

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045242.D
 Acq On : 08 Oct 2021 11:31
 Operator : SY/MD
 Sample : M3996-21
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK001

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: VU045242.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	34	40	53	rBV	18478	31802	2.50%	0.338%
2	1.600	74	81	92	rVB	194158	203104	15.96%	2.161%
3	1.896	164	173	184	rBV	131935	177233	13.93%	1.886%
4	2.562	368	380	403	rBV	252623	428084	33.63%	4.555%
5	2.787	444	450	454	rBV3	540	671	0.05%	0.007%
6	2.825	459	462	466	rBV	188	165	0.01%	0.002%
7	2.887	478	481	485	rBV	194	189	0.01%	0.002%
8	2.919	488	491	495	rVB2	267	211	0.02%	0.002%
9	2.954	495	502	508	rBV3	657	970	0.08%	0.010%
10	2.983	508	511	513	rVB	346	221	0.02%	0.002%
11	3.025	521	524	525	rBV2	258	167	0.01%	0.002%
12	3.047	525	531	540	rVV3	1357	2100	0.16%	0.022%
13	3.141	557	560	565	rBV2	173	214	0.02%	0.002%
14	3.186	565	574	576	rBV4	1083	1387	0.11%	0.015%
15	3.288	604	606	611	rVB2	295	273	0.02%	0.003%
16	3.549	684	687	690	rVB	236	182	0.01%	0.002%
17	3.597	698	702	705	rVB	200	163	0.01%	0.002%
18	3.645	714	717	722	rVB2	200	223	0.02%	0.002%
19	3.726	736	742	745	rBV	217	227	0.02%	0.002%
20	4.105	857	860	865	rVV	185	161	0.01%	0.002%
21	4.369	938	942	946	rBV2	223	211	0.02%	0.002%
22	4.626	1008	1022	1053	rBV	146903	344487	27.07%	3.666%
23	5.067	1143	1159	1184	rBV	218554	480721	37.77%	5.115%
24	5.292	1222	1229	1230	rBV	445	488	0.04%	0.005%
25	5.729	1342	1365	1390	rBV2	468874	1272753	100.00%	13.543%
26	5.838	1397	1399	1403	rVB3	483	308	0.02%	0.003%
27	6.025	1451	1457	1459	rBV2	199	256	0.02%	0.003%
28	6.047	1460	1464	1467	rVB2	498	446	0.04%	0.005%
29	6.111	1481	1484	1487	rVV3	273	229	0.02%	0.002%
30	6.253	1513	1528	1550	rBV	334872	623230	48.97%	6.632%
31	6.417	1574	1579	1583	rBV2	197	251	0.02%	0.003%
32	6.478	1595	1598	1604	rVB2	160	168	0.01%	0.002%
33	6.536	1605	1616	1630	rVV9	5169	10596	0.83%	0.113%
34	6.616	1636	1641	1643	rBV2	151	172	0.01%	0.002%
35	6.697	1650	1666	1692	rBV	299090	583424	45.84%	6.208%
36	6.809	1698	1701	1713	rVB4	723	961	0.08%	0.010%

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 Title : VOC Analysis

37	7.044	1768	1774	1776	rBV3	433	379	0.03%	0.004%
38	7.179	1810	1816	1821	rVV3	781	945	0.07%	0.010%
39	7.362	1862	1873	1878	rVB2	234	503	0.04%	0.005%
40	7.388	1878	1881	1884	rBV2	272	221	0.02%	0.002%
41	7.568	1924	1937	1953	rBV	167531	287229	22.57%	3.056%
42	7.668	1964	1968	1970	rBV2	234	196	0.02%	0.002%
43	7.690	1970	1975	1976	rBV2	461	383	0.03%	0.004%
44	7.738	1986	1990	1992	rBV	170	172	0.01%	0.002%
45	7.800	2004	2009	2015	rVB3	296	332	0.03%	0.004%
46	7.902	2026	2041	2056	rBV	567528	956285	75.14%	10.176%
47	7.973	2058	2063	2073	rVB	8335	12299	0.97%	0.131%
48	8.182	2115	2128	2151	rBV	116532	194294	15.27%	2.067%
49	8.381	2186	2190	2193	rBV2	161	173	0.01%	0.002%
50	8.636	2254	2269	2301	rBV	425321	751637	59.06%	7.998%
51	8.880	2342	2345	2347	rBV2	189	165	0.01%	0.002%
52	9.420	2500	2513	2542	rBV	491864	792293	62.25%	8.431%
53	9.571	2553	2560	2564	rBV	678	822	0.06%	0.009%
54	9.697	2591	2599	2615	rVB4	2491	4204	0.33%	0.045%
55	9.889	2655	2659	2661	rBV	184	162	0.01%	0.002%
56	9.976	2680	2686	2689	rBV2	203	230	0.02%	0.002%
57	10.102	2722	2725	2731	rVB3	537	566	0.04%	0.006%
58	10.185	2742	2751	2756	rBV2	210	295	0.02%	0.003%
59	10.359	2802	2805	2809	rBV2	274	262	0.02%	0.003%
60	10.443	2825	2831	2837	rBV	246	358	0.03%	0.004%
61	10.674	2895	2903	2911	rBV2	3414	4815	0.38%	0.051%
62	10.761	2915	2930	2950	rBV	427508	692566	54.41%	7.369%
63	10.873	2957	2965	2969	rBV3	607	929	0.07%	0.010%
64	10.896	2969	2972	2975	rVB	363	204	0.02%	0.002%
65	10.989	2998	3001	3004	rBV	225	214	0.02%	0.002%
66	11.098	3032	3035	3037	rVV2	282	202	0.02%	0.002%
67	11.118	3037	3041	3048	rVV3	663	753	0.06%	0.008%
68	11.195	3061	3065	3068	rVB2	214	189	0.01%	0.002%
69	11.217	3068	3072	3077	rBV2	339	382	0.03%	0.004%
70	11.381	3120	3123	3125	rBV2	232	175	0.01%	0.002%
71	11.462	3140	3148	3160	rVB6	2079	3544	0.28%	0.038%
72	11.578	3180	3184	3186	rBV	276	188	0.01%	0.002%
73	11.664	3207	3211	3214	rVB2	173	164	0.01%	0.002%
74	11.700	3214	3222	3229	rVB4	1251	1928	0.15%	0.021%
75	11.815	3245	3258	3277	rBV	436750	687857	54.04%	7.319%
76	11.944	3293	3298	3301	rBV2	959	1157	0.09%	0.012%

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77	11.976	3304	3308	3316	rVB2	2630	3229	0.25%	0.034%
78	12.118	3350	3352	3357	rVB	333	206	0.02%	0.002%
79	12.198	3359	3377	3397	rBV	505960	820125	64.44%	8.727%
80	12.311	3409	3412	3415	rBV2	405	271	0.02%	0.003%
81	12.336	3415	3420	3423	rVV3	769	550	0.04%	0.006%
82	12.433	3447	3450	3456	rBV2	212	226	0.02%	0.002%
83	12.642	3512	3515	3520	rVB2	383	309	0.02%	0.003%
84	12.774	3548	3556	3559	rBV	199	255	0.02%	0.003%
85	12.828	3569	3573	3577	rBV	240	274	0.02%	0.003%
86	13.095	3654	3656	3662	rVB2	187	164	0.01%	0.002%
87	13.159	3669	3676	3679	rVB3	242	290	0.02%	0.003%
88	13.632	3820	3823	3827	rBV	199	218	0.02%	0.002%
89	14.095	3959	3967	3976	rBV	1106	1639	0.13%	0.017%
90	14.211	3997	4003	4007	rBV2	241	271	0.02%	0.003%
91	14.227	4007	4008	4013	rVB2	339	193	0.02%	0.002%
92	14.253	4013	4016	4017	rBV	300	196	0.02%	0.002%
93	14.301	4027	4031	4035	rBV	327	362	0.03%	0.004%
94	14.339	4039	4043	4048	rVV2	385	425	0.03%	0.005%
95	14.442	4073	4075	4079	rVB2	412	264	0.02%	0.003%
96	14.741	4165	4168	4171	rBV2	280	193	0.02%	0.002%
97	14.889	4210	4214	4219	rBV3	406	484	0.04%	0.005%
98	14.976	4238	4241	4243	rBV2	281	208	0.02%	0.002%
99	15.159	4294	4298	4304	rBV2	471	686	0.05%	0.007%
100	15.876	4517	4521	4525	rBV2	589	587	0.05%	0.006%

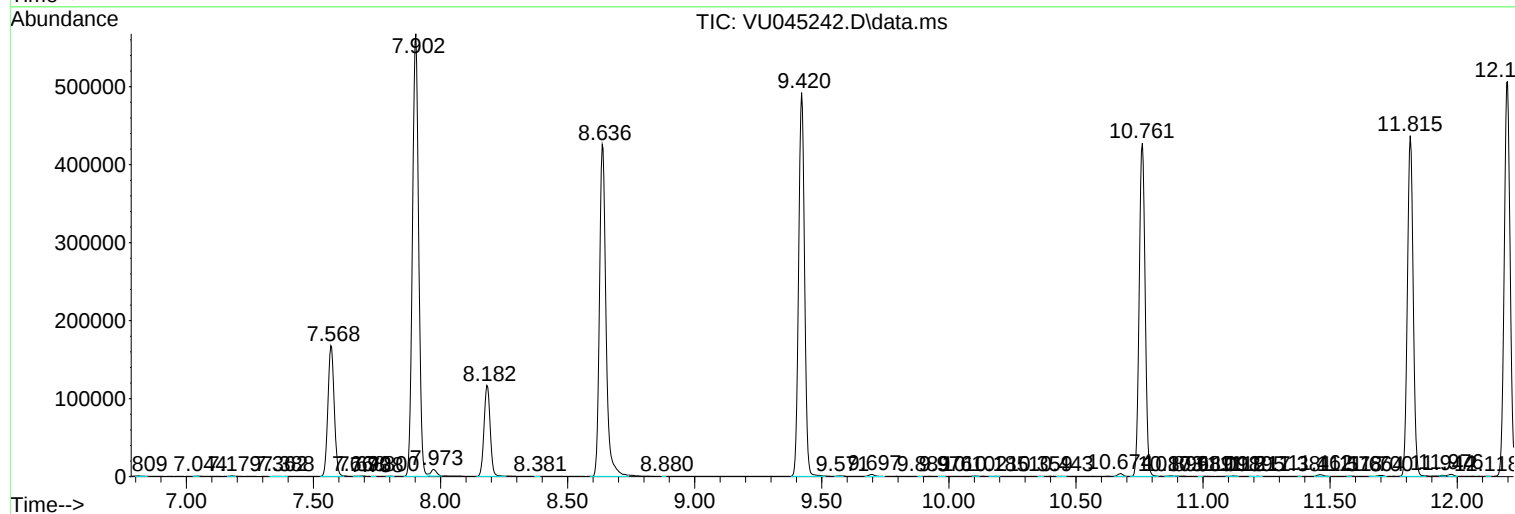
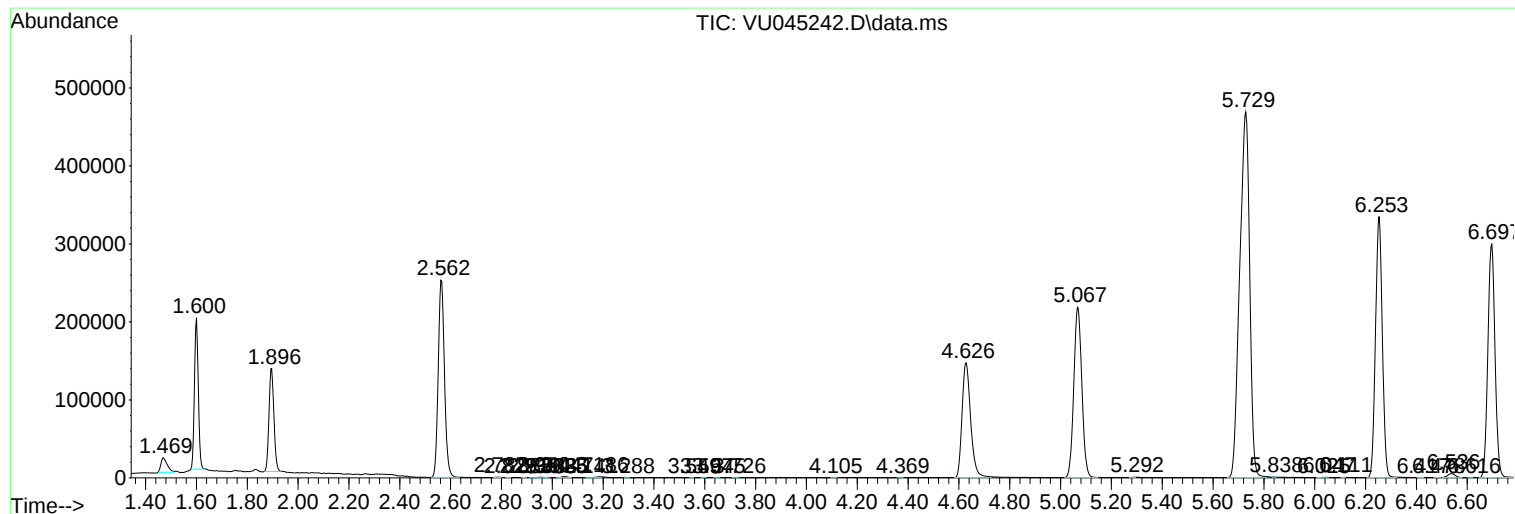
Sum of corrected areas: 9397745

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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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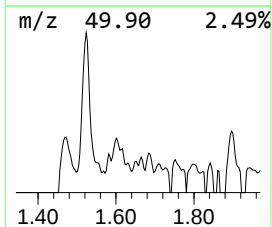
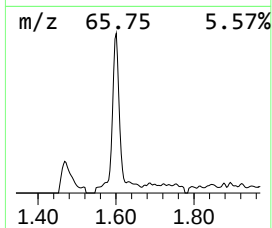
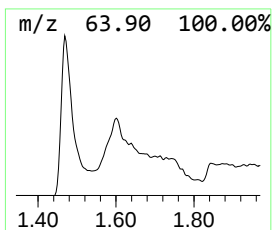
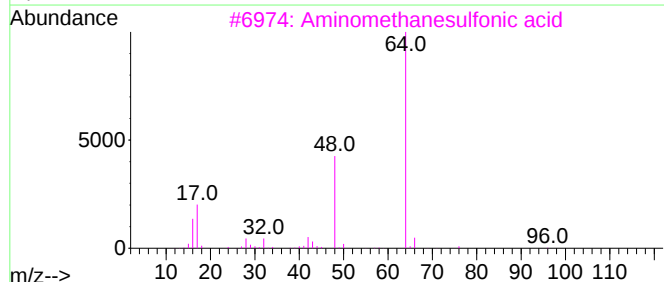
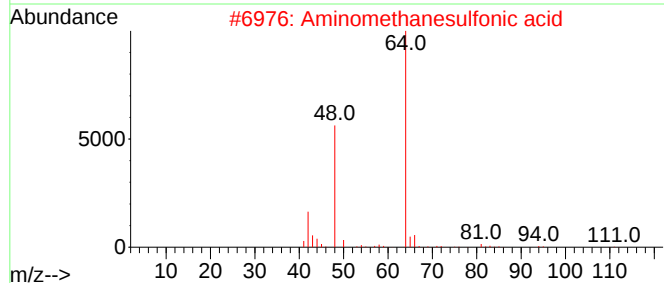
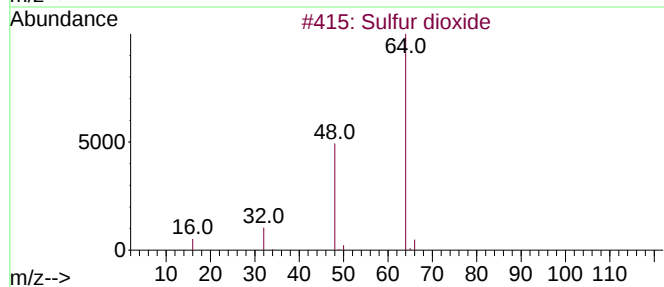
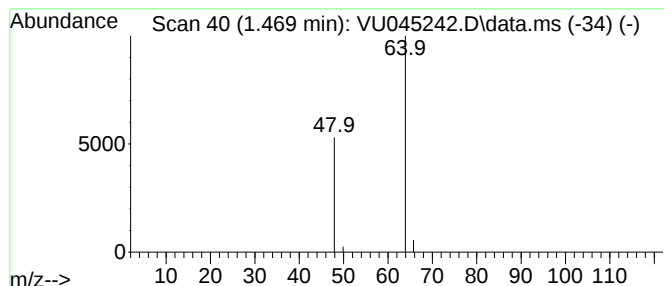
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	2.55 ug/L	31802	1,4-Difluorobenzene	6.253

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



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	2.5	ug/L	31802	1	6.253	623230	50.0