

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037073.D
 Acq On : 27 Aug 2024 10:31
 Operator : SY/MD
 Sample : P3691-02
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K44

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: VV037073.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	35	41	55	rBV	62098	103235	4.33%	0.583%
2	1.278	68	74	91	rVB	316219	331291	13.88%	1.870%
3	1.532	146	153	169	rVB	273933	327053	13.71%	1.847%
4	2.056	308	316	331	rVB	565438	814364	34.13%	4.598%
5	3.474	750	757	759	rBV7	2022	2294	0.10%	0.013%
6	3.571	784	787	793	rVB8	1919	1685	0.07%	0.010%
7	3.600	793	796	797	rBV2	744	302	0.01%	0.002%
8	3.629	802	805	807	rBV3	2110	1121	0.05%	0.006%
9	3.641	807	809	810	rBV2	542	196	0.01%	0.001%
10	3.693	823	825	827	rVB3	719	295	0.01%	0.002%
11	3.719	831	833	834	rBV2	835	317	0.01%	0.002%
12	3.764	846	847	848	rBV	611	199	0.01%	0.001%
13	3.796	848	857	889	rVV	125874	361424	15.15%	2.041%
14	4.243	981	996	1028	rVB	382078	959551	40.21%	5.418%
15	4.538	1085	1088	1089	rBV3	1028	485	0.02%	0.003%
16	4.609	1108	1110	1114	rVB5	752	403	0.02%	0.002%
17	4.628	1114	1116	1118	rBV3	614	236	0.01%	0.001%
18	4.645	1118	1121	1124	rBV6	1537	1378	0.06%	0.008%
19	4.670	1127	1129	1131	rVV3	1099	514	0.02%	0.003%
20	4.699	1134	1138	1141	rBV5	1059	899	0.04%	0.005%
21	4.841	1178	1182	1185	rBV6	1287	1385	0.06%	0.008%
22	4.876	1191	1193	1194	rBV2	817	419	0.02%	0.002%
23	4.950	1201	1216	1248	rBV2	948829	2386163	100.00%	13.472%
24	5.304	1322	1326	1328	rBV4	1425	1232	0.05%	0.007%
25	5.529	1385	1396	1431	rBV	711420	1467289	61.49%	8.284%
26	5.985	1526	1538	1574	rBV	525170	1094543	45.87%	6.180%
27	6.426	1673	1675	1678	rVB3	1390	771	0.03%	0.004%
28	6.458	1683	1685	1688	rVB3	1081	656	0.03%	0.004%
29	6.554	1713	1715	1717	rBV3	900	490	0.02%	0.003%
30	6.796	1788	1790	1791	rBV2	638	264	0.01%	0.001%
31	6.908	1816	1825	1859	rBV	269959	516170	21.63%	2.914%
32	7.239	1917	1928	1964	rBV	1075848	1911152	80.09%	10.790%
33	7.551	2016	2025	2054	rBV2	169794	322841	13.53%	1.823%
34	7.963	2147	2153	2158	rBV9	1194	1364	0.06%	0.008%
35	8.024	2164	2172	2201	rBV	351724	731666	30.66%	4.131%
36	8.471	2308	2311	2313	rBV4	1748	1205	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037073.D
 Acq On : 27 Aug 2024 10:31
 Operator : SY/MD
 Sample : P3691-02
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K44

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	8.718	2386	2388	2390	rBV3	1395	762	0.03%	0.004%
38	8.779	2396	2407	2435	rBV	1121687	1822200	76.37%	10.288%
39	9.252	2552	2554	2557	rVB3	1092	471	0.02%	0.003%
40	9.500	2626	2631	2635	rBV6	1735	1834	0.08%	0.010%
41	9.606	2659	2664	2666	rBV5	1702	1505	0.06%	0.008%
42	9.622	2666	2669	2670	rBV3	1167	605	0.03%	0.003%
43	9.696	2686	2692	2696	rBV7	1842	2533	0.11%	0.014%
44	9.738	2702	2705	2706	rBV2	670	336	0.01%	0.002%
45	9.757	2709	2711	2715	rVV4	773	566	0.02%	0.003%
46	9.821	2724	2731	2733	rBV4	1394	1433	0.06%	0.008%
47	9.911	2755	2759	2761	rVB5	1284	983	0.04%	0.006%
48	9.927	2761	2764	2766	rBV4	740	367	0.02%	0.002%
49	9.982	2778	2781	2782	rBV3	942	347	0.01%	0.002%
50	10.001	2782	2787	2792	rVB6	1740	2014	0.08%	0.011%
51	10.033	2792	2797	2799	rBV5	1180	1233	0.05%	0.007%
52	10.085	2807	2813	2816	rBV7	1337	1204	0.05%	0.007%
53	10.101	2816	2818	2820	rBV3	889	499	0.02%	0.003%
54	10.149	2821	2833	2851	rBV	634873	1019589	42.73%	5.757%
55	10.371	2898	2902	2903	rBV4	720	407	0.02%	0.002%
56	10.474	2932	2934	2936	rVB3	1122	473	0.02%	0.003%
57	10.596	2969	2972	2974	rBV4	960	718	0.03%	0.004%
58	10.760	3016	3023	3029	rBV8	2255	3554	0.15%	0.020%
59	10.860	3050	3054	3056	rBV5	1656	1336	0.06%	0.008%
60	10.937	3076	3078	3080	rBV3	666	274	0.01%	0.002%
61	10.992	3091	3095	3099	rVB6	1103	1140	0.05%	0.006%
62	11.017	3099	3103	3109	rBV9	1851	2111	0.09%	0.012%
63	11.062	3115	3117	3118	rBV2	783	215	0.01%	0.001%
64	11.123	3130	3136	3137	rBV7	1902	2071	0.09%	0.012%
65	11.181	3142	3154	3186	rVV	1099346	1782328	74.69%	10.063%
66	11.435	3231	3233	3234	rBV2	919	411	0.02%	0.002%
67	11.554	3258	3270	3292	rBV	1050330	1689853	70.82%	9.541%
68	11.866	3362	3367	3371	rBV8	1722	2150	0.09%	0.012%
69	11.934	3385	3388	3390	rBV4	1423	817	0.03%	0.005%
70	12.011	3410	3412	3415	rBV4	1140	559	0.02%	0.003%
71	12.082	3430	3434	3435	rBV4	1281	864	0.04%	0.005%
72	12.091	3435	3437	3441	rVB4	1461	907	0.04%	0.005%
73	12.123	3441	3447	3450	rVB6	1992	1930	0.08%	0.011%
74	12.246	3482	3485	3488	rBV4	1301	900	0.04%	0.005%
75	12.342	3511	3515	3516	rBV4	734	436	0.02%	0.002%
76	12.483	3556	3559	3562	rBV4	1578	1046	0.04%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037073.D
Acq On : 27 Aug 2024 10:31
Operator : SY/MD
Sample : P3691-02
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K44

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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	12.538	3574	3576	3577	rBV2	890	396	0.02%	0.002%
78	12.664	3613	3615	3616	rBV2	756	305	0.01%	0.002%
79	12.831	3663	3667	3670	rVB4	1347	1098	0.05%	0.006%
80	12.918	3691	3694	3697	rBV3	1359	930	0.04%	0.005%
81	13.188	3776	3778	3779	rBV	1305	569	0.02%	0.003%
82	13.361	3828	3832	3834	rBV4	1342	1210	0.05%	0.007%
83	13.409	3845	3847	3850	rBV3	1353	788	0.03%	0.004%
84	13.435	3853	3855	3857	rBV2	1368	676	0.03%	0.004%
85	13.451	3857	3860	3862	rBV4	2618	1906	0.08%	0.011%
86	13.795	3965	3967	3970	rBV4	1186	675	0.03%	0.004%
87	14.075	4045	4054	4057	rBV9	2071	2709	0.11%	0.015%
88	14.194	4089	4091	4094	rBV4	944	496	0.02%	0.003%
89	14.258	4109	4111	4113	rBV3	1297	642	0.03%	0.004%
90	14.663	4234	4237	4241	rBV4	1476	1316	0.06%	0.007%

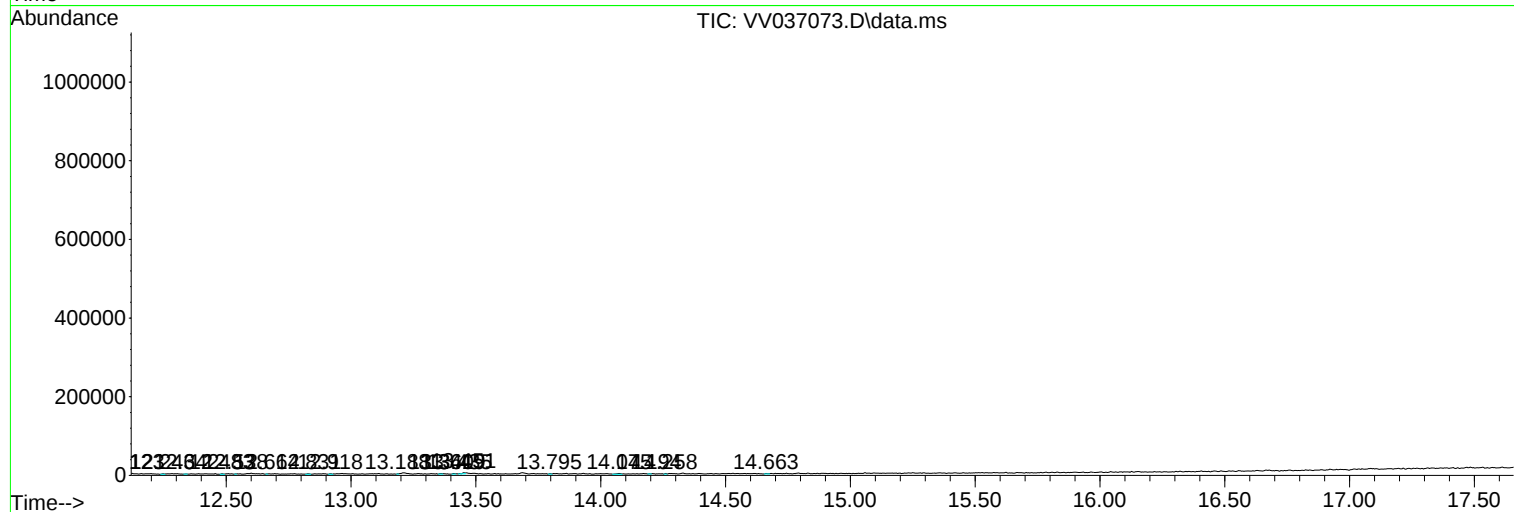
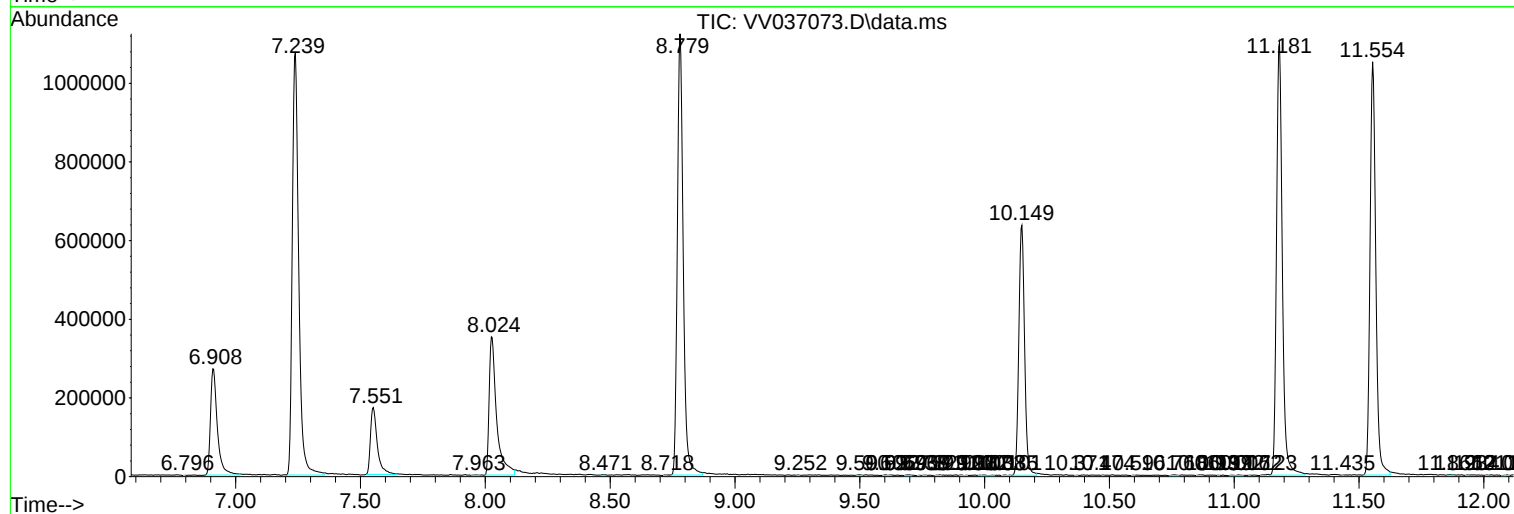
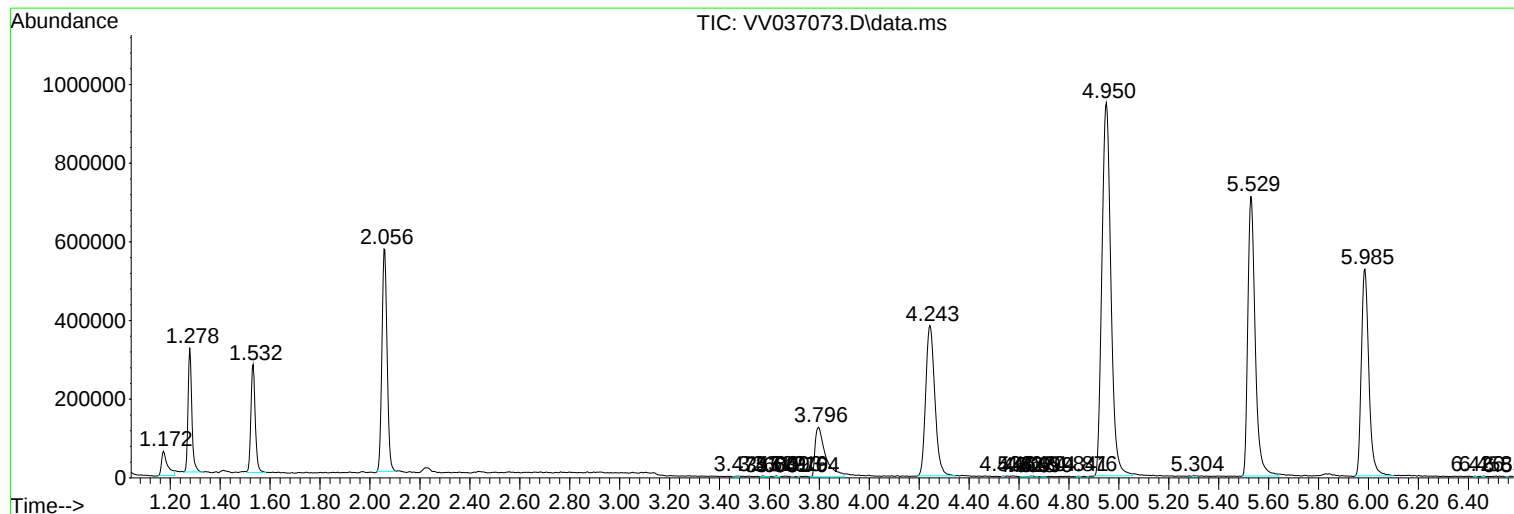
Sum of corrected areas: 17711549

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037073.D
Acq On : 27 Aug 2024 10:31
Operator : SY/MD
Sample : P3691-02
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K44

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 : VV037073.D
Acq On : 27 Aug 2024 10:31
Operator : SY/MD
Sample : P3691-02
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K44

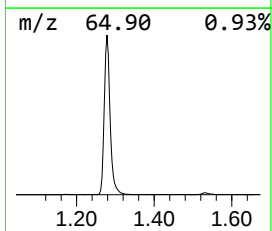
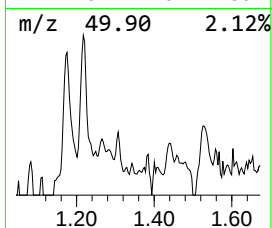
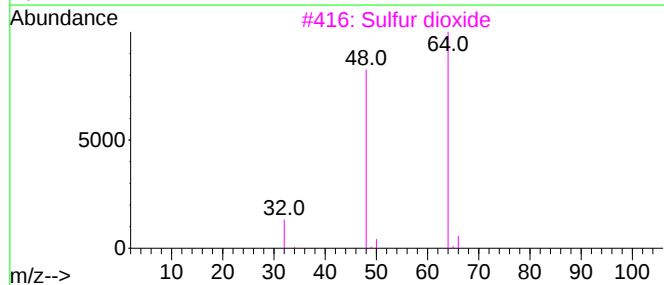
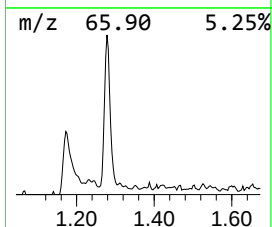
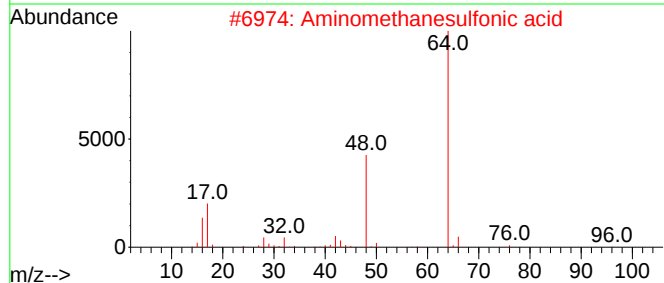
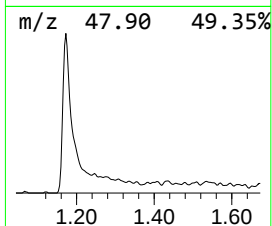
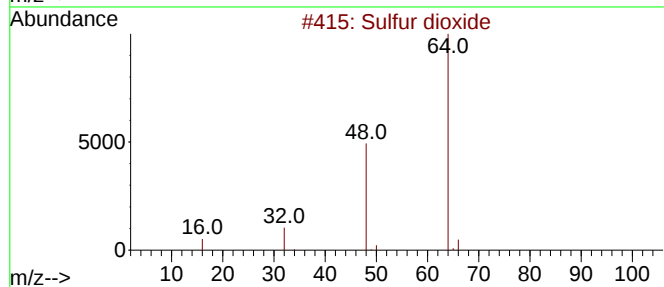
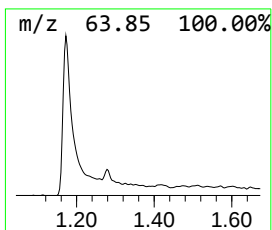
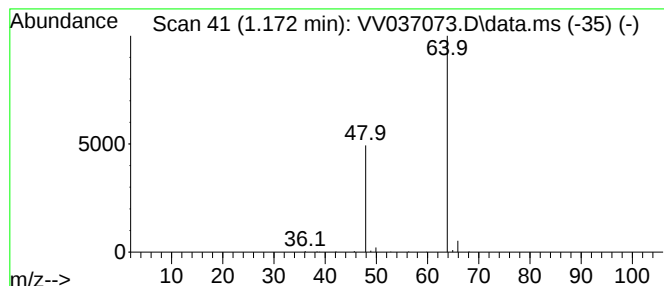
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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	3.52 ug/L	103235	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			Sulfur dioxide	64	O2S	007446-09-5	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037073.D
Acq On : 27 Aug 2024 10:31
Operator : SY/MD
Sample : P3691-02
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K44

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	3.5	ug/L	103235	1	5.529	1467290	50.0