

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048003.D
 Acq On : 13 Apr 2022 15:02
 Operator : SY/MD
 Sample : N2345-17 20X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JB0

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\SFAMULM032422WMA.M

Title : VOC Analysis

Signal : TIC: VU048003.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	102	rBV	155301	185574	14.40%	1.739%
2	1.916	170	179	200	rBV	126408	179241	13.91%	1.680%
3	2.569	370	382	399	rBV	266263	437632	33.96%	4.101%
4	2.710	423	426	428	rBV	402	249	0.02%	0.002%
5	2.768	438	444	451	rBV5	1062	1852	0.14%	0.017%
6	2.848	465	469	476	rVB3	503	549	0.04%	0.005%
7	2.909	485	488	490	rBV	321	268	0.02%	0.003%
8	3.051	524	532	543	rVB6	2771	5457	0.42%	0.051%
9	3.157	562	565	569	rVB3	545	461	0.04%	0.004%
10	3.186	569	574	577	rBV3	620	495	0.04%	0.005%
11	3.205	577	580	585	rVB3	458	368	0.03%	0.003%
12	3.234	585	589	591	rBV2	294	271	0.02%	0.003%
13	3.424	643	648	649	rBV2	388	291	0.02%	0.003%
14	3.546	683	686	692	rVV2	435	405	0.03%	0.004%
15	3.655	715	720	723	rBV2	404	402	0.03%	0.004%
16	3.726	735	742	745	rBV2	498	396	0.03%	0.004%
17	3.832	772	775	779	rBV2	408	341	0.03%	0.003%
18	3.884	786	791	793	rVB	334	284	0.02%	0.003%
19	4.160	874	877	882	rVB2	298	282	0.02%	0.003%
20	4.189	882	886	888	rBV	318	270	0.02%	0.003%
21	4.247	901	904	907	rVV2	297	238	0.02%	0.002%
22	4.559	996	1001	1005	rBV3	405	363	0.03%	0.003%
23	4.626	1006	1022	1045	rBV	131176	320371	24.86%	3.002%
24	4.938	1116	1119	1126	rBV2	277	335	0.03%	0.003%
25	5.067	1142	1159	1180	rBV	229492	500359	38.83%	4.689%
26	5.295	1222	1230	1232	rBV3	423	578	0.04%	0.005%
27	5.453	1275	1279	1281	rBV2	333	247	0.02%	0.002%
28	5.482	1285	1288	1297	rVB2	347	555	0.04%	0.005%
29	5.530	1297	1303	1306	rBV3	430	458	0.04%	0.004%
30	5.617	1325	1330	1334	rBV3	355	352	0.03%	0.003%
31	5.726	1339	1364	1395	rBV2	471772	1288494	100.00%	12.074%
32	5.893	1411	1416	1420	rBV3	366	395	0.03%	0.004%
33	6.035	1456	1460	1462	rBV2	599	418	0.03%	0.004%
34	6.170	1499	1502	1507	rVB2	422	311	0.02%	0.003%
35	6.250	1512	1527	1551	rBV	402106	765849	59.44%	7.176%
36	6.421	1575	1580	1582	rBV2	567	601	0.05%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	6.527	1608	1613	1621	rBV4	1407	2140	0.17%	0.020%
38	6.694	1650	1665	1686	rBV	291983	570702	44.29%	5.348%
39	6.806	1693	1700	1701	rBV5	473	523	0.04%	0.005%
40	7.048	1768	1775	1776	rBV2	593	610	0.05%	0.006%
41	7.057	1776	1778	1786	rVB4	830	716	0.06%	0.007%
42	7.099	1786	1791	1793	rBV	377	270	0.02%	0.003%
43	7.183	1808	1817	1830	rBV2	3922	6847	0.53%	0.064%
44	7.282	1845	1848	1852	rVB	315	253	0.02%	0.002%
45	7.565	1922	1936	1954	rBV	151354	267517	20.76%	2.507%
46	7.687	1968	1974	1975	rBV2	2182	1871	0.15%	0.018%
47	7.752	1992	1994	1999	rBV2	388	350	0.03%	0.003%
48	7.800	2006	2009	2015	rVB4	452	411	0.03%	0.004%
49	7.900	2026	2040	2056	rBV	580394	1011477	78.50%	9.478%
50	8.179	2115	2127	2141	rBV	108753	182938	14.20%	1.714%
51	8.356	2177	2182	2188	rVB4	988	1205	0.09%	0.011%
52	8.446	2207	2210	2212	rBV2	469	298	0.02%	0.003%
53	8.469	2213	2217	2227	rVV4	1328	2281	0.18%	0.021%
54	8.507	2227	2229	2232	rVB2	502	281	0.02%	0.003%
55	8.633	2256	2268	2303	rBV	418229	756069	58.68%	7.085%
56	8.880	2341	2345	2347	rBV3	328	252	0.02%	0.002%
57	9.022	2384	2389	2391	rBV3	563	405	0.03%	0.004%
58	9.160	2428	2432	2433	rBV	387	329	0.03%	0.003%
59	9.334	2483	2486	2491	rVB2	370	274	0.02%	0.003%
60	9.417	2498	2512	2537	rBV	608410	1075908	83.50%	10.082%
61	9.617	2571	2574	2579	rBV2	376	362	0.03%	0.003%
62	9.649	2579	2584	2588	rVB3	410	364	0.03%	0.003%
63	9.694	2589	2598	2602	rBV4	1353	1503	0.12%	0.014%
64	10.115	2727	2729	2732	rVB2	465	260	0.02%	0.002%
65	10.199	2750	2755	2758	rBV	224	257	0.02%	0.002%
66	10.298	2783	2786	2791	rBV2	262	257	0.02%	0.002%
67	10.446	2829	2832	2839	rVV3	310	317	0.02%	0.003%
68	10.671	2894	2902	2909	rBV7	2180	3049	0.24%	0.029%
69	10.713	2910	2915	2916	rVV3	781	735	0.06%	0.007%
70	10.758	2917	2929	2950	rVB	445205	711176	55.19%	6.664%
71	10.893	2965	2971	2977	rVV5	1695	2215	0.17%	0.021%
72	10.989	2998	3001	3008	rBV3	397	483	0.04%	0.005%
73	11.227	3070	3075	3079	rBV3	392	406	0.03%	0.004%
74	11.269	3082	3088	3093	rBV2	292	284	0.02%	0.003%
75	11.433	3137	3139	3142	rBV2	310	239	0.02%	0.002%
76	11.581	3179	3185	3187	rBV2	576	732	0.06%	0.007%

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77	11.690	3215	3219	3220	rBV	723	447	0.03%	0.004%
78	11.752	3230	3238	3244	rVB5	1601	2453	0.19%	0.023%
79	11.813	3244	3257	3279	rBV	679806	1092436	84.78%	10.236%
80	11.951	3292	3300	3314	rVB8	3536	7502	0.58%	0.070%
81	12.067	3330	3336	3343	rBV4	1452	1902	0.15%	0.018%
82	12.105	3345	3348	3353	rVB3	711	609	0.05%	0.006%
83	12.192	3361	3375	3399	rBV	611000	1020444	79.20%	9.562%
84	12.314	3410	3413	3416	rBV3	376	265	0.02%	0.002%
85	12.340	3418	3421	3424	rVV3	600	318	0.02%	0.003%
86	12.459	3455	3458	3462	rVB2	373	302	0.02%	0.003%
87	12.481	3462	3465	3470	rBV	375	369	0.03%	0.003%
88	12.636	3511	3513	3519	rVV2	452	377	0.03%	0.004%
89	12.742	3543	3546	3550	rBV2	458	446	0.03%	0.004%
90	12.838	3574	3576	3579	rVB2	561	307	0.02%	0.003%
91	12.973	3606	3618	3627	rVB4	5538	9833	0.76%	0.092%
92	13.173	3677	3680	3684	rVB3	540	407	0.03%	0.004%
93	13.263	3705	3708	3710	rBV2	596	337	0.03%	0.003%
94	13.333	3722	3730	3738	rBV4	3630	5338	0.41%	0.050%
95	13.378	3738	3744	3754	rBV4	4144	5577	0.43%	0.052%
96	13.845	3882	3889	3898	rBV6	2911	4621	0.36%	0.043%
97	14.330	4038	4040	4044	rBV4	929	654	0.05%	0.006%
98	15.314	4342	4346	4352	rVB3	1853	2160	0.17%	0.020%
99	15.546	4408	4418	4432	rBV2	48296	75638	5.87%	0.709%
100	16.388	4670	4680	4692	rBV	84295	137724	10.69%	1.291%

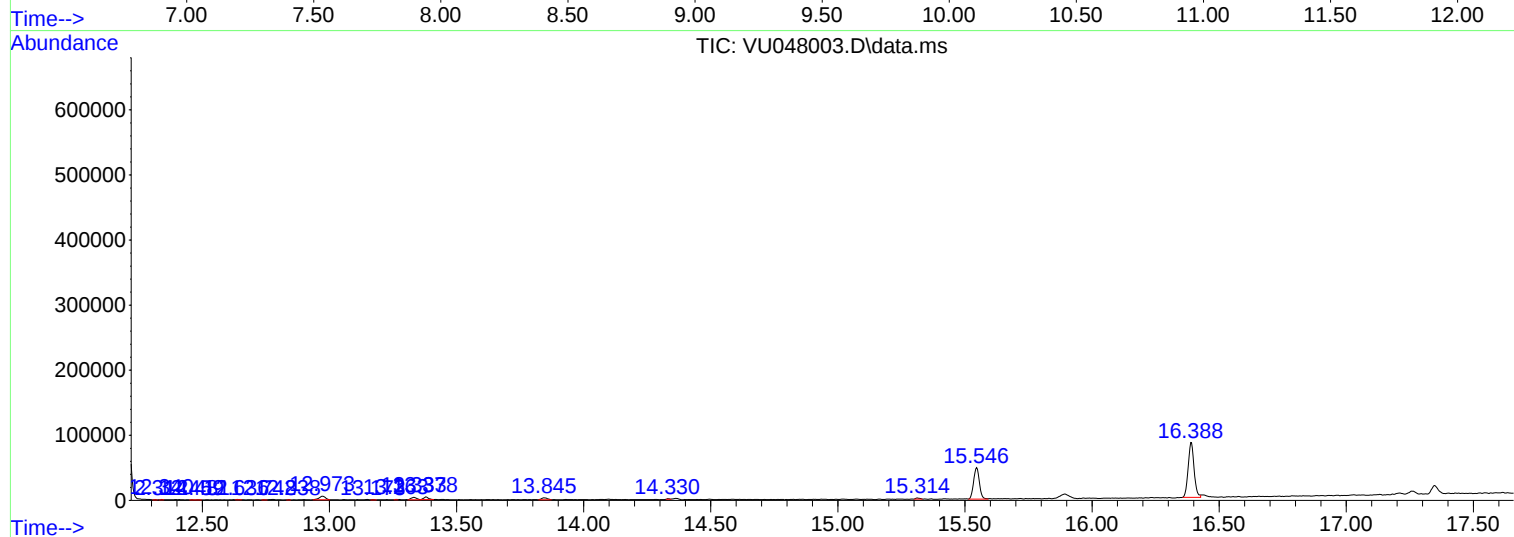
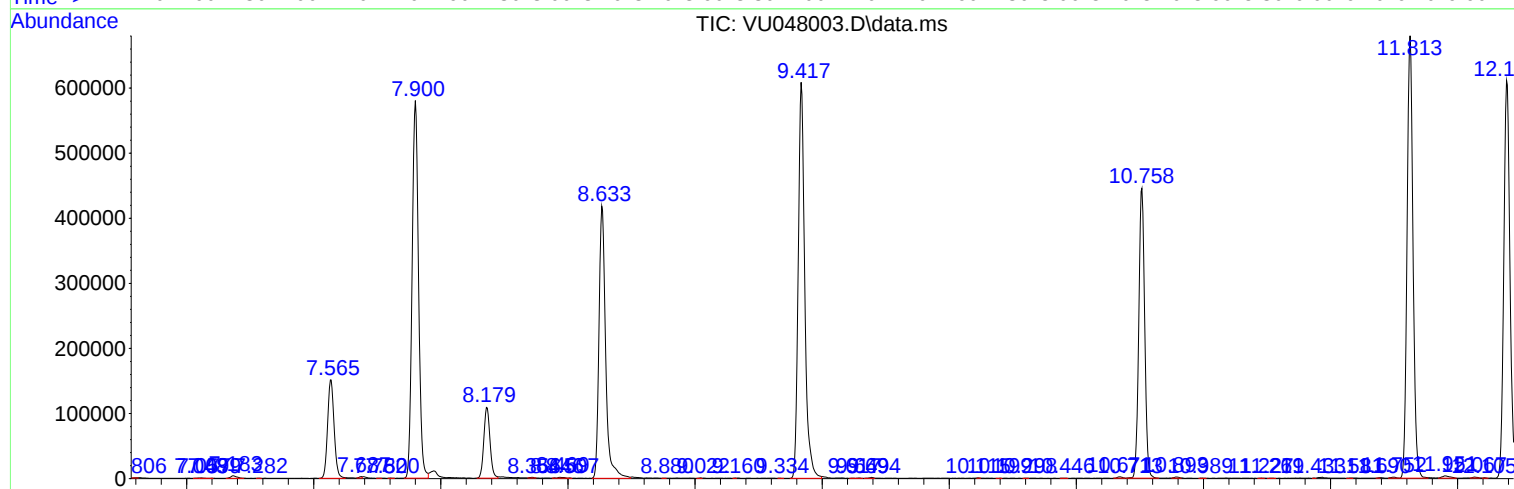
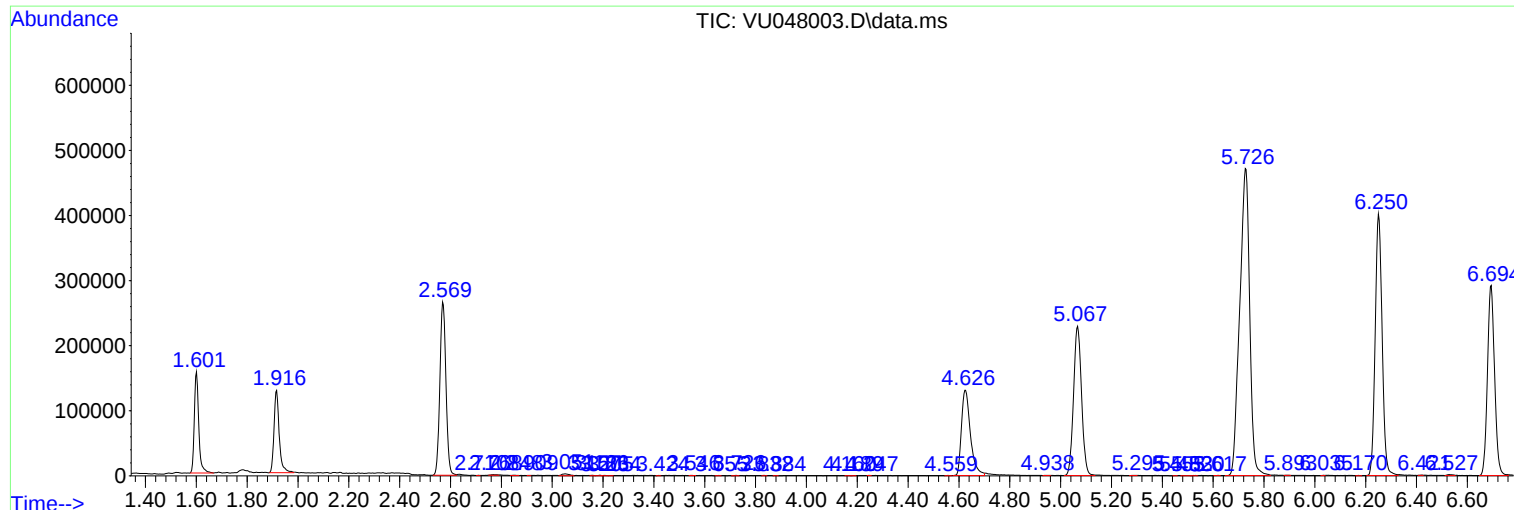
Sum of corrected areas: 10672044

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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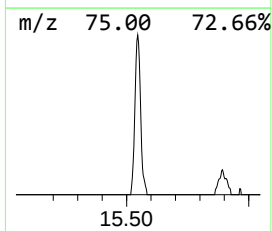
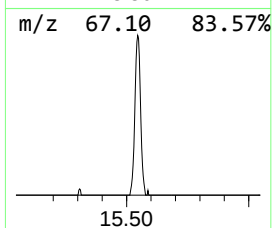
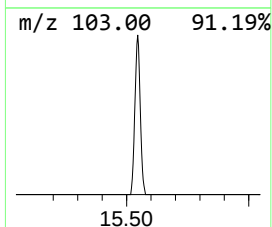
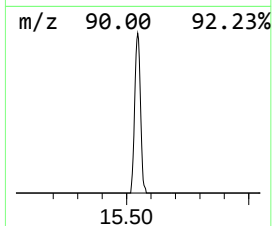
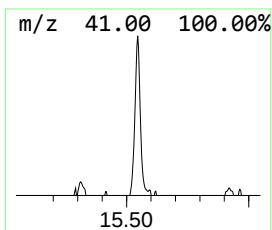
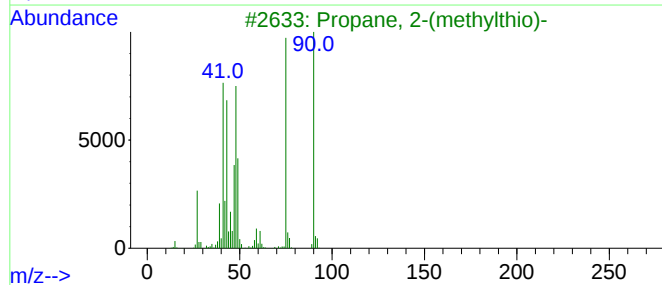
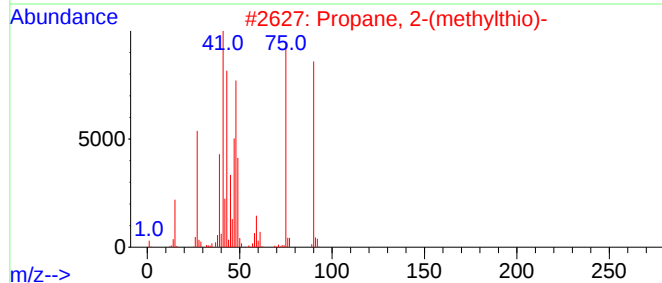
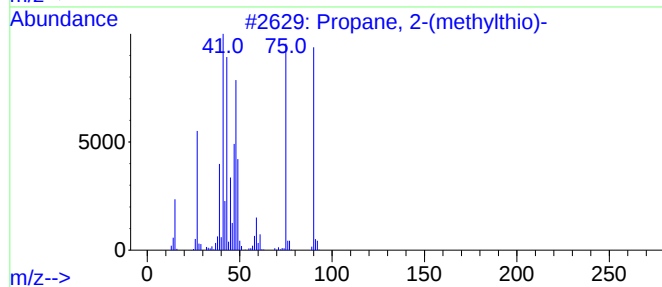
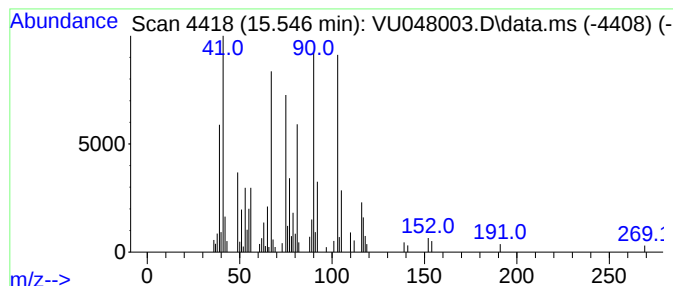
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Propane, 2-(methylthio)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.546	3.46 ug/L	75638	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	52
2			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	52
3			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	40
4			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
5			Pyrophosphoric acid, P,P'-dimeth...	203	C4H12FN03P2	1000226-54-0	37



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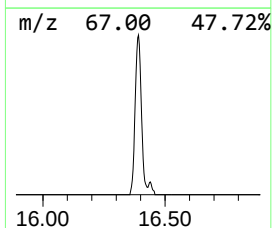
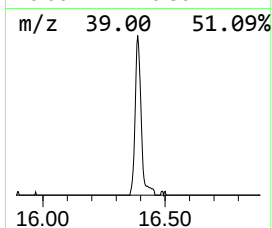
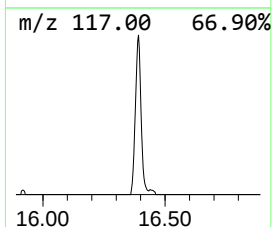
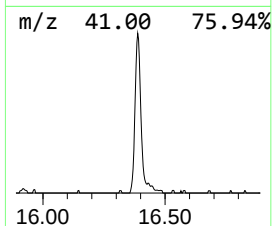
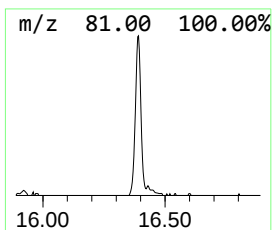
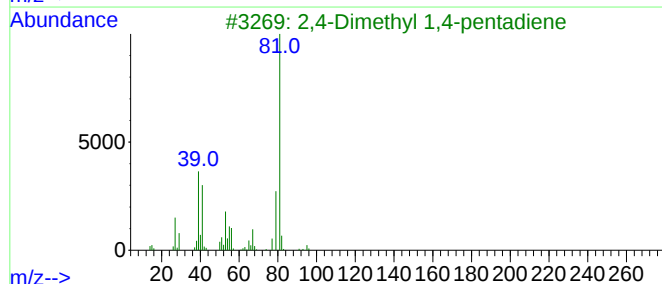
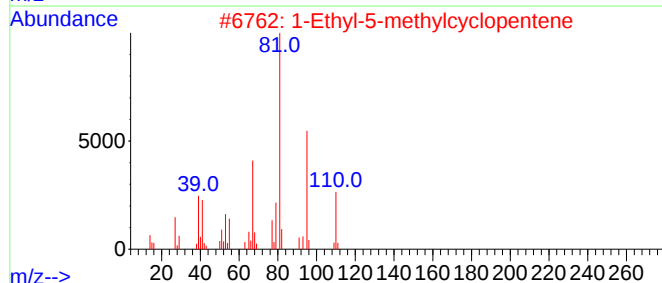
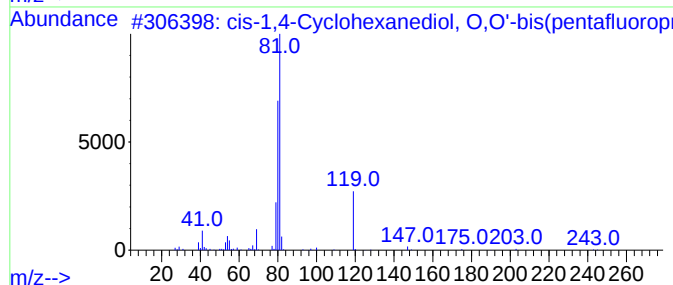
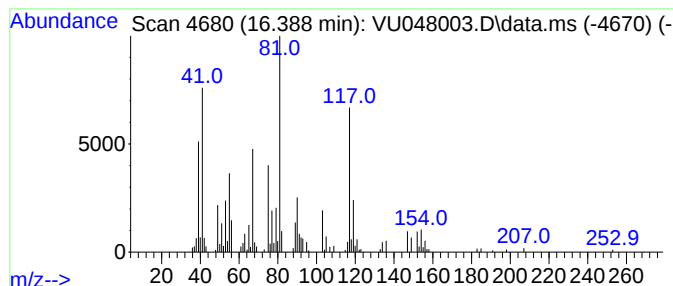
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Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	6.30 ug/L	137724	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-1,4-Cyclohexanediol, 0,0'-bi...	408	C12H10F10O4	1000385-95-0	14
2			1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	14
3			2,4-Dimethyl 1,4-pentadiene	96	C7H12	004161-65-3	11
4			1,2-Dibromo-5-hexene	240	C6H10Br2	004285-48-7	10
5			Isomycorene	136	C10H16	006876-07-9	10



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2-(met...	15.546	3.5	ug/L	75638	3	11.813	1092440	50.0
unknown-01	16.388	6.3	ug/L	137724	3	11.813	1092440	50.0