

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041524\
 Data File : VX041076.D
 Acq On : 15 Apr 2024 14:21
 Operator : JC/MD
 Sample : P2098-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MC0R73

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_X\Method\SFAMXML041024WMA.M
 Title : VOC Analysis

Signal : TIC: VX041076.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	6	10	22	rVB	44592	52139	5.37%	0.657%
2	1.270	27	30	36	rBV2	5098	6689	0.69%	0.084%
3	1.368	41	46	54	rBV	139697	183883	18.94%	2.316%
4	1.673	92	96	105	rVB	89277	122088	12.57%	1.538%
5	2.307	194	200	208	rBV	194979	306705	31.59%	3.863%
6	2.532	230	237	248	rBV2	4357	8739	0.90%	0.110%
7	2.636	253	254	256	rBV	227	202	0.02%	0.003%
8	2.654	256	257	260	rVB	332	236	0.02%	0.003%
9	2.703	260	265	274	rBV3	2688	6333	0.65%	0.080%
10	2.788	274	279	293	rVB2	4265	9753	1.00%	0.123%
11	2.947	300	305	312	rBV4	757	1434	0.15%	0.018%
12	3.099	322	330	336	rBV4	808	1610	0.17%	0.020%
13	3.178	340	343	345	rBV	144	165	0.02%	0.002%
14	3.258	351	356	357	rVV2	100	174	0.02%	0.002%
15	3.331	364	368	375	rVV4	1398	3091	0.32%	0.039%
16	3.453	382	388	395	rVB4	1021	2371	0.24%	0.030%
17	3.587	408	410	413	rVB2	182	192	0.02%	0.002%
18	3.672	422	424	427	rVV2	232	277	0.03%	0.003%
19	3.940	465	468	476	rVV3	277	607	0.06%	0.008%
20	4.264	519	521	525	rBV2	121	195	0.02%	0.002%
21	4.459	543	553	571	rBV	69880	219831	22.64%	2.769%
22	4.873	618	621	623	rBV2	200	237	0.02%	0.003%
23	5.056	638	651	673	rBV	127778	394465	40.63%	4.968%
24	5.239	679	681	685	rVB2	191	223	0.02%	0.003%
25	5.337	694	697	699	rBV2	156	167	0.02%	0.002%
26	5.391	701	706	709	rBV3	444	821	0.08%	0.010%
27	5.477	717	720	723	rBV	155	209	0.02%	0.003%
28	5.544	726	731	732	rBV2	542	554	0.06%	0.007%
29	5.617	742	743	745	rBV	187	156	0.02%	0.002%
30	5.708	755	758	761	rVB	191	188	0.02%	0.002%
31	5.794	769	772	776	rBV2	106	184	0.02%	0.002%
32	5.971	789	801	828	rBV2	319086	970892	100.00%	12.228%
33	6.269	848	850	853	rVB2	214	229	0.02%	0.003%
34	6.300	853	855	858	rVB	192	162	0.02%	0.002%
35	6.355	858	864	865	rBV2	231	369	0.04%	0.005%
36	6.464	880	882	884	rVB2	256	183	0.02%	0.002%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041024WMA.M
 Title : VOC Analysis

37	6.635	907	910	911	rBV2	194	209	0.02%	0.003%
38	6.763	921	931	950	rBV	248855	598082	61.60%	7.532%
39	7.117	985	989	997	rVB3	1001	2324	0.24%	0.029%
40	7.306	1011	1020	1036	rBV	196923	433203	44.62%	5.456%
41	7.489	1045	1050	1055	rVB5	602	1127	0.12%	0.014%
42	7.903	1113	1118	1119	rBV	179	206	0.02%	0.003%
43	7.940	1121	1124	1125	rBV2	264	238	0.02%	0.003%
44	8.324	1181	1187	1206	rVV	125817	215110	22.16%	2.709%
45	8.647	1234	1240	1251	rBV	488445	777042	80.03%	9.786%
46	8.952	1284	1290	1300	rBV	95071	142136	14.64%	1.790%
47	9.092	1311	1313	1316	rVB2	508	556	0.06%	0.007%
48	9.141	1316	1321	1322	rBV2	220	314	0.03%	0.004%
49	9.226	1331	1335	1336	rVV	136	161	0.02%	0.002%
50	9.275	1338	1343	1349	rVB2	2220	3845	0.40%	0.048%
51	9.385	1355	1361	1378	rBV	306917	475845	49.01%	5.993%
52	9.604	1396	1397	1399	rBV	293	181	0.02%	0.002%
53	9.775	1423	1425	1427	rBV2	162	159	0.02%	0.002%
54	9.982	1457	1459	1461	rVB2	174	172	0.02%	0.002%
55	10.055	1465	1471	1485	rBV	540993	772867	79.60%	9.734%
56	10.256	1501	1504	1506	rBV2	244	256	0.03%	0.003%
57	10.287	1506	1509	1510	rBV2	197	199	0.02%	0.003%
58	10.305	1510	1512	1517	rVV2	683	822	0.08%	0.010%
59	10.409	1527	1529	1533	rBV2	144	188	0.02%	0.002%
60	10.640	1563	1567	1568	rBV2	194	206	0.02%	0.003%
61	10.689	1572	1575	1576	rBV2	415	407	0.04%	0.005%
62	10.781	1585	1590	1593	rBV3	627	1009	0.10%	0.013%
63	10.866	1600	1604	1606	rBV3	791	1152	0.12%	0.015%
64	10.964	1618	1620	1623	rVB4	382	435	0.04%	0.005%
65	11.092	1636	1641	1647	rVB2	1115	1459	0.15%	0.018%
66	11.189	1652	1657	1671	rVV	410956	526206	54.20%	6.627%
67	11.311	1673	1677	1683	rVV	3631	5137	0.53%	0.065%
68	11.500	1704	1708	1713	rBV3	492	746	0.08%	0.009%
69	11.579	1715	1721	1723	rBV3	382	436	0.04%	0.005%
70	11.616	1725	1727	1732	rVB	164	241	0.02%	0.003%
71	11.713	1740	1743	1747	rVB3	345	363	0.04%	0.005%
72	11.750	1747	1749	1751	rBV	295	348	0.04%	0.004%
73	11.811	1757	1759	1762	rVB2	195	225	0.02%	0.003%
74	11.884	1766	1771	1775	rVB2	6790	8358	0.86%	0.105%
75	11.976	1782	1786	1789	rBV2	6878	8580	0.88%	0.108%
76	12.024	1789	1794	1809	rVB	596872	788656	81.23%	9.933%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

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Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041024WMA.M
Title : VOC Analysis

77	12.219	1821	1826	1837	rBV	21367	49666	5.12%	0.626%
78	12.317	1837	1842	1853	rVB	641881	814822	83.93%	10.262%
79	12.768	1912	1916	1919	rBV6	1379	2063	0.21%	0.026%
80	12.860	1928	1931	1938	rVB3	1476	1794	0.18%	0.023%
81	13.018	1954	1957	1960	rBV3	319	491	0.05%	0.006%
82	13.164	1980	1981	1984	rBV2	178	178	0.02%	0.002%
83	13.347	2008	2011	2012	rBV	126	152	0.02%	0.002%
84	13.524	2037	2040	2042	rBV	221	179	0.02%	0.002%
85	13.591	2047	2051	2053	rBV2	1996	2168	0.22%	0.027%
86	13.664	2061	2063	2065	rBV	223	156	0.02%	0.002%
87	13.780	2080	2082	2083	rBV2	423	380	0.04%	0.005%
88	13.878	2096	2098	2100	rVB	266	198	0.02%	0.002%
89	13.908	2100	2103	2104	rBV2	225	200	0.02%	0.003%
90	13.926	2104	2106	2109	rVB2	352	282	0.03%	0.004%
91	13.963	2109	2112	2116	rBV3	517	509	0.05%	0.006%
92	14.054	2125	2127	2130	rVB	218	181	0.02%	0.002%
93	14.085	2130	2132	2133	rBV	198	178	0.02%	0.002%
94	14.323	2167	2171	2172	rBV	232	279	0.03%	0.004%
95	14.359	2175	2177	2179	rBV2	218	188	0.02%	0.002%
96	14.414	2184	2186	2187	rVV	288	179	0.02%	0.002%
97	14.451	2190	2192	2195	rBV	255	236	0.02%	0.003%
98	14.823	2251	2253	2254	rBV2	269	184	0.02%	0.002%
99	14.951	2271	2274	2275	rBV2	387	348	0.04%	0.004%
100	15.371	2341	2343	2344	rBV	314	179	0.02%	0.002%

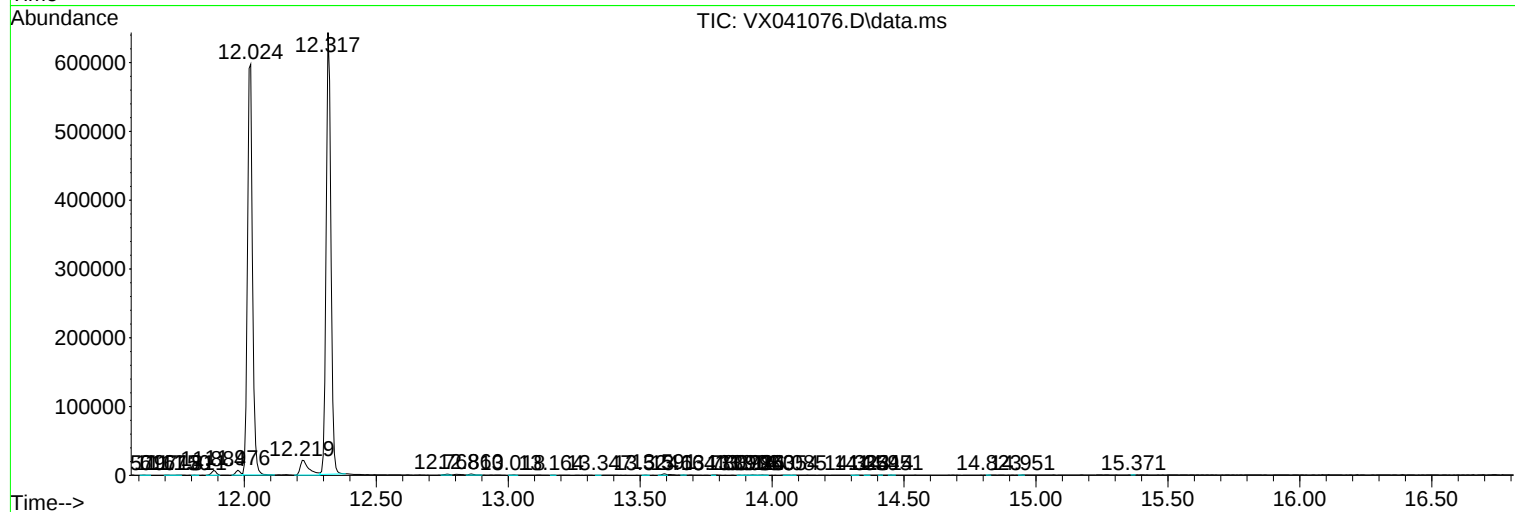
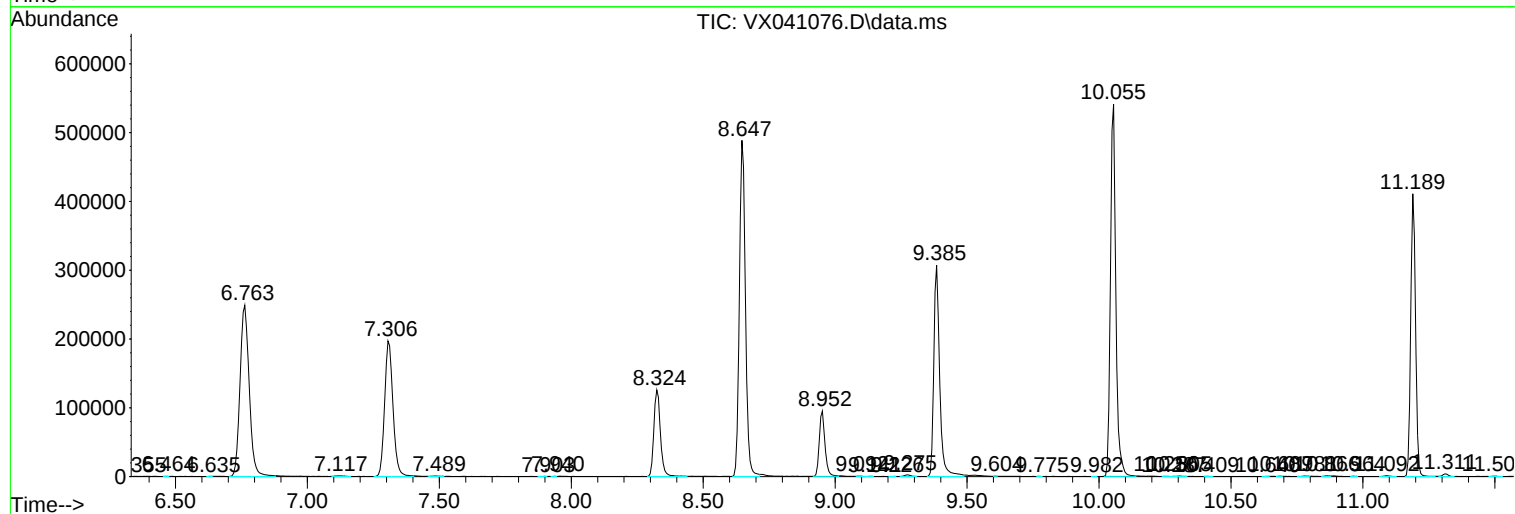
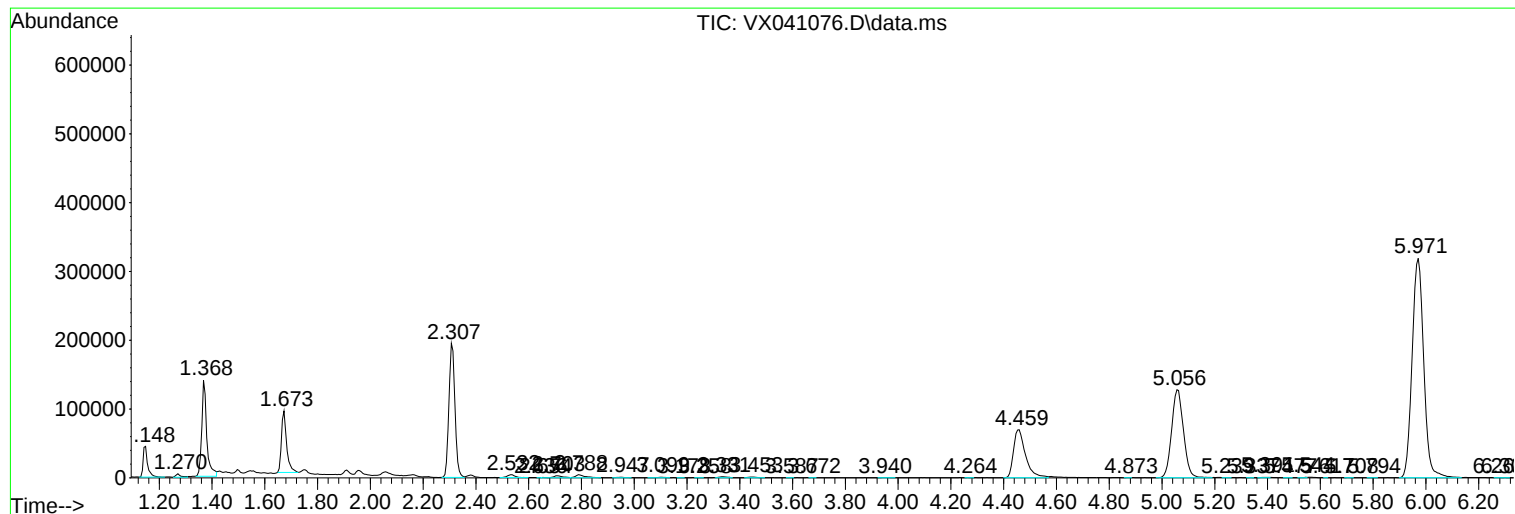
Sum of corrected areas: 7940149

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041024WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO41524\
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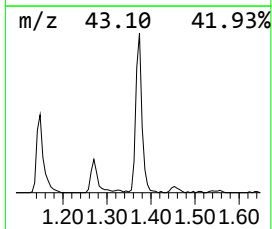
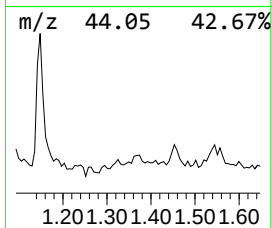
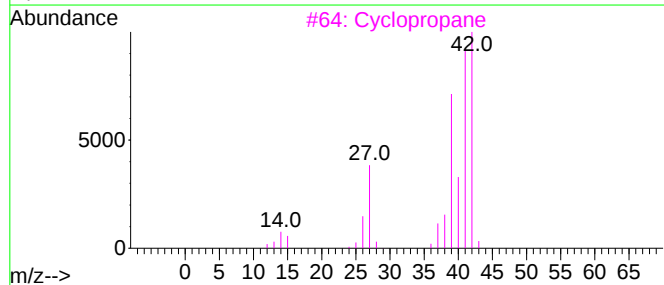
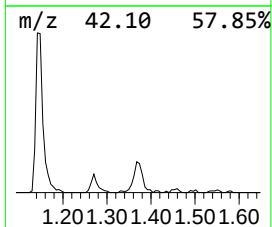
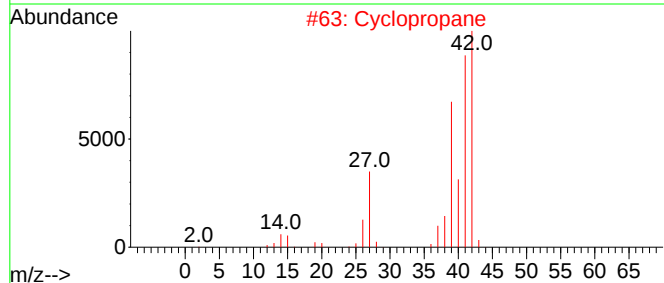
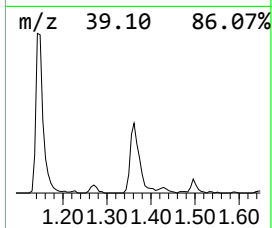
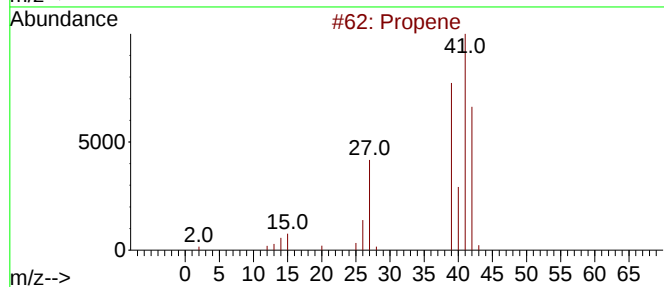
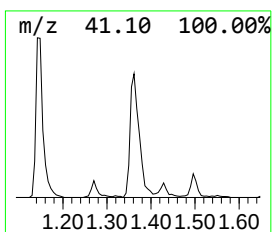
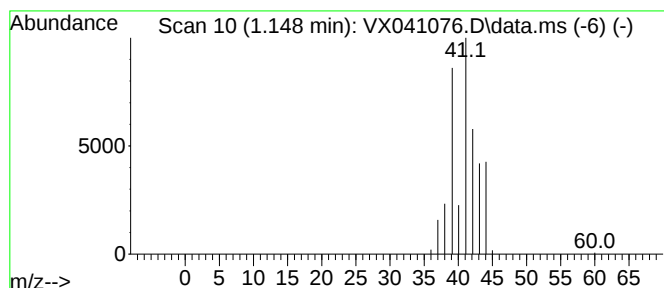
Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.148	4.36 ug/L	52139	1,4-Difluorobenzene	6.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	42
2	Cyclopropane	42	C3H6	000075-19-4	10
3	Cyclopropane	42	C3H6	000075-19-4	7
4	Propene	42	C3H6	000115-07-1	7
5	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4



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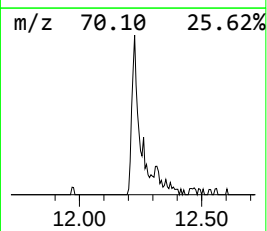
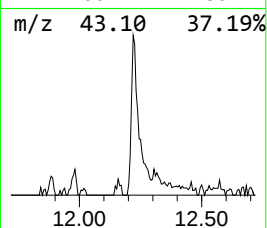
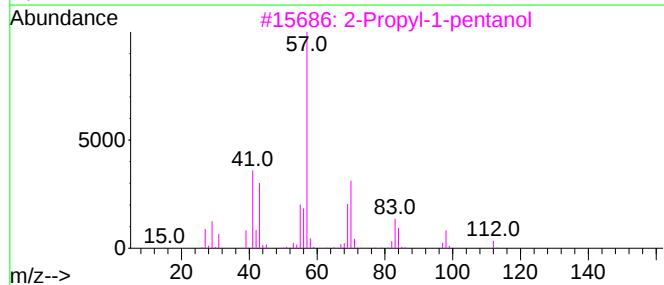
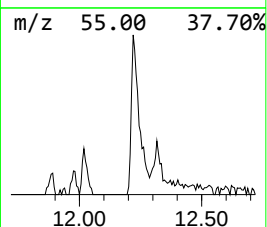
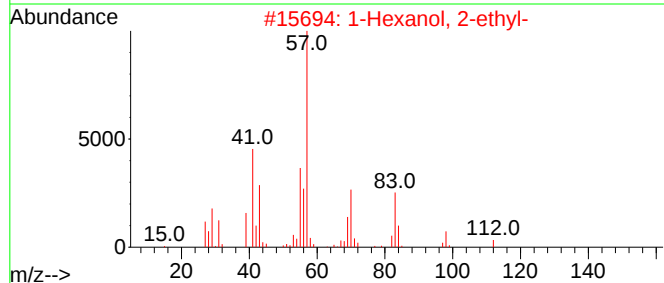
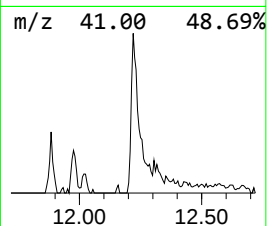
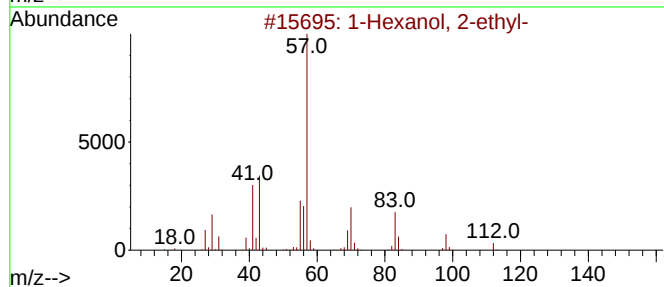
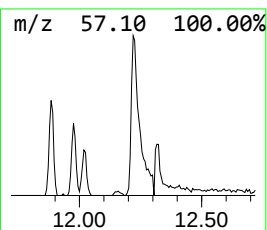
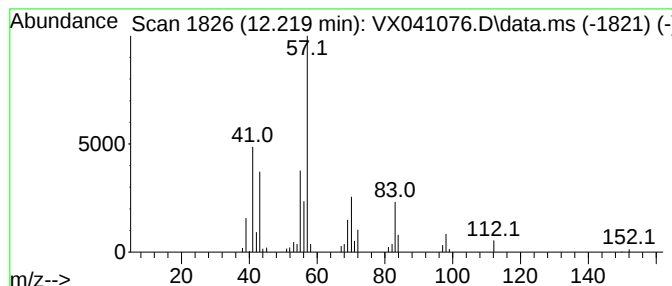
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Quant Title : VOC Analysis

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	3.15 ug/L	49666	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.148	4.4	ug/L	52139	1	6.763	598082	50.0
1-Hexanol, 2-et...	12.219	3.1	ug/L	49666	3	12.024	788656	50.0