

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121818\
 Data File : VU028775.D
 Acq On : 18 Dec 2018 17:23
 Operator : MD/SY
 Sample : J6422-12
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COLD6

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\SOMULM120718WMA.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	1.398	63	70	82	rBV	117628	118617	16.04%	2.132%
2	1.665	146	153	171	rVB	83684	105816	14.31%	1.902%
3	2.267	330	340	353	rBV	166665	255073	34.50%	4.584%
4	2.450	386	397	414	rBV	15141	30645	4.14%	0.551%
5	2.623	443	451	457	rBV2	712	1122	0.15%	0.020%
6	2.697	472	474	475	rBV2	255	87	0.01%	0.002%
7	2.836	505	517	533	rVB	9245	19710	2.67%	0.354%
8	3.154	613	616	620	rBV	117	76	0.01%	0.001%
9	3.177	620	623	625	rBV	116	84	0.01%	0.002%
10	3.376	682	685	688	rVB	237	133	0.02%	0.002%
11	3.414	694	697	703	rBV	101	111	0.02%	0.002%
12	3.559	738	742	744	rBV	87	71	0.01%	0.001%
13	3.730	792	795	800	rVB	172	140	0.02%	0.003%
14	3.755	800	803	805	rBV	100	73	0.01%	0.001%
15	3.932	856	858	863	rVB	206	109	0.01%	0.002%
16	4.176	919	934	961	rBV2	77001	221716	29.99%	3.985%
17	4.469	1022	1025	1027	rBV2	267	141	0.02%	0.003%
18	4.569	1053	1056	1058	rBV	108	79	0.01%	0.001%
19	4.578	1058	1059	1063	rVB	204	86	0.01%	0.002%
20	4.646	1063	1080	1109	rBV	120063	276750	37.43%	4.974%
21	4.781	1120	1122	1125	rVB	276	100	0.01%	0.002%
22	4.884	1148	1154	1164	rVB3	370	619	0.08%	0.011%
23	4.987	1184	1186	1190	rVB3	342	254	0.03%	0.005%
24	5.009	1190	1193	1199	rVB	102	76	0.01%	0.001%
25	5.131	1227	1231	1234	rBV	139	99	0.01%	0.002%
26	5.337	1271	1295	1318	rBV2	256429	739407	100.00%	13.289%
27	5.527	1351	1354	1356	rBV	164	133	0.02%	0.002%
28	5.652	1390	1393	1396	rBV	142	65	0.01%	0.001%
29	5.668	1396	1398	1400	rVB	172	68	0.01%	0.001%
30	5.816	1437	1444	1446	rBV	285	213	0.03%	0.004%
31	5.884	1451	1465	1485	rBV	206015	399807	54.07%	7.186%
32	6.167	1550	1553	1558	rBV	240	135	0.02%	0.002%
33	6.196	1560	1562	1564	rBV2	253	84	0.01%	0.002%
34	6.328	1589	1603	1624	rBV	171770	340785	46.09%	6.125%

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Integrator: RTE
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 Title : VOC Analysis

35	6.453	1637	1642	1644	rBV2	247	232	0.03%	0.004%
36	6.610	1689	1691	1695	rVB	207	99	0.01%	0.002%
37	6.784	1743	1745	1747	rVB	221	75	0.01%	0.001%
38	6.922	1784	1788	1790	rBV2	151	97	0.01%	0.002%
39	6.938	1790	1793	1799	rVB	143	108	0.01%	0.002%
40	7.035	1815	1823	1826	rBV	166	212	0.03%	0.004%
41	7.173	1863	1866	1869	rBV	212	83	0.01%	0.001%
42	7.225	1870	1882	1901	rBV	97658	172404	23.32%	3.099%
43	7.347	1917	1920	1923	rVB	192	94	0.01%	0.002%
44	7.389	1929	1933	1937	rBV	376	451	0.06%	0.008%
45	7.446	1949	1951	1954	rVB	192	84	0.01%	0.002%
46	7.469	1954	1958	1962	rBV	227	225	0.03%	0.004%
47	7.562	1973	1987	2025	rBV	340165	600772	81.25%	10.798%
48	7.803	2059	2062	2065	rBV2	206	129	0.02%	0.002%
49	7.848	2065	2076	2099	rVV	68470	113336	15.33%	2.037%
50	7.987	2117	2119	2123	rVB2	296	197	0.03%	0.004%
51	8.012	2126	2127	2129	rVB2	202	71	0.01%	0.001%
52	8.035	2132	2134	2138	rBV	149	79	0.01%	0.001%
53	8.061	2138	2142	2145	rBV2	242	161	0.02%	0.003%
54	8.157	2169	2172	2174	rBV	286	223	0.03%	0.004%
55	8.241	2195	2198	2201	rBV	253	199	0.03%	0.004%
56	8.308	2206	2219	2243	rBV	251316	419468	56.73%	7.539%
57	8.514	2281	2283	2286	rVB	115	83	0.01%	0.001%
58	8.536	2286	2290	2293	rBV2	195	135	0.02%	0.002%
59	8.565	2296	2299	2301	rBV2	153	94	0.01%	0.002%
60	8.643	2321	2323	2325	rBV2	160	81	0.01%	0.001%
61	8.774	2361	2364	2365	rBV	158	98	0.01%	0.002%
62	8.845	2384	2386	2388	rVB	163	84	0.01%	0.002%
63	8.893	2399	2401	2406	rVB	223	101	0.01%	0.002%
64	8.922	2408	2410	2414	rVV	154	74	0.01%	0.001%
65	8.954	2417	2420	2424	rVB	242	160	0.02%	0.003%
66	8.996	2431	2433	2436	rBV	152	89	0.01%	0.002%
67	9.086	2450	2461	2484	rBV	284495	480435	64.98%	8.635%
68	9.263	2513	2516	2518	rVB2	169	93	0.01%	0.002%
69	9.343	2537	2541	2544	rBV	183	166	0.02%	0.003%
70	9.382	2550	2553	2556	rBV	208	177	0.02%	0.003%
71	9.459	2575	2577	2579	rVB	272	70	0.01%	0.001%

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 Title : VOC Analysis

72	9.520	2594	2596	2599	rVB2	161	87	0.01%	0.002%
73	9.588	2615	2617	2622	rVB	211	109	0.01%	0.002%
74	9.909	2714	2717	2720	rVB2	199	144	0.02%	0.003%
75	9.990	2739	2742	2744	rBV	165	106	0.01%	0.002%
76	10.167	2791	2797	2800	rBV2	404	298	0.04%	0.005%
77	10.324	2843	2846	2849	rBV	209	150	0.02%	0.003%
78	10.369	2857	2860	2863	rBV	139	100	0.01%	0.002%
79	10.430	2867	2879	2900	rVB	232038	366223	49.53%	6.582%
80	10.559	2917	2919	2922	rVB	199	97	0.01%	0.002%
81	10.585	2922	2927	2928	rBV	372	347	0.05%	0.006%
82	10.684	2953	2958	2961	rBV3	463	486	0.07%	0.009%
83	10.970	3045	3047	3050	rBV	164	102	0.01%	0.002%
84	11.086	3081	3083	3086	rBB	203	86	0.01%	0.002%
85	11.122	3090	3094	3096	rBV2	243	166	0.02%	0.003%
86	11.218	3122	3124	3125	rBV2	161	69	0.01%	0.001%
87	11.482	3194	3206	3229	rBV	264350	411748	55.69%	7.400%
88	11.736	3282	3285	3288	rBV2	312	205	0.03%	0.004%
89	11.765	3290	3294	3297	rBV2	351	213	0.03%	0.004%
90	11.781	3297	3299	3302	rBV2	256	148	0.02%	0.003%
91	11.858	3311	3323	3340	rBV	301047	478290	64.69%	8.596%
92	11.974	3356	3359	3363	rBV2	451	291	0.04%	0.005%
93	12.093	3393	3396	3397	rBV2	174	83	0.01%	0.001%
94	12.141	3409	3411	3412	rBV2	225	71	0.01%	0.001%
95	12.482	3514	3517	3520	rBV	241	165	0.02%	0.003%
96	12.613	3556	3558	3563	rVB	177	78	0.01%	0.001%
97	12.703	3583	3586	3588	rBV	361	229	0.03%	0.004%
98	12.752	3598	3601	3605	rBV2	279	259	0.04%	0.005%
99	12.771	3605	3607	3611	rVV2	281	148	0.02%	0.003%
100	12.790	3611	3613	3616	rVB2	249	137	0.02%	0.002%

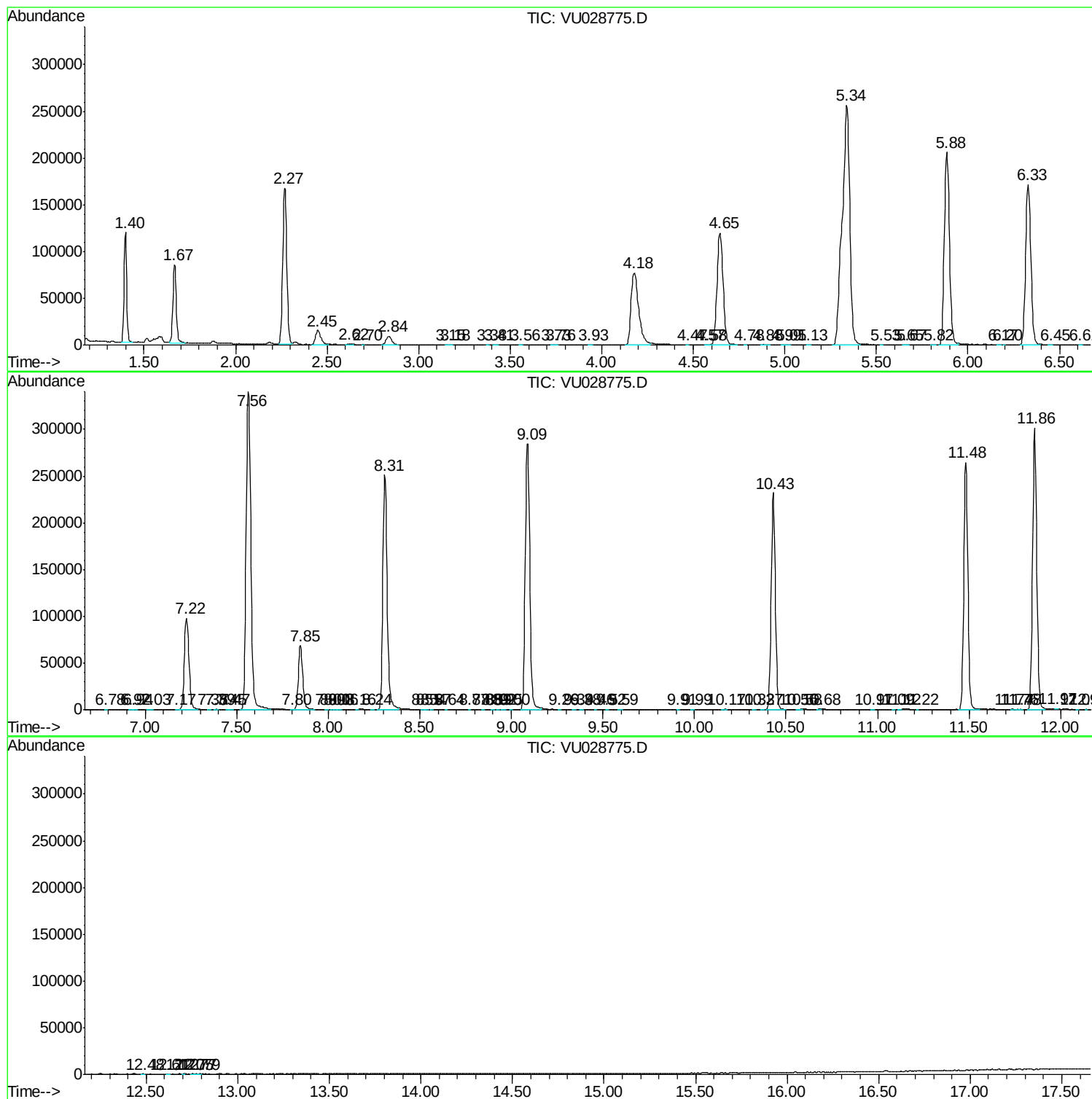
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Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM120718WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU121818\
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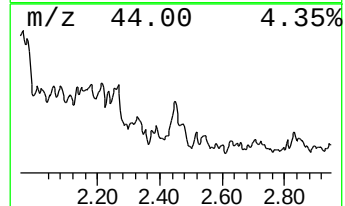
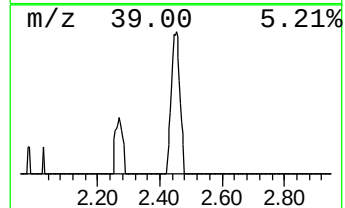
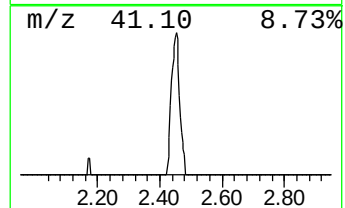
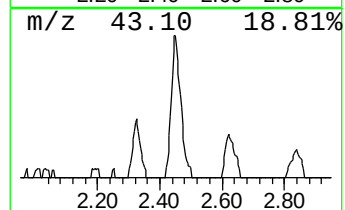
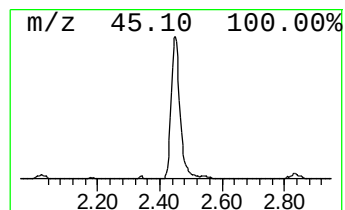
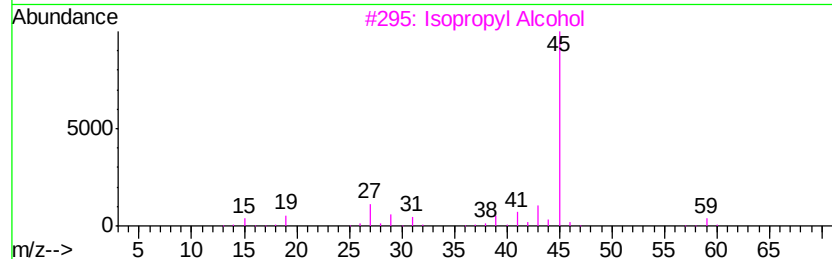
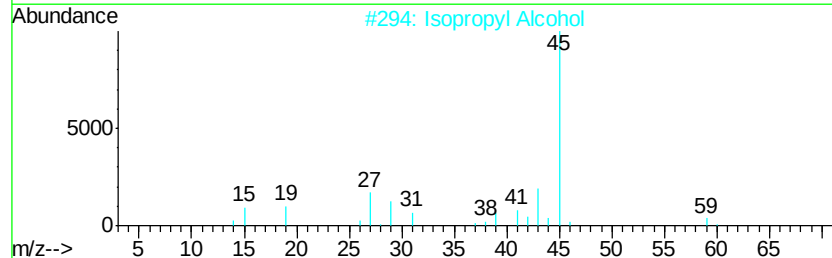
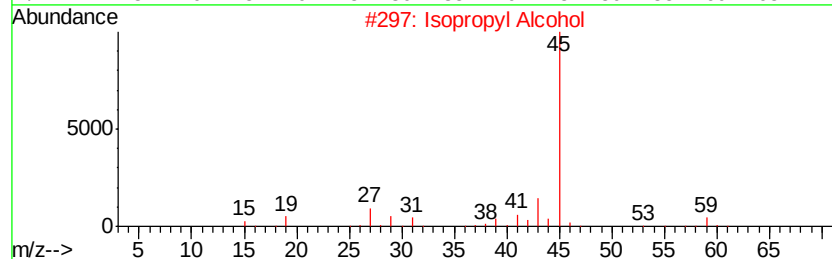
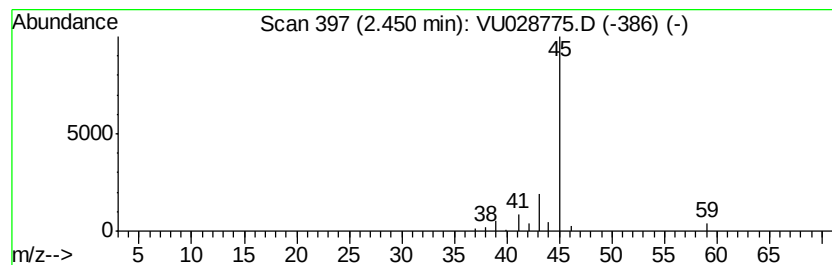
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM120718WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	3.83 ug/L	30645	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Formamide	45	CH3NO	000075-12-7	7
5			Ethylamine	45	C2H7N	000075-04-7	5



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C0LD6

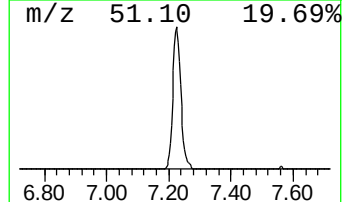
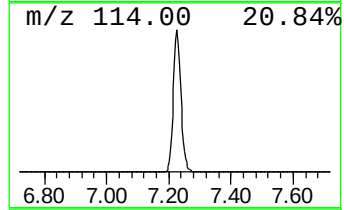
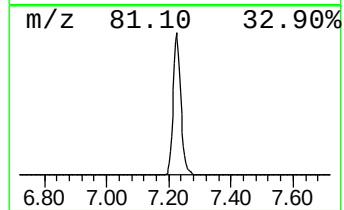
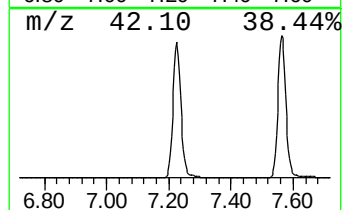
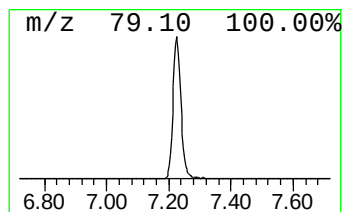
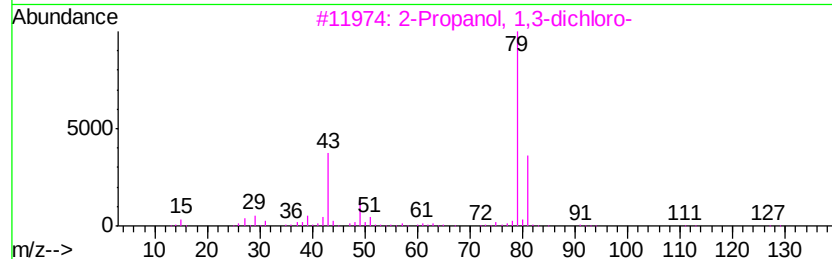
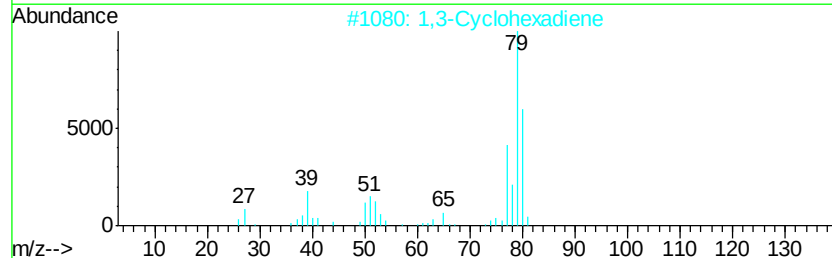
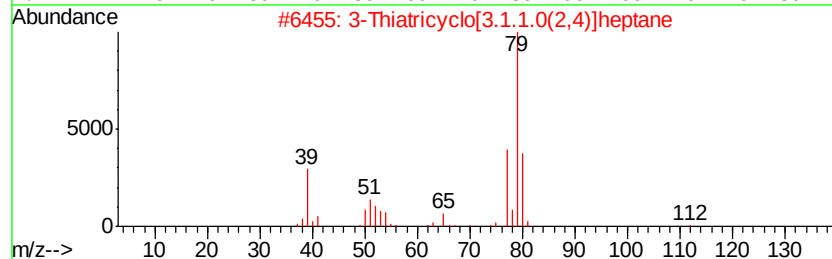
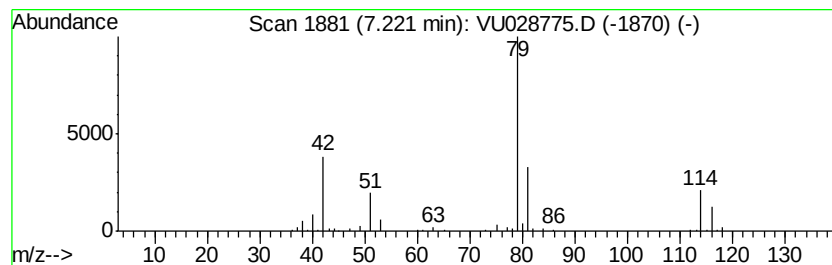
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Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	21.56 ug/L	172404	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	37
2		1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
3		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	23
4		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	9
5		1,3,5-Hexatriene, (Z)-	80	C6H8	002612-46-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.45	3.8	ug/L	30645	1	5.88	399807	50.0
unknown-01	7.22	21.6	ug/L	172404	1	5.88	399807	50.0