Analysis Information

Item name:	CCM SST Sep 02, 2022	Analysis Method Item name:	CCM SST Analysis Method
Version:	1	Analysis Method Version:	1
Modified date:	Sep 02, 2022 08:55:47 W. Europe Daylight Time	Sample Set Created date:	
Modified by:	Administrator, waters_connect	Sample Set Instrument system name:	
Folder:	Company/SST CCM		

SST PASS: Complete

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The BioAccord LC-MS system is fully operational. The quality criteria for mass accuracy, RT stability, MS response and reproducibility are within expectations across five replicates injections for each positive and negative polarities.

The analysis results meets the following criteria:
1). Identified components mass accuracy is within +/- 5 mDa
2). Observed RT %RSD is better than 1.00%
3). MS Response %RSD is better than 10.0%
4). Sulfadimethoxine mean response is greater than 5'000 counts for positive polarity
5). Sulfadimethoxine mean response is greater than 1'000 counts for negative polarity

SST FAIL: Complete with Error

The BioAccord LC-MS system requires user attention before acquiring new data. One or more quality criteria are not meeting expected results across five replicates injections for each positive and negative polarities. The following page of the report will show red flags where passing criteria have not been achieved.

Here are some tips for troubleshooting the system:
1). Mass error flags will require a new RDa detector setup to be performed.
2). Observed RT %RSD and MS Response %RSD flags indicates an issue on the chromatographic system. This requires to check the flow path for leaks, prepare fresh solvents and prime the system.
3). A flag on sulfadimethoxine response indicates a sensitivity issue with the RDa detector. This may require to make a fresh sample or change the apperture disc.
4). The limit status column of the analysis injection list allows to review which specific injection is causing issues.

Addionnal informations can be found on the KCS article WKB231508
https://support.waters.com/KB_Inst/Mass_Spectrometry/WKB231508_BioAccord_cell_culture_media_system_suitability_test

Analysis injection list

	Sample name	Sample type	Replicate number	Sample position	Injection volume (µL)	Acquisition status	Polarity	Acquisition start time	Limit status
1	Blank 1	Blank	1	1:A,1	2.00	Complete	Positive	Apr 01, 2022 10:29:12 W. Europe Daylight Time	No Checks Performed
2	Blank 2	Blank	1	1:A,1	2.00	Complete	Positive	Apr 01, 2022 10:41:37 W. Europe Daylight Time	No Checks Performed
3	SST 1	QC	1	1:A,2	0.50	Complete	Positive	Apr 01, 2022 10:53:02 W. Europe Daylight Time	Complete
4	SST 2	QC	1	1:A,2	0.50	Complete	Positive	Apr 01, 2022 11:04:16 W. Europe Daylight Time	Complete
5	SST 3	QC	1	1:A,2	0.50	Complete	Positive	Apr 01, 2022 11:15:40 W. Europe Daylight Time	Complete
6	SST 4	QC	1	1:A,2	0.50	Complete	Positive	Apr 01, 2022 11:26:52 W. Europe Daylight Time	Complete
7	SST 5	QC	1	1:A,2	0.50	Complete	Positive	Apr 01, 2022 11:38:15 W. Europe Daylight Time	Complete
8	Blank 1	Blank	1	1:A,1	2.00	Complete	Negative	Apr 01, 2022 12:03:35 W. Europe Daylight Time	No Checks Performed
9	Blank 2	Blank	1	1:A,1	2.00	Complete	Negative	Apr 01, 2022 12:15:27 W. Europe Daylight Time	No Checks Performed
10	SST 1	QC	1	1:A,2	0.50	Complete	Negative	Apr 01, 2022 12:27:08 W. Europe Daylight Time	Complete
11	SST 2	QC	1	1:A,2	0.50	Complete	Negative	Apr 01, 2022 12:39:05 W. Europe Daylight Time	Complete
12	SST 3	QC	1	1:A,2	0.50	Complete	Negative	Apr 01, 2022 12:50:25 W. Europe Daylight Time	Complete
13	SST 4	QC	1	1:A,2	0.50	Complete	Negative	Apr 01, 2022 13:02:58 W. Europe Daylight Time	Complete
14	SST 5	QC	1	1:A,2	0.50	Complete	Negative	Apr 01, 2022 13:14:23 W. Europe Daylight Time	Complete

Summarized by: Mass error (mDa)

.	Item name	Replicate number	Polarity	Acetaminophen	Caffeine	Leucine enkephalin	Reserpine	Sulfadimethoxine	Sulfaguanidine	Terfenadine	Val-tyr-val	Verapamil
1	SST 1	1	Positive	-0.9	-1.0	0.3	0.1	-0.9	0.0	0.0	-0.4	-0.4
2	SST 2	1	Positive	-0.8	-1.2	0.2	0.3	-1.2	-0.4	0.1	-0.7	-0.5
3	SST 3	1	Positive	-1.0	-1.5	-0.6	-0.6	-1.2	-0.5	-0.6	-1.0	-0.8
4	SST 4	1	Positive	-1.2	-1.5	-0.7	-0.9	-1.6	-0.4	-1.0	-0.9	-1.4
5	SST 5	1	Positive	-0.6	-1.1	-0.1	-0.4	-1.5	-0.6	-0.5	-0.2	-0.4
6	SST 1	1	Negative			-0.1		-1.1	-0.7		-0.2	
7	SST 2	1	Negative			0.0		-0.4	-0.9		-0.7	
8	SST 3	1	Negative			0.7		-0.7	-0.4		-0.1	
9	SST 4	1	Negative			0.4		-0.8	0.1		-0.6	
10	SST 5	1	Negative			-0.6		-0.9	-0.4		-0.2	

Category: QC
Summarized by: Observed RT
Sample position: 1:A,2

.	Component name	Mean	Std dev	% RSD (%)	Minimum	Maximum	Count
1	Sulfaguanidine	2.403	0.008	0.31	2.388	2.412	10
2	Acetaminophen	3.666	0.000	0.01	3.665	3.666	5
3	Val-tyr-val	3.827	0.001	0.04	3.825	3.829	10
4	Caffeine	4.057	0.001	0.01	4.056	4.057	5
5	Leucine enkephalin	4.596	0.002	0.03	4.593	4.599	10
6	Verapamil	5.578	0.001	0.03	5.576	5.580	5
7	Sulfadimethoxine	5.728	0.002	0.03	5.726	5.730	10
8	Reserpine	5.737	0.001	0.02	5.736	5.739	5
9	Terfenadine	6.398	0.001	0.02	6.397	6.400	5

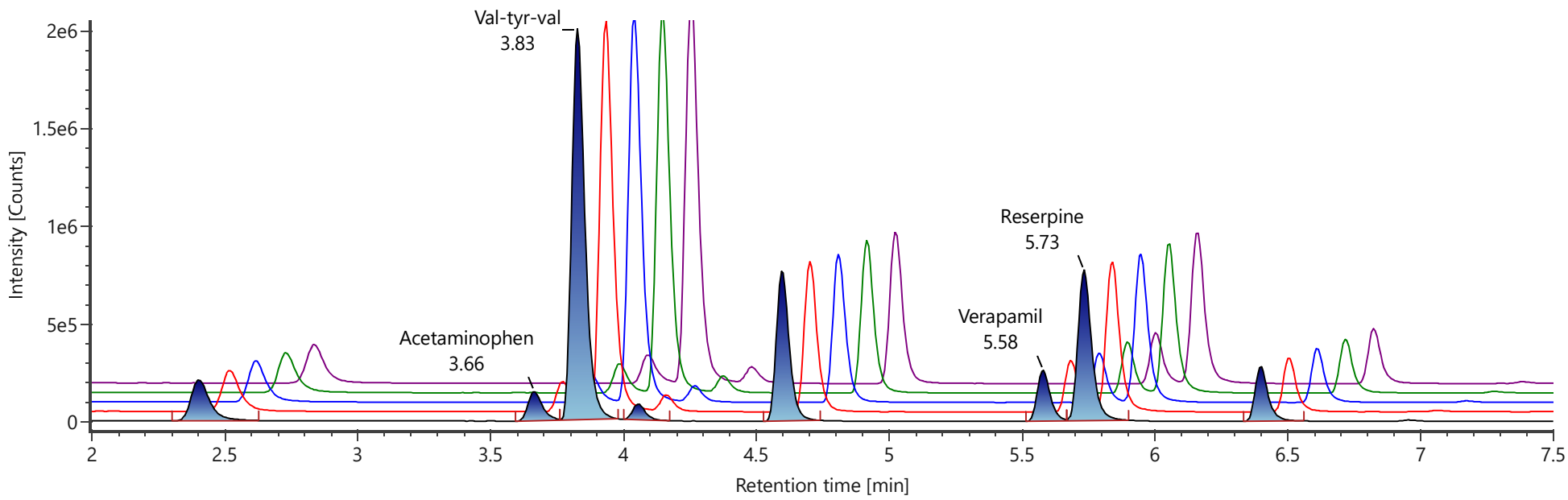
Category: QC
Summarized by: MS Response
Level: POS

.	Component name	Mean	% RSD (%)	Std dev	Minimum	Maximum	Count
1	Sulfaguanidine	52531.292	3.92	2060.400	49631.934	54899.988	5
2	Acetaminophen	27929.755	2.78	775.492	27180.670	29137.484	5
3	Val-tyr-val	452019.681	2.45	11064.989	441615.656	465440.750	5
4	Caffeine	16024.871	3.01	482.334	15495.789	16563.342	5
5	Leucine enkephalin	197313.341	1.47	2904.330	193682.281	201803.250	5
6	Verapamil	63855.601	1.99	1273.520	61987.867	65226.938	5
7	Sulfadimethoxine	87811.178	2.25	1973.478	86050.078	90774.977	5
8	Reserpine	106283.153	1.21	1285.116	104899.766	107688.594	5
9	Terfenadine	65578.288	1.90	1245.587	64178.426	66807.055	5

Category: QC
Summarized by: MS Response
Level: NEG

.	Component name	Mean	% RSD (%)	Std dev	Minimum	Maximum	Count
1	Sulfaguanidine	4680.008	2.76	129.128	4541.799	4877.313	5
2	Val-tyr-val	27445.479	1.62	443.922	26972.820	28001.469	5
3	Leucine enkephalin	23104.554	1.13	261.128	22870.646	23549.754	5
4	Sulfadimethoxine	6383.295	2.78	177.515	6155.365	6614.938	5

Extracted ion chromatogram of all compounds identified in positive mode



Item name: SST 1
Channel name: Identified Components

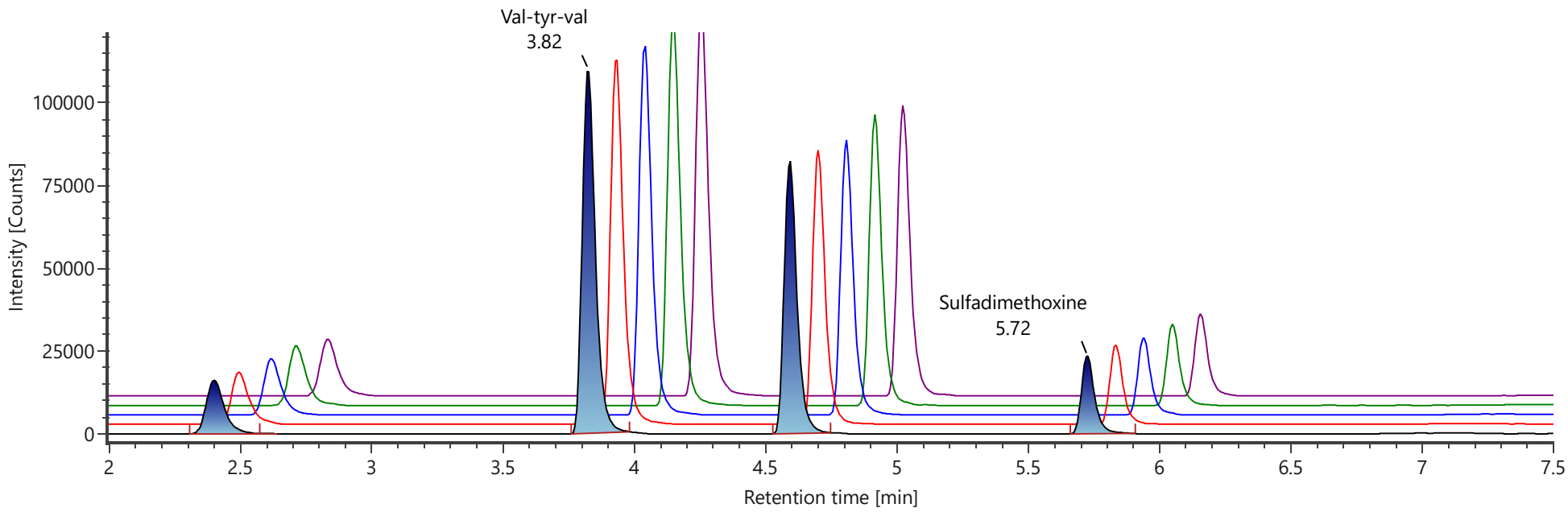
Item name: SST 2
Channel name: Identified Components

Item name: SST 3
Channel name: Identified Components

Item name: SST 4
Channel name: Identified Components

Item name: SST 5
Channel name: Identified Components

Extracted ion chromatogram of all compounds identified in negative mode



Item name: SST 1
Channel name: Identified Components

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Channel name: Identified Components

Item name: SST 3
Channel name: Identified Components

Item name: SST 4
Channel name: Identified Components

Item name: SST 5
Channel name: Identified Components