

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092622\
 Data File : VU050945.D
 Acq On : 26 Sep 2022 14:32
 Operator : JC/MD
 Sample : N4747-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E45A7

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\SFAMULM092022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050945.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	16	rVB2	16449	17358	1.27%	0.158%
2	1.488	43	46	52	rVB2	14788	12918	0.94%	0.118%
3	1.600	73	81	94	rVB	172096	203548	14.88%	1.857%
4	1.845	150	157	165	rBV	56988	71796	5.25%	0.655%
5	1.912	171	178	193	rVB	144930	193367	14.14%	1.764%
6	2.356	313	316	320	rBV5	1347	1134	0.08%	0.010%
7	2.568	367	382	397	rBV	254084	427241	31.24%	3.897%
8	2.793	446	452	454	rBV2	1471	1520	0.11%	0.014%
9	3.044	522	530	538	rBV4	3234	5509	0.40%	0.050%
10	3.124	550	555	556	rBV3	704	525	0.04%	0.005%
11	3.186	568	574	575	rBV	577	519	0.04%	0.005%
12	3.227	581	587	593	rVB4	637	892	0.07%	0.008%
13	3.356	621	627	636	rVB6	3420	5527	0.40%	0.050%
14	3.430	647	650	655	rVB2	427	321	0.02%	0.003%
15	3.584	689	698	702	rBV5	1100	1747	0.13%	0.016%
16	3.694	725	732	742	rVV4	1400	2192	0.16%	0.020%
17	3.874	768	788	804	rBV	19247	47537	3.48%	0.434%
18	4.231	893	899	900	rBV2	358	379	0.03%	0.003%
19	4.459	964	970	973	rBV3	517	493	0.04%	0.004%
20	4.536	982	994	998	rBV6	1268	2476	0.18%	0.023%
21	4.629	1010	1023	1031	rBV	171796	430409	31.47%	3.926%
22	4.896	1102	1106	1108	rBV2	480	410	0.03%	0.004%
23	5.063	1139	1158	1187	rVV2	251406	560513	40.98%	5.113%
24	5.378	1243	1256	1258	rBV5	2261	3199	0.23%	0.029%
25	5.584	1318	1320	1326	rBV2	342	310	0.02%	0.003%
26	5.726	1340	1364	1397	rBV2	494660	1367730	100.00%	12.476%
27	5.944	1428	1432	1434	rBV3	514	409	0.03%	0.004%
28	5.986	1441	1445	1447	rVV4	446	379	0.03%	0.003%
29	6.121	1483	1487	1489	rBV2	530	448	0.03%	0.004%
30	6.163	1496	1500	1506	rVB2	674	816	0.06%	0.007%
31	6.250	1513	1527	1547	rBV	349510	661109	48.34%	6.031%
32	6.346	1555	1557	1561	rVB3	560	339	0.02%	0.003%
33	6.542	1598	1618	1635	rBV	249559	486090	35.54%	4.434%
34	6.690	1649	1664	1681	rBV	327094	639596	46.76%	5.834%
35	6.867	1716	1719	1721	rBV4	840	596	0.04%	0.005%
36	6.890	1721	1726	1733	rVB5	1987	2581	0.19%	0.024%

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37	6.957	1742	1747	1750	rVB3	514	491	0.04%	0.004%
38	6.999	1750	1760	1761	rBV5	1414	1721	0.13%	0.016%
39	7.121	1795	1798	1806	rVB2	359	411	0.03%	0.004%
40	7.182	1812	1817	1830	rBV6	1853	3130	0.23%	0.029%
41	7.234	1830	1833	1838	rBV4	583	597	0.04%	0.005%
42	7.565	1924	1936	1956	rBV	156202	286336	20.94%	2.612%
43	7.690	1968	1975	1982	rBV5	1276	1843	0.13%	0.017%
44	7.787	2003	2005	2010	rBV2	373	360	0.03%	0.003%
45	7.809	2010	2012	2017	rVB3	582	343	0.03%	0.003%
46	7.848	2018	2024	2026	rBV3	417	453	0.03%	0.004%
47	7.896	2026	2039	2055	rBV	547131	958673	70.09%	8.745%
48	8.176	2112	2126	2151	rBV2	127340	260156	19.02%	2.373%
49	8.365	2181	2185	2188	rVB3	752	570	0.04%	0.005%
50	8.475	2210	2219	2222	rBV3	1237	1761	0.13%	0.016%
51	8.549	2236	2242	2246	rVB2	370	422	0.03%	0.004%
52	8.574	2246	2250	2252	rBV2	382	358	0.03%	0.003%
53	8.635	2256	2269	2299	rBV3	449562	954412	69.78%	8.706%
54	8.787	2307	2316	2333	rVB2	37052	63168	4.62%	0.576%
55	8.922	2351	2358	2361	rBV5	718	835	0.06%	0.008%
56	9.037	2391	2394	2398	rBV	481	315	0.02%	0.003%
57	9.105	2409	2415	2418	rVB2	565	442	0.03%	0.004%
58	9.144	2424	2427	2431	rBV	508	468	0.03%	0.004%
59	9.240	2453	2457	2461	rVB2	369	341	0.02%	0.003%
60	9.417	2498	2512	2531	rBV	514255	848478	62.04%	7.740%
61	9.568	2555	2559	2562	rBV4	855	726	0.05%	0.007%
62	9.635	2577	2580	2581	rBV	465	321	0.02%	0.003%
63	9.693	2590	2598	2609	rVV4	1811	3350	0.24%	0.031%
64	9.806	2630	2633	2637	rVB	416	329	0.02%	0.003%
65	10.343	2795	2800	2808	rVB6	1438	1732	0.13%	0.016%
66	10.414	2816	2822	2826	rBV2	355	376	0.03%	0.003%
67	10.571	2867	2871	2880	rVB2	430	491	0.04%	0.004%
68	10.671	2895	2902	2910	rBV6	1616	2280	0.17%	0.021%
69	10.754	2914	2928	2948	rBV	510449	811715	59.35%	7.404%
70	10.851	2955	2958	2961	rBV3	409	359	0.03%	0.003%
71	10.999	2998	3004	3008	rBV3	568	673	0.05%	0.006%
72	11.057	3018	3022	3027	rBV2	358	390	0.03%	0.004%
73	11.086	3027	3031	3035	rBV2	622	577	0.04%	0.005%
74	11.118	3038	3041	3045	rBV3	536	486	0.04%	0.004%
75	11.182	3058	3061	3071	rVB	465	563	0.04%	0.005%
76	11.304	3094	3099	3105	rVB4	689	750	0.05%	0.007%

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77	11.471	3140	3151	3159	rVB8	2070	3846	0.28%	0.035%
78	11.693	3214	3220	3226	rVB5	1322	1667	0.12%	0.015%
79	11.751	3235	3238	3244	rVB3	474	386	0.03%	0.004%
80	11.809	3244	3256	3279	rBV	425064	683685	49.99%	6.237%
81	11.973	3303	3307	3311	rBV3	460	388	0.03%	0.004%
82	12.063	3325	3335	3350	rBV4	18134	34281	2.51%	0.313%
83	12.192	3362	3375	3392	rBV	531099	864679	63.22%	7.888%
84	12.481	3462	3465	3469	rBV2	443	330	0.02%	0.003%
85	12.594	3495	3500	3501	rBV3	598	539	0.04%	0.005%
86	12.770	3551	3555	3562	rVB3	818	904	0.07%	0.008%
87	12.893	3586	3593	3600	rBV4	1556	2136	0.16%	0.019%
88	13.098	3653	3657	3658	rVV	522	369	0.03%	0.003%
89	13.124	3662	3665	3669	rVB2	482	339	0.02%	0.003%
90	13.147	3669	3672	3674	rBV2	549	366	0.03%	0.003%
91	13.285	3711	3715	3717	rBV2	607	421	0.03%	0.004%
92	13.420	3754	3757	3760	rBV	550	311	0.02%	0.003%
93	13.851	3887	3891	3899	rBV4	907	913	0.07%	0.008%
94	14.375	4050	4054	4058	rBV2	717	724	0.05%	0.007%
95	14.561	4109	4112	4113	rBV	686	416	0.03%	0.004%
96	14.822	4189	4193	4196	rBV2	779	746	0.05%	0.007%
97	14.954	4231	4234	4237	rBV3	537	344	0.03%	0.003%
98	14.995	4245	4247	4251	rBV3	731	393	0.03%	0.004%
99	15.494	4400	4402	4404	rBV2	754	420	0.03%	0.004%
100	15.568	4421	4425	4427	rBV4	874	821	0.06%	0.007%

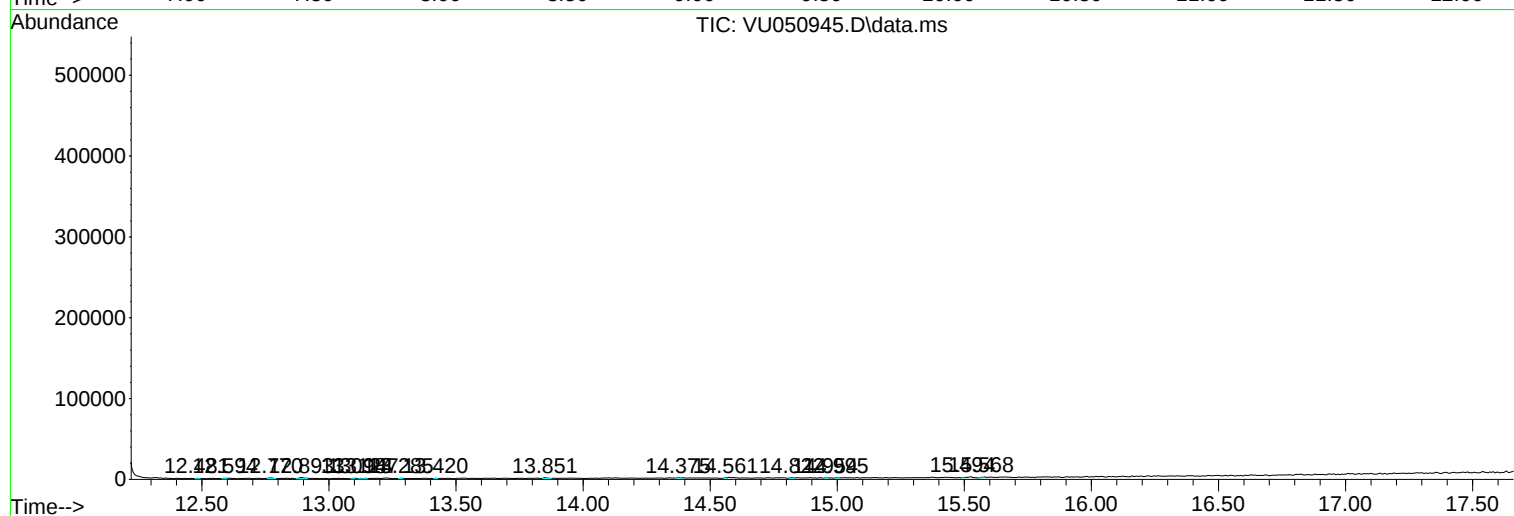
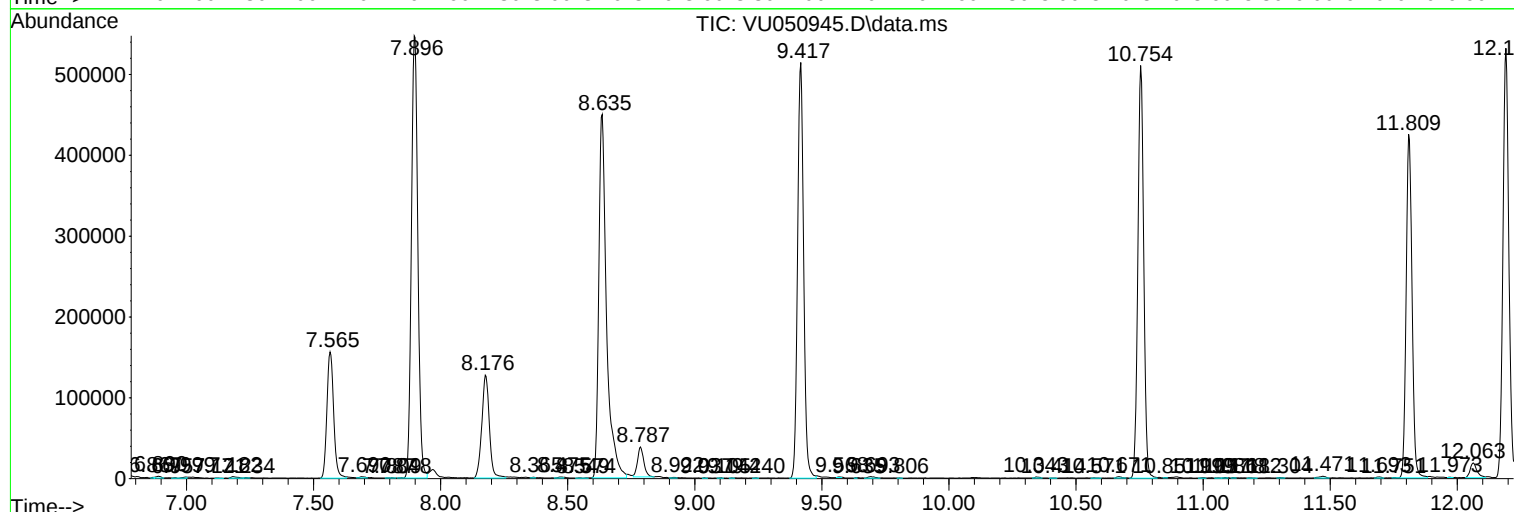
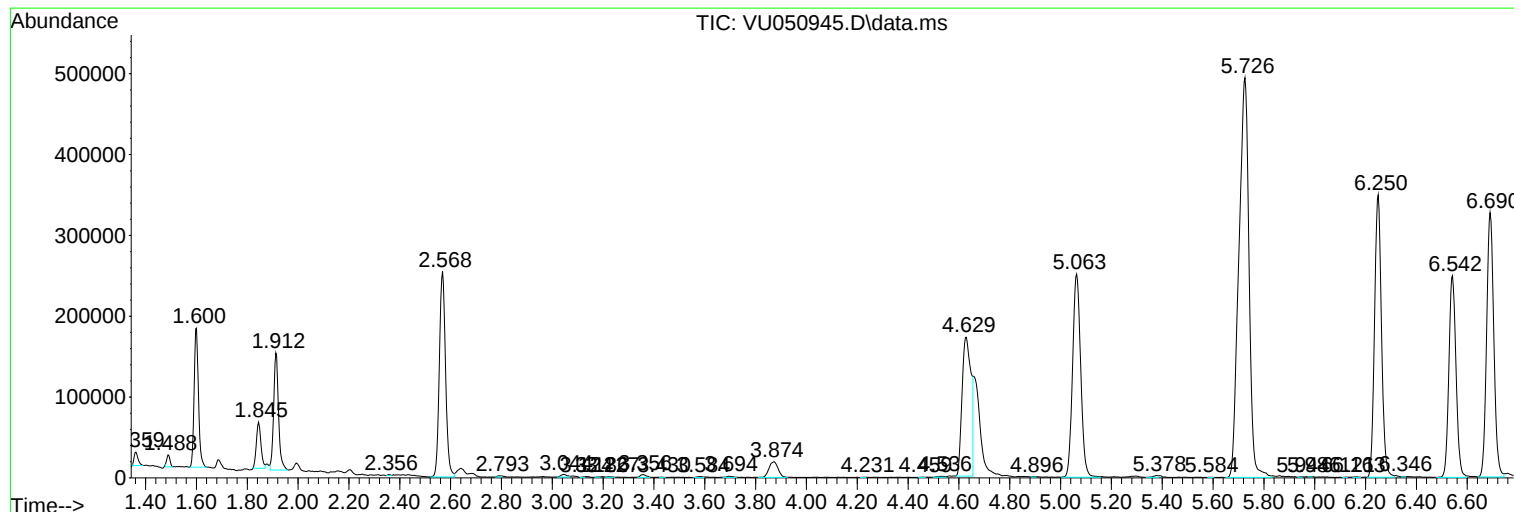
Sum of corrected areas: 10962559

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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



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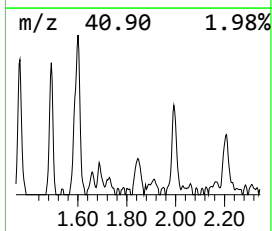
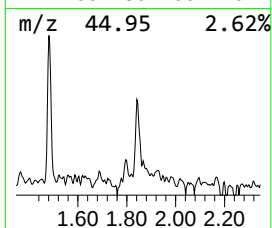
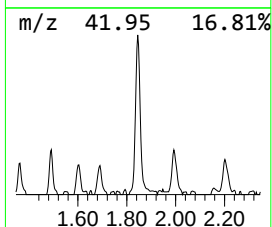
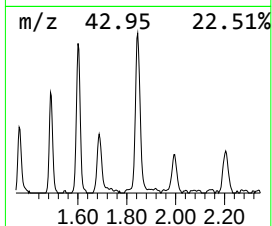
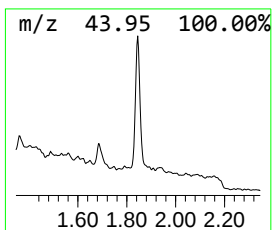
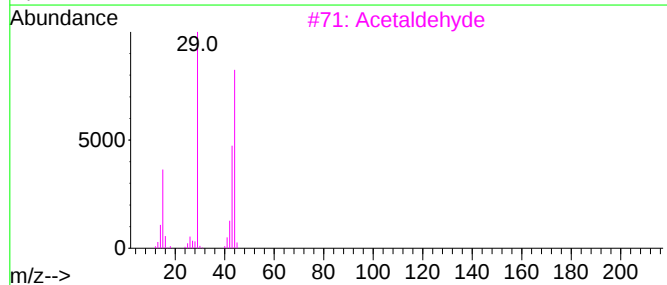
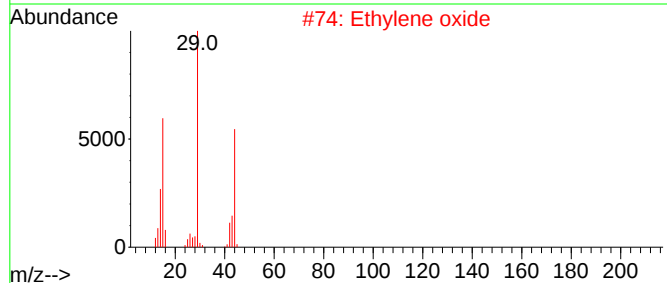
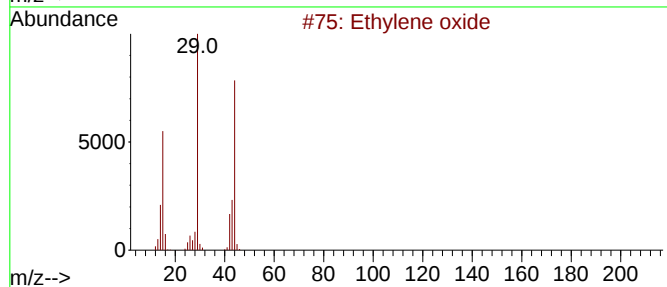
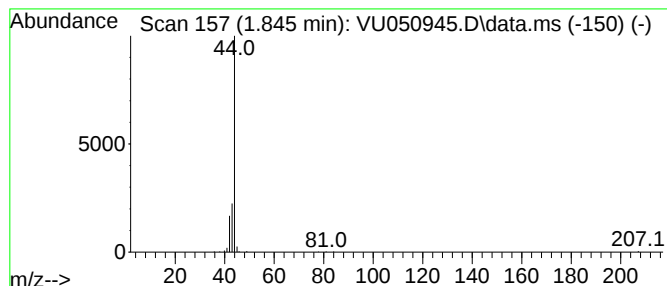
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.845	5.43 ug/L	71796	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene oxide	44	C2H4O	000075-21-8	9
2			Ethylene oxide	44	C2H4O	000075-21-8	9
3			Acetaldehyde	44	C2H4O	000075-07-0	5
4			Acetaldehyde	44	C2H4O	000075-07-0	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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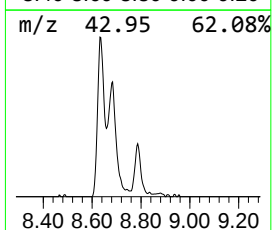
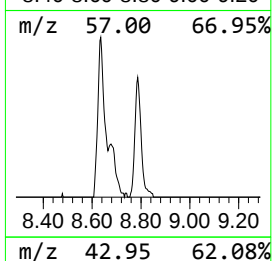
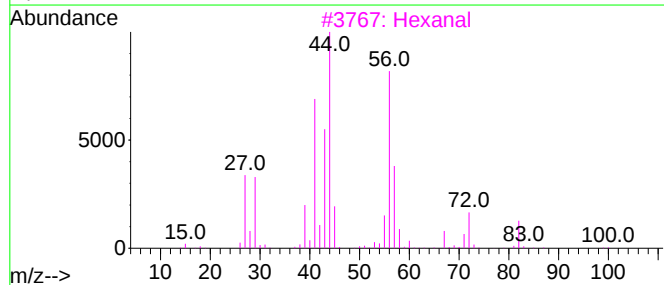
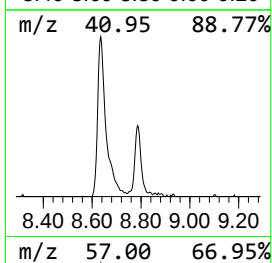
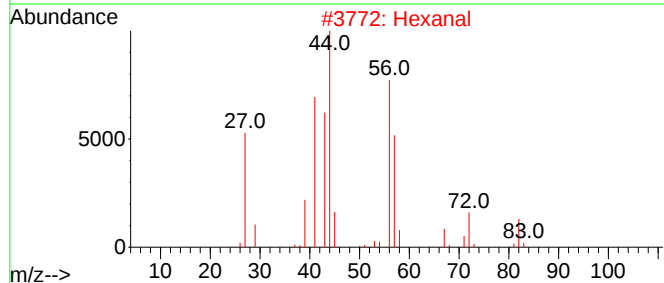
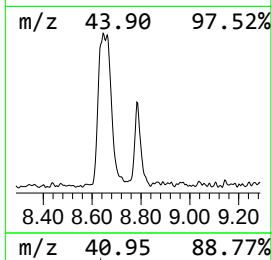
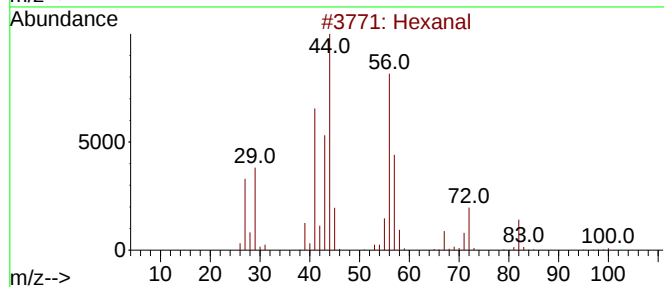
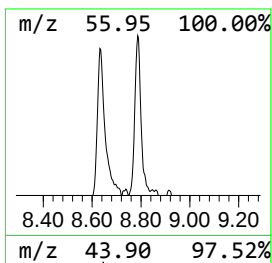
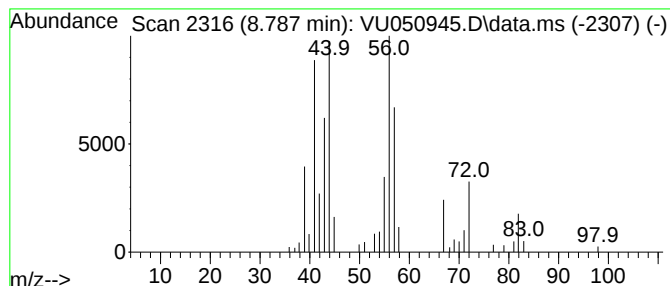
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	3.72 ug/L	63168	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	59
2	Hexanal			100	C6H12O	000066-25-1	59
3	Hexanal			100	C6H12O	000066-25-1	59
4	1-Pentene, 2-methyl-			84	C6H12	000763-29-1	35
5	1-Pentene, 2-methyl-			84	C6H12	000763-29-1	32



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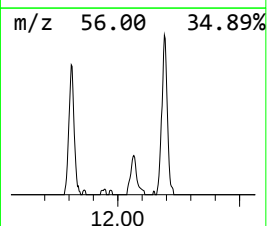
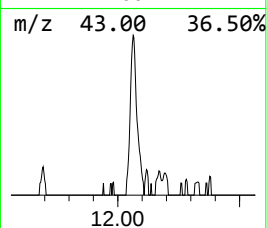
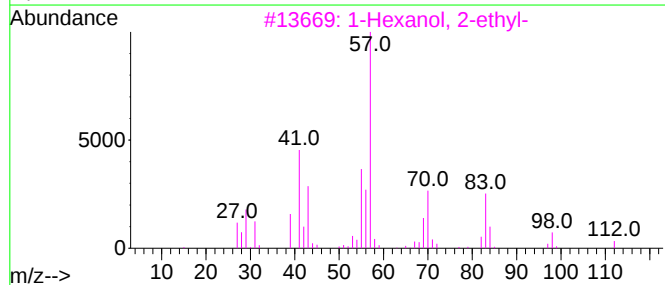
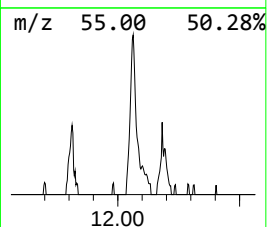
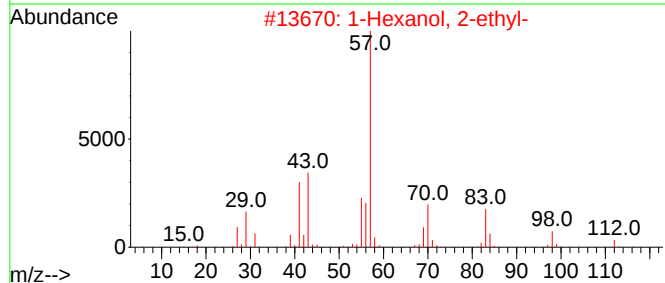
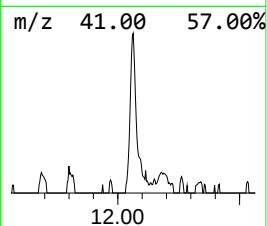
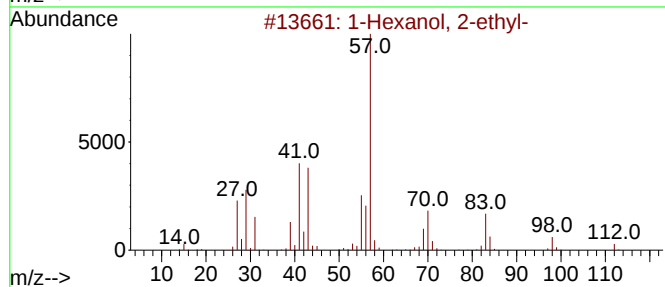
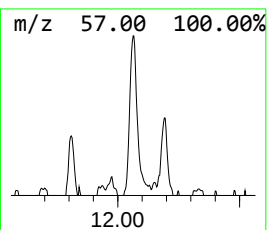
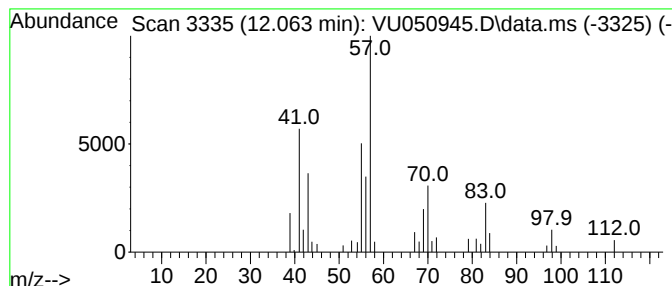
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	2.51 ug/L	34281	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	64
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	53
4	2-Octene			112	C8H16	000111-67-1	52
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092622\
Data File : VU050945.D
Acq On : 26 Sep 2022 14:32
Operator : JC/MD
Sample : N4747-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E45A7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.845	5.4	ug/L	71796	1	6.250	661109	50.0
Hexanal	8.787	3.7	ug/L	63168	2	9.417	848478	50.0
1-Hexanol, 2-et...	12.063	2.5	ug/L	34281	3	11.809	683685	50.0