

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045262.D
 Acq On : 08 Oct 2021 19:26
 Operator : SY/MD
 Sample : M4026-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP7

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: VU045262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	33	40	54	rBV	23951	46092	3.49%	0.471%
2	1.600	74	81	92	rVB	203650	220722	16.71%	2.256%
3	1.896	165	173	184	rVB	142107	187411	14.19%	1.915%
4	2.562	367	380	397	rBV	272085	456501	34.57%	4.666%
5	2.739	431	435	437	rBV	301	226	0.02%	0.002%
6	2.784	437	449	462	rVV3	7143	15187	1.15%	0.155%
7	2.951	496	501	502	rBV2	501	427	0.03%	0.004%
8	2.986	510	512	517	rVB2	169	123	0.01%	0.001%
9	3.044	526	530	534	rBV3	762	879	0.07%	0.009%
10	3.192	561	576	594	rBV2	17287	41022	3.11%	0.419%
11	3.285	602	605	610	rBV2	153	174	0.01%	0.002%
12	3.353	622	626	629	rBV	228	221	0.02%	0.002%
13	3.423	645	648	652	rBV2	216	201	0.02%	0.002%
14	3.472	660	663	666	rBV2	148	152	0.01%	0.002%
15	3.603	701	704	710	rVB2	176	165	0.01%	0.002%
16	3.632	710	713	718	rBV2	251	188	0.01%	0.002%
17	3.671	720	725	732	rBV2	206	280	0.02%	0.003%
18	3.751	747	750	752	rBV	193	166	0.01%	0.002%
19	3.835	773	776	780	rBV2	222	234	0.02%	0.002%
20	3.896	792	795	797	rBV	172	150	0.01%	0.002%
21	3.948	808	811	813	rBV	166	126	0.01%	0.001%
22	3.996	824	826	831	rVB2	207	134	0.01%	0.001%
23	4.025	831	835	837	rBV	164	142	0.01%	0.001%
24	4.089	852	855	861	rVB	172	207	0.02%	0.002%
25	4.205	885	891	893	rBV2	162	224	0.02%	0.002%
26	4.507	980	985	989	rBV2	164	212	0.02%	0.002%
27	4.629	1007	1023	1050	rBV	146683	344357	26.08%	3.519%
28	4.854	1091	1093	1096	rBV2	208	150	0.01%	0.002%
29	4.915	1109	1112	1117	rBV2	154	173	0.01%	0.002%
30	4.980	1129	1132	1140	rVB	373	409	0.03%	0.004%
31	5.070	1140	1160	1179	rBV	228707	501274	37.96%	5.123%
32	5.201	1199	1201	1202	rBV	484	219	0.02%	0.002%
33	5.295	1223	1230	1237	rVB2	474	858	0.06%	0.009%
34	5.491	1287	1291	1293	rBV2	191	126	0.01%	0.001%
35	5.729	1343	1365	1393	rBV2	493736	1320587	100.00%	13.497%
36	5.964	1434	1438	1443	rBV2	437	512	0.04%	0.005%

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37	6.079	1471	1474	1477	rBV	249	214	0.02%	0.002%
38	6.253	1512	1528	1553	rBV	364415	678578	51.38%	6.935%
39	6.439	1583	1586	1589	rBV2	209	183	0.01%	0.002%
40	6.539	1606	1617	1634	rVB6	3979	7435	0.56%	0.076%
41	6.607	1634	1638	1644	rBB3	179	149	0.01%	0.002%
42	6.697	1651	1666	1690	rBV	309381	596782	45.19%	6.099%
43	6.812	1696	1702	1711	rVB3	717	1165	0.09%	0.012%
44	6.851	1711	1714	1717	rBV	373	196	0.01%	0.002%
45	6.915	1730	1734	1738	rBV2	154	154	0.01%	0.002%
46	7.041	1768	1773	1774	rBV2	311	215	0.02%	0.002%
47	7.182	1811	1817	1826	rVB5	1094	1808	0.14%	0.018%
48	7.378	1873	1878	1880	rBV2	125	126	0.01%	0.001%
49	7.568	1924	1937	1957	rBV	168879	289874	21.95%	2.963%
50	7.687	1971	1974	1975	rBV	490	256	0.02%	0.003%
51	7.774	1997	2001	2005	rVV2	141	167	0.01%	0.002%
52	7.902	2026	2041	2056	rBV	596688	1009502	76.44%	10.317%
53	7.973	2056	2063	2075	rVB	9188	15619	1.18%	0.160%
54	8.182	2116	2128	2144	rBV	118681	194146	14.70%	1.984%
55	8.307	2164	2167	2171	rVB	191	173	0.01%	0.002%
56	8.356	2180	2182	2189	rVB2	284	267	0.02%	0.003%
57	8.407	2189	2198	2204	rBV2	352	459	0.03%	0.005%
58	8.436	2204	2207	2210	rBV	133	122	0.01%	0.001%
59	8.475	2210	2219	2221	rVB3	1114	1281	0.10%	0.013%
60	8.639	2257	2270	2309	rBV	416230	739839	56.02%	7.561%
61	8.992	2377	2380	2385	rVB	226	175	0.01%	0.002%
62	9.246	2456	2459	2464	rBV2	207	195	0.01%	0.002%
63	9.346	2487	2490	2493	rBV	159	159	0.01%	0.002%
64	9.420	2500	2513	2550	rBV	511698	840176	63.62%	8.587%
65	9.571	2554	2560	2568	rVB3	597	851	0.06%	0.009%
66	9.696	2591	2599	2607	rVB2	1583	2300	0.17%	0.024%
67	9.758	2614	2618	2620	rBV	235	224	0.02%	0.002%
68	9.857	2643	2649	2655	rBV2	234	419	0.03%	0.004%
69	10.092	2715	2722	2723	rBV2	298	289	0.02%	0.003%
70	10.108	2724	2727	2732	rVB3	534	426	0.03%	0.004%
71	10.674	2895	2903	2911	rBV2	3249	4452	0.34%	0.046%
72	10.761	2916	2930	2950	rBV	424923	674827	51.10%	6.897%
73	10.877	2957	2966	2969	rBV4	857	1033	0.08%	0.011%
74	10.902	2969	2974	2979	rVV3	898	1061	0.08%	0.011%
75	10.925	2979	2981	2987	rVB2	373	294	0.02%	0.003%
76	10.954	2987	2990	2995	rBV2	139	134	0.01%	0.001%

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77	11.040	3015	3017	3021	rBV2	146	122	0.01%	0.001%
78	11.082	3027	3030	3032	rBV2	172	128	0.01%	0.001%
79	11.121	3037	3042	3046	rVV2	755	803	0.06%	0.008%
80	11.404	3127	3130	3133	rVB	198	128	0.01%	0.001%
81	11.462	3139	3148	3157	rVB4	1980	3565	0.27%	0.036%
82	11.500	3157	3160	3166	rVB2	164	138	0.01%	0.001%
83	11.577	3180	3184	3190	rBV2	550	563	0.04%	0.006%
84	11.696	3215	3221	3228	rBV3	1449	1693	0.13%	0.017%
85	11.815	3245	3258	3273	rBV	459241	724122	54.83%	7.401%
86	11.944	3294	3298	3302	rBV4	849	981	0.07%	0.010%
87	11.979	3303	3309	3318	rVB5	2298	3156	0.24%	0.032%
88	12.085	3339	3342	3347	rVB3	311	280	0.02%	0.003%
89	12.198	3360	3377	3398	rBV	509104	839612	63.58%	8.581%
90	12.291	3404	3406	3413	rVB2	287	238	0.02%	0.002%
91	12.333	3414	3419	3425	rBV4	598	742	0.06%	0.008%
92	12.407	3436	3442	3445	rVB4	427	447	0.03%	0.005%
93	12.635	3509	3513	3520	rBV2	339	515	0.04%	0.005%
94	13.073	3645	3649	3650	rBV	195	156	0.01%	0.002%
95	13.150	3669	3673	3674	rBV	237	183	0.01%	0.002%
96	13.712	3843	3848	3851	rBV2	194	260	0.02%	0.003%
97	14.143	3977	3982	3983	rBV	338	219	0.02%	0.002%
98	14.256	4014	4017	4021	rVB	323	245	0.02%	0.003%
99	14.298	4028	4030	4032	rBV	198	129	0.01%	0.001%
100	14.436	4070	4073	4080	rBV3	258	221	0.02%	0.002%

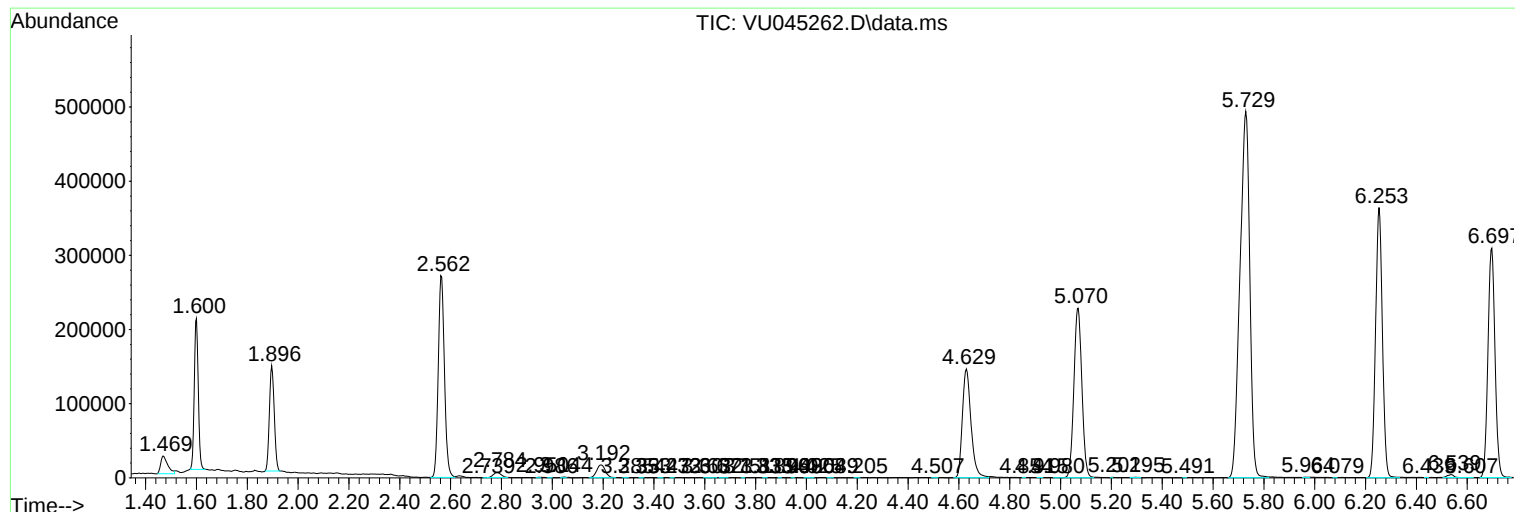
Sum of corrected areas: 9784602

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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



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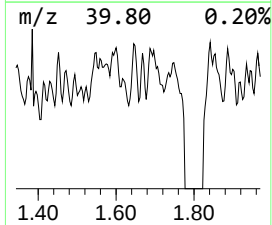
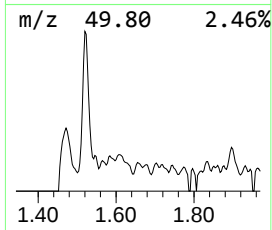
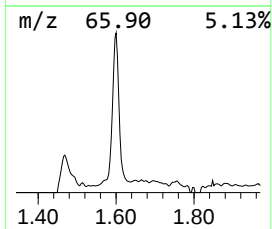
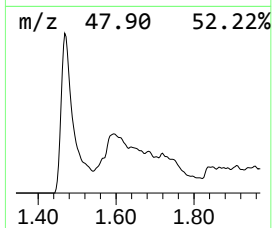
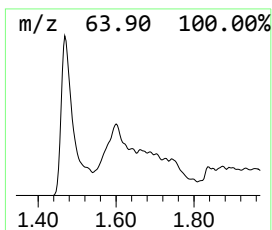
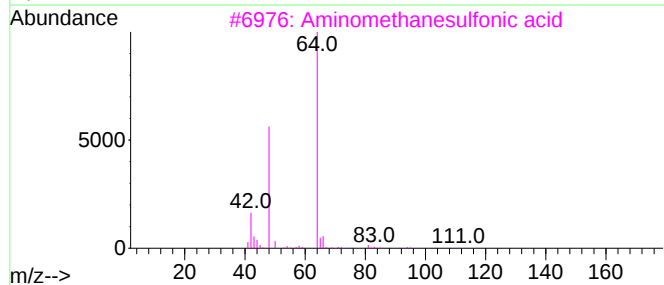
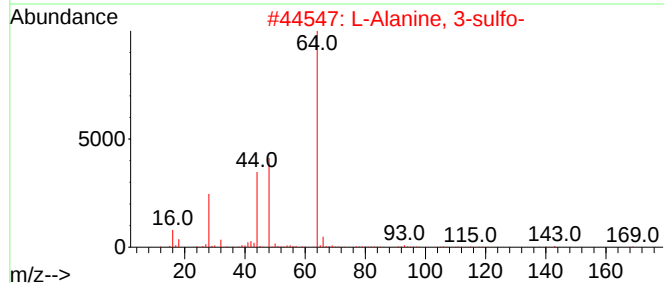
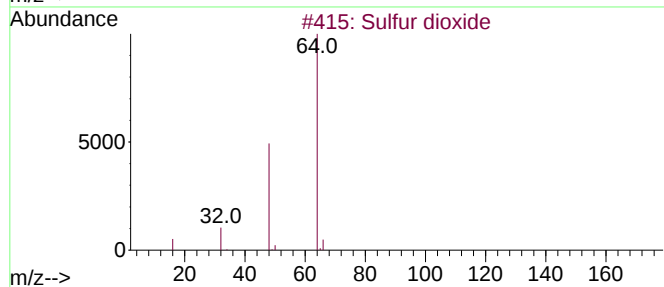
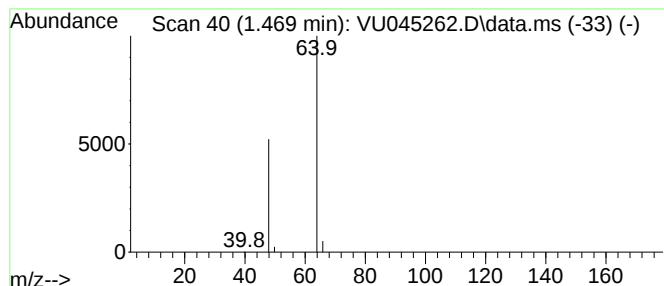
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.469	3.40 ug/L	46092	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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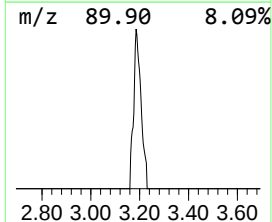
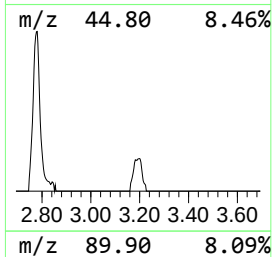
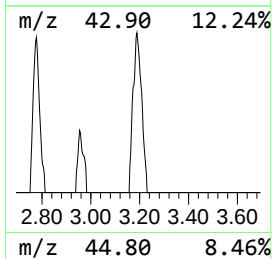
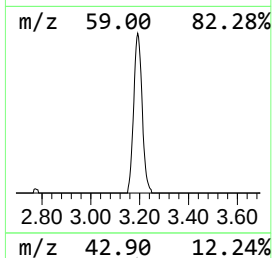
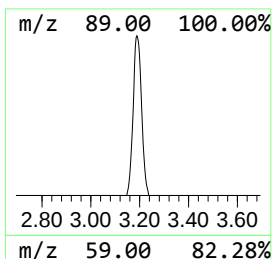
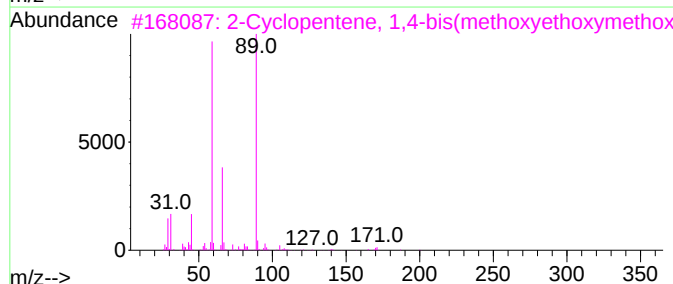
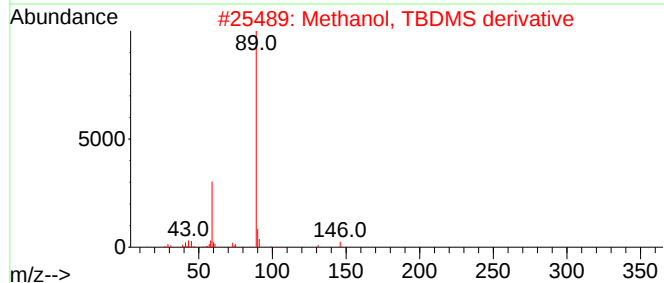
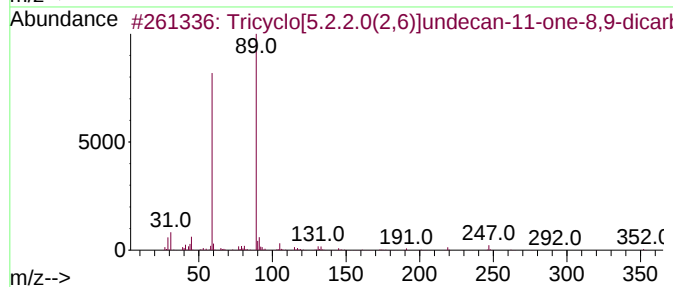
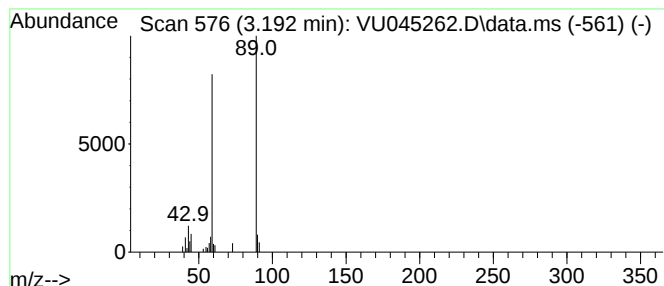
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tricyclo[5.2.2.0(2,6)]undec... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.192	3.02 ug/L	41022	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[5.2.2.0(2,6)]undecan-11...	352	C18H24O7	1000155-17-7	74
2			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
3			2-Cyclopentene, 1,4-bis(methoxye...	276	C13H24O6	1000156-00-3	64
4			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	56
5			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	39



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.4	ug/L	46092	1	6.253	678578	50.0
Tricyclo[5.2.2....	3.192	3.0	ug/L	41022	1	6.253	678578	50.0