

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
 Data File : VU027836.D
 Acq On : 26 Oct 2018 16:15
 Operator : MD/SY
 Sample : J5668-10
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETBS0

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\SOMULM102218WMA.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	1.402	64	71	84	rBV2	62720	70903	4.47%	1.382%
2	1.685	151	159	174	rVB	39526	50291	3.17%	0.980%
3	2.276	333	343	355	rBV	79093	123215	7.77%	2.402%
4	2.447	384	396	413	rBV	20088	35120	2.22%	0.685%
5	2.620	446	450	459	rVB	171	237	0.01%	0.005%
6	2.833	509	516	526	rVB2	483	896	0.06%	0.017%
7	2.987	555	564	576	rBV2	5361	9537	0.60%	0.186%
8	3.193	619	628	631	rBV3	394	519	0.03%	0.010%
9	3.456	706	710	713	rBV	162	161	0.01%	0.003%
10	4.106	908	912	919	rBV2	173	262	0.02%	0.005%
11	4.231	921	951	991	rVV2	603115	1584875	100.00%	30.891%
12	4.472	1024	1026	1031	rVB	186	127	0.01%	0.002%
13	4.652	1066	1082	1106	rBV	68803	161163	10.17%	3.141%
14	4.800	1126	1128	1134	rVB	183	191	0.01%	0.004%
15	4.833	1134	1138	1142	rBV2	200	236	0.01%	0.005%
16	4.881	1150	1153	1162	rVB2	258	231	0.01%	0.005%
17	4.990	1185	1187	1193	rVB	157	109	0.01%	0.002%
18	5.058	1206	1208	1211	rBV2	158	87	0.01%	0.002%
19	5.099	1218	1221	1223	rBV	133	78	0.00%	0.002%
20	5.138	1227	1233	1236	rBV	183	255	0.02%	0.005%
21	5.215	1251	1257	1261	rVB	154	144	0.01%	0.003%
22	5.234	1261	1263	1265	rBV	147	80	0.01%	0.002%
23	5.344	1271	1297	1318	rBV3	137264	407947	25.74%	7.951%
24	5.418	1318	1320	1324	rVB	221	116	0.01%	0.002%
25	5.697	1404	1407	1412	rVB	193	211	0.01%	0.004%
26	5.723	1412	1415	1417	rBB	123	89	0.01%	0.002%
27	5.742	1418	1421	1423	rBB	236	118	0.01%	0.002%
28	5.791	1424	1436	1438	rBV2	484	673	0.04%	0.013%
29	5.816	1442	1444	1447	rVB	218	149	0.01%	0.003%
30	5.890	1453	1467	1486	rBV	155318	302614	19.09%	5.898%
31	6.151	1544	1548	1555	rBV	87	131	0.01%	0.003%
32	6.183	1555	1558	1559	rBV	544	319	0.02%	0.006%
33	6.199	1559	1563	1567	rVB3	996	1021	0.06%	0.020%
34	6.244	1571	1577	1581	rVB	104	115	0.01%	0.002%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
 Title : VOC Analysis

35	6.334	1591	1605	1621	rBV	97289	194277	12.26%	3.787%
36	6.556	1671	1674	1677	rVB	213	156	0.01%	0.003%
37	6.585	1678	1683	1684	rBV	154	163	0.01%	0.003%
38	6.643	1697	1701	1704	rVB	165	170	0.01%	0.003%
39	6.681	1708	1713	1715	rBV	158	196	0.01%	0.004%
40	6.829	1754	1759	1760	rBV	161	109	0.01%	0.002%
41	6.861	1763	1769	1780	rVB2	1230	1995	0.13%	0.039%
42	7.176	1864	1867	1871	rVB	190	179	0.01%	0.003%
43	7.228	1871	1883	1905	rBV	56167	99473	6.28%	1.939%
44	7.389	1923	1933	1943	rBV6	2286	3598	0.23%	0.070%
45	7.566	1975	1988	2008	rBV	179964	310319	19.58%	6.048%
46	7.852	2066	2077	2095	rBV	38464	65010	4.10%	1.267%
47	8.183	2166	2180	2188	rBV	31301	65563	4.14%	1.278%
48	8.311	2212	2220	2251	rVB	167047	293034	18.49%	5.711%
49	8.472	2264	2270	2276	rVB5	651	855	0.05%	0.017%
50	8.652	2322	2326	2333	rBV	126	140	0.01%	0.003%
51	8.688	2334	2337	2342	rVB	95	88	0.01%	0.002%
52	8.893	2397	2401	2403	rBV	104	89	0.01%	0.002%
53	9.090	2450	2462	2481	rBV	224039	364936	23.03%	7.113%
54	9.186	2490	2492	2496	rVB2	437	233	0.01%	0.005%
55	9.202	2496	2497	2500	rVB	307	101	0.01%	0.002%
56	9.228	2503	2505	2510	rVB	324	283	0.02%	0.006%
57	9.254	2510	2513	2517	rBV2	269	237	0.01%	0.005%
58	9.299	2523	2527	2530	rBV2	374	384	0.02%	0.007%
59	9.334	2534	2538	2540	rBV2	154	143	0.01%	0.003%
60	9.472	2577	2581	2586	rVB2	330	274	0.02%	0.005%
61	9.524	2593	2597	2599	rBV2	206	176	0.01%	0.003%
62	9.569	2606	2611	2614	rBV3	233	205	0.01%	0.004%
63	9.585	2614	2616	2618	rVB	311	130	0.01%	0.003%
64	9.601	2618	2621	2622	rBV	207	135	0.01%	0.003%
65	9.684	2644	2647	2652	rBV3	255	288	0.02%	0.006%
66	9.871	2702	2705	2708	rVB2	159	112	0.01%	0.002%
67	9.955	2728	2731	2733	rBV	262	152	0.01%	0.003%
68	10.250	2820	2823	2830	rVB	128	119	0.01%	0.002%
69	10.430	2868	2879	2894	rBV	130249	205720	12.98%	4.010%
70	10.617	2923	2937	2951	rVB4	18908	38844	2.45%	0.757%
71	10.877	3010	3018	3025	rBV2	732	1129	0.07%	0.022%

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 Title : VOC Analysis

72	11.485	3195	3207	3225	rBV	212268	330980	20.88%	6.451%
73	11.569	3231	3233	3235	rBV	145	94	0.01%	0.002%
74	11.749	3282	3289	3299	rBV4	1962	3047	0.19%	0.059%
75	11.861	3312	3324	3346	rBV	173293	277863	17.53%	5.416%
76	12.128	3401	3407	3408	rBV	439	375	0.02%	0.007%
77	12.160	3414	3417	3418	rBV	624	375	0.02%	0.007%
78	12.482	3510	3517	3531	rVB	11674	19781	1.25%	0.386%
79	12.533	3531	3533	3535	rBV2	238	97	0.01%	0.002%
80	12.659	3570	3572	3577	rBV2	255	162	0.01%	0.003%
81	12.797	3611	3615	3616	rBV	195	110	0.01%	0.002%
82	13.176	3729	3733	3735	rBV2	249	200	0.01%	0.004%
83	13.208	3741	3743	3749	rVB3	336	299	0.02%	0.006%
84	13.237	3749	3752	3758	rVB3	400	326	0.02%	0.006%
85	13.273	3758	3763	3765	rBV2	158	168	0.01%	0.003%
86	13.710	3895	3899	3902	rBV2	275	204	0.01%	0.004%
87	13.842	3937	3940	3941	rBV2	201	121	0.01%	0.002%
88	14.060	4005	4008	4010	rBV2	181	131	0.01%	0.003%
89	14.077	4010	4013	4015	rVB2	225	125	0.01%	0.002%
90	14.122	4025	4027	4030	rBV	143	89	0.01%	0.002%
91	14.199	4042	4051	4052	rBV3	970	1204	0.08%	0.023%
92	14.279	4068	4076	4087	rVB	14052	23203	1.46%	0.452%
93	14.321	4087	4089	4093	rVB2	247	189	0.01%	0.004%
94	14.363	4093	4102	4105	rBV3	676	606	0.04%	0.012%
95	14.385	4106	4109	4110	rBV	215	133	0.01%	0.003%
96	14.443	4124	4127	4132	rBV2	193	237	0.01%	0.005%
97	14.591	4144	4173	4174	rBV4	13565	30687	1.94%	0.598%
98	14.794	4234	4236	4239	rBV	388	223	0.01%	0.004%
99	15.880	4564	4574	4588	rBV3	7958	13113	0.83%	0.256%
100	16.462	4741	4755	4765	rBV7	8833	25233	1.59%	0.492%

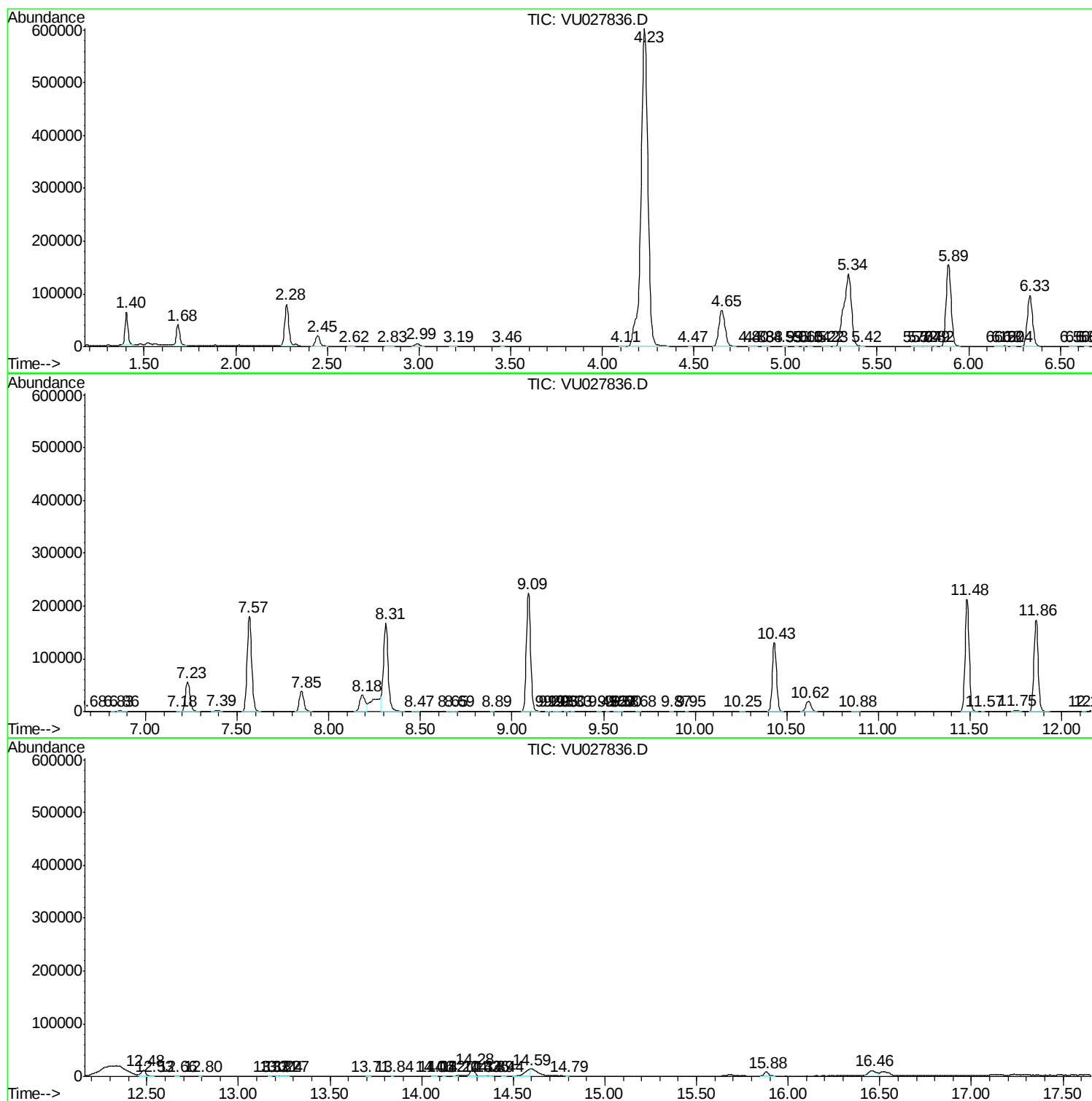
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
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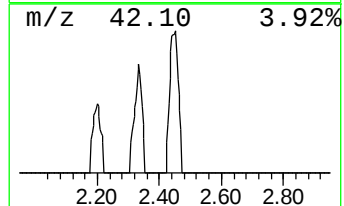
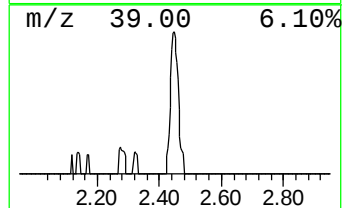
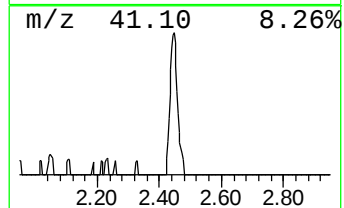
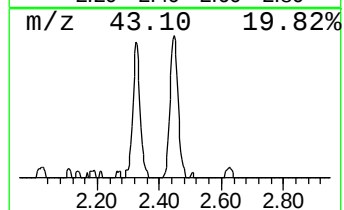
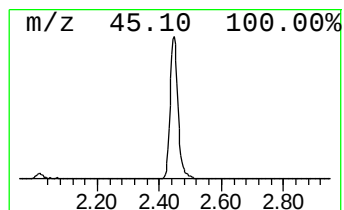
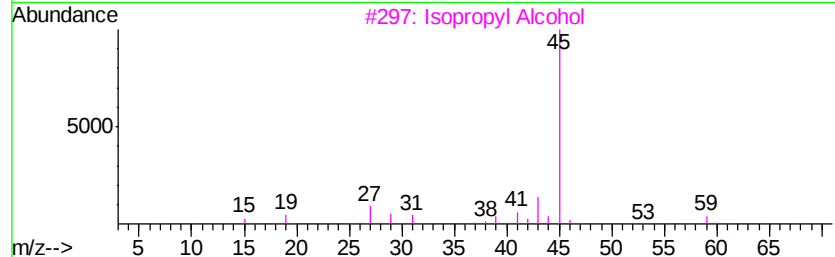
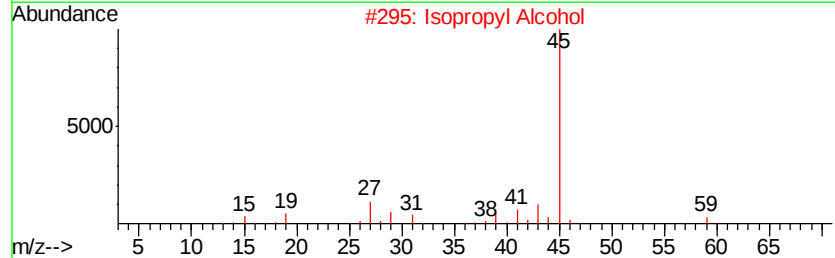
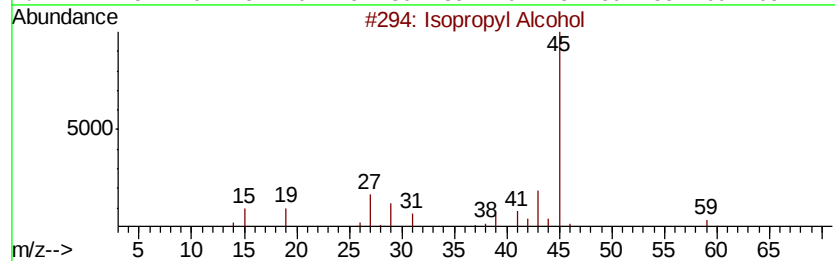
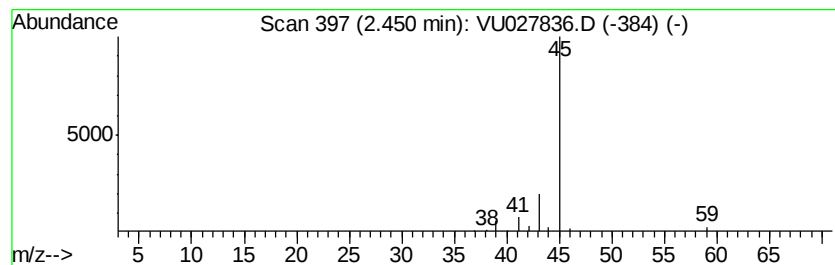
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	5.80 ug/L	35120	1,4-Difluorobenzene	5.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Formamide	45	CH3NO	000075-12-7	5
5			Formamide	45	CH3NO	000075-12-7	5



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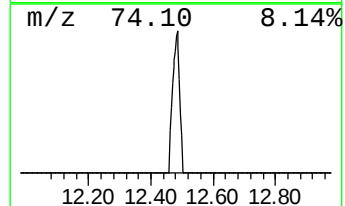
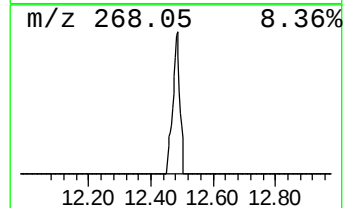
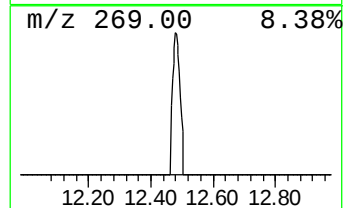
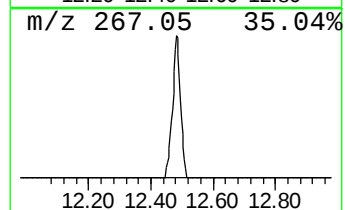
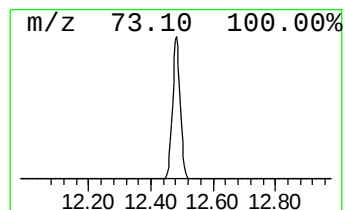
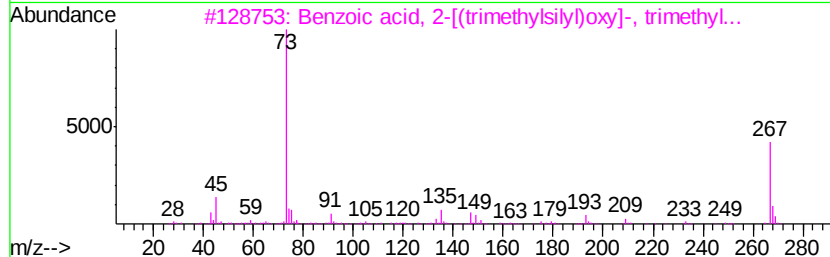
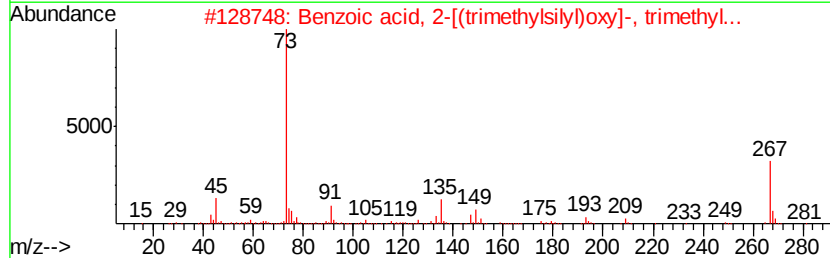
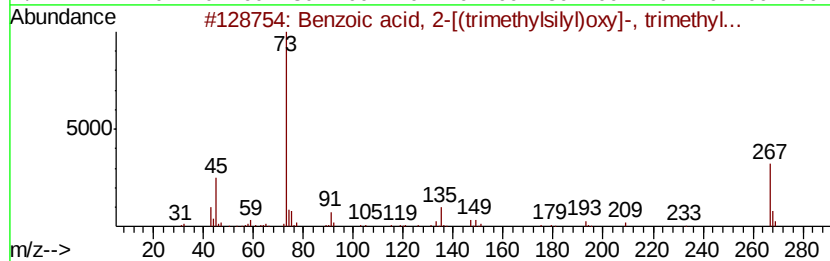
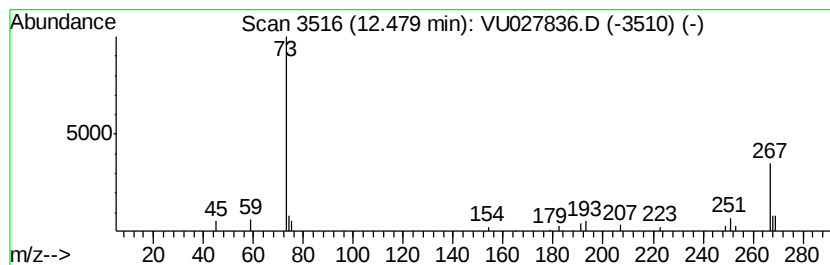
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	2.99 ug/L	19781	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3	45
2		Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3	38
3		Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3	38
4		Benzeneethanamine, N-[(pentafluoroethyl)oxy]-, trimethyl...	475	C21H26F5NO2Si2	055429-85-1	9
5		Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3	9



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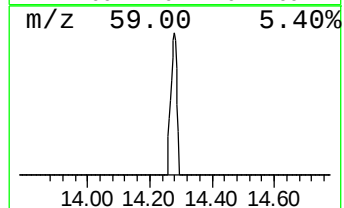
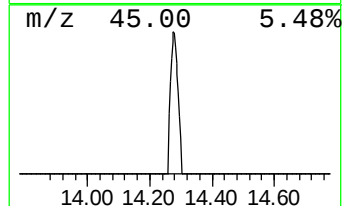
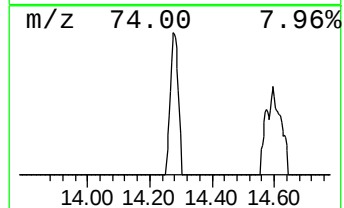
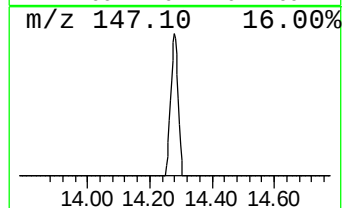
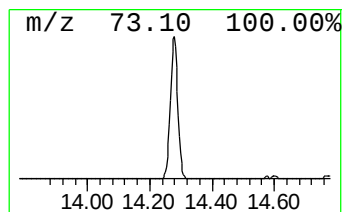
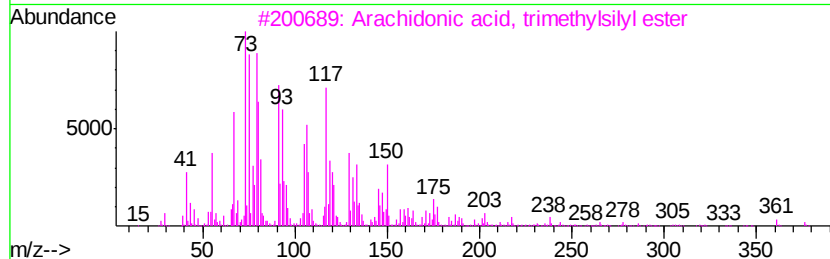
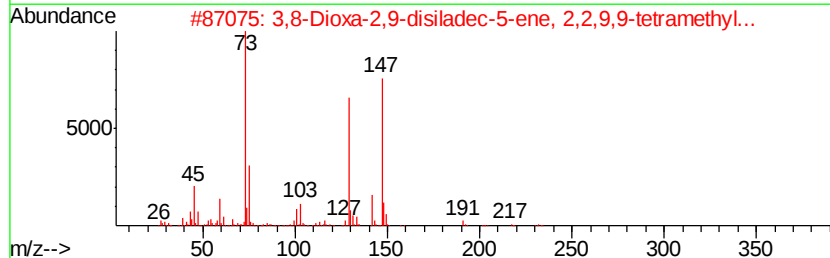
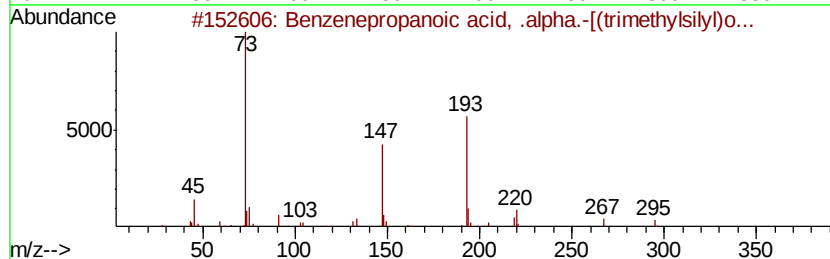
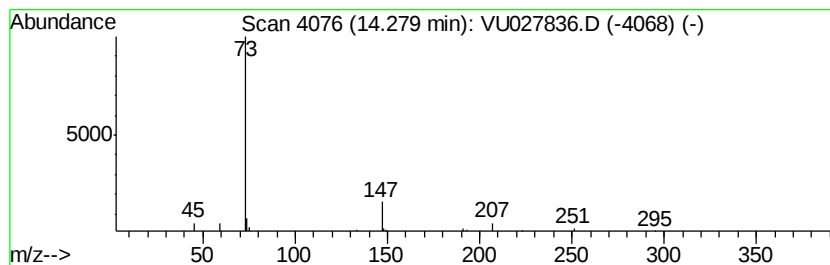
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	3.51 ug/L	23203	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenepropanoic acid, .alpha.-[...	310	C15H26O3Si2	027750-45-4	33
2		3,8-Dioxa-2,9-disiladec-5-ene, 2...	232	C10H24O2Si2	053326-59-3	9
3		Arachidonic acid, trimethylsilyl...	376	C23H40O2Si	113516-18-0	9
4		Inosose, 2-desoxy-, 0-methylxim...	479	C19H45NO5Si4	1000149-50-8	9
5		Propanoic acid, 2-[(trimethylsil...	234	C9H22O3Si2	017596-96-2	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027836.D
Acq On : 26 Oct 2018 16:15
Operator : MD/SY
Sample : J5668-10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETBS0

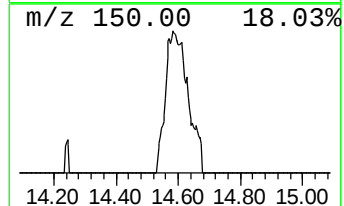
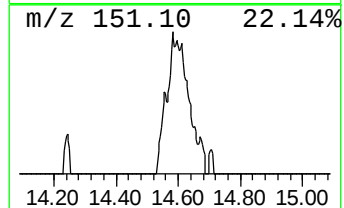
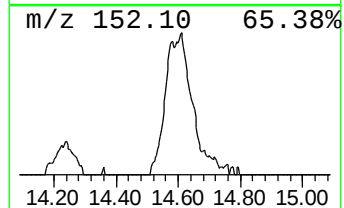
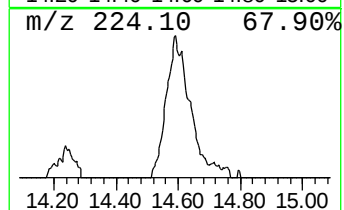
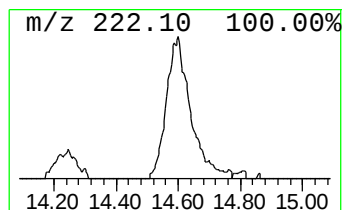
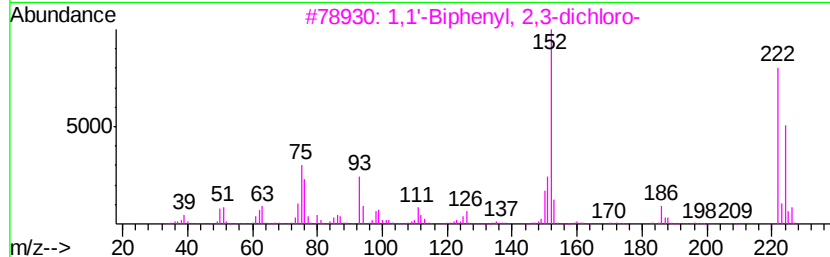
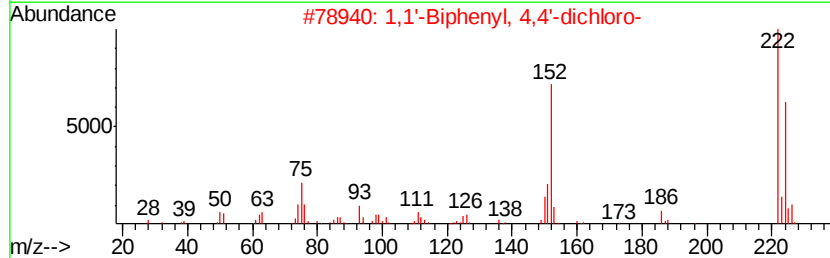
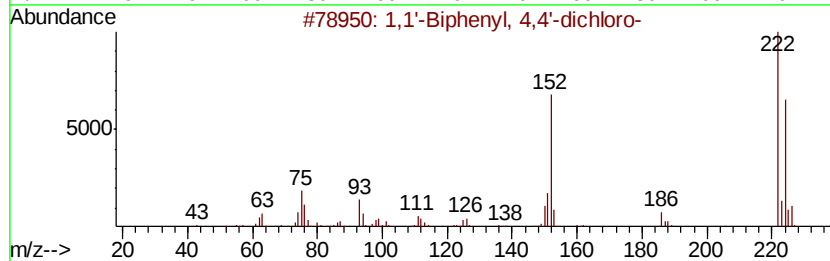
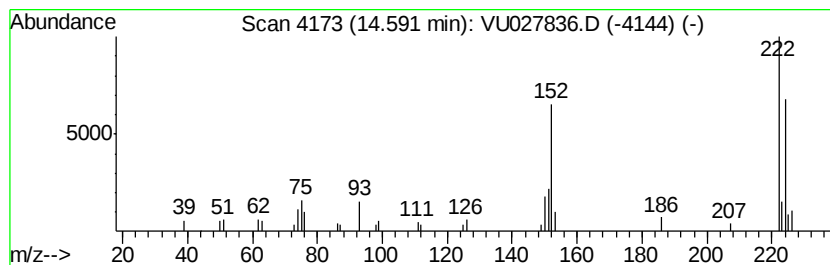
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Quant Title : VOC Analysis

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

Peak Number 7 1,1'-Biphenyl, 4,4'-dichloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	4.64 ug/L	30687	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 4,4'-dichloro-	222	C12H8Cl2	002050-68-2	98
2		1,1'-Biphenyl, 4,4'-dichloro-	222	C12H8Cl2	002050-68-2	98
3		1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	97
4		1,1'-Biphenyl, 3,3'-dichloro-	222	C12H8Cl2	002050-67-1	97
5		1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	97



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027836.D
Acq On : 26 Oct 2018 16:15
Operator : MD/SY
Sample : J5668-10
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETBS0

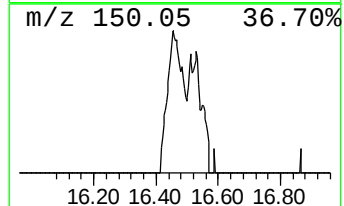
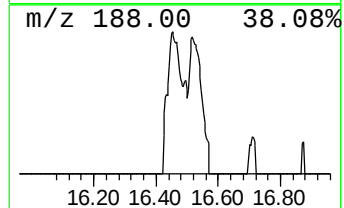
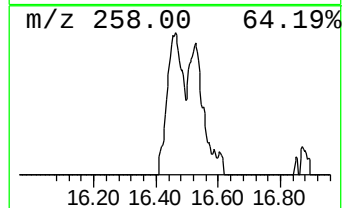
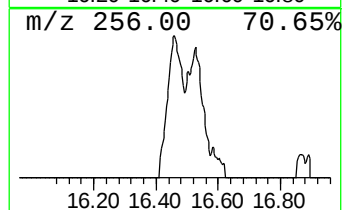
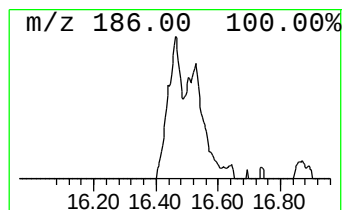
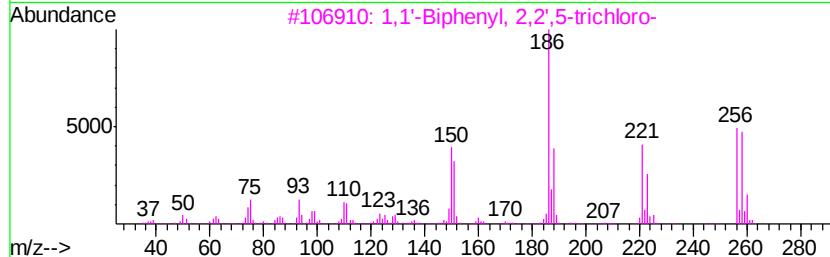
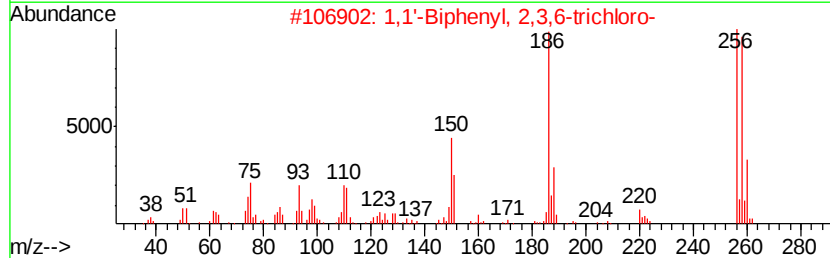
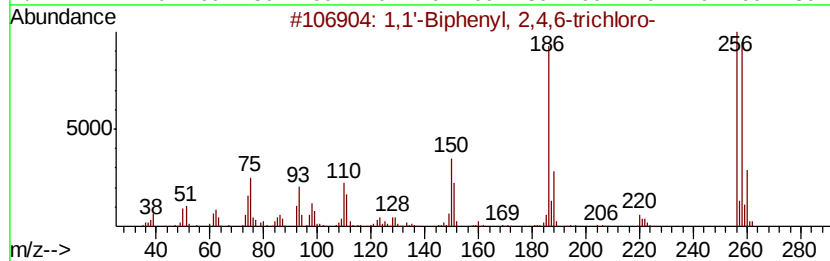
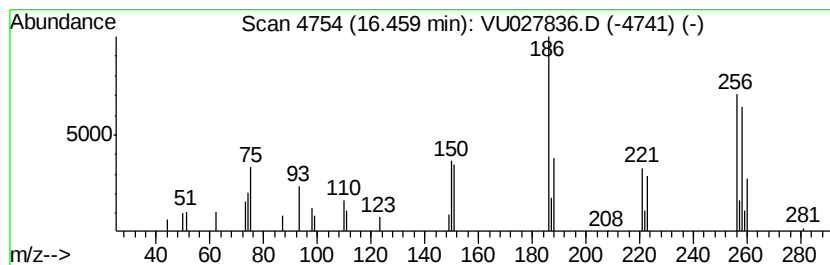
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 1,1'-Biphenyl, 2,4,6-trichl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	3.81 ug/L	25233	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,4,6-trichloro-	256	C12H7Cl3	035693-92-6	92
2		1,1'-Biphenyl, 2,3,6-trichloro-	256	C12H7Cl3	055702-45-9	92
3		1,1'-Biphenyl, 2,2',5-trichloro-	256	C12H7Cl3	037680-65-2	91
4		1,1'-Biphenyl, 2,4,4'-trichloro-	256	C12H7Cl3	007012-37-5	90
5		1,1'-Biphenyl, 2,4',5-trichloro-	256	C12H7Cl3	016606-02-3	81



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU102618\
Data File : VU027836.D
Acq On : 26 Oct 2018 16:15
Operator : MD/SY
Sample : J5668-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETBS0

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.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	2.45	5.8	ug/L	35120	1	5.89	302614	50.0
unknown-01	12.48	3.0	ug/L	19781	3	11.48	330980	50.0
unknown-02	14.28	3.5	ug/L	23203	3	11.48	330980	50.0
1,1'-Biphenyl, 4,...	14.59	4.6	ug/L	30687	3	11.48	330980	50.0
1,1'-Biphenyl, 2,...	16.46	3.8	ug/L	25233	3	11.48	330980	50.0