

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092022\
 Data File : VV027973.D
 Acq On : 20 Sep 2022 19:39
 Operator : SY/MD
 Sample : N4619-09
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0E25

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\SFAMVLM092022WMA.M
 Title : VOC Analysis

Signal : TIC: VV027973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	76	81	99	rVB	226174	238412	16.21%	2.107%
2	1.558	155	161	178	rVB	163309	195256	13.27%	1.725%
3	2.098	320	329	342	rBV	363291	525394	35.71%	4.643%
4	2.375	413	415	416	rBV	250	110	0.01%	0.001%
5	2.413	425	427	428	rBV	396	171	0.01%	0.002%
6	2.436	428	434	436	rVV4	1052	944	0.06%	0.008%
7	2.494	448	452	454	rBV4	1598	1282	0.09%	0.011%
8	2.545	466	468	471	rBV2	429	238	0.02%	0.002%
9	2.674	505	508	509	rBV2	320	200	0.01%	0.002%
10	2.703	515	517	520	rVB2	450	233	0.02%	0.002%
11	2.722	520	523	525	rBV3	440	244	0.02%	0.002%
12	2.741	527	529	530	rBV2	319	115	0.01%	0.001%
13	2.770	536	538	540	rVB2	468	200	0.01%	0.002%
14	2.786	540	543	544	rBV2	315	142	0.01%	0.001%
15	2.812	549	551	553	rBV2	271	127	0.01%	0.001%
16	2.828	555	556	560	rVB2	431	188	0.01%	0.002%
17	2.870	566	569	573	rVB3	844	656	0.04%	0.006%
18	2.896	574	577	580	rBV2	466	349	0.02%	0.003%
19	2.925	584	586	588	rVB	691	286	0.02%	0.003%
20	2.941	588	591	593	rBV2	296	137	0.01%	0.001%
21	2.957	593	596	600	rBV3	721	589	0.04%	0.005%
22	3.008	608	612	614	rBV2	921	677	0.05%	0.006%
23	3.082	633	635	637	rBV	536	249	0.02%	0.002%
24	3.150	654	656	658	rBV2	781	437	0.03%	0.004%
25	3.162	658	660	664	rVB4	1008	630	0.04%	0.006%
26	3.233	679	682	684	rBV2	720	516	0.04%	0.005%
27	3.278	694	696	699	rVB3	985	535	0.04%	0.005%
28	3.294	699	701	702	rBV	430	187	0.01%	0.002%
29	3.304	702	704	707	rVB2	803	377	0.03%	0.003%
30	3.323	707	710	713	rBV2	700	478	0.03%	0.004%
31	3.346	713	717	719	rBV	1078	741	0.05%	0.007%
32	3.375	724	726	728	rBV	377	136	0.01%	0.001%
33	3.445	745	748	751	rVB3	651	416	0.03%	0.004%
34	3.590	790	793	795	rBV4	1007	689	0.05%	0.006%
35	3.658	811	814	816	rBV3	635	340	0.02%	0.003%
36	3.680	819	821	822	rBV	377	147	0.01%	0.001%

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37	3.757	843	845	847	rBV2	523	243	0.02%	0.002%
38	3.773	847	850	852	rVB4	835	437	0.03%	0.004%
39	3.828	864	867	870	rBV4	837	574	0.04%	0.005%
40	3.870	870	880	915	rBV	124913	347568	23.63%	3.071%
41	4.339	1011	1026	1054	rBV	242396	591387	40.20%	5.226%
42	4.802	1168	1170	1174	rBV4	737	461	0.03%	0.004%
43	4.889	1191	1197	1198	rBV4	1305	1271	0.09%	0.011%
44	4.944	1212	1214	1216	rBV2	629	253	0.02%	0.002%
45	5.037	1226	1243	1274	rBV2	570494	1471099	100.00%	13.000%
46	5.326	1331	1333	1337	rBV3	951	690	0.05%	0.006%
47	5.526	1393	1395	1397	rBV2	1126	605	0.04%	0.005%
48	5.609	1410	1421	1448	rBV	405804	836425	56.86%	7.391%
49	5.915	1504	1516	1536	rBV3	37397	80864	5.50%	0.715%
50	6.063	1548	1562	1594	rBV	328197	671871	45.67%	5.937%
51	6.387	1662	1663	1666	rBV2	623	379	0.03%	0.003%
52	6.445	1678	1681	1684	rBV4	740	400	0.03%	0.004%
53	6.619	1733	1735	1737	rBV3	650	359	0.02%	0.003%
54	6.735	1768	1771	1775	rBV4	1145	845	0.06%	0.007%
55	6.828	1797	1800	1803	rBV5	746	690	0.05%	0.006%
56	6.895	1818	1821	1822	rBV2	691	366	0.02%	0.003%
57	6.928	1829	1831	1834	rBV2	248	122	0.01%	0.001%
58	6.982	1835	1848	1874	rBV	167637	317330	21.57%	2.804%
59	7.310	1938	1950	1971	rBV	626058	1092003	74.23%	9.650%
60	7.619	2036	2046	2067	rBV	118770	211184	14.36%	1.866%
61	7.844	2114	2116	2118	rBV2	744	394	0.03%	0.003%
62	7.892	2130	2131	2133	rBV2	558	279	0.02%	0.002%
63	8.085	2181	2191	2225	rBV	429341	771901	52.47%	6.821%
64	8.497	2315	2319	2321	rBV5	979	863	0.06%	0.008%
65	8.625	2357	2359	2361	rBV2	1017	530	0.04%	0.005%
66	8.770	2400	2404	2407	rBV3	1061	797	0.05%	0.007%
67	8.847	2417	2428	2453	rBV	620476	1016970	69.13%	8.987%
68	9.371	2588	2591	2593	rBV	620	413	0.03%	0.004%
69	9.445	2610	2614	2619	rVB5	876	759	0.05%	0.007%
70	9.468	2619	2621	2623	rBV	360	151	0.01%	0.001%
71	9.481	2623	2625	2629	rVB3	488	197	0.01%	0.002%
72	9.503	2629	2632	2634	rVB2	624	310	0.02%	0.003%
73	9.529	2634	2640	2641	rBV3	795	610	0.04%	0.005%
74	9.651	2676	2678	2681	rVB3	463	234	0.02%	0.002%
75	9.673	2683	2685	2686	rVB	325	102	0.01%	0.001%
76	9.683	2686	2688	2689	rBV	277	107	0.01%	0.001%

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77	9.715	2693	2698	2700	rBV2	1320	1094	0.07%	0.010%
78	9.866	2743	2745	2750	rBV4	1193	764	0.05%	0.007%
79	9.905	2754	2757	2760	rVB2	594	336	0.02%	0.003%
80	9.944	2760	2769	2773	rBV7	1059	1364	0.09%	0.012%
81	10.001	2784	2787	2789	rBV2	557	349	0.02%	0.003%
82	10.014	2789	2791	2794	rBV2	569	414	0.03%	0.004%
83	10.046	2799	2801	2804	rVB2	738	422	0.03%	0.004%
84	10.124	2817	2825	2834	rBV7	2122	3628	0.25%	0.032%
85	10.214	2841	2853	2874	rBV	467675	728075	49.49%	6.434%
86	10.432	2918	2921	2924	rBV2	1093	906	0.06%	0.008%
87	10.493	2938	2940	2942	rBV3	772	420	0.03%	0.004%
88	11.024	3104	3105	3106	rBV2	719	209	0.01%	0.002%
89	11.153	3138	3145	3153	rBV9	5888	9447	0.64%	0.083%
90	11.246	3163	3174	3194	rBV	587266	899435	61.14%	7.948%
91	11.529	3252	3262	3279	rBV	88731	179889	12.23%	1.590%
92	11.622	3281	3291	3309	rVB	630740	1000604	68.02%	8.842%
93	11.995	3399	3407	3422	rBV6	14665	35046	2.38%	0.310%
94	12.918	3691	3694	3696	rBV3	1316	885	0.06%	0.008%
95	13.069	3739	3741	3746	rBV4	1069	935	0.06%	0.008%
96	13.133	3753	3761	3769	rBV4	3877	7253	0.49%	0.064%
97	13.439	3850	3856	3865	rVB9	2673	3361	0.23%	0.030%
98	13.869	3989	3990	3992	rBV2	780	284	0.02%	0.003%
99	14.030	4038	4040	4044	rBV3	1135	752	0.05%	0.007%
100	14.400	4147	4155	4167	rVB5	27049	46827	3.18%	0.414%

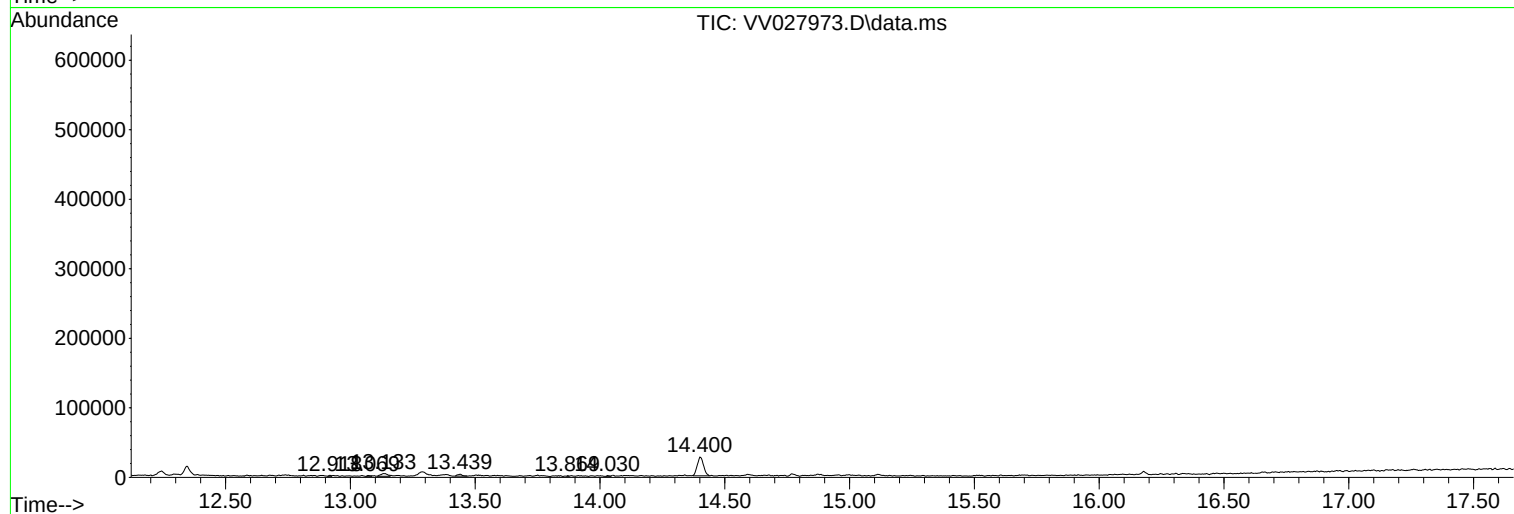
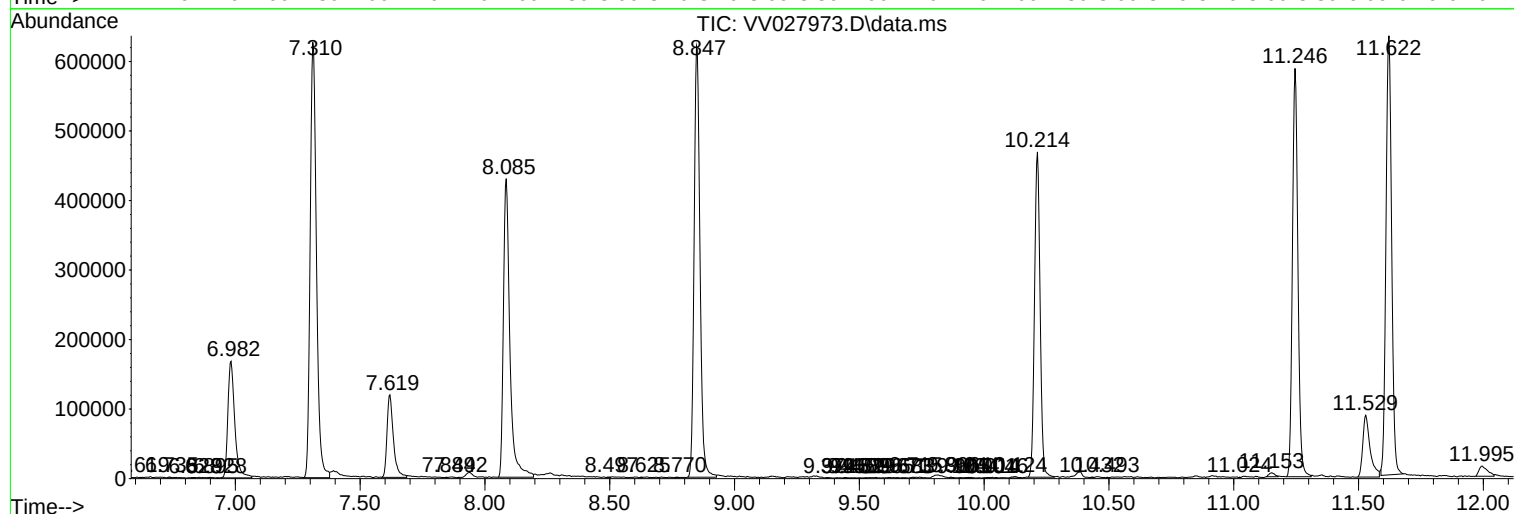
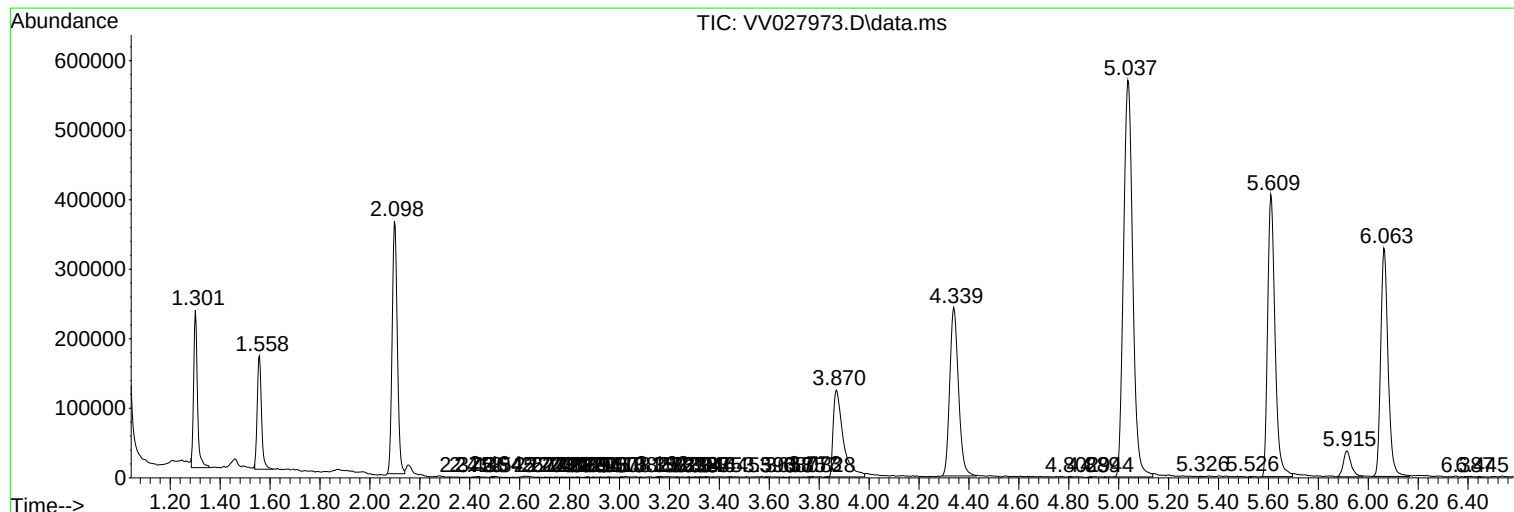
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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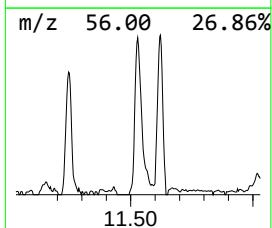
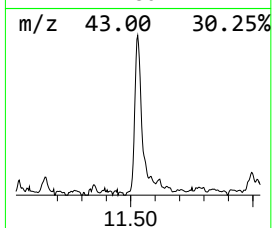
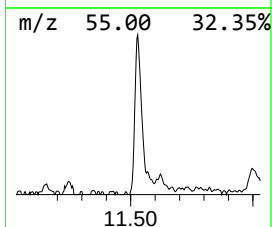
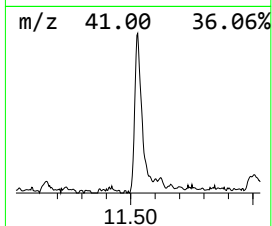
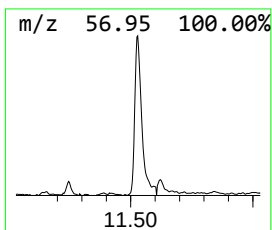
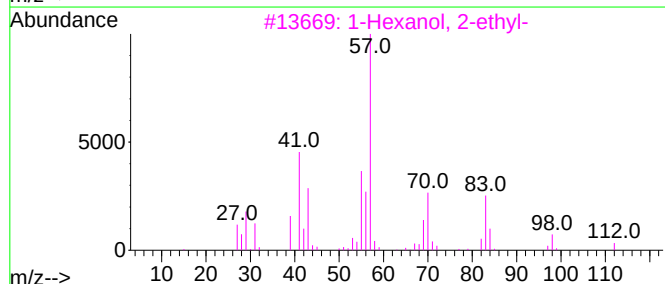
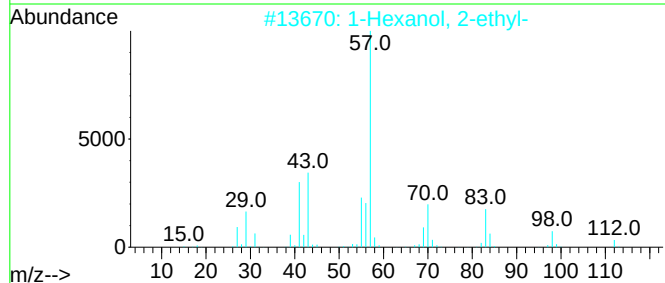
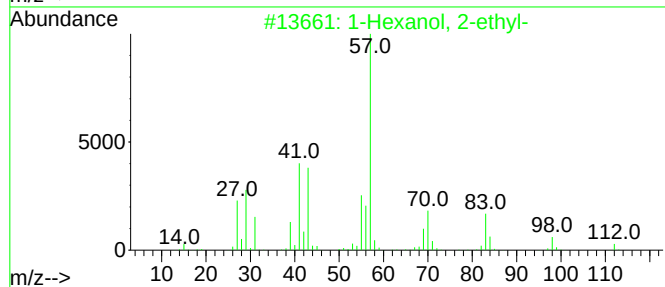
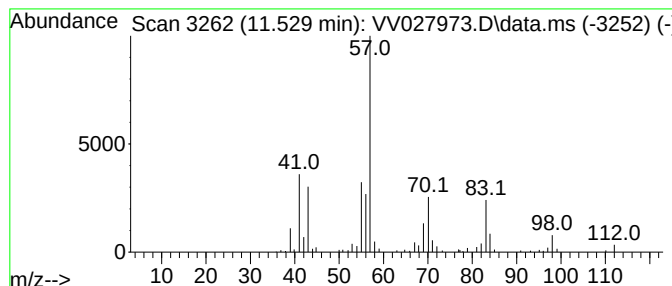
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	10.00 ug/L	179889	1,4-Dichlorobenzene-d4	11.246

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
5		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	59



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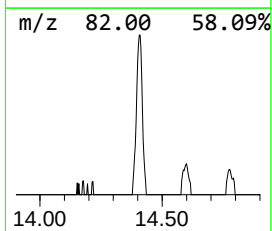
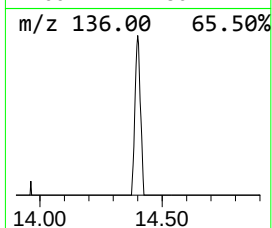
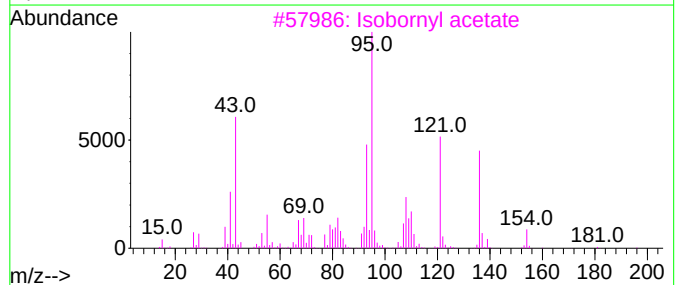
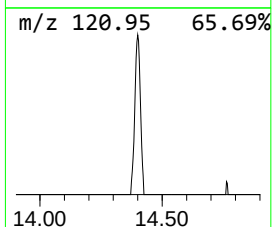
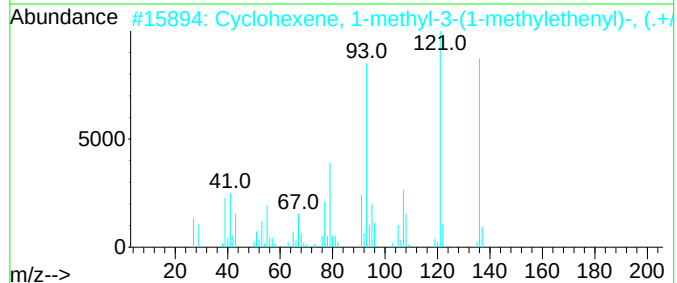
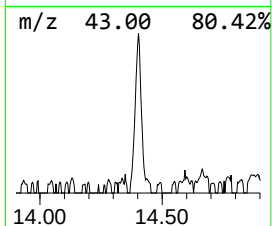
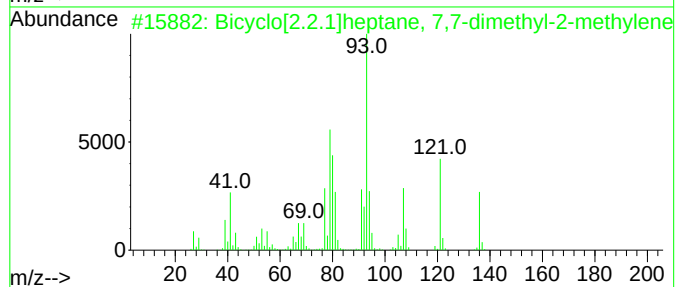
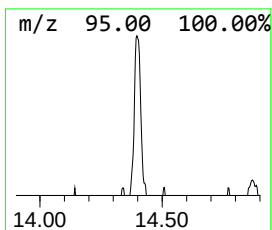
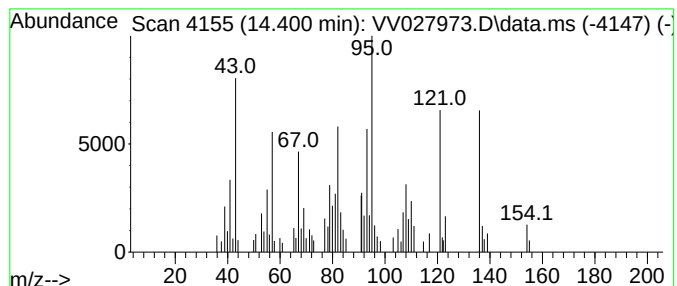
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Bicyclo[2.2.1]heptane, 7,7-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.400	2.60 ug/L	46827	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	81
2			Cyclohexene, 1-methyl-3-(1-methy...	136	C10H16	000499-03-6	70
3			Isobornyl acetate	196	C12H20O2	000125-12-2	58
4			Isobornyl thiocyanoacetate	253	C13H19NO2S	000115-31-1	52
5			Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	196	C12H20O2	005655-61-8	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	11.529	10.0	ug/L	179889	3	11.246	899435	50.0
Bicyclo[2.2.1]h...	14.400	2.6	ug/L	46827	3	11.246	899435	50.0