

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU041319\
 Data File : VU031155.D
 Acq On : 13 Apr 2019 14:44
 Operator : JC/SP
 Sample : K2299-29
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB709

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\SOMULM040519WMA.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	23	28	37	rVB2	17424	17613	1.40%	0.148%
2	1.395	89	95	106	rVB	128661	137485	10.90%	1.159%
3	1.469	112	118	127	rVB	56320	62538	4.96%	0.527%
4	1.675	175	182	199	rVB	128632	172372	13.67%	1.453%
5	2.264	350	365	375	rBV2	183020	377683	29.96%	3.183%
6	2.318	375	382	400	rVB	48778	80390	6.38%	0.678%
7	2.440	409	420	441	rBV2	30880	60694	4.81%	0.512%
8	2.540	447	451	453	rBV5	784	610	0.05%	0.005%
9	2.694	487	499	511	rBV	12989	23205	1.84%	0.196%
10	2.833	525	542	560	rBV	60213	134049	10.63%	1.130%
11	2.929	569	572	574	rBV	816	466	0.04%	0.004%
12	3.058	609	612	616	rVV3	669	462	0.04%	0.004%
13	3.138	631	637	639	rBV3	725	651	0.05%	0.005%
14	3.177	642	649	661	rVV7	2893	5876	0.47%	0.050%
15	3.469	738	740	745	rVB4	637	438	0.03%	0.004%
16	3.505	748	751	754	rVB2	715	449	0.04%	0.004%
17	3.649	791	796	798	rBV2	660	587	0.05%	0.005%
18	3.855	854	860	863	rBV2	459	460	0.04%	0.004%
19	3.878	864	867	873	rVB	575	504	0.04%	0.004%
20	3.993	893	903	906	rBV4	5995	8571	0.68%	0.072%
21	4.173	941	959	992	rBV2	201277	672012	53.30%	5.664%
22	4.546	1072	1075	1077	rBV2	827	469	0.04%	0.004%
23	4.643	1088	1105	1133	rBV3	218309	597331	47.38%	5.034%
24	4.829	1157	1163	1166	rVB5	527	616	0.05%	0.005%
25	4.878	1172	1178	1179	rBV4	1412	1374	0.11%	0.012%
26	4.939	1191	1197	1203	rVB6	604	855	0.07%	0.007%
27	4.980	1207	1210	1213	rBV3	879	548	0.04%	0.005%
28	5.071	1234	1238	1241	rBV3	964	707	0.06%	0.006%
29	5.122	1249	1254	1261	rVB6	905	954	0.08%	0.008%
30	5.334	1295	1320	1352	rBV2	388816	1260794	100.00%	10.626%
31	5.543	1383	1385	1391	rBV6	1080	862	0.07%	0.007%
32	5.595	1398	1401	1404	rBV3	1319	974	0.08%	0.008%
33	5.714	1435	1438	1441	rVB2	835	571	0.05%	0.005%
34	5.759	1447	1452	1453	rBV3	505	445	0.04%	0.004%

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35	5.788	1458	1461	1466	rBV4	715	623	0.05%	0.005%
36	5.881	1477	1490	1518	rVV	384944	775662	61.52%	6.537%
37	6.189	1574	1586	1603	rVB5	21779	47948	3.80%	0.404%
38	6.324	1615	1628	1652	rBV	311770	631276	50.07%	5.320%
39	6.530	1683	1692	1714	rBV3	53078	109860	8.71%	0.926%
40	6.685	1735	1740	1745	rVB6	1496	1502	0.12%	0.013%
41	6.755	1753	1762	1773	rBV4	11933	23124	1.83%	0.195%
42	7.013	1837	1842	1845	rVB4	964	702	0.06%	0.006%
43	7.041	1845	1851	1854	rBV5	961	1128	0.09%	0.010%
44	7.225	1897	1908	1927	rBV	138057	252972	20.06%	2.132%
45	7.466	1979	1983	1991	rBV7	1785	2292	0.18%	0.019%
46	7.562	1999	2013	2030	rBV	385421	692406	54.92%	5.835%
47	7.784	2080	2082	2086	rVB2	1132	615	0.05%	0.005%
48	7.849	2092	2102	2124	rBV2	93564	173441	13.76%	1.462%
49	8.074	2168	2172	2177	rBV3	797	744	0.06%	0.006%
50	8.103	2180	2181	2187	rVB3	746	475	0.04%	0.004%
51	8.141	2187	2193	2194	rBV3	850	724	0.06%	0.006%
52	8.170	2197	2202	2210	rBV6	2274	3697	0.29%	0.031%
53	8.225	2211	2219	2231	rVB5	15636	29362	2.33%	0.247%
54	8.308	2234	2245	2276	rBV2	461641	933594	74.05%	7.868%
55	8.459	2281	2292	2322	rVV	587215	999951	79.31%	8.427%
56	8.758	2383	2385	2390	rVB3	1045	680	0.05%	0.006%
57	8.877	2419	2422	2423	rBV3	939	554	0.04%	0.005%
58	8.887	2423	2425	2428	rVV3	1075	715	0.06%	0.006%
59	8.906	2428	2431	2433	rVV3	882	516	0.04%	0.004%
60	8.951	2443	2445	2451	rVB3	1533	971	0.08%	0.008%
61	9.041	2470	2473	2475	rBV3	822	573	0.05%	0.005%
62	9.086	2475	2487	2526	rVV	557485	973121	77.18%	8.201%
63	9.331	2560	2563	2568	rBV6	814	712	0.06%	0.006%
64	9.453	2598	2601	2606	rVB4	1266	954	0.08%	0.008%
65	9.485	2606	2611	2615	rBV3	764	758	0.06%	0.006%
66	9.636	2656	2658	2664	rVB3	1221	829	0.07%	0.007%
67	9.662	2664	2666	2674	rVB4	1052	1154	0.09%	0.010%
68	9.713	2679	2682	2684	rBV3	755	507	0.04%	0.004%
69	9.820	2712	2715	2717	rBV4	665	443	0.04%	0.004%
70	9.932	2744	2750	2751	rBV3	1828	1403	0.11%	0.012%
71	10.028	2770	2780	2798	rBV5	43030	82454	6.54%	0.695%

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72	10.234	2840	2844	2847	rBV4	1104	862	0.07%	0.007%
73	10.299	2862	2864	2869	rVB3	673	493	0.04%	0.004%
74	10.328	2869	2873	2876	rBV3	573	498	0.04%	0.004%
75	10.427	2892	2904	2926	rVV	482229	812640	64.45%	6.849%
76	10.607	2949	2960	2968	rBV8	2832	4772	0.38%	0.040%
77	10.707	2988	2991	2993	rBV3	1275	646	0.05%	0.005%
78	10.858	3035	3038	3040	rVB2	942	603	0.05%	0.005%
79	10.881	3040	3045	3046	rBV3	563	549	0.04%	0.005%
80	10.922	3054	3058	3061	rBV3	1123	964	0.08%	0.008%
81	10.990	3073	3079	3091	rBV8	4089	6073	0.48%	0.051%
82	11.234	3152	3155	3158	rBV2	928	615	0.05%	0.005%
83	11.369	3185	3197	3220	rBV2	69985	131784	10.45%	1.111%
84	11.482	3220	3232	3253	rVV	441495	724777	57.49%	6.108%
85	11.758	3307	3318	3321	rBV4	6442	8906	0.71%	0.075%
86	11.858	3337	3349	3368	rBV	416329	698236	55.38%	5.885%
87	12.247	3465	3470	3473	rBV6	3215	3315	0.26%	0.028%
88	12.488	3542	3545	3549	rBV4	988	663	0.05%	0.006%
89	12.569	3561	3570	3587	rBV4	45646	88625	7.03%	0.747%
90	13.073	3723	3727	3733	rBV6	1394	1299	0.10%	0.011%
91	13.109	3736	3738	3743	rVB4	1107	852	0.07%	0.007%
92	13.131	3743	3745	3748	rVB2	850	469	0.04%	0.004%
93	13.157	3749	3753	3755	rBV2	1163	815	0.06%	0.007%
94	13.340	3808	3810	3817	rVB5	1038	980	0.08%	0.008%
95	13.382	3821	3823	3826	rBV4	717	451	0.04%	0.004%
96	13.453	3842	3845	3848	rBV3	961	631	0.05%	0.005%
97	13.472	3848	3851	3852	rBV2	1047	475	0.04%	0.004%
98	13.614	3891	3895	3897	rBV2	1104	859	0.07%	0.007%
99	13.755	3936	3939	3942	rBV2	1123	981	0.08%	0.008%
100	14.237	4087	4089	4092	rVB2	1261	613	0.05%	0.005%

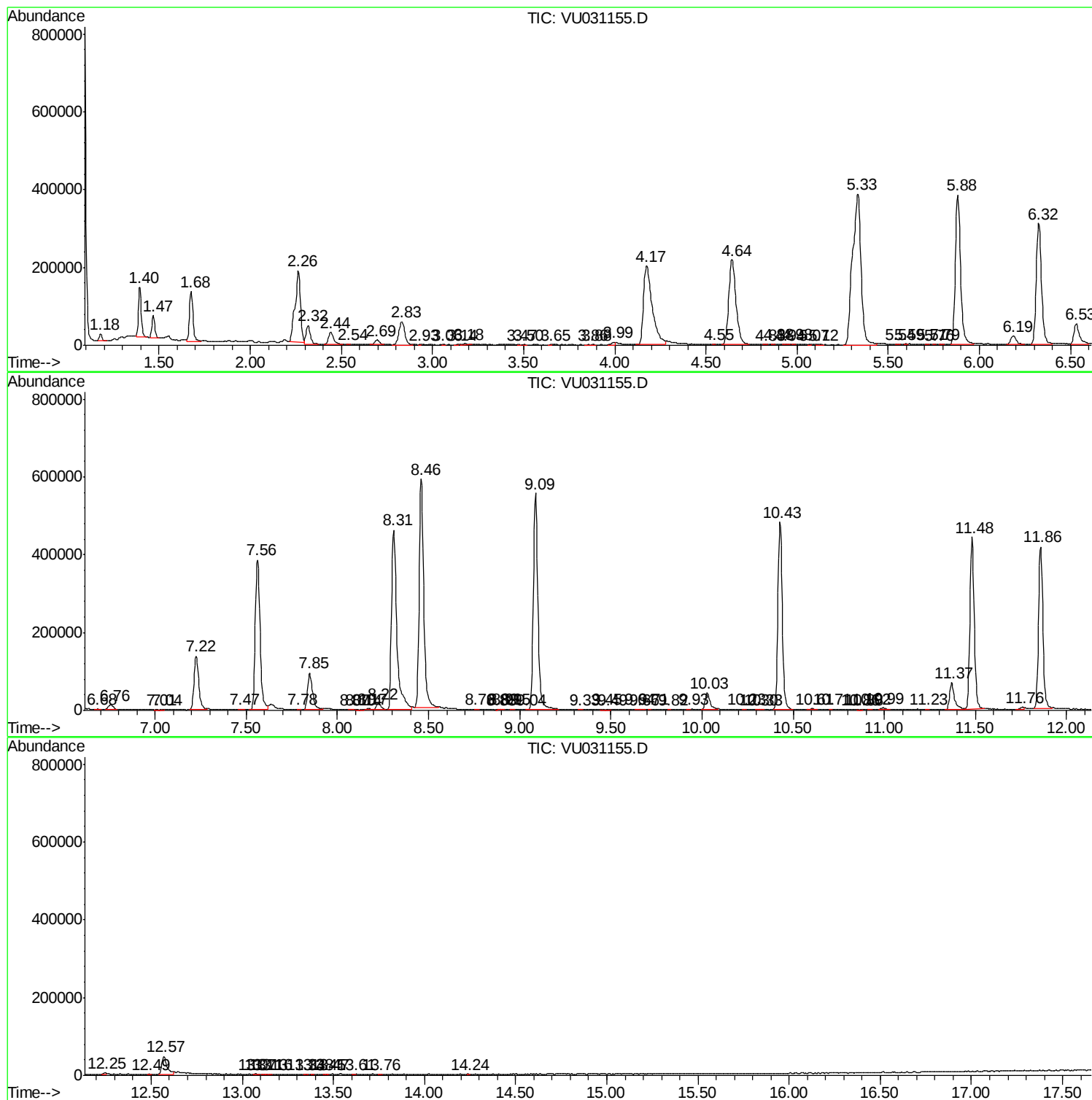
Sum of corrected areas: 11865503

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

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



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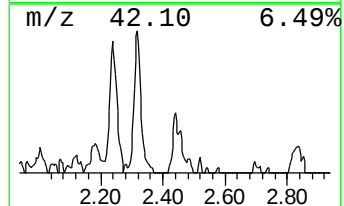
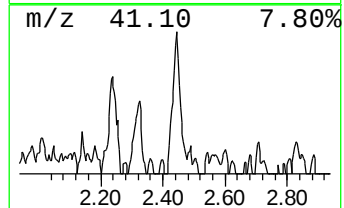
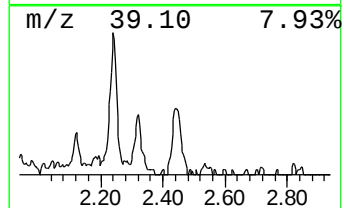
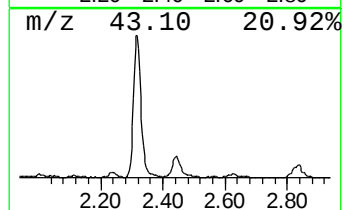
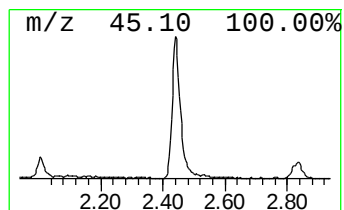
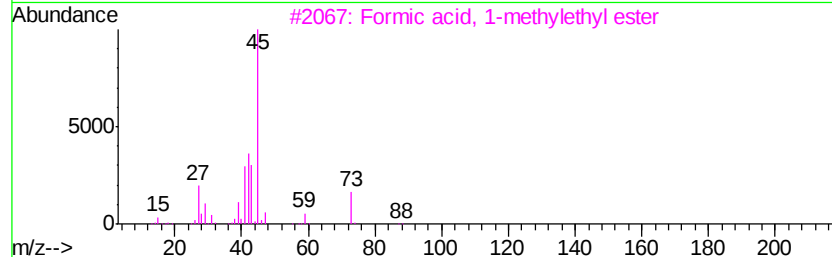
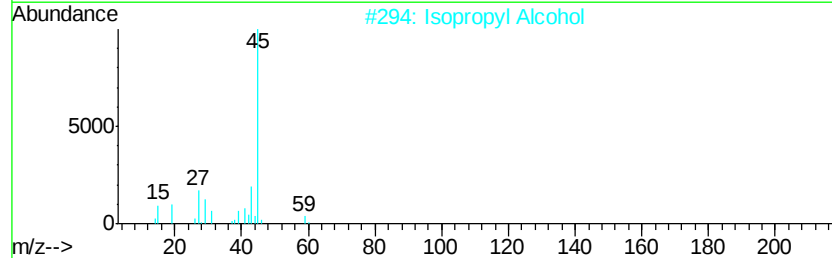
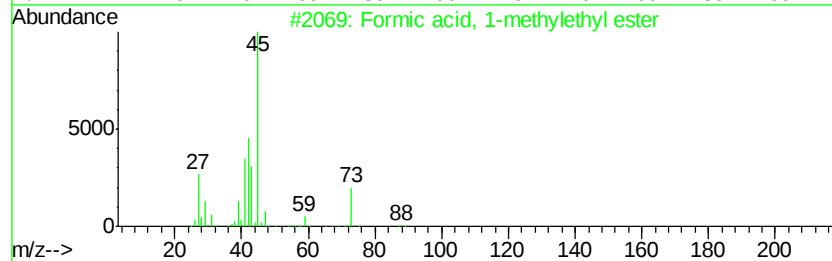
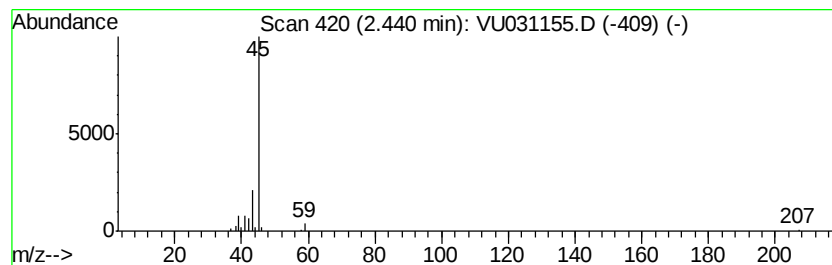
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	3.91 ug/L	60694	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	43
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	43
3		Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9



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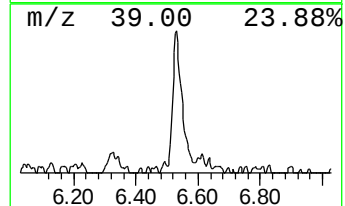
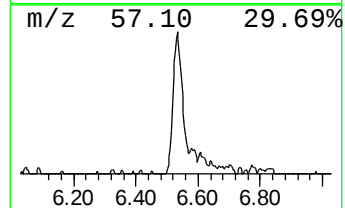
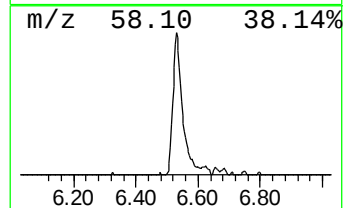
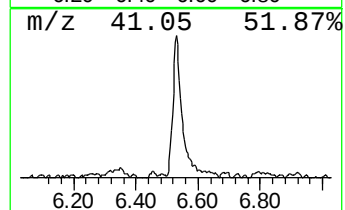
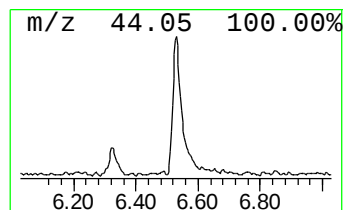
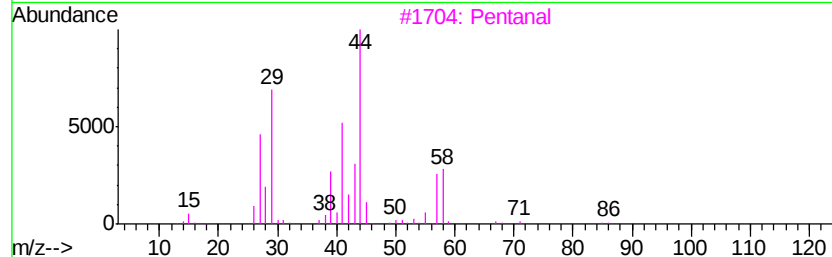
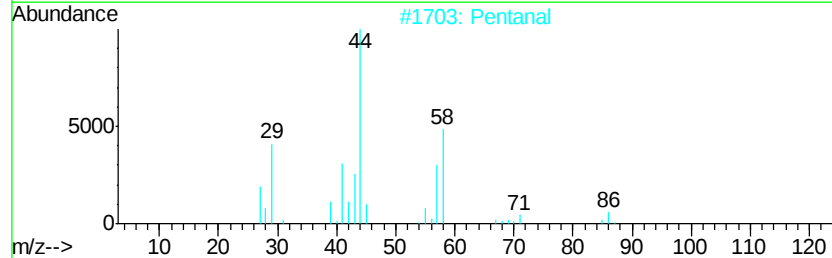
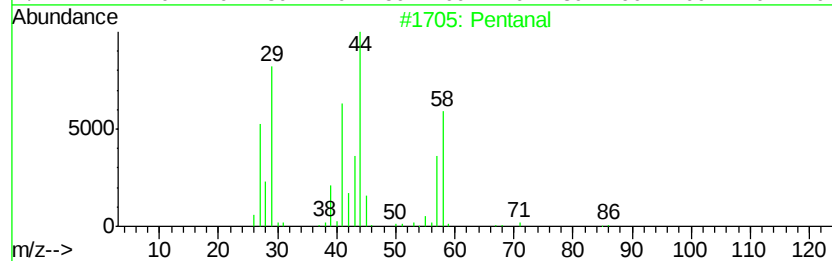
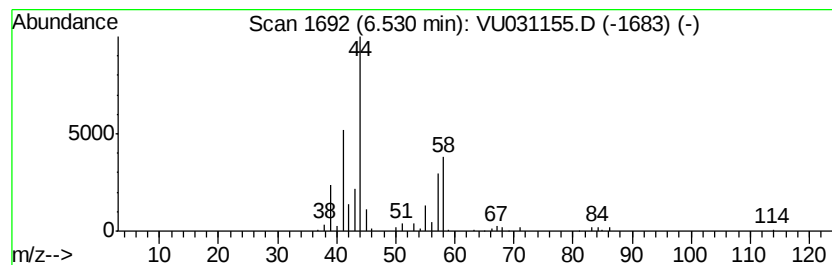
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Pentanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	7.08 ug/L	109860	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	78
2		Pentanal	86	C5H10O	000110-62-3	64
3		Pentanal	86	C5H10O	000110-62-3	64
4		1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	43
5		Cyclopropyl carbinol	72	C4H8O	002516-33-8	40



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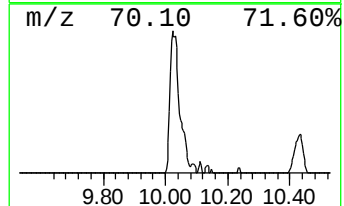
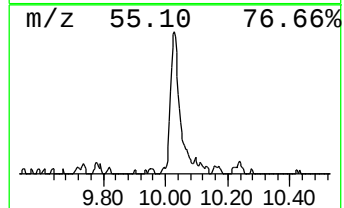
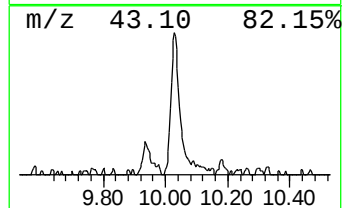
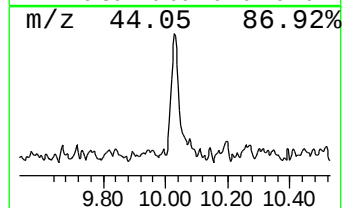
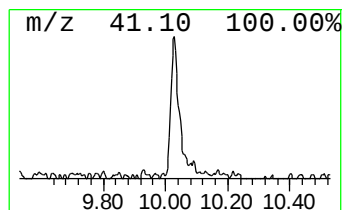
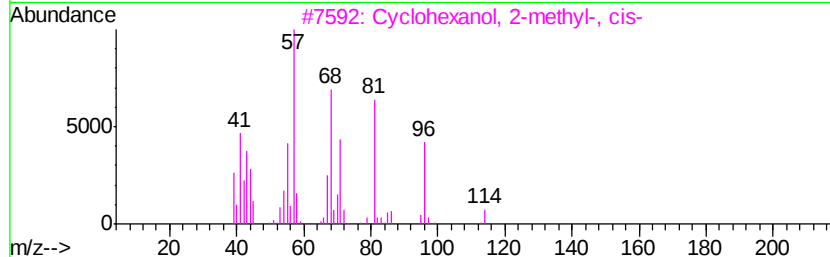
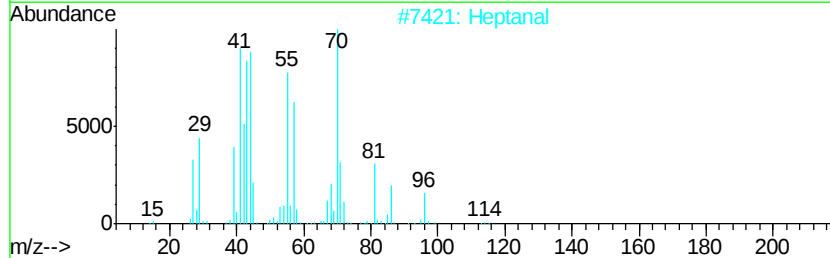
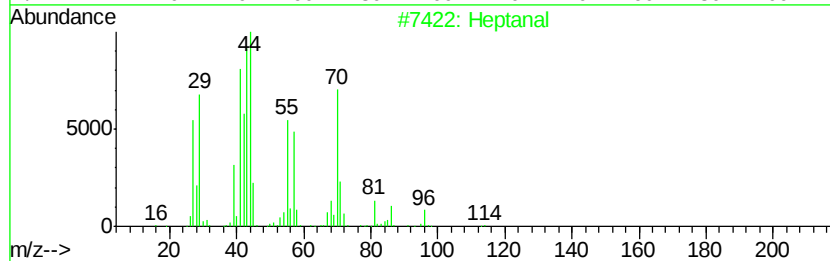
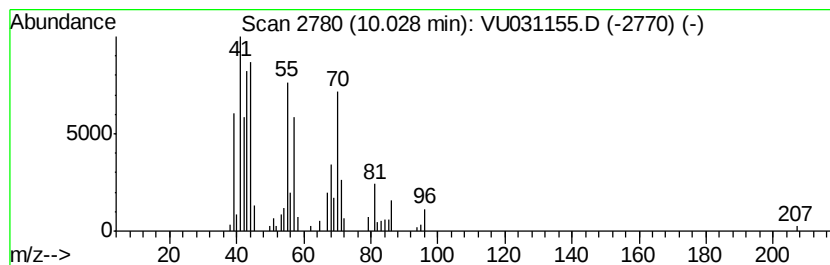
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	4.24 ug/L	82454	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanal	114	C7H14O	000111-71-7	45
2		Heptanal	114	C7H14O	000111-71-7	43
3		Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	38
4		Hexanal, 3-methyl-	114	C7H14O	019269-28-4	32
5		Pentane, 2-chloro-	106	C5H11Cl	000625-29-6	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU041319\
Data File : VU031155.D
Acq On : 13 Apr 2019 14:44
Operator : JC/SP
Sample : K2299-29
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB709

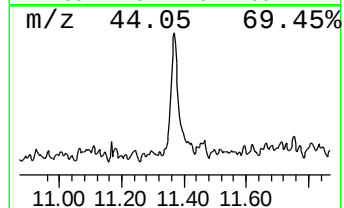
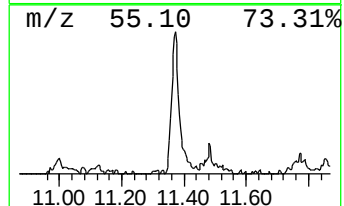
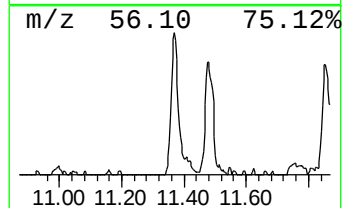
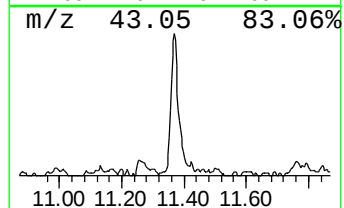
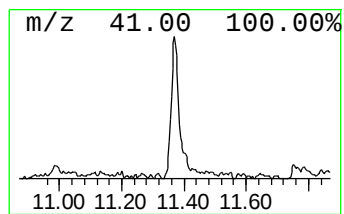
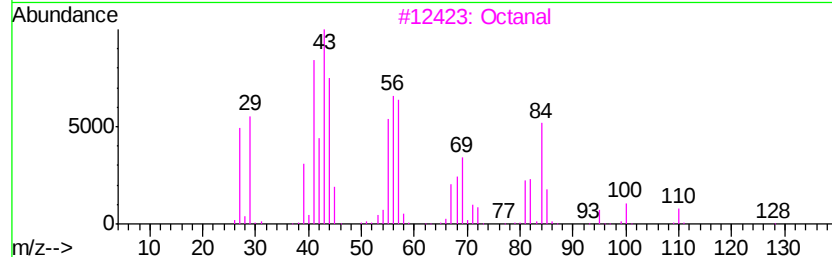
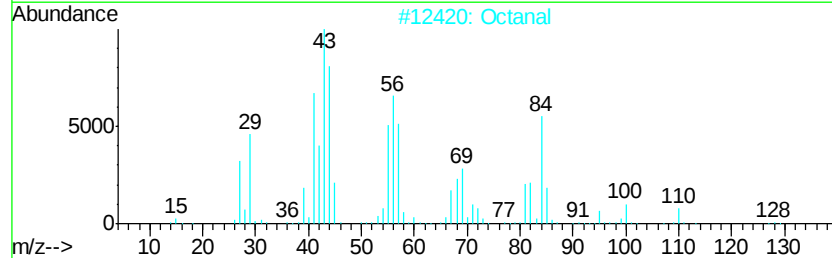
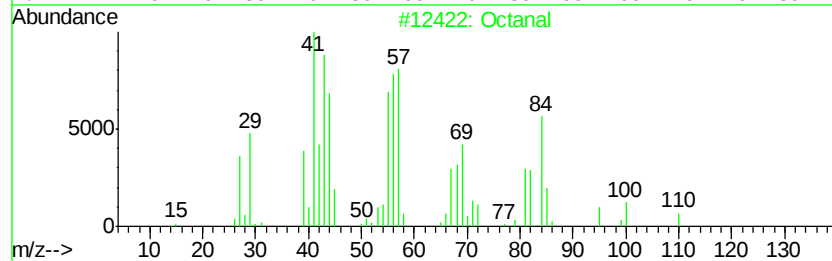
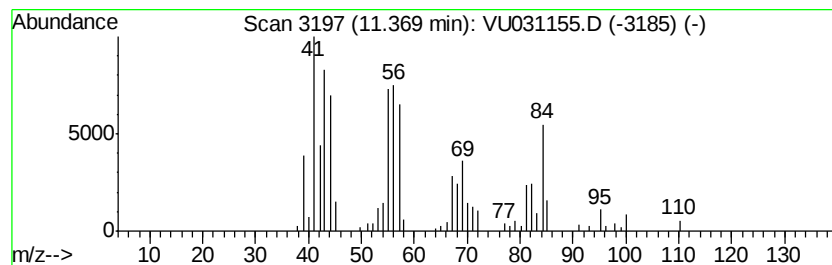
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Quant Title : VOC Analysis

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

Peak Number 7 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.37	9.09 ug/L	131784	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanal	128	C8H16O	000124-13-0	87
2		Octanal	128	C8H16O	000124-13-0	72
3		Octanal	128	C8H16O	000124-13-0	64
4		2-Amino-oxazole	84	C3H4N2O	004570-45-0	47
5		1-Pentene, 3-methyl-	84	C6H12	000760-20-3	46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU041319\
Data File : VU031155.D
Acq On : 13 Apr 2019 14:44
Operator : JC/SP
Sample : K2299-29
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 5 Sample Multiplier: 1

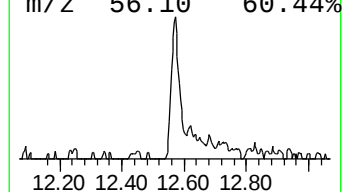
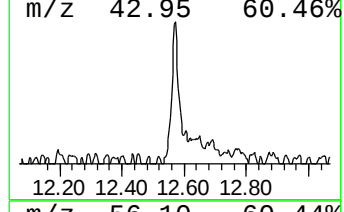
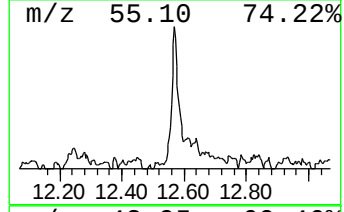
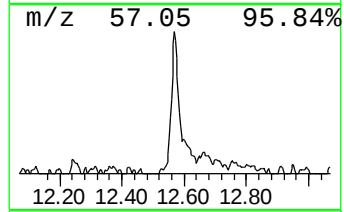
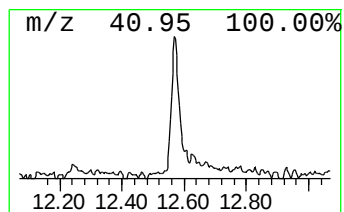
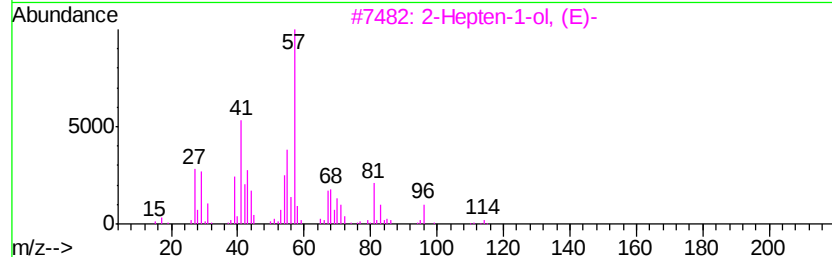
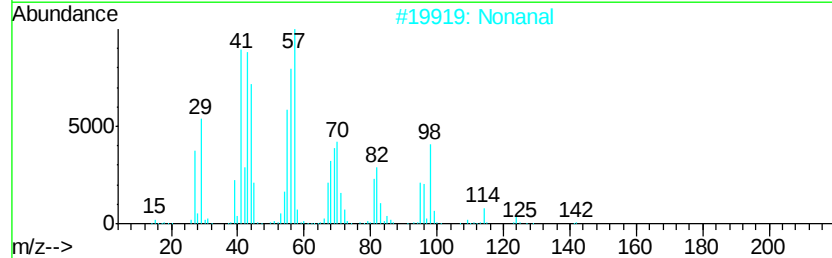
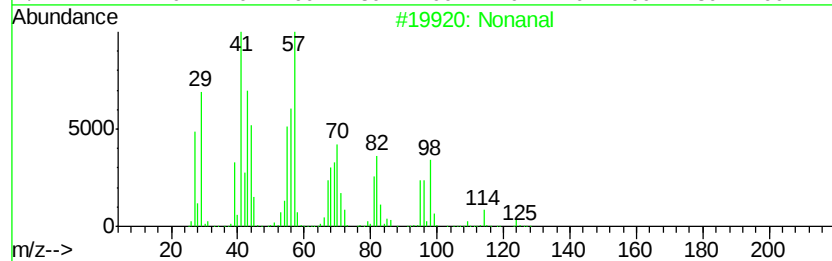
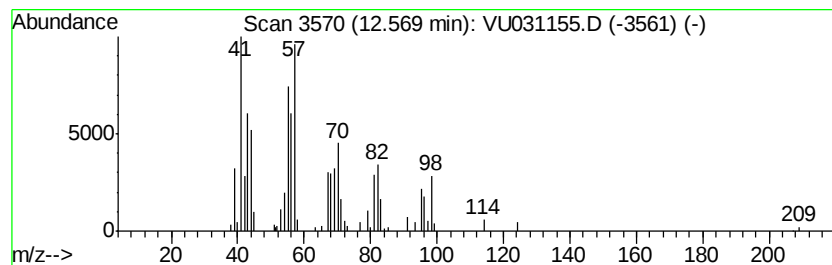
Instrument :
MSVOA_U
ClientSampleId :
DB709

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Nonanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	6.11 ug/L	88625	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonanal		142 C9H18O	000124-19-6 80
2	Nonanal		142 C9H18O	000124-19-6 72
3	2-Hepten-1-ol, (E)-		114 C7H14O	033467-76-4 38
4	Carbonic acid, 2,2,2-trichloroet...		344 C14H23Cl3O3	1000314-55-7 30
5	2,3-Dimethyl-aziridine		71 C4H9N	002549-68-0 22



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU041319\
Data File : VU031155.D
Acq On : 13 Apr 2019 14:44
Operator : JC/SP
Sample : K2299-29
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB709

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.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	3.9	ug/L	60694	1	5.88	775662	50.0
Pentanal	6.53	7.1	ug/L	109860	1	5.88	775662	50.0
unknown-02	10.03	4.2	ug/L	82454	2	9.09	973121	50.0
Octanal	11.37	9.1	ug/L	131784	3	11.48	724777	50.0
Nonanal	12.57	6.1	ug/L	88625	3	11.48	724777	50.0