

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071522\
 Data File : VU049735.D
 Acq On : 15 Jul 2022 14:38
 Operator : SY/MD
 Sample : N3748-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH0E6

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: VU049735.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	41	46	50	rVB3	1387	1365	0.18%	0.023%
2	1.597	72	80	97	rVB	76218	85676	11.52%	1.452%
3	1.899	165	174	192	rVB	62170	82800	11.13%	1.403%
4	2.038	215	217	221	rBV3	594	370	0.05%	0.006%
5	2.295	285	297	298	rBV5	2011	2913	0.39%	0.049%
6	2.366	317	319	324	rBV3	678	415	0.06%	0.007%
7	2.562	368	380	391	rBV	118379	188950	25.41%	3.203%
8	2.626	392	400	413	rVB	21223	34923	4.70%	0.592%
9	2.761	439	442	446	rBV3	195	190	0.03%	0.003%
10	2.919	488	491	497	rBV2	191	172	0.02%	0.003%
11	2.951	498	501	504	rBV2	259	222	0.03%	0.004%
12	3.022	520	523	525	rBV	246	205	0.03%	0.003%
13	3.038	525	528	535	rVB3	583	642	0.09%	0.011%
14	3.079	535	541	544	rBV2	242	261	0.04%	0.004%
15	3.121	550	554	557	rBV2	295	261	0.04%	0.004%
16	3.179	564	572	576	rBV2	1501	2299	0.31%	0.039%
17	3.375	630	633	636	rVB2	255	169	0.02%	0.003%
18	3.996	821	826	831	rBV2	207	277	0.04%	0.005%
19	4.620	1005	1020	1038	rBV	100682	241674	32.50%	4.096%
20	4.886	1100	1103	1106	rBV3	421	343	0.05%	0.006%
21	5.060	1142	1157	1175	rVV	152484	335311	45.09%	5.683%
22	5.211	1200	1204	1207	rVB2	278	237	0.03%	0.004%
23	5.295	1219	1230	1241	rVB3	940	1757	0.24%	0.030%
24	5.346	1241	1246	1249	rBV2	294	303	0.04%	0.005%
25	5.365	1249	1252	1253	rBV2	358	177	0.02%	0.003%
26	5.423	1265	1270	1275	rBV	200	197	0.03%	0.003%
27	5.510	1292	1297	1300	rBV2	240	263	0.04%	0.004%
28	5.636	1329	1336	1338	rBV2	220	273	0.04%	0.005%
29	5.722	1342	1363	1392	rVV3	272105	743704	100.00%	12.605%
30	5.886	1410	1414	1416	rBV2	358	271	0.04%	0.005%
31	5.899	1416	1418	1420	rVV2	329	165	0.02%	0.003%
32	5.919	1420	1424	1430	rVB3	297	314	0.04%	0.005%
33	5.960	1434	1437	1440	rBV3	293	248	0.03%	0.004%
34	5.976	1440	1442	1446	rVB	289	211	0.03%	0.004%
35	6.102	1474	1481	1485	rVB2	269	414	0.06%	0.007%
36	6.246	1510	1526	1545	rBV	237449	449174	60.40%	7.613%

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 Title : VOC Analysis

37	6.365	1561	1563	1565	rVB	423	199	0.03%	0.003%
38	6.526	1604	1613	1622	rVB6	1572	2676	0.36%	0.045%
39	6.690	1650	1664	1686	rBV	188752	360422	48.46%	6.109%
40	6.787	1691	1694	1696	rBV2	232	191	0.03%	0.003%
41	6.851	1709	1714	1716	rBV2	241	228	0.03%	0.004%
42	7.179	1811	1816	1820	rBV3	1010	992	0.13%	0.017%
43	7.288	1845	1850	1855	rBV2	221	340	0.05%	0.006%
44	7.365	1870	1874	1879	rVB2	264	229	0.03%	0.004%
45	7.446	1890	1899	1904	rVB2	257	359	0.05%	0.006%
46	7.513	1915	1920	1923	rBV2	186	210	0.03%	0.004%
47	7.565	1923	1936	1953	rBV	91658	158921	21.37%	2.694%
48	7.639	1957	1959	1965	rVB2	450	377	0.05%	0.006%
49	7.690	1969	1975	1976	rBV2	880	699	0.09%	0.012%
50	7.783	1999	2004	2007	rBV2	348	375	0.05%	0.006%
51	7.896	2025	2039	2057	rBV	297633	510859	68.69%	8.659%
52	8.179	2112	2127	2141	rBV	61682	103074	13.86%	1.747%
53	8.317	2164	2170	2174	rBV2	269	347	0.05%	0.006%
54	8.372	2183	2187	2190	rVB2	303	213	0.03%	0.004%
55	8.410	2195	2199	2203	rVB2	264	180	0.02%	0.003%
56	8.459	2210	2214	2216	rBV	302	167	0.02%	0.003%
57	8.478	2216	2220	2224	rVB2	266	227	0.03%	0.004%
58	8.632	2256	2268	2308	rBV2	267067	532409	71.59%	9.024%
59	8.790	2308	2317	2327	rVB7	6789	11801	1.59%	0.200%
60	8.883	2343	2346	2351	rVB	221	190	0.03%	0.003%
61	8.922	2352	2358	2361	rBV2	302	245	0.03%	0.004%
62	8.976	2372	2375	2384	rVV2	428	561	0.08%	0.010%
63	9.121	2417	2420	2426	rBV2	191	204	0.03%	0.003%
64	9.417	2500	2512	2530	rBV	325934	538797	72.45%	9.132%
65	9.725	2605	2608	2616	rVB2	321	362	0.05%	0.006%
66	9.783	2621	2626	2633	rVB2	483	648	0.09%	0.011%
67	9.918	2660	2668	2671	rBV2	218	324	0.04%	0.005%
68	10.079	2713	2718	2723	rVB2	207	263	0.04%	0.004%
69	10.124	2727	2732	2734	rBV3	571	407	0.05%	0.007%
70	10.240	2758	2768	2776	rBV3	2433	3777	0.51%	0.064%
71	10.343	2797	2800	2803	rBV2	809	660	0.09%	0.011%
72	10.455	2831	2835	2837	rBV	242	197	0.03%	0.003%
73	10.568	2860	2870	2891	rVV2	21531	38726	5.21%	0.656%
74	10.754	2916	2928	2947	rVV	270333	431635	58.04%	7.316%
75	11.413	3130	3133	3136	rBV2	216	167	0.02%	0.003%
76	11.475	3147	3152	3154	rBV3	719	662	0.09%	0.011%

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77	11.536	3169	3171	3177	rVB2	188	169	0.02%	0.003%
78	11.674	3210	3214	3216	rBV	273	249	0.03%	0.004%
79	11.693	3217	3220	3227	rVV3	671	684	0.09%	0.012%
80	11.812	3244	3257	3280	rBV	299413	474047	63.74%	8.035%
81	12.063	3325	3335	3356	rBV3	23417	45604	6.13%	0.773%
82	12.192	3364	3375	3392	rVB	297024	475169	63.89%	8.054%
83	12.333	3417	3419	3423	rVB2	316	188	0.03%	0.003%
84	12.593	3494	3500	3510	rVB5	1503	2721	0.37%	0.046%
85	12.645	3510	3516	3523	rBV2	355	638	0.09%	0.011%
86	12.783	3548	3559	3567	rBV4	7163	10694	1.44%	0.181%
87	12.828	3568	3573	3583	rVV3	1973	3038	0.41%	0.051%
88	12.889	3586	3592	3598	rVB6	1869	2295	0.31%	0.039%
89	12.950	3608	3611	3614	rBV2	311	180	0.02%	0.003%
90	13.574	3800	3805	3808	rBV2	413	364	0.05%	0.006%
91	13.738	3854	3856	3863	rVB2	276	174	0.02%	0.003%
92	13.860	3891	3894	3898	rBV2	314	324	0.04%	0.005%
93	14.037	3946	3949	3952	rBV2	273	207	0.03%	0.004%
94	14.085	3957	3964	3966	rBV2	397	518	0.07%	0.009%
95	14.429	4068	4071	4075	rBV	443	393	0.05%	0.007%
96	14.548	4105	4108	4110	rBV	434	305	0.04%	0.005%
97	15.031	4255	4258	4259	rBV	542	339	0.05%	0.006%
98	16.050	4573	4575	4579	rVB2	625	397	0.05%	0.007%
99	16.069	4579	4581	4585	rBV3	494	296	0.04%	0.005%
100	16.098	4588	4590	4597	rVB3	567	529	0.07%	0.009%

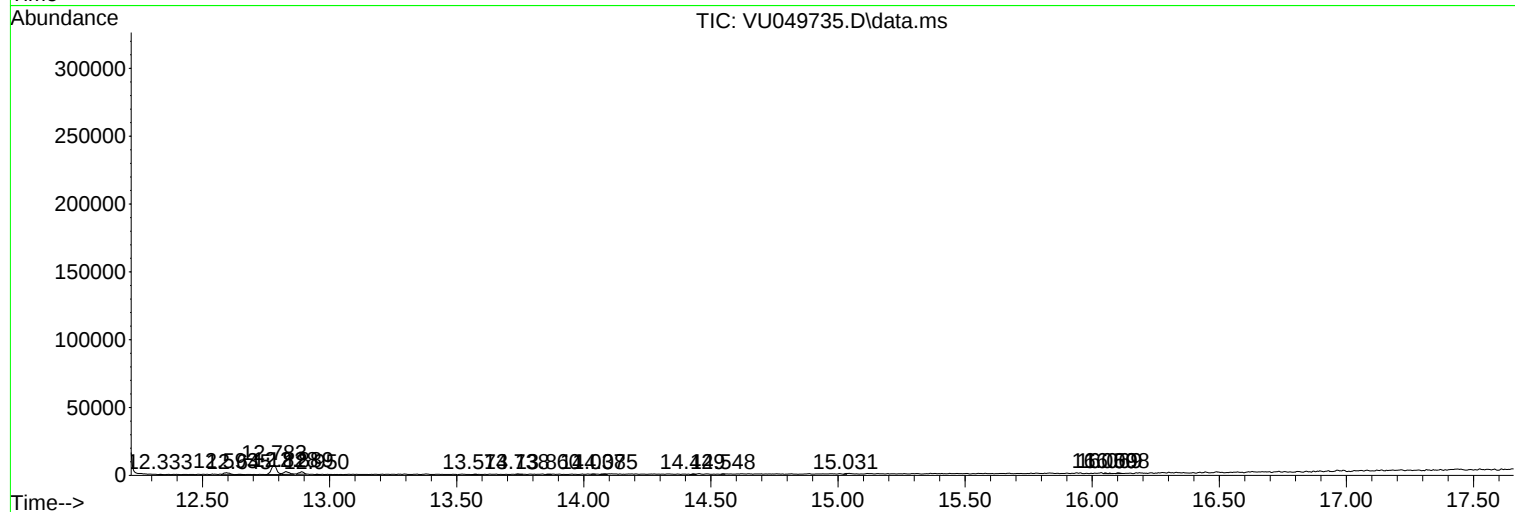
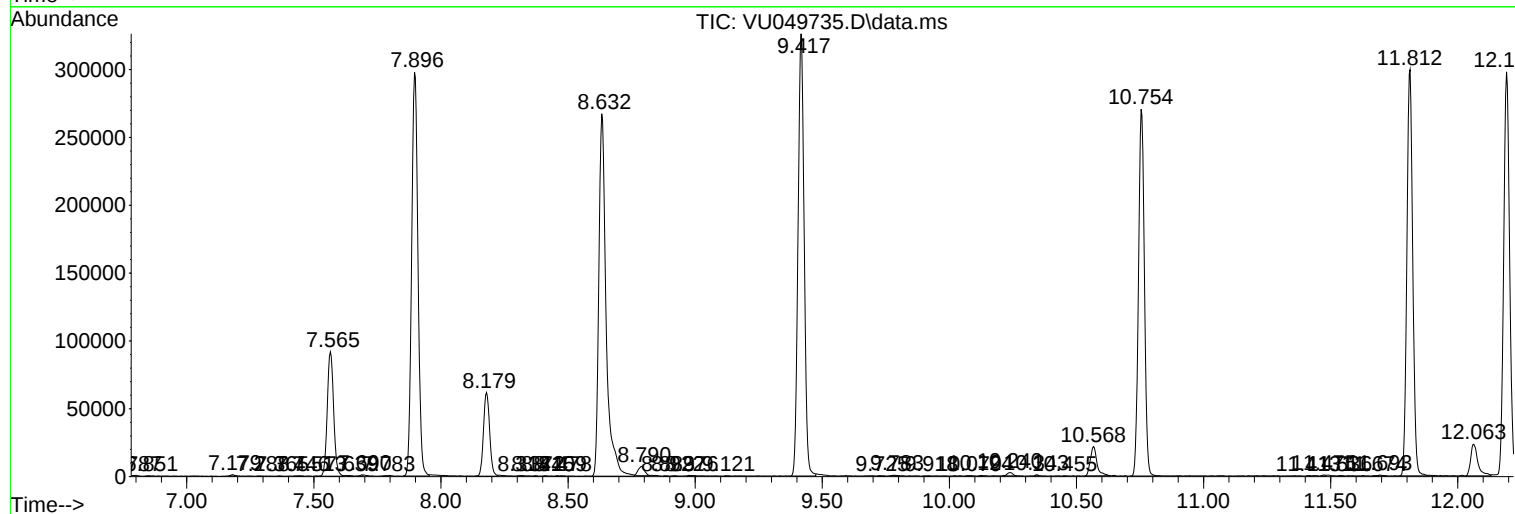
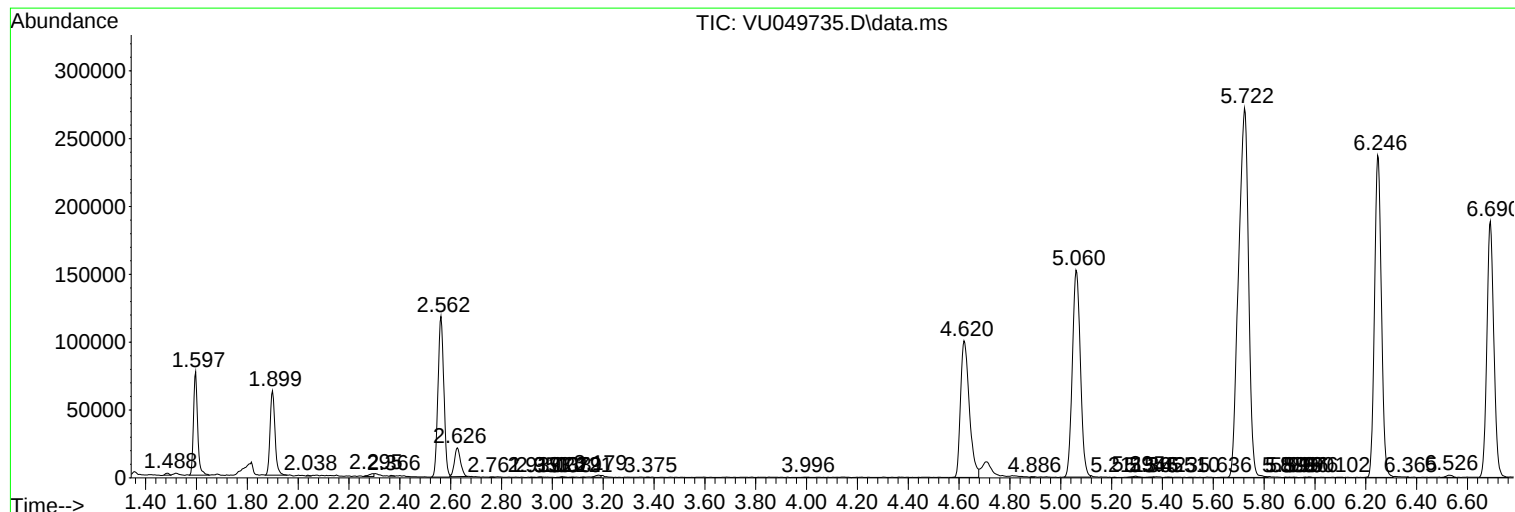
Sum of corrected areas: 5899988

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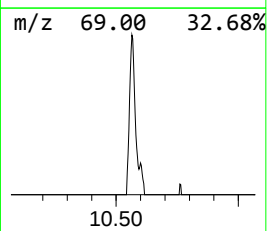
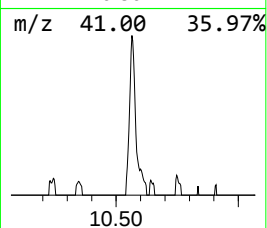
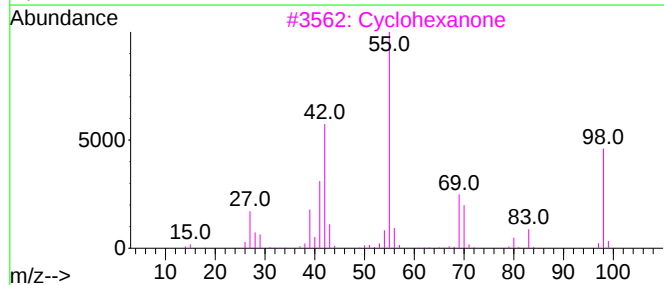
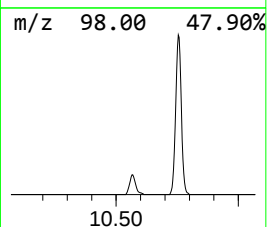
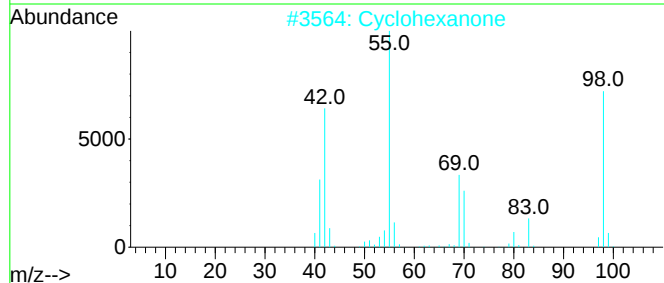
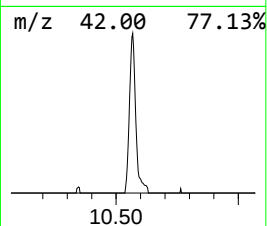
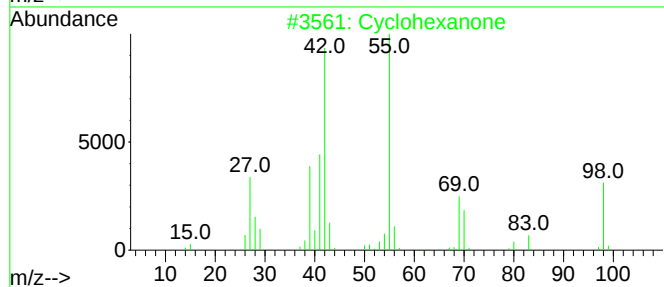
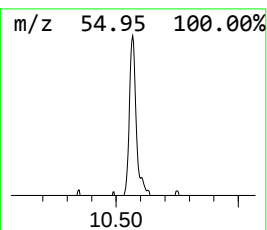
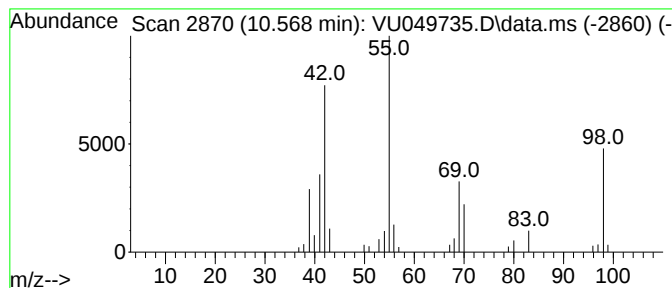
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Cyclohexanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.568	3.59 ug/L	38726	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	94
2			Cyclohexanone	98	C6H10O	000108-94-1	91
3			Cyclohexanone	98	C6H10O	000108-94-1	91
4			Cyclohexanone	98	C6H10O	000108-94-1	91
5			Cyclohexanone	98	C6H10O	000108-94-1	83



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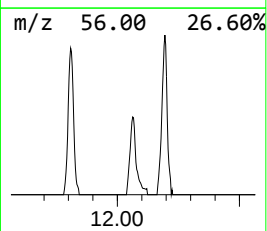
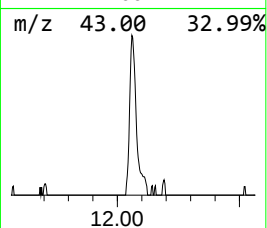
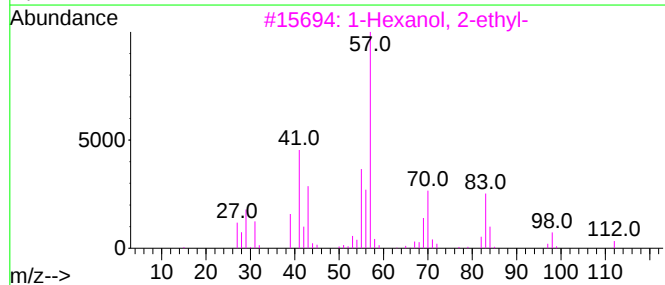
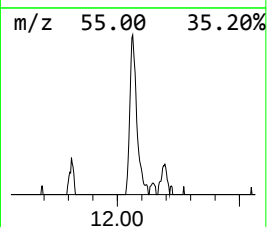
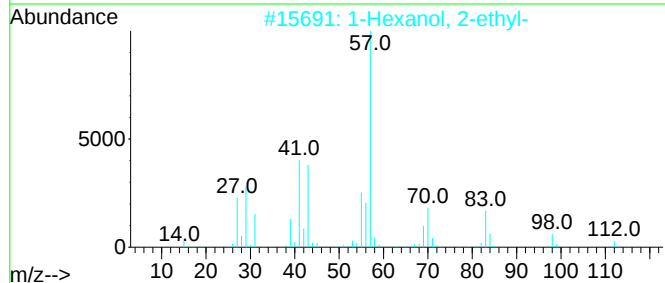
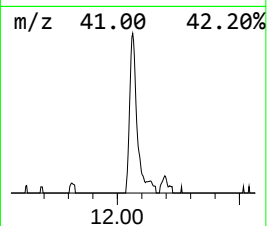
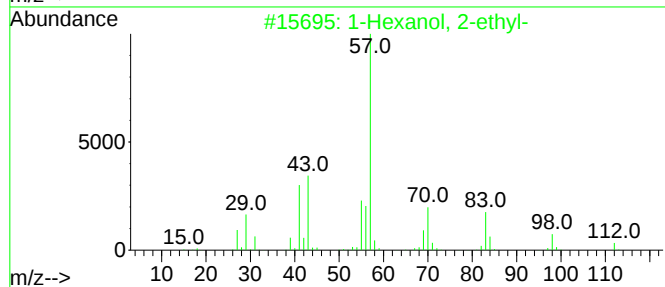
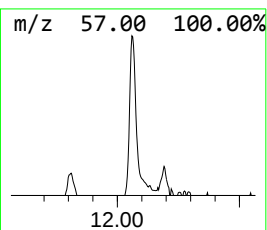
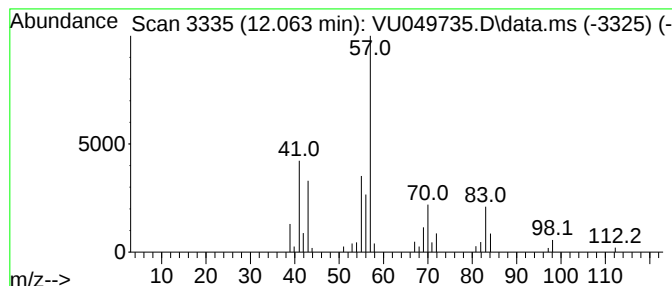
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Quant Title : VOC Analysis

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.
12.063	4.81 ug/L	45604	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	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	56



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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	3.6	ug/L	38726	2	9.417	538797	50.0
1-Hexanol, 2-et...	12.063	4.8	ug/L	45604	3	11.812	474047	50.0