

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030665.D
 Acq On : 17 Aug 2022 17:12
 Operator : JC/MD
 Sample : N4221-18
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KP0

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: VX030665.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	32	rBV	17380	38158	0.45%	0.171%
2	1.367	42	46	53	rVB	181339	189711	2.24%	0.850%
3	1.666	91	95	104	rVB	132540	158006	1.87%	0.708%
4	2.306	194	200	210	rBV2	372390	684797	8.09%	3.069%
5	2.703	263	265	269	rBV3	387	519	0.01%	0.002%
6	2.800	274	281	286	rVB5	1068	2478	0.03%	0.011%
7	2.861	288	291	294	rBV3	723	784	0.01%	0.004%
8	2.946	300	305	311	rVV2	3244	6912	0.08%	0.031%
9	2.995	311	313	316	rVB2	668	537	0.01%	0.002%
10	3.093	324	329	338	rVB2	6357	10899	0.13%	0.049%
11	3.178	342	343	346	rBV2	438	461	0.01%	0.002%
12	3.269	357	358	362	rVB	663	375	0.00%	0.002%
13	3.452	385	388	391	rBV3	348	499	0.01%	0.002%
14	3.489	391	394	395	rBV3	440	398	0.00%	0.002%
15	3.611	405	414	426	rVB	24894	61372	0.73%	0.275%
16	3.971	470	473	475	rBV2	490	436	0.01%	0.002%
17	4.062	486	488	490	rVB2	465	361	0.00%	0.002%
18	4.111	490	496	498	rBV3	626	957	0.01%	0.004%
19	4.318	527	530	532	rVB3	276	310	0.00%	0.001%
20	4.379	537	540	542	rVB3	503	585	0.01%	0.003%
21	4.495	545	559	585	rBV2	768029	2282756	26.97%	10.231%
22	4.781	601	606	610	rVB4	703	1369	0.02%	0.006%
23	5.062	639	652	669	rBV	168570	514756	6.08%	2.307%
24	5.391	692	706	718	rBV3	32345	98152	1.16%	0.440%
25	5.519	724	727	728	rBV	586	427	0.01%	0.002%
26	5.543	728	731	732	rBV3	1212	1315	0.02%	0.006%
27	5.720	758	760	763	rVB2	512	451	0.01%	0.002%
28	5.745	763	764	767	rVB2	376	338	0.00%	0.002%
29	5.775	767	769	770	rBV2	418	379	0.00%	0.002%
30	5.806	772	774	777	rVB2	383	359	0.00%	0.002%
31	5.860	781	783	785	rVB	578	431	0.01%	0.002%
32	5.976	789	802	818	rBV2	442997	1301316	15.38%	5.832%
33	6.190	835	837	840	rVB2	463	496	0.01%	0.002%
34	6.226	842	843	846	rVB2	655	404	0.00%	0.002%
35	6.348	861	863	865	rBV2	465	485	0.01%	0.002%
36	6.452	879	880	883	rVB	521	442	0.01%	0.002%

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

37	6.769	922	932	946	rBV	311790	750432	8.87%	3.363%
38	6.964	962	964	968	rVB2	614	831	0.01%	0.004%
39	7.001	968	970	971	rBV2	583	421	0.00%	0.002%
40	7.129	981	991	1013	rBV	713787	1577835	18.64%	7.071%
41	7.311	1013	1021	1035	rVB	264679	582027	6.88%	2.608%
42	7.482	1047	1049	1052	rVB3	791	815	0.01%	0.004%
43	7.622	1071	1072	1075	rBV2	423	445	0.01%	0.002%
44	7.671	1078	1080	1084	rVV3	878	1029	0.01%	0.005%
45	7.836	1103	1107	1110	rVV2	553	645	0.01%	0.003%
46	7.939	1119	1124	1127	rBV5	1210	1983	0.02%	0.009%
47	8.086	1144	1148	1149	rBV2	406	403	0.00%	0.002%
48	8.330	1182	1188	1199	rVV	177388	290067	3.43%	1.300%
49	8.549	1223	1224	1226	rVB2	464	307	0.00%	0.001%
50	8.586	1229	1230	1233	rBV2	378	451	0.01%	0.002%
51	8.653	1234	1241	1256	rVV	665537	1056916	12.49%	4.737%
52	8.787	1261	1263	1265	rBV2	618	497	0.01%	0.002%
53	8.860	1272	1275	1276	rVB	699	597	0.01%	0.003%
54	8.872	1276	1277	1278	rBV	444	315	0.00%	0.001%
55	8.951	1285	1290	1303	rBV	126021	191506	2.26%	0.858%
56	9.153	1320	1323	1331	rVB6	2040	4108	0.05%	0.018%
57	9.281	1337	1344	1356	rBV	5607632	8463037	100.00%	37.929%
58	9.390	1356	1362	1373	rVB	444631	649508	7.67%	2.911%
59	9.738	1417	1419	1421	rVB2	1249	960	0.01%	0.004%
60	9.781	1424	1426	1429	rBV	526	518	0.01%	0.002%
61	9.927	1448	1450	1451	rVB	485	309	0.00%	0.001%
62	10.055	1466	1471	1485	rVV	667396	956368	11.30%	4.286%
63	10.171	1486	1490	1494	rVB3	1799	2282	0.03%	0.010%
64	10.335	1515	1517	1520	rBV	390	450	0.01%	0.002%
65	10.372	1520	1523	1526	rVV2	1110	1521	0.02%	0.007%
66	10.591	1555	1559	1560	rBV2	510	606	0.01%	0.003%
67	10.610	1560	1562	1563	rVB2	535	331	0.00%	0.001%
68	10.640	1565	1567	1571	rVV2	340	360	0.00%	0.002%
69	10.780	1587	1590	1592	rBV2	436	397	0.00%	0.002%
70	11.055	1633	1635	1637	rBV2	449	422	0.00%	0.002%
71	11.128	1645	1647	1649	rVB2	530	413	0.00%	0.002%
72	11.195	1652	1658	1665	rVV	465546	581145	6.87%	2.605%
73	11.317	1673	1678	1683	rVB3	8986	12382	0.15%	0.055%
74	11.457	1699	1701	1703	rBV2	436	481	0.01%	0.002%
75	11.481	1703	1705	1708	rVB3	498	453	0.01%	0.002%
76	11.512	1708	1710	1712	rBV	423	438	0.01%	0.002%

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77	11.609	1723	1726	1727	rBV	557	569	0.01%	0.003%
78	11.707	1741	1742	1745	rVB2	723	392	0.00%	0.002%
79	11.762	1749	1751	1752	rVV2	613	382	0.00%	0.002%
80	11.792	1752	1756	1760	rVV4	4047	5636	0.07%	0.025%
81	11.884	1769	1771	1776	rVB2	413	482	0.01%	0.002%
82	12.024	1788	1794	1804	rBV	698092	851451	10.06%	3.816%
83	12.176	1815	1819	1821	rBV2	432	574	0.01%	0.003%
84	12.219	1821	1826	1834	rBV2	25104	43411	0.51%	0.195%
85	12.323	1838	1843	1854	rVB	718932	897291	10.60%	4.021%
86	12.463	1864	1866	1868	rBV2	746	425	0.01%	0.002%
87	12.585	1885	1886	1890	rVB3	566	472	0.01%	0.002%
88	12.640	1893	1895	1896	rBV	540	418	0.00%	0.002%
89	12.768	1912	1916	1920	rVB4	3052	4399	0.05%	0.020%
90	13.115	1972	1973	1974	rBV	806	489	0.01%	0.002%
91	13.280	1999	2000	2003	rBV2	722	455	0.01%	0.002%
92	13.512	2036	2038	2041	rVV2	416	319	0.00%	0.001%
93	13.597	2050	2052	2055	rVB2	705	661	0.01%	0.003%
94	14.133	2134	2140	2143	rBV3	3217	4854	0.06%	0.022%
95	15.078	2293	2295	2299	rBV3	626	943	0.01%	0.004%
96	15.773	2407	2409	2412	rVB2	1071	948	0.01%	0.004%
97	15.871	2423	2425	2426	rBV2	734	429	0.01%	0.002%
98	16.212	2479	2481	2485	rBV2	828	626	0.01%	0.003%
99	16.401	2510	2512	2513	rVB2	771	319	0.00%	0.001%
100	16.474	2522	2524	2526	rVB2	1090	687	0.01%	0.003%

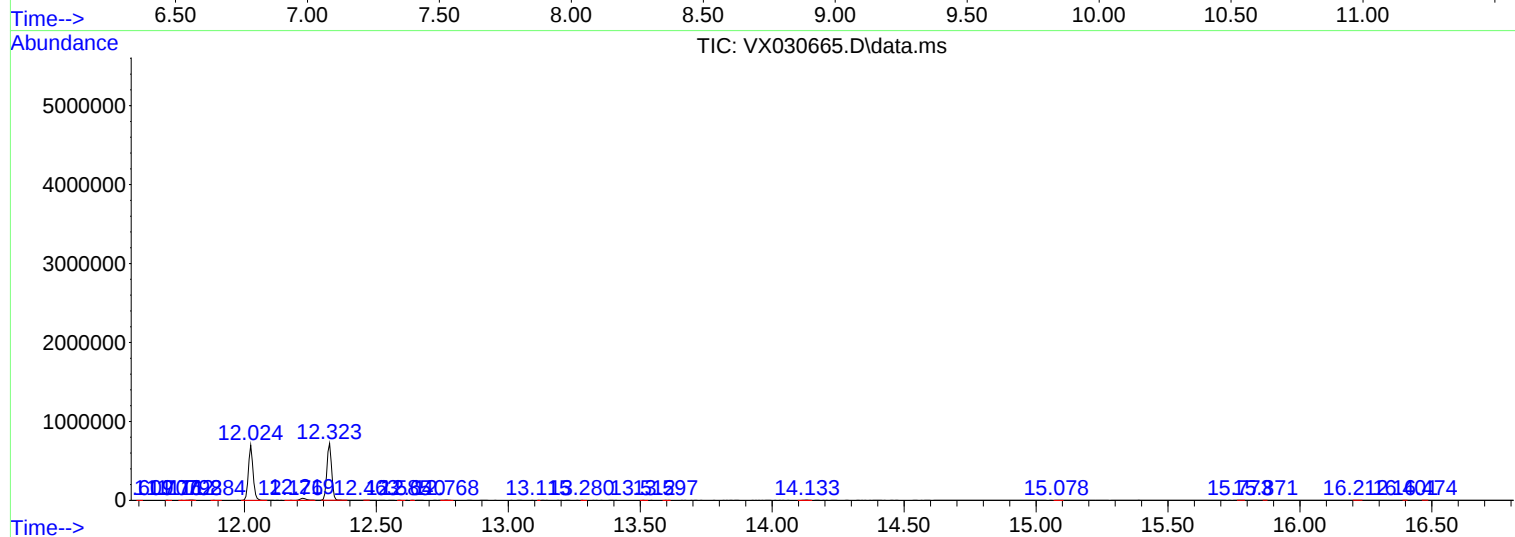
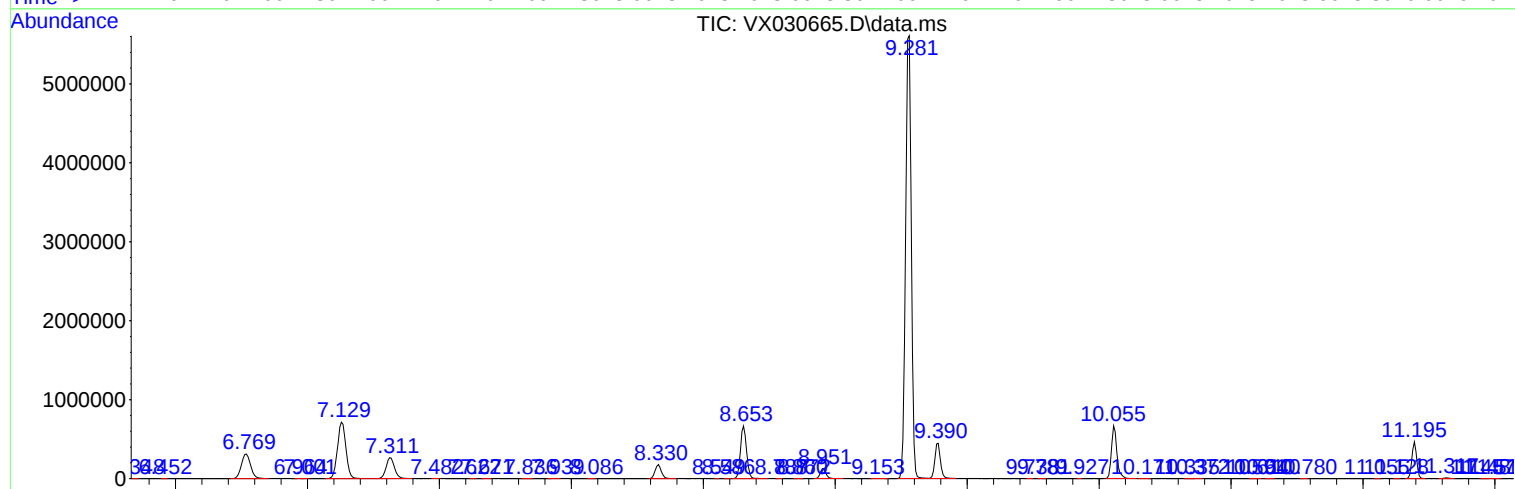
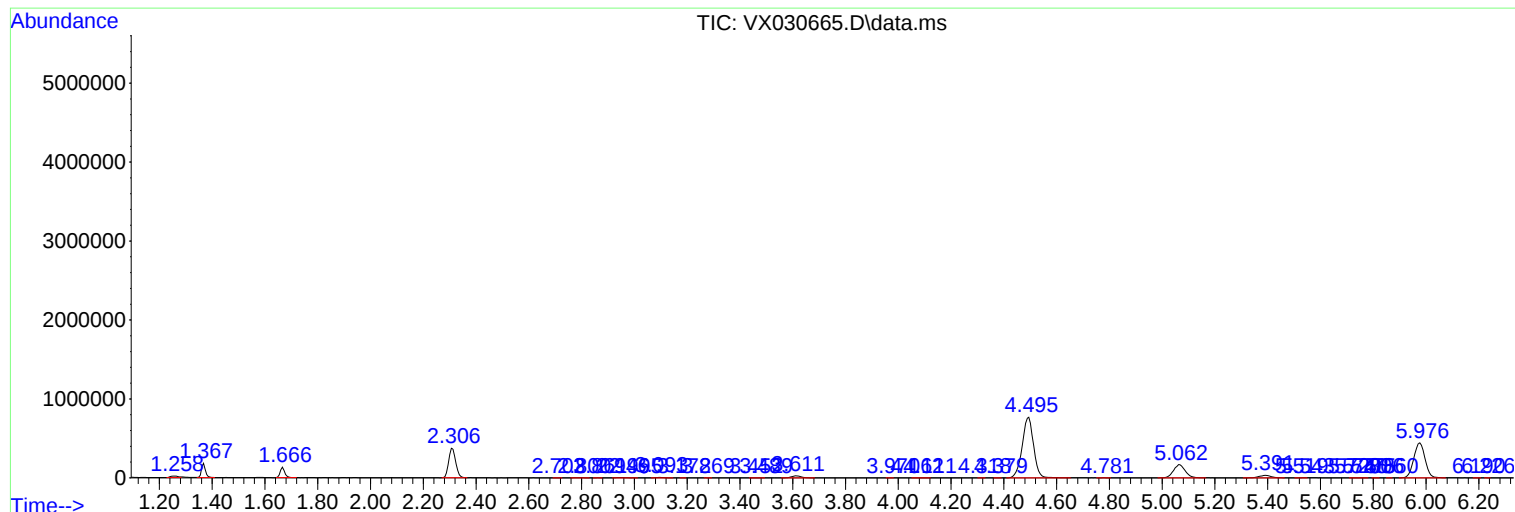
Sum of corrected areas: 22313074

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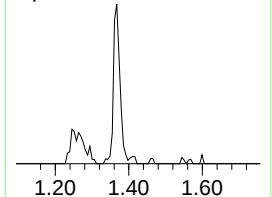
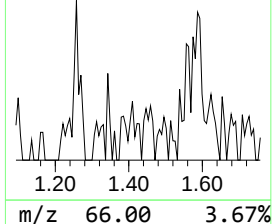
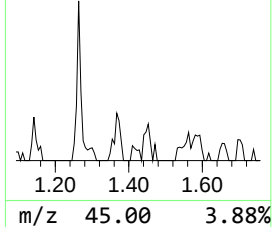
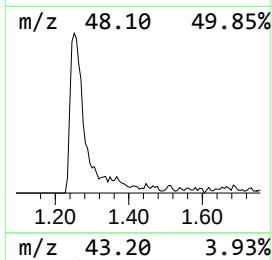
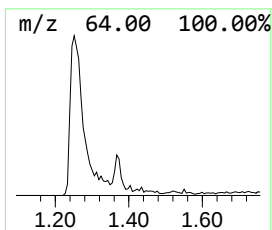
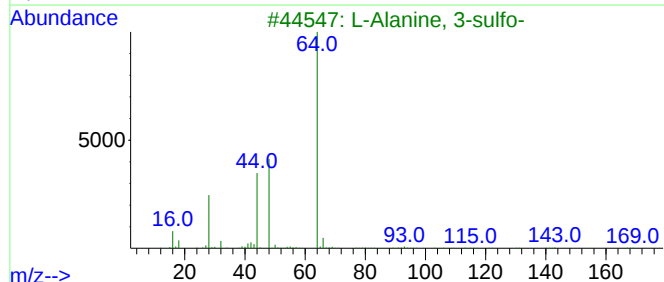
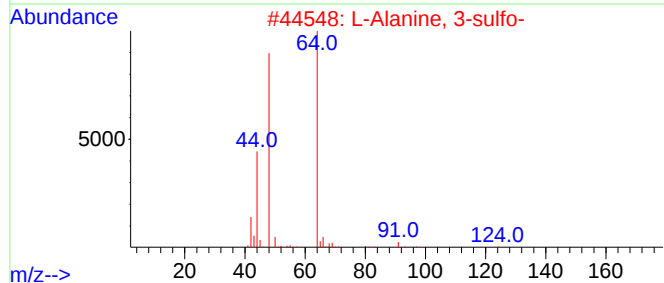
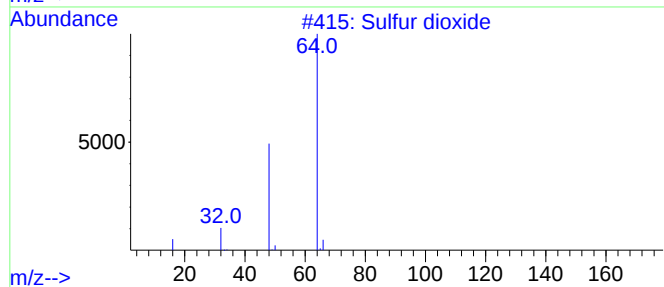
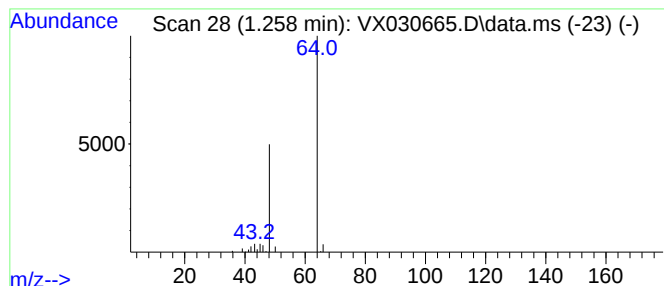
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	2.54 ug/L	38158	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	9
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5



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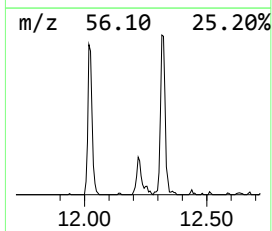
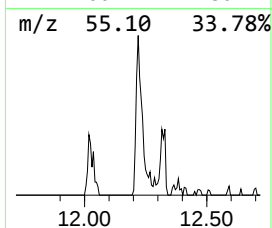
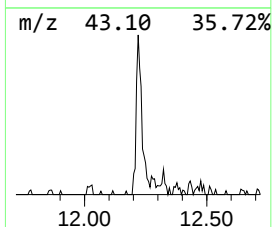
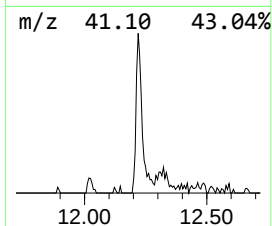
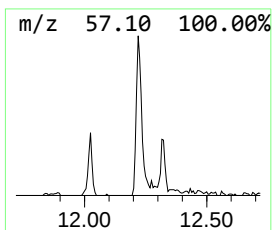
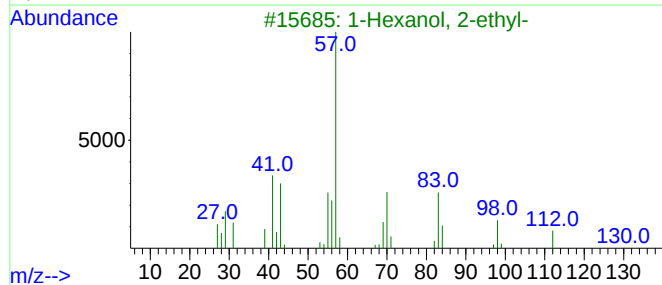
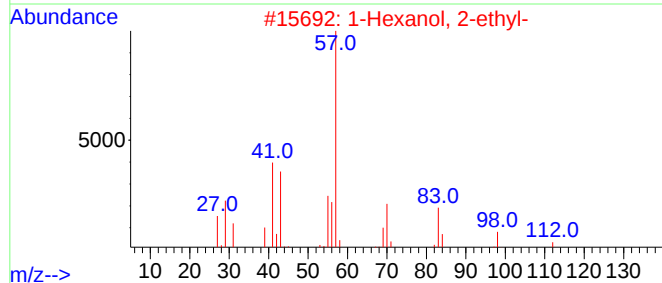
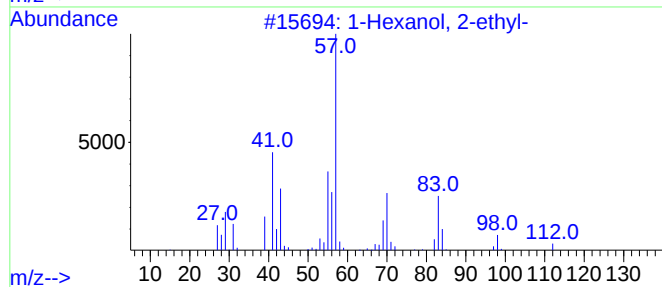
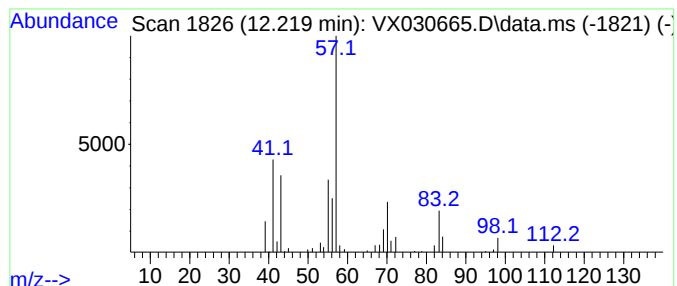
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	2.55 ug/L	43411	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	72
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.258	2.5	ug/L	38158	1	6.769	750432	50.0
1-Hexanol, 2-et...	12.219	2.5	ug/L	43411	3	12.024	851451	50.0