

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061019\
 Data File : VU032578.D
 Acq On : 10 Jun 2019 20:25
 Operator : JC/SP
 Sample : K3277-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB8B9

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	39	rVB2	5960	5875	0.42%	0.076%
2	1.395	88	95	105	rVB	95125	99749	7.20%	1.284%
3	1.469	111	118	129	rBV	59710	66591	4.80%	0.857%
4	1.672	174	181	195	rVB	74336	92902	6.70%	1.196%
5	2.267	351	366	376	rBV	164029	264269	19.07%	3.403%
6	2.318	376	382	398	rVB	19101	30529	2.20%	0.393%
7	2.440	411	420	438	rBV	33622	58569	4.23%	0.754%
8	2.826	533	540	541	rBV	786	728	0.05%	0.009%
9	2.939	570	575	579	rBV3	355	414	0.03%	0.005%
10	2.961	579	582	589	rVV2	183	224	0.02%	0.003%
11	3.193	644	654	660	rVB5	600	1178	0.08%	0.015%
12	3.357	700	705	708	rBV2	228	214	0.02%	0.003%
13	3.415	721	723	729	rVV2	283	243	0.02%	0.003%
14	3.440	729	731	740	rVB2	319	384	0.03%	0.005%
15	3.482	740	744	748	rBV2	256	225	0.02%	0.003%
16	3.617	783	786	792	rBV2	307	288	0.02%	0.004%
17	3.997	894	904	920	rBV4	3808	9825	0.71%	0.127%
18	4.170	945	958	992	rBV	74856	199210	14.37%	2.565%
19	4.434	1037	1040	1046	rVB2	308	273	0.02%	0.004%
20	4.640	1088	1104	1128	rBV	117408	273150	19.71%	3.517%
21	4.890	1174	1182	1190	rVB3	440	708	0.05%	0.009%
22	5.334	1297	1320	1350	rBV2	242517	703703	50.77%	9.061%
23	5.569	1390	1393	1396	rBV2	287	253	0.02%	0.003%
24	5.698	1427	1433	1436	rBV3	280	311	0.02%	0.004%
25	5.794	1458	1463	1465	rBV3	422	340	0.02%	0.004%
26	5.881	1476	1490	1516	rBV	226868	441482	31.85%	5.685%
27	6.180	1569	1583	1615	rBV	724193	1386039	100.00%	17.847%
28	6.325	1616	1628	1656	rVB	155658	314044	22.66%	4.044%
29	6.443	1662	1665	1666	rBV2	699	462	0.03%	0.006%
30	6.534	1686	1693	1709	rVB4	5193	10657	0.77%	0.137%
31	6.733	1751	1755	1760	rVV	291	243	0.02%	0.003%
32	6.839	1785	1788	1793	rVB	349	240	0.02%	0.003%
33	6.929	1813	1816	1820	rVV2	199	223	0.02%	0.003%
34	7.032	1843	1848	1854	rVB	162	215	0.02%	0.003%

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

35	7.222	1896	1907	1931	rBV	89789	162942	11.76%	2.098%
36	7.476	1983	1986	1989	rVB2	309	216	0.02%	0.003%
37	7.559	2000	2012	2037	rBV	325146	573992	41.41%	7.391%
38	7.845	2090	2101	2120	rBV	60298	105731	7.63%	1.361%
39	8.135	2187	2191	2195	rVB2	326	311	0.02%	0.004%
40	8.164	2195	2200	2202	rBV2	449	458	0.03%	0.006%
41	8.228	2212	2220	2228	rVB3	2526	3696	0.27%	0.048%
42	8.305	2233	2244	2277	rBV	225783	432844	31.23%	5.573%
43	8.463	2284	2293	2315	rVB2	30259	54336	3.92%	0.700%
44	8.733	2374	2377	2382	rVB2	339	271	0.02%	0.003%
45	8.762	2382	2386	2390	rBV	265	210	0.02%	0.003%
46	8.861	2412	2417	2423	rVB2	203	256	0.02%	0.003%
47	9.083	2474	2486	2524	rBV	327072	546820	39.45%	7.041%
48	9.350	2564	2569	2573	rBV	231	260	0.02%	0.003%
49	9.482	2607	2610	2615	rVB2	269	260	0.02%	0.003%
50	9.527	2620	2624	2627	rVB2	220	202	0.01%	0.003%
51	9.553	2627	2632	2638	rBV3	338	366	0.03%	0.005%
52	9.730	2683	2687	2688	rVV3	278	226	0.02%	0.003%
53	9.929	2741	2749	2759	rBV2	2462	4170	0.30%	0.054%
54	9.987	2764	2767	2769	rVV2	301	206	0.01%	0.003%
55	10.029	2769	2780	2802	rVV2	18125	32406	2.34%	0.417%
56	10.160	2817	2821	2824	rBV2	327	292	0.02%	0.004%
57	10.376	2882	2888	2892	rBV2	200	222	0.02%	0.003%
58	10.427	2892	2904	2920	rBV	226127	361946	26.11%	4.660%
59	10.601	2952	2958	2960	rBV2	460	457	0.03%	0.006%
60	10.726	2992	2997	2999	rBV2	876	759	0.05%	0.010%
61	10.739	2999	3001	3007	rVB4	1106	1000	0.07%	0.013%
62	10.803	3012	3021	3025	rBV3	923	1338	0.10%	0.017%
63	10.829	3025	3029	3040	rVB4	1057	1401	0.10%	0.018%
64	10.945	3056	3065	3068	rBV4	610	905	0.07%	0.012%
65	10.961	3068	3070	3072	rVV2	459	292	0.02%	0.004%
66	10.980	3072	3076	3083	rVB4	1306	1695	0.12%	0.022%
67	11.041	3089	3095	3097	rBV4	1313	1491	0.11%	0.019%
68	11.160	3124	3132	3139	rBV6	1823	2777	0.20%	0.036%
69	11.254	3154	3161	3175	rBV3	7755	13274	0.96%	0.171%
70	11.366	3186	3196	3219	rBV2	72615	116885	8.43%	1.505%
71	11.479	3219	3231	3252	rBV	359190	565750	40.82%	7.285%

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72	11.633	3276	3279	3281	rBV3	554	361	0.03%	0.005%
73	11.749	3305	3315	3329	rBV3	6867	15424	1.11%	0.199%
74	11.855	3336	3348	3379	rVB	348054	562466	40.58%	7.242%
75	12.067	3409	3414	3423	rVB5	1282	1914	0.14%	0.025%
76	12.122	3423	3431	3439	rBV3	6086	8910	0.64%	0.115%
77	12.173	3440	3447	3455	rVB6	4298	5937	0.43%	0.076%
78	12.241	3460	3468	3472	rBV4	4222	6499	0.47%	0.084%
79	12.456	3527	3535	3545	rBV3	4065	6619	0.48%	0.085%
80	12.565	3554	3569	3582	rBV	56447	94741	6.84%	1.220%
81	12.681	3598	3605	3614	rVB4	8114	11566	0.83%	0.149%
82	12.842	3652	3655	3657	rBV3	578	392	0.03%	0.005%
83	12.893	3668	3671	3673	rBV3	536	387	0.03%	0.005%
84	12.958	3682	3691	3703	rVB8	8356	15154	1.09%	0.195%
85	13.038	3709	3716	3725	rBV5	2608	3412	0.25%	0.044%
86	13.093	3730	3733	3736	rBV4	478	281	0.02%	0.004%
87	13.215	3768	3771	3772	rBV	550	281	0.02%	0.004%
88	13.234	3773	3777	3779	rVV3	690	640	0.05%	0.008%
89	13.292	3790	3795	3806	rVB5	1433	1999	0.14%	0.026%
90	13.389	3817	3825	3835	rVV5	4850	7525	0.54%	0.097%
91	13.495	3849	3858	3868	rBV3	16156	28116	2.03%	0.362%
92	13.598	3884	3890	3896	rBV5	3205	4083	0.29%	0.053%
93	13.668	3905	3912	3923	rVB5	12685	21947	1.58%	0.283%
94	13.855	3967	3970	3972	rBV3	298	200	0.01%	0.003%
95	13.929	3987	3993	4006	rVB7	6110	9764	0.70%	0.126%
96	14.160	4059	4065	4073	rVV6	1111	1691	0.12%	0.022%
97	14.292	4102	4106	4109	rBV3	733	645	0.05%	0.008%
98	14.379	4130	4133	4135	rBV2	358	205	0.01%	0.003%
99	15.006	4324	4328	4331	rBV2	471	445	0.03%	0.006%
100	16.215	4701	4704	4705	rBV2	627	339	0.02%	0.004%

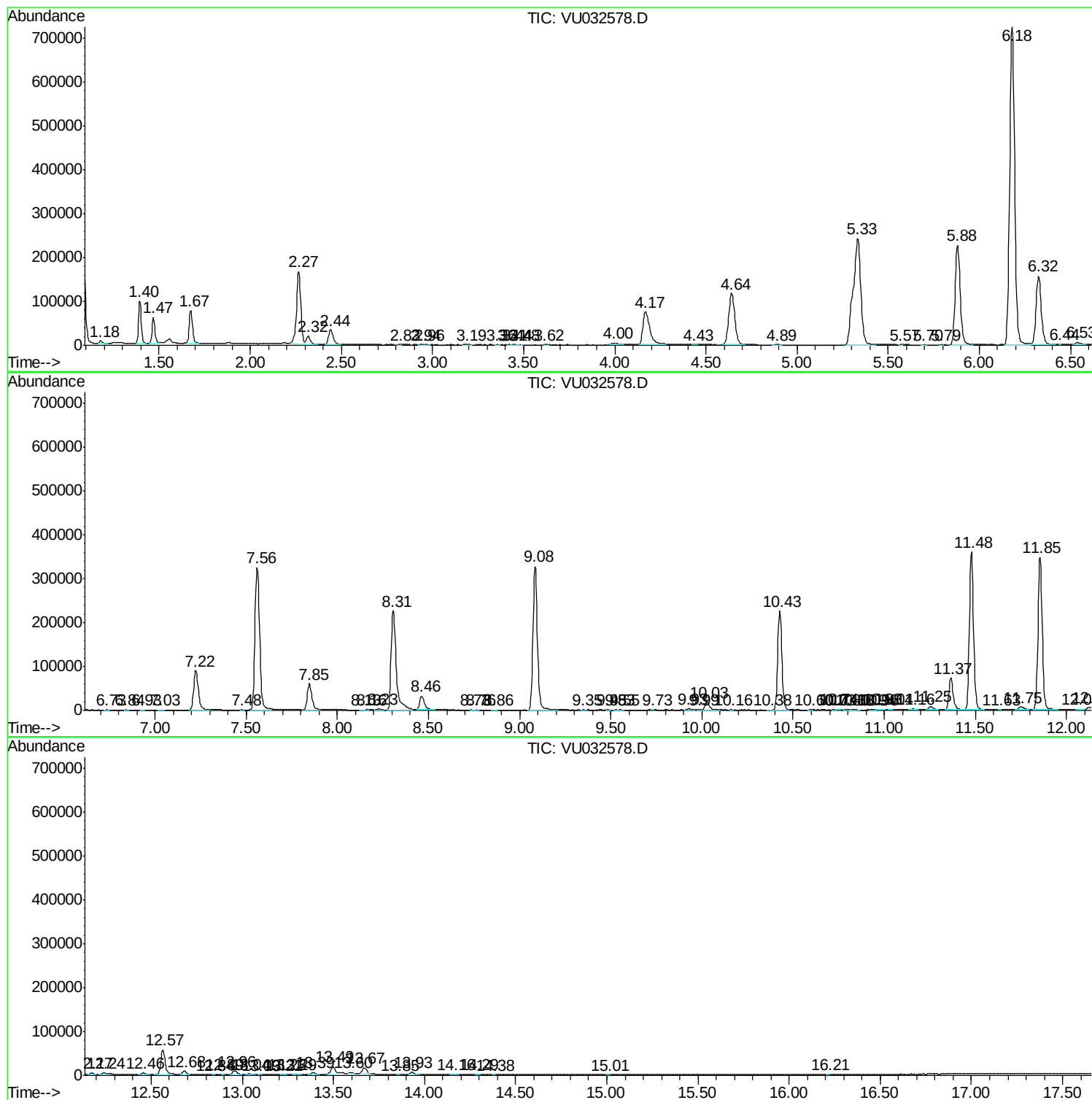
Sum of corrected areas: 7766366

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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



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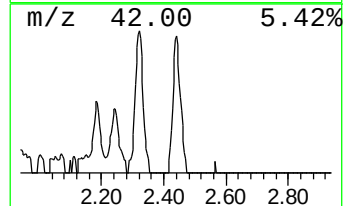
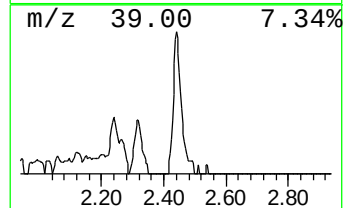
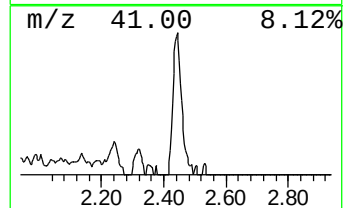
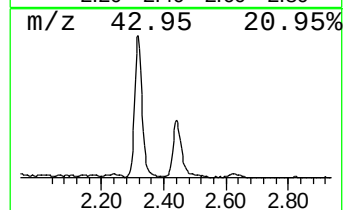
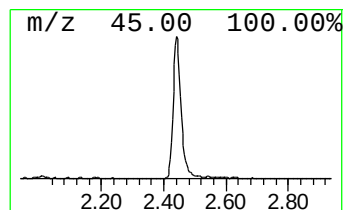
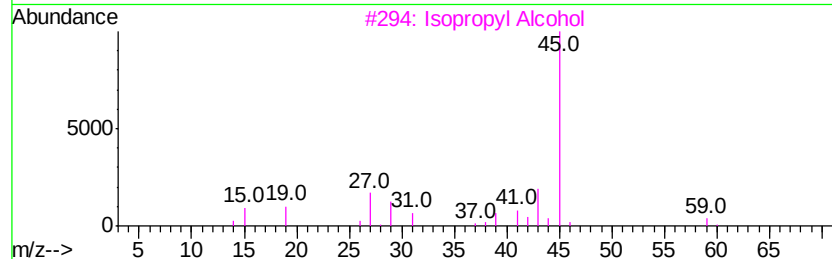
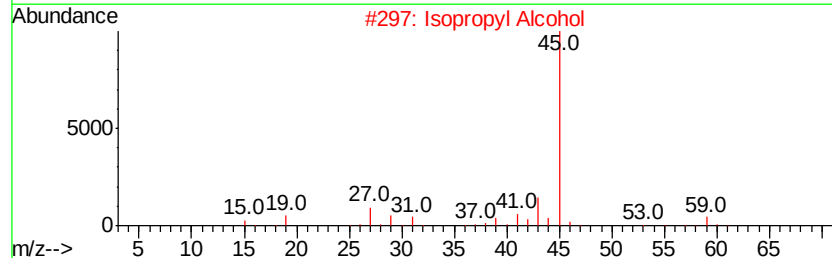
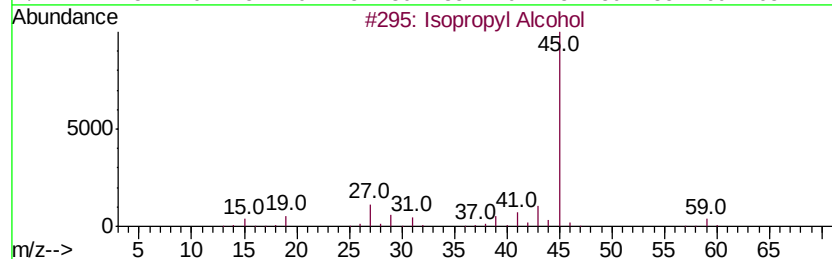
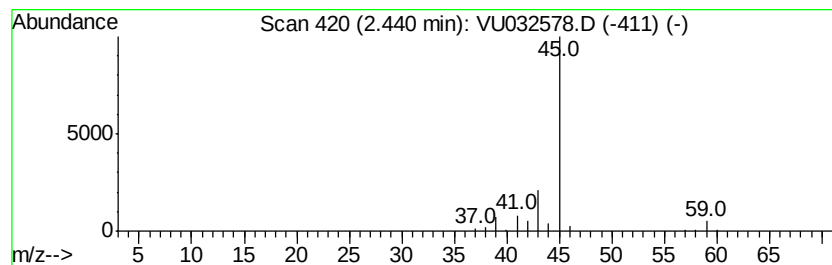
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	6.63 ug/L	58569	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	90
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40



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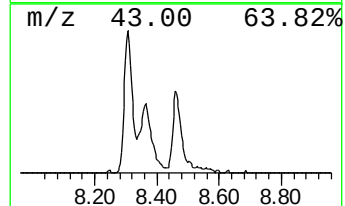
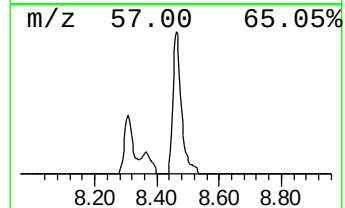
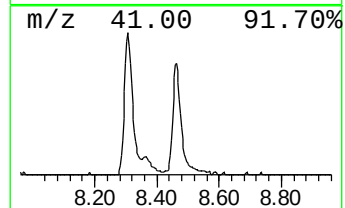
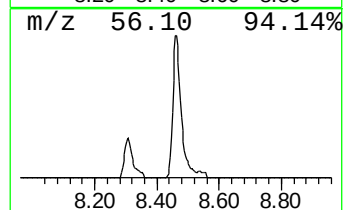
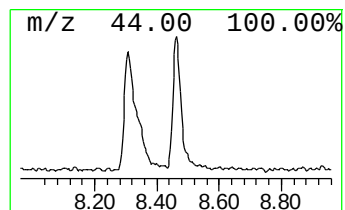
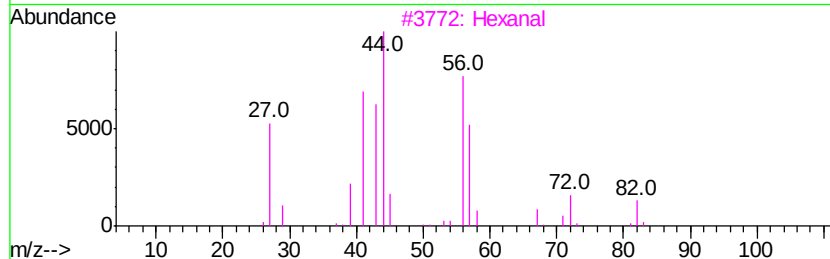
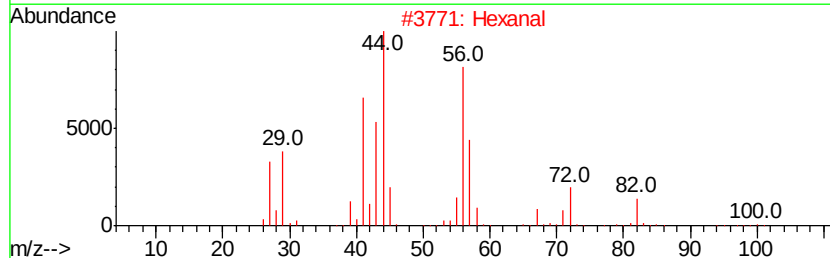
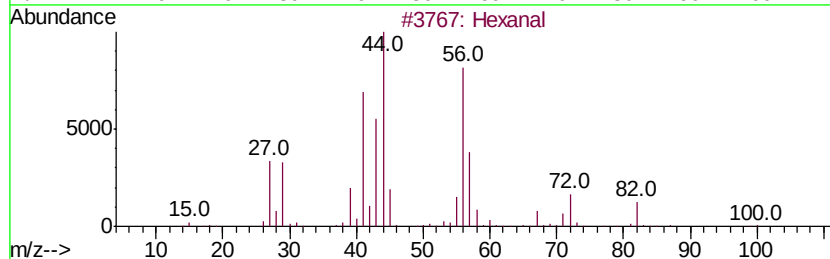
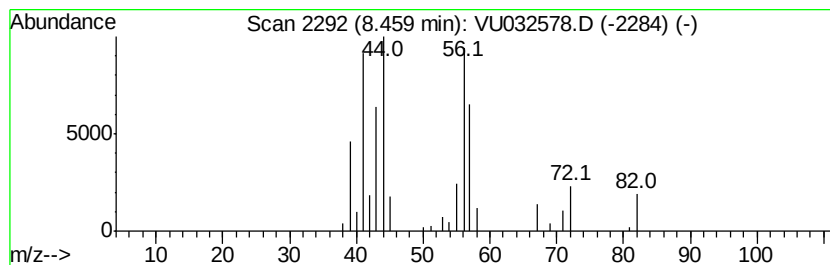
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	4.97 ug/L	54336	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	72
2		Hexanal	100	C6H12O	000066-25-1	72
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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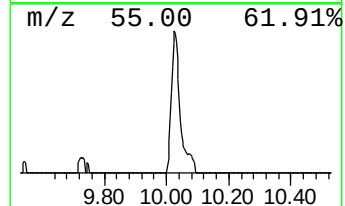
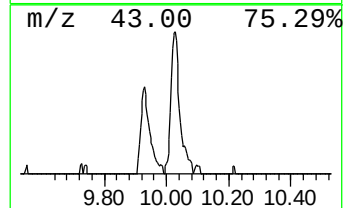
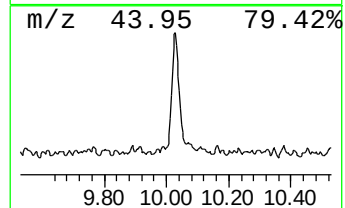
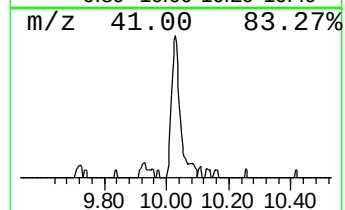
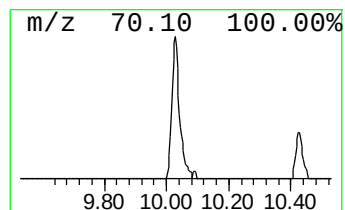
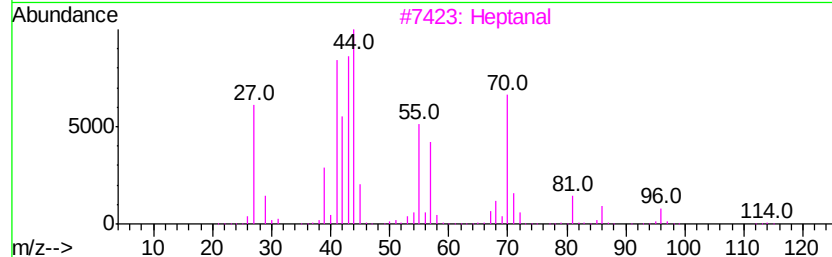
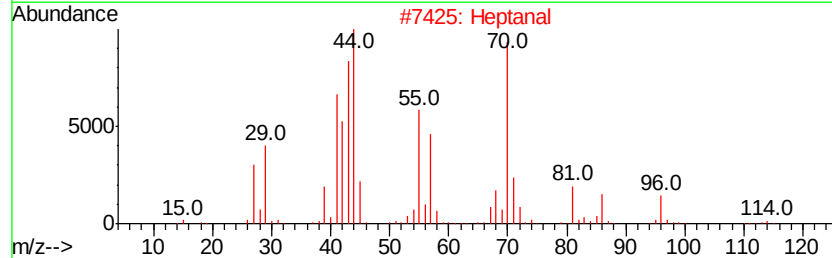
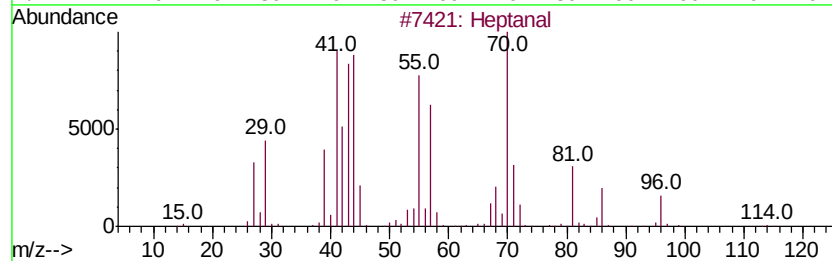
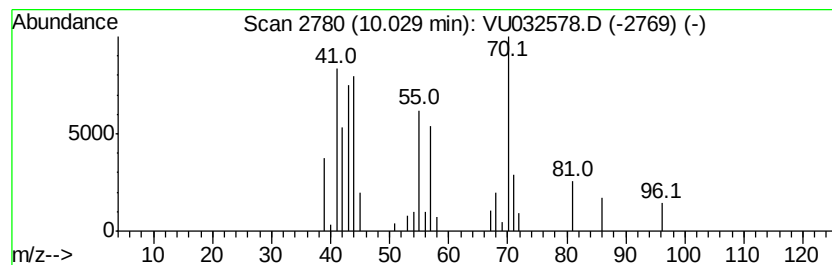
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Quant Title : VOC Analysis

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

Peak Number 5 Heptanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	2.96 ug/L	32406	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanal	114	C7H14O	000111-71-7	91
2		Heptanal	114	C7H14O	000111-71-7	86
3		Heptanal	114	C7H14O	000111-71-7	83
4		Heptanal	114	C7H14O	000111-71-7	83
5		Heptanal	114	C7H14O	000111-71-7	59



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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 27 Sample Multiplier: 1

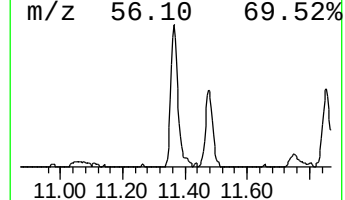
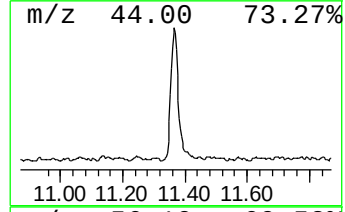
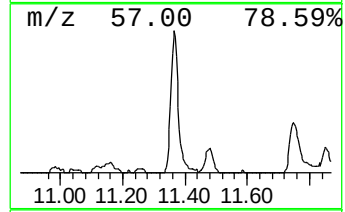
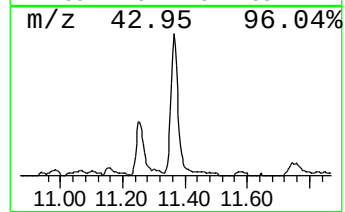
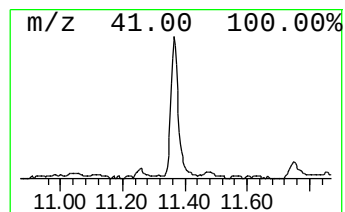
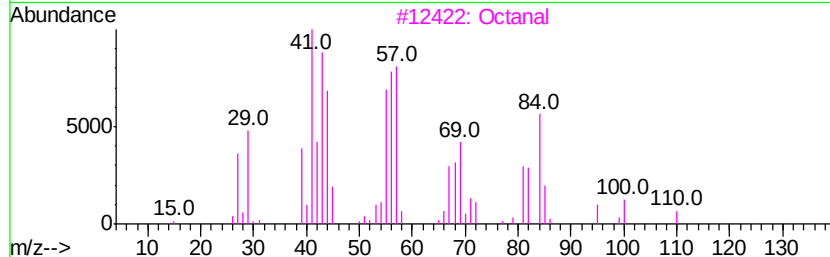
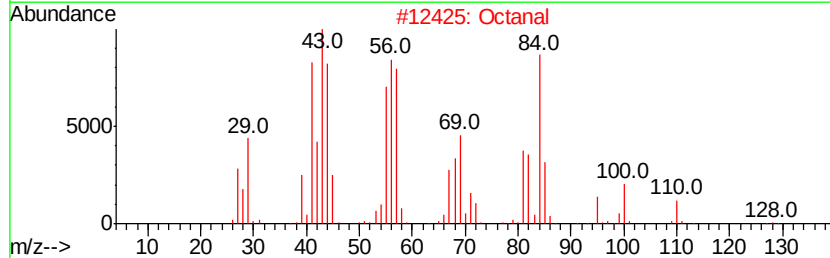
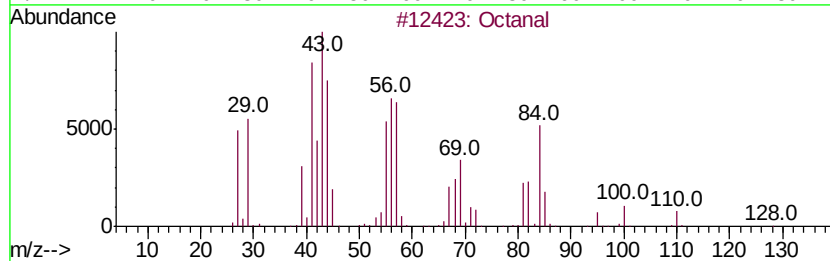
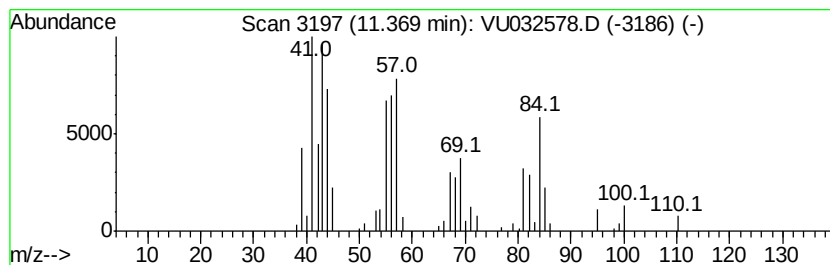
Instrument :
MSVOA_U
ClientSampleId :
DB8B9

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 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.37	10.33 ug/L	116885	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octanal		128 C8H16O	000124-13-0 91
2	Octanal		128 C8H16O	000124-13-0 91
3	Octanal		128 C8H16O	000124-13-0 87
4	Octanal		128 C8H16O	000124-13-0 80
5	Hydroperoxide, hexyl		118 C6H14O2	004312-76-9 35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061019\
Data File : VU032578.D
Acq On : 10 Jun 2019 20:25
Operator : JC/SP
Sample : K3277-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB8B9

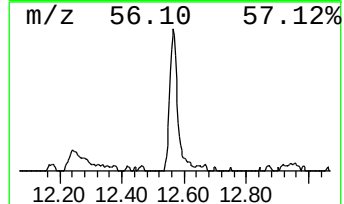
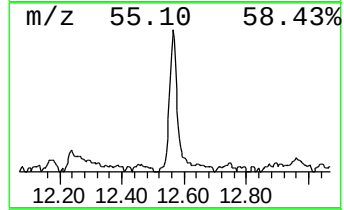
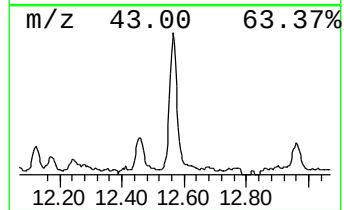
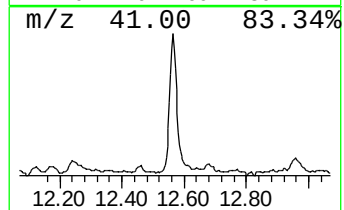
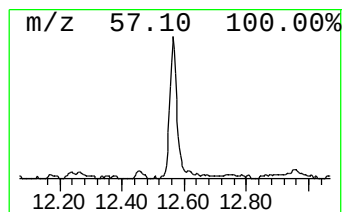
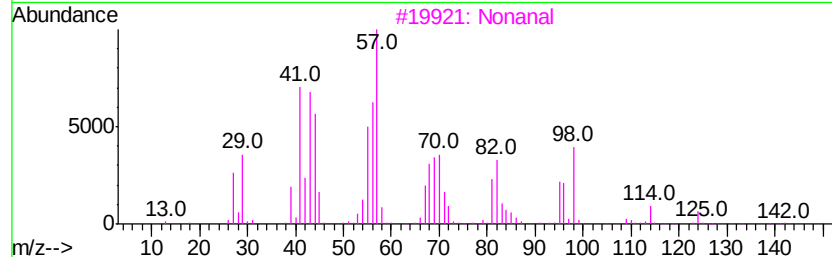
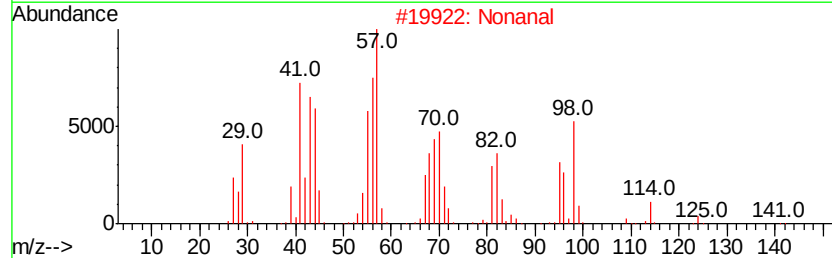
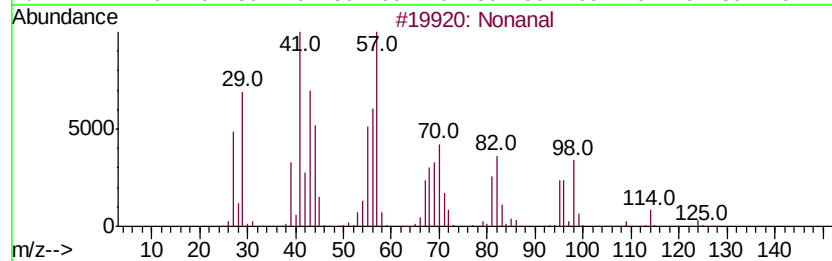
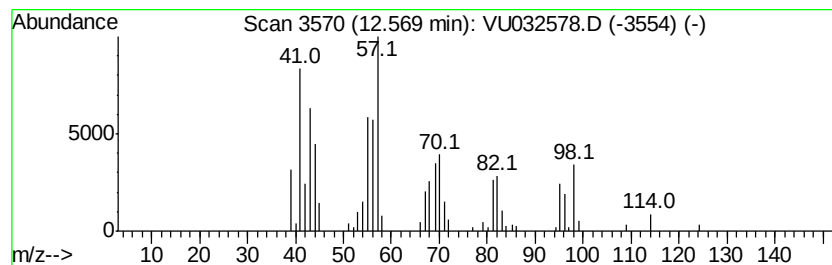
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	8.37 ug/L	94741	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	86
5		2-Heptene	98	C7H14	000592-77-8	30



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU061019\
Data File : VU032578.D
Acq On : 10 Jun 2019 20:25
Operator : JC/SP
Sample : K3277-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB8B9

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
Isopropyl Alcohol	2.44	6.6	ug/L	58569	1	5.88	441482	50.0
Hexanal	8.46	5.0	ug/L	54336	2	9.08	546820	50.0
Heptanal	10.03	3.0	ug/L	32406	2	9.08	546820	50.0
Octanal	11.37	10.3	ug/L	116885	3	11.48	565750	50.0
Nonanal	12.57	8.4	ug/L	94741	3	11.48	565750	50.0