

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070621\
 Data File : VV021612.D
 Acq On : 06 Jul 2021 13:57
 Operator : SY/MD
 Sample : VIBLK201
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VIBLK201

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\SFAMVLM062921WMA.M

Title : VOC Analysis

Signal : TIC: VV021612.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.191	41	47	74	rBV	41397	87024	5.44%	0.629%
2	1.304	75	82	92	rBV	165051	164672	10.30%	1.190%
3	1.359	92	99	116	rBV	34929	83443	5.22%	0.603%
4	1.561	155	162	176	rVB	141424	167274	10.46%	1.209%
5	2.105	321	331	345	rVB	311129	450526	28.17%	3.257%
6	2.291	383	389	400	rVB	6680	10193	0.64%	0.074%
7	2.442	432	436	439	rBV5	666	554	0.03%	0.004%
8	2.503	447	455	464	rBV2	5180	8642	0.54%	0.062%
9	2.593	479	483	485	rBV4	441	371	0.02%	0.003%
10	2.664	501	505	508	rBV3	485	347	0.02%	0.003%
11	2.786	540	543	547	rBV2	557	321	0.02%	0.002%
12	2.912	578	582	586	rBV5	674	603	0.04%	0.004%
13	3.124	645	648	650	rBV3	583	435	0.03%	0.003%
14	3.204	669	673	676	rBV4	534	508	0.03%	0.004%
15	3.256	685	689	695	rVB3	409	373	0.02%	0.003%
16	3.391	728	731	733	rBV3	435	337	0.02%	0.002%
17	3.404	733	735	737	rVV2	537	312	0.02%	0.002%
18	3.490	758	762	767	rBV3	448	408	0.03%	0.003%
19	3.587	790	792	796	rVB2	562	320	0.02%	0.002%
20	3.651	806	812	815	rBV3	423	364	0.02%	0.003%
21	3.722	826	834	838	rBV5	1781	2609	0.16%	0.019%
22	3.870	869	880	917	rBV	139500	361256	22.59%	2.612%
23	4.195	977	981	983	rBV3	456	328	0.02%	0.002%
24	4.346	1012	1028	1058	rBV	255953	633925	39.63%	4.583%
25	4.506	1076	1078	1086	rVB6	645	558	0.03%	0.004%
26	4.635	1116	1118	1121	rVB3	636	355	0.02%	0.003%
27	4.748	1148	1153	1155	rBV4	443	377	0.02%	0.003%
28	4.828	1174	1178	1181	rBV3	432	346	0.02%	0.003%
29	5.047	1228	1246	1282	rVV2	620858	1599448	100.00%	11.563%
30	5.281	1317	1319	1324	rVB4	602	324	0.02%	0.002%
31	5.326	1331	1333	1335	rBV3	653	412	0.03%	0.003%
32	5.413	1358	1360	1364	rBV5	609	322	0.02%	0.002%
33	5.465	1370	1376	1378	rVB4	395	358	0.02%	0.003%
34	5.497	1378	1386	1389	rBV7	853	1128	0.07%	0.008%
35	5.616	1410	1423	1461	rBV	522179	1060485	66.30%	7.667%
36	5.912	1500	1515	1530	rBV3	7936	16685	1.04%	0.121%

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Integrator: RTE

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
 Title : VOC Analysis

37	5.998	1536	1542	1545	rBV4	481	467	0.03%	0.003%
38	6.069	1550	1564	1591	rVV	354518	721786	45.13%	5.218%
39	6.211	1605	1608	1609	rBV2	660	405	0.03%	0.003%
40	6.281	1627	1630	1634	rVV3	941	708	0.04%	0.005%
41	6.313	1638	1640	1644	rVB4	677	466	0.03%	0.003%
42	6.336	1644	1647	1652	rVB4	609	492	0.03%	0.004%
43	6.365	1652	1656	1658	rBV3	532	473	0.03%	0.003%
44	6.426	1671	1675	1682	rVB3	648	686	0.04%	0.005%
45	6.558	1713	1716	1719	rBV3	598	426	0.03%	0.003%
46	6.619	1726	1735	1746	rBV4	4685	10812	0.68%	0.078%
47	6.735	1768	1771	1775	rVB3	626	398	0.02%	0.003%
48	6.895	1819	1821	1826	rBV2	349	366	0.02%	0.003%
49	6.985	1838	1849	1873	rBV	209191	381193	23.83%	2.756%
50	7.159	1894	1903	1911	rBV6	2436	5466	0.34%	0.040%
51	7.239	1923	1928	1930	rBV3	981	1002	0.06%	0.007%
52	7.317	1939	1952	1971	rBV	770118	1329378	83.11%	9.611%
53	7.622	2036	2047	2074	rBV	144678	252758	15.80%	1.827%
54	7.796	2098	2101	2106	rBV4	965	613	0.04%	0.004%
55	7.953	2148	2150	2154	rBV4	555	333	0.02%	0.002%
56	7.976	2154	2157	2159	rBV3	582	428	0.03%	0.003%
57	8.011	2166	2168	2173	rBV2	718	520	0.03%	0.004%
58	8.040	2173	2177	2178	rBV2	686	446	0.03%	0.003%
59	8.085	2181	2191	2231	rBV	483024	836321	52.29%	6.046%
60	8.854	2417	2430	2459	rBV	767140	1270885	79.46%	9.188%
61	9.313	2571	2573	2577	rBV3	769	597	0.04%	0.004%
62	9.339	2577	2581	2585	rVB5	801	731	0.05%	0.005%
63	9.378	2590	2593	2595	rBV3	588	454	0.03%	0.003%
64	9.551	2642	2647	2653	rVB4	1846	2192	0.14%	0.016%
65	9.619	2662	2668	2670	rBV4	567	621	0.04%	0.004%
66	9.635	2670	2673	2677	rVB5	751	590	0.04%	0.004%
67	9.670	2679	2684	2685	rBV3	681	648	0.04%	0.005%
68	9.815	2726	2729	2731	rBV3	731	471	0.03%	0.003%
69	10.027	2793	2795	2799	rVB3	918	533	0.03%	0.004%
70	10.127	2820	2826	2834	rBV7	2008	3414	0.21%	0.025%
71	10.217	2842	2854	2872	rBV	544246	843019	52.71%	6.094%
72	10.342	2885	2893	2908	rBV6	6208	13109	0.82%	0.095%
73	10.696	2992	3003	3014	rBV3	13291	21718	1.36%	0.157%
74	10.853	3047	3052	3055	rBV5	1198	1278	0.08%	0.009%
75	10.918	3064	3072	3084	rVB3	7925	12056	0.75%	0.087%
76	11.021	3094	3104	3123	rBV5	21308	49813	3.11%	0.360%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

77	11.249	3159	3175	3190	rBV	842801	1307711	81.76%	9.454%
78	11.445	3228	3236	3245	rVB3	4929	8248	0.52%	0.060%
79	11.529	3252	3262	3280	rBV	116709	221339	13.84%	1.600%
80	11.625	3281	3292	3309	rVB	802374	1274792	79.70%	9.216%
81	11.921	3376	3384	3394	rVB2	31444	48297	3.02%	0.349%
82	12.185	3459	3466	3469	rBV5	1647	2155	0.13%	0.016%
83	12.291	3485	3499	3512	rBV5	7959	16936	1.06%	0.122%
84	12.464	3546	3553	3566	rVB7	12604	20269	1.27%	0.147%
85	12.554	3574	3581	3587	rBV5	5821	8325	0.52%	0.060%
86	12.779	3641	3651	3665	rBV5	14858	43664	2.73%	0.316%
87	13.185	3771	3777	3794	rVB5	5787	10942	0.68%	0.079%
88	13.384	3832	3839	3842	rBV5	9445	12358	0.77%	0.089%
89	13.416	3843	3849	3858	rVB2	25292	39825	2.49%	0.288%
90	13.509	3873	3878	3889	rVB3	15587	24147	1.51%	0.175%
91	13.596	3900	3905	3912	rBV7	4719	7488	0.47%	0.054%
92	13.763	3947	3957	3964	rBV4	33751	54522	3.41%	0.394%
93	13.812	3964	3972	3987	rVB6	28825	53940	3.37%	0.390%
94	13.963	4016	4019	4021	rBV4	2578	1831	0.11%	0.013%
95	14.024	4031	4038	4046	rBV5	11120	15852	0.99%	0.115%
96	14.197	4084	4092	4108	rVB5	18377	31806	1.99%	0.230%
97	15.303	4428	4436	4448	rBV3	19818	33924	2.12%	0.245%
98	15.512	4494	4501	4511	rBV4	39271	61076	3.82%	0.442%
99	15.914	4619	4626	4642	rVB2	30604	54053	3.38%	0.391%
100	17.098	4987	4994	5005	rBV3	32154	55042	3.44%	0.398%

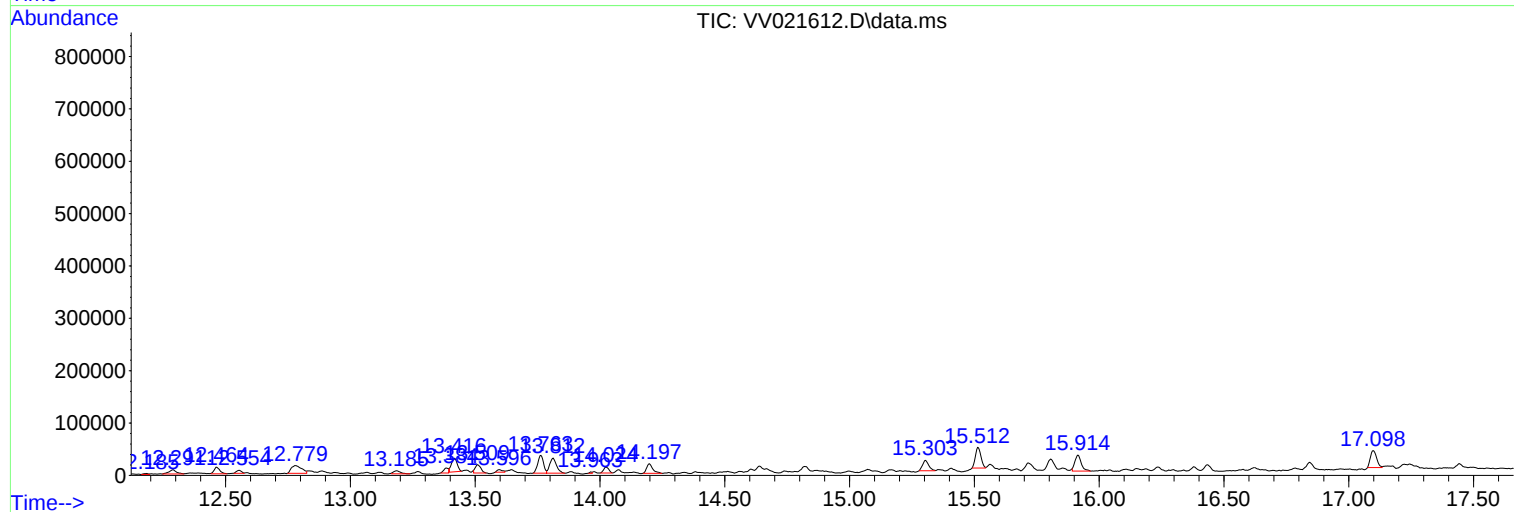
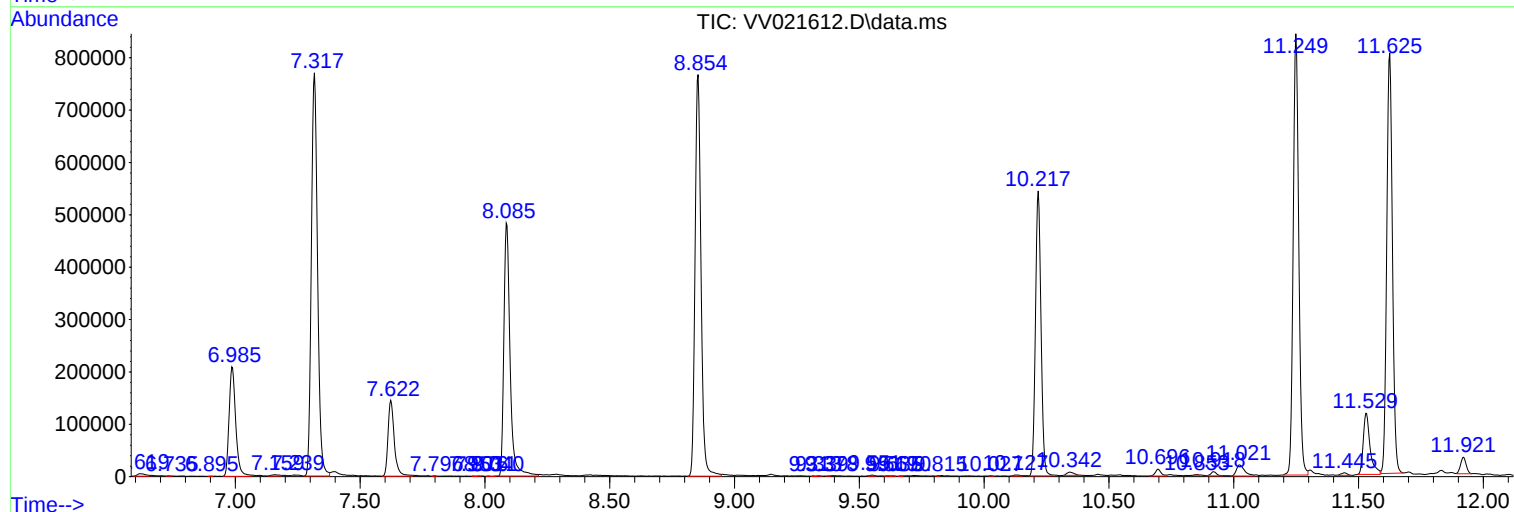
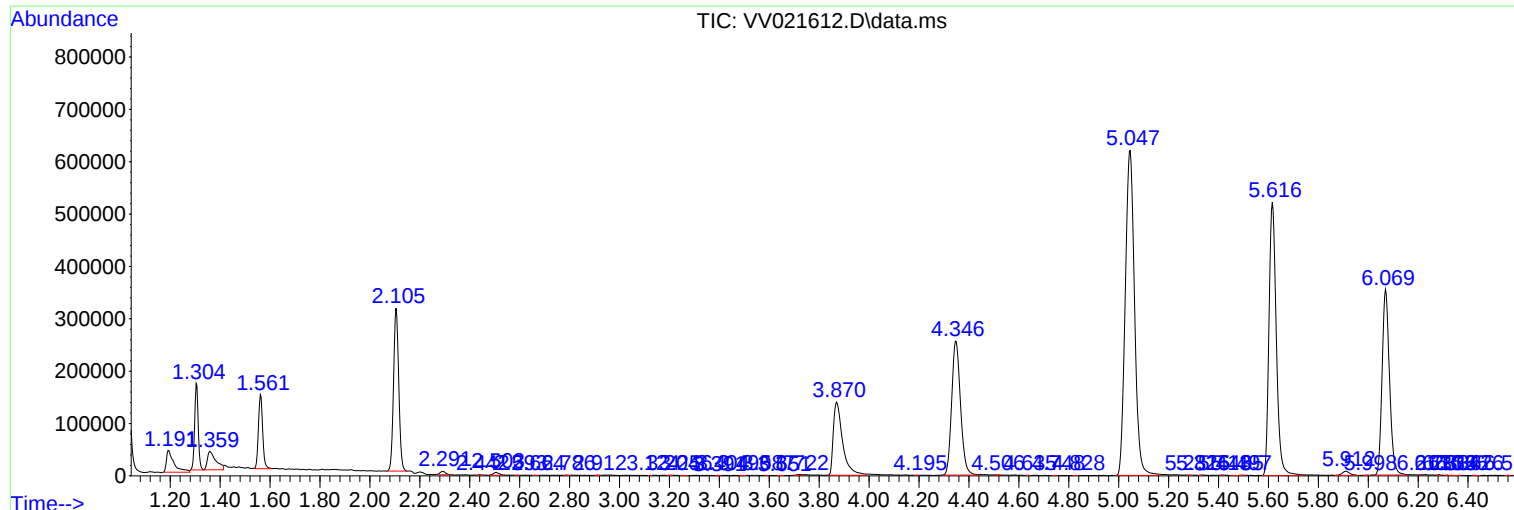
Sum of corrected areas: 13832557

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VIBLK201

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VIBLK201

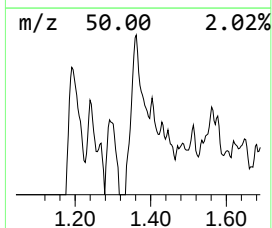
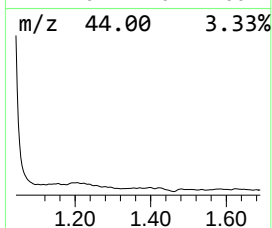
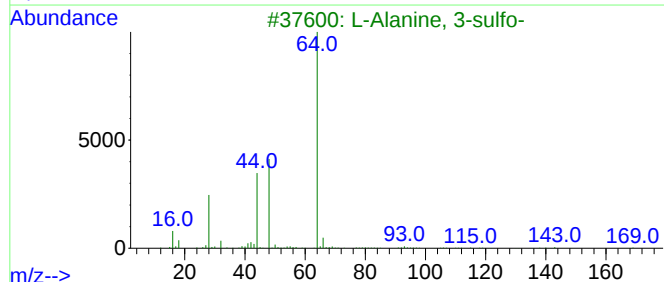
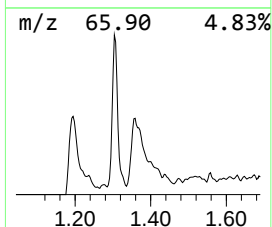
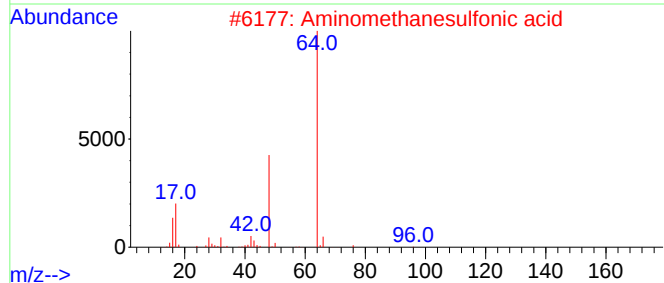
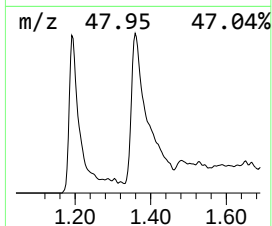
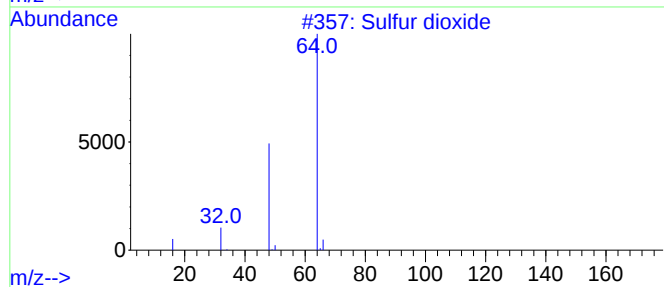
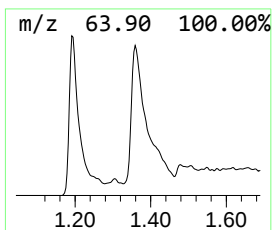
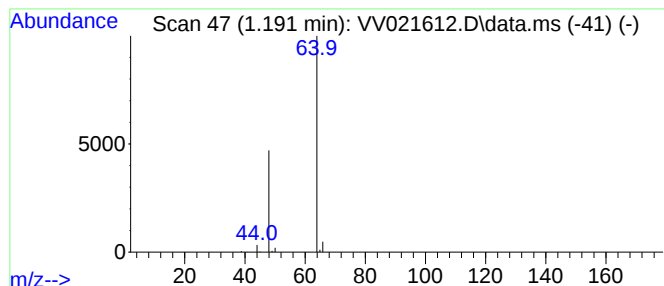
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.191	4.10 ug/L	87024	1,4-Difluorobenzene	5.616

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	4



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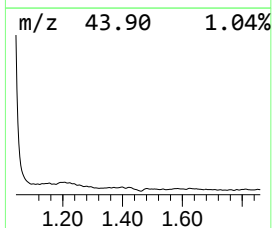
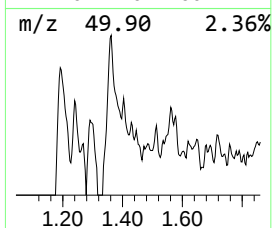
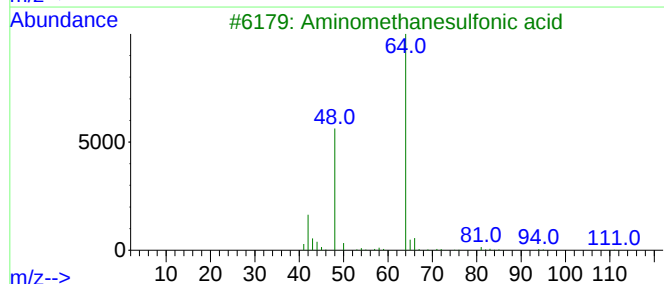
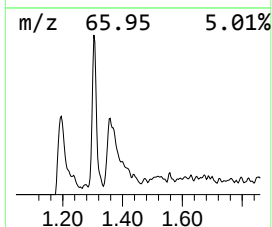
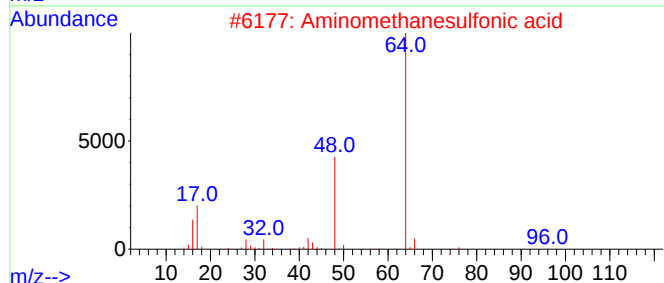
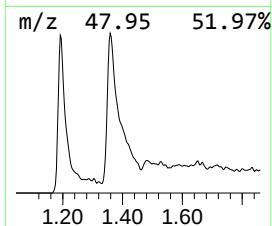
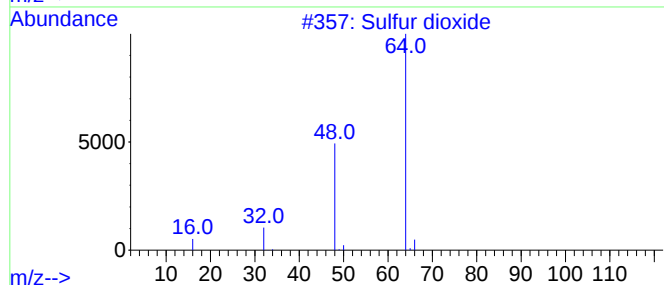
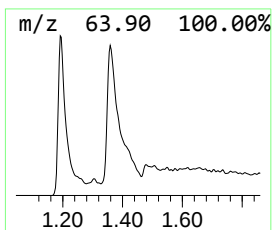
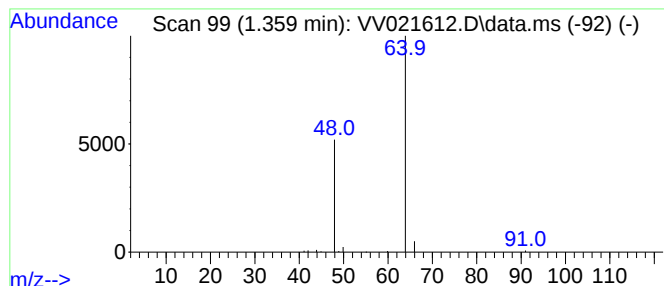
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	3.93 ug/L	83443	1,4-Difluorobenzene	5.616

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	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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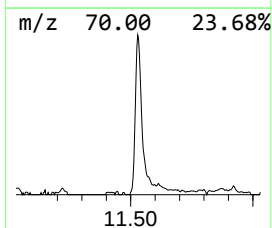
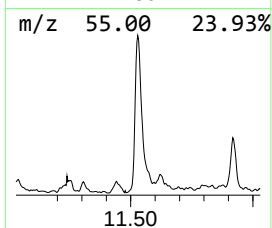
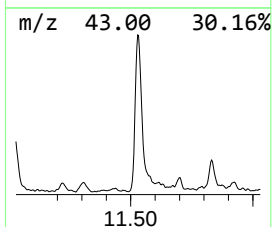
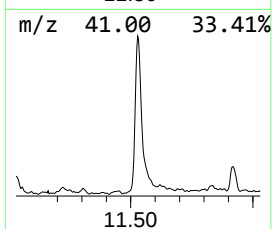
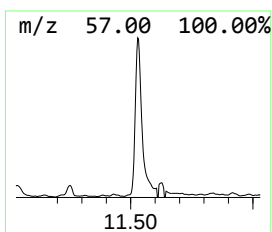
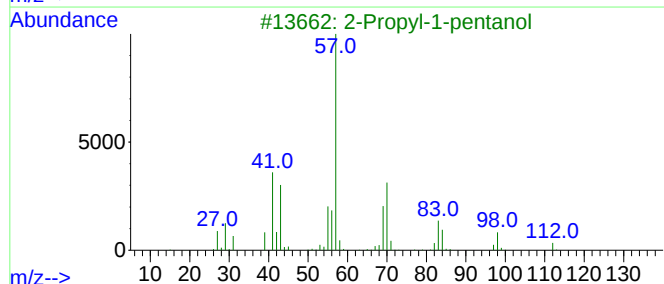
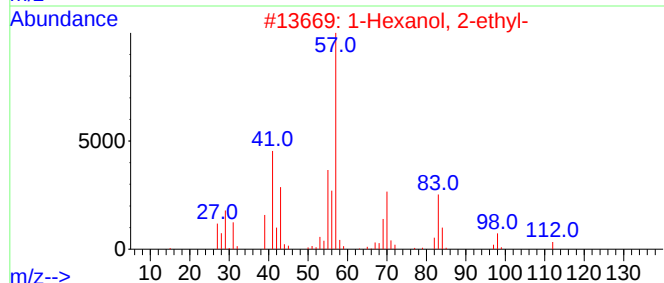
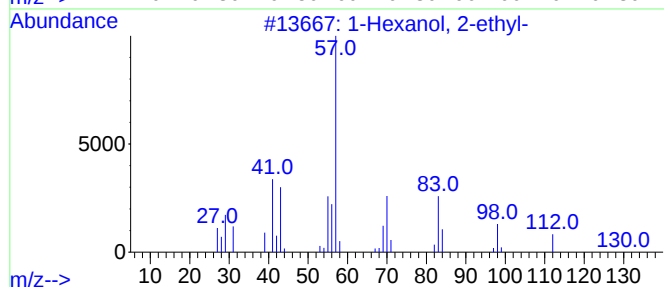
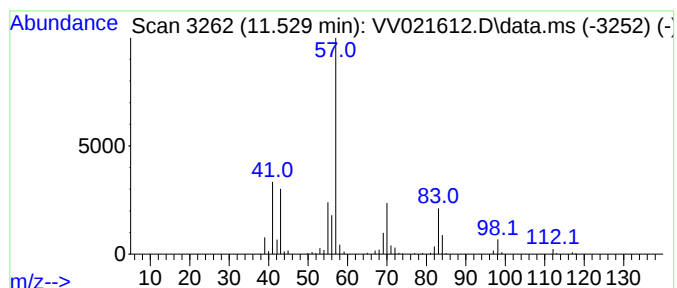
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	8.46 ug/L	221339	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	74
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
3	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	59
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	53
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070621\
Data File : VV021612.D
Acq On : 06 Jul 2021 13:57
Operator : SY/MD
Sample : VIBLK201
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VIBLK201

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062921WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.191	4.1	ug/L	87024	1	5.616	1060490	50.0
Aminomethanesul...	1.359	3.9	ug/L	83443	1	5.616	1060490	50.0
1-Hexanol, 2-et...	11.529	8.5	ug/L	221339	3	11.249	1307710	50.0