

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045183.D
 Acq On : 06 Oct 2021 14:15
 Operator : SY/MD
 Sample : M3996-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A17

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: VU0451183.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.479	34	43	54	rBV	30853	79016	5.87%	0.737%
2	1.601	75	81	94	rVB	214018	236644	17.57%	2.208%
3	1.903	167	175	194	rVB	148559	212867	15.80%	1.986%
4	2.565	368	381	396	rBV	287261	478547	35.53%	4.466%
5	2.633	397	402	413	rVB	5456	8585	0.64%	0.080%
6	2.675	413	415	417	rBV	222	121	0.01%	0.001%
7	2.687	417	419	425	rVB3	504	367	0.03%	0.003%
8	2.729	428	432	437	rBV2	365	362	0.03%	0.003%
9	2.797	442	453	463	rBV2	2824	6540	0.49%	0.061%
10	3.192	561	576	592	rVB	19273	44035	3.27%	0.411%
11	3.842	774	778	780	rBV2	190	180	0.01%	0.002%
12	3.906	795	798	803	rBV	150	184	0.01%	0.002%
13	3.993	820	825	832	rBV2	448	567	0.04%	0.005%
14	4.096	854	857	868	rVB2	230	222	0.02%	0.002%
15	4.626	1007	1022	1053	rBV	145824	367337	27.27%	3.428%
16	4.957	1121	1125	1128	rBV2	253	183	0.01%	0.002%
17	5.067	1143	1159	1185	rBV	238318	521535	38.72%	4.867%
18	5.205	1198	1202	1204	rBV3	253	190	0.01%	0.002%
19	5.221	1204	1207	1210	rVB3	439	273	0.02%	0.003%
20	5.289	1219	1228	1231	rBV2	808	1126	0.08%	0.011%
21	5.385	1251	1258	1265	rBV4	402	565	0.04%	0.005%
22	5.617	1326	1330	1332	rBV2	190	171	0.01%	0.002%
23	5.729	1343	1365	1395	rBV2	501411	1346896	100.00%	12.568%
24	6.047	1459	1464	1470	rBV4	207	262	0.02%	0.002%
25	6.115	1481	1485	1494	rVB3	337	538	0.04%	0.005%
26	6.253	1513	1528	1548	rVV	377241	707359	52.52%	6.601%
27	6.346	1554	1557	1561	rBV3	324	201	0.01%	0.002%
28	6.543	1608	1618	1630	rVB6	6280	11481	0.85%	0.107%
29	6.594	1630	1634	1635	rBV2	231	135	0.01%	0.001%
30	6.697	1650	1666	1687	rBV	313875	612031	45.44%	5.711%
31	6.858	1713	1716	1718	rVB2	257	135	0.01%	0.001%
32	6.912	1732	1733	1738	rVB2	256	175	0.01%	0.002%
33	6.941	1738	1742	1745	rBV2	163	158	0.01%	0.001%
34	6.973	1750	1752	1755	rVB2	187	124	0.01%	0.001%
35	6.999	1755	1760	1762	rBV	225	173	0.01%	0.002%
36	7.041	1769	1773	1774	rBV	384	295	0.02%	0.003%

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Integrator: RTE

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

37	7.109	1786	1794	1805	rBV3	3076	4898	0.36%	0.046%
38	7.176	1811	1815	1816	rBV	608	533	0.04%	0.005%
39	7.250	1833	1838	1841	rBV	213	220	0.02%	0.002%
40	7.330	1856	1863	1866	rBV2	190	292	0.02%	0.003%
41	7.366	1870	1874	1877	rBV	257	281	0.02%	0.003%
42	7.491	1910	1913	1916	rBV2	176	184	0.01%	0.002%
43	7.568	1924	1937	1954	rBV	175900	305204	22.66%	2.848%
44	7.797	2004	2008	2017	rVB2	601	769	0.06%	0.007%
45	7.903	2026	2041	2056	rBV	616364	1054678	78.30%	9.842%
46	7.973	2057	2063	2073	rVB	9012	13809	1.03%	0.129%
47	8.182	2116	2128	2146	rBV	125079	202933	15.07%	1.894%
48	8.372	2184	2187	2191	rBV2	174	120	0.01%	0.001%
49	8.398	2192	2195	2200	rVB2	149	129	0.01%	0.001%
50	8.555	2231	2244	2257	rBV	289488	489819	36.37%	4.571%
51	8.636	2257	2269	2308	rVB	419882	730267	54.22%	6.814%
52	8.842	2331	2333	2335	rBV2	264	123	0.01%	0.001%
53	9.009	2383	2385	2391	rVB2	280	206	0.02%	0.002%
54	9.038	2391	2394	2398	rBV2	201	213	0.02%	0.002%
55	9.102	2411	2414	2417	rBV	187	177	0.01%	0.002%
56	9.144	2424	2427	2430	rBV2	227	204	0.02%	0.002%
57	9.179	2435	2438	2441	rVV2	192	174	0.01%	0.002%
58	9.372	2494	2498	2500	rBV2	222	182	0.01%	0.002%
59	9.420	2500	2513	2550	rVB	547538	882755	65.54%	8.237%
60	9.578	2558	2562	2565	rVB3	289	173	0.01%	0.002%
61	9.697	2591	2599	2609	rVB3	2676	3645	0.27%	0.034%
62	9.835	2639	2642	2645	rBV2	186	163	0.01%	0.002%
63	10.034	2700	2704	2706	rBV	196	207	0.02%	0.002%
64	10.105	2722	2726	2729	rBV2	367	271	0.02%	0.003%
65	10.144	2733	2738	2741	rBV	151	198	0.01%	0.002%
66	10.214	2754	2760	2761	rBV	251	274	0.02%	0.003%
67	10.388	2812	2814	2821	rBV2	165	202	0.01%	0.002%
68	10.423	2821	2825	2829	rVB2	182	195	0.01%	0.002%
69	10.446	2829	2832	2839	rVB2	214	228	0.02%	0.002%
70	10.478	2839	2842	2845	rBV	179	164	0.01%	0.002%
71	10.520	2852	2855	2857	rBV	185	129	0.01%	0.001%
72	10.674	2895	2903	2911	rBV2	4024	5709	0.42%	0.053%
73	10.761	2917	2930	2951	rBV	430853	688767	51.14%	6.427%
74	10.874	2959	2965	2971	rBV4	613	909	0.07%	0.008%
75	10.903	2971	2974	2977	rVB2	561	360	0.03%	0.003%
76	11.086	3027	3031	3033	rBV	194	162	0.01%	0.002%

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Instrument :
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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoother: 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

77	11.121	3036	3042	3048	rVV3	721	1016	0.08%	0.009%
78	11.153	3048	3052	3056	rVB3	527	435	0.03%	0.004%
79	11.256	3081	3084	3086	rBV	240	177	0.01%	0.002%
80	11.327	3101	3106	3109	rBV2	262	265	0.02%	0.002%
81	11.369	3116	3119	3124	rVB2	245	169	0.01%	0.002%
82	11.459	3140	3147	3158	rVB6	2489	4028	0.30%	0.038%
83	11.523	3164	3167	3169	rBV	153	122	0.01%	0.001%
84	11.578	3180	3184	3187	rBV3	503	462	0.03%	0.004%
85	11.697	3214	3221	3232	rVB3	1518	2099	0.16%	0.020%
86	11.816	3245	3258	3278	rVV	494794	780725	57.96%	7.285%
87	11.890	3278	3281	3283	rBV3	295	216	0.02%	0.002%
88	11.980	3302	3309	3316	rVB4	2395	3363	0.25%	0.031%
89	12.070	3324	3337	3348	rBV4	2228	4170	0.31%	0.039%
90	12.195	3360	3376	3398	rBV	544661	886466	65.82%	8.272%
91	12.327	3413	3417	3419	rBV2	655	576	0.04%	0.005%
92	12.394	3434	3438	3440	rBV2	402	339	0.03%	0.003%
93	12.642	3506	3515	3519	rVB3	449	578	0.04%	0.005%
94	12.661	3519	3521	3523	rVV2	230	135	0.01%	0.001%
95	12.684	3526	3528	3537	rVB2	240	283	0.02%	0.003%
96	12.803	3562	3565	3568	rBV	281	225	0.02%	0.002%
97	13.343	3726	3733	3736	rBV2	222	331	0.02%	0.003%
98	13.716	3847	3849	3852	rVB	202	131	0.01%	0.001%
99	14.205	3998	4001	4005	rBV2	252	203	0.02%	0.002%
100	16.581	4737	4740	4742	rBV2	737	468	0.03%	0.004%

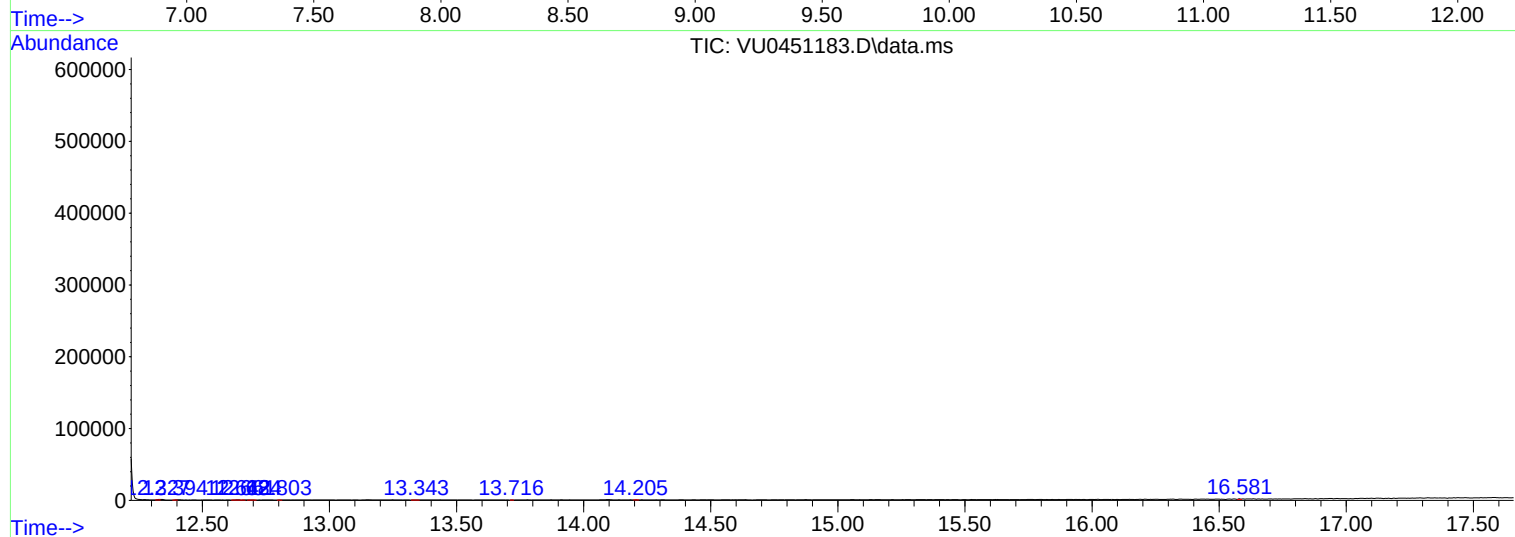
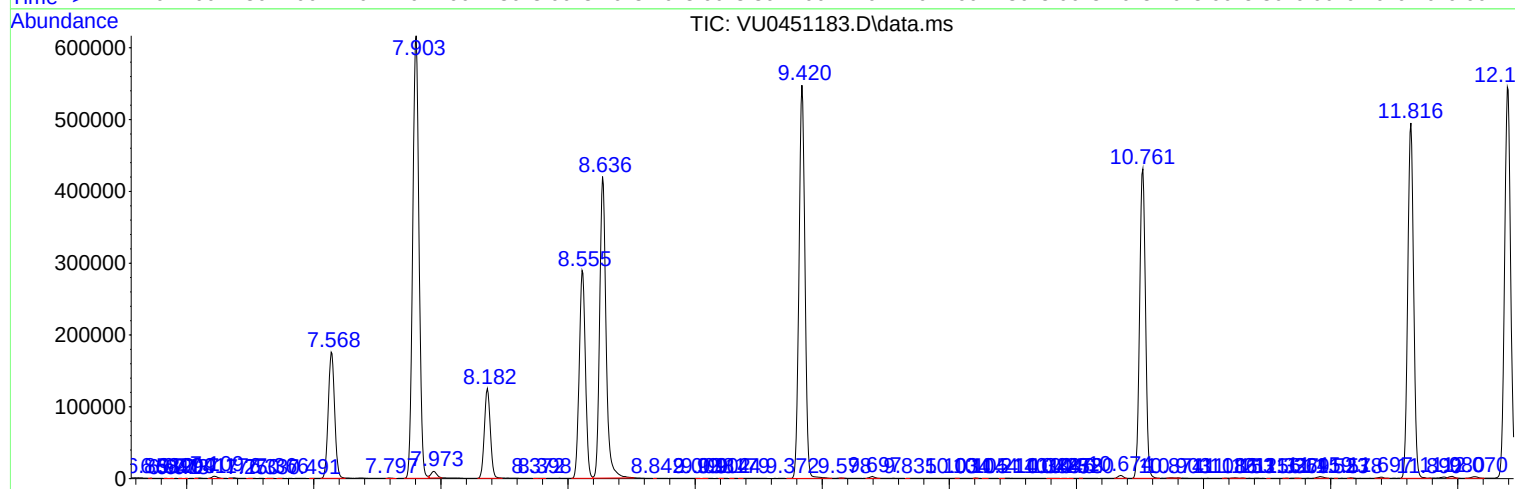
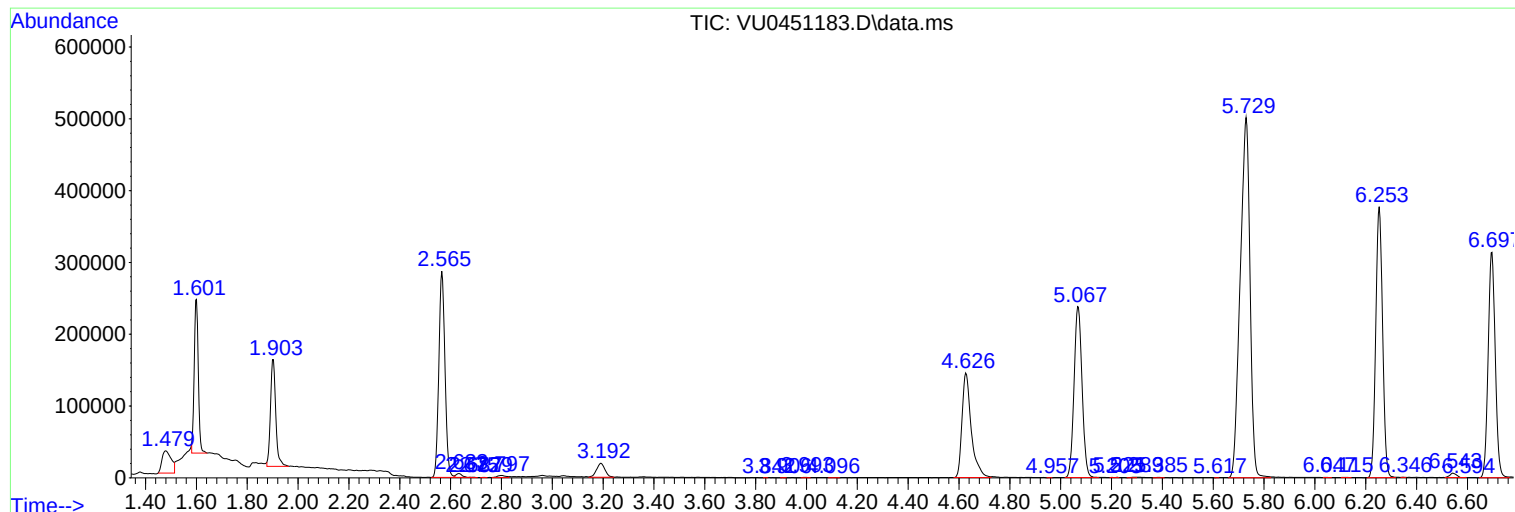
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MSVOA_U
ClientSampled :
F4A17

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 : 12 Sample Multiplier: 1

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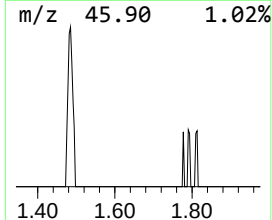
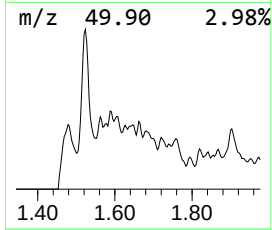
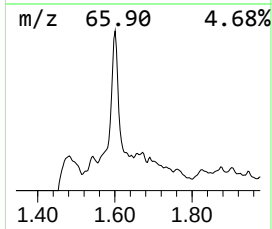
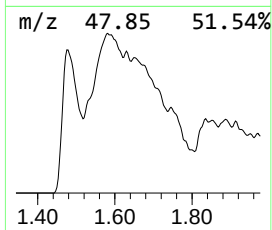
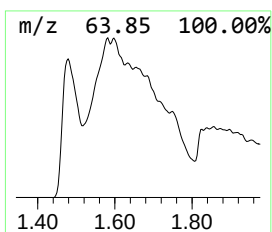
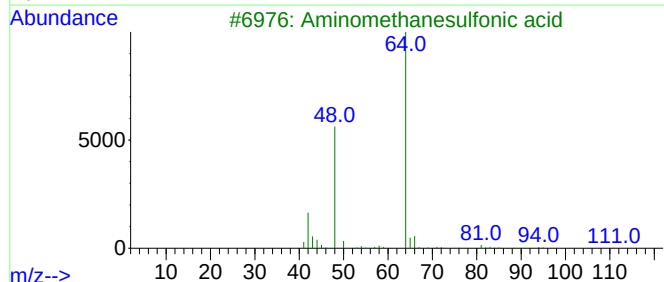
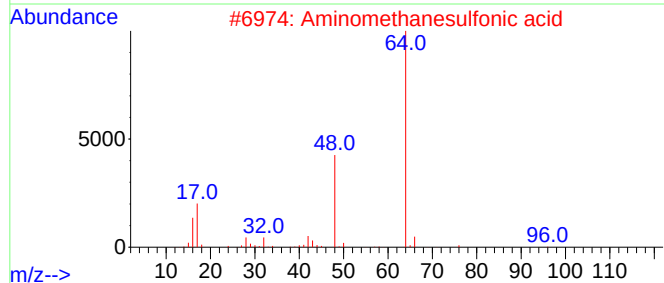
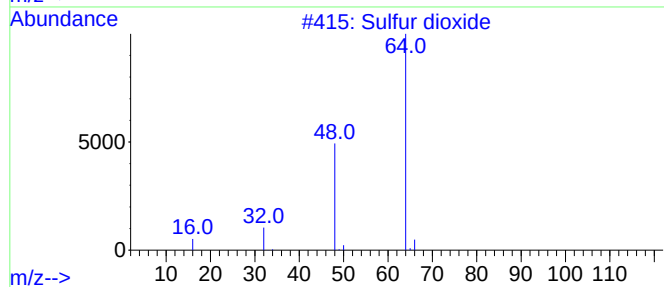
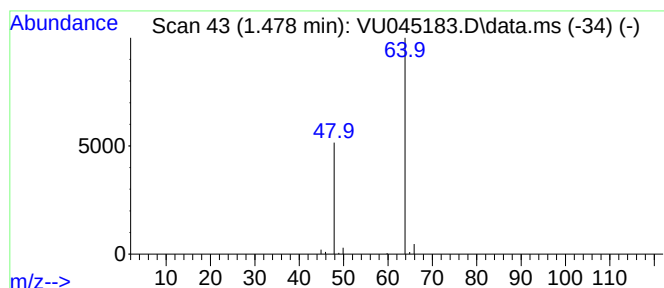
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	5.59 ug/L	79016	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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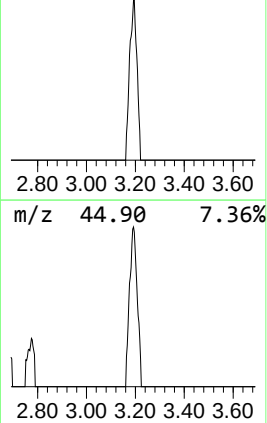
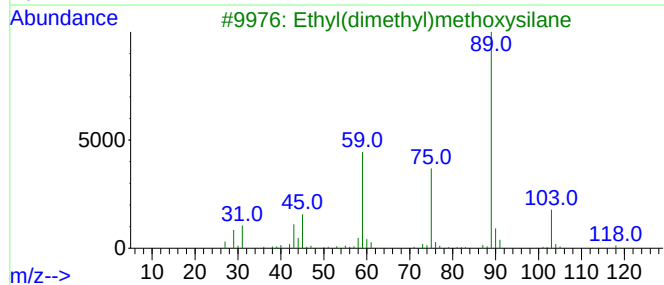
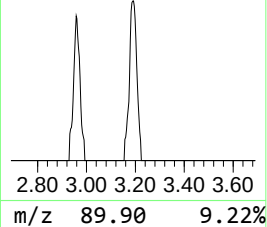
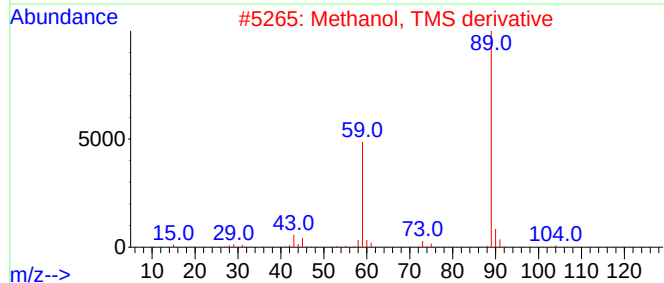
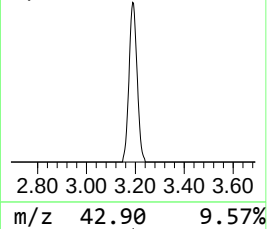
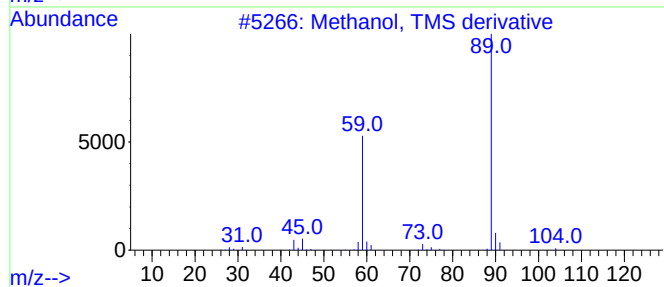
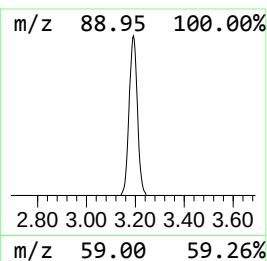
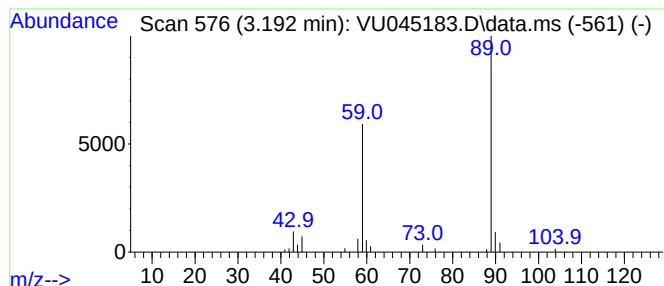
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Methanol, TMS derivative Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.192	3.11 ug/L	44035	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	91
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	91
3			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	83
4			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	74
5			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	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	1.478	5.6	ug/L	79016	1	6.253	707359	50.0
Methanol, TMS d...	3.192	3.1	ug/L	44035	1	6.253	707359	50.0