

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
 Data File : VU049282.D
 Acq On : 18 Jun 2022 15:37
 Operator : SY/MD
 Sample : N3313-05DL 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 YB7L3DL

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: VU049282.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	34	42	55	rBV	34289	75515	7.00%	0.769%
2	1.597	74	80	103	rVB	135137	160723	14.89%	1.637%
3	1.912	170	178	194	rVB	103647	133674	12.38%	1.362%
4	2.568	370	382	396	rBV	209355	343956	31.87%	3.504%
5	2.671	412	414	418	rBV3	367	305	0.03%	0.003%
6	2.758	436	441	445	rBV3	977	1209	0.11%	0.012%
7	2.883	478	480	483	rBV2	363	250	0.02%	0.003%
8	3.044	524	530	533	rBV4	1005	1025	0.09%	0.010%
9	3.186	560	574	590	rVV2	14390	30414	2.82%	0.310%
10	3.343	621	623	626	rVB2	469	293	0.03%	0.003%
11	3.369	626	631	638	rBV2	337	511	0.05%	0.005%
12	3.671	722	725	728	rBV2	331	280	0.03%	0.003%
13	3.735	743	745	750	rVB2	404	287	0.03%	0.003%
14	3.835	772	776	779	rBV3	264	240	0.02%	0.002%
15	3.932	801	806	814	rVB2	410	642	0.06%	0.007%
16	4.125	863	866	871	rVB	387	365	0.03%	0.004%
17	4.160	871	877	882	rBV2	337	422	0.04%	0.004%
18	4.231	895	899	902	rBV2	264	251	0.02%	0.003%
19	4.279	908	914	917	rBV2	319	350	0.03%	0.004%
20	4.446	963	966	972	rBV2	280	310	0.03%	0.003%
21	4.620	1005	1020	1061	rBV	149419	368540	34.14%	3.755%
22	5.063	1139	1158	1177	rBV	197428	434494	40.25%	4.427%
23	5.215	1200	1205	1206	rBV3	302	251	0.02%	0.003%
24	5.301	1224	1232	1236	rVB3	637	1040	0.10%	0.011%
25	5.372	1236	1254	1275	rBV	238916	497511	46.09%	5.069%
26	5.726	1342	1364	1387	rBV2	399712	1079363	100.00%	10.997%
27	5.883	1410	1413	1416	rBV2	341	231	0.02%	0.002%
28	5.903	1417	1419	1422	rVB3	563	327	0.03%	0.003%
29	5.925	1422	1426	1429	rBV2	653	450	0.04%	0.005%
30	5.996	1444	1448	1455	rVB3	292	323	0.03%	0.003%
31	6.095	1475	1479	1481	rBV2	565	367	0.03%	0.004%
32	6.250	1512	1527	1551	rBV	365293	693424	64.24%	7.065%
33	6.430	1578	1583	1587	rBV3	295	335	0.03%	0.003%
34	6.542	1604	1618	1635	rBV3	208639	389155	36.05%	3.965%
35	6.620	1641	1642	1650	rVB5	716	809	0.07%	0.008%
36	6.690	1650	1664	1688	rBV	265716	517056	47.90%	5.268%

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

37	6.796	1694	1697	1699	rBV3	677	479	0.04%	0.005%
38	6.841	1708	1711	1716	rVB3	480	348	0.03%	0.004%
39	7.079	1781	1785	1786	rBV2	283	232	0.02%	0.002%
40	7.102	1790	1792	1797	rVV2	321	261	0.02%	0.003%
41	7.185	1809	1818	1829	rVV4	1813	3275	0.30%	0.033%
42	7.523	1917	1923	1924	rBV	375	328	0.03%	0.003%
43	7.565	1924	1936	1955	rBV	146975	256342	23.75%	2.612%
44	7.722	1982	1985	1989	rVB3	583	407	0.04%	0.004%
45	7.784	2001	2004	2006	rBV2	396	275	0.03%	0.003%
46	7.899	2025	2040	2057	rBV	497075	856390	79.34%	8.725%
47	8.092	2097	2100	2106	rVB3	710	776	0.07%	0.008%
48	8.179	2115	2127	2151	rBV	100596	169939	15.74%	1.731%
49	8.288	2159	2161	2165	rVB3	455	252	0.02%	0.003%
50	8.388	2188	2192	2197	rVB2	438	358	0.03%	0.004%
51	8.552	2234	2243	2255	rBV3	15963	26525	2.46%	0.270%
52	8.632	2255	2268	2300	rBV	387427	724550	67.13%	7.382%
53	8.851	2334	2336	2340	rVB3	374	278	0.03%	0.003%
54	9.211	2444	2448	2450	rBV	374	298	0.03%	0.003%
55	9.224	2450	2452	2457	rVB	377	296	0.03%	0.003%
56	9.259	2457	2463	2471	rVB3	464	650	0.06%	0.007%
57	9.298	2471	2475	2478	rBV	384	393	0.04%	0.004%
58	9.365	2492	2496	2499	rVB2	454	353	0.03%	0.004%
59	9.417	2499	2512	2536	rBV	501624	839409	77.77%	8.552%
60	9.581	2560	2563	2570	rVB2	539	540	0.05%	0.006%
61	9.619	2570	2575	2577	rBV3	266	278	0.03%	0.003%
62	9.661	2583	2588	2593	rBV3	748	650	0.06%	0.007%
63	9.722	2604	2607	2612	rVB2	488	412	0.04%	0.004%
64	9.745	2612	2614	2618	rBV2	315	279	0.03%	0.003%
65	9.806	2630	2633	2635	rBV2	324	277	0.03%	0.003%
66	9.864	2646	2651	2654	rVB3	288	260	0.02%	0.003%
67	10.111	2725	2728	2734	rVB2	496	454	0.04%	0.005%
68	10.150	2734	2740	2742	rBV2	308	332	0.03%	0.003%
69	10.330	2790	2796	2801	rVB3	269	367	0.03%	0.004%
70	10.433	2822	2828	2831	rBV2	345	338	0.03%	0.003%
71	10.488	2841	2845	2848	rBV	282	293	0.03%	0.003%
72	10.536	2854	2860	2863	rBV2	441	392	0.04%	0.004%
73	10.568	2866	2870	2873	rVV2	300	247	0.02%	0.003%
74	10.754	2916	2928	2950	rVV	366793	602072	55.78%	6.134%
75	11.025	3009	3012	3014	rBV2	328	265	0.02%	0.003%
76	11.314	3098	3102	3104	rBV2	357	296	0.03%	0.003%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.471	3147	3151	3154	rVV3	355	362	0.03%	0.004%
78	11.652	3204	3207	3213	rVB3	242	271	0.03%	0.003%
79	11.751	3233	3238	3241	rVB2	557	504	0.05%	0.005%
80	11.812	3241	3257	3282	rBV	485579	783808	72.62%	7.986%
81	12.098	3342	3346	3352	rVB2	459	383	0.04%	0.004%
82	12.192	3362	3375	3399	rBV	483546	793571	73.52%	8.085%
83	12.343	3419	3422	3427	rVB3	439	247	0.02%	0.003%
84	12.391	3434	3437	3440	rBV2	344	236	0.02%	0.002%
85	12.623	3505	3509	3513	rBV2	293	308	0.03%	0.003%
86	12.658	3518	3520	3525	rVB	417	292	0.03%	0.003%
87	12.909	3595	3598	3603	rBV3	320	385	0.04%	0.004%
88	13.076	3644	3650	3655	rBV3	465	773	0.07%	0.008%
89	13.143	3668	3671	3680	rVV3	413	456	0.04%	0.005%
90	13.224	3692	3696	3698	rBV3	429	367	0.03%	0.004%
91	13.452	3764	3767	3772	rBV2	325	340	0.03%	0.003%
92	13.484	3772	3777	3781	rBV3	322	438	0.04%	0.004%
93	13.844	3884	3889	3899	rBV5	1376	1783	0.17%	0.018%
94	14.095	3959	3967	3969	rBV3	2475	2563	0.24%	0.026%
95	14.333	4038	4041	4047	rVB3	1056	1046	0.10%	0.011%
96	14.645	4134	4138	4140	rBV	370	295	0.03%	0.003%
97	14.909	4217	4220	4223	rBV2	514	451	0.04%	0.005%
98	15.571	4421	4426	4429	rBV3	531	491	0.05%	0.005%
99	15.815	4498	4502	4505	rBV2	703	634	0.06%	0.006%
100	16.372	4672	4675	4676	rBV4	694	405	0.04%	0.004%

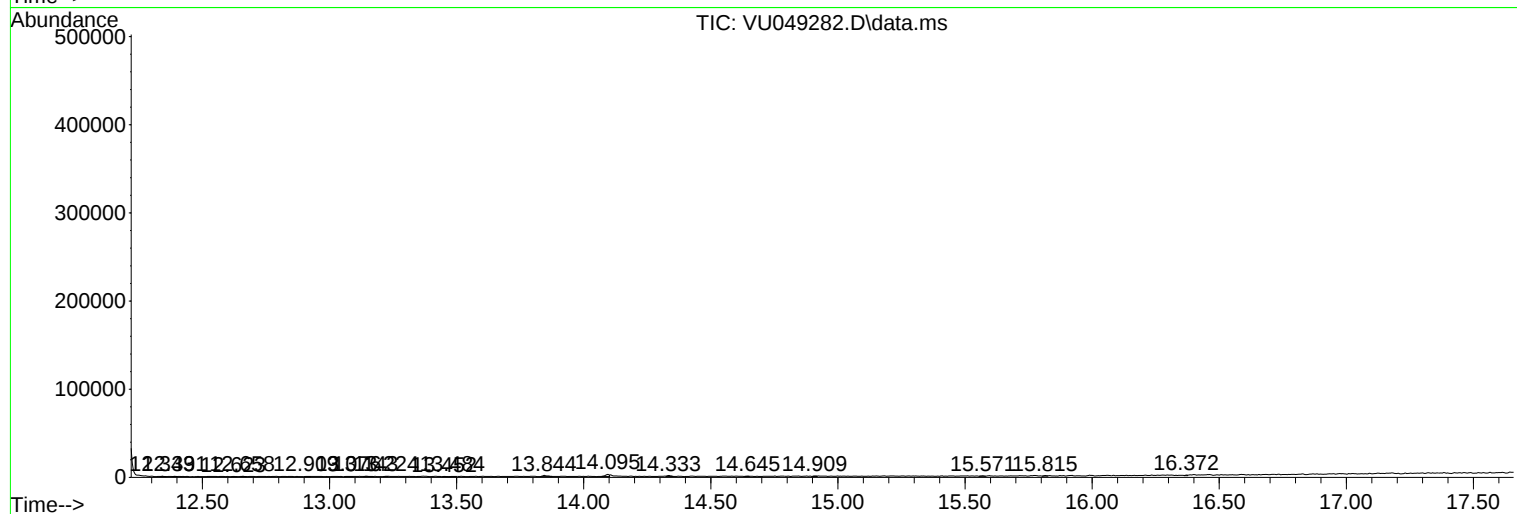
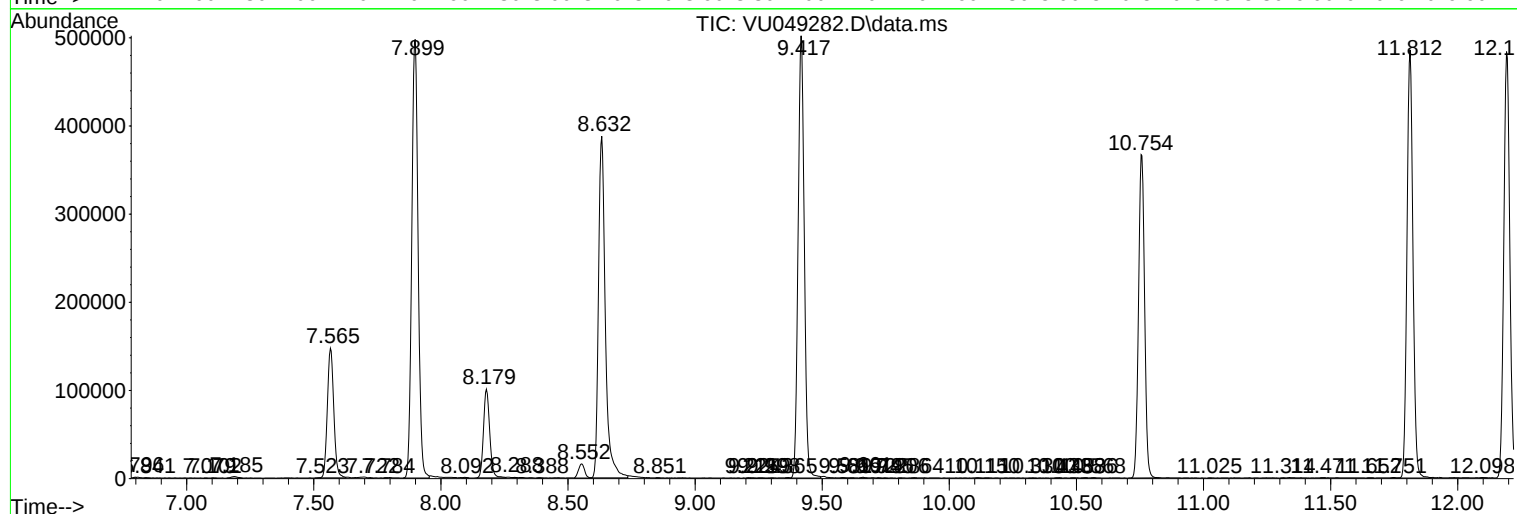
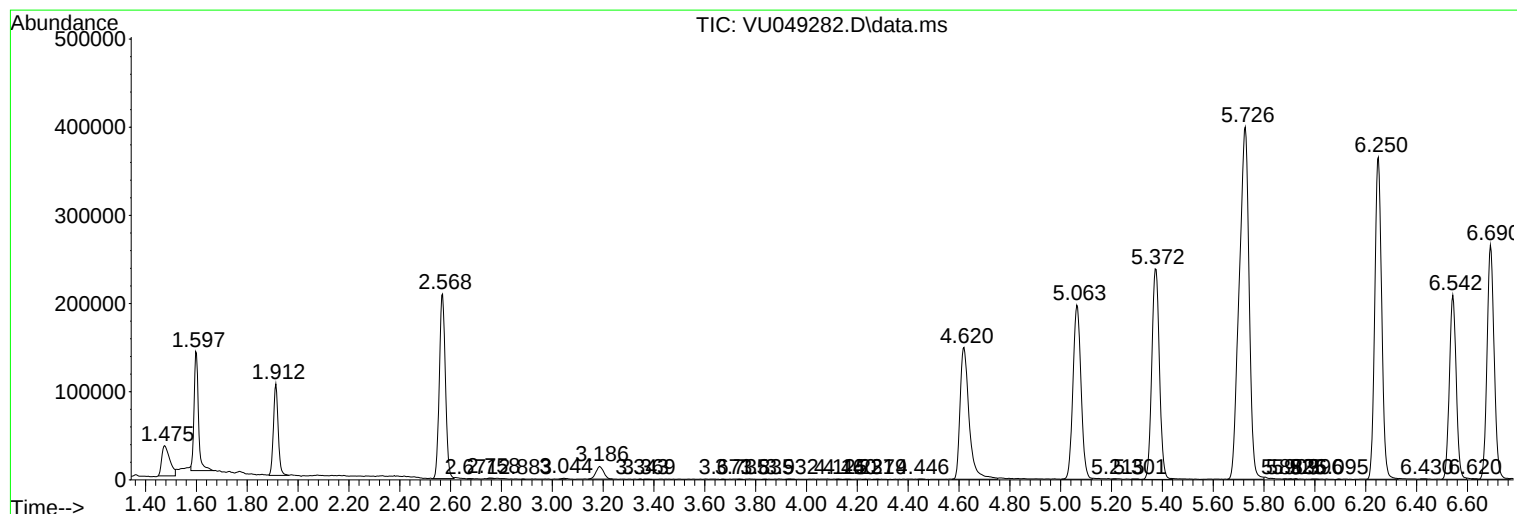
Sum of corrected areas: 9815273

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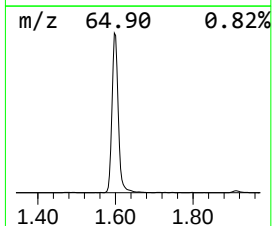
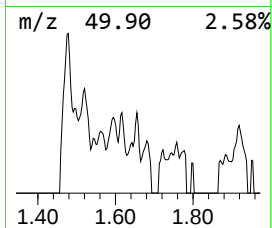
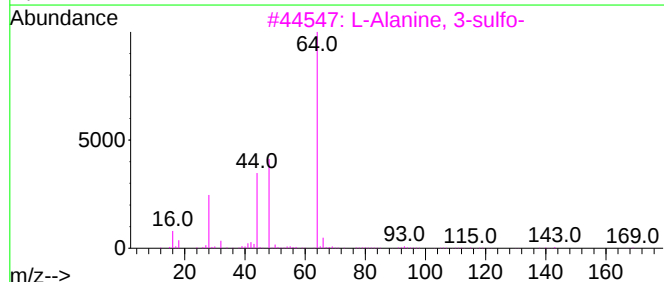
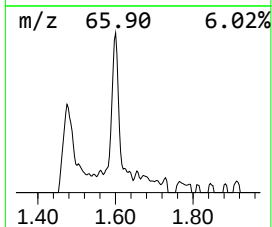
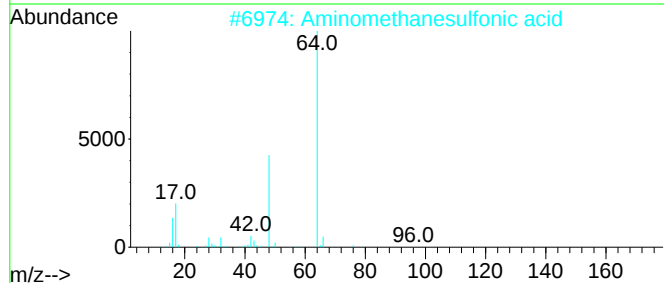
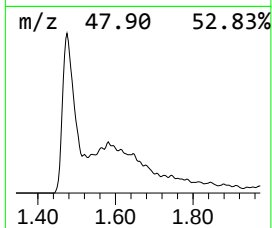
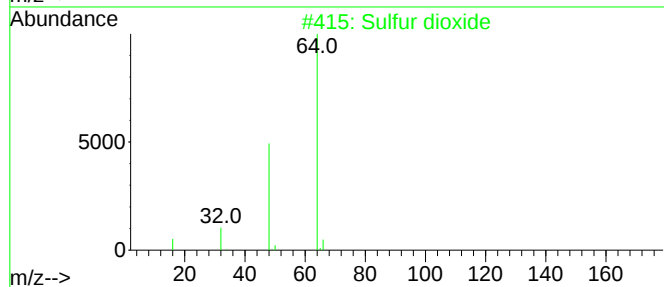
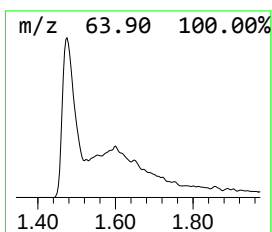
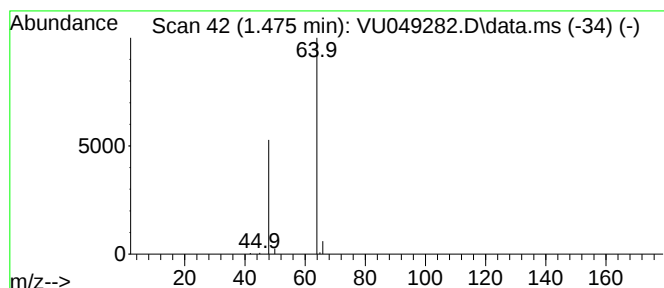
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	5.45 ug/L	75515	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.475	5.5	ug/L	75515	1	6.250	693424	50.0