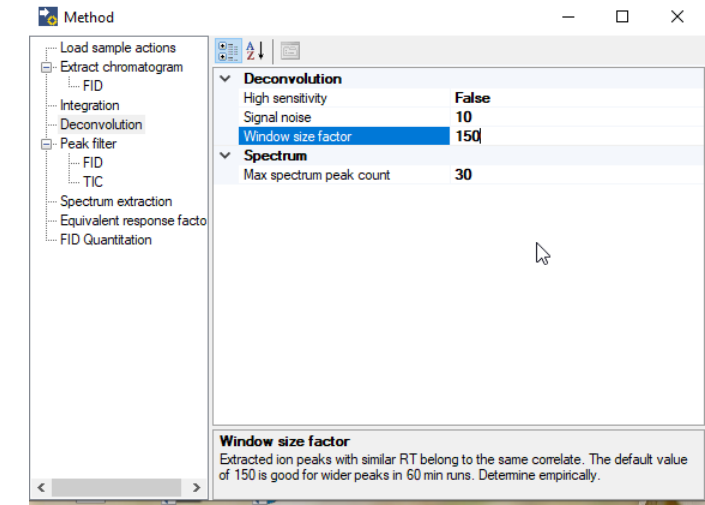
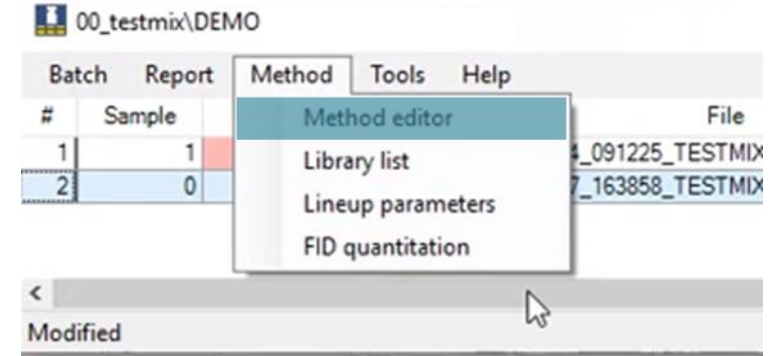
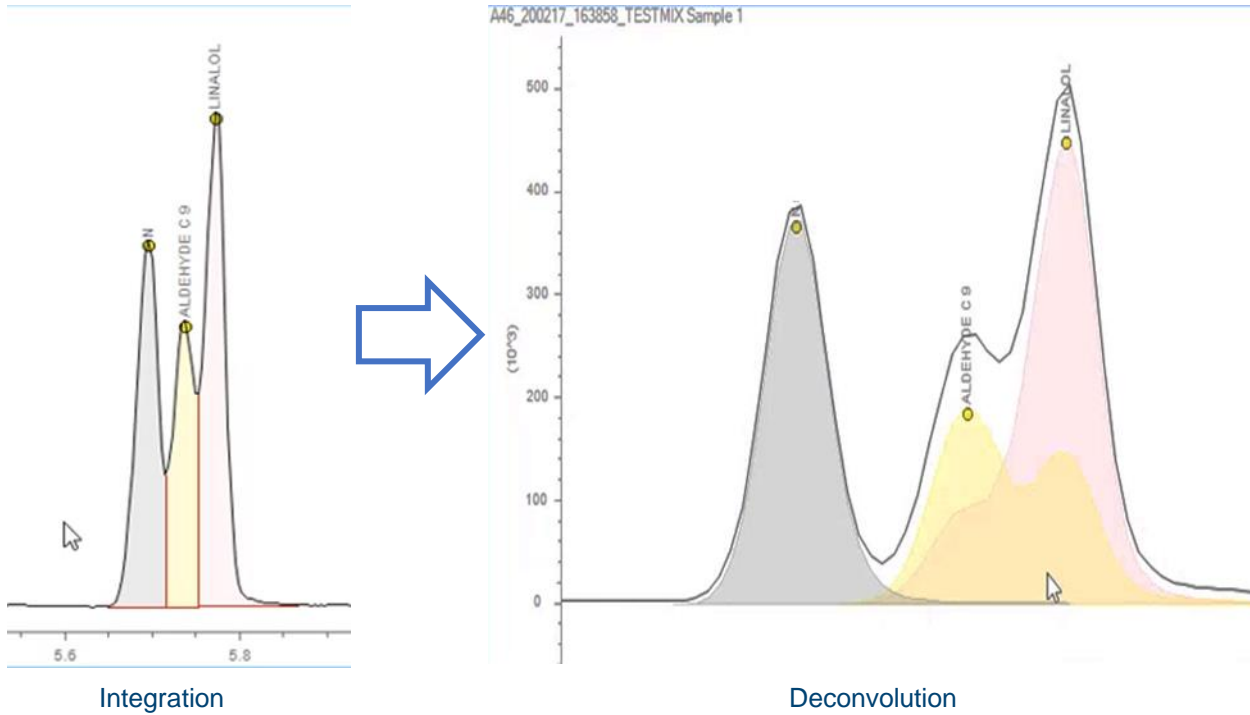
Integrate	
Deconvolute	
<hr/>	
Manual correlate	K
Break correlation	Shift+K
Reset manual correlation	Ctrl+K
<hr/>	
Match	
<hr/>	
Manual lineup	L
Break lineup	Shift+L
Reset lineup	Ctrl+L
<hr/>	
Exclude	Ctrl+1
Report	Ctrl+2
Highlight	Ctrl+3
<hr/>	
Unknown	Ctrl+4
Tentative	Ctrl+5
Approved	Ctrl+6
<hr/>	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



Data Reviewing – Chromatogram

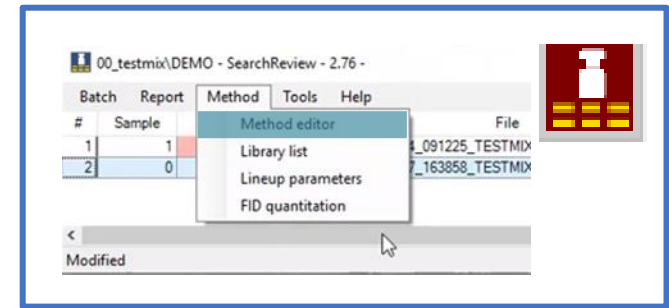


Local deconvolution: right click → deconvolute

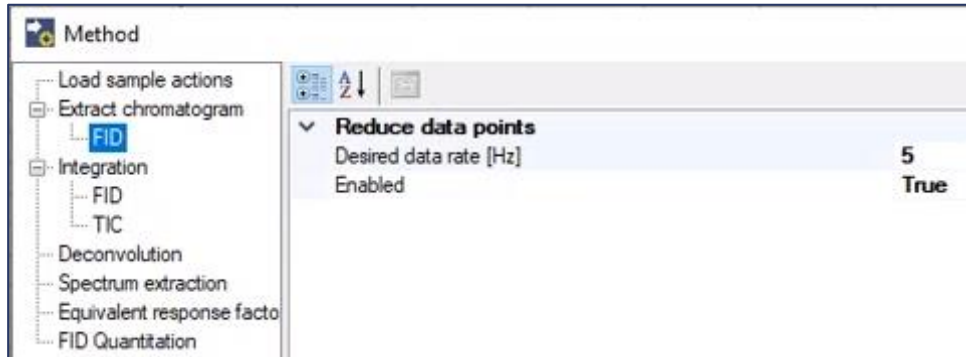


Adjust deconvolution parameters: in the main window, click on Method → Method editor → Deconvolution Tab

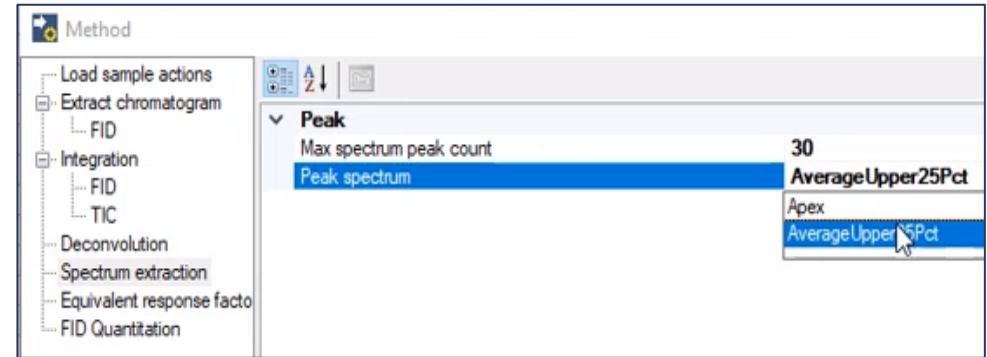
Data Reviewing – Chromatogram



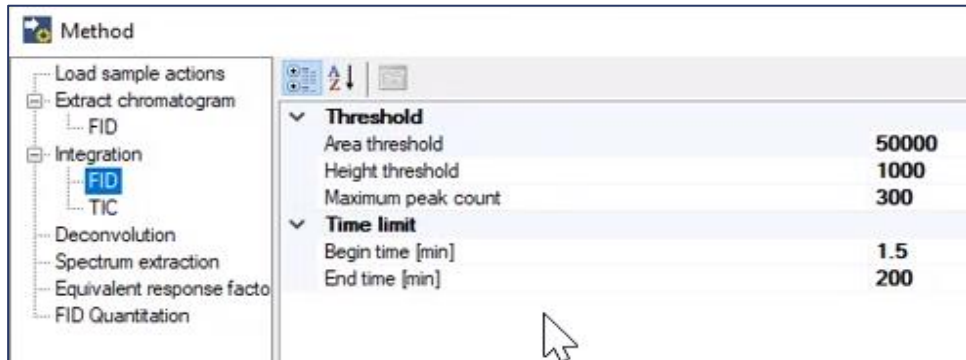
Several other parameters can be adjusted through the Main window:



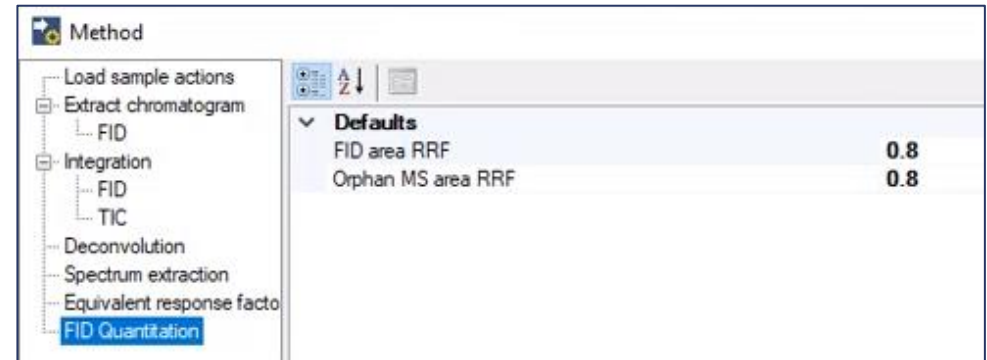
FID: desired data rate for extraction and do we went to extract FID or not



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



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 – Review Peak



Review peak - A46_201207_123018_TESTMIX - - 12.134

12.13-12.14 (12.08)

Selected peak spectrum

Library spectrum

#	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

Report Status

Exclude

Report

Highlight

Review status

Unknown

Tentative

Approved

Accept

Accept for lineup

Delete peak

Peak

Prev Next

Appr + Prev Appr + Next

Unk + Prev Unk + Next

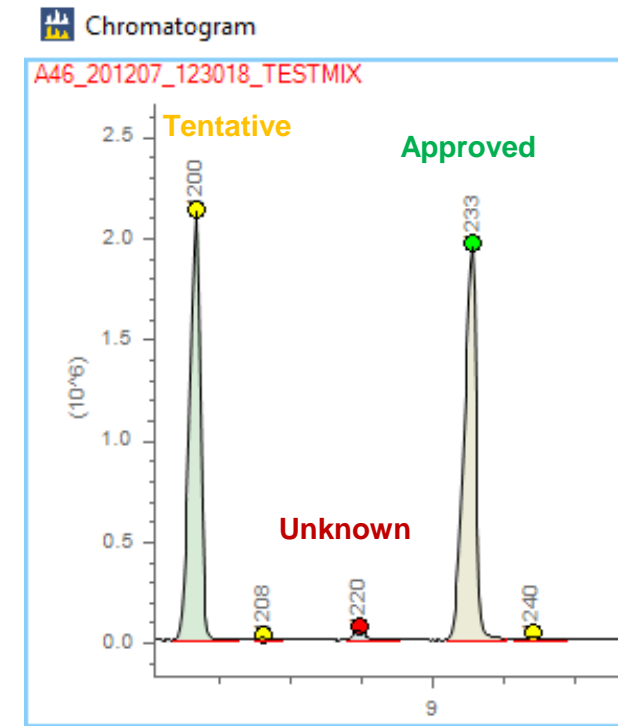
RT and LRI

Right click on the first row
→ Show/Hide columns

Switch from a peak to another

Library hits

- 1) Select the best hit, if available
 - 2) Select the status
 - 3) Click on accept
- It updates the chromatogram colors



Data Reviewing – Review Peak



Review peak - A46_201207_123018_TESTMIX - - 12.134

12.13-12.14 (12.08)

Sample

Library

#	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

12.134 1359

Fixed X scale

10 450

Zoom out

Search

Add to library

Lib DEMO.mslibrary

Report Status

Exclude

Report

Highlight

Review status

Unknown

Tentative

Approved

Accept

Accept for lineup

Delete peak

Peak

Prev Next

Appr + Appr +
Prev Next

Unk + Unk +
Prev Next

Add a peak to your own editable library

Ken\TestMix_Ken_MRSG

Batch Report Method Tools Help

#	Sample	Type
1	0 A4	
2	1 A4	

Method editor

Library list

Lineup parameters

FID quantitation

Access libraries parameters at any time via the Main Window

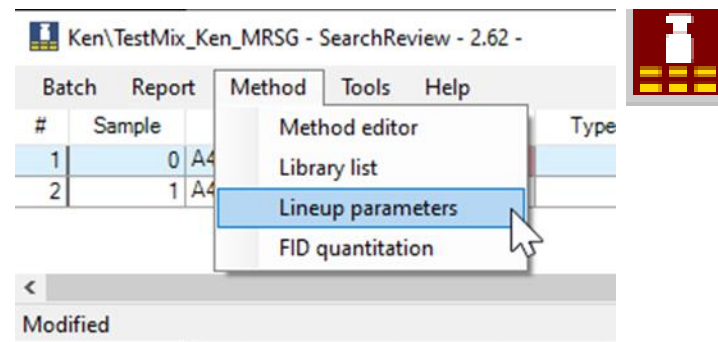
Data Reviewing – Lineup



#	Compound	Formula	MW	Curve	A46_201207_123018_TESTMIX	A46_210201_123528_TESTMIX
54	PINENE ALPHA	C10H16	136.2		PINENE ALPHA 96 FID+MS 0	PINENE ALPHA 96 FID+MS -63
55	CAMPHENE	C10H16	136.2		945 CAMPHENE 94 FID+MS 0	945 CAMPHENE 89 FID+MS -64
56	DECANE	C10H22	142.3		1000 DECANE 98 FID+MS 0	1000 DECANE 99 FID+MS -65
57	ALCOHOL C 8	C8H18O	130.2		1050 ALCOHOL C 8 99 FID+MS 0	1050 ALCOHOL C 8 99 FID+MS -67
58	CIS-LINALOOL OXIDE (furan deriv.)	C10H18O2	170.2			1056 CIS-LINALOOL OXIDE (furan deriv.) 80 FID+MS
59	ALDEHYDE	C8H10O	122.2		1078 N 96 FID+MS 0	1078 N 96 FID+MS -67
60	ALDEHYDE C 9	C9H18O	142.2		1081 ALDEHYDE C 9 91 FID+MS 0	1081 ALDEHYDE C 9 95 FID+MS -68
61	LINALOL	C10H18O	154.2		1083 LINALOL 90 FID+MS 0	1083 LINALOL 90 FID+MS -65
62	(+)-2-ETHYLHEXANOIC ACID	C8H16O2	144.2		1110 (+)-2-ETHYLHEXANOIC ACID 96 FID+MS 0	1105 (+)-2-ETHYLHEXANOIC ACID 95 FID+MS -67
63	2,6-DIMETHYLANILINE	C8H11N	121.2		1133 2,6-DIMETHYLANILINE 96 FID+MS 0	1133 2,6-DIMETHYLANILINE 96 FID+MS -67
64	dodecane	C12H26	170.3		1200 dodecane 97 FID+MS 0	1200 dodecane 97 FID+MS -66
65	PENTYLENDOL (+)-	C10H18O	154.2			1220 PENTYLENDOL (+)- 80 FID+MS
66	GERANIOL	C10H18O	154.2		1233 GERANIOL 89 FID+MS 0	1233 GERANIOL 83 FID+MS -67
					1306 METHYL CAPRATE 0	1306 METHYL CAPRATE 0

Peaks lineup/comparison between chromatograms

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



Lineup parameters

#	On	Phase	Signal	DRT	DRI	Match	Main hit	Hit list	Comment
1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		2.0	80			

Buttons: Add row, Delete row, Reload, Test, OK, Cancel

Delta Retention Time / Index

Data Reviewing – Lineup



Sample 1	Sample 1	Sample 1
2020-01-14 11:52:44	2020-01-27 13:20:56	
1.000	1.000	
1306 10.820 2128527 THYL CAPRATE 95 FID+MS	1306 10.808 2236443 METHYL CAPRATE 93 FID+MS	METHY
1315 11.030 47737 szole, 5-ethyl-4-phenyl- 61 FID+MS	1315 11.021 19203 1-Methyl-3-acetylindole 58 MS	
1360 12.099 1779568 RANYL ACETATE 91 FID+MS	1359 12.085 1826993 GERANYL ACETATE 91 FID+MS	GERAP
1400 13.077 2669575 TRADECANE 96 FID+MS	1400 13.065 2884227 TETRADECANE 95 FID+MS	TETRA
1867 23.286 131935 noline, 1,2,3,4-tetrahydro-2-meth 65 FID+MS	1867 23.286 131935 Quinoline, 1,2,3,4-tetrahydro- 68 FID+MS	
	3618 43 MS	
1220 8.765 42661 VITYLENDOL (+) 83 FID+MS		
2308 31.193 50075 FID+MS		
932 3.383 2075983 ENE ALPHA 96 FID+MS	932 3.383 2075983 PINENE ALPHA 96 FID+MS	
1000 4.275 1604582 CANE 99 FID+MS	1000 4.275 1604582 DECANE 99 FID+MS	
1050 5.180 2107116 COHOL C 8 99 FID+MS	1050 5.180 2107116 ALCOHOL C 8 99 FID+MS	
1078 5.695 1321917 N 96 FID+MS	1078 5.695 1321917 N 96 FID+MS	
1083 5.781 1878612 ALOL 91 FID+MS	1083 5.781 1878612 Linalool 86 FID+MS	
1134 6.832 1753428 DIMETHYLANILINE 97 FID+MS	1133 6.832 1753428 2,6-DIMETHYLANILINE 97 FID+MS	
1200 8.296 2160656 ecane 97 FID+MS	1200 8.296 2160656 dodecane 97 FID+MS	
1233 9.071 2089688 RANIOL 88 FID+MS	1233 9.071 2089688 GERANIOL 87 FID+MS	
1562 16.827 704229	1561 16.827 704229	

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



Lineup

#	Compound	Formula	MW	Curve	A46_201207_123018_TESTMIX	A46_210201_123528_TESTMIX
56	AMPHENE	C10H16	136.2		CAMPHERE 94 FID+MS 0	CAMPHERE 89 FID+MS -64
57	ECANE	C10H22	142.3		DECANE 1000 4.306 3118323 98 FID+MS 0	DECANE 1000 4.291 1057183 99 FID+MS -65
58	ALCOHOL C 8	C8H18O	130.2		ALCOHOL C 8 1050 5.216 4223225 99 FID+MS 0	ALCOHOL C 8 1050 5.192 99 FID+MS -67
59	CIS-LINALOOL OXIDE (furan deriv.)	C10H18O2	170.2			CIS-LINALOOL OXIDE (furan 1056 5.309 80 FID+MS
60	ALDEHYDE	C8H10O	122.2		ALDEHYDE C 9 1078 5.727 2323865 96 FID+MS 0	ALDEHYDE C 9 1078 5.703 96 FID+MS -67
61	ALDEHYDE C 9	C9H18O	142.2		ALDEHYDE C 9 1081 5.781 1191547 91 FID+MS 0	ALDEHYDE C 9 1081 5.761 95 FID+MS -68
62	LINALOL	C10H18O	154.2		LINALOL 1083 5.815 2550477 90 FID+MS 0	LINALOL 1083 5.791 90 FID+MS -65
63	(+)-2-ETHYLHEXANOIC ACID	C8H16O2	144.2		(+)-2-ETHYLHEXANOIC ACID 1110 6.355 1847979 96 FID+MS 0	(+)-2-ETHYLHEXANOIC ACID 1105 6.219 95 FID+MS -67
64	2,6-DIMETHYLANILINE	C8H11N	121.2		2,6-DIMETHYLANILINE 1133 6.862 1915248 96 FID+MS 0	2,6-DIMETHYLANILINE 1133 6.842 96 FID+MS -67
65	dodecane	C12H26	170.3		dodecane 1200 8.337 4589974 97 FID+MS 0	dodecane 1200 8.312 97 FID+MS -66
66	PENTYLENDOL (+)-	C10H18O	154.2			PENTYLENDOL (+)- 1220 8.785 80 FID+MS
67	GERANIOL	C10H18O	154.2		GERANIOL 1233 9.116 4548783 89 FID+MS 0	GERANIOL 1233 9.082 83 FID+MS -67
68	METHYL CAPRATE	C11H22O2	186.3		METHYL CAPRATE 1306 10.864 4461957 92 FID+MS 0	METHYL CAPRATE 1306 10.834 91 FID+MS -66
69	TETRADECANE	C14H30	198.4		TETRADECANE 1401 13.128 4994266 95 FID+MS 0	TETRADECANE 1400 13.098 95 FID+MS

Chromatogr. A46_201207_1230

Freeze row Ctrl+Shift+T
Freeze column Ctrl+T
Cut Ctrl+X
Copy Ctrl+C
Copy with header Ctrl+Shift+C
Paste Ctrl+V
Clear Del
Select all Ctrl+A
Fill down Ctrl+D
Find text Ctrl+F
Search spectra
Review hit
Accept hit info for all in line Ctrl+Enter
Delete selected peaks Ctrl+Del
Delete all smaller than selected
Delete all smaller than 20% of selected
Delete all after selected
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

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

Retention Index - Retention Time - Area

1200	8.337	4589974
dodecane		
97	FID+MS	90
	0	

Library Match

05 Quantitation

Quantitation

The screenshot displays a chromatography software interface with three main panels:

- Top Panel (Sample Table):** A table with columns: #, Sample, Folder, DataPath, RelativePath, File, Sample, Amount, IS key, IS Amount, IS Resp, Ref, Level, Operator, Inst, Acquired, AcqMethod, Type, and FD. It lists 8 samples, with sample 4 (Q98TC) highlighted.
- Bottom Left Panel (Well known compounds):** A table with columns: #, On, Name, CAS, RI, Formula, Mw, Comment, IS Amount, IS, and IS key. It lists Toluene, Toluene-D8, and p-Xylene with their respective CAS numbers and IS keys (TOL, DTOL, PX).
- Bottom Right Panel (Peaks - Q98TC_openlab2_ - Q98TC):** A table with columns: #, tY, EndY, StartBl, EndBl, Rel, Report, Area, Rsp, Rsp%, Amt, Amt%, %ofRef%, %ofRef, Dominant, Dom%, RT, CAS, and Name. It lists 20 peaks, with peak 648 (Toluene) highlighted in yellow.

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



TestMix_Ken_MRSG_Lineup_20210210095501



TestMix_KEN_MRSG_Samples_20210203134944



TestMix_Ken_MRSG_A46_210201_123528_TESTMIX_Peaks_202102101016

Report

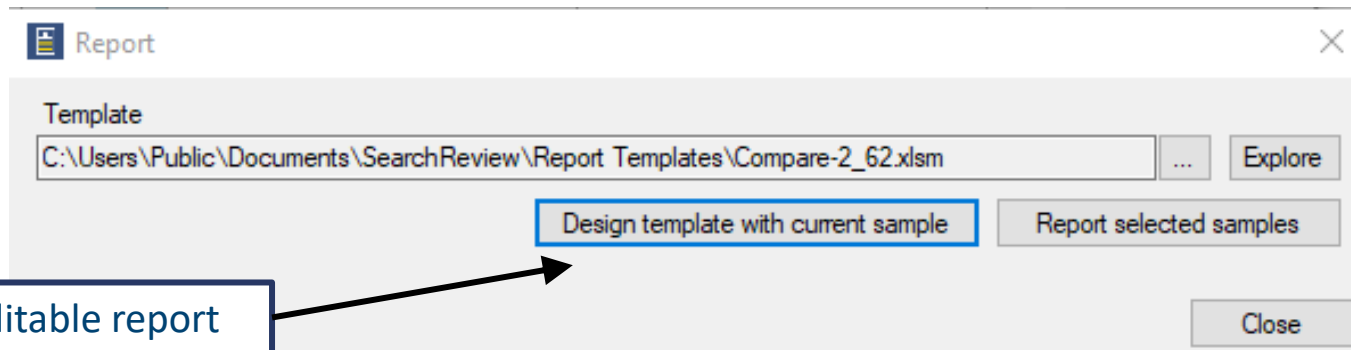


from the Samples window

Ken\TestMix_Ken_MRSG

Batch	Report	Method	Tools	Help	File	Inst	Sample
#	0		<input checked="" type="checkbox"/>		A46_200217_163858_TESTMIX	Ken	Sample 1
			<input checked="" type="checkbox"/>		A46_200203_114447_TESTMIX	Ken	Sample 1

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



Select a template

Editable report

Report



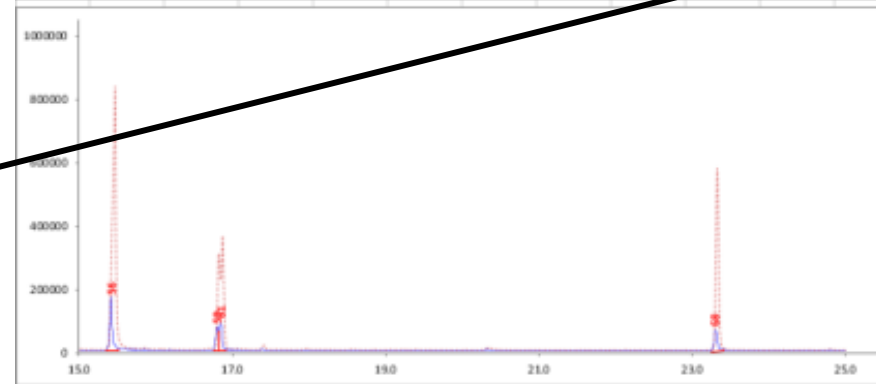
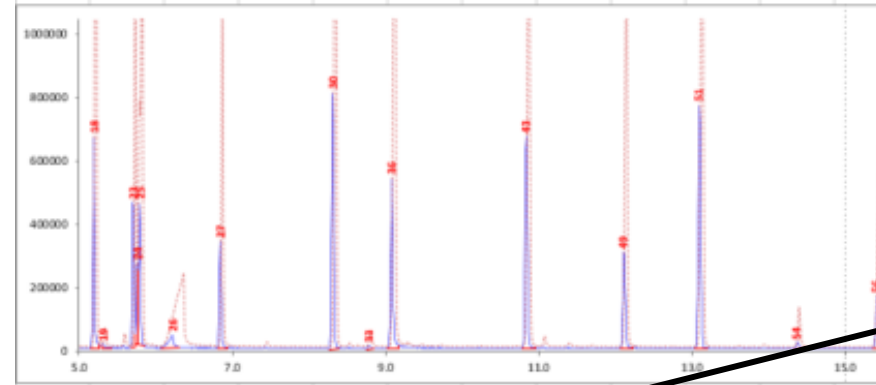
Sample and ref data

Chromatogram

Template settings

Compound data

Reported	2021-02-10 09:58
Comparison mode	Perfume
Sample	Z:\vest_mkt_lgal\KeriA46_210201_123528_TESTMX.D
Item	
LotNr	
LIMS_ID	
Runtime	01.02.2021 12:35
Channel	
Timebase	HPIPE_B
Reference	Z:\vest_mkt_lgal\KeriA46_201207_123018_TESTMX.D
Item	
LotNr	
LIMS_ID	
Runtime	07.12.2020 12:30
Channel	
Timebase	HPIPE_B



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	NaN
3	1.362		777		0.009		Extra peak	NaN
4		1.392		778		0.005	Peak missing	NaN
5	1.392		779		0.002		Extra peak	NaN
6		1.435		782		99.893	Peak missing	NaN
7	1.435		782		99.923		Extra peak	NaN
8		1.908		818		0.012	Peak missing	NaN
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	NaN
12		2.182		838		0.000	Peak missing	NaN
13	2.485		861		0.000		Extra peak	NaN

Reformat	Create PDF
Names	Save as template ...

Signal selection	MS
MS	n/a
FDI	n/a

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

Label selection	ReportIndex
Ampl	n/a
Comment	Format
Name	Format
CAS	Format
ReportIndex	Format
RetentionIndex	Format
RetentionTime	Format

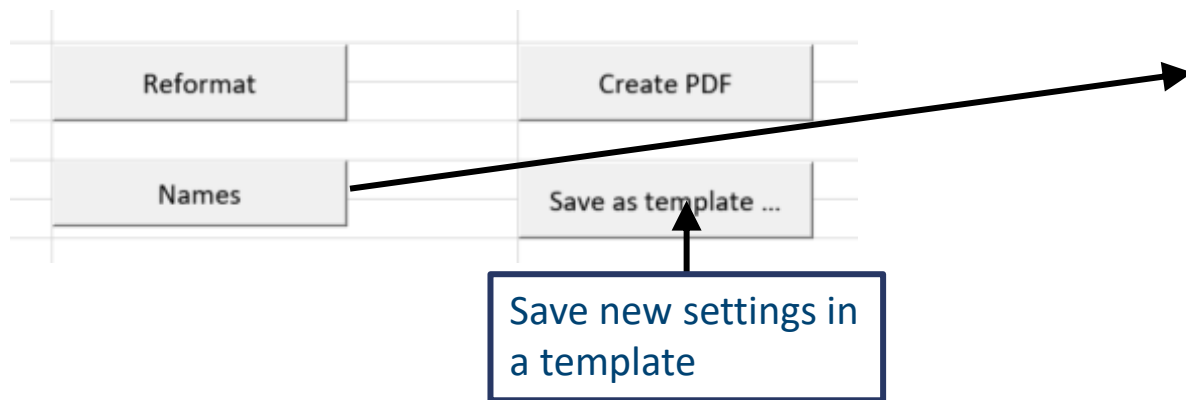
Response Max selection	HighestPointAfter
HighestPointAfter	0
Fixed	800000
ChartNumber	2
ChartIndividual	n/a
SetInChartAxisScale	n/a

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

Report



Top right corner of the report



- 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

Names

Sample | Compound | RefSample | RefCompound

DataFile
DataPath
BatchName
FileName
AnalysisMethod
AnalysisMethodName
SampleName
IsReference
SampleType
LevelName
OperatorName
InstrumentName
AcqDateTime
SampleComment
SampleInformation
Barcode
ExpectedBarcode
SampleAmount
Volume
Dilution
RefAmount
RefResponse
Istd1Amount
Istd1Area
Istd1Rt
CompoundOfInterestKeyword
InterestArea
FidAmount
FinalFidConcentration
FidPeakCount
TicPeakCount
FidRiCalValid
TicRiCalValid
FidDataPointCount
TicDataPointCount
ColumnPhase
PlateCode
RackCode
PlatePosition
RackPosition
SamplePosition
Vial
ActualFidOverTicAreaRatio
ManualFidOverTicAreaRatio
ReportTime

Select a cell and double click on a name.

Names

Sample | Compound | RefSample | RefCompound

RetentionTime
RetentionIndex
Area
FidCorrectedAreaPercent
AreaPercent
Width
Height
Deconvoluted
ReportCalculation
ManualReportCalculation
ReportHighlight
ReviewStatus
StartX
EndX
FidCorrectedRetentionTime
ChildrenArea
FidCorrectedArea
Amount
FinalFidConcentration
ReportIndex
AmountByRef
AmountByRefPercent
DegreeOfUnsaturation
AromaticRingCount
CalculatedRrf
ManualRrf
IstdConc
ManualIstdConc
IstdName
IsIstd
ReferencePercentDifference
Rrf
Name
HitName
HitCoc
HitCid
HitIupac
FirmenichFema
FirmenichRrf
FirmenichItemNumber
HitCas
HitFormula
MolWeight
HitMatchScore
HitRetentionIndex
HitDeltaRetentionIndex
HitRetentionIndexDependability
Comment
DetectorType
HitLibrary

Select a cell and double click on a name.

Report



Signal selection	MS	MS
MS	n/a	
FID	n/a	FID
Time selection	BothLimit	LowerLimit
LowerLimit	5	UpperLimit
UpperLimit	25	BothLimit
BothLimit	n/a	Full
Full	n/a	SetInChartAxisScale
SetInChartAxisScale	n/a	SetInChartAxisScale
Overlap	0.5	
Label selection	ReportIndex	Any
Any	n/a	Comment
Comment	format	Name
Name	format	CAS
CAS	format	ReportIndex
ReportIndex	format	RetentionIndex
RetentionIndex	format	RetentionTime
RetentionTime	format	
Response Max selection	HighestPointAfter	HighestPointAfter
HighestPointAfter	0	Fixed
Fixed	800000	ChartNumber
ChartNumber	2	ChartsIndividual
ChartsIndividual	n/a	SetInChartAxisScale
SetInChartAxisScale	n/a	
Response Min selection	SetInChartAxisScale	LowestPointAfter
LowestPointAfter	0	Fixed
Fixed	0	ChartNumber
ChartNumber	2	ChartsIndividual
ChartsIndividual	n/a	SetInChartAxisScale
SetInChartAxisScale	n/a	

Select the signal you want to display

Scaling options for x axis

Chromatogram labelling options

Scaling options for y axis

Reformat

Click on reformat to apply the new settings