Masshunter Quant Software
Dioxin Reporting

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Example of Level 4 Reporting

Required Reports Dioxins

The use of GC/MS/MS platforms has been accepted as an alternate testing procedure by USEPA for analyzing polychlorinated dioxin and furans in wastewater, soil, and biotas.

The use of a GC/MS/MS allows labs to analyze samples offering versatility, robustness, reliability and familiarity to environmental lab.

Magnetic Sector systems are very costly and require significant expertise in maintenance and operation. As a greater number of GC/MS/MS systems are installed in Analytical Laboratories the capacity for analyzing dioxins and PCBs has increased exponentially.

The quantification and reporting needs for these compounds can be complex. This presentation focuses on the tools needed for reporting this data.

Example of Level 4 Reporting

Required Reports Dioxins

The question is how we are currently reporting data and how can we improve that process.

Large laboratories historically incorporate a LIMS system to generate reports. Smaller labs traditionally create reports in Excel or similar.

Working with several laboratories we have designed a series of reports to help improve & streamline this process. This approach gives the bench chemist & lab manager the ability to generate repots in real time enabling them to make several critical decisions.

Example of Level 4 Reporting

Required Reports Dioxins

1. Are dilutions necessary?
2. Does the sample require re-extraction?
3. Does the sample need to be re-injected?
4. Are there Diphenyl Ethers present?
5. What are the Estimated Maximum Possible Concentrations?
6. What is the total Toxic Equivalency of the sample?
7. Does the sample meet all the QA/QC requirements?

Required Reports Dioxins

Calibration Report Summary

Calibration RRF Summary Report

Batch Path: E:\MassHunter\Data\QQQ\DioxinCanada\Dioxin data-BV Oct 2023\TQ2_231005A_1613\

Analysis Time: 12/21/2023 4:45:33 PM

Level Name	Sample Name	Calibration File	Acq. Time
L0	CSL_1613_13CSL 1021	D:\MassHunter\GCMS\1\data\2023\TQ2_231005A_1613TQ2_231005A06.D	10/5/2023 1:25:57 AM
L1	CS1_1613_13CS1 1021	D:\MassHunter\GCMS\1\data\2023\TQ2_231005A_1613TQ2_231005A07.D	10/5/2023 2:14:56 AM
L2	CS2_1613_13CS2 1021	D:\MassHunter\GCMS\1\data\2023\TQ2_231005A_1613TQ2_231005A08.D	10/5/2023 3:03:55 AM
L3	CS3_1613_13CS3 1021	D:\MassHunter\GCMS\1\data\2023\TQ2_231005A_1613TQ2_231005A09.D	10/5/2023 3:52:53 AM
L4	CS4_1613_13CS4 1021	D:\MassHunter\GCMS\1\data\2023\TQ2_231005A_1613TQ2_231005A10.D	10/5/2023 4:41:52 AM
L5	CS5_1613_13CS5 1021	D:\MassHunter\GCMS\1\data\2023\TQ2_231005A_1613TQ2_231005A11.D	10/5/2023 5:30:52 AM

No	Compound	Av-RRF	SD	%RSD	OK (%RSD)	L0	L1	L2	L3	L4	L5
1	2378-TCDF	1.2072	4.0657	3.4	OK(20)	1.2851	1.1822	1.1769	1.1828	1.2027	1.2134
2	12378-PeCDF	1.1159	3.3616	3.0	OK(20)	1.1669	1.0736	1.0993	1.0943	1.1373	1.1237
3	23478-PeCDF	1.2277	2.6739	2.2	OK(20)	1.2581	1.1880	1.2092	1.2223	1.2357	1.2530
4	123478-HxCDF	1.0379	1.4553	1.4	OK(20)	1.0487	1.0519	1.0170	1.0223	1.0427	1.0447
5	123678-HxCDF	1.0140	1.7294	1.7	OK(20)	1.0403	1.0095	0.9883	1.0089	1.0238	1.0132
6	234678-HxCDF	1.0507	1.6959	1.6	OK(20)	1.0394	1.0372	1.0337	1.0649	1.0758	1.0533
7	123789-HxCDF	0.9821	1.9174	2.0	OK(20)	0.9951	0.9937	0.9484	0.9738	1.0003	0.9814
8	1234678-HpCDF	0.9891	0.9350	0.9	OK(20)	0.9990	0.9768	0.9808	0.9916	0.9996	0.9868
9	1234789-HpCDF	0.9873	1.5827	1.6	OK(20)	0.9969	1.0059	0.9641	0.9790	0.9988	0.9789
10	OCDF	1.1880	9.9533	8.4	OK(20)	1.0170	1.1215	1.2526	1.2327	1.2795	1.2247
11	2378-TCDD	1.2024	6.3054	5.2	OK(20)	1.3190	1.1271	1.1931	1.1833	1.2019	1.1899
12	12378-PeCDD	1.1130	2.4874	2.2	OK(20)	1.0992	1.1059	1.0847	1.1039	1.1538	1.1304
13	123478-HxCDD	0.9767	7.6103	7.8	OK(20)	0.9806	1.0390	0.9710	1.0314	0.8314	1.0069
14	123678-HxCDD	1.0162	1.0016	1.0	OK(20)	1.0128	1.0186	1.0191	1.0047	1.0088	1.0333
15	123789-HxCDD	1.0320	4.8516	4.7	OK(20)	1.0793	0.9833	1.1041	1.0166	1.0143	0.9943
16	1234678-HpCDD	1.0344	1.4908	1.4	OK(20)	1.0618	1.0176	1.0272	1.0310	1.0316	1.0371
17	OCDD	0.9085	0.9099	1.0	OK(20)	0.9202	0.9016	0.9022	0.8994	0.9188	0.9086
18	13C-2378-TCDF	2.7652	17.7093	6.4	OK(20)	2.7708	3.0375	2.7248	2.6796	2.5130	2.8655
19	13C-12378-PeCDF	1.6781	26.4795	15.8	OK(20)	1.4232	1.6602	1.5195	1.6827	1.6009	2.1823
20	13C-23478-PeCDF	1.6441	24.4623	14.9	OK(20)	1.3678	1.5915	1.5206	1.6172	1.6721	2.0950
21	13C-123478-HxCDF	1.5164	8.3335	5.5	OK(20)	1.4371	1.6087	1.3994	1.5717	1.5722	1.5091
22	13C-123678-HxCDF	1.5848	8.5184	5.4	OK(20)	1.5171	1.6393	1.4512	1.6731	1.6403	1.5879
23	13C-234678-HxCDF	1.4449	8.6294	6.0	OK(20)	-	1.5038	1.3191	1.5302	1.4748	1.3966
24	13C-123789-HxCDF	1.4376	3.6617	2.5	OK(20)	-	1.4832	1.3877	1.4518	1.4161	1.4490
25	13C-1234678-HpCDF	1.5922	16.0604	10.1	OK(20)	1.8863	1.6575	1.4966	1.5665	1.4691	1.4771
26	13C-1234789-HpCDF	1.4931	10.2409	6.9	OK(20)	1.5468	1.4513	1.6493	1.4961	1.3414	1.4735
27	13C-2378-TCDD	1.7373	9.5410	5.5	OK(20)	1.6124	1.7878	1.7670	1.7073	1.6679	1.8814
28	13C-12378-PeCDD	0.9305	16.1766	17.4	OK(20)	0.7656	0.9130	0.8529	0.8888	0.9230	1.2396
29	13C-123478-HxCDD	0.9137	4.0410	4.4	OK(20)	0.9461	0.9459	0.8532	0.8826	0.9041	0.9505
30	13C-123678-HxCDD	0.9971	6.4866	6.5	OK(20)	0.9333	1.0723	0.9030	1.0287	1.0137	1.0316
31	13C-1234678-HpCDD	0.9725	3.7296	3.8	OK(20)	1.0201	0.9230	1.0118	0.9595	0.9497	0.9711
32	13C-OCDD	1.0370	7.8322	7.6	OK(20)	1.1168	0.9680	0.9311	1.0152	1.0733	1.1178

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Required Reports Dioxins

Calibration RRF AVG RRF

Dioxin Quantitative Analysis Calibrator Report

Data Path	E:\MassHunter\Data\QQQ\DioxinCanada\Dioxin data-BV Oct 2023\TQ2_231005A_1613\		
Data File	TQ2_231005A06.D	Sample Name	CSL_1613_13CSL 1021
Acq. Method	TQDF_MRM	Acq. Time	10/5/2023 1:25:57 AM
Acq. Operator		Quant Method	
Analysis Time	12/21/2023 4:45:33 PM	Analyst Name	AGILENT\lisun

No	Compound	RT[min]	Exp Conc[ng/ml]	Area	Q-Area	Sum Area	Resp Ratio	%Ratio Error	OK(Ratio)	Av-RRF	RRF
1	2378-TCDF	24.885	0.100	1176	1166	2341	0.991	4.9	OK(15)	1.2072	1.2851
2	12378-PeCDF	32.300	0.500	3133	2326	5459	0.742	-7.0	OK(15)	1.1159	1.1669
3	23478-PeCDF	33.420	0.500	3115	2542	5657	0.816	2.2	OK(15)	1.2277	1.2581
4	123478-HxCDF	37.040	0.500	2422	1547	3969	0.639	0.7	OK(15)	1.0379	1.0487
5	123678-HxCDF	37.154	0.500	2518	1638	4156	0.650	0.9	OK(15)	1.0140	1.0403
6	234678-HxCDF	37.732	0.500	2403	1611	4014	0.670	4.1	OK(15)	1.0507	1.0394
7	123789-HxCDF	38.492	0.500	2331	1522	3853	0.653	-1.6	OK(15)	0.9821	0.9951
8	1234678-HpCDF	40.134	0.500	2790	2173	4962	0.779	-3.1	OK(15)	0.9891	0.9990
9	1234789-HpCDF	41.620	0.500	2322	1739	4061	0.749	-7.5	OK(15)	0.9873	0.9969
10	OCDF	44.862	1.000	3078	2904	5982	0.944	-1.7	OK(15)	1.1880	1.0170
11	2378-TCDD	26.097	0.100	675	723	1398	1.071	11.7	OK(15)	1.2024	1.3190
12	12378-PeCDD	33.949	0.500	1563	1203	2766	0.770	-3.1	OK(15)	1.1130	1.0992
13	123478-HxCDD	37.884	0.500	1473	970	2443	0.658	3.7	OK(15)	0.9767	0.9806
14	123678-HxCDD	37.975	0.500	1556	933	2489	0.599	-12.1	OK(15)	1.0162	1.0128
15	123789-HxCDD	38.289	0.500	1670	1001	2671	0.599	-9.1	OK(15)	1.0320	1.0793
16	1234678-HpCDD	41.189	0.500	1553	1299	2852	0.837	4.0	OK(15)	1.0344	1.0618
17	OCDD	44.709	1.000	2679	2734	5413	1.020	4.5	OK(15)	0.9085	0.9202
18	13C-2378-TCDF	24.860	100.000	943349	878350	1821699	0.931	-1.1	OK(15)	2.7652	2.7708
19	13C-12378-PeCDF	32.288	100.000	519475	416237	935712	0.801	-1.0	OK(15)	1.6781	1.4232
20	13C-23478-PeCDF	33.408	100.000	499939	399347	899286	0.799	-1.6	OK(15)	1.6441	1.3678
21	13C-123478-HxCDF	37.027	100.000	463070	293813	756882	0.634	0.9	OK(15)	1.5164	1.4371
22	13C-123678-HxCDF	37.142	100.000	494939	304078	799017	0.614	-1.5	OK(15)	1.5848	1.5171
23	13C-234678-HxCDF	37.725	100.000	476469	295837	772306	0.621	-1.5	OK(15)	1.4449	
24	13C-123789-HxCDF	38.479	100.000	476016	298374	774390	0.627	-1.0	OK(15)	1.4376	
25	13C-1234678-HpCDF	40.127	100.000	555943	437527	993470	0.787	-1.6	OK(15)	1.5922	1.8863
26	13C-1234789-HpCDF	41.613	100.000	454433	360223	814656	0.793	-0.4	OK(15)	1.4931	1.5468
27	13C-2378-TCDD	26.071	100.000	547318	512786	1060104	0.937	0.0	OK(15)	1.7373	1.6124
28	13C-12378-PeCDD	33.931	100.000	280135	223249	503384	0.797	-0.8	OK(15)	0.9305	0.7656
29	13C-123478-HxCDD	37.876	100.000	306646	191634	498281	0.625	0.1	OK(15)	0.9137	0.9461
30	13C-123678-HxCDD	37.968	100.000	300023	191516	491539	0.638	-2.0	OK(15)	0.9971	0.9333
31	13C-1234678-HpCDD	41.182	100.000	301204	236045	537249	0.784	-2.3	OK(15)	0.9725	1.0201
32	13C-OCDD	44.701	200.000	598786	577567	1176353	0.965	-0.8	OK(15)	1.0370	1.1168
33	Cl37-2378-TCDD	26.095	0.100	1418		1418				2.0156	2.1574
42	HexaDPE / TCDF	22.101	1.000	108		108				114.8409	107.8866
43	HeptaDPE / PeCDF	31.999	1.000	103		103				154.8071	103.0561
44	OctaDPE / HxCDF		1.000							120.9631	
45	NonaDPE / HpCDF		1.000							100.9802	
46	DecaDPE / OCDF		1.000								
47	PFTBA	32.633	1.000	40		40				44.7322	39.6907
48	Average 13C-123678HxCDD/13C-123478HxCDD	37.922	100.000	303335		494910				6157.1648	4949.0979
49	13C-1234-TCDD	25.750	100.000	340583	316879	657462	0.930	-2.3	OK(15)		

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Required Reports Dioxins

Continuing Calibration

Continuing Calibration Report

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Batch Name	C:\MassHunter\Data\TQ2_230711A_1613\QuantResults\DRW Short list.batch.bin
Method File	
Daily CC	C:\MassHunter\Data\TQ2_230711A_1613TQ2_230711A12.D

Level name	Injection Time	Calibration Files	
L0	7/11/2023 12:42:35 PM	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_230711A05.D	
L1	7/11/2023 1:31:39 PM	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_230711A06.D	
L2	7/11/2023 2:20:42 PM	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_230711A07.D	
L3	7/11/2023 3:09:46 PM	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_230711A08.D	
L4	7/11/2023 3:58:50 PM	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_230711A09.D	
L5	7/11/2023 4:47:54 PM	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_230711A10.D	
CC	7/11/2023 6:26:03 PM	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_230711A12.D	<=======

ISTD Compound:	Avg Resp	Mid Resp	CC Resp	Area%	A/M
13C-1234-TCDD	735746	748854	1239223	168.43	A
Average 13C-123678HxCDD/13C-123478HxCDD	654127	616205	991563	151.59	A
13C-2378-TCDD	1335392	1365958	2096695	157.01	A
13C-2378-TCDF	2138079	2180875	3508515	164.10	A
13C-23478-PeCDF	1262428	1246203	1999420	158.38	A
13C-12378-PeCDF	1298036	1312490	2085687	160.68	A
13C-123678-HxCDF	1080501	1129028	1622880	150.20	A
13C-12378-PeCDD	708291	667894	1080589	152.56	A
13C-234678-HxCDF	1024725	1004808	1510018	147.36	A
13C-123478-HxCDD	622571	591959	963574	154.77	A
13C-123789-HxCDF	1004710	909498	1416792	141.01	A
13C-123478-HxCDF	999578	989364	1426068	142.67	A
13C-123678-HxCDD	685683	640451	1019553	148.69	A
13C-1234678-HpCDD	605427	583592	818363	135.17	A
13C-1234678-HpCDF	965887	888694	1479191	153.14	A
13C-1234789-HpCDF	921298	870054	1362599	147.90	A
13C-OCDD	1236585	1129284	1930657	156.13	A

Target Compound	AvgRF/R2	CC RF	Exp. Conc	Calc. Conc	%Dev	Area%	Curve Fit
13C-1234-TCDD	----------ISTD----------						
Cl37-2378-TCDD	2.1019	1.8311	10.00	8.71	12.88	27.18	Avg RF
Average 13C-123678HxCDD/13C-123478HxCDD	----------ISTD----------						
123789-HxCDD	1.0336	0.9419	50.00	45.57	8.87	21.45	Avg RF
13C-2378-TCDD	----------ISTD----------						
2378-TCDD	1.1839	1.1624	10.00	9.82	1.82	27.41	Avg RF
13C-2378-TCDF	----------ISTD----------						
2378-TCDF	1.2034	1.1994	10.00	9.97	0.33	30.15	Avg RF
8.50 x 11.00 in 3478-PeCDF	----------ISTD----------						

Required Reports Dioxins

Surrogate Recovery

Quantitation Results Report (Not Reviewed)

Agilent

Data File	TQ2_230711A05.D	Operator	
Acq. Method	TQDF_M_MRM	Acq. Date-Time	7/11/2023 11:42:35 AM
Sample Name	CSL_1613_13CSL 1021	Instrument	TQ 02
Vial	3	Multiplier	1.00
DA Method File	Shortlist 4.m	Comment	
Tune File	atunes.eihs_DF.tune.xml	Tune Date	6/12/2023 3:09:28 PM
Batch Name	DRW Short list.batch.bin	Last Calib Update	7/18/2023 6:40:26 AM
Ref Library			

Compound	RT	QIon	Resp.	Conc.	Units		Dev(Min)
Internal Standards							
System Monitoring Compounds							
24) 13C-2378-TCDF	24.390	315.9 -> 252.0, 254.0	2010620	100.0000	ng/ml	+	0.018
Spiked Amount: 100.000	Range: 24.0 - 169.0%			Recovery = 95.59%			
18) 13C-2378-TCDD	25.583	331.9 -> 268.0, 270.0	1182925	100.0000	ng/ml	+	0.018
Spiked Amount: 100.000	Range: 25.0 - 164.0%			Recovery = 90.17%			
25) 13C-12378-PeCDF	31.911	351.9 -> 287.9, 285.9	1186453	100.0000	ng/ml	+	0.011
Spiked Amount: 100.000	Range: 24.0 - 185.0%			Recovery = 93.50%			
26) 13C-23478-PeCDF	33.088	351.9 -> 287.9, 285.9	1123836	100.0000	ng/ml	+	0.006
Spiked Amount: 100.000	Range: 21.0 - 178.0%			Recovery = 91.06%			
19) 13C-12378-PeCDD	33.646	367.9 -> 303.9, 301.9	622059	100.0000	ng/ml	+	0.006
Spiked Amount: 100.000	Range: 25.0 - 181.0%			Recovery = 90.15%			
27) 13C-123478-HxCDF	36.848	385.9 -> 321.9, 323.9	935539	100.0000	ng/ml	+	0.006
Spiked Amount: 100.000	Range: 26.0 - 152.0%			Recovery = 103.46%			
28) 13C-123678-HxCDF	36.962	385.9 -> 321.9, 323.9	997882	100.0000	ng/ml	+	0.000
Spiked Amount: 100.000	Range: 26.0 - 123.0%			Recovery = 102.20%			
29) 13C-234678-HxCDF	37.562	385.9 -> 321.9, 323.9	907714	100.0000	ng/ml	+	0.006
Spiked Amount: 100.000	Range: 28.0 - 136.0%			Recovery = 99.20%			
20) 13C-123478-HxCDD	37.725	401.9 -> 337.9, 339.9	564702	100.0000	ng/ml	+	0.006
Spiked Amount: 100.000	Range: 26.0 - 152.0%			Recovery = 101.16%			
21) 13C-123678-HxCDD	37.817	401.9 -> 337.9, 339.9	621143	100.0000	ng/ml	+	0.006
Spiked Amount: 100.000	Range: 28.0 - 130.0%			Recovery = 101.11%			
Average 13C-123678HxCDD/13C-123478HxCDD	37.771	401.9 -> 0.0	592923	100.0000	ng/ml		-0.560
Spiked Amount:	Range: - %			Recovery = NA%			
30) 13C-123789-HxCDF	38.334	385.9 -> 321.9, 323.9	930533	100.0000	ng/ml	+	0.006
Spiked Amount: 100.000	Range: 29.0 - 147.0%			Recovery = 103.73%			
31) 13C-1234678-HpCDF	40.007	419.8 -> 355.9, 357.9	875165	100.0000	ng/ml	+	0.000
Spiked Amount: 100.000	Range: 28.0 - 143.0%			Recovery = 100.91%			
22) 13C-1234678-HpCDD	41.073	435.8 -> 371.9, 373.9	565447	100.0000	ng/ml	+	0.000
Spiked Amount: 100.000	Range: 23.0 - 140.0%			Recovery = 103.95%			
32) 13C-1234789-HpCDF	41.499	419.8 -> 355.9, 357.9	889018	100.0000	ng/ml	+	0.000
Spiked Amount: 100.000	Range: 26.0 - 138.0%			Recovery = 107.40%			
23) 13C-OCDD	44.619	469.8 -> 405.8, 407.8	1197294	200.0000	ng/ml	+	0.006
Spiked Amount: 200.000	Range: 34.0 - 313.0%			Recovery = 107.39%			

Required Reports Dioxins

Matrix Spike Recovery Report

Matrix Spike/Duplicate Recovery and RPD Summary Report

Agilent

Batch Name	C:\BV Canada\Things to do for BV\BV_DIOXIN\TQ2_230218A_1613_MDL\QuantResults\msd 07182023.batch.bin
Last Calib Update	7/12/2023 11:38:09 AM
Method File	
Data Path	C:\BV Canada\Things to do for BV\BV_DIOXIN\TQ2_230218A_1613_MDL

Sample Name	Sample Type	Matrix Spike Group	Acq. Date Time
8351624:SPIKE	Matrix		12/22/2022 3:48:16 AM
8351624:SPIKE	Matrix Dup		12/22/2022 4:37:26 AM

Compound	Sample Conc	Spike Amt	Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Rec
2378-TCDF	0.000	10.000	10.155	10.123	101.55	101.23	0.31	50	30 - 130
2378-TCDD	0.000	10.000	11.075	11.057	110.75	110.57	0.16	50	30 - 130
12378-PeCDF	0.000	50.000	47.762	45.156	95.52	90.31	5.61	50	30 - 130
12378-PeCDD	0.000	50.000	49.761	49.117	99.52	98.23	1.30	50	30 - 130
23478-PeCDF	0.000	50.000	51.699	51.922	103.40	103.84	0.43	50	30 - 130
123678-HxCDF	0.000	50.000	52.688	52.046	105.38	104.09	1.23	50	30 - 130
123478-HxCDD	0.000	50.000	50.036	51.050	100.07	102.10	2.01	50	30 - 130
234678-HxCDF	0.000	50.000	49.704	49.261	99.41	98.52	0.90	50	30 - 130
123789-HxCDF	0.000	50.000	52.026	51.370	104.05	102.74	1.27	50	30 - 130
123678-HxCDD	0.000	50.000	51.404	49.304	102.81	98.61	4.17	50	30 - 130
123789-HxCDD	0.000	50.000	49.081	47.860	98.16	95.72	2.52	50	30 - 130
123478-HxCDF	0.000	50.000	49.392	48.374	98.78	96.75	2.08	50	30 - 130
1234678-HpCDF	0.000	50.000	54.468	53.365	108.94	106.73	2.05	50	30 - 130
1234678-HpCDD	0.000	50.000	53.373	52.457	106.75	104.91	1.73	50	30 - 130
1234789-HpCDF	0.000	50.000	59.752	54.912	119.50	109.82	8.44	50	30 - 130
OCDD	0.000	100.000	125.374	111.042	125.37	111.04	12.12	50	30 - 130
OCDF	0.000	100.000	147.240	111.551	147.24 #	111.55	27.58	50	30 - 130

(#) = out of Range

Required Reports Dioxins

LCS and LCSD

LCS Spike Report

Agilent

Batch Name	C:\BV Canada\Things to do for BV\BV_DIOXIN\TQ2_230218A_1613_MDL\QuantResults\msd 07182023.batch.bin
Last Calib Update	7/12/2023 11:38:09 AM
Method File	
Data Path	C:\BV Canada\Things to do for BV\BV_DIOXIN\TQ2_230218A_1613_MDL

Data File	Sample Name	Sample Type	LCS Type	Acq. Date Time
TQ2_221221A12.D	8351624:SPIKE	QC	LCSA	12/22/2022 3:48:16 AM
TQ2_221221A13.D	8351624:SPIKE	QC	LCSB	12/22/2022 4:37:26 AM

Data File = TQ2_221221A12.D, Sample Name = 8351624:SPIKE, Type = LCSA

Compound	Spike Amt	Spike Res	Spike Rec	QC LCS Min %Rec	QC LCS Max %Rec
2378-TCDF	10.000	10.155	101.55	75	158
2378-TCDD	10.000	11.075	110.75	67	158
12378-PeCDF	50.000	47.762	95.52	80	134
12378-PeCDD	50.000	49.761	99.52	70	142
23478-PeCDF	50.000	51.699	103.40	68	160
123678-HxCDF	50.000	52.688	105.38	84	130
123478-HxCDD	50.000	50.036	100.07	70	164
234678-HxCDF	50.000	49.704	99.41	70	156
123789-HxCDF	50.000	52.026	104.05	78	130
123678-HxCDD	50.000	51.404	102.81	76	134
123789-HxCDD	50.000	49.081	98.16	64	162
123478-HxCDF	50.000	49.392	98.78	72	134
1234678-HpCDF	50.000	54.468	108.94	82	122
1234678-HpCDD	50.000	53.373	106.75	70	140
1234789-HpCDF	50.000	59.752	119.50	78	138
OCDD	100.000	125.374	125.37	78	144
OCDF	100.000	147.240	147.24	63	170

Data File = TQ2_221221A13.D, Sample Name = 8351624:SPIKE, Type = LCSB

Compound	Spike Amt	Spike Res	Spike Rec	QC LCS Min %Rec	QC LCS Max %Rec
2378-TCDF	10.000	10.123	101.23	75	158
2378-TCDD	10.000	11.057	110.57	67	158
12378-PeCDF	50.000	45.156	90.31	80	134
12378-PeCDD	50.000	49.117	98.23	70	142
23478-PeCDF	50.000	51.922	103.84	78	160
123678-HxCDF	50.000	52.046	104.09	84	130
123478-HxCDD	50.000	51.050	102.10	70	164
234678-HxCDF	50.000	49.261	98.52	70	156
123789-HxCDF	50.000	51.370	102.74	78	130
123678-HxCDD	50.000	49.304	98.61	76	134
123789-HxCDD	50.000	47.860	95.72	64	162
123478-HxCDF	50.000	48.374	96.75	72	134
1234678-HpCDF	50.000	53.365	106.73	82	122
1234678-HpCDD	50.000	52.457	104.91	70	140
1234789-HpCDF	50.000	54.912	109.82	78	138
OCDD	100.000	111.042	111.04	78	144
OCDF	100.000	111.551	111.55	63	170

Required Reports Dioxins

Window Defining Mix

Dioxin Quantitative Analysis Sample Report

Agilent

Data Path	C:\MassHunter\GCMS\1\data\TQ2_231005A_1613\TQ2_231005A03.D		
Sample Name	Window Defining Mix	Acq. Method	TQDF_MRM
Acq. Time	2023-10-05 1:59:02 AM	Quant Method	16130_Quant12_Dale (1).m
Sample Type	Sample	Sample Amt	
Analysis Time	2023-11-09 3:55:38 PM	Analyst Name	AGILENT\shotoole

No	Type	Compound	RT [min]	RRT [min]	Area	Q-Area	S/N	Q-S/N	Resp. Ratio	%Ratio Error	Av-RRF	Conc. [pg/g]	Mod.	LOQ (pg/g)	%Rec
1	Target	2378-TCDD	26.079	0.020	219957	210311	8529.5	17291.9	0.956	-0.2	0.2395	174.029			
2	Target	12378-PeCDD	34.572	*0.647*	135621	108003	7136.3	7623.3	0.796	2.1	1.1135	3221.389			
3	Target	123478-HxCDD	38.244	*0.373*	122926	79861	4662.8	4206.4	0.650	6.3	0.9767	36.324			
4	Target	123678-HxCDD	38.244	*0.373*	122926	79861	4662.8	4206.4	0.650	3.9	0.9719	36.487			
5	Target	123789-HxCDD	38.244	*0.373*	122926	79881	4931.2	5273.9	0.650	3.1	1.0802	32.840			
6	Target	1234678-HpCDD	41.189	0.013	112280	90893	4388.9	2923.8	0.810	0.5	1.0347	3409.607			
7	Target	OCDD	44.709	0.002	99952	96789	20303.5	4797.0	0.968	0.9	9.0856	13727.567			
8	Target	2378-TCDF	24.891	0.019	173	165	2.8	3.5	0.952	-0.9	0.2414	196.529			
9	Target	12378-PeCDF	32.294	0.018	733	586	36.1	25.0	0.799	1.8	1.1168	330.631			
10	Target	23478-PeCDF	33.649	*-0.251*	133	109	12.7	12.4	0.816	3.4	1.2270	142.384			
11	Target	234678-HxCDF	38.567	*0.167*	193450	120118	5967.6	6082.6	0.621	-10.1	0.9809	1330558.470			
12	Target	123478-HxCDF	35.868	*-0.873*	165725	104993	3846.0	3505.5	0.634	-1.0	1.0379	762807.653			
13	Target	123678-HxCDF	37.034	0.013	5707	3597	249.6	239.5	0.630	-0.5	1.0377	12370.346			
14	Target	123789-HxCDF	38.567	*0.842*	193344	119997	7943.0	3619.7	0.621	-2.4	1.0499	437771.134			
15	Target	1234678-HpCDF	40.134	0.013	183653	146042	44175.3	5538.4	0.795	-0.3	0.9892	212051.092			
16	Target	1234789-HpCDF	41.620	0.024	175686	139729	3622.1	2531.6	0.795	-0.6	0.9873	263222.296			
17	Target	OCDF	44.862	*0.154*	137692	131271	7049.7	11687.5	0.953	-0.7	11.8713	14363.019			
18	Surrogate	13C-2378-TCDD	26.059		532490	499743	7674.2	15535.0	0.939	0.5	1.7377	95.695			95.7
19	Surrogate	13C-12378-PeCDD	33.926		4048	2743	119.4	79.2	0.678	-13.1	0.9303	1.176			*1.2*
20	Surrogate	13C-123478-HxCDD	37.871		350801	220783	18212.3	15111.3	0.629	0.3	1.0000	99.955			100.0
21	Surrogate	13C-123678-HxCDD	37.871		351060	220787	14751.6	12096.9	0.629	-3.0	0.9999	100.008			100.0
22	Surrogate	13C-1234678-HpCDD	41.176		3192	2567	149.3	107.4	0.804	0.5	1.0661	0.945			*0.9*
23	Surrogate	13C-OCDD	44.707		175	141	20.4	*2.7*	*0.806*	*-16.1*	1.1346	0.049			*0.0*
24	Surrogate	13C-2378-TCDF	24.872		425	286	25.5	29.9	*0.674*	*-29.8*	2.7649	0.041			*0.0*
25	Surrogate	13C-12378-PeCDF	32.276		221	136	*6.6*	12.4	*0.615*	*-22.8*	1.6777	0.034			*0.0*
26	Surrogate	13C-23478-PeCDF	33.900		18	121	*1.6*	*6.0*	*6.799*	*754.1*	1.6449	0.014			*0.0*
27	Surrogate	13C-123478-HxCDF	36.741		34	0	*4.0*		*0*		1.6612	0.004			*0.0*
28	Surrogate	13C-123678-HxCDF	37.022		72	0	20.7		*0*		1.6615	0.008			*0.0*
29	Surrogate	13C-234678-HxCDF	38.399		24	0	*3.1*		*0*		1.5807	0.003			*0.0*
30	Surrogate	13C-123789-HxCDF	37.725		68	0	13.2		*0*		1.5855	0.008			*0.0*
31	Surrogate	13C-1234678-HpCDF	40.121		92	65	17.7	*2.3*	0.706	-9.9	1.7422	0.016			*0.0*
32	Surrogate	13C-1234789-HpCDF	41.596		83	39	*1.9*	*1.0*	*0.468*	*-41.0*	1.6385	0.013			*0.0*
41	IS	13C-1234-TCDD	25.738		320300	300454	4218.2	9440.2	0.938	0.2	-	-			
42	IS	13C-123789-HxCDD	37.871		351059	220779	11838.8	7614.5	0.629	0.2	-	-			

Required Reports Dioxins

Calibration Standard

Dioxin Quantitative Analysis Sample Report

Data Path	C:\MassHunter\GCMS\1\data\TQ2_231005A_1613\TQ2_231005A11.D		
Sample Name	CS5_1613_13CS5 1021	Acq. Method	TQDF_MRM
Acq. Time	2023-10-05 8:30:52 AM	Quant Method	16130_Quant12_Dale (1).m
Sample Type	Cal	Sample Amt	
Analysis Time	2023-11-09 3:55:38 PM	Analyst Name	AGILENT\shotoole

No	Type	Compound	RT [min]	RRT [min]	Area	Q-Area	S/N	Q-S/N	Resp. Ratio	%Ratio Error	Av-RRF	Conc. [pg/g]	Mod.	LOQ (pg/g)	%Rec
1	Target	2378-TCDD	26.085	0.020	1732354	1649243	307483.5	291861.5	0.952	-0.6	0.2395	992.628			
2	Target	12378-PeCDD	33.943	0.018	5932093	4668020	422241.1	137687.3	0.787	0.9	1.1135	1015.167			
3	Target	123478-HxCDD	37.884	0.007	5238742	3337896	462453.4	66215.7	0.637	4.2	0.9767	1030.885			
4	Target	123678-HxCDD	37.884	0.007	5238712	3337888	111284.1	66215.7	0.637	1.9	0.9719	1035.950			
5	Target	123789-HxCDD	38.284	*0.407*	5379447	3451326	367625.1	104116.9	0.642	1.7	1.0802	959.729			
6	Target	1234678-HpCDD	41.189	0.007	5003575	4021505	140129.1	41185.1	0.804	-0.2	1.0347	1002.365			
7	Target	OCDD	44.721	0.008	9243960	8960145	456536.0	478328.0	0.969	1.0	9.0856	200.132			
8	Target	2378-TCDF	24.873	0.019	2706542	2554209	66043.5	34932.2	0.944	-1.7	0.2414	1005.576			
9	Target	12378-PeCDF	32.294	0.012	10344862	8205703	161965.5	754736.7	0.793	1.1	1.1168	1006.301			
10	Target	23478-PeCDF	33.414	0.012	11089409	8769739	36885.0	37669.2	0.791	0.2	1.2270	1020.964			
11	Target	234678-HxCDF	38.487	0.007	7822685	4920889	40585.2	14626.1	0.629	-8.9	0.9809	1000.465			
12	Target	123478-HxCDF	37.040	0.013	8637628	5490805	330252.2	752120.9	0.636	-0.7	1.0379	1006.545			
13	Target	123678-HxCDF	37.040	0.013	8637628	5490805	330252.2	752120.9	0.636	0.4	1.0377	1006.677			
14	Target	123789-HxCDF	37.732	0.007	8060400	5122632	153611.3	308319.8	0.636	0.0	1.0499	1005.563			
15	Target	1234678-HpCDF	40.134	0.007	7281183	5782552	764323.3	244094.3	0.794	-0.4	0.9892	997.526			
16	Target	1234789-HpCDF	41.620	0.007	7168117	5759252	106543.6	47204.6	0.803	0.4	0.9873	991.894			
17	Target	OCDF	44.874	*0.160*	12599231	11939474	609372.8	581268.8	0.948	-1.3	11.8713	206.468			
18	Surrogate	13C-2378-TCDD	26.065		732362	689950	14267.6	33732.5	0.942	0.9	1.7377	108.206			108.2
19	Surrogate	13C-12378-PeCDD	33.926		522684	415033	17403.1	13885.6	0.794	1.8	0.9303	133.254			133.3
20	Surrogate	13C-123478-HxCDD	37.876		523821	327988	13690.9	18960.6	0.626	-0.2	1.0000	99.999			100.0
21	Surrogate	13C-123678-HxCDD	37.876		523836	327988	15136.1	18960.6	0.626	-3.4	0.9999	100.007			100.0
22	Surrogate	13C-1234678-HpCDD	41.182		484304	385841	10144.9	8574.3	0.797	-0.4	1.0661	95.816			95.8
23	Surrogate	13C-OCDD	44.713		1019514	982796	25064.9	24371.1	0.964	0.4	1.1346	207.170			103.6
24	Surrogate	13C-2378-TCDF	24.854		1114394	1053139	9147.7	10893.9	0.945	-1.6	2.7649	103.635			103.6
25	Surrogate	13C-12378-PeCDF	32.282		915827	734881	9996.0	7912.0	0.802	0.8	1.6777	130.074			130.1
26	Surrogate	13C-23478-PeCDF	33.402		878311	706969	6467.5	12372.9	0.805	1.1	1.6449	127.402			127.4
27	Surrogate	13C-123478-HxCDF	37.027		833017	519400	29937.2	24221.1	0.624	0.0	1.6612	95.573			95.6
28	Surrogate	13C-123678-HxCDF	37.027		833030	519400	19594.8	16894.5	0.624	1.2	1.6615	95.560			95.6
29	Surrogate	13C-234678-HxCDF	38.479		796390	502134	4224.2	4976.8	0.631	0.4	1.5807	96.438			96.4
30	Surrogate	13C-123789-HxCDF	37.725		768764	479904	41131.3	6055.1	0.624	0.7	1.5855	92.458			92.5
31	Surrogate	13C-1234678-HpCDF	40.127		742643	581301	19020.8	28925.4	0.783	-0.1	1.7422	89.212			89.2
32	Surrogate	13C-1234789-HpCDF	41.613		739246	580755	18290.1	5061.0	0.786	-0.9	1.6385	94.578			94.6
41	IS	13C-1234-TCDD	25.738		389380	367064	7570.1	3591.7	0.943	0.7	-	-			
42	IS	13C-123789-HxCDD	37.876		523825	327994	12040.5	8153.7	0.626	-0.2	-	-			

Required Reports Dioxins

Dioxin Quantitative Analysis Sample Report

Agilent

Data Path	C:\MassHunter\Data\TQ2_230711A_1613\TQ2_221221A08.D		
Sample Name	UHH389	Acq. Method	TQDF_MRM
Acq. Time	12/22/2022 1:31:30 AM	Quant Method	
Sample Type	Sample	Sample Amt	10.00 g
Analysis Time	7/12/2023 4:43:41 PM	Analyst Name	AME\kuxu

No	Type	Compound	RT [min]	RRT [min]	Area	Q-Area	S/N	Q-S/N	Resp. Ratio	%Ratio Error	Av-RRF	Conc. [pg/g]	Mod.	LOQ (pg/g)	%Rec
1	IS	2378-TCDD	26.109		2167	2482	44.5	35.6	*1.145*	*19.3*	1.1839	0.192			
2	IS	12378-PeCDD	34.672		33786	26995	1764.2	1183.0	0.799	2.4	1.1139	3.983			
3	IS	123478-HxCDD	37.603		423287	271616	20820.8	7826.2	0.642	-1.9	1.0199	62.949			
4	IS	123678-HxCDD	37.603		423287	271616	20820.8	7375.3	0.642	1.8	1.0421	61.607			
5	IS	123789-HxCDD	38.461		1112868	713830	54835.8	20317.0	0.641	0.2	1.0336	163.289			
6	IS	1234678-HpCDD	41.685		14795633	11937121	591546.4	464684.4	0.807	0.9	1.0762	2638.260			
7	IS	OCDD	-		0	0			*0*		0.9179	ND			*0.0*
8	IS	2378-TCDF	24.986		30965	29180	1191.6	321.2	0.942	-1.8	1.2034	1.446			
9	IS	12378-PeCDF	32.606		135029	107256	1680.8	2403.5	0.794	1.8	1.0942	10.206			
10	IS	23478-PeCDF	34.023		104508	82672	1992.2	1194.2	0.791	1.4	1.2095	6.962			
11	IS	123478-HxCDF	36.880		871474	547771	14295.2	11619.9	0.629	-10.4	1.0510	83.294			
12	IS	123678-HxCDF	38.155		305235	197227	5287.6	4300.9	0.646	1.4	1.0253	30.227			
13	IS	234678-HxCDF	38.155		305235	197227	7028.6	4300.9	0.646	2.4	1.0719	28.255			
14	IS	123789-HxCDF	38.281		244663	156498	4272.5	2724.9	0.640	-0.1	0.9880	22.542			
15	IS	1234678-HpCDF	41.379		2610135	2086926	27368.7	15677.4	0.800	0.2	1.0213	308.602			
16	IS	1234789-HpCDF	41.379		2610135	2086926	27368.7	15677.4	0.800	-0.1	0.9932	308.231			
17	IS	OCDF	45.877		1425056	1382657	18365.1	31670.0	0.970	1.1	1.1599	467.321			
18	Surrogate	13C-2378-TCDD	26.089		1055097	986210	5276.8	10016.8	0.935	-2.6	1.8039	66.199			66.2
19	Surrogate	13C-12378-PeCDD	34.655		762705	607198	27398.7	10248.7	0.796	2.1	0.9488	84.464			84.5
20	Surrogate	13C-123478-HxCDD	39.083		664438	417888	8815.0	5024.9	0.629	0.0	0.9094	109.957			110.0
21	Surrogate	13C-123678-HxCDD	39.083		664512	417895	13275.0	4164.9	0.629	-3.4	1.0007	99.933			99.9
22	Surrogate	13C-1234678-HpCDD	42.387		524519	417039	20910.3	10990.2	0.795	-0.6	0.8861	98.169			98.2
23	Surrogate	13C-OCDD	45.752		529631	506313	9393.6	5960.9	0.956	-0.4	0.9081	105.395			52.7
24	Surrogate	13C-2378-TCDF	24.967		1784699	1672543	10798.8	5239.8	0.937	-2.4	2.8920	69.934			69.9
25	Surrogate	13C-12378-PeCDF	32.577		1206766	962981	9255.4	14930.1	0.798	2.3	1.7449	72.745			72.7
26	Surrogate	13C-23478-PeCDF	34.006		1236589	986316	6322.6	8501.8	0.798	2.3	1.6969	76.634			76.6
27	Surrogate	13C-123478-HxCDF	38.142		997960	623252	45785.7	9927.5	0.625	-13.8	1.4730	101.681			101.7
28	Surrogate	13C-123678-HxCDF	38.142		997971	623252	25583.0	7592.7	0.625	0.3	1.5905	94.172			94.2
29	Surrogate	13C-234678-HxCDF	38.268		1024430	634558	25708.3	7582.5	0.619	-0.8	1.4906	102.826			102.8
30	Surrogate	13C-123789-HxCDF	38.903		1103616	697637	29227.2	8794.6	0.632	-0.6	1.4613	113.880			113.9
31	Surrogate	13C-1234678-HpCDF	41.372		836691	653557	42061.7	13658.1	0.781	-0.4	1.4128	97.452			97.5
32	Surrogate	13C-1234789-HpCDF	42.773		861261	673080	40668.8	7797.6	0.782	-1.1	1.3484	105.128			105.1

"L"--Below LOQ/LOD/MDL

Required Reports Dioxins

Sample Report Unknowns

Dioxin Quantitative Analysis Sample Report

Agilent

Unknowns	RT [min]	Resp.	Av-RRF	Conc. [pg/g]	Area	Q-Area	Resp. Ratio	S/N	Q-S/N	Mod.	Fail
Total Tetra-Dioxins(0)	-	-	0.6005	ND							
Unknowns	25.954	522	-	-	277	245	0.883	15.3	19.3		
Unknowns	26.109	4729	-	-	2218	2511	1.132	103.1	163.2		
Unknowns	26.365	192	-	-	91	101	1.114	5.1	6.0		
Unknowns	25.305	1551	-	-	807	744	0.922	40.6	51.4		
Unknowns	26.656	2445	-	-	1189	1256	1.056	55.0	79.7		
Unknowns	24.901	1146	-	-	691	454	*0.658*	25.4	35.6		*Fail*
Unknowns	27.019	417	-	-	188	228	*1.214*	9.4	12.7		*Fail*
Unknowns	24.770	1788	-	-	918	870	0.948	35.1	52.7		
Unknowns	24.412	6214	-	-	3190	3023	0.948	126.3	166.8		
Unknowns	23.526	1769	-	-	936	833	0.890	49.8	55.8		
Unknowns	23.180	2240	-	-	1153	1087	0.943	63.8	74.7		
Unknowns	22.758	3113	-	-	1661	1452	0.875	92.8	111.3		
Total Penta-Dioxins(0)	-	-	1.1139	ND							
Unknowns	34.672	60781	-	-	33786	26995	0.799	1764.2	1183.0		
Unknowns	34.907	4656	-	-	2565	2092	0.816	132.6	86.1		
Unknowns	34.341	825	-	-	474	351	0.742	24.6	16.2		
Unknowns	34.147	934	-	-	424	509	*1.201*	19.1	16.2		*Fail*
Unknowns	35.404	5417	-	-	2975	2442	0.821	171.1	115.5		
Unknowns	33.792	13646	-	-	7592	6054	0.797	261.1	177.1		
Unknowns	33.638	3337	-	-	1705	1632	*0.957*	86.4	61.6		*Fail*
Unknowns	33.312	9600	-	-	5309	4291	0.808	247.7	167.8		
Unknowns	32.998	35594	-	-	19593	16001	0.817	833.2	566.4		
Unknowns	32.712	14620	-	-	7910	6710	0.848	461.6	313.6		
Total Hexa-Dioxins(0)	-	-	0.3620	ND							
Unknowns	38.187	63469	-	-	38904	24566	0.631	546.4	400.4		
Unknowns	38.461	1825386	-	-	1111608	713778	0.642	15171.3	11324.8		
Unknowns	38.621	22899	-	-	13655	9243	0.677	134.3	102.3		
Unknowns	37.603	692608	-	-	421740	270868	0.642	5762.8	4319.6		
Unknowns	39.090	155541	-	-	95717	59824	0.625	1495.4	1102.6		
Unknowns	39.187	1842443	-	-	1124251	718192	0.639	16249.1	12095.1		
Unknowns	39.513	366866	-	-	223359	143507	0.642	3013.3	2258.5		
Total Hepta-Dioxins(0)	-	-	1.0762	ND							
Unknowns	41.685	26732754	-	-	14795633	11937121	0.807	591546.4	464684.4		
Unknowns	42.400	35317540	-	-	19566833	15750707	0.805	726855.0	573552.0		
Total Tetra-Furans(0)	-	-	1.2021	ND							
Unknowns	24.986	60375	-	-	31132	29243	0.939	1824.3	897.4		
Unknowns	24.403	21705	-	-	11273	10431	0.925	694.6	344.3		
Unknowns	25.623	915	-	-	520	395	*0.760*	22.7	14.2		*Fail*
Unknowns	24.135	9761	-	-	4945	4815	0.974	310.0	167.9		
Unknowns	25.992	815	-	-	463	352	*0.761*	20.0	10.2		*Fail*
Unknowns	23.975	2881	-	-	1570	1311	0.835	81.7	34.3		
Unknowns	23.635	25467	-	-	13119	12348	0.941	876.0	439.9		
Unknowns	23.183	44632	-	-	23068	21564	0.935	1439.9	707.0		
Unknowns	26.980	2930	-	-	1518	1411	0.930	86.6	39.4		
Unknowns	22.850	24073	-	-	12443	11630	0.935	824.7	403.0		
Unknowns	22.600	1115	-	-	599	516	0.862	41.7	19.9		
Unknowns	27.486	2161	-	-	1121	1039	0.927	66.5	29.4		
Unknowns	22.463	1442	-	-	757	685	0.905	54.0	24.9		

UHH389 Page 2 of 14 Generated at 5:30 PM on 7/12/2023

Failure Codes: "RT"-- Quantifier RT out of range

"SN"-- Quantifier or Qualifier Signal To Noise Ratio l

"NQ"-- Qualifier not found; "QRT"-- Qualifier RT ou

"QR"-- Qualifier Ratio out of range; "DPE"-- DPE int

"T"--Target;

"L"--Below LOQ/LOD/MDL

Required Reports Dioxins

Sample Report Unknowns

Dioxin Quantitative Analysis Sample Report

Unknowns	RT [min]	Resp.	Av-RRF	Conc. [pg/g]	Area	Q-Area	Resp. Ratio	S/N	Q-S/N	Mod.	Fail
Unknowns	27.718	1827	-	-	946	881	0.932	50.5	27.7		
Unknowns	22.094	54475	-	-	28081	26395	0.940	2032.5	1027.1		
Unknowns	21.844	4609	-	-	2298	2312	1.006	169.5	89.8		
Unknowns	21.344	1133	-	-	533	601	1.127	43.4	25.9		
Total Penta-Furans(0)	-	-	0.5618	ND							
Unknowns	32.606	242771	-	-	135029	107742	0.798	2497.9	3029.7		
Unknowns	32.440	41822	-	-	23640	18182	0.769	459.4	550.9		
Unknowns	33.206	208492	-	-	116032	92460	0.797	2369.8	2919.5		
Unknowns	32.017	32392	-	-	18009	14384	0.799	326.6	426.6		
Unknowns	31.874	73104	-	-	40944	32160	0.785	666.6	779.5		
Unknowns	34.023	187578	-	-	104343	83235	0.798	2342.1	2851.1		
Unknowns	34.315	301401	-	-	167049	134352	0.804	3805.8	4658.1		
Unknowns	31.057	23440	-	-	13301	10139	0.762	213.6	259.4		
Total Hexa_Furans(0)	-	-	0.2461	ND							
Unknowns	38.281	406031	-	-	249658	156373	0.626	1507.1	843.6		
Unknowns	38.155	505351	-	-	309670	195681	0.632	1864.7	1033.5		
Unknowns	38.835	354257	-	-	219017	135240	0.617	1394.4	772.4		
Unknowns	38.915	294802	-	-	180352	114450	0.635	1134.3	629.5		
Unknowns	37.669	5401165	-	-	3299408	2101757	0.637	25103.1	14027.6		
Unknowns	39.796	330328	-	-	201907	128420	0.636	1302.2	729.4		
Total Hepta-Furans(0)	-	-	0.4739	ND							
Unknowns	42.780	263425	-	-	145363	118062	0.812	1701.7	955.0		
Unknowns	41.757	9785930	-	-	5416383	4369547	0.807	67356.1	37488.9		
Unknowns	41.379	4697073	-	-	2610130	2086943	0.800	32539.2	18025.9		

Failure Codes: "RT"-- Quantifier RT out of range

"SN"-- Quantifier or Qualifier Signal To Noise Ratio low;

"NQ"-- Qualifier not found; "QRT"-- Qualifier RT out of range;

"QR"-- Qualifier Ratio out of range; "DPE"-- DPE interference;

"T"--Target;

"L"--Below LOQ/LOD/MDL

Required Reports Dioxins

Sample Report Blank

Dioxin Quantitative Analysis Sample Report

Agilent

Data Path	C:\MassHunter\GCMS\1\data\TQ2_231005A_1613\TQ2_231005A12.D		
Sample Name	solvent	Acq. Method	TQDF_MRM
Acq. Time	2023-10-05 9:19:50 AM	Quant Method	16130_Quant12_Dale (1).m
Sample Type	Sample	Sample Amt	
Analysis Time	2023-11-09 3:55:38 PM	Analyst Name	AGILENT\shotoole

No	Type	Compound	RT [min]	RRT [min]	Area	Q-Area	S/N	Q-S/N	Resp. Ratio	%Ratio Error	Av-RRF	Conc. [pg/g]	Mod.	LOQ (pg/g)	%Rec
1	Target	2378-TCDD	25.912	0.139	73	36	2.9	1.4	0.500	-47.8	0.2395	102.403			
2	Target	12378-PeCDD	33.966	0.023	1116	767	42.9	26.9	0.688	-11.8	1.1135	399.933			
3	Target	123478-HxCDD	37.895	0.013	465	322	58.8	16.6	0.691	13.1	0.9767	292.372			
4	Target	123678-HxCDD	37.895	0.013	474	321	79.1	16.6	0.678	8.5	0.9719	296.468			
5	Target	123789-HxCDD	37.981	0.099	598	404	53.9	29.4	0.675	7.0	1.0802	336.400			
6	Target	1234678-HpCDD	41.200	0.224	587	478	85.9	83.4	0.814	1.0	1.0347	923.089			
7	Target	OCDD	44.733	0.026	586	612	24.6	53.0	1.045	8.8	9.0856	86.060			
8	Target	2378-TCDF	24.897	0.019	1434	1286	41.6	38.6	0.897	-6.6	0.2414	649.407			
9	Target	12378-PeCDF	32.323	0.018	1786	1650	57.5	81.1	0.924	17.7	1.1168	467.814			
10	Target	23478-PeCDF	33.437	0.206	1538	1234	71.2	69.5	0.802	1.7	1.2270	7620.332			
11	Target	234678-HxCDF	38.504	0.270	1083	743	55.2	27.4	0.686	-0.6	0.9809	3765.542			
12	Target	123478-HxCDF	37.052	0.024	1301	899	34.6	492.9	0.691	8.0	1.0379	134.602			
13	Target	123678-HxCDF	37.052	0.024	1301	899	34.6	492.9	0.691	9.2	1.0377	132.895			
14	Target	123789-HxCDF	37.749	0.019	1011	656	32.1	62.6	0.649	2.1	1.0499	379.755			
15	Target	1234678-HpCDF	40.145	0.207	661	651	45.1	54.5	0.985	23.5	0.9892	2115.924			
16	Target	1234789-HpCDF	41.632	0.322	677	613	36.6	22.3	0.906	13.3	0.9873	2603.465			
17	Target	OCDF	44.880	0.172	883	847	96.5	54.4	0.960	0.0	11.8713	95.115			
18	Surrogate	13C-2378-TCDD	25.774		241	204	6.4	9.0	0.849	-9.1	1.7377	263.022			263.0
19	Surrogate	13C-12378-PeCDD	33.943		232	190	9.9	41.9	0.819	5.0	0.9303	466.537			466.5
20	Surrogate	13C-123478-HxCDD	37.882		163	112	11.7	32.7	0.688	9.6	1.0000	100.200			100.2
21	Surrogate	13C-123678-HxCDD	37.882		164	112	11.7	32.6	0.686	5.8	0.9999	100.341			100.3
22	Surrogate	13C-1234678-HpCDD	40.976		75	37	7.6	2.4	0.492	-38.5	1.0661	38.015			38.0
23	Surrogate	13C-OCDD	44.707		151	156	4.6	11.8	1.036	7.9	1.1346	98.185			49.1
24	Surrogate	13C-2378-TCDF	24.878		910	825	10.6	11.3	0.907	-5.6	2.7649	644.243			644.2
25	Surrogate	13C-12378-PeCDF	32.305		379	279	41.9	15.4	0.737	-7.4	1.6777	402.394			402.4
26	Surrogate	13C-23478-PeCDF	33.231		30	0	4.7		0		1.6449	18.501			18.5
27	Surrogate	13C-123478-HxCDF	37.027		835	740	17.9	22.9	0.886	42.1	1.6612	344.666			344.7
28	Surrogate	13C-123678-HxCDF	37.027		840	755	23.7	19.4	0.900	45.9	1.6615	349.092			349.1
29	Surrogate	13C-234678-HxCDF	38.234		30	20	1.9	4.2	0.652	3.8	1.5807	11.370			11.4
30	Surrogate	13C-123789-HxCDF	37.731		237	181	17.6	7.6	0.762	23.0	1.5855	95.914			95.9
31	Surrogate	13C-1234678-HpCDF	39.938		22	40	1.9	14.2	1.796	129.2	1.7422	13.080			13.1
32	Surrogate	13C-1234789-HpCDF	41.310		37	13	3.7	2.3	0.351	-55.8	1.6385	11.137			11.1
41	IS	13C-1234-TCDD	25.423		37	60	2.1	4.5	1.622	73.2	-	-			
42	IS	13C-123789-HxCDD	37.882		164	111	11.7	32.3	0.673	7.2	-	-			

Required Reports Dioxins

Sample Report Blank

Dioxin Quantitative Analysis Sample Report

Agilent

Unknowns	RT [min]	Resp.	Av-RRF	Conc. [pg/g]	Area	Q-Area	Resp. Ratio	S/N	Q-S/N	Mod.	Fail
Total Tetra-Dioxins(0)	-	-	0.2395	ND							
Unknowns	24.133	25	-	356.743	14	11	*0.764*	2.6	5.1		*QR*
Unknowns	25.900	62	-	878.849	9	53	*6.012*	3.4	6.9		*QR*
Unknowns	27.954	102	-	1444.738	72	30	*0.409*	9.4	6.1		*QR*
Total Penta-Dioxins(3)	-	217	1.1135	235.696							
Unknowns	31.148	36	-	39.396	24	12	0.522	7.6	8.0		*DPE*
Unknowns	31.365	36	-	38.628	29	6	*0.220*	7.8	4.7		*QR*
Unknowns	31.462	29	-	31.948	23	7	*0.296*	5.8	4.6		*QR*
Unknowns	31.685	29	-	31.749	12	18	*1.507*	4.2	5.2		*QR*
Unknowns	32.303	113	-	122.117	59	53	0.896	5.8	11.7		
Unknowns	32.612	83	-	90.286	46	37	0.801	5.9	9.4		
Unknowns	33.366	31	-	33.451	20	11	*0.558*	7.1	6.1		*QR*
Unknowns	33.886	22	-	24.044	11	11	*1.013*	3.3	3.7		*QR*
Unknowns	34.578	21	-	23.293	12	9	0.789	2.8	5.7		
Unknowns	34.721	18	-	19.722	6	12	*2.039*	2.8	4.9		*QR*
Total Hexa-Dioxins(0)	-	-	1.0096	ND							
Total Hepta-Dioxins(0)	-	-	1.0347	ND							
Unknowns	40.000	33	-	116.442	9	24	2.721	*1.7*	1.3		*SN*
Unknowns	40.874	29	-	100.885	7	22	3.377	*1.5*	1.6		*SN*
Total Tetra-Furans(0)	-	-	0.2414	ND							
Unknowns	20.332	24	-	51.668	9	15	*1.704*	4.4	2.8		*QR*
Unknowns	20.499	26	-	56.618	16	10	*0.585*	12.1	3.2		*QR*
Total Penta-Furans(0)	-	-	1.1719	ND							
Unknowns	28.350	21	-	29.209	6	15	*2.615*	4.2	5.7		*QR*
Unknowns	32.346	134	-	190.068	89	45	*0.505*	13.2	12.3		*QR*
Unknowns	32.889	39	-	55.004	29	9	*0.318*	6.8	5.9		*QR*
Total Hexa_Furans(1)	-	19	1.0266	20.354							
Unknowns	35.559	43	-	45.701	16	26	*1.604*	98.5	10.5		*QR*
Unknowns	35.885	49	-	52.834	16	33	*2.095*	135.5	12.8		*QR*
Unknowns	36.063	9	-	9.638	9			66.9			*NQ*
Unknowns	36.125	65	-	69.658	10	55	*5.536*	70.8	14.3		*QR*
Unknowns	36.657	25	-	26.922	9	16	*1.659*	51.1	10.9		*QR*
Unknowns	37.160	58	-	62.095	29	29	*0.982*	101.9	12.2		*QR*
Unknowns	38.069	46	-	49.673	13	33	*2.609*	76.7	9.1		*QR*
Unknowns	38.321	19	-	20.354	12	7	0.647	61.8	7.4		
Total Hepta-Furans(0)	-	-	0.9883	ND							
Unknowns	40.140	24	-	27.331	12	12	1.041	*1.3*	3.6		*SN*
Unknowns	40.391	34	-	38.639	20	14	0.687	*1.7*	2.4		*SN*
Unknowns	40.894	27	-	31.110	13	14	1.140	*1.1*	4.2		*SN*
Unknowns	41.226	50	-	57.697	33	18	0.549	*1.7*	2.8		*SN*
1234789-HpCDF	*41.620*	66	-	75.633	44	22	0.510	*2.1*	3.6		*SN*
Unknowns	41.969	14	-	16.303	9	5	0.564	*1.3*	4.1		*SN*

Failure Codes: "RT"-- Quantifier RT out of range

"SN"-- Quantifier or Qualifier Signal To Noise Ratio low;

"NQ"-- Qualifier not found; "QRT"-- Qualifier RT out of range;

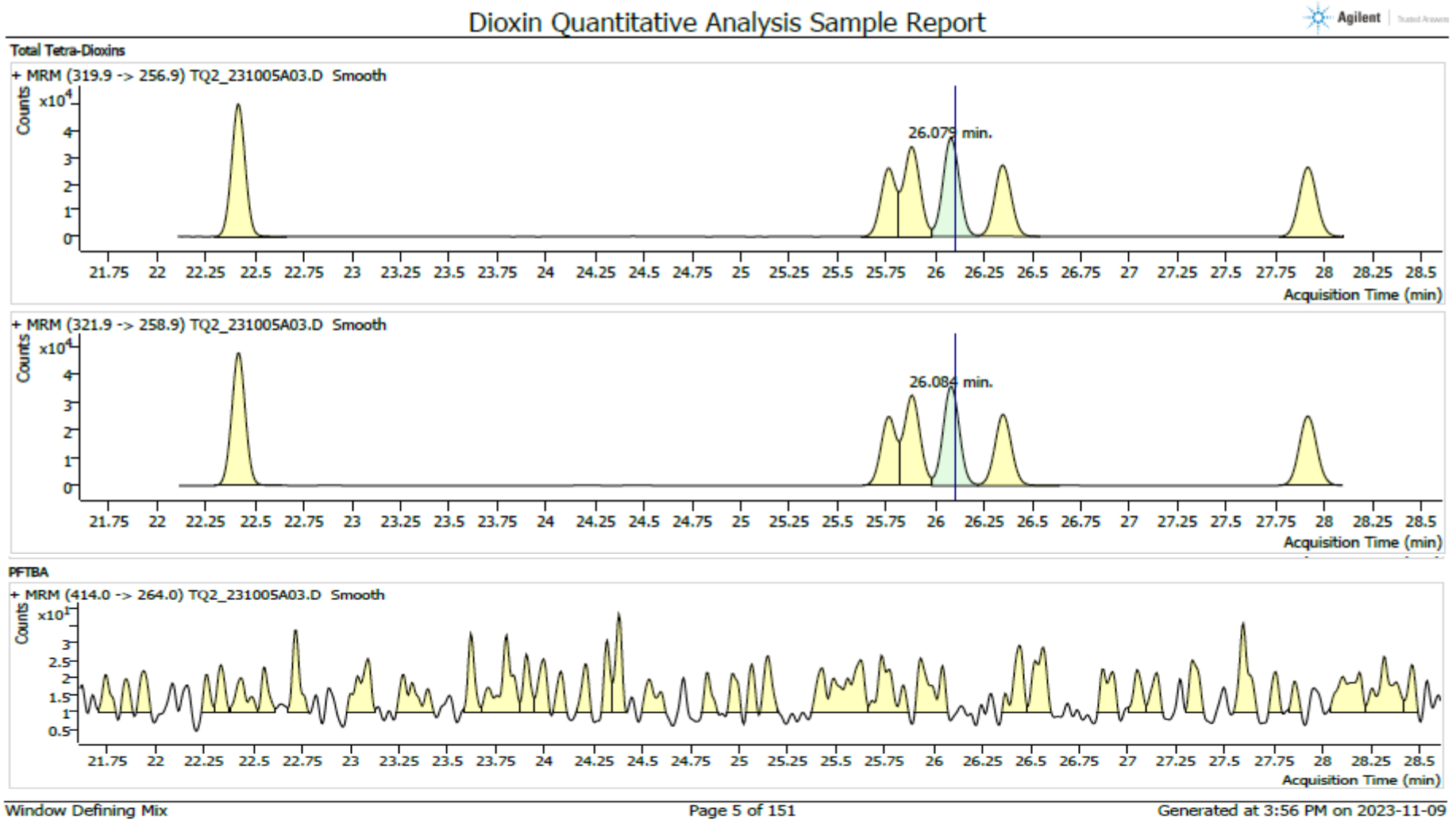
"QR"-- Qualifier Ratio out of range; "DPE"-- DPE interference;

"T"--Target;

"L"--Below LOQ/LOD/MDL

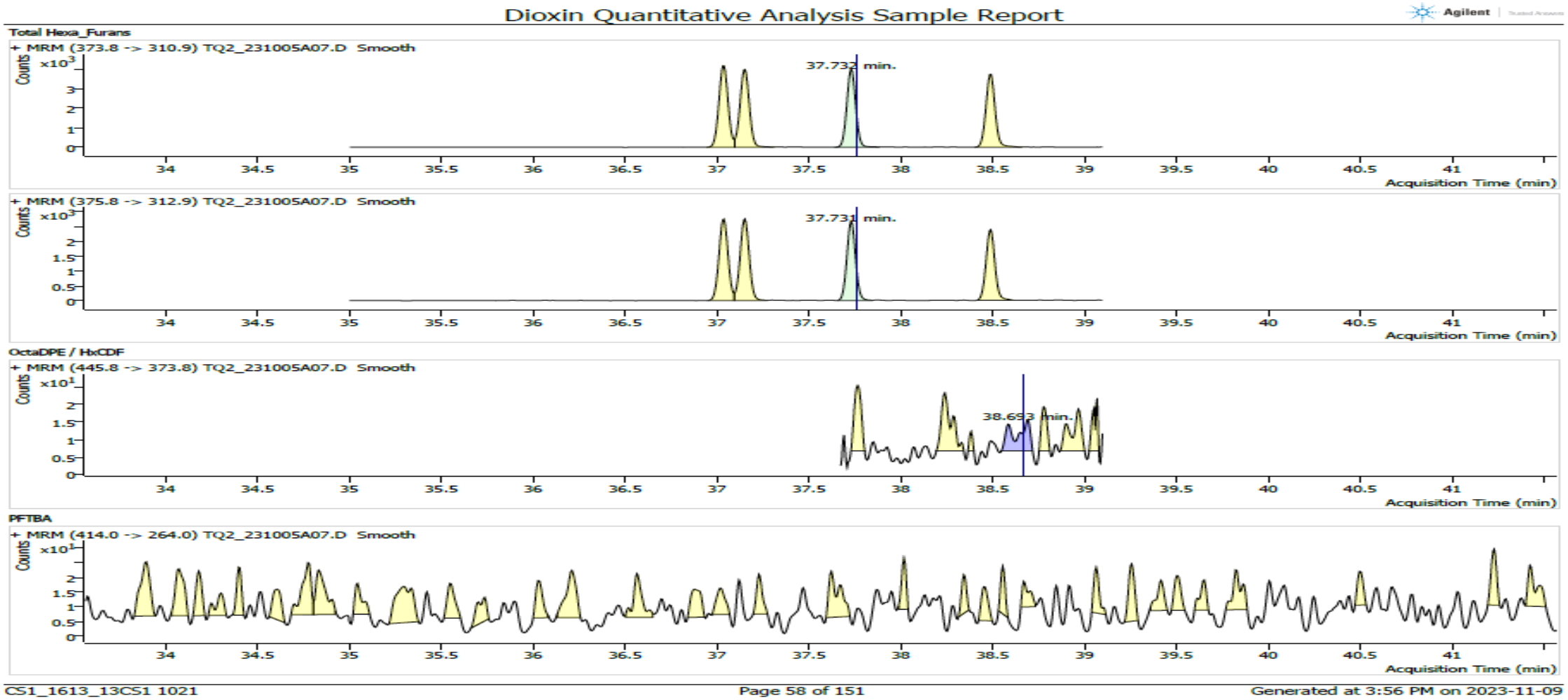
Required Reports Dioxins

Window Defining Mix



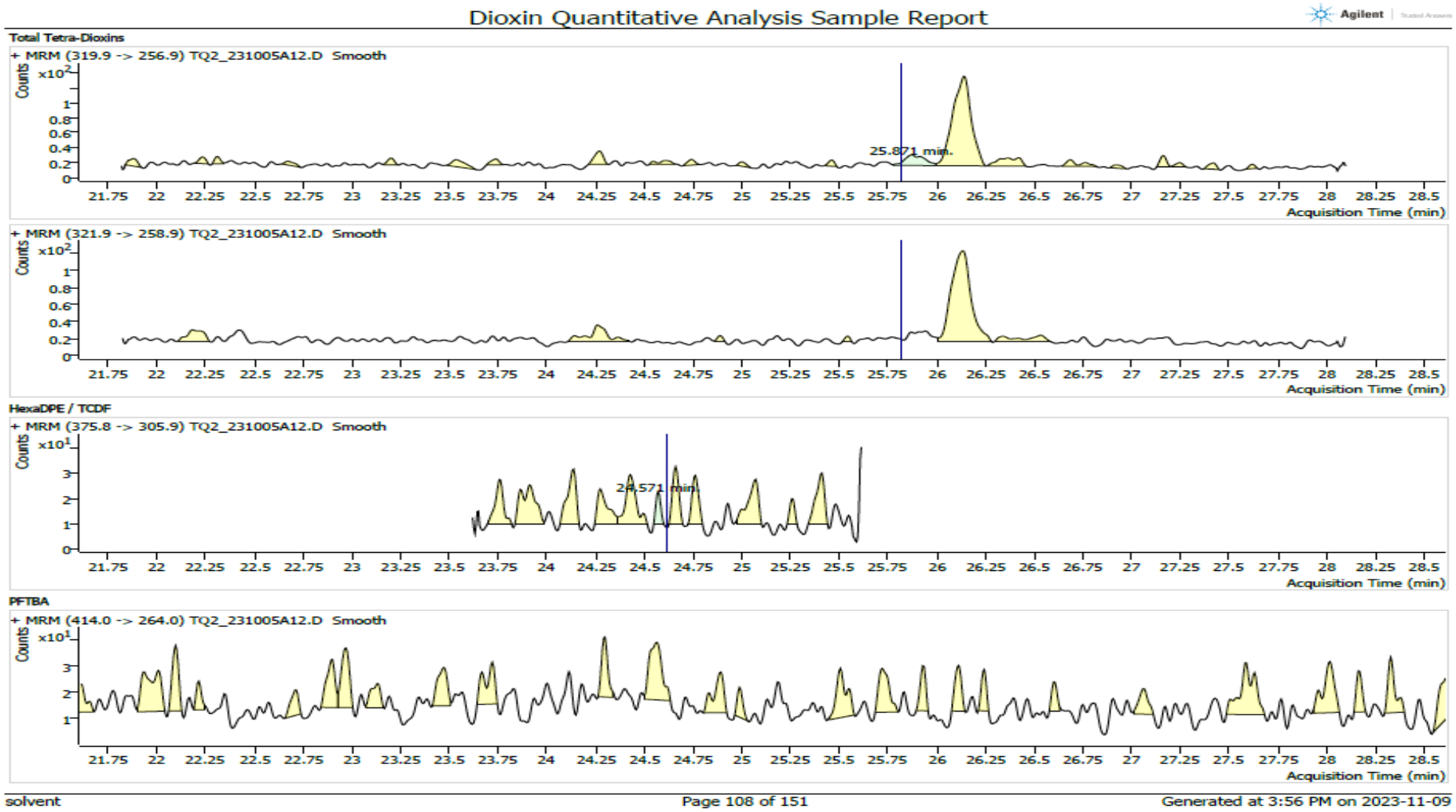
Required Reports Dioxins

Calibration Standard



Required Reports Dioxins

Sample



Required Reports Dioxins

Installation

Part I: Installation instructions:

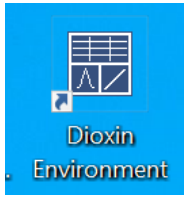
Link to the package installation file Dioxin_Environment.msi

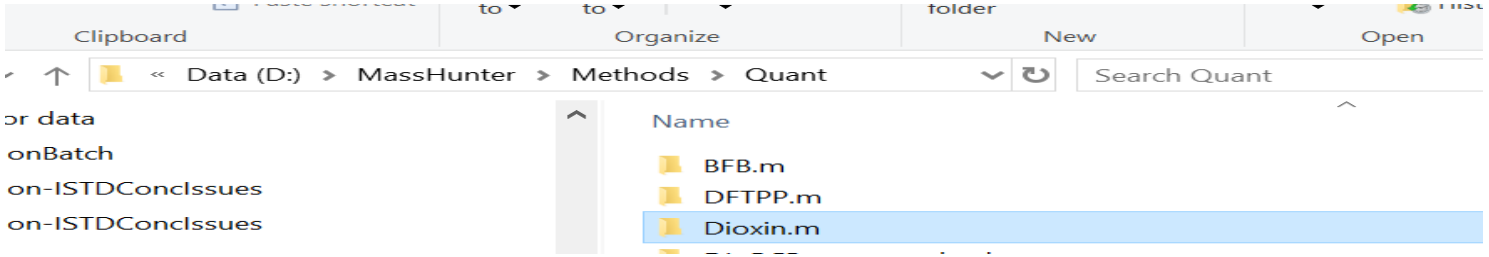
Download the installation file and install it on your computer.

(Prerequisite: MH Quant 12.0 or later need to be installed already)

After successful installation, you will see the following icon on the desktop

Location of installed files Quant DA method

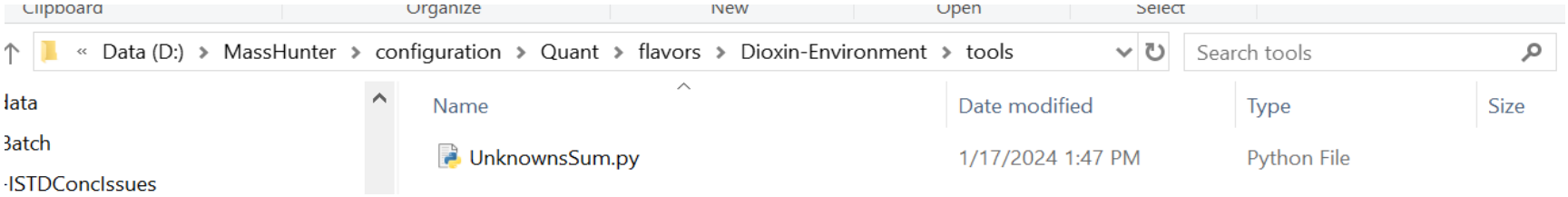




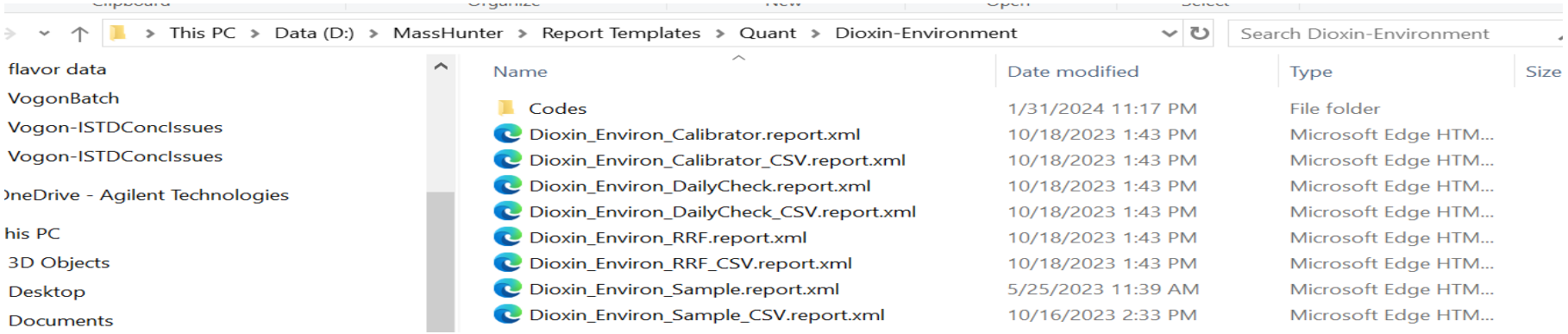
Required Reports Dioxins

Installations

Script for unknown isomers summation UnknownsSum.py



Report templates specially designed for Dioxin Environment



Required Reports Dioxins

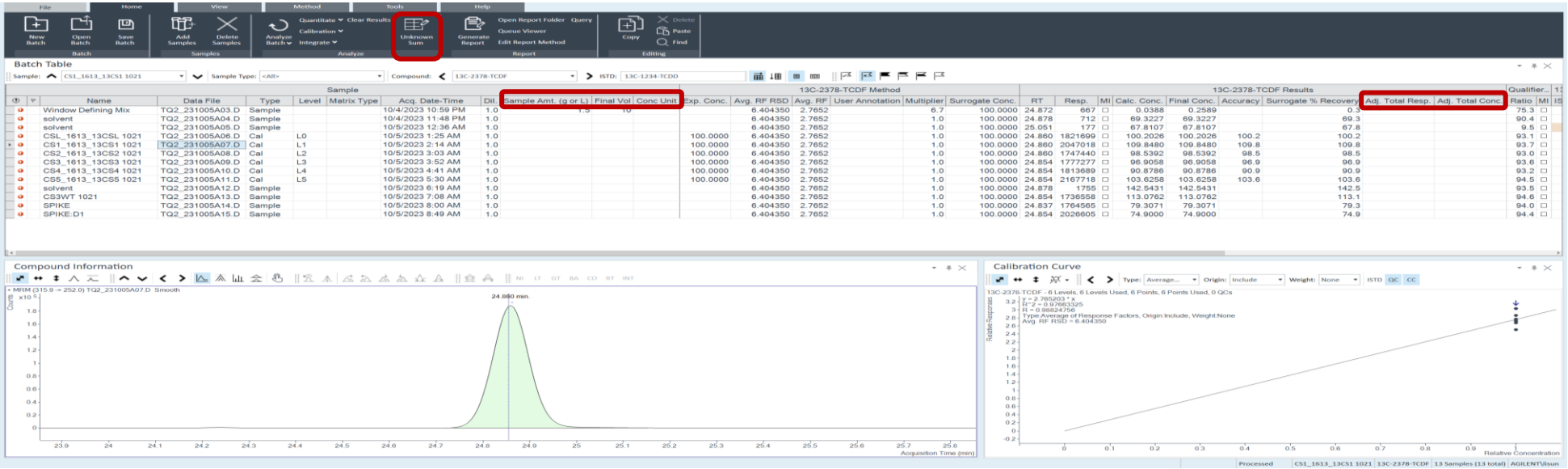
Unknowns

Customized UI for the Dioxin Environment workflow

Customized default columns

Customized column headers

Customized button for quick access to the UnknownsSum.py script



Required Reports Dioxins

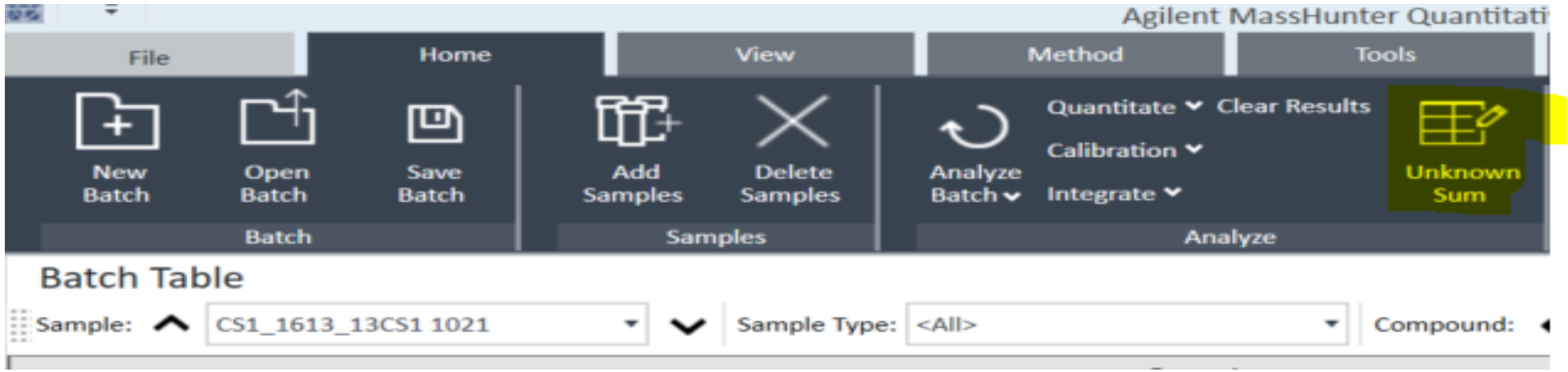
Sample

Part II: Steps for analysis and report

Create a new batch, load the *Dioxin.m* and make necessary adjustment to the method.

Apply method to the batch and analyze.

Click the “Unknown Sum” button to run the script Save batch and generate reports



Required Reports Dioxins

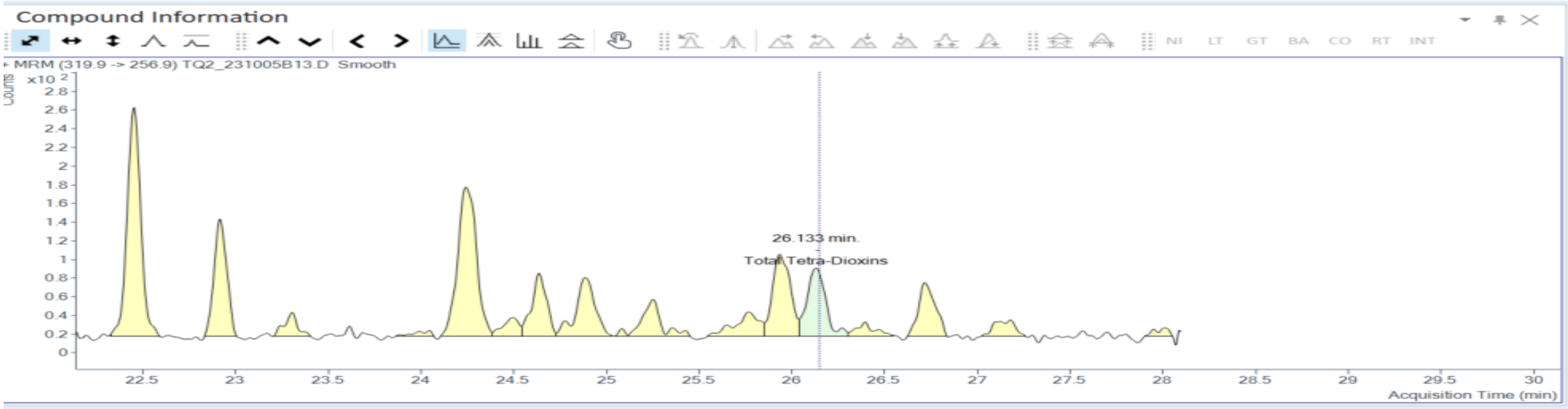
Sample

FAQ about script:

How does the Unknown Sum script work?

For any “total” compound (identified by the keyword “Total” in the compound name), the EIC usually looks like the following

In Quant UI, green represents primary peak and yellow represents alternative peaks.



Required Reports Dioxins

Unknowns

For unknowns total, the color doesn't have any meaning, every peak are treated equally in the script. When the script is run after analyzing the whole batch, for each *total* compound, the script loops through all peaks, and checks the following criteria to determine if it's a qualified isomer:

1a) RT of the peak (check if it is overlapping with RT of any calibrated target compound, <0.004 min is the threshold by default)

1b) RT of the qualifier peak (check if it coelutes with the quantifier peak, <0.0333 min is the threshold by default)

1c) S/N of both quantifier peak and qualifier peak (>2.5 is the default threshold, S/N outlier limit set up in the Quant method will override

1d) Qualifier ratio (use Relative Response and Uncertainty in the Quant method as expected ratio and threshold)

Required Reports Dioxins

Sample

If enabled (change the constant on the top of the script *DPE_INTERFERENCE_REMOVAL = False* to *DPE_INTERFERENCE_REMOVAL = True*)

The script will also check if the isomer peak is interfered by a DPE compound, the DPE peak is considered real if its S/N>2.5, Area > 10% of the native peak area, and if the RT difference between the DPE peak and the isomer peak is <0.0333 min, the isomer peak is determined as interfered by a DPE compound and hence non-qualified.

1f) If enabled (change constant on the top of the script EXCLUDE_LOD/EXCLUDE_LOQ/EXCLUDE_MDL to *True*) and have corresponding LOD/LOQ/MDL outlier limit set up in the Quant method, the script will also check if the calculated concentration of each isomer peak is below LOD/LOQ/MDL, and if yes, the isomer peak is considered as non-qualified).

Required Reports Dioxins

Changing Variables

How to change the peak qualification criteria values?

The constants described above are listed on the top of the UnknownsSum.py (see below for the screenshot),

User may use Notepad to open it and adjust the values.

Some criteria are controlled by the corresponding outlier limit as described in the comments of the code.

UnknownsSum.py | CompoundCalibration.cs | CalibrationSetup.cs | Quantifier.cs | CalibrationCurveFit.cs | DailyCheck_CSV.py

```
clr.AddReference("QuantUIScriptIF")
clr.AddReference("QuantUIScriptIFImpls")
clr.AddReference("AppCommandContext")
clr.AddReference("System.Windows.Forms")
from System.Collections.Generic import List
from System import Array

import Agilent
import _commands
from Agilent.MassSpectrometry.DataAnalysis.Quantitative.UIScriptIF import *

SAME_CPD_RT_DIFF_THRESHOLD = 0.004 #min
DPE_INTERFERENCE_RT_DIFF_THRESHOLD = 0.0333 #min
DPE_SN_THRESHOLD = 2.5
DPE_AREA_THRESHOLD_RELATIVE_TO_NATIVE =0.1 #10%
QUANT_QUAL_SN_THRESHOLD =2.5 #method specified limit will overide it if exist
QUANT_QUAL_RT_DIFF_THRESHOLD = 0.0333 #min
#QUAL_RATIO_THRESHOLD = 0.2 #use method specified limit instead for reporting purpose
EXCLUDE_LOD = False #change to True if unknown calculated concentration < LOD needs to be excluded in total
EXCLUDE_LOQ = False #change to True if unknown calculated concentration < LOQ needs to be excluded in total
EXCLUDE_MDL = False #change to True if unknown calculated concentration < MDL needs to be excluded in total
DPE_INTERFERENCE_REMOVAL = False #switch to turn on/off automatic DPE interference removal

def SetState(ToolState, UIState):
    ToolState.Enabled = True
```

Required Reports Dioxins

EMPC Report

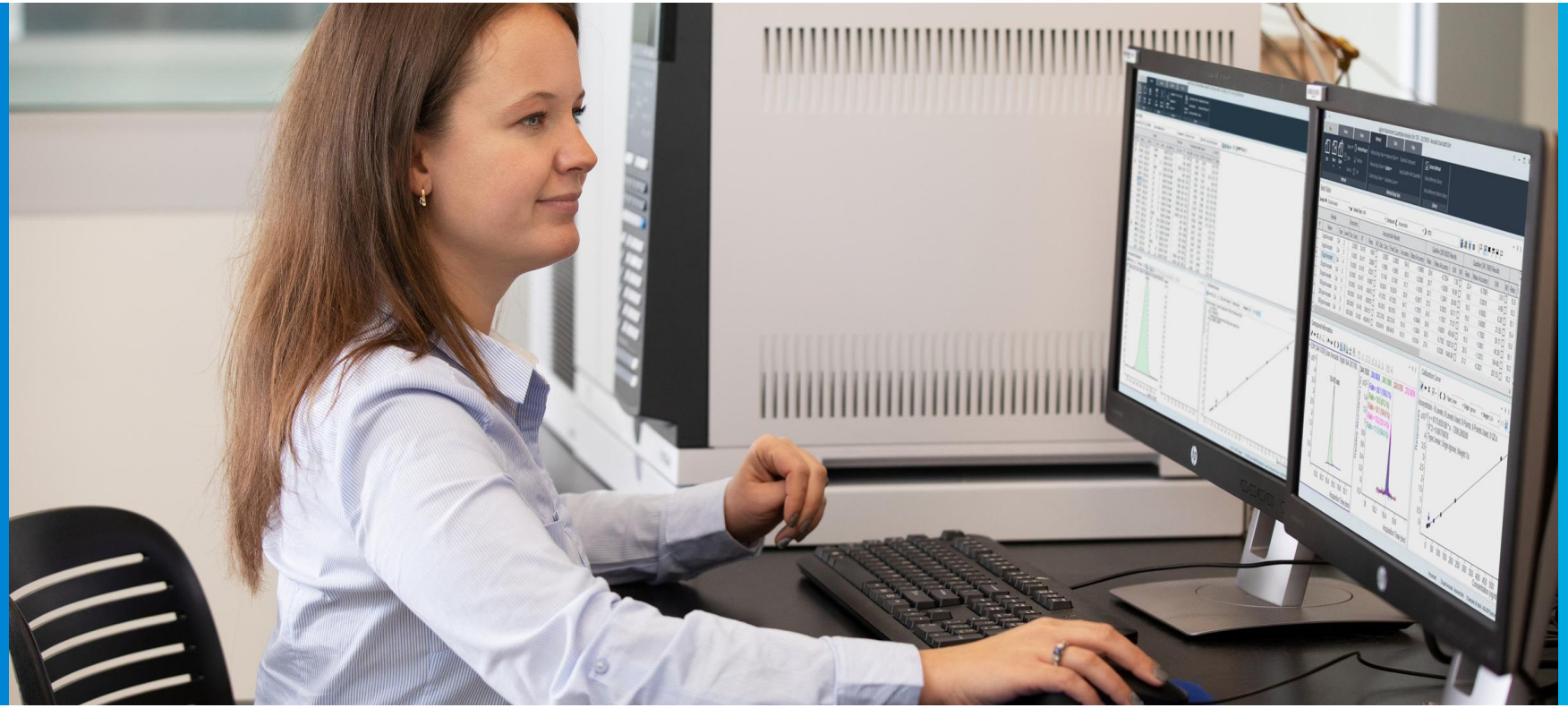
Dioxin Quantitative Analysis Sample Report

Data Path	E:\MassHunter\Data\QQQ\DioxinCanada\Dioxin data-BV Oct 2023\TQ2_231005B_1613\TQ2_231005B10.D		
Sample Name	SAMPLE	**Acq. Method**	TQDF_MRM
Acq. Time	10/6/2023 3:18:47 AM	**Acq. Operator**	
Quant Method	Li.batch.bin	**Sample Type**	Sample
Sample Amt (g or L)		**Final Vol (uL)**	
Analysis Time	1/31/2024 12:14:19 PM	**Analyst Name**	AGILENT\lisun

No	Compound	RT[min]	QRT[min]	Area	Q-Area	Sum Area	Resp Ratio	OK(Ratio)	Av-RRF	Surr Conc	Calc Conc[ng/mL]	Final Conc [ng/ml]	EMPC [ng/ml]	%Rec	Fail	Status	Mod
1	2378-TCDD	26.121	26.096	166	312	477	*1.878*	Fail(15)	0.2395	-	0.204	0.204	0.139		*QR*	Fail	
2	12378-PeCDD	33.966	33.967	223	198	421	0.886	OK(15)	1.1135	-	0.056	0.056				Pass	
3	123478-HxCDD	37.889	37.888	187	126	313	0.672	OK(15)	0.9767	-	0.060	0.060				Pass	
4	123678-HxCDD	37.981	37.980	590	299	889	*0.508*	Fail(15)	0.9719	-	0.174	0.174	0.152		*QR*	Fail	
5	123789-HxCDD	38.289	38.294	493	312	805	0.632	OK(15)	1.0802	-	0.141	0.141				Pass	
6	1234678-HpCDD	41.200	41.199	6091	4896	10986	0.804	OK(15)	1.0347	-	2.768	2.768				Pass	
7	OCDD	44.739	44.738	29974	29412	59386	0.981	OK(15)	9.0856	-	1.793	1.793				Pass	
8	2378-TCDF	24.909	24.920	1872	1704	3577	0.910	OK(15)	0.2414	-	0.900	0.900				Pass	
9	12378-PeCDF	32.311	32.301	500	350	851	0.700	OK(15)	1.1168	-	0.079	0.079				Pass	
10	23478-PeCDF	33.432	33.438	573	446	1019	0.778	OK(15)	1.2270	-	0.078	0.078				Pass	
11	234678-HxCDF	38.572	38.371	192	35	227	*0.185*	Fail(15)	0.9809	-	0.033	0.033	0.013		*QR*	Fail	
12	123478-HxCDF	37.034	37.033	759	489	1247	0.644	OK(15)	1.0379	-	0.155	0.155				Pass	
13	123678-HxCDF	37.160	37.153	429	278	707	0.648	OK(15)	1.0377	-	0.085	0.085				Pass	
14	123789-HxCDF	37.738	37.742	520	302	822	0.582	OK(15)	1.0499	-	0.095	0.095				Pass	
15	1234678-HpCDF	40.151	40.150	3560	2868	6427	0.806	OK(15)	0.9892	-	1.004	1.004				Pass	
16	1234789-HpCDF	41.632	41.642	142	129	271	0.908	OK(15)	0.9873	-	0.052	0.052				Pass	
17	OCDF	44.892	44.891	2531	2367	4899	0.935	OK(15)	11.8713	-	0.113	0.113				Pass	
18	13C-2378-TCDD	26.083	26.083	503611	474661	978272	0.943	OK(15)	1.7377	100.0	80.747	80.747		80.7		Pass	
19	13C-12378-PeCDD	33.943	33.943	376400	299663	676063	0.796	OK(15)	0.9303	100.0	104.233	104.233		104.2		Pass	
20	13C-123478-HxCDD	37.882	37.882	328208	205688	533897	0.627	OK(15)	1.0000	100.0	99.991	99.991		100.0		Pass	
21	13C-123678-HxCDD	37.968	37.973	319392	207252	526644	0.649	OK(15)	0.9999	100.0	98.639	98.639		98.6		Pass	
22	13C-1234678-HpCDD	41.193	41.193	213412	170213	383625	0.798	OK(15)	1.0661	100.0	67.392	67.392		67.4		Pass	
23	13C-OCDD	44.732	44.731	372109	356958	729068	0.959	OK(15)	1.1346	200.0	120.342	120.342		60.2		Pass	
24	13C-2378-TCDF	24.866	24.866	851229	795088	1646317	0.934	OK(15)	2.7649	100.0	85.402	85.402		85.4		Pass	
25	13C-12378-PeCDF	32.288	32.288	533014	428303	961317	0.804	OK(15)	1.6777	100.0	82.186	82.186		82.2		Pass	
26	13C-23478-PeCDF	33.414	33.414	587843	470825	1058669	0.801	OK(15)	1.6449	100.0	92.309	92.309		92.3		Pass	
27	13C-123478-HxCDF	37.033	37.033	473821	300378	774199	0.634	OK(15)	1.6612	100.0	87.283	87.283		87.3		Pass	
28	13C-123678-HxCDF	37.147	37.147	497144	302404	799549	0.608	OK(15)	1.6615	100.0	90.129	90.129		90.1		Pass	
29	13C-234678-HxCDF	38.485	38.485	427458	270012	697470	0.632	OK(15)	1.5807	100.0	82.638	82.638		82.6		Pass	
30	13C-123789-HxCDF	37.731	37.730	509055	316522	825577	0.622	OK(15)	1.5855	100.0	97.524	97.524		97.5		Pass	
31	13C-1234678-HpCDF	40.144	40.144	361683	285501	647184	0.789	OK(15)	1.7422	100.0	69.572	69.572		69.6		Pass	
32	13C-1234789-HpCDF	41.625	41.624	293084	231614	524698	0.790	OK(15)	1.6385	100.0	59.976	59.976		60.0		Pass	
41	13C-1234-TCDD	25.756	25.762	360048	337163	697212	0.936	OK(15)	-	-	-	-			*RT*	Fail	
42	13C-123789-HxCDD	37.882	37.882	328220	205721	533941	0.627	OK(15)	-	-	-	-			*RT*	Fail	
43	Cl37-2378-TCDD	26.107	0	131641	0	131641			2.0155	-	9.368	9.368				Pass	

Level 4 Reporting

While not Covered During this presentation I have attached the reports needed for Level Four reporting using Masshunter Quant software.



Questions?

Thank you!

DE21978995

Agilent

Masshunter Quant Software
Level 4 Reporting

D. R. Walker
Agilent Technologies
Application Scientist
July 8 2024

Example of Level 4 Reporting

Based on ISO/IEC 17025:2017(E)

NELAC Institute (TNI) Standards Volume 1, Sept 2009

DOD Quality Systems Manual version 5.4 2001

Department of Defense (DoD) Department of Energy (DOE) Consolidated Quality Systems Manual (QSM) for Environmental Laboratories

Example of Level 4 Reporting

Required Reports

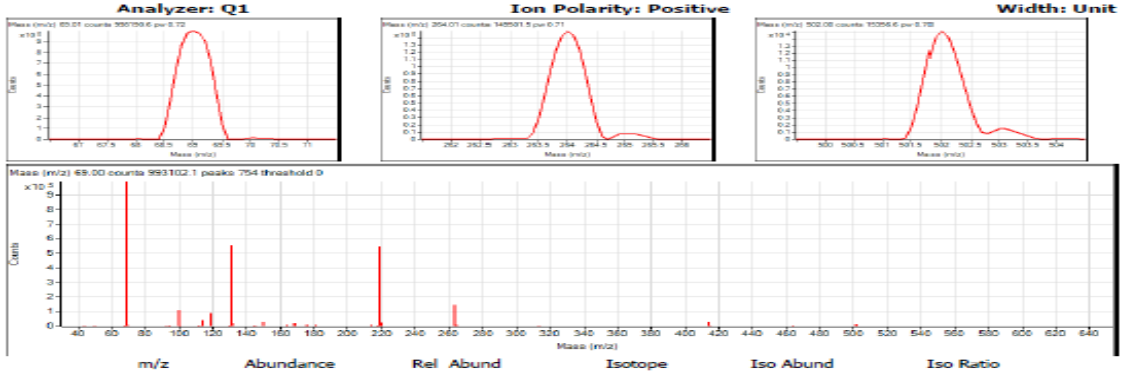
1. Instrument Tunning and Calibration
2. DFTPP or BFB Tuning
3. Sequence Run Log
4. Initial Calibration
5. Second Source Calibration
6. Continuing Calibration
7. Internal Standards Area and Retention Time Surrogate Recovery
8. Laboratory Controls and Laboratory Duplicate Control Sample
9. Matrix Spike and Matrix Spike Duplicate
10. System Blank
11. Method Blank
12. Manual Integrations
13. Raw Data
14. Dilutions

Initial System Tuning

Triple Quadrupole GC/MS Autotune Report

Instrument Name	GC-QQQ / US10015004	**MS Model**	7000
Tune Date & Time	2/1/2021 12:49:01 PM	**Source**	EI with Extractor
Tune File	D:\MassHunter\GCMS\1\7000\atunes.eiex.tune.xml		

Analyzer: Q1 **Ion Polarity: Positive** **Width: Unit**



m/z	Abundance	Rel Abund	Isotope	Iso Abund	Iso Ratio
69.00	993102.1	100.0%	70.10	10665.3	1.1%
219.00	546334.4	55.0%	220.00	23340.7	4.3%
264.00	144838.8	14.6%	265.00	8305.8	5.7%
414.00	26044.4	2.6%	415.00	2392.1	9.2%
502.00	14272.8	1.4%	503.00	1339.3	9.4%

Analyzer: Q2 **Ion Polarity: Positive** **Width: Unit**

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Initial System Tuning

Triple Quadrupole GC/MS Autotune Report

Instrument Name	GC-QQQ / US10015004	**MS Model**	7000
Tune Date & Time	2/1/2021 12:49:01 PM	**Source**	EI with Extractor
Tune File	D:\MassHunter\GCMS\1\7000\atunes.eiex.tune.xml		

Instrument Actuals		**Vacuum**	
Source Temp.	300 °C	Rough Vac	1.51E+2 mTorr
MS1 Quad Temp.	150 °C	High Vac	7.52E-5 Torr
MS2 Quad Temp.	150 °C	Turbo 1 Speed	100.0 %
Filament Current	35.0 µA	Turbo 1 Power	46.0 W
Ion Source			
Type/mode	EI+	Repeller	10.1 V
Source Temp.	300 °C	Ion Body	12.4 V
Emission	35.0 µA	Ion Focus	-75.0 V
Energy	70 eV	Entrance Lens	Dynamic V
Filament	2		

Quadrupoles		**Q1**			**Q2**	
DC		7.2 V			-3.8 V	
Post/Pre Filter		7.2 V			-13.8 V	
Temperature		150 °C			150 °C	
Polarity		Negative			Positive	
DIP Mass	100.00	1000.00 m/z		100.00	1000.00 m/z	
DIP Value	4.8	64.9 %		4.5	63.6 %	
Resolution	**Unit**	**Wide**	**Widest**	**Unit**	**Wide**	**Widest**
Mass Gain	-6.43	-6.46	-6.82	31.01	30.66	30.47
Mass Offset	Dynamic	-1.957	-1.494	Dynamic	-1.922	-1.467
Width Gain	30.0	30.0	30.0	-6.8	-6.8	-6.8
Width Offset	Dynamic	-0.401	-0.921	Dynamic	-0.327	-0.847

Collision Cell		**Detector**	
Cell Entrance	8.2 V	Detector Type	Triple Axis
Hex DC	7.2 V	Iris	-35.0 V
Hex RF	400 V	HED	-10.0 kV
Hex Accel	-5.0 V	EMV (Gain=1.0E+005)	1502 V
Cell Exit	1.2 V	Gain Parameter a	11.88225
Collision Energy	0 eV	Gain Parameter b	-75.39713
		Max Gain Factor	3728

Fast Scan			
Fast Scan Offset	-4.0 V		
Q1 Mass Gain	15.78	Q2 Mass Gain	38.36
Q1 Mass Offset	1.767	Q2 Mass Offset	-1.753
Q1 Width Gain	30.0	Q2 Width Gain	-6.3
Q1 Width Offset	-0.921	Q2 Width Offset	-0.783

Initial System Tuning

Triple Quadrupole GC/MS Autotune Report

Instrument Name	GC-QQQ / US10015004	**MS Model**	7000
Tune Date & Time	2/1/2021 12:49:01 PM	**Source**	EI with Extractor
Tune File	D:\MassHunter\GCMS\1\7000\atunes.eiex.tune.xml		

Dynamic Ramp Tables

MS1 Mass Axis Offset

m/z	69.00	219.00	264.00	414.00	502.00
Setting	-2.098	-2.097	-2.103	-2.088	-2.055

MS1 Width Offset

m/z	69.00	219.00	264.00	414.00	502.00
Setting	-0.203	-0.197	-0.195	-0.195	-0.204

MS2 Mass Axis Offset

m/z	69.00	219.00	264.00	414.00	502.00
Setting	-2.152	-2.066	-2.106	-2.150	-2.122

MS2 Width Offset

m/z	69.00	219.00	264.00	414.00	502.00
Setting	-0.125	-0.123	-0.124	-0.122	-0.125

Entrance Lens

m/z	69.00	219.00	264.00	414.00	502.00
Setting	-8.600	-11.000	-11.000	-11.000	-11.000

Scan Speed Correction Factor

	Q1	Q2
a0	-0.001039	0.004487
a1	1.464329	0.508332
a2	-0.122525	-0.152576
b0	-0.062982	-0.062575
b1	6.888017	1.701859
b2	1.034112	0.848692

Diagnostic Information

Air/Water Check: H20 2.71% (<=20.00%), O2 0.71% (<=2.50%), N2 2.64% (<=10.00%)

Detector Dark Current Check: Baseline 42, Threshold 41, HED On Pulse Count 12, HED Off Pulse Count 16

Initial System Tuning

Triple Quadrupole GC/MS System Verification - Tune

Instrument Name	GC-QQQ / US10015004	**MS Model**	7000
Tune Date & Time	2/1/2021 1:56:49 PM	**Source**	EI with Extractor
Tune File	D:\MassHunter\GCMS\1\7000\atunes.eiex.tune.xml		

Instrument Actuals

Ionization mode	EI+	Rough Vacuum	1.51E+2 mTorr
Source Temperature	230 °C	High Vacuum	7.47E-5 Torr
Quad. 1 Temperature	150 °C	Turbo Speed	100.0 %
Quad. 2 Temperature	150 °C	Turbo Power	45.2 W
Emission Current	35.0 µA		

MS1 Checktune Results	Value	Limit	Result
Low mass assignment (target 69.00, actual 69.00)	0.00	<= 0.20	OK
Mid mass assignment (target 264.00, actual 264.00)	0.00	<= 0.20	OK
High mass assignment (target 502.00, actual 502.00)	0.00	<= 0.20	OK
Low mass isotope position (target 70.00, actual 70.10)	0.10	<= 0.20	OK
Mid mass isotope position (target 265.00, actual 265.00)	0.00	<= 0.20	OK
High mass isotope position (target 503.00, actual 503.00)	0.00	<= 0.20	OK
Low mass isotope ratio	1.07%	>= 0.5% and <= 1.6%	OK
Mid mass isotope ratio	5.71%	>= 4.2% and <= 6.9%	OK
High mass isotope ratio	9.63%	>= 7.9% and <= 12.3%	OK
Ratio of mid mass to low mass	19.44%	>= 5.0%	OK
Ratio of high mass to low mass	3.67%	>= 0.8%	OK
Low mass precursor ratio	0.54%	<= 3.00%	OK
Mid mass precursor ratio	0.08%	<= 6.00%	OK
High mass precursor ratio	0.08%	<= 12.00%	OK

MS2 Checktune Results			
Low mass assignment (target 69.00, actual 69.00)	0.00	<= 0.20	OK
Mid mass assignment (target 264.00, actual 264.00)	0.00	<= 0.20	OK
High mass assignment (target 502.00, actual 502.05)	0.05	<= 0.20	OK
Low mass isotope position (target 70.00, actual 70.00)	0.00	<= 0.20	OK
Mid mass isotope position (target 265.00, actual 265.05)	0.05	<= 0.20	OK
High mass isotope position (target 503.00, actual 503.02)	0.02	<= 0.20	OK
Low mass isotope ratio	1.09%	>= 0.5% and <= 1.6%	OK
Mid mass isotope ratio	5.55%	>= 4.2% and <= 6.9%	OK
High mass isotope ratio	10.94%	>= 7.9% and <= 12.3%	OK
Low mass precursor ratio	0.00%	<= 3.00%	OK
Mid mass precursor ratio	0.04%	<= 6.00%	OK
High mass precursor ratio	0.26%	<= 12.00%	OK

Detector			
EMV	1492	<= 2900	OK
Maximum gain factor	3997	>= 100	OK

Air and Water Check	Abundance	Relative Abundance	Limit	Result
PFTBA (69.00)	708438			
Water	5405	0.76%	<= 20.00%	OK
Oxygen	4503	0.64%	<= 2.50%	OK
Nitrogen	16784	2.37%	<= 10.00%	OK

* Nitrogen values are calculated from oxygen abundance

Analytical Sequence

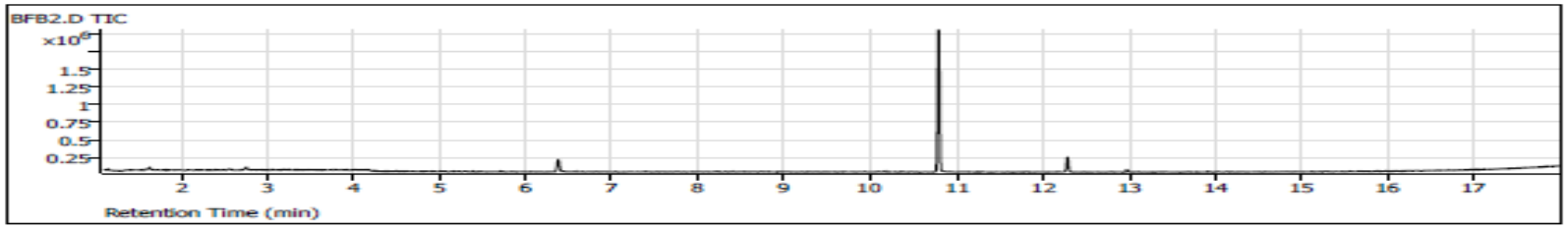
Injection Log - C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\IDC MDL ICAL.batch.bin

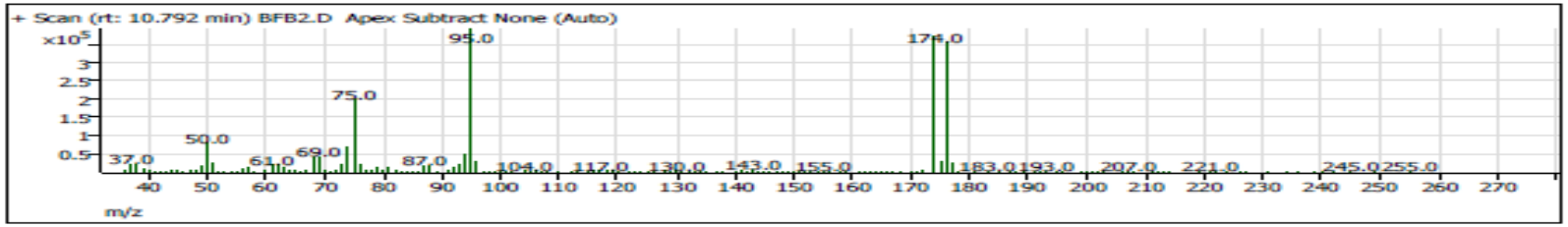
SampleName	MiscInfo	Vial	Mult.	Injection Time
LFB001.D LFB 5.0 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/3/2017 4:55:25 PM
BFB2.D BFB2	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 10:03:02 AM
ICALG0025.D 0.25 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 10:52:03 AM
ICALG005.D 0.50 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 11:23:48 AM
ICALG010.D 1.0 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 11:55:33 AM
ICALG050.D 5.0 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 12:27:17 PM
ICALG100.D 10.0 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 12:59:03 PM
ICALG250.D 25.0 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 1:30:48 PM
ICALG500.D 50.0 ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 2:02:36 PM
VBLK01.D Blank	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 2:33:46 PM
MDL1_10_10_17.D MDL 0.5ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 3:05:28 PM
MDL2_10_10_17.D MDL 0.5ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 3:37:11 PM
MDL3_10_10_17.D MDL 0.5ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 4:08:56 PM
IDC001.D IDC 5.0ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 4:40:42 PM
IDC002.D IDC 5.0ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 5:12:26 PM
IDC003.D IDC 5.0ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 5:44:14 PM
IDC004.D IDC 5.0ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 6:15:58 PM
IDC005.D IDC 5.0ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/10/2017 6:47:41 PM
MDL4_10_11_17.D MDL 0.5ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/11/2017 2:51:31 PM
MDL5_10_11_17.D MDL 0.5ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/11/2017 3:23:16 PM
MDL6_10_12_17.D MDL 0.5ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/12/2017 2:52:21 PM
MDL7_10_12_17.D MDL 0.5ppb	GF=5.0 | 150:1 Split | 25mL	-1	1	10/12/2017 3:24:07 PM

Tuning Criteria

Tune Evaluation Report

Data Path:	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\BFB2.D
Acq on:	10/10/2017 10:03:02 AM
Operator:	Nicolae Popescu
Sample:	BFB2
Inst Name:	Agilent VOC System
ALS Vial:	1
Method:	C:\masshunter\Methods\Quant\BFB.m





Target Mass	Rel. To Mass	Lower Limit%	Upper Limit%	Rel. Abn%	Raw Abn	Pass/Fail
50	95	15	40	19.8	78034	Pass
75	95	30	60	50.4	198468	Pass
95	95	100	100	100.0	393975	Pass
96	95	5	9	6.7	26554	Pass
173	174	0	2	0.0	0	Pass
174	95	50	100	94.6	372737	Pass
175	174	5	9	7.3	27155	Pass
176	174	95	101	95.8	356963	Pass
177	176	5	9	6.2	22300	Pass

Initial Calibration Summary

Initial Calibration Report - Agilent VOC System

Agilent

Method Path
Method File
Batch Name C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\QuantResults\IDC MDL ICAL.batch.bin
Last Calib Update 10/18/2023 6:58:54 AM

Level Name	Calibration Files	Acq. Date-Time	Level Last Update Time
1	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG0025.D	10/10/2017 10:52:03 AM	10/18/2023 6:58:54 AM
2	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG005.D	10/10/2017 11:23:48 AM	10/18/2023 6:58:54 AM
3	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG010.D	10/10/2017 11:55:33 AM	10/18/2023 6:58:54 AM
4	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG050.D	10/10/2017 12:27:17 PM	10/18/2023 6:58:54 AM
5	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG100.D	10/10/2017 12:59:03 PM	10/18/2023 6:58:54 AM
6	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG250.D	10/10/2017 1:30:48 PM	10/18/2023 6:58:54 AM
7	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG500.D	10/10/2017 2:02:36 PM	10/18/2023 6:58:54 AM

Compound	Curve Fit	1	2	3	4	5	6	7	Avg RF	%RSD
I Fluorobenzene				---------- ISTD ----------						
M Dichlorodifluoromethane	Avg RF	0.1565	0.2171	0.2110	0.2032	0.2119	0.2051	0.1996	0.2006	10.127
M Vinyl Chloride	Avg RF	0.2368	0.2844	0.2651	0.2610	0.2581	0.2531	0.2477	0.2580	5.775
M Trichlorofluoromethane	Avg RF	0.3314	0.4323	0.3883	0.3730	0.3804	0.3692	0.3623	0.3767	8.084
M 1,1-Dichloroethene	Avg RF	0.3054	0.3304	0.3243	0.3236	0.3249	0.3209	0.3157	0.3207	2.528
M FREON 113	Avg RF	0.2414	0.2532	0.2430	0.2384	0.2386	0.2356	0.2293	0.2399	3.066
M Methylene Chloride	Avg RF	0.2781	0.3163	0.3055	0.2883	0.2768	0.2772	0.2596	0.2860	6.737
M trans-1,2-Dichloroethene	Avg RF	0.2864	0.3549	0.3310	0.3190	0.3122	0.3170	0.3076	0.3183	6.627
M Methyl tert-butyl ether [MTBE]	Avg RF	0.4461	0.4149	0.4200	0.4101	0.4053	0.4205	0.3955	0.4161	3.819
M 1,1-Dichloroethane	Avg RF	0.4482	0.4811	0.4617	0.4514	0.4200	0.4271	0.4140	0.4434	5.467
M DIPE	Avg RF	0.6101	0.6594	0.6680	0.6860	0.6562	0.6788	0.6490	0.6582	3.772
M ETBE	Avg RF	0.5603	0.5335	0.5101	0.5182	0.5232	0.5510	0.5312	0.5325	3.353
M 2,2-Dichloropropane	Avg RF	0.3813	0.3423	0.3197	0.3267	0.3230	0.3258	0.3283	0.3353	6.414
M cis-1,2-Dichloroethene	Avg RF	0.4162	0.3766	0.3875	0.3725	0.3745	0.3839	0.3639	0.3822	4.419
M Bromochloromethane	Avg RF	0.1453	0.1469	0.1408	0.1318	0.1289	0.1335	0.1290	0.1366	5.581
M Chloroform	Avg RF	0.4311	0.4464	0.4164	0.4205	0.4251	0.4270	0.4113	0.4254	2.677
M 1,1,1-Trichloroethane	Avg RF	0.3563	0.3923	0.3598	0.3668	0.3691	0.3855	0.3822	0.3732	3.665
M Carbon Tetrachloride	Avg RF	0.2879	0.3168	0.3059	0.3047	0.3248	0.3368	0.3395	0.3166	5.881
M 1,1-Dichloro-1-propene	Avg RF	0.2771	0.3261	0.3263	0.3187	0.3157	0.3226	0.3241	0.3158	5.535
M Benzene	Avg RF	0.9061	1.0024	0.9739	0.9580	0.9518	0.9679	0.9422	0.9575	3.103
M 1,2-Dichloroethane	Avg RF	0.2923	0.3205	0.2671	0.2577	0.2514	0.2551	0.2411	0.2693	10.285
M TAME	Avg RF	0.3522	0.4219	0.4176	0.4232	0.4302	0.4581	0.4411	0.4206	7.898
M Trichloroethene	Avg RF	0.2873	0.3221	0.2693	0.2758	0.2694	0.2766	0.2707	0.2816	6.716
M 1,2-Dichloropropane	Avg RF	0.2333	0.2705	0.2266	0.2298	0.2254	0.2300	0.2233	0.2341	7.000
M Dibromomethane	Avg RF	0.0984	0.1388	0.1214	0.1190	0.1199	0.1227	0.1186	0.1198	9.815
M Bromodichloromethane	Avg RF	0.2955	0.2641	0.2457	0.2542	0.2617	0.2777	0.2779	0.2681	6.255
M cis-1,3-Dichloropropene	Avg RF	0.2744	0.3090	0.2618	0.2828	0.2886	0.3122	0.3137	0.2918	6.968
M 4-methyl-2-pentanone [MIBK]	Avg RF	0.1606	0.1915	0.1622	0.1745	0.1804	0.1942	0.1856	0.1784	7.490
M Toluene	Avg RF	1.0328	1.0882	1.0185	1.0572	1.0657	1.1064	1.0724	1.0630	2.858
M trans-1,3-Dichloropropene	Avg RF	0.2018	0.2296	0.1965	0.2193	0.2222	0.2454	0.2465	0.2230	8.715

Page 1 of 2 Generated at 7:13 AM on 10/18/2023

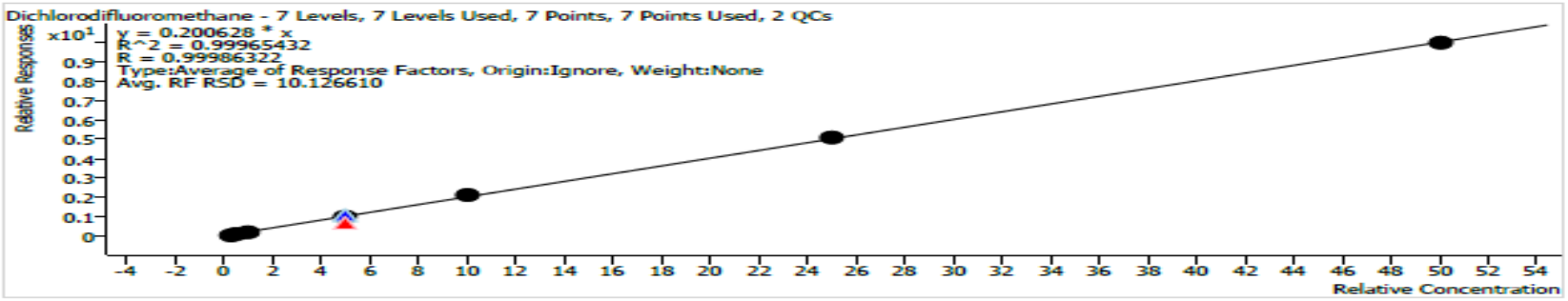
Initial Calibration Detailed

Quantitative Analysis Complete Report

Agilent

Batch Path	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\QuantResults\IDC MDL ICAL.batch.bin		
Analysis Time	10/19/2023 3:25 AM	**Analyst Name**	AGILENT\dalwalke
Report Time	10/19/2023 3:30:29 AM	**Reporter Name**	AGILENT\dalwalke
Last Calib Update	10/19/2023 3:25 AM	**Batch State**	Processed
Analyzed by Quant version	12.0	**Reported by Quant version**	12.0

Dichlorodifluoromethane



Calibration STD Path	Cal Type	Level	Enabled	Resp.	Exp. Conc	Resp. Factor
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG0025.D	Calibration	1	x	6114	0.2500	0.1565
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG005.D	Calibration	2	x	17503	0.5000	0.2171
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG010.D	Calibration	3	x	34185	1.0000	0.2110
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG050.D	Calibration	4	x	173378	5.0000	0.2032
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\IDC003.D	QC	4	x	171582	5.0000	0.2059
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\IDC004.D	QC	4	x	171816	5.0000	0.2087
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\LFB001.D	CC	CC	x	109344	5.0000	0.1301
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG100.D	Calibration	5	x	364977	10.0000	0.2119
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG250.D	Calibration	6	x	854358	25.0000	0.2051
C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG500.D	Calibration	7	x	1727622	50.0000	0.1996

Second Source or Continuing Calibration

Continuing Calibration Report

Agilent

Batch Name	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\QuantResults\IDC MDL ICAL.batch.bin
Method File	
Daily CC	D:\San jose Water\10_10_2017_IDCLFB001.D

Level name	Injection Time	Calibration Files
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2	10/10/2017 11:23:48 AM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG005.D
3	10/10/2017 11:55:33 AM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG010.D
4	10/10/2017 12:27:17 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG050.D
5	10/10/2017 12:59:03 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG100.D
6	10/10/2017 1:30:48 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG250.D
7	10/10/2017 2:02:36 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG500.D
CC	10/3/2017 4:55:25 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\LFB001.D <======

ISTD Compound:	Avg Resp	Mid Resp	CC Resp	Area%	RT	Diff	A/M
Fluorobenzene	166020	170639	168140	98.54	6.380	0.000	M

Target Compound	AvgRF/R2	CC RF	Exp. Conc	Calc. Conc	%Dev	Area%	Curve Fit
Fluorobenzene	ISTD						
Dichlorodifluoromethane	0.2006	0.1301	5.00	3.24	35.17 #	63.07	Avg RF
Vinyl Chloride	0.2580	0.2451	5.00	4.75	4.99	92.54	Avg RF
Trichlorofluoromethane	0.3767	0.3716	5.00	4.93	1.35	98.17	Avg RF
1,1-Dichloroethene	0.3207	0.2896	5.00	4.51	9.71	88.18	Avg RF
FREON 113	0.2399	0.2231	5.00	4.65	7.02	92.18	Avg RF
Methylene Chloride	0.2860	0.2723	5.00	4.76	4.78	93.07	Avg RF
trans-1,2-Dichloroethene	0.3183	0.2992	5.00	4.70	6.00	92.42	Avg RF
Methyl tert-butyl ether [MTBE]	0.4161	0.4165	5.00	5.01	-0.11	100.07	Avg RF
1,1-Dichloroethane	0.4434	0.4377	5.00	4.94	1.28	95.54	Avg RF
DIPE	0.6582	0.6662	5.00	5.06	-1.22	95.70	Avg RF
ETBE	0.5325	0.5407	5.00	5.08	-1.54	102.82	Avg RF
2,2-Dichloropropane	0.3353	0.2542	5.00	3.79	24.18	76.67	Avg RF
cis-1,2-Dichloroethene	0.3822	0.3623	5.00	4.74	5.19	95.84	Avg RF
Bromochloromethane	0.1366	0.1312	5.00	4.80	3.98	98.05	Avg RF
Chloroform	0.4254	0.4513	5.00	5.30	-6.08	105.74	Avg RF
1,1,1-Trichloroethane	0.3732	0.3578	5.00	4.79	4.11	96.13	Avg RF
Carbon Tetrachloride	0.3166	0.2998	5.00	4.73	5.32	96.93	Avg RF
1,1-Dichloro-1-propene	0.3158	0.3003	5.00	4.75	4.92	92.84	Avg RF
Benzene	0.9575	0.9572	5.00	5.00	0.03	98.46	Avg RF
1,2-Dichloroethane	0.2693	0.2716	5.00	5.04	-0.86	103.86	Avg RF
TAME	0.4206	0.4376	5.00	5.20	-4.05	101.90	Avg RF
Trichloroethene	0.2816	0.2844	5.00	5.05	-0.99	101.59	Avg RF
1,2-Dichloropropane	0.2341	0.2444	5.00	5.22	-4.41	104.81	Avg RF
Dibromomethane	0.1198	0.1177	5.00	4.91	1.77	97.46	Avg RF
Bromodichloromethane	0.2681	0.2503	5.00	4.67	6.65	97.02	Avg RF
cis-1,3-Dichloropropene	0.2918	0.2733	5.00	4.68	6.36	95.20	Avg RF
4-methyl-2-pentanone [MIBK]	0.1784	0.1823	5.00	5.11	-2.20	102.97	Avg RF
Toluene	1.0630	1.0960	5.00	5.16	-3.10	102.16	Avg RF
trans-1,3-Dichloropropene	0.2230	0.1973	5.00	4.42	11.52	88.68	Avg RF
1,1,2-Trichloroethane	0.1559	0.1525	5.00	4.89	2.21	99.86	Avg RF
Tetrachloroethene	0.3185	0.3172	5.00	4.98	0.40	100.22	Avg RF

Page 1 of 2 Generated at 7:13 AM on 10/18/2023

Internal Standard and Surrogate Report

ISTD and Surrogate Recovery% Report

Agilent | Trusted Answers

Batch Name	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\QuantResults\IDC MDL ICAL.batch.bin
Data File	D:\San jose Water\10_10_2017_IDC\LFB001.D
Sample Name	LFB 5.0 ppb

Level name		Calibration Files
CC	10/3/2017 4:55:25 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\LFB001.D <=======
1	10/10/2017 10:52:03 AM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG0025.D
2	10/10/2017 11:23:48 AM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG005.D
3	10/10/2017 11:55:33 AM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG010.D
4	10/10/2017 12:27:17 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG050.D
5	10/10/2017 12:59:03 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG100.D
6	10/10/2017 1:30:48 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG250.D
7	10/10/2017 2:02:36 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\ICALG500.D
4	10/10/2017 5:44:14 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\IDC003.D
4	10/10/2017 6:15:58 PM	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\IDC004.D

ISTD Recovery%

Compound Name	Avg Resp	CC Resp	Resp in Sample	Area%_Avg	Area%_CC
Fluorobenzene	166020	168140	168140	101.28%	100.00%

Surrogate Recovery%

Compound Name	Avg Resp	CC Resp	Resp in Sample	Area%_Avg	Area%_CC
Bromofluorobenzene	55922	58688	58688	104.95%	100.00%
1,2-Dichlorobenzene-d4	58093	59293	59293	102.06%	100.00%

LCS and LCSD Report

LCS Spike Report

Batch Name	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\QuantResults\IDC MDL ICAL.batch.bin
Last Calib Update	10/18/2023 6:58:54 AM
Method File	
Data Path	D:\San jose Water\10_10_2017_IDC

Data File	Sample Name	Sample Type	LCS Type	Acq. Date Time
IDC003.D	IDC 5.0ppb	QC	LCSA	10/10/2017 5:44:14 PM
IDC004.D	IDC 5.0ppb	QC	LCSB	10/10/2017 6:15:58 PM

Data File = IDC003.D, Sample Name = IDC 5.0ppb, Type = LCSA

Compound	Spike Amt	Spike Res	Spike Rec	QC LCS Min %Rec	QC LCS Max %Rec
Dichlorodifluoromethane	5.000	5.130	102.60	80	120
Vinyl Chloride	5.000	5.090	101.80	80	120
Trichlorofluoromethane	5.000	5.099	101.98	80	120
1,1-Dichloroethene	5.000	5.199	103.98	80	120
FREON 113	5.000	5.017	100.34	80	120
Methylene Chloride	5.000	5.123	102.47	80	120
trans-1,2-Dichloroethene	5.000	5.052	101.04	80	120
Methyl tert-butyl ether [MTBE]	5.000	5.441	108.82	80	120
1,1-Dichloroethane	5.000	5.167	103.33	80	120
DIPE	5.000	5.300	105.99	80	120
ETBE	5.000	5.210	104.19	80	120
2,2-Dichloropropane	5.000	4.175	83.50	80	120
cis-1,2-Dichloroethene	5.000	4.900	98.00	80	120
Bromochloromethane	5.000	4.974	99.49	80	120
Chloroform	5.000	5.150	103.00	80	120
1,1,1-Trichloroethane	5.000	5.053	101.07	80	120
Carbon Tetrachloride	5.000	4.945	98.91	80	120
1,1-Dichloro-1-propene	5.000	5.033	100.66	80	120
Benzene	5.000	5.119	102.37	80	120
1,2-Dichloroethane	5.000	5.099	101.99	80	120
TAME	5.000	5.236	104.72	80	120
Trichloroethene	5.000	4.942	98.83	80	120
1,2-Dichloropropane	5.000	5.013	100.26	80	120
Dibromomethane	5.000	5.056	101.13	80	120
Bromodichloromethane	5.000	4.921	98.42	80	120
cis-1,3-Dichloropropene	5.000	4.832	96.64	80	120
4-methyl-2-pentanone [MIBK]	5.000	5.518	110.36	80	120
Toluene	5.000	5.053	101.05	80	120
trans-1,3-Dichloropropene	5.000	4.811	96.23	80	120
1,1,2-Trichloroethane	5.000	5.055	101.11	80	120
Tetrachloroethene	5.000	4.937	98.74	80	120
1,3-Dichloropropane	5.000	5.090	101.80	80	120
Dibromochloromethane	5.000	4.750	95.00	80	120
Chlorobenzene	5.000	5.030	100.59	80	120
1,1,1,2-Tetrachloroethane	5.000	5.213	104.26	80	120
Ethylbenzene	5.000	5.183	103.66	80	120
m+p-Xylene	10.000	10.724	107.24	80	120
o-Xylene	5.000	5.141	102.81	80	120
Styrene	5.000	5.321	106.41	80	120
Bromoform	5.000	4.672	93.44	80	120
Isopropylbenzene	5.000	5.231	104.62	80	120
Bromofluorobenzene	5.000	5.233	104.66	80	120
Bromobenzene	5.000	5.242	104.85	80	120
1,1,2,2-Tetrachloroethane	5.000	5.445	108.90	80	120

Page 1 of 3 Generated at 7:13 AM on 10/18/2023

Matrix Spike and Spike Duplicate

Matrix Spike/Duplicate Recovery and RPD Summary Report

Agilent

Batch Name	C:\Users\dalwalke\OneDrive - Agilent Technologies\San jose Water\10_10_2017_IDC\QuantResults\IDC MDL ICAL.batch.bin
Last Calib Update	10/18/2023 6:58:54 AM
Method File	
Data Path	D:\San jose Water\10_10_2017_IDC

Sample Name	Sample Type	Matrix Spike Group	Acq. Date Time
IDC 5.0ppb	Matrix		10/10/2017 4:40:42 PM
IDC 5.0ppb	Matrix Dup		10/10/2017 5:12:28 PM

Compound	Sample Conc	Spike Amt	Spike Res	Dup Res	Spike Rec	Dup Rec	RPD	QC RPD	Limits %Rec
Dichlorodifluoromethane	0.000	5.000	5.142	5.018	102.84	100.36	2.44	20	80 - 120
Vinyl Chloride	0.000	5.000	5.015	4.957	100.29	99.13	1.16	20	80 - 120
Trichlorofluoromethane	0.000	5.000	4.959	5.033	99.19	100.66	1.47	20	80 - 120
1,1-Dichloroethene	0.000	5.000	5.251	5.086	105.03	101.72	3.20	20	80 - 120
FREON 113	0.000	5.000	4.972	5.002	99.43	100.03	0.60	20	80 - 120
Methylene Chloride	0.000	5.000	5.229	5.238	104.58	104.76	0.17	20	80 - 120
trans-1,2-Dichloroethene	0.000	5.000	5.238	5.202	104.75	104.03	0.69	20	80 - 120
Methyl tert-butyl ether [MTBE]	0.000	5.000	5.286	5.374	105.73	107.48	1.64	20	80 - 120
1,1-Dichloroethane	0.000	5.000	5.208	5.032	104.17	100.64	3.44	20	80 - 120
DIPE	0.000	5.000	5.256	5.320	105.11	106.41	1.23	20	80 - 120
ETBE	0.000	5.000	5.104	5.328	102.07	106.56	4.30	20	80 - 120
2,2-Dichloropropane	0.000	5.000	4.207	4.190	84.13	83.79	0.40	20	80 - 120
cis-1,2-Dichloroethene	0.000	5.000	5.034	5.016	100.68	100.31	0.36	20	80 - 120
Bromochloromethane	0.000	5.000	4.991	4.988	99.82	99.76	0.06	20	80 - 120
Chloroform	0.000	5.000	5.177	5.220	103.55	104.41	0.83	20	80 - 120
1,1,1-Trichloroethane	0.000	5.000	5.127	4.866	102.55	97.32	5.23	20	80 - 120
Carbon Tetrachloride	0.000	5.000	4.994	4.894	99.87	97.87	2.02	20	80 - 120
1,1-Dichloro-1-propene	0.000	5.000	5.117	4.990	102.34	99.80	2.51	20	80 - 120
Benzene	0.000	5.000	5.230	5.106	104.60	102.12	2.40	20	80 - 120
1,2-Dichloroethane	0.000	5.000	5.019	5.034	100.39	100.68	0.29	20	80 - 120
TAME	0.000	5.000	5.275	5.391	105.49	107.82	2.18	20	80 - 120
Trichloroethene	0.000	5.000	4.960	4.848	99.21	96.95	2.30	20	80 - 120
1,2-Dichloropropane	0.000	5.000	5.120	5.099	102.39	101.98	0.41	20	80 - 120
Dibromomethane	0.000	5.000	5.227	5.211	104.54	104.22	0.30	20	80 - 120
Bromodichloromethane	0.000	5.000	4.900	4.916	97.99	98.32	0.33	20	80 - 120
cis-1,3-Dichloropropene	0.000	5.000	4.778	4.769	95.56	95.37	0.19	20	80 - 120
4-methyl-2-pentanone [MIBK]	0.000	5.000	5.256	5.488	105.12	109.77	4.32	20	80 - 120
Toluene	0.000	5.000	5.102	5.113	102.04	102.27	0.22	20	80 - 120
trans-1,3-Dichloropropene	0.000	5.000	4.812	4.758	96.24	95.15	1.14	20	80 - 120
1,1,2-Trichloroethane	0.000	5.000	5.058	5.052	101.15	101.04	0.11	20	80 - 120
Tetrachloroethene	0.000	5.000	5.024	5.028	100.47	100.56	0.09	20	80 - 120
1,3-Dichloropropane	0.000	5.000	4.946	5.275	98.92	105.50	6.43	20	80 - 120
Dibromochloromethane	0.000	5.000	4.681	4.807	93.62	96.13	2.65	20	80 - 120
Chlorobenzene	0.000	5.000	5.109	5.069	102.18	101.38	0.79	20	80 - 120
1,1,1,2-Tetrachloroethane	0.000	5.000	5.146	5.098	102.93	101.96	0.95	20	80 - 120
Ethylbenzene	0.000	5.000	5.199	5.226	103.98	104.53	0.53	20	80 - 120
m+p-Xylene	0.000	5.000	10.903	10.890	218.05 #	217.80 #	0.12	20	80 - 120
o-Xylene	0.000	5.000	5.183	5.309	103.65	106.17	2.40	20	80 - 120
Styrene	0.000	5.000	5.291	5.287	105.81	105.74	0.07	20	80 - 120
Bromoform	0.000	5.000	4.894	4.801	97.88	96.02	1.92	20	80 - 120
Isopropylbenzene	0.000	5.000	5.317	5.313	106.33	106.26	0.07	20	80 - 120
Bromobenzene	0.000	5.000	5.273	5.357	105.46	107.14	1.58	20	80 - 120
1,1,2,2-Tetrachloroethane	0.000	5.000	5.236	5.445	104.72	108.90	3.91	20	80 - 120

Page 1 of 2 Generated at 7:13 AM on 10/18/2023

Method Blank

Quantitation Results Report

Agilent

Data File	:	VBLK01.D
Operator	:	Nicolae Popescu
Acq. Method	:	524_2_Nick_100517_MDL
Acq. Date-Time	:	10/10/2017 2:33:46 PM
Sample Name	:	Blank
Vial	:	8
Multiplier	:	1
Sample Info	:	
DA Method File	:	
Tune File	:	BFB_Atune.u
Tune Date	:	9/28/2017 1:43:05 PM
Batch Name	:	IDC MDL ICAL.batch.bin
Last Calib Update	:	10/18/2023 6:58:54 AM

Compound	RT	QIon	Resp.	Conc.	Units		Dev(Min)
Internal Standards							
Fluorobenzene	6.380	96.0	162396	1.0000	ppb		0.000
System Monitoring Compounds							
Bromofluorobenzene	10.792	95.0	54530	4.9840	ppb		-0.003
Spiked Amount: 5.000	Range: 70.0 - 130.0%			Recovery = 99.68%			
1,2-Dichlorobenzene-d4	12.289	152.0	58486	5.1497	ppb		-0.003
Spiked Amount: 5.000	Range: 70.0 - 130.0%			Recovery = 102.99%			
Target Compounds							QValue
Dichlorodifluoromethane	1.182	85.0	1364	N.D.	ppb	#	63
Vinyl Chloride	1.388	62.0	768	N.D.	ppb		86
Trichlorofluoromethane	1.988	101.0	959	N.D.	ppb	#	28
1,1-Dichloroethene	2.479	61.0	800	N.D.	ppb	#	1
FREON 113	2.490	101.0	909	N.D.	ppb	#	33
Methylene Chloride	3.003	49.0	2814	N.D.	ppb	#	47
trans-1,2-Dichloroethene	3.519	61.0	1150	N.D.	ppb		95
Methyl tert-butyl ether [MTBE]	3.410	73.0	914	N.D.	ppb	#	1
1,1-Dichloroethane	3.971	63.0	2642	N.D.	ppb	#	79
DIPE	3.965	45.0	2740	N.D.	ppb	#	44
ETBE	4.852	59.0	1818	N.D.	ppb	#	65
2,2-Dichloropropane	4.793	77.0	1442	N.D.	ppb	#	15
cis-1,2-Dichloroethene	4.855	61.0	1515	N.D.	ppb	#	29
Bromochloromethane	5.181	130.0	1015	N.D.	ppb		53
Chloroform	5.331	83.0	1352	N.D.	ppb	#	25
1,1,1-Trichloroethane	5.750	97.0	1300	N.D.	ppb	#	24
Carbon Tetrachloride	0.000		0	N.D.			
1,1-Dichloro-1-propene	5.752	75.0	1305	N.D.	ppb	#	1
Benzene	0.000		0	N.D.			
1,2-Dichloroethane	6.076	62.0	2033	N.D.	ppb	#	40
TAME	6.377	73.0	1851	N.D.	ppb	#	40
Trichloroethene	6.804	130.0	1180	N.D.	ppb	#	68
1,2-Dichloropropane	7.088	63.0	735	N.D.	ppb	#	58
Dibromomethane	7.200	174.0	856	N.D.	ppb	#	41
Bromodichloromethane	7.409	83.0	850	N.D.	ppb	#	1
cis-1,3-Dichloropropene	7.872	75.0	1770	N.D.	ppb	#	79
4-methyl-2-pentanone [MIBK]	8.081	43.0	1000	N.D.	ppb	#	59
Toluene	8.220	91.0	3229	N.D.	ppb	#	29
trans-1,3-Dichloropropene	8.466	75.0	746	N.D.	ppb		64
1,1,2-Trichloroethane	8.661	97.0	771	N.D.	ppb	#	46
Tetrachloroethene	0.000		0	N.D.			
1,3-Dichloropropane	8.828	76.0	1084	N.D.	ppb		90

VBLK01.D Page 1 of 3 Generated at 1:23 PM on 10/18/2023

Sample Summary Report

Quantitation Results Report (Not Reviewed)

Agilent

Data File	LFB001.D	Operator	Nicolae Popescu
Acq. Method	524_2_Nick_100317	Acq. Date-Time	10/3/2017 4:55:25 PM
Sample Name	LFB 5.0 ppb	Instrument	Agilent VOC System
Vial	12	Multiplier	1.00
DA Method File		Comment	GF=5.0 | 150:1 Split | 25mL
Tune File	BFB_Atune.u	Tune Date	9/28/2017 1:43:05 PM
Batch Name	IDC MDL ICAL.batch.bin	Last Calib Update	10/18/2023 6:58:54 AM
Ref Library			

Compound	RT	QIon	Resp.	Conc.	Units		Dev(Min)
Internal Standards							
1) Fluorobenzene	6.380	96.0	168140	1.0000	ppb		0.000
System Monitoring Compounds							
43) Bromofluorobenzene	10.794	95.0	58688	5.1807	ppb		-0.001
Spiked Amount: 5.000	Range: 70.0 - 130.0%			Recovery = 103.61%			
57) 1,2-Dichlorobenzene-d4	12.292	152.0	59293	5.0424	ppb		0.000
Spiked Amount: 5.000	Range: 70.0 - 130.0%			Recovery = 100.85%			
Target Compounds							QValue
2) Dichlorodifluoromethane	1.184	85.0	109344	3.2414	ppb		94
3) Vinyl Chloride	1.413	62.0	206085	4.7504	ppb		96
4) Trichlorofluoromethane	1.993	101.0	312429	4.9327	ppb		96
5) 1,1-Dichloroethene	2.478	61.0	243479	4.5147	ppb		88
6) FREON 113	2.495	101.0	187538	4.6488	ppb		89
7) Methylene Chloride	3.017	49.0	228930	4.7608	ppb		95
8) trans-1,2-Dichloroethene	3.354	61.0	251518	4.7000	ppb		89
9) Methyl tert-butyl ether [MTBE]	3.407	73.0	350146	5.0053	ppb		93
10) 1,1-Dichloroethane	3.948	63.0	367970	4.9360	ppb		99
11) DIPE	4.151	45.0	560102	5.0609	ppb		98
15) ETBE	4.723	59.0	454577	5.0769	ppb		99
12) 2,2-Dichloropropane	4.840	77.0	213729	3.7910	ppb		93
13) cis-1,2-Dichloroethene	4.851	61.0	304607	4.7406	ppb		90
14) Bromochloromethane	5.189	130.0	110259	4.8010	ppb	#	65
17) Chloroform	5.334	83.0	379378	5.3039	ppb		99
18) 1,1,1-Trichloroethane	5.540	97.0	300830	4.7947	ppb		94
19) Carbon Tetrachloride	5.752	117.0	252015	4.7338	ppb		97
20) 1,1-Dichloro-1-propene	5.763	75.0	252434	4.7540	ppb		92
21) Benzene	6.017	78.0	804735	4.9987	ppb	#	84
22) 1,2-Dichloroethane	6.059	62.0	228363	5.0431	ppb	#	74
16) TAME	6.237	73.0	367920	5.2023	ppb		99
23) Trichloroethene	6.809	130.0	239075	5.0493	ppb		93
24) 1,2-Dichloropropane	7.060	63.0	205496	5.2203	ppb	#	70
25) Dibromomethane	7.186	174.0	98967	4.9115	ppb		93
26) Bromodichloromethane	7.384	83.0	210425	4.6677	ppb		98
27) cis-1,3-Dichloropropene	7.877	75.0	229730	4.6822	ppb		88
28) 4-methyl-2-pentanone [MIBK]	8.084	43.0	153294	5.1098	ppb		81
29) Toluene	8.217	91.0	921409	5.1551	ppb	#	30
30) trans-1,3-Dichloropropene	8.471	75.0	165911	4.4240	ppb		87
31) 1,1,2-Trichloroethane	8.652	97.0	128170	4.8895	ppb		89
32) Tetrachloroethene	8.781	166.0	266668	4.9801	ppb		98
33) 1,3-Dichloropropane	8.817	76.0	223492	4.9945	ppb		92
34) Dibromochloromethane	9.040	129.0	125180	4.5809	ppb		97
35) Chlorobenzene	9.648	112.0	613856	5.1900	ppb	#	85
36) 1,1,1,2-Tetrachloroethane	9.740	131.0	183982	4.9171	ppb		98
37) Ethylbenzene	9.773	91.0	1026520	5.2456	ppb		92
38) m+p-Xylene	9.891	91.0	1640422	10.7134	ppb		72

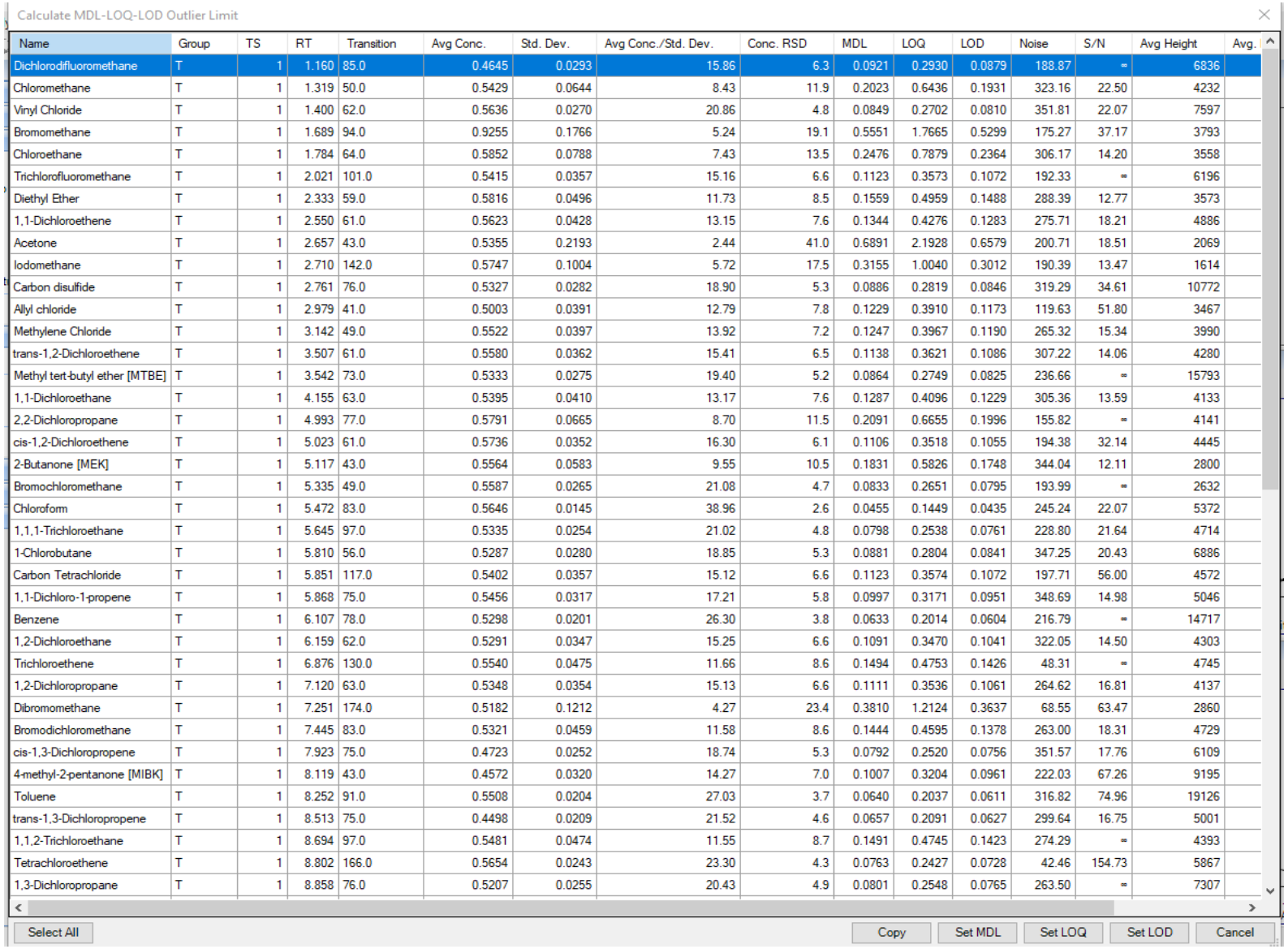
LFB001.D Page 1 of 419 Generated at 7:14 AM on 10/18/2023

MDL Report

	Name	Group	TS	RT	Quant Ion	Rf	Avg Conc.	Std. Dev.	Avg Conc./Std. Dev.	Conc. RSD	MDL	LOQ	LOD	Noise	S/N	Avg Heigh	Avg. Resp	Resp. RSD
2	Dichlorodifluoromethane		1	1.185	85	0.5302, 0.4545, 0.5320, 0.4615, 0.4794, 0.3821, 0.3735	0.459	0.0633	7.25	13.8	0.199	0.6332	0.19	178.05	∞	15097	15160	13.3
3	Vinyl Chloride		1	1.414	62	0.4623, 0.4739, 0.4960, 0.5350, 0.5822, 0.4835, 0.4594	0.4989	0.0447	11.15	9	0.1406	0.4474	0.1342	233.24	394.69	19282	20911	8.3
4	Trichlorofluoromethane		1	1.991	101	0.5292, 0.4609, 0.4963, 0.5152, 0.5499, 0.4739, 0.4835	0.5013	0.0318	15.78	6.3	0.0999	0.3178	0.0953	223.89	206.04	19737	30810	5.7
5	1,1-Dichloroethene		1	2.479	61	0.4878, 0.4945, 0.5511, 0.4805, 0.5066, 0.5009, 0.4886	0.5014	0.0236	21.28	4.7	0.0741	0.2357	0.0707	182.84	∞	15476	26168	3.4
6	FREON 113		1	2.496	101	0.4849, 0.4825, 0.5060, 0.4587, 0.4979, 0.5043, 0.5028	0.491	0.017	28.85	3.5	0.0535	0.1702	0.0511	141.06	111.66	9281	19127	2.4
7	Methylene Chloride		1	3.017	49	0.5118, 0.4970, 0.5889, 0.5348, 0.4910, 0.5908, 0.4917	0.5294	0.044	12.04	8.3	0.1382	0.4397	0.1319	340.32	∞	11900	24807	8
8	trans-1,2-Dichloroethene		1	3.354	61	0.5296, 0.5147, 0.5263, 0.4911, 0.4946, 0.5001, 0.4919	0.5069	0.0164	30.83	3.2	0.0517	0.1644	0.0493	272.23	139.57	12638	26391	3.7
9	Methyl tert-butyl ether [MTBE]		1	3.407	73	0.4995, 0.5070, 0.5879, 0.4911, 0.5088, 0.4978, 0.4664	0.5084	0.0378	13.45	7.4	0.1188	0.3781	0.1134	205.78	69.81	13067	34789	6.4
10	1,1-Dichloroethane		1	3.946	63	0.4942, 0.5172, 0.5550, 0.4472, 0.5500, 0.5729, 0.5062	0.5204	0.043	12.1	8.3	0.1351	0.43	0.129	491.78	57.24	13842	37535	7
11	DIPE		1	4.155	45	0.5111, 0.5104, 0.5232, 0.4828, 0.5287, 0.5189, 0.5339	0.5156	0.0168	30.66	3.3	0.0528	0.1681	0.0504	287.45	88.44	18336	55576	2.4
12	2,2-Dichloropropane		1	4.838	77	0.4215, 0.3895, 0.4348, 0.3862, 0.4452, 0.4234, 0.3900	0.413	0.0241	17.12	5.8	0.0758	0.2413	0.0724	177.9	76.14	8615	23055	3.9
13	cis-1,2-Dichloroethene		1	4.852	61	0.5254, 0.4575, 0.5260, 0.4650, 0.5092, 0.5166, 0.5005	0.5	0.028	17.84	5.6	0.0881	0.2803	0.0841	277.99	124.61	12306	30977	4.1
14	Bromochloromethane		1	5.189	130	0.4762, 0.4769, 0.5734, 0.5097, 0.5207, 0.5203, 0.4550	0.5046	0.0394	12.81	7.8	0.1238	0.3939	0.1182	164.39	43.62	4950	11175	6.6
15	ETBE		1	4.726	59	0.5274, 0.5119, 0.5274, 0.4820, 0.5001, 0.4615, 0.4606	0.4958	0.0285	17.38	5.8	0.0897	0.2853	0.0856	267.01	131.71	15311	42537	5.7
16	TAME		1	6.241	73	0.4829, 0.5124, 0.5321, 0.4569, 0.4747, 0.4544, 0.4503	0.4805	0.0313	15.37	6.5	0.0982	0.3126	0.0938	289.51	129.34	14673	32786	6.4
17	Chloroform		1	5.334	83	0.4677, 0.5078, 0.5357, 0.4621, 0.5274, 0.5482, 0.4806	0.5042	0.0345	14.61	6.8	0.1084	0.345	0.1035	223.14	∞	15274	34933	5.8
18	1,1,1-Trichloroethane		1	5.541	97	0.4936, 0.4633, 0.5227, 0.4763, 0.5261, 0.4819, 0.4688	0.4904	0.0252	19.49	5.1	0.0791	0.2516	0.0755	129.74	∞	12598	29742	3.2
19	Carbon Tetrachloride		1	5.753	117	0.4814, 0.4556, 0.4552, 0.4480, 0.4796, 0.4546, 0.4095	0.4549	0.0239	19.05	5.3	0.075	0.2388	0.0716	131.26	127.09	10249	23348	5.1
20	1,1-Dichloro-1-propene		1	5.764	75	0.4890, 0.4761, 0.4825, 0.5052, 0.5029, 0.5391, 0.4734	0.4955	0.0228	21.69	4.6	0.0718	0.2284	0.0685	263.82	56.01	11744	25372	4.9
21	Benzene		1	6.018	78	0.4996, 0.5010, 0.5587, 0.4866, 0.5202, 0.4928, 0.4757	0.5049	0.0274	18.43	5.4	0.0861	0.2739	0.0822	251.78	307.67	37079	78404	4.1
22	1,2-Dichloroethane		1	6.059	62	0.4875, 0.5409, 0.5496, 0.4813, 0.5220, 0.4691, 0.4653	0.5022	0.0348	14.45	6.9	0.1092	0.3476	0.1043	252.69	58.21	10489	21977	6.6
23	Trichloroethene		1	6.812	130	0.4728, 0.4427, 0.5390, 0.4799, 0.4842, 0.4825, 0.5001	0.4859	0.0292	16.65	6	0.0917	0.2919	0.0876	220.84	126.96	11547	22208	4.7
24	1,2-Dichloropropane		1	7.061	63	0.5316, 0.4899, 0.6058, 0.5183, 0.5304, 0.5175, 0.5308	0.532	0.0356	14.92	6.7	0.112	0.3565	0.1069	224.56	∞	9974	20201	5.3
25	Dibromomethane		1	7.192	174	0.4760, 0.4777, 0.5310, 0.5010, 0.5227, 0.4744, 0.4784	0.4945	0.024	20.6	4.9	0.0754	0.2401	0.072	435.63	12.97	5462	9610	3.7
26	Bromodichloromethane		1	7.387	83	0.4991, 0.4481, 0.4850, 0.4569, 0.4566, 0.4012, 0.4207	0.4525	0.034	13.32	7.5	0.1067	0.3397	0.1019	169.09	102.6	10888	19677	7.4

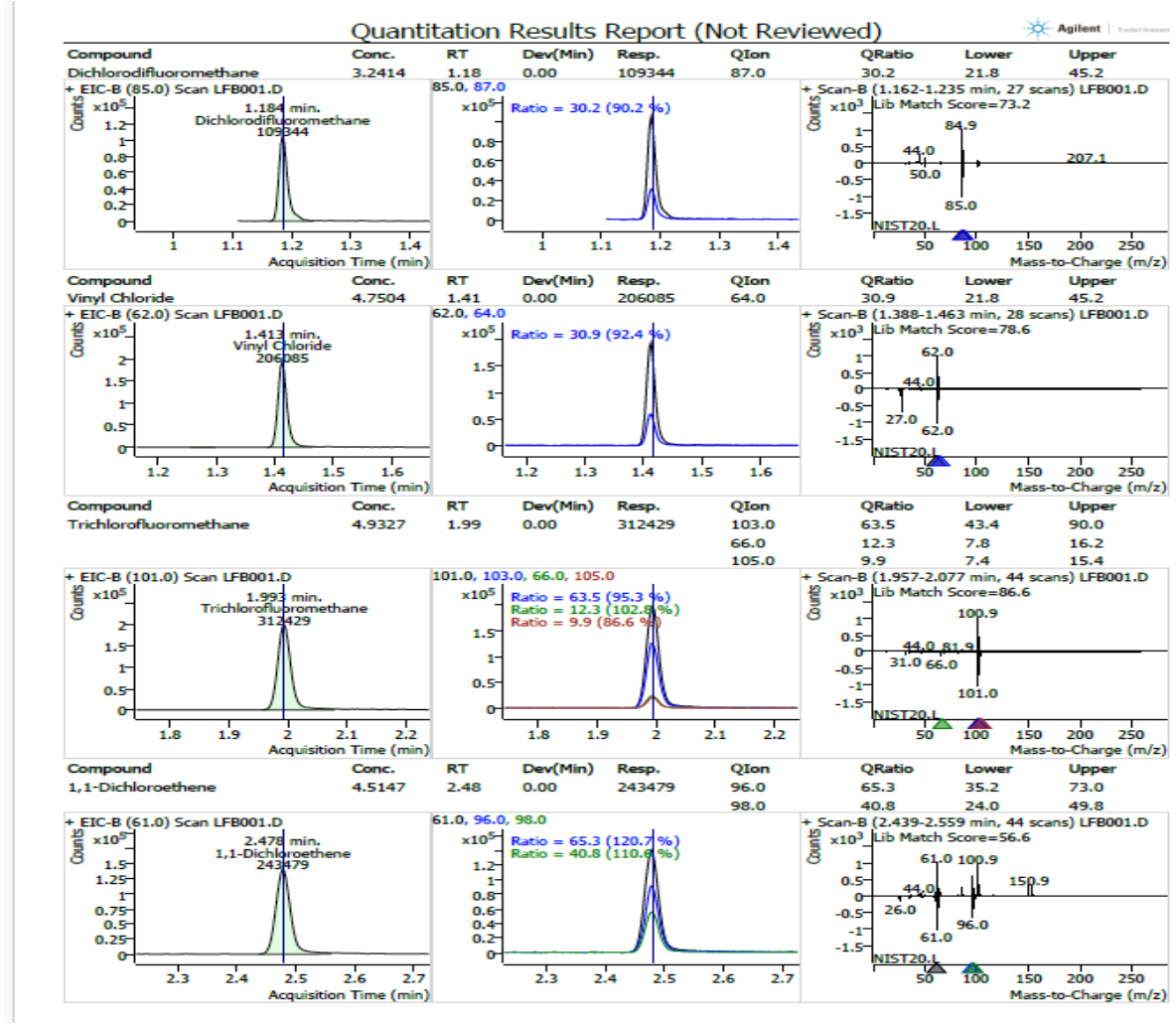
On the upper tool bar go to:
Tools
Actions
Replicate injections MDL LOD LOQ

At the bottom of the table
Select All
Set MDL
Set LOD
Set LOQ



Name	Group	TS	RT	Transition	Avg Conc.	Std. Dev.	Avg Conc./Std. Dev.	Conc. RSD	MDL	LOQ	LOD	Noise	S/N	Avg Height	Avg.
Dichlorodifluoromethane	T	1	1.160	85.0	0.4645	0.0293	15.86	6.3	0.0921	0.2930	0.0879	188.87	∞	6836	
Chloromethane	T	1	1.319	50.0	0.5429	0.0644	8.43	11.9	0.2023	0.6436	0.1931	323.16	22.50	4232	
Vinyl Chloride	T	1	1.400	62.0	0.5636	0.0270	20.86	4.8	0.0849	0.2702	0.0810	351.81	22.07	7597	
Bromomethane	T	1	1.689	94.0	0.9255	0.1766	5.24	19.1	0.5551	1.7665	0.5299	175.27	37.17	3793	
Chloroethane	T	1	1.784	64.0	0.5852	0.0788	7.43	13.5	0.2476	0.7879	0.2364	306.17	14.20	3558	
Trichlorofluoromethane	T	1	2.021	101.0	0.5415	0.0357	15.16	6.6	0.1123	0.3573	0.1072	192.33	∞	6196	
Diethyl Ether	T	1	2.333	59.0	0.5816	0.0496	11.73	8.5	0.1559	0.4959	0.1488	288.39	12.77	3573	
1,1-Dichloroethene	T	1	2.550	61.0	0.5623	0.0428	13.15	7.6	0.1344	0.4276	0.1283	275.71	18.21	4886	
Acetone	T	1	2.657	43.0	0.5355	0.2193	2.44	41.0	0.6891	2.1928	0.6579	200.71	18.51	2069	
Iodomethane	T	1	2.710	142.0	0.5747	0.1004	5.72	17.5	0.3155	1.0040	0.3012	190.39	13.47	1614	
Carbon disulfide	T	1	2.761	76.0	0.5327	0.0282	18.90	5.3	0.0886	0.2819	0.0846	319.29	34.61	10772	
Allyl chloride	T	1	2.979	41.0	0.5003	0.0391	12.79	7.8	0.1229	0.3910	0.1173	119.63	51.80	3467	
Methylene Chloride	T	1	3.142	49.0	0.5522	0.0397	13.92	7.2	0.1247	0.3967	0.1190	265.32	15.34	3990	
trans-1,2-Dichloroethene	T	1	3.507	61.0	0.5580	0.0362	15.41	6.5	0.1138	0.3621	0.1086	307.22	14.06	4280	
Methyl tert-butyl ether [MTBE]	T	1	3.542	73.0	0.5333	0.0275	19.40	5.2	0.0864	0.2749	0.0825	236.66	∞	15793	
1,1-Dichloroethane	T	1	4.155	63.0	0.5395	0.0410	13.17	7.6	0.1287	0.4096	0.1229	305.36	13.59	4133	
2,2-Dichloropropane	T	1	4.993	77.0	0.5791	0.0665	8.70	11.5	0.2091	0.6655	0.1996	155.82	∞	4141	
cis-1,2-Dichloroethene	T	1	5.023	61.0	0.5736	0.0352	16.30	6.1	0.1106	0.3518	0.1055	194.38	32.14	4445	
2-Butanone [MEK]	T	1	5.117	43.0	0.5564	0.0583	9.55	10.5	0.1831	0.5826	0.1748	344.04	12.11	2800	
Bromochloromethane	T	1	5.335	49.0	0.5587	0.0265	21.08	4.7	0.0833	0.2651	0.0795	193.99	∞	2632	
Chloroform	T	1	5.472	83.0	0.5646	0.0145	38.96	2.6	0.0455	0.1449	0.0435	245.24	22.07	5372	
1,1,1-Trichloroethane	T	1	5.645	97.0	0.5335	0.0254	21.02	4.8	0.0798	0.2538	0.0761	228.80	21.64	4714	
1-Chlorobutane	T	1	5.810	56.0	0.5287	0.0280	18.85	5.3	0.0881	0.2804	0.0841	347.25	20.43	6886	
Carbon Tetrachloride	T	1	5.851	117.0	0.5402	0.0357	15.12	6.6	0.1123	0.3574	0.1072	197.71	56.00	4572	
1,1-Dichloro-1-propene	T	1	5.868	75.0	0.5456	0.0317	17.21	5.8	0.0997	0.3171	0.0951	348.69	14.98	5046	
Benzene	T	1	6.107	78.0	0.5298	0.0201	26.30	3.8	0.0633	0.2014	0.0604	216.79	∞	14717	
1,2-Dichloroethane	T	1	6.159	62.0	0.5291	0.0347	15.25	6.6	0.1091	0.3470	0.1041	322.05	14.50	4303	
Trichloroethene	T	1	6.876	130.0	0.5540	0.0475	11.66	8.6	0.1494	0.4753	0.1426	48.31	∞	4745	
1,2-Dichloropropane	T	1	7.120	63.0	0.5348	0.0354	15.13	6.6	0.1111	0.3536	0.1061	264.62	16.81	4137	
Dibromomethane	T	1	7.251	174.0	0.5182	0.1212	4.27	23.4	0.3810	1.2124	0.3637	68.55	63.47	2860	
Bromodichloromethane	T	1	7.445	83.0	0.5321	0.0459	11.58	8.6	0.1444	0.4595	0.1378	263.00	18.31	4729	
cis-1,3-Dichloropropene	T	1	7.923	75.0	0.4723	0.0252	18.74	5.3	0.0792	0.2520	0.0756	351.57	17.76	6109	
4-methyl-2-pentanone [MIBK]	T	1	8.119	43.0	0.4572	0.0320	14.27	7.0	0.1007	0.3204	0.0961	222.03	67.26	9195	
Toluene	T	1	8.252	91.0	0.5508	0.0204	27.03	3.7	0.0640	0.2037	0.0611	316.82	74.96	19126	
trans-1,3-Dichloropropene	T	1	8.513	75.0	0.4498	0.0209	21.52	4.6	0.0657	0.2091	0.0627	299.64	16.75	5001	
1,1,2-Trichloroethane	T	1	8.694	97.0	0.5481	0.0474	11.55	8.7	0.1491	0.4745	0.1423	274.29	∞	4393	
Tetrachloroethene	T	1	8.802	166.0	0.5654	0.0243	23.30	4.3	0.0763	0.2427	0.0728	42.46	154.73	5867	
1,3-Dichloropropane	T	1	8.858	76.0	0.5207	0.0255	20.43	4.9	0.0801	0.2548	0.0765	263.50	∞	7307	

Raw Data

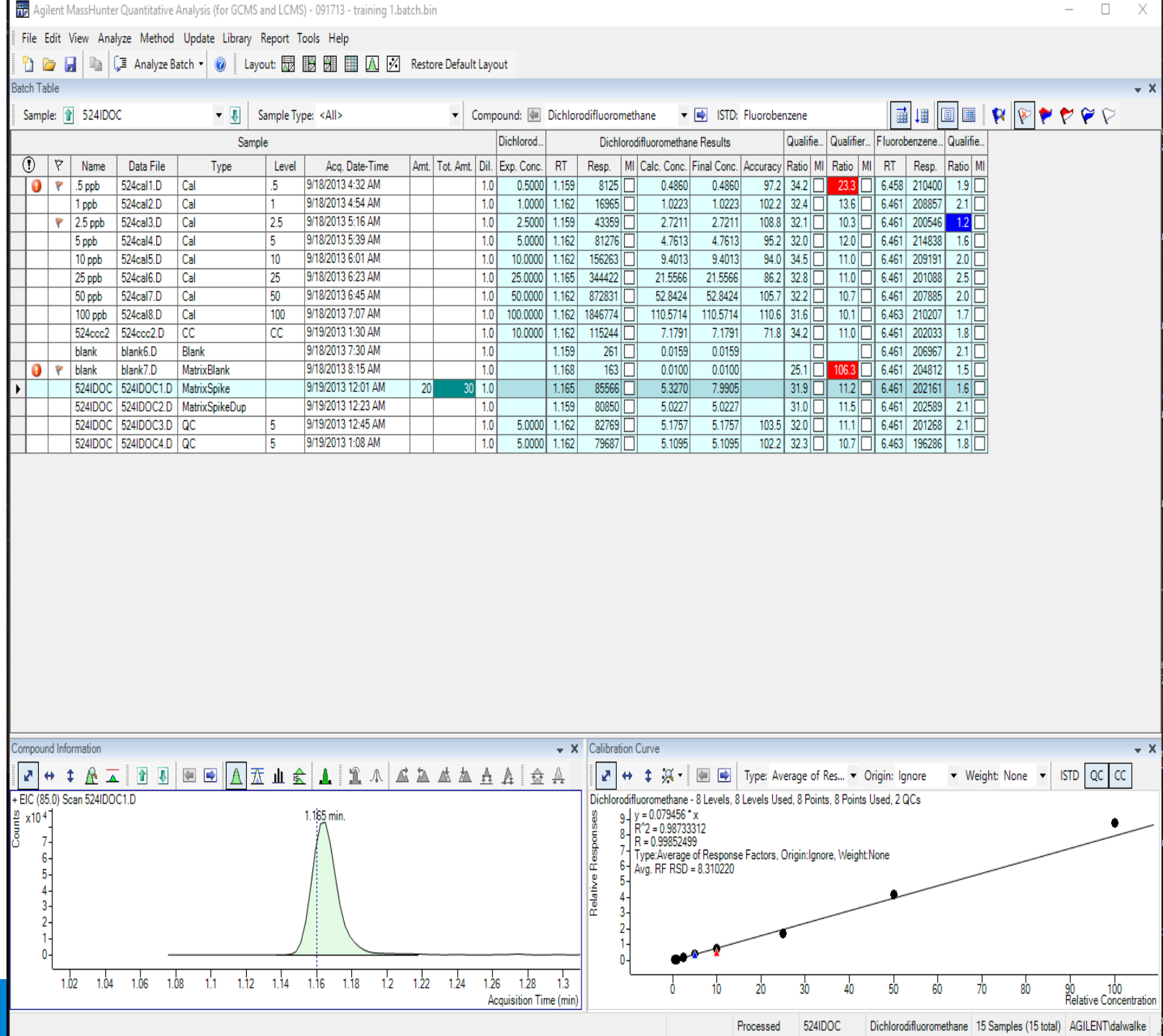

Quantitation Results Report (Not Reviewed)
Agilent
Compound Conc. RT Dev(Min) Resp. QIon QRatio Lower Upper
Dichlorodifluoromethane 3.2414 1.18 0.00 109344 87.0 30.2 21.8 45.2
+ EIC-B (85.0) Scan LFB001.D
1.184 min.
Dichlorodifluoromethane
109344
85.0, 87.0
Ratio = 30.2 (90.2 %)
+ Scan-B (1.162-1.235 min, 27 scans) LFB001.D
Lib Match Score=73.2
84.9
44.0
50.0
207.1
85.0
NIST20.L
Acquisition Time (min)
Mass-to-Charge (m/z)
Compound Conc. RT Dev(Min) Resp. QIon QRatio Lower Upper
Vinyl Chloride 4.7504 1.41 0.00 206085 64.0 30.9 21.8 45.2
+ EIC-B (62.0) Scan LFB001.D
1.413 min.
Vinyl Chloride
206085
62.0, 64.0
Ratio = 30.9 (92.4 %)
+ Scan-B (1.388-1.463 min, 28 scans) LFB001.D
Lib Match Score=78.6
62.0
44.0
27.0
62.0
NIST20.L
Acquisition Time (min)
Mass-to-Charge (m/z)
Compound Conc. RT Dev(Min) Resp. QIon QRatio Lower Upper
Trichlorofluoromethane 4.9327 1.99 0.00 312429 103.0 63.5 43.4 90.0
66.0 12.3 7.8 16.2
105.0 9.9 7.4 15.4
+ EIC-B (101.0) Scan LFB001.D
1.993 min.
Trichlorofluoromethane
312429
101.0, 103.0, 66.0, 105.0
Ratio = 63.5 (95.3 %)
Ratio = 12.3 (102.8 %)
Ratio = 9.9 (86.6 %)
+ Scan-B (1.957-2.077 min, 44 scans) LFB001.D
Lib Match Score=86.6
100.9
44.0
81.9
31.0
66.0
101.0
NIST20.L
Acquisition Time (min)
Mass-to-Charge (m/z)
Compound Conc. RT Dev(Min) Resp. QIon QRatio Lower Upper
1,1-Dichloroethene 4.5147 2.48 0.00 243479 96.0 65.3 35.2 73.0
98.0 40.8 24.0 49.8
+ EIC-B (61.0) Scan LFB001.D
2.478 min.
1,1-Dichloroethene
243479
61.0, 96.0, 98.0
Ratio = 65.3 (120.7 %)
Ratio = 40.8 (110.6 %)
+ Scan-B (2.439-2.559 min, 44 scans) LFB001.D
Lib Match Score=56.6
61.0
100.9
150.9
44.0
26.0
96.0
61.0
NIST20.L
Acquisition Time (min)
Mass-to-Charge (m/z)

Chang the Total Amount to that the method call out to be extracted.

In Amount set the Amount the chemist extracted

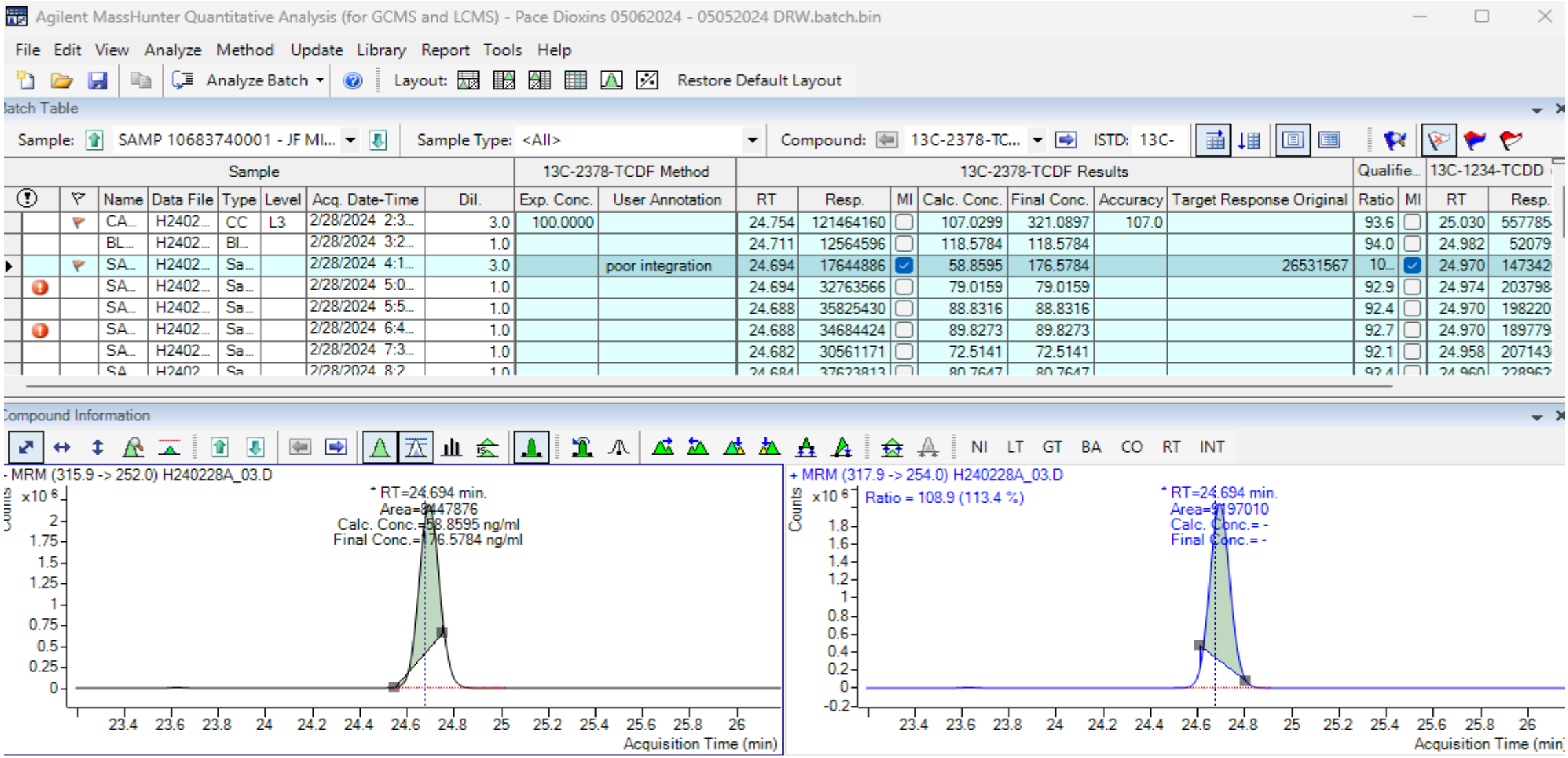
The final concentration now shows the corrected amount based on the two weights

Explanation:
We utilize other applications to perform calculations only to enter them into MassHunter. Time is lost during data processing, and validation steps due to this. The dilution factor column for soil batches is a prime example;
When calculating dilution factor, we use the formula:
DF = Final weight / Initial weight
All the client samples have different initial weights, so we enter them into Microsoft Excel to calculate the dilution factor. We then copy it from Excel and paste it into MassHunter. However, we already enter initial weight into a User Defined column for reporting purposes (



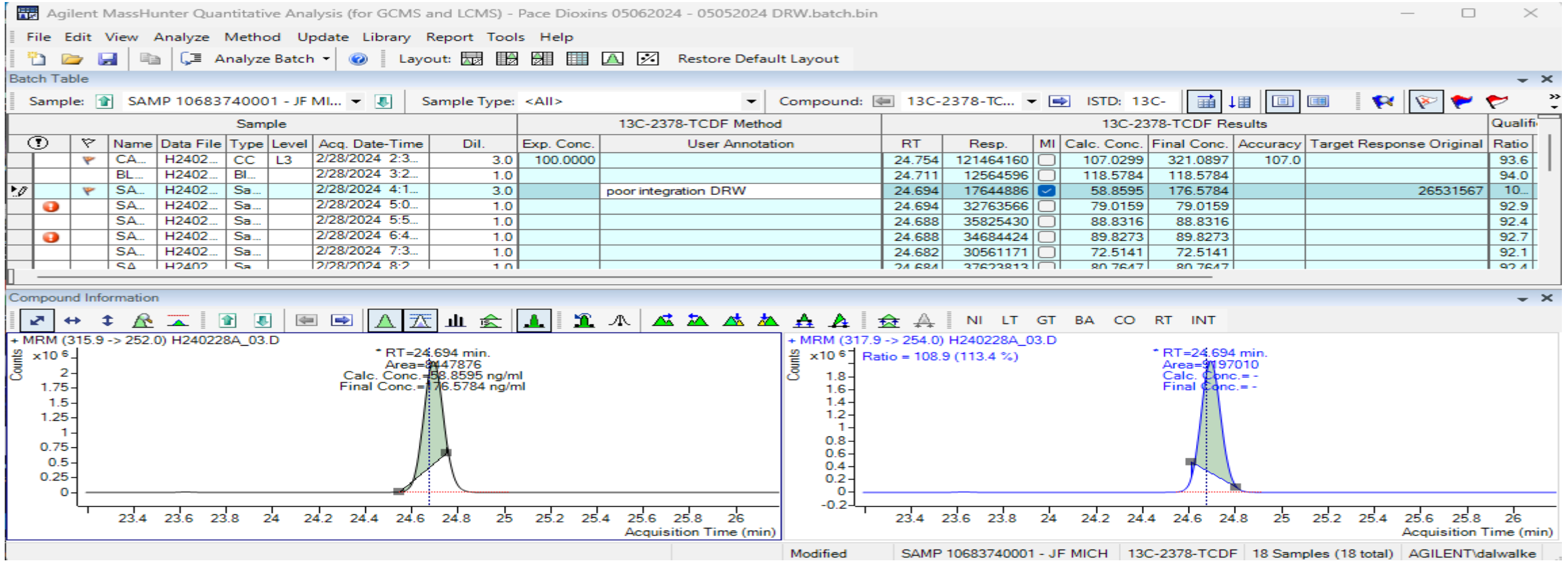
Sample									Dichlorod...	Dichlorodifluoromethane Results						Qualifie...	Qualifier...		Fluorobenzene...		Qualifie...	
		Name	Data File	Type	Level	Acq. Date-Time	Amt.	Tot. Amt.	Dil.	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	Ratio	MI	RT	Resp.	Ratio	MI
		.5 ppb	524cal1.D	Cal	.5	9/18/2013 4:32 AM			1.0	0.5000	1.159	8125		0.4860	0.4860	97.2	34.2		23.3		6.458	210400	1.9	
		1 ppb	524cal2.D	Cal	1	9/18/2013 4:54 AM			1.0	1.0000	1.162	16965		1.0223	1.0223	102.2	32.4		13.6		6.461	208857	2.1	
		2.5 ppb	524cal3.D	Cal	2.5	9/18/2013 5:16 AM			1.0	2.5000	1.159	43359		2.7211	2.7211	108.8	32.1		10.3		6.461	200546	1.2	
		5 ppb	524cal4.D	Cal	5	9/18/2013 5:39 AM			1.0	5.0000	1.162	81276		4.7613	4.7613	95.2	32.0		12.0		6.461	214838	1.6	
		10 ppb	524cal5.D	Cal	10	9/18/2013 6:01 AM			1.0	10.0000	1.162	156263		9.4013	9.4013	94.0	34.5		11.0		6.461	209191	2.0	
		25 ppb	524cal6.D	Cal	25	9/18/2013 6:23 AM			1.0	25.0000	1.165	344422		21.5566	21.5566	86.2	32.8		11.0		6.461	201088	2.5	
		50 ppb	524cal7.D	Cal	50	9/18/2013 6:45 AM			1.0	50.0000	1.162	872831		52.8424	52.8424	105.7	32.2		10.7		6.461	207885	2.0	
		100 ppb	524cal8.D	Cal	100	9/18/2013 7:07 AM			1.0	100.0000	1.162	1846774		110.5714	110.5714	110.6	31.6		10.1		6.463	210207	1.7	
		524ccc2	524ccc2.D	CC	CC	9/19/2013 1:30 AM			1.0	10.0000	1.162	115244		7.1791	7.1791	71.8	34.2		11.0		6.461	202033	1.8	
		blank	blank6.D	Blank		9/18/2013 7:30 AM			1.0		1.159	261		0.0159	0.0159						6.461	206967	2.1	
		blank	blank7.D	MatrixBlank		9/18/2013 8:15 AM			1.0		1.168	163		0.0100	0.0100		25.1		106.3		6.461	204812	1.5	
▸		524IDOC	524IDOC1.D	MatrixSpike		9/19/2013 12:01 AM	20	30	1.0		1.165	85566		5.3270	7.9905		31.9		11.2		6.461	202161	1.6	
		524IDOC	524IDOC2.D	MatrixSpikeDup		9/19/2013 12:23 AM			1.0		1.159	80850		5.0227	5.0227		31.0		11.5		6.461	202589	2.1	
		524IDOC	524IDOC3.D	QC	5	9/19/2013 12:45 AM			1.0	5.0000	1.162	82769		5.1757	5.1757	103.5	32.0		11.1		6.461	201268	2.1	
		524IDOC	524IDOC4.D	QC	5	9/19/2013 1:08 AM			1.0	5.0000	1.162	79687		5.1095	5.1095	102.2	32.3		10.7		6.463	196286	1.8	

Diluted amount and recalculated amount



Manual Integration Before and After

The Red line Below the Green integrated peaks show where the data system set the integration. The annotation gives a reason for the annotation and the reviewers initials .



Agilent CrossLab

From Insight to Outcome

DE21978995