

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV071918\
 Data File : VV006646.D
 Acq On : 19 Jul 2018 16:51
 Operator : SY/MD
 Sample : J3983-06
 Misc : 25 mL/MSVOA V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DB171

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_V\METHOD\SOMVTR071918WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.029	29	43	57	rBV	3156924	3795292	100.00%	18.858%
2	1.112	57	69	94	rVV	965593	2630828	69.32%	13.072%
3	1.218	95	102	124	rVV	260325	721892	19.02%	3.587%
4	1.318	129	133	151	rVB2	188242	271854	7.16%	1.351%
5	1.472	175	181	192	rVB	1443404	1379844	36.36%	6.856%
6	2.051	353	361	375	rVV	531693	709096	18.68%	3.523%
7	2.128	377	385	395	rVV	231264	323972	8.54%	1.610%
8	2.193	397	405	412	rVV	125108	190132	5.01%	0.945%
9	2.231	412	417	434	rVB	75444	107593	2.83%	0.535%
10	2.318	439	444	452	rVB	31385	39777	1.05%	0.198%
11	2.459	482	488	499	rVB	94346	137426	3.62%	0.683%
12	2.688	550	559	581	rVV	183022	338091	8.91%	1.680%
13	2.791	582	591	605	rVB	150754	260955	6.88%	1.297%
14	3.961	938	955	972	rBV2	239926	630421	16.61%	3.132%
15	4.405	1074	1093	1117	rVB	139063	327885	8.64%	1.629%
16	5.099	1291	1309	1323	rBV2	347560	794513	20.93%	3.948%
17	5.170	1324	1331	1350	rVB4	28537	65243	1.72%	0.324%
18	5.668	1466	1486	1514	rBV	349584	1042564	27.47%	5.180%
19	6.122	1616	1627	1647	rVB	188512	378412	9.97%	1.880%
20	7.035	1899	1911	1927	rVB	95553	166116	4.38%	0.825%
21	7.363	1999	2013	2026	rBV	421030	712228	18.77%	3.539%
22	7.569	2066	2077	2092	rBV	25133	43008	1.13%	0.214%
23	7.668	2097	2108	2122	rVV	56922	95477	2.52%	0.474%
24	7.987	2191	2207	2215	rBV	21810	42209	1.11%	0.210%
25	8.138	2242	2254	2279	rBV	389983	646093	17.02%	3.210%
26	8.395	2322	2334	2362	rBV2	39828	172020	4.53%	0.855%
27	8.852	2461	2476	2479	rBV3	31557	77846	2.05%	0.387%
28	8.900	2481	2491	2522	rVB	442360	785871	20.71%	3.905%
29	9.353	2623	2632	2644	rBV	28426	44011	1.16%	0.219%
30	9.610	2697	2712	2731	rBV4	19357	71054	1.87%	0.353%
31	10.266	2906	2916	2930	rVB	129178	197870	5.21%	0.983%
32	10.427	2956	2966	2978	rBV	27200	45467	1.20%	0.226%
33	10.983	3125	3139	3160	rBV	109590	178697	4.71%	0.888%
34	11.102	3163	3176	3185	rBV3	35614	73631	1.94%	0.366%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Title : TRACE VOA SOM01.0

35	11.298	3226	3237	3260	rBV	432949	689851	18.18%	3.428%
36	11.578	3314	3324	3340	rBV	25754	48960	1.29%	0.243%
37	11.678	3343	3355	3377	rVB	376284	591187	15.58%	2.937%
38	12.285	3533	3544	3553	rBV2	70100	124793	3.29%	0.620%
39	12.330	3554	3558	3572	rVB3	21942	41950	1.11%	0.208%
40	14.385	4186	4197	4215	rBV	79141	134275	3.54%	0.667%
41	16.372	4803	4815	4840	rBV	682383	997594	26.29%	4.957%

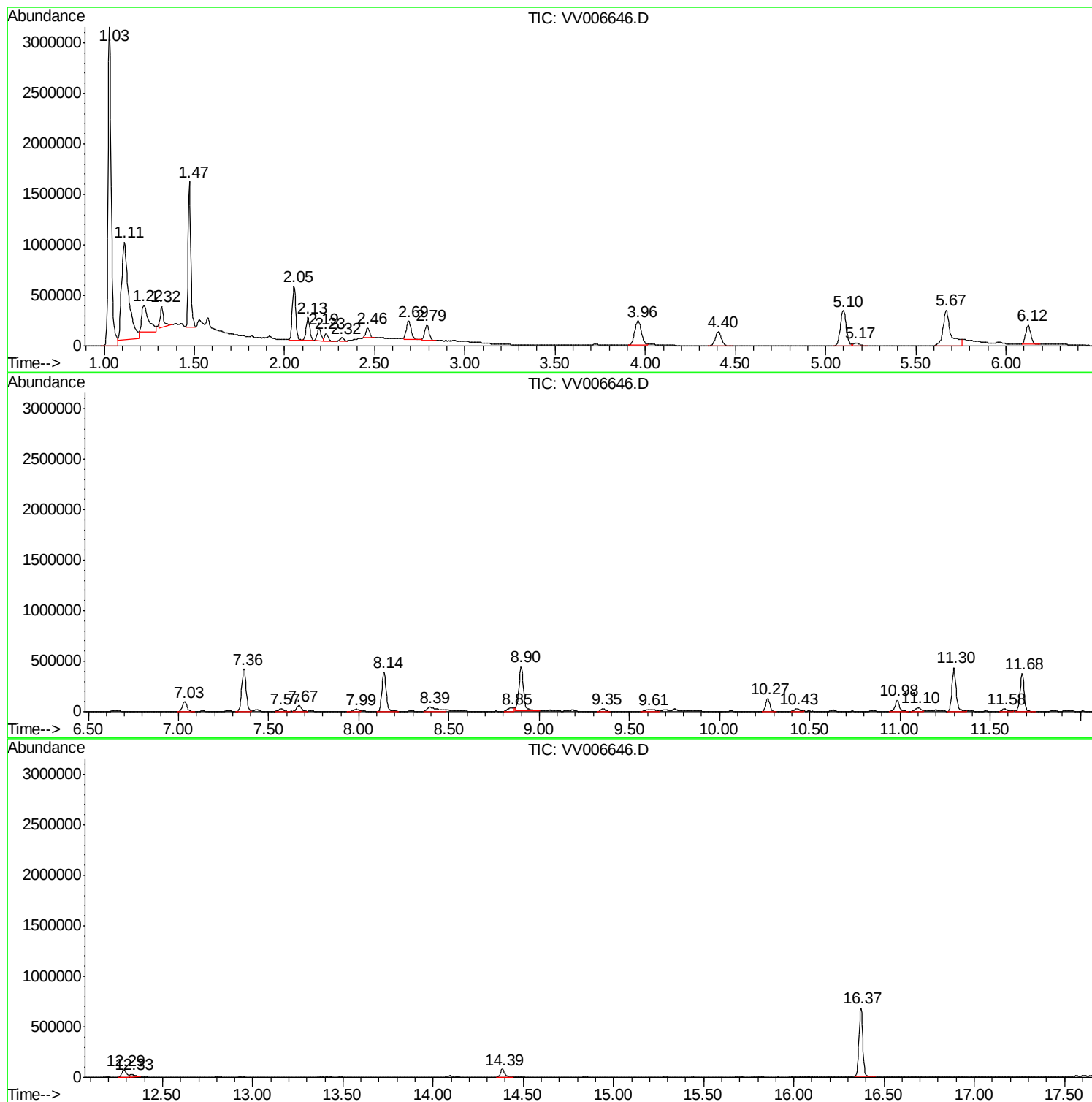
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

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



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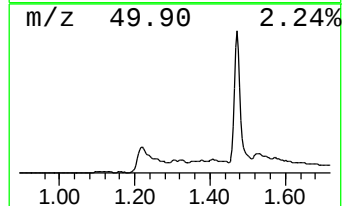
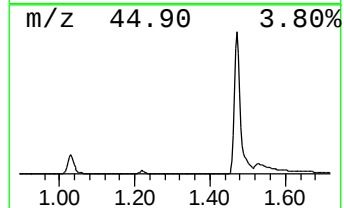
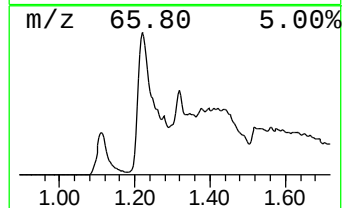
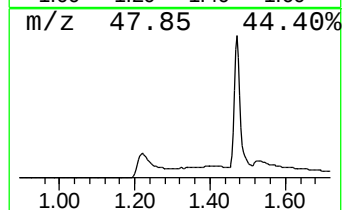
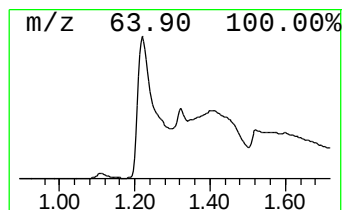
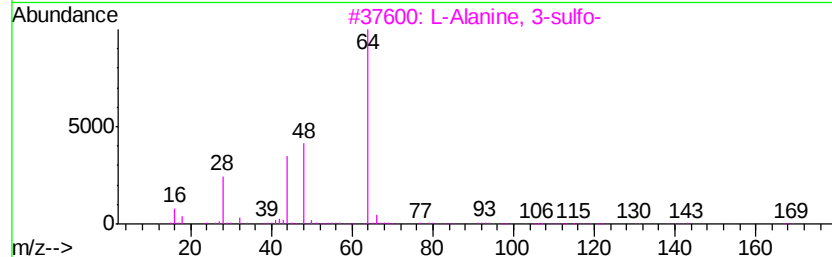
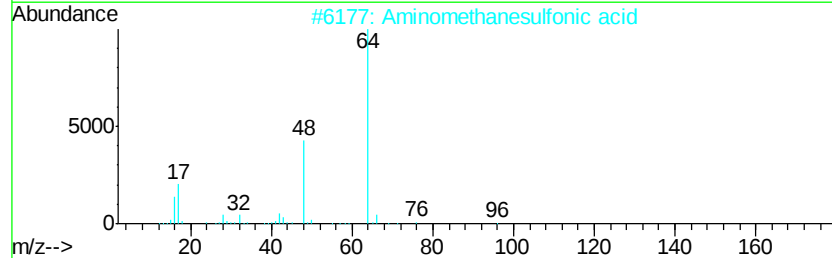
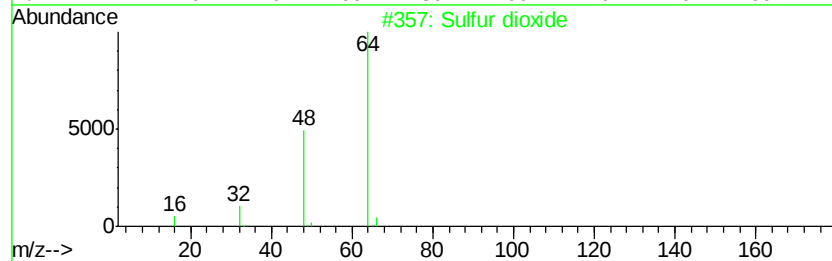
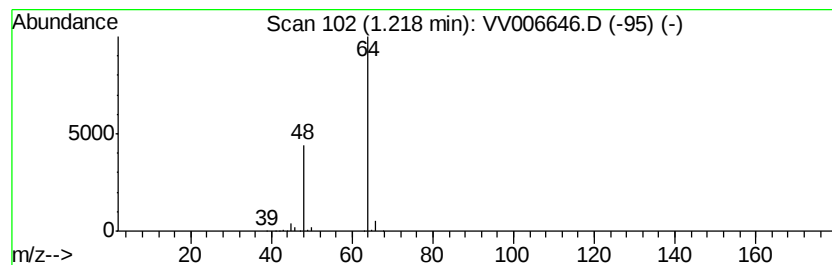
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.22	3.46 ug/L	721892	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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Instrument :
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ClientSampleId :
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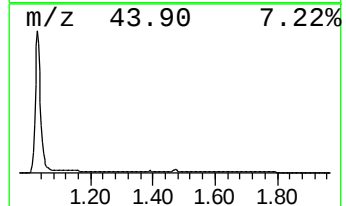
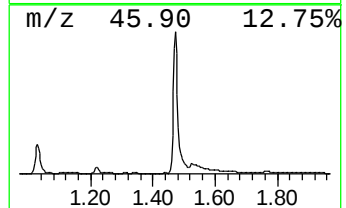
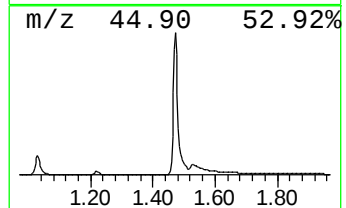
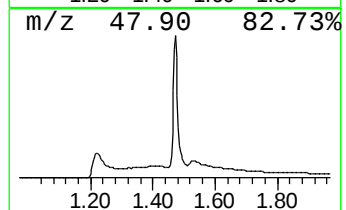
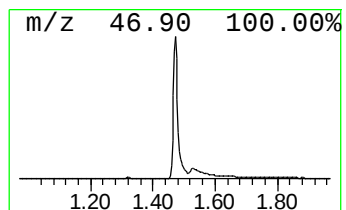
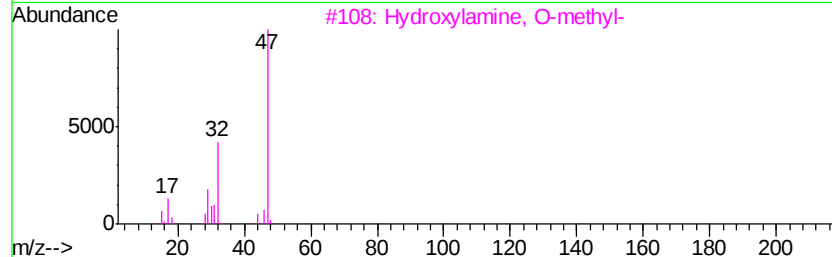
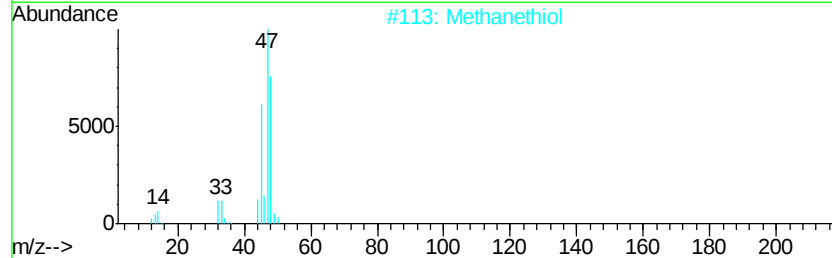
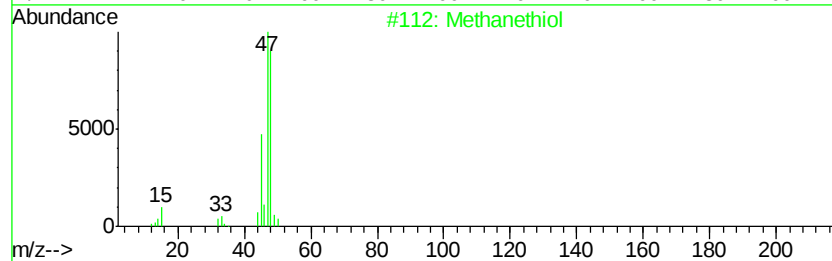
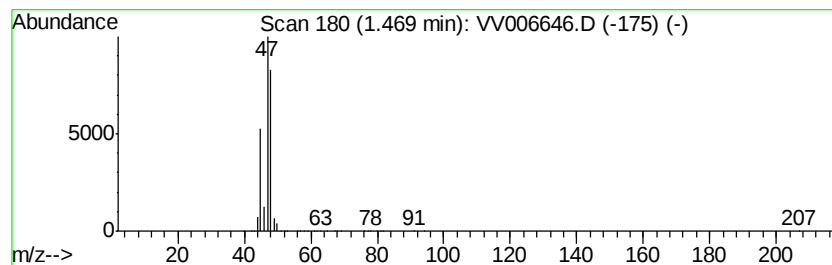
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Methanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	6.62 ug/L	1379840	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	90
2		Methanethiol	48	CH4S	000074-93-1	90
3		Hvdroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4		Hvdroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5		Methane, nitroso-	45	CH3NO	000865-40-7	5



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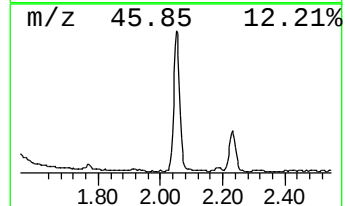
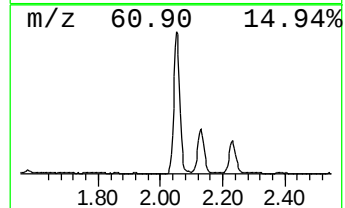
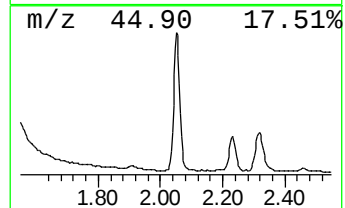
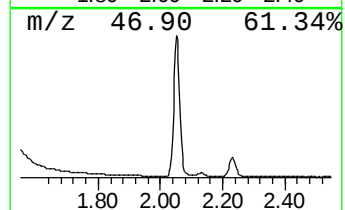
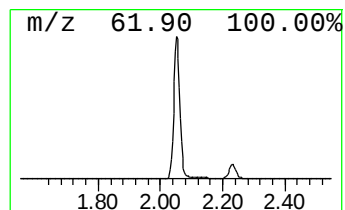
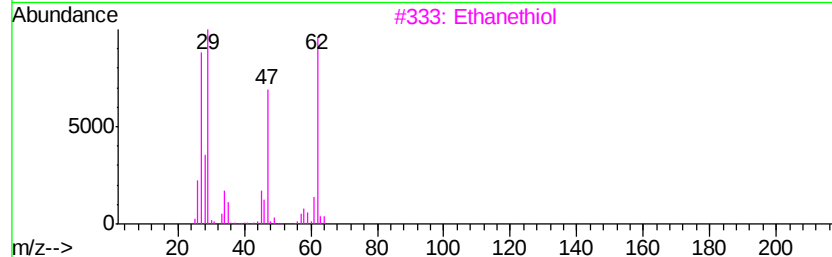
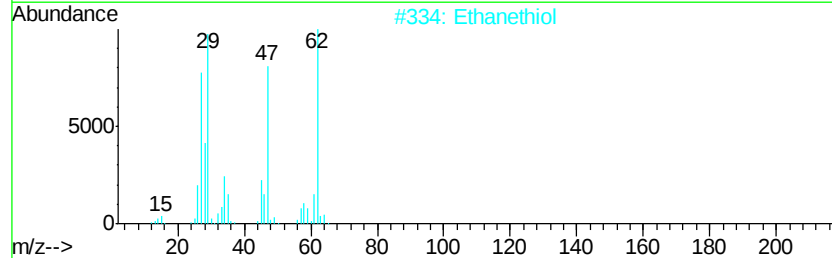
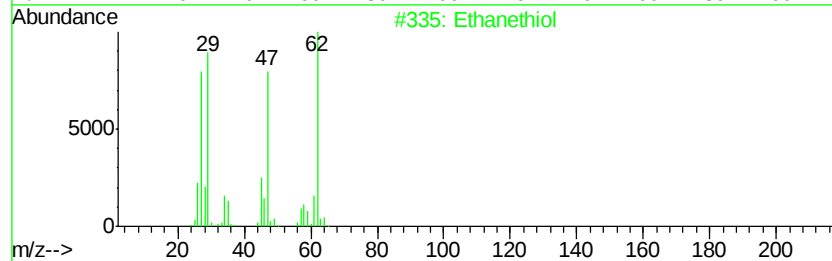
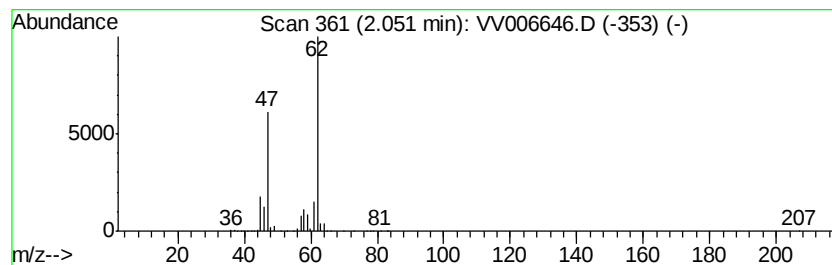
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Ethanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	3.40 ug/L	709096	1,4-Difluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol		62	C2H6S	000075-08-1	91
2	Ethanethiol		62	C2H6S	000075-08-1	91
3	Ethanethiol		62	C2H6S	000075-08-1	91
4	Ethanethiol		62	C2H6S	000075-08-1	91
5	Ethanethiol		62	C2H6S	000075-08-1	91



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ALS Vial : 11 Sample Multiplier: 1

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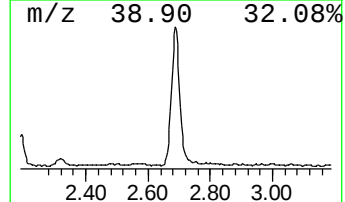
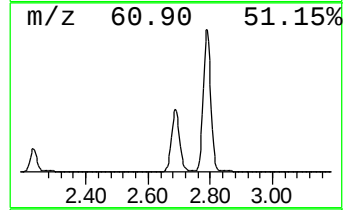
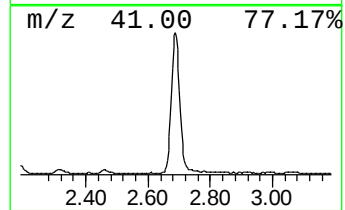
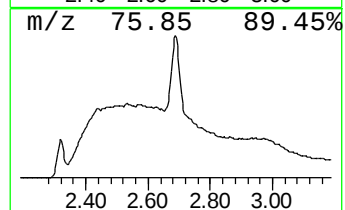
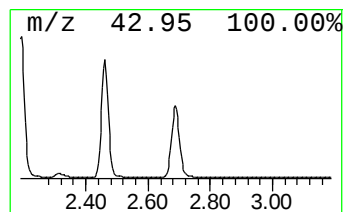
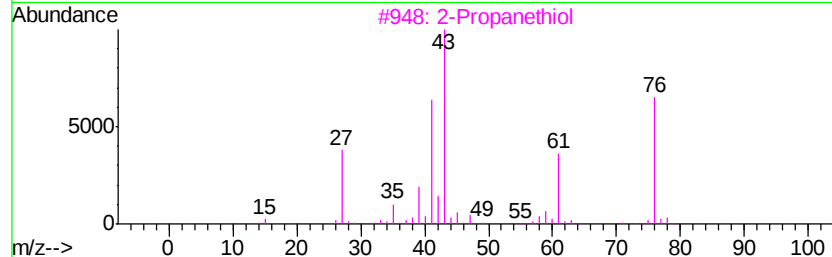
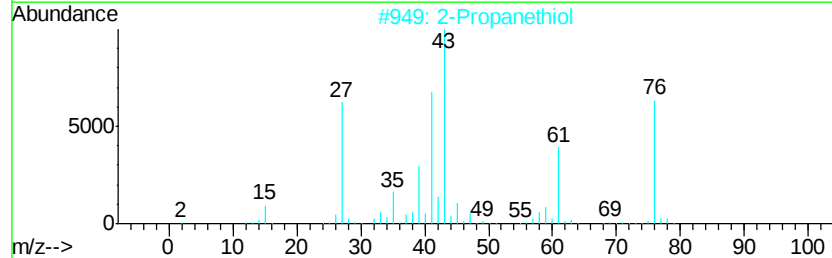
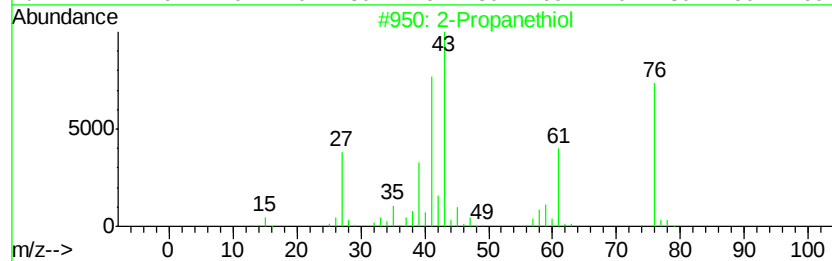
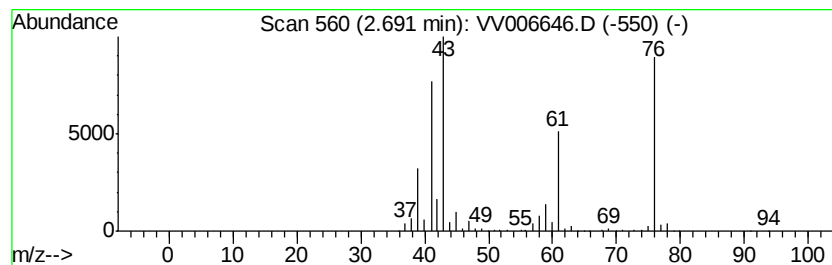
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Propanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.69	1.62 ug/L	338091	1,4-Difluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol	76	C3H8S	000075-33-2	94
2			2-Propanethiol	76	C3H8S	000075-33-2	91
3			2-Propanethiol	76	C3H8S	000075-33-2	91
4			Trimethylphosphine	76	C3H9P	000594-09-2	64
5			Thiourea	76	CH4N2S	000062-56-6	56



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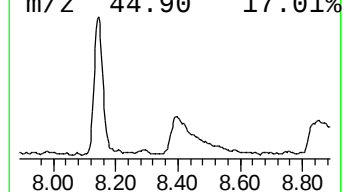
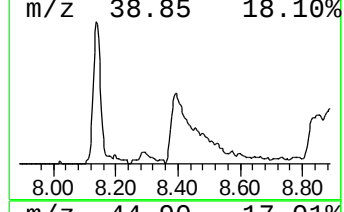
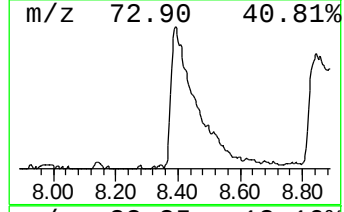
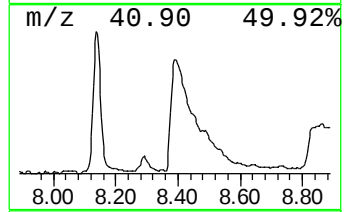
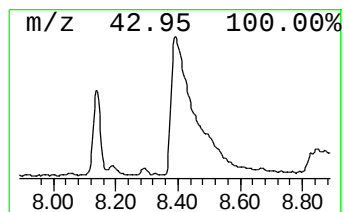
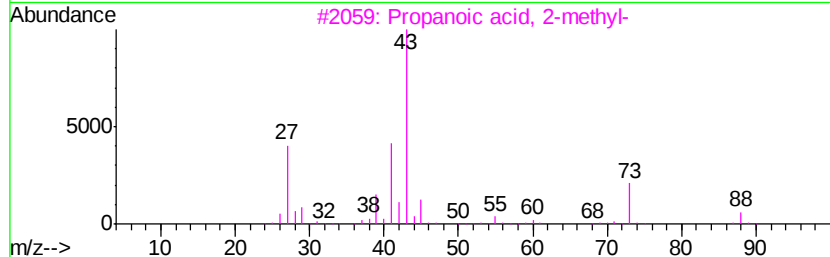
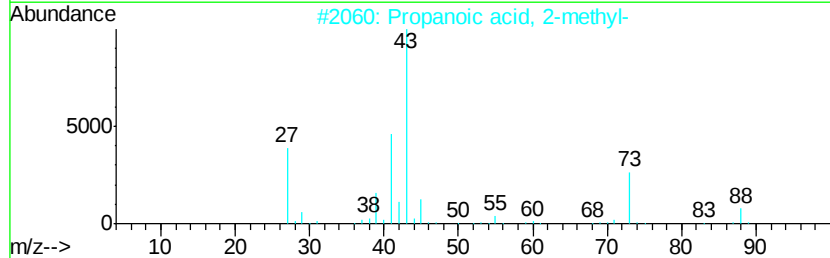
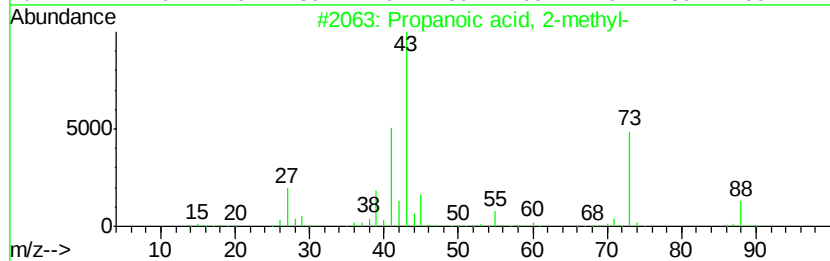
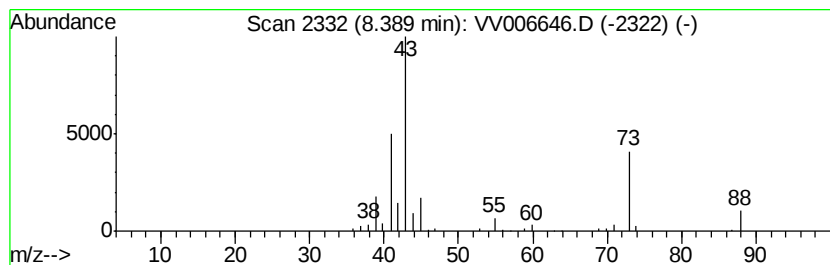
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Propanoic acid, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.39	1.09 ug/L	172020	Chlorobenzene-d5	8.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	91
2			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	90
3			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	87
4			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	83
5			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV071918\
Data File : VV006646.D
Acq On : 19 Jul 2018 16:51
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 11 Sample Multiplier: 1

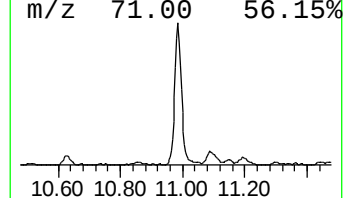
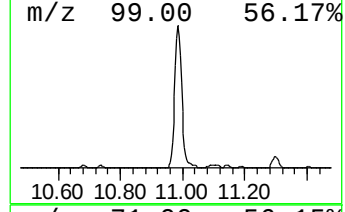
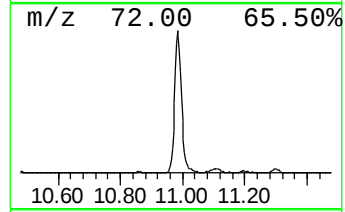
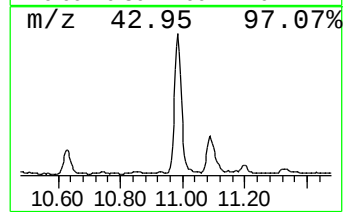
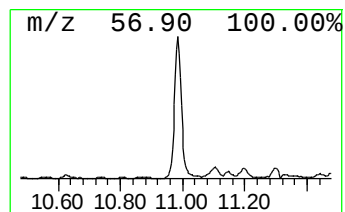
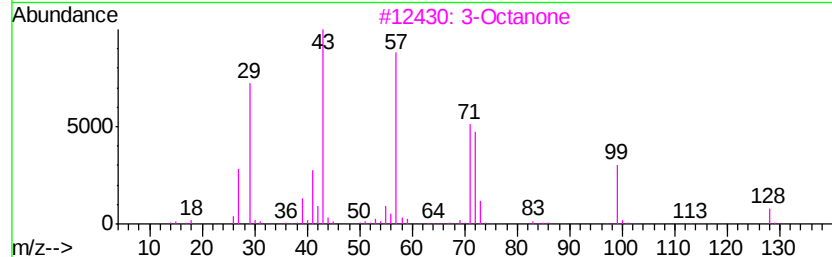
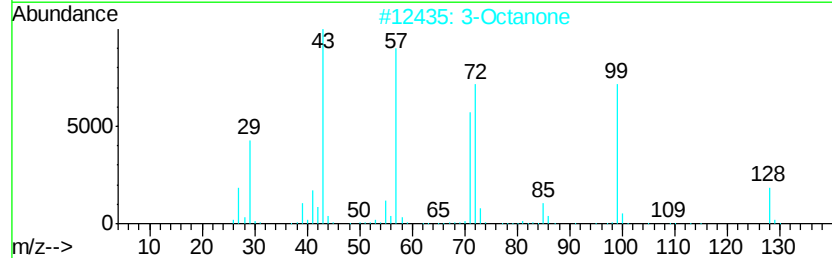
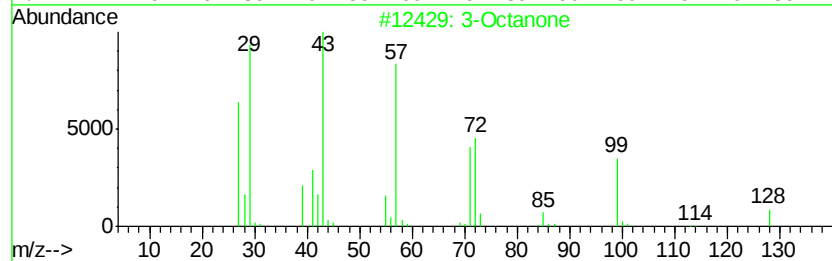
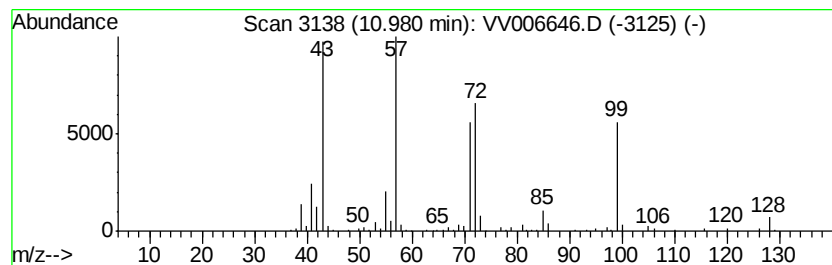
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MSVOA_V
ClientSampleId :
DB171

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 3-Octanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	1.30 ug/L	178697	1,4-Dichlorobenzene-d4	11.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Octanone	128 C8H16O	000106-68-3	91
2	3-Octanone	128 C8H16O	000106-68-3	90
3	3-Octanone	128 C8H16O	000106-68-3	64
4	3-Heptanone, 6-methyl-	128 C8H16O	000624-42-0	53
5	3-Octanone	128 C8H16O	000106-68-3	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV071918\
Data File : VV006646.D
Acq On : 19 Jul 2018 16:51
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DB171

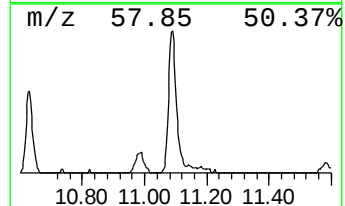
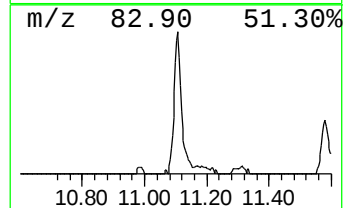
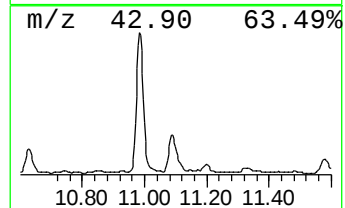
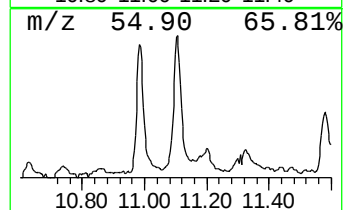
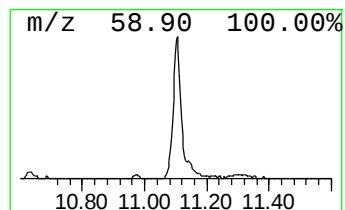
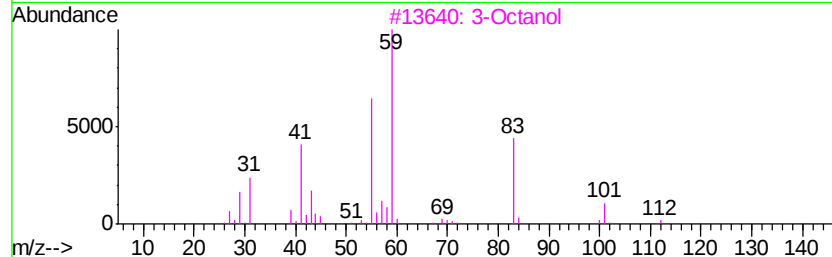
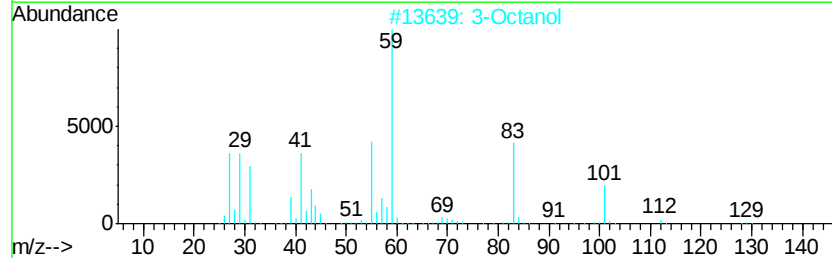
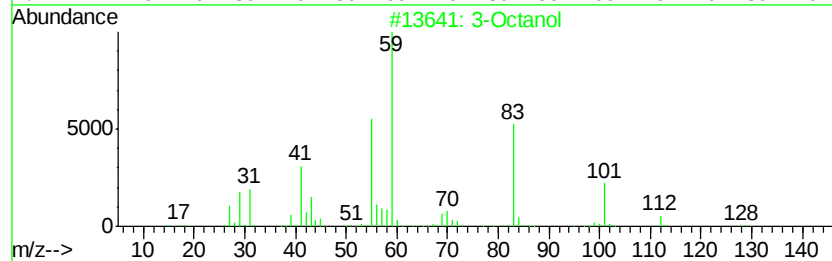
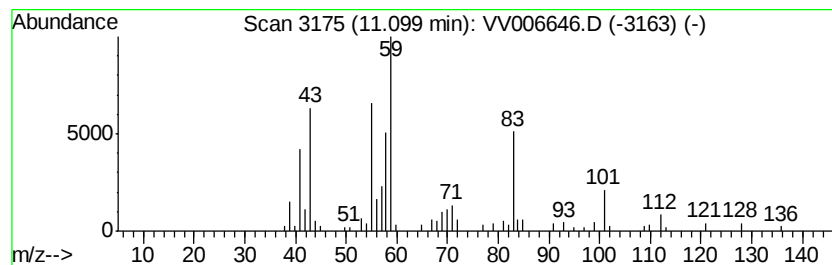
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 3-Octanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	0.53 ug/L	73631	1,4-Dichlorobenzene-d4	11.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanol	130	C8H18O	000589-98-0	64
2			3-Octanol	130	C8H18O	000589-98-0	64
3			3-Octanol	130	C8H18O	000589-98-0	59
4			Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	43
5			Oxetane, 2,2,3-trimethyl-	100	C6H12O	023120-43-6	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV071918\
Data File : VV006646.D
Acq On : 19 Jul 2018 16:51
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DB171

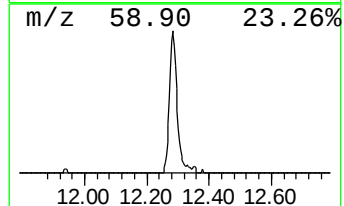
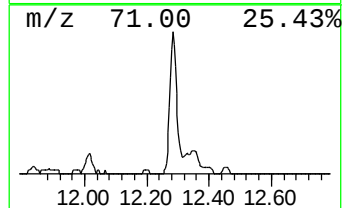
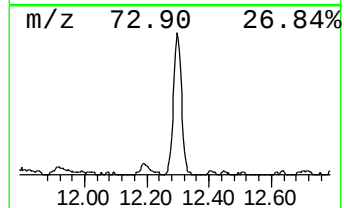
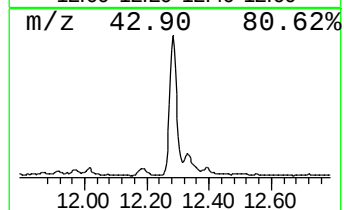
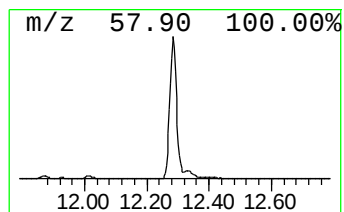
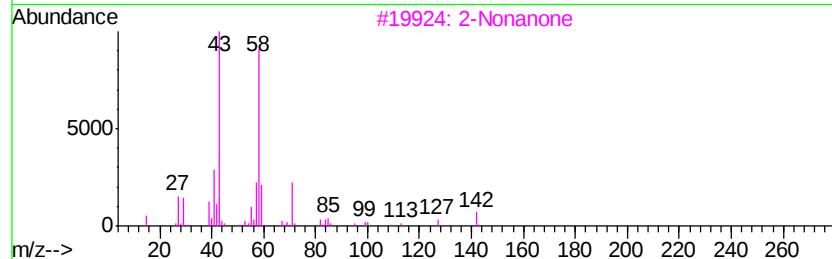
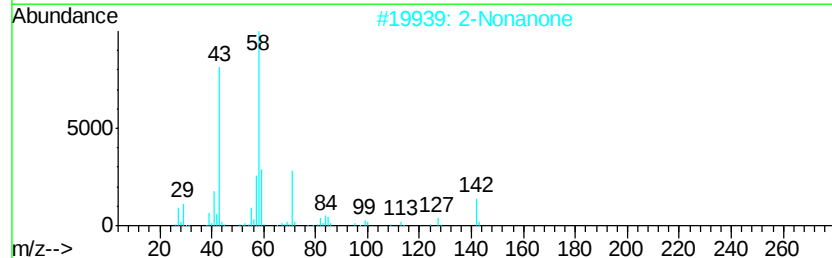
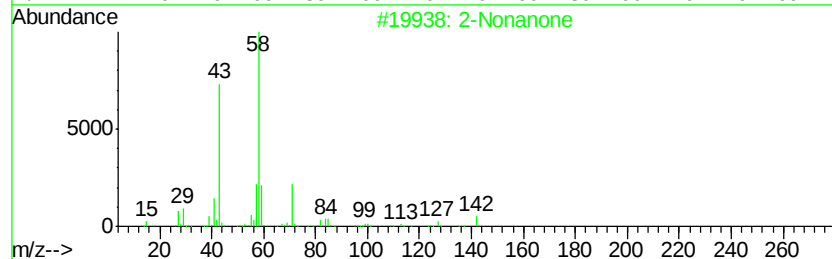
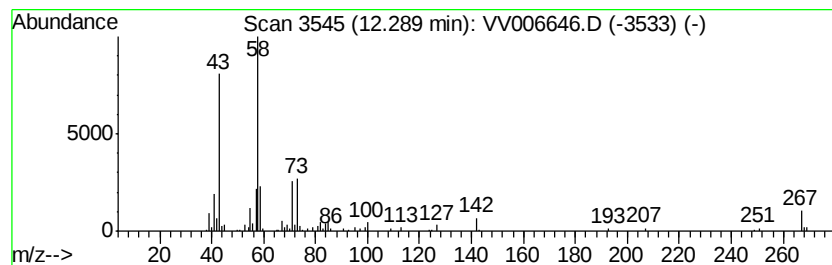
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 2-Nonanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	0.90 ug/L	124793	1,4-Dichlorobenzene-d4	11.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone			142	C9H18O	000821-55-6	93
2	2-Nonanone			142	C9H18O	000821-55-6	87
3	2-Nonanone			142	C9H18O	000821-55-6	87
4	2-Nonanone			142	C9H18O	000821-55-6	81
5	2-Undecanone			170	C11H22O	000112-12-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV071918\
Data File : VV006646.D
Acq On : 19 Jul 2018 16:51
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DB171

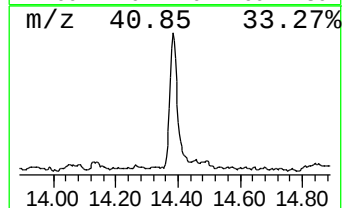
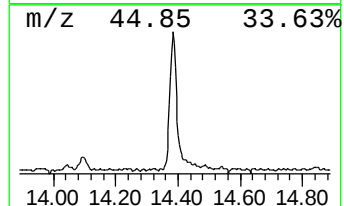
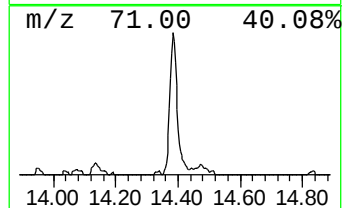
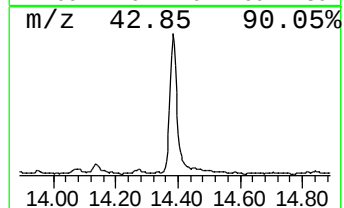
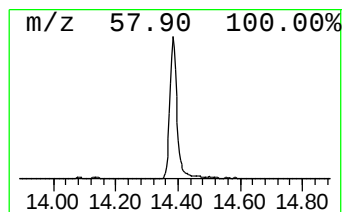
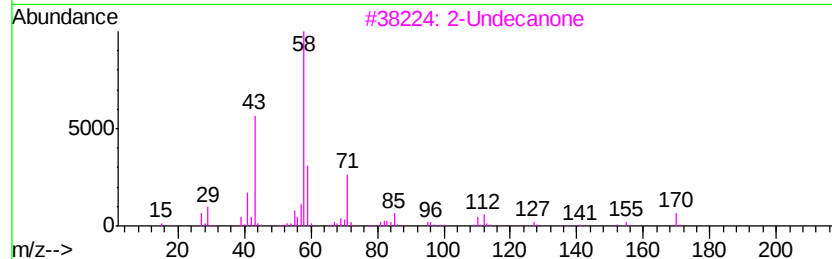
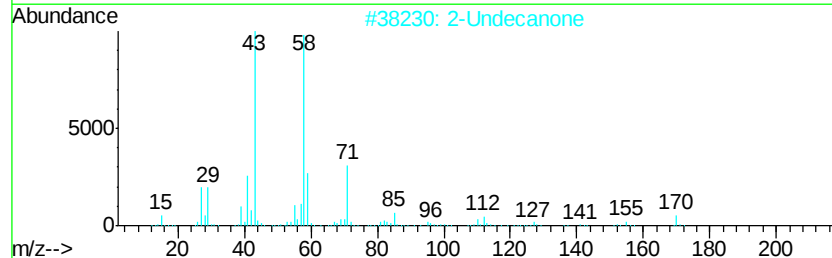
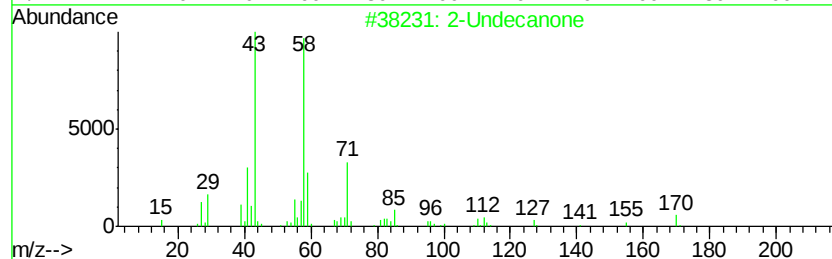
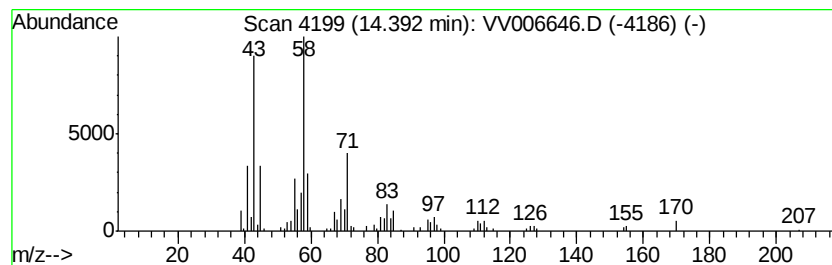
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 12 2-Undecanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	0.97 ug/L	134275	1,4-Dichlorobenzene-d4	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Undecanone	170	C11H22O	000112-12-9	93
2		2-Undecanone	170	C11H22O	000112-12-9	87
3		2-Undecanone	170	C11H22O	000112-12-9	81
4		11-Dodecen-2-one	182	C12H22O	005009-33-6	64
5		2-Tridecanone	198	C13H26O	000593-08-8	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV071918\
Data File : VV006646.D
Acq On : 19 Jul 2018 16:51
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DB171

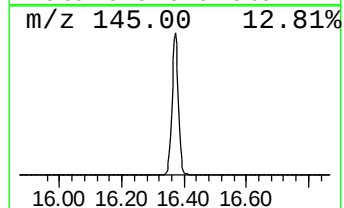
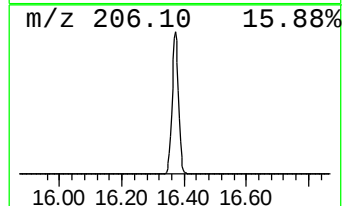
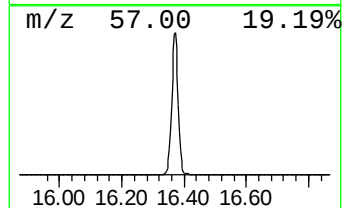
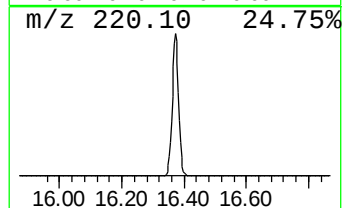
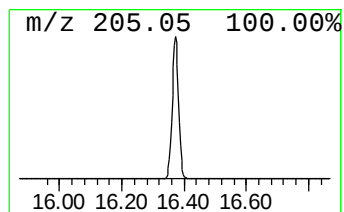
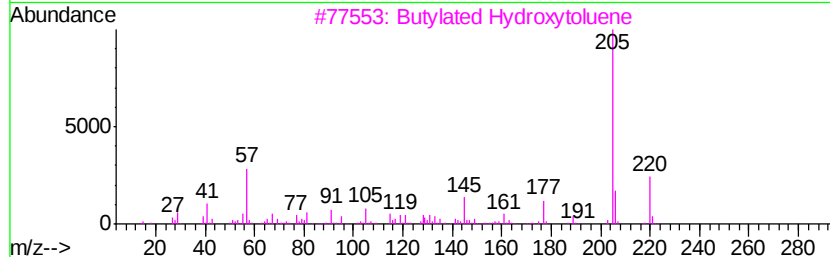
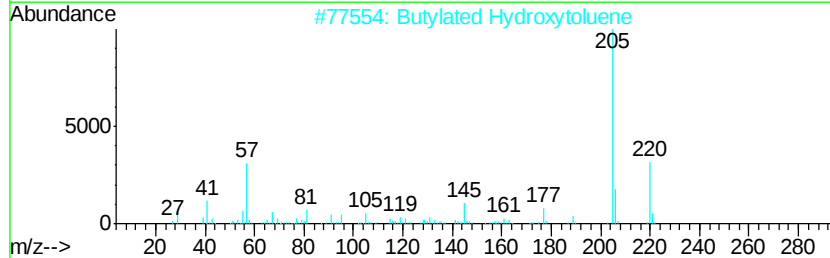
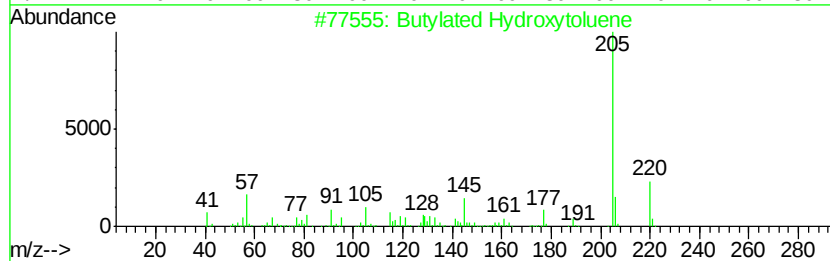
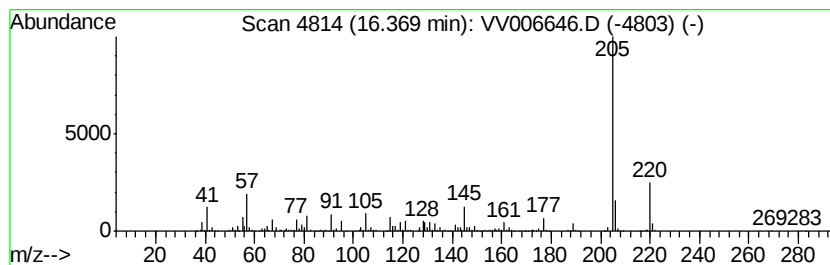
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 13 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	7.23 ug/L	997594	1,4-Dichlorobenzene-d4	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
3		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
4		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5		Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV071918\
Data File : VV006646.D
Acq On : 19 Jul 2018 16:51
Operator : SY/MD
Sample : J3983-06
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DB171

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

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	1.22	3.5	ug/L	721892	1	5.67	1042560	5.0
Methanethiol	1.47	6.6	ug/L	1379840	1	5.67	1042560	5.0
Ethanethiol	2.05	3.4	ug/L	709096	1	5.67	1042560	5.0
2-Propanethiol	2.69	1.6	ug/L	338091	1	5.67	1042560	5.0
Propanoic acid, 2...	8.39	1.1	ug/L	172020	2	8.90	785871	5.0
3-Octanone	10.98	1.3	ug/L	178697	3	11.30	689851	5.0
3-Octanol	11.10	0.5	ug/L	73631	3	11.30	689851	5.0
2-Nonanone	12.29	0.9	ug/L	124793	3	11.30	689851	5.0
2-Undecanone	14.39	1.0	ug/L	134275	3	11.30	689851	5.0
Butylated Hydroxy...	16.37	7.2	ug/L	997594	3	11.30	689851	5.0