

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062022\
 Data File : VU049299.D
 Acq On : 20 Jun 2022 12:41
 Operator : SY/MD
 Sample : N3395-08
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0155

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\SFAMULM061022WMA.M
 Title : VOC Analysis

Signal : TIC: VU049299.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	37	46	62	rBV	16615	43065	4.47%	0.515%
2	1.597	74	80	99	rVB	115167	131707	13.68%	1.576%
3	1.912	170	178	190	rVB	93688	118572	12.32%	1.419%
4	2.568	369	382	395	rBV	182357	294719	30.62%	3.526%
5	2.748	437	438	441	rBV	275	197	0.02%	0.002%
6	2.787	447	450	453	rBV2	443	404	0.04%	0.005%
7	2.880	474	479	482	rBV3	405	450	0.05%	0.005%
8	2.941	493	498	499	rBV	304	251	0.03%	0.003%
9	3.041	525	529	530	rBV2	315	200	0.02%	0.002%
10	3.186	570	574	578	rBV3	411	329	0.03%	0.004%
11	3.620	705	709	712	rBV2	272	235	0.02%	0.003%
12	3.768	753	755	760	rVB3	280	228	0.02%	0.003%
13	3.803	760	766	770	rBV2	336	311	0.03%	0.004%
14	3.903	793	797	803	rVB3	246	249	0.03%	0.003%
15	4.166	876	879	883	rVV2	298	204	0.02%	0.002%
16	4.195	885	888	893	rVB3	265	200	0.02%	0.002%
17	4.327	924	929	931	rBV2	432	381	0.04%	0.005%
18	4.401	945	952	957	rBV2	228	272	0.03%	0.003%
19	4.546	991	997	1000	rBV	328	378	0.04%	0.005%
20	4.623	1007	1021	1057	rBV	115891	296853	30.84%	3.552%
21	5.063	1142	1158	1183	rBV	175692	387622	40.27%	4.638%
22	5.208	1200	1203	1205	rBV3	445	254	0.03%	0.003%
23	5.282	1221	1226	1231	rBV4	493	652	0.07%	0.008%
24	5.372	1239	1254	1272	rBV	218665	446438	46.38%	5.342%
25	5.472	1283	1285	1291	rVB3	421	311	0.03%	0.004%
26	5.514	1293	1298	1300	rBV2	354	338	0.04%	0.004%
27	5.636	1333	1336	1340	rVB	247	214	0.02%	0.003%
28	5.726	1342	1364	1389	rBV2	354054	962624	100.00%	11.518%
29	5.948	1430	1433	1437	rBV3	397	289	0.03%	0.003%
30	5.973	1437	1441	1445	rVV3	368	300	0.03%	0.004%
31	6.057	1463	1467	1470	rBV3	353	271	0.03%	0.003%
32	6.176	1499	1504	1506	rBV2	256	219	0.02%	0.003%
33	6.250	1512	1527	1550	rBV	345781	653566	67.89%	7.820%
34	6.523	1603	1612	1615	rBV7	1737	1960	0.20%	0.023%
35	6.690	1649	1664	1692	rBV	235643	463496	48.15%	5.546%
36	6.800	1693	1698	1699	rBV3	566	491	0.05%	0.006%

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 Title : VOC Analysis

37	6.999	1757	1760	1769	rVB3	507	567	0.06%	0.007%
38	7.038	1769	1772	1776	rBV	309	328	0.03%	0.004%
39	7.063	1776	1780	1782	rBV2	255	213	0.02%	0.003%
40	7.096	1786	1790	1795	rBV2	250	283	0.03%	0.003%
41	7.118	1795	1797	1802	rVB	268	214	0.02%	0.003%
42	7.144	1802	1805	1809	rBV3	349	305	0.03%	0.004%
43	7.186	1810	1818	1828	rBV4	1784	3163	0.33%	0.038%
44	7.227	1828	1831	1832	rBV	331	205	0.02%	0.002%
45	7.343	1863	1867	1870	rVB2	235	210	0.02%	0.003%
46	7.420	1887	1891	1895	rBV2	321	277	0.03%	0.003%
47	7.468	1895	1906	1912	rVV3	295	638	0.07%	0.008%
48	7.510	1914	1919	1923	rBV3	245	294	0.03%	0.004%
49	7.565	1923	1936	1955	rBV	104046	184449	19.16%	2.207%
50	7.684	1969	1973	1976	rBV3	712	726	0.08%	0.009%
51	7.784	2001	2004	2006	rBV2	360	231	0.02%	0.003%
52	7.896	2026	2039	2060	rBV	440961	762281	79.19%	9.121%
53	8.179	2112	2127	2144	rBV	73531	124815	12.97%	1.493%
54	8.391	2190	2193	2198	rVB2	230	214	0.02%	0.003%
55	8.417	2198	2201	2204	rVB2	374	259	0.03%	0.003%
56	8.533	2233	2237	2240	rVB2	328	249	0.03%	0.003%
57	8.632	2256	2268	2308	rBV2	336810	659458	68.51%	7.891%
58	8.806	2320	2322	2326	rVB4	555	260	0.03%	0.003%
59	8.919	2354	2357	2362	rBV2	338	284	0.03%	0.003%
60	9.005	2381	2384	2387	rBV2	322	234	0.02%	0.003%
61	9.063	2398	2402	2407	rVB2	362	334	0.03%	0.004%
62	9.105	2412	2415	2418	rBV2	329	256	0.03%	0.003%
63	9.166	2429	2434	2435	rBV2	324	259	0.03%	0.003%
64	9.362	2489	2495	2499	rBV2	316	357	0.04%	0.004%
65	9.417	2499	2512	2534	rBV	475940	791142	82.19%	9.466%
66	9.565	2555	2558	2561	rBV2	360	291	0.03%	0.003%
67	9.623	2574	2576	2580	rVB3	318	217	0.02%	0.003%
68	9.697	2595	2599	2602	rBV3	445	493	0.05%	0.006%
69	9.739	2606	2612	2619	rBV3	352	482	0.05%	0.006%
70	9.915	2663	2667	2670	rBV2	300	285	0.03%	0.003%
71	9.964	2675	2682	2685	rBV2	389	526	0.05%	0.006%
72	10.147	2736	2739	2743	rVB3	233	200	0.02%	0.002%
73	10.308	2783	2789	2791	rBV2	458	454	0.05%	0.005%
74	10.378	2806	2811	2815	rBV2	386	420	0.04%	0.005%
75	10.433	2825	2828	2832	rVB	521	438	0.05%	0.005%
76	10.468	2832	2839	2840	rBV	446	413	0.04%	0.005%

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 Title : VOC Analysis

77	10.755	2915	2928	2950	rBV	336179	541209	56.22%	6.476%
78	10.976	2994	2997	3000	rVB2	344	222	0.02%	0.003%
79	11.092	3027	3033	3038	rBV2	439	454	0.05%	0.005%
80	11.291	3092	3095	3098	rVB3	386	227	0.02%	0.003%
81	11.340	3105	3110	3112	rBV	412	324	0.03%	0.004%
82	11.427	3134	3137	3144	rVB3	289	288	0.03%	0.003%
83	11.510	3157	3163	3166	rBV3	371	432	0.04%	0.005%
84	11.726	3227	3230	3234	rBV2	252	269	0.03%	0.003%
85	11.812	3243	3257	3277	rBV	463714	743489	77.24%	8.896%
86	11.951	3298	3300	3306	rVB2	554	405	0.04%	0.005%
87	12.192	3362	3375	3402	rBV	446168	718165	74.60%	8.593%
88	12.510	3467	3474	3476	rBV2	362	406	0.04%	0.005%
89	12.748	3544	3548	3549	rBV2	347	246	0.03%	0.003%
90	12.771	3549	3555	3563	rVB2	973	1281	0.13%	0.015%
91	13.021	3629	3633	3635	rBV2	433	439	0.05%	0.005%
92	13.140	3668	3670	3676	rVB2	327	268	0.03%	0.003%
93	13.221	3692	3695	3702	rVB3	455	536	0.06%	0.006%
94	13.298	3713	3719	3724	rBV2	291	407	0.04%	0.005%
95	13.388	3744	3747	3749	rBV2	316	236	0.02%	0.003%
96	13.793	3868	3873	3877	rBV3	418	473	0.05%	0.006%
97	13.844	3883	3889	3897	rBV4	1165	1717	0.18%	0.021%
98	14.327	4037	4039	4041	rBV2	444	267	0.03%	0.003%
99	14.725	4160	4163	4166	rBV	360	276	0.03%	0.003%
100	15.983	4551	4554	4556	rBV2	578	451	0.05%	0.005%

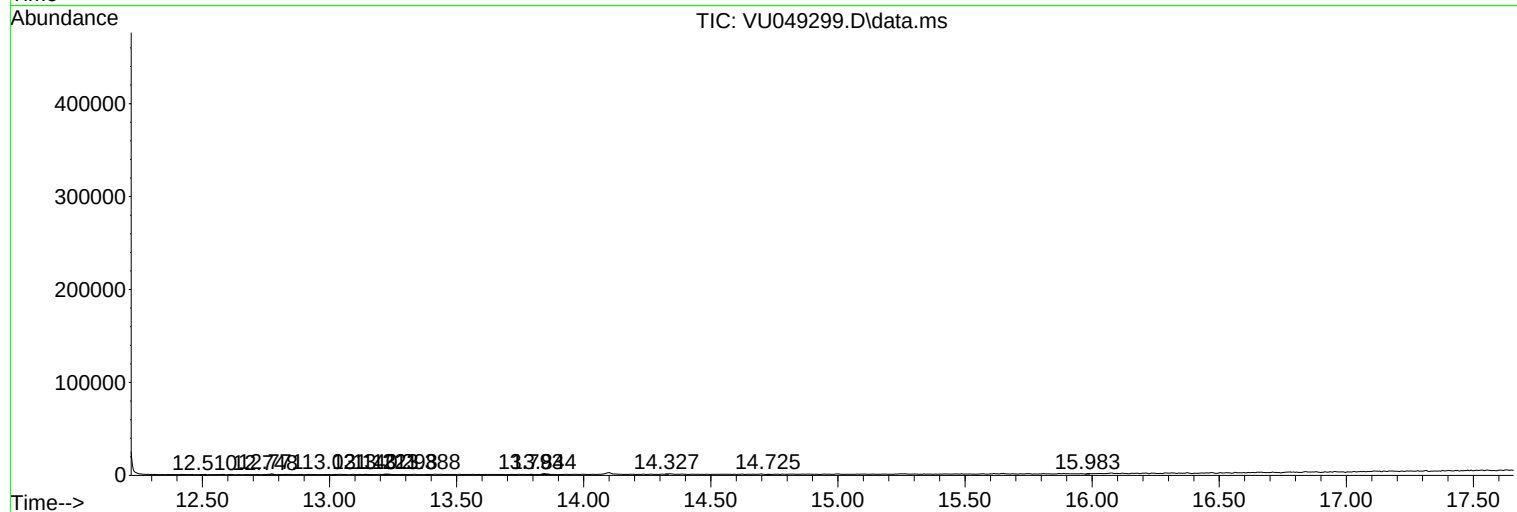
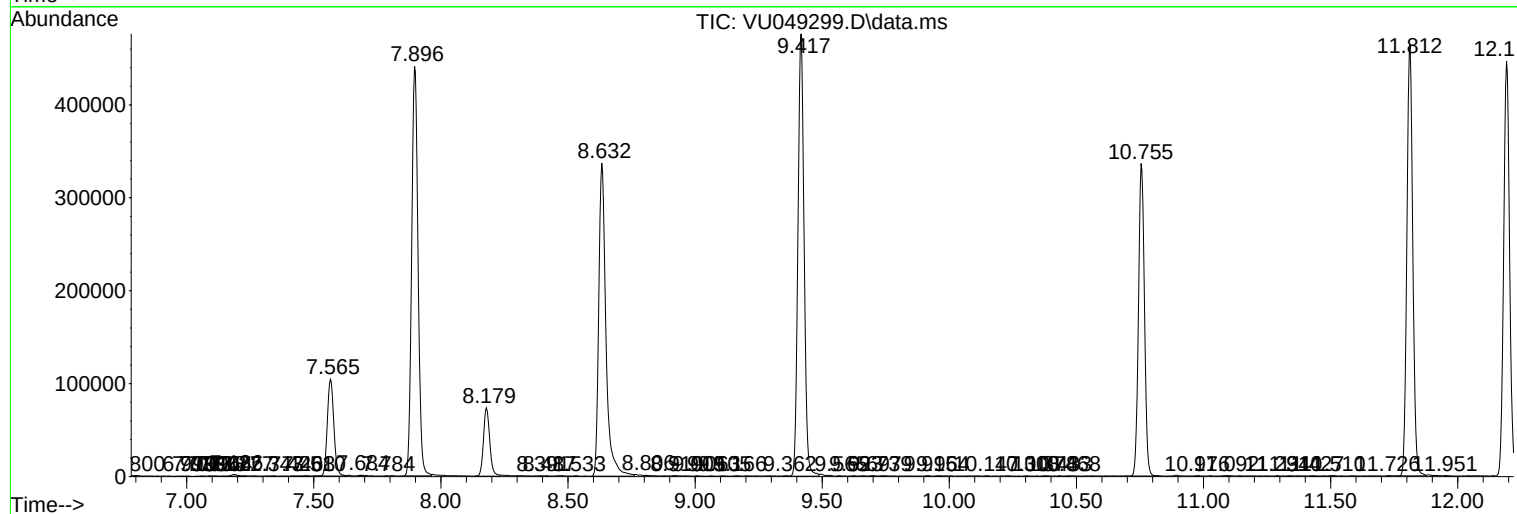
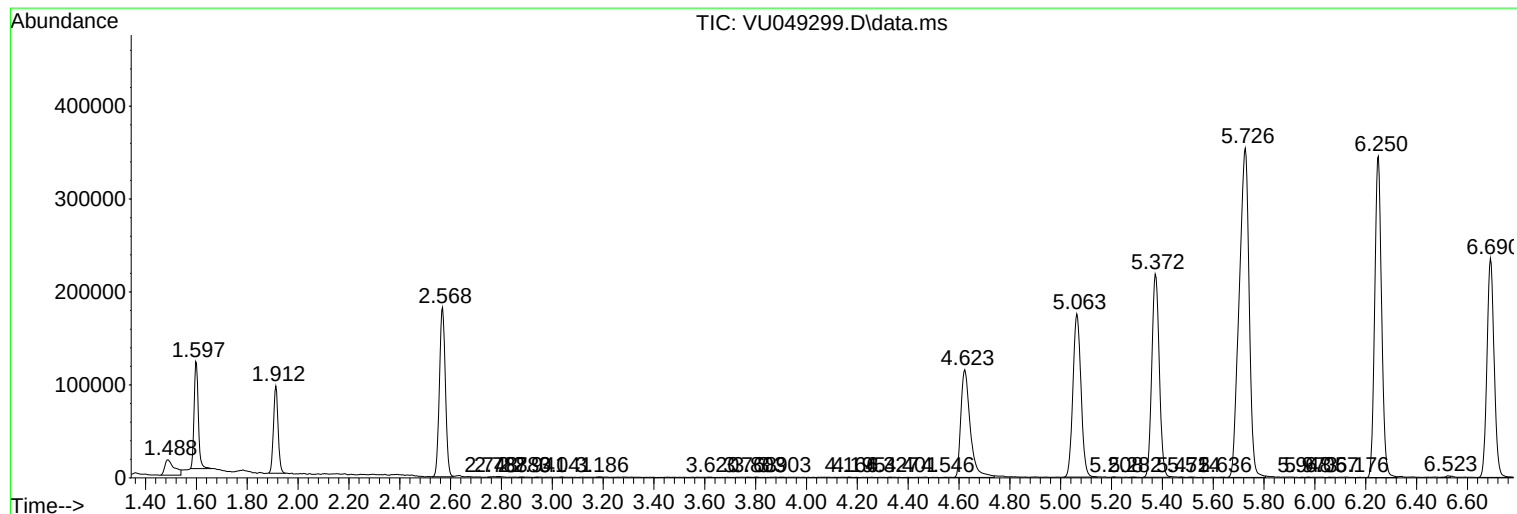
Sum of corrected areas: 8357461

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



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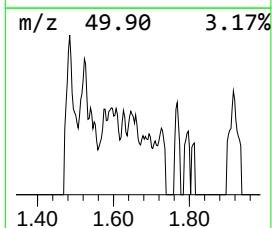
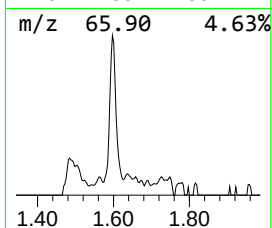
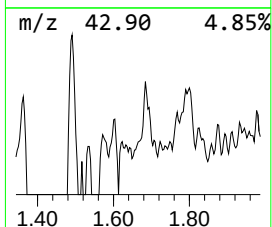
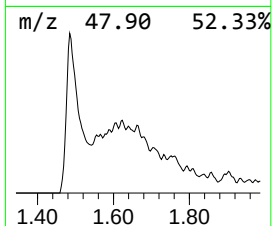
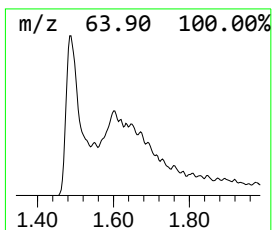
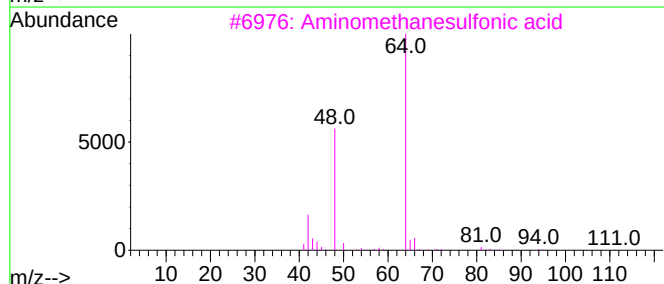
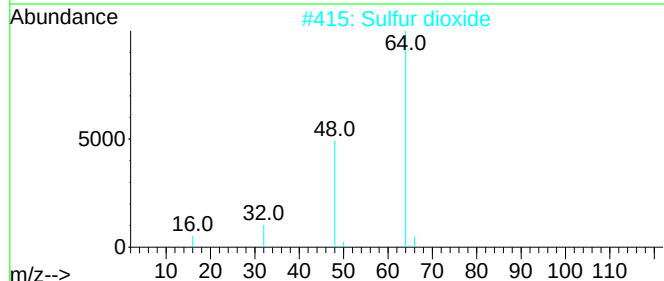
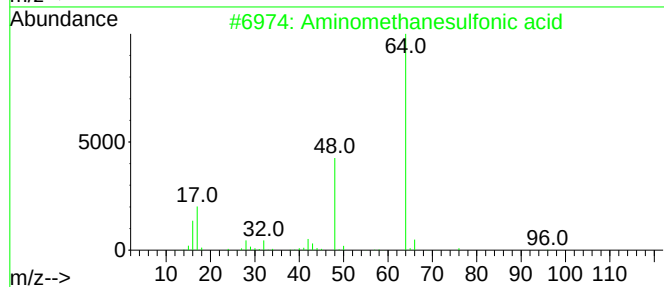
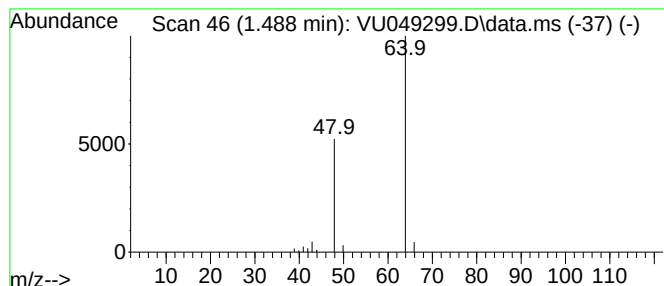
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.488	3.29 ug/L	43065	1,4-Difluorobenzene	6.250

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



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.488	3.3	ug/L	43065	1	6.250	653566	50.0