

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV052423\
 Data File : VV031214.D
 Acq On : 24 May 2023 14:47
 Operator : SY/MD
 Sample : 02865-16
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GBX71

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\SFAMVLM051923WMA.M
 Title : VOC Analysis

Signal : TIC: VV031214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.281	70	75	89	rVB	93593	101172	12.85%	1.575%
2	1.535	148	154	166	rVB	108206	123493	15.68%	1.923%
3	2.063	309	318	332	rBV	196014	290486	36.88%	4.523%
4	2.420	424	429	432	rBV6	2406	2071	0.26%	0.032%
5	2.757	532	534	536	rVB3	1734	793	0.10%	0.012%
6	2.777	538	540	543	rBV4	861	622	0.08%	0.010%
7	2.815	547	552	555	rBV5	2251	2267	0.29%	0.035%
8	2.841	559	560	561	rBV	985	281	0.04%	0.004%
9	2.940	588	591	592	rBV2	1255	810	0.10%	0.013%
10	2.982	602	604	607	rBV3	2198	1413	0.18%	0.022%
11	3.095	637	639	640	rBV2	882	330	0.04%	0.005%
12	3.140	650	653	654	rBV3	764	390	0.05%	0.006%
13	3.169	660	662	664	rBV3	1396	870	0.11%	0.014%
14	3.217	674	677	679	rBV4	1739	887	0.11%	0.014%
15	3.240	679	684	687	rBV7	1715	1596	0.20%	0.025%
16	3.317	706	708	710	rBV3	890	451	0.06%	0.007%
17	3.330	710	712	715	rBV4	1371	950	0.12%	0.015%
18	3.362	720	722	725	rVV4	1075	604	0.08%	0.009%
19	3.461	752	753	756	rBV3	1250	525	0.07%	0.008%
20	3.516	768	770	773	rBV4	1221	599	0.08%	0.009%
21	3.532	773	775	776	rVV2	1292	405	0.05%	0.006%
22	3.548	777	780	781	rVB3	1403	612	0.08%	0.010%
23	3.596	794	795	800	rBV5	1496	954	0.12%	0.015%
24	3.641	806	809	810	rBV3	1696	975	0.12%	0.015%
25	3.703	826	828	829	rBV2	1307	437	0.06%	0.007%
26	3.767	845	848	849	rBV2	1403	864	0.11%	0.013%
27	3.799	849	858	880	rVV	63093	169505	21.52%	2.639%
28	3.989	913	917	920	rBV6	1992	1514	0.19%	0.024%
29	4.259	988	1001	1020	rBV	124297	306364	38.90%	4.770%
30	4.696	1135	1137	1140	rBV3	1165	604	0.08%	0.009%
31	4.870	1189	1191	1193	rBV3	1117	598	0.08%	0.009%
32	4.889	1195	1197	1200	rVV4	1876	1076	0.14%	0.017%
33	4.966	1204	1221	1250	rBV3	281891	787633	100.00%	12.263%
34	5.458	1373	1374	1378	rBV4	1529	1012	0.13%	0.016%
35	5.542	1388	1400	1424	rBV	220561	461173	58.55%	7.180%
36	5.799	1473	1480	1484	rBV9	2311	2836	0.36%	0.044%

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Integrator: RTE

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 Title : VOC Analysis

37	5.828	1484	1489	1490	rBV5	2292	1803	0.23%	0.028%
38	5.995	1525	1541	1561	rBV	171793	359536	45.65%	5.598%
39	6.236	1609	1616	1618	rBV6	3249	3415	0.43%	0.053%
40	6.439	1677	1679	1680	rBV2	1015	334	0.04%	0.005%
41	6.542	1709	1711	1712	rBV2	1182	341	0.04%	0.005%
42	6.651	1743	1745	1748	rVB4	1112	562	0.07%	0.009%
43	6.670	1748	1751	1754	rBV4	1336	1121	0.14%	0.017%
44	6.686	1754	1756	1758	rVB3	1520	575	0.07%	0.009%
45	6.812	1793	1795	1796	rBV2	1743	569	0.07%	0.009%
46	6.918	1820	1828	1847	rBV2	83728	148929	18.91%	2.319%
47	7.059	1871	1872	1874	rBV2	1514	500	0.06%	0.008%
48	7.249	1920	1931	1945	rBV	324522	559404	71.02%	8.710%
49	7.558	2020	2027	2043	rBV	63659	107496	13.65%	1.674%
50	7.763	2088	2091	2094	rBV5	1930	1510	0.19%	0.024%
51	7.863	2120	2122	2123	rBV3	1743	875	0.11%	0.014%
52	8.034	2166	2175	2209	rBV	201678	420049	53.33%	6.540%
53	8.329	2265	2267	2268	rBV2	1504	614	0.08%	0.010%
54	8.635	2361	2362	2365	rVB3	1848	697	0.09%	0.011%
55	8.648	2365	2366	2368	rBV2	1098	475	0.06%	0.007%
56	8.689	2376	2379	2382	rBV4	2287	1777	0.23%	0.028%
57	8.792	2399	2411	2430	rBV	347168	587411	74.58%	9.146%
58	8.953	2453	2461	2473	rVB2	24529	43018	5.46%	0.670%
59	9.336	2578	2580	2581	rBV2	1868	568	0.07%	0.009%
60	9.654	2672	2679	2689	rBV2	17145	28616	3.63%	0.446%
61	9.824	2727	2732	2739	rBV10	3080	4013	0.51%	0.062%
62	9.853	2739	2741	2744	rBV4	2069	1124	0.14%	0.018%
63	9.959	2764	2774	2788	rBV	89686	164381	20.87%	2.559%
64	10.159	2826	2836	2853	rVB	256527	403973	51.29%	6.290%
65	10.275	2870	2872	2873	rBV2	1983	989	0.13%	0.015%
66	10.609	2974	2976	2977	rBV2	1375	428	0.05%	0.007%
67	10.770	3024	3026	3029	rBV4	1184	586	0.07%	0.009%
68	10.834	3044	3046	3049	rBV5	1864	1272	0.16%	0.020%
69	11.191	3148	3157	3173	rVB	364533	574535	72.94%	8.945%
70	11.490	3242	3250	3263	rBV	54167	99046	12.58%	1.542%
71	11.567	3265	3274	3289	rVB	377542	595452	75.60%	9.271%
72	11.844	3358	3360	3365	rBV6	2347	1826	0.23%	0.028%
73	11.950	3390	3393	3397	rBV5	2876	1919	0.24%	0.030%
74	12.027	3414	3417	3418	rBV3	1872	976	0.12%	0.015%
75	12.146	3452	3454	3457	rBV4	1846	1134	0.14%	0.018%
76	12.381	3525	3527	3528	rBV2	1411	635	0.08%	0.010%

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77	12.535	3572	3575	3579	rBV5	1729	1530	0.19%	0.024%
78	12.554	3579	3581	3584	rVV4	1624	764	0.10%	0.012%
79	12.738	3634	3638	3640	rBV5	2310	1784	0.23%	0.028%
80	12.776	3647	3650	3651	rBV3	1339	876	0.11%	0.014%
81	13.075	3741	3743	3747	rBV5	2068	1296	0.16%	0.020%
82	13.236	3789	3793	3795	rBV5	2155	1754	0.22%	0.027%
83	13.281	3805	3807	3808	rBV2	1733	748	0.09%	0.012%
84	13.426	3849	3852	3854	rBV3	2081	1404	0.18%	0.022%
85	13.615	3909	3911	3913	rVB3	2466	972	0.12%	0.015%
86	13.731	3945	3947	3950	rBV4	1816	1236	0.16%	0.019%
87	13.837	3979	3980	3981	rBV	1550	478	0.06%	0.007%
88	13.863	3985	3988	3996	rVB9	2433	3015	0.38%	0.047%
89	13.930	4004	4009	4010	rBV5	1829	1403	0.18%	0.022%
90	13.998	4028	4030	4034	rVB5	2279	1353	0.17%	0.021%
91	14.088	4055	4058	4061	rBV5	2031	1468	0.19%	0.023%
92	14.155	4074	4079	4084	rBV10	2014	1961	0.25%	0.031%
93	14.188	4084	4089	4091	rBV6	1537	1511	0.19%	0.024%
94	14.352	4134	4140	4144	rBV7	2555	3696	0.47%	0.058%
95	14.483	4179	4181	4185	rBV4	2396	1592	0.20%	0.025%
96	14.647	4228	4232	4235	rBV5	2198	1865	0.24%	0.029%
97	14.734	4257	4259	4261	rBV4	1409	721	0.09%	0.011%
98	14.811	4281	4283	4284	rBV2	1845	603	0.08%	0.009%
99	15.004	4339	4343	4344	rBV4	1533	1117	0.14%	0.017%

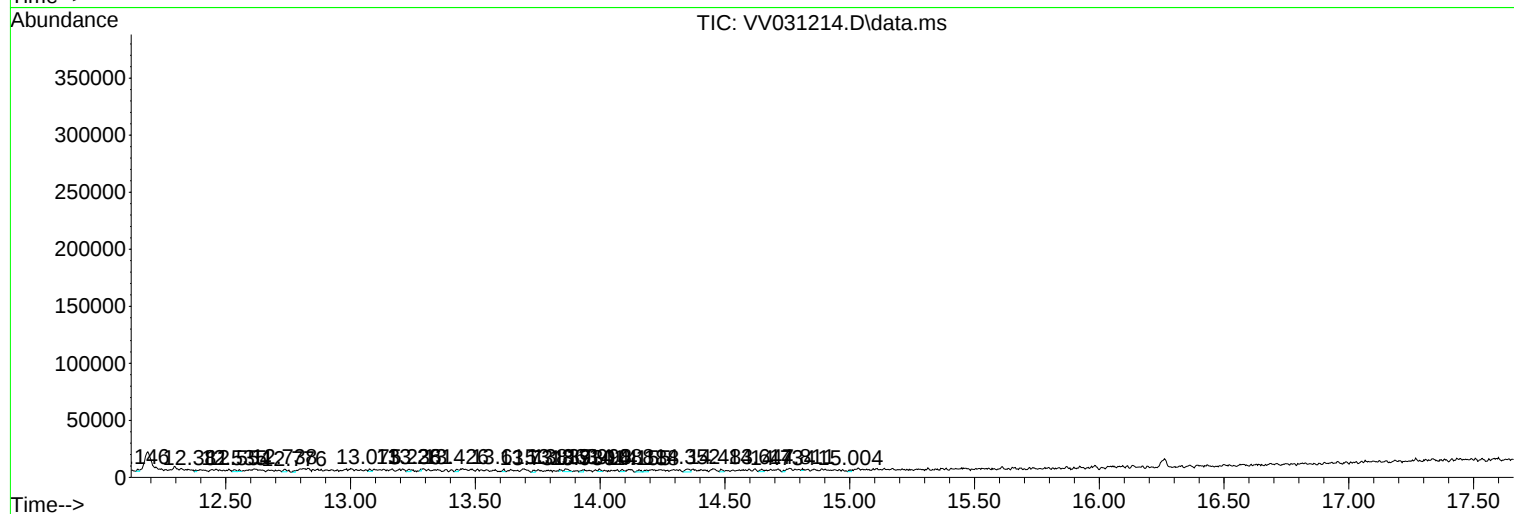
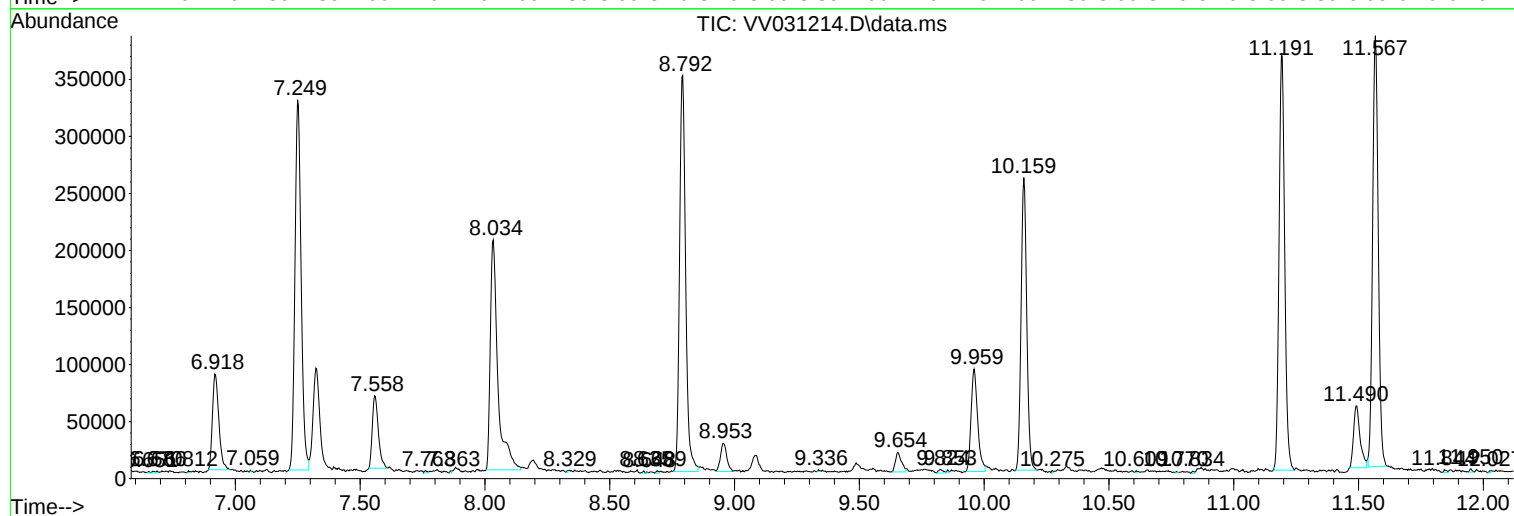
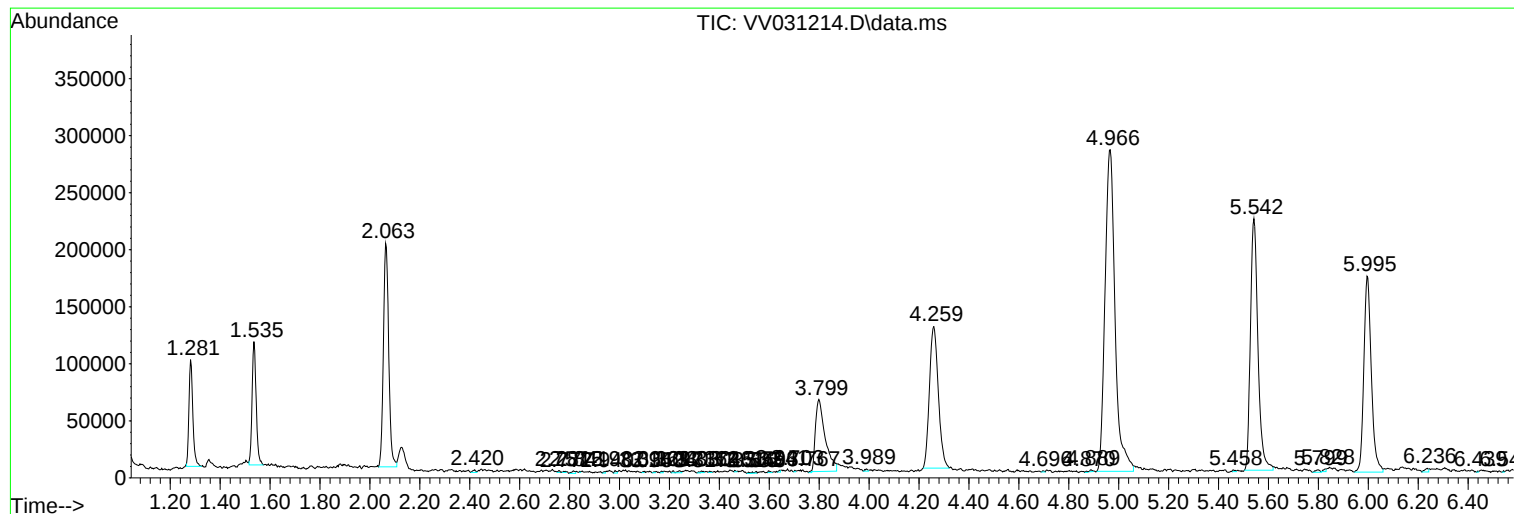
Sum of corrected areas: 6422803

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

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



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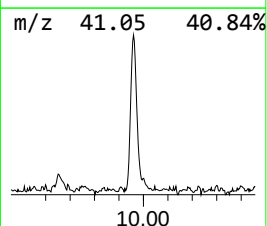
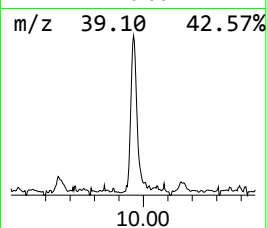
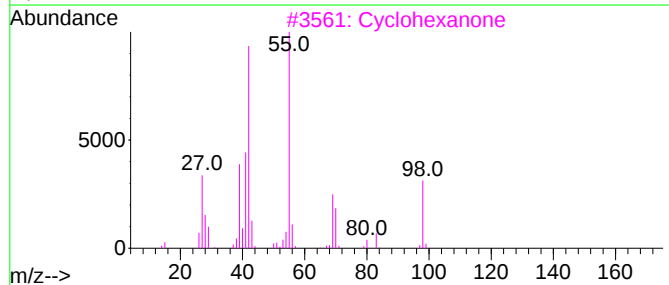
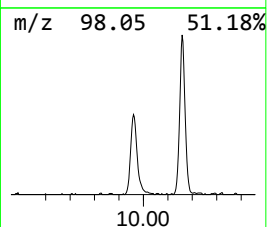
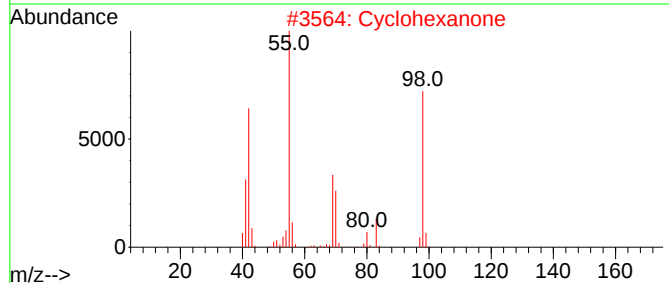
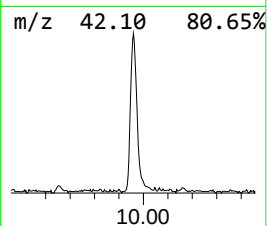
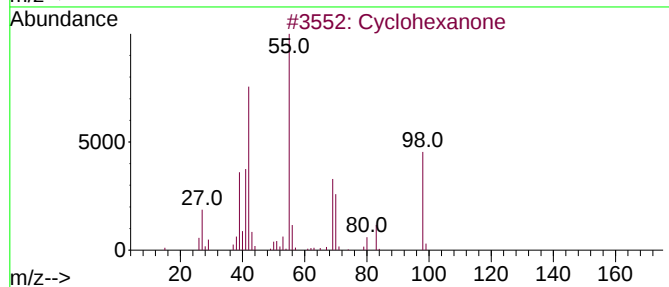
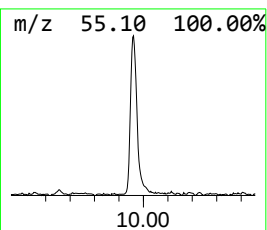
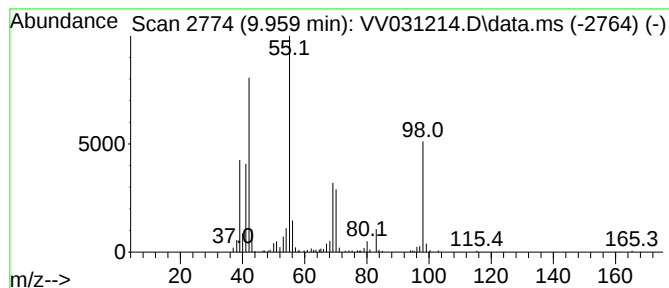
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Cyclohexanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.959	13.99 ug/L	164381	Chlorobenzene-d5	8.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	93
2			Cyclohexanone	98	C6H10O	000108-94-1	91
3			Cyclohexanone	98	C6H10O	000108-94-1	87
4			Cyclohexanone	98	C6H10O	000108-94-1	81
5			Cyclohexanone	98	C6H10O	000108-94-1	74



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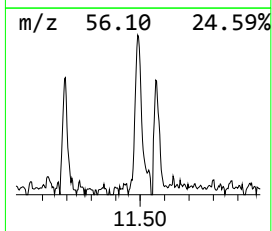
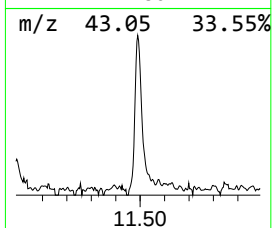
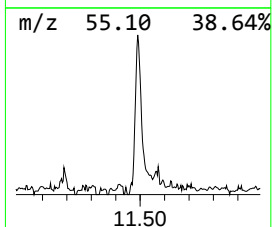
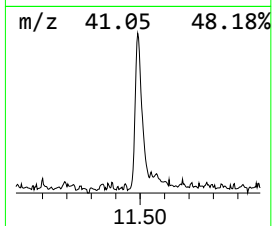
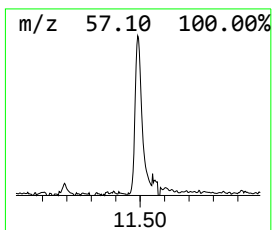
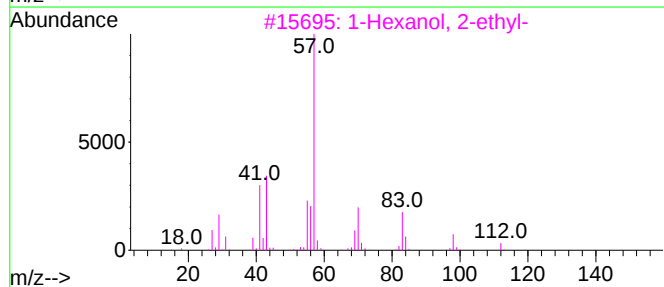
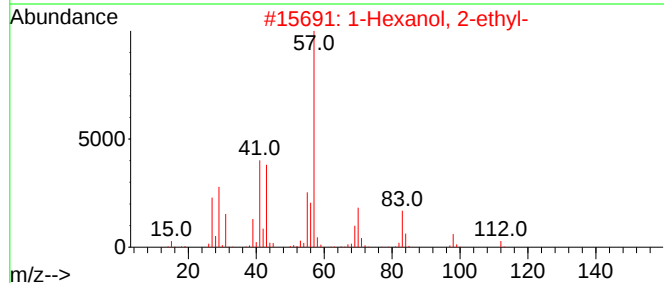
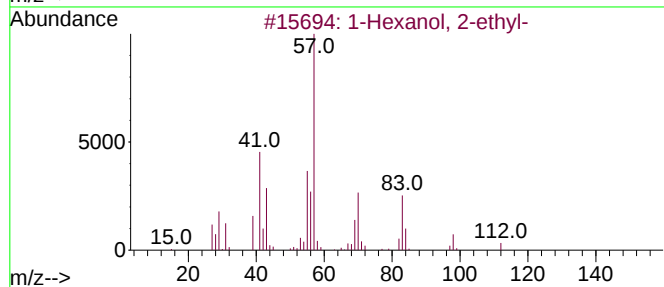
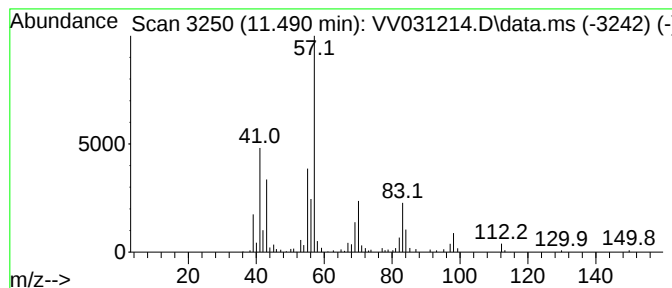
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.490	8.62 ug/L	99046	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64



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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	9.959	14.0	ug/L	164381	2	8.792	587411	50.0
1-Hexanol, 2-et...	11.490	8.6	ug/L	99046	3	11.194	574535	50.0