What‘s new in TASQ 2024b

TASQ 2024B Main Feature

- Library Search
- Direct MS Data workflow for TQ fullscan data,
- Direct MS Data workflow for TOF and timsTOF data w/ and w/o autoMSMS/PASEF (library search)
- Minor updates in TASQ RealTimeQC 2024b -> described in What‘s new in TASQ RealTimeQC 2024b

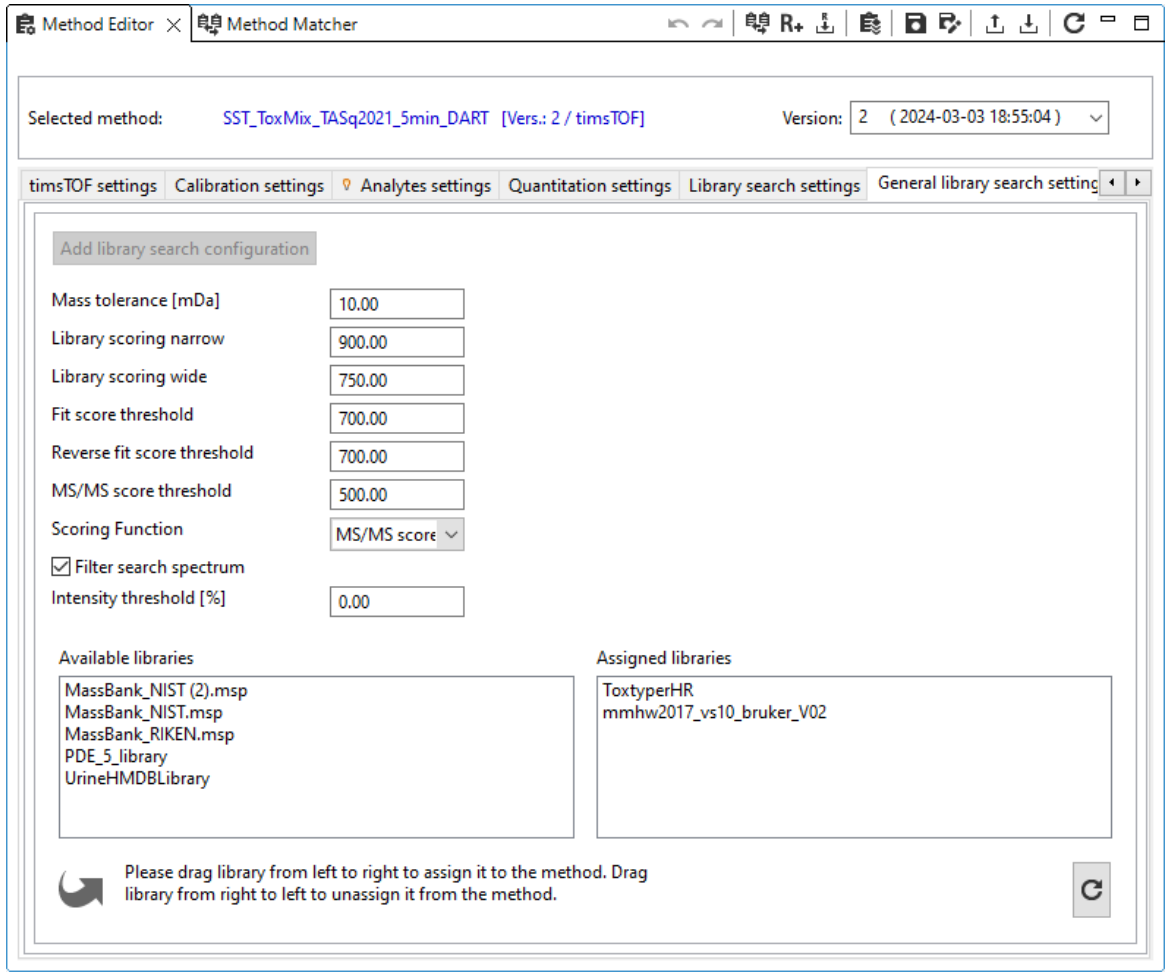
TASQ 2024B Main Feature

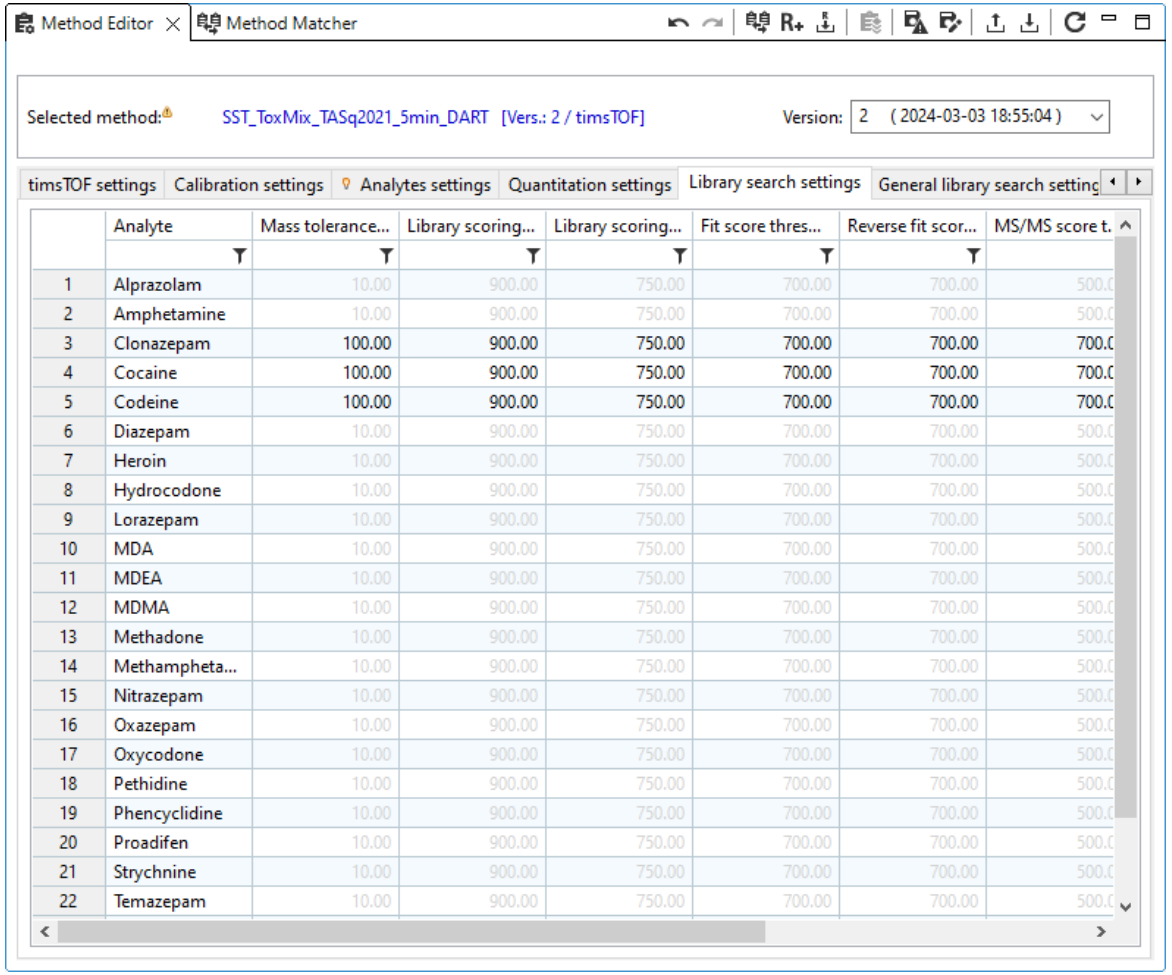
- Library Search
  - Manual workflow supported first
  - User selects a batch, data set, or determination and invokes library search
  - User reviews library search results
  - User specifies parameters for library search in library search parameters section of TASQ method/profile
  - The found determinations will be used for the library search
  - Library search parameters from TASQ method are applied to the library search
  - Library search results are shown:
    - Results table as libary search score
    - Detailed library search results view
    - Butterfly view

TASQ 2024B: Library Search

- For a specific determination all relevant acquired MS/MS spectra are retrieved
- Selection of MS/MS spectra is done by lookup of all MS/MS spectra events in the region of interest
- Region of interest is specified by the screening result for principle ion
  - Chromatogram peak retention time start to end
  - Mobilogram peak start to end
  - Assumed precursor *m/z* value derived from the principal ion information or prm-PASEF precursor
- Equivalent MS/MS spectra are summed up, equal precursor *m/z*, equal collision energy, same polarity, and same mobility
- Retrieved MS/MS spectra are stored and can be reviewed in Detailed Library Search Results view and Butterfly view, even if no library match was found
- Library search is performed and found matches are stored
- Finally a library search score is derived from the found library spectra

TASQ 2024B: Library Search Parameters – Manage Parameters on Analyte Level

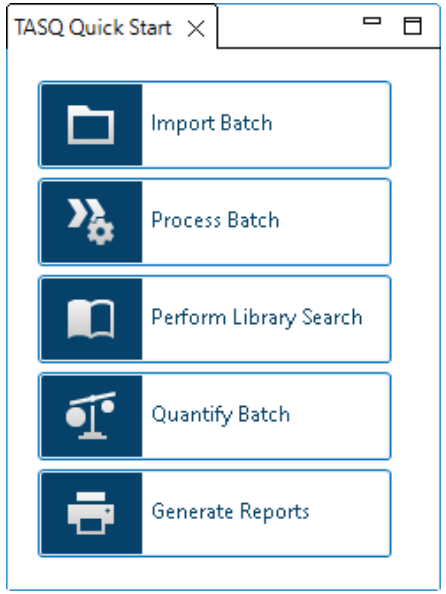


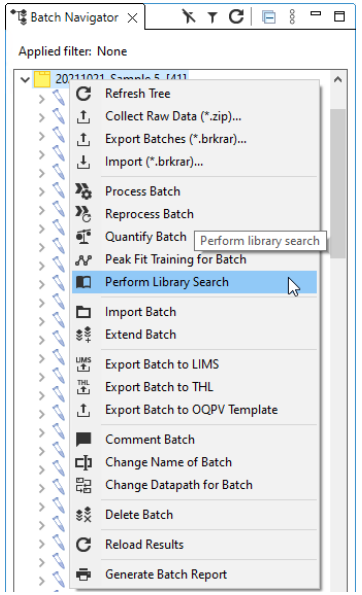


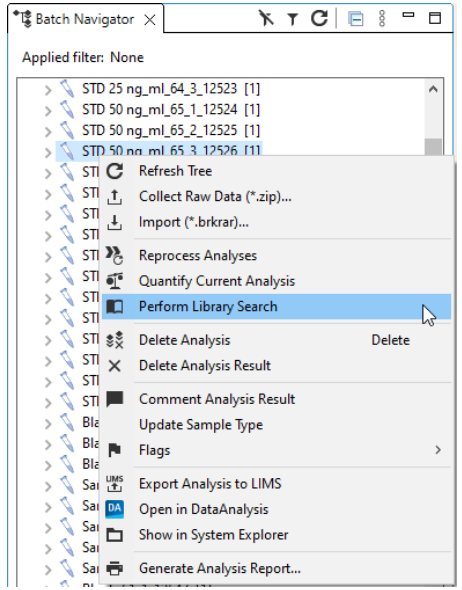
	Analyte	Mass tolerance...	Library scoring...	Library scoring...	Fit score thres...	Reverse fit scor...	MS/MS score t.
1	Alprazolam	10.00	900.00	750.00	700.00	700.00	500.0
2	Amphetamine	10.00	900.00	750.00	700.00	700.00	500.0
3	Clonazepam	100.00	900.00	750.00	700.00	700.00	700.0
4	Cocaine	100.00	900.00	750.00	700.00	700.00	700.0
5	Codeine	100.00	900.00	750.00	700.00	700.00	700.0
6	Diazepam	10.00	900.00	750.00	700.00	700.00	500.0
7	Heroin	10.00	900.00	750.00	700.00	700.00	500.0
8	Hydrocodone	10.00	900.00	750.00	700.00	700.00	500.0
9	Lorazepam	10.00	900.00	750.00	700.00	700.00	500.0
10	MDA	10.00	900.00	750.00	700.00	700.00	500.0
11	MDEA	10.00	900.00	750.00	700.00	700.00	500.0
12	MDMA	10.00	900.00	750.00	700.00	700.00	500.0
13	Methadone	10.00	900.00	750.00	700.00	700.00	500.0
14	Methampheta...	10.00	900.00	750.00	700.00	700.00	500.0
15	Nitrazepam	10.00	900.00	750.00	700.00	700.00	500.0
16	Oxazepam	10.00	900.00	750.00	700.00	700.00	500.0
17	Oxycodone	10.00	900.00	750.00	700.00	700.00	500.0
18	Pethidine	10.00	900.00	750.00	700.00	700.00	500.0
19	Phencyclidine	10.00	900.00	750.00	700.00	700.00	500.0
20	Proadifen	10.00	900.00	750.00	700.00	700.00	500.0
21	Strychnine	10.00	900.00	750.00	700.00	700.00	500.0
22	Temazepam	10.00	900.00	750.00	700.00	700.00	500.0

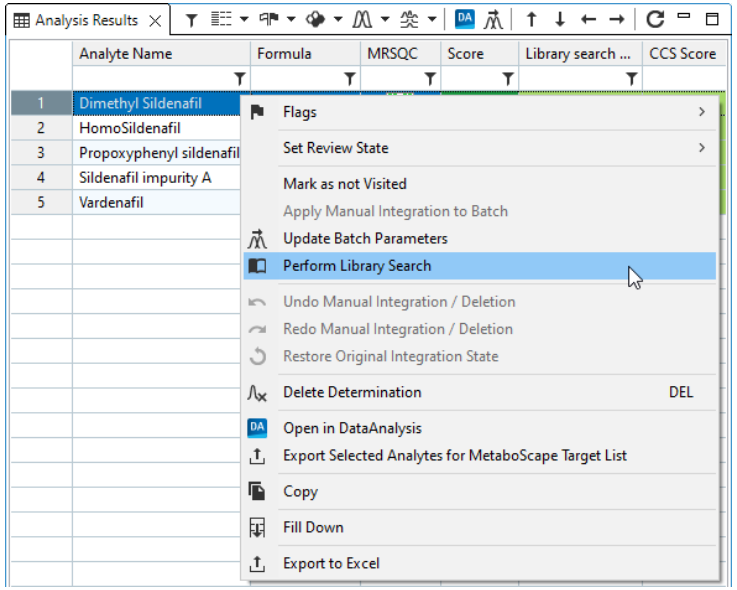
TASQ 2024B: Library Search: Commands

- New library search button in TASQ Quick start view
- Context menu on batch level, data set level in Batch Navigator
- Context menu on determination level in Results views









TASQ 2024B: Library Search Results – Scores

- New columns for library search results
- Score columns gets an extra + for library search results, up to 6+
- MRSQLC, MRSQL, RQL column added with an extral battery symbol for library score
- Scoring Score columns with highlighting whether there is another search result with a higher score value than the principle search result
- Detailed library search result view highlights principle library search result

Analysis Results

	Analyte Name	Formula	#Analytes (LS)	#MS/MS Spectra (LS)	Scoring Function (LS)	Scoring Score (LS)	Score	MRSQLC	m/z Score	RT Score	mSigma Score	Ions Score	Library search score	CCS Score
1	Dimethyl Sildenafil	$C_{23}H_{32}N_6O_4S$	5	1	SCORE_BY_FIT_SCORE	977.04	+++++		++	++	+	++	++	++
2	HomoSildenafil	$C_{23}H_{32}N_6O_4S$	5	1	SCORE_BY_FIT_SCORE	945.73	++++++		++	++	++	++	++	++
3	Propoxyphenyl sildenafil	$C_{23}H_{32}N_6O_4S$	5	1	SCORE_BY_FIT_SCORE	941.84	+++++		++	++	+	++	++	++
4	Sildenafil impurity A	$C_{23}H_{32}N_6O_4S$	5	1	SCORE_BY_FIT_SCORE	941.84	+		++	++	+	++	+	++
5	Vardenafil	$C_{23}H_{32}N_6O_4S$	3	1	SCORE_BY_FIT_SCORE	974.01	+++++		++	++	+	++	++	++

Detailed Ion Results

	Ion Formula	Ion Type	Mandatory	Area	MRSC	CCS [Å²]	Δm/z [mDa]	ΔRT [min]	mSigma	m/z Score	RT Score	CCS Score
1	$C_{23}H_{33}N_6O_4S^{1+}$	M+nH	☑	3120972		215.25	0.24	-0.00	46.7	++	++	++
2	$C_{23}H_{33}N_6O_4S^{1+}$	M+nH+1	☑	746129			0.46	-0.00	46.4	++	++	++
3		475.212	☐									
4		72.081	☐	4737			0.10	0.00		++	++	+
5		99.092	☐	152978			0.11	0.00		++	++	++
6		Frag 113	☑	203580			0.33	0.00		++	++	++
7		Frag 311	☑	180369			-0.12	0.00		++	++	++

Detailed Library Search Results

	Spectrum Type	Analyte	Result Analyte	Result Formula	Precursor m/z	Coll. Energy Li...	CCS	MS/MS Score	Fit Score	Reverse Fit Score	Instrument
1	bbCiD	HomoSildenafil	⚠ Dimethyl Sildenafil	$C_{23}H_{32}N_6O_4S$	489.2279	40	215.57	945.96	956.42	959.39	timsTOF Pro
2	bbCiD	HomoSildenafil	✔ HomoSildenafil	$C_{23}H_{32}N_6O_4S$	489.2279	40	214.73	925.81	945.73	942.58	timsTOF Pro
3	bbCiD	HomoSildenafil	⚠ Propoxyphenyl sildenafil	$C_{23}H_{32}N_6O_4S$	489.2279	40	216.09	534.30	680.14	562.56	timsTOF Pro
4	bbCiD	HomoSildenafil	⚠ Sildenafil impurity A	$C_{23}H_{32}N_6O_4S$	489.2279	40	216.09	255.44	328.93	316.93	timsTOF Pro
5	bbCiD	HomoSildenafil	⚠ Vardenafil	$C_{23}H_{32}N_6O_4S$	489.2279	40	226.26	172.32	175.28	337.37	timsTOF Pro

TASQ 2024B: Library Search –Summary Statistics in Results View

- #Analytes (LS) and #MS/MS spectra (LS) column gives information whether a library search was performed or not
- If no library search was performed for that determination the cells will be empty. Ohterwise a number >= 0 will be presented

Analysis Results

	Analyte Name	Formula	MRSQLC	Scoring Score (LS)	Scoring Function (LS)	#Analytes (LS)	#MS/MS Spectra (LS)	
1	Amitriptyline	$C_{20}H_{23}N$		846.59	SCORE_BY_MSMS_SCORE	5	1	Search performed and retrieved results
2	7-Aminoclonazepam	$C_{15}H_{12}ClN_3O$				0	0	Search performed and retrieved **no** results and **no** MS/MS spectra
3	Citalopram	$C_{20}H_{21}FN_2O$						**No** search performed
4	Doxylamine	$C_{17}H_{22}N_2O$						**No** search performed

Analysis Results

	Analyte Name	Formula	MRSQLC	Scoring Score (LS)	Scoring Function (LS)	#Analytes (LS)	#MS/MS Spectra (LS)	
7	Nordiazepam	$C_{15}H_{11}ClN_2O$		808.81	SCORE_BY_MSMS_SCORE	10	1	
8	7-Aminoclonazepam	$C_{15}H_{12}ClN_3O$				0	0	
9	Mirtazapine	$C_{17}H_{19}N_3$				7	1	Search performed and retrieved **no** matching results
10	Zolpidem	$C_{19}H_{21}N_3O$		747.55	SCORE_BY_MSMS_SCORE	4	1	

TASQ 2024B: Library Search – Detailed Library Search Result

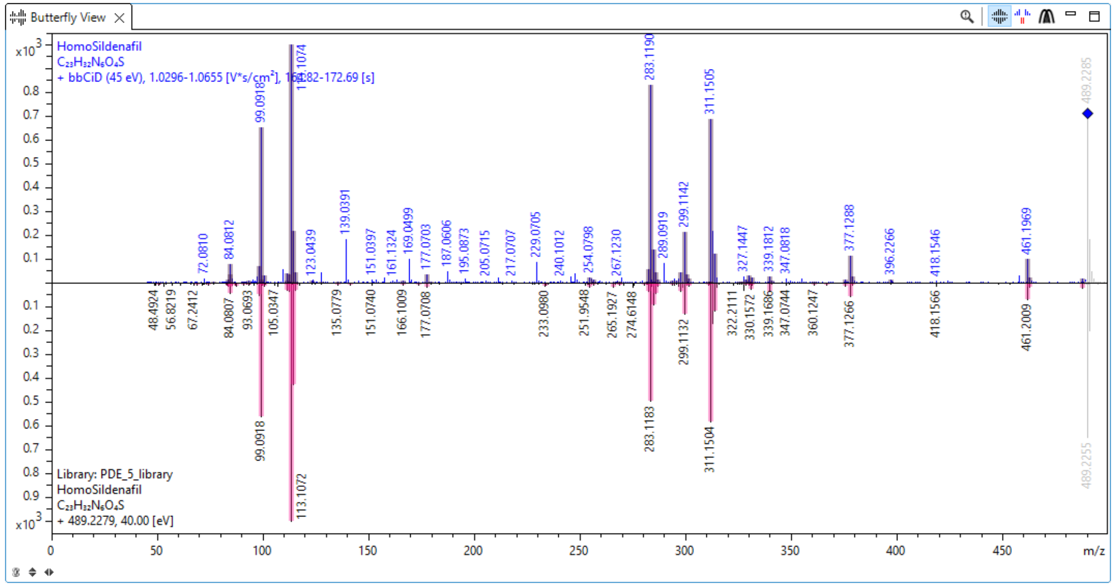
- Green check mark indicates the principle library search result spectrum
- Yellow exclamation mark indicates that the name of analyte in TASQ method and name of analyte of library compound differs, nevertheless the library spectrum was assigned as a positive match
- Score value with a background color indicates that in the list of found library spectra there are candidates with a better score value than the assigned principle library search result spectrum

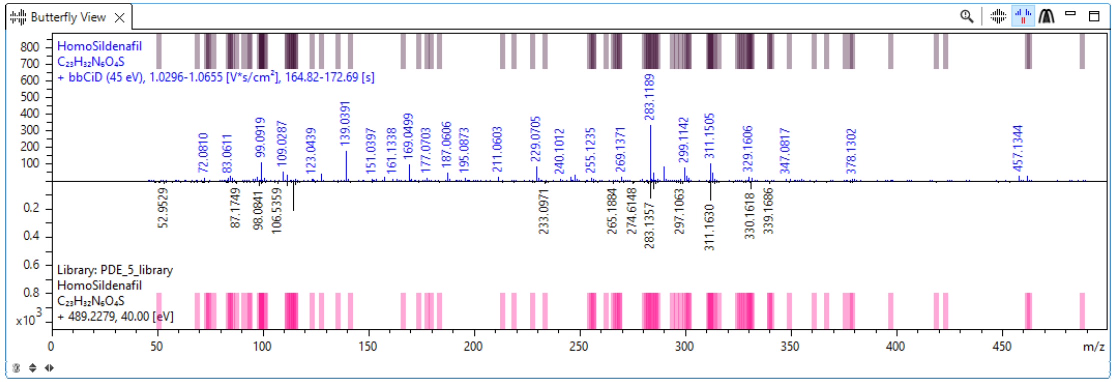
TASQ 2024B: Library Search – New Columns in Result Views

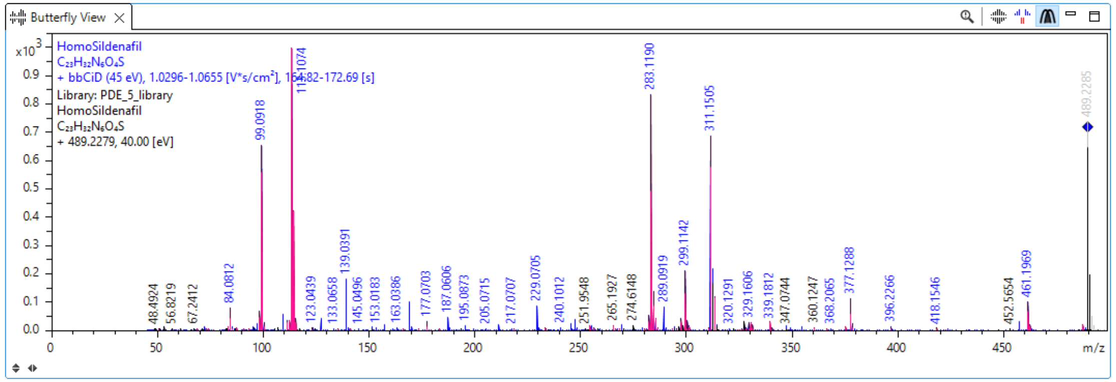
Library search score	Library search score
#Analytes (LS)	Number of found analytes in library search
#MS/MS Spectra (LS)	Number of retrieved acquired MS/MS spectra which are used for library search
Scoring Function (LS)	The type of the score value (MS/MS score, Fit score, or RFit score) used for identifying the best resulting library spectrum
Scoring Score (LS)	Score value calculated for the query spectrum and the best hit found in library search
MRSQLC	[Δm/z - Retention Time - mSigma - Diagnostic Ions - Library Search - CCS Ω]
MRSQL	[Δm/z - Retention Time - mSigma - Diagnostic Ions - Library Search]
RQL	[Retention Time - Diagnostic Ions - Library Search]

TASQ 2024B: Libray Search – Butterfly View

- Compare acquired MS/MS spectrum together with library spectrum
- Show most important information of both spectra in legend
- Acquired spectrum can be normalized to 1000 or raw intensities can be shown → to see whether this is in noise level or not
- Show both spectra in difference or overlay mode

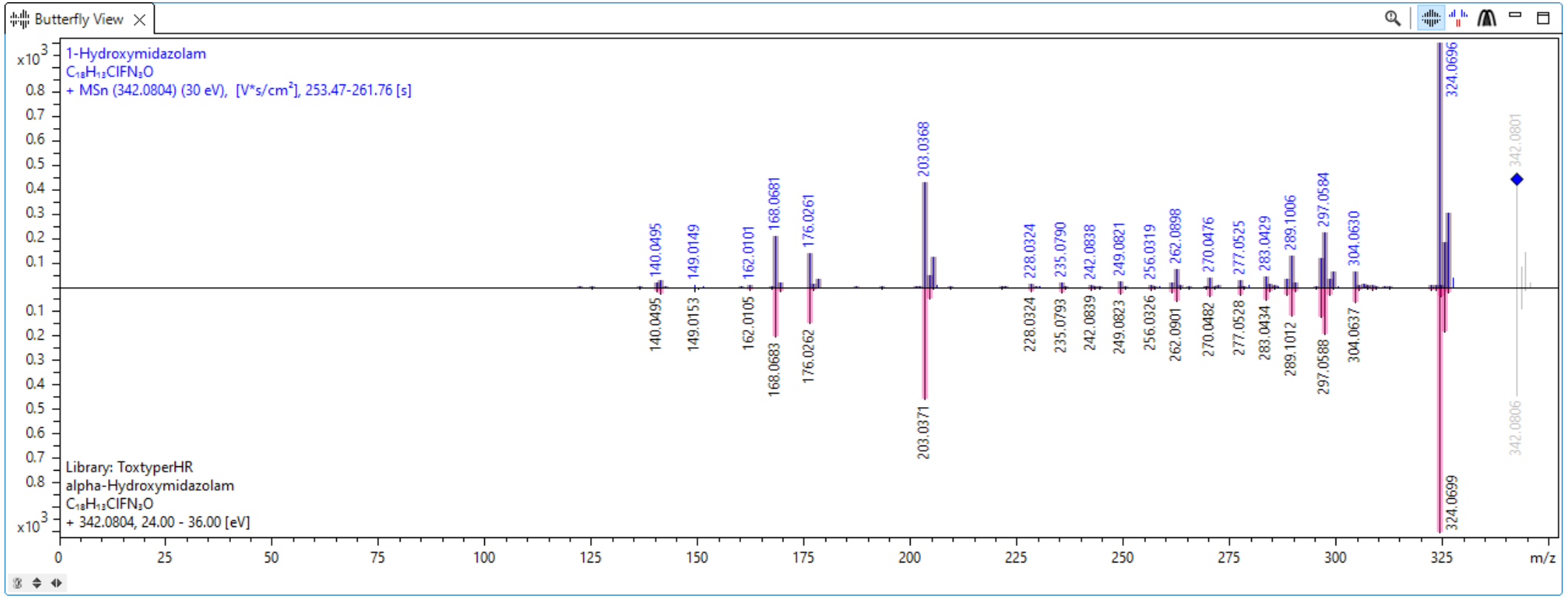






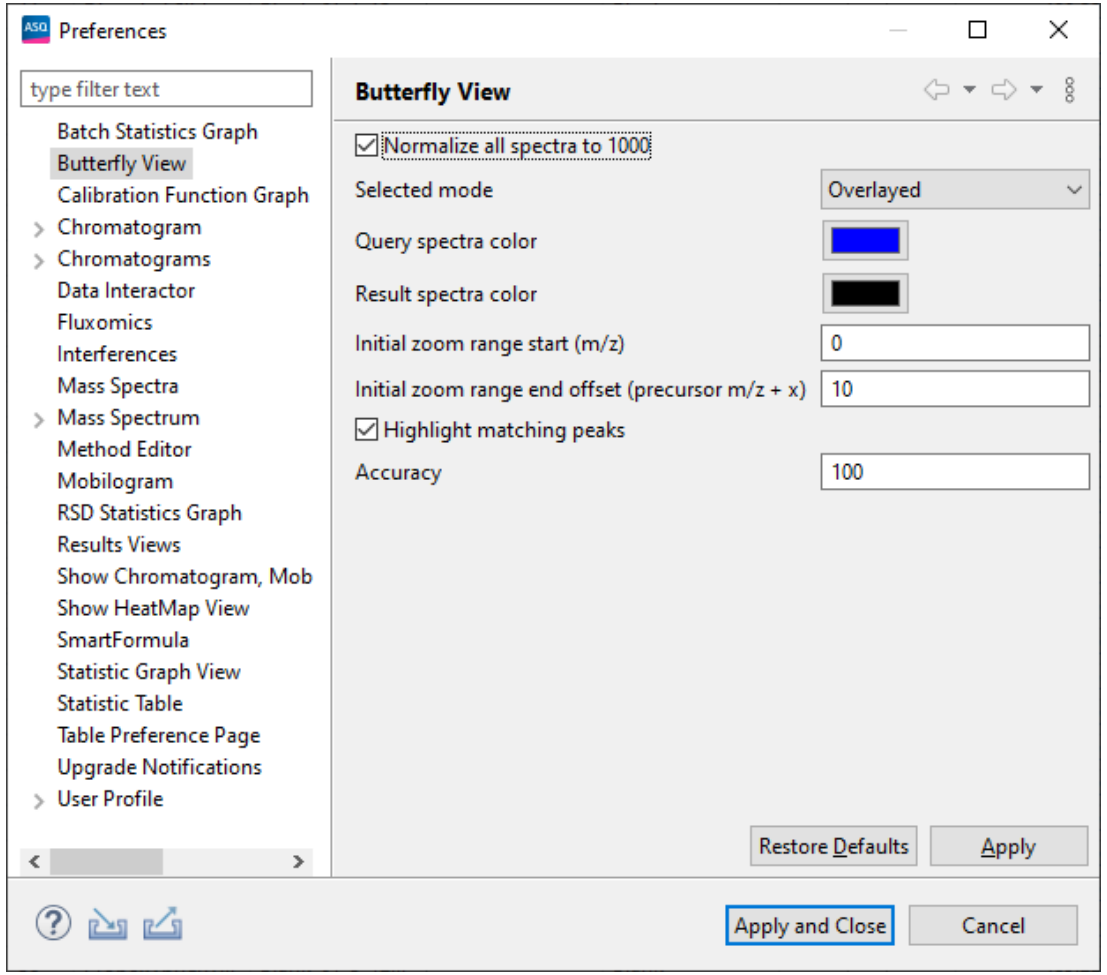
TASQ 2024B: Visual Inspection which Peaks Contributes to Score Value

- Unknown spectrum: Blackberry
- Library spectrum: Liloc



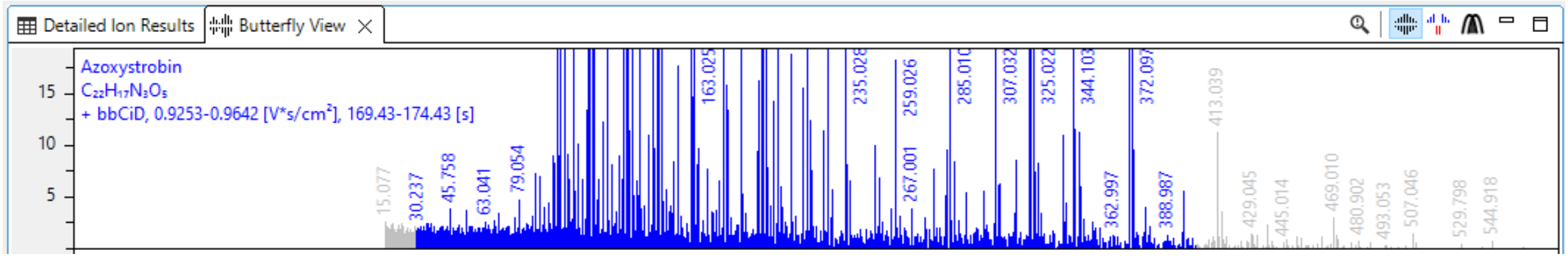
TASQ 2024B: Butterfly View – Preference settings

- Change options on how to display the measured spectra and found library spectrum
- Change colors, zooming, normalization and highlight peaks used for scoring



TASQ 2024B: Library Search – Preparation of Query Spectrum

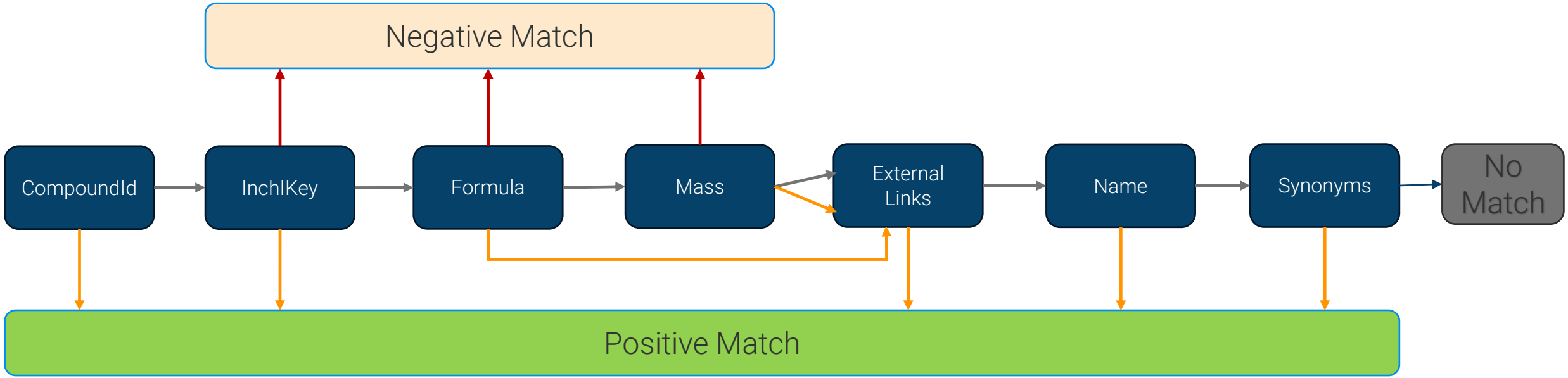
- The observed spectrum will be filtered prior to library search
  - The interval where the isotopic pattern of the precursor resides will be removed
  - The tail of spectrum with *m/z* greater than mass of precursor / z with z=1 will be removed
  - Peaks with *m/z* < 30 will be removed
  - Peaks with an intensity less than the specified intensity threshold will be removed
  - Filtered peaks will be shown in light grey



TASQ 2024B: Library Search – Matching Analytes of found Library Spectra

- A determination is assigned to an analyte in TASQ method
- A found library spectrum is assigned to an analyte, which may be the same chemical compound as in the TASQ method
- To test whether the analyte of the determination is the same as the analyte of the library spectrum a series of comparison are performed

TASQ 2024B: Library Search – Matching Analytes



- CompoundId: The match is positive if both AnalyteDB compoundIds are equal.
- InchIKey: If an InchIKey exists on both sides, the match is positive if the keys are the same. Otherwise the match is negative.
- Formula: If a formula is present on both sides, the match is neutral if they are identical. Otherwise the match is negative.
- Mass: If a mass is present on both sides, the masses must be equal (a threshold is applied) to trigger a positive match. Otherwise the match is negative.
- External Links: Check registry numbers like: CAS, KEGG, PubChem, Chemspider if available
- Name: If the names are similar enough (JaroWinklerSimilarity) , a positive match is triggered.
- Synonym: If one synonym matches the name, a positive match is triggered.

TASQ 2024B: Library Search – Assign a Score

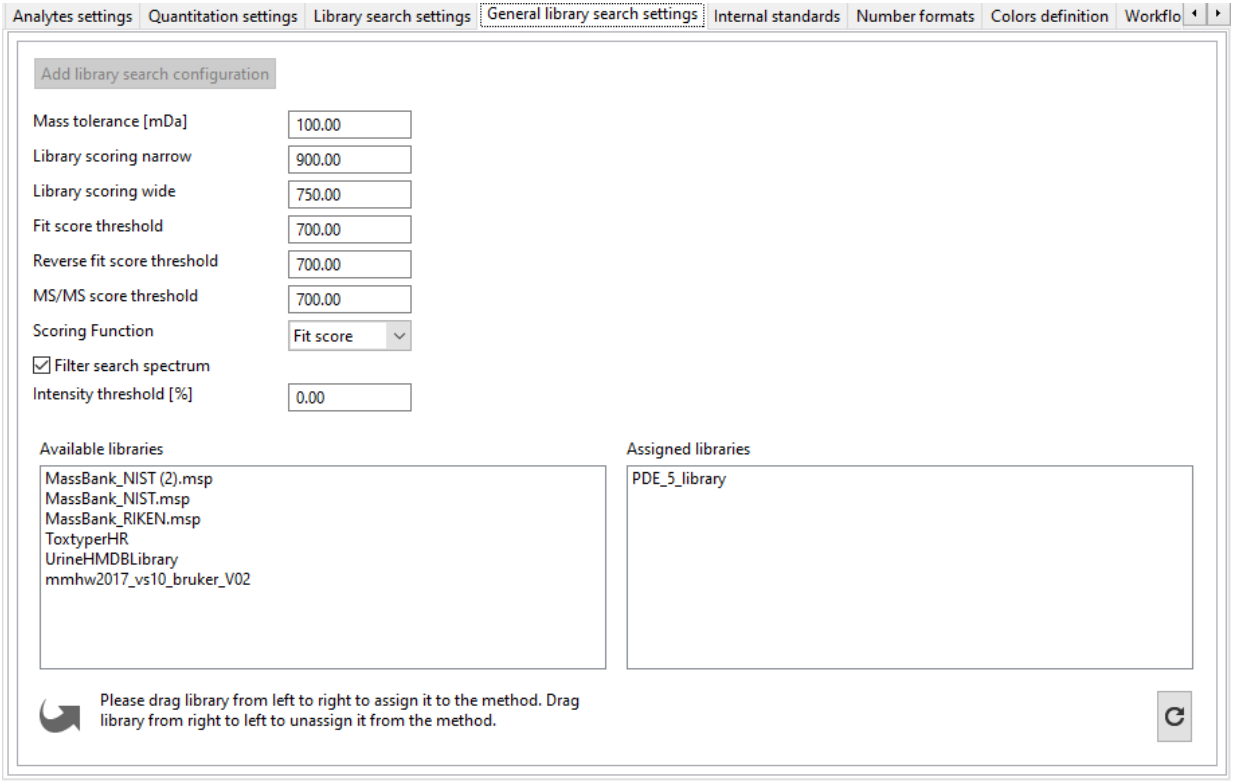
- SCORENA: If no search spectra could be generated – No MS/MS spectra acquired or retrieved
- Score.ZERO: Either the library search gives not results, or the compound matching is negative
- Score.ONE:
  - Either the compound match is positive and the score is below the wide threshold and above the narrow score
  - or the match is neutral and the score is above the narrow threshold.
- Score.TWO: The compound match is positive and the score is above the wide threshold.
- Score narrow and wide score are specified in the TASQ method

TASQ 2024B: Library Search – Assign a Score

```
ScoreType.SCORENA => no ms/ms spectra (or search not yet performed)
 This case is handled outside of this routine.

ScoreType.ZERO    => matching compound and score below scoringWideTolerance
                     or no match
                     or negative match

ScoreType.ONE     => matching compound and score below scoringNarrowTolerance
                    or no match and score above scoringWideTolerance

ScoreType.TWO     => matching compound and score above scoringNarrowTolerance
```

TASQ 2024B: Library Search – Assign a Score

- Specify which score category shall be presented as library score value
- Scoring narrow/wide tolerance for assigning library score rate



TASQ 2024B: Detailed Library Search Results View: Columns

Analyte	Name of determination compound
CCS	Collision cross section of the library compound
CDR Spectrum Id	CDR Spectrum Id
Coll. Energy Library [eV]	Collision energy applied for generation of MS/MS library spectrum
Fit Score	Fit score of acquired spectrum in this data set and matched library spectrum
Formula	Elemental composition of the determination compound
Formula Difference	Difference of elemental composition of the determination and library compound
Instrument	Instrument used for recording the library spectrum
Label	Description of the found library spectrum
Library Label	Library which contains the matched library spectrum
Library Score	Score value (MS/MS score, Fit score, or RFit score) of the best library spectrum
Library Score Description	Information how the library scoring was derived
Library Scoring Function	Score type used for identifying the best library search hit
Library Scoring Score	Score value retrieved from library search. Score is one of MS/MS score, Fit score, or RFit score value
MS/MS Score	Overall MS/MS score of acquired spectrum in this data set and matched library spectrum
Matching Description	Information of how good the analyte in the TASQ method was matched with the analyte assigned to the library spectrum.

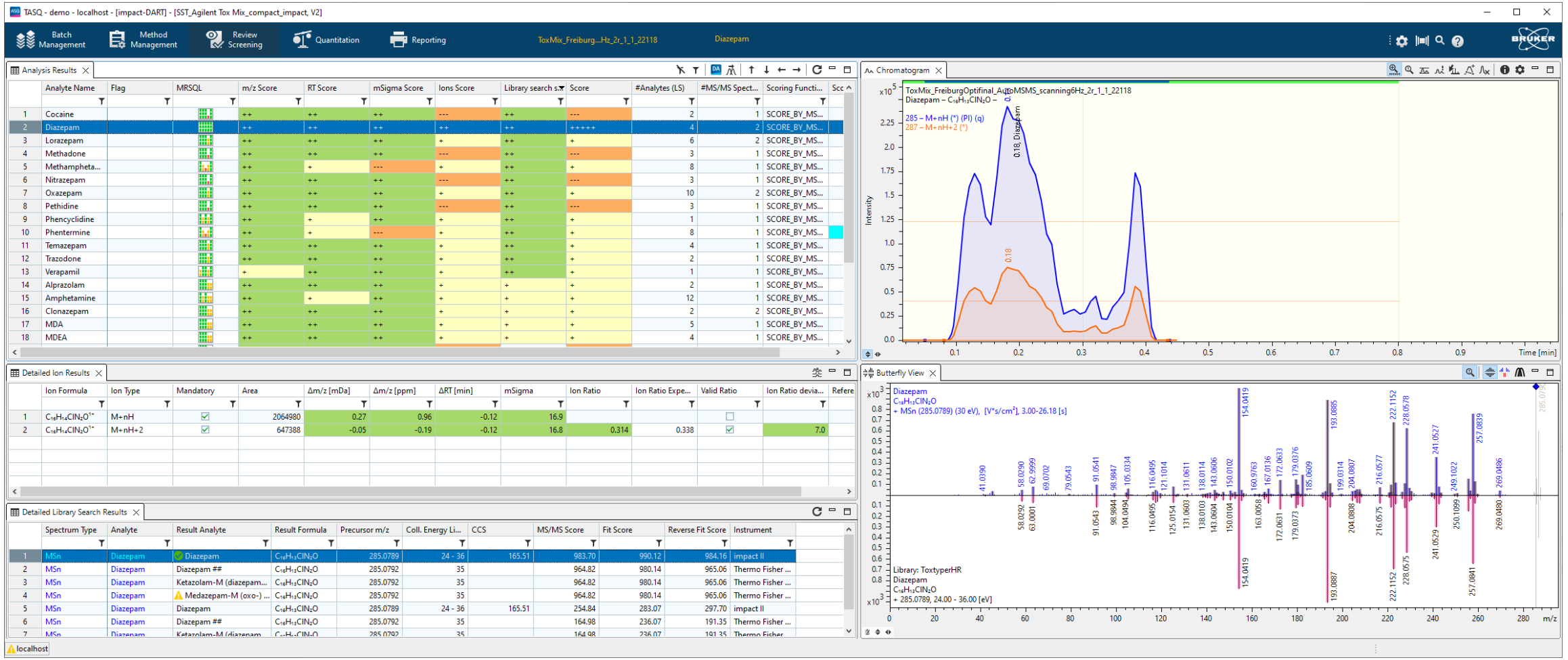
TASQ 2024B: Detailed Library Search Results View: Columns cont.

Matching Score	Information of how good the analyte in the TASQ method was matched with the analyte assigned to the library spectrum.
Matching Type	Category which matching was successful to assign the analyte of the TASQ method and the analyte assigned to the library spectrum, or for which reason it wasn't matched.
Max Intensity	Max intensity of Query Spectrum (precursor range excluded)
Mob. Interval	Mob. Interval
Origin Label	Origin label giving information of used instrument, ionization source and polarity to generate the library spectrum.
Polarity	Polarity
Precursor Deviation *m/z*	Precursor Deviation *m/z*
Precursor *m/z*	*m/z* value of the ion isolated and fragmented to create the MS/MS library spectrum
Result Analyte	Name of library compound
Result Formula	Elemental composition of the library compound
Reverse Fit Score	Revers fit score of acquired spectrum in this data set and matched library spectrum
Review State	The review state of that library finding.
Rt Interval [s]	Rt Interval [s]
Search Precursor m/z	Search Precursor m/z
Spectrum Type	Spectrum Type
Sum Intensity	Intensity sum of Query Spectrum (precursor range excluded)

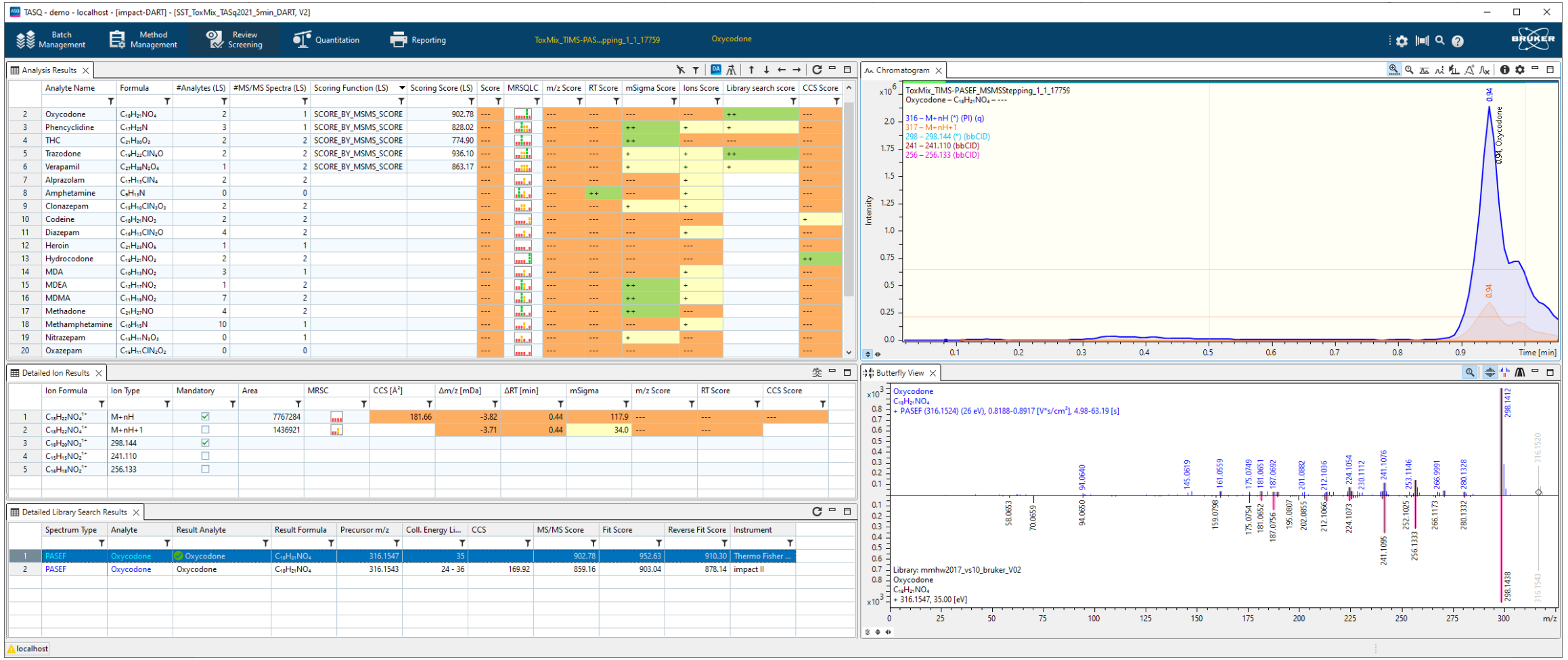
Library Search – Supported Data Types

Instrument type	Spectrum type	Tested / Smoke test
TQ	Fullscan	
	Product ion	
TOF	bbCID	yes – does not reveal results, due to high background
	AutoMSn	yes
	MRM	no – not tested
timsTOF	bbCID	yes
	PASEF	yes
	prm-PASEF	yes
	dia-PASEF	no

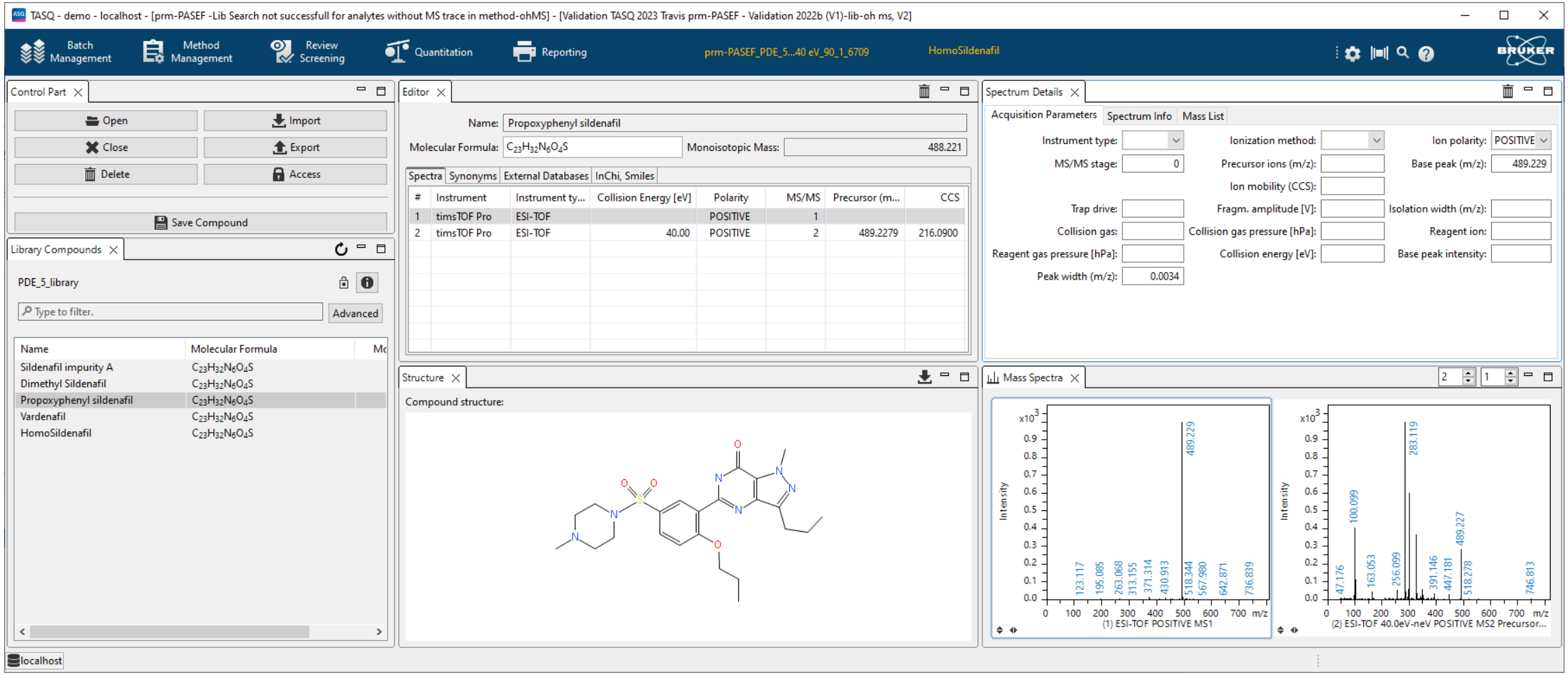
TASQ 2024B: DART impact AutoMS/MS– Library Search Example – Tox Screening



TASQ 2024B: DART timsTOF-PASEF– Library Search Example – Tox Screening

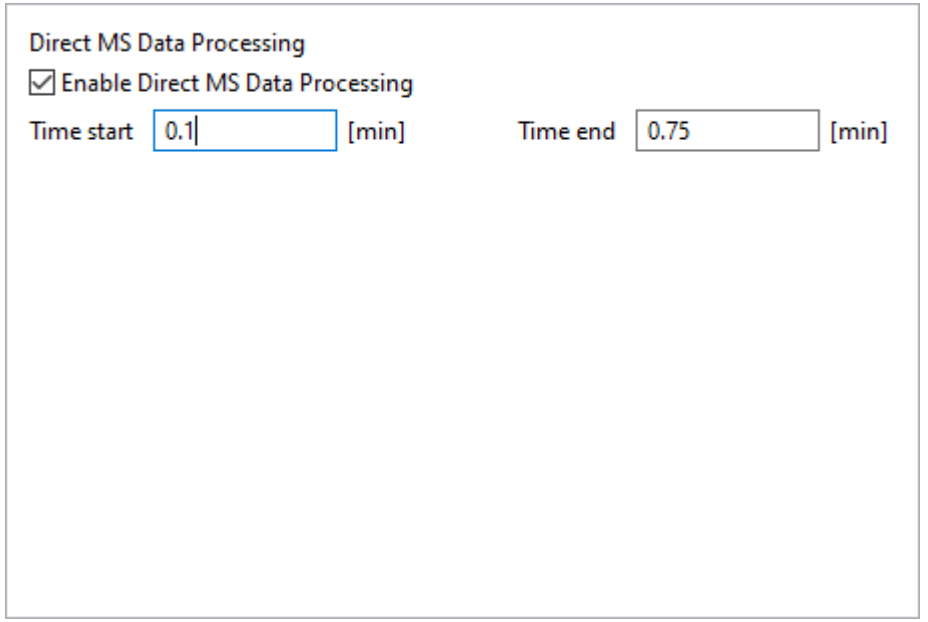


TASQ 2024B: Library Management Perspective



TASQ 2024b: ChromatograFree Processing

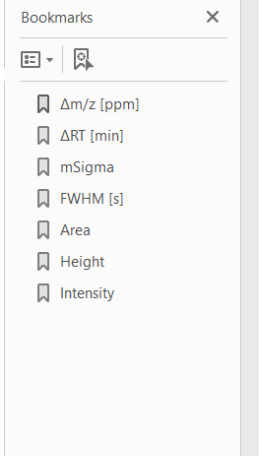
- New parameters for Direct MS Data processing
  - Perform processing for chronogram or direct infusion measurements
  - Create chronograms for the entire acquisition time range
  - Process data in acquisition time range from – to
  - Time range 0. – 0. will use the entire acquisitions time range for processing
- Checks for chromatographic peak type data are switched off
  - SignalToNoise
  - MinNumberOfPoints
  - RetentionTime
  - MinPeakOverlap
  - PeaksCloseness
  - PeakApexWithinOtherPeaks
  - CrossCorrelation
  - A/H filter



TASQ 2024B: Supported Instruments for Direct MS Processing

- Supported instruments
  - TQ fullscan
  - TOF - autoMS/MS data can be used for library searching
  - timsTOF - PASEF data can be used for library searching

TASQ RealTimeQC: Batch Report Available from TASQ and RTQC



Demo Data Quantitation – RealTimeQC Sample Type Statistics

Operator	bdal@de	Station Name	NBBRE01-5V7J1T3
Instrument Name	impact HDII	Instrument SN	1825153.10011
TASQ Method	Demo Data Quant (3)		

Δm/z [ppm]

Alprazolam

Δm/z [ppm]

Statistic	Blank	QC Sample	Calibrant	Sample
n	0	0	18	2
%RSD			57.65	44.09
Mean			2.00	1.57
StdDev			1.15	0.69
Max			4.55	2.06
Min			0.63	1.08

Alprazolam D5

Δm/z [ppm]

Statistic	Blank	QC Sample	Calibrant	Sample
n	0	3	18	4
%RSD		28.75	35.92	41.92
Mean		1.01	1.61	1.07
StdDev		0.29	0.58	0.45

ΔRT [min]

Alprazolam

ΔRT [min]

Statistic	Blank	QC Sample	Calibrant	Sample
n	0	0	18	2
%RSD			-135.57	-90.15
Mean			-0.01	-0.01
StdDev			0.01	0.01
Max			0.00	-0.00
Min			-0.05	-0.01

Alprazolam D5

ΔRT [min]

Statistic	Blank	QC Sample	Calibrant	Sample
n	0	3	18	4
%RSD		-1615.18	-121.73	-63.16
Mean		-0.00	-0.01	-0.01
StdDev		0.01	0.01	0.00
Max		0.01	0.00	-0.00
Min		-0.02	-0.05	-0.01

Diazepam

ΔRT [min]

Nordiazepam

Area

Statistic	Blank	QC Sample	Calibrant	Sample
n	1	3	18	2
%RSD	0	2	111	0
Mean	10082	792724	1762192	1947523
StdDev	0	11938	1956985	1176
Max	10082	806169	5658428	1948355
Min	10082	783370	143128	1946692

Nordiazepam D5

Area

Statistic	Blank	QC Sample	Calibrant	Sample
n	0	3	18	4
%RSD		4	4	9
Mean		1138370	1146265	1177203
StdDev		41129	45260	101969
Max		1185402	1251075	1291798
Min		1109146	1057500	1086509

Oxazepam

Area

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Nordiazepam

FWHM [s]

Statistic	Blank	QC Sample	Calibrant	Sample
n	1	3	18	2
%RSD	0.0000	1.8882	1.6852	3.2959
Mean	4.5078	3.3729	3.3429	3.3747
StdDev	0.0000	0.0637	0.0563	0.1112
Max	4.5078	3.4443	3.5101	3.4534
Min	4.5078	3.3219	3.2895	3.2961

Nordiazepam D5

FWHM [s]

Statistic	Blank	QC Sample	Calibrant	Sample
n	0	3	18	4
%RSD		2.3011	1.3815	2.2731
Mean		3.3616	3.3379	3.3535
StdDev		0.0774	0.0461	0.0762
Max		3.4458	3.4721	3.4677
Min		3.2937	3.2850	3.3110

Oxazepam

FWHM [s]

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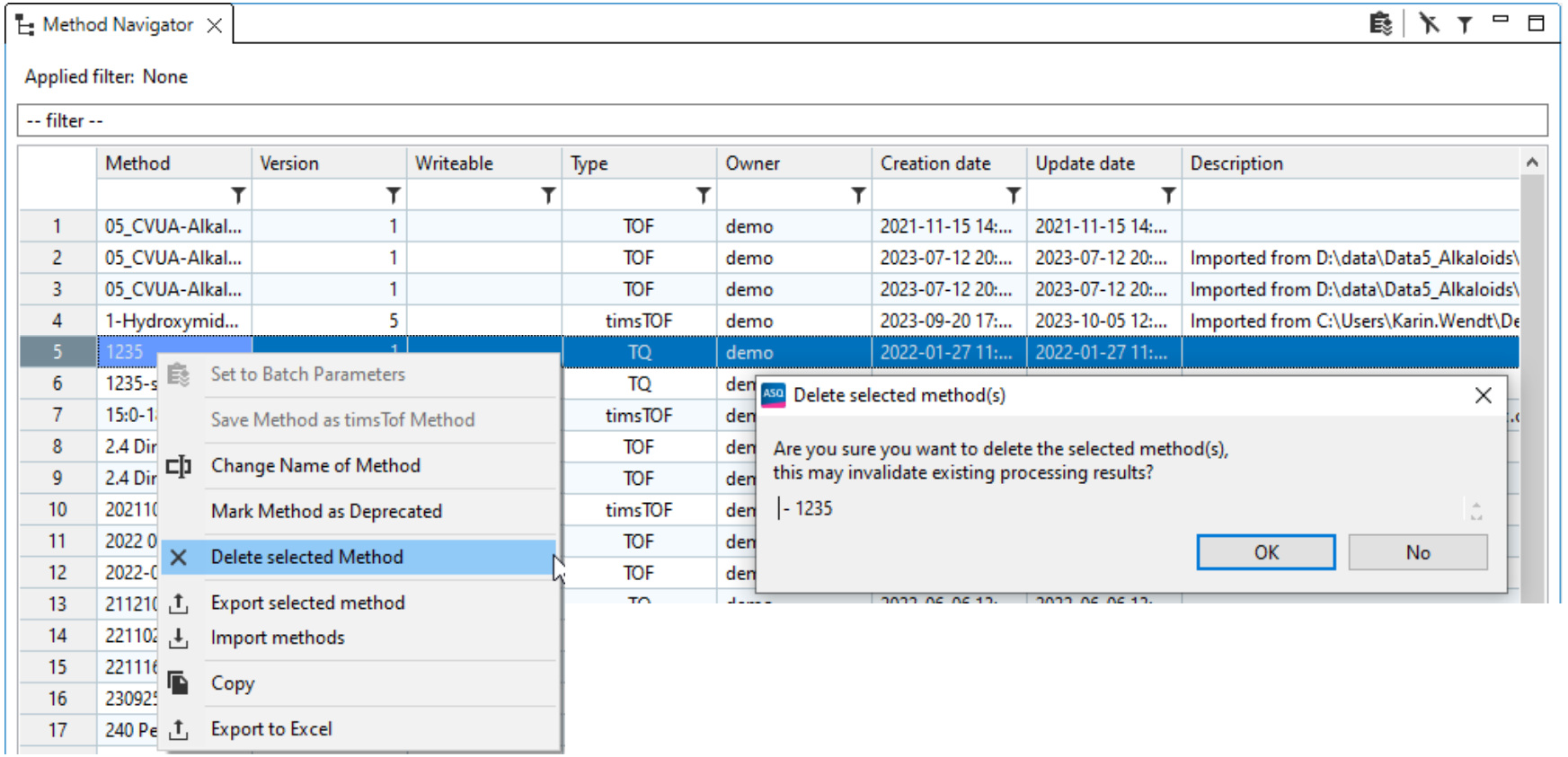
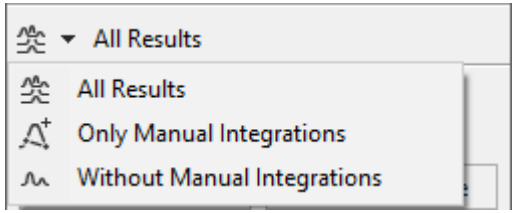
TASQ 2024B: Delete TASQ Method Removes it from Database

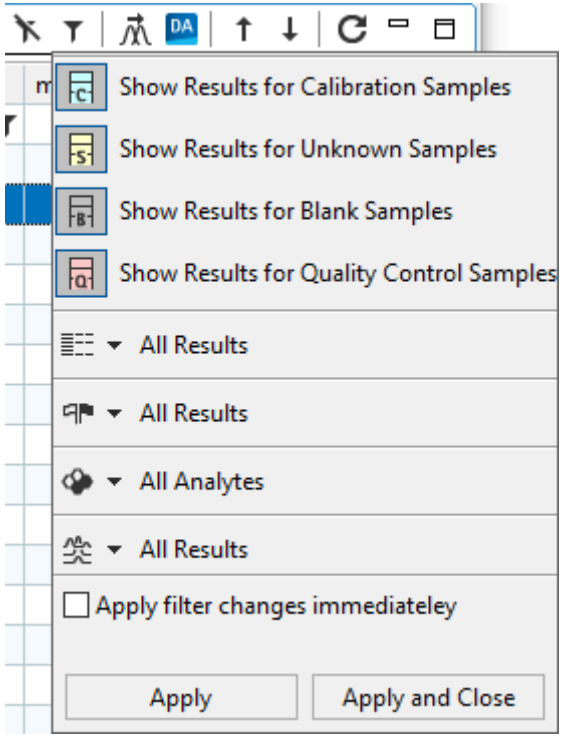
- Delete method in method navigatore removes the method from data base irrevocable
  - May create invalid results if the user acts thoughtless



TASQ 2024B: Filter Options in Result Views

- New filter option dialog for filtering result tables, all filters are available in the new dialog
- The filter toolbar button changes if data is filtered
- The filter can be switched off in the toolbar
- New filter option: manually integrated
  - show all – show manually integrated – show not manually integrated

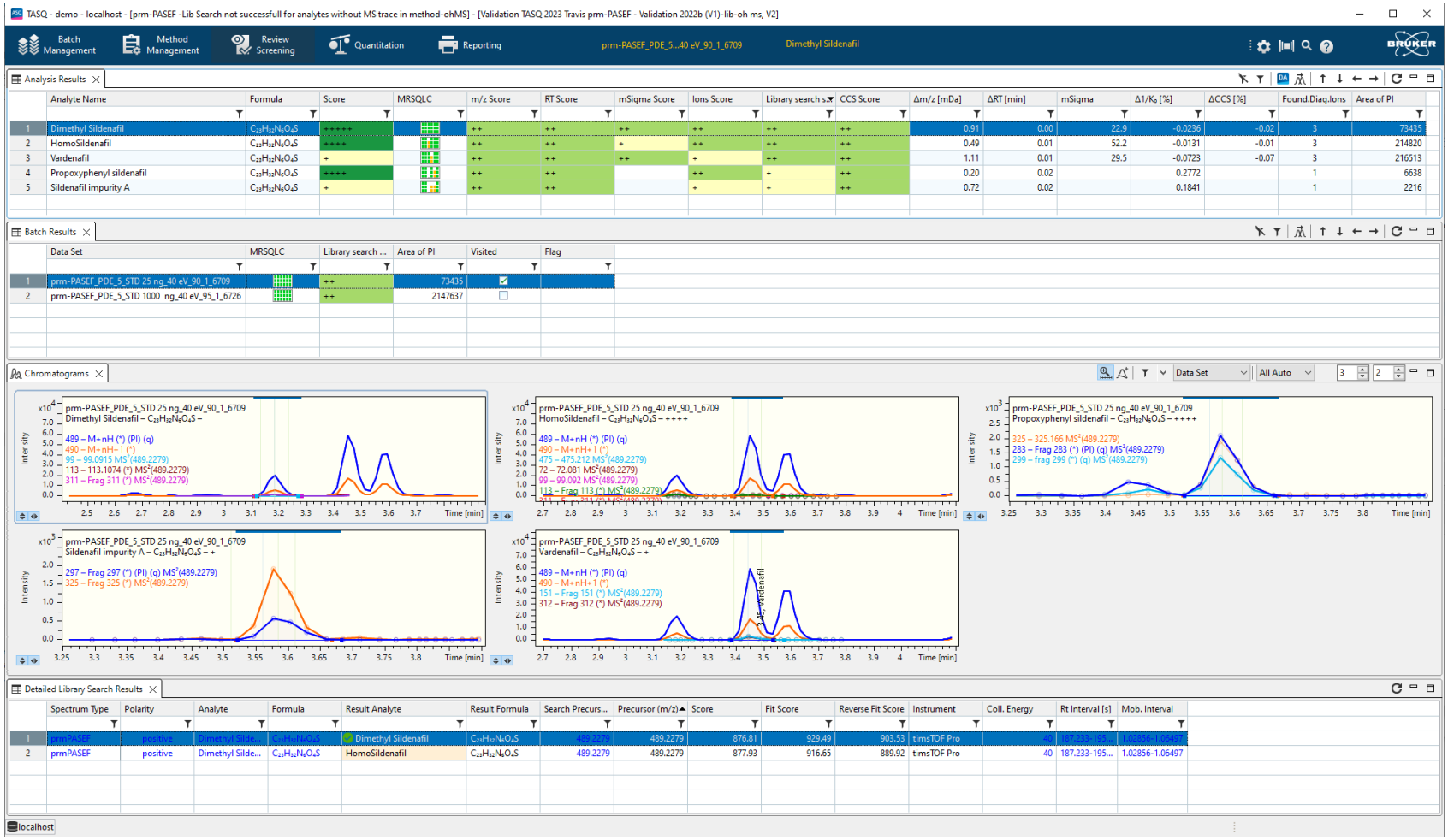




  - Filters can be applied immediately on change, or explicitly by pressing Apply or Apply and Close

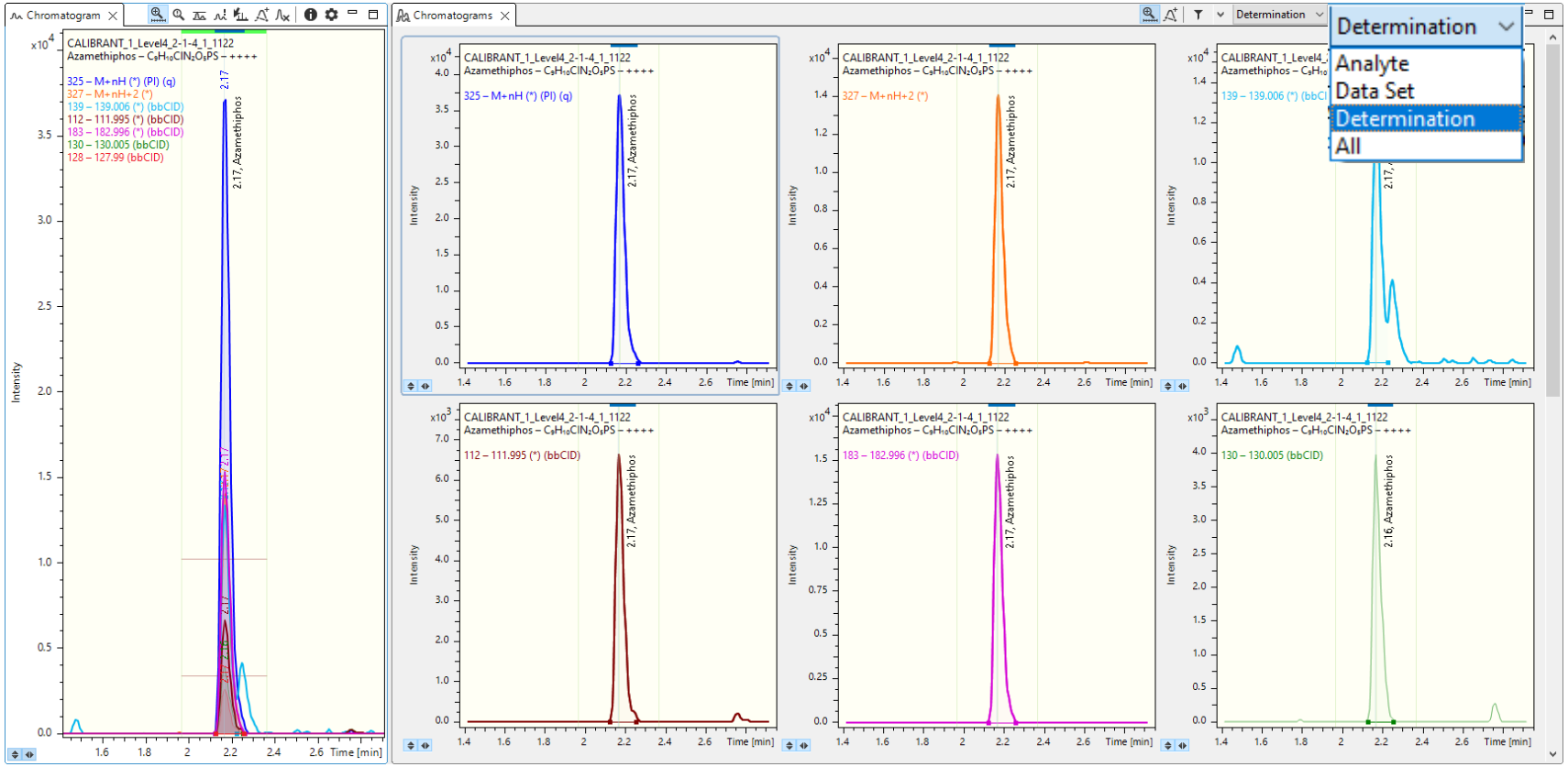
TASQ 2024B: Cleaned up Toolbar – Reduced Number of Icons

- Filter buttons are moved to a filter dialog
- All other buttons to toggle information shown in the Chromatogram/s views are moved to the preference dialog



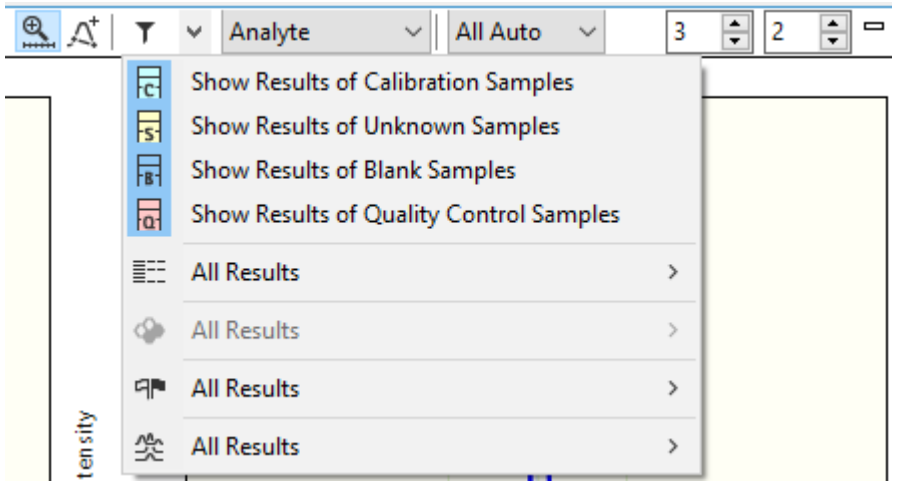
TASQ 2024B:Chromatograms View – Select Data Source

- Show chromatograms of selected determinations – list chromatograms of all ions seperately – same list as in Detailed Ion Results view
- Analyte: show all findings for selected analyte – same list as Batch Results view
- Data Set: show all findings for selected data set – same list as Analysis Results view
- All: show all findings for selected batch – same list as Global Results view



TASQ 2024B:Chromatograms View – New Options

- New filter option dialog, used in all other result views
- Individual filter buttons were removed from the toolbar to give a cleaner appearance

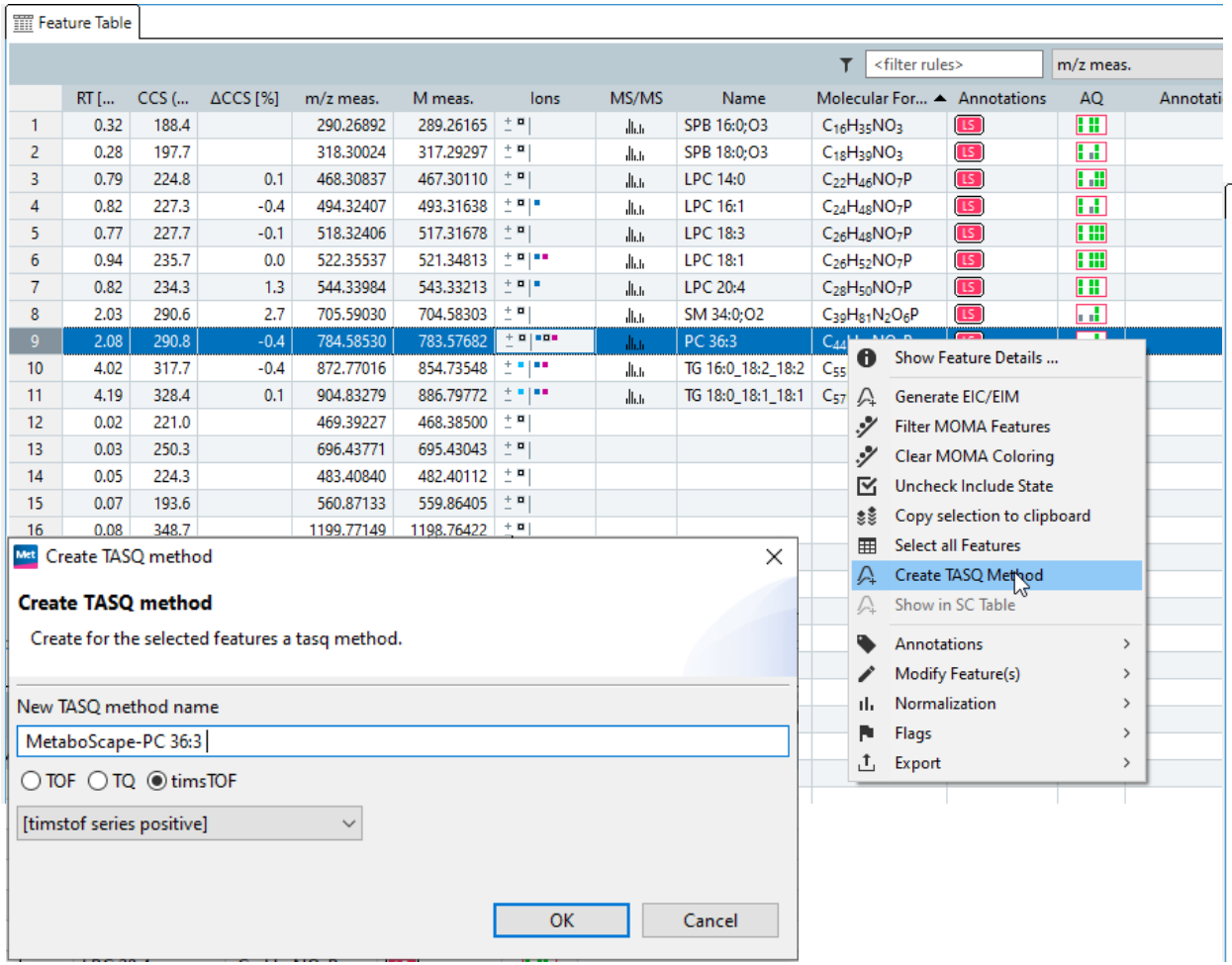


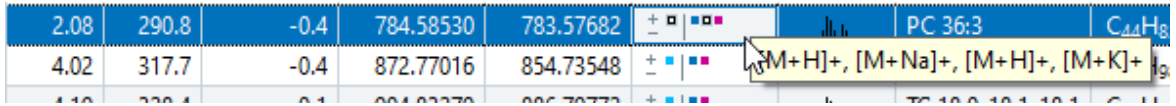
- Manual integration is available in Chromatograms view, no need to change to the Chromatogram view for changing the peak boundaries

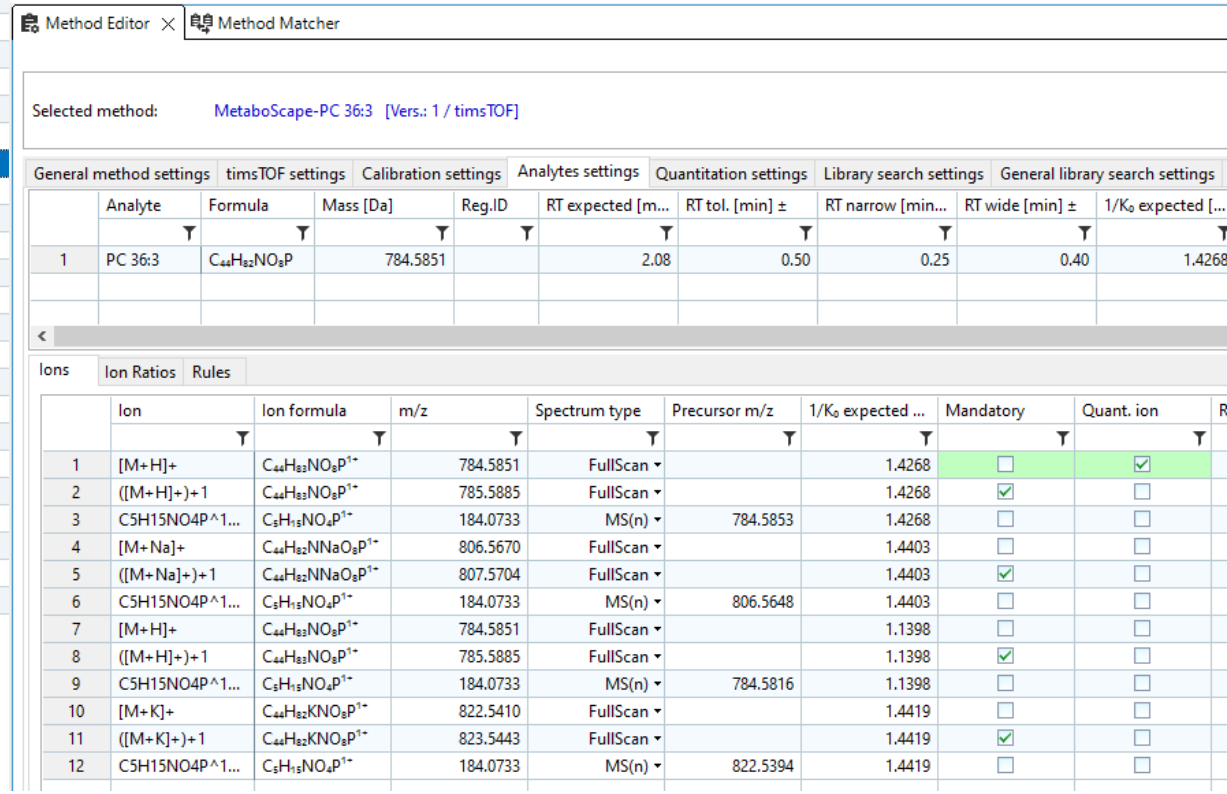
MetaboScape 2024B: Create TASQ Method of Selected Features Available

- Select one or more features in MetaboScape feature table
- Select **Create TASQ Method** from context menu
- Enter name for new TASQ method
- Specify the instrument type for which the method shall be created
- Select from a list of available method profiles for the selected instrument type
- For each selected feature an analyte will be added to the new TASQ method
- For each ion in the selected feature an ion will be added to the analyte in the TASQ method
- For each detected adduct all isotopologues will be created as specified in the selected method profile
- In case of timsTOF data for each ion with different $1/K_0$ value in the detected feature a separate ion will be added to the list of ions

MetaboScape 2024B: Create TASQ Method of Selected Features Available

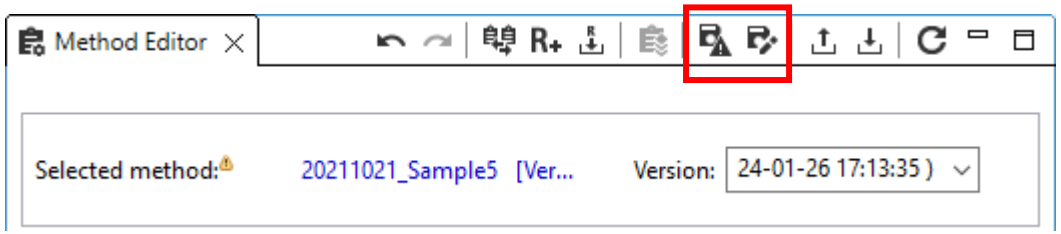






TASQ 2024B: Miscellaneous

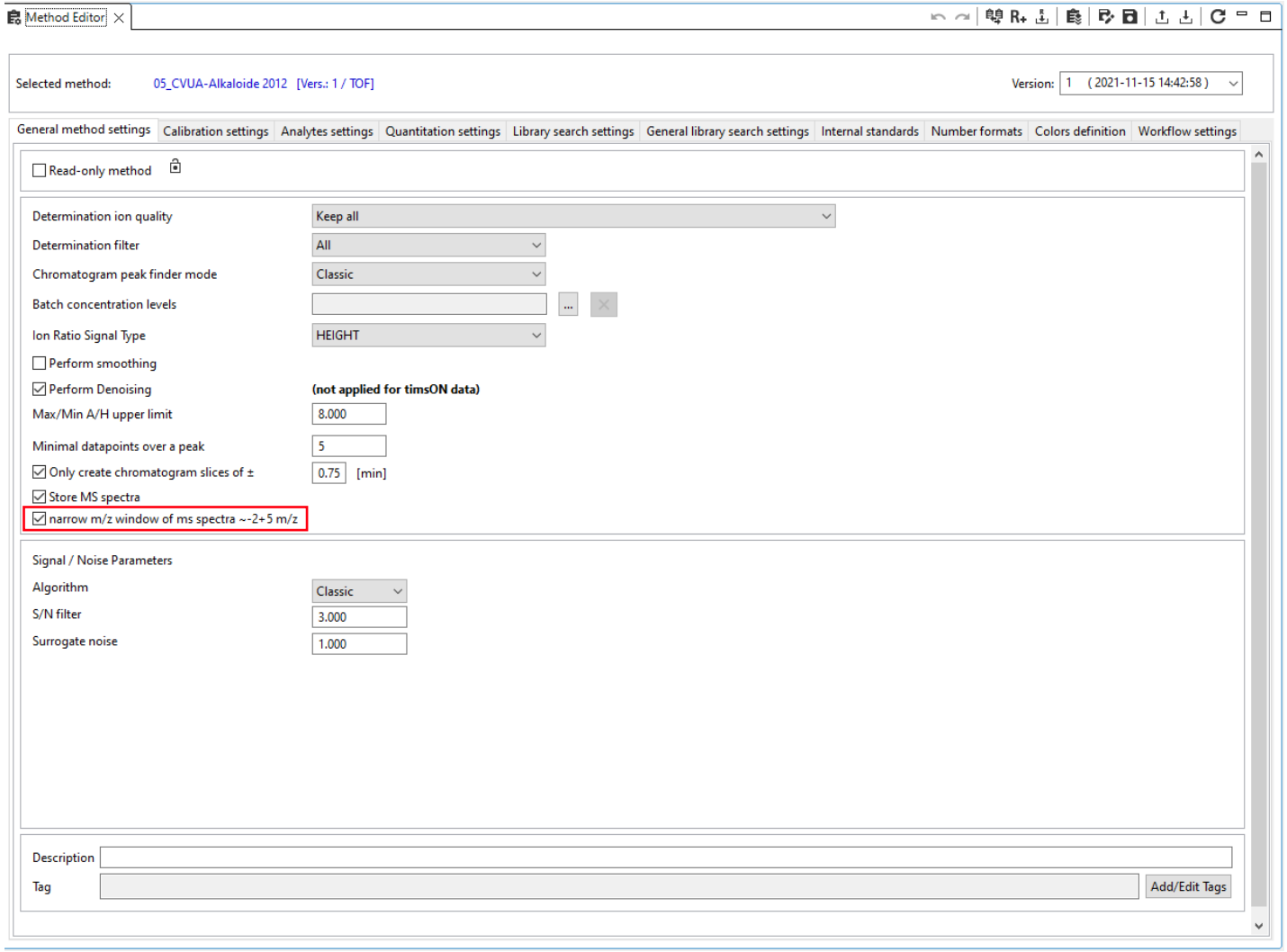
- Improvements in Heat Map
  - Point selection mode – scroll mouse wheel: zoom image – Ctrl scroll: enlarge selection box width – Shift scroll : enlarge selection box heigth
  - Zoom: showing box containing all determinations
- Improvements in selection behaviour of tables in wizards
- Method matcher handles library search parameters
- Method profile editor manages library search parameters



- Swapped order of Save and Save as… toolbar item
- Improved zooming on butterfly view – normalize excluding precursor peaks – zoom y axis automatically to 1000
- Show matched peaks always in butterfly view – preferences
- Stable sorting of tables: order of null or <empty> cells

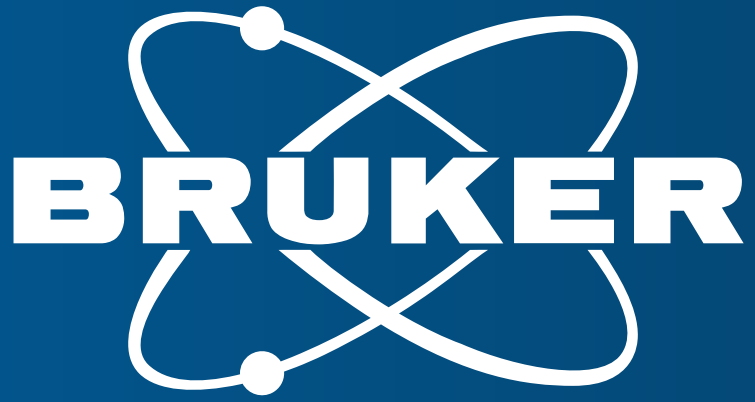
Known Problems

- Automatic workflow fails to process.
- Processing is aborted
- A very high memory consumption to be observed which makes the processing task to abort and potentially will stop the acquisition
- To circumvent that problem make sure that the option „**narrow *m/z* window of MS spectra**“ is switched on!



Known Problems: Slow Performance Quantitation, Delete Determinations

- A customer performed an upgrade from TASQ 2022B to TASQ 2023B
- Database update took 7 days, ~90,000 data set results
- After that quantification was such slow that it finally was aborted
- Same to delete determination
- The customer used TASQ for a very long period
- Postgre 10 was still installed
- Database comprised 450 GB
- Solution: Create a backup of DB, uninstall TASQ SW and postgre. Reinstall TASQ and new postgre version. Restore the data base
- Performance was restored
- Database size after restore was only 380 GB, backup size is 170 GB ~ 200 GB of index size



Innovation with Integrity