

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045186.D
 Acq On : 06 Oct 2021 15:27
 Operator : SY/MD
 Sample : M4024-16
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AM8

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_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

Signal : TIC: VU0451186.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.462	31	38	54	rBV	340463	517749	41.04%	4.858%
2	1.597	76	80	103	rVB	176476	225238	17.85%	2.113%
3	1.896	166	173	196	rVB	127769	182360	14.45%	1.711%
4	2.565	368	381	395	rBV	227326	388440	30.79%	3.645%
5	2.633	396	402	415	rVB	8720	14451	1.15%	0.136%
6	2.736	429	434	437	rVB2	344	303	0.02%	0.003%
7	3.051	525	532	537	rVB4	834	1263	0.10%	0.012%
8	3.189	560	575	593	rBV2	47215	106826	8.47%	1.002%
9	3.507	668	674	677	rBV	261	280	0.02%	0.003%
10	3.584	689	698	711	rVB4	1504	3625	0.29%	0.034%
11	3.639	712	715	722	rBV2	201	284	0.02%	0.003%
12	3.999	814	827	828	rBV4	812	1282	0.10%	0.012%
13	4.154	870	875	880	rBV2	229	271	0.02%	0.003%
14	4.626	1007	1022	1052	rBV	163098	404101	32.03%	3.792%
15	5.067	1143	1159	1184	rBV	231588	504402	39.98%	4.733%
16	5.160	1185	1188	1193	rVV4	274	241	0.02%	0.002%
17	5.295	1224	1230	1237	rBV4	612	1114	0.09%	0.010%
18	5.491	1287	1291	1295	rVB2	218	253	0.02%	0.002%
19	5.584	1317	1320	1324	rBV	230	236	0.02%	0.002%
20	5.729	1343	1365	1392	rBV2	466579	1261663	100.00%	11.839%
21	5.829	1392	1396	1400	rBV3	1165	1334	0.11%	0.013%
22	5.970	1434	1440	1449	rVB6	1462	2467	0.20%	0.023%
23	6.047	1459	1464	1467	rBV3	204	231	0.02%	0.002%
24	6.131	1486	1490	1492	rBV4	704	574	0.05%	0.005%
25	6.147	1493	1495	1509	rVB4	1262	1906	0.15%	0.018%
26	6.253	1513	1528	1554	rBV	380338	711489	56.39%	6.676%
27	6.536	1608	1616	1628	rVB7	2011	3275	0.26%	0.031%
28	6.594	1631	1634	1639	rVB4	342	228	0.02%	0.002%
29	6.697	1648	1666	1683	rBV	301088	585785	46.43%	5.497%
30	6.977	1748	1753	1757	rBV2	450	537	0.04%	0.005%
31	7.044	1770	1774	1782	rVB3	525	681	0.05%	0.006%
32	7.182	1808	1817	1827	rVB4	2059	3493	0.28%	0.033%
33	7.485	1905	1911	1914	rBV2	205	282	0.02%	0.003%
34	7.568	1925	1937	1952	rVV	152478	262529	20.81%	2.463%
35	7.636	1956	1958	1964	rVV3	572	436	0.03%	0.004%
36	7.694	1964	1976	1984	rVV5	1619	2838	0.22%	0.027%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.903	2022	2041	2055	rBV	568293	973351	77.15%	9.133%
38	7.973	2056	2063	2076	rVB2	9028	14783	1.17%	0.139%
39	8.182	2115	2128	2146	rBV2	108964	178670	14.16%	1.677%
40	8.247	2146	2148	2150	rVV2	424	241	0.02%	0.002%
41	8.269	2153	2155	2161	rVB4	317	347	0.03%	0.003%
42	8.481	2217	2221	2222	rBV	525	383	0.03%	0.004%
43	8.559	2238	2245	2249	rVB4	907	894	0.07%	0.008%
44	8.636	2256	2269	2305	rBV	480582	831456	65.90%	7.802%
45	8.787	2306	2316	2332	rVB2	14965	27046	2.14%	0.254%
46	8.964	2368	2371	2374	rBV3	521	404	0.03%	0.004%
47	9.028	2385	2391	2394	rBV2	201	252	0.02%	0.002%
48	9.420	2500	2513	2547	rBV	547438	906665	71.86%	8.508%
49	9.575	2552	2561	2573	rVB	3293	4647	0.37%	0.044%
50	9.697	2589	2599	2614	rVB	9930	15508	1.23%	0.146%
51	9.790	2625	2628	2634	rBV2	197	261	0.02%	0.002%
52	9.874	2650	2654	2656	rBV3	486	403	0.03%	0.004%
53	9.915	2663	2667	2673	rBV2	287	380	0.03%	0.004%
54	9.944	2673	2676	2684	rVV	272	403	0.03%	0.004%
55	9.980	2684	2687	2689	rVV	314	252	0.02%	0.002%
56	10.054	2699	2710	2719	rVV5	2402	4709	0.37%	0.044%
57	10.102	2719	2725	2736	rVB4	1631	2613	0.21%	0.025%
58	10.488	2839	2845	2850	rVV	981	974	0.08%	0.009%
59	10.575	2869	2872	2874	rBV	547	353	0.03%	0.003%
60	10.645	2889	2894	2896	rVV4	964	877	0.07%	0.008%
61	10.674	2898	2903	2907	rVB5	1069	1265	0.10%	0.012%
62	10.761	2918	2930	2947	rVV	442840	705902	55.95%	6.624%
63	10.874	2961	2965	2967	rBV2	305	282	0.02%	0.003%
64	11.211	3067	3070	3074	rVB2	310	242	0.02%	0.002%
65	11.394	3125	3127	3133	rBV	232	254	0.02%	0.002%
66	11.472	3138	3151	3158	rVB5	1847	3685	0.29%	0.035%
67	11.513	3158	3164	3168	rBV2	220	281	0.02%	0.003%
68	11.629	3194	3200	3201	rBV2	494	425	0.03%	0.004%
69	11.639	3201	3203	3211	rVB3	440	502	0.04%	0.005%
70	11.684	3214	3217	3218	rBV	500	240	0.02%	0.002%
71	11.816	3245	3258	3278	rBV	523365	819914	64.99%	7.694%
72	11.909	3286	3287	3292	rVB	509	238	0.02%	0.002%
73	11.967	3295	3305	3314	rVB7	4815	8637	0.68%	0.081%
74	12.012	3316	3319	3328	rVB5	485	542	0.04%	0.005%
75	12.054	3328	3332	3333	rBV	532	414	0.03%	0.004%
76	12.073	3333	3338	3342	rBV5	421	443	0.04%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

77	12.092	3342	3344	3347	rBV4	329	226	0.02%	0.002%
78	12.195	3361	3376	3403	rBV	532583	864545	68.52%	8.112%
79	12.337	3415	3420	3426	rVB4	1356	1541	0.12%	0.014%
80	12.404	3433	3441	3447	rBV6	3439	4874	0.39%	0.046%
81	12.513	3468	3475	3479	rBV4	655	793	0.06%	0.007%
82	12.925	3600	3603	3604	rBV2	433	264	0.02%	0.002%
83	13.079	3645	3651	3656	rBV5	1762	1998	0.16%	0.019%
84	13.237	3693	3700	3708	rVB3	2847	4005	0.32%	0.038%
85	13.285	3709	3715	3717	rBV4	918	888	0.07%	0.008%
86	13.436	3757	3762	3764	rBV3	412	371	0.03%	0.003%
87	13.517	3781	3787	3796	rBV3	432	614	0.05%	0.006%
88	13.745	3854	3858	3863	rVB2	862	722	0.06%	0.007%
89	14.089	3953	3965	3977	rBV2	23042	38147	3.02%	0.358%
90	14.211	3994	4003	4010	rBV5	1038	1738	0.14%	0.016%
91	14.291	4022	4028	4031	rBV4	769	918	0.07%	0.009%
92	14.327	4036	4039	4044	rBV2	271	229	0.02%	0.002%
93	14.571	4112	4115	4119	rBV2	247	226	0.02%	0.002%
94	14.703	4152	4156	4158	rBV3	308	300	0.02%	0.003%
95	14.738	4163	4167	4168	rBV2	369	223	0.02%	0.002%
96	15.073	4268	4271	4275	rBV3	339	309	0.02%	0.003%
97	15.227	4310	4319	4331	rBV	4881	7851	0.62%	0.074%
98	15.414	4369	4377	4391	rVB2	3870	5964	0.47%	0.056%
99	15.960	4540	4547	4554	rBV3	1340	1824	0.14%	0.017%
100	17.102	4893	4902	4914	rBV3	10038	16977	1.35%	0.159%

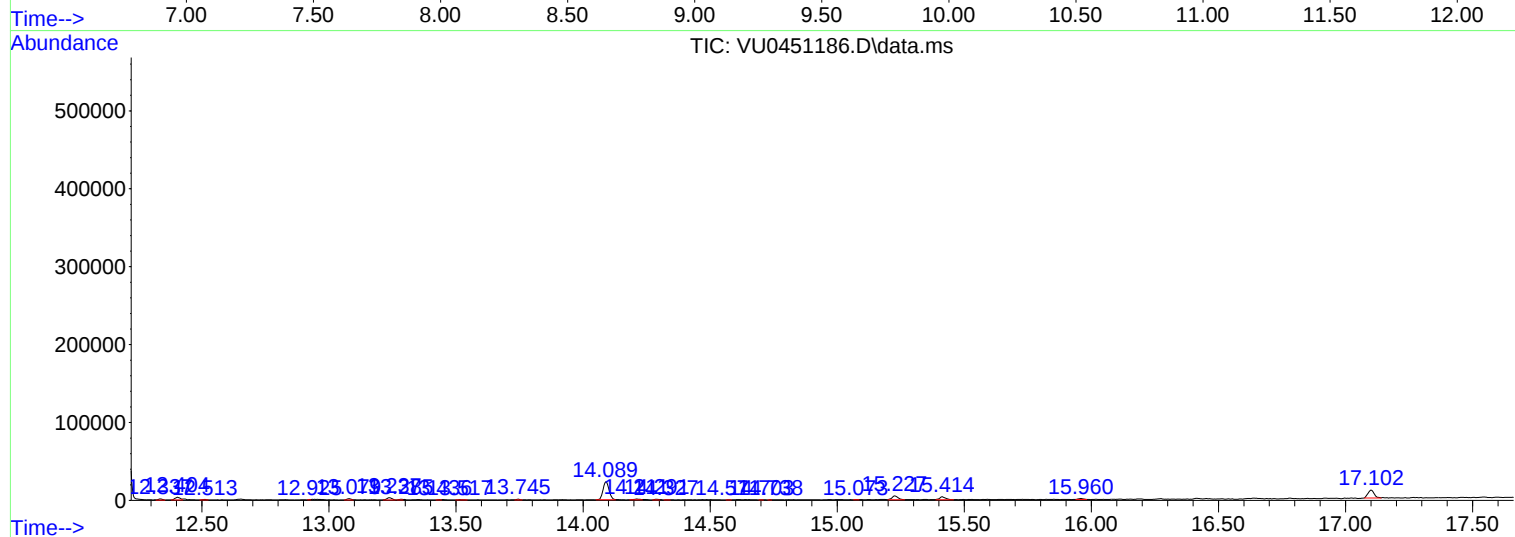
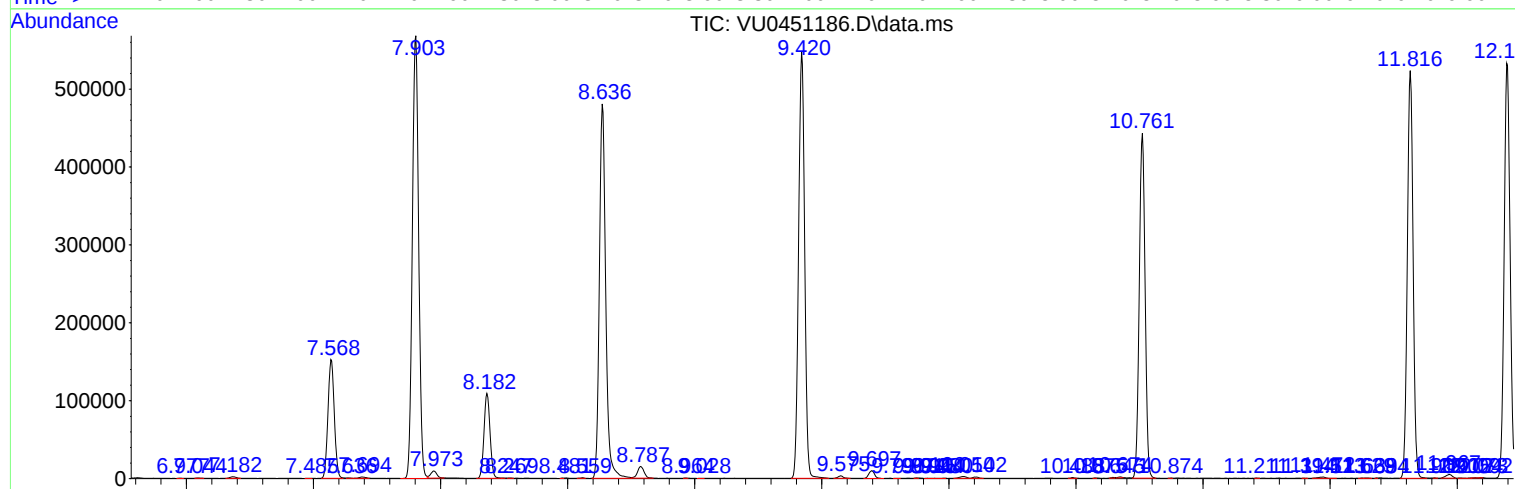
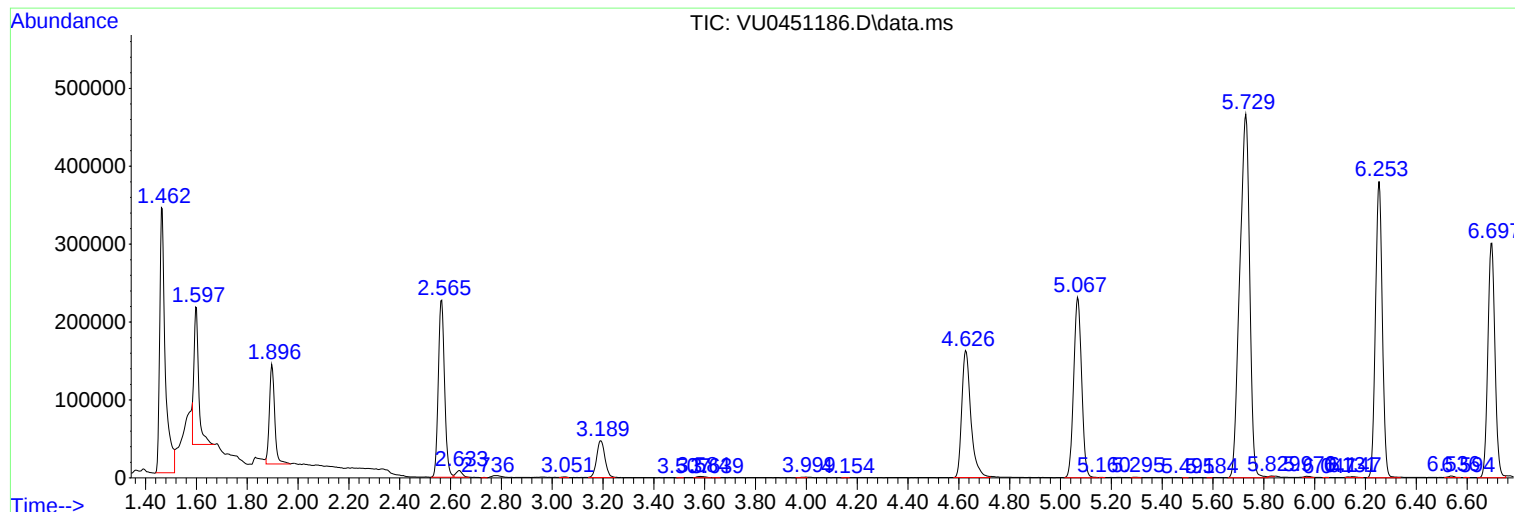
Sum of corrected areas: 10657152

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COAM8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AM8

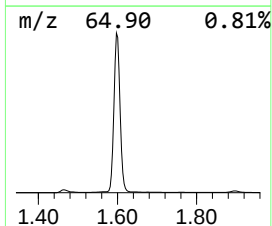
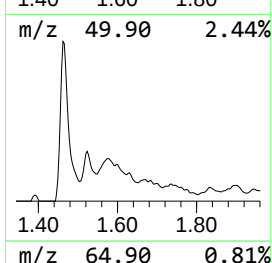
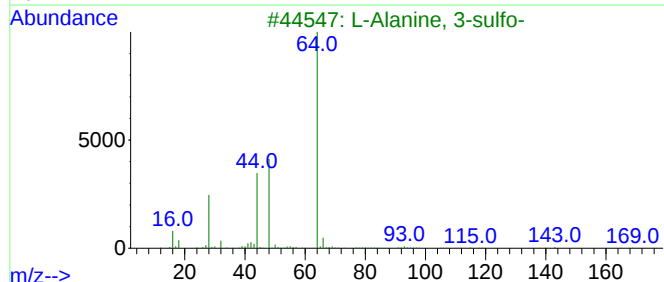
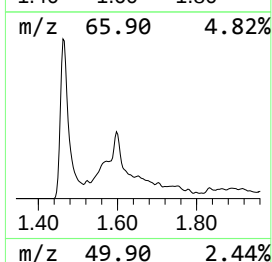
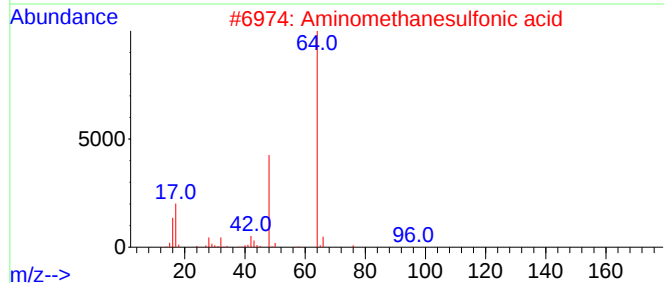
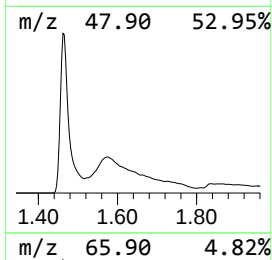
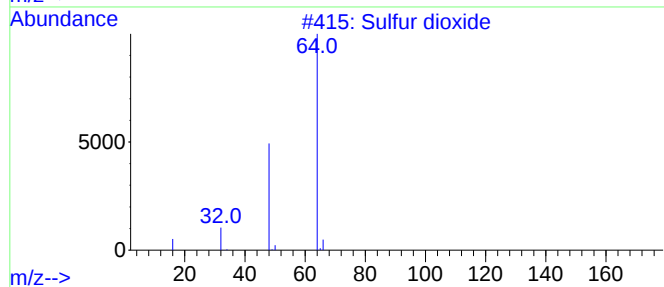
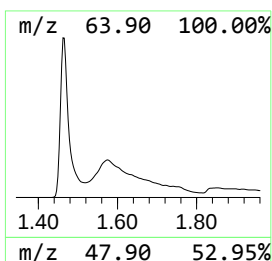
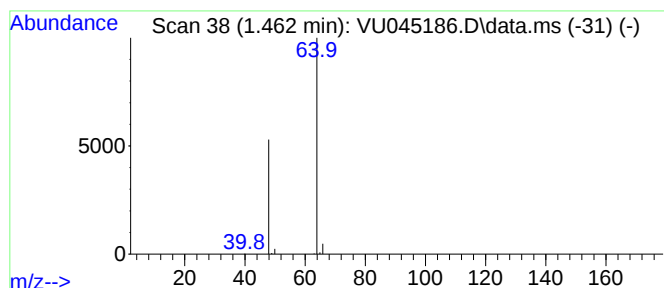
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.462	36.38 ug/L	517749	1,4-Difluorobenzene	6.253

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



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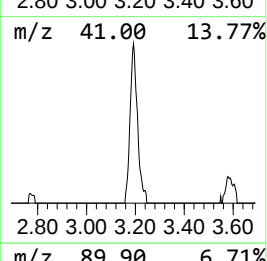
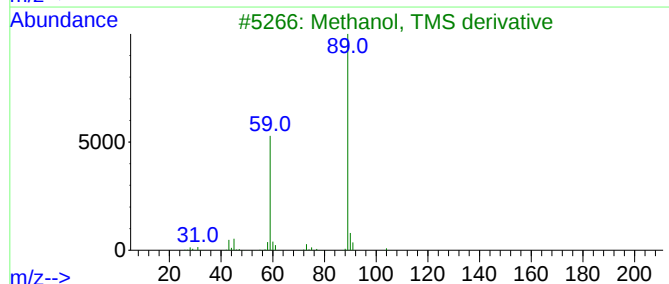
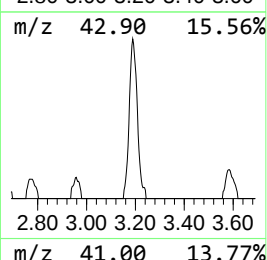
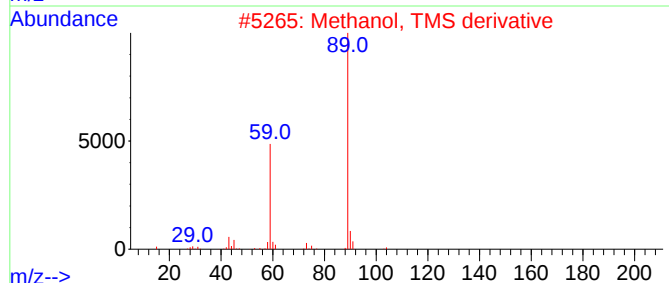
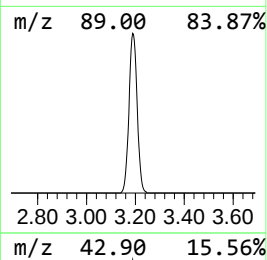
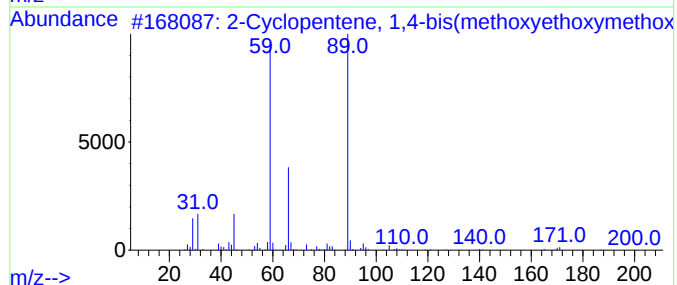
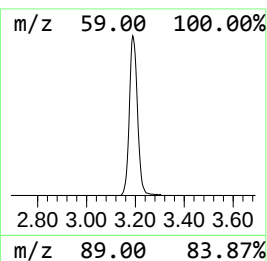
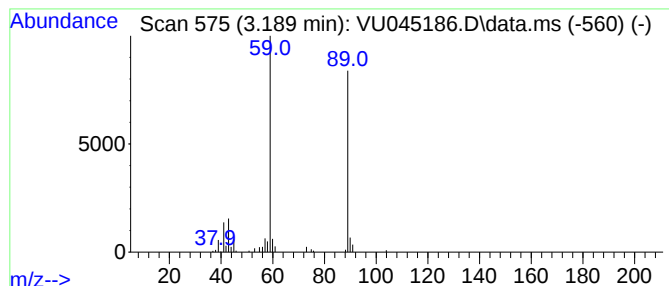
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Cyclopentene, 1,4-bis(met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	7.51 ug/L	106826	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclopentene, 1,4-bis(methoxye...	276	C13H24O6	1000156-00-3	83
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	80
3			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	80
4			3-(2-Methoxyethoxymethoxy)-2-met...	206	C10H22O4	097991-45-2	74
5			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	74



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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	1.462	36.4	ug/L	517749	1	6.253	711489	50.0
2-Cyclopentene,...	3.189	7.5	ug/L	106826	1	6.253	711489	50.0