

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
 Data File : VU049285.D
 Acq On : 18 Jun 2022 16:48
 Operator : SY/MD
 Sample : N3313-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 YB7N1

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: VU049285.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	36	45	63	rBV	36034	94097	9.26%	1.059%
2	1.597	74	80	100	rVB	125411	144144	14.18%	1.622%
3	1.912	169	178	190	rVB	96082	125282	12.33%	1.410%
4	2.565	369	381	395	rBV	198816	322434	31.73%	3.629%
5	2.764	439	443	444	rBV2	804	519	0.05%	0.006%
6	2.948	497	500	503	rBV3	481	265	0.03%	0.003%
7	3.035	522	527	529	rBV2	313	279	0.03%	0.003%
8	3.179	564	572	574	rBV5	825	921	0.09%	0.010%
9	3.420	643	647	653	rVB3	328	334	0.03%	0.004%
10	3.600	700	703	706	rBV3	326	292	0.03%	0.003%
11	3.723	738	741	744	rBV	305	210	0.02%	0.002%
12	3.819	768	771	779	rVB2	303	389	0.04%	0.004%
13	3.861	779	784	787	rBV2	401	379	0.04%	0.004%
14	3.916	798	801	806	rVB2	343	283	0.03%	0.003%
15	3.944	806	810	812	rBV	324	239	0.02%	0.003%
16	4.051	838	843	846	rVB	422	383	0.04%	0.004%
17	4.076	846	851	853	rBV2	273	227	0.02%	0.003%
18	4.237	894	901	904	rBV2	391	545	0.05%	0.006%
19	4.308	920	923	929	rBV2	172	224	0.02%	0.003%
20	4.571	1002	1005	1008	rBV3	323	230	0.02%	0.003%
21	4.623	1008	1021	1060	rBV	129724	324527	31.93%	3.652%
22	4.803	1073	1077	1080	rBV2	644	574	0.06%	0.006%
23	5.063	1141	1158	1180	rBV	189816	410861	40.43%	4.624%
24	5.292	1223	1229	1232	rVB4	429	389	0.04%	0.004%
25	5.372	1239	1254	1276	rBV	231643	478360	47.07%	5.384%
26	5.494	1288	1292	1295	rBV2	614	352	0.03%	0.004%
27	5.726	1341	1364	1392	rBV2	380294	1016320	100.00%	11.438%
28	6.038	1458	1461	1467	rVB3	518	442	0.04%	0.005%
29	6.063	1467	1469	1472	rBV	265	195	0.02%	0.002%
30	6.108	1480	1483	1484	rBV2	512	323	0.03%	0.004%
31	6.150	1492	1496	1497	rBV2	299	233	0.02%	0.003%
32	6.250	1511	1527	1546	rBV	349417	663430	65.28%	7.466%
33	6.468	1591	1595	1597	rBV	349	231	0.02%	0.003%
34	6.542	1607	1618	1631	rVB8	7549	15223	1.50%	0.171%
35	6.690	1650	1664	1689	rBV	249499	484636	47.69%	5.454%
36	6.784	1691	1693	1695	rVV	461	259	0.03%	0.003%

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

37	6.877	1717	1722	1724	rBV3	275	246	0.02%	0.003%
38	6.983	1753	1755	1760	rBV3	308	248	0.02%	0.003%
39	7.140	1798	1804	1805	rBV2	307	328	0.03%	0.004%
40	7.182	1811	1817	1829	rVB6	1552	3050	0.30%	0.034%
41	7.372	1872	1876	1878	rBV2	340	249	0.02%	0.003%
42	7.565	1923	1936	1960	rVV	134090	241440	23.76%	2.717%
43	7.693	1967	1976	1981	rBV6	1017	1610	0.16%	0.018%
44	7.796	2005	2008	2015	rVB3	411	451	0.04%	0.005%
45	7.896	2025	2039	2057	rBV	462471	803999	79.11%	9.048%
46	8.121	2106	2109	2115	rBV2	260	244	0.02%	0.003%
47	8.179	2115	2127	2147	rBV	91667	158882	15.63%	1.788%
48	8.398	2193	2195	2202	rVB2	482	477	0.05%	0.005%
49	8.468	2202	2217	2219	rBV3	924	1567	0.15%	0.018%
50	8.552	2237	2243	2245	rBV	355	350	0.03%	0.004%
51	8.632	2252	2268	2296	rBV	372642	702985	69.17%	7.911%
52	8.922	2353	2358	2365	rVB3	308	382	0.04%	0.004%
53	8.964	2365	2371	2373	rBV	241	257	0.03%	0.003%
54	8.980	2373	2376	2378	rVV2	385	280	0.03%	0.003%
55	9.124	2417	2421	2424	rBV2	404	419	0.04%	0.005%
56	9.417	2499	2512	2540	rBV	484689	801194	78.83%	9.017%
57	9.616	2571	2574	2580	rBV2	346	423	0.04%	0.005%
58	9.664	2583	2589	2594	rBV2	640	686	0.07%	0.008%
59	9.709	2599	2603	2607	rVV3	258	248	0.02%	0.003%
60	9.735	2608	2611	2616	rVB2	276	259	0.03%	0.003%
61	10.153	2735	2741	2744	rBV3	370	368	0.04%	0.004%
62	10.182	2746	2750	2752	rBV2	299	269	0.03%	0.003%
63	10.272	2770	2778	2784	rBV2	370	620	0.06%	0.007%
64	10.324	2791	2794	2798	rVB	255	208	0.02%	0.002%
65	10.626	2881	2888	2891	rBV3	368	377	0.04%	0.004%
66	10.754	2916	2928	2948	rBV	345823	562681	55.36%	6.332%
67	10.877	2964	2966	2967	rBV	418	213	0.02%	0.002%
68	10.896	2968	2972	2981	rVV3	1437	1717	0.17%	0.019%
69	11.060	3020	3023	3027	rVB3	445	357	0.04%	0.004%
70	11.086	3027	3031	3033	rBV	440	327	0.03%	0.004%
71	11.234	3072	3077	3082	rBV2	233	281	0.03%	0.003%
72	11.378	3119	3122	3124	rBV2	287	204	0.02%	0.002%
73	11.536	3168	3171	3175	rBV2	318	236	0.02%	0.003%
74	11.587	3183	3187	3190	rBV2	235	242	0.02%	0.003%
75	11.616	3194	3196	3200	rVB2	388	270	0.03%	0.003%
76	11.658	3205	3209	3210	rBV	349	237	0.02%	0.003%

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77	11.754	3236	3239	3244	rBV4	541	480	0.05%	0.005%
78	11.812	3244	3257	3278	rBV	472718	750032	73.80%	8.441%
79	11.906	3284	3286	3291	rBV3	480	300	0.03%	0.003%
80	11.963	3302	3304	3313	rVB2	202	224	0.02%	0.003%
81	12.005	3313	3317	3320	rBV	352	267	0.03%	0.003%
82	12.076	3329	3339	3343	rBV5	2010	3383	0.33%	0.038%
83	12.192	3362	3375	3394	rBV	461961	746900	73.49%	8.406%
84	12.481	3463	3465	3471	rVB2	304	256	0.03%	0.003%
85	12.754	3545	3550	3551	rBV2	327	243	0.02%	0.003%
86	12.774	3551	3556	3564	rVB3	978	1375	0.14%	0.015%
87	13.221	3692	3695	3702	rBV3	271	244	0.02%	0.003%
88	13.349	3732	3735	3738	rBV2	316	269	0.03%	0.003%
89	13.844	3886	3889	3893	rBV3	480	329	0.03%	0.004%
90	13.995	3933	3936	3943	rVB2	397	421	0.04%	0.005%
91	14.028	3943	3946	3947	rBV2	428	255	0.03%	0.003%
92	14.086	3962	3964	3966	rBV2	349	198	0.02%	0.002%
93	14.504	4091	4094	4096	rBV2	338	218	0.02%	0.002%
94	14.777	4176	4179	4180	rBV	467	235	0.02%	0.003%
95	14.970	4235	4239	4243	rBV2	468	403	0.04%	0.005%
96	15.076	4269	4272	4275	rBV2	435	313	0.03%	0.004%
97	15.465	4391	4393	4396	rBV	439	229	0.02%	0.003%
98	15.510	4404	4407	4409	rBV3	530	302	0.03%	0.003%
99	15.825	4503	4505	4510	rVB3	794	533	0.05%	0.006%
100	16.365	4669	4673	4678	rBV4	1054	1305	0.13%	0.015%

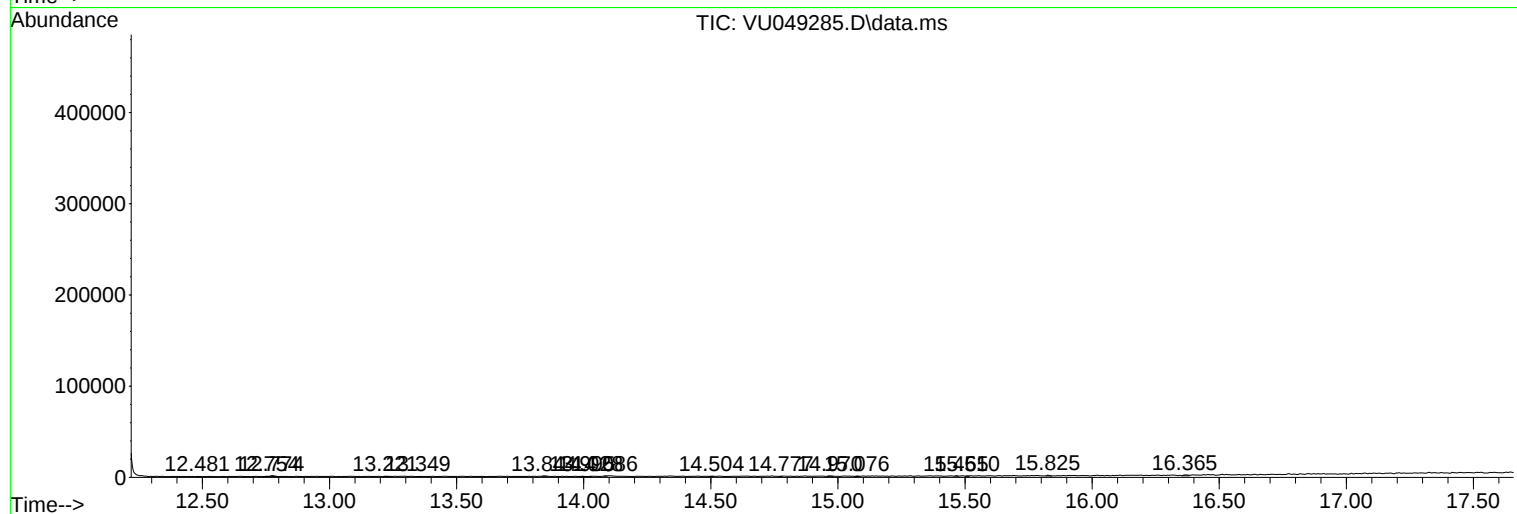
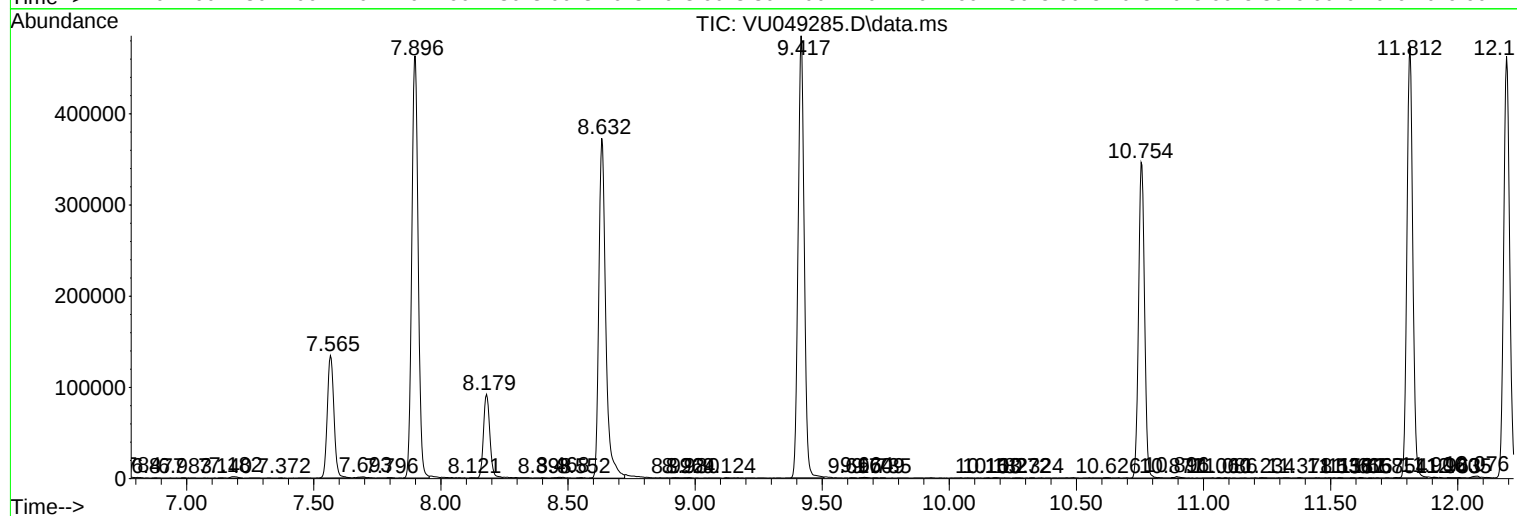
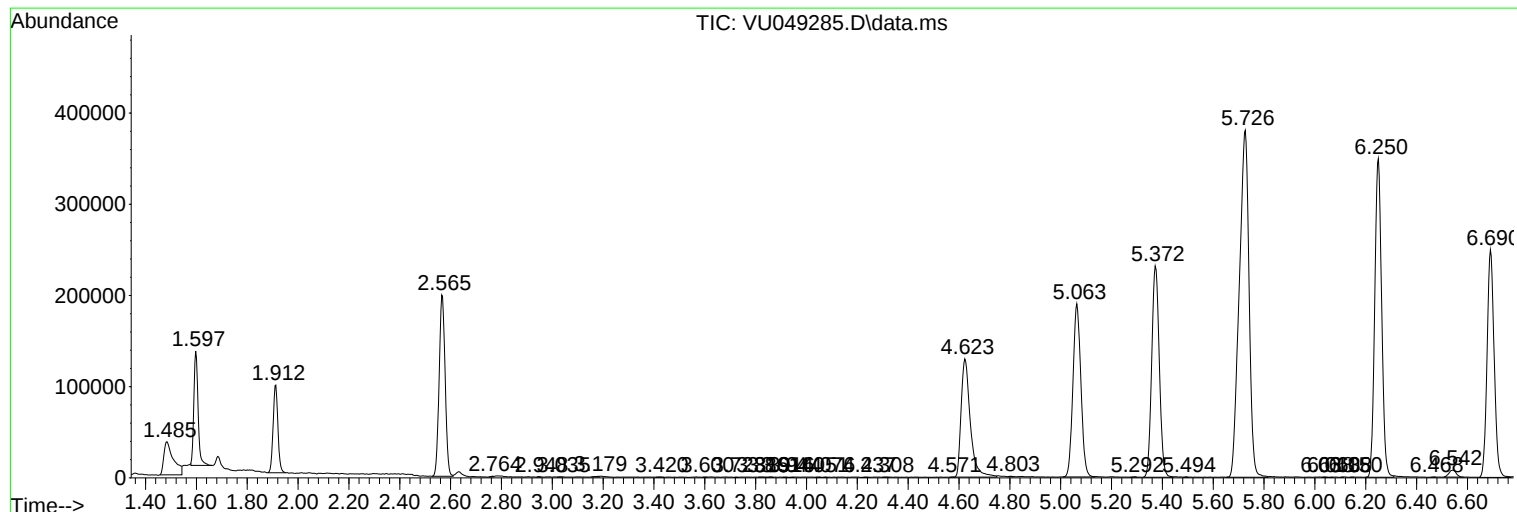
Sum of corrected areas: 8885626

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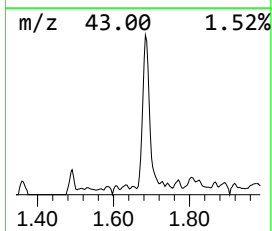
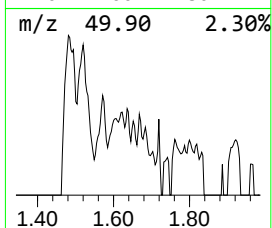
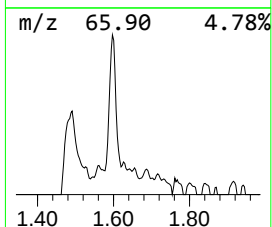
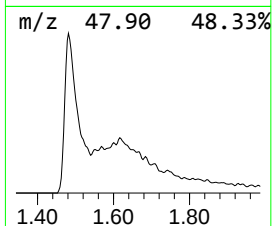
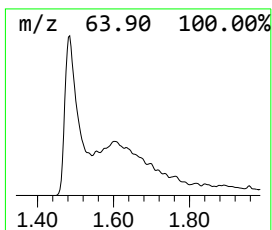
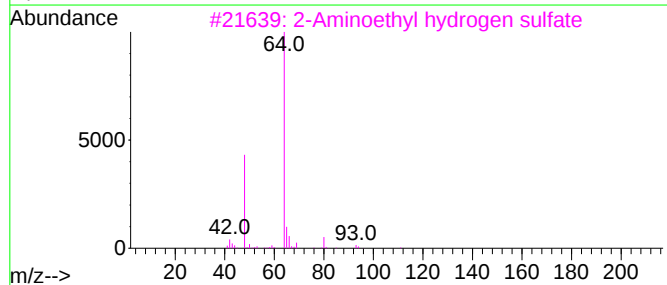
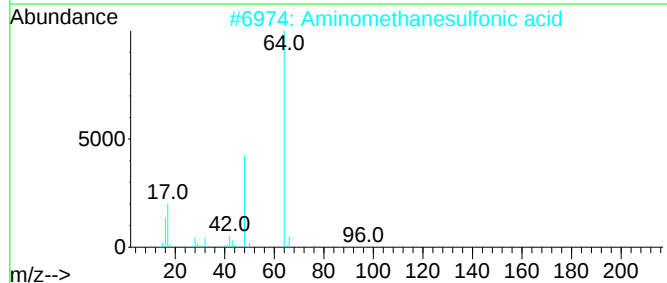
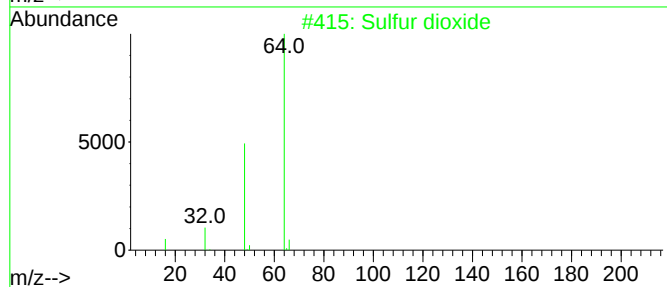
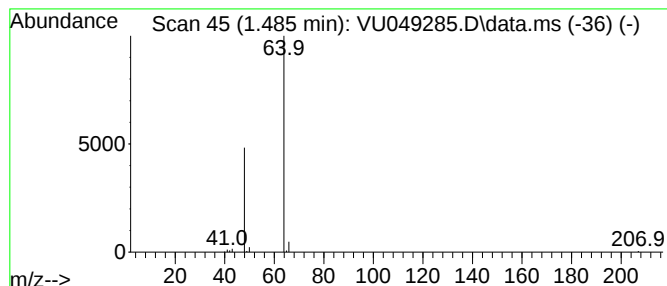
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.485	7.09 ug/L	94097	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			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecafluoro...	602	C10F22O2S	1000486-78-5	64
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.485	7.1	ug/L	94097	1	6.250	663430	50.0