

TASQ 2025

What is new in TASQ 2025

TASQ 2025 – Features

- User Workflows
 - More complex processing workflows, e.g., process, quantify, evaluate results, export
 - Check batch and method which steps can be executed successfully
 - New tsq-processing workflow implemented
- Library Search continued
 - Library Compound Matcher: match tasq method compounds and library compounds store matches in tasqMethod
 - Improved score calculation – matching approach instead of binning
 - Loading raw MS/MS spectra improved
 - Data provider of library search results available
 - LIMS export contains library search results
- Support sample sub types

TASQ 2025 – Features

- Improved viewers
 - List viewer for chromatograms
 - Show traces for determination
 - Show traces for BPC
 - Show pressure traces
 - Show UV traces
 - List viewer for MS library search results
 - Mobilograms viewer
 - Support manual integration in Chromatograms / Mobilograms view
 - Show and edit flags and review state in all views (table, graph)

TASQ 2025: Improvements

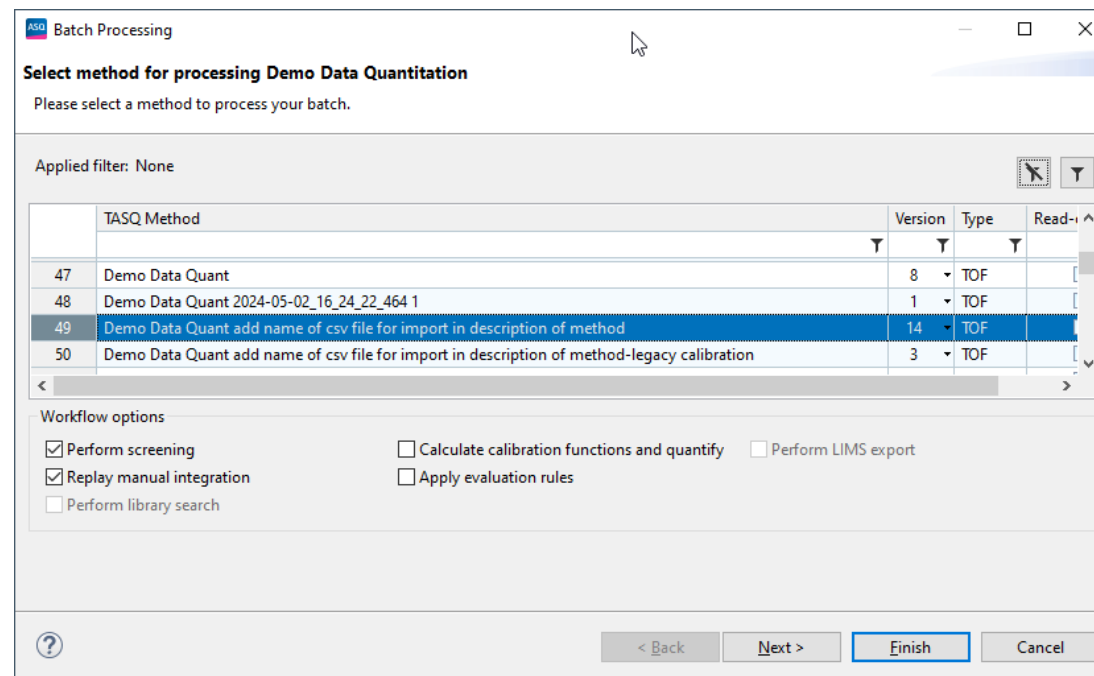
- QSee Performance Test finalized as part of the QSee product family
- Analyte tags in statistics table for grouping
- Statistics table sends notification of selected analyte
- Extended options for m/z and 1/K0 calibration
 - User can use calibration created by DataAnalysis or MetaboScape (only for tsf and tdf data sets)
- Clear indication if Bruker MS Data Processing server is connected to the station where batch data is located
- Drag & Drop of .tasqMethod files from file explorer into Batch Summary view imports the TASQ method
- Change order of ions in ion table by [ALT] Arrow Up | Down
- Improved performance for storing of concentrations
- Method editor include 1/K0 and precursor m/z for interference detection
- Improved SmartFormula View

TASQ 2025: Improvements

- If audit trail or user actions rights are active client checks whether Compass Regulatory toolkit license is activated – otherwise TASQ client does not work – clear indication given if license is required
- Bug fixes and improvements

TASQ 2025: User Workflows

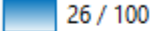

- When reprocessing a batch perform quantification and evaluate rules automatically
- Perform individual activities optionally
 - Perform screening
 - Replay manual integration
 - Perform library search
 - Calculate calibration functions and quantify
 - Apply evaluation rules
 - Perform LIMS export



- When quantifying a batch calibration functions will be calculated, quantitative values generated and evaluation rules applied

TASQ 2025: User Workflows

- On some occasions a user workflow can't be started again, as the task queue is in a bad state
- An option is available to purge the task queues, and the user is able to start the user workflow again
- This option will be offered if the state of batch is bad
- Single tasks can be canceled in Task Progress view

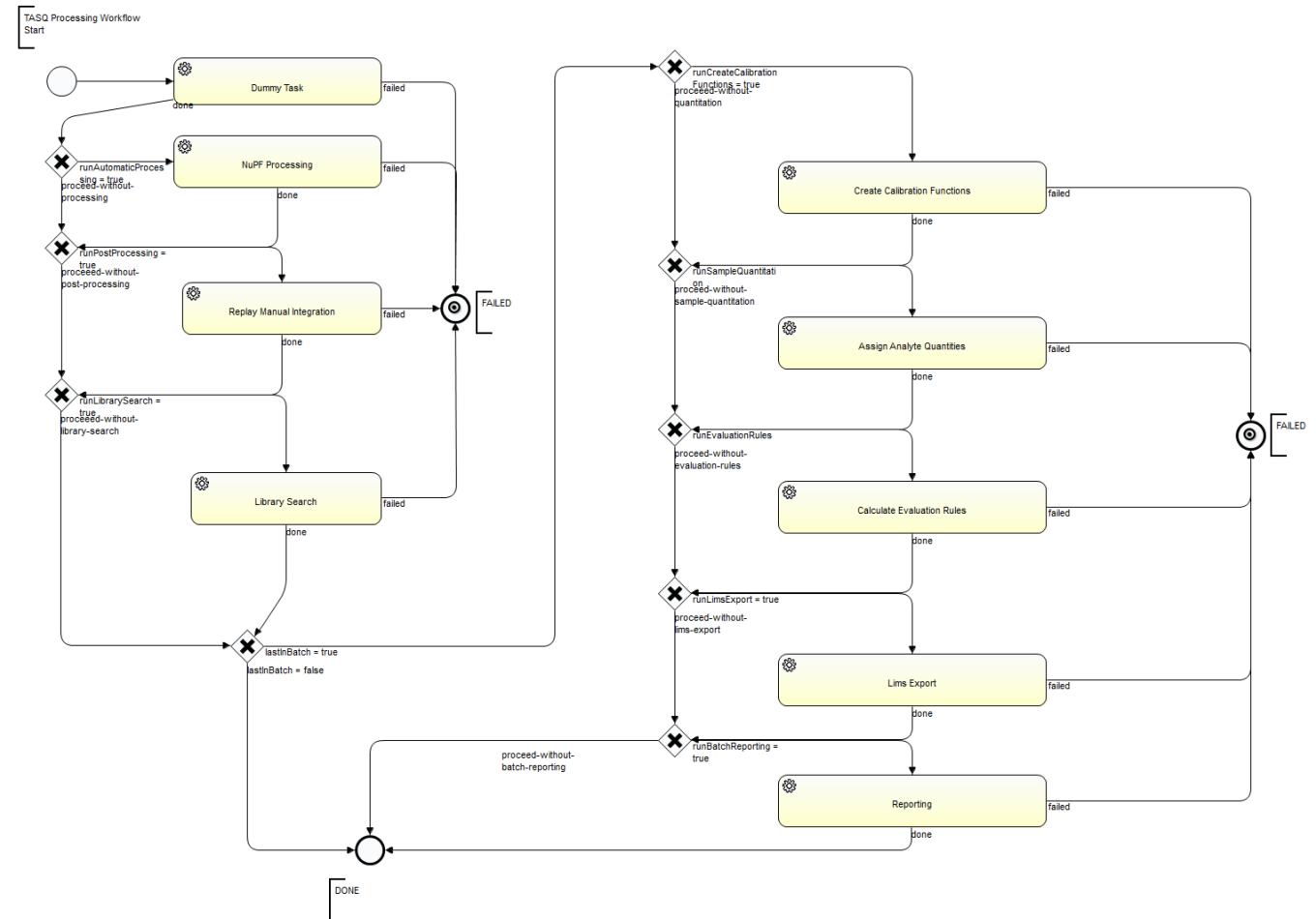
Batch	Data Set	Station	Type	W..	Status	Started	Progress
Demo Data Quantitation	Serum Std Level 4_RB7_01_2547	WSBRE01-HCGB5N3	NuPF automatic pro...		<i>RUNNING</i>	2024-08...	 26 / 100
Demo Data Quantitation	Serum Std Level 4_RB7_02_2548	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum Std Level 4_RB7_03_2549	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum Std Level 5_RB8_01_2550	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum Std Level 5_RB8_02_2551	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum Std Level 5_RB8_03_2552	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum Std Level 6_RC1_04_2553	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum Std Level 6_RC1_06_2554	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum Std Level 6_RC1_07_2555	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	blank_RE6_02_2556	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum A_RC5_01_2557	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	Serum A_RC5_03_2558	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		
Demo Data Quantitation	blank_RE1_01_2559	WSBRE01-HCGB5N3	NuPF automatic pro...		QUEUED		

TASQ 2025: User Workflows

- In case of reprocessing check which steps can be performed based on batch and method
 - If no concentrations are stored for analytes quantification shall not be performed
 - If no spectral libraries are assigned to the method library search shall not be performed
 - All options will be offered if the steps are possible or they will be greyed out

TASQ 2025: tsq-processing Workflow

- This workflow will be started when user choose Process Batch or Reprocess Batch from TASQ client
 - Screening process
 - Replay manual integration
 - Library search
 - Calibration functions for quantification calculated
 - Quantities calculated
 - Calculate evaluation rules
 - LIMS export
 - Report generation – currently disabled

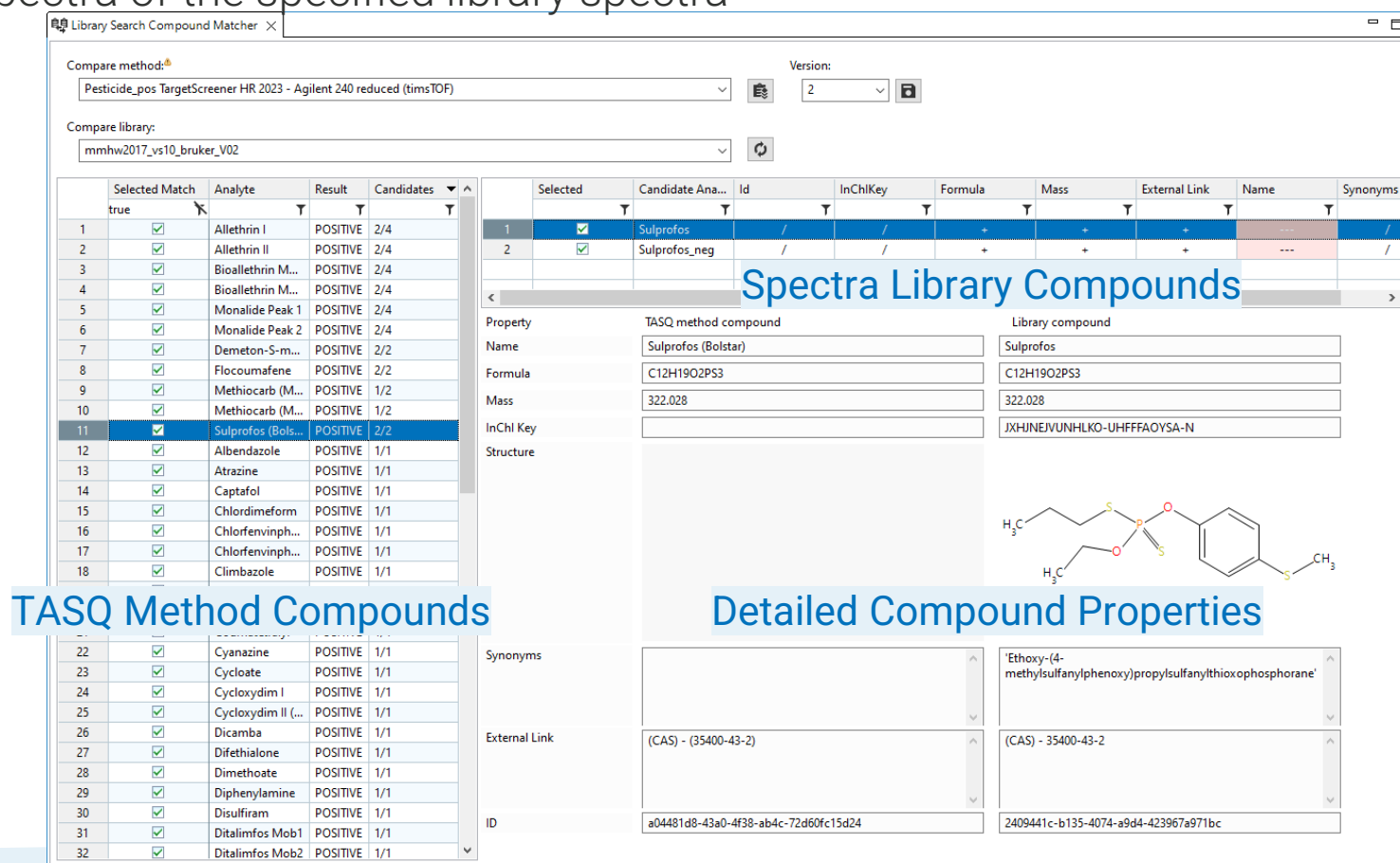


TASQ 2025 – Library Search

- Improved peak matching for score calculation
- Matching of compounds during method development and matched pairs stored in tasq method
- Library search results are filtered by looking up the list the matched pairs in the tasq method
- If for an analyte and a library no compounds are matched all library search results in that library will be reported
- Improved retrieval of MS/MS spectra

TASQ 2025: Library Compound Matcher

- Store compound pairs – TASQ method compound and spectrum library compound – in method
- Use that relation to only check for spectra of the specified library spectra
- Matcher shows all candidates for TASQ method compound
- User selects the correct one from list, if available
- For matching same criteria are applied as for library search
- Multiple library compounds can be assigned to an method compound
- Do not match automatically
- Select method of selected batch



Library Search Compound Matcher


Compare method: Pesticide_pos TargetScreener HR 2023 - Agilent 240 reduced (timsTOF) | Version: 2

Compare library: mmhw2017_vs10_bruker_V02

Selected Match	Analyte	Result	Candidates
1	Allethrin I	POSITIVE	2/4
2	Allethrin II	POSITIVE	2/4
3	Bioallethrin M...	POSITIVE	2/4
4	Bioallethrin M...	POSITIVE	2/4
5	Monalide Peak 1	POSITIVE	2/4
6	Monalide Peak 2	POSITIVE	2/4
7	Demeton-S-m...	POSITIVE	2/2
8	Flocoumafene	POSITIVE	2/2
9	Methiocarb (M...	POSITIVE	1/2
10	Methiocarb (M...	POSITIVE	1/2
11	Sulprofos (Bols...	POSITIVE	2/2
12	Albendazole	POSITIVE	1/1
13	Atrazine	POSITIVE	1/1
14	Captafol	POSITIVE	1/1
15	Chlordimeform	POSITIVE	1/1
16	Chlorfenvinph...	POSITIVE	1/1
17	Chlorfenvinph...	POSITIVE	1/1
18	Climbazole	POSITIVE	1/1

Selected	Candidate Ana...	Id	InChIKey	Formula	Mass	External Link	Name	Synonyms
1	Sulprofos	/	/	+	+	+	---	/
2	Sulprofos_neg	/	/	+	+	+	---	/

Spectra Library Compounds

Property	TASQ method compound	Library compound
Name	Sulprofos (Bolstar)	Sulprofos
Formula	C12H19O2PS3	C12H19O2PS3
Mass	322.028	322.028
InChI Key		JXHJNEJVUNHLKO-UHFFFAOYSA-N
Structure		
Synonyms		'Ethoxy-(4-methylsulfanylphenoxy)propylsulfanythioxophosphorane'
External Link	(CAS) - (35400-43-2)	(CAS) - 35400-43-2
ID	a04481d8-43a0-4f38-ab4c-72d60fc15d24	2409441c-b135-4074-a9d4-423967a971bc

TASQ Method Compounds

22	Cyanazine	POSITIVE	1/1
23	Cycloate	POSITIVE	1/1
24	Cycloxydim I	POSITIVE	1/1
25	Cycloxydim II (...)	POSITIVE	1/1
26	Dicamba	POSITIVE	1/1
27	Difethialone	POSITIVE	1/1
28	Dimethoate	POSITIVE	1/1
29	Diphenylamine	POSITIVE	1/1
30	Disulfiram	POSITIVE	1/1
31	Ditalimfos Mob1	POSITIVE	1/1
32	Ditalimfos Mob2	POSITIVE	1/1

Detailed Compound Properties

TASQ 2025: Library Compound Matcher

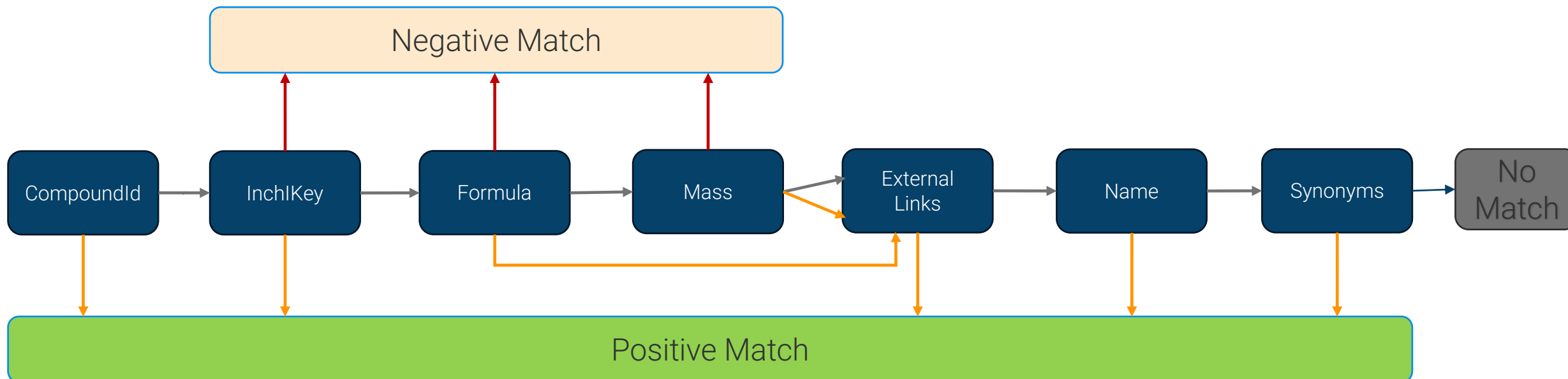
- Compounds are compared by AnalyteDB Id, InChiKey, Formula, Mass, External Link (CAS, PubChem, ...), Name, and Synonyms.
- Comparison results are shown by + (matched), / neutral, --- different
- Id, InChiKey, Name, Synonyms, or External Link will give a positive assignment if one of these matches.
- If elemental composition differs the library compound will be removed from further comparison

36	<input checked="" type="checkbox"/>	Chlorfenvinphos (E/Z) Peak 1 (Main)	POSITIVE	3
37	<input checked="" type="checkbox"/>	Chlorfenvinphos (E/Z) Peak 2 (Minor)	POSITIVE	3

	Selected	Candidate Analyte	Id	InChiKey	Formula	Mass	External Link	Name	Synonyms
	▾	▾	▾	▾	▾	▾	▾	▾	▾
1	<input checked="" type="checkbox"/>	Chlorfenvinphos	/	/	+	+	+	---	/
2	<input type="checkbox"/>	alpha-Chlorfenvinphos	/	/	+	+	/	---	/
3	<input type="checkbox"/>	beta-Chlorfenvinphos	/	/	+	+	/	---	/

- To compare analyte names is non trivial. Wrong spelling, trivial names, ...
- caffeine – Koffein – Kofeiini – Cafeína – 咖啡因 – Tein – Guaranin – 1,3,7-Trimethyl-3,7-dihydro-1H-purin-2,6-dion

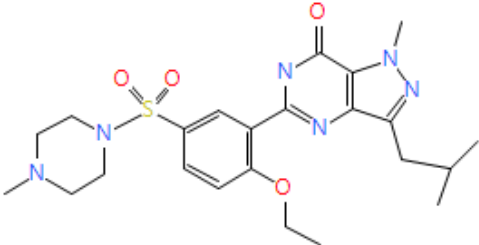
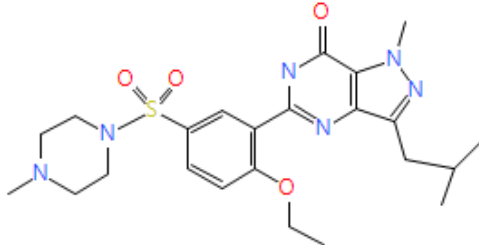
TASQ 2025: Library Search – Matching Analytes



- 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, Chempider if available
- Name: If the names are similar enough (JaroWinklerSimilarity) , a positive match is triggered. Otherwise, it is considered as no match.
- Synonym: If one synonym matches the name, a positive match is triggered.

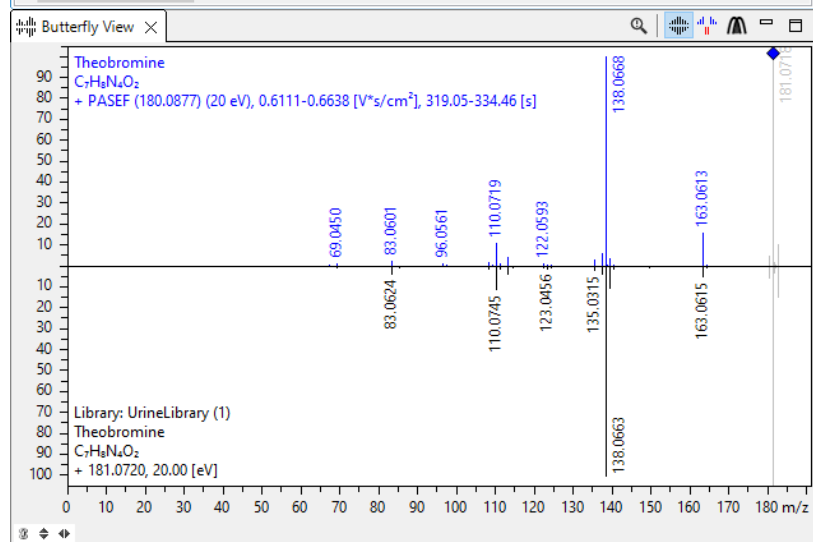
TASQ 2025: Library Compound Matcher

- If available the chemical structure will be shown

Property	TASQ method compound	Library compound
Name	<input type="text" value="Sildenafil impurity A"/>	<input type="text" value="Sildenafil impurity A"/>
Formula	<input type="text" value="C23H32N6O4S"/>	<input type="text" value="C23H32N6O4S"/>
Mass	<input type="text" value="488.221"/>	<input type="text" value="488.221"/>
InChI Key	<input type="text"/>	<input type="text"/>
Structure		
Synonyms	<input type="text"/>	<input type="text"/>
External Link	<input type="text"/>	<input type="text"/>
ID	<input type="text" value="59cf390a-1e4e-4271-b3f7-66a98cff7c6d"/>	<input type="text" value="59cf390a-1e4e-4271-b3f7-66a98cff7c6d"/>

TASQ 2025: Library Search Results Data Provider Available

	Spectrum Type	Polarity	Analyte	Formula	Result Analyte	Result Form
1	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	⚠ Paraxanthine	C ₇ H ₈ N ₄ O ₂
2	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	✅ Theobromine	C ₇ H ₈ N ₄ O ₂
3	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
4	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
5	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
6	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
7	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
8	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
9	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	⚠ Caffeine-M (...)	C ₇ H ₈ N ₄ O ₂
10	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine #	C ₇ H ₈ N ₄ O ₂
11	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	⚠ Paraxanthine	C ₇ H ₈ N ₄ O ₂
12	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
13	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
14	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂
15	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	⚠ D-Fructose	C ₆ H ₁₂ O ₆
16	PASEF	positive	Theobromine	C ₇ H ₈ N ₄ O ₂	Theobromine	C ₇ H ₈ N ₄ O ₂



Determination-Library-Results

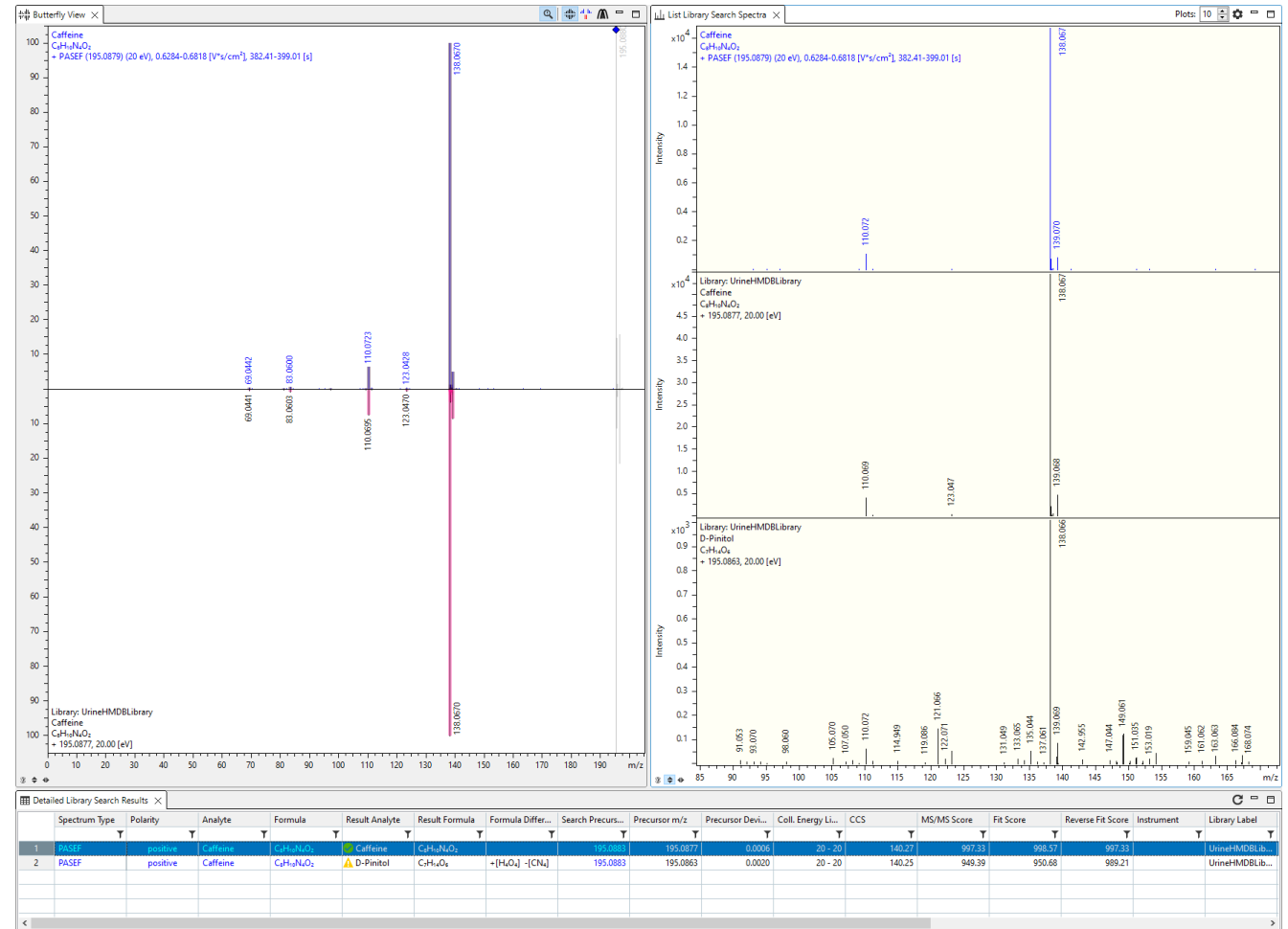
- CCS
- CDR Spectrum ID
- Coll. Energy [eV]
- Coll. Energy Library [eV]
- Fit Score
- Hybrid Score
- Instrument
- Label
- Library CDR Spectrum ID
- Library Label
- Library Score
- Library Score Description
- Library Scoring Function
- Library Scoring Score
- Matching Description
- Matching Score
- Matching Type
- Max Intensity
- Mob. Interval
- MS/MS Score
- Origin Label
- Polarity
- Precursor m/z
- Result Analyte
- Result Formula
- Retention Time Interval [s]
- Reverse Fit Score
- Review State
- Search Precursor m/z
- Spectrum Type
- Sum Intensity
- Used for Scoring

Urine MET_PASEF pos 20CE_2_1_4421 – LibrarySearchResults

Result Analyte	Fit Score	RFit Score	MS/MS Score	Review State	Library Score
Paraxanthine	986.28	986.74	984.28	NONE	+
Theobromine	986.28	986.74	984.28	NONE	++
Theobromine	989.34	979.48	979.48	NONE	++
4-Fluoro-phenylpiperazine #	987.06	969.33	963.15	NONE	---

TASQ 2025: Library Search – List Viewer for Library Search Results

- List all spectra for library search
- Get a quick overview on which spectra are available



TASQ 2025: Support Sample Sub Types

User can define new sample sub types, e.g., for QC pooled QC

Editor available in administration preferences

Assign sample sub type in Batch Summary view, Batch Navigator, Batch Setup wizard

Additional column in results views

Batch statistics view discerns the sub type as well

In statistics table the sub type can be used for grouping and calculation of sample sub type specific statistics

TASQ RealTimeQC supports sample sub types and show for each sample / sub type a different symbol in statistics graph

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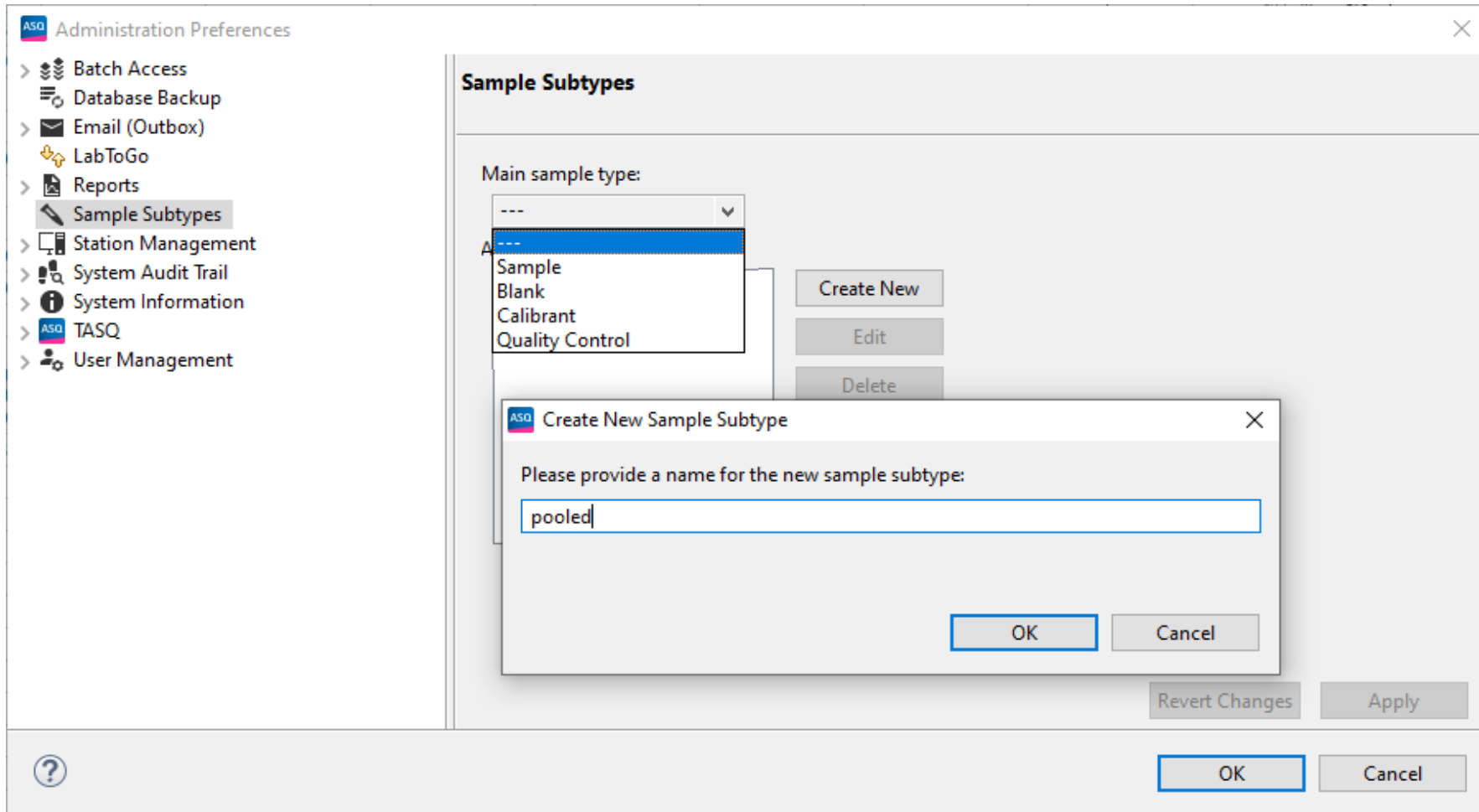
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TASQ RealTimeQC supports sample sub types and show for each sample / sub type a different symbol in statistics graph

TASQ 2025: Create Sample Subtypes



The screenshot shows the 'Administration Preferences' window with the 'Sample Subtypes' section selected in the left-hand navigation pane. The 'Main sample type' dropdown menu is open, showing options: 'Sample', 'Blank', 'Calibrant', and 'Quality Control'. The 'Create New' button is highlighted. A secondary dialog box titled 'Create New Sample Subtype' is overlaid on top, with the text 'Please provide a name for the new sample subtype:' and a text input field containing the word 'pooled'. The 'OK' button in this dialog is highlighted. At the bottom of the main window, there are 'Revert Changes', 'Apply', 'OK', and 'Cancel' buttons.

TASQ 2025: Assign Sample Sub Types in Batch Summary View

	Data Set	Flag	Sample Type	Sample Subtype	C
7	std 2-1 matrix_...		Calibration Sa...		
8	std 5-1 matrix_...		Calibration Sa...		
9	std 10-1 matrix...		Calibration Sa...		
10	std 50-1 matrix...		Calibration Sa...		
11	IS-oplossing1_...		Blank		
12	std_50-1 solve...		Sample		
13	Level0_1_5 min...		Qualitycontrol...		
14	Level1_1_5 min...		Qualitycontrol...		
15	Level2_1_5 min...		Qualitycontrol...	pooled	

	Data Set	Flag	Sample Type	Sample Subtype	Concentration ...
1	test inj std 10_...		Sample		
2	test inj std 5_5 ...		Sample		
3	test inj std 2_5 ...		Sample		
4	test inj std 1_5 ...		Sample		
5	IS oplossing0_...		Blank	solvent	
6	std 1-1 matrix_...		Calibration Sa...		1
7	std 2-1 matrix_...		Calibration Sa...		2
8	std 5-1 matrix_...		Calibration Sa...		3
9	std 10-1 matrix...		Calibration Sa...		4
10	std 50-1 matrix...		Calibration Sa...		5
11	IS-oplossing1_...		Blank	matrix	
12	std_50-1 solve...		Sample		
13	Level0_1_5 min...		Qualitycontrol...	pooled	0
14	Level1_1_5 min...		Qualitycontrol...		1
15	Level2_1_5 min...		Qualitycontrol...		2
16	Level3_1_5 min...		Qualitycontrol...		3
17	Level3_2_5 min...		Qualitycontrol...		3
18	Level2_2_5 min...		Qualitycontrol...	pooled	2

TASQ 2025: Assign Sample Sub Type

Batch Navigator | Batch Summary

Applied filter: None

- NVWA Validation in Wheat 5min_2 [61]
 - test inj std 10_5 min_4_1_4421 [1]
 - test inj std 5_5 min_3_1_4422 [1]
 - test inj std 2_5 min_2_1_4423 [1]
 - test inj std 1_5 min_1_1_4424 [1]
 - IS oplossing0_5 min_6_1_4425 [1]
 - std 1-1 matrix_5 min_1_1_4426 [1]
 - std 2-1 matrix_5 min_1_1_4427 [1]
 - std 5-1 matrix_5 min_1_1_4428 [1]
 - std 10-1 matrix_5 min_1_1_4429 [1]
 - std 50-1 matrix_5 min_1_1_4430 [1]
 - IS-oplossing1_5 min_1_1_4431 [1]
 - std_50-1 solve_5 min_1_1_4432 [1]
 - Level0
 - Level1
 - Level2
 - Level3
 - Level3
 - Level2
 - Level1
 - Level0

Refresh Tree

Collect Raw Data (*.zip)...

Import (*.brkrar)...

Reprocess Analyses

Quantify Current Analysis

Perform Library Search

Delete Analysis

Delete Analysis Result

Comment Analysis Result

Update Sample Type

Flags

	Data Set	Flag	Sample Type	Sample Subtype
1	test inj std 10_...		Sample	
2	test inj std 5_5 ...		Sample	
3	test inj std 2_5 ...		Sample	
4	test inj std 1_5 ...		Sample	
5	IS oplossing0_...		Blank	solvent
6	std 1-1 matrix_...		Qualitycontrol...	
	std 2-1 matrix_...		Calibration Sa...	
	std 5-1 matrix_...		Calibration Sa...	
	std 10-1 matrix...		Calibration Sa...	
	std 50-1 matrix...		Calibration Sa...	
	IS-oplossing1_...		Blank	matrix
	std_50-1 solve...		Sample	
	Level0_1_5 min...		Qualitycontrol...	pooled
	Level1_1_5 min...		Qualitycontrol...	
	Level2_1_5 min...		Qualitycontrol...	
	Level3_1_5 min...		Qualitycontrol...	
	Level3_2_5 min...		Qualitycontrol...	
	Level2_2_5 min...		Qualitycontrol...	pooled
	Level1_2_5 min...		Qualitycontrol...	

ASQ

Sample Type

Please select sample type for current analysis.

Sample Type: QUALITYCONTROL

Sample Subtype: pooled

OK Cancel

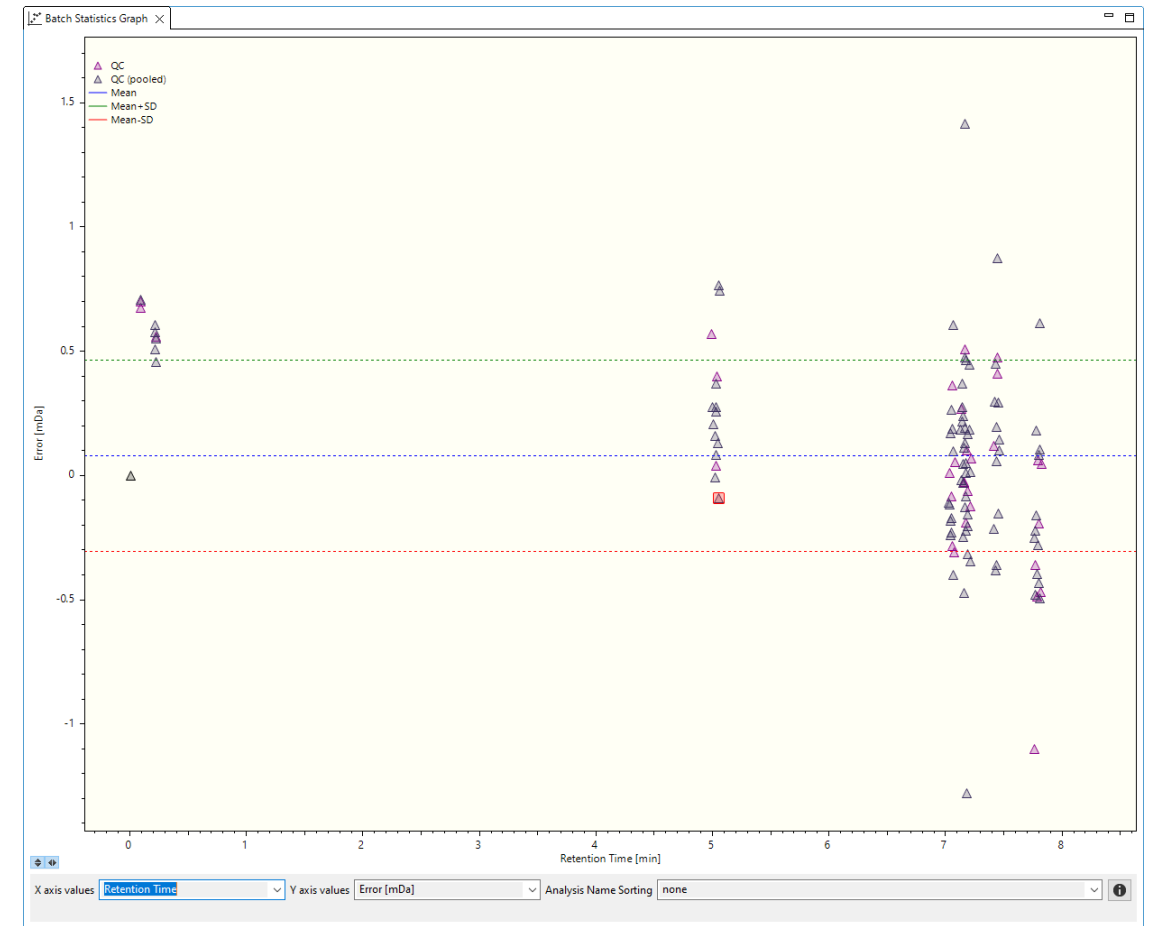
- Changing sample sub type is available in „Update Sample Type“ wizard from context menu of Batch Navigator

TASQ 2025: Sample Sub Type in Batch Statistics Graph

- LHS: show for all sample / sub sample types

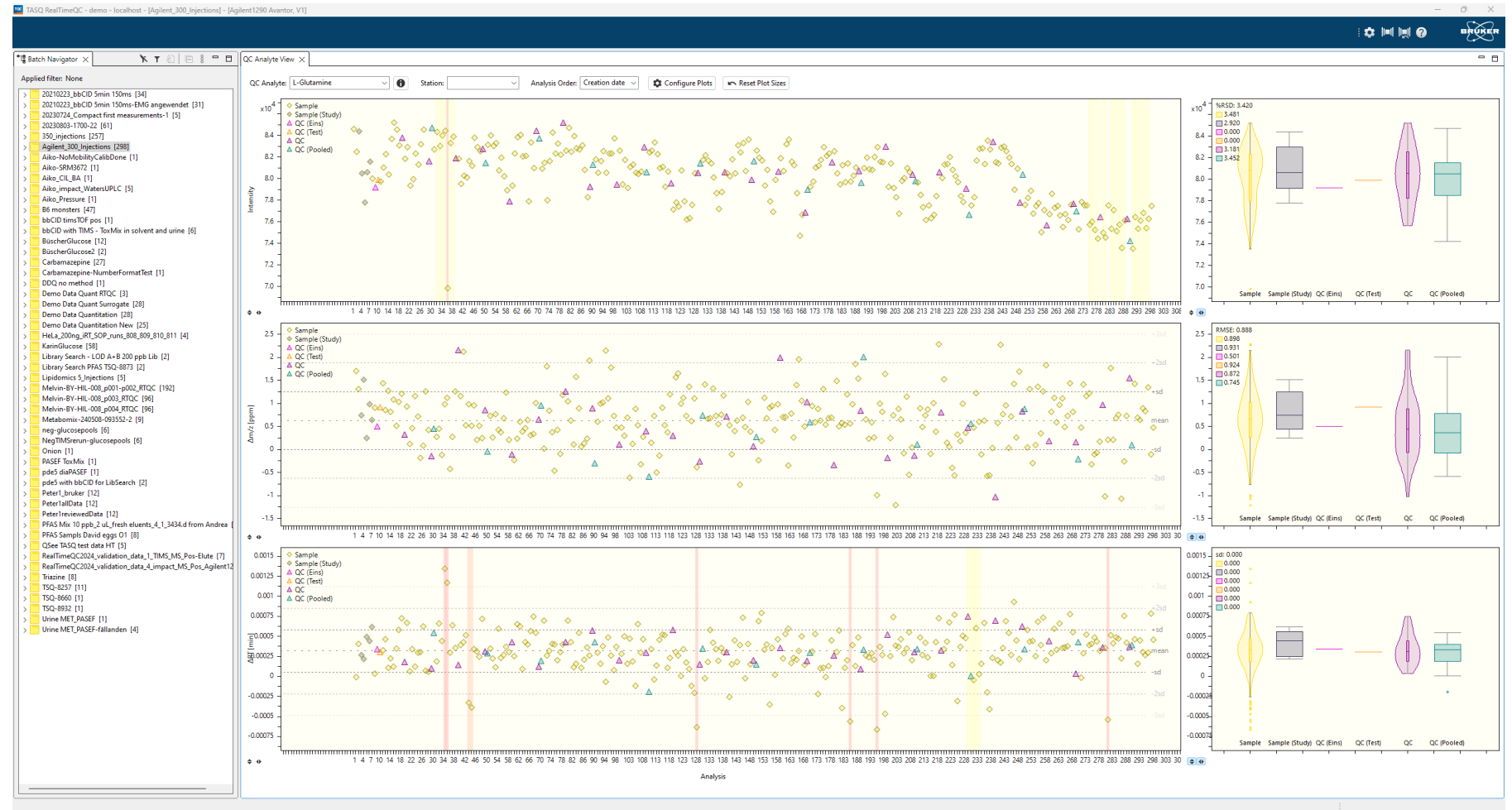


- RHS: show only QC sample type



TASQ 2025: RealTimeQC – Support of Subsample Type

- Statistics is calculated for each sample / subsample types

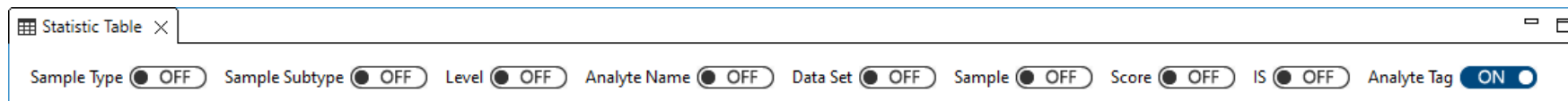


TASQ 2025: Sample Sub Type in Statistics Table

- Additional grouping by Sample Sub Type

Statistic Table									
Sample Type <input checked="" type="checkbox"/> Sample Subtype <input checked="" type="checkbox"/> Level <input type="checkbox"/> Analyte Name <input type="checkbox"/> Data Set <input type="checkbox"/> Sample <input type="checkbox"/> Score <input type="checkbox"/> IS <input type="checkbox"/>									
	SampleType	Sample Subtype	Property	ΔRT [min]	Δm/z [mDa]	mSigma	FWHM [s]	Area for Quant...	
1	BLANK		nrDatapoints	9	12	12	12	12	
2	BLANK		mean	-0.1227	0.701	143	7.33	3936	
3	BLANK		median	-0.0237	0.614	57.5	2.33	2823	
4	BLANK		sd	0.154	0.534	174	9.16	2943	
5	BLANK		minimum	-0.3816	-0.1263	8.62	2.10	932	
6	BLANK		maximum	-0.0032	1.92	518	22.7	10899	
7	BLANK		%RSD	-125.8037	76.2	122	125	74.8	
8	CALIBRANT		nrDatapoints	156	173	173	173	173	
9	CALIBRANT		mean	-0.0097	0.165	30.6	2.70	880228	
10	CALIBRANT		median	-0.0059	0.137	9.89	2.28	304071	
11	CALIBRANT		sd	0.0154	0.534	71.1	2.26	1614784	
12	CALIBRANT		minimum	-0.0804	-2.2479	0.497	1.79	1056	
13	CALIBRANT		maximum	0.0374	2.51	438	22.2	11863570	
14	CALIBRANT		%RSD	-159.3077	323	232	83.9	183	
15	QUALITYCONTROL	pooled	nrDatapoints	78	84	84	84	84	
16	QUALITYCONTROL	pooled	mean	-0.0120	0.0913	17.5	2.54	913098	
17	QUALITYCONTROL	pooled	median	-0.0113	0.104	9.08	2.30	356117	
18	QUALITYCONTROL	pooled	sd	0.0108	0.383	31.0	0.910	1651499	
19	QUALITYCONTROL	pooled	minimum	-0.0435	-1.2782	0.250	2.08	3711	
20	QUALITYCONTROL	pooled	maximum	0.00503	1.42	250	6.07	11927893	
21	QUALITYCONTROL	pooled	%RSD	-90.2672	420	177	35.8	181	
22	QUALITYCONTROL		nrDatapoints	28	31	31	31	31	
23	QUALITYCONTROL		mean	0.00738	0.0567	20.7	3.68	943198	
24	QUALITYCONTROL		median	0.00343	0.0487	12.5	2.30	819525	
25	QUALITYCONTROL		sd	0.0587	0.392	25.9	4.97	855712	
26	QUALITYCONTROL		minimum	-0.0547	-1.0996	2.05	2.17	916	
27	QUALITYCONTROL		maximum	0.296	0.700	126	22.7	2507380	
28	QUALITYCONTROL		%RSD	795	692	125	135	90.7	
29	SAMPLE		nrDatapoints	42	46	46	46	46	
30	SAMPLE		mean	-0.0217	0.441	25.2	2.60	840092	
31	SAMPLE		median	-0.0088	0.395	9.97	2.30	324697	
32	SAMPLE		sd	0.0583	0.519	55.4	0.993	1033371	
33	SAMPLE		minimum	-0.3371	-0.3302	1.28	2.19	906	
34	SAMPLE		maximum	0.00855	1.87	337	5.90	4203948	
35	SAMPLE		%RSD	-268.1505	117	220	38.2	123	

TASQ 2025: Analyte Tags in Statistics Table

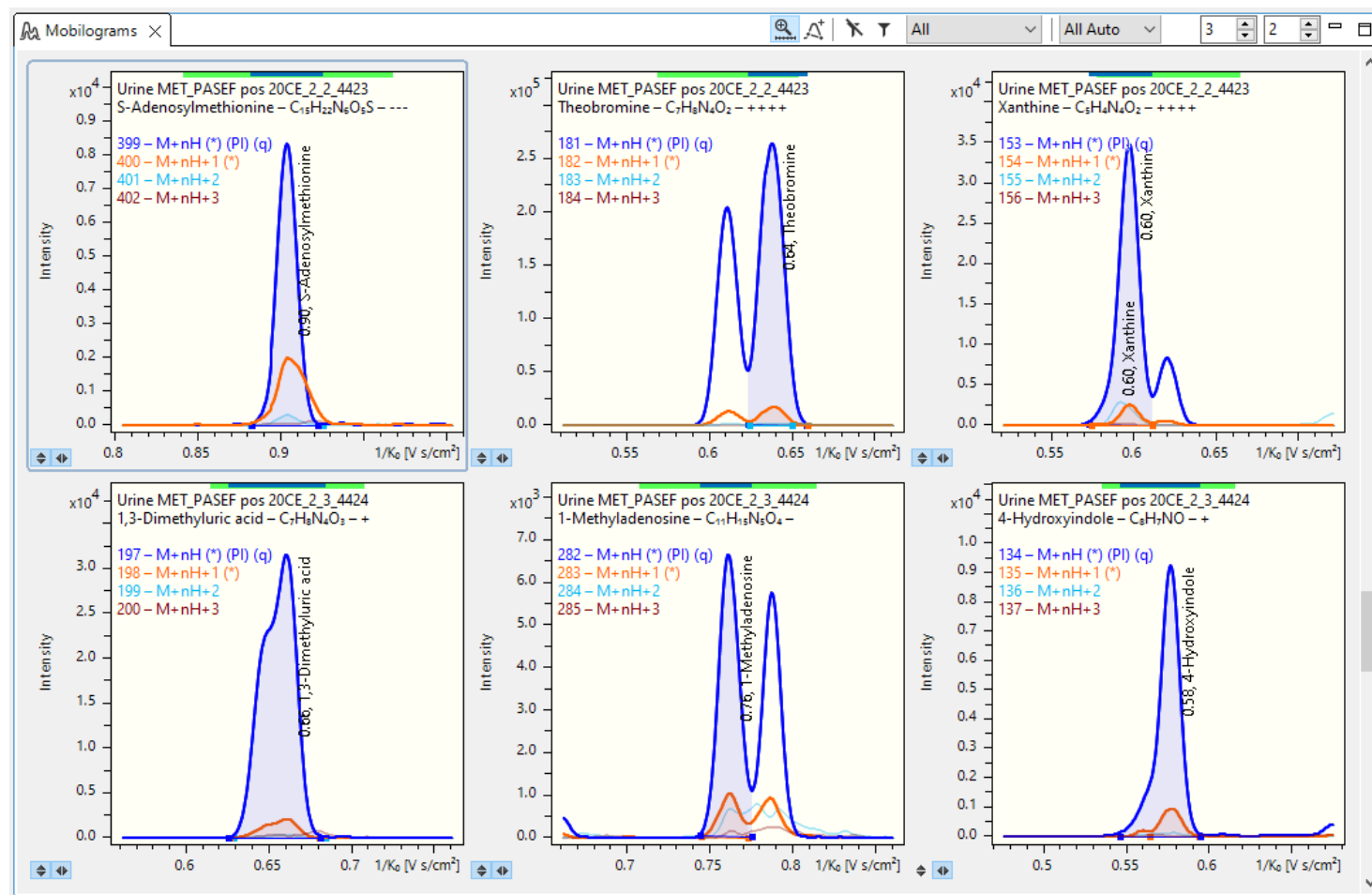
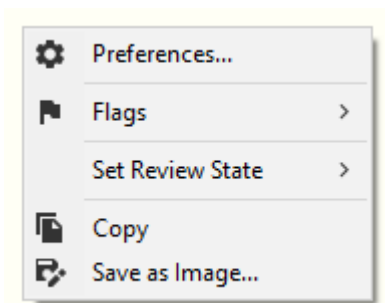


- Use Analyte Tab for grouping
- E.g., Morphine metabolites for all metabolites

	Analyte Tag ▼	Property ▼	Δ RT [min] ▼	Δ m/z [mDa] ▼	mSigma ▼
1	test	nrDatapoints	71	71	71
2	test	mean	-0.0132	0.233	30.5
3	test	median	-0.0042	0.174	12.7
4	test	sd	0.0630	0.556	73.3
5	test	minimum	-0.3371	-1.0996	1.27
6	test	maximum	0.296	1.87	518
7	test	%RSD	-476.6717	238	241
8	bla	nrDatapoints	70	70	70
9	bla	mean	-0.0135	0.101	37.2
10	bla	median	-0.0042	0.0511	12.3
11	bla	sd	0.0464	0.471	79.4
12	bla	minimum	-0.3816	-1.2782	0.748
13	bla	maximum	0.0134	1.92	438
14	bla	%RSD	-343.3577	465	213
15		nrDatapoints	172	205	205
16		mean	-0.0138	0.210	26.9
17		median	-0.0101	0.199	9.33
18		sd	0.0312	0.499	62.4
19		minimum	-0.3739	-2.2479	0.250
20		maximum	0.0374	2.51	482
21		%RSD	-226.6918	238	232

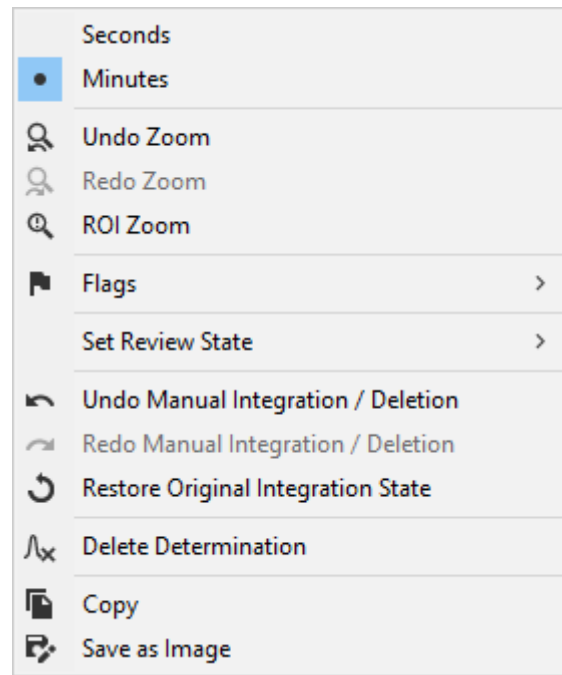
TASQ 2025: Multi Mobilogram Viewer

- Mobilograms view to present mobilograms of data set, batch results, determination or mobilograms of all findings in batch in tile view. It has the same behaviour as Chromatograms view



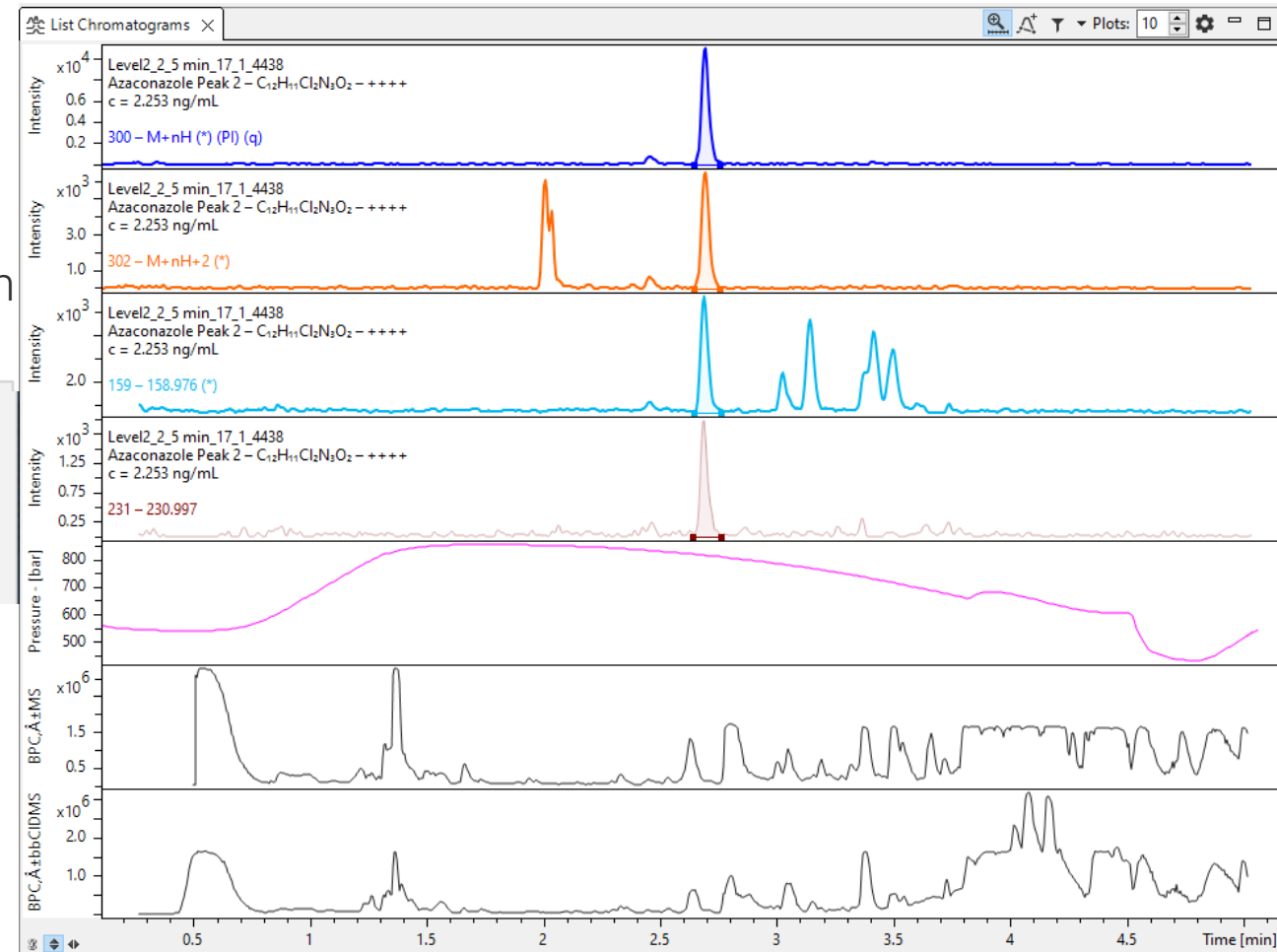
TASQ 2025: Chromatogram List Viewer

- Show chromatograms of selected determination as a list
- Show additionally BPC, pressure and UV traces
- Zoom, Manual Integration, Select traces to be shown

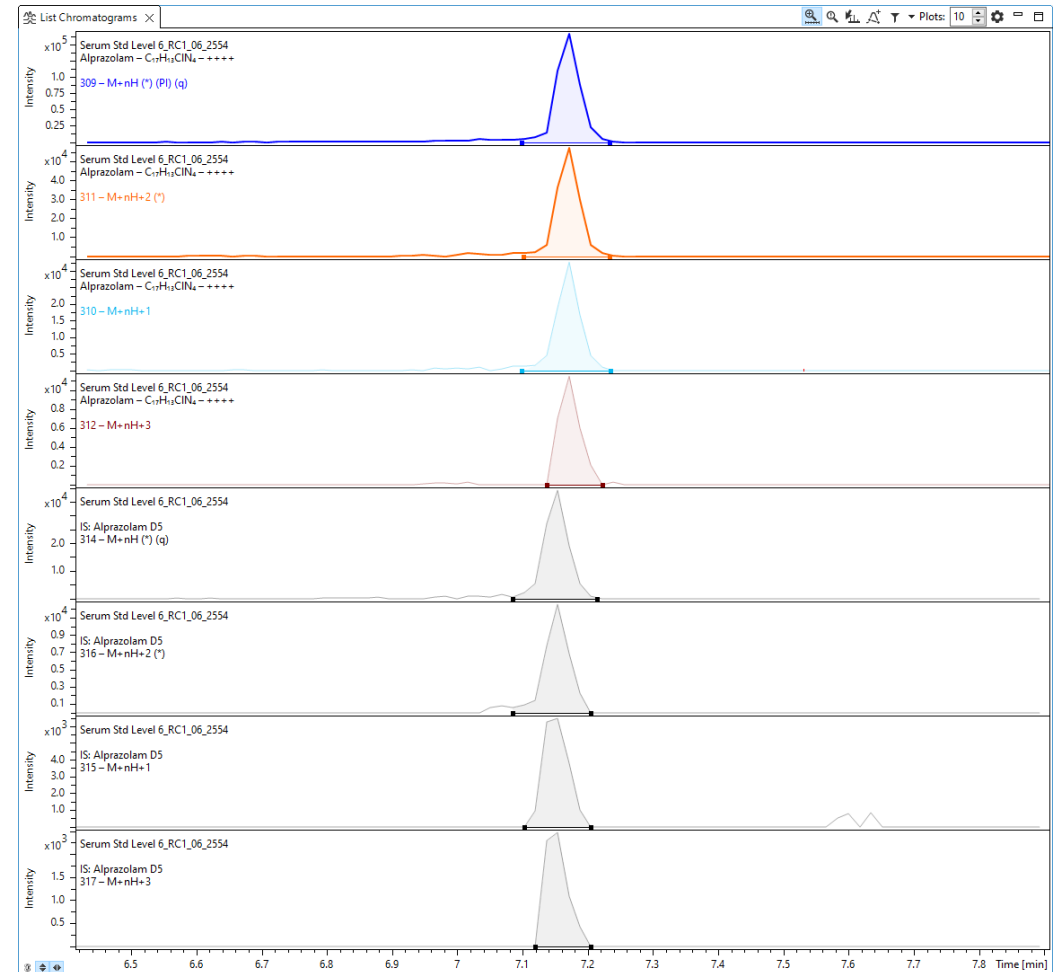
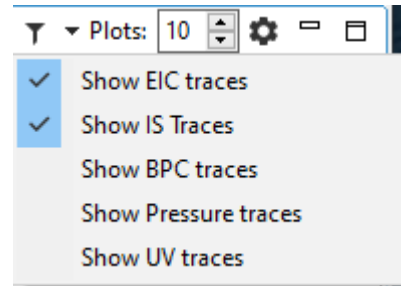
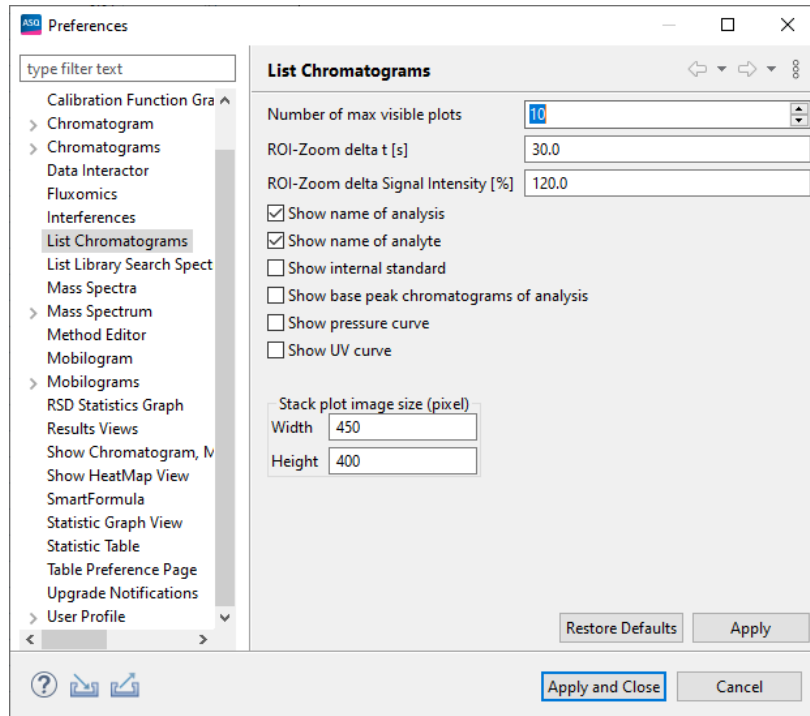


Seconds
 Minutes
 Undo Zoom
 Redo Zoom
 ROI Zoom
 Flags >
 Set Review State >
 Undo Manual Integration / Deletion
 Redo Manual Integration / Deletion
 Restore Original Integration State
 Delete Determination
 Copy
 Save as Image

Show EIC traces
 Show IS Traces
 Show BPC traces
 Show Pressure traces
 Show UV traces



TASQ 2025: Chromatogram List Viewer – Show Chromatograms of Internal Standard

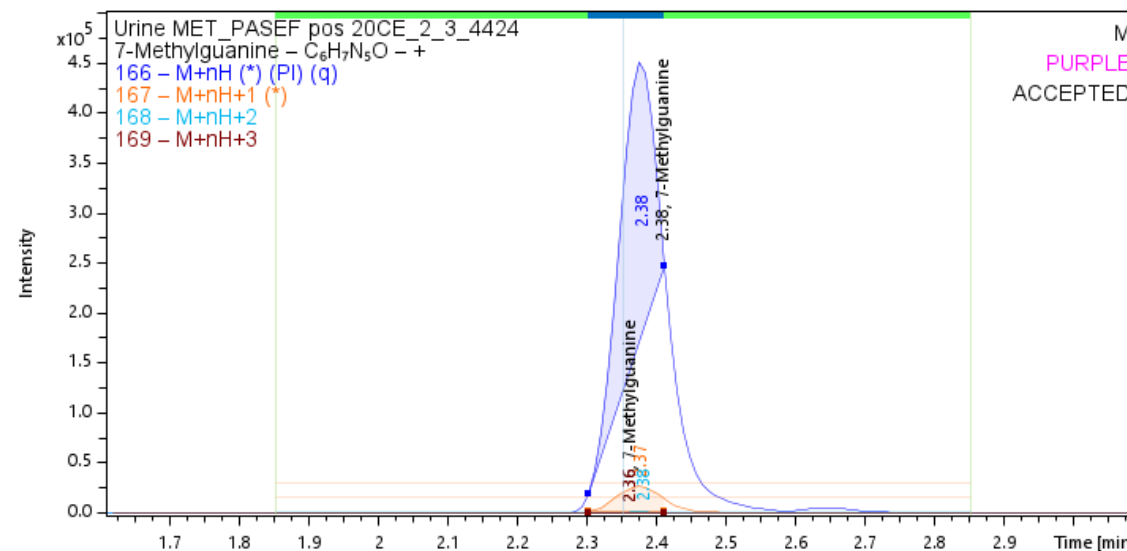
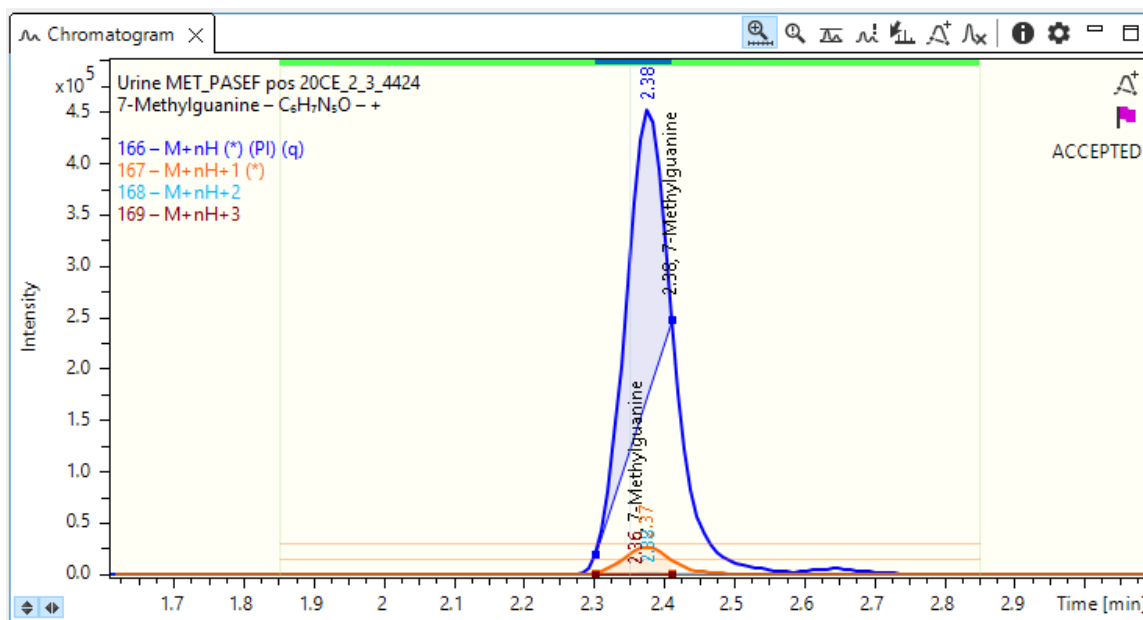
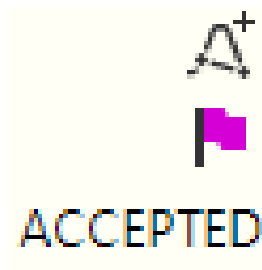


TASQ 2025: Faster Data Review

- Setting flags and review state can be done in all result views
 - Analysis, Batch, and Global Results
 - Additionally available now in
 - Detailed Ion Results view
 - Chromatograms view
 - Mobilograms view
 - List Chromatogram view
 - List Library Search Spectra view
 - Butterfly view
- No need to switch views to be able to set flags or review state

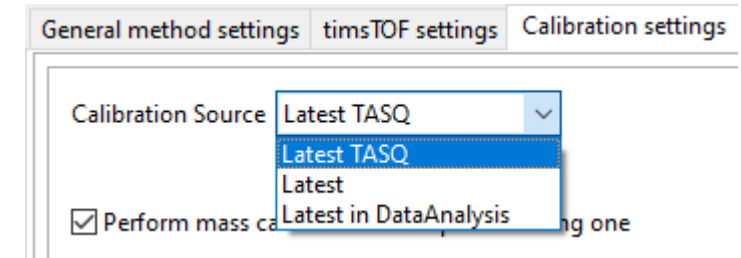
TASQ 2025: Faster Data Review – Extended Graph Views

- Show status of manual integration
- Show user flags
- Show review state
- Set these states directly in the graph views



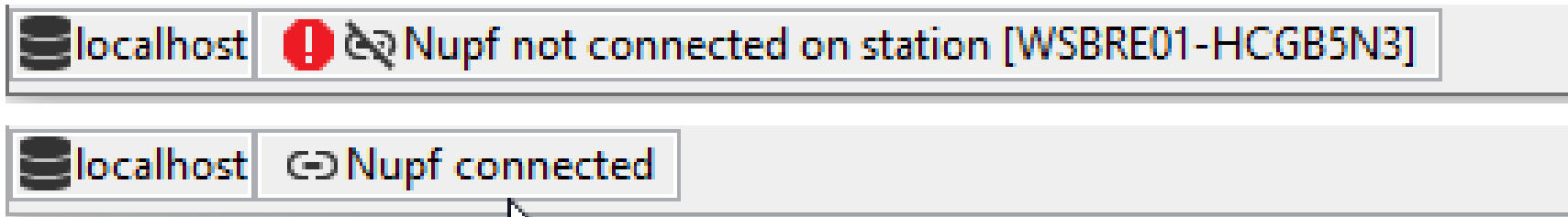
TASQ 2025: New Option for Calibration: use Other Sources

- Sometimes the calibration algorithm in TASQ does not give the best possible results
- In that situation data can be calibrated with DataAnalysis and this calibration result can be used for processing in TASQ
- New option **Calibration Source** is available
- User can specify: **Latest TASQ**, **Latest**, **Latest in DataAnalysis**
- If a user performs a calibration in DataAnalysis and stores the results, this calibration state can be used in TASQ processing by choosing the option **Latest in DataAnalysis**, alternatively the calibration state of MetaboScape can be chosen by setting the option **Latest** if MetaboScape was the last program to create the calibration state
- The calibration of tsf, and tdf data sets can be used
- DataAnalysis does not store the calibration for baf data sets in calibration.sqlite format



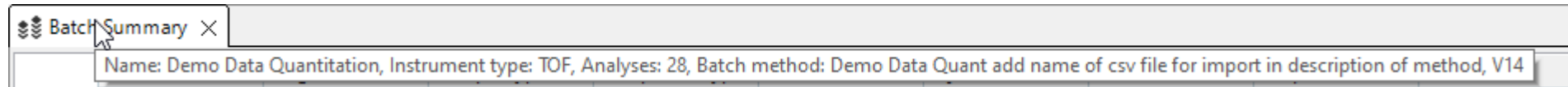
TASQ 2025: Indicator if NUPF is not connected

- For processing of data the Bruker MS Data Processing service (NUPF) has to be connected on a station to the compass server. If it is not connected processing of data is not possible. This state was not clearly visible in the past.
- No a clear indication whether TASQ is able to start a processing is given
- For each batch the assigned station will be checked



TASQ 2025: Miscellaneous

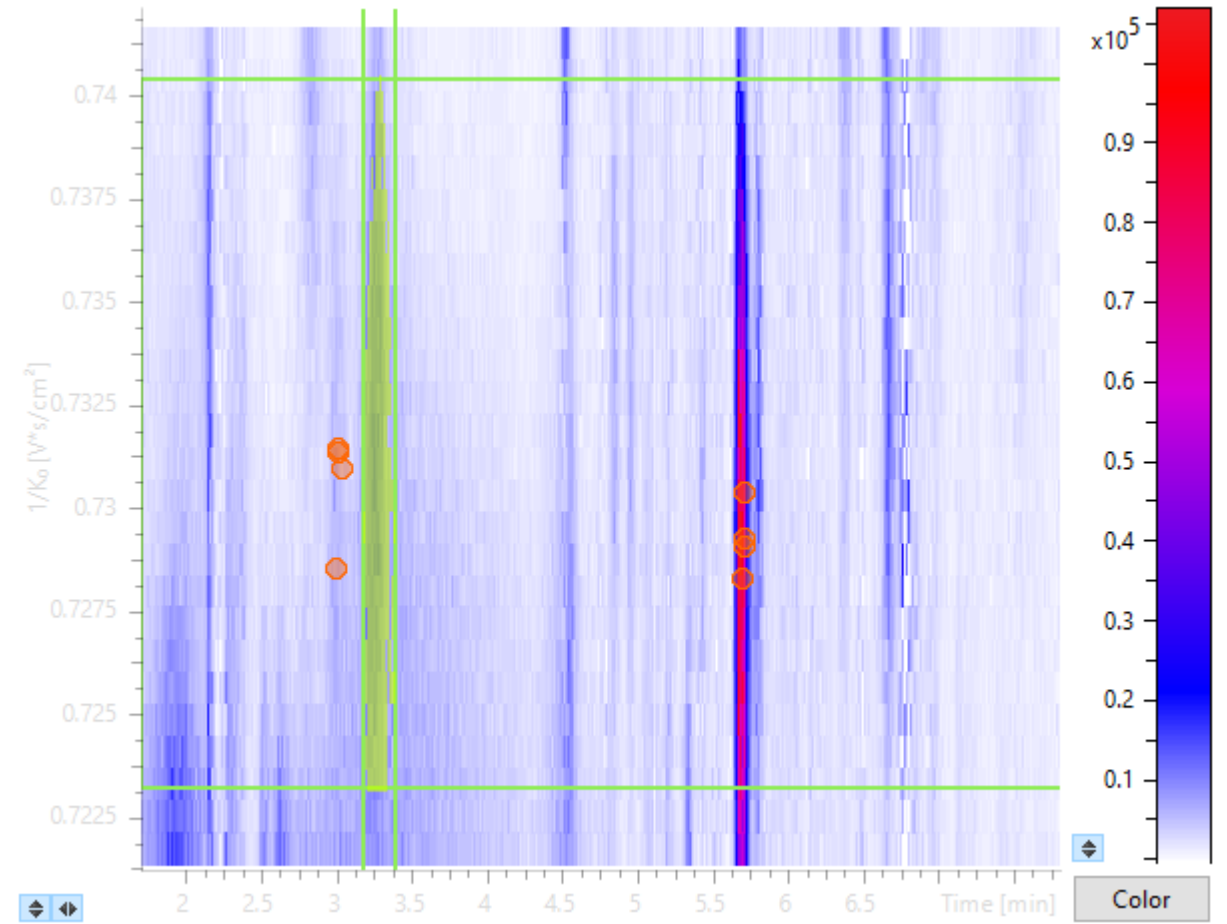
- Drag & Drop of .tasqMethod files from explorer to Batch Summary view imports the TASQ method
- Improvements/ Fixes for generation of TASQ method from MetaboScape
- Fix for generation of prmPASEF.csv from TASQ method
- Batch Summary view: tooltip with information of batch, including instrument type



- Contour detection in HeatMap view: Click on a peak in the heatmap RT / 1/K₀ and the bounding box will be detected automatically. This shall be used in future for manual integration of peaks in the RT / 1/K₀

TASQ 2025: Peak Detection in HeatMap

- Contours are detected automatically in the selected rectangle
- The peak with the largest area will be selected and highlighted by green color
- The bounds of the contour can be enlarged or shrunk by [STRG] mouse wheel



TASQ 2025: Miscellaneous

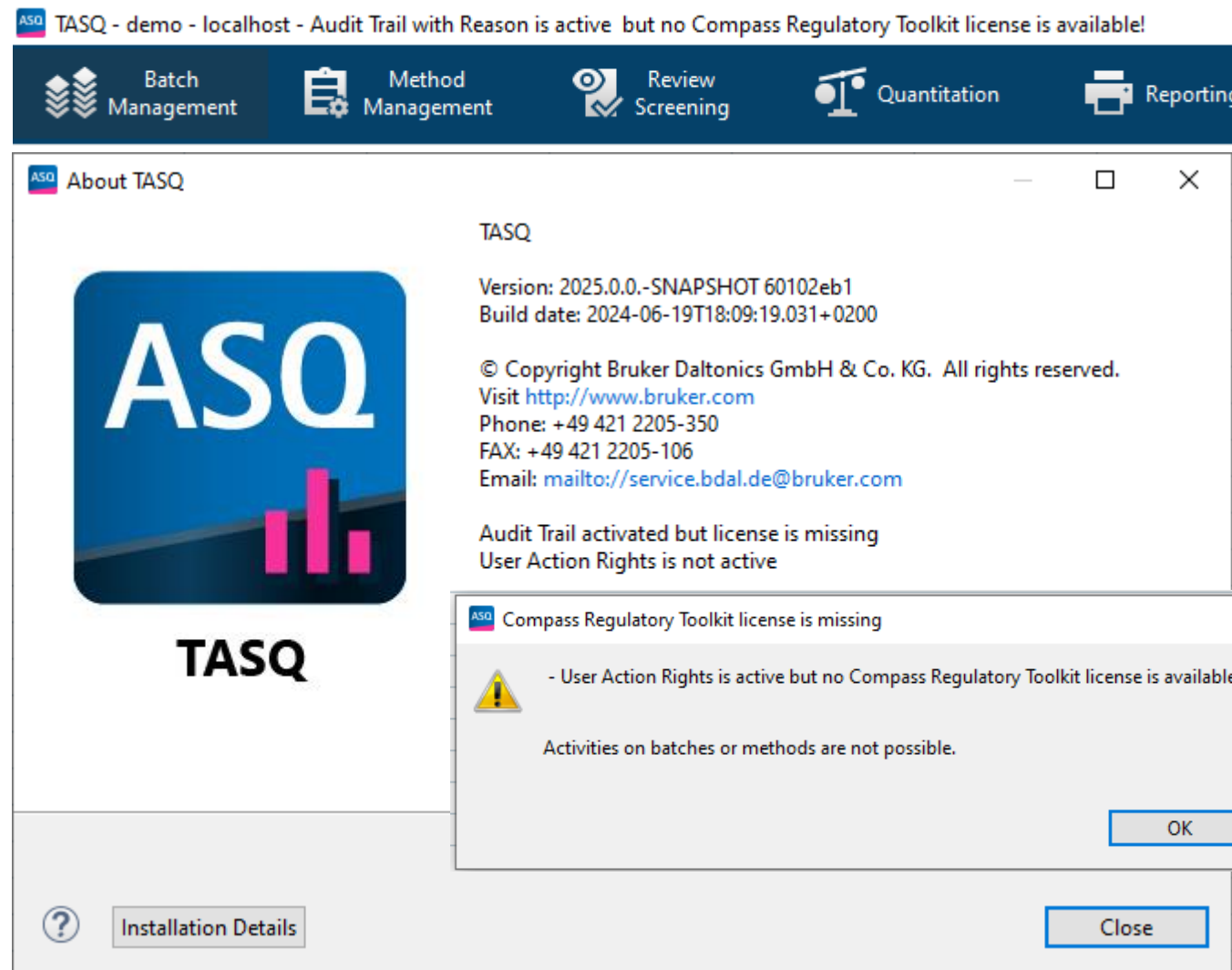
- Lims export extended to store library search results on determination level (analysis / batch results view)
- Storing of concentrations to samples – performance improved
- Improvement in Add ion wizard: switch automatically the polarity of charge specified in wizard when user selects a PMI of other polarity, e.g., set charge to -1 if user selects [M-H]⁻
- Change order of ions in ions table of method editor by [ALT] Arrow Up|Down
- Copy and Save as Image added to all list viewers
- Selecting determinations and data sets in chromatogram / mobilogram view by ↑↓ <> keys

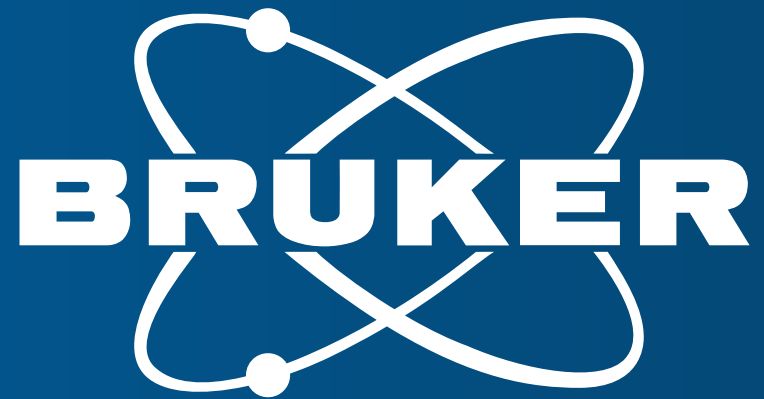
TASQ 2025: Miscellaneous

- Method editor view: interferences detection considers mobility information
- Method editor view: interferences detection considers precursor m/z information
- TQ data processing: matching of analyte names of TASQ method compounds and chromatogram names in analysis.qqq is case insensitive now.
- Bug fixes of nat tables
- Bug fixes context sensitive help
- Improved SmartFormula View
 - Upper formula constrained considered correctly
 - Setting spectrum type for ion parameter settings
- Improvements for Update Parameters wizard
- Statistics table send notification of analyte selection change

TASQ 2025: More Stringent Check for Compass Regulatory Toolkit License

- Activating Audit Trail and/or User Action Rights requires a valid Compass Regulatory Toolkit License during setup
- TASQ Client checks now whether the license is available or not in case that Audit Trail or User Action Rights is activated in the Compass Server.
- If no Compass Regulatory Toolkit is available TASQ client is not usable
 - Batches can't be loaded
 - Methods can't be loaded
- A hint is given in About TASQ dialog and in windows title bar





Innovation with Integrity