

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037076.D
 Acq On : 27 Aug 2024 11:36
 Operator : SY/MD
 Sample : P3691-19
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K72

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: VV037076.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.175	35	42	53	rBV	47384	93475	4.55%	0.620%
2	1.278	69	74	90	rVB	234965	248576	12.11%	1.649%
3	1.532	146	153	168	rVB	214437	255289	12.43%	1.694%
4	2.056	308	316	329	rVB	417240	592813	28.87%	3.934%
5	3.352	717	719	722	rBV4	1703	977	0.05%	0.006%
6	3.613	797	800	801	rBV3	660	321	0.02%	0.002%
7	3.632	803	806	809	rVB4	1217	739	0.04%	0.005%
8	3.745	838	841	844	rBV6	1378	878	0.04%	0.006%
9	3.764	844	847	848	rBV2	731	451	0.02%	0.003%
10	3.796	848	857	887	rBV	129437	361874	17.63%	2.401%
11	4.243	981	996	1024	rBV	321180	810719	39.49%	5.380%
12	4.606	1107	1109	1113	rBV4	1655	1303	0.06%	0.009%
13	4.677	1128	1131	1133	rBV4	778	518	0.03%	0.003%
14	4.725	1144	1146	1147	rBV2	1131	437	0.02%	0.003%
15	4.767	1156	1159	1163	rBV5	998	629	0.03%	0.004%
16	4.838	1178	1181	1183	rBV4	1118	654	0.03%	0.004%
17	4.851	1183	1185	1189	rBV5	619	408	0.02%	0.003%
18	4.880	1191	1194	1196	rBV3	1210	592	0.03%	0.004%
19	4.950	1200	1216	1254	rBV2	807323	2053141	100.00%	13.624%
20	5.281	1317	1319	1320	rBV2	1312	562	0.03%	0.004%
21	5.529	1385	1396	1434	rBV	559953	1173267	57.14%	7.785%
22	5.986	1526	1538	1564	rBV	453885	940849	45.82%	6.243%
23	6.272	1624	1627	1628	rBV3	883	536	0.03%	0.004%
24	6.571	1718	1720	1723	rVV3	1312	779	0.04%	0.005%
25	6.600	1727	1729	1730	rBV2	938	514	0.03%	0.003%
26	6.709	1761	1763	1766	rBV3	1110	740	0.04%	0.005%
27	6.912	1816	1826	1853	rBV	225270	433961	21.14%	2.880%
28	7.240	1917	1928	1956	rBV	884031	1558642	75.92%	10.343%
29	7.551	2016	2025	2045	rBV	149542	278527	13.57%	1.848%
30	7.863	2120	2122	2124	rBV2	1607	1078	0.05%	0.007%
31	7.895	2126	2132	2135	rBV7	2057	1878	0.09%	0.012%
32	7.937	2143	2145	2146	rBV2	991	378	0.02%	0.003%
33	8.024	2164	2172	2208	rBV	368483	768977	37.45%	5.103%
34	8.384	2282	2284	2292	rBV8	1713	1937	0.09%	0.013%
35	8.629	2359	2360	2362	rBV2	785	324	0.02%	0.002%
36	8.728	2389	2391	2394	rBV4	779	613	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037076.D
 Acq On : 27 Aug 2024 11:36
 Operator : SY/MD
 Sample : P3691-19
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K72

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	8.780	2397	2407	2439	rVV	908528	1510605	73.58%	10.024%
38	9.050	2487	2491	2495	rBV4	2295	2455	0.12%	0.016%
39	9.355	2580	2586	2587	rBV6	1793	1788	0.09%	0.012%
40	9.413	2601	2604	2607	rBV4	653	431	0.02%	0.003%
41	9.542	2642	2644	2646	rBV3	980	594	0.03%	0.004%
42	9.616	2664	2667	2670	rBV5	1102	819	0.04%	0.005%
43	9.674	2679	2685	2688	rBV6	2023	2300	0.11%	0.015%
44	9.709	2693	2696	2700	rBV5	1307	1057	0.05%	0.007%
45	9.735	2702	2704	2705	rBV3	965	399	0.02%	0.003%
46	9.796	2721	2723	2724	rBV2	698	260	0.01%	0.002%
47	9.805	2724	2726	2729	rBV3	1060	689	0.03%	0.005%
48	9.905	2751	2757	2760	rBV6	1318	1155	0.06%	0.008%
49	9.989	2779	2783	2784	rBV4	1217	608	0.03%	0.004%
50	10.053	2800	2803	2804	rBV2	1067	569	0.03%	0.004%
51	10.092	2812	2815	2816	rBV3	1068	521	0.03%	0.003%
52	10.149	2821	2833	2856	rBV	614314	979554	47.71%	6.500%
53	10.561	2958	2961	2964	rBV5	1084	851	0.04%	0.006%
54	10.616	2976	2978	2980	rVB3	873	326	0.02%	0.002%
55	10.719	3008	3010	3013	rVB3	1145	537	0.03%	0.004%
56	10.747	3017	3019	3021	rBV3	553	270	0.01%	0.002%
57	10.757	3021	3022	3024	rBV	913	465	0.02%	0.003%
58	10.857	3049	3053	3054	rBV4	1368	1035	0.05%	0.007%
59	10.902	3065	3067	3069	rBV3	1451	771	0.04%	0.005%
60	10.934	3075	3077	3081	rBV4	996	728	0.04%	0.005%
61	10.979	3088	3091	3095	rVB6	1694	1233	0.06%	0.008%
62	11.008	3095	3100	3102	rBV4	1111	1051	0.05%	0.007%
63	11.024	3102	3105	3107	rBV3	752	431	0.02%	0.003%
64	11.108	3123	3131	3132	rBV6	1401	1372	0.07%	0.009%
65	11.182	3143	3154	3185	rBV	900413	1470361	71.62%	9.757%
66	11.452	3236	3238	3239	rBV2	1034	259	0.01%	0.002%
67	11.554	3258	3270	3293	rBV	915458	1468929	71.55%	9.747%
68	11.998	3406	3408	3411	rBV3	1125	543	0.03%	0.004%
69	12.117	3442	3445	3448	rBV5	1107	850	0.04%	0.006%
70	12.146	3452	3454	3458	rBV4	1290	799	0.04%	0.005%
71	12.217	3473	3476	3479	rBV4	1120	764	0.04%	0.005%
72	12.246	3483	3485	3486	rBV2	937	483	0.02%	0.003%
73	12.317	3503	3507	3510	rVB5	2692	1932	0.09%	0.013%
74	12.329	3510	3511	3512	rBV	996	347	0.02%	0.002%
75	12.342	3512	3515	3518	rVV5	1001	755	0.04%	0.005%
76	12.442	3542	3546	3548	rBV5	1534	1233	0.06%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037076.D
 Acq On : 27 Aug 2024 11:36
 Operator : SY/MD
 Sample : P3691-19
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K72

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	12.468	3552	3554	3556	rVB3	1450	596	0.03%	0.004%
78	12.587	3588	3591	3597	rBV5	2913	3042	0.15%	0.020%
79	12.651	3608	3611	3616	rBV6	1327	883	0.04%	0.006%
80	12.683	3619	3621	3625	rVB3	985	655	0.03%	0.004%
81	12.770	3645	3648	3649	rBV3	1085	598	0.03%	0.004%
82	12.985	3713	3715	3718	rBV5	1097	491	0.02%	0.003%
83	13.024	3725	3727	3728	rBV2	1009	499	0.02%	0.003%
84	13.053	3733	3736	3737	rBV3	1136	620	0.03%	0.004%
85	13.098	3747	3750	3752	rBV4	1426	851	0.04%	0.006%
86	13.114	3753	3755	3756	rBV2	1654	627	0.03%	0.004%
87	13.149	3765	3766	3768	rBV2	1124	486	0.02%	0.003%
88	13.210	3778	3785	3787	rBV7	2400	2757	0.13%	0.018%
89	13.320	3816	3819	3820	rBV3	1288	743	0.04%	0.005%
90	13.355	3827	3830	3831	rBV3	1495	927	0.05%	0.006%
91	13.381	3836	3838	3843	rBV6	1119	801	0.04%	0.005%
92	13.403	3843	3845	3849	rBV5	787	692	0.03%	0.005%
93	13.545	3887	3889	3890	rBV	1135	347	0.02%	0.002%
94	13.622	3911	3913	3916	rBV4	1288	958	0.05%	0.006%
95	13.963	4015	4019	4021	rBV5	1310	1215	0.06%	0.008%
96	13.979	4022	4024	4030	rVB5	2475	1856	0.09%	0.012%
97	14.079	4052	4055	4056	rBV3	1321	670	0.03%	0.004%
98	14.246	4105	4107	4109	rBV3	1256	614	0.03%	0.004%
99	14.307	4123	4126	4128	rBV3	1497	1060	0.05%	0.007%
100	14.500	4183	4186	4187	rBV3	1428	643	0.03%	0.004%

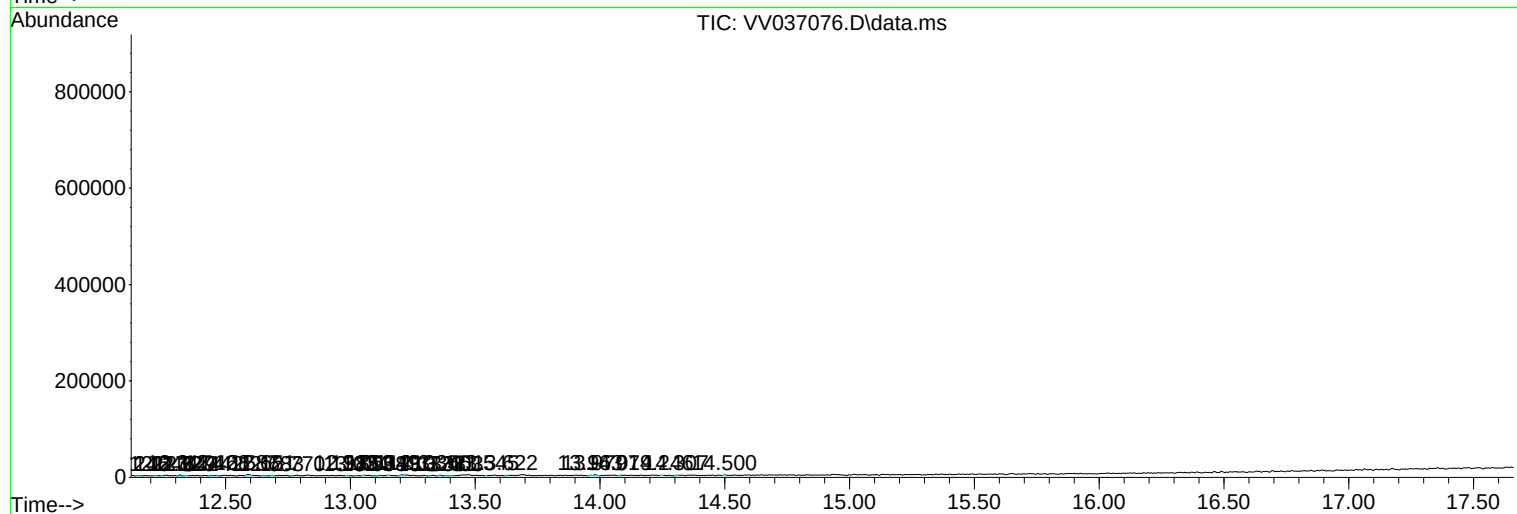
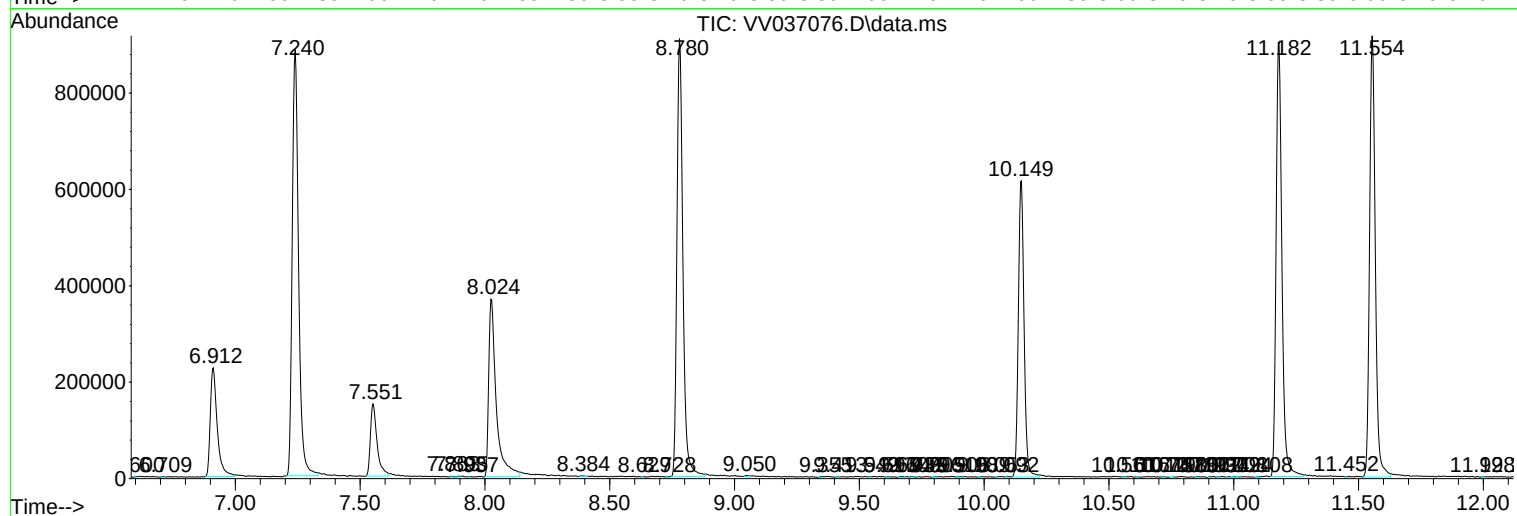
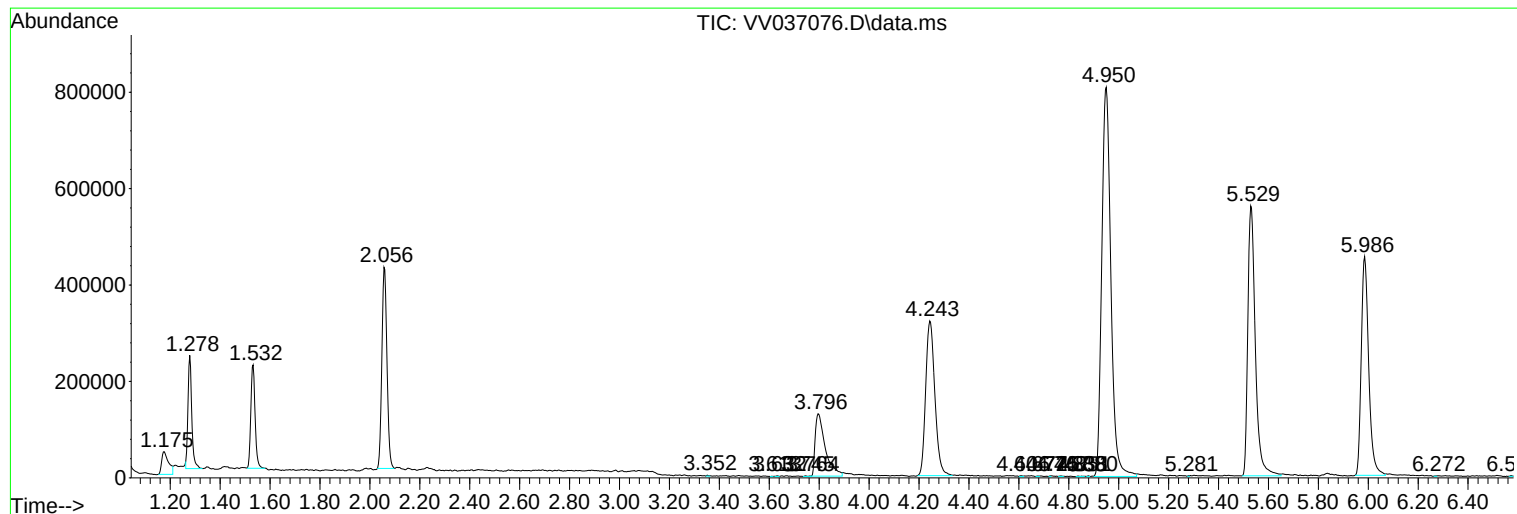
Sum of corrected areas: 15070116

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037076.D
Acq On : 27 Aug 2024 11:36
Operator : SY/MD
Sample : P3691-19
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K72

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 : VV037076.D
Acq On : 27 Aug 2024 11:36
Operator : SY/MD
Sample : P3691-19
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K72

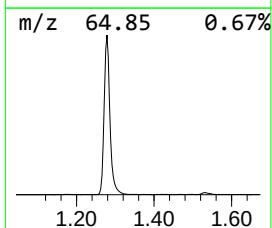
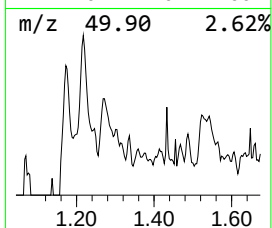
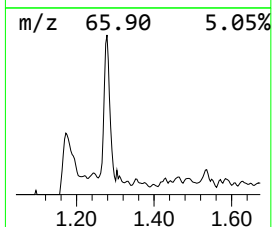
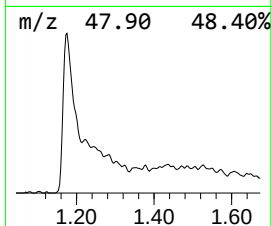
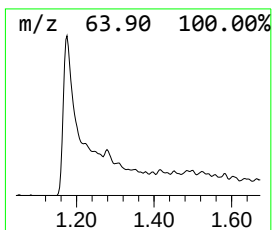
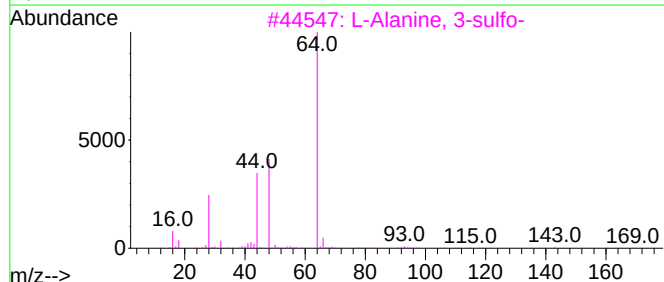
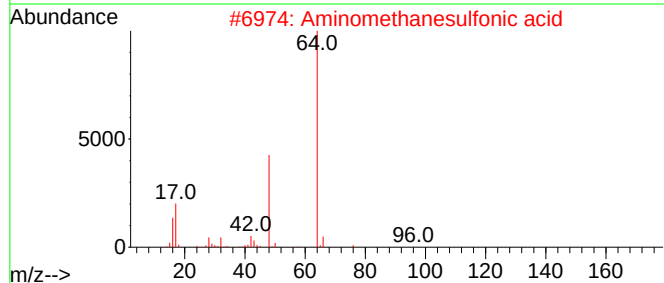
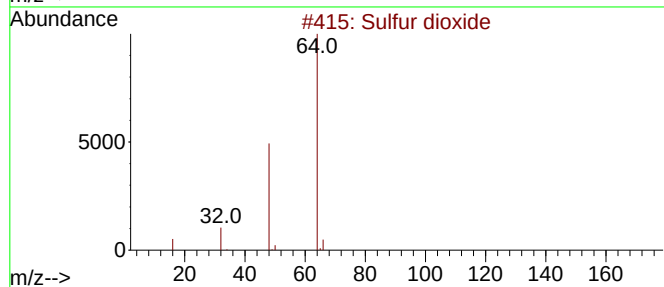
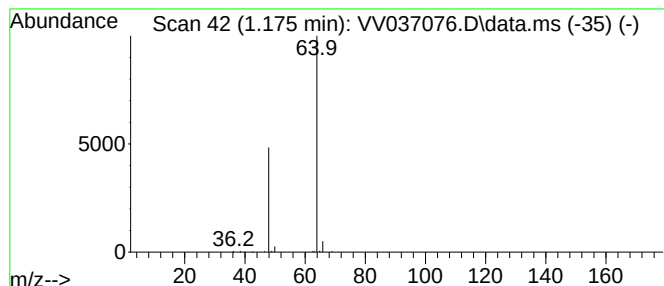
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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.
1.175	3.98 ug/L	93475	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
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			Sulfur dioxide	64	O2S	007446-09-5	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037076.D
Acq On : 27 Aug 2024 11:36
Operator : SY/MD
Sample : P3691-19
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K72

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	1.175	4.0	ug/L	93475	1	5.529	1173270	50.0