

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU031119\
 Data File : VU029907.D
 Acq On : 08 Mar 2019 22:48
 Operator : JC/SP
 Sample : K1763-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0957

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\SOMULM021519WMA.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	1.177	22	27	37	rBV3	33464	38220	0.31%	0.098%
2	1.277	52	58	68	rBV	36807	56171	0.46%	0.145%
3	1.328	68	74	87	rVB	123654	132047	1.08%	0.340%
4	1.399	88	96	104	rBV	196325	225617	1.85%	0.581%
5	1.473	114	119	126	rVV	40673	42219	0.35%	0.109%
6	1.518	129	133	143	rVB	41202	46510	0.38%	0.120%
7	1.679	177	183	208	rVB	174522	261435	2.14%	0.673%
8	2.270	353	367	376	rBV2	361924	586563	4.80%	1.510%
9	2.318	376	382	410	rVB2	80521	175921	1.44%	0.453%
10	2.441	411	420	427	rBV2	8945	14597	0.12%	0.038%
11	2.560	445	457	465	rBV3	2436	4517	0.04%	0.012%
12	2.621	468	476	485	rVB3	3059	5010	0.04%	0.013%
13	2.698	485	500	530	rBV	3876730	6930846	56.72%	17.846%
14	2.833	533	542	553	rVB3	9644	20762	0.17%	0.053%
15	3.183	638	651	659	rBV6	3828	7511	0.06%	0.019%
16	3.437	718	730	745	rVB4	3428	8036	0.07%	0.021%
17	3.621	770	787	799	rBV3	4402	11655	0.10%	0.030%
18	3.990	889	902	903	rBV4	8135	10534	0.09%	0.027%
19	4.170	942	958	967	rBV	163282	393868	3.22%	1.014%
20	4.646	1089	1106	1147	rVV3	318249	985977	8.07%	2.539%
21	5.132	1248	1257	1271	rVB4	3911	8478	0.07%	0.022%
22	5.338	1296	1321	1357	rBV2	546494	1643460	13.45%	4.232%
23	5.595	1390	1401	1412	rBV10	2308	4824	0.04%	0.012%
24	5.781	1455	1459	1473	rVB9	2283	4133	0.03%	0.011%
25	5.881	1473	1490	1514	rBV	536488	1061000	8.68%	2.732%
26	6.183	1566	1584	1617	rBV	6286037	12218752	100.00%	31.462%
27	6.325	1617	1628	1654	rVV	364624	785888	6.43%	2.024%
28	6.424	1654	1659	1683	rVV5	7439	20804	0.17%	0.054%
29	6.540	1687	1695	1704	rVB7	2583	4454	0.04%	0.011%
30	6.611	1710	1717	1734	rVB6	5061	11716	0.10%	0.030%
31	6.755	1751	1762	1774	rBV6	7719	13347	0.11%	0.034%
32	6.862	1786	1795	1804	rVB10	1890	3261	0.03%	0.008%
33	7.225	1896	1908	1932	rBV	170890	308661	2.53%	0.795%
34	7.460	1971	1981	1997	rBV3	10189	18925	0.15%	0.049%

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Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
 Title : VOC Analysis

35	7.563	1998	2013	2029	rBV	757807	1325724	10.85%	3.414%
36	7.633	2031	2035	2050	rVB2	14230	28012	0.23%	0.072%
37	7.845	2091	2101	2125	rBV	120049	217881	1.78%	0.561%
38	8.064	2159	2169	2187	rVB7	11928	23307	0.19%	0.060%
39	8.164	2187	2200	2209	rBV6	10275	21782	0.18%	0.056%
40	8.225	2209	2219	2233	rVB2	60788	104539	0.86%	0.269%
41	8.308	2233	2245	2282	rBV	593500	1042456	8.53%	2.684%
42	8.469	2288	2295	2310	rVB5	9300	18777	0.15%	0.048%
43	8.575	2322	2328	2335	rBV7	1851	2940	0.02%	0.008%
44	9.087	2474	2487	2520	rBV	795141	1316677	10.78%	3.390%
45	9.254	2529	2539	2548	rBV	8675	13998	0.11%	0.036%
46	9.325	2554	2561	2570	rVV3	8913	14730	0.12%	0.038%
47	9.373	2570	2576	2589	rVB2	9752	16756	0.14%	0.043%
48	9.611	2643	2650	2660	rVB7	1723	3258	0.03%	0.008%
49	9.778	2691	2702	2711	rBV	113709	182516	1.49%	0.470%
50	9.923	2732	2747	2758	rBV4	7805	16552	0.14%	0.043%
51	10.025	2764	2779	2791	rBV10	8972	22406	0.18%	0.058%
52	10.077	2791	2795	2804	rVB5	3494	4625	0.04%	0.012%
53	10.157	2804	2820	2823	rBV7	7430	11989	0.10%	0.031%
54	10.299	2856	2864	2873	rBV8	4407	6947	0.06%	0.018%
55	10.427	2887	2904	2922	rVV	638469	1030423	8.43%	2.653%
56	10.601	2948	2958	2967	rBV5	5577	10086	0.08%	0.026%
57	10.659	2967	2976	2987	rBV3	14848	25799	0.21%	0.066%
58	10.730	2988	2998	3008	rBV3	58111	95250	0.78%	0.245%
59	10.945	3055	3065	3069	rBV9	9111	13034	0.11%	0.034%
60	11.029	3085	3091	3096	rBV7	3016	4453	0.04%	0.011%
61	11.144	3117	3127	3137	rVB4	12539	21609	0.18%	0.056%
62	11.218	3137	3150	3153	rBV8	6710	11651	0.10%	0.030%
63	11.251	3158	3160	3172	rVB8	7399	11485	0.09%	0.030%
64	11.366	3188	3196	3207	rVB4	23654	35377	0.29%	0.091%
65	11.479	3218	3231	3250	rVB	883019	1390673	11.38%	3.581%
66	11.569	3250	3259	3273	rBV3	20964	39975	0.33%	0.103%
67	11.636	3275	3280	3290	rVB4	10268	15495	0.13%	0.040%
68	11.739	3299	3312	3337	rBV	1720128	2731409	22.35%	7.033%
69	11.855	3337	3348	3368	rVB	852568	1400188	11.46%	3.605%
70	12.122	3427	3431	3434	rBV5	3724	3652	0.03%	0.009%
71	12.228	3455	3464	3485	rBV5	19056	47569	0.39%	0.122%

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72	12.379	3502	3511	3519	rBV5	6858	10902	0.09%	0.028%
73	12.453	3523	3534	3538	rBV3	19692	31610	0.26%	0.081%
74	12.562	3556	3568	3590	rBV	395783	636692	5.21%	1.639%
75	12.675	3599	3603	3610	rVB8	5061	6590	0.05%	0.017%
76	12.855	3652	3659	3662	rBV8	6261	7855	0.06%	0.020%
77	12.894	3662	3671	3680	rVV2	49474	77878	0.64%	0.201%
78	13.057	3713	3722	3731	rBV6	12333	20835	0.17%	0.054%
79	13.119	3737	3741	3757	rVB7	7789	14404	0.12%	0.037%
80	13.292	3785	3795	3796	rBV8	4997	6612	0.05%	0.017%
81	13.324	3800	3805	3810	rVV6	6741	9210	0.08%	0.024%
82	13.453	3839	3845	3851	rBV7	4740	7117	0.06%	0.018%
83	13.511	3856	3863	3866	rBV7	10104	13418	0.11%	0.035%
84	13.659	3900	3909	3921	rBV5	42032	73481	0.60%	0.189%
85	13.742	3927	3935	3950	rVB	22485	45867	0.38%	0.118%
86	13.810	3950	3956	3967	rBV4	11361	15437	0.13%	0.040%
87	13.948	3991	3999	4006	rBV10	7912	13759	0.11%	0.035%
88	14.074	4029	4038	4053	rVB	38301	57580	0.47%	0.148%
89	14.565	4181	4191	4205	rBV9	10180	23020	0.19%	0.059%
90	14.649	4209	4217	4231	rVV9	14209	34361	0.28%	0.088%
91	14.713	4234	4237	4241	rVB4	4173	3621	0.03%	0.009%
92	14.819	4265	4270	4280	rVB10	6719	9629	0.08%	0.025%
93	14.890	4281	4292	4305	rVB10	8252	20622	0.17%	0.053%
94	15.028	4322	4335	4361	rVV	101728	224426	1.84%	0.578%
95	15.218	4388	4394	4401	rVB8	4901	7174	0.06%	0.018%
96	15.353	4427	4436	4448	rVB3	22750	37898	0.31%	0.098%
97	15.614	4509	4517	4519	rBV9	3334	4228	0.03%	0.011%
98	15.713	4540	4548	4551	rBV5	10681	14502	0.12%	0.037%
99	16.424	4759	4769	4778	rBV7	18899	31874	0.26%	0.082%
100	17.504	5097	5105	5118	rVB5	13754	25982	0.21%	0.067%

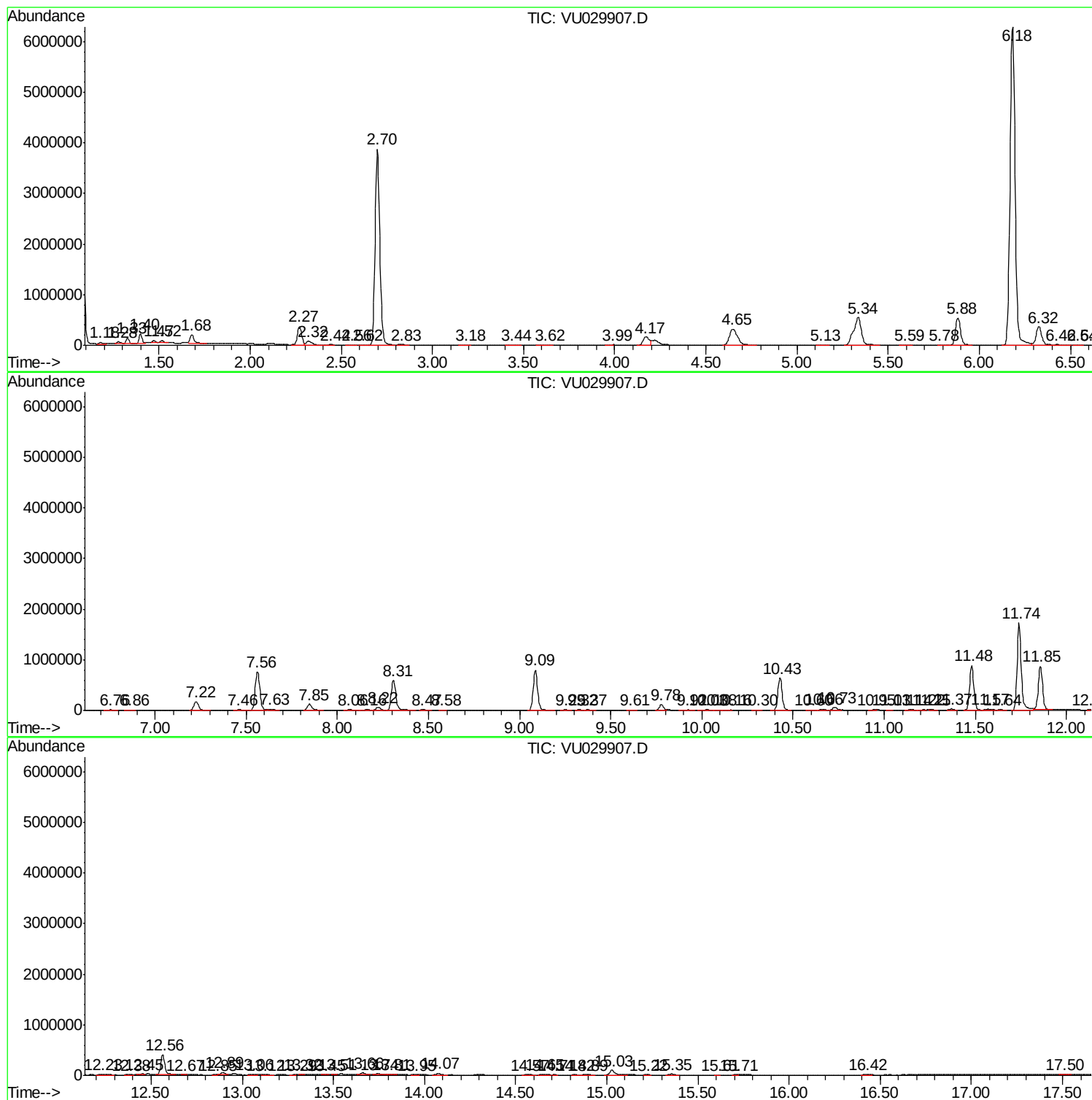
Sum of corrected areas: 38836303

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ClientSampled :
C0957

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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



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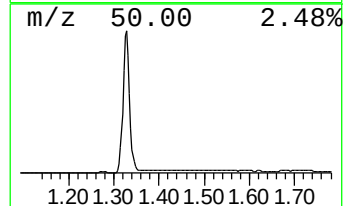
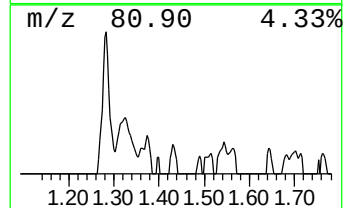
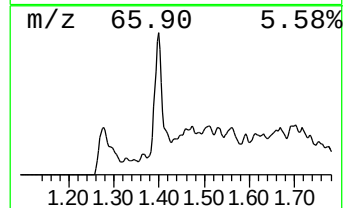
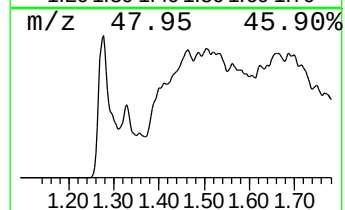
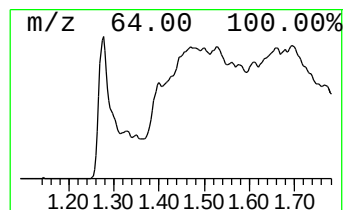
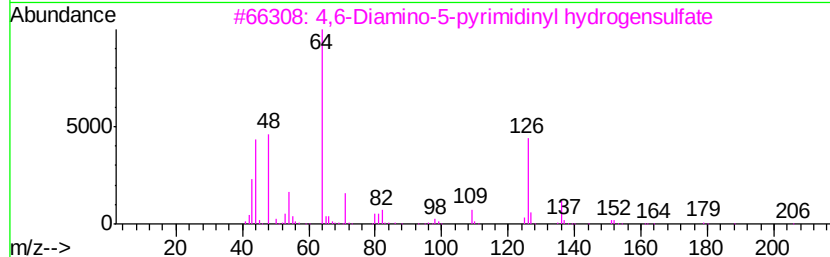
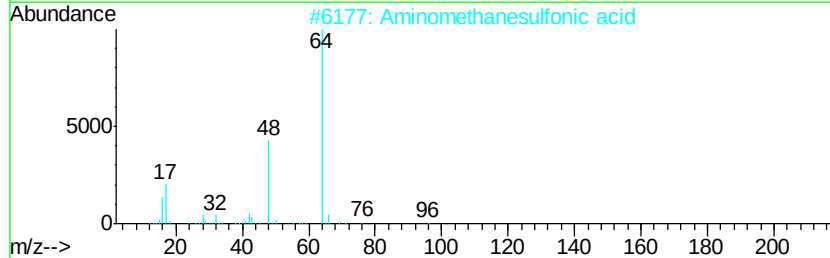
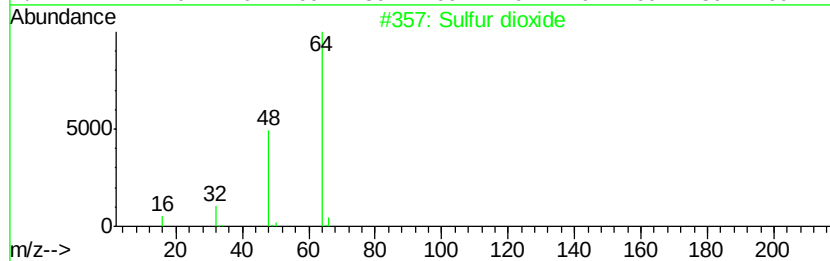
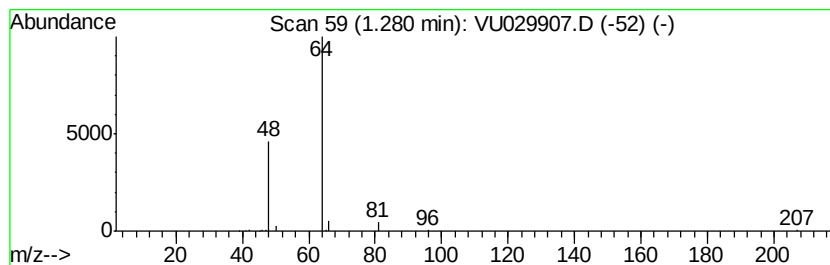
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	2.65 ug/L	56171	1,4-Difluorobenzene	5.88
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Sulfur dioxide	64 O2S	007446-09-5 90
2		Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9 64
3		4,6-Diamino-5-pyrimidinyl hydrog...	206 C4H6N4O4S	071525-41-2 9
4		Thiosulfuric acid (H2S2O3), S-(2...	320 C11H16N2O3S3	040284-00-2 9
5		S-2-[4-Glutarimidobutylamino]eth...	324 C11H20N2O5S2	031701-78-7 9



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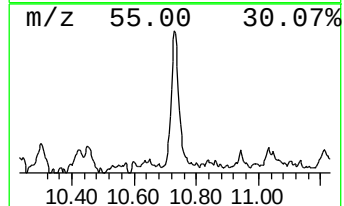
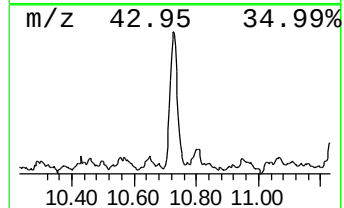
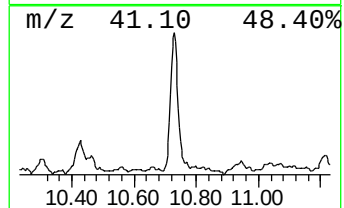
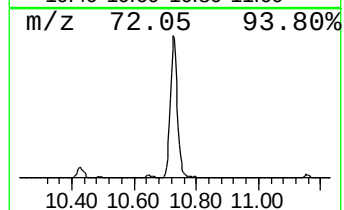
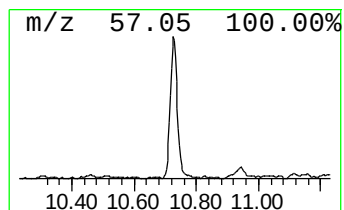
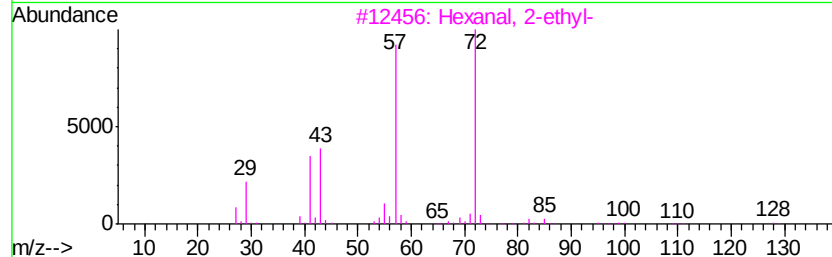
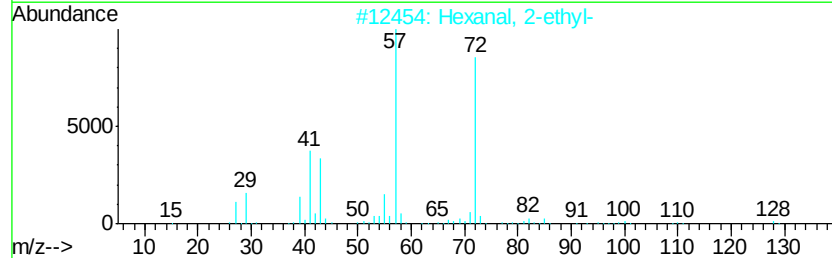
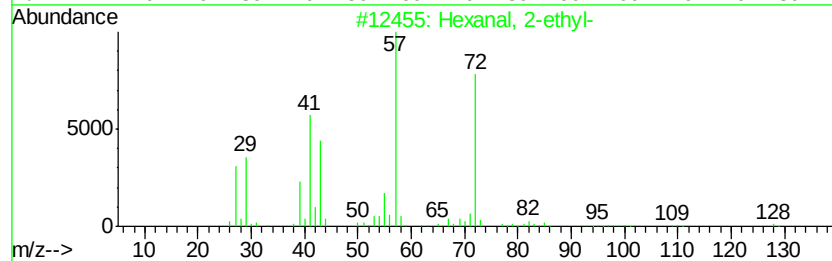
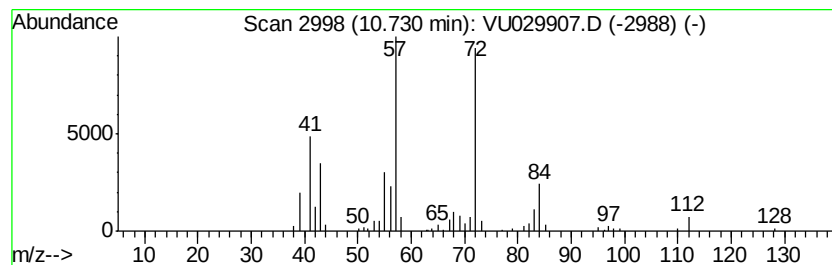
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexanal, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.42 ug/L	95250	1,4-Dichlorobenzene-d4	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	64	
2	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	52	
3	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	49	
4	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	49	
5	trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	47	



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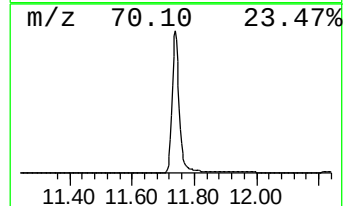
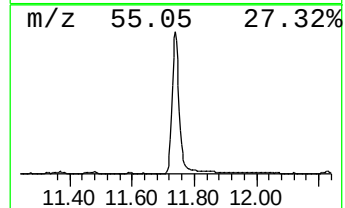
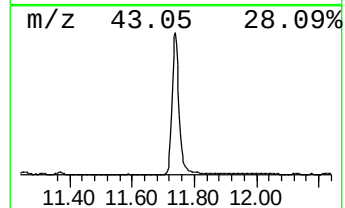
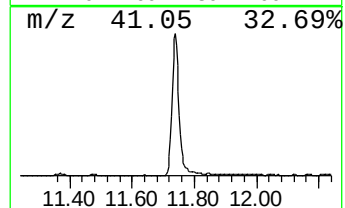
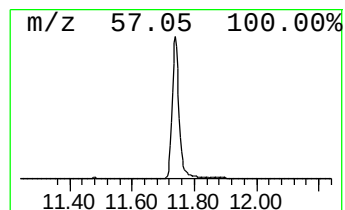
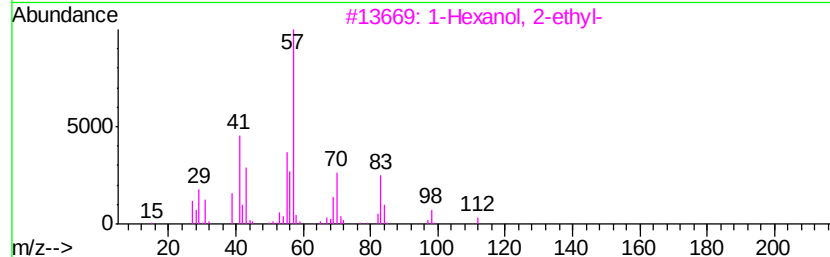
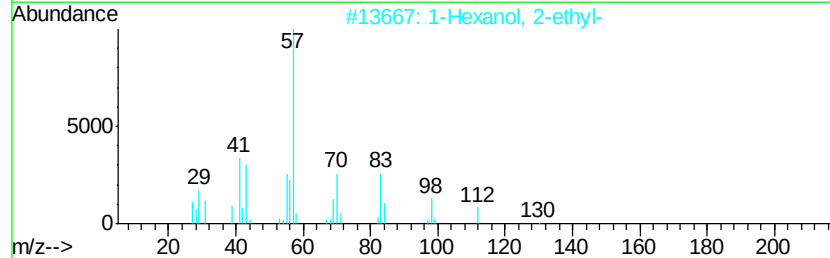
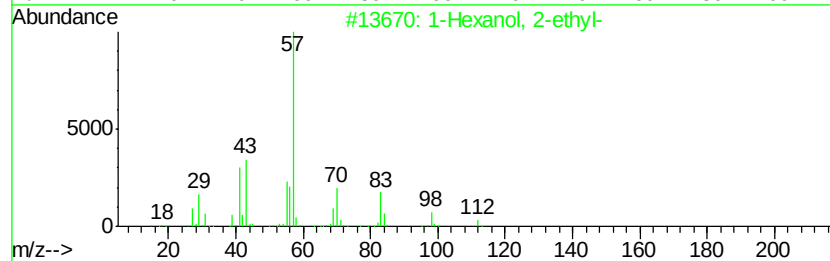
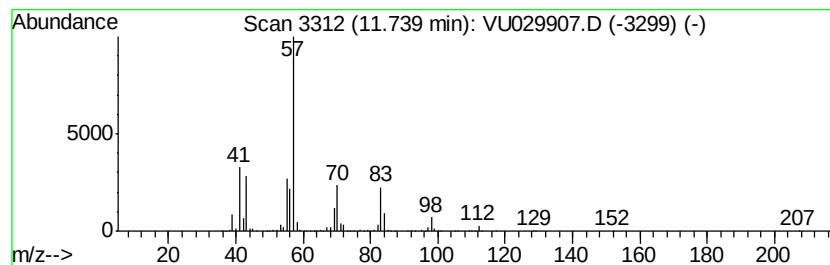
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	98.20 ug/L	2731410	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4		Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	59
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU031119\
Data File : VU029907.D
Acq On : 08 Mar 2019 22:48
Operator : JC/SP
Sample : K1763-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0957

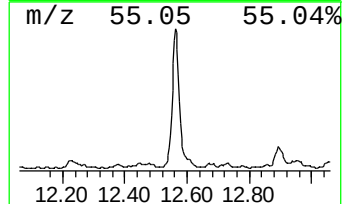
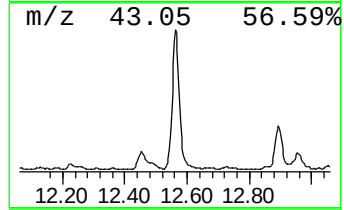
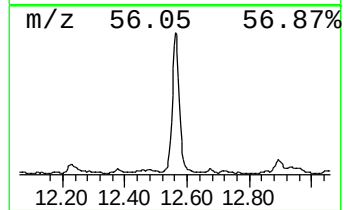
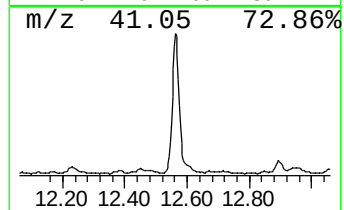
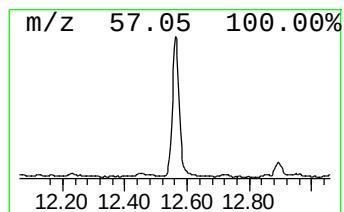
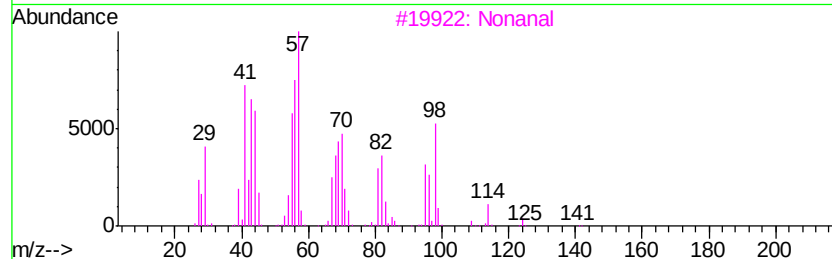
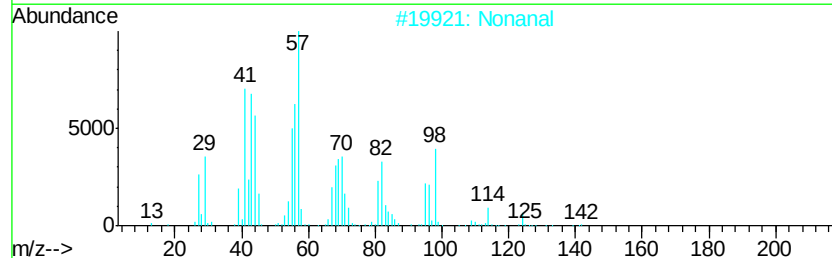
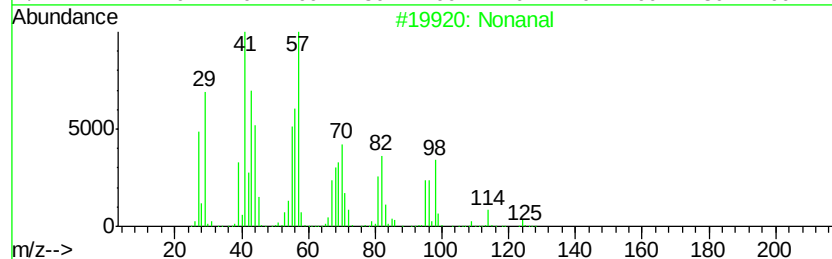
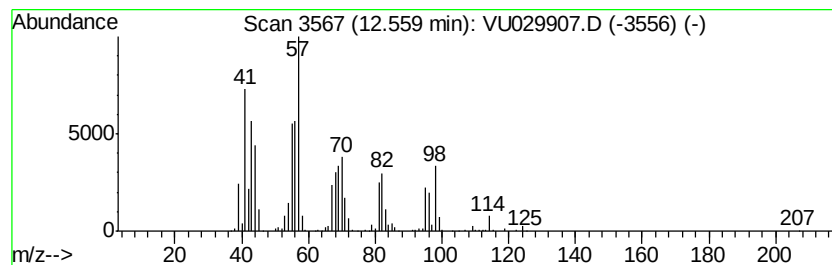
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Quant Title : VOC Analysis

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

Peak Number 5 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	22.89 ug/L	636692	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		Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	30
5		Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU031119\
Data File : VU029907.D
Acq On : 08 Mar 2019 22:48
Operator : JC/SP
Sample : K1763-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0957

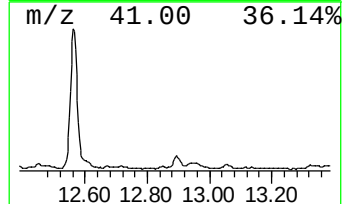
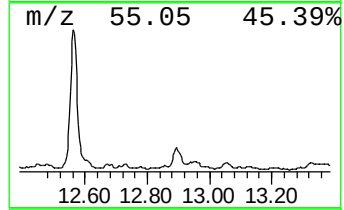
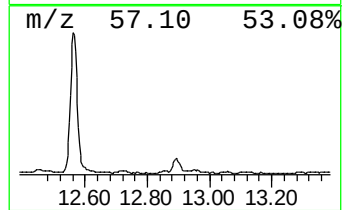
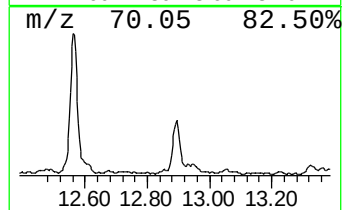
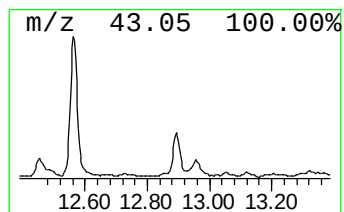
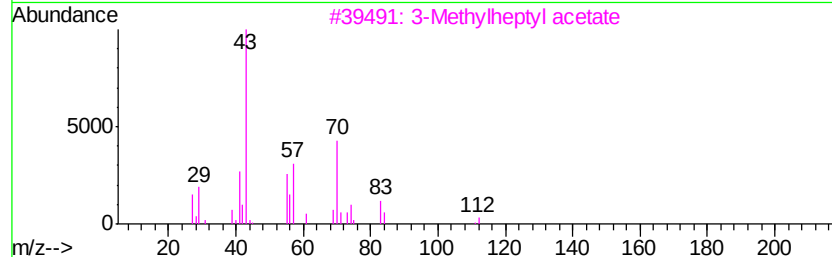
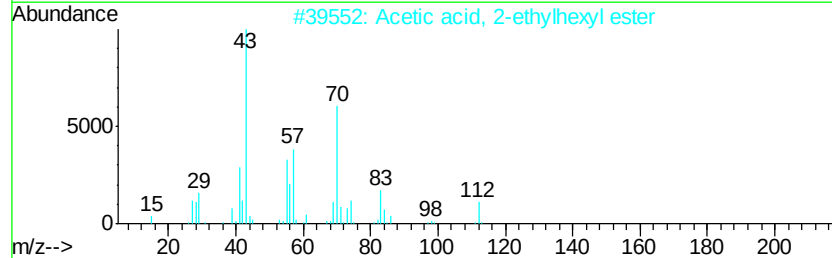
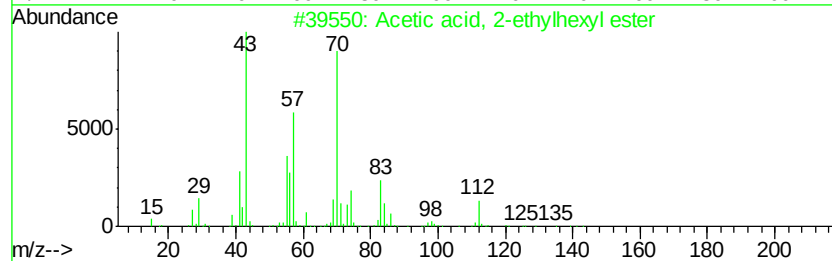
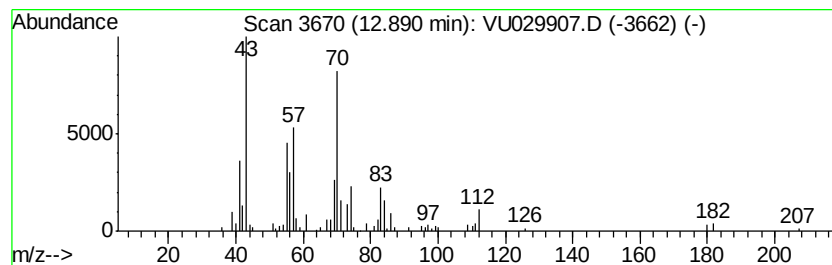
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, 2-ethylhexyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	2.80 ug/L	77878	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	90
2		Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	90
3		3-Methylheptyl acetate	172	C10H20O2	072218-58-7	83
4		Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	72
5		1-Octene	112	C8H16	000111-66-0	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU031119\
Data File : VU029907.D
Acq On : 08 Mar 2019 22:48
Operator : JC/SP
Sample : K1763-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0957

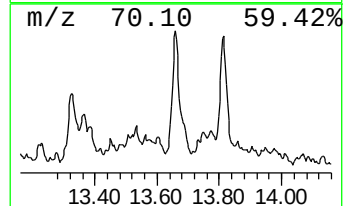
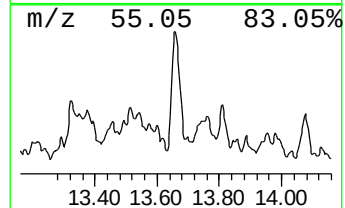
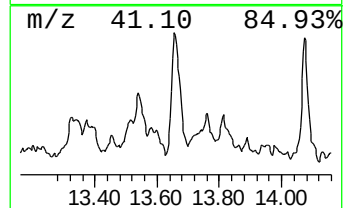
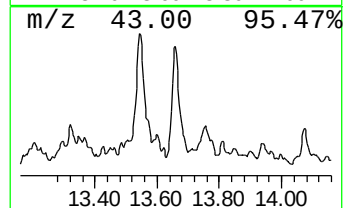
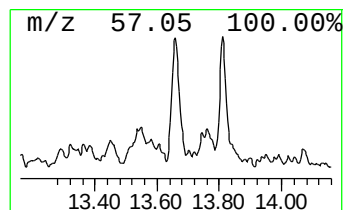
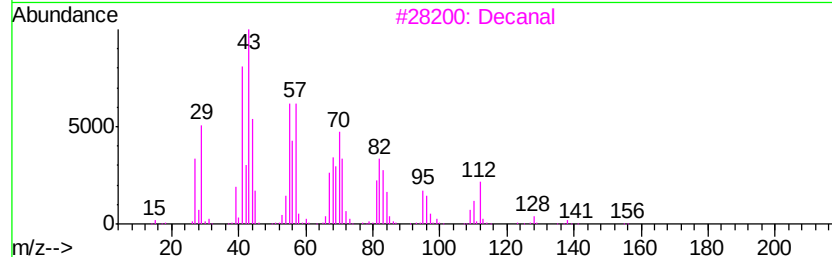
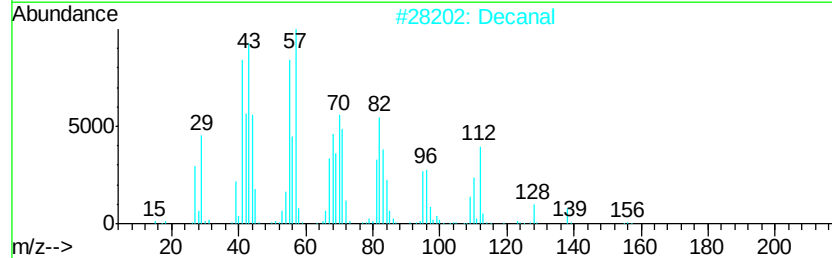
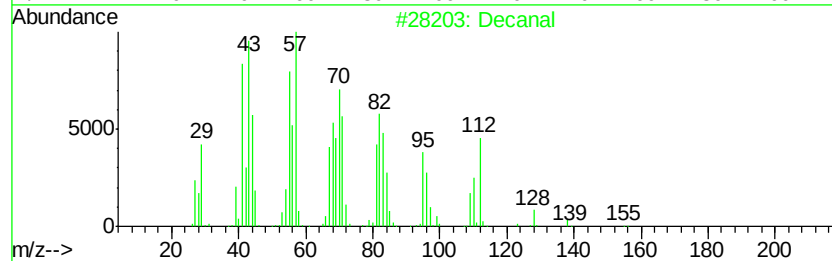
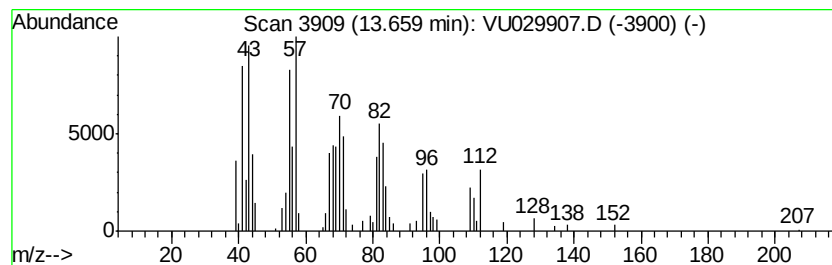
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Quant Title : VOC Analysis

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

Peak Number 7 Decanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	2.64 ug/L	73481	1,4-Dichlorobenzene-d4	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanal		156	C10H20O	000112-31-2	90
2	Decanal		156	C10H20O	000112-31-2	87
3	Decanal		156	C10H20O	000112-31-2	86
4	Oxirane, decyl-		184	C12H24O	002855-19-8	74
5	11-Dodecen-1-yl acetate		226	C14H26O2	035153-10-7	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU031119\
Data File : VU029907.D
Acq On : 08 Mar 2019 22:48
Operator : JC/SP
Sample : K1763-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 26 Sample Multiplier: 1

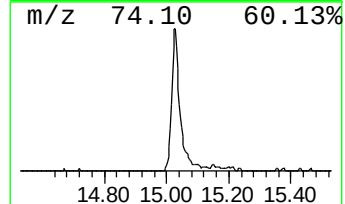
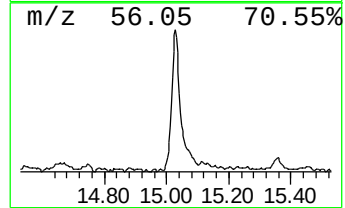
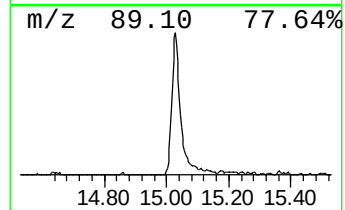
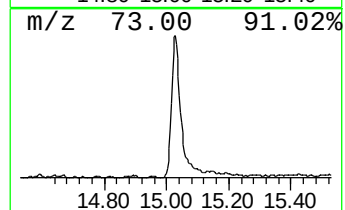
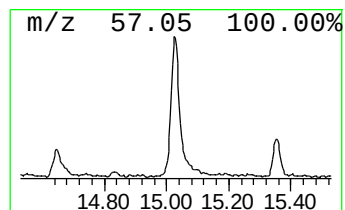
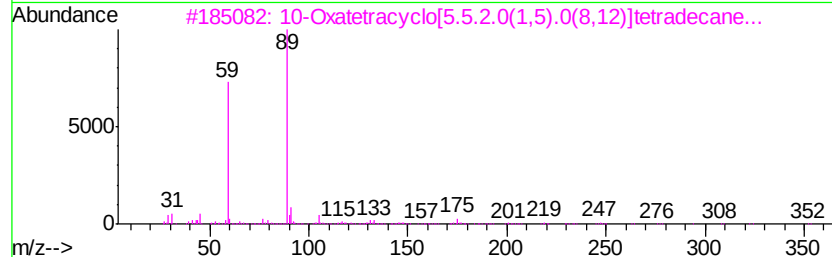
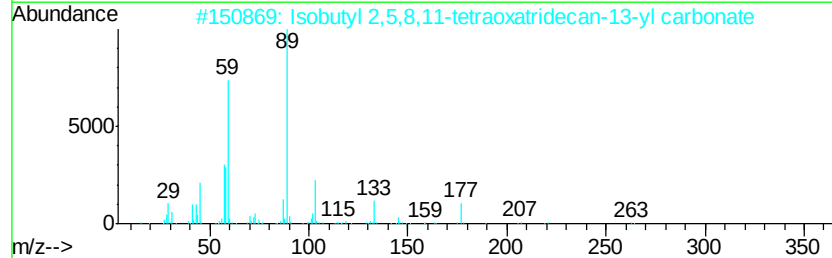
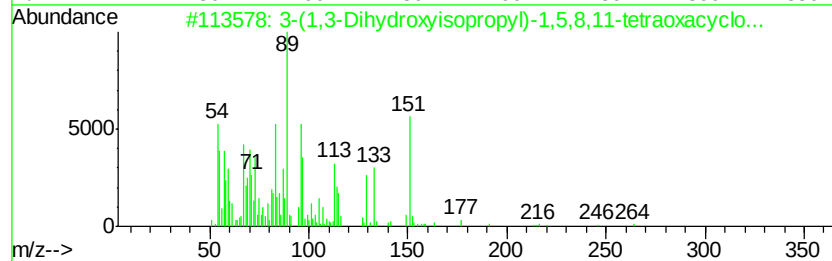
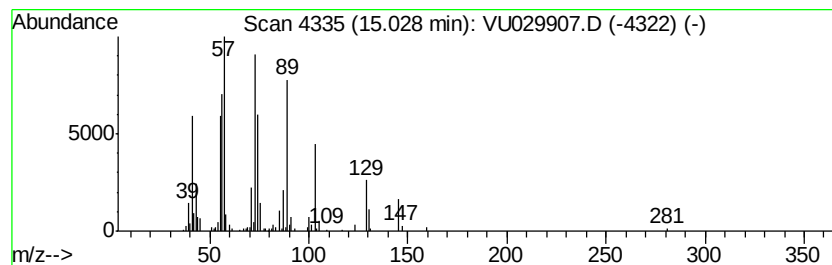
Instrument :
MSVOA_U
ClientSampleId :
C0957

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 3-(1,3-Dihydroxyisopropyl)-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	8.07 ug/L	224426	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-(1,3-Dihydroxyisopropyl)-1,5,8...	264 C12H24O6	109773-63-9	53
2	Isobutyl 2,5,8,11-tetraoxatridec...	308 C14H28O7	1000378-27-9	50
3	10-Oxatetracyclo[5.5.2.0(1,5).0(...	352 C18H24O7	1000154-01-5	47
4	Propanoic acid, 2-methyl-, 2-eth...	216 C12H24O3	074367-31-0	42
5	1-Methoxy-3-trimethylsilyloxymet...	232 C12H28O2Si	1000216-84-0	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU031119\
Data File : VU029907.D
Acq On : 08 Mar 2019 22:48
Operator : JC/SP
Sample : K1763-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0957

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.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
Sulfur dioxide	1.28	2.6	ug/L	56171	1	5.88	1061000	50.0
Hexanal, 2-ethyl-	10.73	3.4	ug/L	95250	3	11.48	1390670	50.0
1-Hexanol, 2-ethyl-	11.74	98.2	ug/L	2731410	3	11.48	1390670	50.0
Nonanal	12.56	22.9	ug/L	636692	3	11.48	1390670	50.0
Acetic acid, 2-et...	12.89	2.8	ug/L	77878	3	11.48	1390670	50.0
Decanal	13.66	2.6	ug/L	73481	3	11.48	1390670	50.0
3-(1,3-Dihydroxyi...	15.03	8.1	ug/L	224426	3	11.48	1390670	50.0