

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061724\
 Data File : VV036102.D
 Acq On : 17 Jun 2024 16:32
 Operator : SY/MD
 Sample : P2909-05
 Misc : 4.89g/10.0mL/MSVOA_V/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A4B84

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_V\Method\SFAMVLM053024SMA.M

Title : VOC Analysis

Signal : TIC: VV036102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.272	67	72	92	rVB	193265	216045	21.66%	3.330%
2	1.526	146	151	167	rVB	157106	187491	18.80%	2.890%
3	2.050	306	314	331	rVB	311777	441487	44.27%	6.805%
4	2.442	425	436	457	rBV	197665	330331	33.12%	5.092%
5	2.680	507	510	514	rBV3	960	813	0.08%	0.013%
6	2.815	547	552	553	rBV	228	188	0.02%	0.003%
7	2.841	558	560	564	rVV2	363	262	0.03%	0.004%
8	2.960	580	597	621	rBV2	31781	68472	6.87%	1.055%
9	3.127	644	649	652	rBV2	380	300	0.03%	0.005%
10	3.185	665	667	671	rBV3	257	151	0.02%	0.002%
11	3.230	679	681	686	rVB	411	314	0.03%	0.005%
12	3.256	686	689	692	rVB2	298	142	0.01%	0.002%
13	3.285	696	698	700	rBV	312	148	0.01%	0.002%
14	3.333	709	713	719	rVB4	472	428	0.04%	0.007%
15	3.359	719	721	722	rBV4	139	77	0.01%	0.001%
16	3.368	722	724	727	rVV2	310	164	0.02%	0.003%
17	3.413	735	738	741	rBV2	229	170	0.02%	0.003%
18	3.446	746	748	752	rVB	259	162	0.02%	0.002%
19	3.526	770	773	774	rBV	207	85	0.01%	0.001%
20	3.568	785	786	788	rBV	126	41	0.00%	0.001%
21	3.616	795	801	804	rBV	277	279	0.03%	0.004%
22	3.671	815	818	819	rBV	249	145	0.01%	0.002%
23	3.703	827	828	829	rBV	226	78	0.01%	0.001%
24	3.745	839	841	844	rBV	192	138	0.01%	0.002%
25	3.761	844	846	849	rVB2	438	225	0.02%	0.003%
26	3.806	858	860	861	rBV	202	72	0.01%	0.001%
27	3.860	864	877	881	rBV3	11518	24248	2.43%	0.374%
28	4.246	983	997	1028	rBV	172957	454242	45.55%	7.001%
29	4.606	1106	1109	1110	rBV3	288	166	0.02%	0.003%
30	4.732	1145	1148	1151	rVB	215	131	0.01%	0.002%
31	4.751	1151	1154	1156	rBV	159	81	0.01%	0.001%
32	4.764	1156	1158	1161	rVB2	234	102	0.01%	0.002%
33	4.812	1170	1173	1175	rBV2	385	241	0.02%	0.004%
34	4.847	1181	1184	1185	rBV	221	118	0.01%	0.002%
35	4.892	1196	1198	1200	rBV2	146	87	0.01%	0.001%
36	4.953	1202	1217	1255	rBV2	383516	997315	100.00%	15.372%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
 Title : VOC Analysis

37	5.307	1326	1327	1328	rBV2	219	74	0.01%	0.001%
38	5.349	1338	1340	1343	rBV2	239	143	0.01%	0.002%
39	5.413	1359	1360	1363	rVB	309	138	0.01%	0.002%
40	5.429	1363	1365	1368	rVB2	469	226	0.02%	0.003%
41	5.532	1385	1397	1424	rBV	387671	826183	82.84%	12.734%
42	5.834	1480	1491	1512	rVB3	8608	21551	2.16%	0.332%
43	5.989	1526	1539	1565	rBV	228104	484344	48.56%	7.465%
44	6.320	1639	1642	1643	rBV2	305	166	0.02%	0.003%
45	6.404	1666	1668	1673	rBV4	229	160	0.02%	0.002%
46	6.439	1677	1679	1683	rBV2	319	178	0.02%	0.003%
47	6.468	1686	1688	1689	rBV2	336	113	0.01%	0.002%
48	6.487	1690	1694	1696	rVB2	375	226	0.02%	0.003%
49	6.519	1701	1704	1708	rBV2	405	348	0.03%	0.005%
50	6.542	1708	1711	1713	rBV2	231	127	0.01%	0.002%
51	6.574	1718	1721	1725	rBV2	297	243	0.02%	0.004%
52	6.606	1729	1731	1734	rVB	192	82	0.01%	0.001%
53	6.642	1741	1742	1745	rBV	209	74	0.01%	0.001%
54	6.677	1749	1753	1756	rBV2	584	434	0.04%	0.007%
55	6.699	1759	1760	1762	rBV	111	44	0.00%	0.001%
56	6.712	1762	1764	1767	rVB2	258	90	0.01%	0.001%
57	6.728	1767	1769	1770	rBB2	72	37	0.00%	0.001%
58	6.767	1777	1781	1784	rBV2	202	188	0.02%	0.003%
59	6.783	1784	1786	1788	rVB	323	131	0.01%	0.002%
60	6.796	1788	1790	1791	rBV	255	101	0.01%	0.002%
61	6.815	1793	1796	1798	rBV2	519	255	0.03%	0.004%
62	6.873	1813	1814	1816	rBV2	112	43	0.00%	0.001%
63	6.918	1817	1828	1853	rBV	60178	128136	12.85%	1.975%
64	7.169	1904	1906	1909	rBV	166	113	0.01%	0.002%
65	7.243	1919	1929	1959	rBV	298849	560065	56.16%	8.633%
66	7.561	2018	2028	2053	rBV	41418	86925	8.72%	1.340%
67	7.876	2116	2126	2135	rBV3	11368	19765	1.98%	0.305%
68	8.002	2161	2165	2169	rBV3	247	213	0.02%	0.003%
69	8.040	2169	2177	2213	rBV2	40075	119796	12.01%	1.846%
70	8.342	2269	2271	2276	rVB3	848	579	0.06%	0.009%
71	8.445	2301	2303	2309	rVB4	724	661	0.07%	0.010%
72	8.529	2326	2329	2331	rVB3	346	203	0.02%	0.003%
73	8.542	2331	2333	2334	rBV3	248	101	0.01%	0.002%
74	8.596	2348	2350	2352	rBV	362	149	0.01%	0.002%
75	8.712	2383	2386	2389	rBV	326	276	0.03%	0.004%
76	8.783	2398	2408	2436	rBV	390747	673572	67.54%	10.382%

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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_V\Method\SFAMVLM053024SMA.M
 Title : VOC Analysis

77	9.082	2497	2501	2503	rBV4	587	435	0.04%	0.007%
78	9.288	2560	2565	2568	rBV2	581	553	0.06%	0.009%
79	9.323	2574	2576	2579	rVB2	443	244	0.02%	0.004%
80	9.413	2600	2604	2606	rBV2	373	310	0.03%	0.005%
81	9.526	2634	2639	2641	rBV	275	275	0.03%	0.004%
82	9.590	2654	2659	2662	rBV4	440	482	0.05%	0.007%
83	9.838	2731	2736	2744	rVB6	3305	4217	0.42%	0.065%
84	10.056	2800	2804	2806	rBV3	1253	1130	0.11%	0.017%
85	10.153	2823	2834	2857	rBV	133596	219271	21.99%	3.380%
86	10.284	2873	2875	2877	rBV2	430	252	0.03%	0.004%
87	10.323	2877	2887	2905	rVB2	43095	71083	7.13%	1.096%
88	10.391	2905	2908	2910	rBV	298	169	0.02%	0.003%
89	10.461	2927	2930	2935	rBV3	570	461	0.05%	0.007%
90	10.564	2960	2962	2967	rVB3	454	276	0.03%	0.004%
91	10.628	2979	2982	2984	rBV2	383	220	0.02%	0.003%
92	11.185	3145	3155	3173	rBV	170876	285114	28.59%	4.395%
93	11.416	3222	3227	3230	rBV5	1015	941	0.09%	0.015%
94	11.490	3240	3250	3263	rBV4	15608	36596	3.67%	0.564%
95	11.561	3264	3272	3295	rVB2	104799	178111	17.86%	2.745%
96	12.191	3463	3468	3482	rVB	11918	18748	1.88%	0.289%
97	12.616	3593	3600	3612	rBV3	8214	13341	1.34%	0.206%
98	12.825	3660	3665	3677	rVB6	2955	4399	0.44%	0.068%

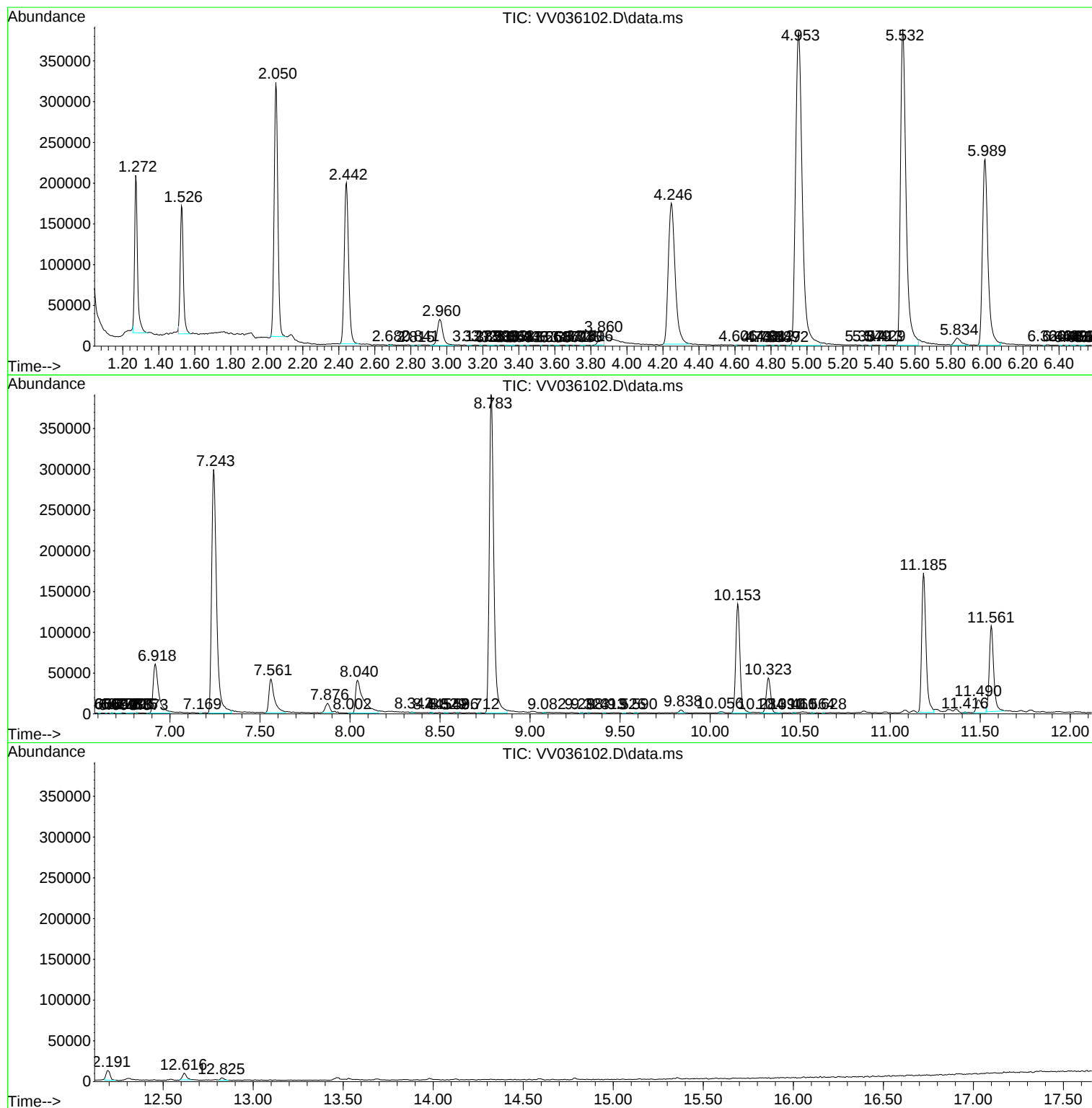
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
Quant Title : VOC Analysis

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



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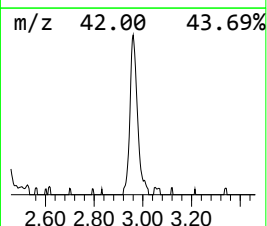
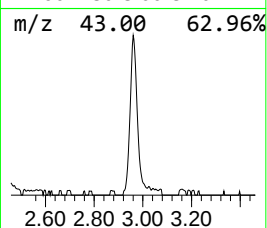
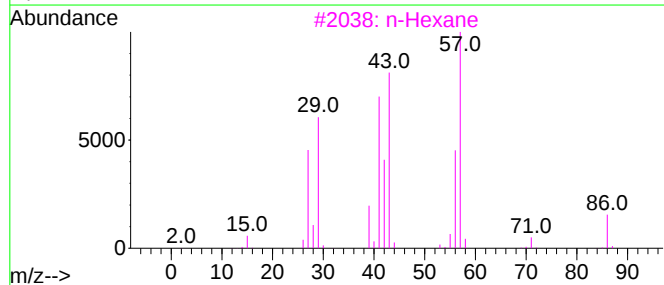
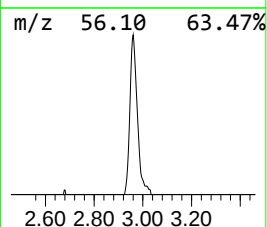
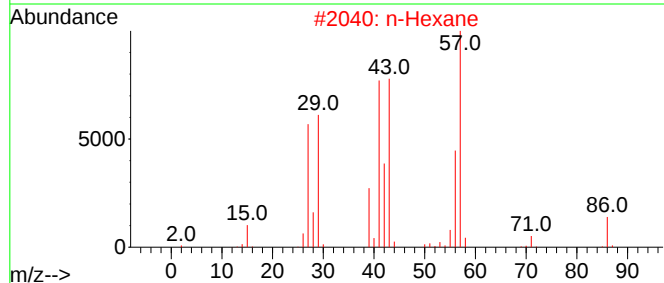
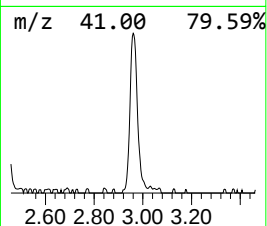
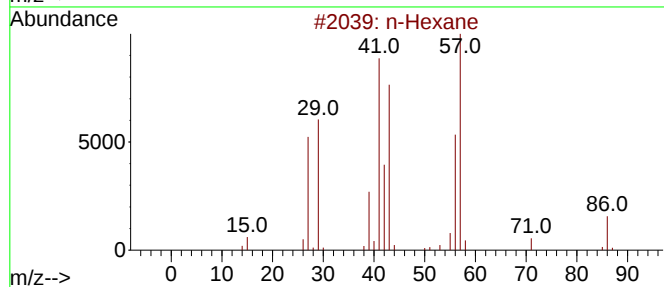
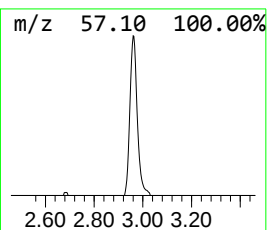
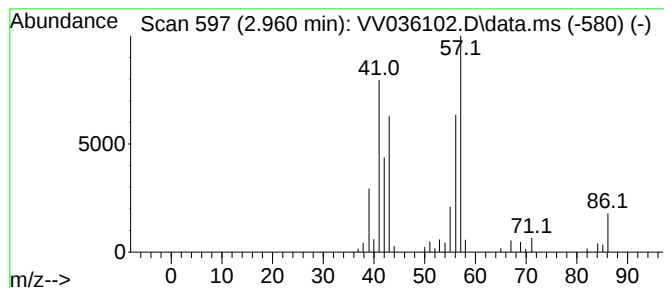
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.960	2.07 ug/L	68472	1,4-Difluorobenzene	5.532

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane		86	C6H14	000110-54-3	80
2	n-Hexane		86	C6H14	000110-54-3	80
3	n-Hexane		86	C6H14	000110-54-3	64
4	Azetidine		57	C3H7N	000503-29-7	52
5	Butane, 2,2,3-trimethyl-		100	C7H16	000464-06-2	47



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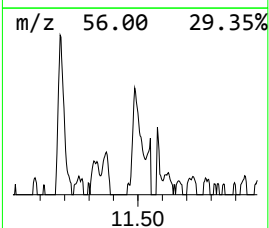
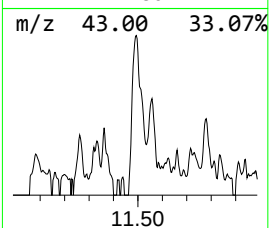
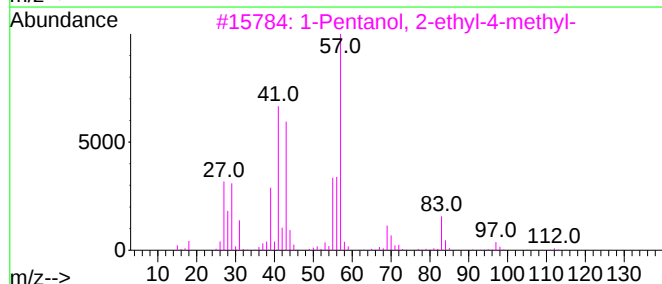
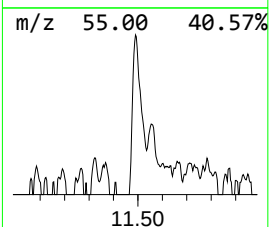
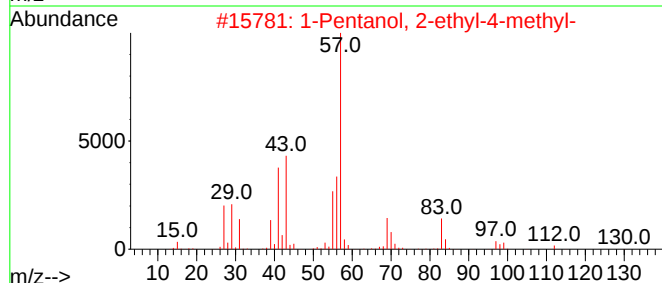
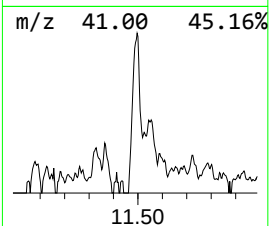
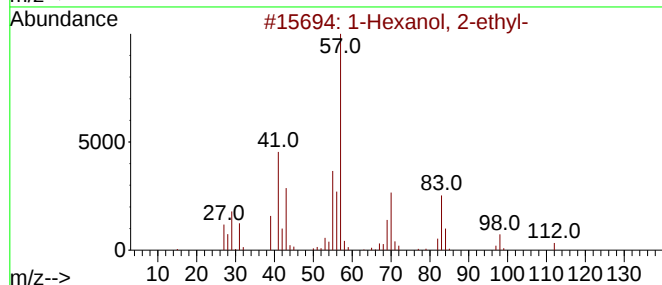
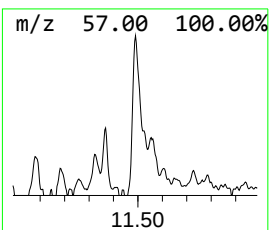
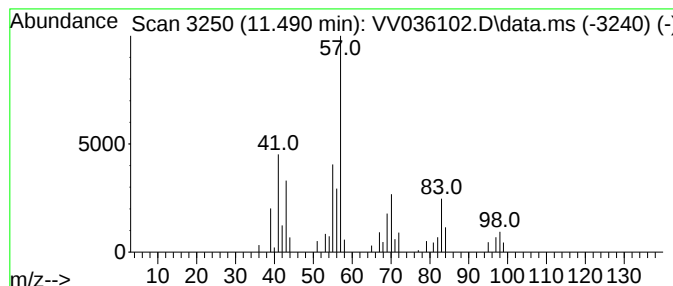
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.490	3.21 ug/L	36596	1,4-Dichlorobenzene-d4	11.185

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.960	2.1	ug/L	68472	1	5.532	826183	25.0
1-Hexanol, 2-et...	11.490	3.2	ug/L	36596	3	11.185	285114	25.0