

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
 Data File : VU033919.D
 Acq On : 22 Aug 2019 23:02
 Operator : JC/SP
 Sample : K4485-08
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F2B68

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.174	22	26	34	rBV2	7641	7444	0.31%	0.041%
2	1.280	52	59	73	rBV	37242	72782	3.03%	0.403%
3	1.389	86	93	108	rVB	345070	367025	15.27%	2.035%
4	1.669	172	180	199	rVB	270398	343148	14.28%	1.902%
5	2.254	352	362	373	rBV	565426	840818	34.99%	4.661%
6	2.678	490	494	495	rBV2	707	468	0.02%	0.003%
7	2.810	523	535	548	rBV4	7346	16417	0.68%	0.091%
8	2.952	575	579	582	rBV3	335	325	0.01%	0.002%
9	2.971	582	585	591	rVB4	635	586	0.02%	0.003%
10	3.023	598	601	604	rBV	340	275	0.01%	0.002%
11	3.045	604	608	610	rVV2	485	288	0.01%	0.002%
12	3.106	624	627	630	rBV3	495	419	0.02%	0.002%
13	3.161	636	644	646	rBV3	615	725	0.03%	0.004%
14	3.219	659	662	665	rBV2	451	282	0.01%	0.002%
15	3.357	701	705	710	rBV3	511	527	0.02%	0.003%
16	3.408	718	721	724	rBV2	417	307	0.01%	0.002%
17	3.453	733	735	740	rVB2	583	436	0.02%	0.002%
18	3.482	740	744	745	rBV	602	353	0.01%	0.002%
19	3.521	751	756	759	rBV3	302	292	0.01%	0.002%
20	3.695	807	810	817	rVB3	316	334	0.01%	0.002%
21	3.955	880	891	896	rBV5	1280	2242	0.09%	0.012%
22	4.000	903	905	908	rVB	395	239	0.01%	0.001%
23	4.151	939	952	1001	rBV2	192339	595072	24.76%	3.299%
24	4.524	1066	1068	1074	rVB3	662	537	0.02%	0.003%
25	4.550	1074	1076	1079	rBV3	351	244	0.01%	0.001%
26	4.621	1079	1098	1131	rVV	381777	939986	39.12%	5.211%
27	4.865	1165	1174	1182	rVB10	1505	3038	0.13%	0.017%
28	4.971	1198	1207	1210	rBV6	865	1100	0.05%	0.006%
29	5.022	1220	1223	1227	rBV2	350	334	0.01%	0.002%
30	5.055	1227	1233	1239	rVB6	592	916	0.04%	0.005%
31	5.093	1239	1245	1248	rBV4	405	427	0.02%	0.002%
32	5.145	1259	1261	1265	rBV2	411	284	0.01%	0.002%
33	5.177	1265	1271	1275	rBV4	416	440	0.02%	0.002%
34	5.315	1289	1314	1342	rBV2	811679	2403072	100.00%	13.321%

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 Title : VOC Analysis

35	5.653	1411	1419	1423	rBV4	1166	1675	0.07%	0.009%
36	5.862	1470	1484	1511	rBV	703374	1399778	58.25%	7.759%
37	6.151	1562	1574	1596	rVB	63171	127851	5.32%	0.709%
38	6.309	1608	1623	1647	rBV	553817	1116613	46.47%	6.190%
39	6.437	1660	1663	1671	rVB5	1537	1760	0.07%	0.010%
40	6.585	1706	1709	1711	rBV3	557	316	0.01%	0.002%
41	6.601	1712	1714	1716	rVV2	597	320	0.01%	0.002%
42	6.614	1716	1718	1721	rVB3	639	265	0.01%	0.001%
43	6.717	1746	1750	1757	rVB3	487	636	0.03%	0.004%
44	6.772	1764	1767	1768	rBV3	415	255	0.01%	0.001%
45	6.807	1768	1778	1786	rBV6	2587	5199	0.22%	0.029%
46	6.862	1792	1795	1797	rBV2	472	323	0.01%	0.002%
47	6.894	1803	1805	1808	rVB2	668	392	0.02%	0.002%
48	6.964	1825	1827	1831	rVB3	420	234	0.01%	0.001%
49	7.019	1839	1844	1848	rVB4	435	421	0.02%	0.002%
50	7.071	1856	1860	1862	rBV2	385	234	0.01%	0.001%
51	7.100	1866	1869	1873	rVV	331	311	0.01%	0.002%
52	7.125	1874	1877	1880	rVB2	495	336	0.01%	0.002%
53	7.209	1889	1903	1923	rBV	270284	501520	20.87%	2.780%
54	7.546	1993	2008	2042	rBV	1049456	1847842	76.89%	10.243%
55	7.829	2085	2096	2117	rBV	195164	346099	14.40%	1.919%
56	8.157	2194	2198	2202	rBV3	416	368	0.02%	0.002%
57	8.209	2209	2214	2218	rBV6	2014	2724	0.11%	0.015%
58	8.296	2228	2241	2275	rBV3	559237	1197777	49.84%	6.640%
59	8.659	2352	2354	2358	rVB3	674	347	0.01%	0.002%
60	8.739	2375	2379	2382	rVB4	682	560	0.02%	0.003%
61	8.759	2382	2385	2388	rBV2	504	417	0.02%	0.002%
62	8.826	2401	2406	2411	rBV4	880	1121	0.05%	0.006%
63	8.884	2420	2424	2426	rVB2	523	417	0.02%	0.002%
64	8.907	2426	2431	2434	rBV4	639	540	0.02%	0.003%
65	9.070	2468	2482	2510	rBV	1064579	1779707	74.06%	9.866%
66	9.363	2569	2573	2582	rVB7	1279	1928	0.08%	0.011%
67	9.402	2582	2585	2589	rBV2	524	403	0.02%	0.002%
68	9.453	2597	2601	2602	rBV	525	326	0.01%	0.002%
69	9.591	2641	2644	2651	rBV3	640	552	0.02%	0.003%
70	9.636	2655	2658	2662	rBV2	494	400	0.02%	0.002%
71	9.697	2673	2677	2680	rBV3	420	323	0.01%	0.002%

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72	9.861	2725	2728	2731	rBV2	459	236	0.01%	0.001%
73	9.923	2740	2747	2759	rBV5	1627	3229	0.13%	0.018%
74	9.990	2766	2768	2771	rBV2	446	248	0.01%	0.001%
75	10.077	2793	2795	2798	rBV3	357	243	0.01%	0.001%
76	10.109	2801	2805	2810	rVV4	458	438	0.02%	0.002%
77	10.206	2830	2835	2840	rBV3	635	632	0.03%	0.004%
78	10.231	2840	2843	2846	rBV3	424	289	0.01%	0.002%
79	10.347	2877	2879	2882	rBV3	377	274	0.01%	0.002%
80	10.415	2887	2900	2923	rBV	627898	1021982	42.53%	5.665%
81	10.540	2935	2939	2940	rBV3	613	419	0.02%	0.002%
82	10.607	2958	2960	2966	rVB4	600	483	0.02%	0.003%
83	10.640	2966	2970	2980	rBV3	916	1329	0.06%	0.007%
84	10.717	2987	2994	2998	rBB4	468	598	0.02%	0.003%
85	10.897	3048	3050	3053	rVB3	596	277	0.01%	0.002%
86	10.919	3053	3057	3062	rBV3	564	760	0.03%	0.004%
87	10.945	3063	3065	3068	rVV	497	311	0.01%	0.002%
88	10.964	3068	3071	3074	rVV4	597	360	0.01%	0.002%
89	10.996	3078	3081	3083	rVV2	531	383	0.02%	0.002%
90	11.035	3087	3093	3097	rBV3	458	502	0.02%	0.003%
91	11.058	3098	3100	3109	rVV4	483	638	0.03%	0.004%
92	11.144	3121	3127	3130	rBV2	618	728	0.03%	0.004%
93	11.199	3141	3144	3145	rBV2	467	245	0.01%	0.001%
94	11.337	3179	3187	3190	rBV3	653	925	0.04%	0.005%
95	11.466	3215	3227	3250	rBV	949132	1499806	62.41%	8.314%
96	11.842	3331	3344	3366	rBV	958639	1561221	64.97%	8.654%
97	12.379	3509	3511	3517	rBV4	663	593	0.02%	0.003%
98	12.524	3553	3556	3559	rVB3	668	401	0.02%	0.002%
99	12.691	3605	3608	3610	rBV2	528	318	0.01%	0.002%
100	14.102	4045	4047	4048	rBV	679	317	0.01%	0.002%

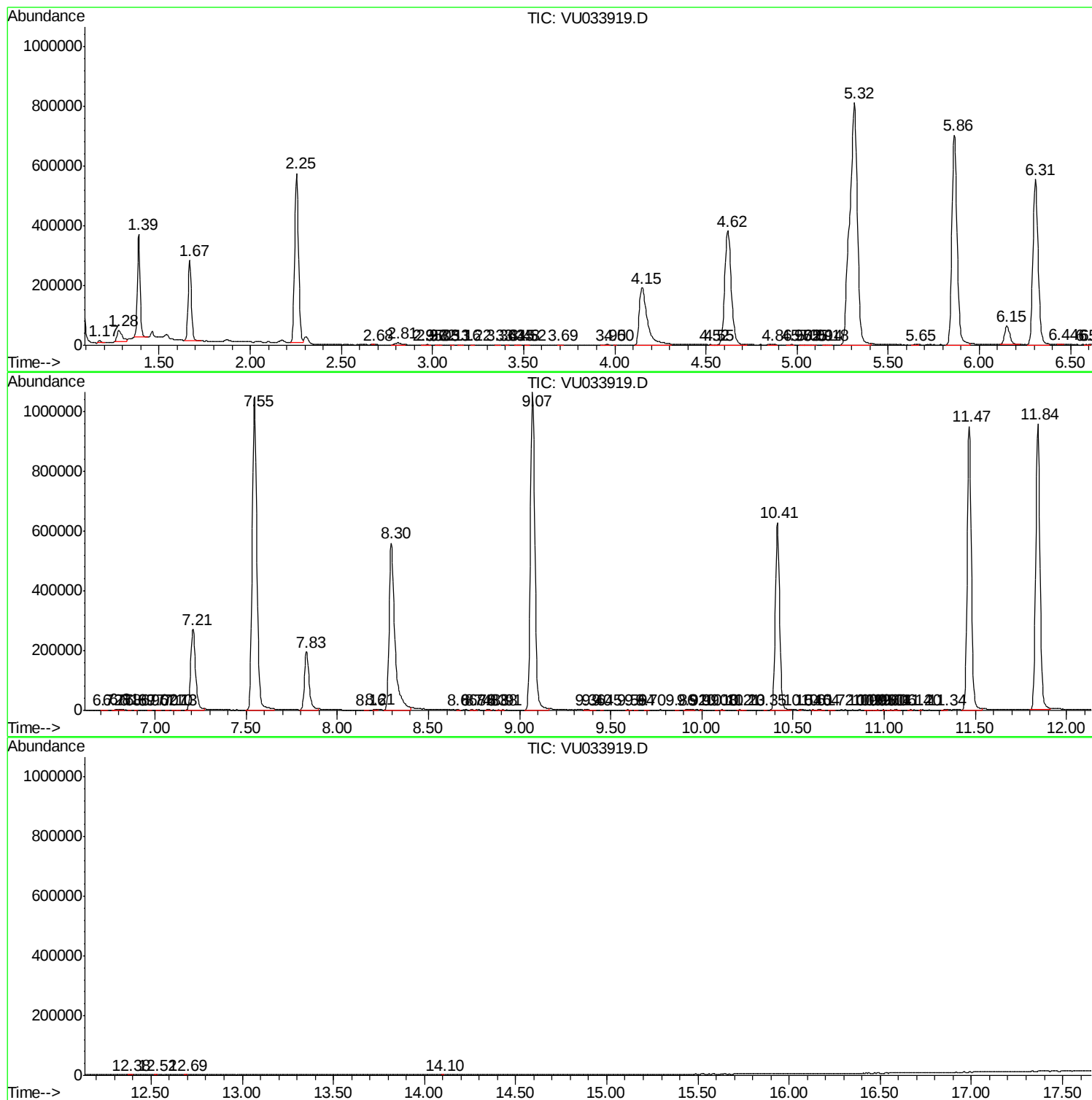
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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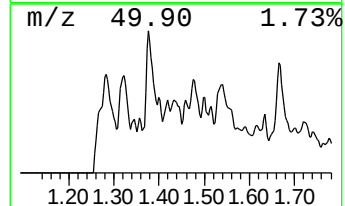
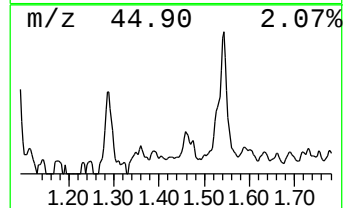
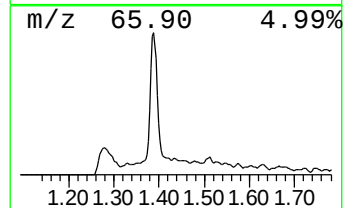
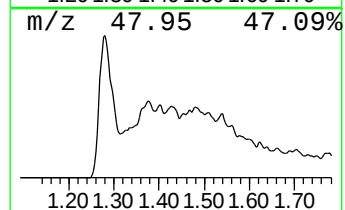
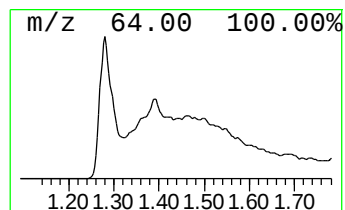
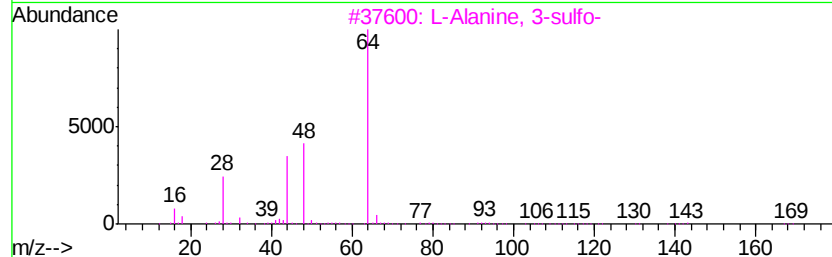
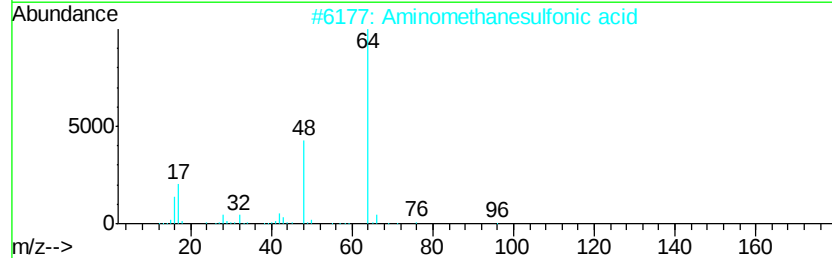
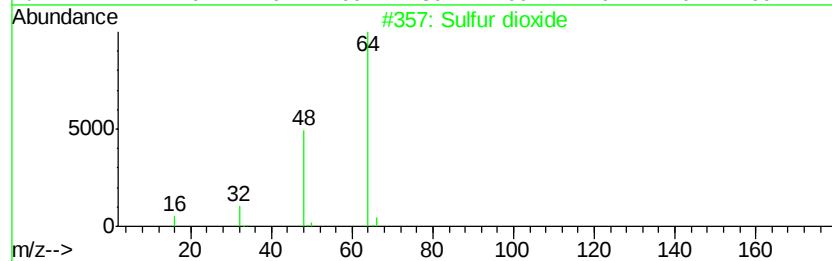
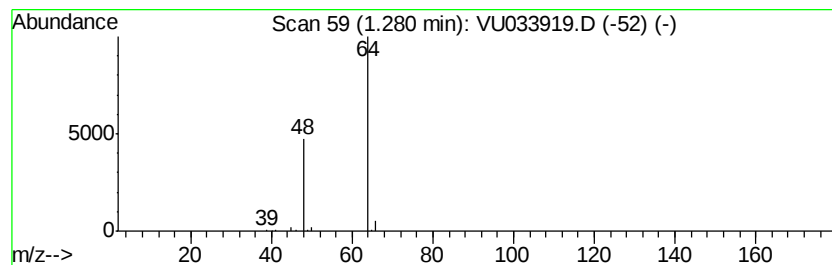
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	2.60 ug/L	72782	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	90
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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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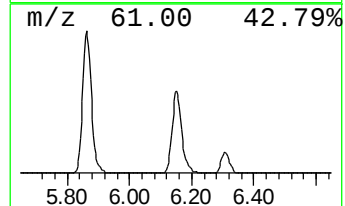
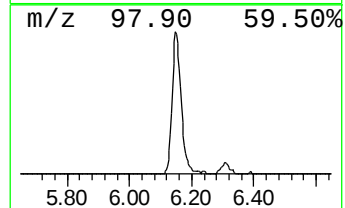
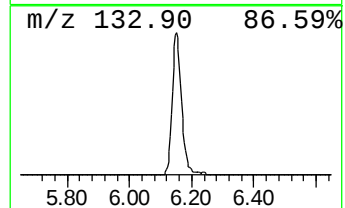
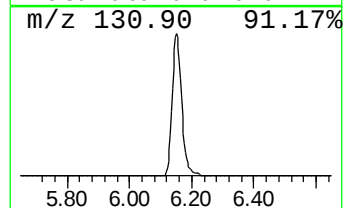
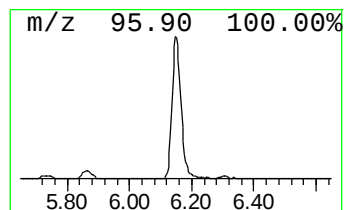
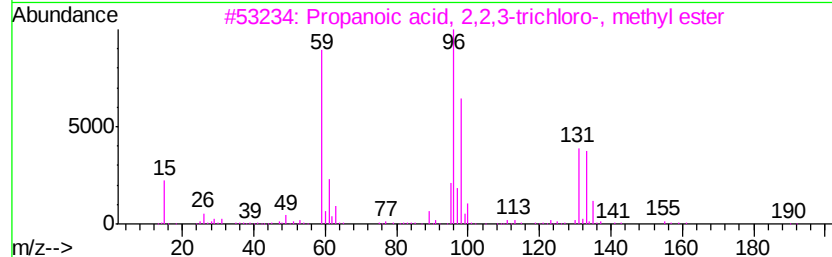
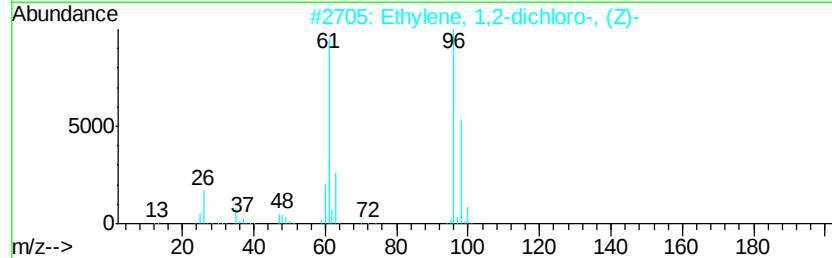
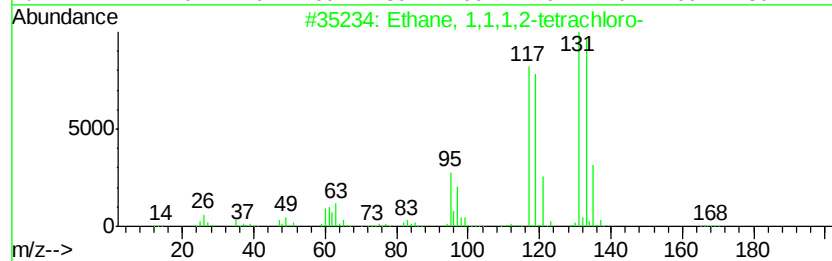
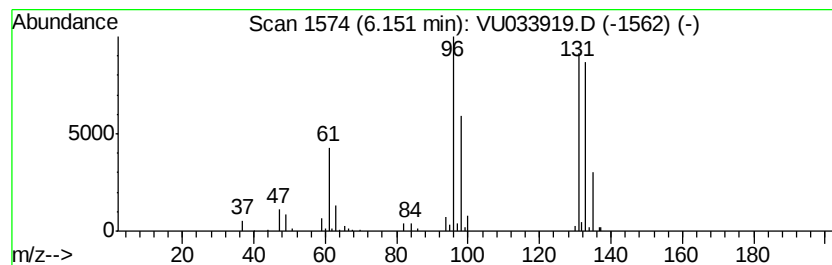
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.15	4.57 ug/L	127851	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
2		Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
3		Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	23
4		Difluoro(methylamino)phosphine s...	131	CH4F2NPS	1000306-16-8	9
5		1H-Imidazole, 1-ethyl-	96	C5H8N2	007098-07-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.28	2.6	ug/L	72782	1	5.86	1399780	50.0
unknown-01	6.15	4.6	ug/L	127851	1	5.86	1399780	50.0