

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037078.D
 Acq On : 27 Aug 2024 12:20
 Operator : SY/MD
 Sample : P3691-20
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K63

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M

Title : VOC Analysis

Signal : TIC: VV037078.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.172	34	41	47	rBV	150847	208205	0.92%	0.369%
2	1.282	68	75	102	rVB	15287490	16904075	74.41%	29.933%
3	1.532	147	153	175	rVB	259256	327218	1.44%	0.579%
4	2.057	308	316	330	rVB	557810	802528	3.53%	1.421%
5	3.433	741	744	747	rBV5	1338	1283	0.01%	0.002%
6	3.471	754	756	759	rBV4	1153	601	0.00%	0.001%
7	3.626	801	804	805	rBV3	924	465	0.00%	0.001%
8	3.635	805	807	810	rVV4	1198	694	0.00%	0.001%
9	3.658	812	814	816	rVV3	957	443	0.00%	0.001%
10	3.690	822	824	829	rBV4	1120	944	0.00%	0.002%
11	3.806	842	860	899	rBV	9756335	22717173	100.00%	40.226%
12	4.243	984	996	1025	rVB	369191	921386	4.06%	1.632%
13	4.616	1109	1112	1115	rBV4	1319	1025	0.00%	0.002%
14	4.825	1175	1177	1180	rBV3	1176	710	0.00%	0.001%
15	4.889	1194	1197	1200	rBV3	936	545	0.00%	0.001%
16	4.950	1200	1216	1252	rBV2	936527	2347915	10.34%	4.158%
17	5.529	1385	1396	1430	rBV	694949	1431236	6.30%	2.534%
18	5.986	1521	1538	1564	rBV	520975	1084275	4.77%	1.920%
19	6.243	1615	1618	1620	rBV4	1401	776	0.00%	0.001%
20	6.407	1666	1669	1673	rBV7	1239	1224	0.01%	0.002%
21	6.426	1673	1675	1677	rBV3	1055	628	0.00%	0.001%
22	6.474	1687	1690	1692	rBV3	1621	916	0.00%	0.002%
23	6.539	1708	1710	1712	rBV3	1098	657	0.00%	0.001%
24	6.574	1718	1721	1723	rBV3	825	466	0.00%	0.001%
25	6.597	1725	1728	1731	rVB5	1709	1173	0.01%	0.002%
26	6.619	1731	1735	1737	rBV5	2095	1746	0.01%	0.003%
27	6.670	1749	1751	1754	rVB4	1412	703	0.00%	0.001%
28	6.767	1776	1781	1784	rBV5	1356	1417	0.01%	0.003%
29	6.857	1805	1809	1812	rVB6	1462	1207	0.01%	0.002%
30	6.873	1812	1814	1815	rBV2	978	472	0.00%	0.001%
31	6.908	1815	1825	1853	rBV	258293	506760	2.23%	0.897%
32	7.240	1917	1928	1961	rBV	1047082	1855421	8.17%	3.285%
33	7.551	2016	2025	2053	rBV	173821	319543	1.41%	0.566%
34	8.024	2163	2172	2211	rBV	378846	790437	3.48%	1.400%
35	8.468	2307	2310	2311	rBV3	1543	891	0.00%	0.002%
36	8.535	2328	2331	2334	rBV4	1387	842	0.00%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037078.D
 Acq On : 27 Aug 2024 12:20
 Operator : SY/MD
 Sample : P3691-20
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K63

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
 Title : VOC Analysis

37	8.651	2365	2367	2371	rBV5	1667	943	0.00%	0.002%
38	8.780	2395	2407	2431	rBV	1058980	1772436	7.80%	3.139%
39	9.214	2540	2542	2545	rBV3	1414	892	0.00%	0.002%
40	9.355	2584	2586	2588	rBV3	945	504	0.00%	0.001%
41	9.420	2601	2606	2607	rBV4	1381	1218	0.01%	0.002%
42	9.452	2614	2616	2621	rVB6	1002	496	0.00%	0.001%
43	9.477	2621	2624	2625	rBV3	1401	642	0.00%	0.001%
44	9.612	2663	2666	2668	rVB3	1082	618	0.00%	0.001%
45	9.690	2688	2690	2695	rVB6	1184	868	0.00%	0.002%
46	9.767	2711	2714	2716	rBV3	674	411	0.00%	0.001%
47	9.838	2733	2736	2737	rBV3	1261	654	0.00%	0.001%
48	9.924	2762	2763	2769	rVB5	1294	1022	0.00%	0.002%
49	9.950	2769	2771	2773	rBV3	990	532	0.00%	0.001%
50	9.963	2773	2775	2777	rVB3	1495	671	0.00%	0.001%
51	9.979	2777	2780	2781	rBV3	1001	655	0.00%	0.001%
52	9.989	2781	2783	2786	rBV3	844	438	0.00%	0.001%
53	10.050	2801	2802	2806	rVB3	1622	647	0.00%	0.001%
54	10.072	2806	2809	2810	rBV2	1213	602	0.00%	0.001%
55	10.149	2821	2833	2850	rBV	638564	1029893	4.53%	1.824%
56	10.317	2882	2885	2887	rBV4	1286	824	0.00%	0.001%
57	10.329	2887	2889	2892	rVV3	1407	761	0.00%	0.001%
58	10.487	2934	2938	2939	rBV3	1579	932	0.00%	0.002%
59	10.593	2969	2971	2974	rVB4	962	551	0.00%	0.001%
60	10.629	2980	2982	2989	rVB7	1532	1516	0.01%	0.003%
61	10.667	2989	2994	2995	rBV4	1299	1094	0.00%	0.002%
62	10.915	3068	3071	3074	rVV4	1355	851	0.00%	0.002%
63	10.950	3078	3082	3083	rBV4	960	610	0.00%	0.001%
64	11.182	3141	3154	3182	rBV	1093407	1727370	7.60%	3.059%
65	11.555	3259	3270	3294	rBV	1034675	1660224	7.31%	2.940%
66	11.818	3350	3352	3354	rBV3	904	462	0.00%	0.001%
67	12.114	3440	3444	3446	rBV5	1132	834	0.00%	0.001%
68	12.207	3471	3473	3475	rBV3	1374	595	0.00%	0.001%
69	12.220	3475	3477	3479	rBV3	1023	506	0.00%	0.001%
70	12.291	3496	3499	3501	rBV3	1354	822	0.00%	0.001%
71	12.352	3514	3518	3520	rBV3	1391	1257	0.01%	0.002%
72	12.439	3541	3545	3547	rBV5	988	746	0.00%	0.001%
73	12.461	3550	3552	3554	rBV3	998	429	0.00%	0.001%
74	12.477	3554	3557	3558	rBV2	851	417	0.00%	0.001%
75	12.535	3572	3575	3576	rBV2	651	392	0.00%	0.001%
76	12.574	3585	3587	3589	rBV3	698	428	0.00%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037078.D
 Acq On : 27 Aug 2024 12:20
 Operator : SY/MD
 Sample : P3691-20
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K63

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
 Title : VOC Analysis

77	12.673	3615	3618	3620	rBV3	1167	741	0.00%	0.001%
78	12.722	3628	3633	3635	rBV4	1396	1241	0.01%	0.002%
79	12.776	3648	3650	3651	rBV2	1162	515	0.00%	0.001%
80	12.808	3657	3660	3662	rVB4	1058	533	0.00%	0.001%
81	12.825	3663	3665	3668	rBV4	950	647	0.00%	0.001%
82	12.947	3698	3703	3707	rBV7	1316	1517	0.01%	0.003%
83	13.088	3743	3747	3749	rBV4	1230	1062	0.00%	0.002%
84	13.117	3754	3756	3762	rVV7	1716	1320	0.01%	0.002%
85	13.198	3778	3781	3784	rBV4	1776	1222	0.01%	0.002%
86	13.255	3796	3799	3800	rBV4	1293	849	0.00%	0.002%
87	13.326	3818	3821	3823	rBV4	1074	638	0.00%	0.001%
88	13.419	3845	3850	3853	rBV6	1197	1329	0.01%	0.002%
89	13.561	3892	3894	3896	rBV3	973	472	0.00%	0.001%
90	13.635	3915	3917	3919	rBV3	1078	512	0.00%	0.001%
91	13.808	3968	3971	3974	rVB5	1467	932	0.00%	0.002%
92	13.825	3974	3976	3979	rBV4	863	587	0.00%	0.001%
93	13.908	3999	4002	4007	rBV7	1564	1364	0.01%	0.002%
94	13.937	4007	4011	4012	rBV3	926	689	0.00%	0.001%
95	14.027	4038	4039	4043	rBV3	732	420	0.00%	0.001%
96	14.127	4066	4070	4073	rBV5	1025	857	0.00%	0.002%
97	14.355	4138	4141	4145	rBV5	1727	1573	0.01%	0.003%
98	14.696	4245	4247	4251	rVB4	2004	1100	0.00%	0.002%
99	14.760	4265	4267	4270	rBV4	1875	1198	0.01%	0.002%
100	14.828	4286	4288	4289	rBV2	1045	426	0.00%	0.001%

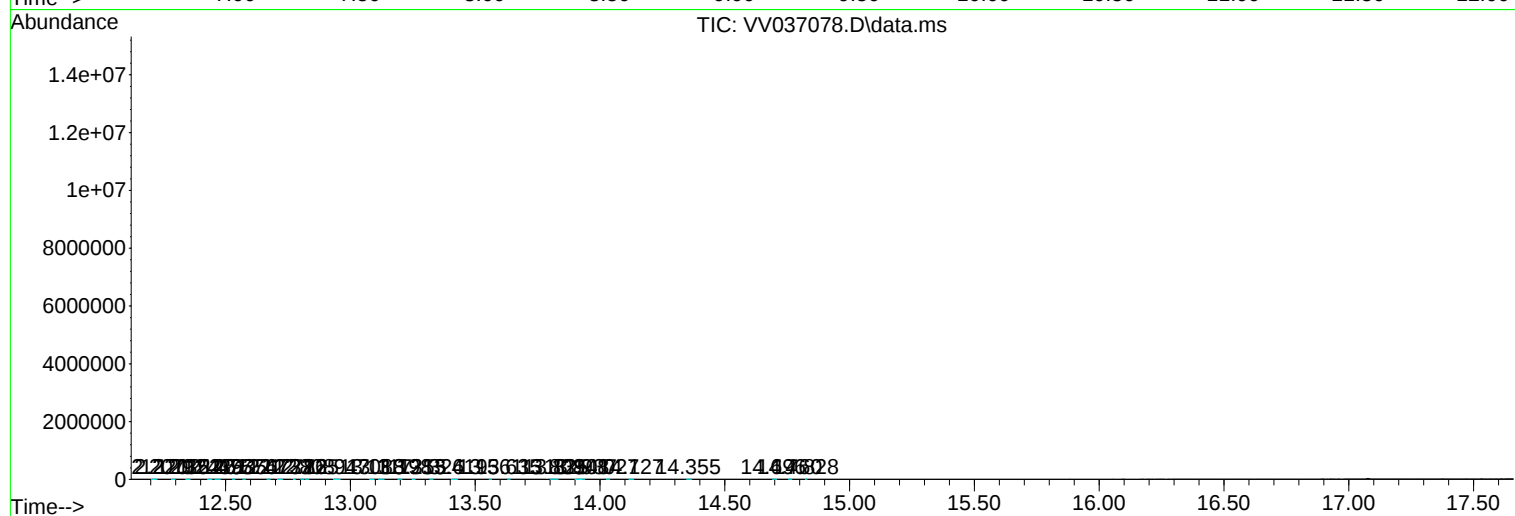
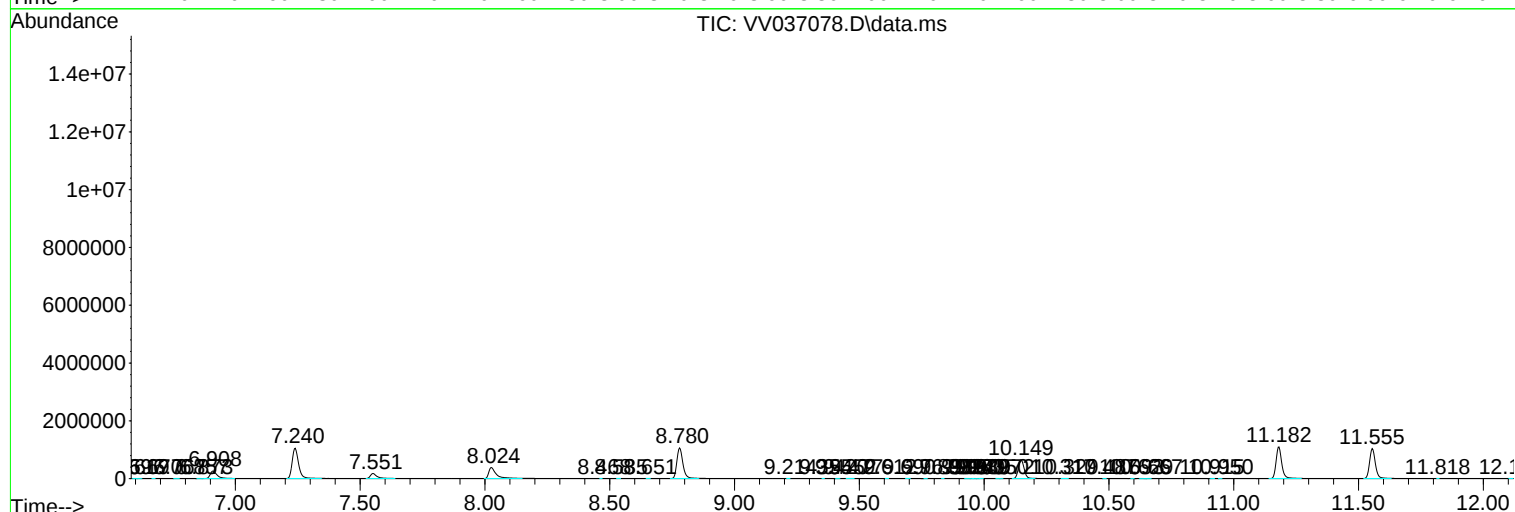
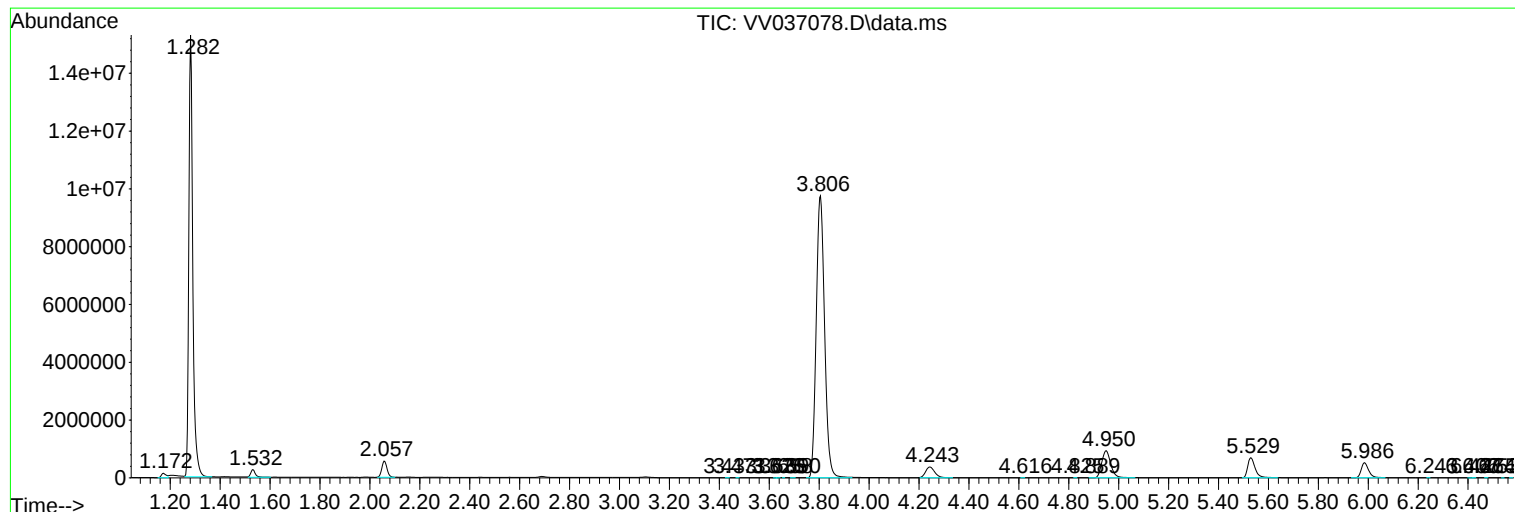
Sum of corrected areas: 56473507

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037078.D
Acq On : 27 Aug 2024 12:20
Operator : SY/MD
Sample : P3691-20
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K63

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037078.D
Acq On : 27 Aug 2024 12:20
Operator : SY/MD
Sample : P3691-20
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K63

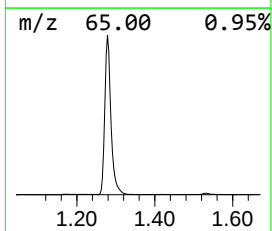
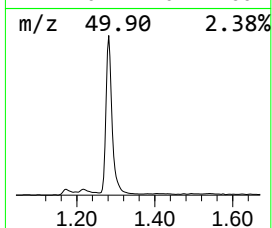
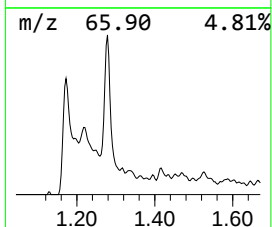
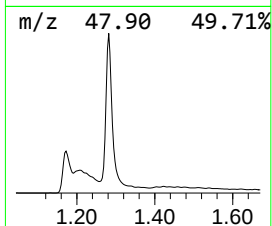
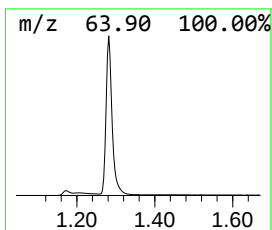
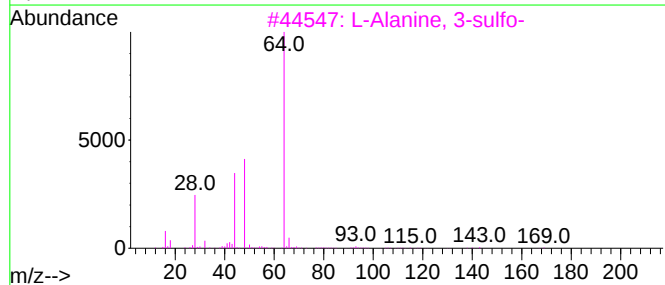
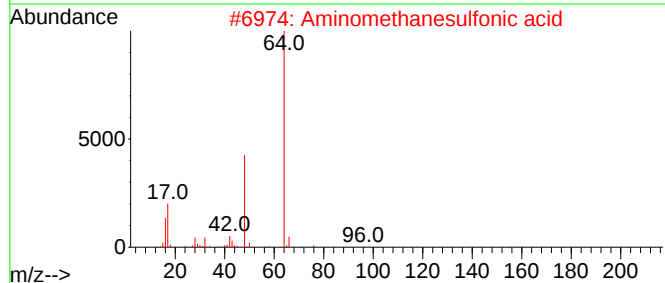
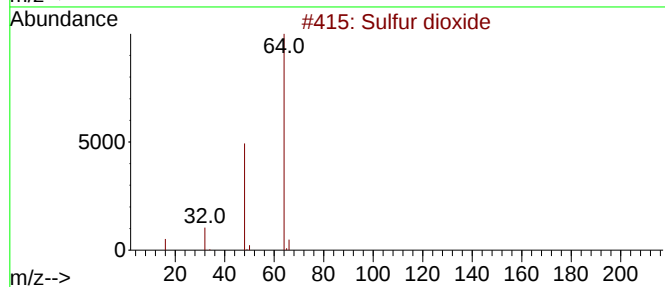
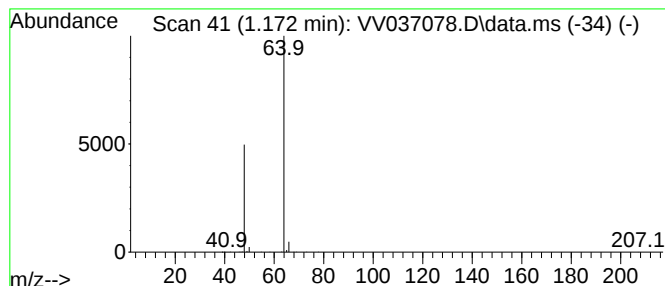
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.172	7.27 ug/L	208205	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037078.D
Acq On : 27 Aug 2024 12:20
Operator : SY/MD
Sample : P3691-20
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K63

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.172	7.3	ug/L	208205	1	5.529	1431240	50.0