

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092519\
 Data File : VU034801.D
 Acq On : 25 Sep 2019 14:30
 Operator : JC/SP
 Sample : K4948-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEDM8

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\SOMULM091919WMA.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	1.177	22	27	44	rVB2	32141	36290	1.57%	0.191%
2	1.395	88	95	104	rBV	344761	371983	16.12%	1.953%
3	1.672	174	181	196	rVB	276950	348218	15.09%	1.828%
4	2.257	354	363	376	rVB	496988	760995	32.99%	3.996%
5	2.431	408	417	439	rVB	30990	62404	2.71%	0.328%
6	2.688	488	497	506	rBV8	6532	12567	0.54%	0.066%
7	2.739	510	513	520	rVB6	2581	1918	0.08%	0.010%
8	2.768	520	522	523	rBV2	1419	691	0.03%	0.004%
9	2.820	527	538	553	rVB	55748	121522	5.27%	0.638%
10	2.981	576	588	604	rVB	38329	79989	3.47%	0.420%
11	3.080	615	619	623	rBV6	1616	1378	0.06%	0.007%
12	3.103	623	626	628	rBV4	1578	959	0.04%	0.005%
13	3.173	643	648	652	rBV7	1732	1781	0.08%	0.009%
14	3.688	806	808	812	rVB5	1343	994	0.04%	0.005%
15	3.730	812	821	825	rBV6	2037	2587	0.11%	0.014%
16	3.778	831	836	837	rBV3	1319	1017	0.04%	0.005%
17	3.788	837	839	841	rVV2	1221	563	0.02%	0.003%
18	3.804	841	844	846	rVV3	978	650	0.03%	0.003%
19	3.829	850	852	856	rVB3	1211	735	0.03%	0.004%
20	3.900	872	874	879	rVB3	781	676	0.03%	0.004%
21	3.923	879	881	884	rBV2	1181	655	0.03%	0.003%
22	4.080	926	930	934	rVB4	696	661	0.03%	0.003%
23	4.103	934	937	939	rVB2	947	552	0.02%	0.003%
24	4.151	939	952	984	rBV	239891	701610	30.41%	3.684%
25	4.517	1064	1066	1068	rBV3	1320	689	0.03%	0.004%
26	4.559	1076	1079	1080	rBV3	1211	538	0.02%	0.003%
27	4.624	1083	1099	1124	rVV	367097	876652	38.00%	4.603%
28	4.958	1200	1203	1204	rBV3	1680	869	0.04%	0.005%
29	5.170	1265	1269	1270	rBV2	1355	871	0.04%	0.005%
30	5.196	1274	1277	1279	rVB2	1400	752	0.03%	0.004%
31	5.315	1291	1314	1334	rBV2	784433	2306962	100.00%	12.113%
32	5.865	1470	1485	1507	rBV	577285	1160325	50.30%	6.092%
33	6.308	1609	1623	1645	rBV	532316	1089523	47.23%	5.720%
34	6.691	1740	1742	1745	rBV3	1259	670	0.03%	0.004%

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 Title : VOC Analysis

35	6.762	1760	1764	1767	rBV3	1264	1203	0.05%	0.006%
36	6.871	1796	1798	1803	rVB3	1565	1180	0.05%	0.006%
37	7.003	1837	1839	1842	rVB2	1365	687	0.03%	0.004%
38	7.029	1843	1847	1853	rBV7	1212	1535	0.07%	0.008%
39	7.154	1884	1886	1888	rBV3	1062	595	0.03%	0.003%
40	7.205	1888	1902	1923	rBV	297172	564606	24.47%	2.964%
41	7.543	1993	2007	2025	rBV	1076949	1898584	82.30%	9.968%
42	7.829	2086	2096	2122	rBV2	197584	366036	15.87%	1.922%
43	8.038	2159	2161	2164	rBV4	1117	542	0.02%	0.003%
44	8.151	2190	2196	2200	rBV5	3623	5060	0.22%	0.027%
45	8.205	2200	2213	2229	rVV	802222	1363397	59.10%	7.158%
46	8.289	2229	2239	2277	rVV	690198	1334484	57.85%	7.007%
47	8.649	2348	2351	2354	rBV4	1900	946	0.04%	0.005%
48	8.739	2376	2379	2385	rBV8	1284	1298	0.06%	0.007%
49	8.826	2404	2406	2411	rVB4	2021	1367	0.06%	0.007%
50	8.926	2433	2437	2438	rBV4	1041	629	0.03%	0.003%
51	8.977	2449	2453	2455	rBV4	1313	985	0.04%	0.005%
52	9.067	2469	2481	2516	rBV	850312	1470735	63.75%	7.722%
53	9.312	2553	2557	2560	rBV5	1758	1285	0.06%	0.007%
54	9.353	2567	2570	2572	rBV4	1333	830	0.04%	0.004%
55	9.379	2576	2578	2584	rVV7	1439	982	0.04%	0.005%
56	9.414	2587	2589	2592	rBV4	971	639	0.03%	0.003%
57	9.572	2635	2638	2640	rBV2	1047	608	0.03%	0.003%
58	9.810	2709	2712	2716	rBV4	1372	1213	0.05%	0.006%
59	9.916	2742	2745	2748	rVB4	1129	589	0.03%	0.003%
60	9.935	2748	2751	2752	rBV2	1268	674	0.03%	0.004%
61	9.980	2761	2765	2767	rBV2	1177	834	0.04%	0.004%
62	10.003	2770	2772	2775	rVB3	1455	678	0.03%	0.004%
63	10.022	2776	2778	2781	rBV3	1217	712	0.03%	0.004%
64	10.057	2786	2789	2791	rBV3	962	614	0.03%	0.003%
65	10.119	2805	2808	2811	rBV3	1432	1009	0.04%	0.005%
66	10.144	2814	2816	2826	rVB8	1541	2215	0.10%	0.012%
67	10.212	2835	2837	2840	rBV4	993	688	0.03%	0.004%
68	10.276	2854	2857	2860	rVB4	1573	988	0.04%	0.005%
69	10.318	2867	2870	2874	rVB3	1635	930	0.04%	0.005%
70	10.344	2876	2878	2881	rVB4	1051	695	0.03%	0.004%
71	10.408	2881	2898	2921	rBV	709860	1167553	50.61%	6.130%

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72	10.553	2941	2943	2946	rVV4	1658	1145	0.05%	0.006%
73	10.588	2947	2954	2964	rVB10	5597	9465	0.41%	0.050%
74	10.649	2971	2973	2978	rVB3	1131	653	0.03%	0.003%
75	10.819	3024	3026	3031	rBV	1075	799	0.03%	0.004%
76	11.009	3083	3085	3090	rVB3	1519	1071	0.05%	0.006%
77	11.270	3163	3166	3168	rBV4	1160	741	0.03%	0.004%
78	11.366	3194	3196	3198	rBV2	960	582	0.03%	0.003%
79	11.459	3214	3225	3247	rBV	774251	1288115	55.84%	6.763%
80	11.836	3330	3342	3366	rBV	938479	1573134	68.19%	8.260%
81	12.167	3443	3445	3447	rBV3	1402	718	0.03%	0.004%
82	12.244	3466	3469	3471	rBV4	2030	1343	0.06%	0.007%
83	12.427	3523	3526	3528	rBV4	1208	849	0.04%	0.004%
84	12.681	3603	3605	3607	rVB	1463	580	0.03%	0.003%
85	12.694	3607	3609	3614	rVB5	1207	824	0.04%	0.004%
86	12.720	3614	3617	3619	rBV3	2187	1351	0.06%	0.007%
87	12.810	3641	3645	3646	rBV3	1542	1124	0.05%	0.006%
88	12.884	3666	3668	3672	rBV3	1394	1127	0.05%	0.006%
89	12.909	3673	3676	3678	rBV4	1869	1268	0.05%	0.007%
90	12.945	3685	3687	3692	rVB4	1924	1215	0.05%	0.006%
91	13.170	3754	3757	3760	rVB5	1770	974	0.04%	0.005%
92	13.485	3853	3855	3859	rVB3	1280	780	0.03%	0.004%
93	13.604	3889	3892	3894	rBV4	1136	758	0.03%	0.004%
94	13.623	3896	3898	3906	rVB6	1445	1340	0.06%	0.007%
95	13.742	3930	3935	3938	rBV6	1652	2011	0.09%	0.011%
96	14.379	4131	4133	4136	rBV4	1474	786	0.03%	0.004%
97	14.604	4201	4203	4205	rBV3	1678	885	0.04%	0.005%
98	14.826	4269	4272	4273	rBV3	2013	1075	0.05%	0.006%
99	15.093	4351	4355	4360	rBV7	2107	2360	0.10%	0.012%
100	15.244	4400	4402	4407	rVB5	3145	2177	0.09%	0.011%

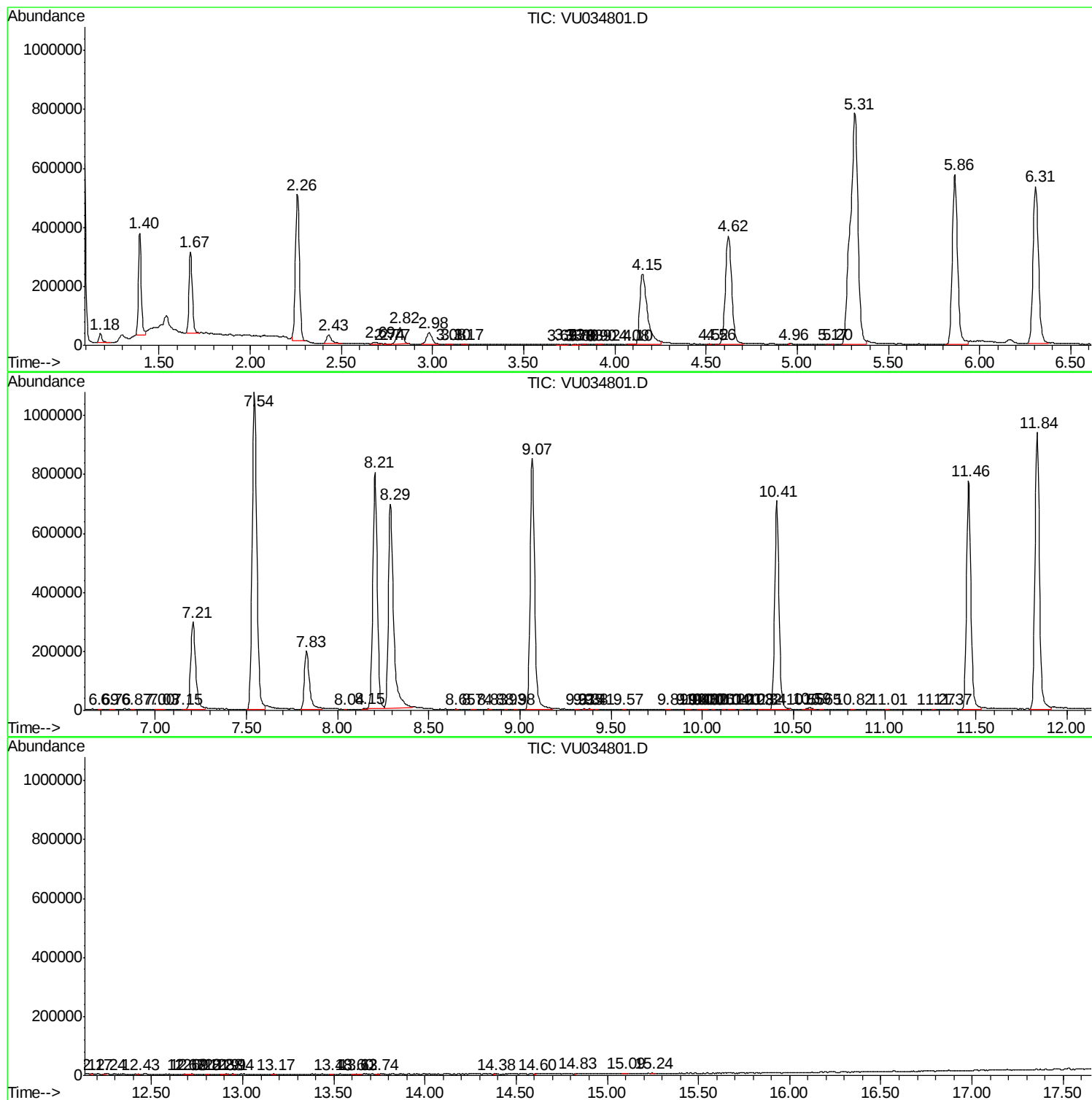
Sum of corrected areas: 19046101

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



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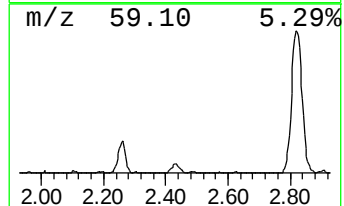
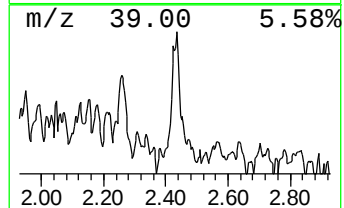
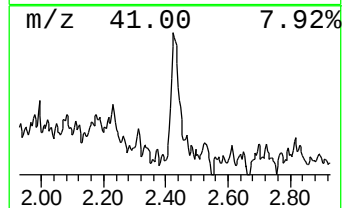
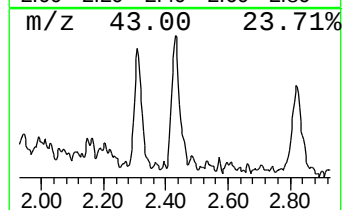
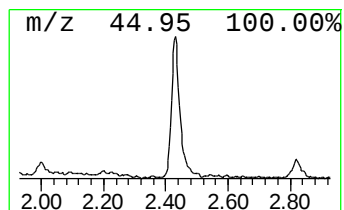
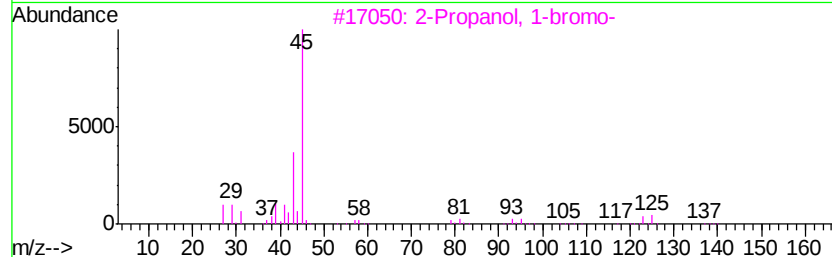
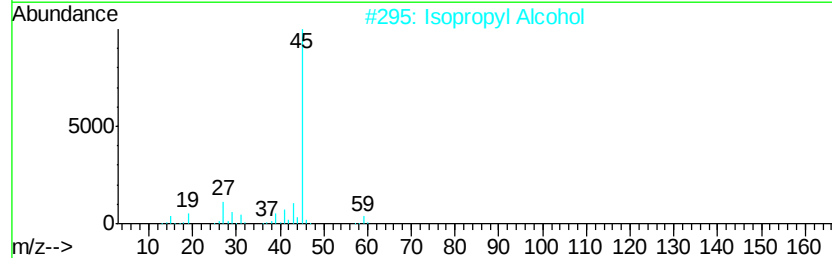
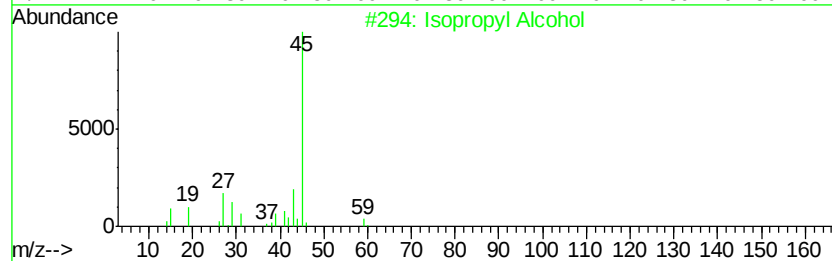
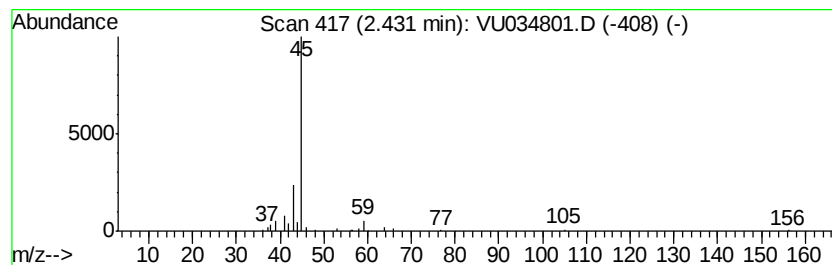
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	2.69 ug/L	62404	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3		2-Propanol, 1-bromo-	138	C3H7BrO	019686-73-8	40
4		2-Pentanol	88	C5H12O	006032-29-7	40
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40



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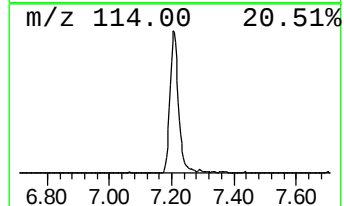
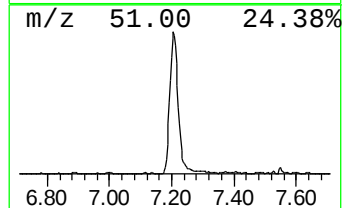
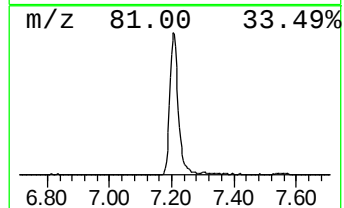
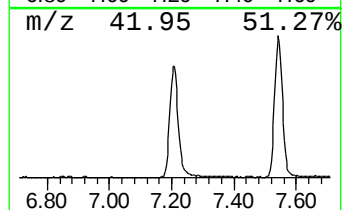
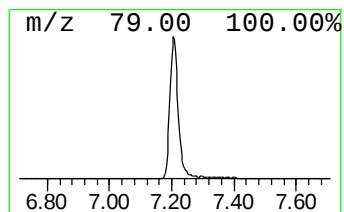
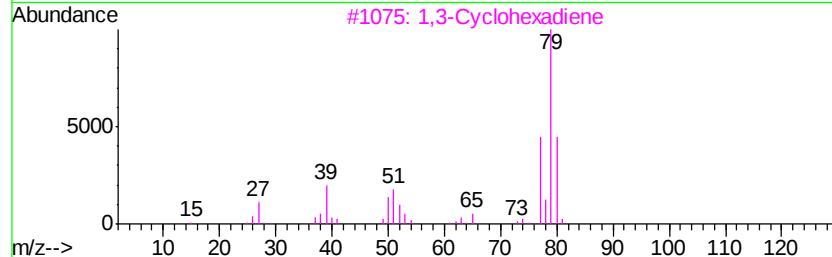
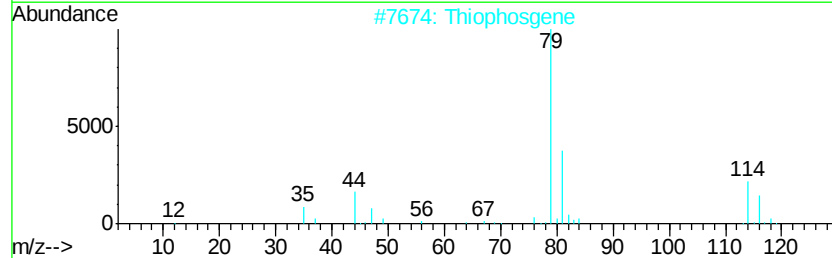
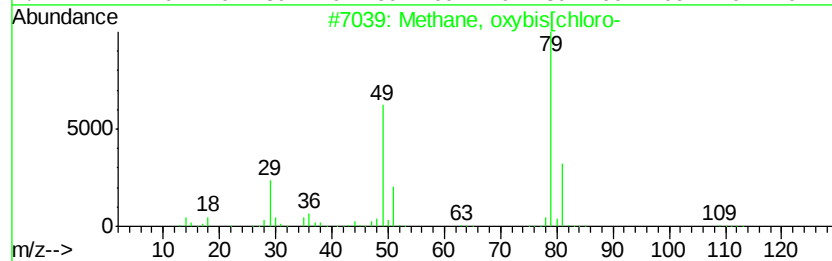
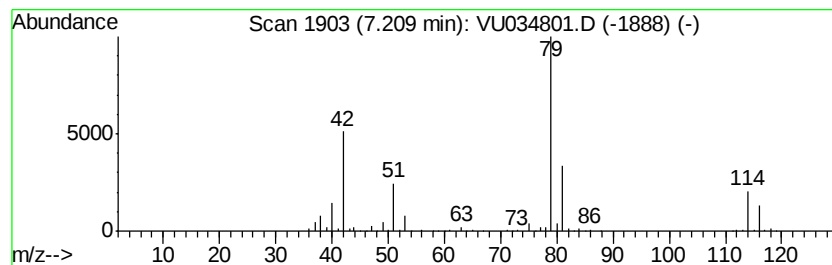
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Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	24.33 ug/L	564606	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	38
2		Thiophosgene	114	CCl2S	000463-71-8	38
3		1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
4		1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
5		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.43	2.7	ug/L	62404	1	5.86	1160330	50.0
unknown-01	7.21	24.3	ug/L	564606	1	5.86	1160330	50.0