

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045181.D
 Acq On : 06 Oct 2021 13:25
 Operator : SY/MD
 Sample : M3996-04 4X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A16

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: VU0451181.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	53	rBV2	57301	75843	2.25%	0.517%
2	1.601	74	81	97	rVB	241725	265806	7.89%	1.811%
3	1.906	168	176	198	rVB	162791	229144	6.80%	1.561%
4	2.565	368	381	400	rBV	327200	551883	16.38%	3.761%
5	2.771	439	445	447	rBV	333	360	0.01%	0.002%
6	2.954	496	502	512	rVV3	418	790	0.02%	0.005%
7	3.051	523	532	542	rBV3	3014	5228	0.16%	0.036%
8	3.189	563	575	592	rVB	8213	18703	0.56%	0.127%
9	3.372	620	632	645	rVB2	4841	10574	0.31%	0.072%
10	3.517	672	677	681	rBV2	175	204	0.01%	0.001%
11	3.758	748	752	758	rVB2	249	342	0.01%	0.002%
12	3.790	759	762	770	rVB2	181	262	0.01%	0.002%
13	3.999	821	827	832	rVB2	215	262	0.01%	0.002%
14	4.028	832	836	842	rBV	191	293	0.01%	0.002%
15	4.144	866	872	875	rBV2	207	280	0.01%	0.002%
16	4.211	890	893	897	rBV2	204	218	0.01%	0.001%
17	4.626	1008	1022	1031	rBV	165898	388005	11.51%	2.644%
18	4.832	1084	1086	1094	rVB2	265	196	0.01%	0.001%
19	4.900	1104	1107	1110	rBV2	282	253	0.01%	0.002%
20	5.070	1142	1160	1184	rBV	270552	592803	17.59%	4.039%
21	5.266	1218	1221	1224	rBV2	230	222	0.01%	0.002%
22	5.324	1224	1239	1249	rVV5	3894	8732	0.26%	0.059%
23	5.375	1253	1255	1259	rVV	244	173	0.01%	0.001%
24	5.729	1343	1365	1394	rBV2	574304	1539113	45.67%	10.487%
25	6.035	1457	1460	1464	rBV2	231	193	0.01%	0.001%
26	6.115	1482	1485	1492	rVB	342	369	0.01%	0.003%
27	6.253	1513	1528	1546	rBV	378076	704573	20.91%	4.801%
28	6.543	1606	1618	1629	rVB5	10096	20094	0.60%	0.137%
29	6.588	1629	1632	1635	rBV	252	194	0.01%	0.001%
30	6.697	1650	1666	1686	rBV	358396	696010	20.65%	4.743%
31	6.809	1698	1701	1710	rVB5	1226	1445	0.04%	0.010%
32	6.973	1746	1752	1758	rBV4	486	692	0.02%	0.005%
33	7.047	1764	1775	1781	rBV3	821	1458	0.04%	0.010%
34	7.073	1781	1783	1789	rVB2	320	236	0.01%	0.002%
35	7.189	1809	1819	1826	rVB4	1098	1840	0.05%	0.013%
36	7.243	1830	1836	1844	rVV2	205	390	0.01%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.279	1844	1847	1852	rVV2	153	178	0.01%	0.001%
38	7.317	1856	1859	1863	rBV2	257	232	0.01%	0.002%
39	7.436	1892	1896	1902	rBV2	196	233	0.01%	0.002%
40	7.488	1909	1912	1917	rBV2	204	240	0.01%	0.002%
41	7.568	1925	1937	1956	rBV	205739	354718	10.53%	2.417%
42	7.903	2025	2041	2056	rBV	719657	1219742	36.20%	8.311%
43	7.973	2056	2063	2076	rVB2	10509	18894	0.56%	0.129%
44	8.182	2116	2128	2145	rBV	143094	234885	6.97%	1.600%
45	8.427	2197	2204	2209	rBV2	225	374	0.01%	0.003%
46	8.555	2230	2244	2258	rBV	1980947	3369896	100.00%	22.962%
47	8.636	2259	2269	2297	rVB	485391	848496	25.18%	5.782%
48	8.890	2343	2348	2351	rBV2	279	241	0.01%	0.002%
49	9.022	2385	2389	2394	rVB3	206	192	0.01%	0.001%
50	9.108	2410	2416	2421	rBV2	221	286	0.01%	0.002%
51	9.231	2450	2454	2457	rBV2	191	208	0.01%	0.001%
52	9.288	2467	2472	2479	rBV2	179	195	0.01%	0.001%
53	9.346	2486	2490	2493	rBV2	241	247	0.01%	0.002%
54	9.420	2500	2513	2549	rBV	542033	880005	26.11%	5.996%
55	9.575	2553	2561	2572	rVB	4254	6226	0.18%	0.042%
56	9.642	2572	2582	2587	rBV2	231	450	0.01%	0.003%
57	9.697	2587	2599	2610	rBV	19824	31184	0.93%	0.212%
58	9.742	2610	2613	2617	rBV3	220	175	0.01%	0.001%
59	9.957	2677	2680	2684	rBV2	246	185	0.01%	0.001%
60	9.986	2687	2689	2694	rVB2	267	221	0.01%	0.002%
61	10.031	2699	2703	2706	rBV	211	196	0.01%	0.001%
62	10.102	2718	2725	2736	rBV	2477	3225	0.10%	0.022%
63	10.423	2822	2825	2829	rBV2	253	220	0.01%	0.001%
64	10.462	2829	2837	2839	rBV2	220	295	0.01%	0.002%
65	10.485	2840	2844	2856	rVB3	959	1241	0.04%	0.008%
66	10.607	2875	2882	2885	rBV2	236	280	0.01%	0.002%
67	10.632	2885	2890	2892	rBV	188	200	0.01%	0.001%
68	10.674	2895	2903	2911	rVB2	4501	6517	0.19%	0.044%
69	10.761	2916	2930	2949	rBV	473442	760979	22.58%	5.185%
70	10.874	2957	2965	2967	rVV	891	1197	0.04%	0.008%
71	10.903	2971	2974	2987	rVB3	1152	1940	0.06%	0.013%
72	10.980	2994	2998	3001	rVB2	230	190	0.01%	0.001%
73	11.118	3036	3041	3043	rBV3	1066	1141	0.03%	0.008%
74	11.153	3049	3052	3058	rVB2	777	705	0.02%	0.005%
75	11.205	3064	3068	3070	rBV2	352	232	0.01%	0.002%
76	11.243	3075	3080	3083	rBV	588	510	0.02%	0.003%

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Title : VOC Analysis

77	11.292	3092	3095	3102	rVB3	305	299	0.01%	0.002%
78	11.366	3113	3118	3120	rBV	176	192	0.01%	0.001%
79	11.382	3120	3123	3127	rVB2	299	224	0.01%	0.002%
80	11.465	3139	3149	3160	rVB4	3074	5615	0.17%	0.038%
81	11.584	3181	3186	3194	rVB2	761	815	0.02%	0.006%
82	11.703	3214	3223	3229	rBV4	1568	2389	0.07%	0.016%
83	11.816	3246	3258	3275	rBV	495960	782860	23.23%	5.334%
84	11.944	3293	3298	3301	rBV5	1220	1382	0.04%	0.009%
85	11.976	3304	3308	3318	rVB3	3035	3680	0.11%	0.025%
86	12.195	3361	3376	3395	rBV	623767	1007063	29.88%	6.862%
87	12.327	3414	3417	3418	rBV2	879	533	0.02%	0.004%
88	12.449	3449	3455	3459	rBV	221	297	0.01%	0.002%
89	12.642	3510	3515	3521	rBV3	683	660	0.02%	0.004%
90	12.980	3616	3620	3621	rBV2	378	293	0.01%	0.002%
91	13.208	3688	3691	3696	rBV2	206	197	0.01%	0.001%
92	13.446	3761	3765	3767	rBV2	428	312	0.01%	0.002%
93	13.517	3780	3787	3791	rBV3	308	531	0.02%	0.004%
94	13.732	3851	3854	3856	rBV	293	207	0.01%	0.001%
95	13.915	3905	3911	3915	rBV2	326	464	0.01%	0.003%
96	13.935	3915	3917	3922	rVV2	274	226	0.01%	0.002%
97	14.092	3962	3966	3982	rVB2	1540	2429	0.07%	0.017%
98	14.574	4114	4116	4118	rBV2	288	188	0.01%	0.001%
99	14.922	4221	4224	4226	rBV2	269	216	0.01%	0.001%
100	15.410	4373	4376	4383	rBV3	689	756	0.02%	0.005%

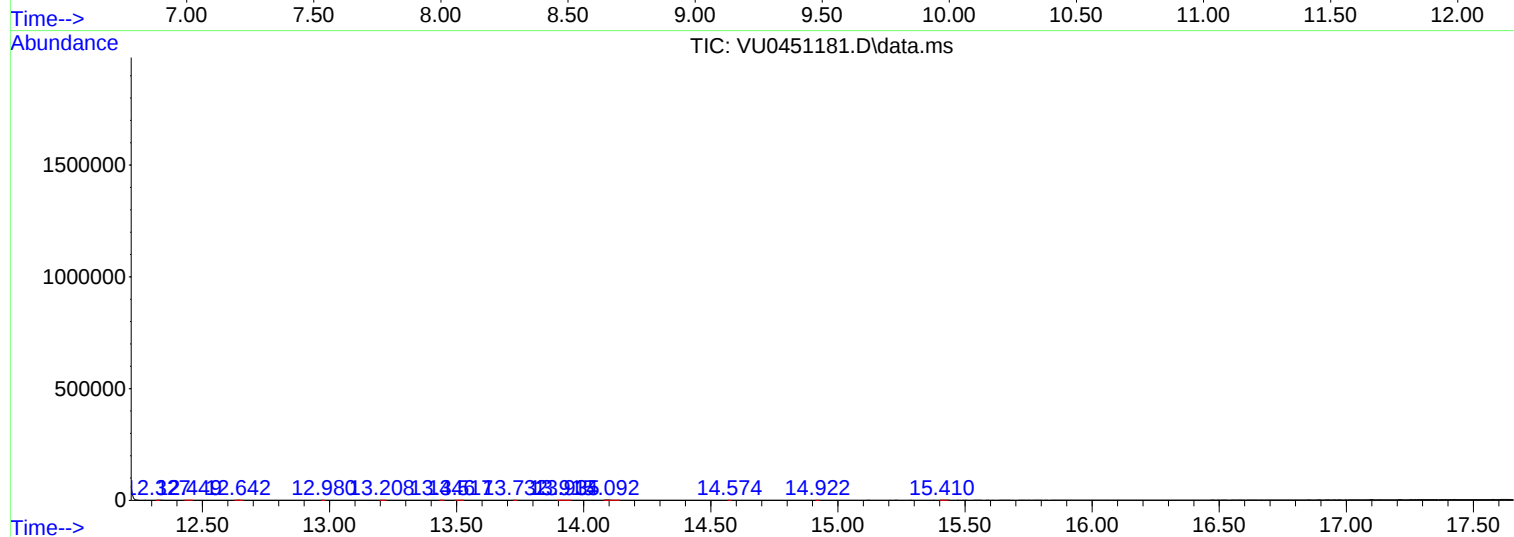
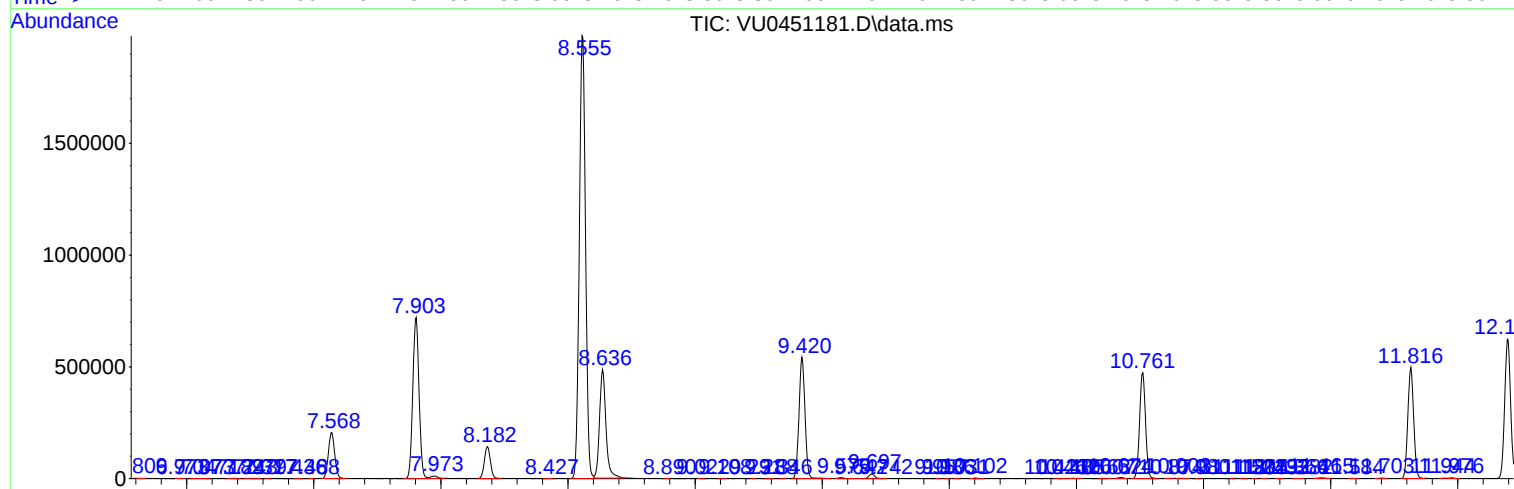
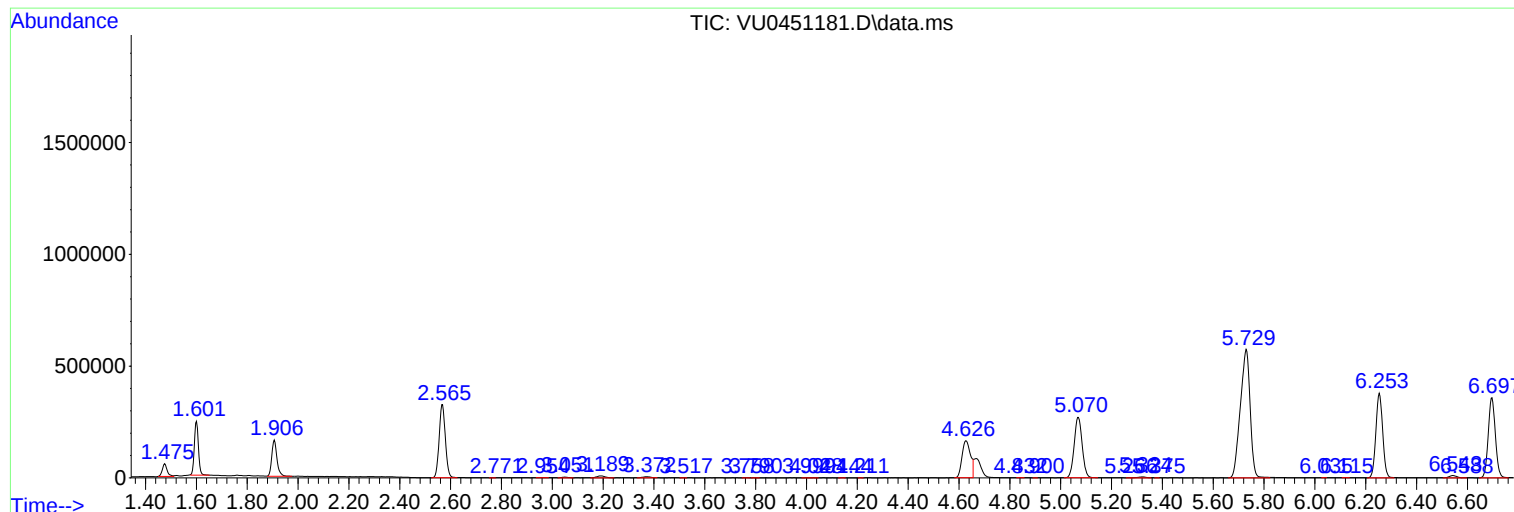
Sum of corrected areas: 14675782

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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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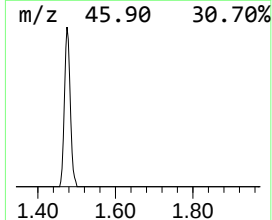
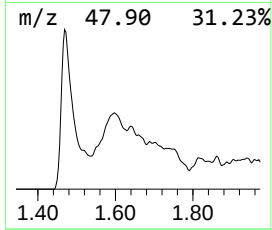
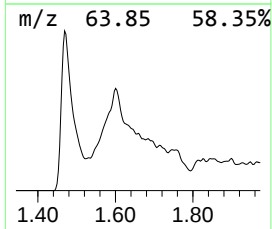
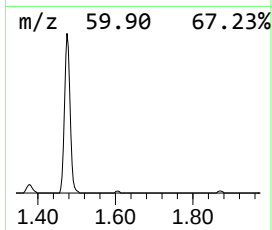
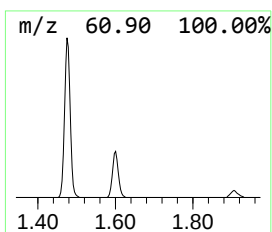
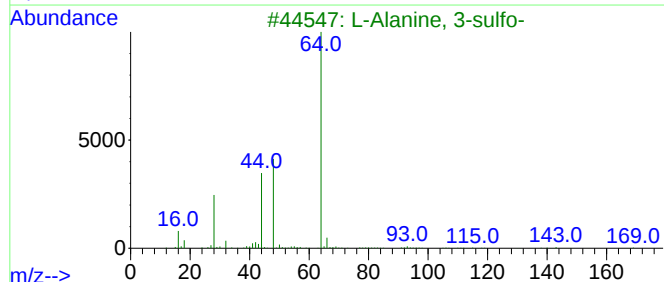
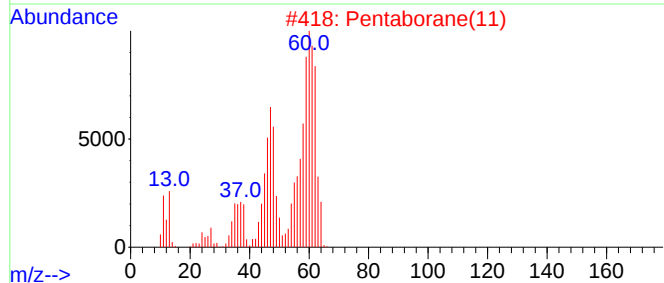
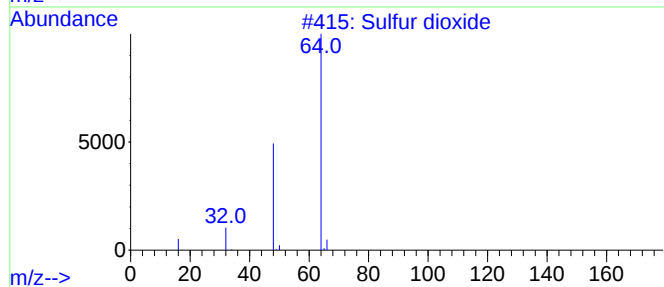
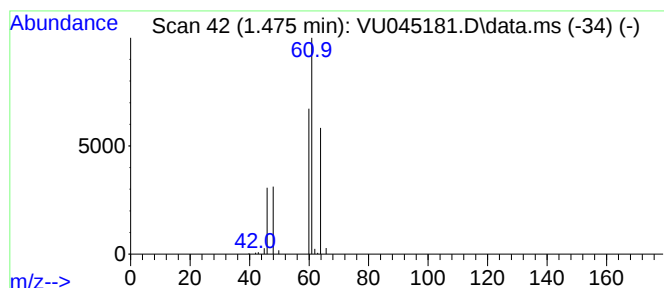
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	5.38 ug/L	75843	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	37
2			Pentaborane(11)	66	B5H11	018433-84-6	9
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.475	5.4	ug/L	75843	1	6.253	704573	50.0