

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU032419\
 Data File : VU030377.D
 Acq On : 24 Mar 2019 17:48
 Operator : JC/SP
 Sample : K2016-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0988

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\SOMULM032319WMA.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	1.183	23	29	36	rBV3	17146	17288	0.01%	0.003%
2	1.328	69	74	82	rBV3	4999	6942	0.00%	0.001%
3	1.395	88	95	106	rBV	207426	208299	0.08%	0.035%
4	1.473	112	119	125	rBV2	7268	11020	0.00%	0.002%
5	1.514	127	132	137	rVV2	7916	9534	0.00%	0.002%
6	1.675	174	182	199	rVB	157174	210152	0.08%	0.035%
7	1.846	231	235	238	rBV2	2487	2229	0.00%	0.000%
8	1.945	260	266	272	rVV4	5589	7187	0.00%	0.001%
9	2.186	334	341	348	rBV4	4993	7420	0.00%	0.001%
10	2.270	353	367	375	rBV	334864	510118	0.20%	0.086%
11	2.318	375	382	394	rVB	136802	220471	0.09%	0.037%
12	2.444	411	421	440	rVB	60466	108965	0.04%	0.018%
13	2.701	491	501	508	rBV4	15726	30158	0.01%	0.005%
14	2.733	508	511	515	rVV3	7248	8678	0.00%	0.001%
15	2.788	517	528	533	rVV	85670	159000	0.06%	0.027%
16	2.836	534	543	561	rVV	196906	434696	0.17%	0.073%
17	2.916	565	568	573	rVB	2352	2526	0.00%	0.000%
18	2.997	573	593	610	rVB5	10183	30017	0.01%	0.005%
19	3.157	637	643	647	rBV	1676	2189	0.00%	0.000%
20	3.186	647	652	659	rVB	2982	3351	0.00%	0.001%
21	3.302	675	688	703	rBV5	6266	15988	0.01%	0.003%
22	3.498	746	749	754	rBV2	1615	1673	0.00%	0.000%
23	4.090	915	933	948	rBV	226851	613153	0.24%	0.103%
24	4.186	948	963	989	rVV4	474370	1419141	0.55%	0.238%
25	4.386	1016	1025	1044	rVB	25790	64095	0.02%	0.011%
26	4.495	1056	1059	1062	rVV2	1813	1683	0.00%	0.000%
27	4.669	1089	1113	1134	rBV	2597930	6530259	2.54%	1.095%
28	4.993	1199	1214	1232	rBV	119174	281016	0.11%	0.047%
29	5.132	1240	1257	1276	rBV	986176	2327466	0.91%	0.390%
30	5.418	1301	1346	1392	rBV4	83793571	256736082	100.00%	43.055%
31	5.884	1481	1491	1510	rVB	606489	1259111	0.49%	0.211%
32	6.186	1570	1585	1595	rBV4	24149	50307	0.02%	0.008%
33	6.328	1612	1629	1641	rBV	370109	741702	0.29%	0.124%
34	6.408	1643	1654	1674	rVB6	60045	176619	0.07%	0.030%

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 Title : VOC Analysis

35	6.534	1689	1693	1699	rVB	1633	1750	0.00%	0.000%
36	6.643	1716	1727	1740	rVB4	9342	20143	0.01%	0.003%
37	6.755	1749	1762	1777	rBV2	38778	75691	0.03%	0.013%
38	6.823	1780	1783	1788	rVB3	2085	1615	0.00%	0.000%
39	6.910	1806	1810	1815	rVB	1734	1929	0.00%	0.000%
40	7.070	1848	1860	1867	rBV4	4570	7001	0.00%	0.001%
41	7.225	1895	1908	1937	rVV	195811	370352	0.14%	0.062%
42	7.389	1952	1959	1969	rVB7	4592	7965	0.00%	0.001%
43	7.469	1977	1984	1985	rBV3	3744	3451	0.00%	0.001%
44	7.562	1997	2013	2028	rBV	707754	1301903	0.51%	0.218%
45	7.636	2029	2036	2057	rVB	77758	162043	0.06%	0.027%
46	7.849	2091	2102	2123	rBV2	136510	250005	0.10%	0.042%
47	7.923	2123	2125	2131	rVV	2297	2730	0.00%	0.000%
48	8.058	2159	2167	2172	rBV4	5164	8827	0.00%	0.001%
49	8.177	2198	2204	2210	rBV2	2156	3253	0.00%	0.001%
50	8.228	2211	2220	2234	rVB3	28071	50341	0.02%	0.008%
51	8.318	2234	2248	2284	rBV	452429	1051995	0.41%	0.176%
52	8.476	2290	2297	2309	rVB3	11893	21418	0.01%	0.004%
53	8.816	2397	2403	2407	rBV	2034	2356	0.00%	0.000%
54	9.032	2463	2470	2475	rBV	1437	2227	0.00%	0.000%
55	9.212	2478	2526	2568	rBV7	151438161	11034634	4.30%	1.851%
56	9.386	2574	2580	2591	rVB3	20948	35476	0.01%	0.006%
57	9.701	2671	2678	2682	rBV4	2816	4138	0.00%	0.001%
58	9.791	2699	2706	2714	rVB6	7517	12331	0.00%	0.002%
59	9.852	2722	2725	2728	rBV	2004	1778	0.00%	0.000%
60	9.961	2754	2759	2769	rVB8	4361	6963	0.00%	0.001%
61	10.254	2846	2850	2853	rVV2	2285	1987	0.00%	0.000%
62	10.270	2853	2855	2862	rVB4	4130	4047	0.00%	0.001%
63	10.434	2891	2906	2936	rBV2	573980	1467735	0.57%	0.246%
64	10.540	2936	2939	2946	rVB3	1796	1779	0.00%	0.000%
65	10.662	2967	2977	2992	rBV2	73433	125307	0.05%	0.021%
66	10.730	2995	2998	3003	rVV3	4163	4132	0.00%	0.001%
67	10.778	3003	3013	3029	rVB	34235	61107	0.02%	0.010%
68	10.971	3067	3073	3077	rVB2	1718	2319	0.00%	0.000%
69	11.102	3103	3114	3124	rVB6	16982	28726	0.01%	0.005%
70	11.167	3125	3134	3138	rBV4	2715	4457	0.00%	0.001%
71	11.209	3144	3147	3155	rVB2	1927	2048	0.00%	0.000%

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72	11.286	3166	3171	3175	rBV2	1467	1678	0.00%	0.000%
73	11.321	3179	3182	3190	rVB	2362	2911	0.00%	0.000%
74	11.430	3196	3216	3230	rBV	36287083	79512090	30.97%	13.334%
75	12.154	3436	3441	3452	rVB6	20338	30053	0.01%	0.005%
76	12.353	3494	3503	3521	rVB	22893	40292	0.02%	0.007%
77	12.575	3565	3572	3579	rBV7	13470	20631	0.01%	0.003%
78	12.633	3579	3590	3604	rVB	718444	1119095	0.44%	0.188%
79	12.816	3634	3647	3653	rBV2	150975	318899	0.12%	0.053%
80	12.861	3653	3661	3684	rVB	430733	830567	0.32%	0.139%
81	12.987	3689	3700	3716	rVB	359919	575239	0.22%	0.096%
82	13.234	3768	3777	3789	rVB4	30511	53602	0.02%	0.009%
83	13.321	3794	3804	3822	rBV3	15122	30468	0.01%	0.005%
84	13.437	3835	3840	3846	rBV2	2167	2869	0.00%	0.000%
85	13.524	3846	3867	3908	rBV2	92665820	174314719	67.90%	29.233%
86	13.745	3927	3936	3949	rVB	39187	67451	0.03%	0.011%
87	13.993	3996	4013	4039	rBV	29043428	46009782	17.92%	7.716%
88	14.382	4124	4134	4157	rBV	89868	168797	0.07%	0.028%
89	14.536	4172	4182	4193	rVB5	26732	61586	0.02%	0.010%
90	14.636	4210	4213	4219	rBV4	2176	2124	0.00%	0.000%
91	14.697	4229	4232	4240	rVB5	6569	8916	0.00%	0.001%
92	14.752	4245	4249	4256	rVB4	8225	10715	0.00%	0.002%
93	14.864	4275	4284	4298	rVB7	13195	24835	0.01%	0.004%
94	15.009	4324	4329	4331	rBV3	3338	3455	0.00%	0.001%
95	15.067	4331	4347	4367	rVB	613716	1122405	0.44%	0.188%
96	15.247	4399	4403	4410	rVB3	5460	6323	0.00%	0.001%
97	15.646	4513	4527	4548	rBV	2211029	3590506	1.40%	0.602%
98	16.475	4781	4785	4789	rBV2	2320	2198	0.00%	0.000%
99	16.903	4913	4918	4929	rVB4	7304	12717	0.00%	0.002%
100	17.015	4950	4953	4956	rBV	2488	1891	0.00%	0.000%

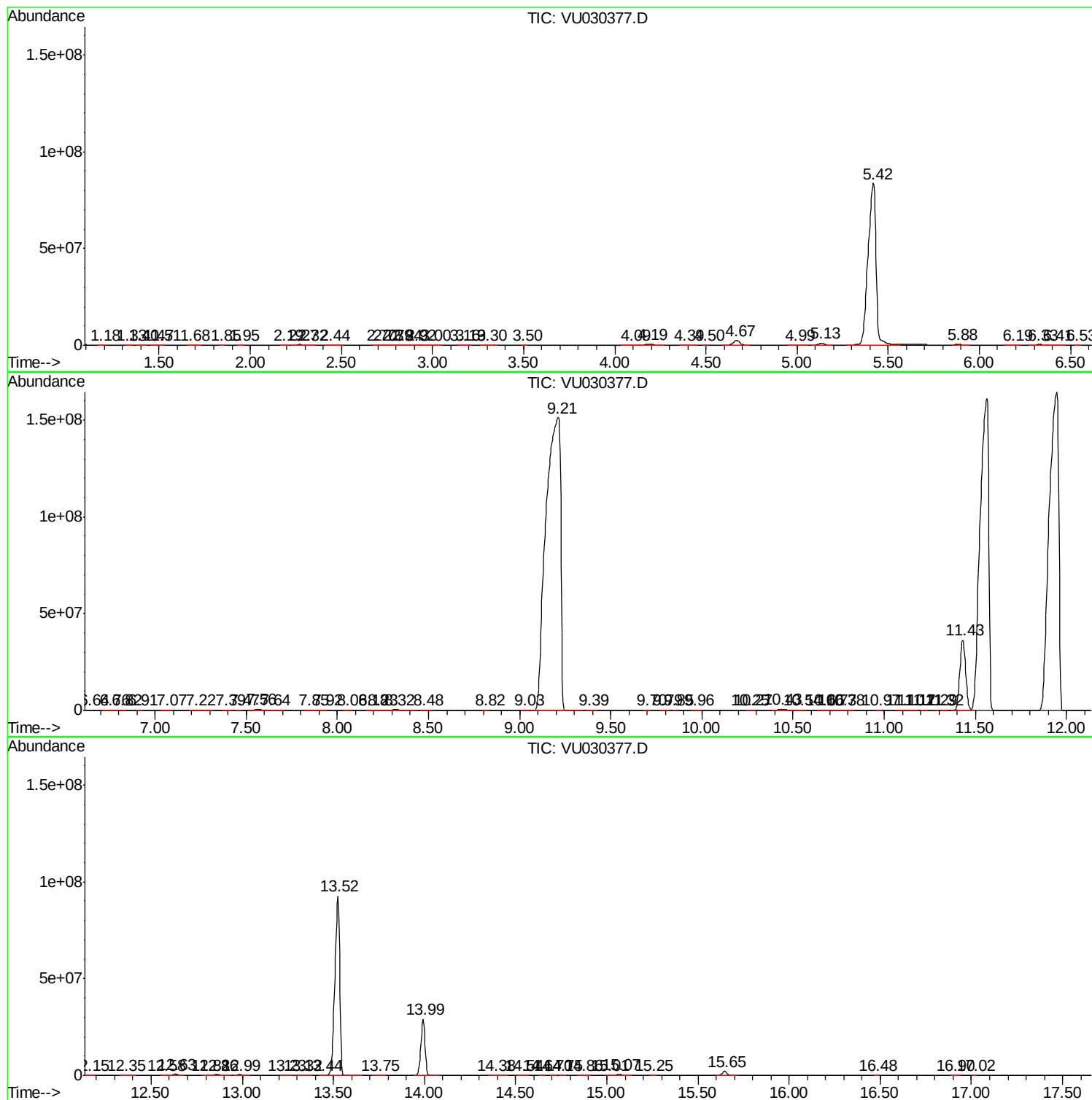
Sum of corrected areas: 596301308

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM032319WMA.M
Quant Title : VOC Analysis

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



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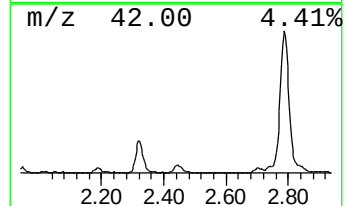
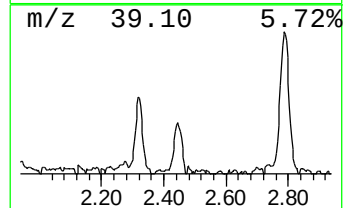
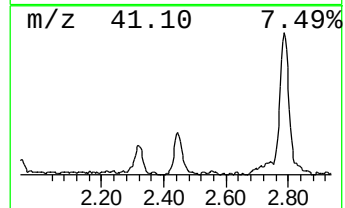
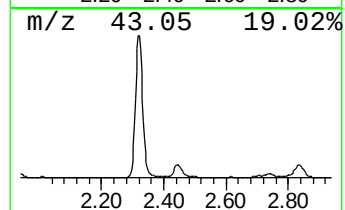
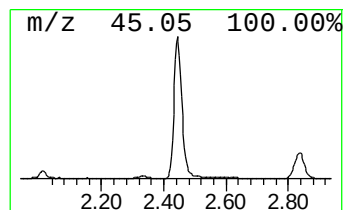
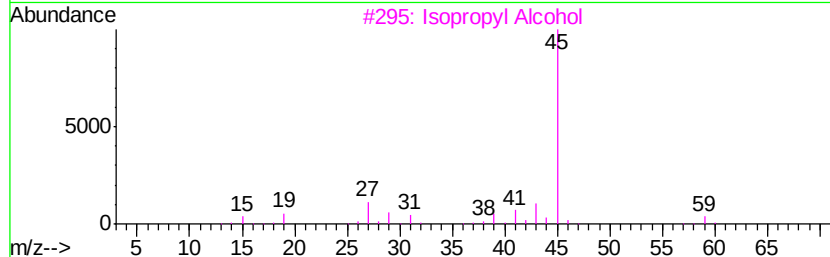
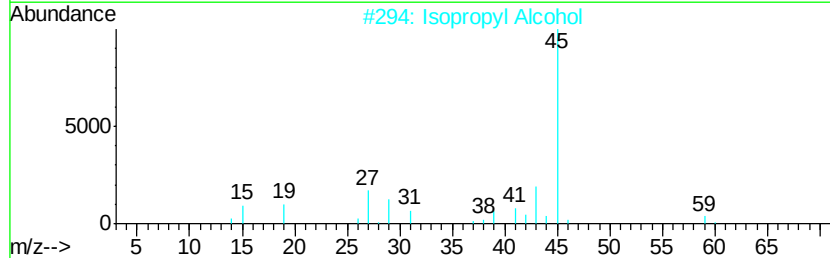
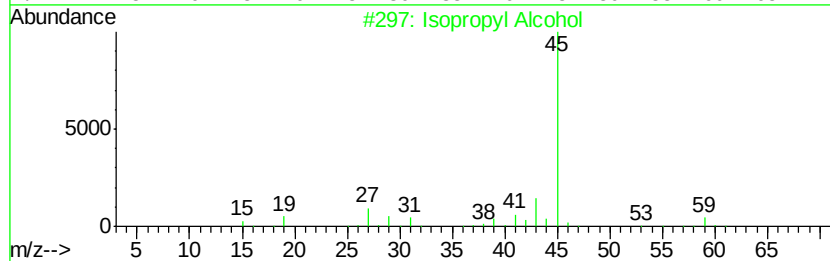
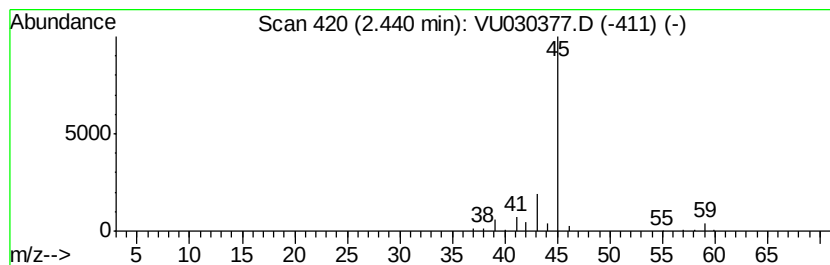
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM032319WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	4.33 ug/L	108965	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	78
3	Isopropyl Alcohol		60	C3H8O	000067-63-0	78
4	Isopropyl Alcohol		60	C3H8O	000067-63-0	56
5	Hydrazine, 1,2-dimethyl-		60	C2H8N2	000540-73-8	9



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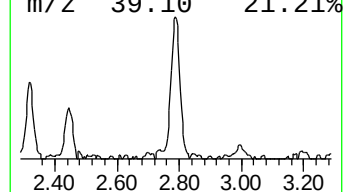
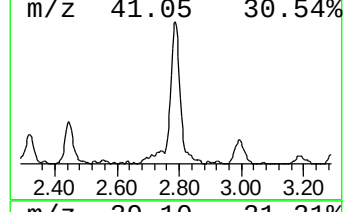
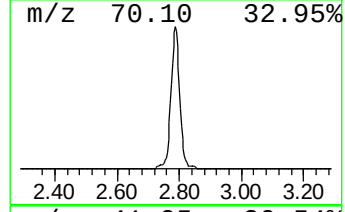
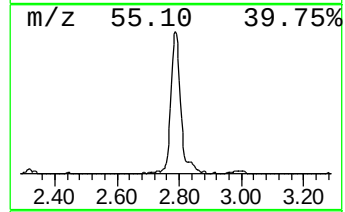
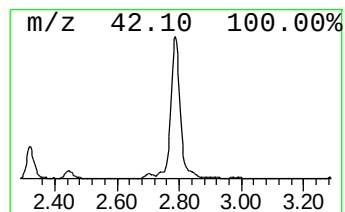
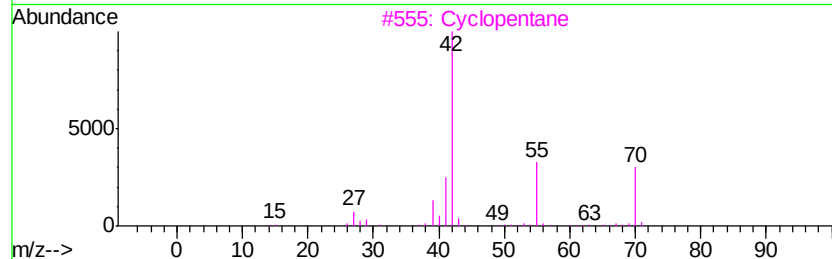
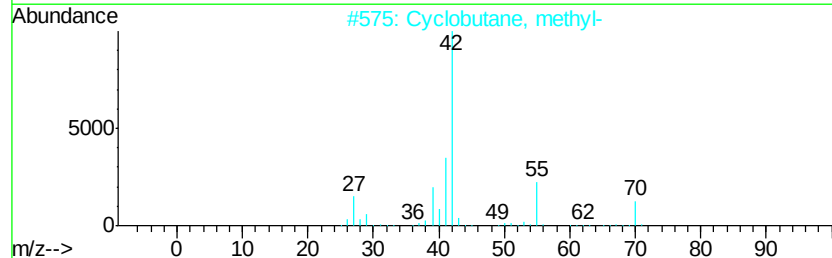
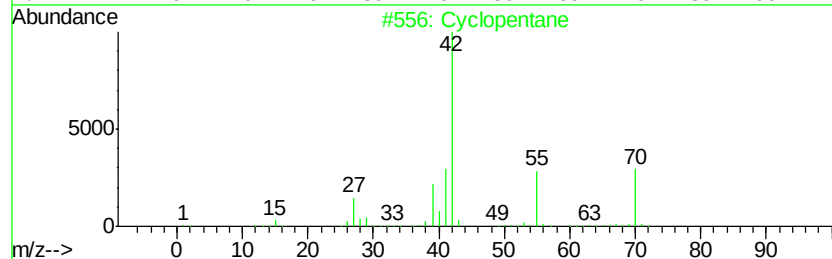
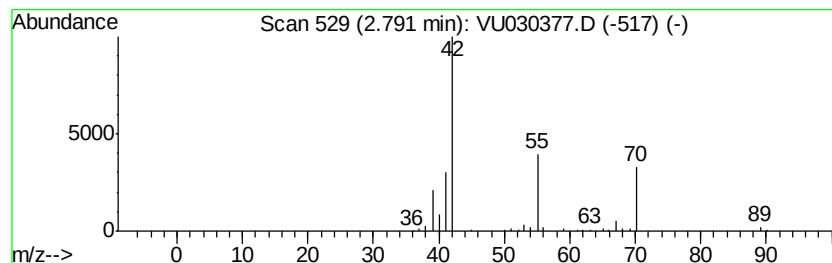
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM032319WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	6.31 ug/L	159000	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane	70	C5H10	000287-92-3	86
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3		Cyclopentane	70	C5H10	000287-92-3	72
4		1-Pentene	70	C5H10	000109-67-1	64
5		Cyclobutane, methyl-	70	C5H10	000598-61-8	50



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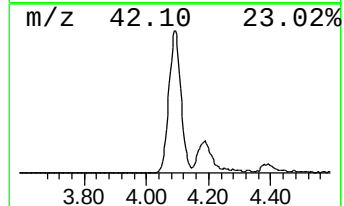
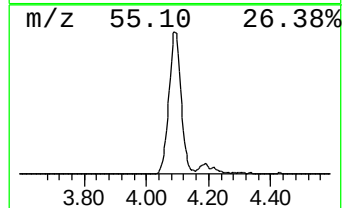
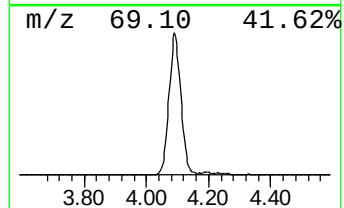
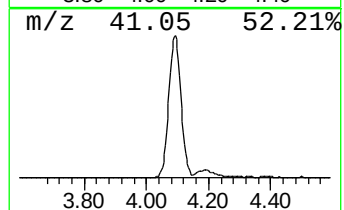
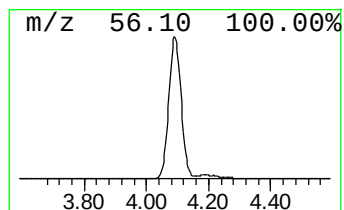
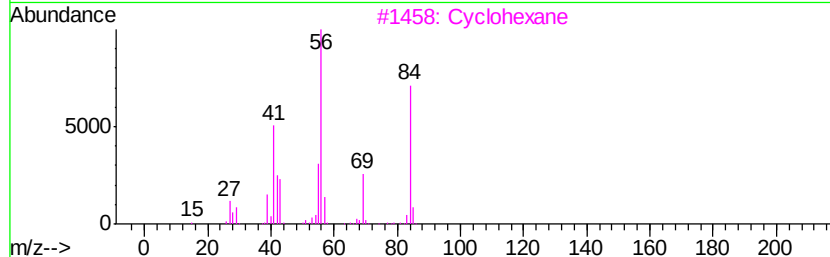
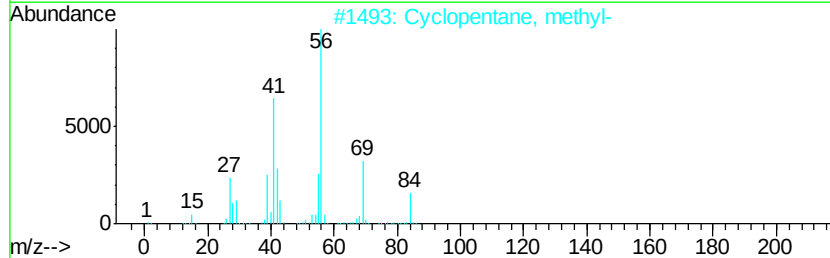
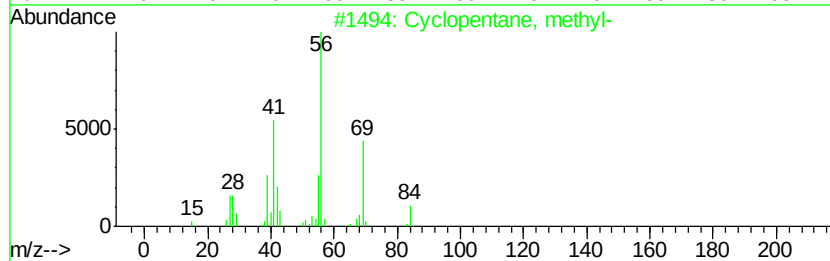
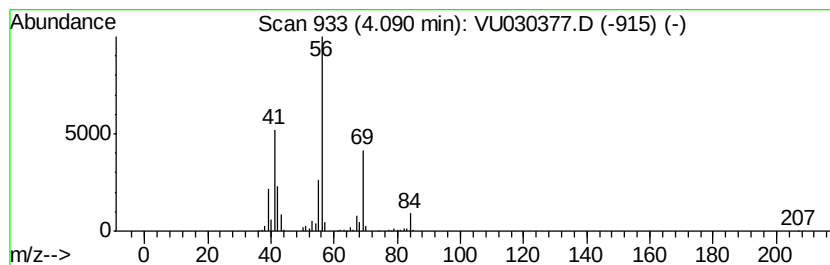
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	24.35 ug/L	613153	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3		Cyclohexane	84	C6H12	000110-82-7	78
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	78
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU032419\
Data File : VU030377.D
Acq On : 24 Mar 2019 17:48
Operator : JC/SP
Sample : K2016-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0988

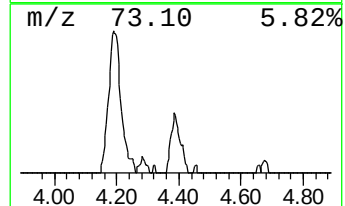
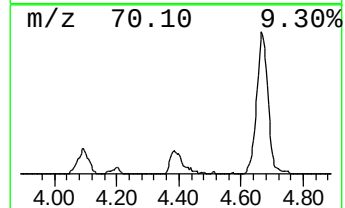
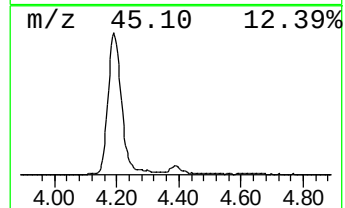
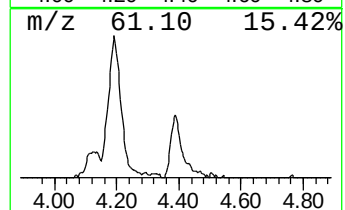
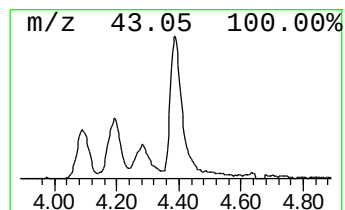
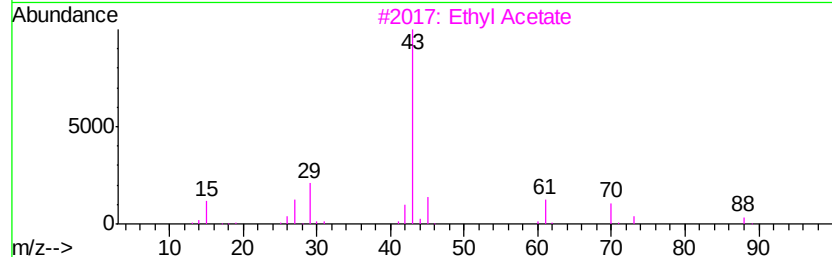
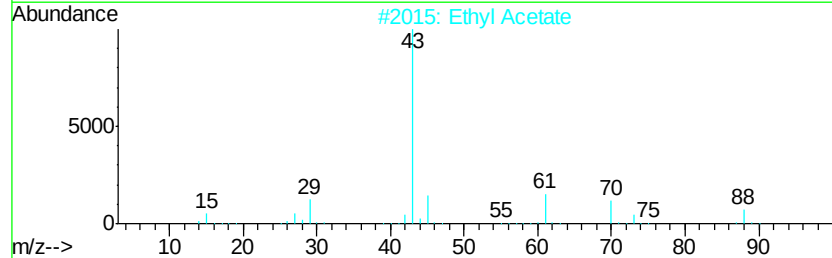
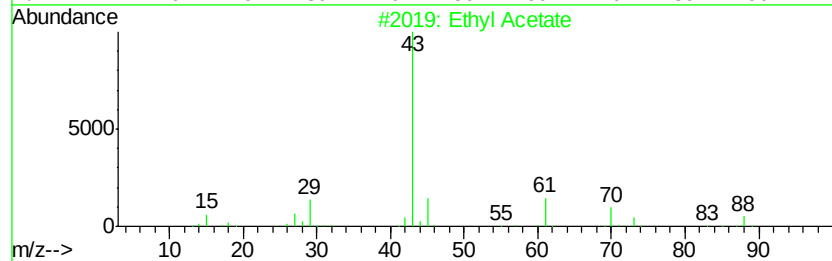
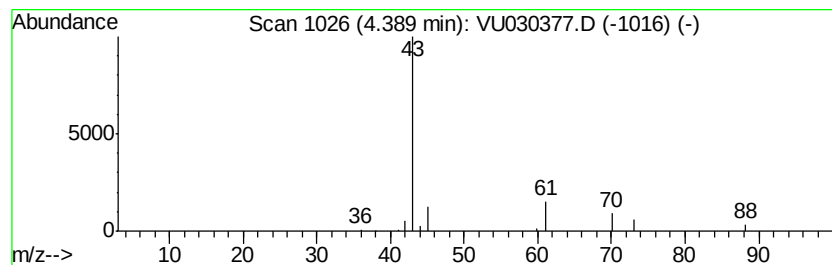
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Quant Title : VOC Analysis

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

Peak Number 5 Ethyl Acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	2.55 ug/L	64095	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2		Ethyl Acetate	88	C4H8O2	000141-78-6	83
3		Ethyl Acetate	88	C4H8O2	000141-78-6	83
4		Ethyl Acetate	88	C4H8O2	000141-78-6	72
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU032419\
Data File : VU030377.D
Acq On : 24 Mar 2019 17:48
Operator : JC/SP
Sample : K2016-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

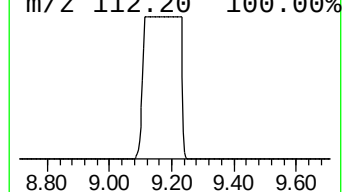
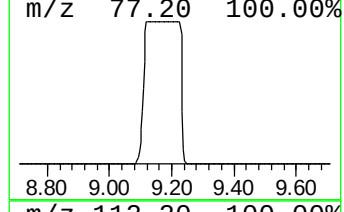
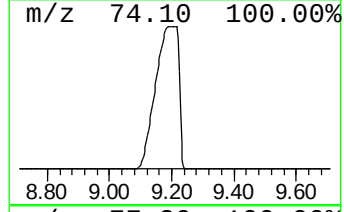
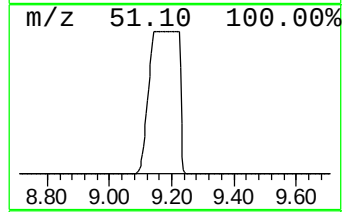
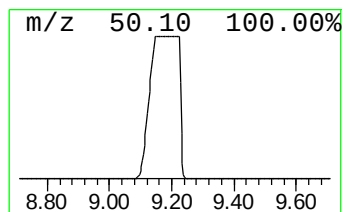
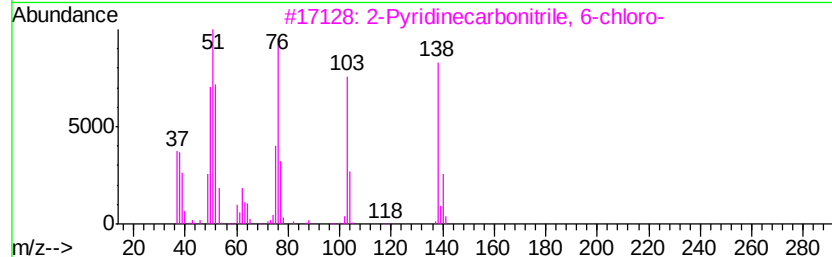
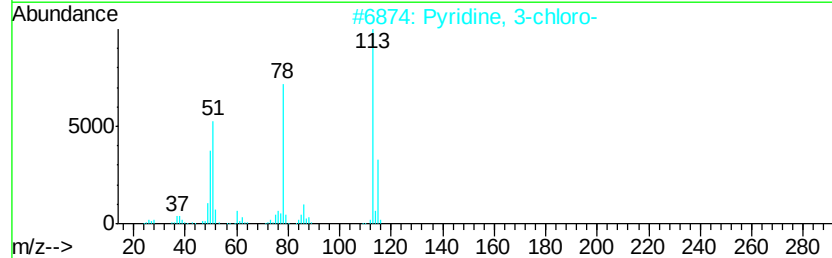
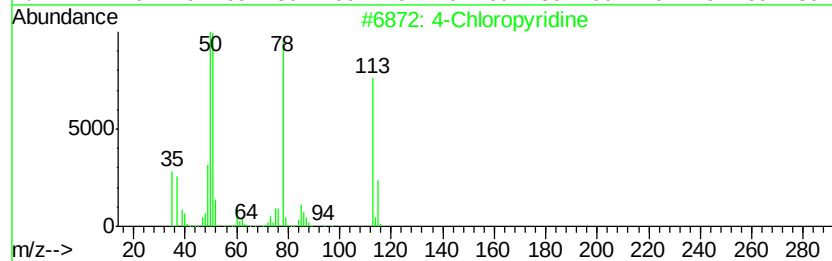
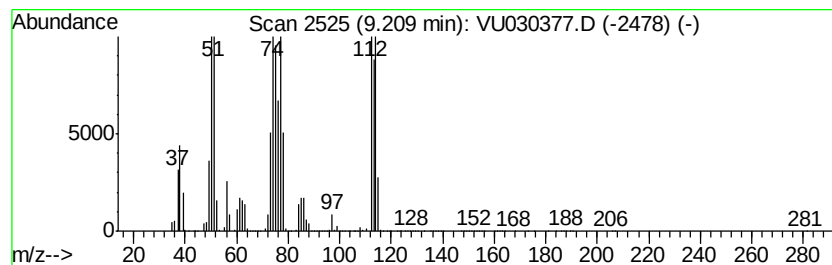
Instrument :
MSVOA_U
ClientSampleId :
C0988

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM032319WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 4-Chloropyridine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.21	50.00 ug/L	11034600	Chlorobenzene-d5	9.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloropyridine	113	C5H4ClN	000626-61-9	83
2	Pyridine, 3-chloro-	113	C5H4ClN	000626-60-8	64
3	2-Pyridinecarbonitrile, 6-chloro-	138	C6H3ClN2	033252-29-8	62
4	1,5-Hexadiyne	78	C6H6	000628-16-0	33
5	4-Chlorobuten-3-yne	86	C4H3Cl	040589-38-6	23



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU032419\
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Sample : K2016-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0988

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM032319WMA.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	4.3	ug/L	108965	1	5.88	1259110	50.0
(DEL) Alkane: Str...	2.79	6.3	ug/L	159000	1	5.88	1259110	50.0
(DEL) Alkane: Str...	4.09	24.4	ug/L	613153	1	5.88	1259110	50.0
Ethyl Acetate	4.39	2.5	ug/L	64095	1	5.88	1259110	50.0
4-Chloropyridine	9.21	50.0	ug/L	11034600	2	9.15	11034600	50.0