

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047956.D
 Acq On : 12 Apr 2022 15:24
 Operator : SY/MD
 Sample : N2345-03DL 40X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J81DL

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: VU047956.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	74	81	97	rVB	182300	213055	15.16%	1.812%
2	1.916	171	179	203	rVB	144120	199262	14.18%	1.695%
3	2.568	370	382	398	rBV	299696	494361	35.18%	4.205%
4	3.018	519	522	523	rBV2	409	219	0.02%	0.002%
5	3.086	541	543	545	rBV2	280	157	0.01%	0.001%
6	3.163	564	567	568	rBV3	230	119	0.01%	0.001%
7	3.475	659	664	666	rBV2	267	239	0.02%	0.002%
8	3.510	672	675	677	rVB2	452	248	0.02%	0.002%
9	3.536	677	683	689	rBV3	383	610	0.04%	0.005%
10	3.607	702	705	708	rBV2	142	122	0.01%	0.001%
11	3.694	729	732	735	rBV2	258	205	0.01%	0.002%
12	3.774	753	757	760	rBV2	260	240	0.02%	0.002%
13	3.819	769	771	772	rVB	203	60	0.00%	0.001%
14	3.829	772	774	777	rBV2	300	190	0.01%	0.002%
15	3.845	777	779	781	rVV	294	147	0.01%	0.001%
16	3.858	781	783	785	rVB2	265	122	0.01%	0.001%
17	3.877	785	789	791	rBV2	170	153	0.01%	0.001%
18	3.925	799	804	809	rBV2	301	346	0.02%	0.003%
19	4.134	866	869	870	rBV	232	148	0.01%	0.001%
20	4.153	872	875	877	rVV	294	193	0.01%	0.002%
21	4.195	886	888	891	rBV2	274	188	0.01%	0.002%
22	4.298	913	920	923	rVB2	405	458	0.03%	0.004%
23	4.330	923	930	934	rBV3	411	462	0.03%	0.004%
24	4.385	942	947	950	rBV2	187	190	0.01%	0.002%
25	4.456	966	969	970	rBV2	268	156	0.01%	0.001%
26	4.517	986	988	991	rBV	294	201	0.01%	0.002%
27	4.623	1008	1021	1062	rBV	140757	346926	24.69%	2.951%
28	5.006	1138	1140	1141	rBV2	227	113	0.01%	0.001%
29	5.063	1142	1158	1180	rVV	252870	551753	39.27%	4.693%
30	5.253	1215	1217	1220	rBV2	137	74	0.01%	0.001%
31	5.269	1220	1222	1224	rBV2	298	159	0.01%	0.001%
32	5.353	1241	1248	1250	rBV	288	212	0.02%	0.002%
33	5.401	1261	1263	1267	rBV2	151	100	0.01%	0.001%
34	5.465	1280	1283	1285	rBV	244	143	0.01%	0.001%
35	5.488	1287	1290	1296	rVB2	378	313	0.02%	0.003%
36	5.517	1296	1299	1301	rBV2	211	132	0.01%	0.001%

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Integrator: RTE

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

37	5.530	1301	1303	1304	rBV	141	39	0.00%	0.000%
38	5.600	1323	1325	1327	rBV	164	81	0.01%	0.001%
39	5.633	1334	1335	1337	rBV	227	88	0.01%	0.001%
40	5.726	1341	1364	1372	rBV2	523855	1405063	100.00%	11.951%
41	6.250	1513	1527	1549	rBV	413064	787018	56.01%	6.694%
42	6.472	1594	1596	1599	rBV	393	241	0.02%	0.002%
43	6.571	1623	1627	1629	rBV3	369	263	0.02%	0.002%
44	6.600	1632	1636	1639	rBV	259	194	0.01%	0.002%
45	6.626	1641	1644	1649	rVB4	250	222	0.02%	0.002%
46	6.690	1649	1664	1686	rBV	317620	625925	44.55%	5.324%
47	6.967	1747	1750	1753	rVB	298	195	0.01%	0.002%
48	6.986	1753	1756	1757	rBV	192	88	0.01%	0.001%
49	7.034	1765	1771	1774	rBV3	438	474	0.03%	0.004%
50	7.089	1786	1788	1789	rVB	175	46	0.00%	0.000%
51	7.108	1791	1794	1796	rBV2	103	70	0.00%	0.001%
52	7.124	1796	1799	1803	rBV2	277	211	0.02%	0.002%
53	7.179	1807	1816	1829	rBV4	3702	6978	0.50%	0.059%
54	7.237	1831	1834	1837	rBV	259	194	0.01%	0.002%
55	7.253	1837	1839	1842	rBV	278	160	0.01%	0.001%
56	7.272	1842	1845	1847	rVB	226	127	0.01%	0.001%
57	7.292	1847	1851	1852	rBV2	139	89	0.01%	0.001%
58	7.366	1870	1874	1879	rBV	184	202	0.01%	0.002%
59	7.404	1883	1886	1889	rVB2	257	180	0.01%	0.002%
60	7.420	1889	1891	1894	rBV	213	137	0.01%	0.001%
61	7.468	1904	1906	1907	rBV	172	54	0.00%	0.000%
62	7.565	1921	1936	1953	rBV	170086	298578	21.25%	2.540%
63	7.687	1968	1974	1984	rVB4	2432	3728	0.27%	0.032%
64	7.899	2026	2040	2056	rBV	641202	1120289	79.73%	9.529%
65	8.179	2116	2127	2146	rBV	118648	201602	14.35%	1.715%
66	8.539	2236	2239	2244	rBV4	465	274	0.02%	0.002%
67	8.632	2255	2268	2307	rBV	444564	813856	57.92%	6.923%
68	9.015	2384	2387	2395	rVB3	1534	1574	0.11%	0.013%
69	9.047	2395	2397	2401	rBV2	184	96	0.01%	0.001%
70	9.275	2465	2468	2471	rBV2	243	184	0.01%	0.002%
71	9.295	2471	2474	2476	rBV2	238	144	0.01%	0.001%
72	9.337	2484	2487	2488	rBV	309	172	0.01%	0.001%
73	9.359	2490	2494	2495	rBV3	676	411	0.03%	0.003%
74	9.417	2499	2512	2518	rBV	634435	1129262	80.37%	9.605%
75	9.578	2557	2562	2567	rVB5	1446	1613	0.11%	0.014%
76	9.687	2592	2596	2597	rBV2	863	556	0.04%	0.005%

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77	9.861	2647	2650	2653	rVB2	476	303	0.02%	0.003%
78	9.947	2674	2677	2679	rBV2	215	132	0.01%	0.001%
79	10.092	2720	2722	2725	rBV4	329	179	0.01%	0.002%
80	10.308	2784	2789	2790	rBV2	401	298	0.02%	0.003%
81	10.420	2821	2824	2825	rBV	322	155	0.01%	0.001%
82	10.671	2894	2902	2910	rBV6	2675	4589	0.33%	0.039%
83	10.758	2917	2929	2947	rVB	468903	761198	54.18%	6.475%
84	11.095	3030	3034	3037	rBV3	398	353	0.03%	0.003%
85	11.150	3048	3051	3052	rBV2	553	285	0.02%	0.002%
86	11.298	3094	3097	3098	rBV	323	211	0.02%	0.002%
87	11.417	3131	3134	3138	rVB	352	201	0.01%	0.002%
88	11.459	3140	3147	3159	rVV8	1937	3533	0.25%	0.030%
89	11.635	3199	3202	3207	rBV3	284	225	0.02%	0.002%
90	11.697	3211	3221	3230	rBV6	1460	2448	0.17%	0.021%
91	11.748	3230	3237	3243	rBV3	997	1256	0.09%	0.011%
92	11.812	3243	3257	3282	rBV	697589	1127965	80.28%	9.594%
93	12.195	3361	3376	3400	rBV	667281	1115281	79.38%	9.486%
94	12.324	3414	3416	3419	rBV3	644	485	0.03%	0.004%
95	12.767	3551	3554	3555	rBV	483	257	0.02%	0.002%
96	12.967	3604	3616	3635	rVB6	9133	17342	1.23%	0.148%
97	13.375	3736	3743	3756	rVB3	19417	30235	2.15%	0.257%
98	14.359	4042	4049	4062	rVB3	15048	22425	1.60%	0.191%
99	15.545	4408	4418	4430	rBV2	80740	124670	8.87%	1.060%
100	16.388	4671	4680	4692	rBV	210525	330154	23.50%	2.808%

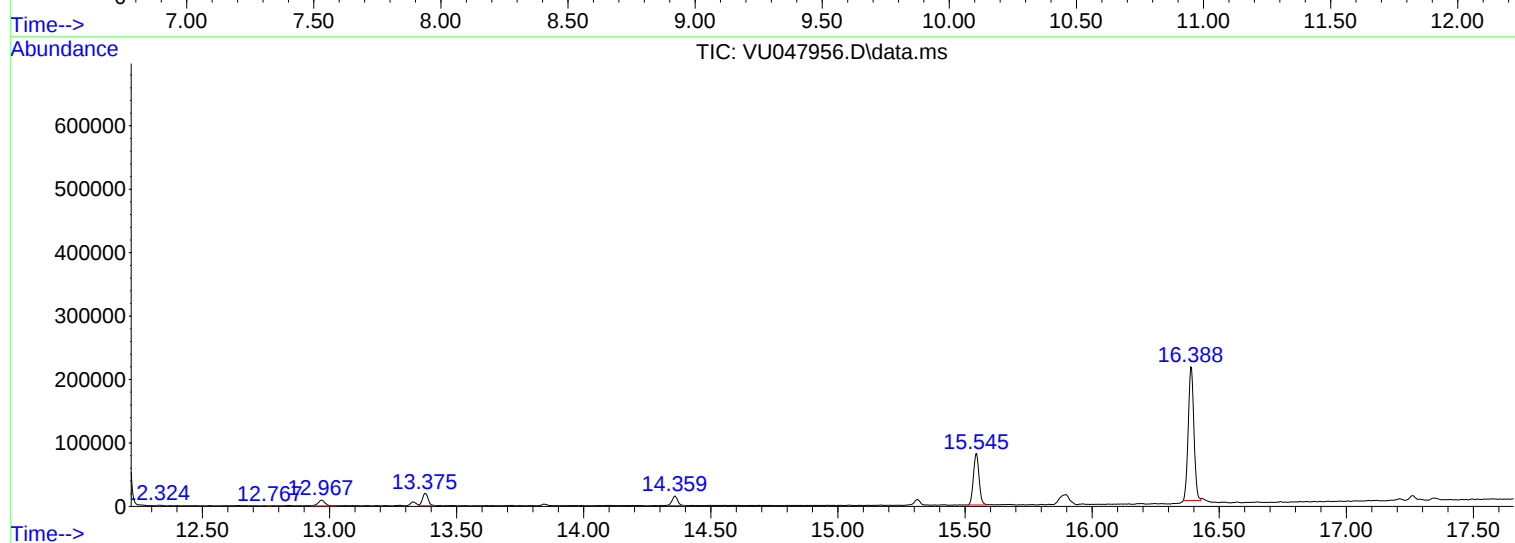
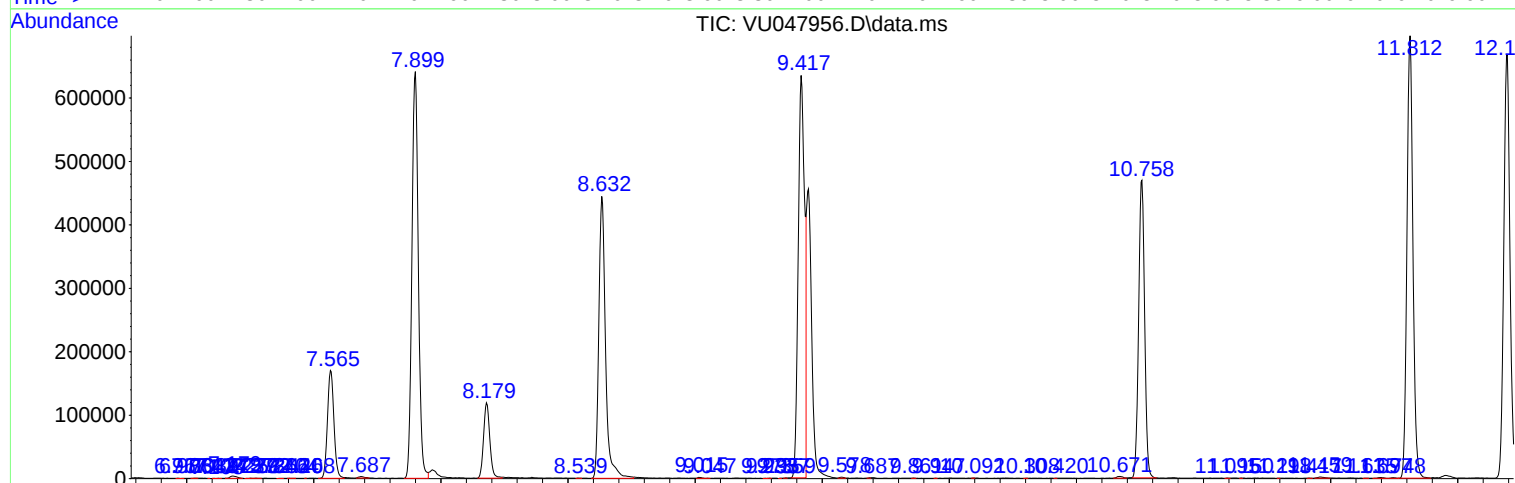
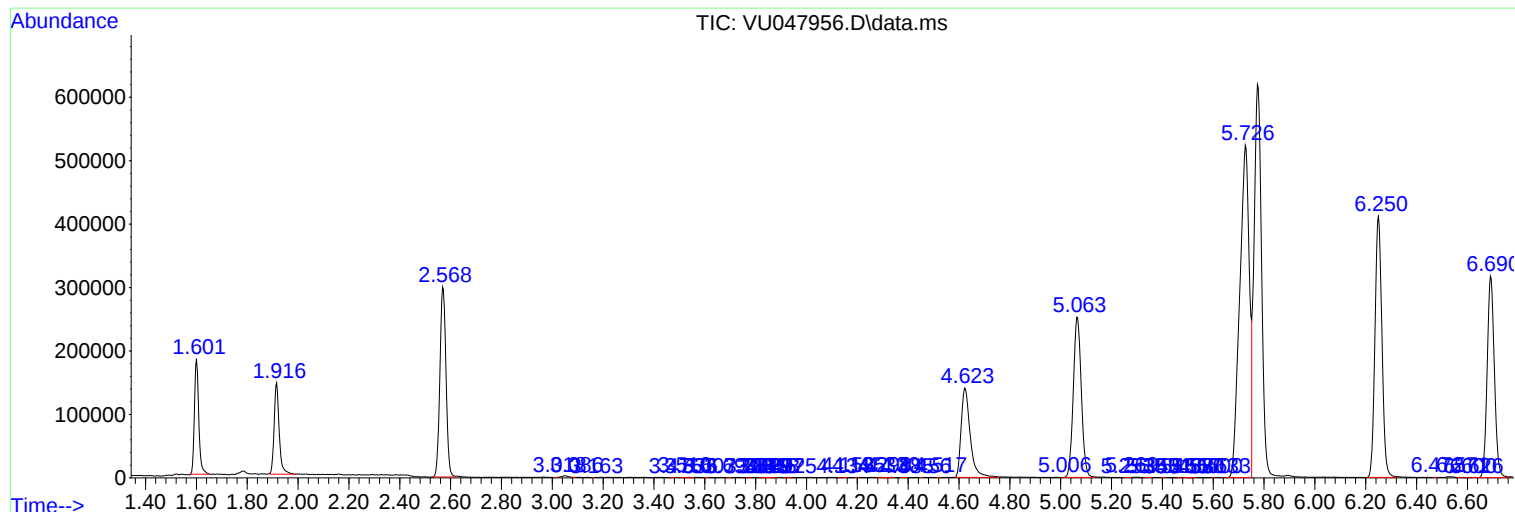
Sum of corrected areas: 11756634

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Instrument :
MSVOA_U
ClientSampleId :
C0J81DL

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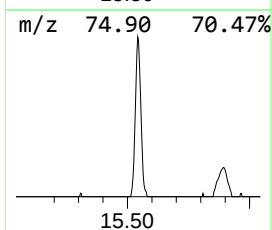
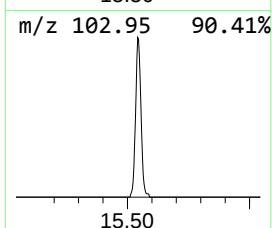
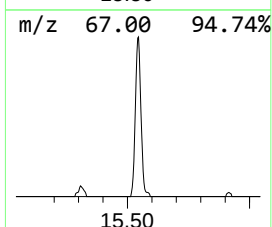
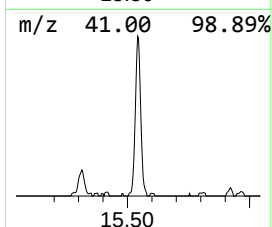
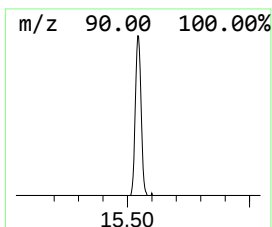
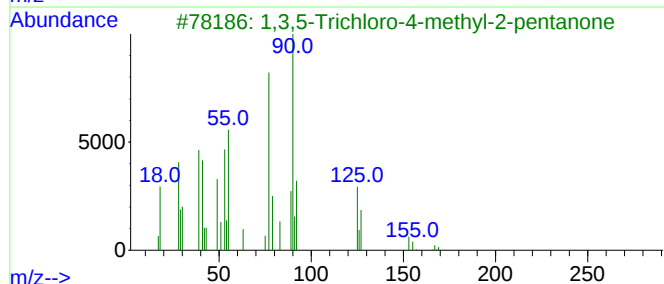
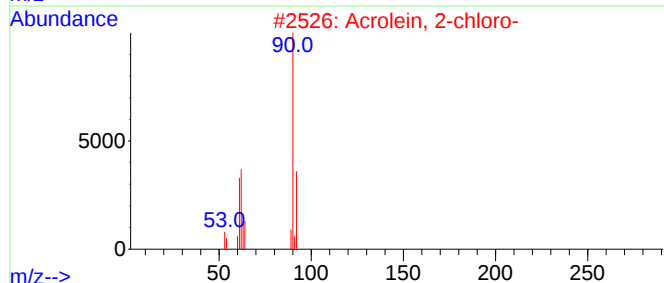
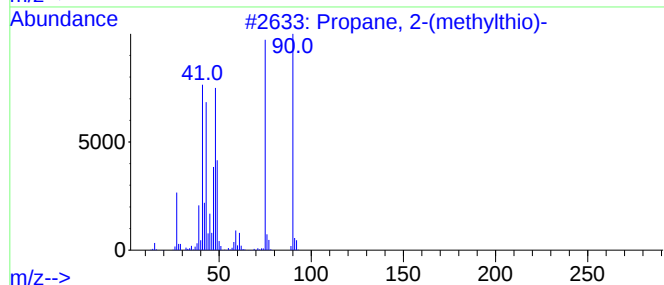
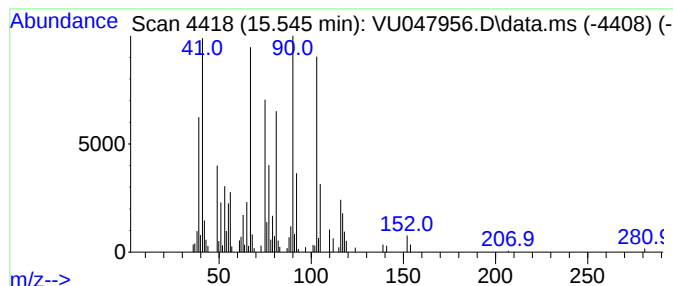
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
15.545	5.53 ug/L	124670	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	52
2			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	43
3			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	33
4			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	27
5			Ethynesulfonamide, 2-phenyl-, N-...	277	C10H6F3N03S	1000452-07-5	17



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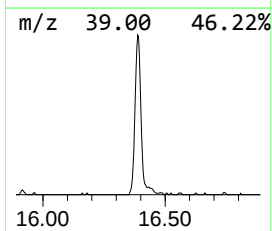
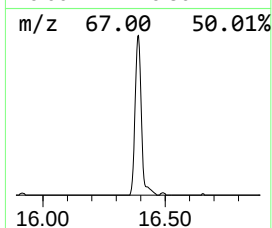
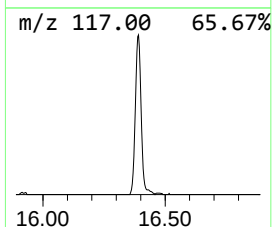
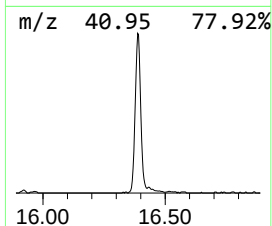
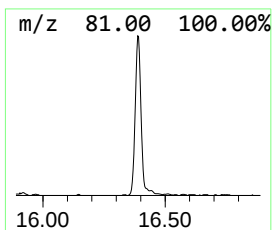
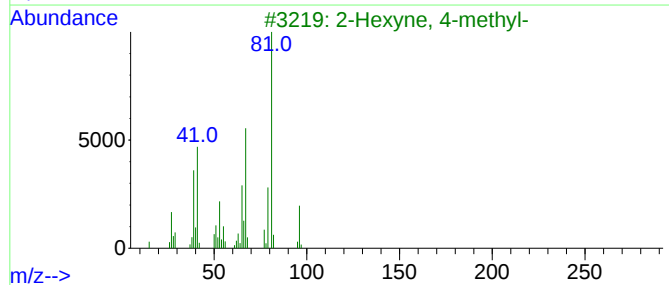
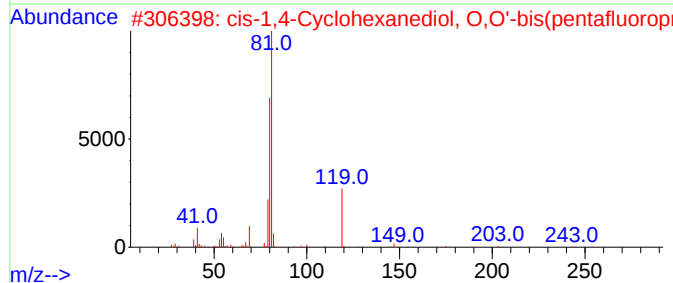
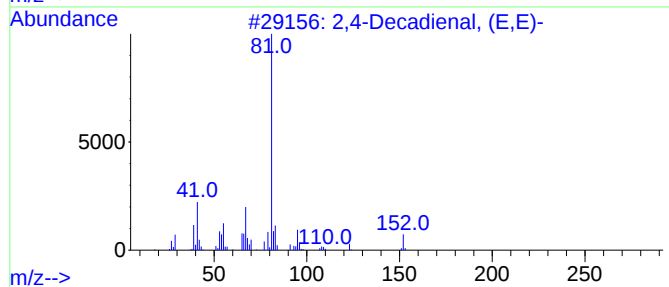
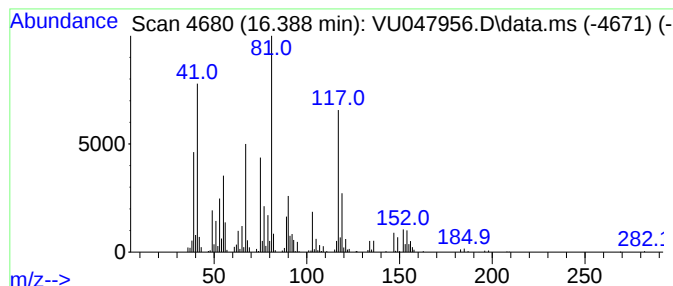
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Quant Title : VOC Analysis

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	14.63 ug/L	330154	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	22
2			cis-1,4-Cyclohexanediol, O,O'-bi...	408	C12H10F10O4	1000385-95-0	14
3			2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	12
4			Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	12
5			Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2-(met...	15.545	5.5	ug/L	124670	3	11.812	1127970	50.0
unknown-01	16.388	14.6	ug/L	330154	3	11.812	1127970	50.0