

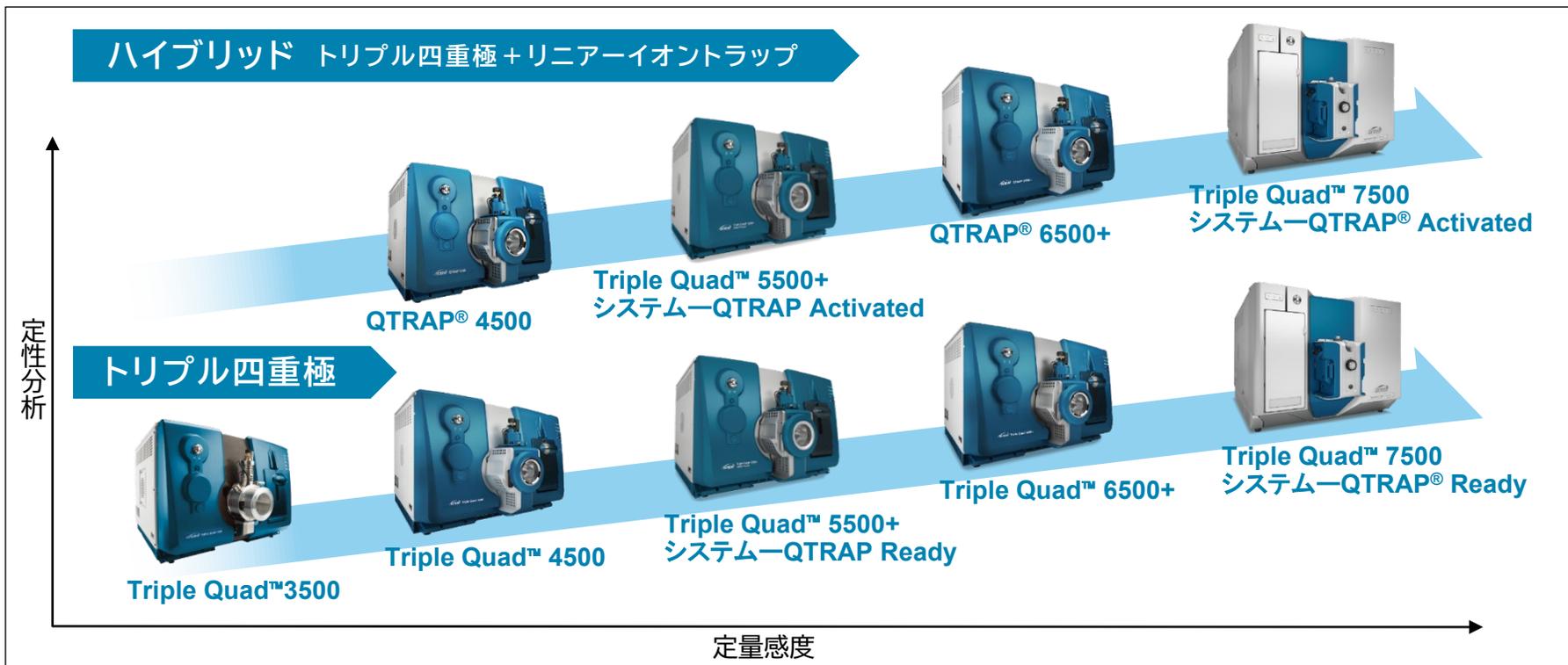


SCIEX 7500システムの測定例と DI対応を含めたSCIEX OSソフトウェアの機能紹介

SCIEX質量分析システムを支えるソフトウェア

2024年02月

SCIEX製品ラインナップ



**キャピラリー
電気泳動システム**



BioPhase 8800



PA 800 Plus



CESI 8000 Plus



P/ACE™ MDQ Plus

QTOFシステム



ZenoTOF 7600



X500 QTOF

Echo®MS



Intabio ZT



新しいレベルの定量

新しいソフトウェア、新しいイオン導入部、新しいイオンソース



- SCIEX 7500 System
 - 様々なサンプル、ワークフローに新しいレベルの定量をもたらします。
- SCIEX OS Software
 - 最新の質量分析制御/解析ソフトウェアは、最良の分析結果を簡単に導き出します

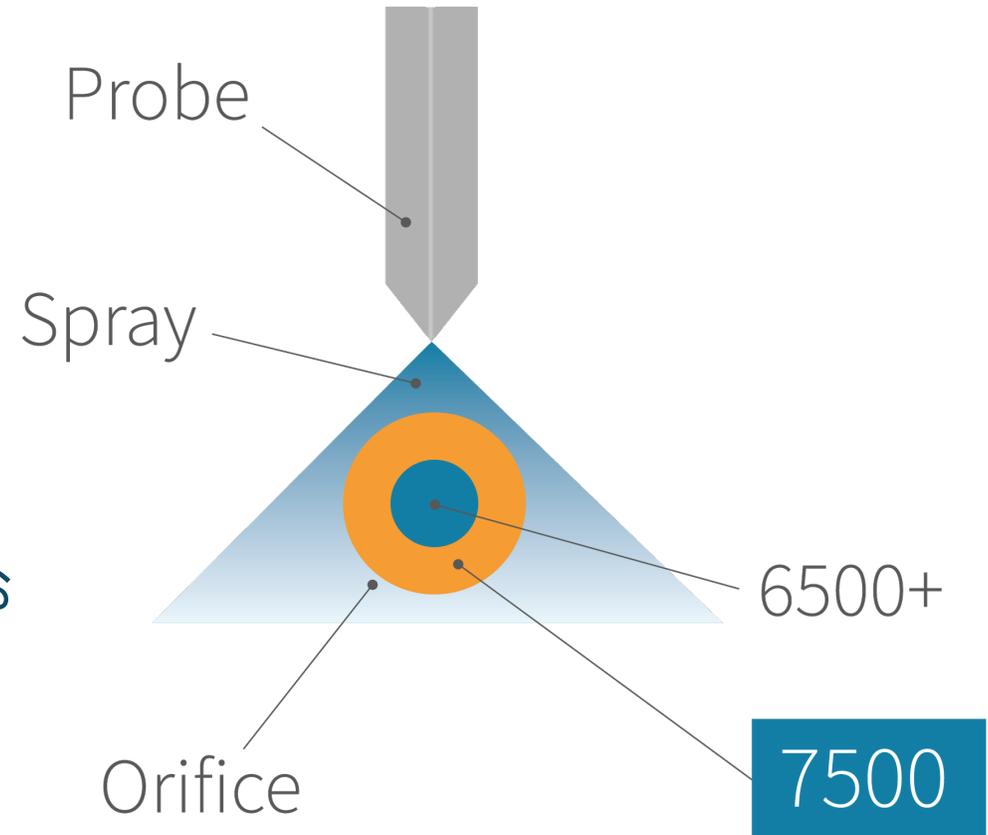


感度を上げるために

- 感度向上は、次の3点を改善することで達成されます
 1. イオンの生成量
 2. イオンの捕捉と受け渡し
 3. イオンの検出効率
 - SCIEX Triple Quad 6500+ system の IonDrive™においても、これらのキーポイントが改善されました

- SCIEX 7500 System では、イオンの捕捉と受け渡しにおいて更なる飛躍を遂げました

- 7500 のサンプリングエリアは、6500の4.3倍に広がりました



新技術 - D Jet イオンガイド

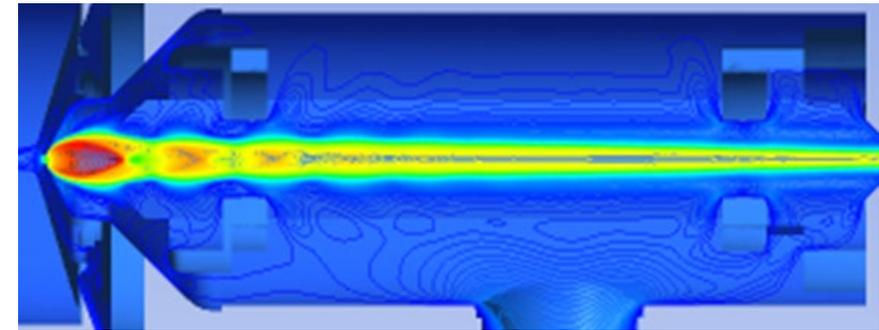
イオン導入部



D Jet イオンガイド

Dual Stage RF Ion Guide

- D Jet Ion Guideは、オリフィス後の高ガスフロー域でのイオンの透過効率を向上させます
- 先が細くなった12極(Dodeca-pole) で構成された D Jet Ion Guideを通じて、イオンは収束され、Q Jetへと導入されます
- Curtain Gasインターフェイスのガス量は、最大 26 L/min に増強されました(18 L/min QTRAP 6500+ System)

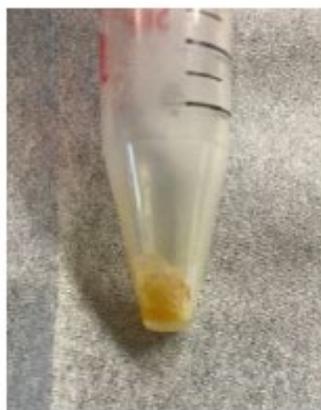


堅牢性について

Injection volume : 3 μ L



Liver homogenate
on right



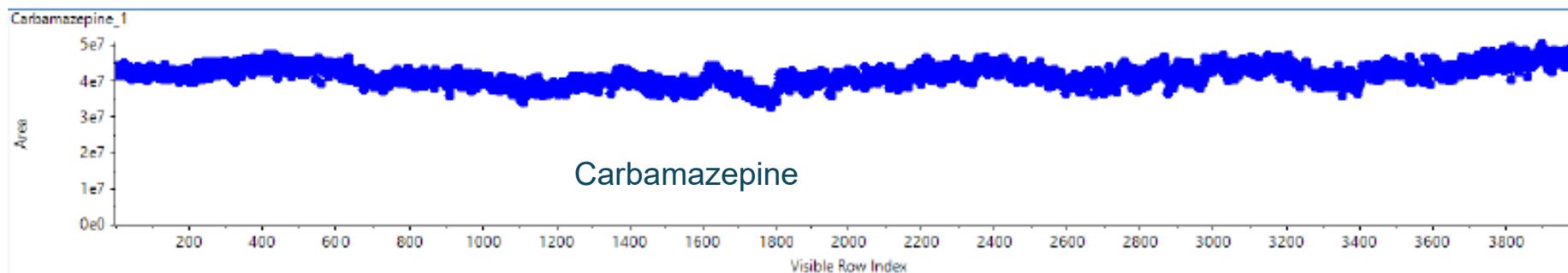
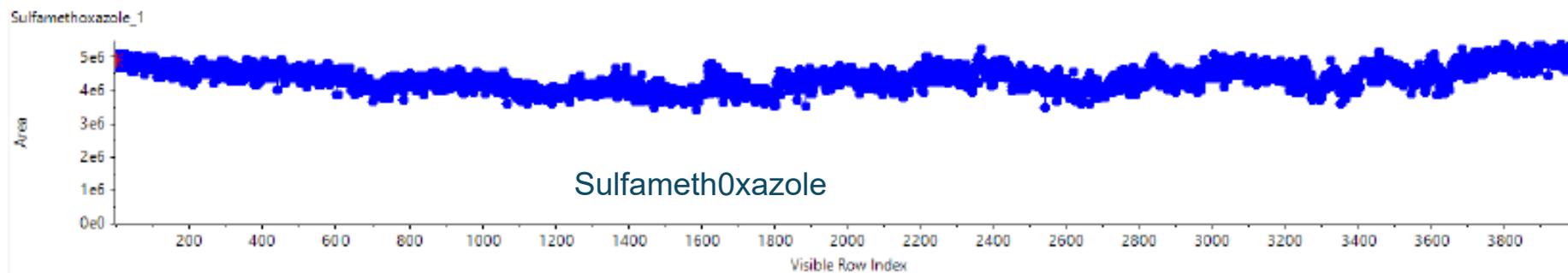
After dry down



After
reconstitution

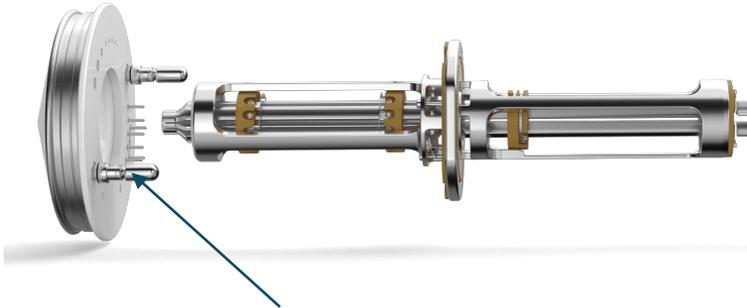


After filtering

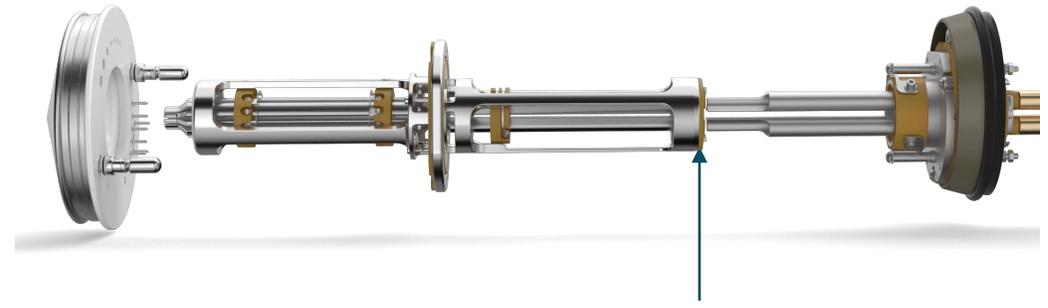


D Jet イオンガイド

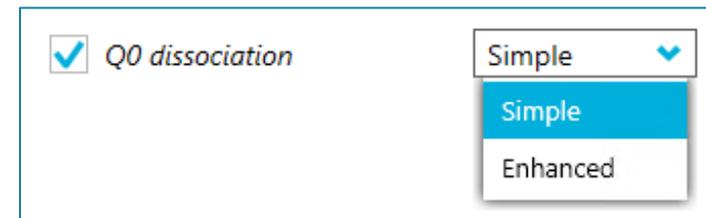
取り込み電圧 (DP)について



- 6500+以前の装置では、オリフィスの電圧 (DP) により、デクラスタリングを制御
- 7500では、DPはフラットとなり、最適化が不要となったため、MSパラメーターから削除



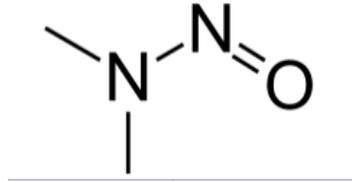
- 7500では、QJet® Ion GuideとIQ0 lens、もしくはIQ0 とQ0 lensの電位差により、デクラスタリングを制御(どちらも設定可能)
- 電位差を増減することにより(Q0D)、予期しないフラグメンテーションの抑制や、夾雑イオンの分解・除去により、S/Nの向上に役立ちます
- 規定値を入れて最適化項目から外すことも可能



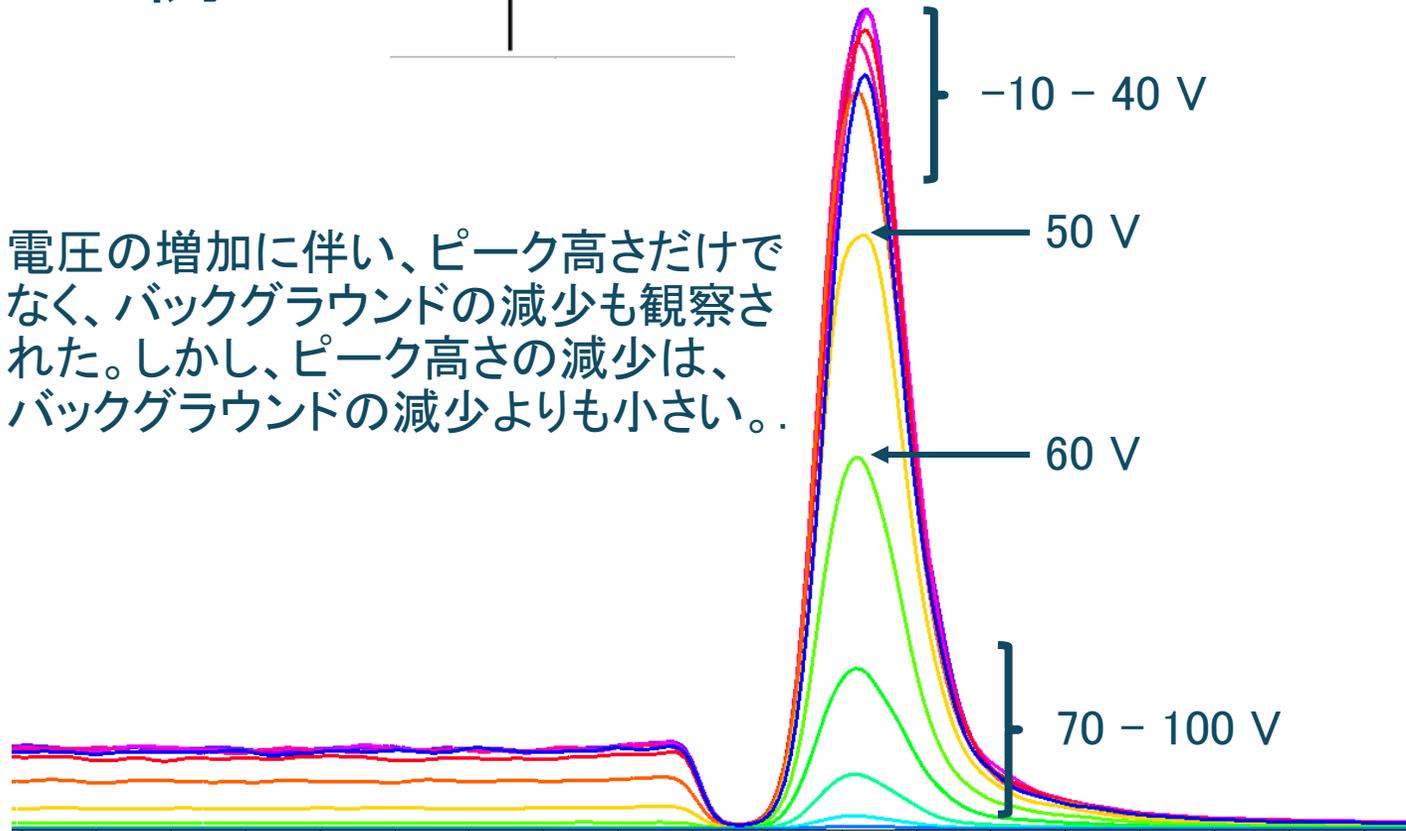
Q0D optimization

Q0Dの感度への影響

NDMAの例



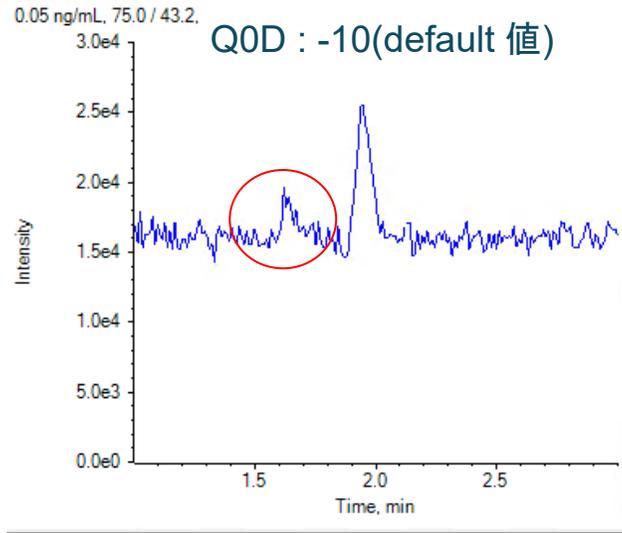
電圧の増加に伴い、ピーク高さだけでなく、バックグラウンドの減少も観察された。しかし、ピーク高さの減少は、バックグラウンドの減少よりも小さい。



Q0D (simple) setting (V)	Signal to noise
-10	105
0	106
10	103
20	118
30	133
40	201
50	284
60	744
70	639
80	376
90	109
100	75

Q0Dを使った測定例 NDMA

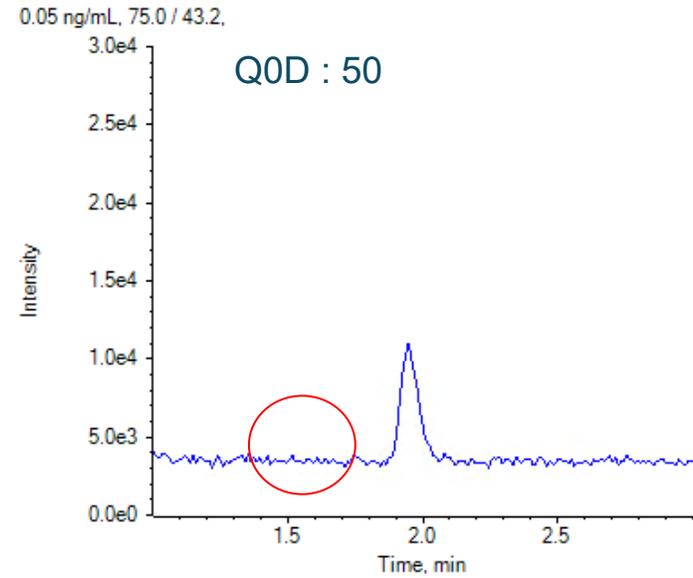
Injection Volume 15 uL



Q0Dを50に設定



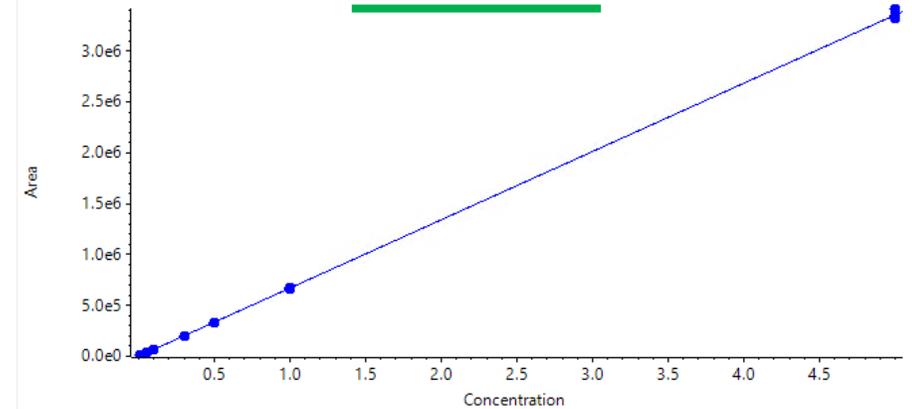
妨害ピークが消失。
Baseline も大幅に減少



0.01ng/mLから再現性の高い直線性が引くことが可能に

Component Name	Actual Concentrati...	Num. Values	Mean	Standard De..	Percent CV	Average A..	Value #1	Value #2	Value #3
NDMA 1	0.01	3 of 3	0.010	0.000	4.76	104.28	0.011	0.010	0.010
NDMA 1	0.03	3 of 3	0.028	0.000	1.39	94.12	0.029	0.028	0.028
NDMA 1	0.05	3 of 3	0.051	0.002	3.31	102.54	0.053	0.051	0.050
NDMA 1	0.10	3 of 3	0.100	0.004	4.39	99.98	0.099	0.105	0.096
NDMA 1	0.30	3 of 3	0.302	0.003	1.10	100.65	0.298	0.304	0.304
NDMA 1	0.50	3 of 3	0.495	0.006	1.27	98.91	0.489	0.493	0.501
NDMA 1	1.00	3 of 3	0.993	0.009	0.93	99.31	0.999	0.983	0.998
NDMA 1	5.00	3 of 3	5.010	0.068	1.36	100.21	5.087	4.956	4.989

Calibration for NDMA 1: $y = 6.71482e5 x + -60.71568$ ($r = 0.99991$, $r^2 = 0.99981$) (weighting: 1 / x)



新技術 – OptiFlow Pro Ion Source

イオンソース



Turbo V イオンソースの進化



Turbo V Ion Source



IonDrive™ Turbo V Ion Source

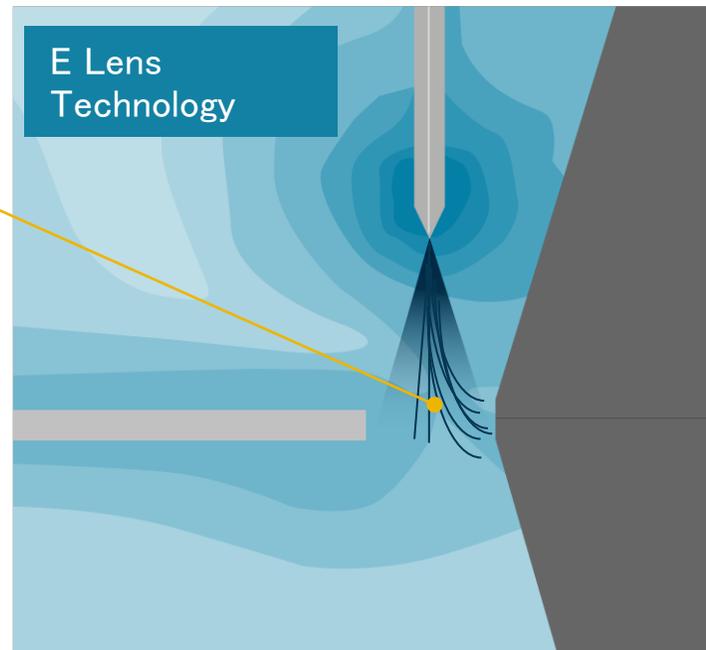
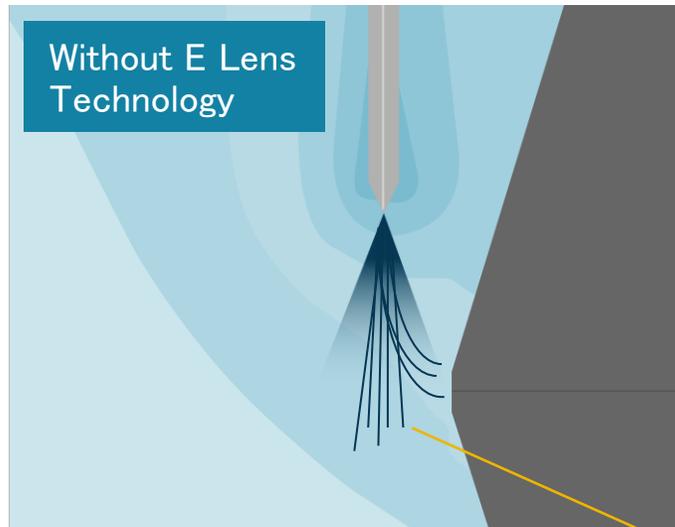


OptiFlow® Ion Source



OptiFlow® Pro Ion Source

信頼性と頑丈さのために



- E Lens™テクノロジーは、イオンをオリフィスへと動かす役割をします
- E Lensは液滴が横断する空間に強い電場を発生させ、液滴を壊すことにより、イオンの液滴からの蒸発を推進します
- E Lens による感度向上は最大2倍となり、マイクロフローでより効果が期待できます

OptiFlow Pro イオンソース

- プローブ位置はあらかじめ最適な位置に設定済
- Ion spray voltage(ISV: エレクトロード電圧)とGas1 (ネブライザーガス)の最適化が必要
 - エレクトロードの位置などの細かいアナログな設定は不必要になりました
- Gas2 (脱溶媒ガス)の最適化は今までと同じ



新しいレベルの定量

新しいソフトウェア、新しいイオン導入部、新しいイオンソース



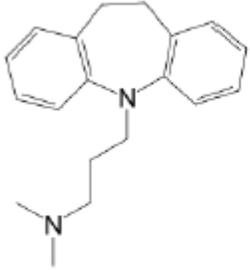
- SCIEX 7500 System
 - 様々なサンプル、ワークフローに新しいレベルの定量をもたらします。
- SCIEX OS Software
 - 最新の質量分析制御/解析ソフトウェアは、最良の分析結果を簡単に導き出します



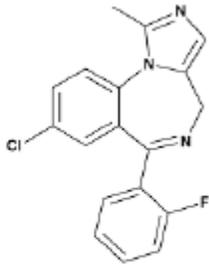
測定例の紹介



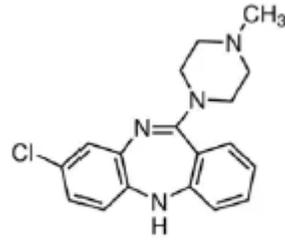
Imipramine, Midazolam and Clozapine



Imipramine



Midazolam



Clozapine

Name	Q1/Q3 (m/z)	Q0D	CE (V)
Imipramine	281.2/86.0	30	22
Midazolam	326.1/291.2	90	36
Clozapine	327.2/270.2	70	32

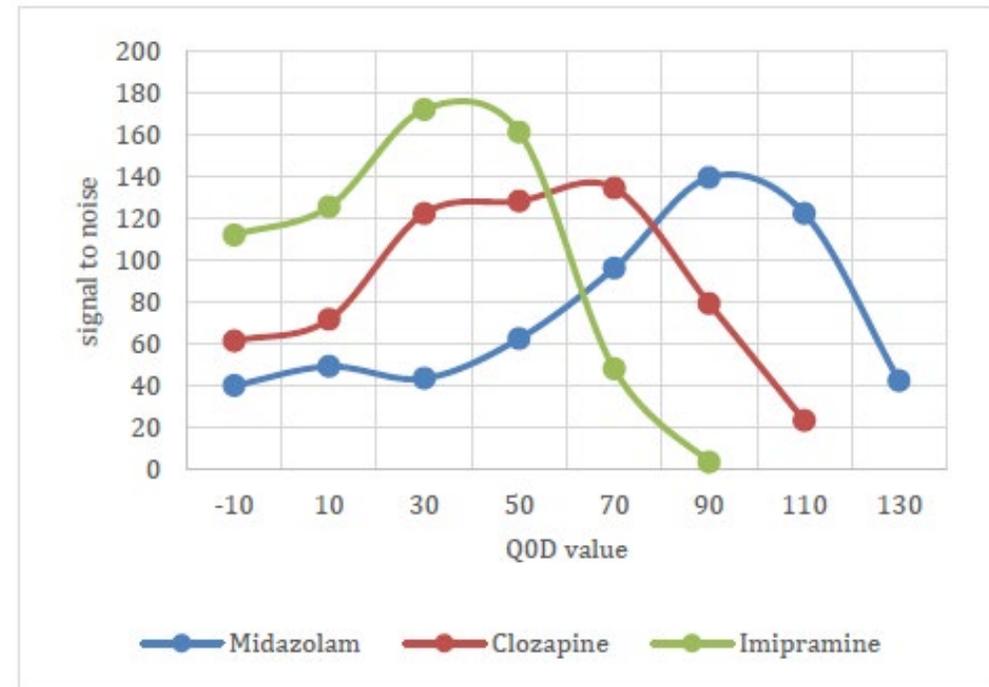
スパイク血漿 100uL (0.05~1000pg/mL)

アセトニトリル 300uL 添加

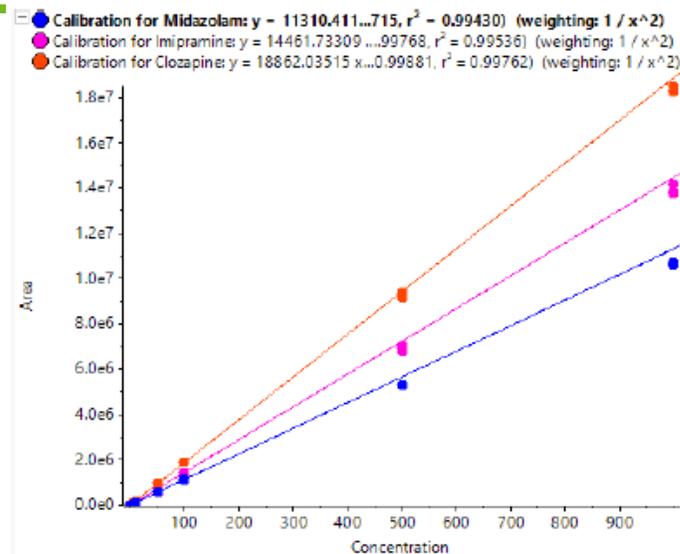
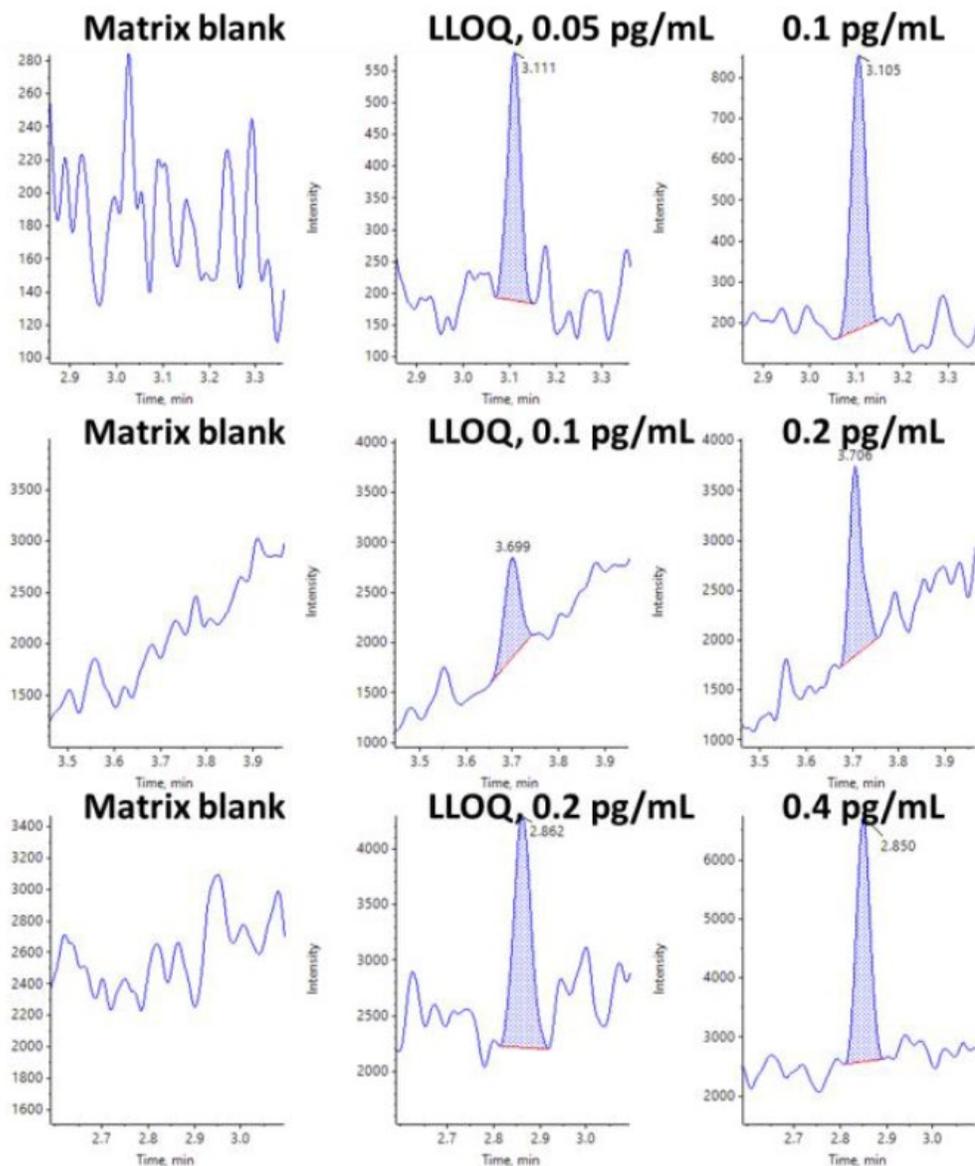
遠沈

上清を回収し、等量の水を添加

10uL 注入



Imipramine, midazolam and clozapine

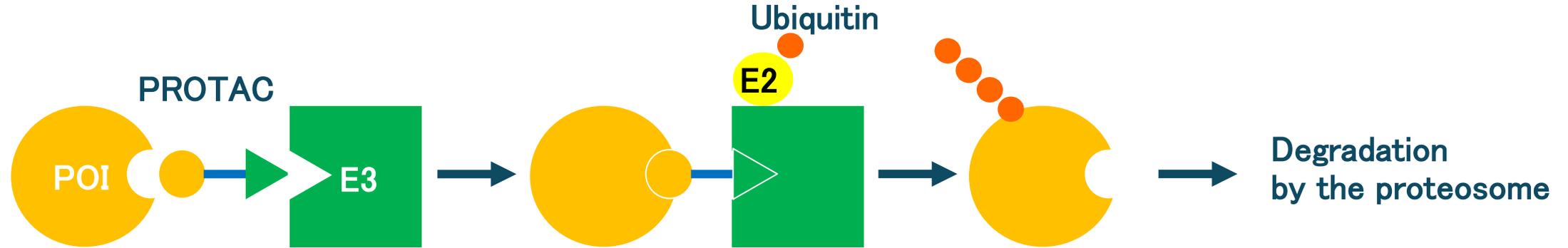


	Midazolam		Imipramine		Clozapine		
	Actual concentration (pg/mL)	Average accuracy (%)	CV (%)	Average accuracy (%)	CV (%)	Average accuracy (%)	CV (%)
0.05		96.6	12.6	N/A	N/A	N/A	N/A
0.1		106	6.08	98.8	5.68	N/A	N/A
0.2		98.2	12.6	101.8	13.4	102	10.0
0.4		104	6.53	99.3	12.5	95.8	4.64
1		101	6.53	104	2.24	99.3	3.06
5		105	1.10	104	1.10	104.9	1.25
10		102	1.91	100	0.94	99.5	1.19
50		99.0	0.48	102	0.91	103	0.42
100		99.1	0.79	98.1	1.17	101	0.52
500		93.9	0.52	95.5	1.94	97.9	1.34
1000		94.3	0.35	96.2	1.49	97.3	0.64

標的型タンパク質分解: PROTAC

PROTEOLYSIS TARGETING CHIMERIC

TPDS



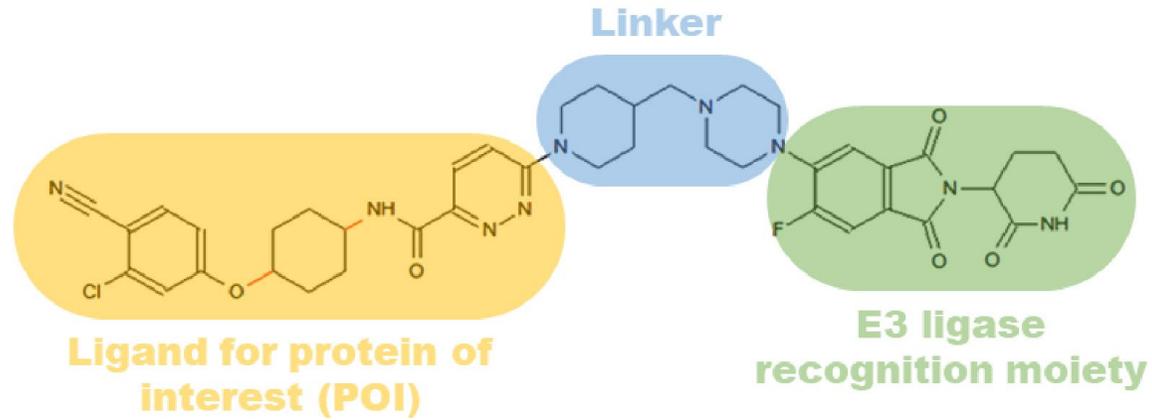
- ARV-110: 転移性去勢抵抗性前立腺がん患者において、引き続き臨床的有用性を示す
- ARV-471: エストロゲン受容体を分解する経口投与可能なプロタック®の乳がん患者への投与

POI: 標的たんぱく質
E3: E3 ligase

POI: 標的タンパク質 E3: ユビキチンリガーゼ

PROTACの高感度な定量化

SCIEX 7500 System



Structure of ARV-110 (bavdegalutamide)
 POIに対するリガンドと、E3ユビキチンリガーゼに対するリガンドが、リンカーで接続されたもの

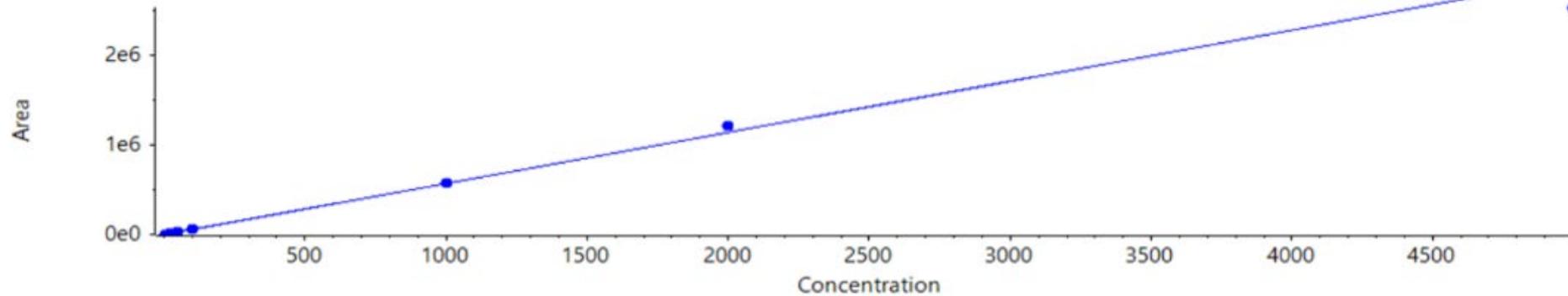
Parameter	Value
Scan mode	MRM
Polarity	Positive
Ion source gas 1	40 psi
Ion source gas 2	60 psi
Curtain gas	42 psi
Source temperature	550°C
Ion spray voltage	4000 V
Declustering potential	40 V
CAD gas	8

ID	Precursor ion (m/z)	Fragment ion (m/z)	CE (V)	CXP (V)
ARV-110_1	812.4	452.2	53	15
ARV-110_2	812.4	562.2	55	15

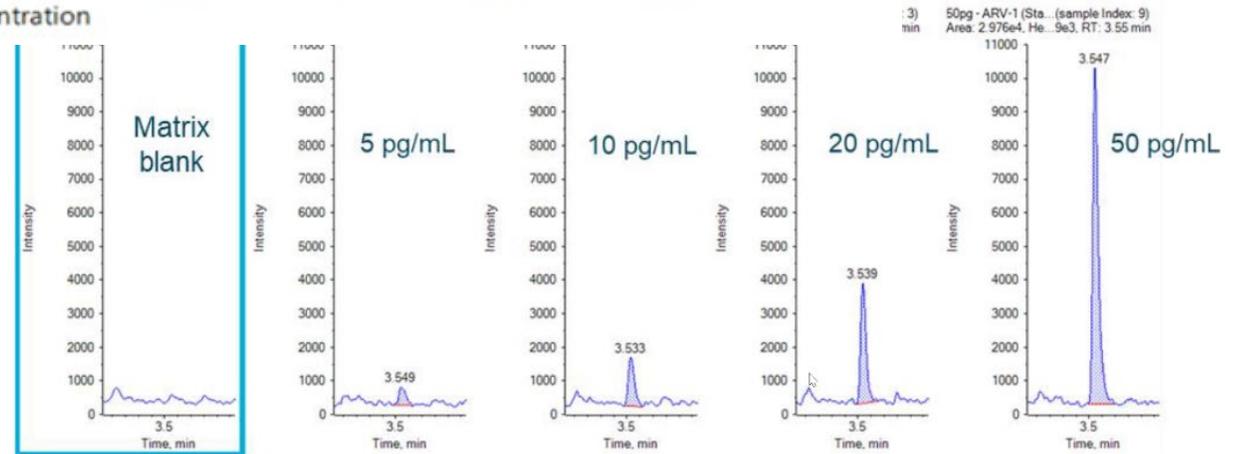
PROTACの高感度な定量化

ARV-110のLLOQは5 pg/mLを達成しました。ブランクではマトリックスとの干渉は認められませんでした。

Calibration for ARV-1: $y = 571.70433x + -814.41724$ ($r = 0.99787, r^2 = 0.99574$) (weighting: $1/x^2$)



Concentration (pg/mL)	Accuracy (%)
5	100
10	99.1
20	98.9
50	107
100	99.0
1000	100
2000	107
5000	88.8





SCIEX OS ソフトウェアの 基本機能の紹介

SCIEX OS ソフトウェア

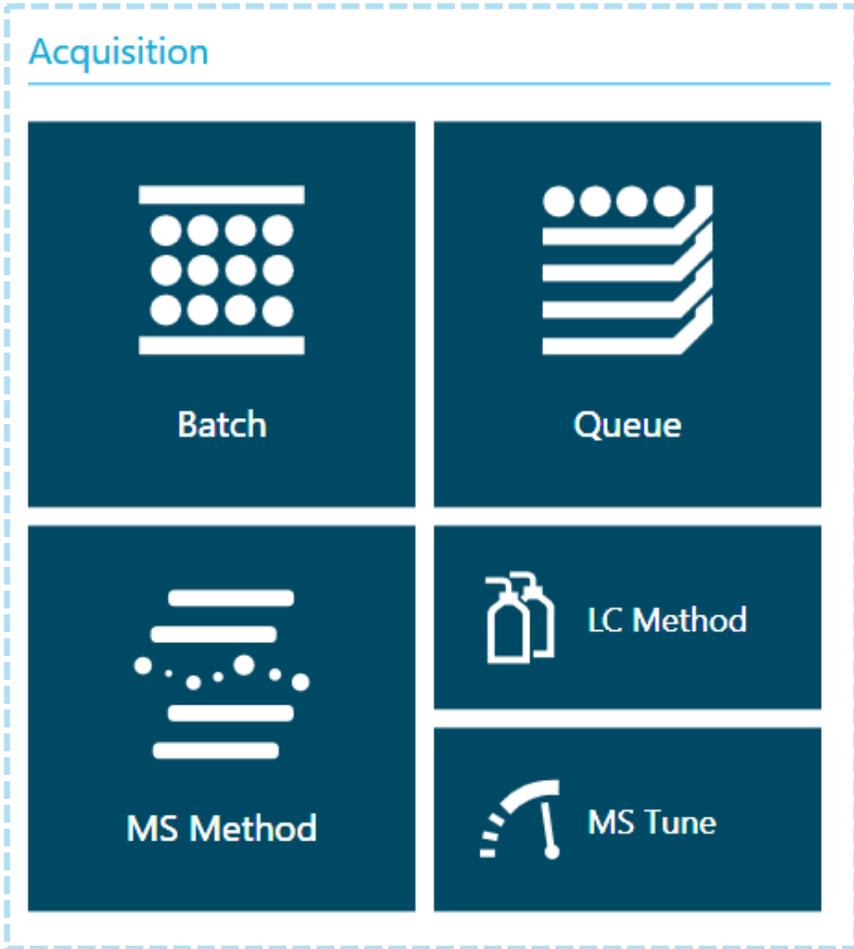
ラボのすべてのシステムに
使いやすさ、高い効率、優れた
インテグリティを実現

すべての SCIEX の LC-MS/MS システムの
ワークフローを単一のソフトウェアプラット
フォームでパワーアップできます。
高度な自動化アルゴリズムが、より多くの
情報に基づいた迅速なデータ解釈を可能に
します。完全なデータインテグリティにより、
正確性、精度および一貫性を強化します。



SCIEX OS ソフトウェア

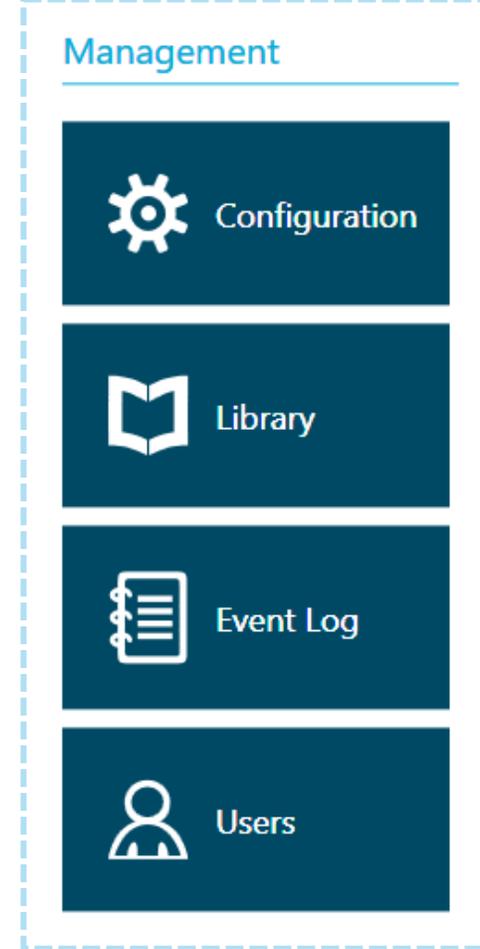
新しい操作画面・より使いやすく



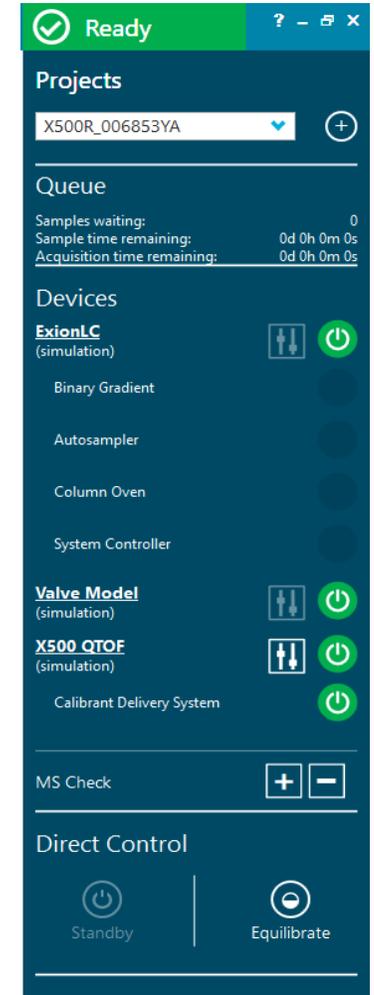
Acquisition
メソッド作成・データ測定



Processing
定量、定性解析

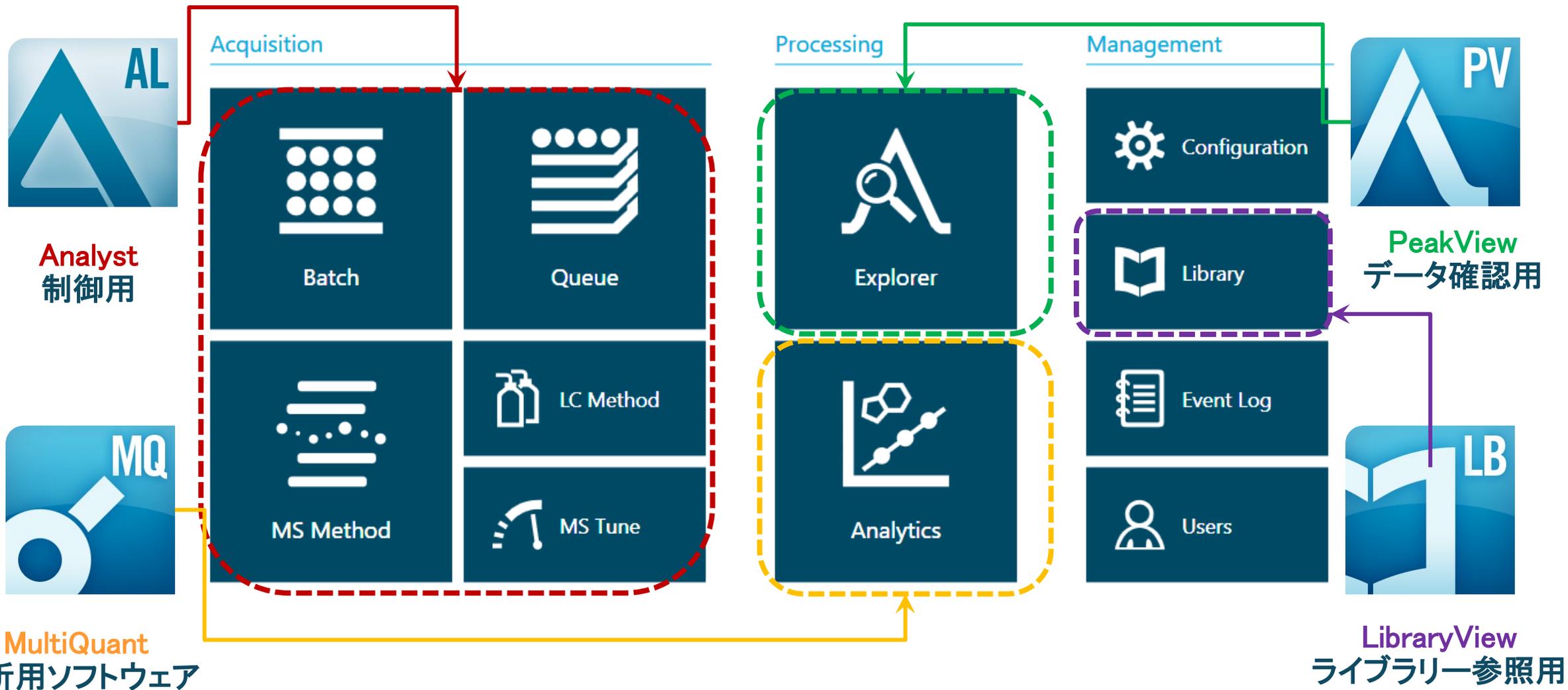


Management
コンフィグ、その他



Status Panel
装置の状態、簡易チェック
装置平衡化・停止

SCIEX OS ソフトウェア



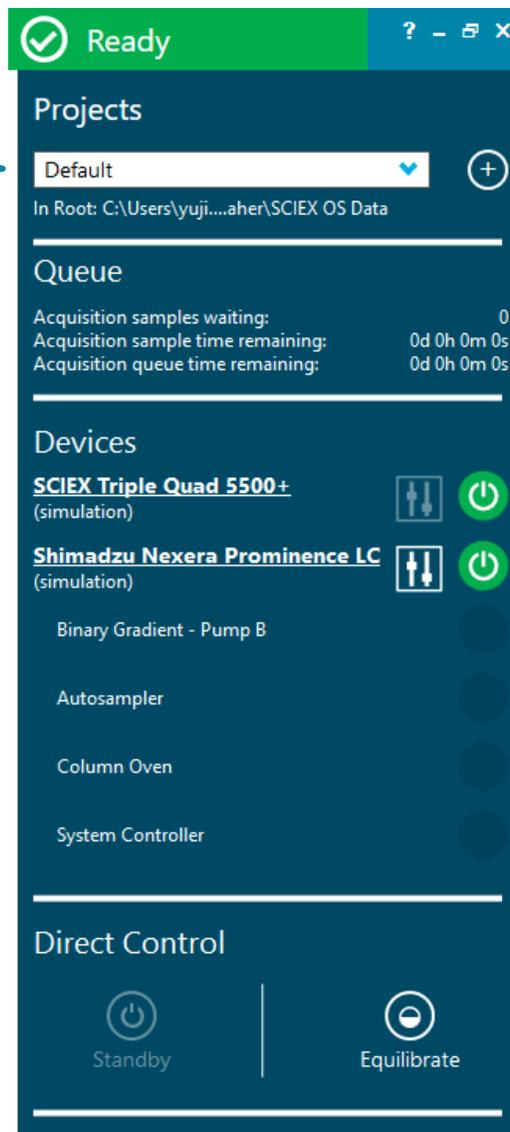
新しい操作画面・より使いやすく

プロジェクト

- プルダウンでプロジェクトの切り替え
- 新規プロジェクトの作成

各機器のステータス
装置状況確認
ポンプ圧を記録可能

- Analyst では Status Bar に該当
- 各デバイスを選択することでステータスの確認やページが可能



測定待ち数
測定時間
トータル測定時間

- 測定状況の表示
(残りのサンプル数や終了までの時間など)

機器平衡化

- 平衡化とスタンバイの操作

MS Tune Calibration の簡便化

MS Tune Running

Tuning Procedures Restore Instrument Data

7500 Low Mass MS Scan Tuning

1. Positive LM Prerequisites

- Introduction
- Achieve Stable Spray Pos
- Optimize Gas1 Pos

2. Positive LM Q3 Unit Resolution Optimization

- Enter Q3 10 Da/sec Tuning
- Tune Q3 Positive 10 Da/sec
- Confirm Q3 Positive 10 Da/sec
- Exit Q3 10 Da/sec Tuning

3. Report

- Report
- Save Tuning Settings

Tune Q3 Positive 10 Da/sec

Run Again Confirm Edit Method View Calibration Reset Mass Points Stop

To calibrate on a peak, select the peak. To better resolve the peaks, use the arrows to increase or decrease the resolution offset. Click Confirm to update the instrument file with the optimized settings. Any unconfirmed settings are discarded when the system advances to the next step.

Auto Calibrate Stop Number of Tries: 2/10 Stage: 1 - Waiting for Count 2 of 5.

Sum of 2 spectra

Item	Min	Max	Actual
Mass	41.934	42.134	42.0365
Width	0.6400	0.7600	0.6764
Intensity	0.00e0	1.00e11	4.00e8

Item	Min	Max	Actual
Mass	132.805	133.005	132.9156
Width	0.6400	0.7600	0.7485
Intensity	0.00e0	1.00e11	1.55e7

Item	Min	Max	Actual
Mass	266.060	266.260	266.1578
Width	0.6400	0.7600	0.6637
Intensity	0.00e0	1.00e11	1.17e7

Item	Min	Max	Actual
Mass	440.900	441.100	440.993
Width	0.6400	0.7600	0.5838
Intensity	0.00e0	1.00e11	7.51e6

Item	Min	Max	Actual
Mass	609.181	609.381	609.2772
Width	0.6400	0.7600	0.7271
Intensity	0.00e0	1.00e11	3.15e7

Item	Min	Max	Actual
Mass	829.440	829.640	829.5386
Width	0.6400	0.7600	0.6314
Intensity	0.00e0	1.00e11	1.87e7

Item	Min	Max	Actual
Mass	921.910	922.110	921.9935
Width	0.6400	0.7600	0.7055
Intensity	0.00e0	1.00e11	1.38e7

Projects: PAL DDK Evaluation

Queue: Acquisition samples waiting: 1, Acquisition sample time remaining: 0d 0h 2m 50s, Acquisition queue time remaining: 0d 0h 2m 50s

Devices: Proto2 Low Mass, Shimadzu Nexera Prominence LC, Binary Gradient, Autosampler, Column Oven, System Controller, Syringe Pump Model

Direct Control: Standby, Equilibrate

Data Acquisition MS Start Stop Save

Windows Taskbar: 3:11 PM 2020-04-02

✓ 簡略化され、簡単に素早くキャリブレーションが出来るようになりました。

MS Method Ready

Method Overview
 Device: SCIEX Triple Quad 5500+
 Ion Source: TurbolonSpray

Source and Gas Parameters

Ion source gas 1: 50 psi
 Ion source gas 2: 60 psi
 Curtain gas: 30 psi
 CAD gas: 8
 Source temperature: 350 °C

Experiment: MRM

Polarity: Negative
 Spray voltage: 4500 V

Advanced Experiment Settings

Settling time: 0 ms
 Pause time: 2 ms
 Q1 resolution: Unit
 Q3 resolution: Unit

Mass Table: Import MRM Mode: MRM

	Group ID	Compound ID	Q1 mass (Da)	Q3 mass (Da)	Dwell time (ms)	DP (V)	EP (V)	CE (V)	CXP (V)
1	Group...	Phenol 1	92.900	64.900	200.000	-38.0	-5.0	-28.0	-12.0
2	Group...	Phenol 2	92.900	41.000	100.000	-38.0	-5.0	-45.0	-12.0
3	Group...	Chlorophenol 1	126.800	34.900	100.000	-41.0	-5.0	-30.0	-5.0
4	Group...	Chlorophenol 2	126.800	90.900	50.000	-41.0	-5.0	-21.0	-5.0
5	Group...	Dichlorophenol 1	160.800	34.900	100.000	-47.0	-5.0	-36.0	-5.0
6	Group...	Dichlorophenol 2	160.800	124.900	50.000	-47.0	-5.0	-24.0	-5.0
7	Group...	2,4,6-Trichlorophenol...	194.800	35.000	100.000	-67.0	-5.0	-42.0	-5.0

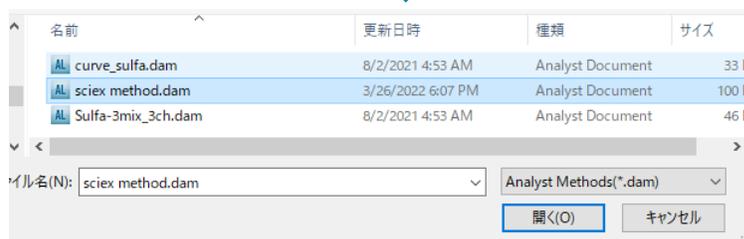
Data Acquisition MS Start Stop Save...

- ・見開きでイオンソースのパラメーター等が確認可能
- ・メソッドを並べて比較可能

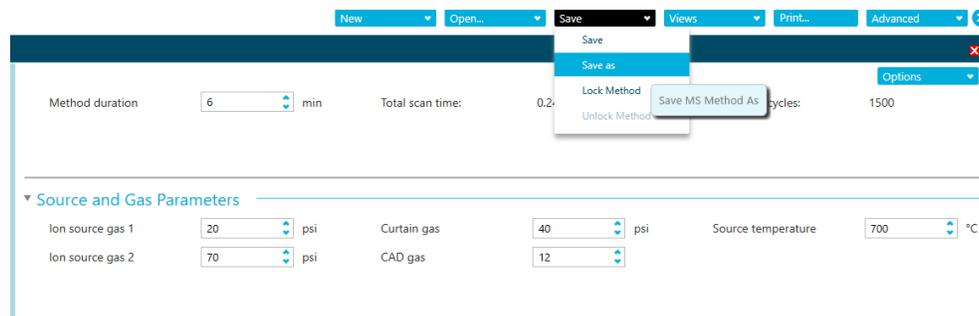
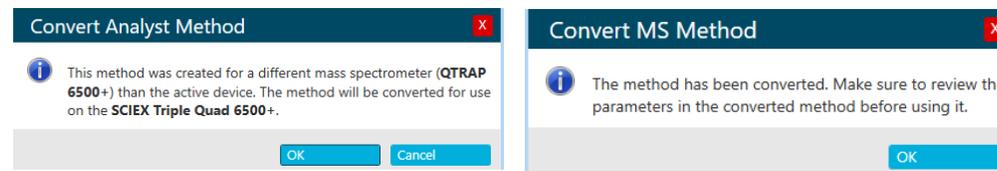
MSメソッド コンバート(Analyst methodのコンバート)



①Open の▼をクリックしてConvert file...を選択



②Convertしたいファイルを選択



③OKを選択してコンバート完了

※ Acquisition Method からコンバートできるのは MS 条件のみになります

MS メソッド 条件の最適化

MS Method

Guided Optimization - MRM FIA

Flow Injection Analysis

- 1. Set Initial Acquisition Values
- 2. Set Initial LC-MS Conditions
- 3. Optimize Parameters
- 4. Review Report

Optimize Parameter

Range: Discrete Intensity: Signal To Noise

Determine step size using: Range Optimize using: Intensity

Initial Parameter Values

Optimize	Parameter Name	Initial Value	Start	Stop	Step
<input type="checkbox"/>	DP (v)	Show all...	80	120	20
<input type="checkbox"/>	CE (v)	Show all...	20	30	5
<input type="checkbox"/>	CXP (v)	Show all...	5	15	5
<input checked="" type="checkbox"/>	Curtain Gas (psi)	35.0	25	40	5
<input checked="" type="checkbox"/>	CAD Gas	9.0	6	11	1
<input checked="" type="checkbox"/>	Spray Voltage (V)	5500.0	4000	5500	500
<input checked="" type="checkbox"/>	Source temperature (°C)	350.0	300	650	50
<input checked="" type="checkbox"/>	Ion Source Gas1 (psi)	60.0	50	80	10
<input checked="" type="checkbox"/>	Ion Source Gas2 (psi)	60.0	50	80	10

Replicate injection for each step: 1 Cycle times

Optimized Parameter Values

Optimize	Compound Name	Vial Position	DP (v)	CE (v)	CXP (v)	Curtain Gas (psi)	CAD Gas	Spray Voltage (V)
<input checked="" type="checkbox"/>	Reserpine 1	1						
<input checked="" type="checkbox"/>	Reserpine 2	1						

Intensity (cps) vs Time (min)

Modeの追加

- ・最適化範囲のStep入力が可能
- ・SN比での最適化が可能

Batch 自動解析

時間の節約: 手動でデータを処理するために待つ必要はありません。
TextもしくはCSV形式でExport及びImportが可能です。
Excelの表をバッチに貼り付けることも可能です。

Sample Name	MS Method	LC Method	Rack Type	Plate Type	Vial Position	Injection Volum...	Sample Type	Data File	Processing Method	Results File
wash	DEMO MS Method	DEMO	Vial Rack	1.5mL (105 vial)	1	10.0	Solvent	demo240110	240110	Demo reuslut 240110
Blak	DEMO MS Method	DEMO	Vial Rack	1.5mL (105 vial)	2	10.0	Blank	demo240110	240110	Demo reuslut 240110
1	DEMO MS Method	DEMO	Vial Rack	1.5mL (105 vial)	3	10.0	Standard	demo240110	240110	Demo reuslut 240110
3	DEMO MS Method	DEMO	Vial Rack	1.5mL (105 vial)	4	10.0	Standard	demo240110	240110	Demo reuslut 240110
10	DEMO MS Method	DEMO	Vial Rack	1.5mL (105 vial)	5	10.0	Standard	demo240110	240110	Demo reuslut 240110
100	DEMO MS Method	DEMO	Vial Rack	1.5mL (105 vial)	6	10.0	Standard	demo240110	240110	Demo reuslut 240110

Export the Batch to a File

Export the batch sample information to a .txt or .csv file

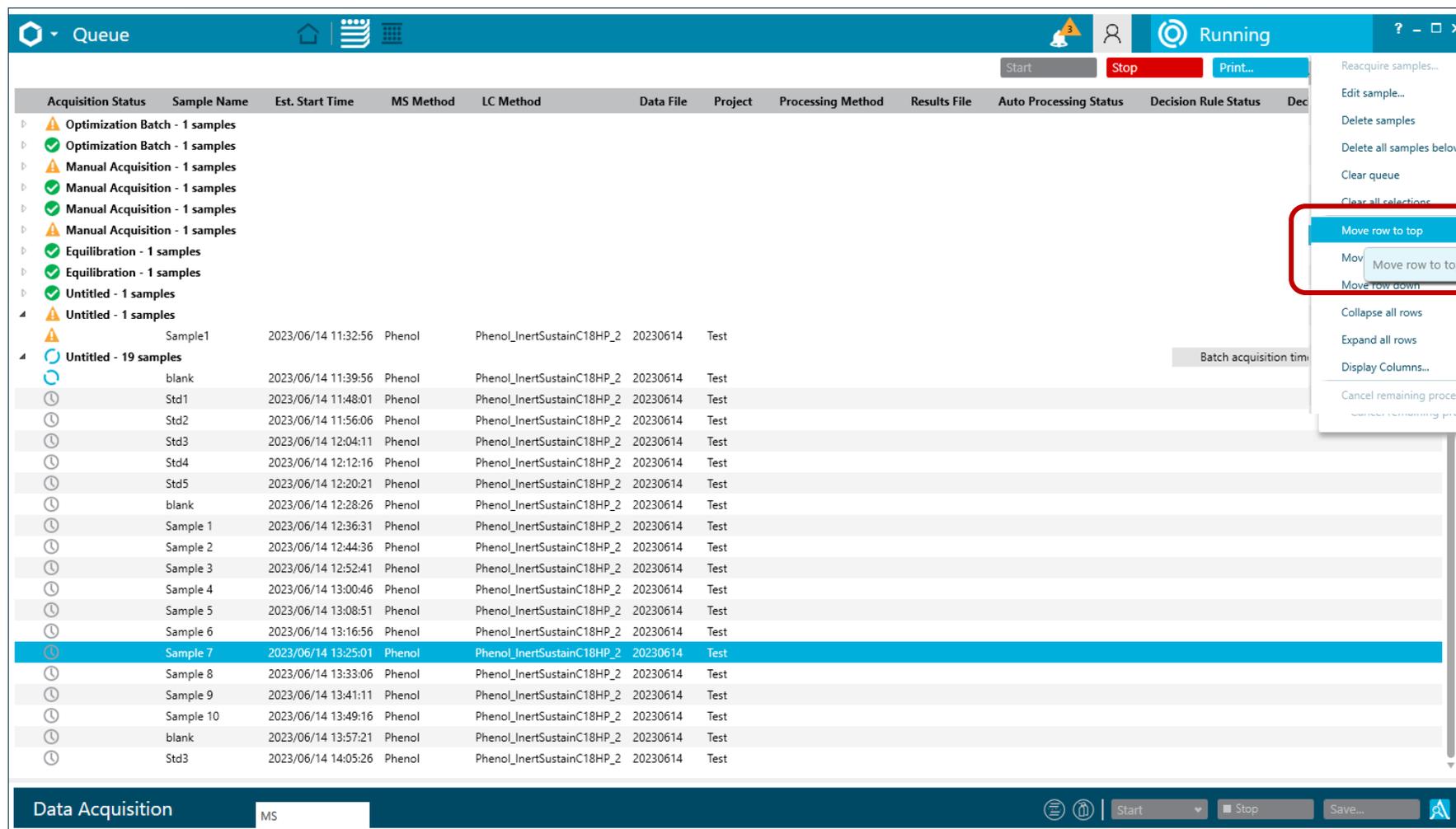
File path

File format .txt .csv

Batchで
解析メソッドを選択

Batchで
結果ファイル名を入力

Queue 測定開始後の測定順番の入れ替え、サンプル名の変更

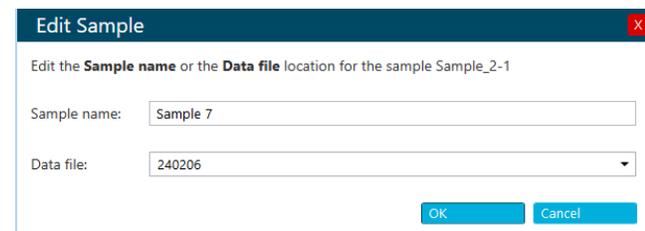


The screenshot shows the 'Queue' window in the SCIEX software. The window title is 'Queue' and it has a 'Running' status. The main area is a table with columns: Acquisition Status, Sample Name, Est. Start Time, MS Method, LC Method, Data File, Project, Processing Method, Results File, Auto Processing Status, Decision Rule Status, and Dec. The table contains several rows, including 'Optimization Batch - 1 samples', 'Manual Acquisition - 1 samples', 'Equilibration - 1 samples', and 'Untitled - 1 samples'. A context menu is open over the table, showing options like 'Reacquire samples...', 'Edit sample...', 'Delete samples', 'Move row to top', and 'Move row down'. The 'Move row to top' option is highlighted with a red box. A blue arrow points to the 'Move row to top' option in the context menu.

Acquisition Status	Sample Name	Est. Start Time	MS Method	LC Method	Data File	Project	Processing Method	Results File	Auto Processing Status	Decision Rule Status	Dec
▲	Optimization Batch - 1 samples										
✓	Optimization Batch - 1 samples										
▲	Manual Acquisition - 1 samples										
✓	Manual Acquisition - 1 samples										
✓	Manual Acquisition - 1 samples										
✓	Manual Acquisition - 1 samples										
▲	Manual Acquisition - 1 samples										
✓	Equilibration - 1 samples										
✓	Equilibration - 1 samples										
✓	Untitled - 1 samples										
▲	Untitled - 1 samples										
▲	Sample1	2023/06/14 11:32:56	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
▲	Untitled - 19 samples										
○	blank	2023/06/14 11:39:56	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Std1	2023/06/14 11:48:01	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Std2	2023/06/14 11:56:06	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Std3	2023/06/14 12:04:11	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Std4	2023/06/14 12:12:16	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Std5	2023/06/14 12:20:21	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	blank	2023/06/14 12:28:26	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 1	2023/06/14 12:36:31	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 2	2023/06/14 12:44:36	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 3	2023/06/14 12:52:41	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 4	2023/06/14 13:00:46	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 5	2023/06/14 13:08:51	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 6	2023/06/14 13:16:56	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 7	2023/06/14 13:25:01	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 8	2023/06/14 13:33:06	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 9	2023/06/14 13:41:11	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Sample 10	2023/06/14 13:49:16	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	blank	2023/06/14 13:57:21	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					
○	Std3	2023/06/14 14:05:26	Phenol	Phenol_InertSustainC18HP_2	20230614	Test					

異なるBatchでもSampleの
順番の入れ替えが可能

測定前であればSample名、
Data file名の変更が可能



The 'Edit Sample' dialog box is shown, allowing users to edit the sample name or data file location for a specific sample. The sample name is currently 'Sample 7' and the data file is '240206'.

Edit the **Sample name** or the **Data file** location for the sample Sample_2-1

Sample name:

Data file:

OK Cancel

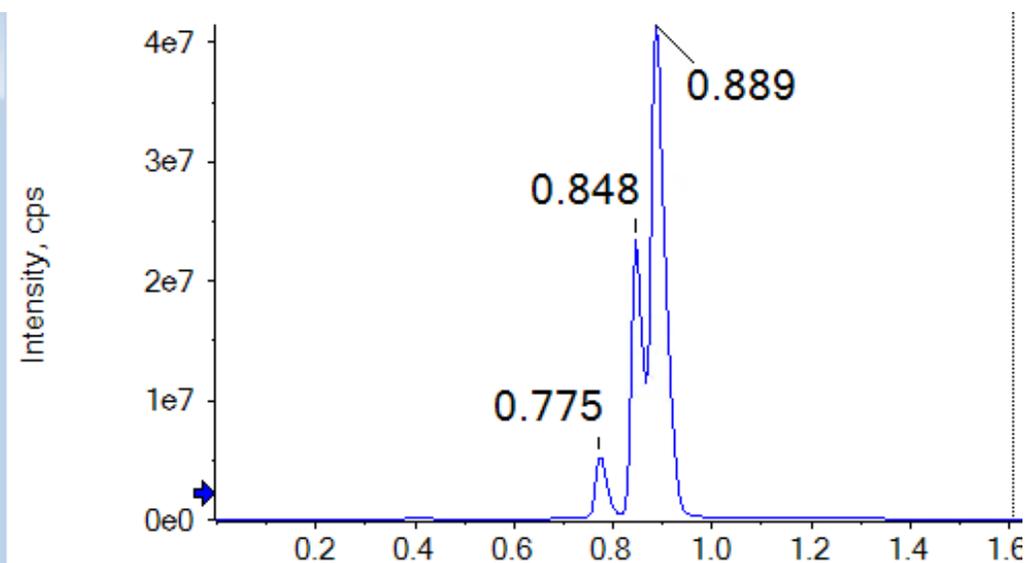
Queue Exploreでのクロマト確認を容易に



Acquisition Status	Sample Name	Est. Start Time	Acquisition Time	Rack Code	Rack Position	Plate Code	Plat
✓	w	2024/01/10 10:28:58	00:31:00	Vial Rack		1.5mL (105 vial)	
✓	w	2024/01/10 11:00:51	00:31:00	Vial Rack		1.5mL (105 vial)	
✓	NC	2024/01/10 11:32:37	00:31:00	Vial Rack		1.5mL (105 vial)	
✓	BL	2024/01/10 12:04:23	00:31:00	Vial Rack		1.5mL (105 vial)	
🔄	Sample_2-1	2024/01/10 12:36:08	00:31:00	Vial Rack		1.5mL (105 vial)	
🕒	Sample_2-2	2024/01/10 13:07:55	00:31:00	Vial Rack		1.5mL (105 vial)	
🕒	Sample_2-3	2024/01/10 13:39:43	00:31:00	Vial Rack		1.5mL (105 vial)	
🕒	Sample_1-1	2024/01/10 14:11:30	00:31:00	Vial Rack		1.5mL (105 vial)	
🕒	Sample_1-2	2024/01/10 14:43:17	00:31:00	Vial Rack		1.5mL (105 vial)	
🕒	Sample_1-3	2024/01/10 15:15:04	00:31:00	Vial Rack		1.5mL (105 vial)	

ダブルクリック

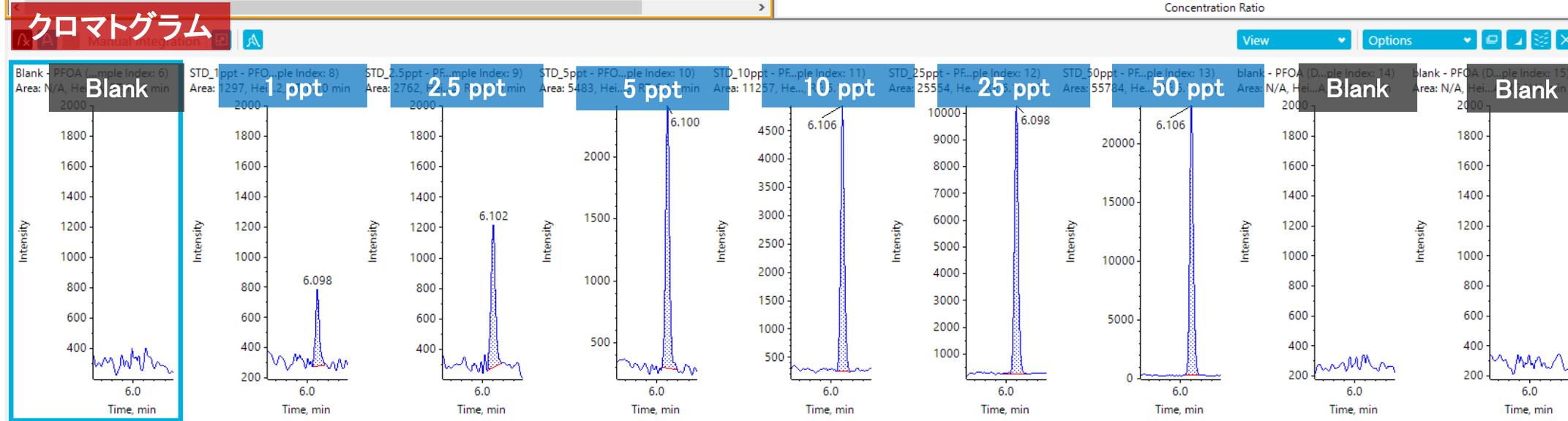
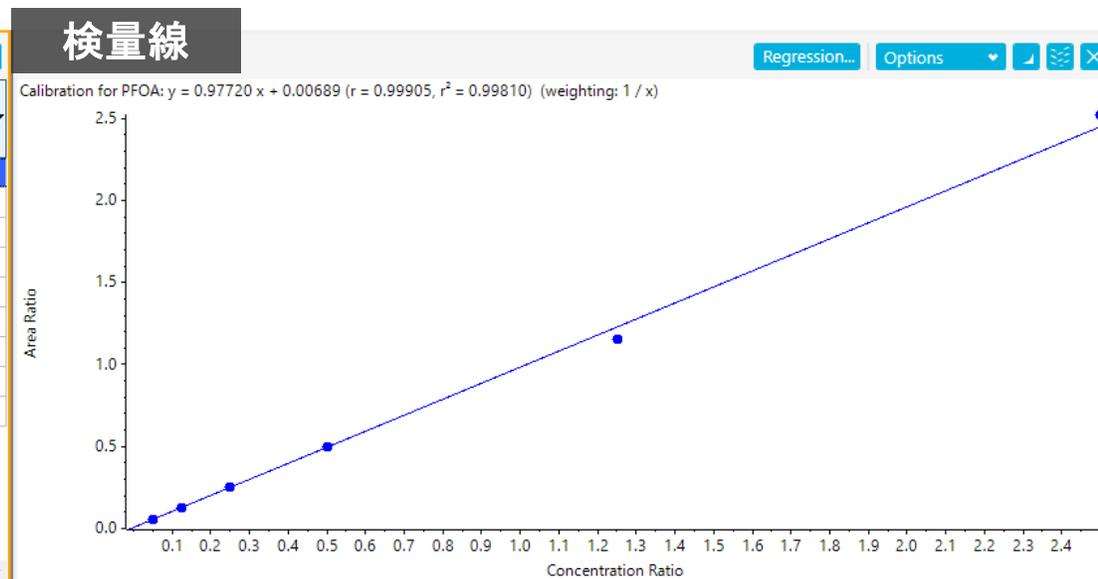
Exploreでファイルを選択しなくても開きます。



Analytics 定量結果の表示

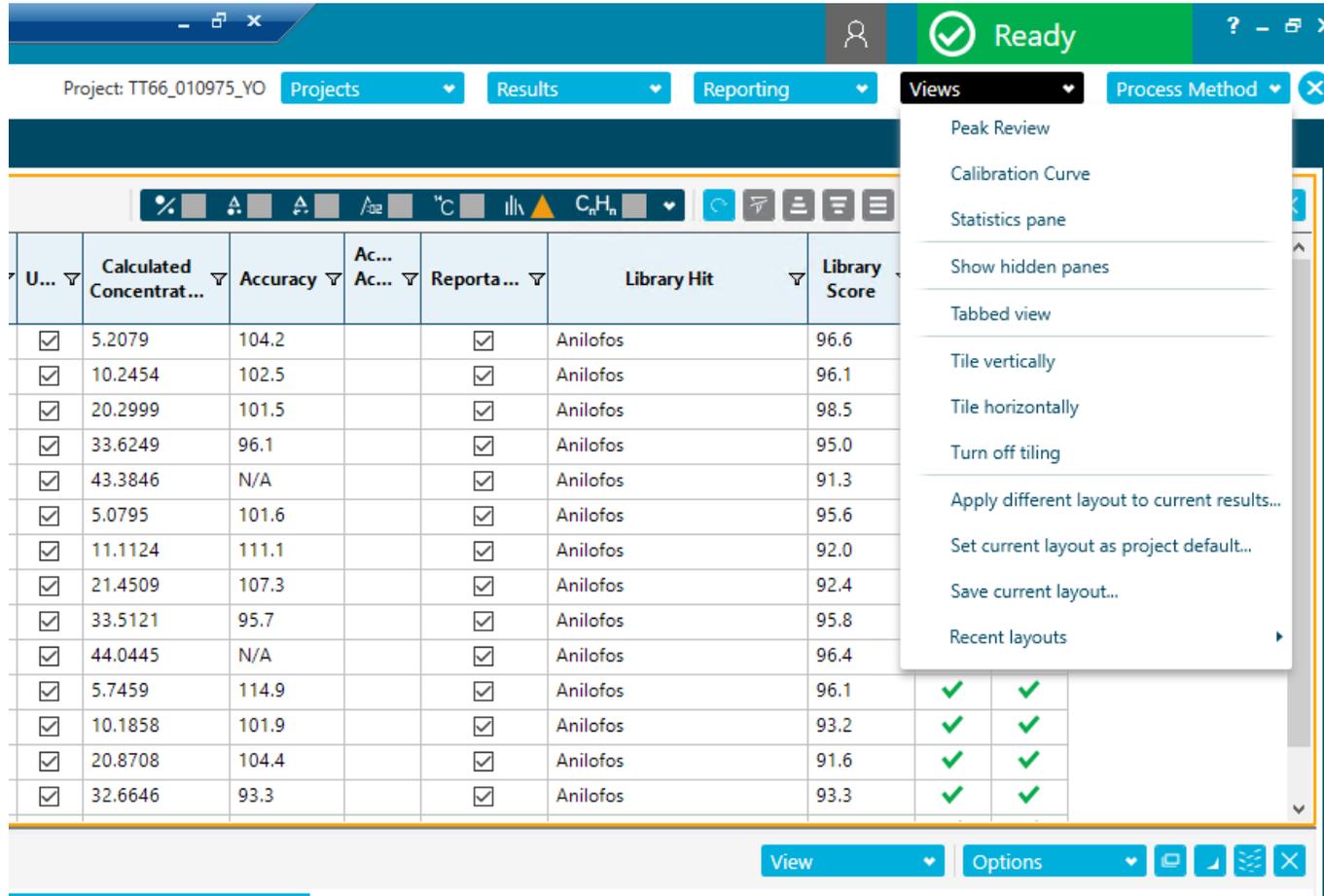
結果表

Sample Name	Sample Type	Actual Concentration	Area	IS Area	Retention Time	Calculated Concentration	Accuracy	Used
Blank	Double Blank	N/A	N/A	N/A	N/A	N/A	N/A	<input checked="" type="checkbox"/>
STD_1ppt	Standard	1.00	1297	22443	6.10	1.0423	104.23	<input checked="" type="checkbox"/>
STD_2.5ppt	Standard	2.50	2762	21958	6.10	2.4331	97.32	<input checked="" type="checkbox"/>
STD_5ppt	Standard	5.00	5483	21507	6.10	5.0771	101.54	<input checked="" type="checkbox"/>
STD_10ppt	Standard	10.00	11257	22708	6.11	10.0049	100.05	<input checked="" type="checkbox"/>
STD_25ppt	Standard	25.00	25554	22136	6.10	23.4858	93.94	<input checked="" type="checkbox"/>
STD_50ppt	Standard	50.00	55784	22127	6.11	51.4568	102.91	<input checked="" type="checkbox"/>
blank	Double Blank	N/A	N/A	N/A	N/A	N/A	N/A	<input checked="" type="checkbox"/>
blank	Double Blank	N/A	N/A	N/A	N/A	N/A	N/A	<input checked="" type="checkbox"/>



Analytics レイアウトの保存

結果画面のレイアウトを保存できます(別プロジェクトでも使用可能)

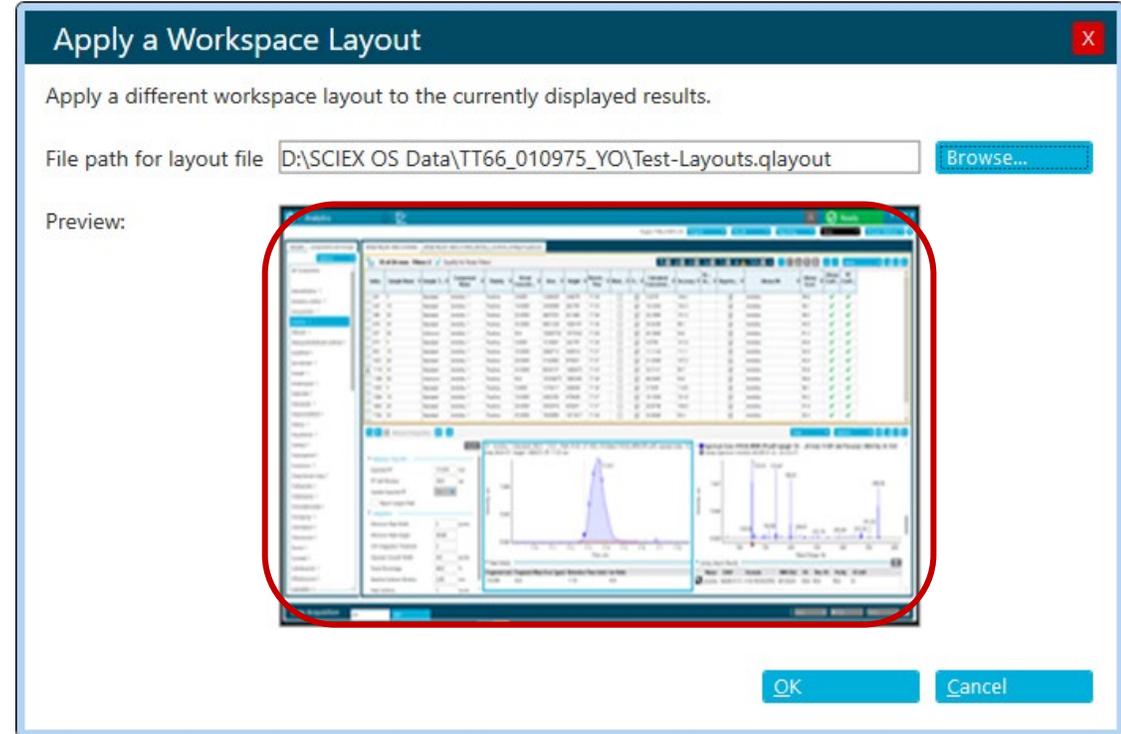


Project: TT66_010975_YO | Projects | Results | Reporting | Views | Process Method

U...	Calculated Concentrat...	Accuracy	Ac...	Reporta...	Library Hit	Library Score
<input checked="" type="checkbox"/>	5.2079	104.2		<input checked="" type="checkbox"/>	Anilofos	96.6
<input checked="" type="checkbox"/>	10.2454	102.5		<input checked="" type="checkbox"/>	Anilofos	96.1
<input checked="" type="checkbox"/>	20.2999	101.5		<input checked="" type="checkbox"/>	Anilofos	98.5
<input checked="" type="checkbox"/>	33.6249	96.1		<input checked="" type="checkbox"/>	Anilofos	95.0
<input checked="" type="checkbox"/>	43.3846	N/A		<input checked="" type="checkbox"/>	Anilofos	91.3
<input checked="" type="checkbox"/>	5.0795	101.6		<input checked="" type="checkbox"/>	Anilofos	95.6
<input checked="" type="checkbox"/>	11.1124	111.1		<input checked="" type="checkbox"/>	Anilofos	92.0
<input checked="" type="checkbox"/>	21.4509	107.3		<input checked="" type="checkbox"/>	Anilofos	92.4
<input checked="" type="checkbox"/>	33.5121	95.7		<input checked="" type="checkbox"/>	Anilofos	95.8
<input checked="" type="checkbox"/>	44.0445	N/A		<input checked="" type="checkbox"/>	Anilofos	96.4
<input checked="" type="checkbox"/>	5.7459	114.9		<input checked="" type="checkbox"/>	Anilofos	96.1
<input checked="" type="checkbox"/>	10.1858	101.9		<input checked="" type="checkbox"/>	Anilofos	93.2
<input checked="" type="checkbox"/>	20.8708	104.4		<input checked="" type="checkbox"/>	Anilofos	91.6
<input checked="" type="checkbox"/>	32.6646	93.3		<input checked="" type="checkbox"/>	Anilofos	93.3

Views menu options:

- Peak Review
- Calibration Curve
- Statistics pane
- Show hidden panes
- Tabbed view
- Tile vertically
- Tile horizontally
- Turn off tiling
- Apply different layout to current results...
- Set current layout as project default...
- Save current layout...
- Recent layouts



Apply a Workspace Layout

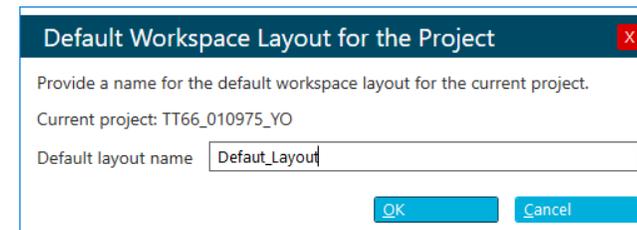
Apply a different workspace layout to the currently displayed results.

File path for layout file: D:\SCIEX OS Data\TT66_010975_YO\Test-Layouts.qlayout

Preview:



OK Cancel



Default Workspace Layout for the Project

Provide a name for the default workspace layout for the current project.

Current project: TT66_010975_YO

Default layout name: Default_Layout

OK Cancel

Analytics Reporter機能によるレポート作成

PDF (Secure PDFの形式も選択可)でレポート作成可能です。

Project: test Project 1 | Projects | Results | **Reporting** | Views | Process Method

[MQ4] Results Table (Demo230424.qsession, locked)

7 rows | Filters: 0 | Qualify for: C_nH_n

Index	Sample Name	Sample T...	Component Name	Component Type	Component Group Name	Actual Concentr...	Expected RT	Area	Retenti... Time	Retention Time D...	Us...	Calcu Conce
1	blank	Blank	251.2 / 108.2	Quantifiers		N/A	1.71	N/A	N/A	N/A	<input checked="" type="checkbox"/>	N/A
4	0.1	Standard	251.2 / 108.2	Quantifiers		0.10	1.71	N/A	N/A	N/A	<input checked="" type="checkbox"/>	N/A

Create Report

Generate a report using a predefined template and specified logo

Template name: MQ Analyte Report 1 Browse...

Template description: MQ Analyte Report 1

- MQ Analyte Report 2
- MQ Analyte Report 3
- MQ Analyte Report condensed table
- MQ Analyte Report with chromatograms
- MQ Blank Template
- MQ Pep Quant

Report format: MQ QC Summary 1 with flags

- MQ Sample Report 1
- MQ Sample Report 2
- MQ Sample Report 3
- MQ Sample Report condensed table
- MQ Sample Report with chromatograms

Report title:

Template View

EXAMPL

Replace Logo... | View Pages...

Browse...

Create | Close

Print Templates Result table

SCIEX OSで解析したResult Tableで表示されたカラム、クロマトグラムをそのまま印刷可能です。

Print Preview

Print Quick Print Page Setup Scale Select Template First Page Previous Page Next Page Last Page Navigation Pane Zoom Out Zoom Zoom In Page Layout Enable Continuous Scrolling

Printing Date: 10/23/2023
Printing Time: 11:45:52 AM

Results Table

Cell Shading Legend

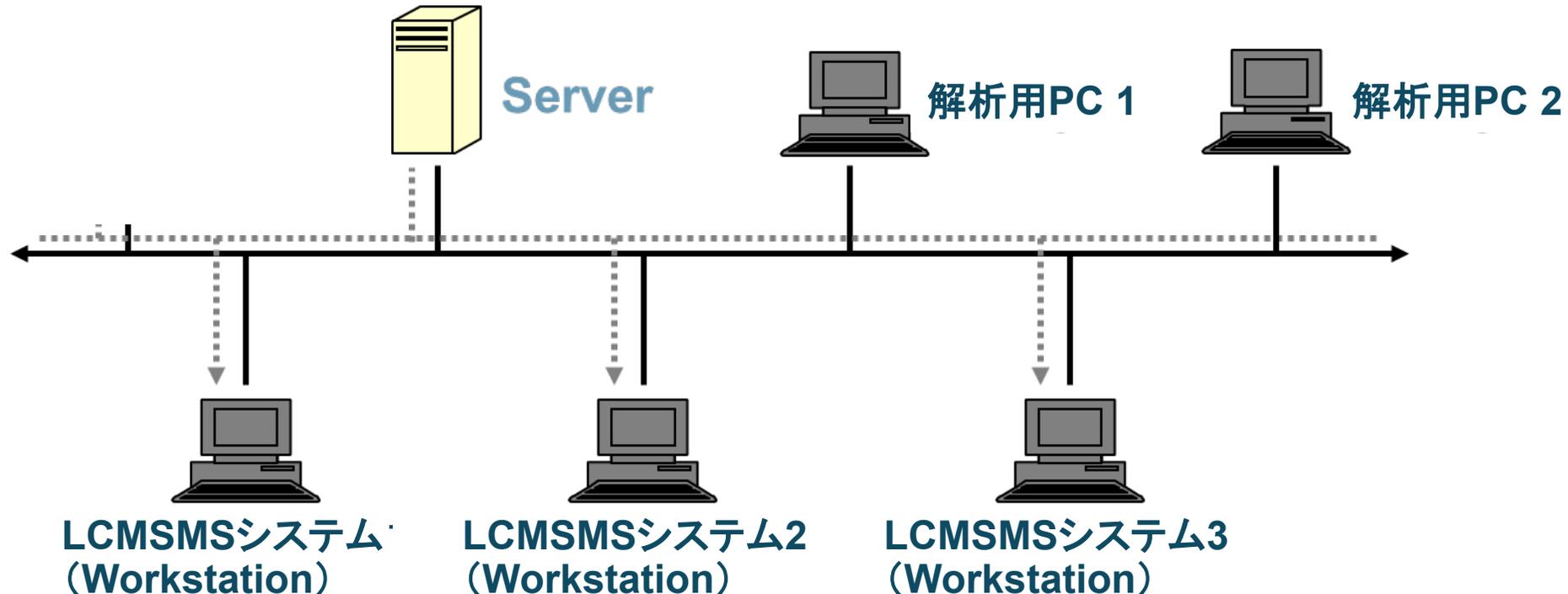
Result	Cell Colour
Passed	
Failed or Above Threshold	
Below Threshold	

Index	Sample Name	Sample Type	Component Name	Actual Concentration	Area	IS Area	Area Ratio	Height	Retention Time	Signal / Noise	Modified	Used	Calculated Concentration	Accuracy
1	Blank	Blank	251.2 / 108.2	N/A	N/A	2152	N/A	N/A	N/A	N/A	<input type="checkbox"/>	<input checked="" type="checkbox"/>	N/A	N/A
4	0.1	Standard	251.2 / 108.2	0.10	1002	13186	0.076	70	1.74	105	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	0.096	96.31
7	1	Standard	251.2 / 108.2	1.00	6279	12014	0.523	542	1.72	815	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1.002	100.23
10	10	Standard	251.2 / 108.2	10.00	66660	12948	5.148	5540	1.71	7072	<input type="checkbox"/>	<input checked="" type="checkbox"/>	10.385	103.85
13	100	Standard	251.2 / 108.2	100.00	575242	11707	49.139	45369	1.71	18274	<input type="checkbox"/>	<input checked="" type="checkbox"/>	99.616	99.62
16	Sample1	Unknown	251.2 / 108.2	N/A	32563	161379	0.202	2814	1.70	3692	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.351	N/A

Printing Date: 10/23/2023
Printing Time: 11:45:52 AM

データの一括管理

- MS (SCIEX OS)に付属する制御末端の測定データを、ネットワークを介して自動で転送することができます。
- ストレージ先を選んで、データを集約することができます。
- 転送後は端末側にデータは残りません。
- ネットワークがダウンした場合、制御末端側にバックアップされています。



Data Integrityの機能紹介



追加機能：承認機能

Reviewerは”Mark results as reviewed and save”を選択します

Project: test Project 1 | Projects | Results | Reporting | Views | Process Method

[MQ4] Results Table (Demo230424.qsession, locked)

7 rows | Filters: 0 | Qualify for

Index	Sample Name	Sample T...	Component Name	Component Type	C	Gr
1	blank	Blank	251.2 / 108.2	Quantifiers		
4	0.1	Standard	251.2 / 108.2	Quantifiers		
7	1	Standard	251.2 / 108.2	Quantifiers		
10	10	Standard	251.2 / 108.2	Quantifiers		
13	100	Standard	251.2 / 108.2	Quantifiers		

- New...
- Open...
- Recent results
- Save
- Save as...
- Unlock results file and save
- Mark results file as reviewed and save**
- Cache all chromatograms for faster peak review

Retenti... Time	Retention Time D...	Us...	Calcu Conce
N/A	N/A	<input checked="" type="checkbox"/>	N/A
N/A	N/A	<input checked="" type="checkbox"/>	N/A
1.72	0.01	<input checked="" type="checkbox"/>	8.834e
1.71	0.01	<input checked="" type="checkbox"/>	1.128e
1.70	0.00	<input checked="" type="checkbox"/>	9.883e



理由とパスワードを入力します。

Confirm Change Events

Change Events

Timestamp	Event Name	Event Description
4/24/2023 5:47:44 PM	Results Table approved	The Results Table, C:\SCIEX OS Data\test Project 1\Quantitation Results\Demo230424.qsession was reviewed

E-Signature

Timestamp: 4/24/2023 5:47:44 PM
 User Name: NETADDS\toshifumi.tohda
 Full User Name: Tohda, Toshifumi

Reason:

Password:

E-signatureにチェックが入り、Event NameにResult Table approvedと表示されます。

Timestamp	Event Name	Description	Reason	E-Signature	Full User Name	User
4/24/2023 5:48:52 PM	File saved	The Results Table, 'C:\SCIEX OS Data\test Project 1\Quantitation Results\Demo230424.qsession', was saved.	Saved	✓	Tohda, Toshifumi	NETADDS\tos
4/24/2023 5:48:53 PM	Results Table approved	The Results Table, C:\SCIEX OS Data\test Project 1\Quantitation Results\Demo230424.qsession was reviewed	Reviewed	✓	Tohda, Toshifumi	NETADDS\tos

メソッド: ロック機能

- ・ロック機能が追加されました。
- ・重要なメソッドを保護できます。



The screenshot displays the 'MS Method' configuration interface. The main area shows a table of parameters for 'DEMO MS Method (QT75-015331_RYa)'. A dropdown menu is open on the right side, highlighting the 'Lock Method' option.

Parameter	Value	Unit
Method duration	30	min
Minimum dwell time	10	ms
Ionization start time	2	min
Target cycle time	600	ms
Maximum dwell time	200	ms
Ionization stop time	13	min

Method Overview
Device: Triple Quad 7500
Ion Source: E-ANLYT 200+ uL
Add Experiment
cMRM

Save
Save as
Lock Method
Unlock Method

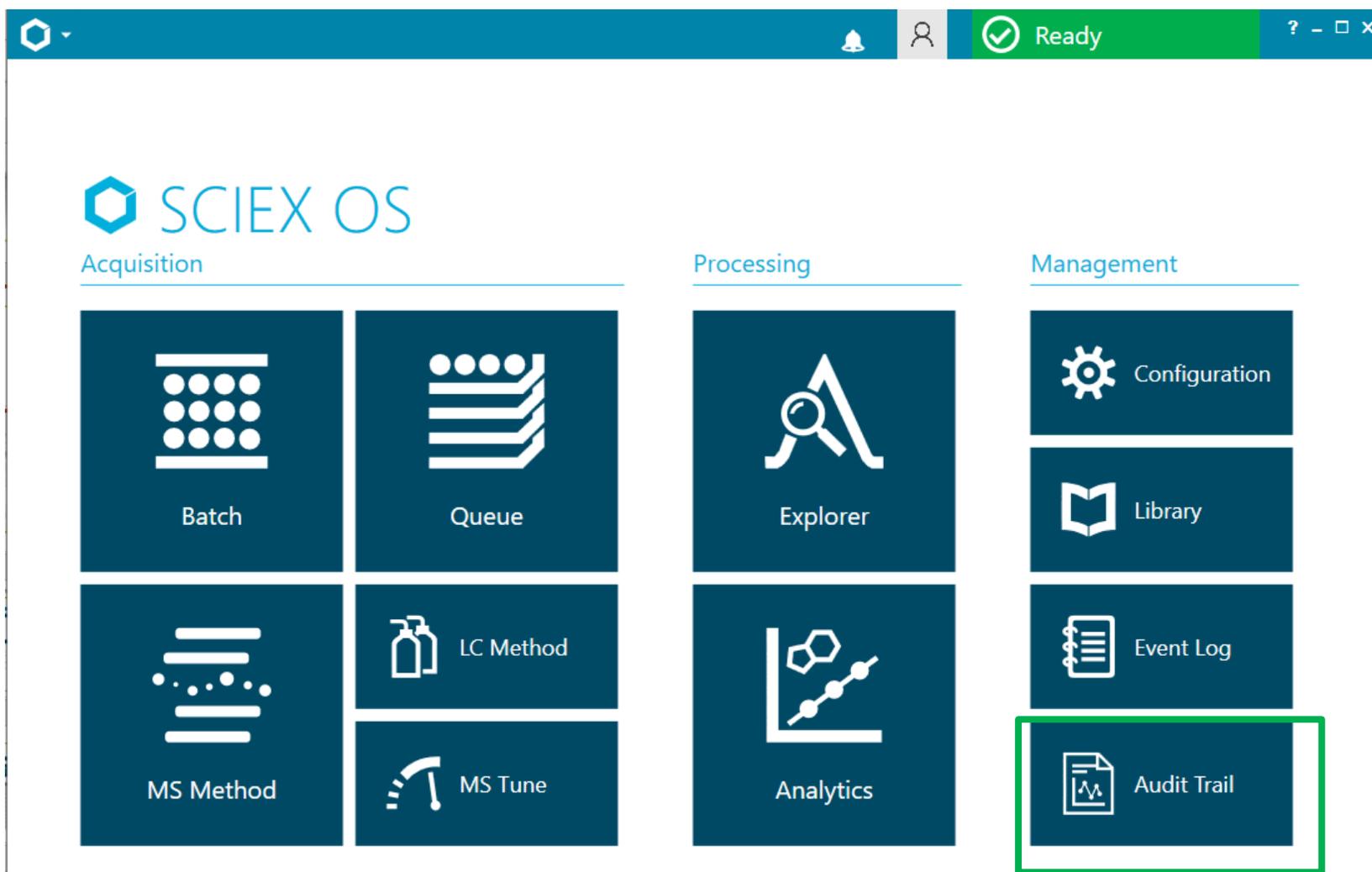
Audit Event の追加

監査証跡イベントがAnalyst に追加され強化されております。
 アーカイブ作成はAnalystでは1000件でしたが20000件と大幅強化されております

Analytics workspace の例

SCIEX OS or CAC	Analyst Software
Analytics Workspace	
Actual Concentration changed	Quantitation Events: 'Concentration' has been changed
Auto-Processing File saved	—
Barcode ID changed	—
Comparison sample changed in non-targeted workflow	—
Custom columns modified	Quantitation Events: 'Custom Title' has changed
Data exploration opened	Project Events: Data File has been opened
Data exported	—
Data transferred to LIMS	—
Dilution Factor changed	Quantitation Events: 'Dilution Factor' has been changed
External calibration changed	—
External calibration exported	—

Audit Trailの確認



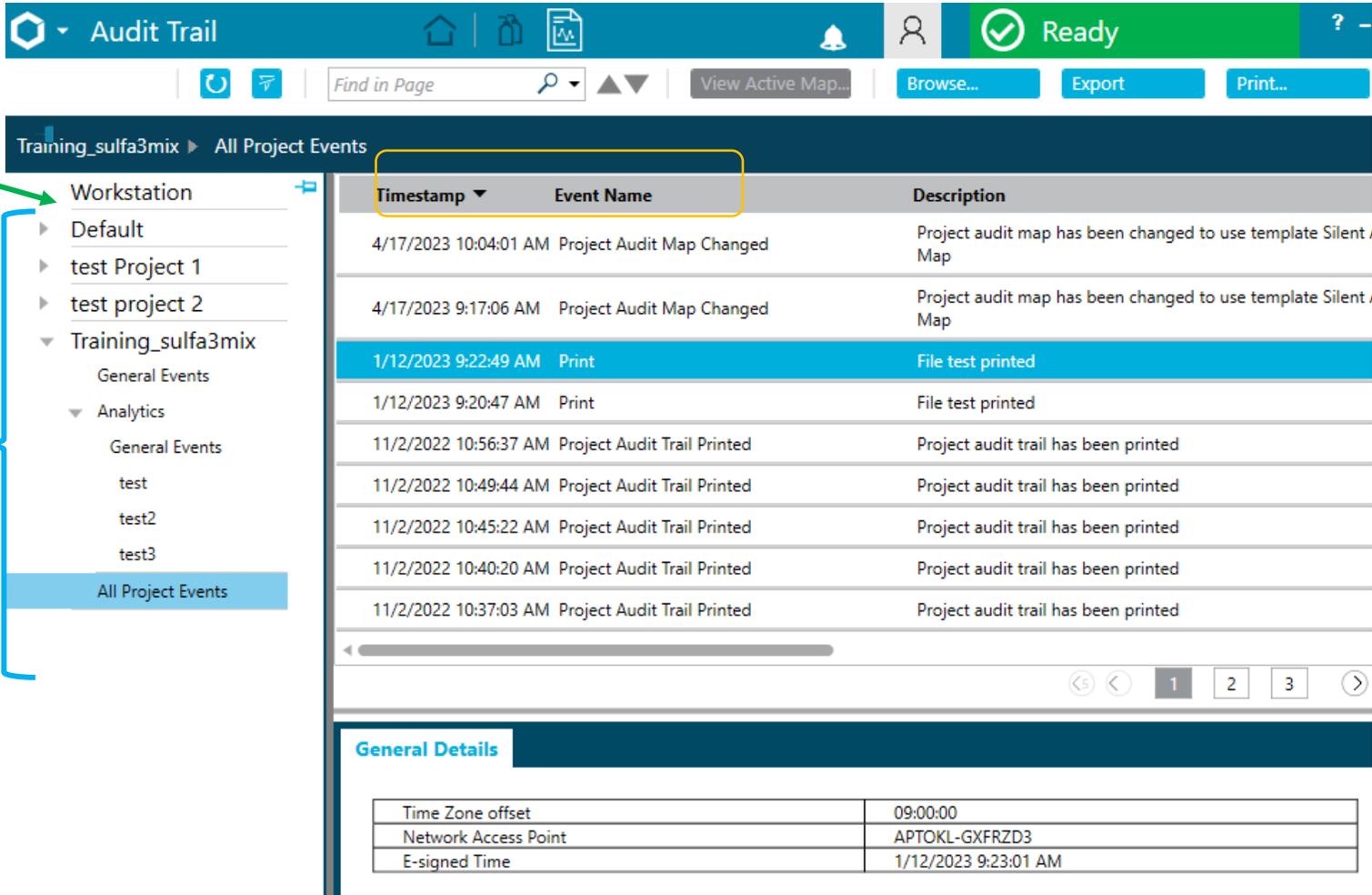
ホーム画面から容易にアクセス可能
(閲覧権限が無い場合は表示されません)

Audit Trail

Workstation*はProject 横断的に記録され、Projectに関してはProjectごとに記録されます。

Workstation

Project

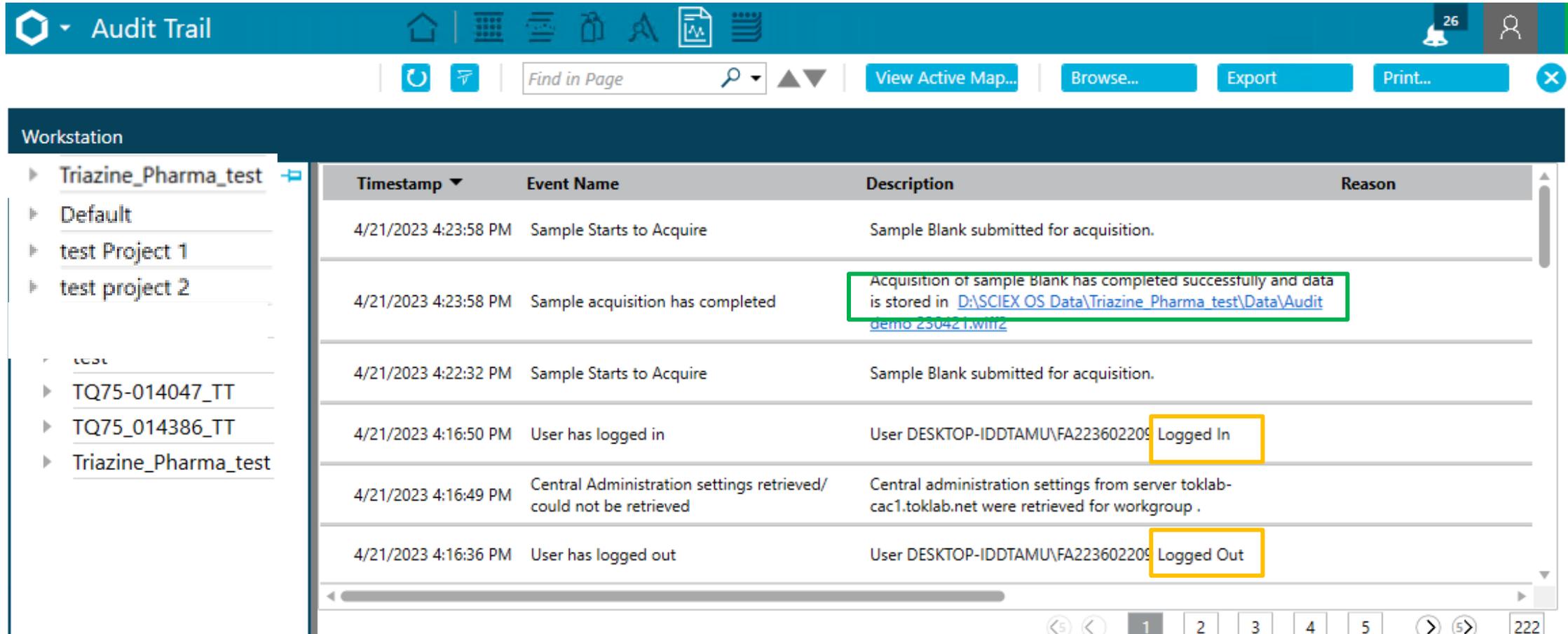


The screenshot shows the 'Audit Trail' interface. The top navigation bar includes a home icon, a refresh icon, a search bar with 'Find in Page', a 'View Active Map...' button, and buttons for 'Browse...', 'Export', and 'Print...'. The main content area is titled 'Training_sulfa3mix > All Project Events'. On the left, a tree view shows the hierarchy: 'Workstation' (with sub-items 'Default', 'test Project 1', 'test project 2', 'Training_sulfa3mix', 'General Events', 'Analytics', 'General Events', 'test', 'test2', 'test3', and 'All Project Events'), and 'Project' (with sub-items 'test', 'test2', 'test3', and 'All Project Events'). A green arrow points to 'Workstation' and a blue arrow points to 'Project'. The main table has columns 'Timestamp', 'Event Name', and 'Description'. The table contains several rows of events, including 'Project Audit Map Changed' and 'File test printed'. At the bottom, a 'General Details' section shows a table with the following data:

General Details	
Time Zone offset	09:00:00
Network Access Point	APTOKL-GXFRZD3
E-signed Time	1/12/2023 9:23:01 AM

Audit Trail Workstation の例

ログイン、ログアウトや測定の記録等、装置全般に関わる記録が保存されます。



The screenshot displays the Audit Trail Workstation interface. At the top, there is a navigation bar with the title "Audit Trail" and various icons. Below this is a toolbar with buttons for "View Active Map...", "Browse...", "Export", and "Print...". The main content area is titled "Workstation" and contains a tree view on the left with folders like "Triazine_Pharma_test", "Default", "test Project 1", and "test project 2". The central part of the interface is a table with the following columns: "Timestamp", "Event Name", "Description", and "Reason".

Timestamp	Event Name	Description	Reason
4/21/2023 4:23:58 PM	Sample Starts to Acquire	Sample Blank submitted for acquisition.	
4/21/2023 4:23:58 PM	Sample acquisition has completed	Acquisition of sample Blank has completed successfully and data is stored in D:\SCIEX OS Data\Triazine Pharma test\Data\Audit demo 250421.wiff2	
4/21/2023 4:22:32 PM	Sample Starts to Acquire	Sample Blank submitted for acquisition.	
4/21/2023 4:16:50 PM	User has logged in	User DESKTOP-IDDTAMU\FA223602209	Logged In
4/21/2023 4:16:49 PM	Central Administration settings retrieved/ could not be retrieved	Central administration settings from server toklab-cac1.toklab.net were retrieved for workgroup .	
4/21/2023 4:16:36 PM	User has logged out	User DESKTOP-IDDTAMU\FA223602209	Logged Out

At the bottom of the interface, there is a pagination control showing page 1 of 222.

Audit Trail Projectの例 (MS Method)

- Methodの変更履歴がAudit Trail上で確認できます。
- 変更前はピンクの、変更後は緑で表示されます。

Timestamp	Event Name	Description	Reason	E-Signature
10/19/2023 2:33:36 PM	MS method saved	MS method changed test.msm		n/a

Change Details
General Details

Side By Side View
Difference View

Experiment

Scan type: MRM

Polarity: Positive

Spray voltage (V): 5500

Q1 resolution: Unit

CAD gas: 9

Q3 resolution: Unit

Pause time (ms): 5

Settling time (ms): 0

Q0 dissociation: False

MRM Mode: MRM

InterQuad1 offset (V): -0.5

Q1 stubbies (V): -10

Mass Table

Group ID	Compound ID	Q1 mass (Da)	Q3 mass (Da)	Dwell time (ms)	EP (V)	CE (V)	CXP (V)
Group 1	Compound 1	500	100900	100	10	30	15

Audit Trail Projectの例 (Result tableの例)

test Project 1 > Analytics > Demo230424

Timestamp	Event Name	Description	Reason	E-Signature	Full User Name	User
4/24/2023 9:49:26 AM	File saved	The Results Table, 'C:\SCIEX OS Data\test Project 1\Quantitation Results\Demo230424.qsession', was modified.	result table update	✓	Tohda, Toshifumi	NETADDS\tos
4/24/2023 9:49:27 AM	Results Table locked	The Results Table, 'C:\SCIEX OS Data\test Project 1\Quantitation Results\Demo230424.qsession' was locked		n/a	Tohda, Toshifumi	NETADDS\tos
4/24/2023 9:47:55 AM	Processing method changed and applied	All samples of component, 265.2 / 92.0, were updated to use the integration parameters from blank of 265.2 / 92.0 (C:\SCIEX OS Data\Training_sulfa3mix\Data\curve_sulfa.wiff, sample 1).	update parameters	✓	Tohda, Toshifumi	NETADDS\tos
4/24/2023 9:46:40 AM	Integration parameters changed	(C:\SCIEX OS Data\Training_sulfa3mix\Data\curve_sulfa.wiff, sample 1). Gaussian Smooth Width was changed from 0 to 4 points. Noise % was changed from 40% to 80%. Area was changed from "423.163" counts to "0" counts (100% decrease).	Parameters changed	✓	Tohda, Toshifumi	NETADDS\tos
4/24/2023 9:34:22 AM	Processing method changed and applied	An Integration parameter for 251.2 / 108.2 was changed: Gaussian Smooth Width was changed from 0 to 3.5 points.	parameter change	✓	Tohda, Toshifumi	NETADDS\tos

Analytics Details
General Details

Results Table Comparison Column Settings... Synchronized

C:\SCIEX OS Data\test Project 1\Quantitation Results\Demo230424.qsession: Results Table of the selected Save Event [4/24/2023 9:49:26 AM]

Index	Sample Name	Sample Ty...	Component Na...	Component T...	Component Group Name	Actual Concentrat...	Expected RT	Area	Retention Time
4	0.1	Standard	251.2 / 108.2	Quantifiers		0.10	1.71	N/A	N/A
5	0.1	Standard	265.2 / 92.0	Quantifiers		0.10	2.70	1.133e3	2.71
6	0.1	Standard	311.2 / 156.3	Quantifiers		0.00	3.48	1.299e4	3.48
7	1	Standard	251.2 / 108.2	Quantifiers		1.00	1.71	6.700e2	1.72

C:\SCIEX OS Data\test Project 1\Quantitation Results\Demo230424.qsession: Previous version of the Results Table of the selected Save Event [4/24/...

Index	Sample Name	Sample Ty...	Component Na...	Component T...	Component Group Name	Actual Concentrat...	Expected RT	Area	Retention Time
4	0.1	Standard	251.2 / 108.2	Quantifiers		0.10	1.71	9.533e2	1.72
5	0.1	Standard	265.2 / 92.0	Quantifiers		0.10	2.70	1.471e3	2.71
6	0.1	Standard	311.2 / 156.3	Quantifiers		0.00	3.48	1.299e4	3.48
7	1	Standard	251.2 / 108.2	Quantifiers		1.00	1.71	6.642e2	1.71

Peak Cal. Curve

blank - 251.2 / 108.2 (Blank 251...ve_sulfa.wiff), (sample Index: 1)
Area: N/A, Height: N/A, RT: N/A min

MPW: 3
MPH: 100.00
S/N: 0
SW: 3.5
Ns%: 40.0
BSW: 2.00
PSF: 2
MACT: 2
ERT: 1.705
RTW: 30.0
URT: No
RLP: No

パラメーターの変更を
クロマトグラムの変化で
確認できます。

Configuration > User ManagementでUserの追加や削除が可能です。

Configuration     

Devices
Projects
User Management
Queue
Print Templates
Audit Maps
Licenses

Users Roles Security

User name or group  

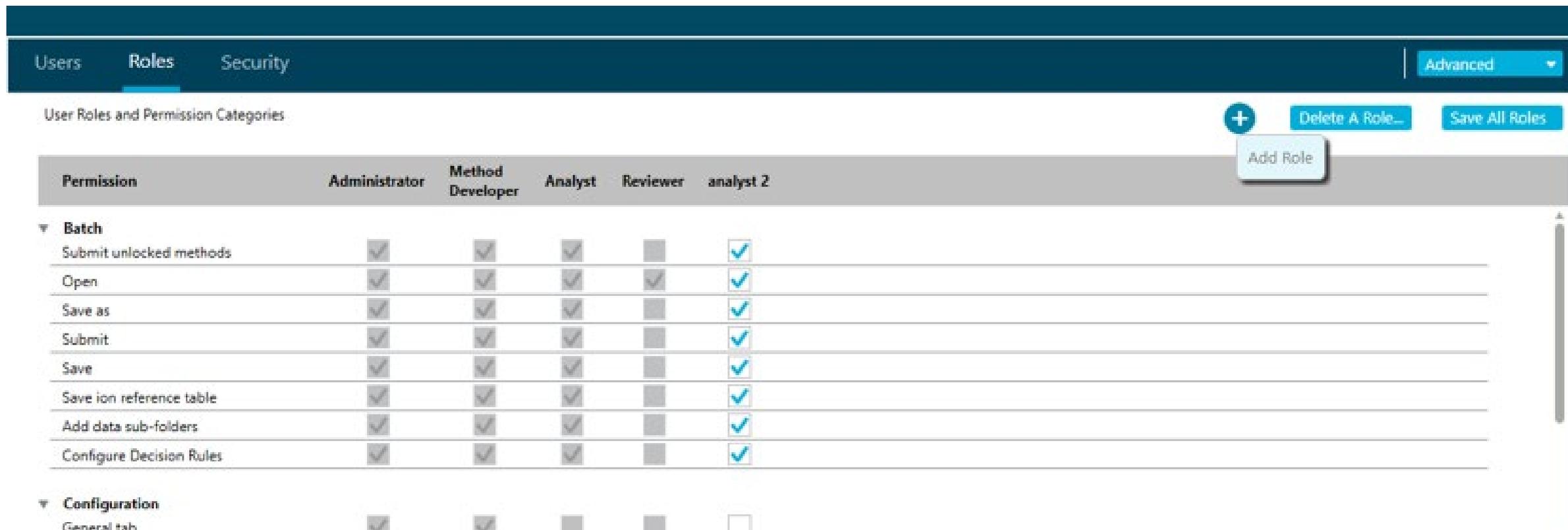
Active user or group **追加** **削除**

Assigned	Role	Role Description
<input type="checkbox"/>	Administrator	Full access. Provides ability to develop methods, run batches, explore data, process and modify settings.
<input type="checkbox"/>	Method Developer	To perform method creation and routine analysis. Provides ability to develop methods, run batches, explore c
<input type="checkbox"/>	Analyst	To perform routine analysis. Provides ability to run batches, review data and process results.
<input type="checkbox"/>	Reviewer	Read-only access. Provides ability to explore data, and process.

Rolesの設定

お客様の使用法に合わせたRolesの作成が可能 (Permissionの追加はできません)

* 作成する際は既にあるRolesを元に作成することが可能です

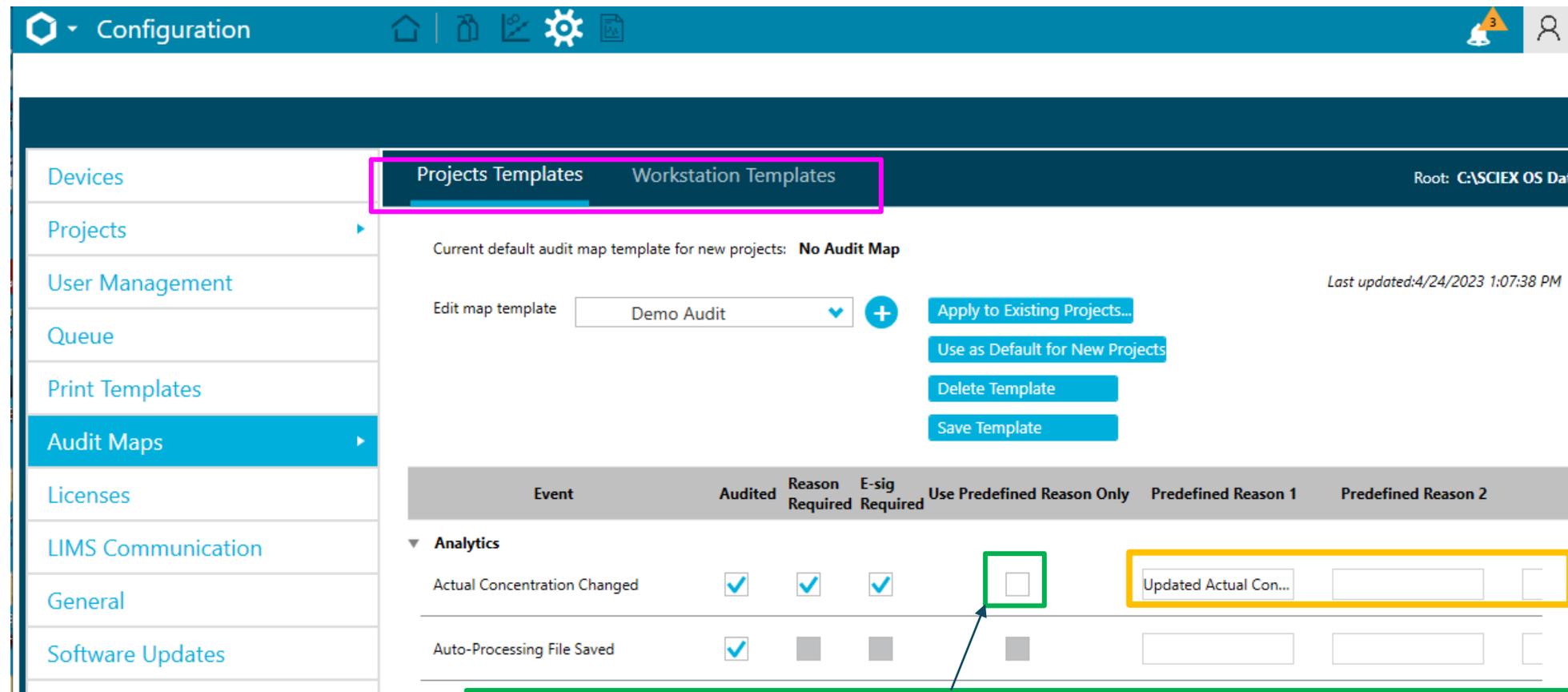


The screenshot shows a web interface for configuring roles. At the top, there are tabs for 'Users', 'Roles', and 'Security', with 'Roles' selected. A dropdown menu is set to 'Advanced'. Below the tabs, there are buttons for '+ Add Role', 'Delete A Role...', and 'Save All Roles'. The main area is a table titled 'User Roles and Permission Categories' with columns for 'Permission', 'Administrator', 'Method Developer', 'Analyst', 'Reviewer', and 'analyst 2'. The table lists permissions under two categories: 'Batch' and 'Configuration'. The 'Batch' category includes 'Submit unlocked methods', 'Open', 'Save as', 'Submit', 'Save', 'Save ion reference table', 'Add data sub-folders', and 'Configure Decision Rules'. The 'Configuration' category includes 'General tab'. Checkmarks indicate which roles have access to each permission.

Permission	Administrator	Method Developer	Analyst	Reviewer	analyst 2
Batch					
Submit unlocked methods	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Open	<input checked="" type="checkbox"/>				
Save as	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Submit	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Save	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Save ion reference table	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Add data sub-folders	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Configure Decision Rules	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Configuration					
General tab	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Audit Maps

- Configuration > Audit Mapsで設定できます。
- Projects Templates とWorkstation Templatesそれぞれの設定が必要です。



Configuration

Devices Projects User Management Queue Print Templates **Audit Maps** Licenses LIMS Communication General Software Updates

Projects Templates Workstation Templates Root: C:\SCIEX OS Data

Current default audit map template for new projects: **No Audit Map** Last updated: 4/24/2023 1:07:38 PM

Edit map template: Demo Audit +

Apply to Existing Projects...
Use as Default for New Projects
Delete Template
Save Template

Event	Audited	Reason Required	E-sig Required	Use Predefined Reason Only	Predefined Reason 1	Predefined Reason 2
▼ Analytics						
Actual Concentration Changed	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Updated Actual Con...	<input type="checkbox"/>
Auto-Processing File Saved	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		<input type="checkbox"/>

入力いただいたコメントがプルダウンで理由として選択可能になります。

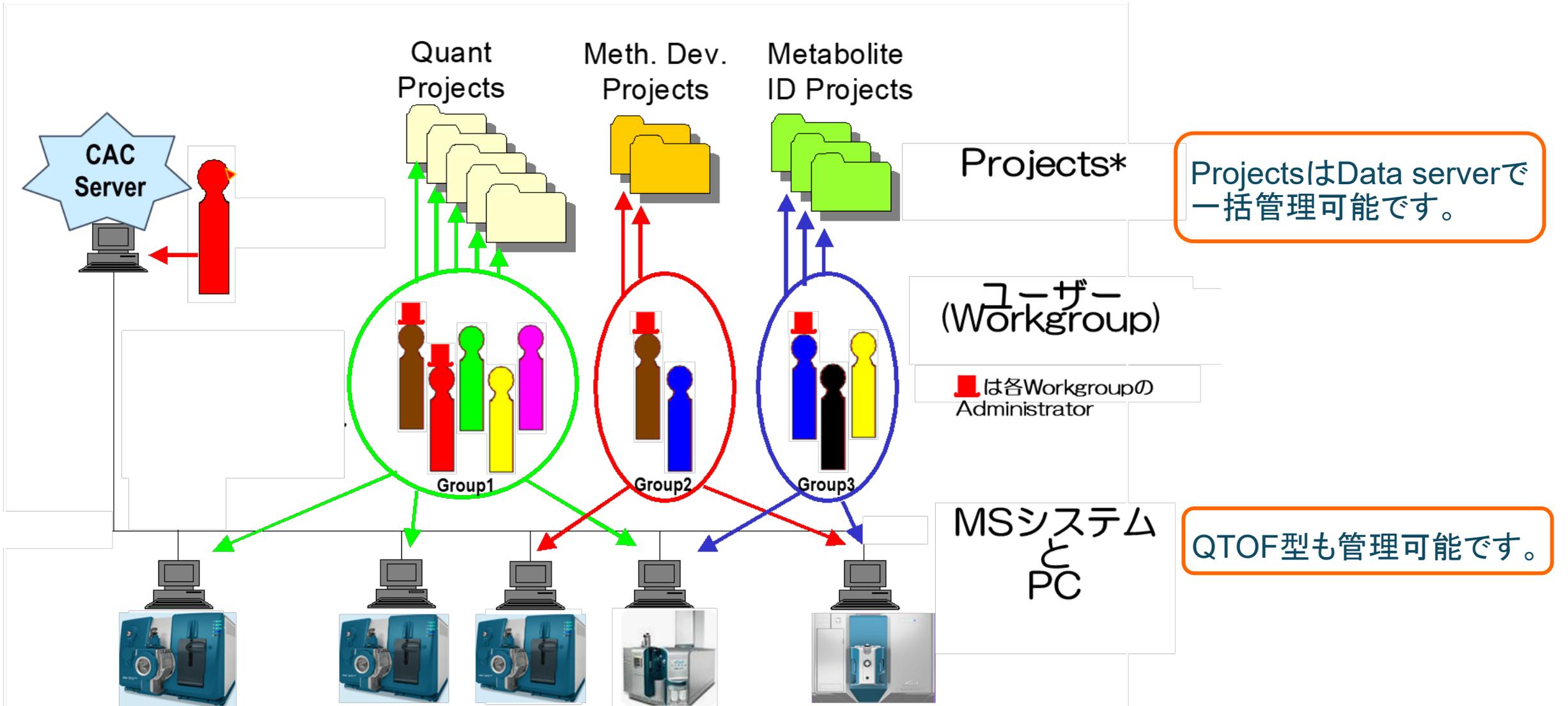
チェックを入れると事前設定したコメントのみ反映可能になります。

Central Administrator Console



Central Administrator Console (CAC) 概要

SCIEX OSで制御する装置をCAC Serverを介して管理するソフトウェアです。



PoolとWorkgroupのイメージ

Work groupを設定することで、Projectごとにユーザーを指定し、Roleを設定できます

