

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030658.D
 Acq On : 17 Aug 2022 14:28
 Operator : JC/MD
 Sample : N4231-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KQ4

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: VX030658.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	56	rVB	186006	192518	14.42%	1.926%
2	1.666	91	95	102	rVB	134335	162360	12.16%	1.625%
3	2.020	151	153	154	rBV2	1368	798	0.06%	0.008%
4	2.306	193	200	209	rBV	328719	489900	36.70%	4.902%
5	2.392	209	214	219	rVB	3964	6490	0.49%	0.065%
6	2.508	231	233	237	rBV2	576	754	0.06%	0.008%
7	2.776	276	277	278	rBV	423	298	0.02%	0.003%
8	2.940	300	304	306	rBV4	842	1434	0.11%	0.014%
9	3.081	325	327	328	rBV	474	387	0.03%	0.004%
10	3.190	342	345	347	rBV2	408	549	0.04%	0.005%
11	3.245	352	354	355	rVV2	453	296	0.02%	0.003%
12	3.690	425	427	429	rVB2	401	298	0.02%	0.003%
13	3.709	429	430	432	rBV	570	444	0.03%	0.004%
14	3.739	432	435	438	rBV	572	821	0.06%	0.008%
15	4.050	484	486	489	rVB2	355	358	0.03%	0.004%
16	4.080	489	491	494	rBV2	479	420	0.03%	0.004%
17	4.208	509	512	513	rBV	380	414	0.03%	0.004%
18	4.227	513	515	517	rVV	651	508	0.04%	0.005%
19	4.251	517	519	523	rVB2	481	565	0.04%	0.006%
20	4.465	545	554	584	rVV	105765	309694	23.20%	3.099%
21	4.721	588	596	614	rVB	30856	88961	6.66%	0.890%
22	4.903	624	626	627	rVB2	630	354	0.03%	0.004%
23	5.062	637	652	670	rBV	176191	559326	41.90%	5.597%
24	5.288	688	689	692	rBV3	583	575	0.04%	0.006%
25	5.312	692	693	696	rVV2	303	297	0.02%	0.003%
26	5.373	701	703	704	rBV	902	700	0.05%	0.007%
27	5.501	723	724	726	rBV2	431	356	0.03%	0.004%
28	5.562	729	734	739	rVB6	1978	4208	0.32%	0.042%
29	5.867	782	784	787	rVB2	324	360	0.03%	0.004%
30	5.976	789	802	817	rBV2	456853	1335048	100.00%	13.358%
31	6.367	864	866	868	rVB2	510	392	0.03%	0.004%
32	6.482	884	885	888	rVB2	501	289	0.02%	0.003%
33	6.531	890	893	896	rBV3	448	665	0.05%	0.007%
34	6.586	900	902	903	rVB	642	416	0.03%	0.004%
35	6.598	903	904	905	rBV	484	304	0.02%	0.003%
36	6.635	909	910	912	rVV	546	352	0.03%	0.004%

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 Title : VOC Analysis

37	6.763	923	931	944	rBV	284387	689506	51.65%	6.899%
38	6.976	964	966	967	rBV	467	306	0.02%	0.003%
39	7.062	977	980	981	rBV	490	597	0.04%	0.006%
40	7.110	981	988	1000	rVB4	12081	29439	2.21%	0.295%
41	7.226	1006	1007	1010	rBV	426	319	0.02%	0.003%
42	7.312	1013	1021	1034	rVB	270412	593352	44.44%	5.937%
43	7.464	1043	1046	1047	rBV2	572	566	0.04%	0.006%
44	7.598	1062	1068	1074	rBV4	1519	3031	0.23%	0.030%
45	7.653	1075	1077	1079	rVB	746	484	0.04%	0.005%
46	7.824	1102	1105	1109	rBV2	620	797	0.06%	0.008%
47	7.946	1120	1125	1131	rVB5	1306	2819	0.21%	0.028%
48	8.257	1175	1176	1181	rBV2	301	415	0.03%	0.004%
49	8.330	1181	1188	1199	rBV	187636	301424	22.58%	3.016%
50	8.653	1234	1241	1250	rBV	685535	1073879	80.44%	10.745%
51	8.952	1284	1290	1300	rBV	137215	197994	14.83%	1.981%
52	9.122	1316	1318	1321	rBV2	657	551	0.04%	0.006%
53	9.147	1321	1322	1324	rVB	634	382	0.03%	0.004%
54	9.171	1324	1326	1327	rBV	561	409	0.03%	0.004%
55	9.275	1337	1343	1349	rBV5	3226	5367	0.40%	0.054%
56	9.384	1356	1361	1374	rBV	457555	679748	50.92%	6.801%
57	9.525	1379	1384	1390	rVB2	25700	38815	2.91%	0.388%
58	9.738	1416	1419	1420	rVB2	733	717	0.05%	0.007%
59	9.793	1425	1428	1429	rBV2	422	403	0.03%	0.004%
60	9.829	1432	1434	1435	rBV	490	444	0.03%	0.004%
61	9.915	1444	1448	1450	rBV	418	531	0.04%	0.005%
62	10.055	1466	1471	1483	rVV	602854	813150	60.91%	8.136%
63	10.250	1501	1503	1507	rBV2	803	969	0.07%	0.010%
64	10.305	1508	1512	1516	rBV3	791	1289	0.10%	0.013%
65	10.384	1523	1525	1530	rVB2	559	647	0.05%	0.006%
66	10.433	1530	1533	1535	rBV2	514	487	0.04%	0.005%
67	10.543	1547	1551	1552	rBV2	322	345	0.03%	0.003%
68	10.646	1564	1568	1578	rVB	9251	13334	1.00%	0.133%
69	10.750	1583	1585	1586	rBV	726	586	0.04%	0.006%
70	10.762	1586	1587	1595	rVB4	1727	2450	0.18%	0.025%
71	10.860	1600	1603	1609	rVB2	3462	4147	0.31%	0.041%
72	11.030	1627	1631	1635	rVB4	2137	3308	0.25%	0.033%
73	11.073	1635	1638	1641	rBV2	848	1093	0.08%	0.011%
74	11.140	1647	1649	1652	rVV	385	335	0.03%	0.003%
75	11.195	1652	1658	1671	rVB	477068	598893	44.86%	5.992%
76	11.317	1674	1678	1681	rVB2	2091	2444	0.18%	0.024%

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77	11.683	1736	1738	1741	rBV4	639	536	0.04%	0.005%
78	11.756	1747	1750	1756	rVB4	4104	5329	0.40%	0.053%
79	11.933	1776	1779	1783	rVB3	2317	2809	0.21%	0.028%
80	11.975	1783	1786	1788	rBV2	628	578	0.04%	0.006%
81	12.024	1789	1794	1803	rVV	609004	748452	56.06%	7.489%
82	12.219	1822	1826	1835	rBV	45168	68668	5.14%	0.687%
83	12.323	1837	1843	1850	rVB	716485	897258	67.21%	8.978%
84	12.719	1907	1908	1912	rBV3	721	654	0.05%	0.007%
85	12.859	1927	1931	1938	rVB5	8115	11161	0.84%	0.112%
86	12.914	1938	1940	1944	rVV3	671	667	0.05%	0.007%
87	13.103	1967	1971	1976	rVB	15593	18813	1.41%	0.188%
88	13.475	2028	2032	2034	rBV5	846	1202	0.09%	0.012%
89	13.591	2049	2051	2054	rVB3	1787	1783	0.13%	0.018%
90	13.725	2071	2073	2078	rBV2	462	782	0.06%	0.008%
91	13.768	2078	2080	2081	rBV2	541	329	0.02%	0.003%
92	13.975	2112	2114	2117	rBV	702	611	0.05%	0.006%
93	14.127	2137	2139	2144	rVB4	1785	2534	0.19%	0.025%
94	14.591	2213	2215	2217	rBV3	508	542	0.04%	0.005%
95	14.664	2226	2227	2230	rVB3	640	316	0.02%	0.003%
96	14.743	2238	2240	2241	rBV	958	585	0.04%	0.006%
97	14.792	2246	2248	2249	rBV	841	459	0.03%	0.005%
98	15.042	2287	2289	2291	rBV2	614	598	0.04%	0.006%
99	15.353	2338	2340	2342	rBV3	1397	1229	0.09%	0.012%
100	15.914	2431	2432	2434	rBV2	850	630	0.05%	0.006%

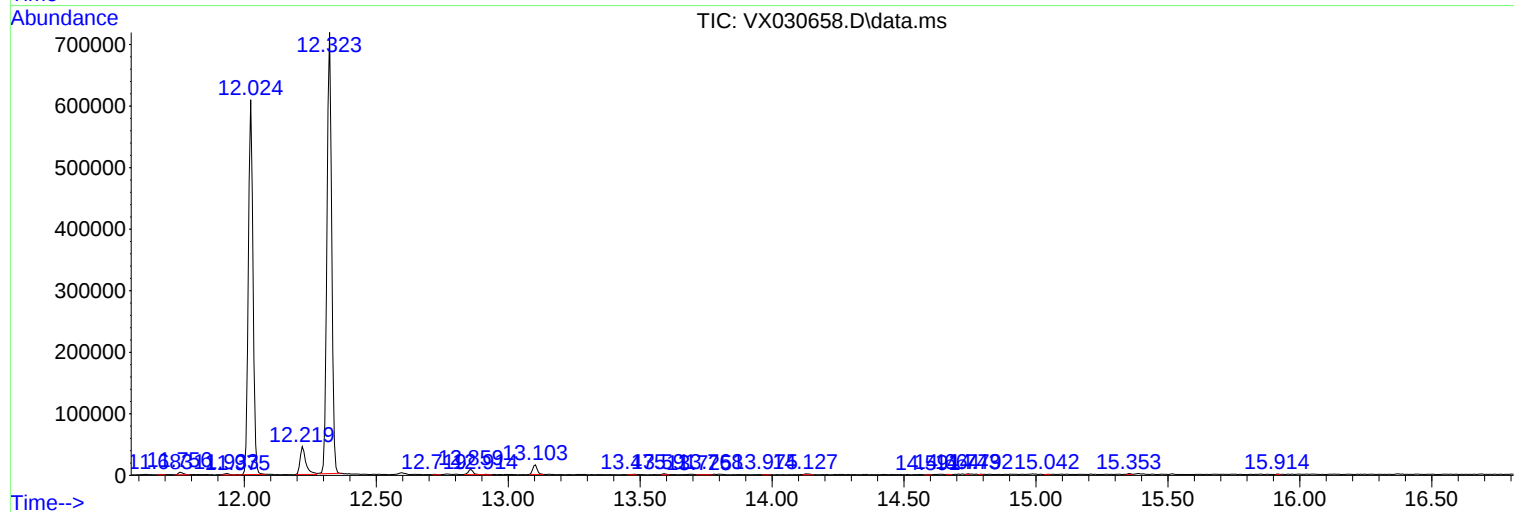
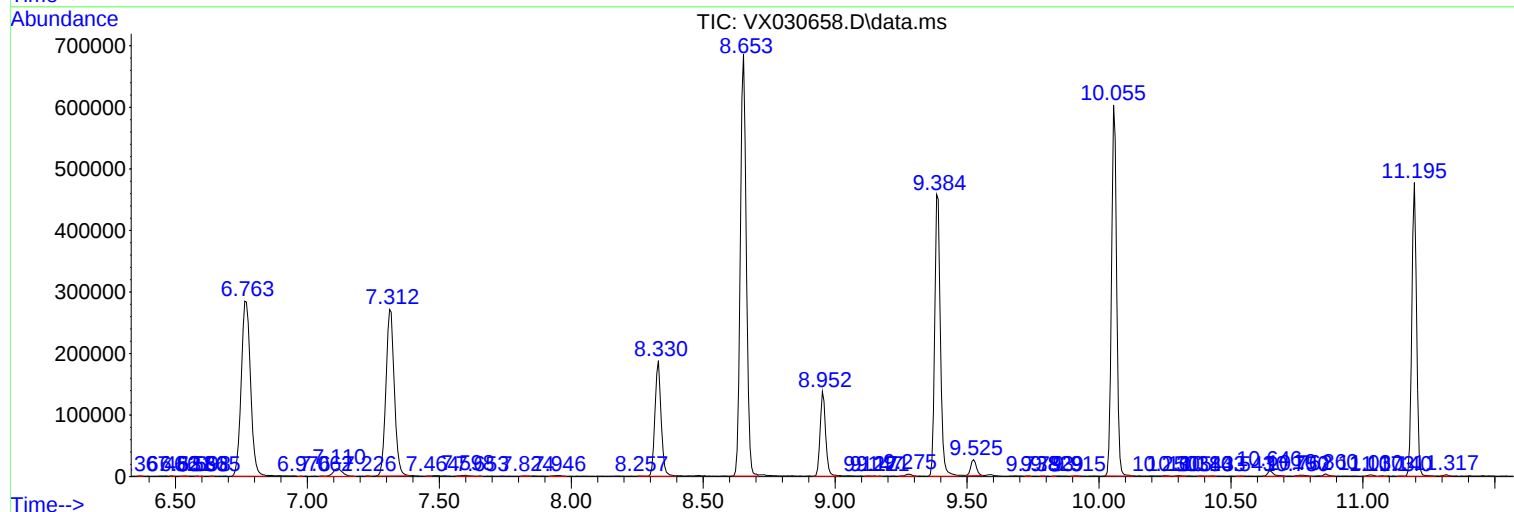
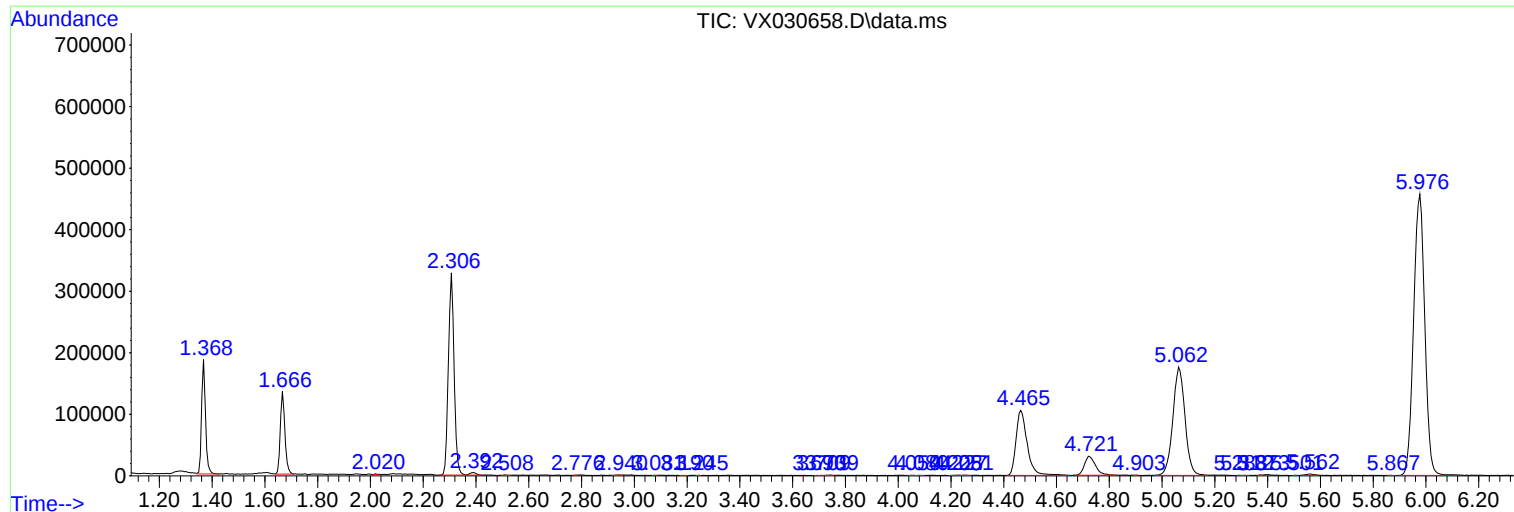
Sum of corrected areas: 9994206

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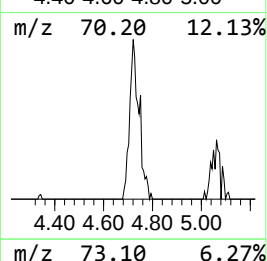
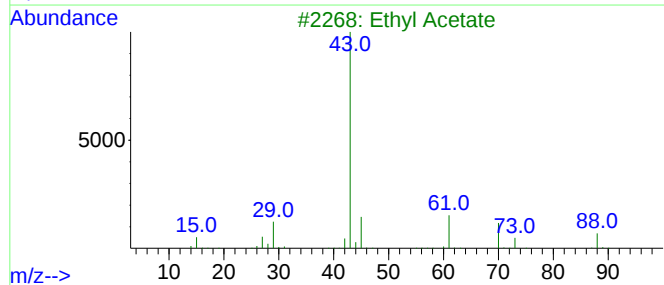
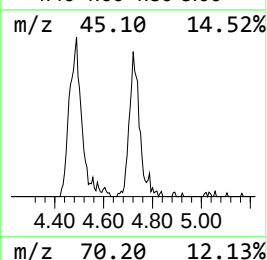
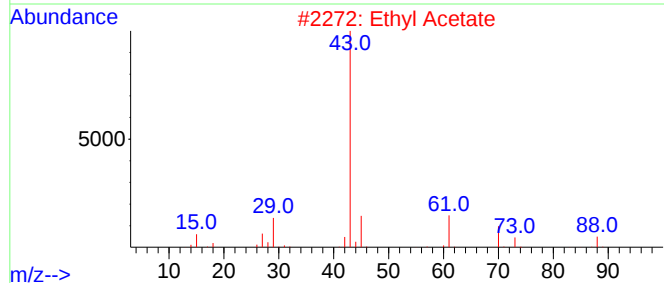
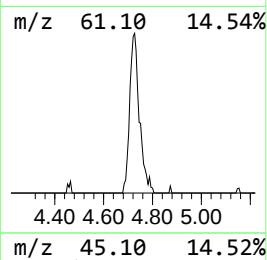
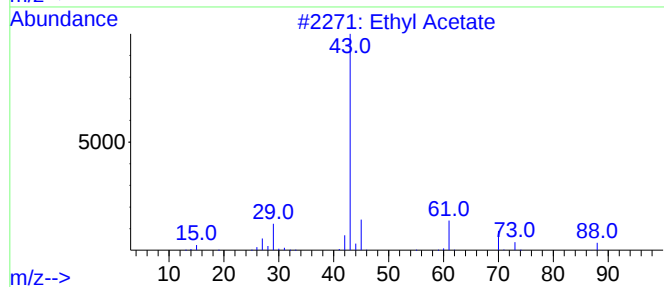
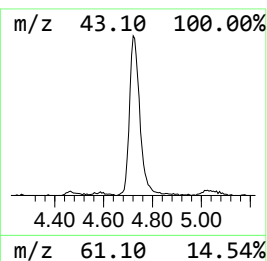
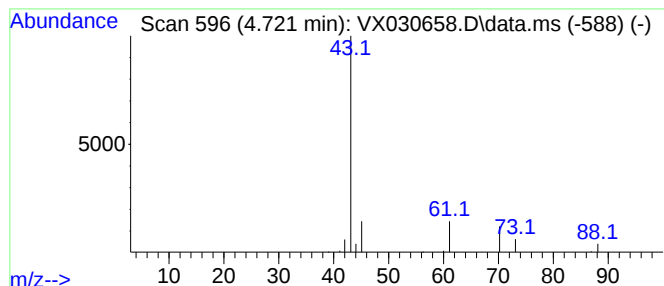
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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.
4.721	6.45 ug/L	88961	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	86
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	78
4			Ethyl Acetate	88	C4H8O2	000141-78-6	53
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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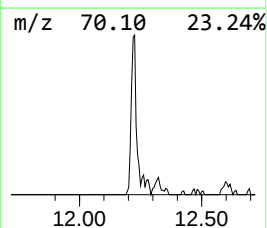
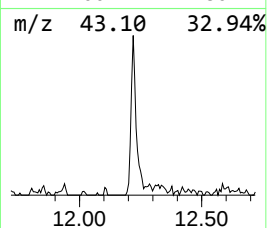
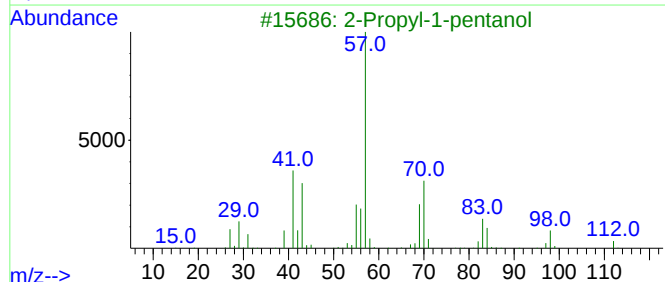
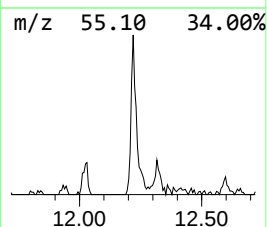
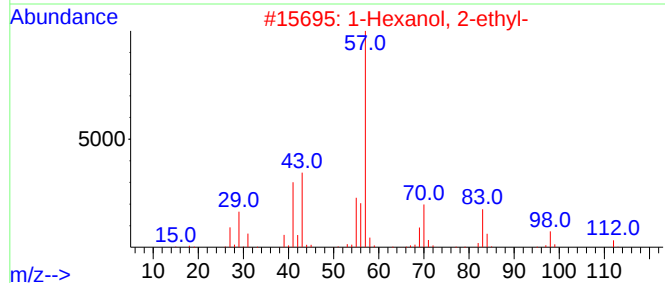
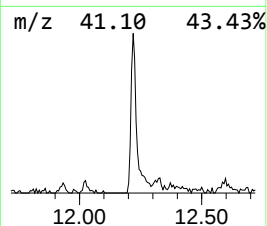
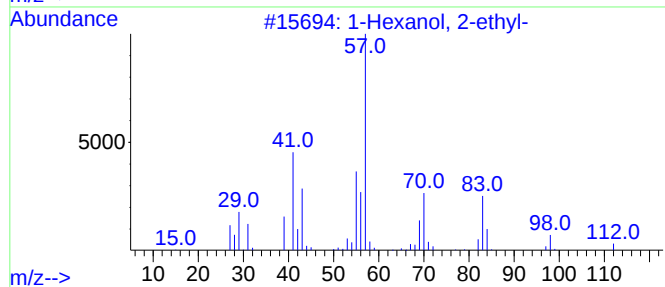
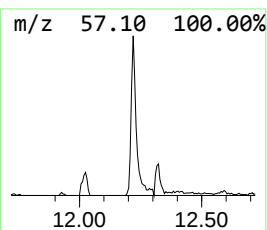
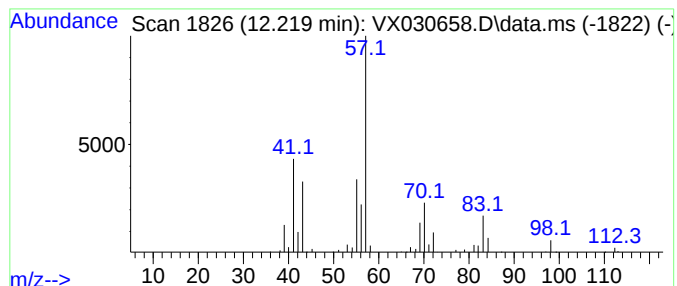
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	4.59 ug/L	68668	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	64
3	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.721	6.5	ug/L	88961	1	6.769	689506	50.0
1-Hexanol, 2-et...	12.219	4.6	ug/L	68668	3	12.024	748452	50.0