

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV093021\
 Data File : VV022463.D
 Acq On : 01 Oct 2021 04:06
 Operator : SY/MD
 Sample : M3996-18
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F4A37

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\SFAMVLM092721WMA.M
 Title : VOC Analysis

Signal : TIC: VV022463.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.201	45	50	58	rVB	40894	38441	4.37%	0.521%
2	1.304	74	82	94	rVB	153389	162936	18.50%	2.210%
3	1.561	155	162	173	rBV	111031	126648	14.38%	1.718%
4	2.105	321	331	342	rBV	224809	323834	36.77%	4.392%
5	2.503	453	455	459	rVB3	556	308	0.03%	0.004%
6	2.574	474	477	478	rBV	286	142	0.02%	0.002%
7	2.700	514	516	519	rBV2	268	191	0.02%	0.003%
8	2.732	523	526	527	rBV2	303	206	0.02%	0.003%
9	2.770	527	538	550	rVB4	5096	10277	1.17%	0.139%
10	2.883	571	573	575	rBV	338	163	0.02%	0.002%
11	3.021	615	616	619	rBV2	330	138	0.02%	0.002%
12	3.037	619	621	624	rBV3	456	273	0.03%	0.004%
13	3.150	654	656	660	rBV	223	150	0.02%	0.002%
14	3.195	668	670	672	rVB	347	123	0.01%	0.002%
15	3.336	712	714	719	rBV	225	131	0.01%	0.002%
16	3.452	748	750	754	rVB2	247	120	0.01%	0.002%
17	3.626	802	804	807	rVV3	513	297	0.03%	0.004%
18	3.654	810	813	816	rVB2	265	175	0.02%	0.002%
19	3.671	816	818	821	rBV	278	120	0.01%	0.002%
20	3.706	826	829	834	rBV3	370	305	0.03%	0.004%
21	3.873	871	881	914	rBV	71664	201957	22.93%	2.739%
22	4.201	980	983	989	rBV3	485	526	0.06%	0.007%
23	4.349	1012	1029	1057	rBV	138808	349793	39.72%	4.744%
24	4.548	1089	1091	1095	rVB3	407	287	0.03%	0.004%
25	4.687	1131	1134	1135	rBV3	394	234	0.03%	0.003%
26	4.706	1138	1140	1144	rVB2	421	270	0.03%	0.004%
27	4.748	1150	1153	1154	rBV	258	134	0.02%	0.002%
28	4.802	1167	1170	1172	rBV	248	164	0.02%	0.002%
29	4.886	1192	1196	1200	rVB3	333	343	0.04%	0.005%
30	4.957	1215	1218	1222	rBV2	348	265	0.03%	0.004%
31	5.047	1229	1246	1280	rBV2	338613	880653	100.00%	11.943%
32	5.445	1368	1370	1374	rVB3	288	166	0.02%	0.002%
33	5.468	1374	1377	1380	rBV3	366	223	0.03%	0.003%
34	5.503	1387	1388	1392	rVB2	385	217	0.02%	0.003%
35	5.616	1412	1423	1445	rBV	250478	508532	57.74%	6.896%
36	5.812	1482	1484	1486	rBV	396	155	0.02%	0.002%

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37	5.918	1504	1517	1532	rBV5	22084	52336	5.94%	0.710%
38	6.011	1544	1546	1548	rVB	326	141	0.02%	0.002%
39	6.069	1548	1564	1590	rBV2	195099	401927	45.64%	5.451%
40	6.359	1652	1654	1658	rVB3	382	208	0.02%	0.003%
41	6.394	1661	1665	1668	rVB3	535	411	0.05%	0.006%
42	6.474	1687	1690	1692	rBV2	278	171	0.02%	0.002%
43	6.548	1709	1713	1716	rVB4	405	245	0.03%	0.003%
44	6.580	1720	1723	1731	rVB4	385	516	0.06%	0.007%
45	6.651	1744	1745	1748	rVB	421	148	0.02%	0.002%
46	6.674	1751	1752	1755	rVV	390	189	0.02%	0.003%
47	6.802	1789	1792	1794	rBV2	330	159	0.02%	0.002%
48	6.831	1799	1801	1804	rBV	338	149	0.02%	0.002%
49	6.989	1838	1850	1869	rBV	95528	173618	19.71%	2.355%
50	7.236	1924	1927	1929	rBV2	529	335	0.04%	0.005%
51	7.317	1941	1952	1971	rBV	397483	697529	79.21%	9.460%
52	7.622	2038	2047	2069	rBV	64367	114525	13.00%	1.553%
53	7.844	2112	2116	2122	rVB3	450	359	0.04%	0.005%
54	7.976	2142	2157	2175	rBV	351605	589902	66.98%	8.000%
55	8.088	2183	2192	2223	rBV	200228	377799	42.90%	5.124%
56	8.423	2294	2296	2299	rVB2	437	233	0.03%	0.003%
57	8.555	2335	2337	2341	rBV2	315	166	0.02%	0.002%
58	8.587	2346	2347	2351	rBV2	249	141	0.02%	0.002%
59	8.725	2388	2390	2392	rBV2	297	157	0.02%	0.002%
60	8.783	2406	2408	2410	rBV2	300	130	0.01%	0.002%
61	8.854	2419	2430	2453	rBV	381484	626345	71.12%	8.494%
62	9.301	2566	2569	2571	rBV	206	128	0.01%	0.002%
63	9.391	2590	2597	2599	rVV2	401	503	0.06%	0.007%
64	9.416	2602	2605	2607	rBV2	520	281	0.03%	0.004%
65	9.555	2645	2648	2651	rBV2	379	306	0.03%	0.004%
66	9.603	2656	2663	2678	rVB3	5161	9462	1.07%	0.128%
67	9.725	2694	2701	2704	rBV5	789	1145	0.13%	0.016%
68	10.034	2795	2797	2802	rVB2	305	240	0.03%	0.003%
69	10.063	2802	2806	2811	rBV2	321	338	0.04%	0.005%
70	10.085	2811	2813	2816	rBV2	270	120	0.01%	0.002%
71	10.120	2819	2824	2826	rBV2	1106	830	0.09%	0.011%
72	10.217	2842	2854	2875	rBV	261155	417239	47.38%	5.658%
73	10.513	2937	2946	2958	rVV3	4238	7072	0.80%	0.096%
74	10.590	2967	2970	2977	rBV2	603	722	0.08%	0.010%
75	10.693	2998	3002	3006	rBV4	334	306	0.03%	0.004%
76	10.847	3045	3050	3056	rBV2	386	430	0.05%	0.006%

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77	10.915	3065	3071	3083	rVB6	1387	2533	0.29%	0.034%
78	10.966	3084	3087	3089	rBV2	224	129	0.01%	0.002%
79	10.979	3089	3091	3094	rVB	335	159	0.02%	0.002%
80	11.046	3104	3112	3123	rBV5	4843	8334	0.95%	0.113%
81	11.130	3136	3138	3141	rVV3	395	247	0.03%	0.003%
82	11.249	3164	3175	3195	rBV	352359	549965	62.45%	7.458%
83	11.532	3253	3263	3281	rBV	45255	88845	10.09%	1.205%
84	11.625	3281	3292	3313	rVB	392581	632216	71.79%	8.574%
85	11.956	3392	3395	3400	rVB3	655	628	0.07%	0.009%
86	11.989	3400	3405	3412	rBV6	802	1158	0.13%	0.016%
87	12.066	3425	3429	3435	rBV4	841	649	0.07%	0.009%
88	12.091	3435	3437	3439	rBV2	432	228	0.03%	0.003%
89	12.130	3445	3449	3450	rBV2	400	286	0.03%	0.004%
90	12.207	3468	3473	3477	rBV3	417	349	0.04%	0.005%
91	12.243	3482	3484	3487	rBV	770	543	0.06%	0.007%
92	12.339	3510	3514	3518	rBV3	453	456	0.05%	0.006%
93	12.500	3562	3564	3565	rBV	395	175	0.02%	0.002%
94	12.866	3676	3678	3681	rBV	282	121	0.01%	0.002%
95	13.098	3747	3750	3752	rBV2	198	134	0.02%	0.002%
96	13.181	3774	3776	3778	rBV3	325	157	0.02%	0.002%
97	13.226	3787	3790	3793	rVV2	265	154	0.02%	0.002%
98	13.802	3967	3969	3971	rBV2	296	120	0.01%	0.002%
99	14.140	4071	4074	4077	rBV	326	221	0.03%	0.003%
100	14.365	4142	4144	4150	rBV2	273	167	0.02%	0.002%

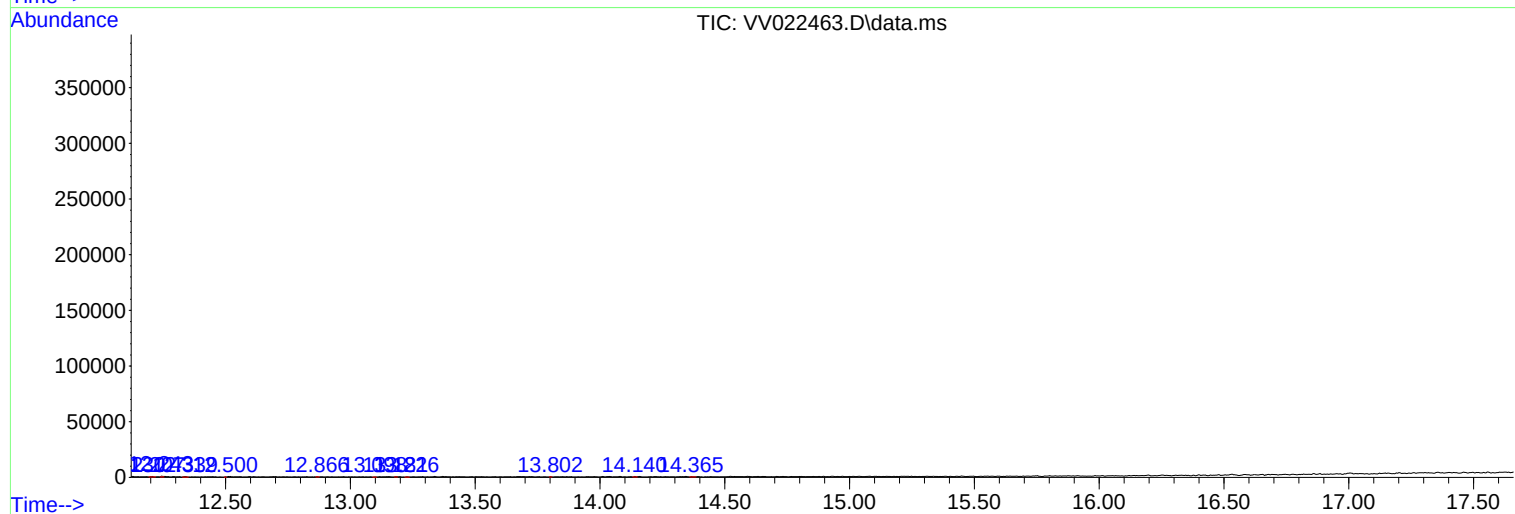
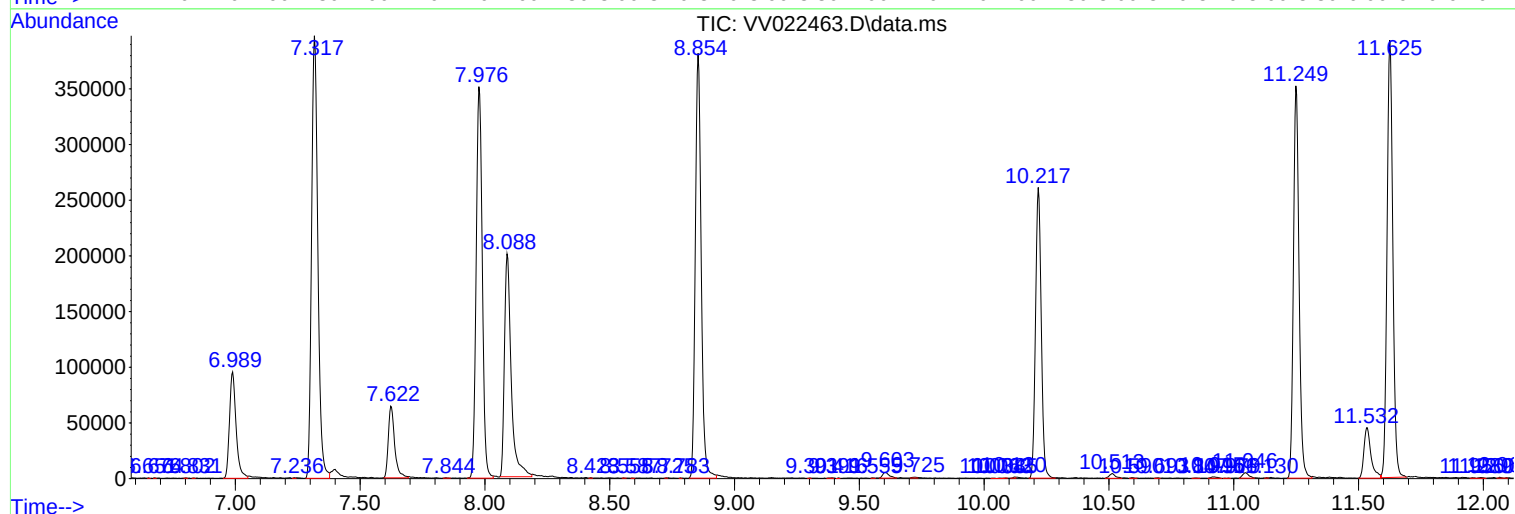
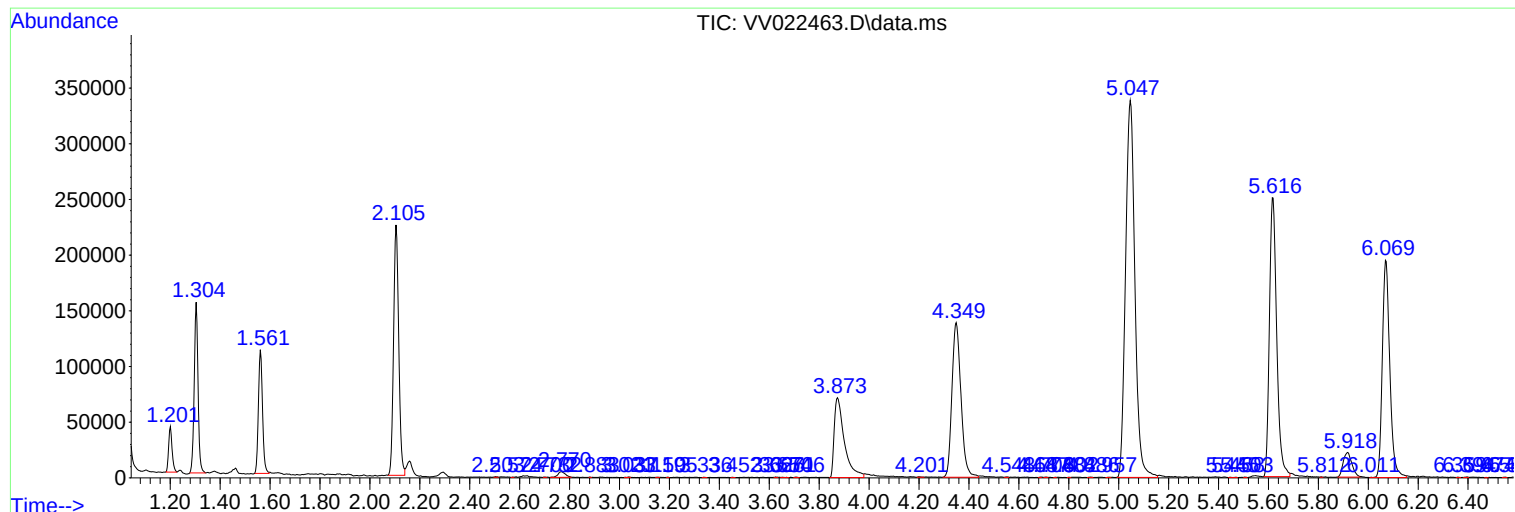
Sum of corrected areas: 7373832

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MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092721WMA.M
Quant Title : VOC Analysis

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



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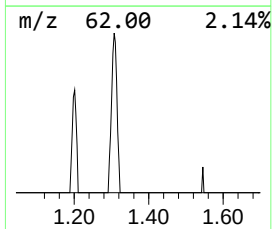
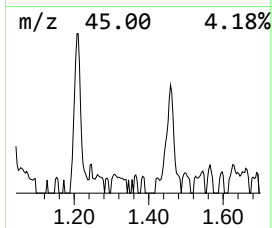
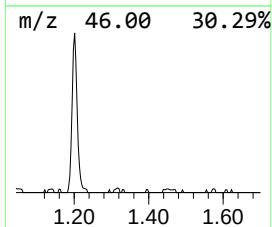
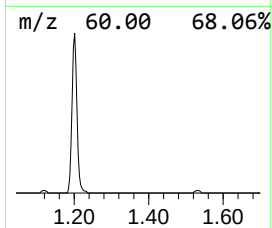
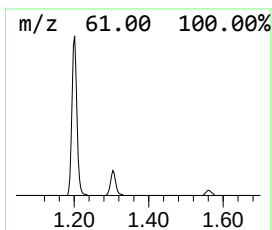
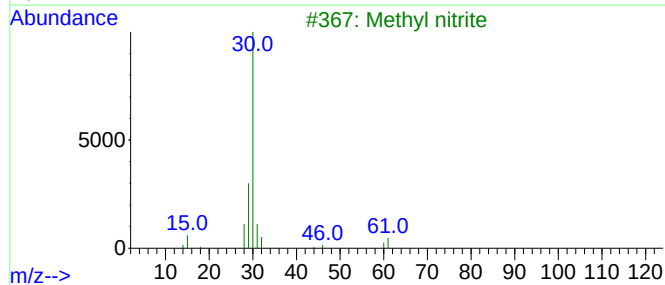
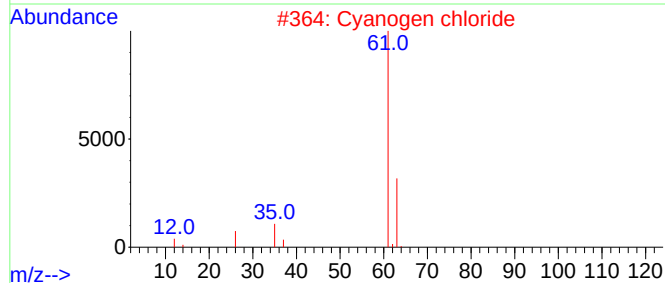
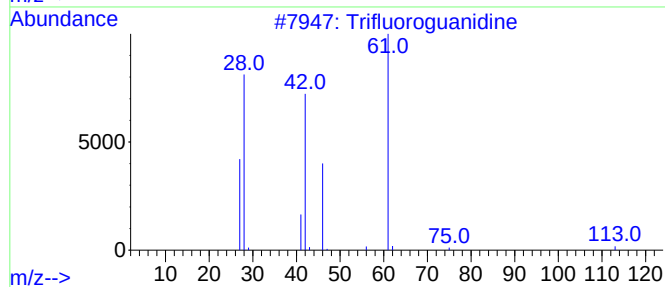
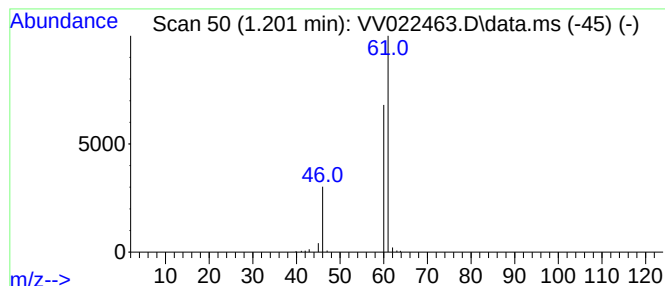
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092721WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.201	3.78 ug/L	38441	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroguanidine	113	CH2F3N3	037950-72-4	9
2			Cyanogen chloride	61	CClN	000506-77-4	5
3			Methyl nitrite	61	CH3NO2	000624-91-9	5
4			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
5			Formamidoxime	60	CH4N2O	000624-82-8	4



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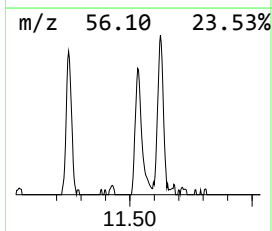
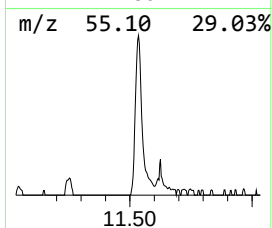
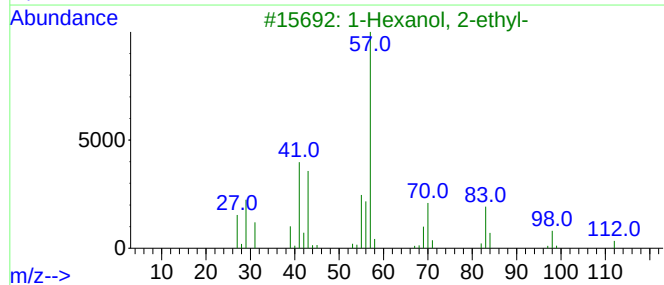
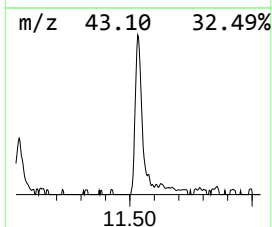
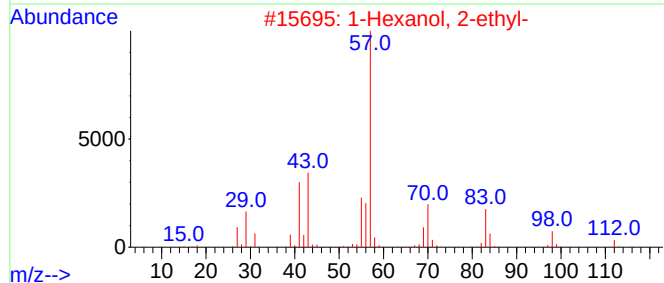
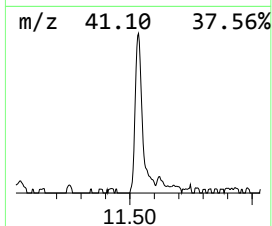
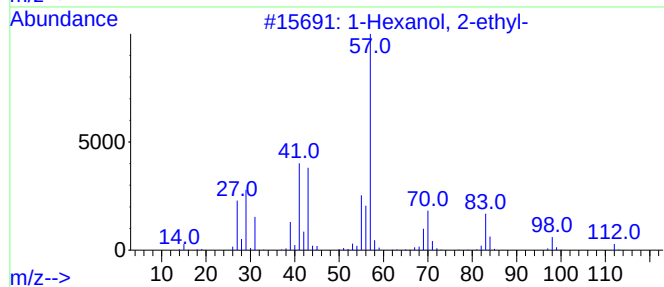
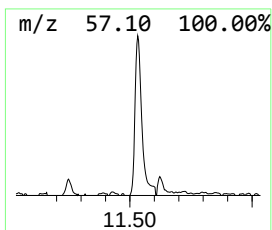
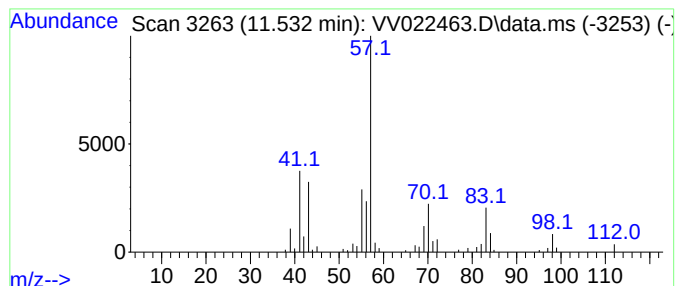
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Quant Title : VOC Analysis

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.
11.532	8.08 ug/L	88845	1,4-Dichlorobenzene-d4	11.249

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	90
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.201	3.8	ug/L	38441	1	5.619	508532	50.0
1-Hexanol, 2-et...	11.532	8.1	ug/L	88845	3	11.249	549965	50.0