

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
 Data File : VV011269.D
 Acq On : 07 Jun 2019 03:47
 Operator : SY/MD
 Sample : K3197-12
 Misc : 25ML/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9P56

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\SOMVTR060419WMA.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	1.232	35	44	62	rBV	511668	1931927	100.00%	22.457%
2	1.579	147	152	166	rVB	79552	105107	5.44%	1.222%
3	2.126	313	322	333	rVB	162671	225906	11.69%	2.626%
4	2.312	370	380	394	rBV	469499	666409	34.49%	7.746%
5	2.650	477	485	496	rVB	21628	39593	2.05%	0.460%
6	3.759	808	830	845	rBV6	23333	73352	3.80%	0.853%
7	3.984	881	900	955	rBV3	43084	274579	14.21%	3.192%
8	4.399	1014	1029	1047	rBV	103453	247593	12.82%	2.878%
9	5.090	1226	1244	1267	rBV3	257369	609931	31.57%	7.090%
10	5.663	1408	1422	1439	rBV	205671	409676	21.21%	4.762%
11	6.116	1544	1563	1589	rBV	138312	297153	15.38%	3.454%
12	6.634	1713	1724	1747	rVB2	46296	105369	5.45%	1.225%
13	7.029	1835	1847	1864	rBV	63653	114558	5.93%	1.332%
14	7.357	1934	1949	1966	rVV	292625	511840	26.49%	5.950%
15	7.666	2034	2045	2059	rBV	36374	67024	3.47%	0.779%
16	8.138	2181	2192	2205	rBV	311478	583223	30.19%	6.780%
17	8.289	2230	2239	2255	rVB2	19592	36461	1.89%	0.424%
18	8.894	2414	2427	2440	rBV	302635	495622	25.65%	5.761%
19	9.142	2497	2504	2513	rBV2	19085	29335	1.52%	0.341%
20	9.752	2684	2694	2707	rBV	20846	40450	2.09%	0.470%
21	9.855	2716	2726	2734	rBV5	13193	22498	1.16%	0.262%
22	10.260	2840	2852	2866	rBV	97034	161312	8.35%	1.875%
23	11.084	3099	3108	3123	rBV2	26627	51153	2.65%	0.595%
24	11.196	3129	3143	3155	rBV3	29985	55992	2.90%	0.651%
25	11.293	3162	3173	3191	rBV	286086	455724	23.59%	5.297%
26	11.572	3248	3260	3273	rBV2	48424	94650	4.90%	1.100%
27	11.669	3279	3290	3312	rVB	266131	434929	22.51%	5.056%
28	12.280	3471	3480	3491	rBV	31493	55940	2.90%	0.650%
29	12.392	3506	3515	3531	rBV2	48418	76828	3.98%	0.893%
30	13.482	3845	3854	3870	rBV6	15237	27939	1.45%	0.325%
31	13.678	3907	3915	3924	rVB3	15219	24970	1.29%	0.290%
32	15.167	4367	4378	4395	rBV3	15371	30501	1.58%	0.355%
33	16.234	4699	4710	4727	rBV5	45971	92575	4.79%	1.076%
34	16.360	4738	4749	4764	rBV2	95521	152607	7.90%	1.774%

LSC Area Percent Report

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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P56

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\SOMVTR060419WMA.M
Title : TRACE VOA SOM01.0

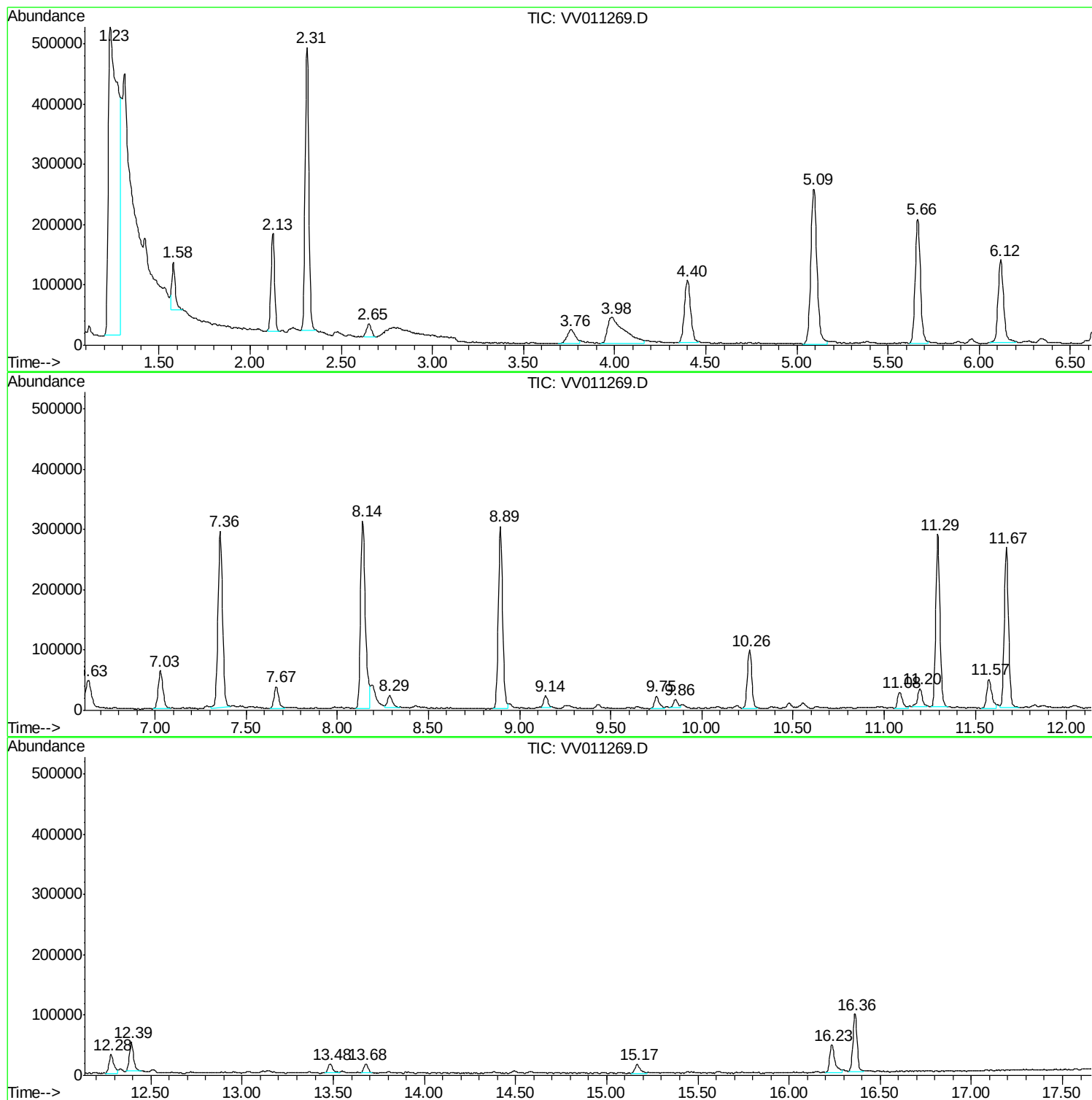
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Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060619\
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Quant Title : TRACE VOA SOM01.0

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



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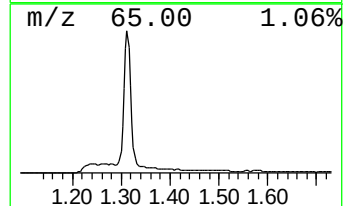
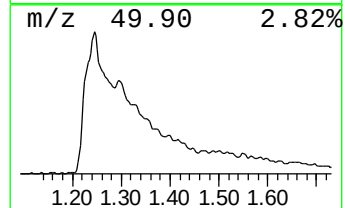
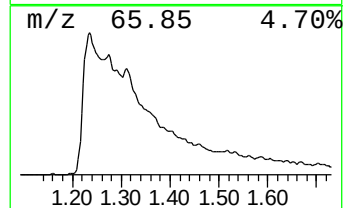
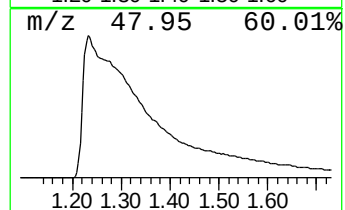
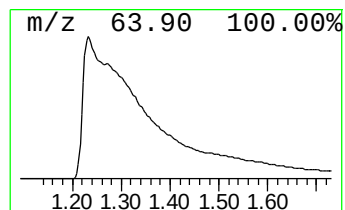
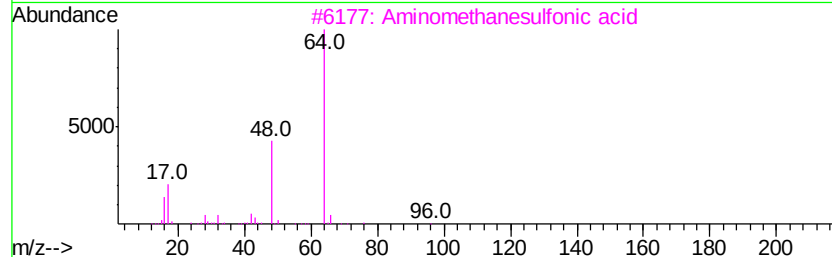
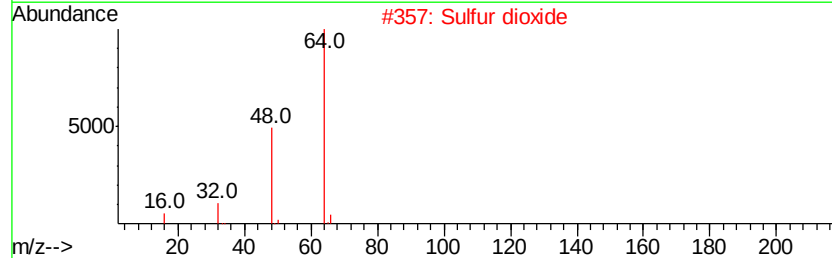
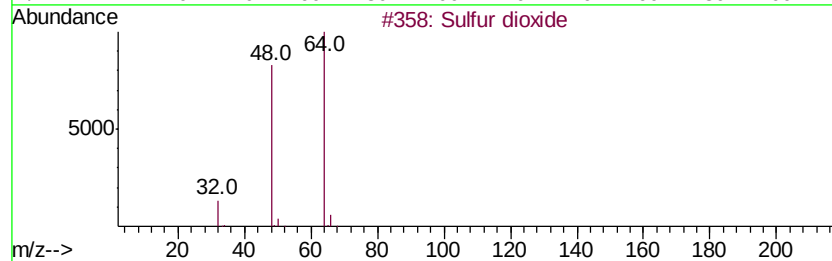
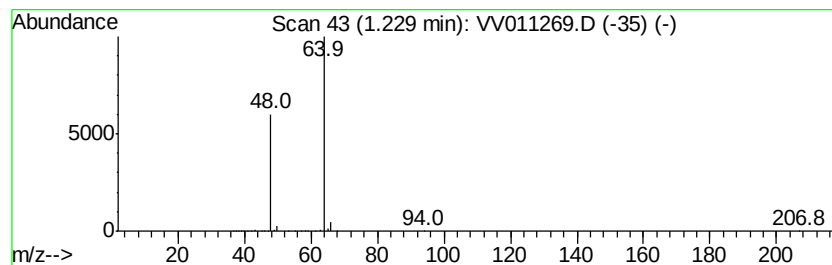
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.23	23.58 ug/L	1931930	1,4-Difluorobenzene	5.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 02S	007446-09-5	83
2	Sulfur dioxide	64 02S	007446-09-5	83
3	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	74
4	L-Alanine, 3-sulfo-	169 C3H7N05S	000498-40-8	9
5	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	9



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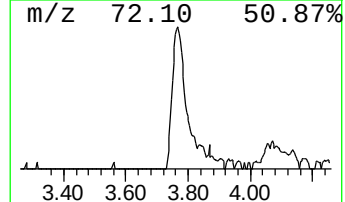
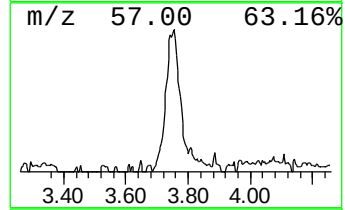
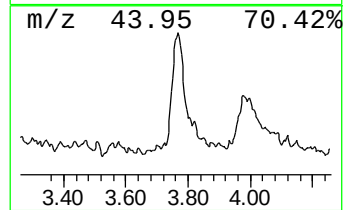
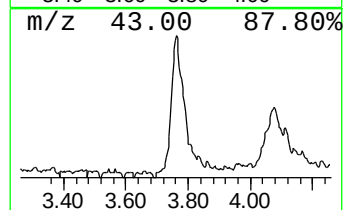
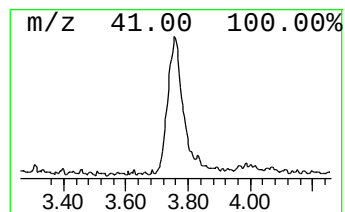
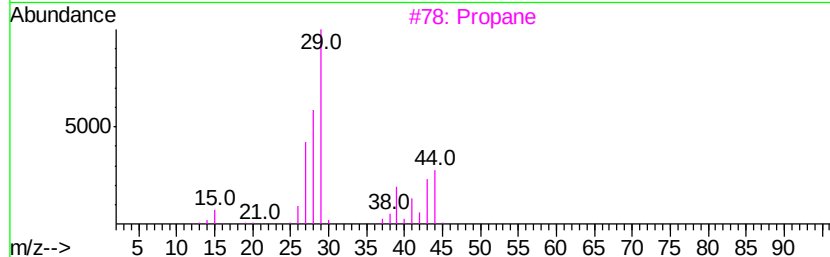
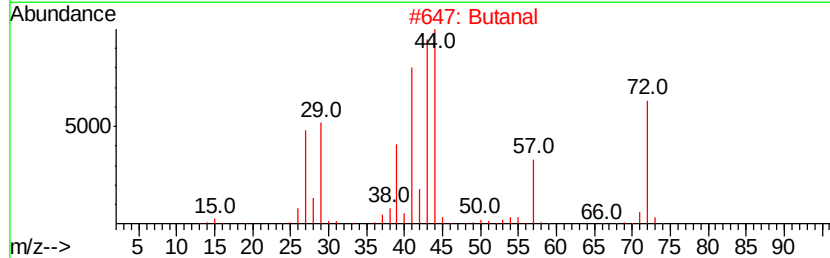
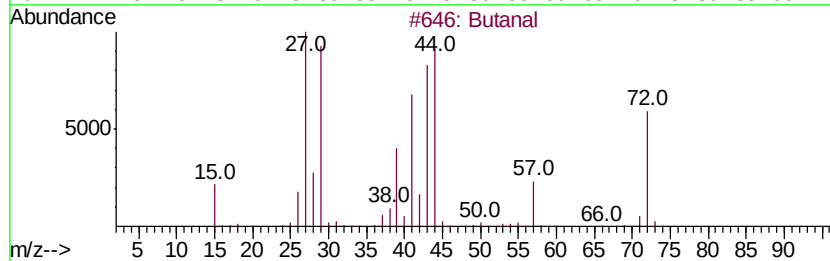
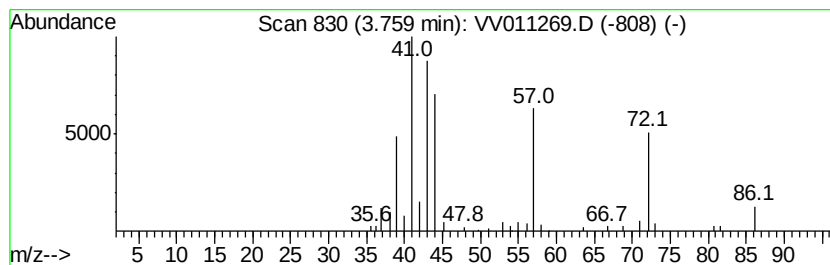
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	0.90 ug/L	73352	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	49
2		Butanal	72	C4H8O	000123-72-8	46
3		Propane	44	C3H8	000074-98-6	40
4		Butanal	72	C4H8O	000123-72-8	38
5		Propane	44	C3H8	000074-98-6	38



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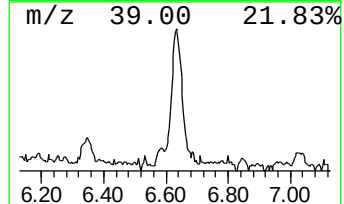
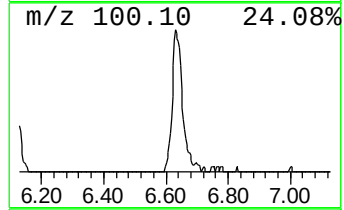
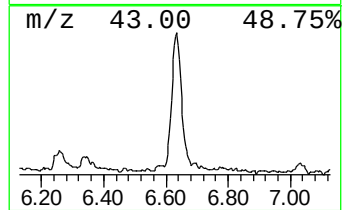
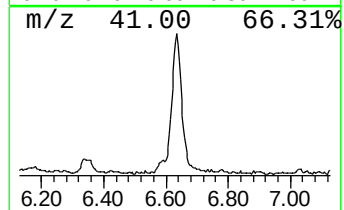
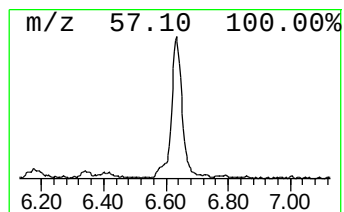
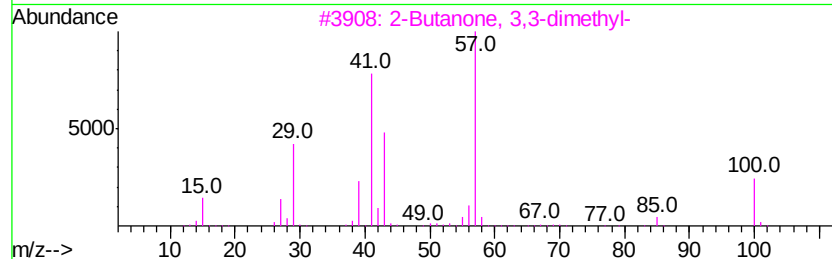
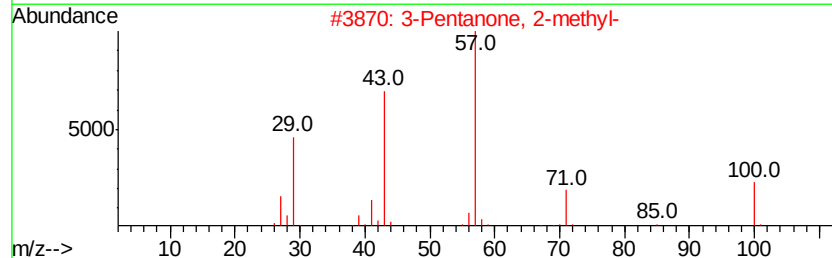
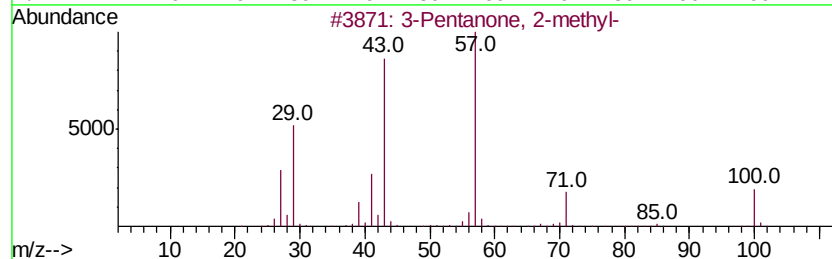
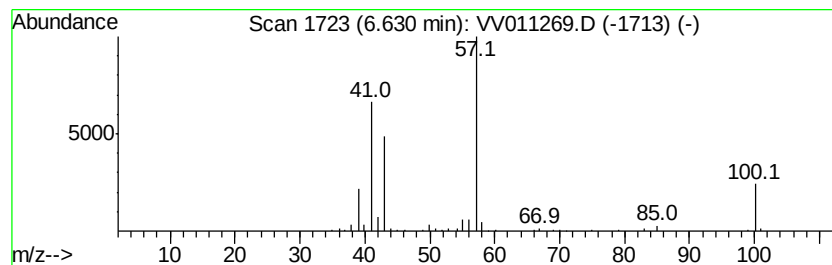
Instrument :
MSVOA_V
ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 3-Pentanone, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.63	1.29 ug/L	105369	1,4-Difluorobenzene	5.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	80
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	58
4	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	56
5	3-Hexanone	100	C6H12O	000589-38-8	53



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ALS Vial : 1 Sample Multiplier: 1

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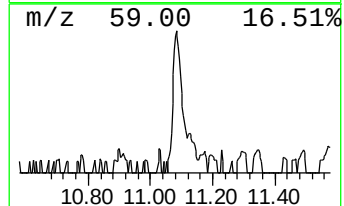
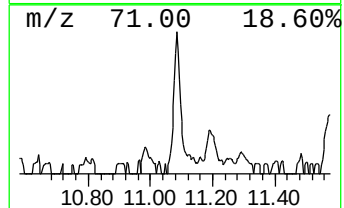
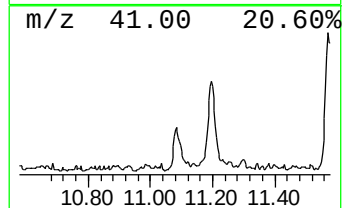
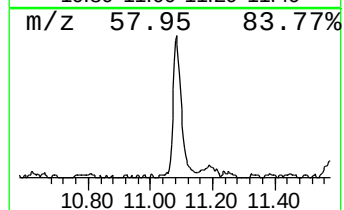
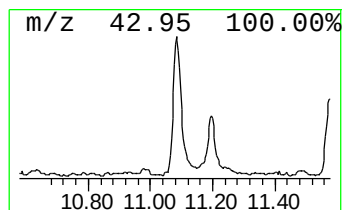
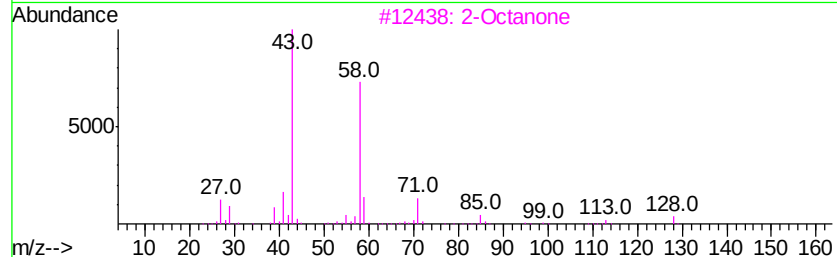
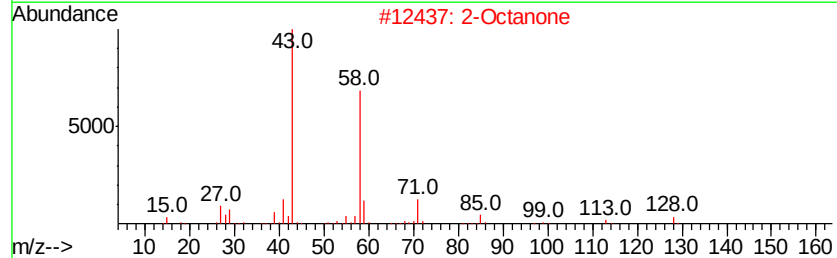
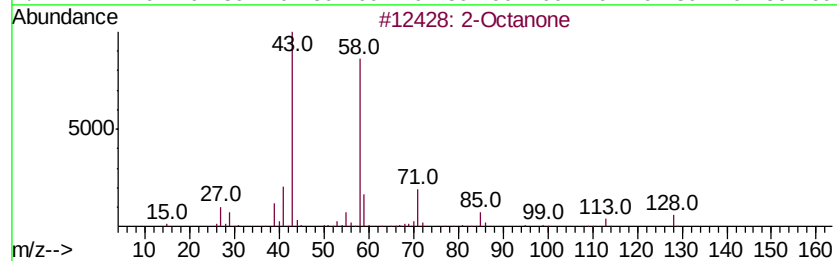
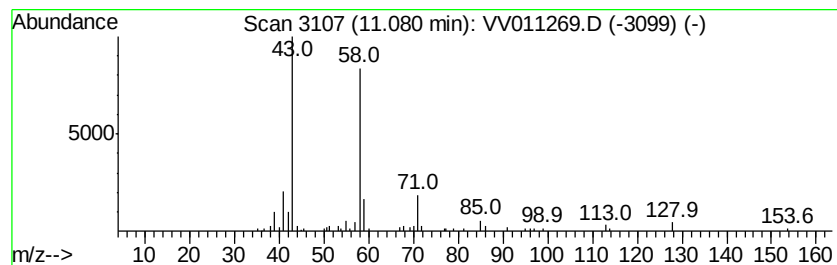
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Octanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	0.56 ug/L	51153	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanone	128	C8H16O	000111-13-7	90
2		2-Octanone	128	C8H16O	000111-13-7	80
3		2-Octanone	128	C8H16O	000111-13-7	80
4		2-Octanone	128	C8H16O	000111-13-7	80
5		2-Heptanone	114	C7H14O	000110-43-0	78



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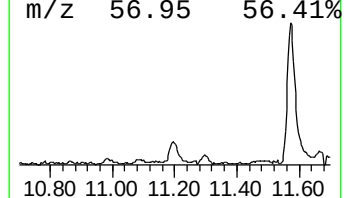
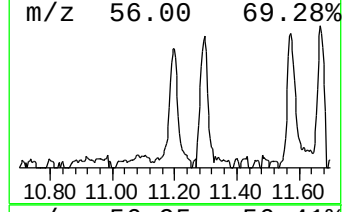
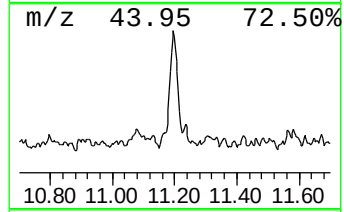
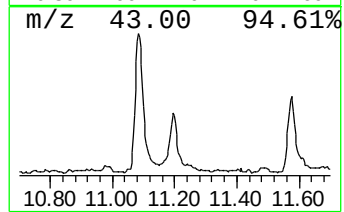
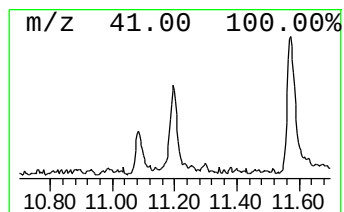
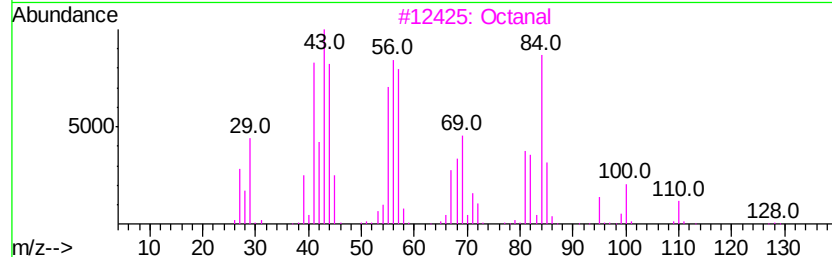
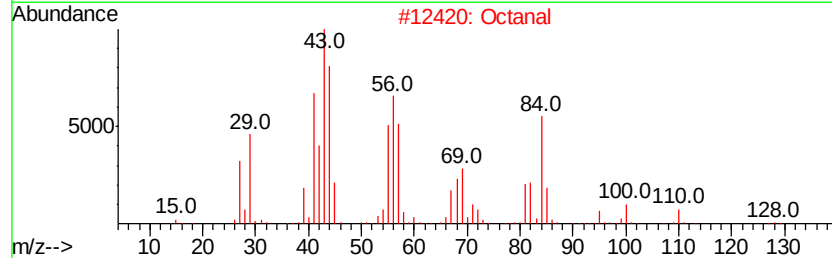
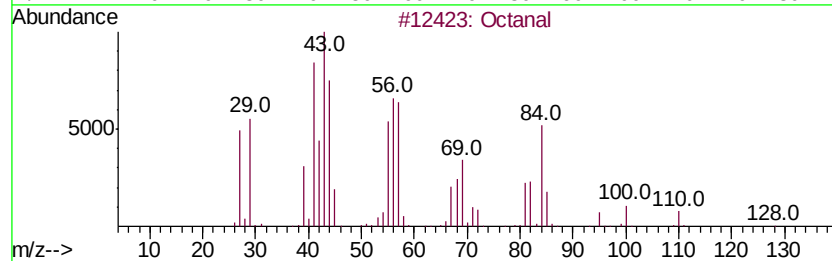
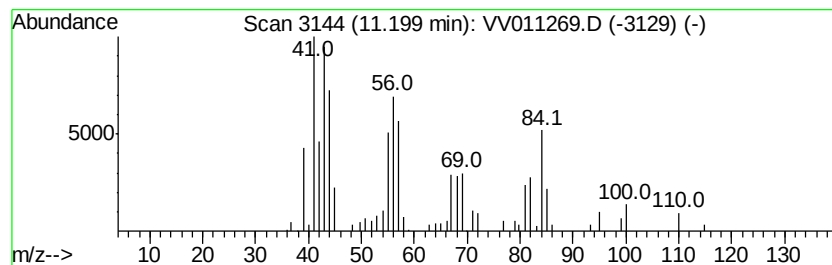
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	0.61 ug/L	55992	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanal	128	C8H16O	000124-13-0	91
2		Octanal	128	C8H16O	000124-13-0	90
3		Octanal	128	C8H16O	000124-13-0	86
4		Octanal	128	C8H16O	000124-13-0	83
5		Octanal	128	C8H16O	000124-13-0	80



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F9P56

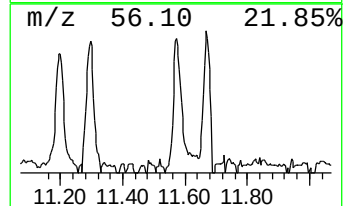
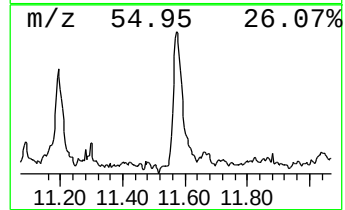
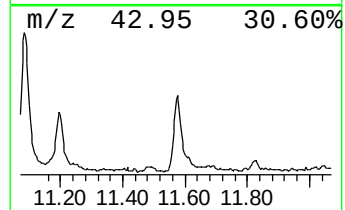
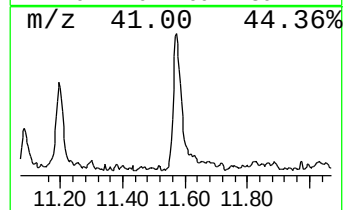
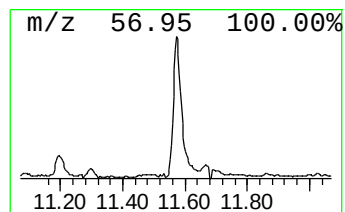
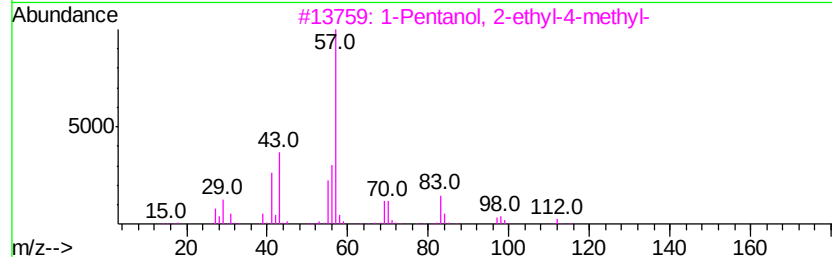
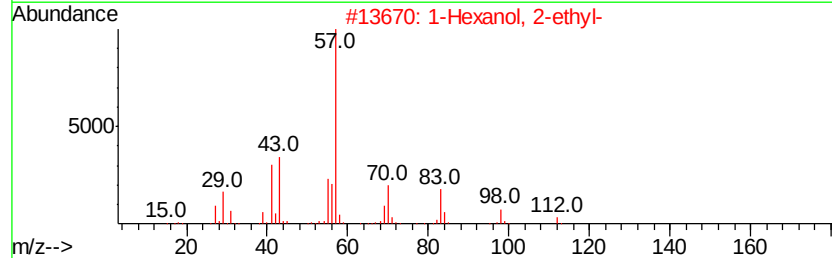
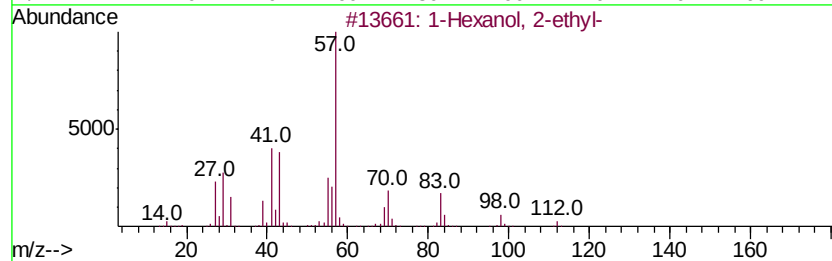
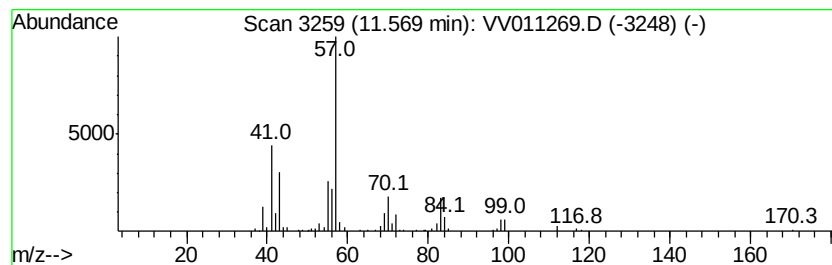
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	1.04 ug/L	94650	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
5		2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011269.D
Acq On : 07 Jun 2019 03:47
Operator : SY/MD
Sample : K3197-12
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

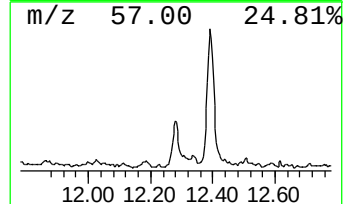
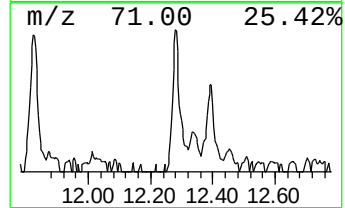
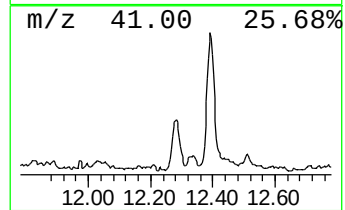
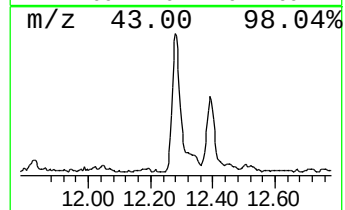
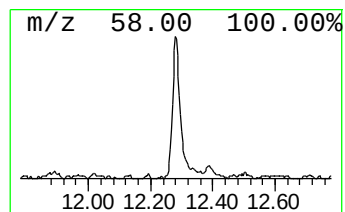
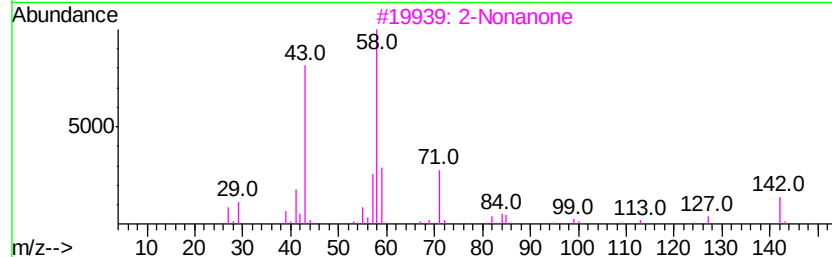
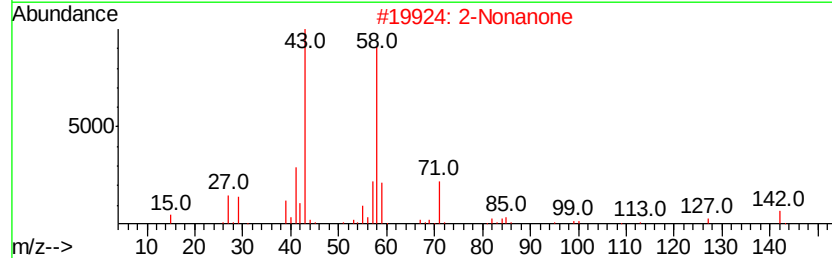
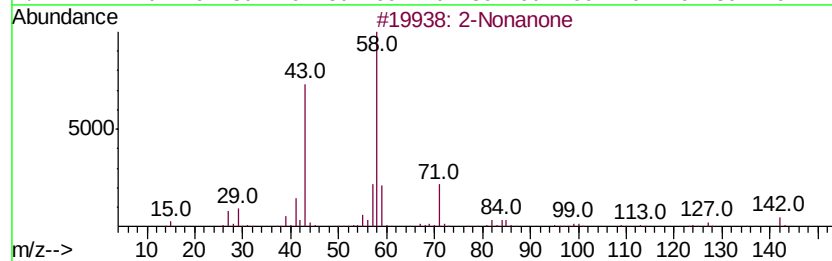
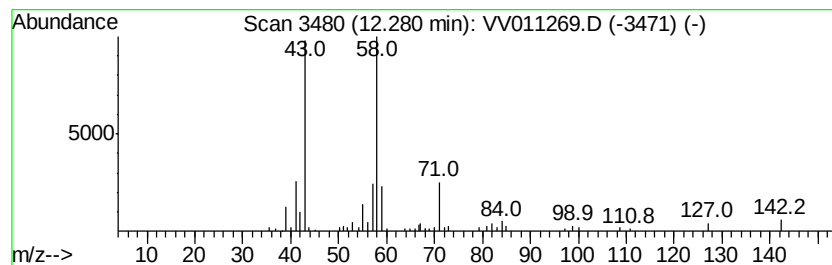
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 2-Nonanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	0.61 ug/L	55940	1,4-Dichlorobenzene-d4	11.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Nonanone		142 C9H18O	000821-55-6 90
2	2-Nonanone		142 C9H18O	000821-55-6 90
3	2-Nonanone		142 C9H18O	000821-55-6 86
4	2-Octanone		128 C8H16O	000111-13-7 64
5	Butanimidamide		86 C4H10N2	000107-90-4 64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011269.D
Acq On : 07 Jun 2019 03:47
Operator : SY/MD
Sample : K3197-12
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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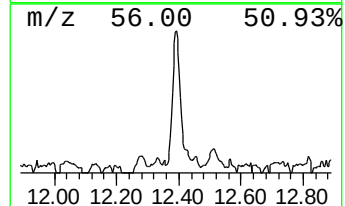
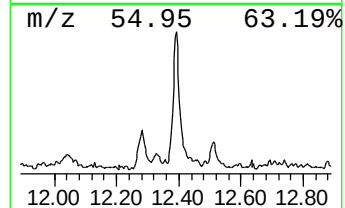
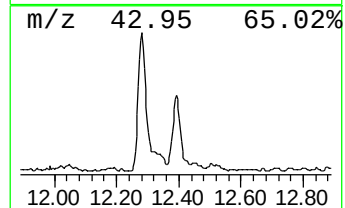
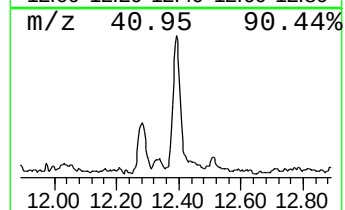
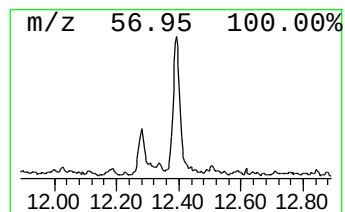
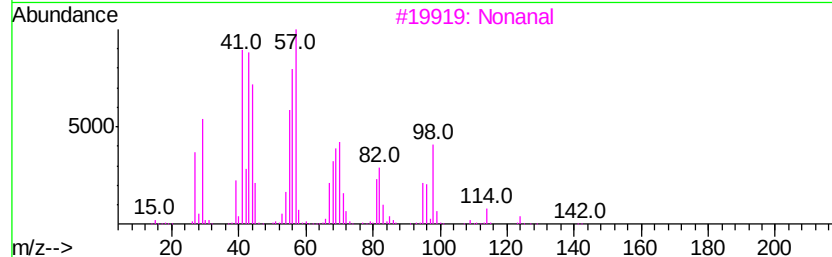
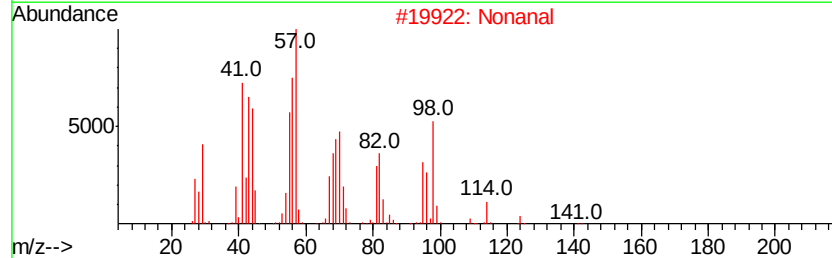
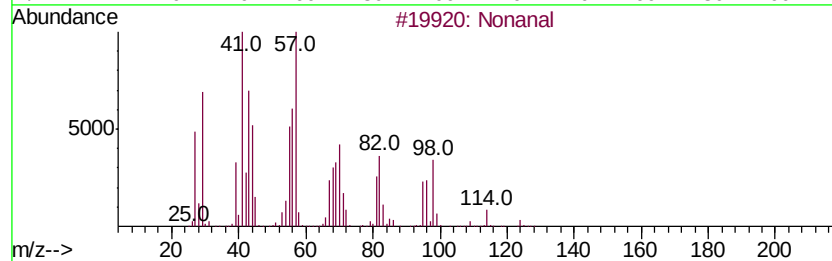
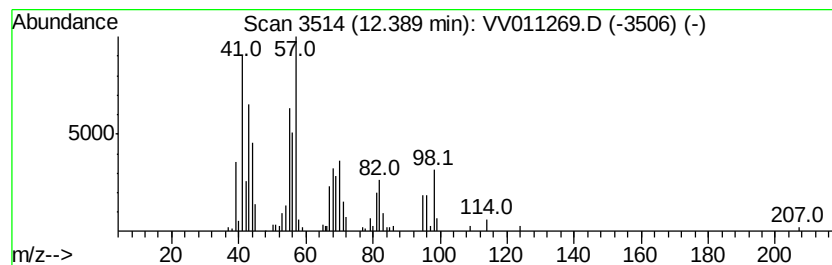
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Nonanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	0.84 ug/L	76828	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	91
2		Nonanal	142	C9H18O	000124-19-6	90
3		Nonanal	142	C9H18O	000124-19-6	90
4		Nonanal	142	C9H18O	000124-19-6	83
5		2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011269.D
Acq On : 07 Jun 2019 03:47
Operator : SY/MD
Sample : K3197-12
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
F9P56

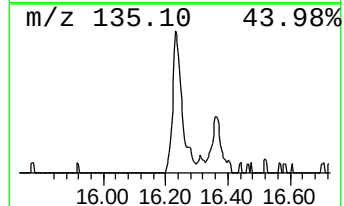
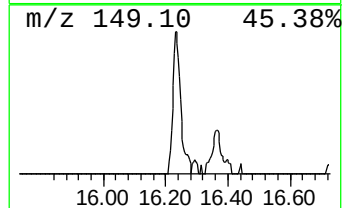
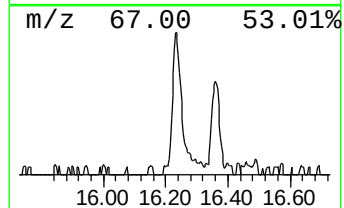
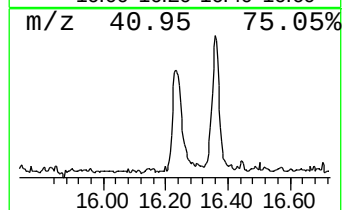
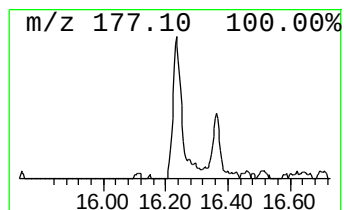
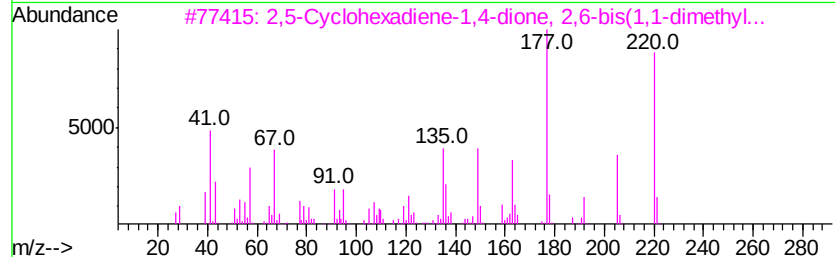
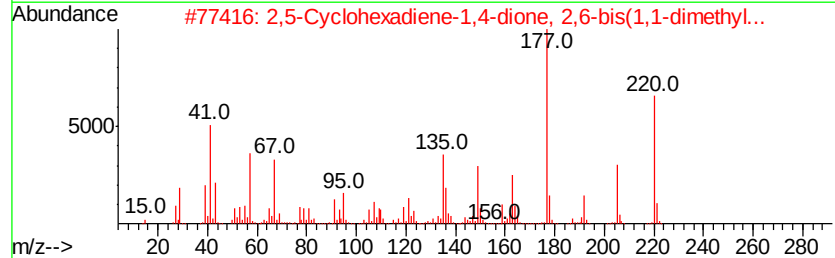
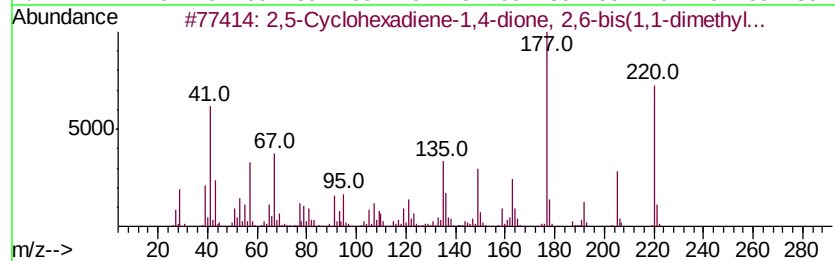
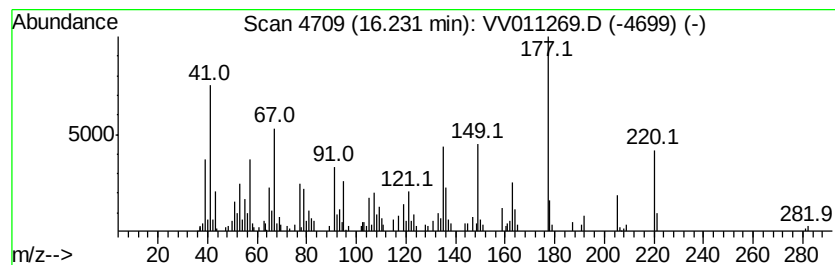
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	1.02 ug/L	92575	1,4-Dichlorobenzene-d4	11.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	90
4			Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	41
5			trans-.beta.-Ionone	192	C13H20O	000079-77-6	30



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011269.D
Acq On : 07 Jun 2019 03:47
Operator : SY/MD
Sample : K3197-12
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
F9P56

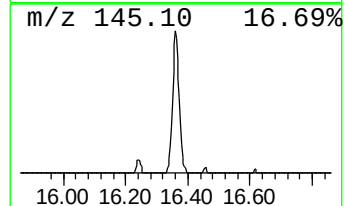
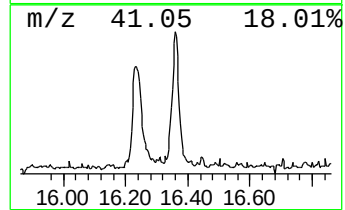
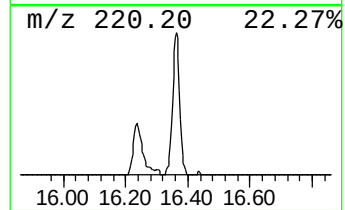
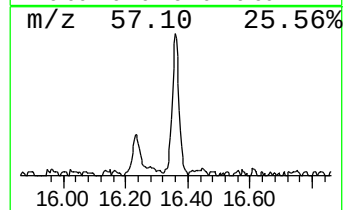
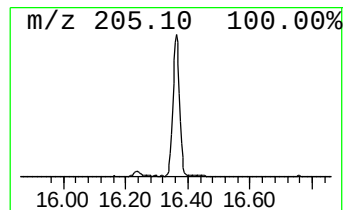
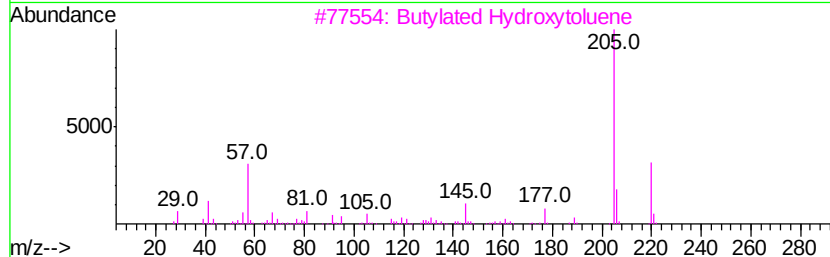
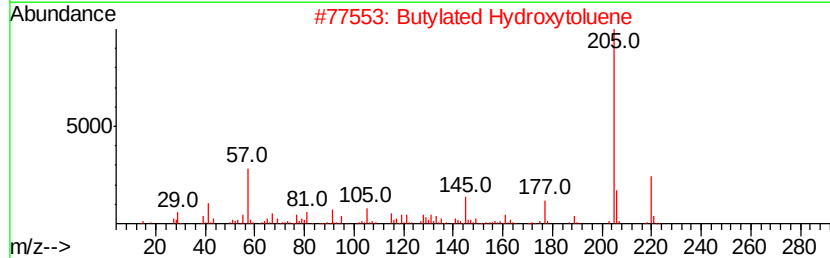
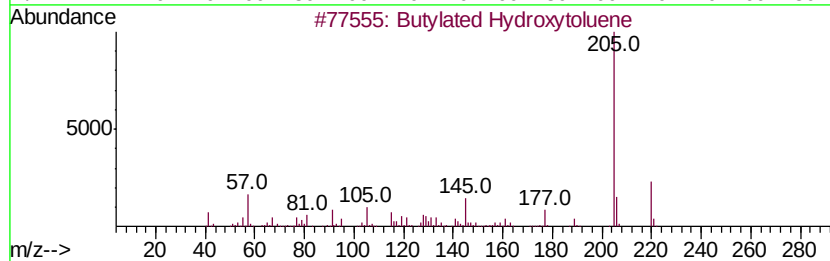
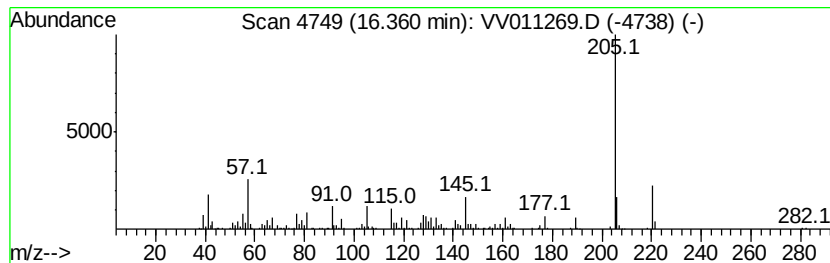
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	1.67 ug/L	152607	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
3		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
4		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5		Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	90



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060619\
Data File : VV011269.D
Acq On : 07 Jun 2019 03:47
Operator : SY/MD
Sample : K3197-12
Misc : 25ML/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P56

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.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	1.23	23.6	ug/L	1931930	1	5.66	409676	5.0
unknown-01	3.76	0.9	ug/L	73352	1	5.66	409676	5.0
3-Pentanone, 2-me...	6.63	1.3	ug/L	105369	1	5.66	409676	5.0
2-Octanone	11.08	0.6	ug/L	51153	3	11.29	455724	5.0
Octanal	11.20	0.6	ug/L	55992	3	11.29	455724	5.0
1-Hexanol, 2-ethyl-	11.57	1.0	ug/L	94650	3	11.29	455724	5.0
2-Nonanone	12.28	0.6	ug/L	55940	3	11.29	455724	5.0
Nonanal	12.39	0.8	ug/L	76828	3	11.29	455724	5.0
2,5-Cyclohexadien...	16.23	1.0	ug/L	92575	3	11.29	455724	5.0
Butylated Hydroxy...	16.36	1.7	ug/L	152607	3	11.29	455724	5.0