

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU031319\
 Data File : VU029986.D
 Acq On : 11 Mar 2019 23:24
 Operator : JC/SP
 Sample : K1763-04 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0959

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\SOMULM031319WMA.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	25	29	41	rBV3	11011	12294	0.69%	0.077%
2	1.270	49	56	69	rBV	215977	278668	15.61%	1.748%
3	1.682	177	184	206	rVB	201886	261041	14.62%	1.638%
4	2.109	309	317	330	rVB	26240	41949	2.35%	0.263%
5	2.321	374	383	399	rVB2	30513	58969	3.30%	0.370%
6	2.479	425	432	442	rVB	5899	8962	0.50%	0.056%
7	2.553	448	455	463	rBV3	3797	6432	0.36%	0.040%
8	2.701	487	501	521	rBV	312401	553323	31.00%	3.471%
9	2.836	533	543	563	rVB	22960	50912	2.85%	0.319%
10	2.942	563	576	588	rVV	6023	12015	0.67%	0.075%
11	2.987	588	590	597	rVB3	902	743	0.04%	0.005%
12	3.058	609	612	619	rVB2	597	641	0.04%	0.004%
13	3.183	643	651	664	rVB4	1837	4259	0.24%	0.027%
14	3.382	708	713	715	rBV2	1025	866	0.05%	0.005%
15	3.395	715	717	722	rVV3	991	763	0.04%	0.005%
16	3.447	725	733	746	rVB3	2202	3864	0.22%	0.024%
17	3.620	780	787	790	rBV3	919	1116	0.06%	0.007%
18	3.685	798	807	812	rBV3	626	1131	0.06%	0.007%
19	3.829	843	852	855	rBV5	1646	2619	0.15%	0.016%
20	4.003	897	906	907	rBV3	2679	3598	0.20%	0.023%
21	4.090	928	933	935	rBV3	614	668	0.04%	0.004%
22	4.170	945	958	981	rBV	155756	410296	22.98%	2.574%
23	4.665	1089	1112	1139	rBV3	548777	1785131	100.00%	11.199%
24	5.048	1227	1231	1232	rBV3	1002	652	0.04%	0.004%
25	5.132	1250	1257	1272	rVB6	3744	8469	0.47%	0.053%
26	5.337	1296	1321	1356	rBV2	553123	1685172	94.40%	10.572%
27	5.569	1389	1393	1396	rBV5	1079	658	0.04%	0.004%
28	5.646	1413	1417	1421	rBV3	856	781	0.04%	0.005%
29	5.733	1438	1444	1446	rBV5	1883	1960	0.11%	0.012%
30	5.791	1459	1462	1466	rBV2	982	684	0.04%	0.004%
31	5.884	1477	1491	1532	rBV	558440	1131240	63.37%	7.097%
32	6.183	1569	1584	1605	rVV2	121505	258631	14.49%	1.623%
33	6.328	1615	1629	1653	rBV	389106	782937	43.86%	4.912%
34	6.543	1690	1696	1697	rBV4	2432	2385	0.13%	0.015%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
 Title : VOC Analysis

35	6.755	1745	1762	1777	rBV	51456	101849	5.71%	0.639%
36	6.813	1777	1780	1784	rVB3	902	658	0.04%	0.004%
37	7.209	1899	1903	1905	rBV3	1245	1124	0.06%	0.007%
38	7.341	1938	1944	1946	rBV4	1048	1077	0.06%	0.007%
39	7.463	1969	1982	1993	rBV2	11826	24095	1.35%	0.151%
40	7.540	1998	2006	2028	rVB3	6876	18840	1.06%	0.118%
41	7.652	2033	2041	2052	rBV4	3621	6361	0.36%	0.040%
42	7.723	2059	2063	2065	rBV3	1049	583	0.03%	0.004%
43	7.855	2093	2104	2120	rVV2	18957	36025	2.02%	0.226%
44	7.990	2141	2146	2149	rBV4	620	711	0.04%	0.004%
45	8.013	2149	2153	2156	rBV4	1331	1500	0.08%	0.009%
46	8.176	2191	2204	2215	rBV	67255	138513	7.76%	0.869%
47	8.308	2235	2245	2281	rVB	514072	918518	51.45%	5.762%
48	8.472	2289	2296	2308	rVB6	14659	26539	1.49%	0.166%
49	8.623	2334	2343	2358	rBV9	1840	4735	0.27%	0.030%
50	8.893	2425	2427	2433	rVB3	1007	753	0.04%	0.005%
51	8.955	2439	2446	2449	rBV2	625	810	0.05%	0.005%
52	9.041	2466	2473	2474	rBV5	1843	2126	0.12%	0.013%
53	9.086	2474	2487	2504	rBV	907062	1541824	86.37%	9.673%
54	9.308	2553	2556	2558	rBV2	900	653	0.04%	0.004%
55	9.328	2559	2562	2567	rVV6	1584	1740	0.10%	0.011%
56	9.392	2580	2582	2586	rVB3	1208	830	0.05%	0.005%
57	9.492	2608	2613	2616	rBV4	1299	1420	0.08%	0.009%
58	9.569	2634	2637	2643	rVB2	857	687	0.04%	0.004%
59	9.820	2710	2715	2727	rVB7	1877	3424	0.19%	0.021%
60	9.938	2744	2752	2754	rVV5	969	1268	0.07%	0.008%
61	9.955	2754	2757	2760	rVB3	891	614	0.03%	0.004%
62	10.035	2774	2782	2798	rVB9	3686	7695	0.43%	0.048%
63	10.099	2798	2802	2808	rVB2	875	658	0.04%	0.004%
64	10.164	2808	2822	2828	rBV2	3922	8493	0.48%	0.053%
65	10.231	2838	2843	2844	rBV2	995	697	0.04%	0.004%
66	10.302	2860	2865	2871	rVB5	1241	1400	0.08%	0.009%
67	10.427	2888	2904	2922	rVV	600801	952268	53.34%	5.974%
68	10.514	2924	2931	2937	rVB2	3151	4562	0.26%	0.029%
69	10.604	2945	2959	2980	rBV	641555	1054874	59.09%	6.618%
70	10.717	2983	2994	3013	rBV	254731	423519	23.72%	2.657%
71	10.803	3020	3021	3027	rVB4	718	599	0.03%	0.004%

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72	11.032	3082	3092	3102	rBV3	9289	16992	0.95%	0.107%
73	11.070	3102	3104	3106	rVV3	1371	822	0.05%	0.005%
74	11.099	3106	3113	3120	rVB7	5280	8744	0.49%	0.055%
75	11.147	3120	3128	3140	rBV6	9125	18164	1.02%	0.114%
76	11.209	3144	3147	3148	rBV2	1321	709	0.04%	0.004%
77	11.315	3173	3180	3182	rBV6	1683	1946	0.11%	0.012%
78	11.373	3189	3198	3206	rBV7	3799	6906	0.39%	0.043%
79	11.418	3207	3212	3219	rVV6	4547	5586	0.31%	0.035%
80	11.479	3219	3231	3250	rVV	917568	1449915	81.22%	9.096%
81	11.691	3294	3297	3301	rBV4	1232	1364	0.08%	0.009%
82	11.749	3307	3315	3320	rBV4	12942	21282	1.19%	0.134%
83	11.855	3336	3348	3373	rBV	876369	1454211	81.46%	9.123%
84	12.263	3472	3475	3478	rBV	1218	962	0.05%	0.006%
85	12.356	3498	3504	3506	rBV5	1871	1955	0.11%	0.012%
86	12.472	3531	3540	3553	rVV3	6835	12856	0.72%	0.081%
87	12.569	3561	3570	3579	rBV3	21951	37685	2.11%	0.236%
88	12.771	3619	3633	3648	rVV4	76541	168637	9.45%	1.058%
89	12.887	3663	3669	3681	rVB7	4825	7303	0.41%	0.046%
90	12.942	3681	3686	3690	rBV4	1121	1343	0.08%	0.008%
91	13.189	3753	3763	3776	rVB3	20711	39303	2.20%	0.247%
92	13.507	3855	3862	3870	rVB6	3928	5887	0.33%	0.037%
93	13.649	3898	3906	3907	rBV5	2723	3125	0.18%	0.020%
94	13.739	3929	3934	3935	rBV3	1210	948	0.05%	0.006%
95	13.990	4006	4012	4021	rVB7	2390	3829	0.21%	0.024%
96	14.250	4087	4093	4094	rBV4	769	722	0.04%	0.005%
97	14.520	4173	4177	4180	rBV3	1205	827	0.05%	0.005%
98	14.684	4224	4228	4234	rBV3	876	944	0.05%	0.006%
99	15.163	4375	4377	4381	rVB3	1202	697	0.04%	0.004%
100	15.424	4455	4458	4460	rBV3	1036	702	0.04%	0.004%

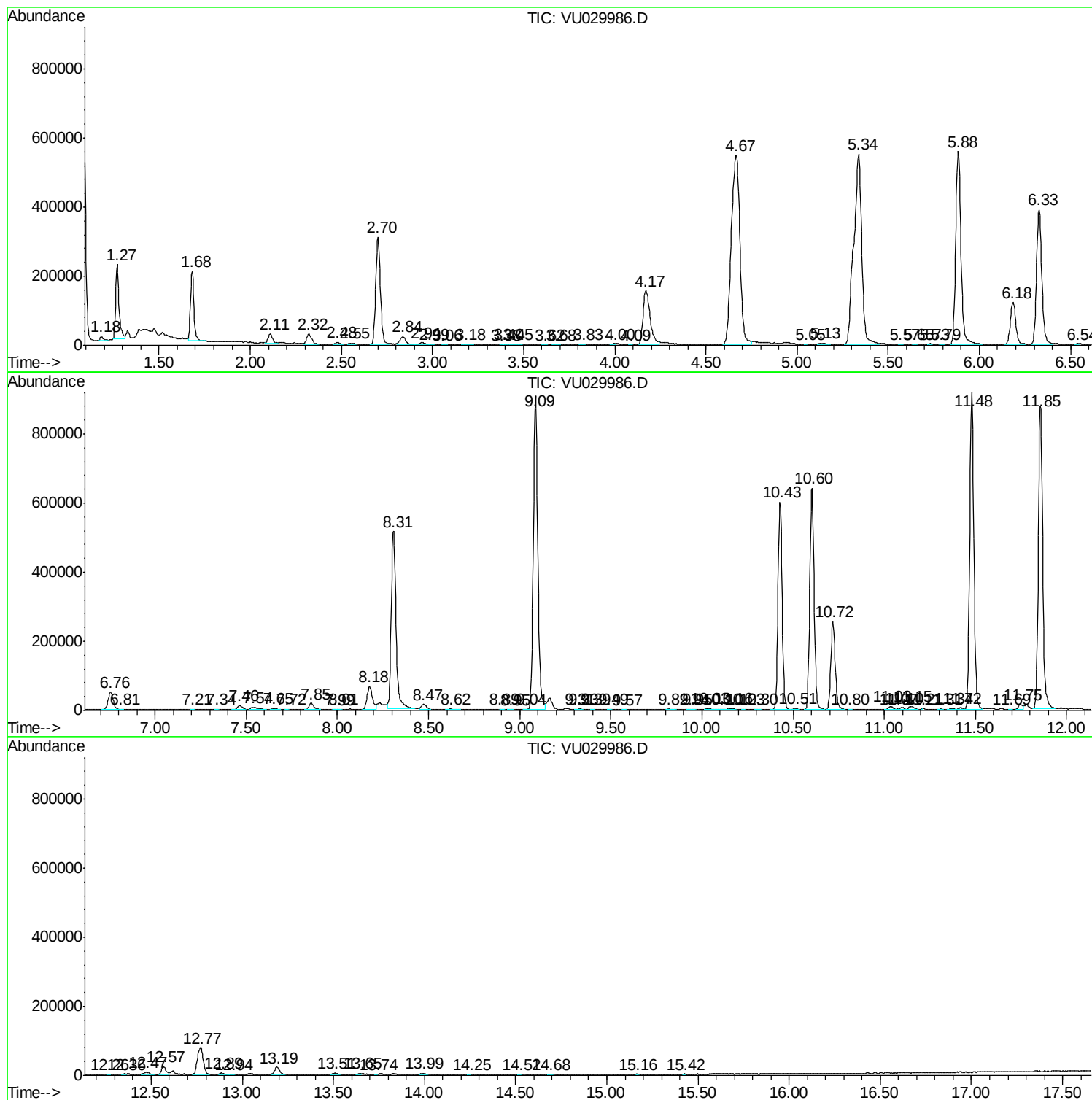
Sum of corrected areas: 15940237

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

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



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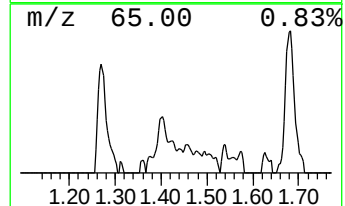
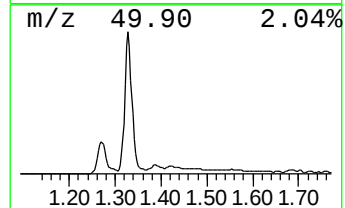
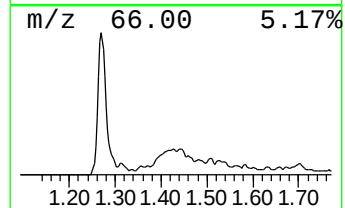
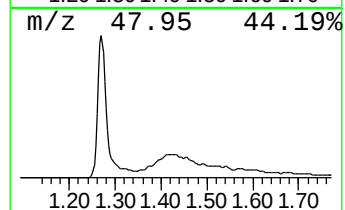
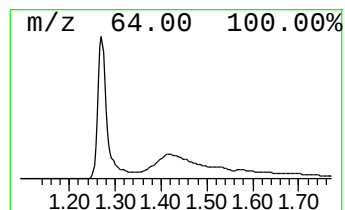
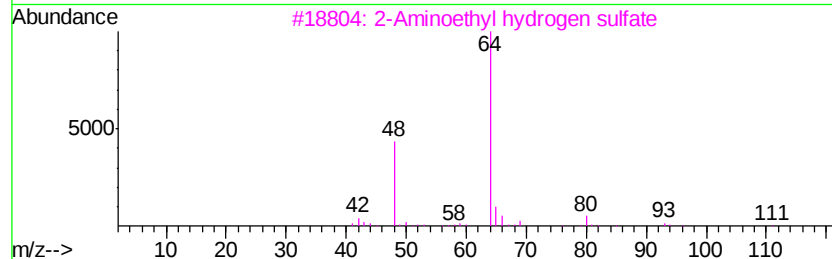
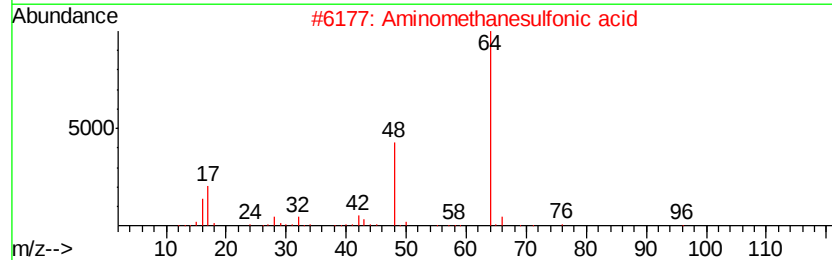
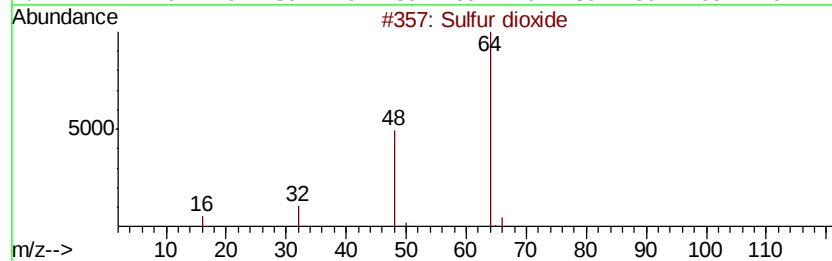
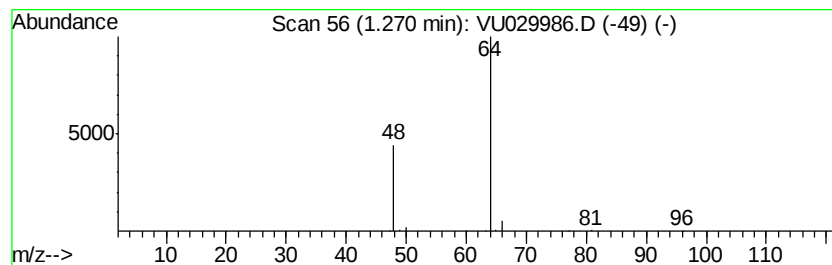
Instrument :
MSVOA_U
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.27	12.32 ug/L	278668	1,4-Difluorobenzene	5.88
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 02S	007446-09-5	83
2	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	74
3	2-Aminoethyl hydrogen sulfate	141 C2H7N04S	000926-39-6	64
4	L-Alanine, 3-sulfo-	169 C3H7N05S	000498-40-8	9
5	Sulfur dioxide	64 02S	007446-09-5	5



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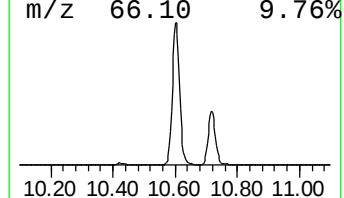
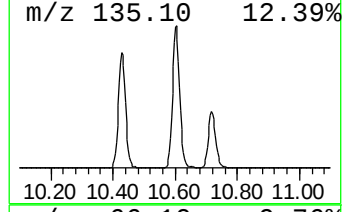
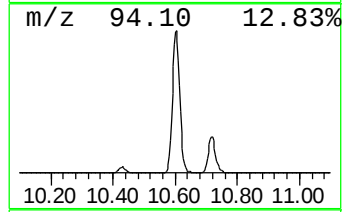
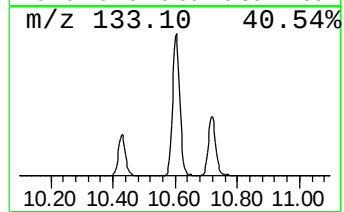
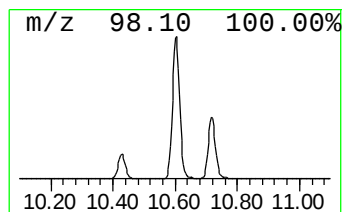
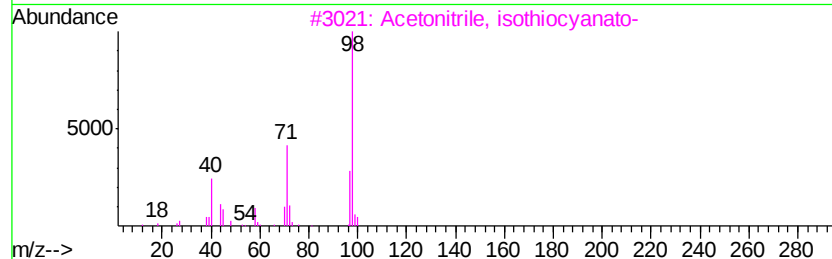
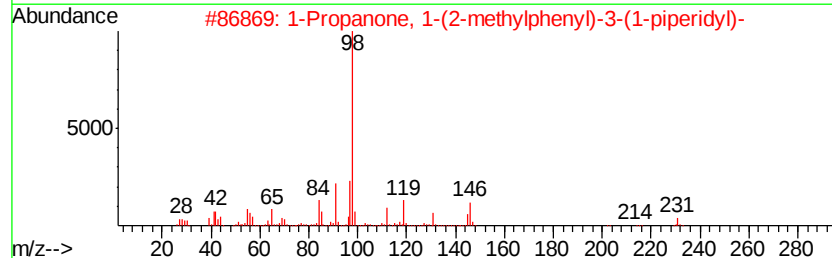
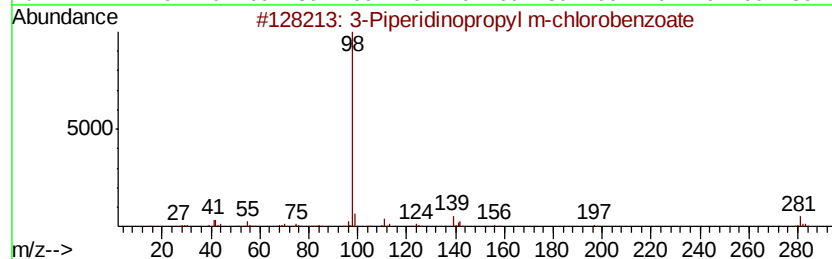
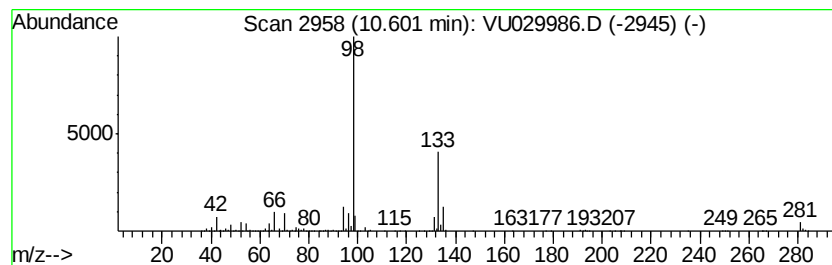
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Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.60	36.38 ug/L	1054870	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Piperidinopropyl m-chlorobenzoate	281	C15H20ClN02	1000240-41-2	38
2	1-Propanone, 1-(2-methylphenyl)-...	231	C15H21NO	125476-98-4	25
3	Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	25
4	Encainide	352	C22H28N2O2	037612-13-8	23
5	3-Piperidinopropyl p-chlorobenzoate	281	C15H20ClN02	1000240-42-7	23



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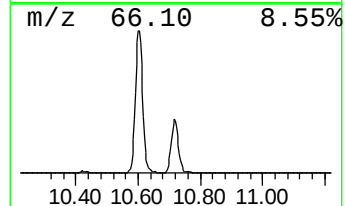
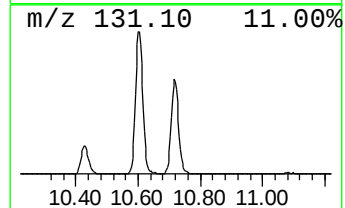
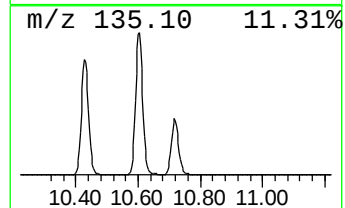
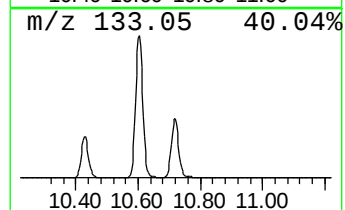
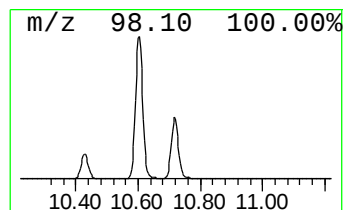
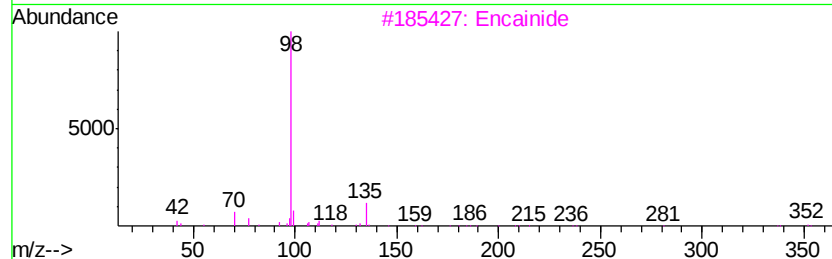
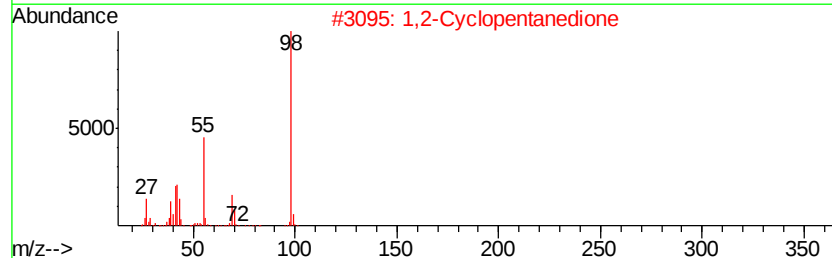
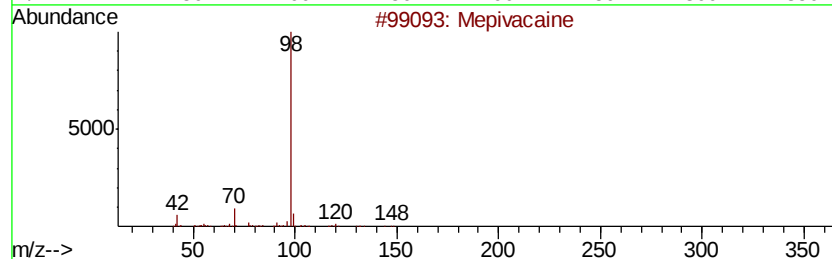
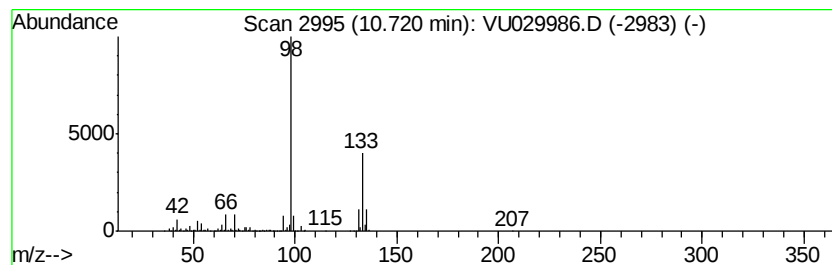
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Quant Title : VOC Analysis

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

Peak Number 4 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	14.61 ug/L	423519	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mepivacaine	246	C15H22N2O	000096-88-8	32
2		1,2-Cyclopentanedione	98	C5H6O2	003008-40-0	32
3		Encainide	352	C22H28N2O2	037612-13-8	25
4		2-[3,4-Dichlorophenyl]-4-[[[1-met...	467	C17H18Cl5N5	061362-15-0	23
5		2-Azabutane, 1-[1-methylazacyclo...	314	C16H24Cl2N2	184637-45-4	23



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU031319\
Data File : VU029986.D
Acq On : 11 Mar 2019 23:24
Operator : JC/SP
Sample : K1763-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

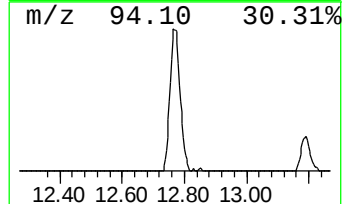
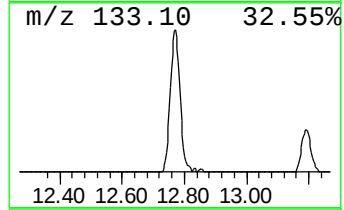
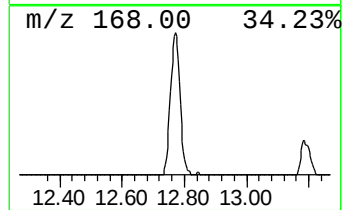
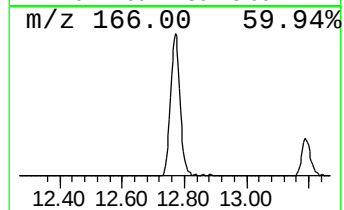
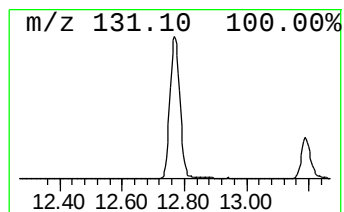
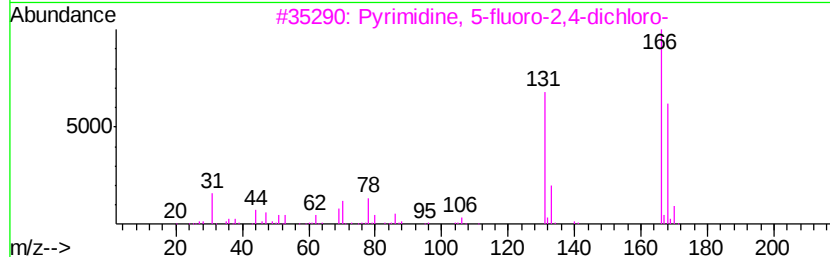
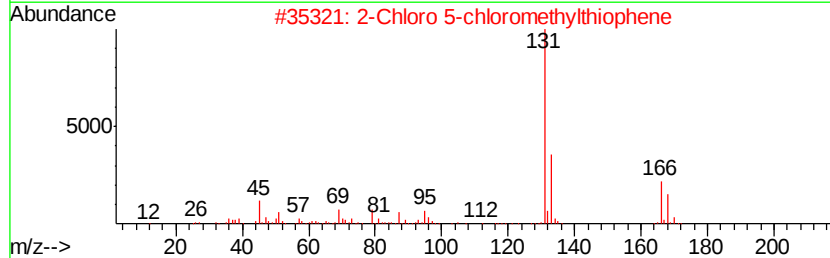
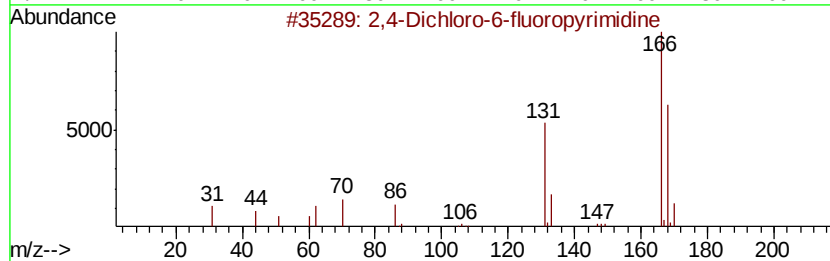
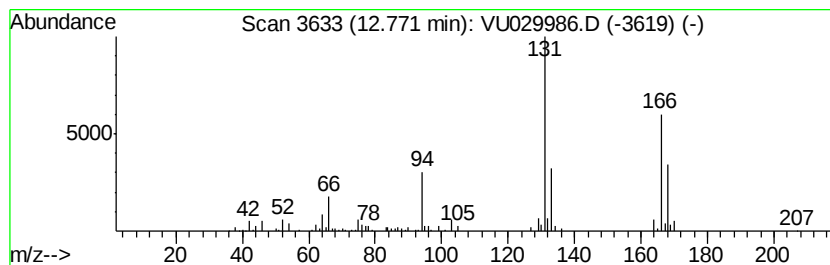
Instrument :
MSVOA_U
ClientSampleId :
C0959

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 2,4-Dichloro-6-fluoropyrimi... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.77	5.82 ug/L	168637	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dichloro-6-fluoropyrimidine	166	C4HCl2FN2	003833-57-6	64
2	2-Chloro 5-chloromethylthiophene	166	C5H4Cl2S	023784-96-5	53
3	Pyrimidine, 5-fluoro-2,4-dichloro-	166	C4HCl2FN2	002927-71-1	50
4	2-Chloromethylbenzimidazole	166	C8H7ClN2	004857-04-9	50
5	4,6-Dichloro-2-fluoropyrimidine	166	C4HCl2FN2	003824-45-1	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU031319\
Data File : VU029986.D
Acq On : 11 Mar 2019 23:24
Operator : JC/SP
Sample : K1763-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0959

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.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	1.27	12.3	ug/L	278668	1	5.88	1131240	50.0
unknown-01	10.60	36.4	ug/L	1054870	3	11.48	1449920	50.0
unknown-02	10.72	14.6	ug/L	423519	3	11.48	1449920	50.0
2,4-Dichloro-6-fl...	12.77	5.8	ug/L	168637	3	11.48	1449920	50.0