

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081822\
 Data File : VX030689.D
 Acq On : 18 Aug 2022 16:48
 Operator : JC/MD
 Sample : N4231-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KQ5

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030689.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	53	rVB	184659	187205	13.90%	1.801%
2	1.666	91	95	107	rVB	134623	165590	12.30%	1.593%
3	2.306	194	200	209	rBV	312126	486876	36.16%	4.684%
4	2.386	211	213	219	rVB	6061	7839	0.58%	0.075%
5	2.648	253	256	257	rBV3	605	563	0.04%	0.005%
6	2.794	274	280	283	rVB3	1009	1739	0.13%	0.017%
7	2.947	301	305	315	rVB6	1246	3417	0.25%	0.033%
8	3.093	327	329	332	rBV	472	361	0.03%	0.003%
9	3.221	348	350	352	rBV2	460	438	0.03%	0.004%
10	3.276	358	359	363	rBV2	404	420	0.03%	0.004%
11	3.312	363	365	368	rVB2	409	435	0.03%	0.004%
12	3.343	368	370	371	rBV2	426	337	0.03%	0.003%
13	3.453	385	388	390	rBV3	407	462	0.03%	0.004%
14	3.477	390	392	395	rBV2	447	471	0.03%	0.005%
15	3.544	402	403	406	rBV	447	388	0.03%	0.004%
16	3.611	412	414	417	rBV	652	710	0.05%	0.007%
17	3.745	431	436	438	rBV2	729	1320	0.10%	0.013%
18	3.843	449	452	454	rVB2	323	376	0.03%	0.004%
19	3.885	454	459	461	rBV2	474	754	0.06%	0.007%
20	4.227	511	515	516	rBV2	542	719	0.05%	0.007%
21	4.355	532	536	538	rBV2	276	365	0.03%	0.004%
22	4.379	538	540	542	rVB	497	325	0.02%	0.003%
23	4.465	542	554	569	rBV	112392	332194	24.67%	3.196%
24	4.647	583	584	587	rBV2	547	398	0.03%	0.004%
25	4.727	588	597	610	rVV2	30790	87880	6.53%	0.845%
26	4.861	617	619	622	rBV3	513	606	0.05%	0.006%
27	4.916	626	628	631	rVB	480	408	0.03%	0.004%
28	5.062	637	652	670	rBV	180327	563235	41.83%	5.418%
29	5.361	699	701	702	rBV	501	333	0.02%	0.003%
30	5.391	702	706	713	rVB4	1557	2527	0.19%	0.024%
31	5.556	729	733	734	rBV3	1739	2174	0.16%	0.021%
32	5.726	758	761	762	rBV	499	380	0.03%	0.004%
33	5.861	779	783	784	rBV	459	470	0.03%	0.005%
34	5.976	789	802	822	rBV2	455790	1346398	100.00%	12.952%
35	6.190	836	837	839	rBV2	381	322	0.02%	0.003%
36	6.348	862	863	865	rBV	430	385	0.03%	0.004%

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37	6.678	913	917	918	rBV2	313	400	0.03%	0.004%
38	6.769	922	932	946	rBV	310853	742097	55.12%	7.139%
39	6.934	958	959	961	rBV	405	386	0.03%	0.004%
40	7.129	981	991	1001	rBV5	30232	79763	5.92%	0.767%
41	7.232	1006	1008	1009	rBV2	383	333	0.02%	0.003%
42	7.312	1013	1021	1037	rVB	276463	605897	45.00%	5.829%
43	7.476	1045	1048	1053	rBV5	831	1534	0.11%	0.015%
44	7.580	1061	1065	1066	rBV2	1284	1314	0.10%	0.013%
45	7.690	1081	1083	1085	rBV3	395	347	0.03%	0.003%
46	7.751	1090	1093	1096	rBV	486	704	0.05%	0.007%
47	7.933	1119	1123	1130	rVB4	1856	3366	0.25%	0.032%
48	8.031	1137	1139	1142	rVB2	322	306	0.02%	0.003%
49	8.141	1155	1157	1160	rBV	557	557	0.04%	0.005%
50	8.238	1172	1173	1180	rVB3	449	478	0.04%	0.005%
51	8.330	1182	1188	1198	rBV	180842	291108	21.62%	2.800%
52	8.567	1225	1227	1228	rBV	414	326	0.02%	0.003%
53	8.653	1234	1241	1251	rBV	716147	1094818	81.31%	10.532%
54	8.952	1285	1290	1297	rBV	127634	187882	13.95%	1.807%
55	9.177	1325	1327	1329	rVB2	553	381	0.03%	0.004%
56	9.244	1333	1338	1339	rBV2	704	1079	0.08%	0.010%
57	9.275	1339	1343	1349	rVB3	17127	27039	2.01%	0.260%
58	9.390	1356	1362	1373	rBV	469265	691078	51.33%	6.648%
59	9.525	1379	1384	1390	rBV	27222	39637	2.94%	0.381%
60	9.726	1415	1417	1419	rBV2	398	367	0.03%	0.004%
61	9.854	1435	1438	1441	rBV2	468	659	0.05%	0.006%
62	9.878	1441	1442	1445	rVV2	460	444	0.03%	0.004%
63	9.915	1447	1448	1453	rVV2	433	533	0.04%	0.005%
64	10.055	1465	1471	1482	rBV	649750	862316	64.05%	8.296%
65	10.250	1499	1503	1505	rBV3	562	731	0.05%	0.007%
66	10.646	1565	1568	1572	rBV	7622	9348	0.69%	0.090%
67	10.768	1586	1588	1594	rVB4	1943	2459	0.18%	0.024%
68	10.860	1598	1603	1608	rVV3	3160	4004	0.30%	0.039%
69	10.939	1614	1616	1618	rBV	468	466	0.03%	0.004%
70	11.037	1626	1632	1637	rVV6	1605	2958	0.22%	0.028%
71	11.091	1639	1641	1643	rBV2	565	353	0.03%	0.003%
72	11.195	1652	1658	1666	rBV	505127	629275	46.74%	6.054%
73	11.317	1674	1678	1682	rVB3	5945	7888	0.59%	0.076%
74	11.390	1688	1690	1694	rVB3	771	862	0.06%	0.008%
75	11.433	1694	1697	1699	rBV2	482	625	0.05%	0.006%
76	11.475	1703	1704	1708	rVB3	868	744	0.06%	0.007%

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77	11.555	1716	1717	1721	rVB	357	371	0.03%	0.004%
78	11.689	1736	1739	1740	rBV2	611	656	0.05%	0.006%
79	11.756	1748	1750	1759	rVB4	2868	5594	0.42%	0.054%
80	11.853	1761	1766	1768	rVB4	816	1261	0.09%	0.012%
81	11.872	1768	1769	1771	rBV	405	347	0.03%	0.003%
82	11.927	1776	1778	1784	rVB4	2289	3225	0.24%	0.031%
83	12.024	1789	1794	1804	rVV	669963	812048	60.31%	7.812%
84	12.225	1822	1827	1837	rVV	50303	94563	7.02%	0.910%
85	12.323	1838	1843	1852	rVB	743647	931856	69.21%	8.965%
86	12.591	1885	1887	1897	rVB4	3106	4888	0.36%	0.047%
87	12.768	1911	1916	1921	rBV5	3029	5063	0.38%	0.049%
88	12.859	1927	1931	1936	rVB3	10293	12877	0.96%	0.124%
89	12.945	1941	1945	1947	rBV3	2905	3272	0.24%	0.031%
90	13.067	1962	1965	1966	rBV3	599	671	0.05%	0.006%
91	13.103	1967	1971	1977	rVB3	11579	15989	1.19%	0.154%
92	13.152	1977	1979	1984	rBV5	782	1250	0.09%	0.012%
93	13.591	2048	2051	2053	rBV3	926	934	0.07%	0.009%
94	13.756	2076	2078	2082	rBV3	782	1040	0.08%	0.010%
95	13.877	2094	2098	2100	rBV2	903	1161	0.09%	0.011%
96	13.951	2107	2110	2112	rBV2	752	825	0.06%	0.008%
97	14.048	2124	2126	2127	rBV	601	344	0.03%	0.003%
98	14.140	2136	2141	2142	rBV3	1514	2163	0.16%	0.021%
99	14.658	2224	2226	2227	rBV	655	358	0.03%	0.003%
100	16.420	2514	2515	2516	rBV	953	507	0.04%	0.005%

Sum of corrected areas: 10394945

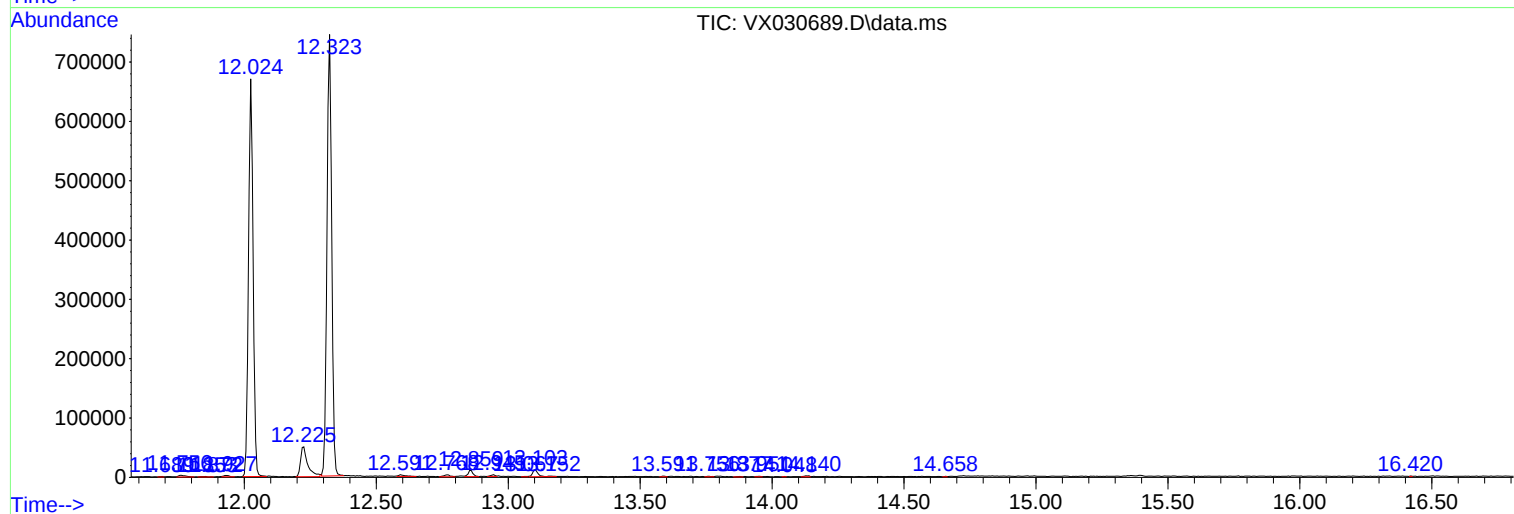
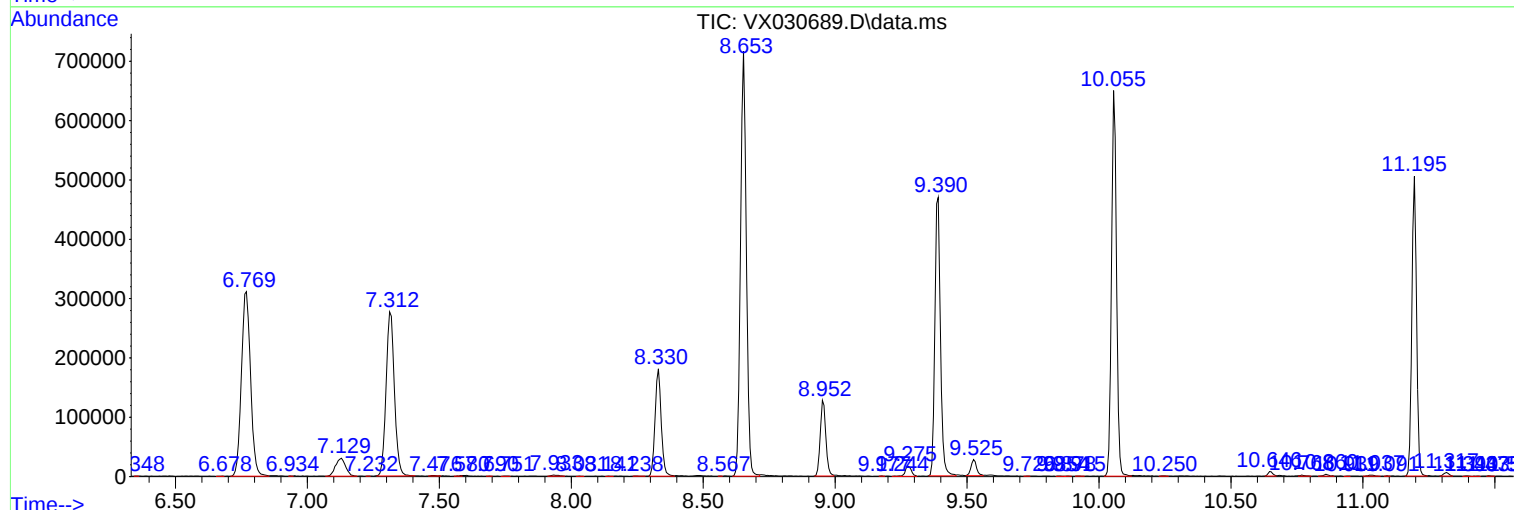
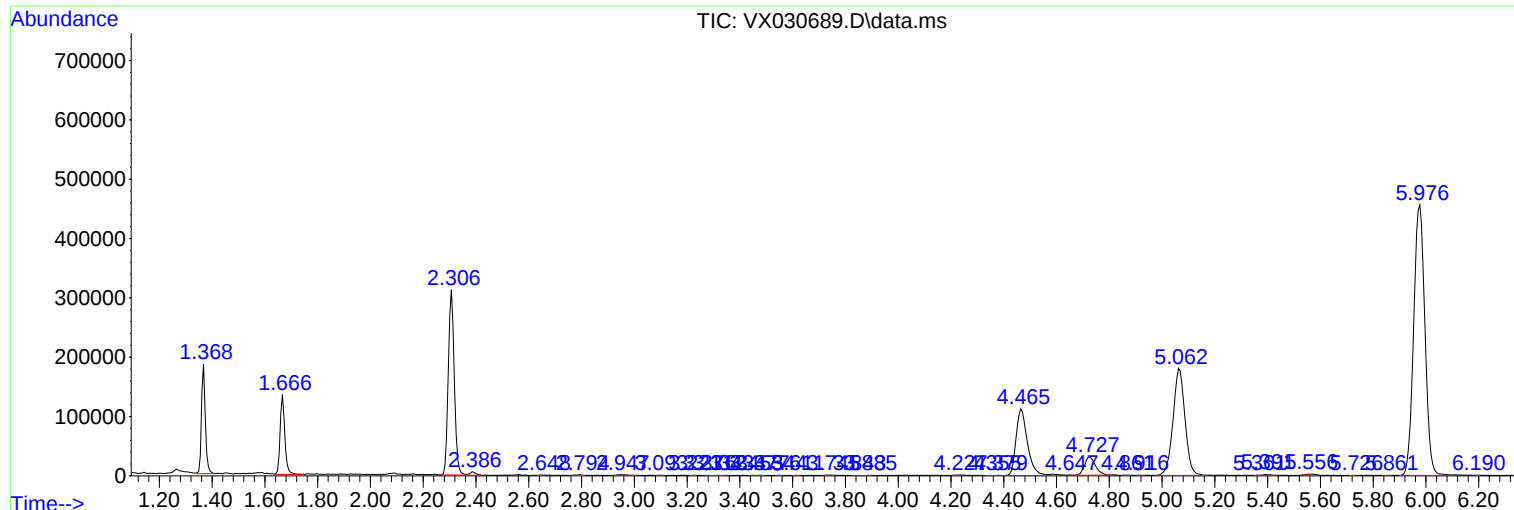
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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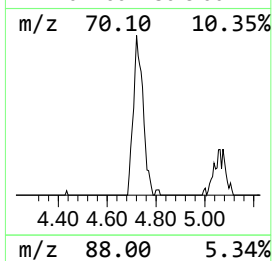
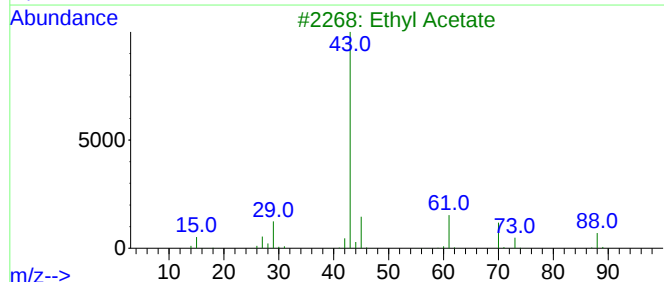
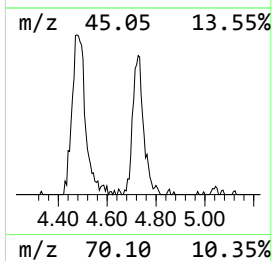
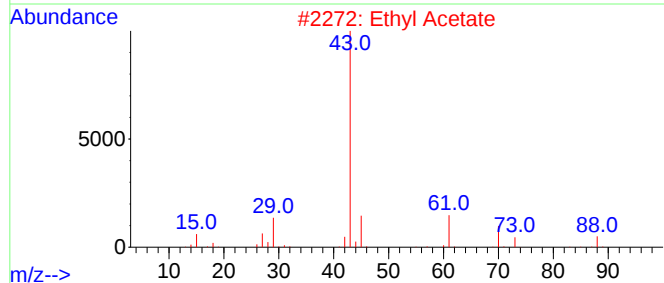
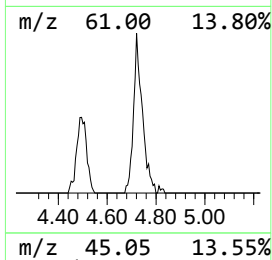
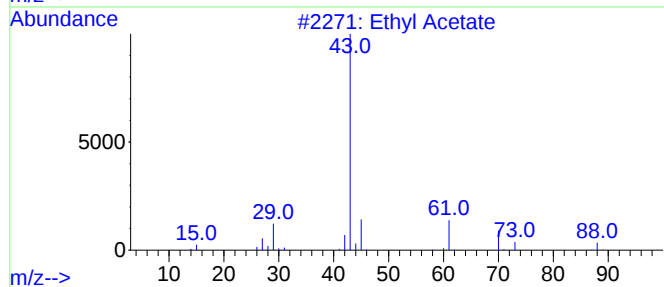
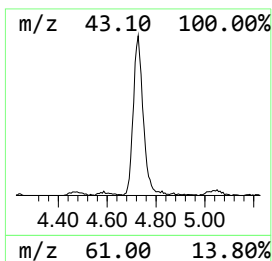
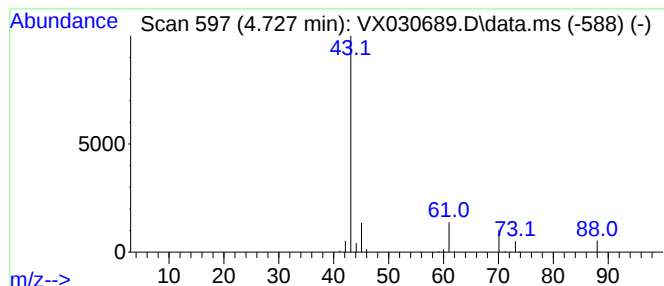
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.727	5.92 ug/L	87880	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	86
4			Ethyl Acetate	88	C4H8O2	000141-78-6	78
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	42



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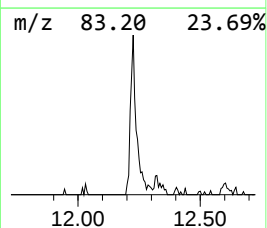
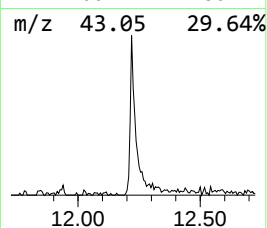
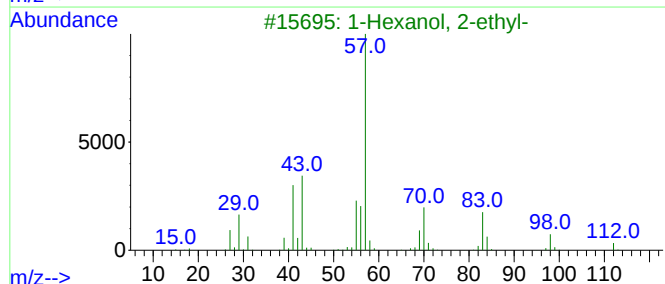
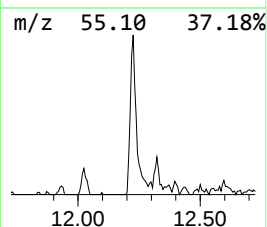
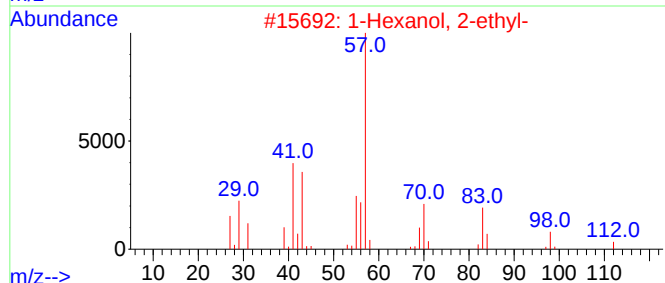
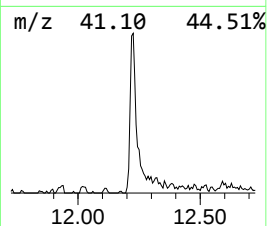
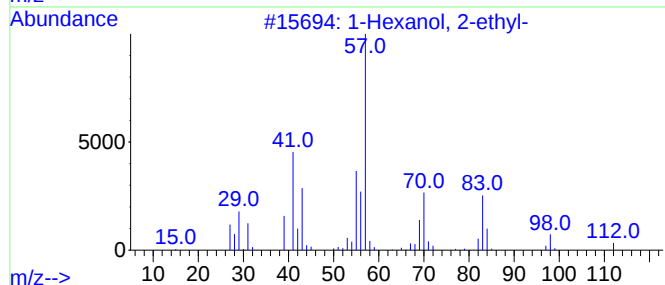
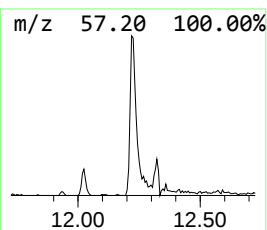
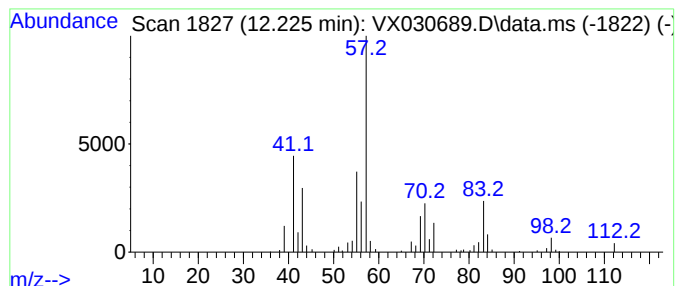
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.225	5.82 ug/L	94563	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	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	59
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.727	5.9	ug/L	87880	1	6.769	742097	50.0
1-Hexanol, 2-et...	12.225	5.8	ug/L	94563	3	12.024	812048	50.0