

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
 Data File : VV011270.D
 Acq On : 07 Jun 2019 04:13
 Operator : SY/MD
 Sample : K3197-13
 Misc : 25ML/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9P57

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	1.116	4	8	20	rVB3	15796	19674	2.52%	0.267%
2	1.274	39	57	59	rBV2	101368	241712	30.99%	3.279%
3	1.312	65	69	79	rVB	110543	114587	14.69%	1.554%
4	1.579	146	152	160	rVB	69593	80760	10.35%	1.096%
5	2.126	313	322	334	rVB	168131	236333	30.30%	3.206%
6	2.312	372	380	395	rVB	52309	82715	10.60%	1.122%
7	2.476	424	431	456	rVB2	16850	42015	5.39%	0.570%
8	2.650	475	485	497	rBV	17463	38217	4.90%	0.518%
9	3.756	806	829	850	rBV7	31593	104753	13.43%	1.421%
10	3.981	883	899	916	rBV2	43082	173023	22.18%	2.347%
11	4.399	1013	1029	1047	rBV2	103202	252587	32.38%	3.427%
12	5.090	1228	1244	1263	rBV3	259780	604124	77.45%	8.196%
13	5.662	1408	1422	1447	rBV	203894	407820	52.28%	5.533%
14	5.958	1495	1514	1527	rVB	7335	19561	2.51%	0.265%
15	6.074	1539	1550	1551	rBV10	7395	9718	1.25%	0.132%
16	6.116	1552	1563	1591	rVV2	144779	307623	39.44%	4.173%
17	6.341	1623	1633	1642	rBV5	8876	15878	2.04%	0.215%
18	6.588	1699	1710	1714	rBV6	7097	12097	1.55%	0.164%
19	6.633	1716	1724	1742	rVB	23605	53651	6.88%	0.728%
20	7.029	1835	1847	1862	rBV	64431	120980	15.51%	1.641%
21	7.286	1918	1927	1932	rBV3	5762	10234	1.31%	0.139%
22	7.357	1935	1949	1963	rVV	295841	509628	65.34%	6.914%
23	7.666	2034	2045	2055	rBV2	37669	66286	8.50%	0.899%
24	8.138	2181	2192	2205	rBV	329037	601801	77.15%	8.164%
25	8.289	2230	2239	2251	rVB3	21940	39411	5.05%	0.535%
26	8.428	2272	2282	2295	rBV7	4354	10222	1.31%	0.139%
27	8.894	2410	2427	2441	rBV	297165	480633	61.62%	6.520%
28	9.145	2495	2505	2514	rBV	36846	57636	7.39%	0.782%
29	9.264	2528	2542	2550	rBV	6626	18717	2.40%	0.254%
30	9.431	2585	2594	2603	rBV10	5540	9911	1.27%	0.134%
31	9.749	2686	2693	2706	rBV2	22008	36436	4.67%	0.494%
32	9.852	2716	2725	2733	rBV5	11980	19710	2.53%	0.267%
33	10.260	2841	2852	2869	rVB	99925	161355	20.69%	2.189%
34	10.556	2936	2944	2957	rVB2	16659	30446	3.90%	0.413%

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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\SOMVTR060419WMA.M
Title : TRACE VOA SOM01.0

35	11.083	3099	3108	3120	rBV	35364	63019	8.08%	0.855%
36	11.196	3128	3143	3158	rBV4	36525	69777	8.95%	0.947%
37	11.292	3162	3173	3193	rVB	280457	447936	57.43%	6.077%
38	11.575	3248	3261	3280	rBV	442354	780017	100.00%	10.582%
39	11.672	3281	3291	3312	rVB	279779	467201	59.90%	6.338%
40	12.280	3467	3480	3492	rBV	78482	139527	17.89%	1.893%
41	12.392	3505	3515	3528	rVB3	40948	64867	8.32%	0.880%
42	13.141	3740	3748	3757	rBV3	5100	8477	1.09%	0.115%
43	13.482	3844	3854	3866	rBV6	16505	29109	3.73%	0.395%
44	13.678	3902	3915	3927	rBV4	17119	29463	3.78%	0.400%
45	15.167	4367	4378	4391	rBV4	10815	22861	2.93%	0.310%
46	16.234	4697	4710	4727	rBV2	81176	169337	21.71%	2.297%
47	16.360	4740	4749	4763	rVB2	57588	89472	11.47%	1.214%

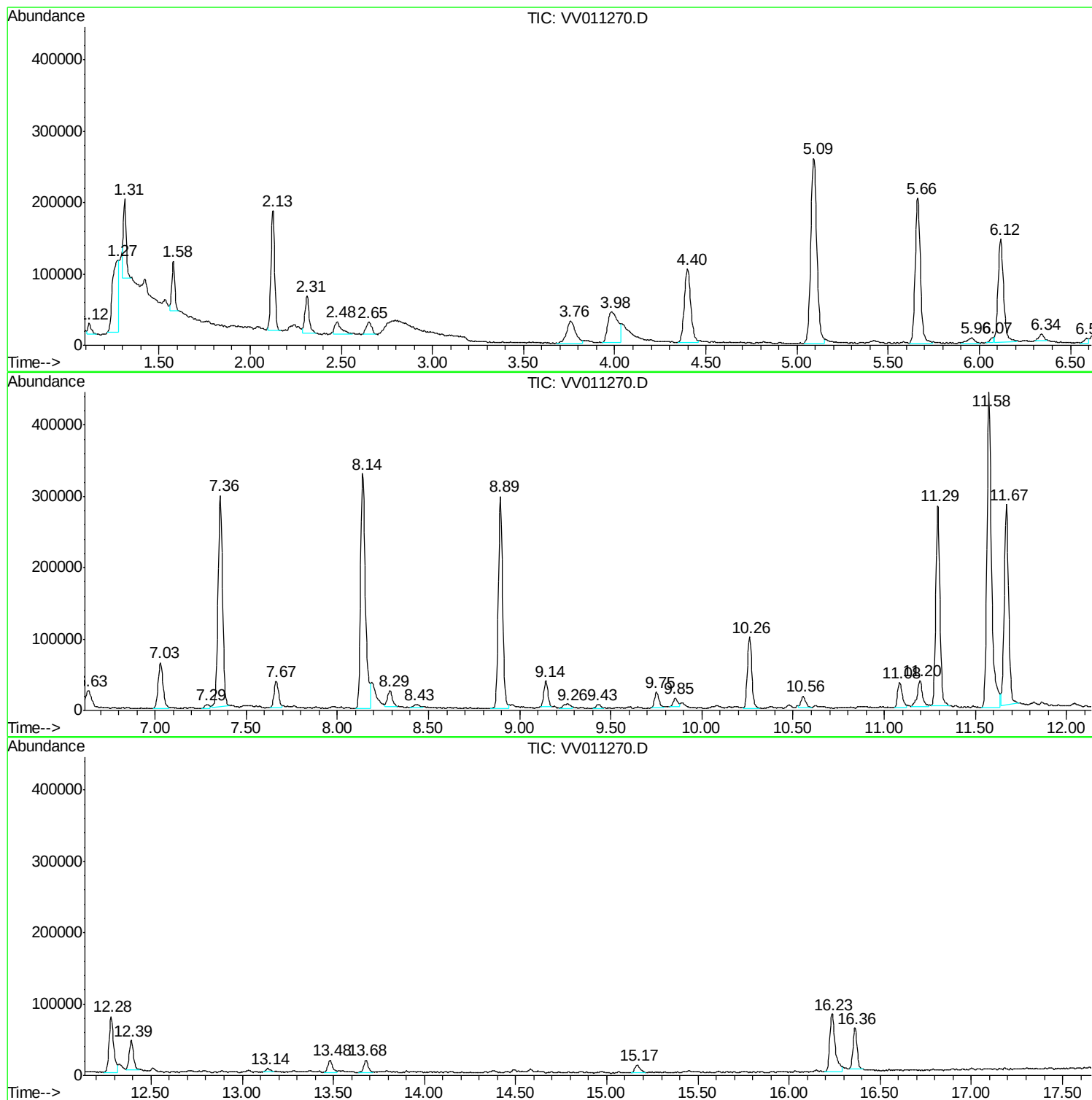
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ClientSampleId :
F9P57

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



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Instrument :
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ClientSampled :
F9P57

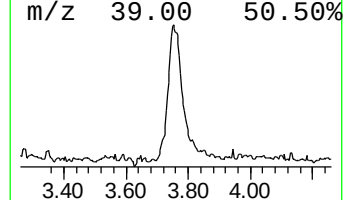
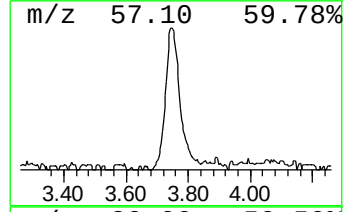
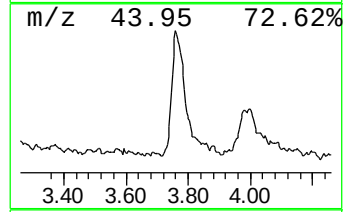
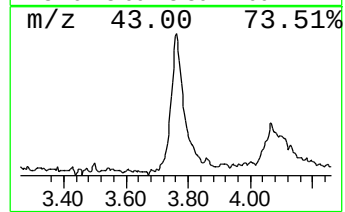
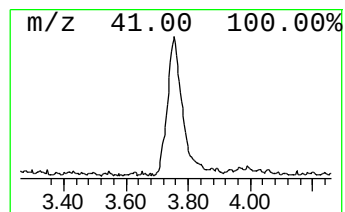
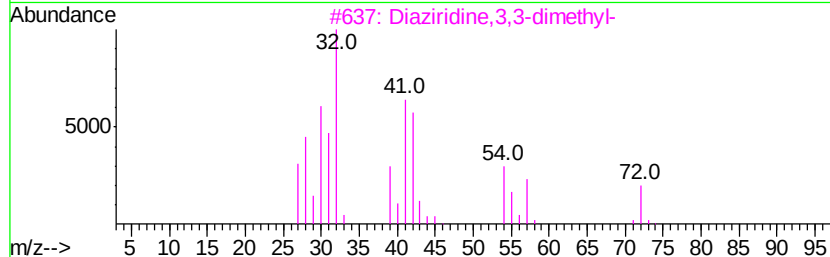
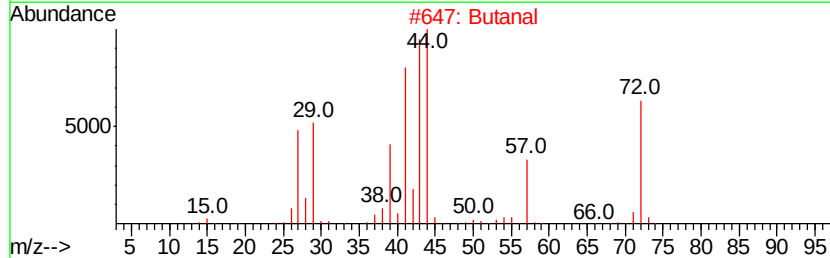
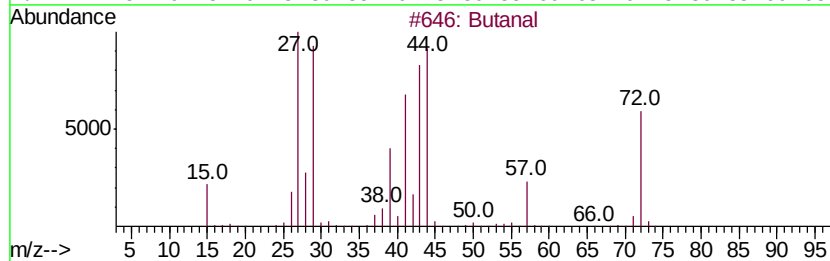
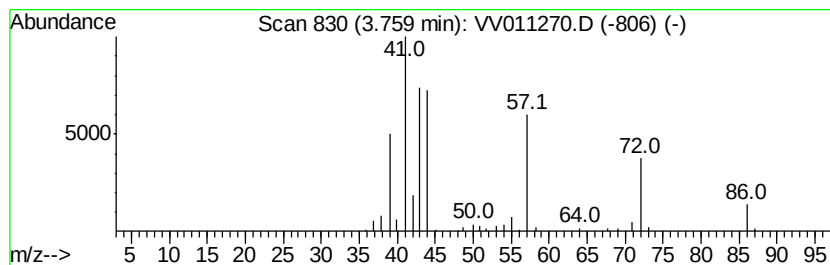
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	1.28 ug/L	104753	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	46
2		Butanal	72	C4H8O	000123-72-8	46
3		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4		Butanal	72	C4H8O	000123-72-8	38
5		Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	38



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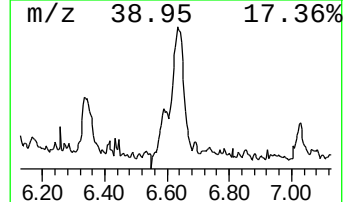
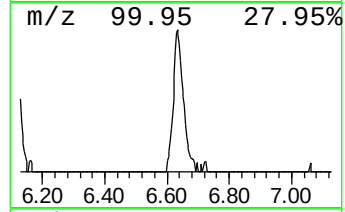
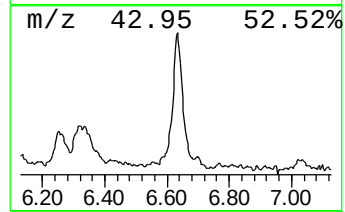
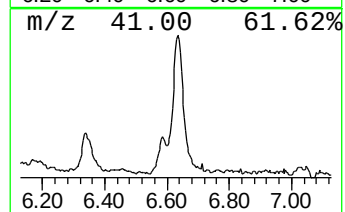
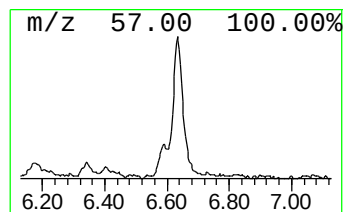
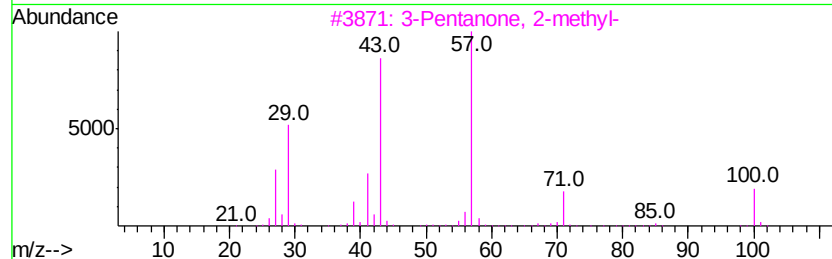
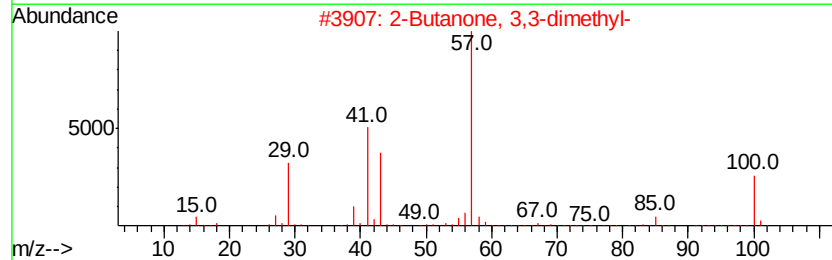
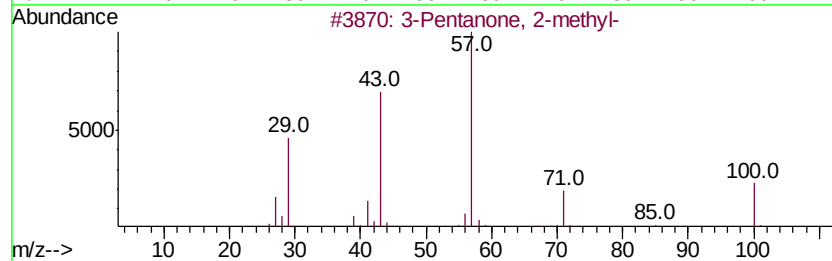
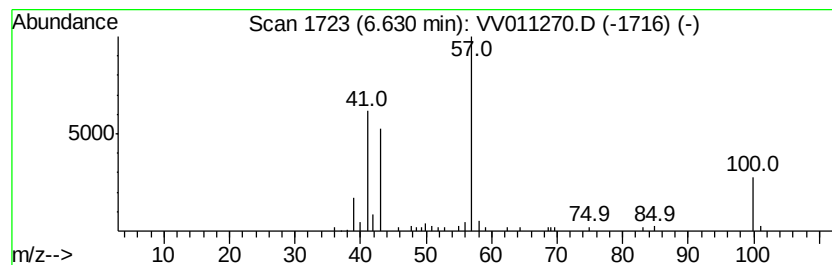
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 3-Pentanone, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	0.66 ug/L	53651	1,4-Difluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
2			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
3			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
4			3-Hexanone	100	C6H12O	000589-38-8	64
5			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	59



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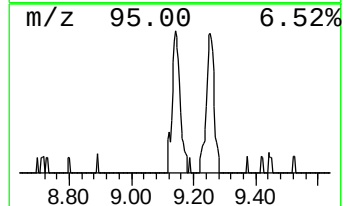
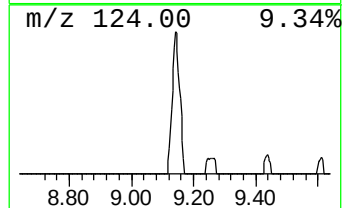
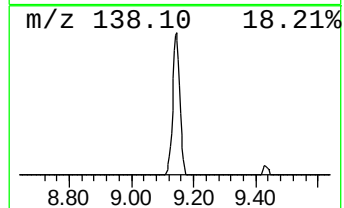
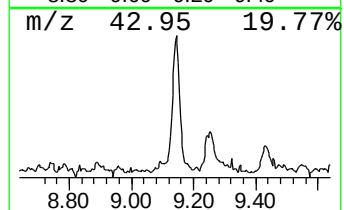
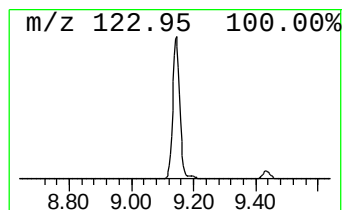
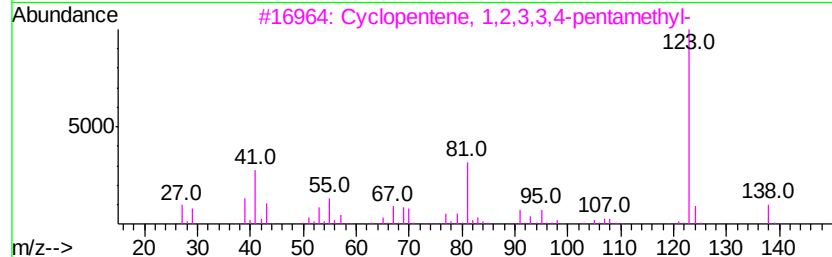
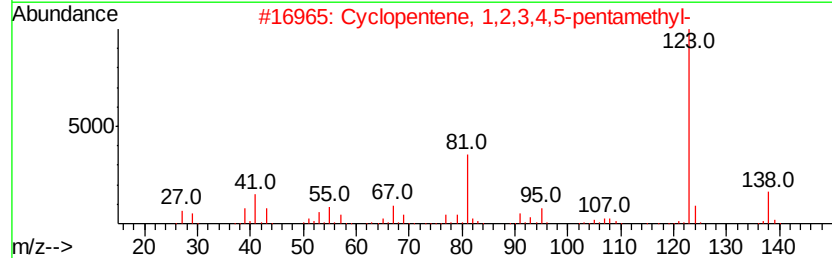
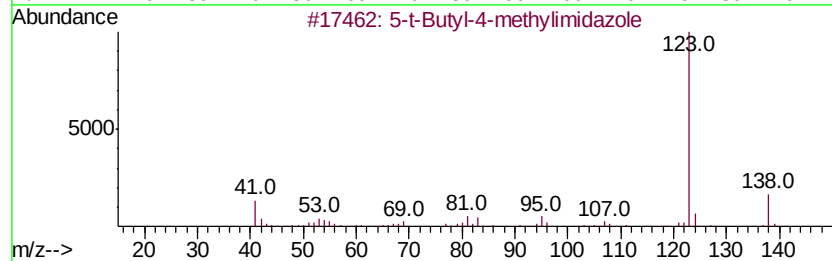
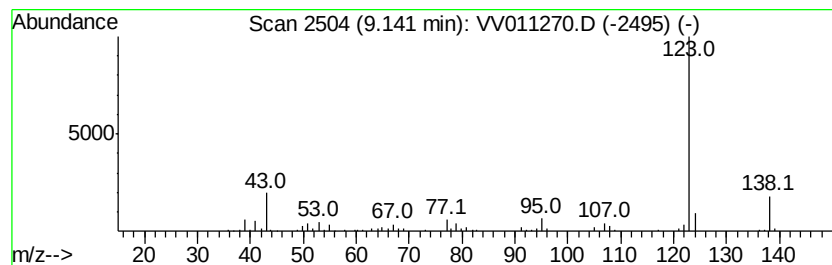
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 5-t-Butyl-4-methylimidazole Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.14	0.60 ug/L	57636	Chlorobenzene-d5	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	91
2		Cyclopentene, 1,2,3,4,5-pentamethyl-	138	C10H18	1000154-28-6	80
3		Cyclopentene, 1,2,3,3,4-pentamethyl-	138	C10H18	197390-29-7	78
4		1,6,6-Trimethyl-7-(3-oxobut-1-en-1-yl)-5-norbornene	236	C13H16O4	1000192-00-9	72
5		o-Fluoroacetophenone	138	C8H7FO	000445-27-2	64



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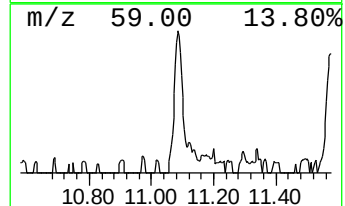
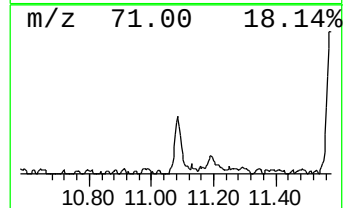
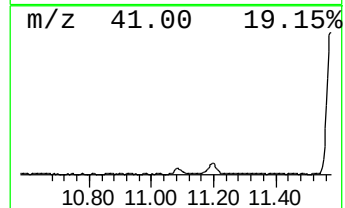
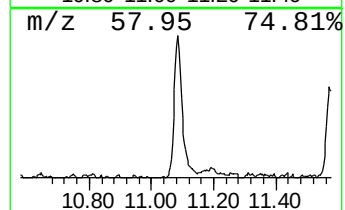
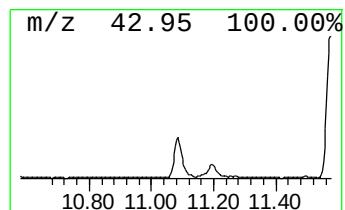
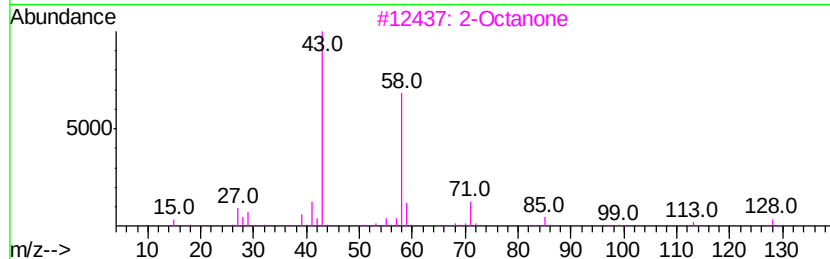
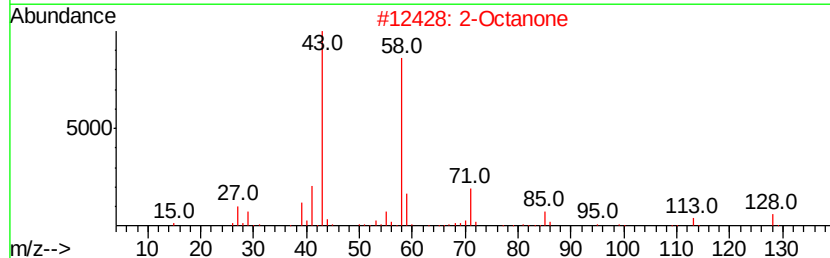
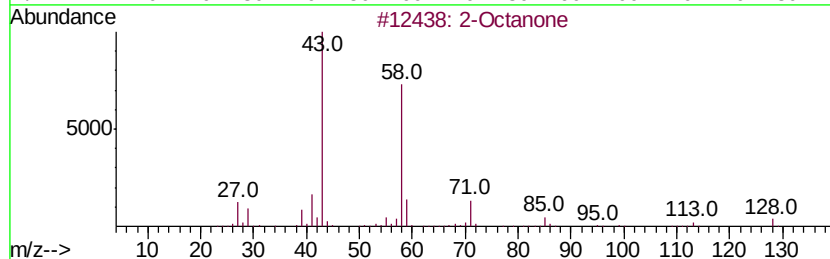
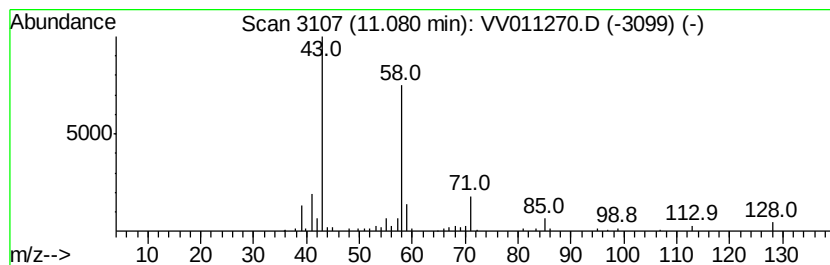
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Octanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	0.70 ug/L	63019	1,4-Dichlorobenzene-d4	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanone	128	C8H16O	000111-13-7	94
2		2-Octanone	128	C8H16O	000111-13-7	91
3		2-Octanone	128	C8H16O	000111-13-7	91
4		2-Octanone	128	C8H16O	000111-13-7	91
5		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	90



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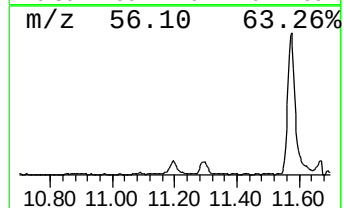
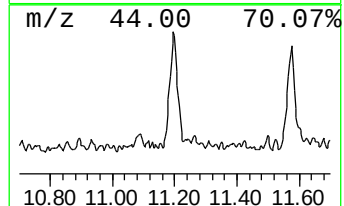
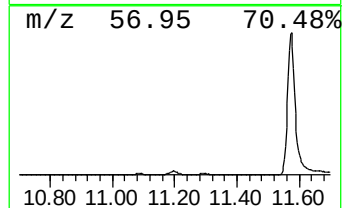
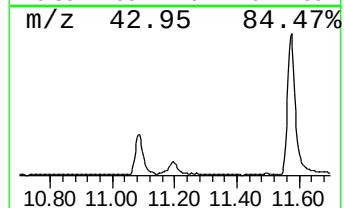
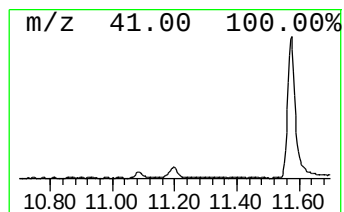
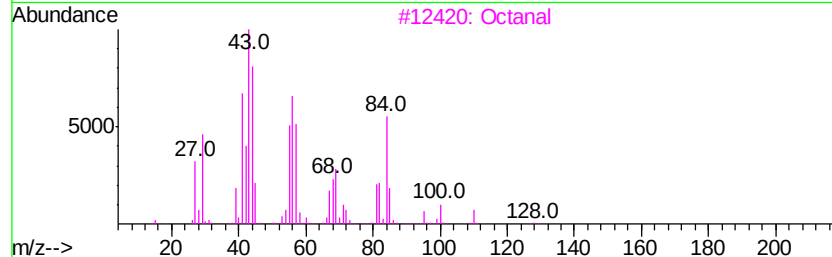
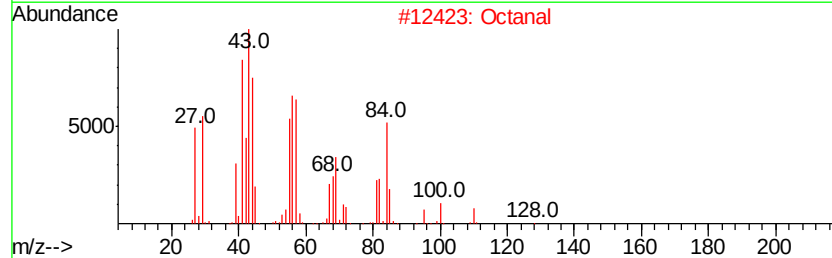
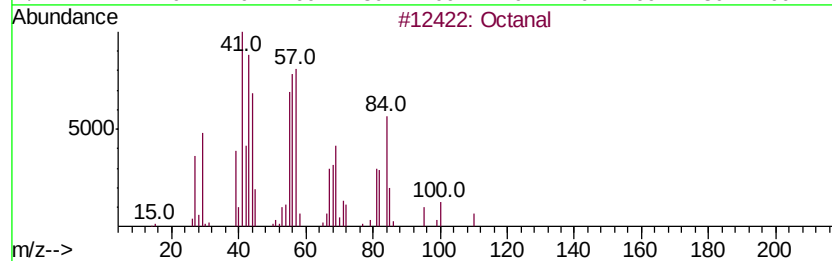
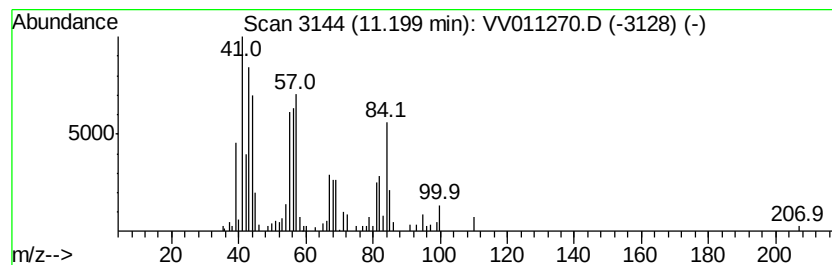
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Octanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	0.78 ug/L	69777	1,4-Dichlorobenzene-d4	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal		128	C8H16O	000124-13-0	91
2	Octanal		128	C8H16O	000124-13-0	91
3	Octanal		128	C8H16O	000124-13-0	90
4	Octanal		128	C8H16O	000124-13-0	87
5	Octanal		128	C8H16O	000124-13-0	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011270.D
Acq On : 07 Jun 2019 04:13
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

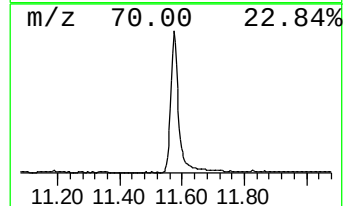
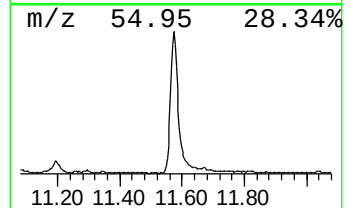
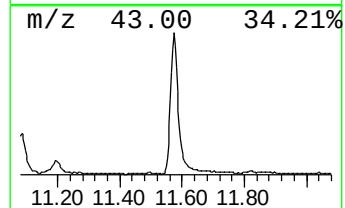
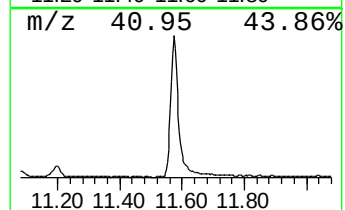
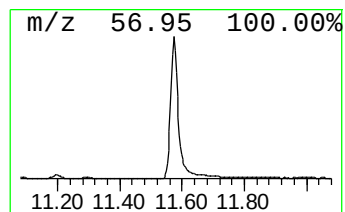
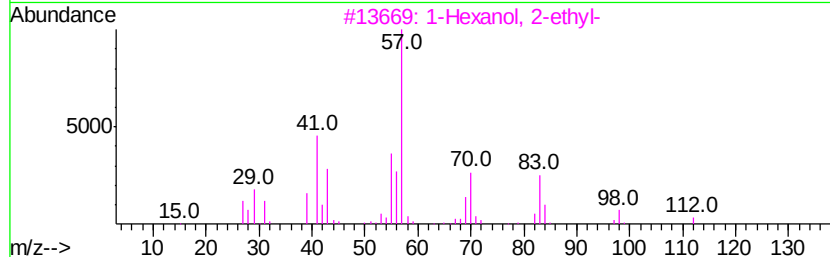
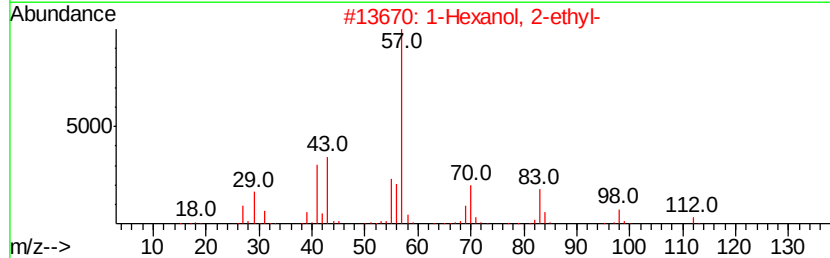
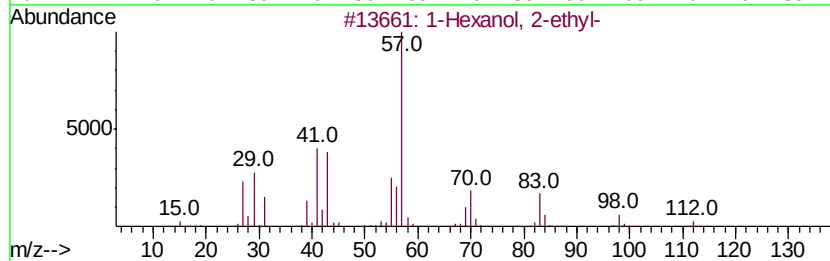
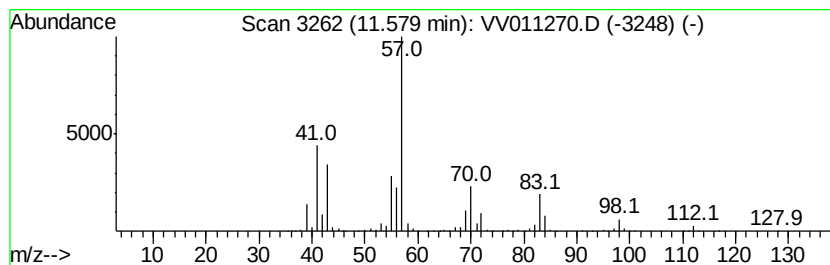
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	8.71 ug/L	780017	1,4-Dichlorobenzene-d4	11.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	72
4	1-Isobutoxy-2-ethylhexane	186 C12H26O	1000139-90-3	64
5	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011270.D
Acq On : 07 Jun 2019 04:13
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

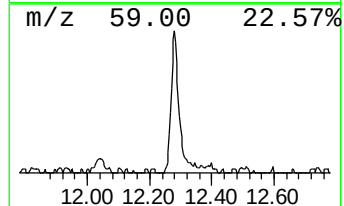
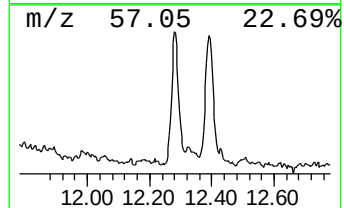
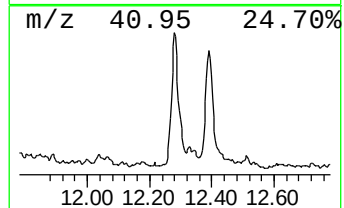
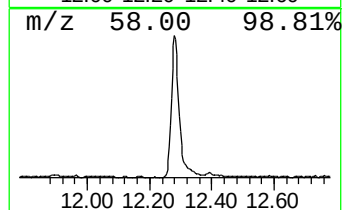
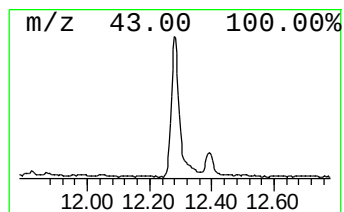
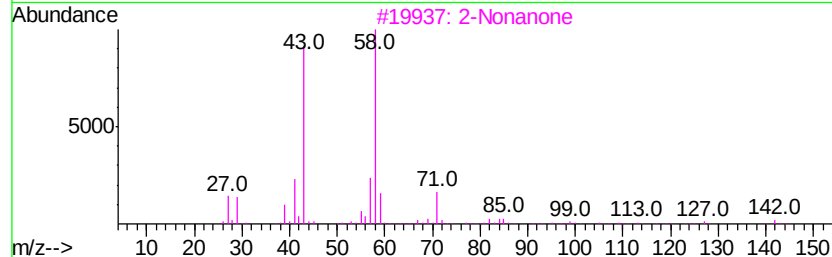
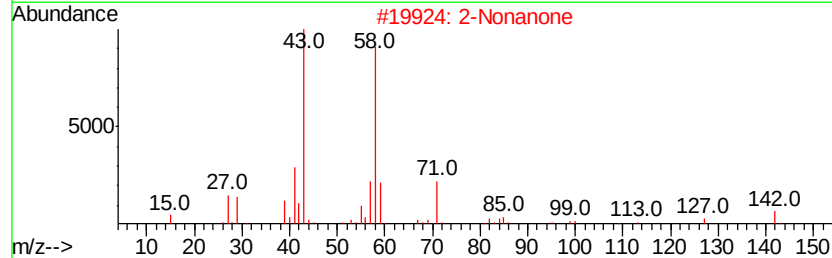
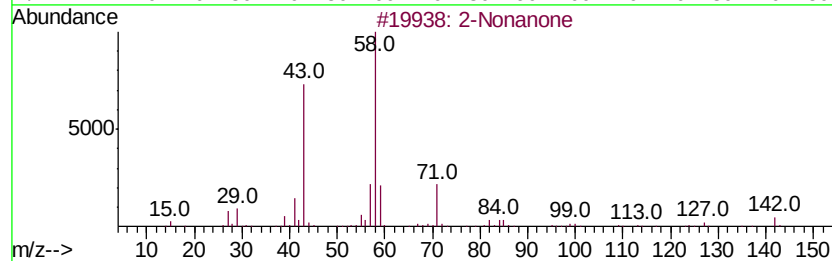
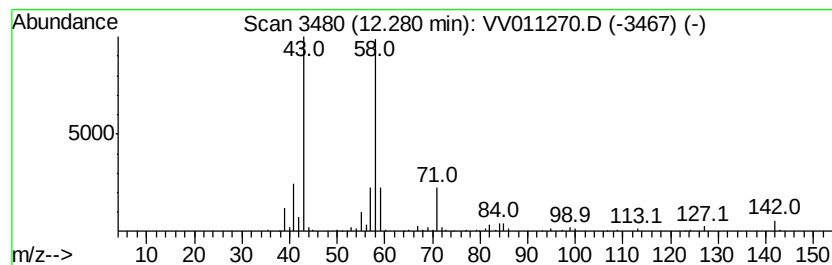
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 2-Nonanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
12.28	1.56 ug/L	139527	1,4-Dichlorobenzene-d4		11.30		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		Nonanone	142	C9H18O	000821-55-6	95
2	2		Nonanone	142	C9H18O	000821-55-6	91
3	2		Nonanone	142	C9H18O	000821-55-6	91
4	2		Nonanone	142	C9H18O	000821-55-6	91
5	2		Octanone	128	C8H16O	000111-13-7	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011270.D
Acq On : 07 Jun 2019 04:13
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P57

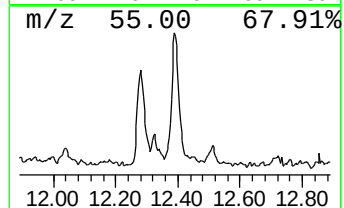
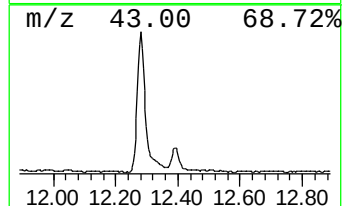
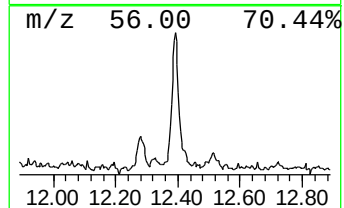
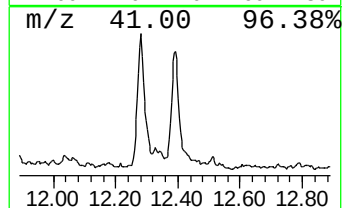
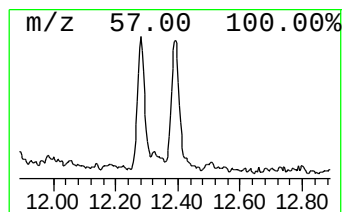
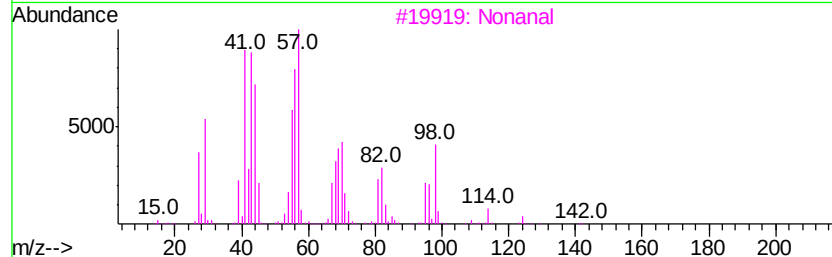
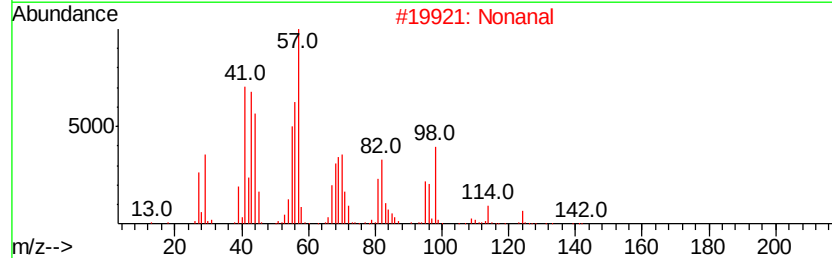
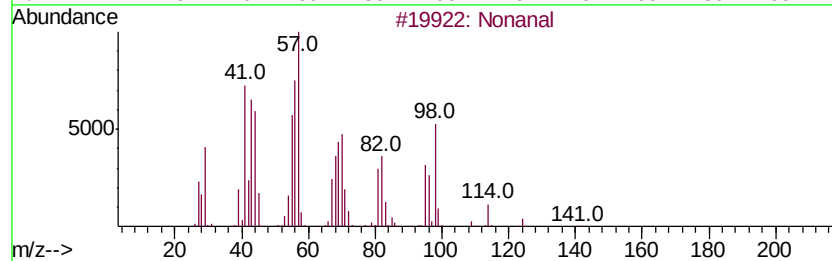
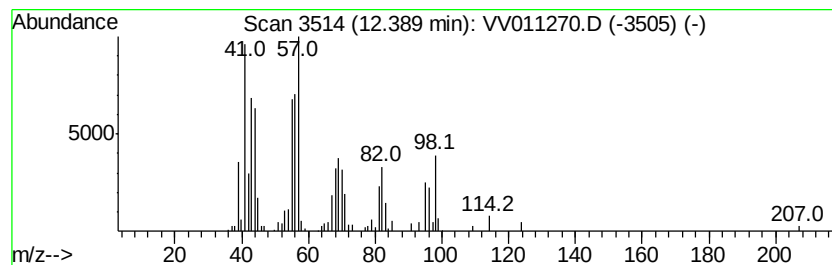
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Quant Title : TRACE VOA SOM01.0

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	0.72 ug/L	64867	1,4-Dichlorobenzene-d4	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	87
2	Nonanal		142	C9H18O	000124-19-6	86
3	Nonanal		142	C9H18O	000124-19-6	80
4	Nonanal		142	C9H18O	000124-19-6	64
5	2-Heptene		98	C7H14	000592-77-8	41



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011270.D
Acq On : 07 Jun 2019 04:13
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

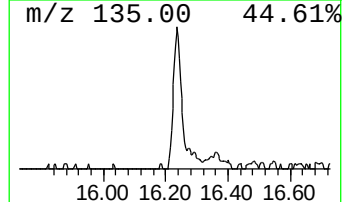
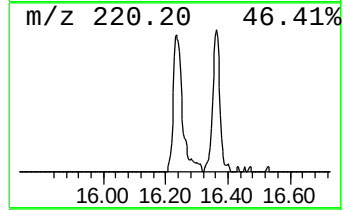
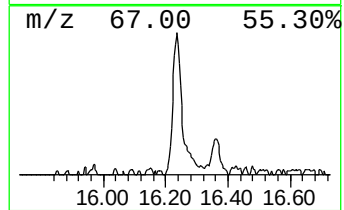
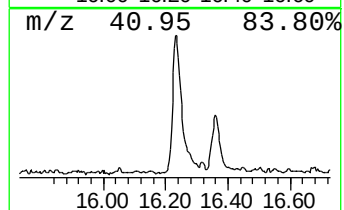
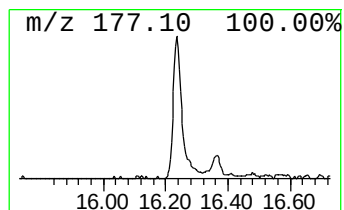
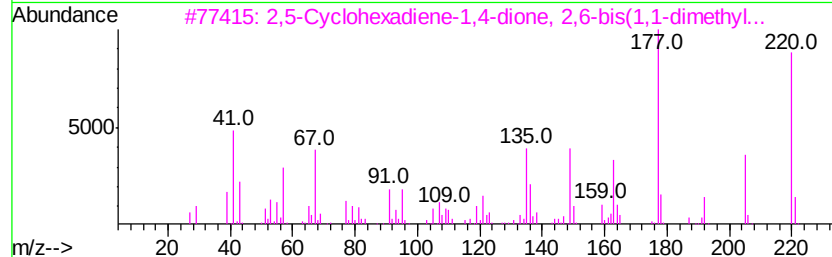
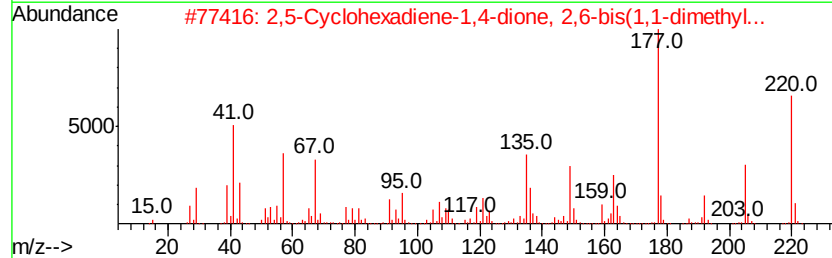
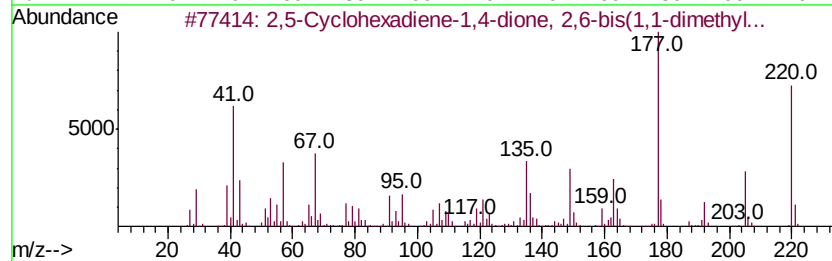
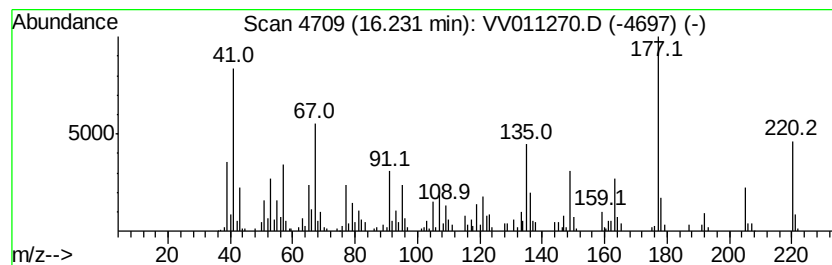
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.23	1.89 ug/L	169337	1,4-Dichlorobenzene-d4	11.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
4	6,8-Dioxabicyclo[3.2.1]octan-4-o...	222	C11H14N2O3	1000362-38-3	43
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011270.D
Acq On : 07 Jun 2019 04:13
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

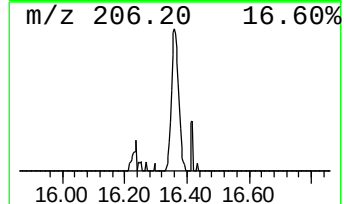
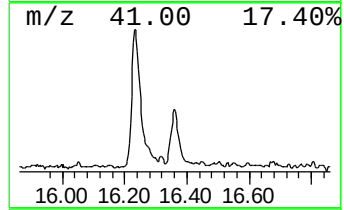
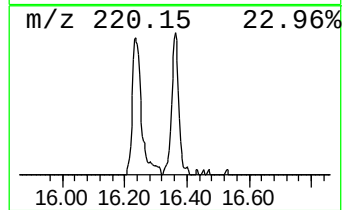
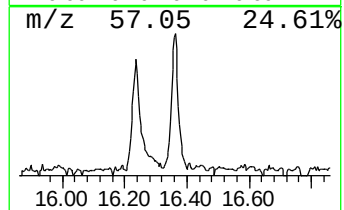
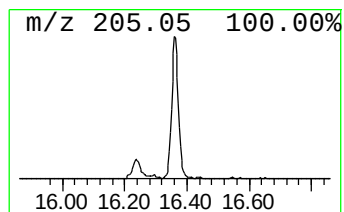
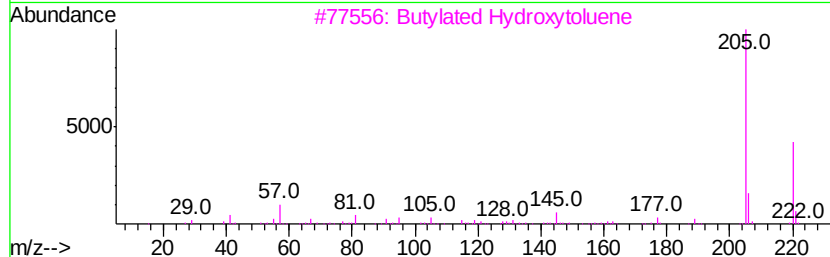
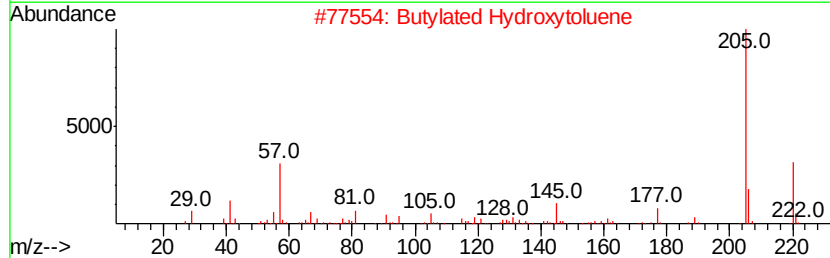
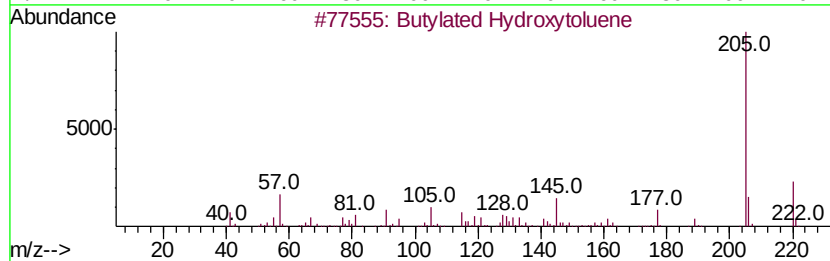
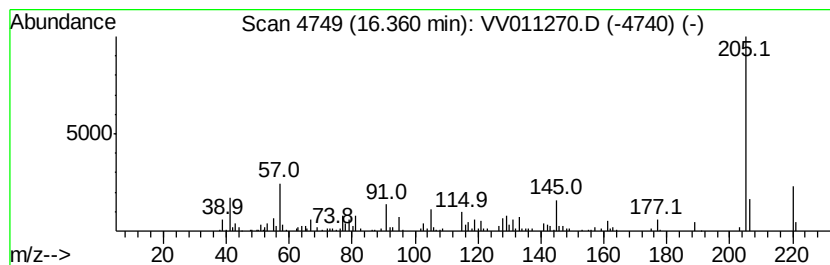
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ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 Butylated Hydroxytoluene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.36	1.00 ug/L	89472	1,4-Dichlorobenzene-d4	11.30		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	95
2	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	95
3	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	94
4	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	93
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 : VV011270.D
Acq On : 07 Jun 2019 04:13
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P57

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
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3-Pentanone, 2-me...	6.63	0.7	ug/L	53651	1	5.66	407820	5.0
5-t-Butyl-4-methy...	9.14	0.6	ug/L	57636	2	8.89	480633	5.0
2-Octanone	11.08	0.7	ug/L	63019	3	11.30	447936	5.0
Octanal	11.20	0.8	ug/L	69777	3	11.30	447936	5.0
1-Hexanol, 2-ethyl-	11.58	8.7	ug/L	780017	3	11.30	447936	5.0
2-Nonanone	12.28	1.6	ug/L	139527	3	11.30	447936	5.0
Nonanal	12.39	0.7	ug/L	64867	3	11.30	447936	5.0
2,5-Cyclohexadien...	16.23	1.9	ug/L	169337	3	11.30	447936	5.0
Butylated Hydroxy...	16.36	1.0	ug/L	89472	3	11.30	447936	5.0