

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
 Data File : VU049284.D
 Acq On : 18 Jun 2022 16:24
 Operator : SY/MD
 Sample : N3313-07DL 40X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 YB7L5DL

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: VU049284.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	58	rBV2	24779	59069	2.83%	0.519%
2	1.597	73	80	94	rBV	128206	140576	6.74%	1.235%
3	1.913	170	178	191	rVB	98843	129137	6.19%	1.135%
4	2.514	363	365	369	rBV3	422	292	0.01%	0.003%
5	2.568	369	382	397	rBV2	211455	359766	17.24%	3.162%
6	2.774	439	446	447	rBV3	626	634	0.03%	0.006%
7	3.006	513	518	519	rBV2	295	249	0.01%	0.002%
8	3.035	524	527	528	rVV	625	328	0.02%	0.003%
9	3.044	528	530	537	rVB4	1286	1447	0.07%	0.013%
10	3.086	537	543	546	rBV3	285	403	0.02%	0.004%
11	3.105	546	549	555	rBV2	506	449	0.02%	0.004%
12	3.189	561	575	591	rBV	8455	19079	0.91%	0.168%
13	3.295	601	608	614	rVB3	371	528	0.03%	0.005%
14	3.359	625	628	633	rVB2	471	395	0.02%	0.003%
15	3.437	650	652	658	rVV2	311	348	0.02%	0.003%
16	3.475	658	664	667	rVB3	239	224	0.01%	0.002%
17	3.504	667	673	676	rBV3	266	297	0.01%	0.003%
18	3.523	677	679	685	rBV2	255	238	0.01%	0.002%
19	4.012	826	831	835	rBV3	225	243	0.01%	0.002%
20	4.121	859	865	868	rBV2	424	518	0.02%	0.005%
21	4.192	881	887	890	rBV3	357	421	0.02%	0.004%
22	4.244	898	903	907	rBV2	276	329	0.02%	0.003%
23	4.346	931	935	942	rVB3	275	274	0.01%	0.002%
24	4.623	1008	1021	1058	rBV2	144187	430340	20.63%	3.782%
25	4.935	1113	1118	1124	rVB3	467	610	0.03%	0.005%
26	4.973	1124	1130	1132	rBV2	355	401	0.02%	0.004%
27	5.064	1142	1158	1178	rBV	191367	417722	20.02%	3.671%
28	5.173	1190	1192	1195	rVB2	537	269	0.01%	0.002%
29	5.189	1195	1197	1200	rBV3	474	357	0.02%	0.003%
30	5.295	1226	1230	1235	rBV3	362	394	0.02%	0.003%
31	5.372	1240	1254	1275	rBV	242560	504435	24.18%	4.433%
32	5.481	1284	1288	1292	rBV2	409	390	0.02%	0.003%
33	5.543	1302	1307	1311	rBV2	344	372	0.02%	0.003%
34	5.591	1318	1322	1325	rBV2	278	246	0.01%	0.002%
35	5.726	1342	1364	1383	rBV2	384026	1038398	49.77%	9.126%
36	5.912	1418	1422	1430	rVB2	336	470	0.02%	0.004%

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 Title : VOC Analysis

37	6.102	1479	1481	1486	rVV3	251	253	0.01%	0.002%
38	6.250	1511	1527	1549	rBV	369064	702580	33.68%	6.175%
39	6.362	1561	1562	1568	rVB3	349	281	0.01%	0.002%
40	6.395	1568	1572	1578	rBV2	322	405	0.02%	0.004%
41	6.543	1603	1618	1644	rBV	1115827	2086241	100.00%	18.335%
42	6.690	1651	1664	1687	rVB	252539	495194	23.74%	4.352%
43	6.803	1696	1699	1701	rBV2	579	357	0.02%	0.003%
44	6.880	1719	1723	1728	rBV4	353	402	0.02%	0.004%
45	6.977	1747	1753	1764	rVB4	1211	2175	0.10%	0.019%
46	7.108	1788	1794	1795	rBV2	299	293	0.01%	0.003%
47	7.186	1811	1818	1829	rVB4	1555	2647	0.13%	0.023%
48	7.260	1837	1841	1846	rVB	531	461	0.02%	0.004%
49	7.433	1892	1895	1898	rBV3	284	247	0.01%	0.002%
50	7.565	1923	1936	1953	rBV2	140090	245012	11.74%	2.153%
51	7.687	1969	1974	1987	rVB5	1179	2070	0.10%	0.018%
52	7.742	1987	1991	1997	rBV3	484	481	0.02%	0.004%
53	7.787	1999	2005	2007	rBV3	278	342	0.02%	0.003%
54	7.835	2015	2020	2024	rBV2	244	248	0.01%	0.002%
55	7.896	2024	2039	2066	rBV	470574	820711	39.34%	7.213%
56	8.028	2078	2080	2083	rVB2	620	327	0.02%	0.003%
57	8.179	2113	2127	2144	rBV	94612	161780	7.75%	1.422%
58	8.375	2181	2188	2191	rBV3	478	584	0.03%	0.005%
59	8.401	2191	2196	2206	rVB5	1164	1536	0.07%	0.013%
60	8.469	2208	2217	2222	rBV5	785	1301	0.06%	0.011%
61	8.552	2234	2243	2254	rBV2	26746	43555	2.09%	0.383%
62	8.632	2256	2268	2301	rBV	390200	716336	34.34%	6.296%
63	8.816	2322	2325	2330	rBV3	218	230	0.01%	0.002%
64	8.993	2373	2380	2384	rBV2	325	439	0.02%	0.004%
65	9.153	2426	2430	2433	rBV2	305	289	0.01%	0.003%
66	9.243	2453	2458	2463	rVB2	358	361	0.02%	0.003%
67	9.269	2463	2466	2469	rBV2	347	312	0.01%	0.003%
68	9.417	2498	2512	2539	rBV	509186	844642	40.49%	7.423%
69	9.665	2583	2589	2597	rBV4	855	1105	0.05%	0.010%
70	9.806	2630	2633	2638	rBV2	305	238	0.01%	0.002%
71	10.108	2718	2727	2729	rBV3	952	1092	0.05%	0.010%
72	10.488	2843	2845	2852	rBV4	358	298	0.01%	0.003%
73	10.755	2915	2928	2948	rBV	353605	569926	27.32%	5.009%
74	10.893	2965	2971	2980	rVB3	1199	1893	0.09%	0.017%
75	11.044	3014	3018	3023	rBV2	512	516	0.02%	0.005%
76	11.089	3026	3032	3037	rVV4	381	494	0.02%	0.004%

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 Title : VOC Analysis

77	11.359	3111	3116	3121	rBV2	253	369	0.02%	0.003%
78	11.475	3148	3152	3155	rBV3	377	313	0.02%	0.003%
79	11.507	3159	3162	3165	rBV	289	224	0.01%	0.002%
80	11.594	3186	3189	3191	rBV2	271	225	0.01%	0.002%
81	11.610	3191	3194	3198	rVB2	366	255	0.01%	0.002%
82	11.726	3226	3230	3233	rBV2	261	246	0.01%	0.002%
83	11.748	3233	3237	3243	rVB2	531	623	0.03%	0.005%
84	11.812	3243	3257	3280	rBV	492586	793931	38.06%	6.977%
85	12.192	3363	3375	3395	rBV	461639	758128	36.34%	6.663%
86	12.510	3468	3474	3476	rBV3	374	396	0.02%	0.003%
87	12.774	3549	3556	3558	rBV4	580	584	0.03%	0.005%
88	12.896	3590	3594	3596	rBV2	299	239	0.01%	0.002%
89	13.005	3625	3628	3631	rBV2	437	353	0.02%	0.003%
90	13.034	3633	3637	3640	rVV2	481	397	0.02%	0.003%
91	13.082	3648	3652	3655	rBV2	607	536	0.03%	0.005%
92	13.221	3692	3695	3697	rBV3	333	239	0.01%	0.002%
93	13.517	3784	3787	3789	rBV2	351	259	0.01%	0.002%
94	13.607	3812	3815	3819	rBV3	376	407	0.02%	0.004%
95	14.095	3961	3967	3973	rBV2	839	1224	0.06%	0.011%
96	14.314	4032	4035	4042	rBV4	475	599	0.03%	0.005%
97	15.333	4350	4352	4355	rBV	497	307	0.01%	0.003%
98	15.375	4362	4365	4372	rBV3	606	701	0.03%	0.006%
99	15.443	4383	4386	4389	rVB	627	403	0.02%	0.004%
100	15.664	4452	4455	4456	rBV2	483	253	0.01%	0.002%

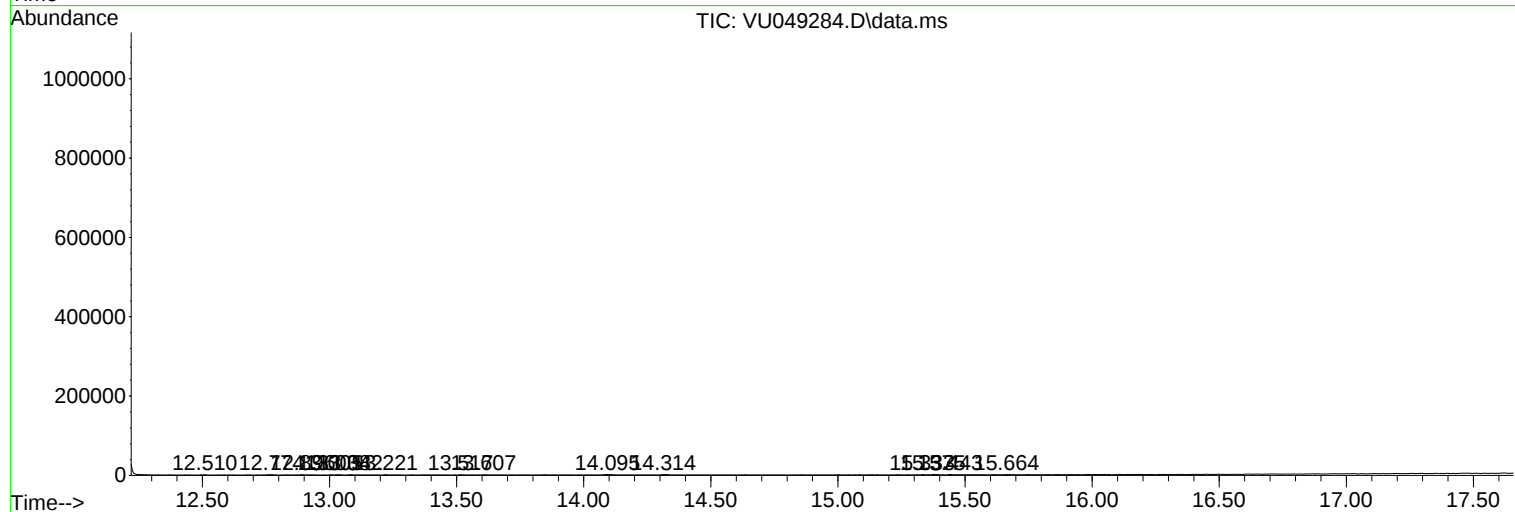
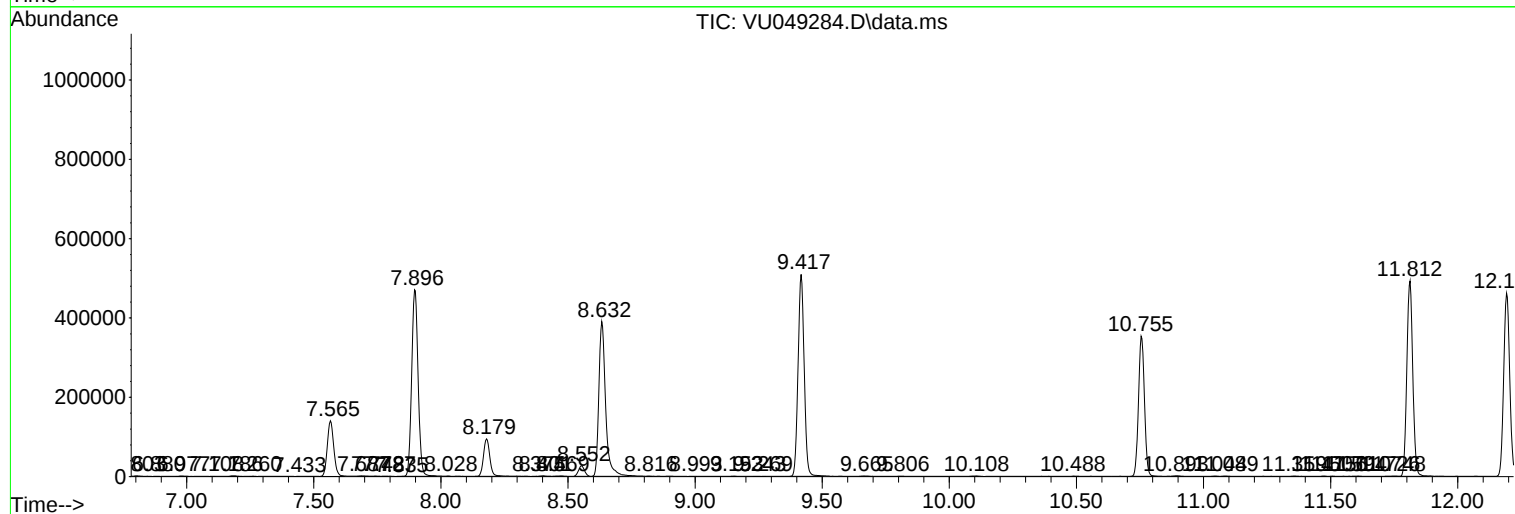
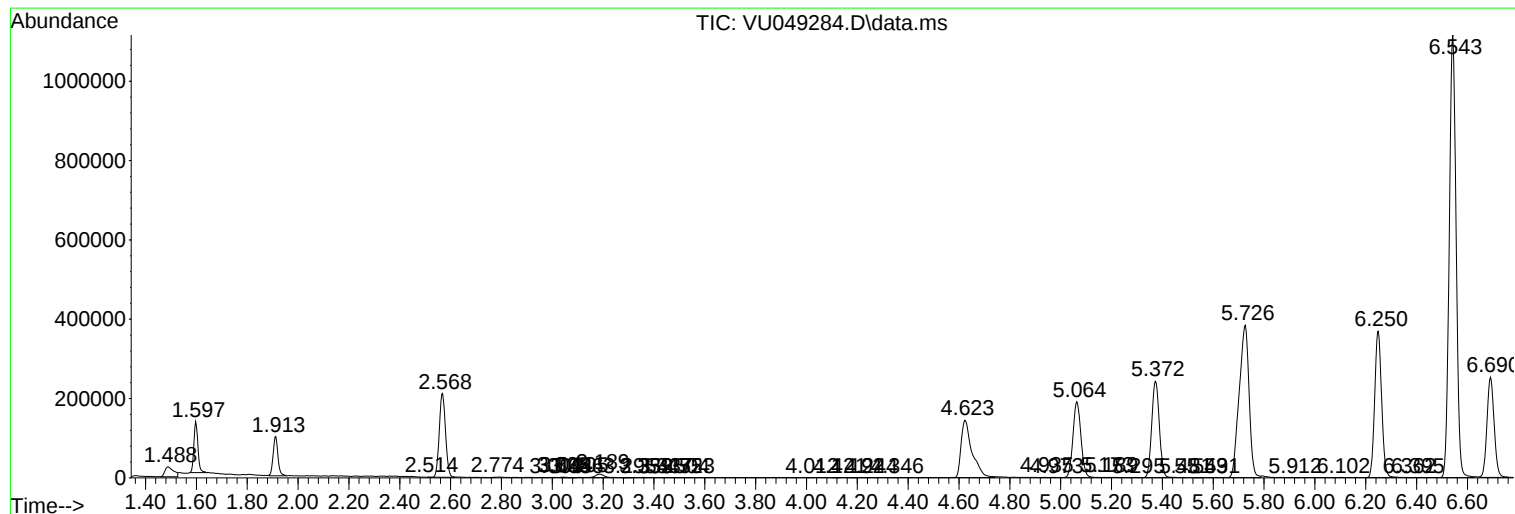
Sum of corrected areas: 11378513

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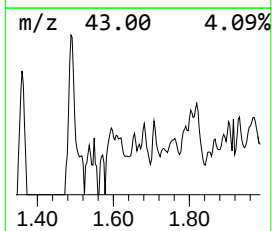
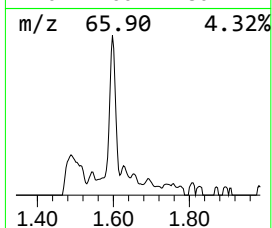
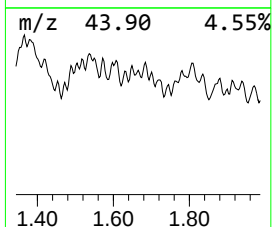
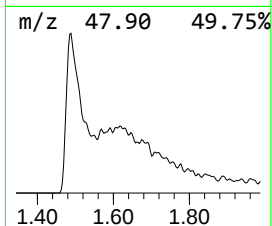
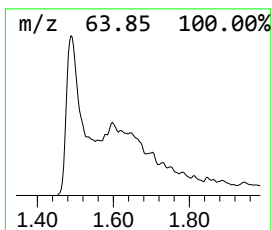
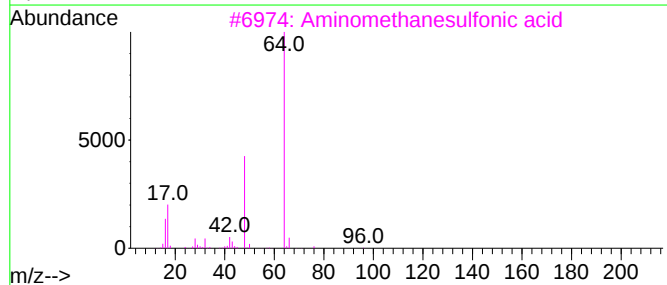
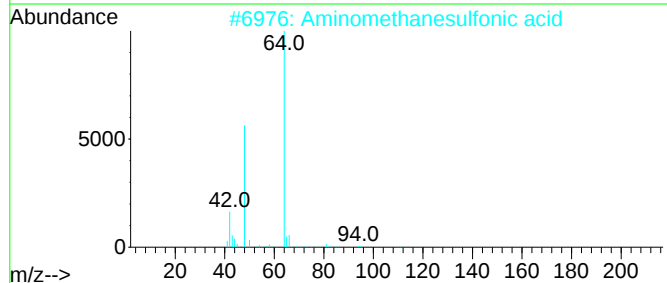
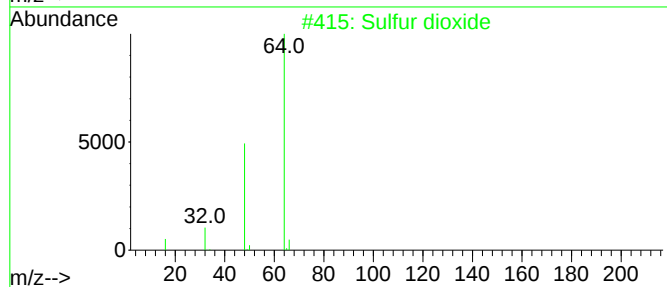
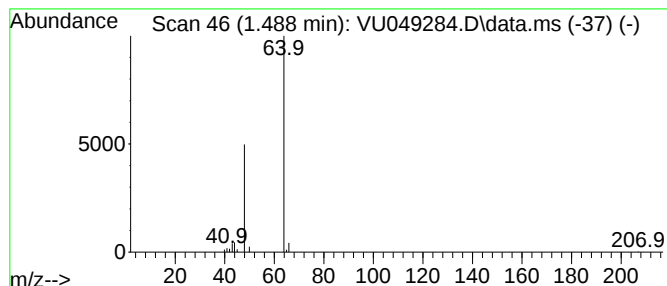
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
1.488	4.20 ug/L	59069	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	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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
Sulfur dioxide	1.488	4.2	ug/L	59069	1	6.250	702580	50.0