

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061119\
 Data File : VU032598.D
 Acq On : 11 Jun 2019 10:42
 Operator : JC/SP
 Sample : K3277-15
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB8C0

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.180	24	28	36	rVB2	5428	5170	0.87%	0.090%
2	1.396	88	95	107	rVB	77723	80808	13.53%	1.412%
3	1.470	112	118	128	rVV	26509	29311	4.91%	0.512%
4	1.675	174	182	197	rVB	63078	79498	13.31%	1.389%
5	2.267	353	366	376	rVV	134613	208659	34.95%	3.647%
6	2.318	377	382	393	rVB2	8115	12472	2.09%	0.218%
7	2.383	399	402	404	rBV	400	230	0.04%	0.004%
8	2.441	409	420	437	rBV	23521	43017	7.20%	0.752%
9	2.563	455	458	462	rVB2	394	274	0.05%	0.005%
10	2.585	462	465	466	rBV2	344	203	0.03%	0.004%
11	2.650	482	485	493	rVB3	485	576	0.10%	0.010%
12	2.695	493	499	503	rBV2	411	405	0.07%	0.007%
13	2.830	534	541	551	rVB2	1156	2008	0.34%	0.035%
14	2.936	567	574	588	rVB2	907	1792	0.30%	0.031%
15	3.186	649	652	654	rBV3	310	203	0.03%	0.004%
16	3.354	698	704	708	rBV	206	272	0.05%	0.005%
17	3.447	726	733	737	rVV2	220	266	0.04%	0.005%
18	3.759	823	830	835	rBV2	196	311	0.05%	0.005%
19	3.997	888	904	921	rBV5	3665	10806	1.81%	0.189%
20	4.167	945	957	999	rVV	66622	178716	29.93%	3.123%
21	4.640	1089	1104	1134	rBV	101231	236682	39.64%	4.136%
22	4.788	1147	1150	1154	rVB3	414	339	0.06%	0.006%
23	4.887	1179	1181	1187	rVB3	415	406	0.07%	0.007%
24	5.019	1213	1222	1233	rBV3	1192	2218	0.37%	0.039%
25	5.109	1244	1250	1253	rBV2	244	231	0.04%	0.004%
26	5.141	1253	1260	1264	rVV	216	235	0.04%	0.004%
27	5.331	1297	1319	1345	rBV2	202371	597060	100.00%	10.434%
28	5.797	1462	1464	1470	rVB2	372	205	0.03%	0.004%
29	5.881	1474	1490	1510	rBV	206964	399839	66.97%	6.988%
30	5.993	1522	1525	1528	rBV2	256	204	0.03%	0.004%
31	6.180	1570	1583	1604	rBV	236509	463907	77.70%	8.107%
32	6.325	1616	1628	1653	rVB2	133819	267602	44.82%	4.677%
33	6.444	1662	1665	1667	rBV2	350	232	0.04%	0.004%
34	6.473	1672	1674	1678	rVV2	405	240	0.04%	0.004%

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 Title : VOC Analysis

35	6.540	1687	1695	1710	rBV3	2699	5977	1.00%	0.104%
36	7.058	1852	1856	1864	rVB2	185	210	0.04%	0.004%
37	7.116	1866	1874	1892	rVB3	2232	4161	0.70%	0.073%
38	7.222	1895	1907	1928	rBV	76339	140639	23.56%	2.458%
39	7.472	1979	1985	1991	rVB2	391	600	0.10%	0.010%
40	7.559	1997	2012	2030	rBV	269767	472042	79.06%	8.249%
41	7.845	2088	2101	2119	rBV	51803	91531	15.33%	1.600%
42	8.116	2178	2185	2188	rVB2	348	315	0.05%	0.006%
43	8.170	2197	2202	2211	rVB4	1161	1566	0.26%	0.027%
44	8.305	2234	2244	2282	rBV2	186619	371243	62.18%	6.488%
45	8.463	2285	2293	2306	rBV3	19589	32966	5.52%	0.576%
46	8.755	2381	2384	2390	rBV2	268	293	0.05%	0.005%
47	8.784	2390	2393	2402	rVB2	200	275	0.05%	0.005%
48	8.993	2451	2458	2463	rBV2	272	318	0.05%	0.006%
49	9.083	2475	2486	2516	rBV	295469	497122	83.26%	8.688%
50	9.238	2530	2534	2537	rBV3	266	236	0.04%	0.004%
51	9.299	2549	2553	2561	rBV3	264	247	0.04%	0.004%
52	9.392	2580	2582	2590	rVB3	302	225	0.04%	0.004%
53	9.530	2622	2625	2632	rBV2	253	208	0.03%	0.004%
54	9.562	2633	2635	2645	rVB2	274	288	0.05%	0.005%
55	9.611	2645	2650	2652	rBV2	205	203	0.03%	0.004%
56	9.720	2676	2684	2689	rBV2	395	528	0.09%	0.009%
57	9.784	2701	2704	2711	rVV3	373	322	0.05%	0.006%
58	10.029	2772	2780	2796	rBV5	8357	14348	2.40%	0.251%
59	10.164	2819	2822	2828	rVB2	392	342	0.06%	0.006%
60	10.234	2839	2844	2846	rBV	317	252	0.04%	0.004%
61	10.302	2859	2865	2872	rBV	273	451	0.08%	0.008%
62	10.427	2891	2904	2927	rVB	204142	328098	54.95%	5.734%
63	10.537	2933	2938	2941	rBV3	305	287	0.05%	0.005%
64	10.601	2951	2958	2969	rVB2	1362	2195	0.37%	0.038%
65	10.746	2995	3003	3016	rVB3	1443	2580	0.43%	0.045%
66	10.807	3017	3022	3023	rBV2	292	226	0.04%	0.004%
67	10.823	3023	3027	3032	rVB4	315	340	0.06%	0.006%
68	10.935	3058	3062	3063	rBV2	349	209	0.04%	0.004%
69	11.035	3089	3093	3096	rBV	306	236	0.04%	0.004%
70	11.099	3109	3113	3115	rVB2	336	282	0.05%	0.005%
71	11.164	3128	3133	3140	rVB3	431	537	0.09%	0.009%

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72	11.228	3149	3153	3155	rBV2	254	212	0.04%	0.004%
73	11.260	3157	3163	3180	rVB5	2057	4308	0.72%	0.075%
74	11.366	3180	3196	3217	rBV2	30222	52645	8.82%	0.920%
75	11.479	3220	3231	3252	rVV	316701	503852	84.39%	8.805%
76	11.611	3270	3272	3275	rBV2	272	215	0.04%	0.004%
77	11.755	3309	3317	3327	rBV5	3030	5854	0.98%	0.102%
78	11.855	3336	3348	3375	rBV	286240	471649	79.00%	8.243%
79	12.070	3409	3415	3425	rVB4	1348	2315	0.39%	0.040%
80	12.151	3437	3440	3445	rVB2	262	238	0.04%	0.004%
81	12.180	3445	3449	3452	rBV2	338	276	0.05%	0.005%
82	12.270	3473	3477	3481	rBV2	350	334	0.06%	0.006%
83	12.295	3482	3485	3488	rBV3	526	378	0.06%	0.007%
84	12.347	3499	3501	3504	rVB2	453	259	0.04%	0.005%
85	12.373	3504	3509	3514	rBV2	405	541	0.09%	0.009%
86	12.418	3519	3523	3526	rBV2	238	213	0.04%	0.004%
87	12.476	3534	3541	3549	rVB4	913	1623	0.27%	0.028%
88	12.566	3559	3569	3593	rBV2	39635	75050	12.57%	1.312%
89	12.890	3665	3670	3674	rVV3	512	698	0.12%	0.012%
90	12.913	3674	3677	3680	rVB2	760	562	0.09%	0.010%
91	12.948	3685	3688	3690	rBV2	356	218	0.04%	0.004%
92	13.170	3753	3757	3758	rBV2	425	281	0.05%	0.005%
93	13.212	3765	3770	3773	rBV3	401	364	0.06%	0.006%
94	13.302	3793	3798	3801	rBV3	373	386	0.06%	0.007%
95	13.344	3806	3811	3814	rBV	347	261	0.04%	0.005%
96	13.559	3875	3878	3880	rBV2	366	267	0.04%	0.005%
97	14.051	4027	4031	4034	rBV2	316	308	0.05%	0.005%
98	14.119	4049	4052	4060	rVB3	392	411	0.07%	0.007%
99	14.279	4093	4102	4108	rBV3	818	1614	0.27%	0.028%
100	15.768	4561	4565	4570	rBV4	445	505	0.08%	0.009%

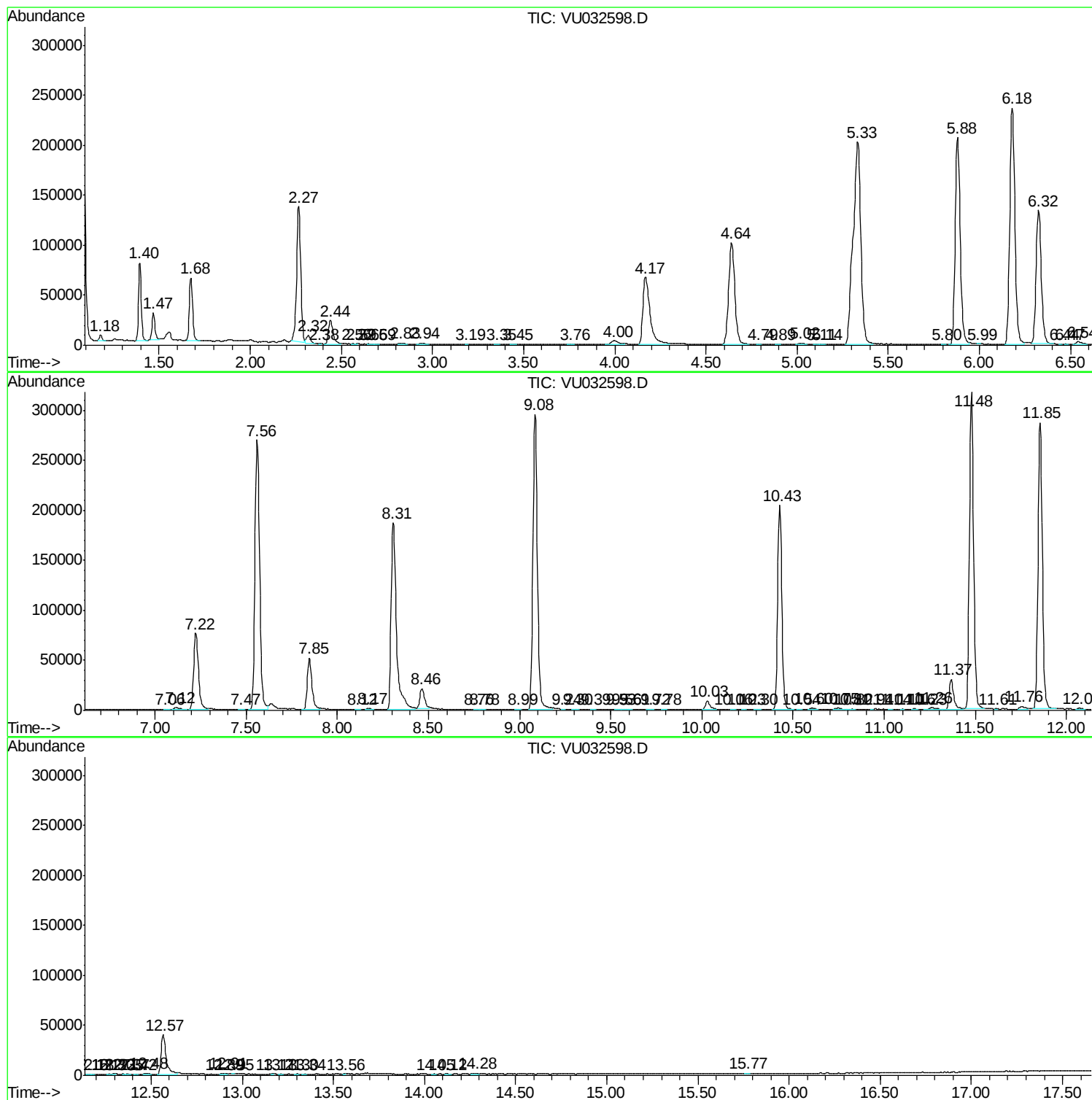
Sum of corrected areas: 5722132

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Quant Title : VOC Analysis

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



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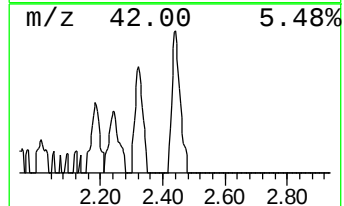
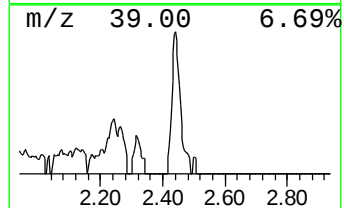
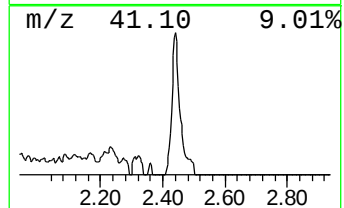
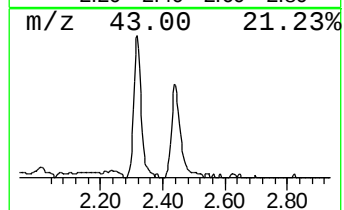
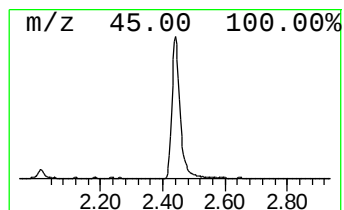
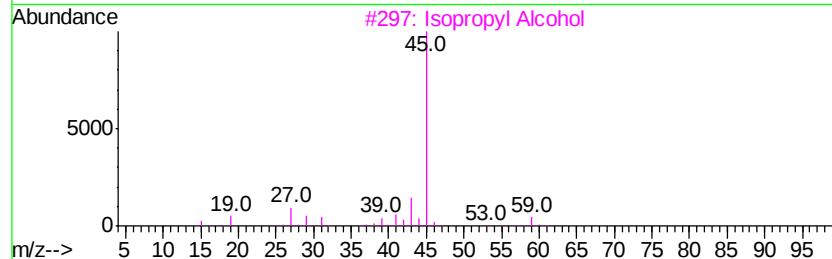
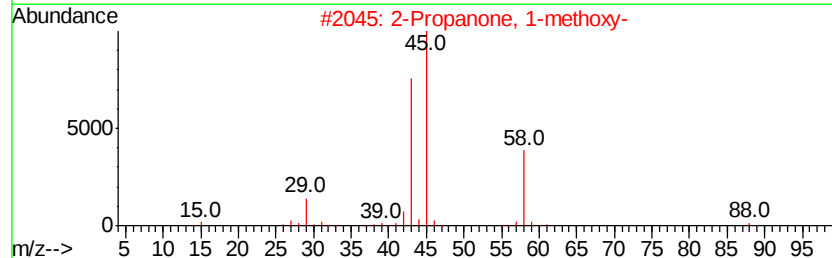
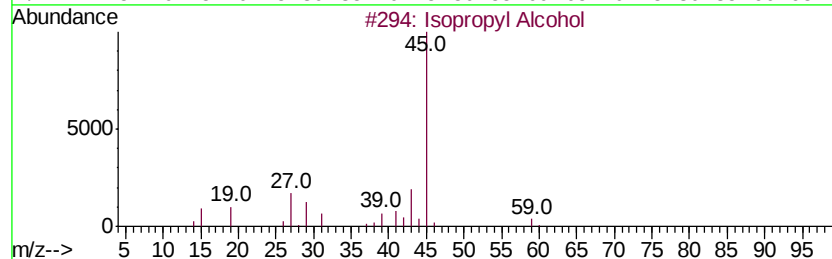
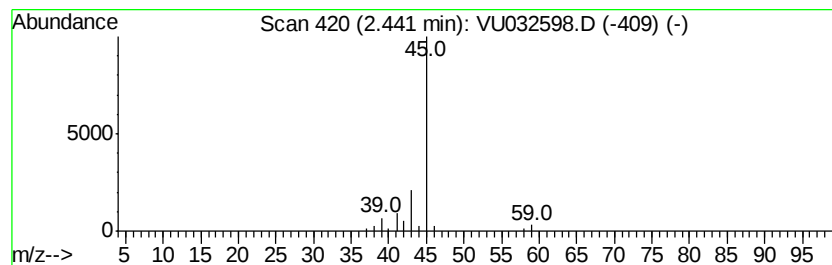
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	5.38 ug/L	43017	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	43
2		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Ethylamine	45	C2H7N	000075-04-7	5



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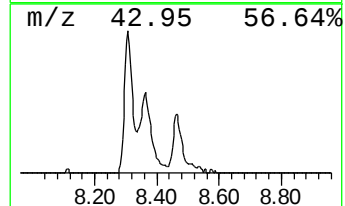
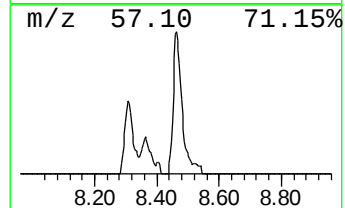
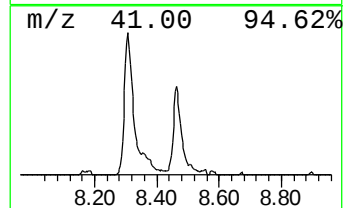
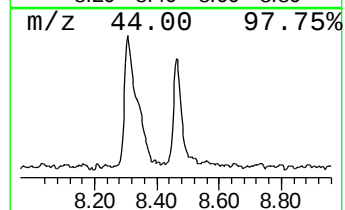
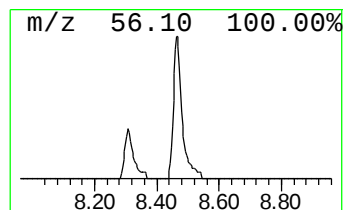
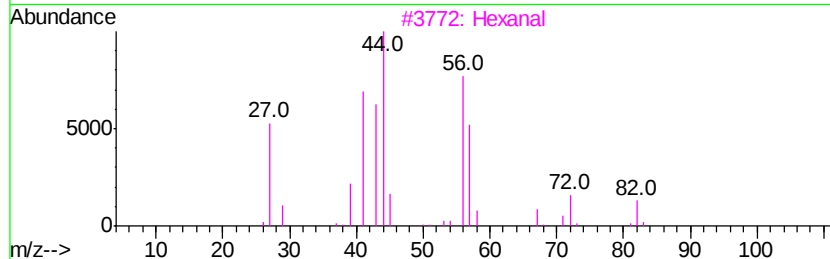
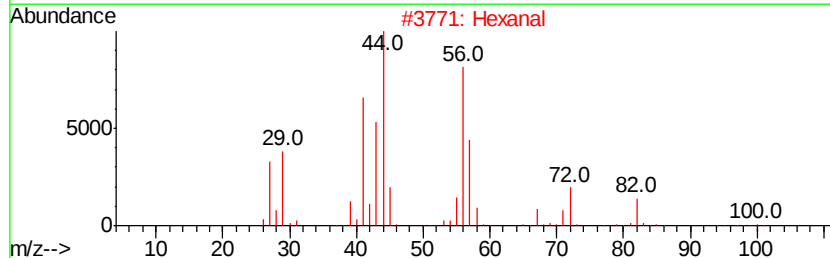
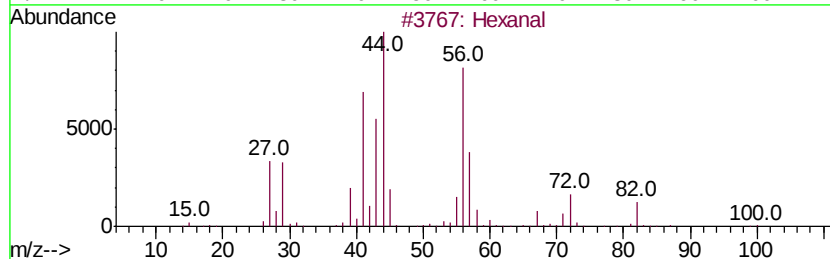
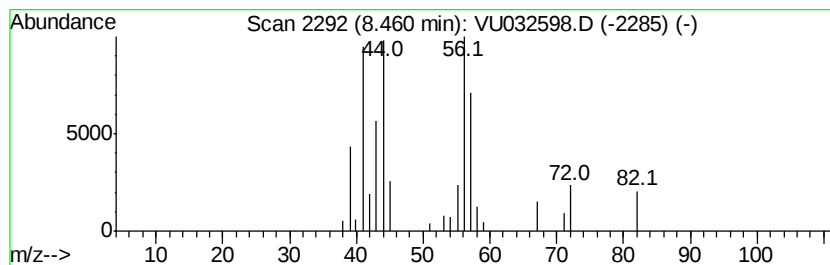
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	3.32 ug/L	32966	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	80
2		Hexanal	100	C6H12O	000066-25-1	64
3		Hexanal	100	C6H12O	000066-25-1	59
4		Hexanal	100	C6H12O	000066-25-1	50
5		2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	32



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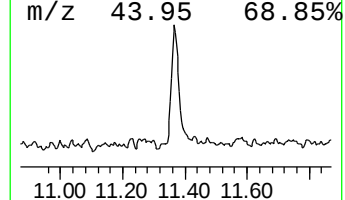
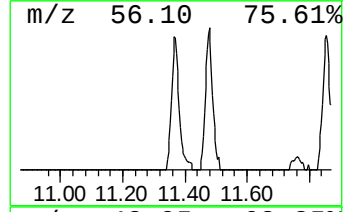
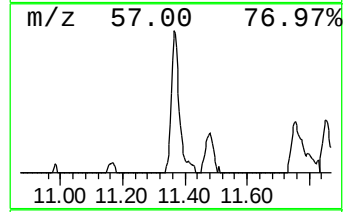
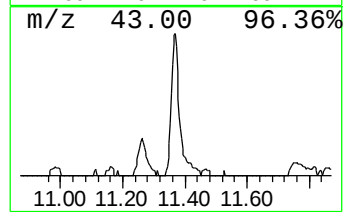
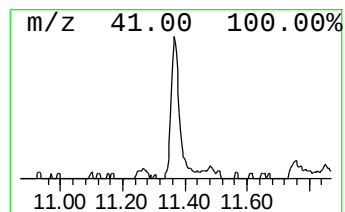
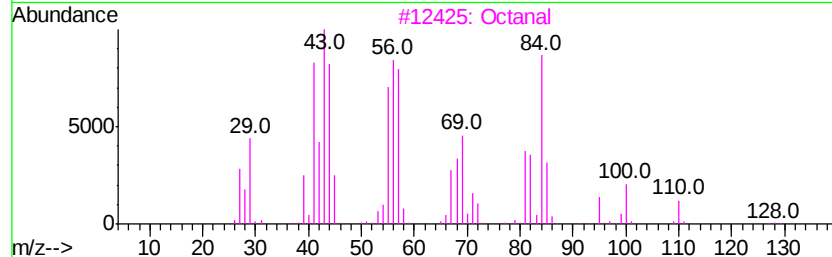
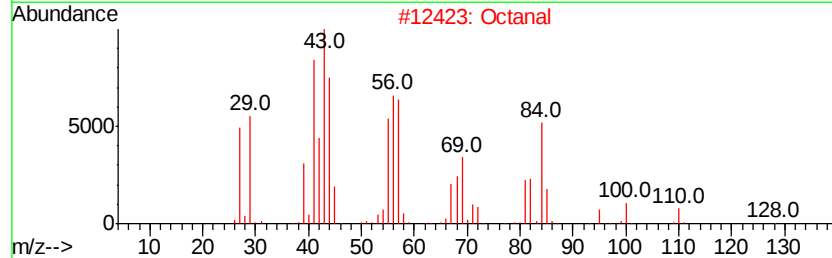
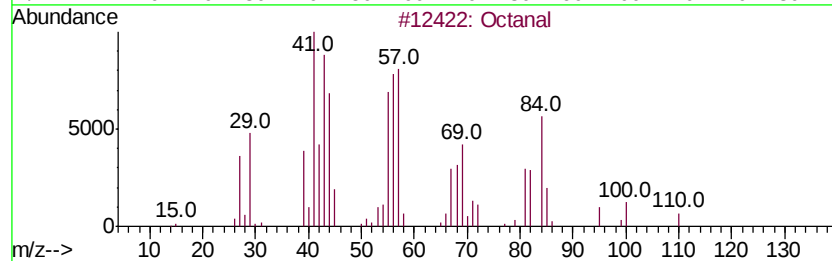
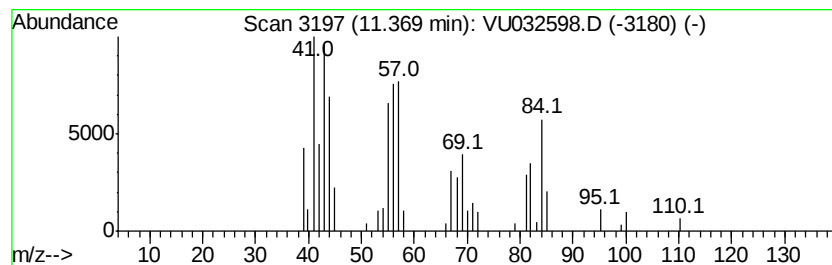
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Quant Title : VOC Analysis

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

Peak Number 5 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.37	5.22 ug/L	52645	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanal	128	C8H16O	000124-13-0	91
2		Octanal	128	C8H16O	000124-13-0	86
3		Octanal	128	C8H16O	000124-13-0	83
4		Octanal	128	C8H16O	000124-13-0	80
5		Octanal	128	C8H16O	000124-13-0	72



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Operator : JC/SP
Sample : K3277-15
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

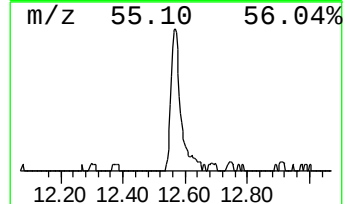
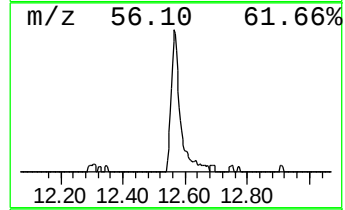
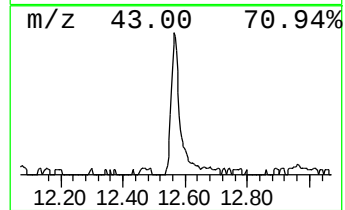
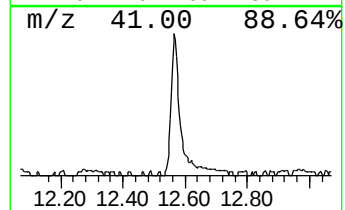
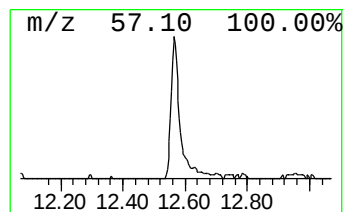
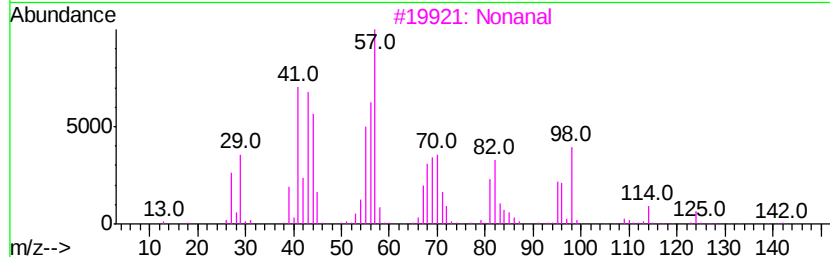
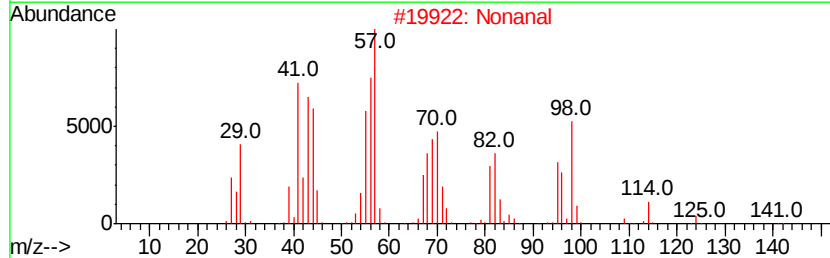
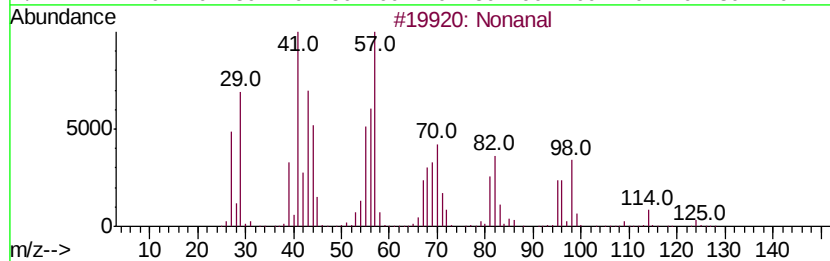
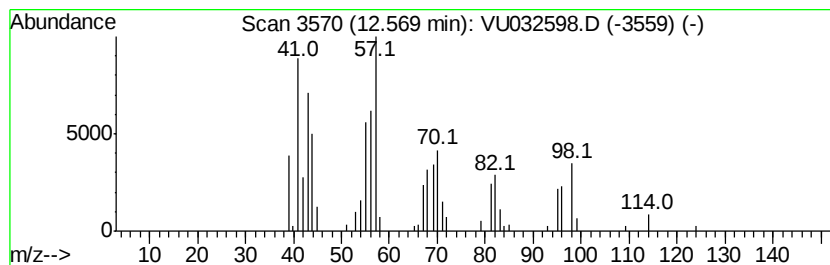
Instrument :
MSVOA_U
ClientSampleId :
DB8C0

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	7.45 ug/L	75050	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonanal		142 C9H18O	000124-19-6 91
2	Nonanal		142 C9H18O	000124-19-6 91
3	Nonanal		142 C9H18O	000124-19-6 91
4	Nonanal		142 C9H18O	000124-19-6 90
5	2-Nonen-1-ol, (E)-		142 C9H18O	031502-14-4 35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU061119\
Data File : VU032598.D
Acq On : 11 Jun 2019 10:42
Operator : JC/SP
Sample : K3277-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB8C0

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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	2.44	5.4	ug/L	43017	1	5.88	399839	50.0
Hexanal	8.46	3.3	ug/L	32966	2	9.08	497122	50.0
Octanal	11.37	5.2	ug/L	52645	3	11.48	503852	50.0
Nonanal	12.57	7.5	ug/L	75050	3	11.48	503852	50.0