

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042576.D
 Acq On : 25 Jul 2024 18:54
 Operator : JC/MD
 Sample : P3334-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20H1

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042576.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	18	rVB	6450	8700	2.11%	0.270%
2	1.239	22	25	36	rBV	30086	38979	9.47%	1.209%
3	1.368	43	46	57	rVB	31436	40579	9.86%	1.259%
4	1.453	57	60	65	rBV	3275	3958	0.96%	0.123%
5	1.648	89	92	101	rVB	30676	39609	9.62%	1.229%
6	1.721	101	104	113	rVB7	2695	4747	1.15%	0.147%
7	1.934	137	139	147	rVB3	994	1637	0.40%	0.051%
8	2.209	182	184	186	rBV2	158	157	0.04%	0.005%
9	2.294	192	198	208	rVV	71209	111862	27.17%	3.471%
10	2.392	208	214	226	rVV	8314	16897	4.10%	0.524%
11	2.495	230	231	233	rBV2	203	162	0.04%	0.005%
12	2.569	238	243	250	rBV2	1574	3031	0.74%	0.094%
13	2.709	263	266	272	rVV3	268	501	0.12%	0.016%
14	2.788	272	279	286	rVV5	1114	2340	0.57%	0.073%
15	2.855	289	290	294	rVB2	204	229	0.06%	0.007%
16	2.947	297	305	320	rVV	9480	23468	5.70%	0.728%
17	3.093	328	329	335	rBV2	157	286	0.07%	0.009%
18	3.264	355	357	359	rBV	140	137	0.03%	0.004%
19	3.300	361	363	365	rBV2	141	150	0.04%	0.005%
20	3.337	366	369	372	rVV2	335	397	0.10%	0.012%
21	3.501	393	396	401	rBV2	168	250	0.06%	0.008%
22	3.593	409	411	412	rBV	158	165	0.04%	0.005%
23	3.861	454	455	457	rBV	224	175	0.04%	0.005%
24	3.885	457	459	460	rVV	177	162	0.04%	0.005%
25	4.068	486	489	490	rBV2	146	180	0.04%	0.006%
26	4.276	520	523	524	rBV	220	185	0.04%	0.006%
27	4.465	545	554	571	rBV	40878	131873	32.03%	4.092%
28	4.745	598	600	603	rVB2	142	155	0.04%	0.005%
29	4.964	634	636	639	rVB2	120	150	0.04%	0.005%
30	5.056	639	651	669	rBV	55981	169362	41.14%	5.255%
31	5.190	671	673	676	rVV3	194	214	0.05%	0.007%
32	5.373	702	703	704	rBV3	250	167	0.04%	0.005%
33	5.416	709	710	711	rVV	266	142	0.03%	0.004%
34	5.464	714	718	721	rVB	371	493	0.12%	0.015%
35	5.641	742	747	748	rBV2	165	206	0.05%	0.006%
36	5.763	765	767	770	rVB	174	197	0.05%	0.006%

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37	5.794	770	772	774	rBV2	138	162	0.04%	0.005%
38	5.964	789	800	821	rBV2	139174	411722	100.00%	12.775%
39	6.361	862	865	866	rVB2	172	137	0.03%	0.004%
40	6.373	866	867	869	rBV	233	150	0.04%	0.005%
41	6.415	871	874	876	rBV2	145	163	0.04%	0.005%
42	6.696	917	920	922	rBV	165	196	0.05%	0.006%
43	6.763	922	931	950	rVV	115526	279781	67.95%	8.681%
44	7.123	983	990	1011	rBV	101397	230257	55.93%	7.144%
45	7.305	1013	1020	1036	rBV	82694	187069	45.44%	5.804%
46	7.781	1096	1098	1103	rVB2	135	215	0.05%	0.007%
47	7.964	1123	1128	1134	rVV2	413	917	0.22%	0.028%
48	8.013	1134	1136	1137	rVB	222	138	0.03%	0.004%
49	8.043	1137	1141	1143	rBV2	194	244	0.06%	0.008%
50	8.208	1166	1168	1172	rBV2	131	166	0.04%	0.005%
51	8.324	1180	1187	1199	rBV	35831	62662	15.22%	1.944%
52	8.506	1215	1217	1218	rBV	194	193	0.05%	0.006%
53	8.586	1228	1230	1234	rBV3	164	184	0.04%	0.006%
54	8.647	1234	1240	1249	rVV	172943	272734	66.24%	8.462%
55	8.726	1250	1253	1263	rVB	2279	4078	0.99%	0.127%
56	8.952	1285	1290	1303	rVV	25435	39388	9.57%	1.222%
57	9.275	1338	1343	1348	rVB3	1983	3008	0.73%	0.093%
58	9.384	1356	1361	1377	rBV	141758	220395	53.53%	6.838%
59	9.701	1410	1413	1416	rVB3	438	525	0.13%	0.016%
60	10.055	1465	1471	1481	rBV	207105	278239	67.58%	8.633%
61	10.165	1487	1489	1492	rVB3	269	216	0.05%	0.007%
62	10.201	1492	1495	1501	rVB2	561	770	0.19%	0.024%
63	10.311	1509	1513	1518	rVB2	660	1108	0.27%	0.034%
64	10.524	1546	1548	1551	rVB	151	153	0.04%	0.005%
65	10.573	1553	1556	1557	rBV2	138	144	0.03%	0.004%
66	10.646	1565	1568	1573	rVB2	454	526	0.13%	0.016%
67	10.787	1589	1591	1593	rBV	245	263	0.06%	0.008%
68	10.805	1593	1594	1596	rVV	259	160	0.04%	0.005%
69	10.829	1596	1598	1601	rVV2	157	145	0.04%	0.004%
70	10.866	1601	1604	1607	rVB2	148	183	0.04%	0.006%
71	10.976	1621	1622	1626	rVB	167	159	0.04%	0.005%
72	11.043	1630	1633	1634	rBV2	146	181	0.04%	0.006%
73	11.189	1652	1657	1669	rVV	168978	228097	55.40%	7.077%
74	11.317	1673	1678	1682	rVV3	274	547	0.13%	0.017%
75	11.451	1698	1700	1704	rBV4	303	404	0.10%	0.013%
76	11.756	1749	1750	1755	rVB3	412	386	0.09%	0.012%

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77	12.024	1789	1794	1805	rBV	143385	183873	44.66%	5.705%
78	12.170	1817	1818	1822	rBV2	214	225	0.05%	0.007%
79	12.219	1822	1826	1837	rVV	8468	12006	2.92%	0.373%
80	12.317	1837	1842	1852	rBV	145079	194128	47.15%	6.023%
81	12.762	1914	1915	1920	rVB2	164	141	0.03%	0.004%
82	13.792	2081	2084	2087	rVV2	255	298	0.07%	0.009%
83	13.859	2093	2095	2099	rVV3	117	187	0.05%	0.006%
84	13.890	2099	2100	2104	rVB	246	222	0.05%	0.007%
85	13.926	2104	2106	2107	rBV	239	153	0.04%	0.005%
86	14.146	2141	2142	2144	rBV	257	238	0.06%	0.007%
87	14.225	2153	2155	2158	rBV2	206	306	0.07%	0.009%
88	14.438	2186	2190	2191	rBV	136	151	0.04%	0.005%
89	14.451	2191	2192	2195	rVB	187	140	0.03%	0.004%
90	14.493	2196	2199	2202	rBV3	144	206	0.05%	0.006%
91	14.524	2202	2204	2206	rVB3	193	188	0.05%	0.006%
92	14.560	2206	2210	2212	rBV2	212	349	0.08%	0.011%
93	14.621	2216	2220	2222	rBV2	288	393	0.10%	0.012%
94	14.902	2265	2266	2268	rBV	267	154	0.04%	0.005%
95	15.286	2327	2329	2330	rBV	197	159	0.04%	0.005%
96	15.304	2330	2332	2337	rVV2	296	349	0.08%	0.011%
97	15.682	2392	2394	2395	rBV	222	191	0.05%	0.006%
98	16.078	2457	2459	2464	rVB4	306	434	0.11%	0.013%
99	16.121	2464	2466	2469	rVB3	242	251	0.06%	0.008%
100	16.475	2522	2524	2525	rBV2	254	143	0.03%	0.004%

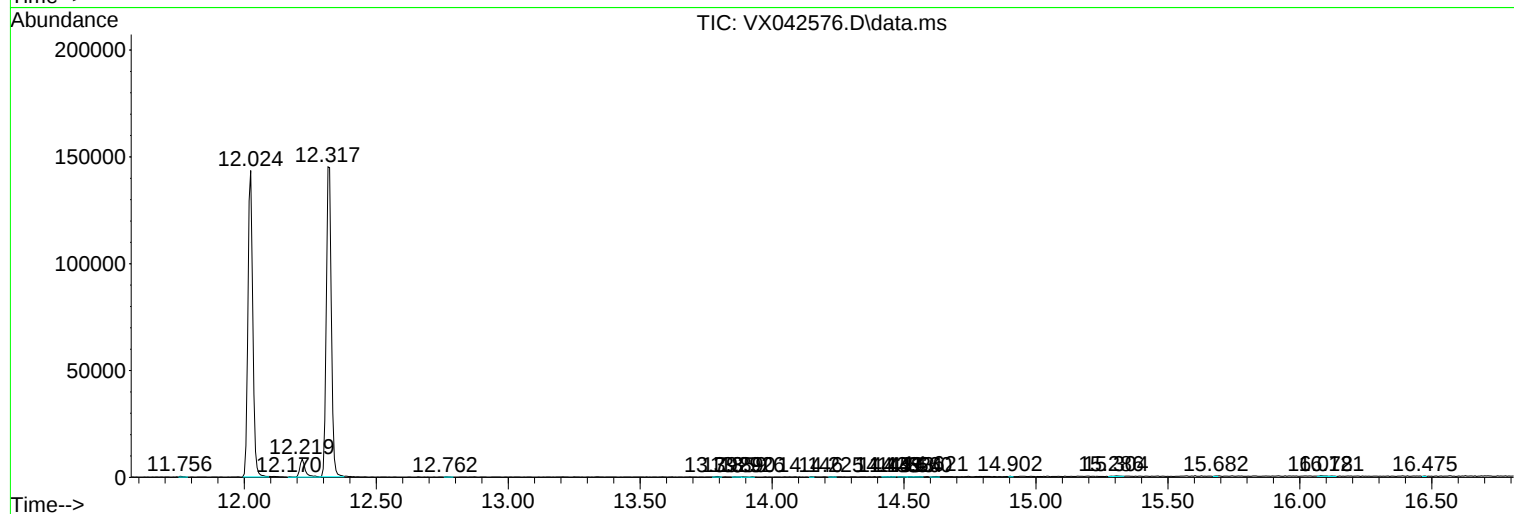
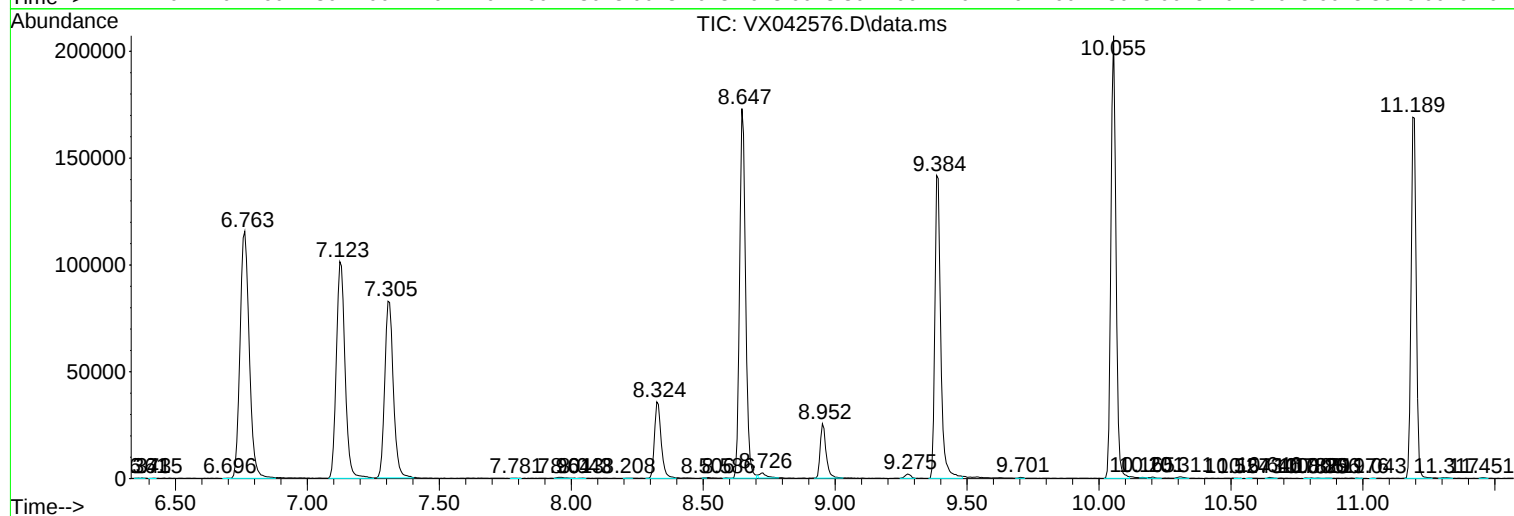
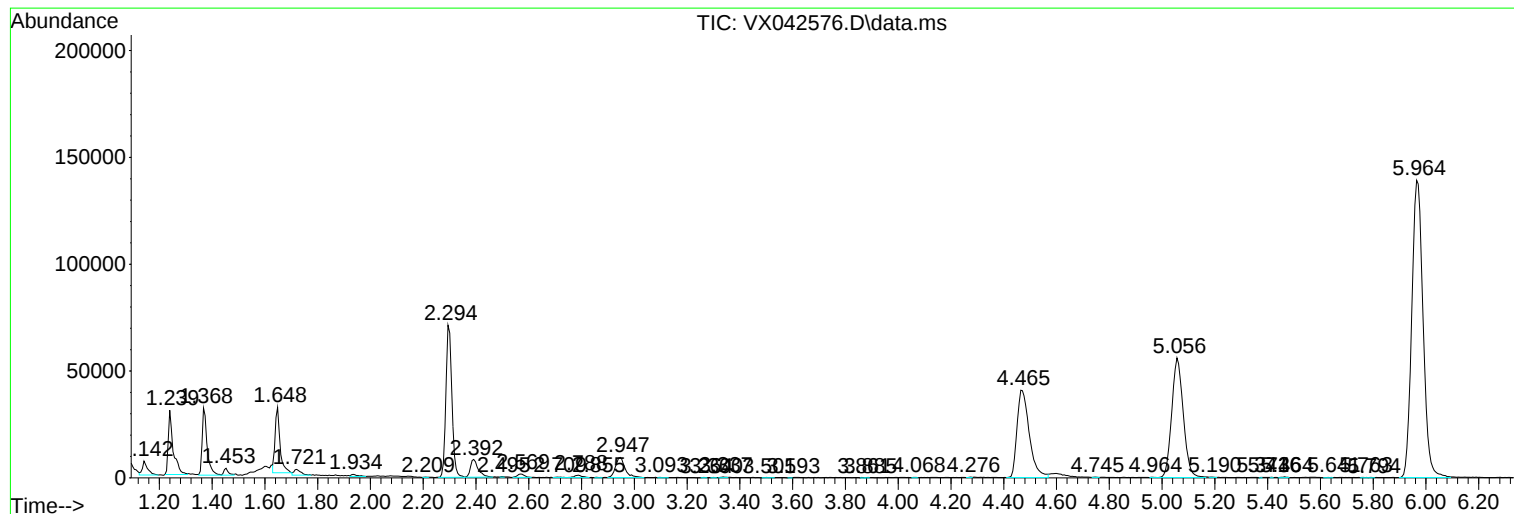
Sum of corrected areas: 3222952

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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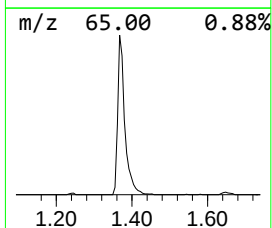
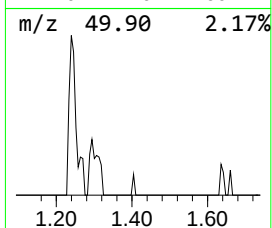
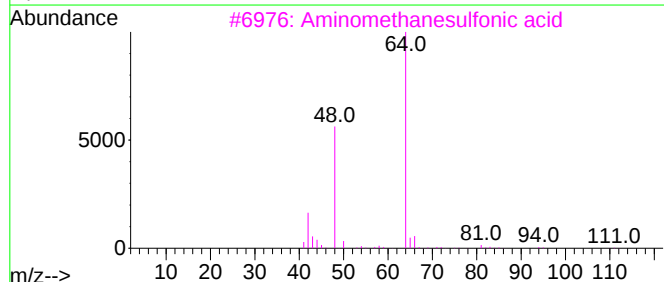
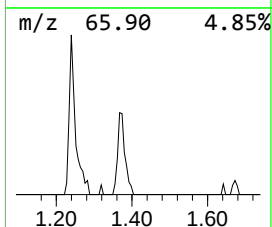
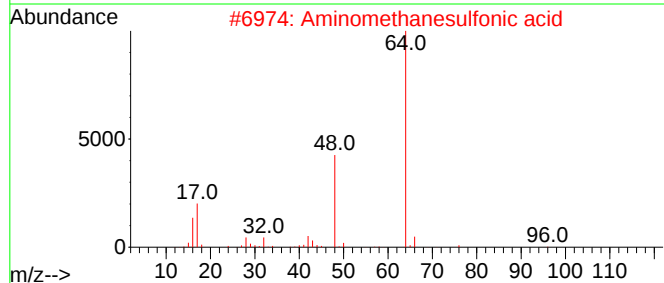
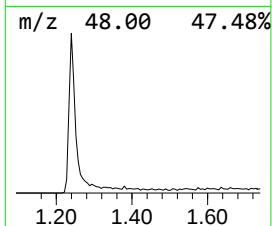
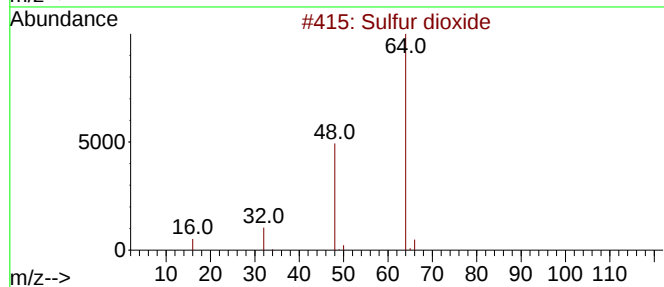
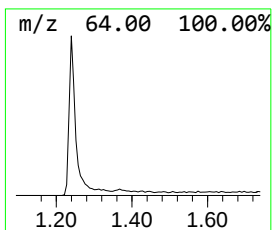
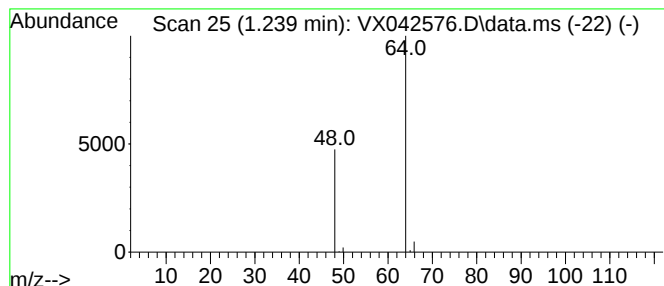
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	6.97 ug/L	38979	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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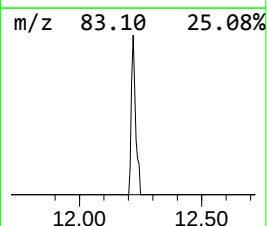
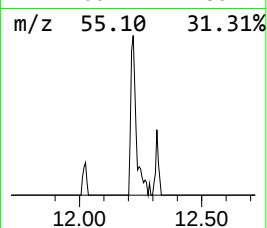
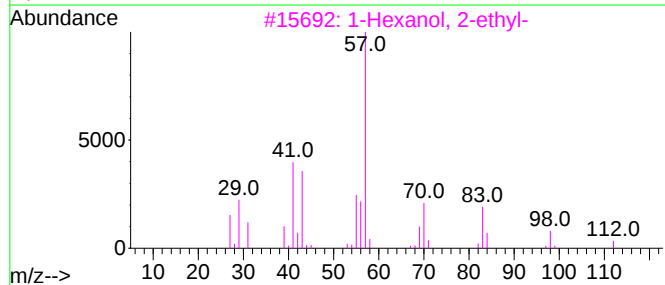
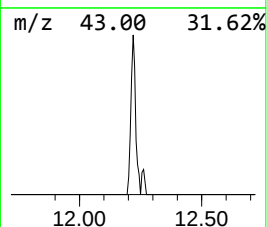
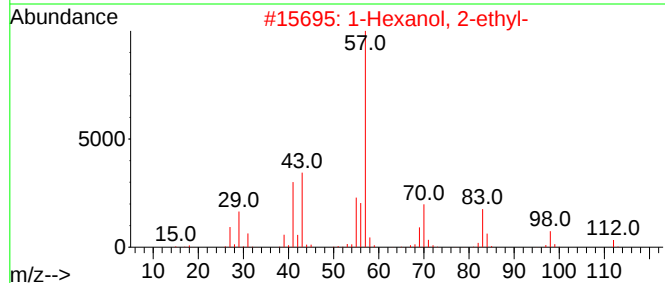
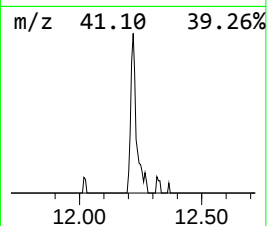
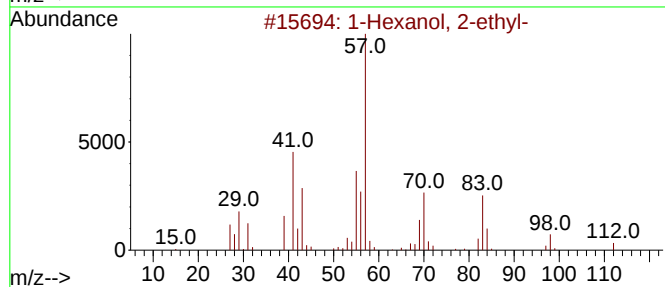
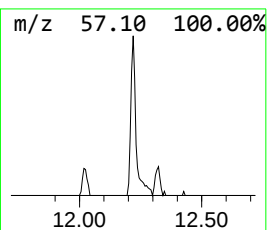
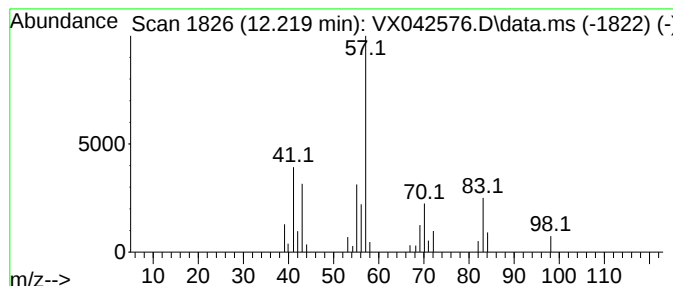
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	3.26 ug/L	12006	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	83
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-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	7.0	ug/L	38979	1	6.763	279781	50.0
1-Hexanol, 2-et...	12.219	3.3	ug/L	12006	3	12.024	183873	50.0