

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071718\
 Data File : VX003426.D
 Acq On : 17 Jul 2018 14:33
 Operator : JC/MD
 Sample : J4006-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RR-BASELINE-WATER

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % 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_X\METHOD\82X071618W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	90	rBV	1448902	1890615	29.24%	6.657%
2	1.313	112	119	146	rBV	477211	2182517	33.75%	7.684%
3	1.581	160	163	178	rVB	50279	88101	1.36%	0.310%
4	2.446	298	305	322	rBV	3742301	6466542	100.00%	22.768%
5	2.623	328	334	343	rBV	227522	438955	6.79%	1.546%
6	4.720	666	678	697	rVB2	704434	1899618	29.38%	6.688%
7	5.172	733	752	773	rBV	1266555	3865746	59.78%	13.611%
8	5.513	795	808	821	rBV	188361	535114	8.28%	1.884%
9	5.671	822	834	850	rVB	274858	774841	11.98%	2.728%
10	6.074	888	900	909	rBV2	190601	501334	7.75%	1.765%
11	6.866	1020	1030	1054	rBV	405314	946812	14.64%	3.334%
12	8.720	1327	1334	1341	rBV	1141949	1750232	27.07%	6.162%
13	8.787	1341	1345	1358	rVB	78710	124757	1.93%	0.439%
14	10.116	1556	1563	1574	rBV	840388	1108979	17.15%	3.905%
15	10.360	1594	1603	1610	rBV	55490	77592	1.20%	0.273%
16	11.091	1718	1723	1726	rBV	76389	102976	1.59%	0.363%
17	11.140	1726	1731	1744	rVB	931577	1152730	17.83%	4.059%
18	12.079	1880	1885	1893	rBV	1098328	1387970	21.46%	4.887%
19	12.274	1912	1917	1931	rBV	135706	201264	3.11%	0.709%
20	13.713	2148	2153	2162	rBV	117500	173535	2.68%	0.611%
21	13.835	2169	2173	2181	rVB	99491	140086	2.17%	0.493%
22	13.926	2183	2188	2192	rBV	281806	393421	6.08%	1.385%
23	13.987	2195	2198	2206	rVB	67895	92089	1.42%	0.324%
24	14.158	2221	2226	2236	rBV	215143	273604	4.23%	0.963%
25	14.310	2248	2251	2258	rVB	69817	92007	1.42%	0.324%
26	14.383	2258	2263	2265	rBV	213881	270596	4.18%	0.953%
27	14.414	2265	2268	2281	rVB	271263	360030	5.57%	1.268%
28	14.585	2291	2296	2298	rBV	229163	294785	4.56%	1.038%
29	14.615	2298	2301	2304	rVV2	269363	399771	6.18%	1.408%
30	14.645	2304	2306	2311	rVV	230276	251410	3.89%	0.885%
31	14.700	2311	2315	2322	rVB2	59122	88887	1.37%	0.313%
32	14.774	2322	2327	2332	rBV2	46392	75163	1.16%	0.265%

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RR-BASELINE-WATER

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : SW846 8260

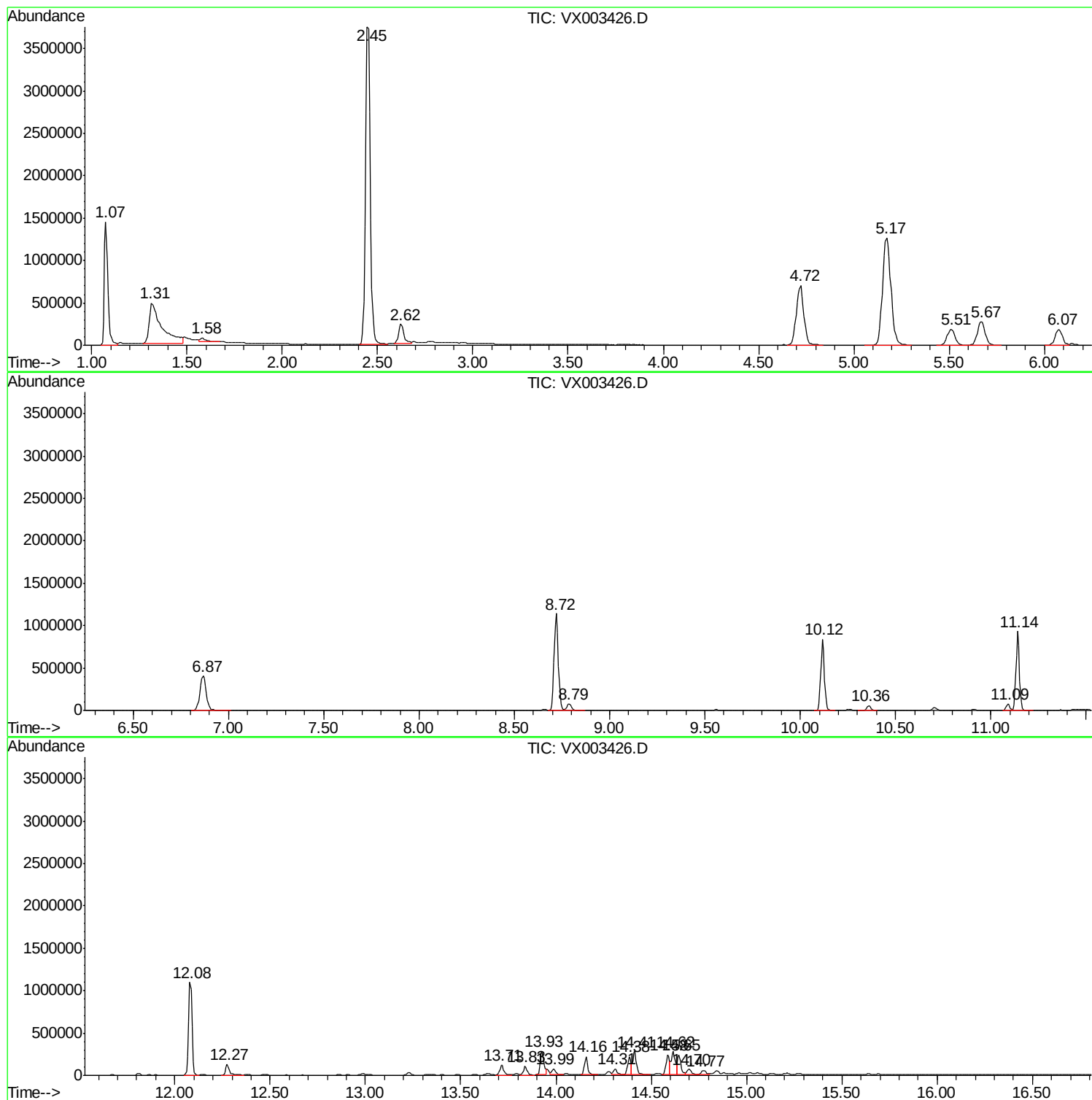
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Quant Title : SW846 8260

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



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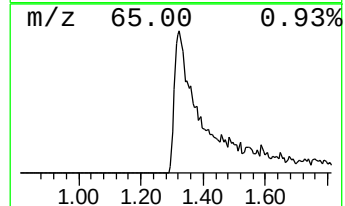
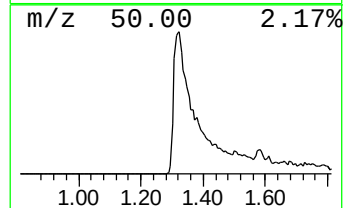
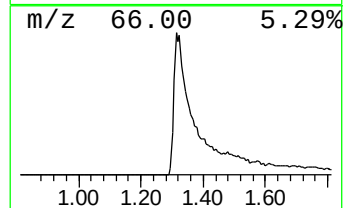
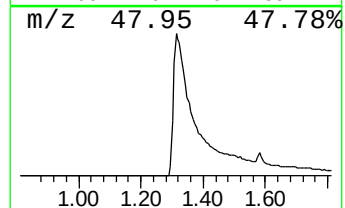
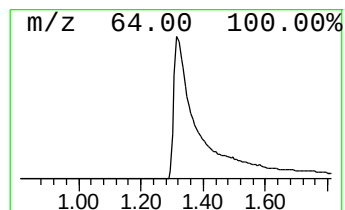
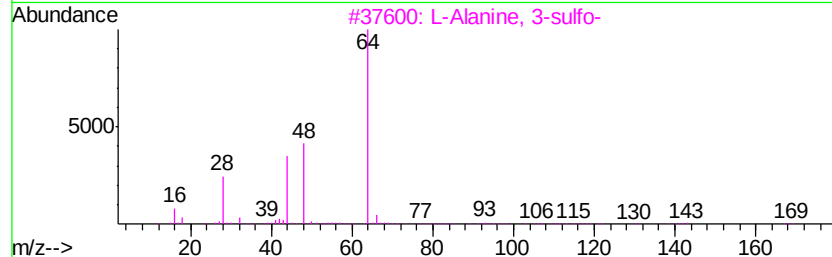
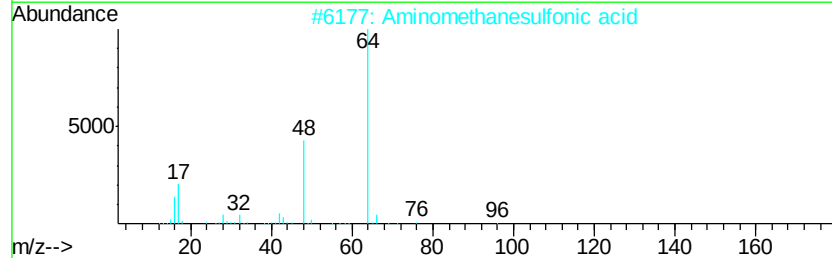
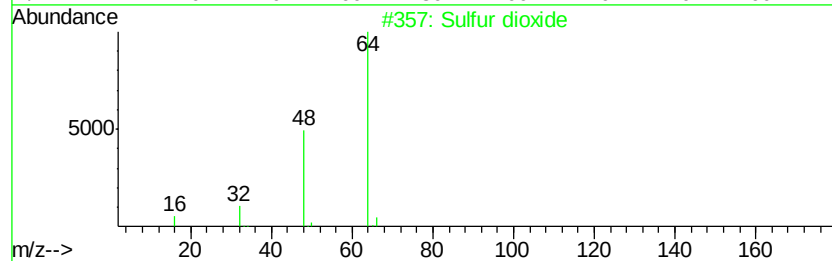
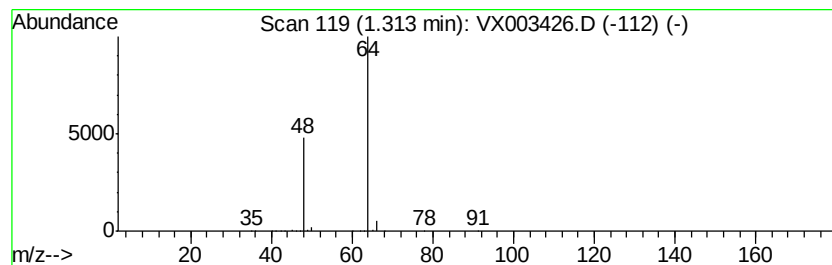
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ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.31	140.84 ug/l	2182520	Pentafluorobenzene	5.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Sulfur dioxide	64 O2S	007446-09-5 83
2		Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9 74
3		L-Alanine, 3-sulfo-	169 C3H7NO5S	000498-40-8 9
4		Ethene, 1,1-difluoro-	64 C2H2F2	000075-38-7 4
5		Ethyl Chloride	64 C2H5Cl	000075-00-3 3



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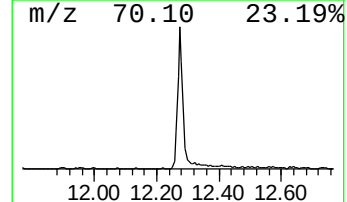
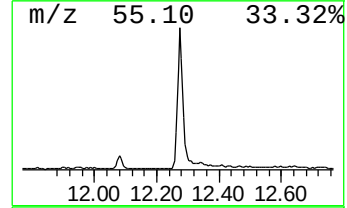
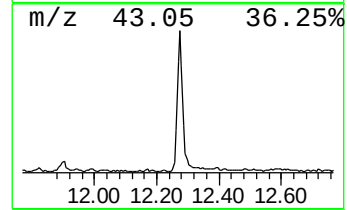
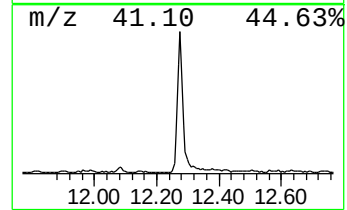
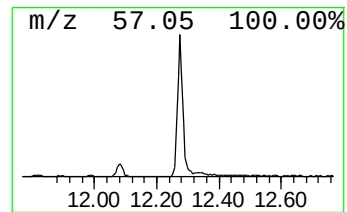
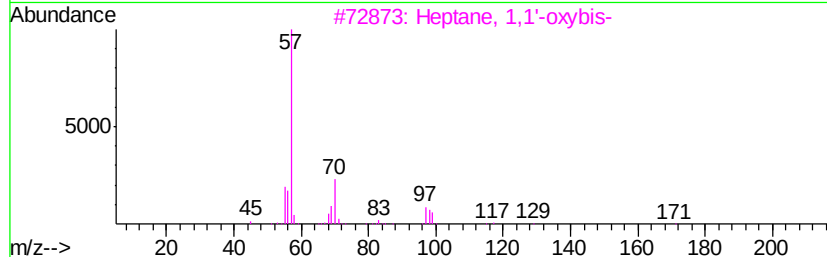
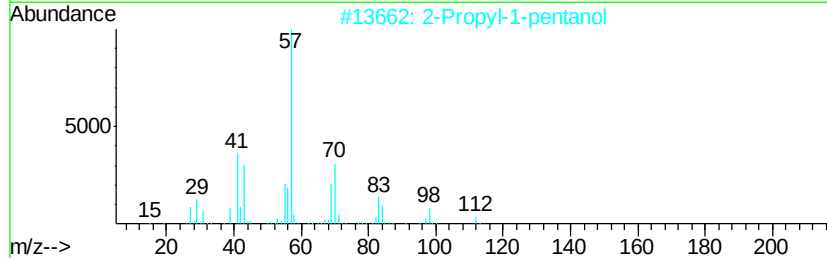
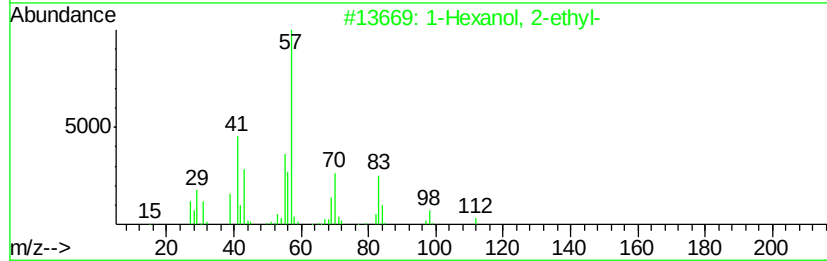
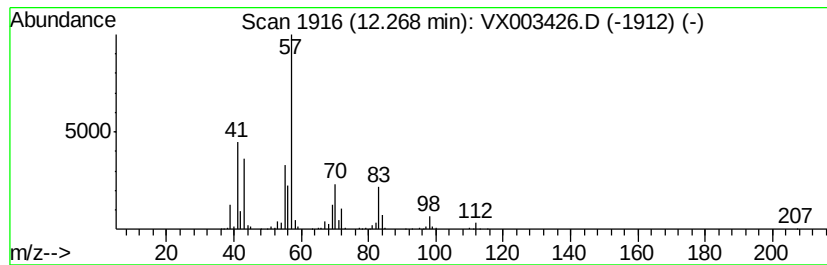
Instrument :
MSVOA_X
ClientSampleId :
RR-BASELINE-WATER

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071618W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	7.25 ug/l	201264	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	86
2	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	53
3	Heptane, 1,1'-oxybis-	214 C14H30O	000629-64-1	50
4	Oxirane, [(2-ethylhexyl)oxyl]met...	186 C11H22O2	002461-15-6	50
5	Carbonic acid, isobutyl 2-ethylh...	230 C13H26O3	1000357-82-9	50



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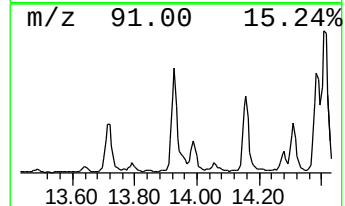
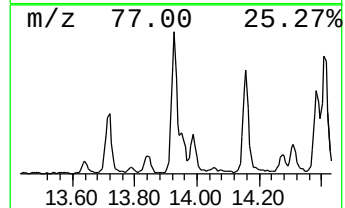
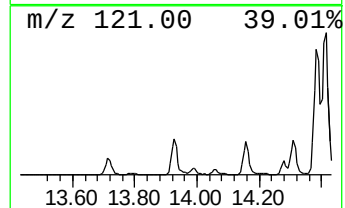
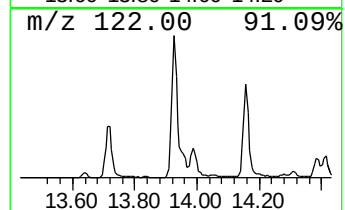
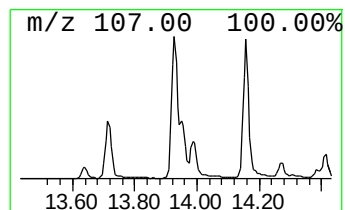
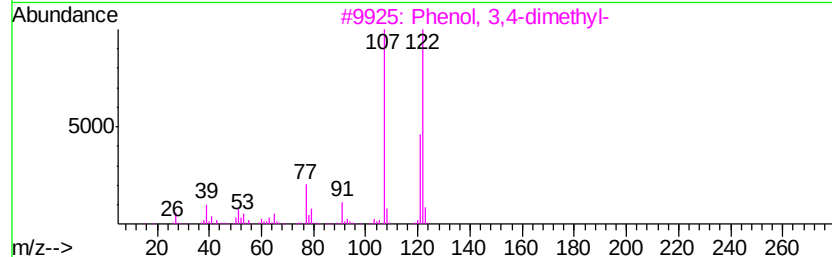
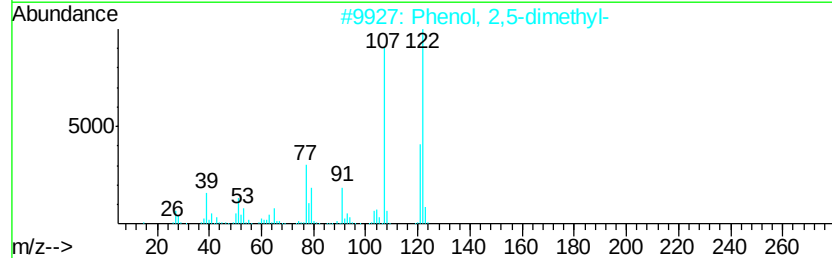
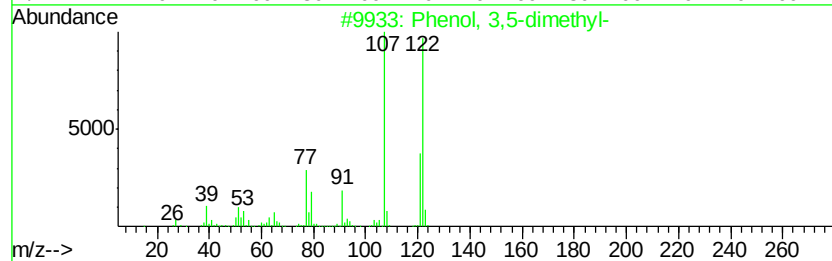
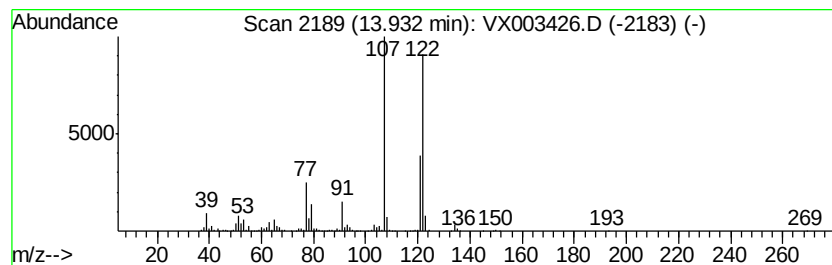
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 3,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	14.17 ug/l	393421	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 3,5-dimethyl-	122	C8H10O	000108-68-9	96
2		Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	94
3		Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	91
4		Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	91
5		Phenol, 2,4-dimethyl-	122	C8H10O	000105-67-9	91



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RR-BASELINE-WATER

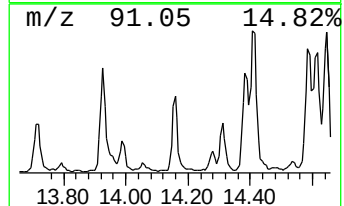
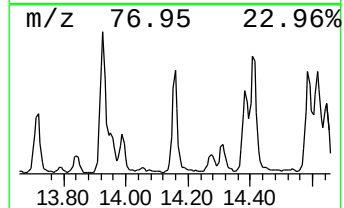
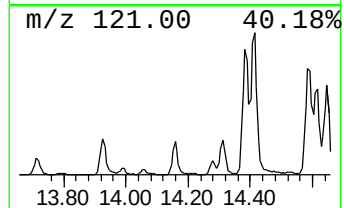
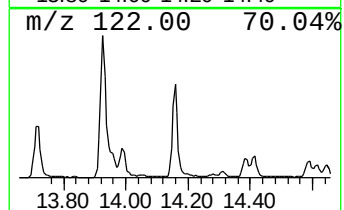
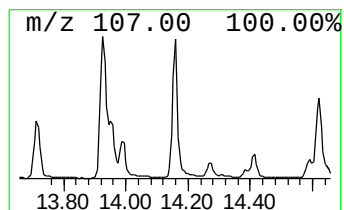
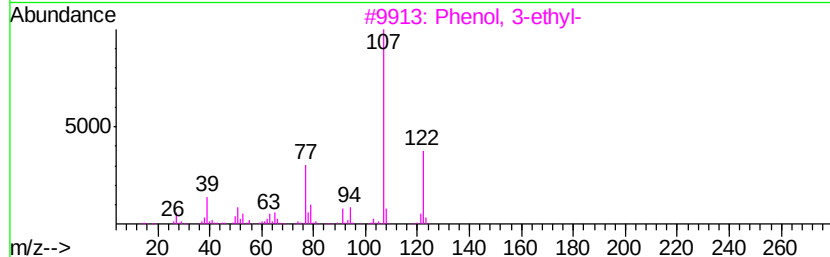
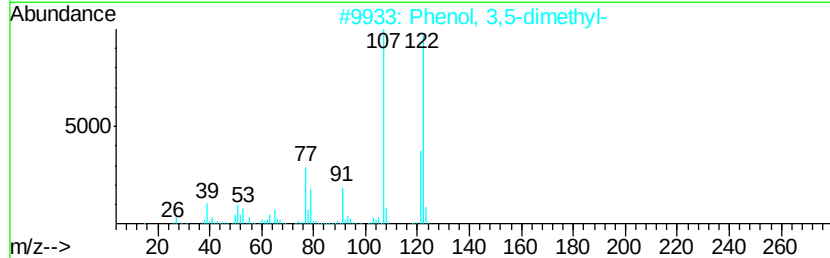
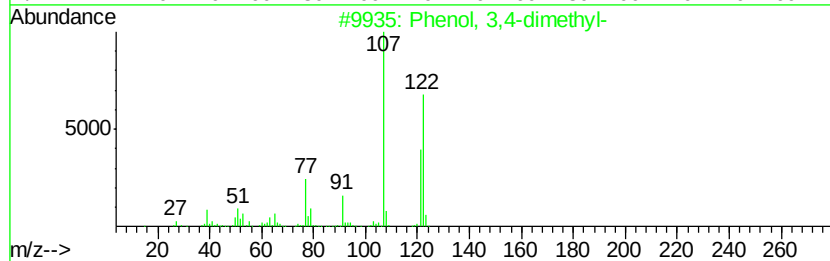
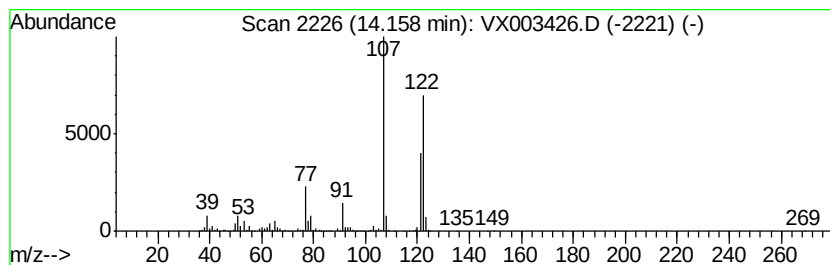
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, 3,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	9.86 ug/l	273604	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol,	3,4-dimethyl-	122	C8H10O	000095-65-8	96
2	Phenol,	3,5-dimethyl-	122	C8H10O	000108-68-9	94
3	Phenol,	3-ethyl-	122	C8H10O	000620-17-7	90
4	Phenol,	2-ethyl-	122	C8H10O	000090-00-6	87
5	Phenol,	4-ethyl-	122	C8H10O	000123-07-9	86



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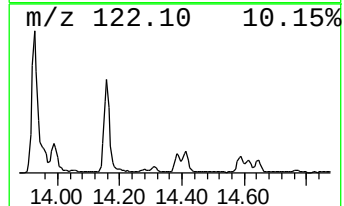
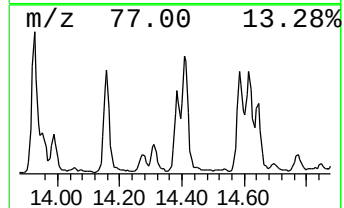
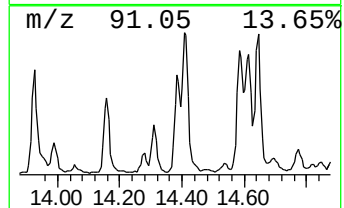
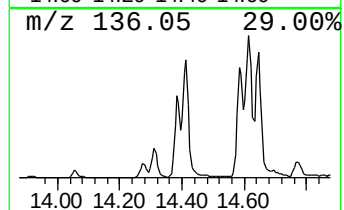
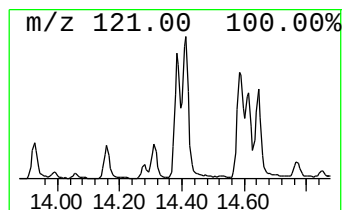
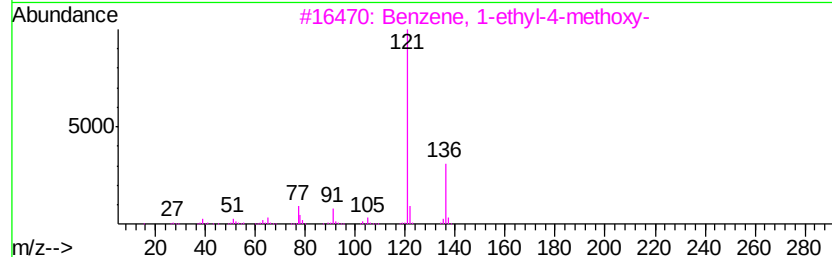
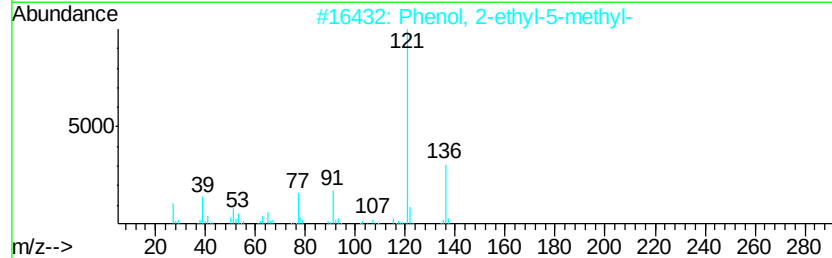
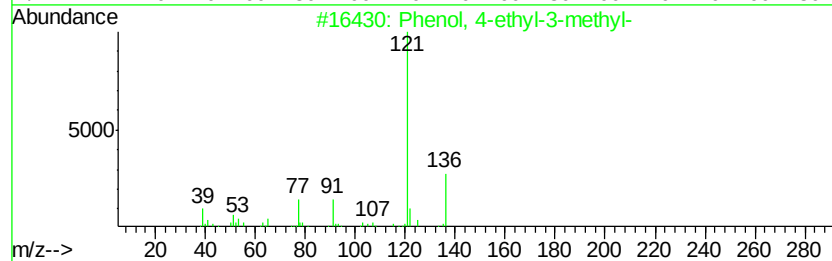
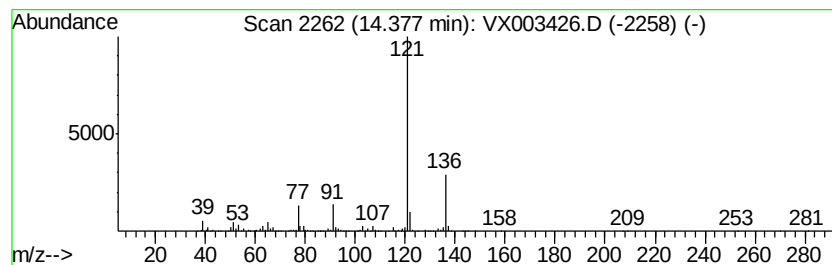
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 4-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.38	9.75 ug/l	270596	1,4-Dichlorobenzene-d4	12.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-3-methyl-		136	C9H12O	001123-94-0	94
2	Phenol, 2-ethyl-5-methyl-		136	C9H12O	001687-61-2	91
3	Benzene, 1-ethyl-4-methoxy-		136	C9H12O	001515-95-3	91
4	Phenol, 2-ethyl-6-methyl-		136	C9H12O	001687-64-5	91
5	Phenol, 2-(1-methylethyl)-		136	C9H12O	000088-69-7	90



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ALS Vial : 14 Sample Multiplier: 1

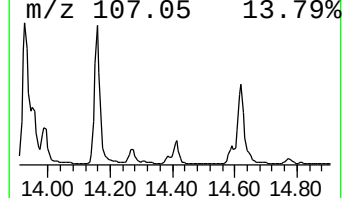
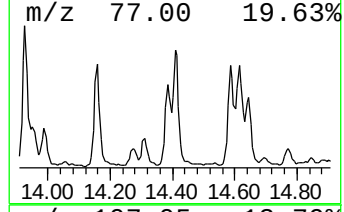
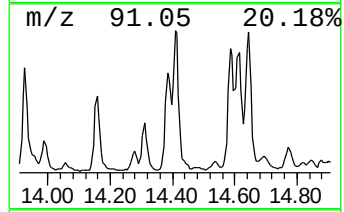
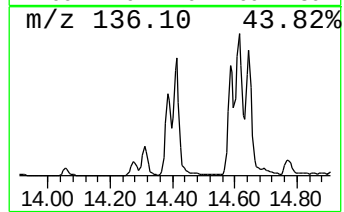
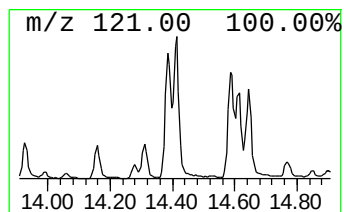
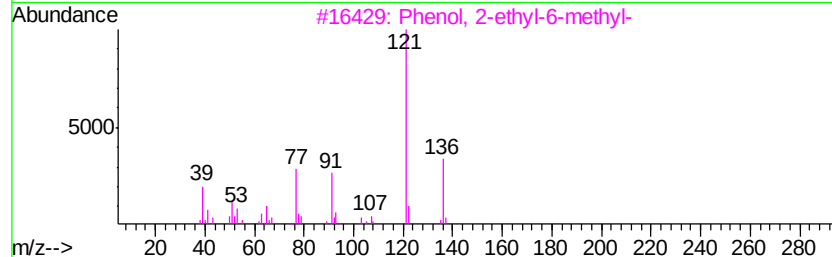
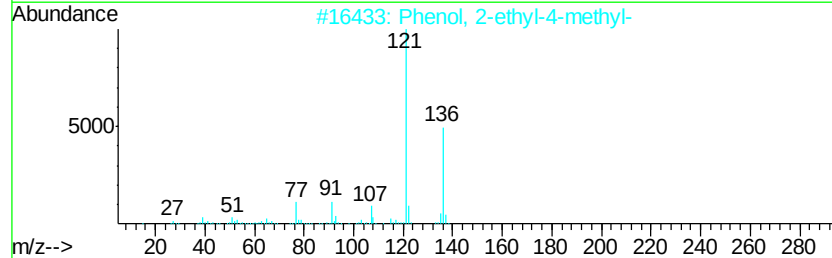
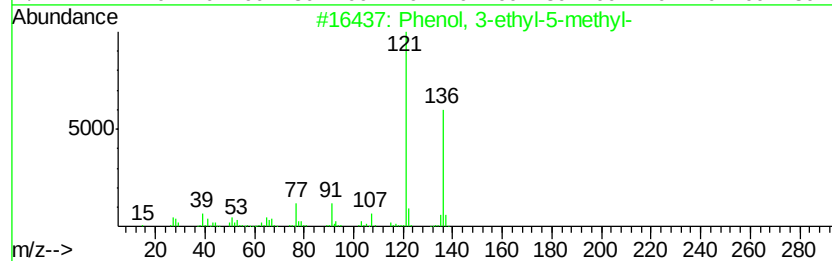
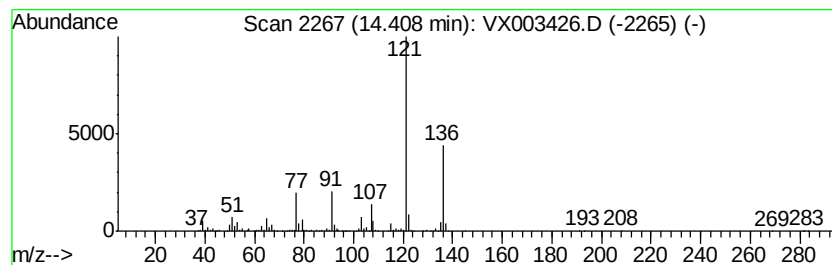
Instrument :
MSVOA_X
ClientSampleId :
RR-BASELINE-WATER

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071618W.M
Quant Title : SW846 8260

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

Peak Number 7 Phenol, 3-ethyl-5-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	12.97 ug/l	360030	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phenol, 3-ethyl-5-methyl-	136 C9H12O	000698-71-5	91
2	Phenol, 2-ethyl-4-methyl-	136 C9H12O	003855-26-3	91
3	Phenol, 2-ethyl-6-methyl-	136 C9H12O	001687-64-5	87
4	Phenol, 3,4,5-trimethyl-	136 C9H12O	000527-54-8	83
5	Phenol, 2-(1-methylethyl)-	136 C9H12O	000088-69-7	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071718\
Data File : VX003426.D
Acq On : 17 Jul 2018 14:33
Operator : JC/MD
Sample : J4006-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

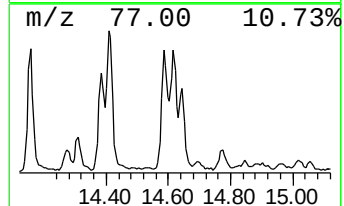
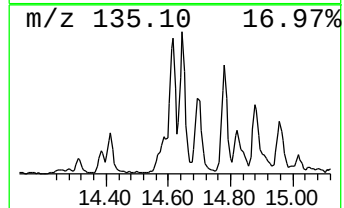
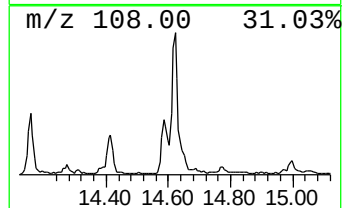
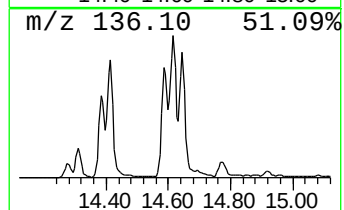
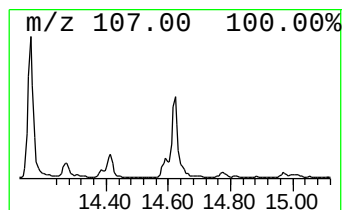
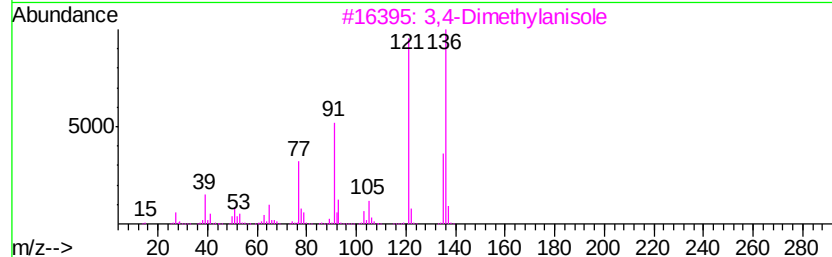
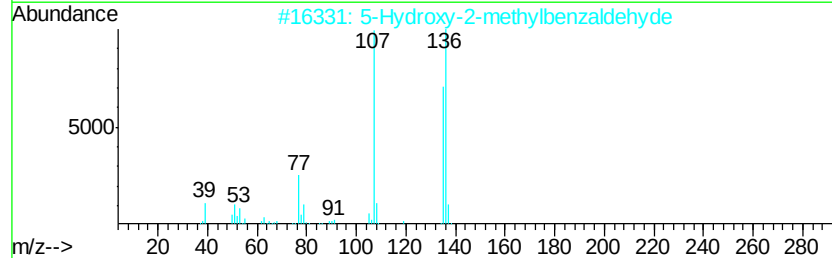
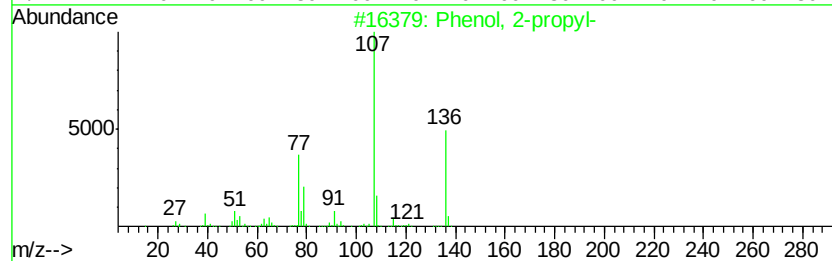
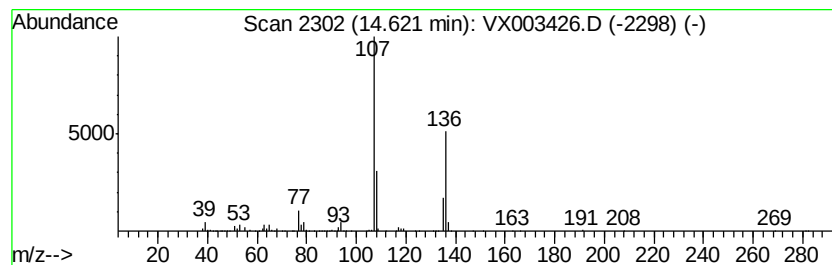
Instrument :
MSVOA_X
ClientSampleId :
RR-BASELINE-WATER

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071618W.M
Quant Title : SW846 8260

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

Peak Number 9 Phenol, 2-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	14.40 ug/l	399771	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phenol, 2-propyl-	136 C9H12O	000644-35-9	64
2	5-Hydroxy-2-methylbenzaldehyde	136 C8H8O2	023942-00-9	62
3	3,4-Dimethylanisole	136 C9H12O	004685-47-6	60
4	1,3-Cyclopentadiene, 5,5-dimethy...	136 C10H16	1000163-57-0	59
5	Phenol, 3-propyl-	136 C9H12O	000621-27-2	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071718\
Data File : VX003426.D
Acq On : 17 Jul 2018 14:33
Operator : JC/MD
Sample : J4006-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RR-BASELINE-WATER

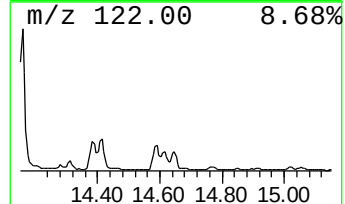
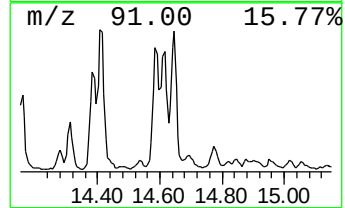
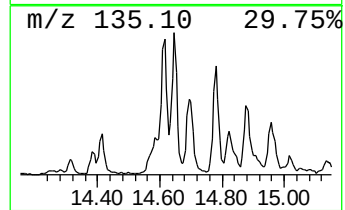
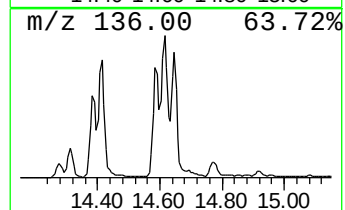
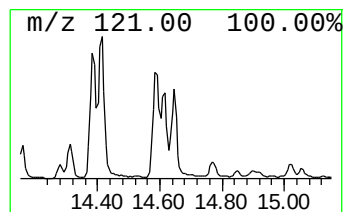
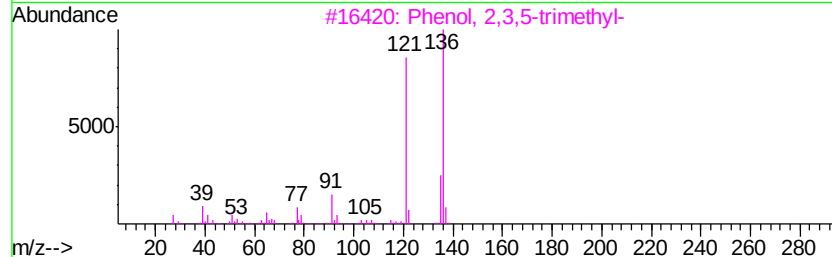
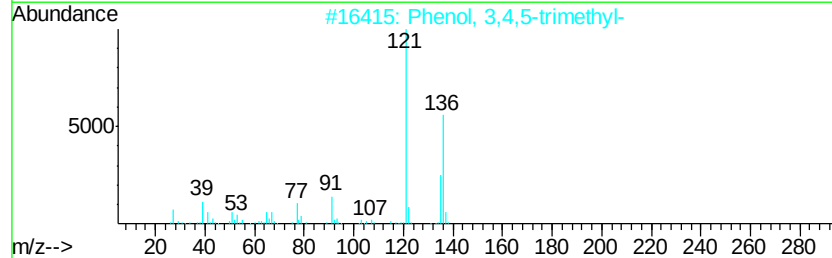
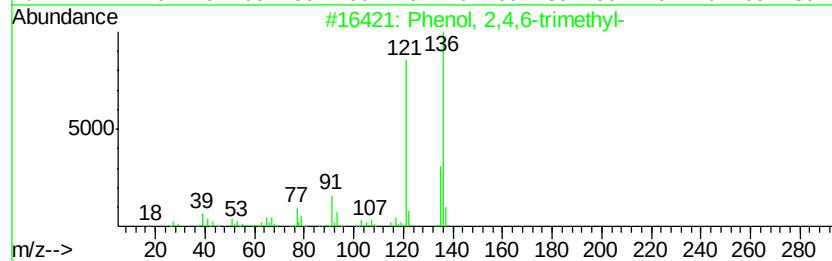
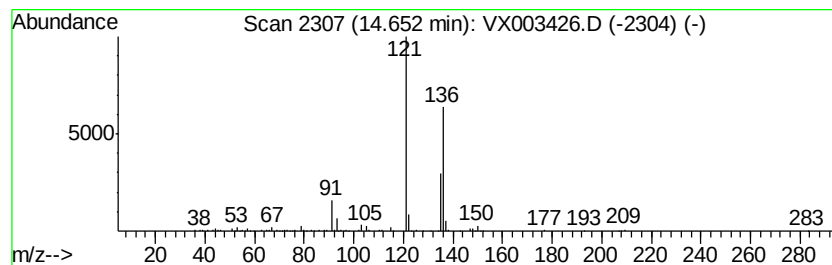
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071618W.M
Quant Title : SW846 8260

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

Peak Number 10 Phenol, 2,4,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	9.06 ug/l	251410	1,4-Dichlorobenzene-d4	12.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol,	2,4,6-trimethyl-		136	C9H12O	000527-60-6	91
2	Phenol,	3,4,5-trimethyl-		136	C9H12O	000527-54-8	91
3	Phenol,	2,3,5-trimethyl-		136	C9H12O	000697-82-5	90
4	Phenol,	2,4,5-trimethyl-		136	C9H12O	000496-78-6	86
5	Phenol,	2,3,6-trimethyl-		136	C9H12O	002416-94-6	83



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071718\
Data File : VX003426.D
Acq On : 17 Jul 2018 14:33
Operator : JC/MD
Sample : J4006-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RR-BASELINE-WATER

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071618W.M
Quant Title : SW846 8260

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	1.31	140.8	ug/l	2182520	1	5.67	774841	50.0
1-Hexanol, 2-ethyl-	12.27	7.3	ug/l	201264	4	12.08	1387970	50.0
Phenol, 3,5-dimet...	13.93	14.2	ug/l	393421	4	12.08	1387970	50.0
Phenol, 3,4-dimet...	14.16	9.9	ug/l	273604	4	12.08	1387970	50.0
Phenol, 4-ethyl-3...	14.38	9.8	ug/l	270596	4	12.08	1387970	50.0
Phenol, 3-ethyl-5...	14.41	13.0	ug/l	360030	4	12.08	1387970	50.0
Phenol, 2-propyl-	14.62	14.4	ug/l	399771	4	12.08	1387970	50.0
Phenol, 2,4,6-tri...	14.65	9.1	ug/l	251410	4	12.08	1387970	50.0