

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050118\
 Data File : VU023553.D
 Acq On : 01 May 2018 15:00
 Operator : MD/SY
 Sample : J2558-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 10 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.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	0.744	46	48	54	rVB2	240	199	0.00%	0.001%
2	0.873	82	88	93	rBV2	183	175	0.00%	0.001%
3	0.989	117	124	127	rBV2	314	383	0.01%	0.002%
4	1.088	135	155	178	rBV	2441695	2744454	67.29%	14.999%
5	1.182	180	184	195	rVB	49785	53905	1.32%	0.295%
6	1.400	245	252	263	rBV	186660	199941	4.90%	1.093%
7	1.683	333	340	351	rVB	123348	153113	3.75%	0.837%
8	2.275	512	524	536	rBV	282969	432296	10.60%	2.363%
9	2.391	557	560	563	rBV2	341	255	0.01%	0.001%
10	2.439	565	575	581	rBV2	3230	5174	0.13%	0.028%
11	2.558	605	612	615	rBV2	406	419	0.01%	0.002%
12	2.616	626	630	631	rBV	351	208	0.01%	0.001%
13	2.706	651	658	666	rBV3	1201	1795	0.04%	0.010%
14	2.754	670	673	675	rVB	360	203	0.00%	0.001%
15	2.841	689	700	710	rVV2	2094	4312	0.11%	0.024%
16	2.921	720	725	728	rBV2	194	232	0.01%	0.001%
17	2.989	734	746	760	rVB	26351	48722	1.19%	0.266%
18	3.149	793	796	800	rBV2	210	175	0.00%	0.001%
19	3.198	808	811	813	rBV2	399	275	0.01%	0.002%
20	3.214	813	816	817	rVB	430	200	0.00%	0.001%
21	3.317	841	848	857	rVB4	631	937	0.02%	0.005%
22	3.362	857	862	864	rBV2	236	254	0.01%	0.001%
23	3.384	867	869	872	rBV2	261	199	0.00%	0.001%
24	3.452	878	890	902	rBV2	5018	10288	0.25%	0.056%
25	3.519	906	911	912	rBV	249	190	0.00%	0.001%
26	4.178	1100	1116	1118	rBV	101815	175357	4.30%	0.958%
27	4.230	1122	1132	1175	rVB	667693	1620649	39.74%	8.857%
28	4.522	1221	1223	1226	rVB2	500	254	0.01%	0.001%
29	4.542	1226	1229	1231	rVB	516	293	0.01%	0.002%
30	4.654	1245	1264	1294	rBV3	168183	470702	11.54%	2.572%
31	4.895	1334	1339	1341	rVV3	269	303	0.01%	0.002%
32	4.963	1358	1360	1364	rVB2	226	180	0.00%	0.001%
33	4.989	1366	1368	1370	rVV2	310	207	0.01%	0.001%
34	5.002	1370	1372	1378	rVB2	394	288	0.01%	0.002%

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 Title : VOC Analysis

35	5.117	1405	1408	1411	rBV2	217	172	0.00%	0.001%
36	5.342	1453	1478	1516	rBV2	415713	1249413	30.64%	6.828%
37	5.625	1562	1566	1571	rBV2	594	576	0.01%	0.003%
38	5.751	1599	1605	1612	rVB2	235	373	0.01%	0.002%
39	5.796	1616	1619	1622	rVB2	303	194	0.00%	0.001%
40	5.818	1622	1626	1630	rVB2	183	202	0.00%	0.001%
41	5.889	1630	1648	1688	rBV	399707	832976	20.42%	4.552%
42	6.111	1715	1717	1724	rVB3	357	217	0.01%	0.001%
43	6.188	1725	1741	1773	rBV	2083140	4078332	100.00%	22.289%
44	6.333	1775	1786	1820	rVB	280338	582380	14.28%	3.183%
45	6.516	1840	1843	1847	rVB3	583	319	0.01%	0.002%
46	6.535	1847	1849	1851	rBV2	389	225	0.01%	0.001%
47	6.571	1857	1860	1869	rVB3	218	353	0.01%	0.002%
48	6.609	1869	1872	1880	rVB2	233	196	0.00%	0.001%
49	6.677	1888	1893	1896	rBV3	212	251	0.01%	0.001%
50	6.773	1920	1923	1927	rVV2	266	194	0.00%	0.001%
51	6.828	1936	1940	1946	rVV2	232	185	0.00%	0.001%
52	7.021	1995	2000	2003	rVB2	223	183	0.00%	0.001%
53	7.040	2003	2006	2008	rBV	320	202	0.00%	0.001%
54	7.178	2044	2049	2053	rBV2	306	326	0.01%	0.002%
55	7.230	2053	2065	2093	rBV	153663	278924	6.84%	1.524%
56	7.567	2157	2170	2210	rBV	542245	1012290	24.82%	5.532%
57	7.853	2248	2259	2283	rVV	103038	180949	4.44%	0.989%
58	7.992	2299	2302	2306	rBV3	348	354	0.01%	0.002%
59	8.101	2333	2336	2339	rBV	245	219	0.01%	0.001%
60	8.181	2348	2361	2367	rBV2	8961	15522	0.38%	0.085%
61	8.233	2368	2377	2390	rVB	41363	69391	1.70%	0.379%
62	8.313	2390	2402	2437	rBV	313561	561959	13.78%	3.071%
63	8.728	2528	2531	2537	rBV2	338	325	0.01%	0.002%
64	8.779	2543	2547	2550	rBV	196	170	0.00%	0.001%
65	8.850	2562	2569	2571	rBV2	260	306	0.01%	0.002%
66	9.095	2631	2645	2685	rBV	577943	1011702	24.81%	5.529%
67	9.329	2714	2718	2722	rBV	280	218	0.01%	0.001%
68	9.381	2727	2734	2739	rBV4	652	810	0.02%	0.004%
69	9.487	2763	2767	2773	rVB2	329	434	0.01%	0.002%
70	9.519	2773	2777	2780	rBV	231	197	0.00%	0.001%
71	9.542	2780	2784	2789	rBV	227	197	0.00%	0.001%

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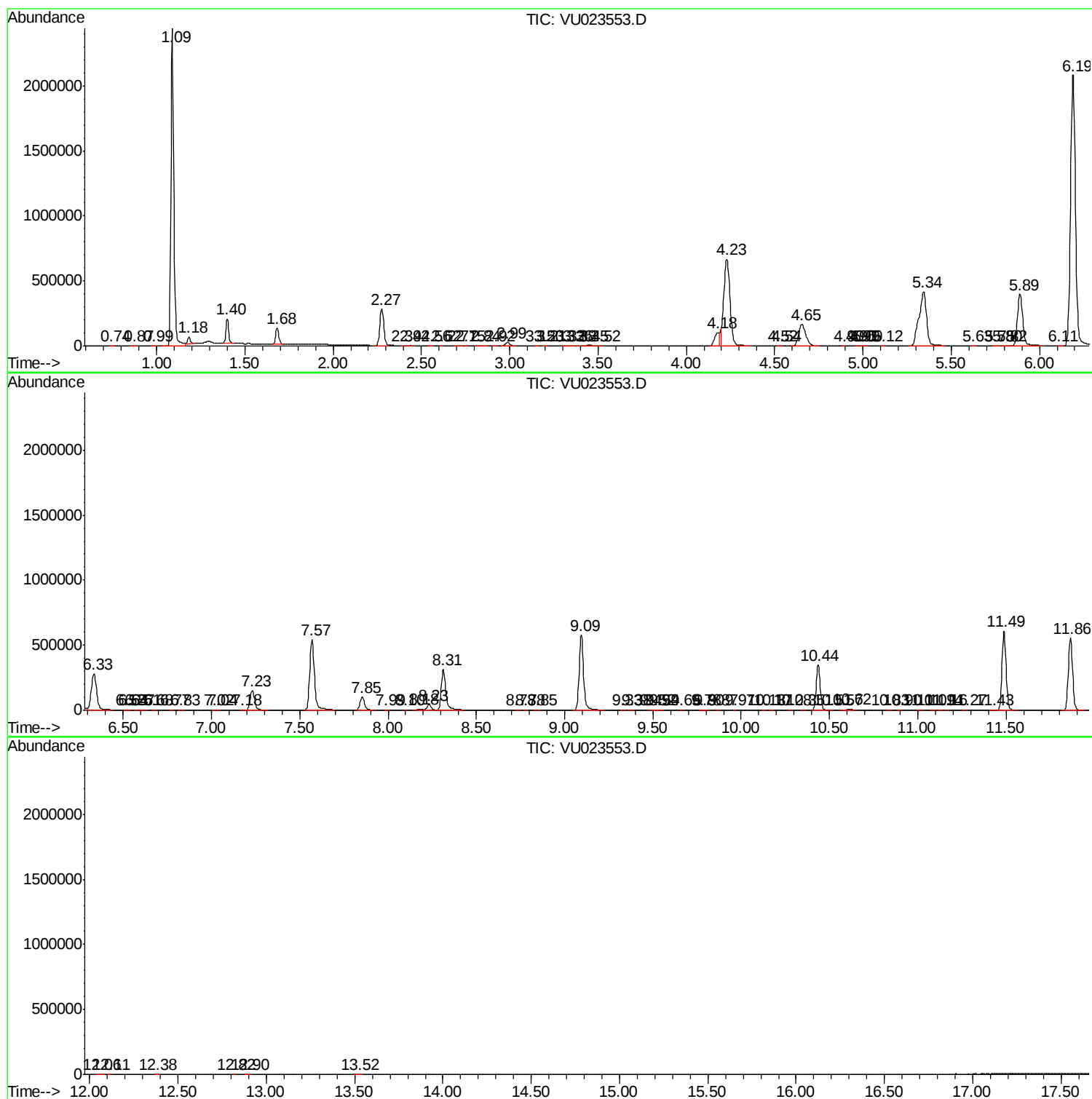
72	9.664	2819	2822	2825	rVB2	293	205	0.01%	0.001%
73	9.776	2852	2857	2860	rBV2	302	359	0.01%	0.002%
74	9.796	2860	2863	2868	rVB4	566	460	0.01%	0.003%
75	9.873	2881	2887	2889	rBV	234	261	0.01%	0.001%
76	9.969	2913	2917	2918	rBV	337	217	0.01%	0.001%
77	10.130	2964	2967	2970	rBV2	365	281	0.01%	0.002%
78	10.169	2975	2979	2984	rVV3	294	308	0.01%	0.002%
79	10.281	3010	3014	3016	rBV2	208	188	0.00%	0.001%
80	10.355	3033	3037	3041	rBV2	165	175	0.00%	0.001%
81	10.435	3050	3062	3083	rBV	347296	564286	13.84%	3.084%
82	10.509	3083	3085	3089	rVB2	365	207	0.01%	0.001%
83	10.570	3101	3104	3107	rVB2	261	181	0.00%	0.001%
84	10.615	3107	3118	3130	rBV2	8064	14166	0.35%	0.077%
85	10.834	3182	3186	3191	rBV	178	266	0.01%	0.001%
86	10.902	3202	3207	3208	rBV2	305	204	0.01%	0.001%
87	11.014	3236	3242	3247	rBV2	265	365	0.01%	0.002%
88	11.091	3259	3266	3268	rVV2	223	255	0.01%	0.001%
89	11.136	3274	3280	3281	rBV	233	203	0.00%	0.001%
90	11.162	3285	3288	3291	rBV	273	173	0.00%	0.001%
91	11.271	3317	3322	3325	rBV	272	277	0.01%	0.002%
92	11.426	3364	3370	3377	rBV3	1090	1387	0.03%	0.008%
93	11.487	3377	3389	3414	rVV	608978	978888	24.00%	5.350%
94	11.863	3490	3506	3533	rBV	555230	921643	22.60%	5.037%
95	12.059	3559	3567	3574	rBV3	600	1041	0.03%	0.006%
96	12.114	3580	3584	3586	rBV3	517	455	0.01%	0.002%
97	12.377	3662	3666	3671	rBV2	595	773	0.02%	0.004%
98	12.818	3800	3803	3804	rBV	357	211	0.01%	0.001%
99	12.898	3822	3828	3832	rBV3	1077	1271	0.03%	0.007%
100	13.519	4014	4021	4028	rVB4	956	1340	0.03%	0.007%

Sum of corrected areas: 18297819

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ALS Vial : 10 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 10 Sample Multiplier: 1

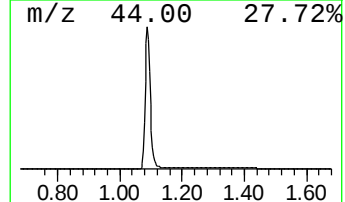
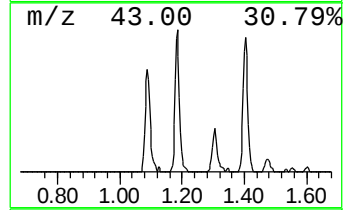
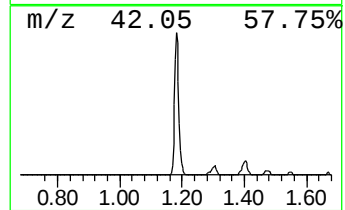
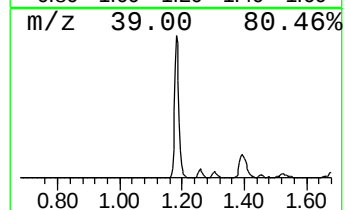
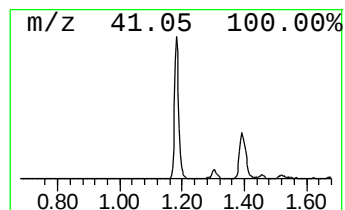
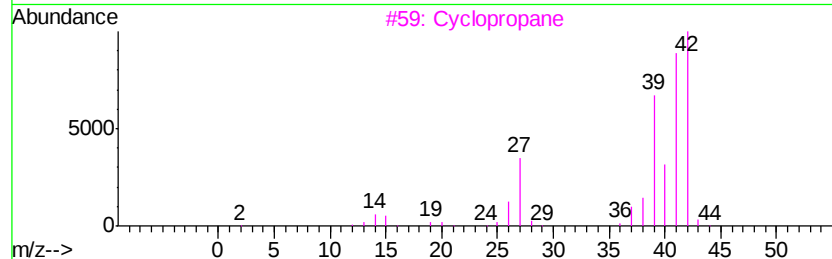
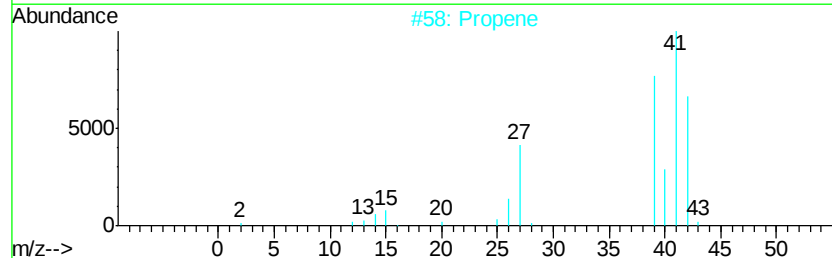
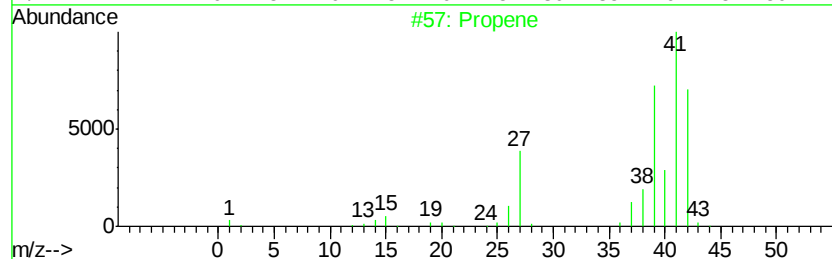
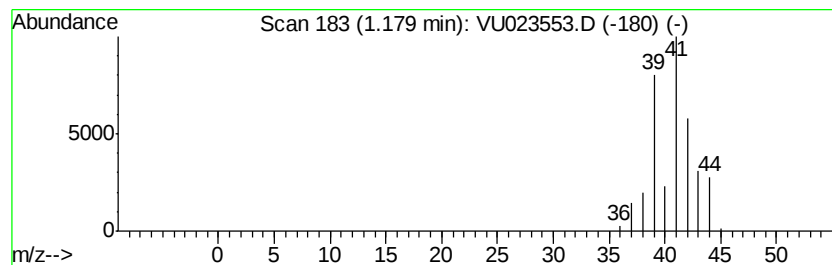
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic1.18 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.18	3.24 ug/L	53905	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propene	42	C3H6	000115-07-1	90
2		Propene	42	C3H6	000115-07-1	42
3		Cyclopropane	42	C3H6	000075-19-4	40
4		Cyclopropene	40	C3H4	002781-85-3	9
5		Cyclopropane	42	C3H6	000075-19-4	7



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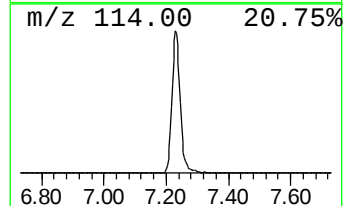
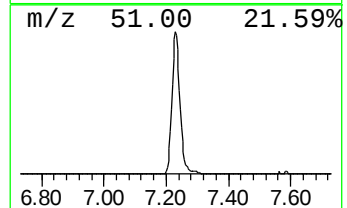
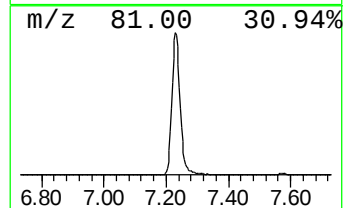
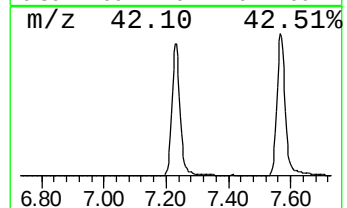
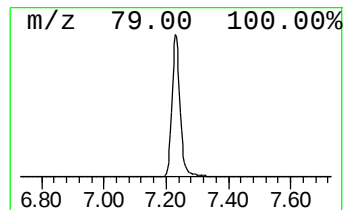
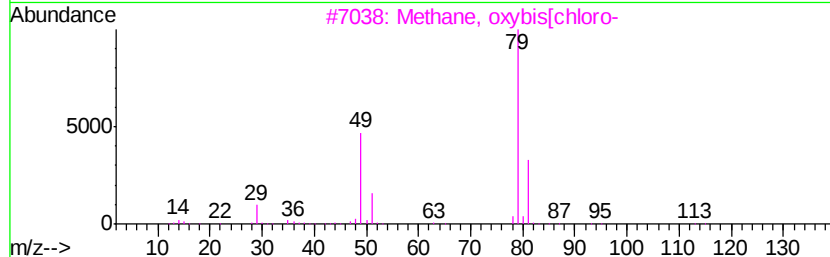
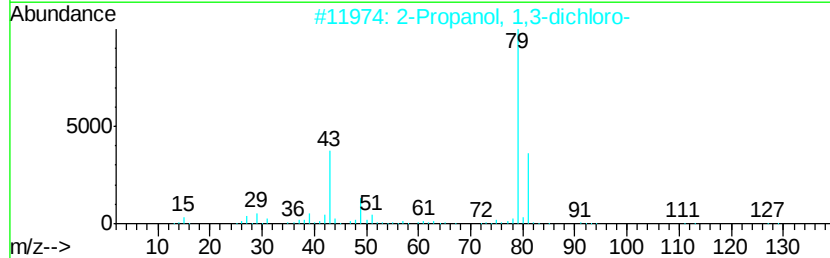
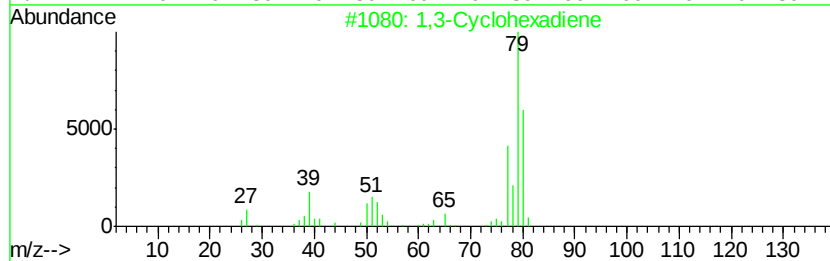
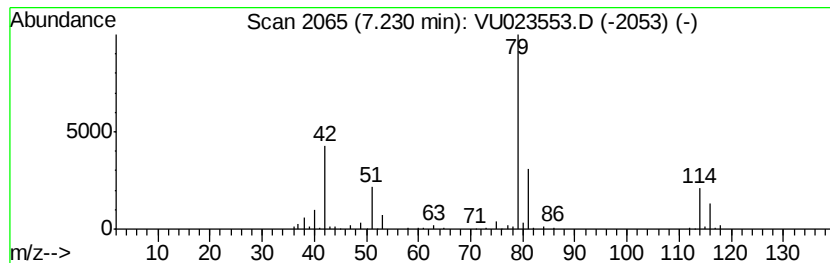
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Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	16.74 ug/L	278924	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
2		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	23
3		Methane, oxvbis[chloro-	114	C2H4Cl2O	000542-88-1	23
4		Thiophosgene	114	CCl2S	000463-71-8	16
5		3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.18	3.2	ug/L	53905	1	5.89	832976	50.0
unknown-01	7.23	16.7	ug/L	278924	1	5.89	832976	50.0