

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045247.D
 Acq On : 08 Oct 2021 13:30
 Operator : SY/MD
 Sample : M4025-14DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN7DL

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: VU045247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	32	41	53	rBV2	87265	125597	9.58%	1.106%
2	1.600	74	81	101	rVB	157875	178199	13.60%	1.569%
3	1.890	163	171	184	rVB	125764	168636	12.87%	1.484%
4	2.562	366	380	399	rBV2	260807	477140	36.41%	4.200%
5	2.777	439	447	458	rBV3	1487	2938	0.22%	0.026%
6	2.948	495	500	502	rBV	375	363	0.03%	0.003%
7	3.047	521	531	544	rVB3	5250	9258	0.71%	0.081%
8	3.189	559	575	596	rVB	30299	69063	5.27%	0.608%
9	3.359	624	628	630	rBV2	251	231	0.02%	0.002%
10	3.555	686	689	693	rVB2	199	189	0.01%	0.002%
11	3.658	715	721	725	rBV2	161	177	0.01%	0.002%
12	3.755	748	751	754	rVB2	220	150	0.01%	0.001%
13	3.780	754	759	764	rBV2	165	151	0.01%	0.001%
14	3.838	773	777	779	rVV2	281	206	0.02%	0.002%
15	3.870	779	787	799	rVV2	1444	2658	0.20%	0.023%
16	4.002	821	828	830	rBV2	213	244	0.02%	0.002%
17	4.108	858	861	868	rBV2	139	202	0.02%	0.002%
18	4.150	870	874	875	rBV	179	158	0.01%	0.001%
19	4.234	897	900	905	rVV	159	171	0.01%	0.002%
20	4.260	905	908	914	rVV2	193	202	0.02%	0.002%
21	4.327	924	929	933	rVB2	156	157	0.01%	0.001%
22	4.485	974	978	981	rBV2	161	140	0.01%	0.001%
23	4.629	1007	1023	1063	rBV2	159912	499822	38.14%	4.399%
24	4.858	1091	1094	1099	rBV3	163	149	0.01%	0.001%
25	4.986	1131	1134	1139	rVB3	309	274	0.02%	0.002%
26	5.067	1142	1159	1181	rVV	235781	508077	38.77%	4.472%
27	5.221	1200	1207	1211	rBV2	506	669	0.05%	0.006%
28	5.317	1223	1237	1252	rVV2	22611	49281	3.76%	0.434%
29	5.597	1319	1324	1327	rBV2	186	210	0.02%	0.002%
30	5.729	1343	1365	1384	rBV2	484651	1310350	100.00%	11.534%
31	5.980	1440	1443	1445	rBV3	217	156	0.01%	0.001%
32	6.034	1457	1460	1467	rVB4	271	316	0.02%	0.003%
33	6.089	1475	1477	1482	rVB2	260	176	0.01%	0.002%
34	6.115	1482	1485	1487	rBV2	240	141	0.01%	0.001%
35	6.253	1513	1528	1546	rBV	353342	657205	50.15%	5.785%
36	6.446	1582	1588	1592	rBV2	234	342	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045247.D
 Acq On : 08 Oct 2021 13:30
 Operator : SY/MD
 Sample : M4025-14DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN7DL

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

37	6.468	1593	1595	1600	rVB2	232	157	0.01%	0.001%
38	6.546	1600	1619	1642	rBV	655467	1231384	93.97%	10.839%
39	6.697	1651	1666	1685	rVB	314442	605461	46.21%	5.329%
40	6.803	1693	1699	1701	rBV4	534	491	0.04%	0.004%
41	7.047	1769	1775	1784	rBV4	663	1157	0.09%	0.010%
42	7.182	1805	1817	1827	rBV3	3003	4948	0.38%	0.044%
43	7.398	1881	1884	1890	rVB2	149	167	0.01%	0.001%
44	7.568	1923	1937	1955	rBV	169760	293278	22.38%	2.581%
45	7.690	1967	1975	1990	rVB3	1853	3416	0.26%	0.030%
46	7.825	2013	2017	2021	rBV2	126	139	0.01%	0.001%
47	7.902	2026	2041	2056	rBV	593213	1008011	76.93%	8.873%
48	7.970	2056	2062	2073	rVB2	7966	13564	1.04%	0.119%
49	8.060	2087	2090	2092	rBV3	185	139	0.01%	0.001%
50	8.095	2099	2101	2103	rBV	229	142	0.01%	0.001%
51	8.182	2115	2128	2150	rBV	118645	195920	14.95%	1.725%
52	8.404	2193	2197	2202	rVB3	711	677	0.05%	0.006%
53	8.475	2215	2219	2222	rBV2	217	183	0.01%	0.002%
54	8.536	2233	2238	2241	rBV2	159	150	0.01%	0.001%
55	8.555	2241	2244	2249	rVB2	172	155	0.01%	0.001%
56	8.639	2256	2270	2301	rBV	436181	783405	59.79%	6.896%
57	9.025	2382	2390	2393	rBV2	149	232	0.02%	0.002%
58	9.131	2420	2423	2427	rVB2	144	131	0.01%	0.001%
59	9.172	2432	2436	2440	rVB2	143	148	0.01%	0.001%
60	9.420	2499	2513	2533	rBV	500192	818290	62.45%	7.203%
61	9.536	2546	2549	2552	rVB2	284	185	0.01%	0.002%
62	9.574	2554	2561	2567	rVB3	654	905	0.07%	0.008%
63	9.693	2589	2598	2606	rBV3	2724	3773	0.29%	0.033%
64	9.793	2625	2629	2634	rBV2	216	293	0.02%	0.003%
65	9.957	2674	2680	2684	rVB2	282	381	0.03%	0.003%
66	9.983	2684	2688	2691	rBV	238	225	0.02%	0.002%
67	10.002	2691	2694	2696	rBV	192	150	0.01%	0.001%
68	10.105	2721	2726	2732	rVB3	551	727	0.06%	0.006%
69	10.304	2784	2788	2791	rVB	176	148	0.01%	0.001%
70	10.330	2791	2796	2799	rBV	184	165	0.01%	0.001%
71	10.571	2867	2871	2878	rBV	198	242	0.02%	0.002%
72	10.677	2895	2904	2912	rVB3	1861	2817	0.21%	0.025%
73	10.761	2917	2930	2949	rVB	458873	728787	55.62%	6.415%
74	10.835	2949	2953	2958	rBV	245	261	0.02%	0.002%
75	10.873	2958	2965	2970	rBV2	580	781	0.06%	0.007%
76	10.947	2986	2988	2990	rBV2	214	145	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045247.D
 Acq On : 08 Oct 2021 13:30
 Operator : SY/MD
 Sample : M4025-14DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN7DL

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

77	11.118	3038	3041	3045	rBV3	290	212	0.02%	0.002%
78	11.330	3103	3107	3111	rBV2	200	235	0.02%	0.002%
79	11.465	3139	3149	3157	rVB3	1613	2607	0.20%	0.023%
80	11.629	3197	3200	3209	rVB3	460	529	0.04%	0.005%
81	11.700	3215	3222	3230	rVV4	929	1332	0.10%	0.012%
82	11.751	3235	3238	3242	rVB2	176	139	0.01%	0.001%
83	11.815	3245	3258	3281	rVV	459990	716710	54.70%	6.309%
84	11.951	3293	3300	3303	rVV5	1027	1356	0.10%	0.012%
85	11.973	3303	3307	3315	rVB4	1772	2327	0.18%	0.020%
86	12.195	3361	3376	3394	rVV	530032	865549	66.05%	7.619%
87	12.394	3435	3438	3439	rBV	295	152	0.01%	0.001%
88	12.542	3481	3484	3486	rBV2	217	150	0.01%	0.001%
89	12.639	3511	3514	3517	rBV2	189	142	0.01%	0.001%
90	12.777	3555	3557	3559	rBV	193	136	0.01%	0.001%
91	12.809	3564	3567	3569	rBV	194	139	0.01%	0.001%
92	13.195	3684	3687	3692	rBV	208	188	0.01%	0.002%
93	13.221	3692	3695	3699	rVV2	190	171	0.01%	0.002%
94	13.375	3738	3743	3746	rBV	182	195	0.01%	0.002%
95	13.552	3794	3798	3799	rBV	306	183	0.01%	0.002%
96	13.716	3840	3849	3856	rBV2	284	595	0.05%	0.005%
97	14.098	3960	3968	3976	rVB2	1101	1904	0.15%	0.017%
98	14.227	4005	4008	4010	rBV	278	234	0.02%	0.002%
99	14.539	4101	4105	4112	rBV3	343	395	0.03%	0.003%
100	14.574	4113	4116	4117	rBV	301	178	0.01%	0.002%

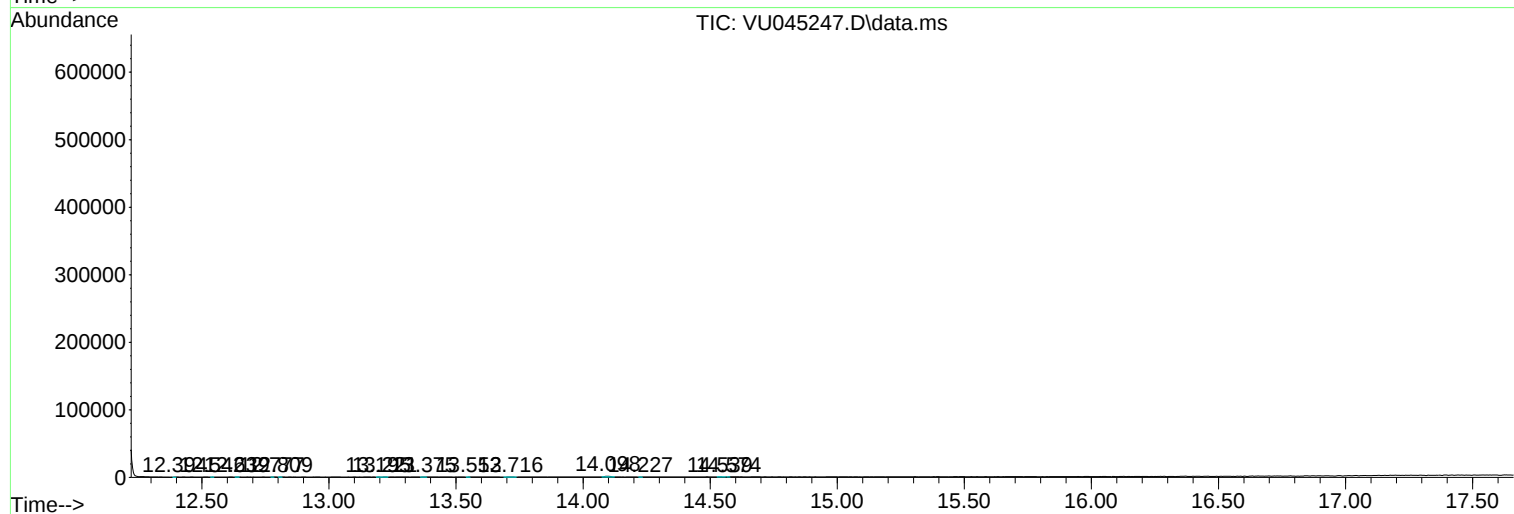
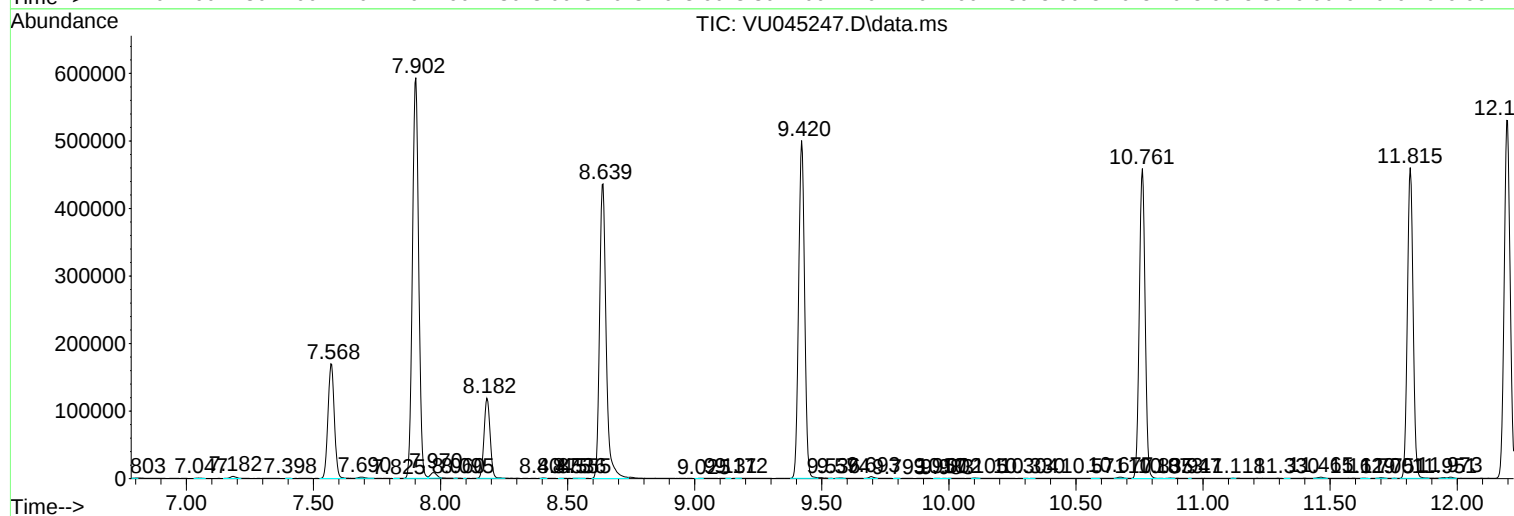
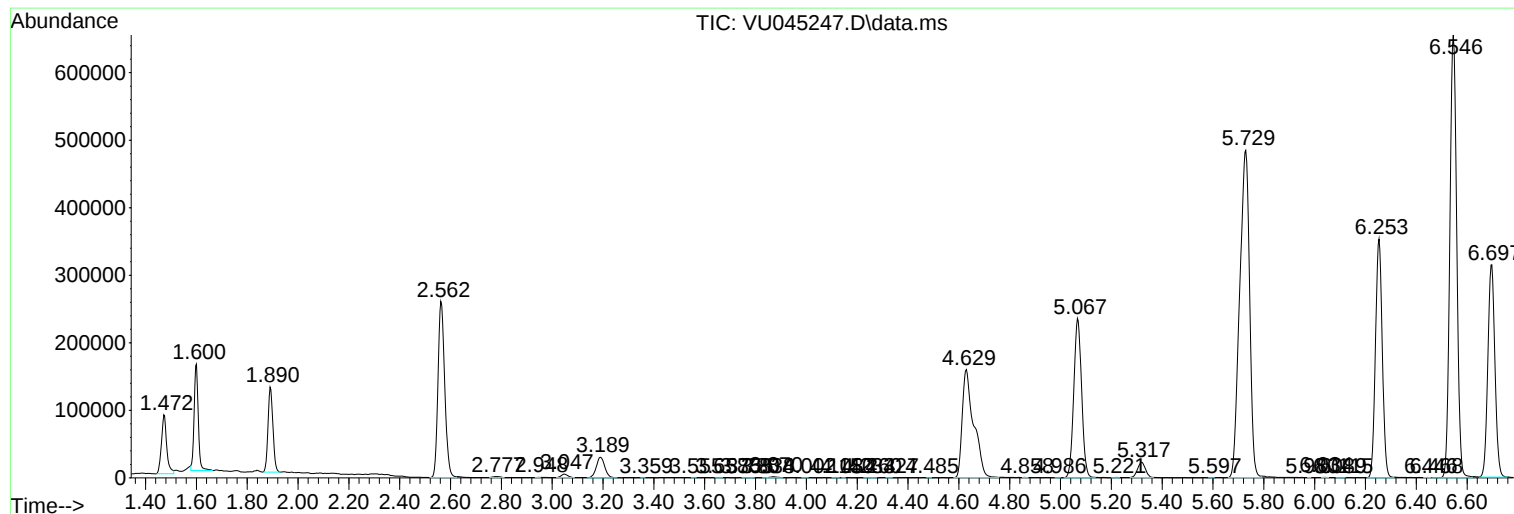
Sum of corrected areas: 11360886

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045247.D
Acq On : 08 Oct 2021 13:30
Operator : SY/MD
Sample : M4025-14DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AN7DL

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045247.D
Acq On : 08 Oct 2021 13:30
Operator : SY/MD
Sample : M4025-14DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AN7DL

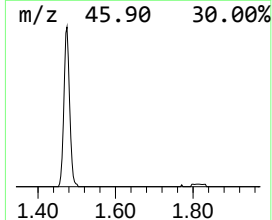
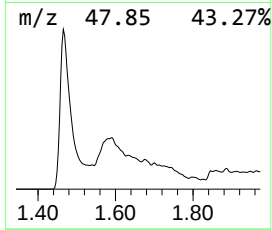
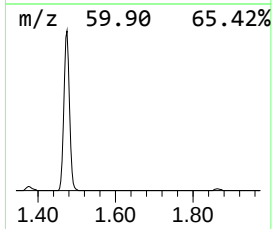
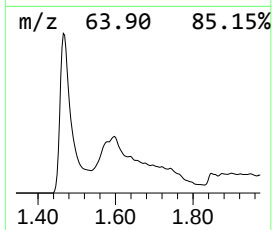
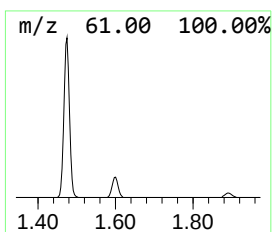
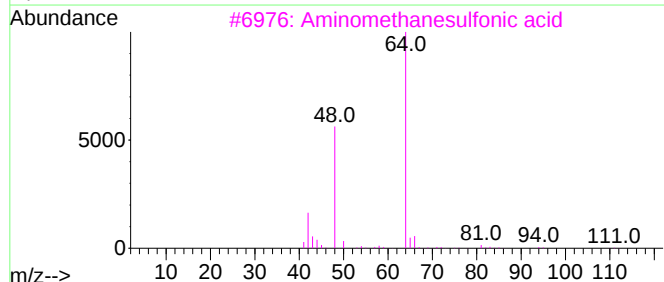
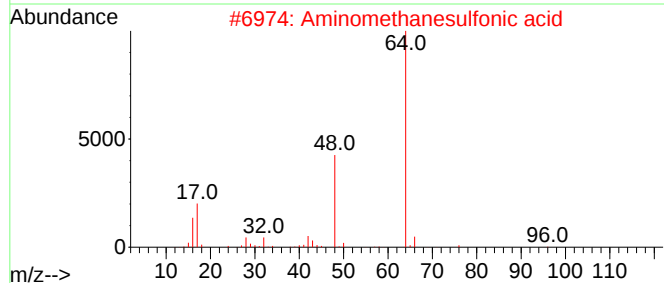
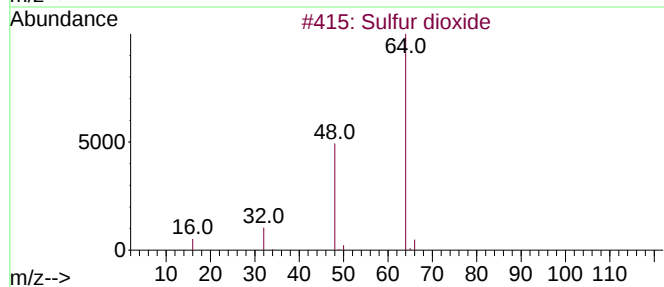
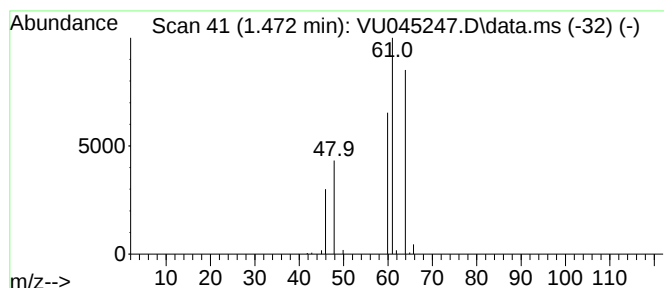
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.472	9.56 ug/L	125597	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	58
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	36
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	36
4			Pentaborane(11)	66	B5H11	018433-84-6	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045247.D
Acq On : 08 Oct 2021 13:30
Operator : SY/MD
Sample : M4025-14DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AN7DL

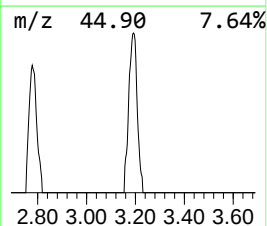
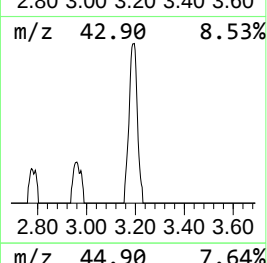
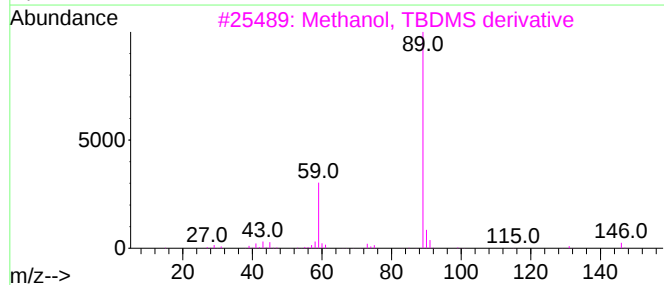
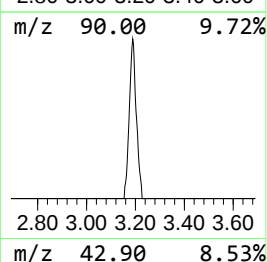
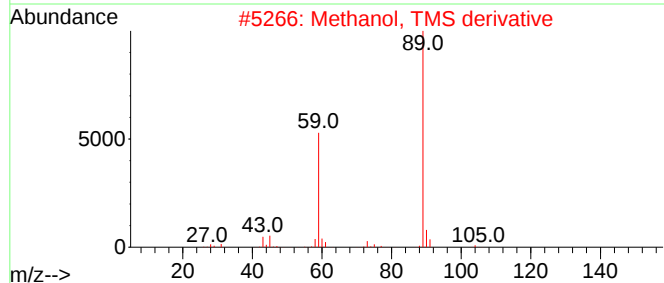
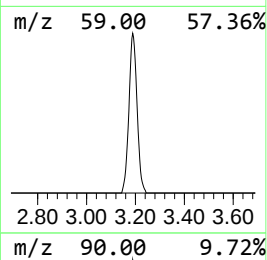
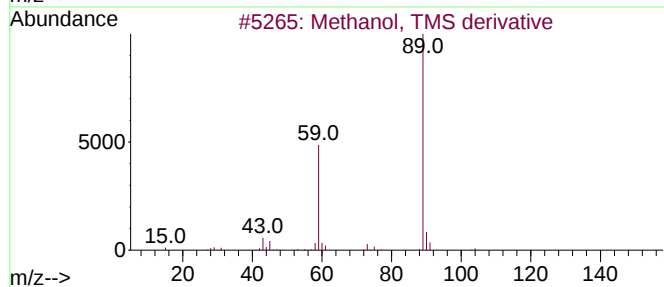
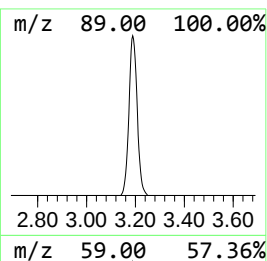
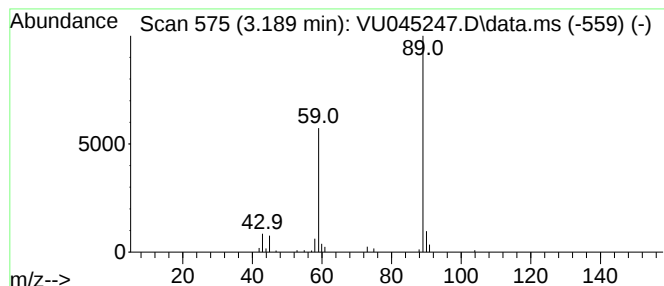
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
3.189	5.25 ug/L	69063	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			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
4			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	74
5			Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045247.D
Acq On : 08 Oct 2021 13:30
Operator : SY/MD
Sample : M4025-14DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AN7DL

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.472	9.6	ug/L	125597	1	6.253	657205	50.0
Methanol, TMS d...	3.189	5.3	ug/L	69063	1	6.253	657205	50.0