

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051202.D
 Acq On : 07 Oct 2022 03:36
 Operator : JC/MD
 Sample : N4893-15
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5J16

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\SFAMULM092922WMA.M
 Title : VOC Analysis

Signal : TIC: VU051202.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	35	41	52	rBV	121487	126892	8.10%	0.973%
2	1.597	71	80	93	rBV2	283249	348794	22.27%	2.676%
3	1.903	167	175	195	rVB	180011	243949	15.57%	1.871%
4	2.562	369	380	392	rBV	313813	502216	32.06%	3.852%
5	3.038	525	528	538	rVB5	1425	1975	0.13%	0.015%
6	3.131	555	557	559	rVB5	366	109	0.01%	0.001%
7	3.244	589	592	596	rBV3	512	410	0.03%	0.003%
8	3.359	619	628	648	rVB2	8167	19420	1.24%	0.149%
9	3.430	648	650	653	rBV2	373	210	0.01%	0.002%
10	3.571	691	694	695	rBV	276	151	0.01%	0.001%
11	3.681	725	728	731	rBV2	323	190	0.01%	0.001%
12	3.700	731	734	737	rBV2	669	370	0.02%	0.003%
13	3.745	746	748	750	rBV	223	138	0.01%	0.001%
14	3.780	755	759	761	rBV2	275	270	0.02%	0.002%
15	3.829	771	774	776	rBV	263	185	0.01%	0.001%
16	3.858	781	783	787	rVB2	407	242	0.02%	0.002%
17	3.916	796	801	802	rBV2	336	304	0.02%	0.002%
18	3.957	810	814	816	rBV	273	174	0.01%	0.001%
19	4.002	824	828	829	rBV	271	146	0.01%	0.001%
20	4.041	838	840	843	rBV	204	128	0.01%	0.001%
21	4.260	904	908	915	rVB2	355	376	0.02%	0.003%
22	4.317	924	926	928	rVB	293	118	0.01%	0.001%
23	4.340	930	933	935	rBV	341	244	0.02%	0.002%
24	4.404	950	953	956	rBV	460	260	0.02%	0.002%
25	4.620	1008	1020	1047	rBV	133145	344685	22.00%	2.644%
26	4.919	1111	1113	1118	rVB3	714	493	0.03%	0.004%
27	5.060	1141	1157	1179	rBV	284556	629394	40.18%	4.828%
28	5.269	1219	1222	1224	rBV2	745	530	0.03%	0.004%
29	5.346	1244	1246	1248	rBV	181	68	0.00%	0.001%
30	5.440	1273	1275	1278	rBV	456	259	0.02%	0.002%
31	5.542	1305	1307	1308	rBV	159	53	0.00%	0.000%
32	5.604	1323	1326	1331	rBV2	213	209	0.01%	0.002%
33	5.723	1341	1363	1391	rBV2	578782	1566437	100.00%	12.016%
34	6.086	1473	1476	1477	rBV2	123	69	0.00%	0.001%
35	6.105	1480	1482	1483	rBV2	382	141	0.01%	0.001%
36	6.160	1490	1499	1509	rBV4	4878	9049	0.58%	0.069%

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 Title : VOC Analysis

37	6.247	1513	1526	1553	rBV	470251	890971	56.88%	6.835%
38	6.395	1570	1572	1575	rBV4	781	403	0.03%	0.003%
39	6.433	1582	1584	1587	rBV2	420	223	0.01%	0.002%
40	6.542	1606	1618	1631	rBV3	32947	63142	4.03%	0.484%
41	6.629	1644	1645	1647	rVB	362	93	0.01%	0.001%
42	6.690	1649	1664	1686	rBV	371975	735150	46.93%	5.639%
43	6.841	1709	1711	1714	rBV4	523	336	0.02%	0.003%
44	6.928	1734	1738	1742	rBV3	617	572	0.04%	0.004%
45	6.986	1754	1756	1759	rBV	328	230	0.01%	0.002%
46	7.057	1775	1778	1781	rBV	173	150	0.01%	0.001%
47	7.108	1791	1794	1797	rBV	323	169	0.01%	0.001%
48	7.166	1805	1812	1814	rBV4	956	1253	0.08%	0.010%
49	7.314	1854	1858	1861	rBV2	250	215	0.01%	0.002%
50	7.349	1867	1869	1870	rBV	222	76	0.00%	0.001%
51	7.407	1882	1887	1890	rBV	352	294	0.02%	0.002%
52	7.472	1905	1907	1908	rBV	234	105	0.01%	0.001%
53	7.565	1923	1936	1957	rBV	167598	294003	18.77%	2.255%
54	7.690	1972	1975	1976	rBV2	817	488	0.03%	0.004%
55	7.774	1999	2001	2004	rBV2	454	260	0.02%	0.002%
56	7.896	2026	2039	2054	rBV	635466	1089479	69.55%	8.357%
57	8.179	2115	2127	2145	rBV	116983	196686	12.56%	1.509%
58	8.272	2153	2156	2157	rBV2	645	390	0.02%	0.003%
59	8.433	2203	2206	2209	rBV2	311	203	0.01%	0.002%
60	8.552	2227	2243	2257	rBV	628889	1063766	67.91%	8.160%
61	8.636	2258	2269	2307	rVB4	307218	751908	48.00%	5.768%
62	9.102	2410	2414	2417	rBV2	538	496	0.03%	0.004%
63	9.140	2423	2426	2430	rBV	354	275	0.02%	0.002%
64	9.195	2441	2443	2444	rBV	172	71	0.00%	0.001%
65	9.208	2444	2447	2451	rVV2	280	237	0.02%	0.002%
66	9.243	2456	2458	2460	rBV	236	135	0.01%	0.001%
67	9.330	2482	2485	2486	rBV	146	77	0.00%	0.001%
68	9.417	2498	2512	2540	rBV	691327	1138426	72.68%	8.733%
69	9.629	2576	2578	2580	rBV2	356	180	0.01%	0.001%
70	9.668	2585	2590	2591	rBV2	564	397	0.03%	0.003%
71	9.755	2614	2617	2622	rVB2	556	491	0.03%	0.004%
72	9.851	2642	2647	2649	rBV	373	338	0.02%	0.003%
73	9.918	2665	2668	2672	rBV2	389	323	0.02%	0.002%
74	9.944	2672	2676	2678	rBV2	204	171	0.01%	0.001%
75	9.957	2678	2680	2682	rBV2	272	159	0.01%	0.001%
76	10.041	2703	2706	2708	rBV3	298	166	0.01%	0.001%

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77	10.237	2761	2767	2776	rBV6	1279	2221	0.14%	0.017%
78	10.385	2809	2813	2814	rBV2	398	268	0.02%	0.002%
79	10.423	2822	2825	2828	rBV2	321	193	0.01%	0.001%
80	10.472	2836	2840	2841	rBV	665	413	0.03%	0.003%
81	10.529	2856	2858	2861	rBV	353	201	0.01%	0.002%
82	10.754	2915	2928	2952	rBV	523076	840642	53.67%	6.448%
83	10.906	2968	2975	2983	rBV4	4038	5193	0.33%	0.040%
84	10.996	2996	3003	3004	rBV	709	677	0.04%	0.005%
85	11.291	3087	3095	3106	rVB3	6218	9160	0.58%	0.070%
86	11.468	3139	3150	3161	rBV	25724	39594	2.53%	0.304%
87	11.545	3171	3174	3175	rBV	556	336	0.02%	0.003%
88	11.574	3175	3183	3197	rVV2	10572	17873	1.14%	0.137%
89	11.809	3244	3256	3275	rBV	518576	829506	52.95%	6.363%
90	12.060	3323	3334	3356	rBV	117513	227747	14.54%	1.747%
91	12.192	3363	3375	3398	rVB	559266	933131	59.57%	7.158%
92	12.571	3486	3493	3501	rVB3	10720	14566	0.93%	0.112%
93	12.684	3518	3528	3531	rBV6	3647	5413	0.35%	0.042%
94	12.973	3610	3618	3626	rBV4	7656	11125	0.71%	0.085%
95	13.024	3627	3634	3648	rVB2	8269	12353	0.79%	0.095%
96	13.452	3760	3767	3782	rVB5	13625	23234	1.48%	0.178%
97	14.089	3957	3965	3982	rVB	18084	31239	1.99%	0.240%

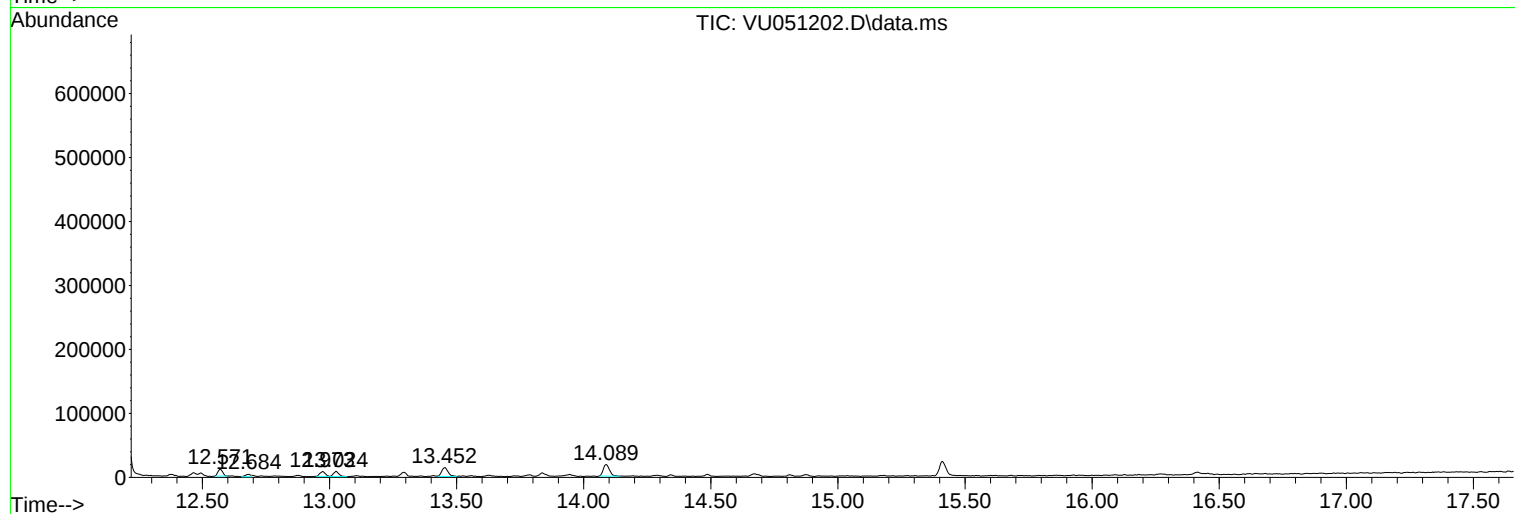
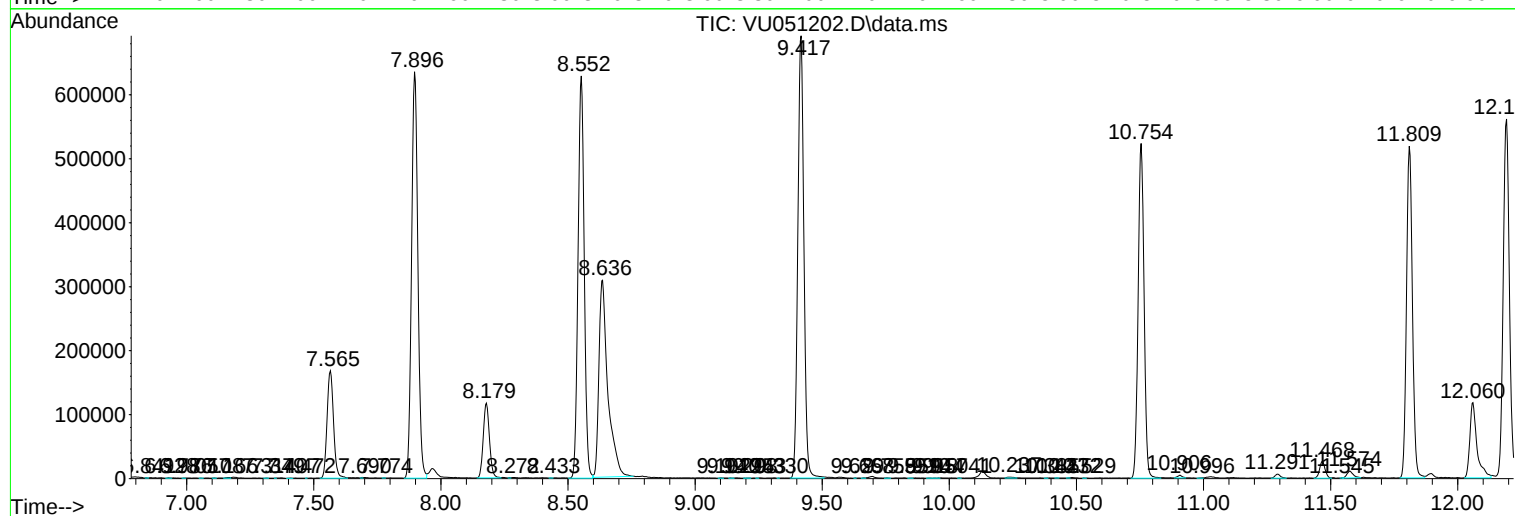
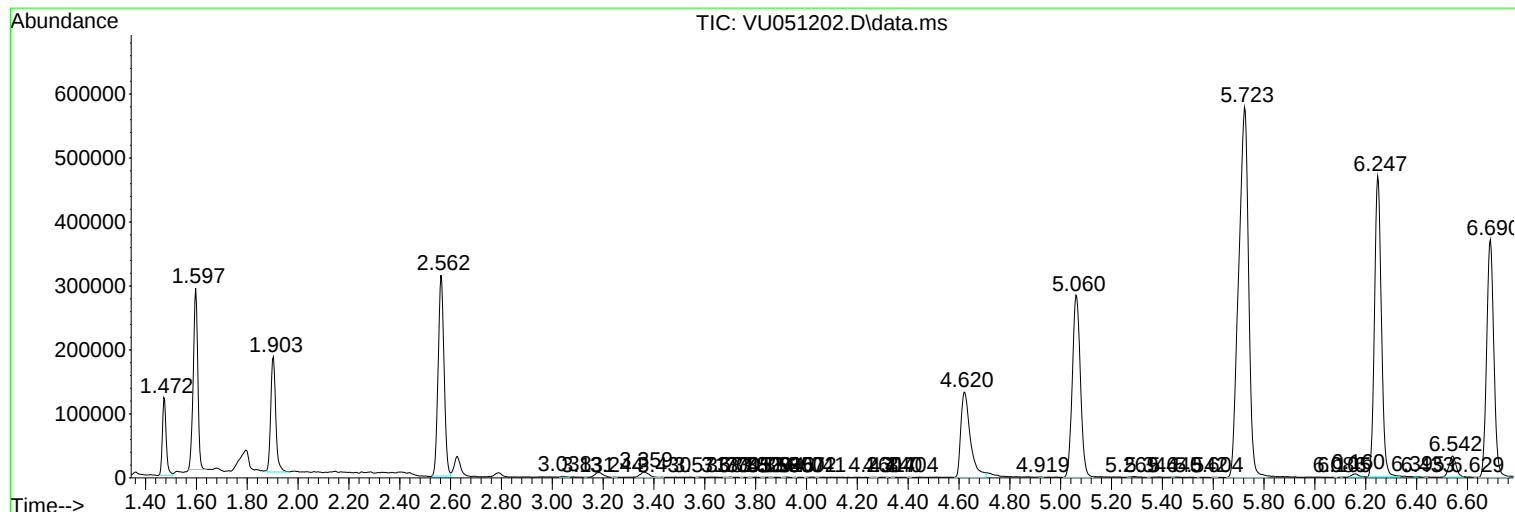
Sum of corrected areas: 13036250

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

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



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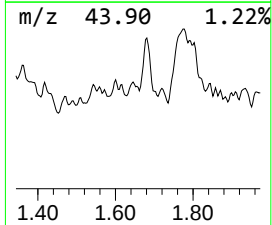
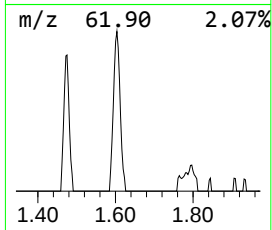
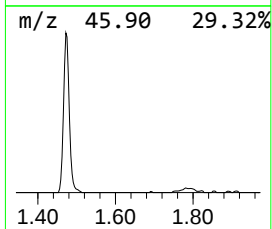
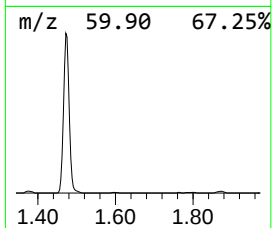
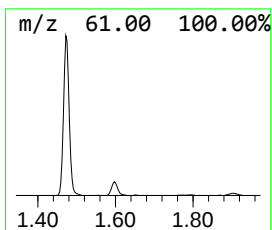
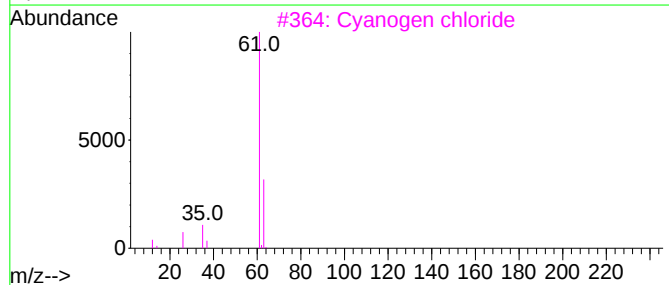
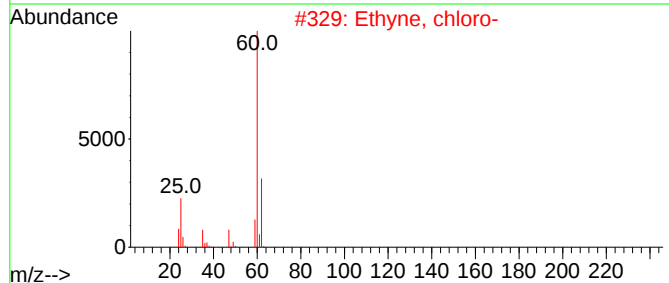
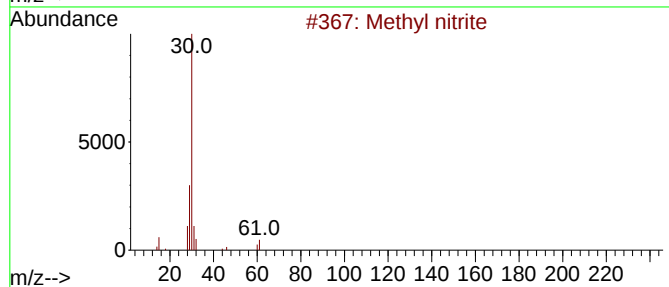
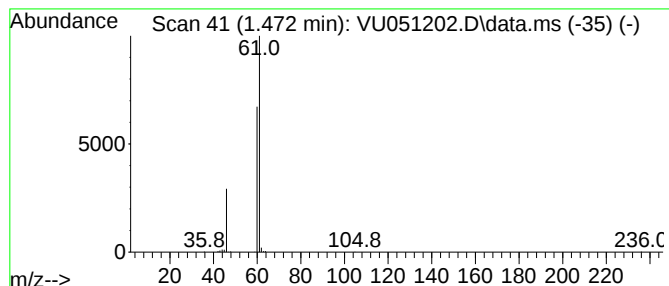
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

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.
1.472	7.12 ug/L	126892	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			Ethyne, chloro-	60	C2HCl	000593-63-5	5
3			Cyanogen chloride	61	CClN	000506-77-4	5
4			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
5			Methanamine, N-methoxy-	61	C2H7NO	001117-97-1	4



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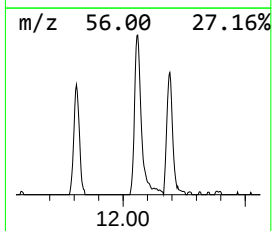
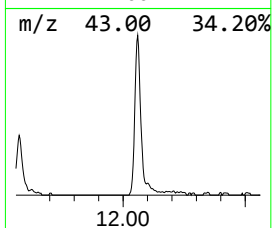
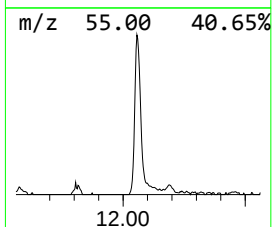
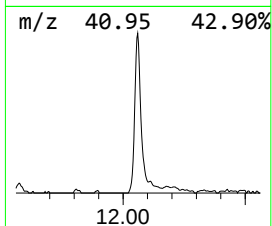
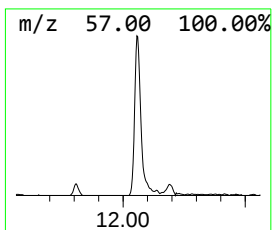
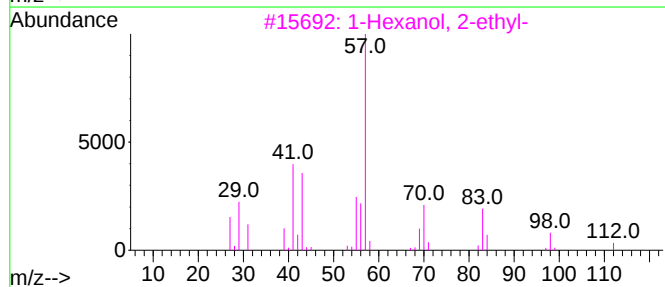
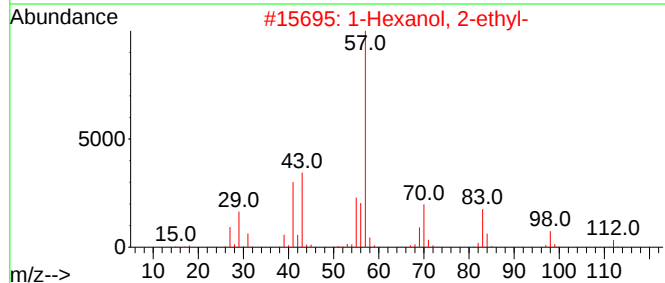
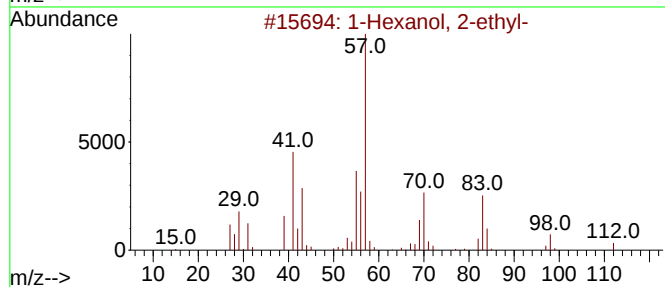
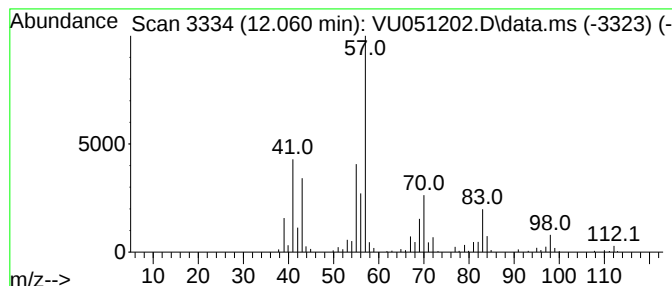
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

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.
12.060	13.73 ug/L	227747	1,4-Dichlorobenzene-d4	11.809

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	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.472	7.1	ug/L	126892	1	6.247	890971	50.0
1-Hexanol, 2-et...	12.060	13.7	ug/L	227747	3	11.809	829506	50.0