

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
 Data File : VU049757.D
 Acq On : 18 Jul 2022 13:40
 Operator : SY/MD
 Sample : N3748-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH0E7

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_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049757.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	72	79	95	rBV	66061	75686	10.72%	1.301%
2	1.809	130	146	154	rVB7	9024	17849	2.53%	0.307%
3	1.899	166	174	187	rBV	56731	73679	10.44%	1.267%
4	2.292	289	296	305	rBV6	2567	4359	0.62%	0.075%
5	2.436	338	341	342	rBV2	460	266	0.04%	0.005%
6	2.562	369	380	391	rBV	107380	169718	24.04%	2.918%
7	2.626	391	400	422	rVB	22175	38874	5.51%	0.668%
8	2.758	436	441	443	rBV3	584	464	0.07%	0.008%
9	3.041	524	529	537	rVB4	926	1148	0.16%	0.020%
10	3.182	559	573	590	rVV2	13093	28841	4.09%	0.496%
11	3.459	656	659	662	rBV2	220	188	0.03%	0.003%
12	3.600	700	703	709	rVB2	354	371	0.05%	0.006%
13	3.629	709	712	715	rBV	196	190	0.03%	0.003%
14	3.690	727	731	737	rBV	225	256	0.04%	0.004%
15	4.414	953	956	959	rBV2	244	225	0.03%	0.004%
16	4.620	1007	1020	1039	rBV	110436	269260	38.14%	4.629%
17	4.822	1080	1083	1085	rBV2	309	213	0.03%	0.004%
18	4.954	1121	1124	1129	rVB3	231	169	0.02%	0.003%
19	5.060	1142	1157	1181	rVV	150938	331761	46.99%	5.703%
20	5.144	1181	1183	1187	rVB3	327	194	0.03%	0.003%
21	5.208	1198	1203	1205	rBV	236	231	0.03%	0.004%
22	5.282	1222	1226	1230	rVV3	360	389	0.06%	0.007%
23	5.369	1249	1253	1254	rBV2	547	454	0.06%	0.008%
24	5.575	1309	1317	1319	rBV2	272	329	0.05%	0.006%
25	5.613	1325	1329	1336	rVB2	236	307	0.04%	0.005%
26	5.722	1342	1363	1383	rBV2	256583	705986	100.00%	12.136%
27	5.980	1440	1443	1451	rVB3	214	216	0.03%	0.004%
28	6.021	1451	1456	1460	rVB	177	160	0.02%	0.003%
29	6.111	1481	1484	1488	rBV3	267	216	0.03%	0.004%
30	6.182	1504	1506	1510	rVB	357	272	0.04%	0.005%
31	6.247	1513	1526	1552	rBV	234391	445378	63.09%	7.656%
32	6.407	1573	1576	1578	rBV	220	175	0.02%	0.003%
33	6.529	1605	1614	1627	rVB5	2080	4073	0.58%	0.070%
34	6.690	1650	1664	1684	rBV	181763	350767	49.68%	6.030%
35	6.886	1719	1725	1727	rBV2	292	310	0.04%	0.005%
36	7.134	1799	1802	1807	rVB3	419	323	0.05%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

37	7.185	1810	1818	1826	rVB5	1590	2504	0.35%	0.043%
38	7.221	1826	1829	1832	rVB	217	165	0.02%	0.003%
39	7.240	1832	1835	1839	rBV2	269	283	0.04%	0.005%
40	7.391	1878	1882	1885	rBV2	228	197	0.03%	0.003%
41	7.468	1903	1906	1914	rVB2	243	275	0.04%	0.005%
42	7.565	1921	1936	1954	rBV	90142	156499	22.17%	2.690%
43	7.655	1960	1964	1969	rVB2	311	264	0.04%	0.005%
44	7.690	1972	1975	1976	rBV3	473	252	0.04%	0.004%
45	7.793	2000	2007	2013	rBV5	946	1349	0.19%	0.023%
46	7.896	2026	2039	2056	rBV	274913	472068	66.87%	8.115%
47	8.082	2093	2097	2100	rVV3	266	220	0.03%	0.004%
48	8.099	2100	2102	2108	rVB2	245	192	0.03%	0.003%
49	8.179	2115	2127	2139	rBV	61062	102398	14.50%	1.760%
50	8.275	2154	2157	2159	rBV3	263	190	0.03%	0.003%
51	8.423	2198	2203	2208	rVB2	434	406	0.06%	0.007%
52	8.497	2223	2226	2230	rBV2	392	277	0.04%	0.005%
53	8.632	2256	2268	2307	rBV2	272353	540177	76.51%	9.286%
54	8.790	2307	2317	2329	rVB5	7076	12471	1.77%	0.214%
55	9.295	2470	2474	2480	rVB	301	226	0.03%	0.004%
56	9.417	2498	2512	2537	rBV	325697	532449	75.42%	9.153%
57	9.629	2574	2578	2581	rBV2	201	188	0.03%	0.003%
58	9.777	2616	2624	2631	rBV2	464	879	0.12%	0.015%
59	9.864	2647	2651	2657	rBV2	297	245	0.03%	0.004%
60	9.951	2676	2678	2681	rVB	270	162	0.02%	0.003%
61	9.979	2681	2687	2694	rBV2	358	574	0.08%	0.010%
62	10.024	2697	2701	2703	rVV2	186	183	0.03%	0.003%
63	10.098	2717	2724	2727	rBV2	257	254	0.04%	0.004%
64	10.134	2731	2735	2743	rBV3	406	424	0.06%	0.007%
65	10.237	2759	2767	2777	rBV6	2534	3859	0.55%	0.066%
66	10.336	2794	2798	2799	rBV3	375	220	0.03%	0.004%
67	10.346	2799	2801	2803	rVB	367	177	0.03%	0.003%
68	10.568	2859	2870	2887	rBV2	22746	41129	5.83%	0.707%
69	10.642	2891	2893	2900	rVB2	517	384	0.05%	0.007%
70	10.754	2916	2928	2948	rVV	273399	442110	62.62%	7.600%
71	10.886	2966	2969	2972	rVB	296	163	0.02%	0.003%
72	10.944	2980	2987	2991	rBV2	283	324	0.05%	0.006%
73	10.996	2998	3003	3007	rBV2	219	234	0.03%	0.004%
74	11.047	3016	3019	3023	rVV3	352	277	0.04%	0.005%
75	11.147	3044	3050	3053	rBV	386	411	0.06%	0.007%
76	11.381	3120	3123	3124	rBV2	332	217	0.03%	0.004%

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77	11.420	3130	3135	3137	rBV	256	193	0.03%	0.003%
78	11.442	3137	3142	3146	rVV2	272	320	0.05%	0.006%
79	11.481	3149	3154	3164	rVB5	884	1156	0.16%	0.020%
80	11.690	3213	3219	3228	rBV4	862	1189	0.17%	0.020%
81	11.812	3245	3257	3274	rBV	283862	453172	64.19%	7.790%
82	12.063	3325	3335	3354	rBV3	24978	49016	6.94%	0.843%
83	12.192	3363	3375	3392	rVB	279685	450602	63.83%	7.746%
84	12.372	3427	3431	3434	rBV3	431	387	0.05%	0.007%
85	12.478	3460	3464	3468	rBV2	312	342	0.05%	0.006%
86	12.542	3481	3484	3487	rBV2	284	234	0.03%	0.004%
87	12.590	3492	3499	3503	rBV5	1363	1781	0.25%	0.031%
88	12.780	3550	3558	3566	rBV5	6220	9582	1.36%	0.165%
89	12.828	3566	3573	3583	rVV5	2653	4712	0.67%	0.081%
90	12.867	3583	3585	3587	rVV	356	255	0.04%	0.004%
91	12.889	3587	3592	3601	rVB4	2392	2981	0.42%	0.051%
92	13.063	3643	3646	3650	rVB2	304	214	0.03%	0.004%
93	13.089	3650	3654	3655	rBV	368	257	0.04%	0.004%
94	13.294	3714	3718	3724	rVB3	490	433	0.06%	0.007%
95	13.426	3755	3759	3763	rBV2	290	322	0.05%	0.006%
96	13.487	3773	3778	3781	rBV	393	348	0.05%	0.006%
97	13.703	3843	3845	3851	rVB2	263	181	0.03%	0.003%
98	13.831	3882	3885	3887	rBV	363	239	0.03%	0.004%
99	14.558	4107	4111	4113	rBV	287	248	0.04%	0.004%
100	16.105	4589	4592	4593	rBV2	533	361	0.05%	0.006%

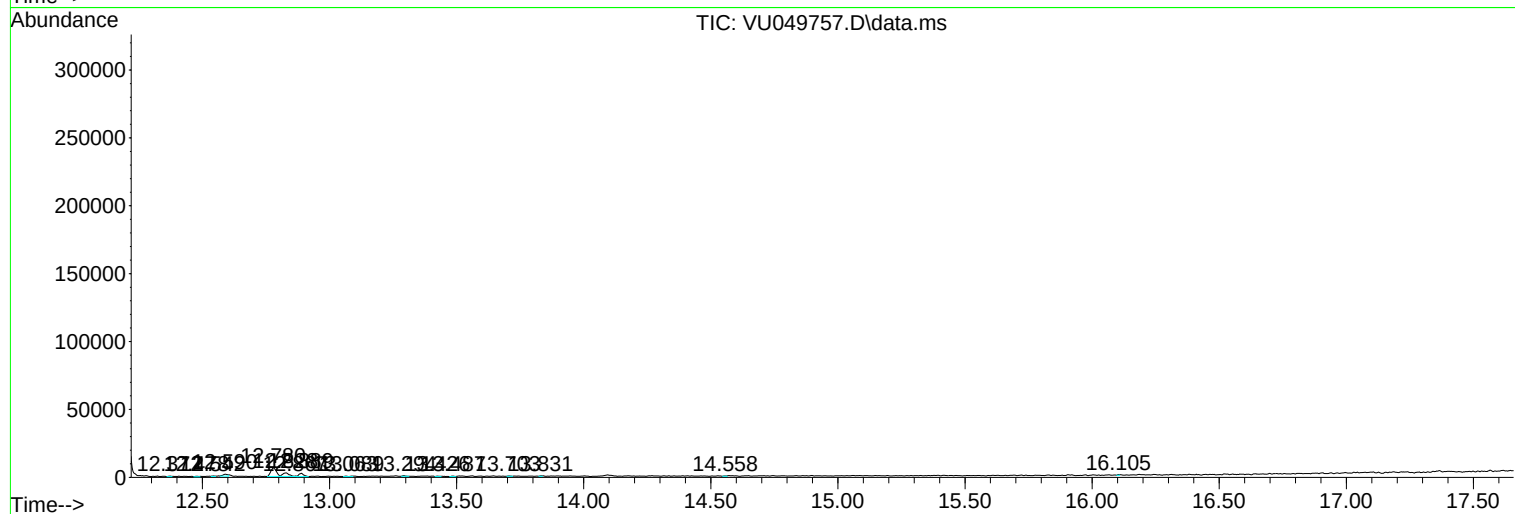
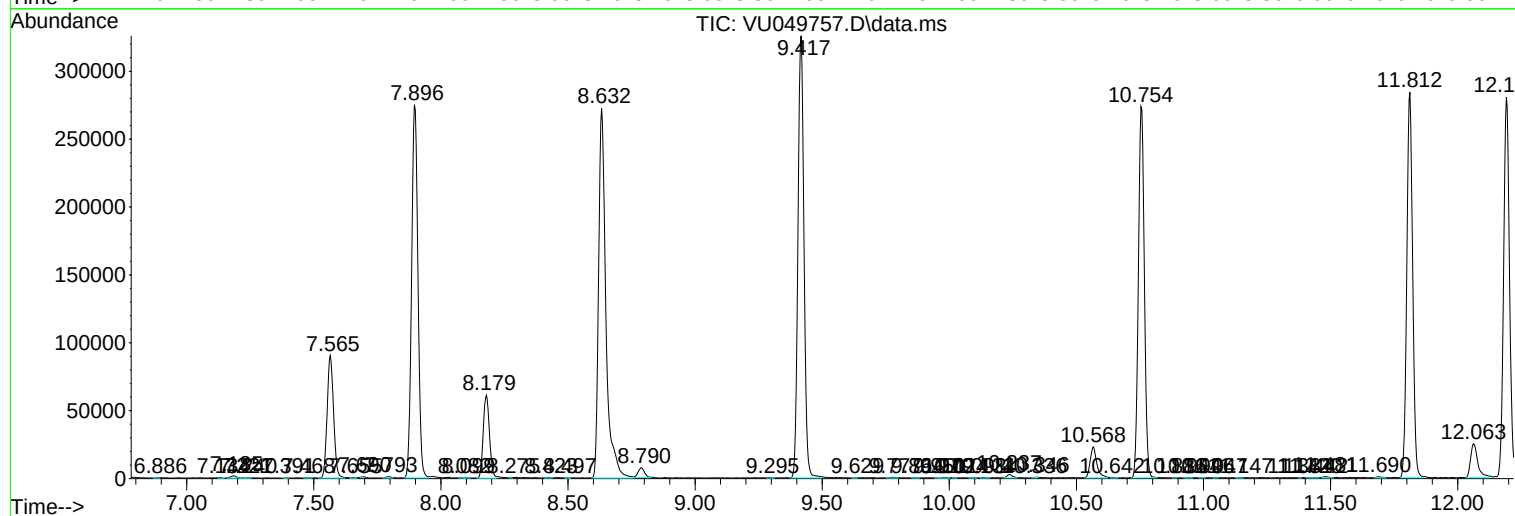
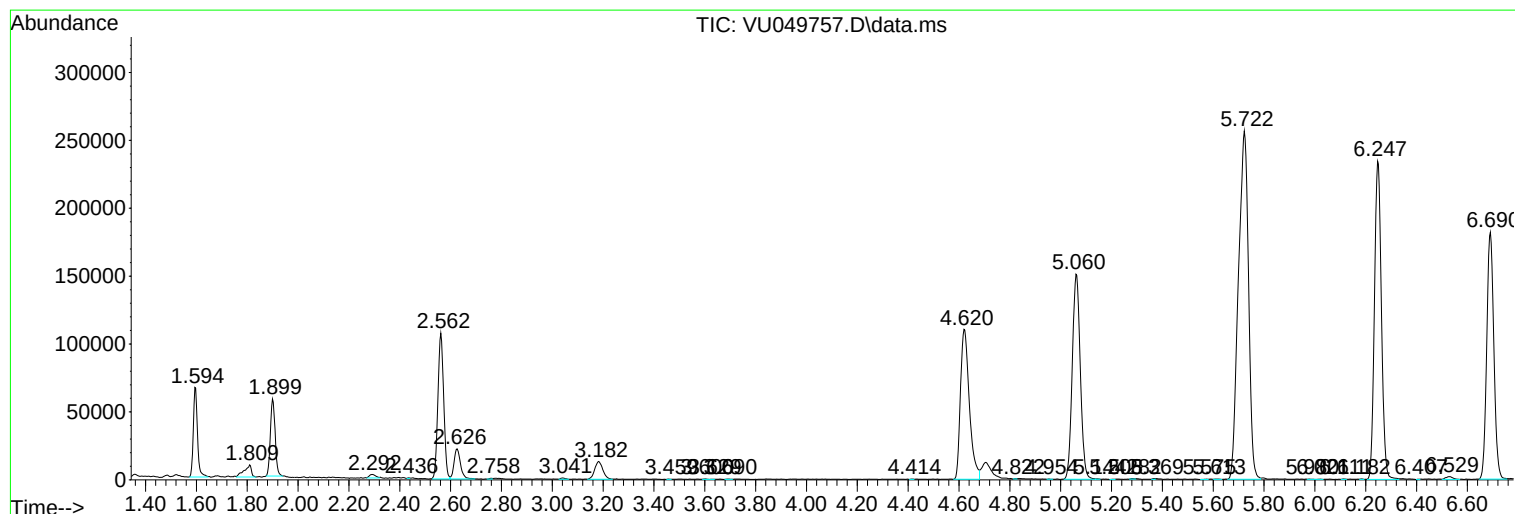
Sum of corrected areas: 5817098

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



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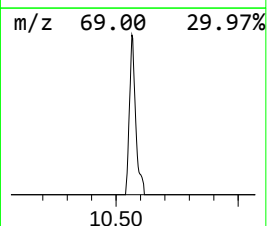
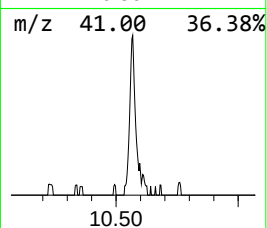
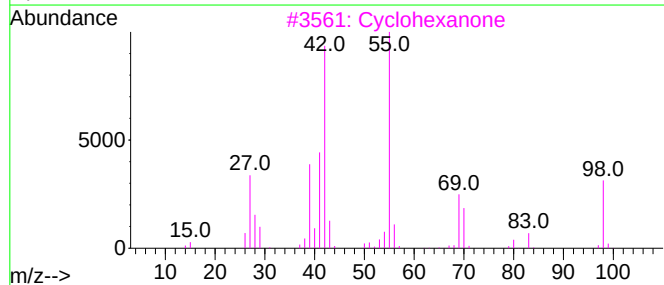
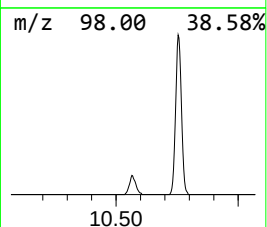
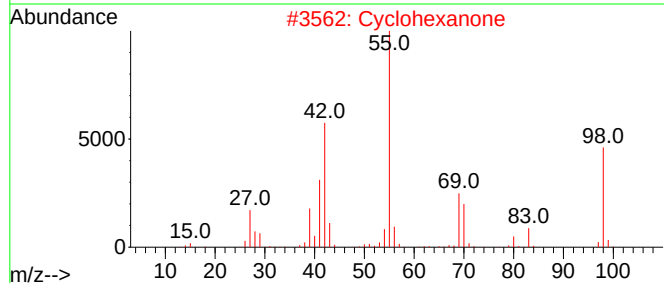
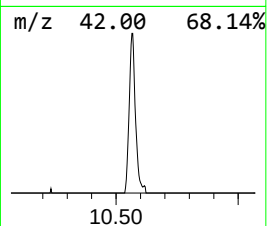
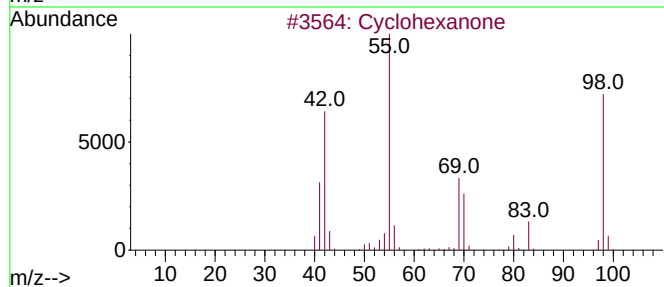
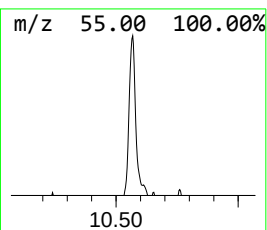
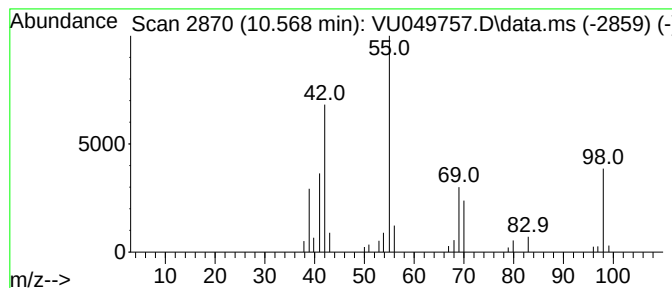
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Cyclohexanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.568	3.86 ug/L	41129	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	91
2			Cyclohexanone	98	C6H10O	000108-94-1	91
3			Cyclohexanone	98	C6H10O	000108-94-1	91
4			Cyclohexanone	98	C6H10O	000108-94-1	74
5			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	72



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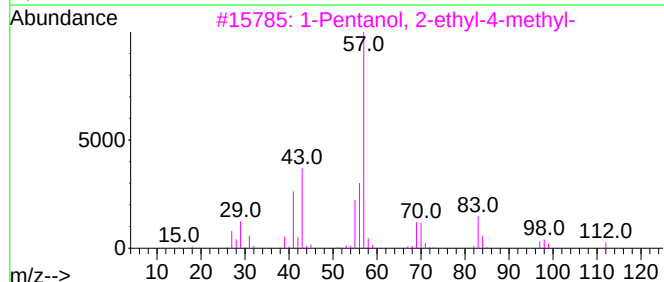
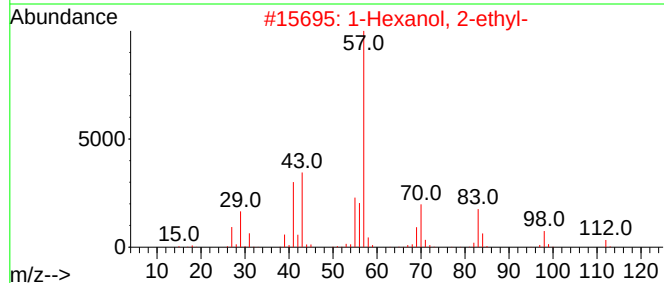
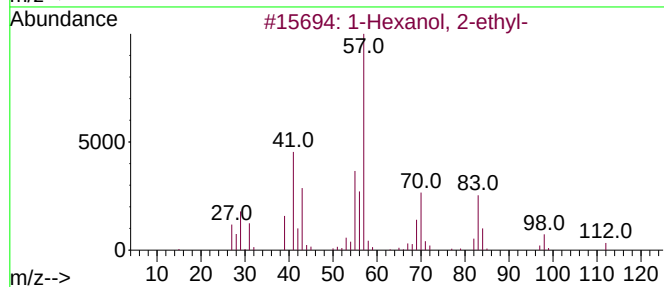
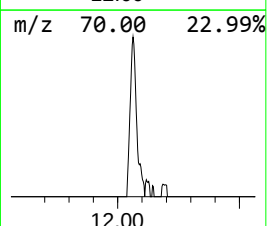
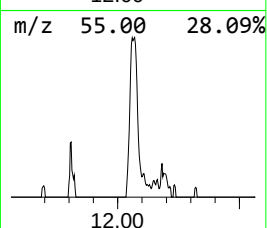
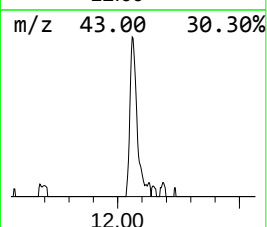
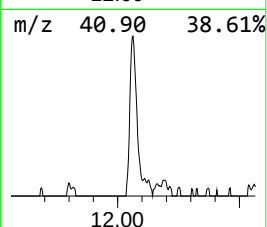
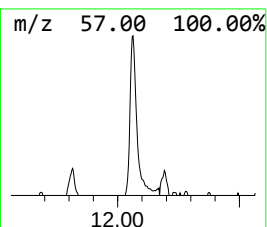
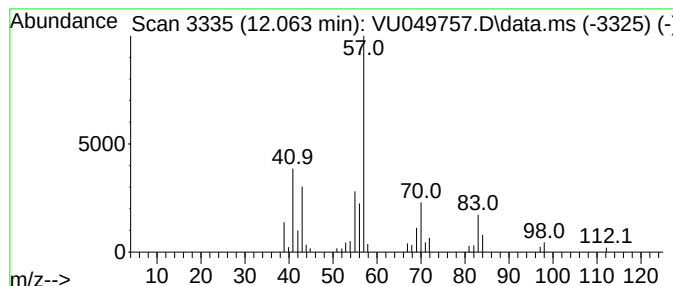
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	5.41 ug/L	49016	1,4-Dichlorobenzene-d4	11.812

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	72
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
5			2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	59



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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
Cyclohexanone	10.568	3.9	ug/L	41129	2	9.417	532449	50.0
1-Hexanol, 2-et...	12.063	5.4	ug/L	49016	3	11.812	453172	50.0