

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017024.D
 Acq On : 22 Jun 2020 18:10
 Operator : SY/MD
 Sample : L3067-03
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXG0

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\SOMVTR061720WMA.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	4.376	1003	1022	1043	rBV	134697	337124	1.04%	0.292%
2	5.071	1222	1238	1252	rBV2	301044	755293	2.34%	0.655%
3	5.640	1397	1415	1435	rBV	231372	468338	1.45%	0.406%
4	6.093	1541	1556	1569	rBV2	167657	344363	1.07%	0.299%
5	6.344	1613	1634	1665	rBV	15514173	32141109	99.52%	27.862%
6	6.955	1809	1824	1834	rBV	359175	650083	2.01%	0.564%
7	7.164	1871	1889	1920	rBV	16188036	31050654	96.15%	26.917%
8	7.338	1933	1943	1959	rVB	360130	613955	1.90%	0.532%
9	8.109	2170	2183	2206	rBV2	350869	630470	1.95%	0.547%
10	8.871	2411	2420	2431	rBV	324036	492942	1.53%	0.427%
11	8.990	2446	2457	2467	rBV	415733	660857	2.05%	0.573%
12	9.762	2680	2697	2728	rBV	19159778	32295194	100.00%	27.996%
13	10.035	2772	2782	2801	rBV	503800	970348	3.00%	0.841%
14	10.376	2873	2888	2910	rVV	2968764	4470754	13.84%	3.876%
15	10.502	2913	2927	2954	rVB	2629016	4326162	13.40%	3.750%
16	11.116	3106	3118	3136	rVB5	209490	435585	1.35%	0.378%
17	11.270	3156	3166	3179	rVB	369014	550843	1.71%	0.478%
18	11.550	3242	3253	3273	rBV	320426	618366	1.91%	0.536%
19	11.646	3273	3283	3303	rVB	393330	654958	2.03%	0.568%
20	11.942	3362	3375	3385	rBV	1865786	2890804	8.95%	2.506%

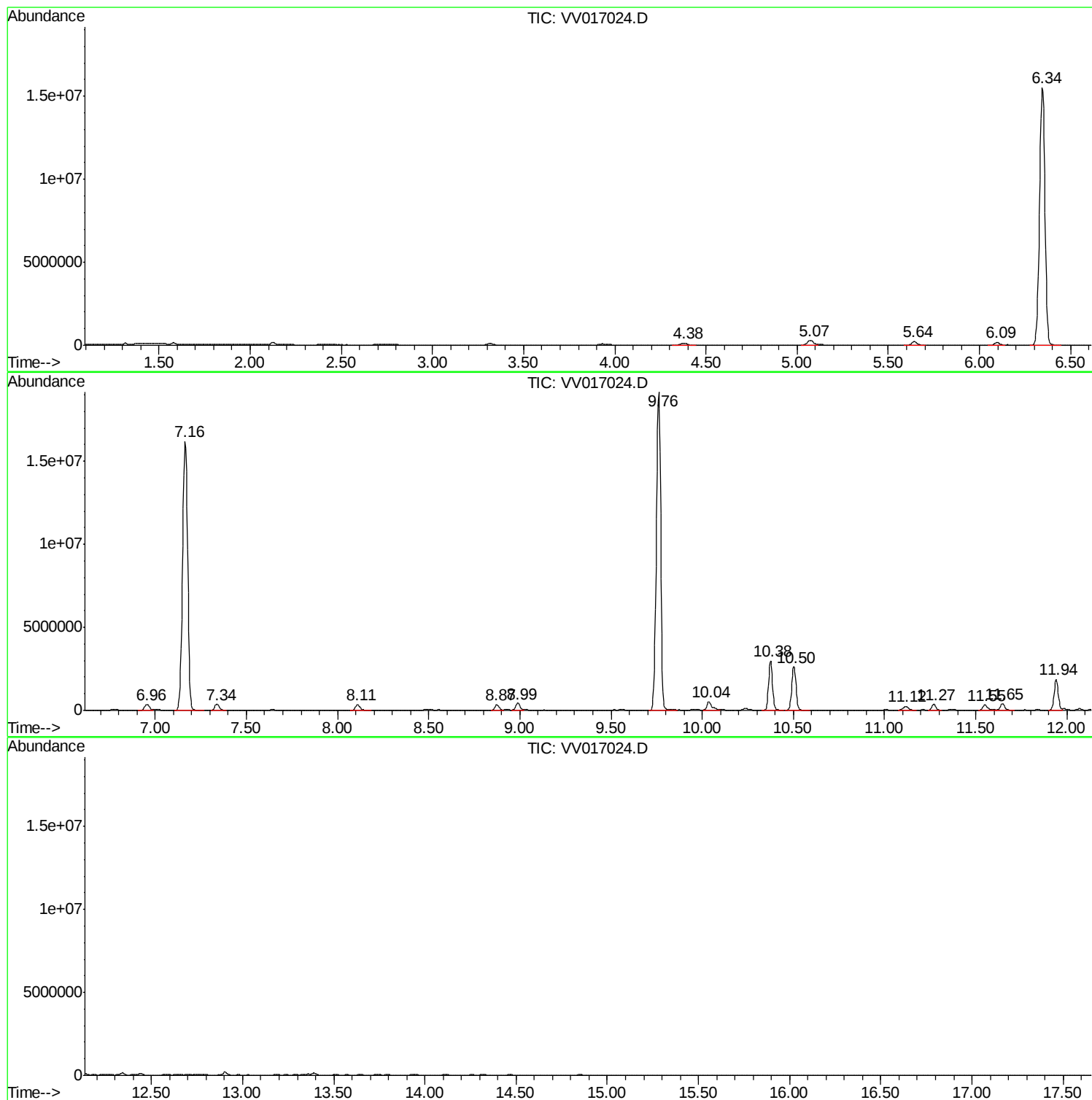
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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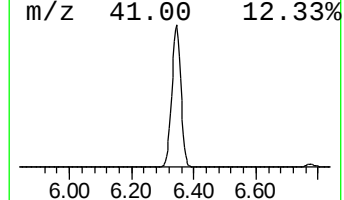
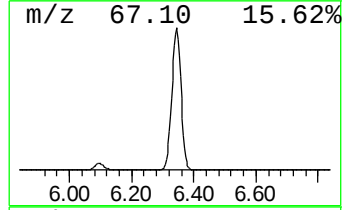
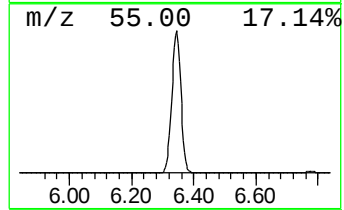
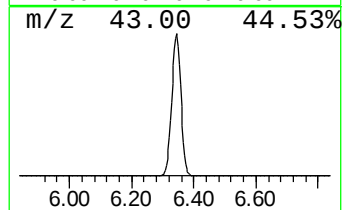
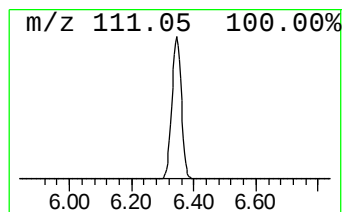
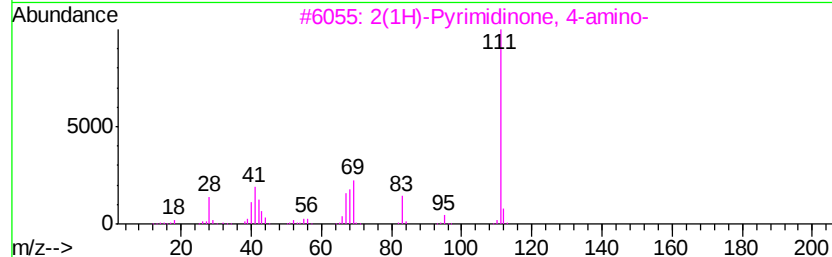
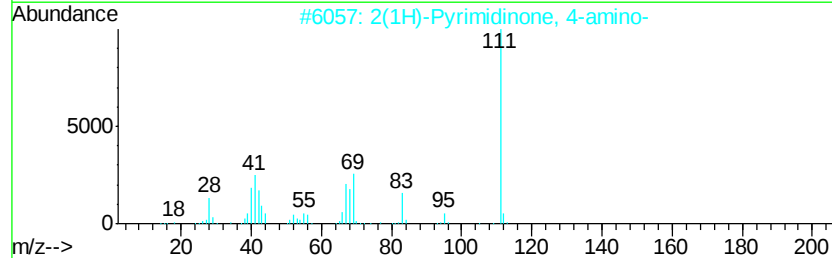
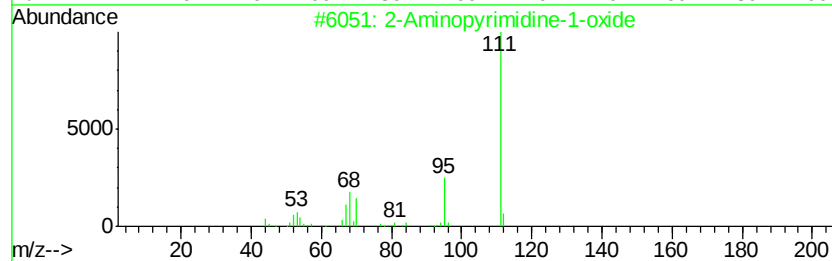
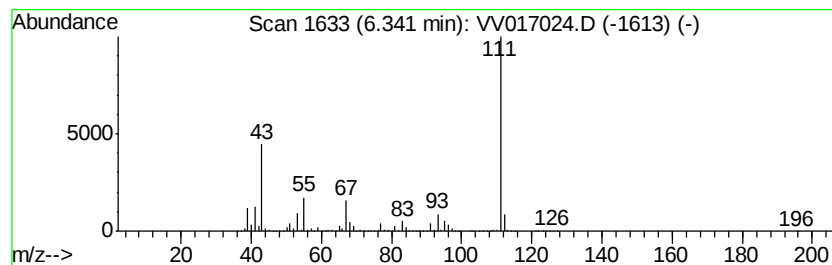
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Aminopyrimidine-1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	343.14 ug/L	32141100	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	72
2		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
3		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
4		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	45
5		2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N2O	016867-04-2	42



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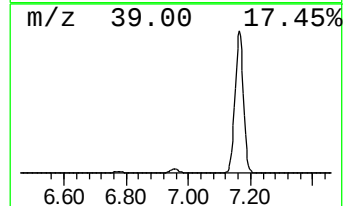
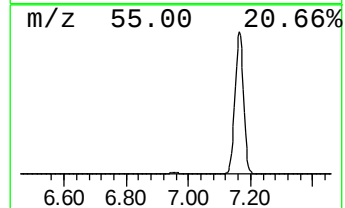
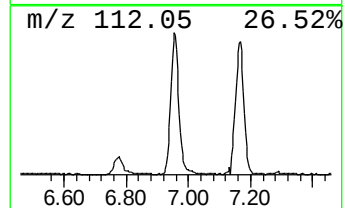
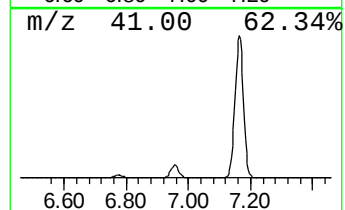
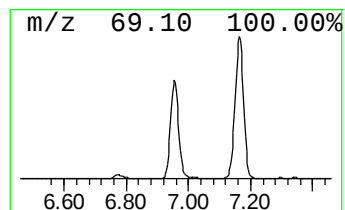
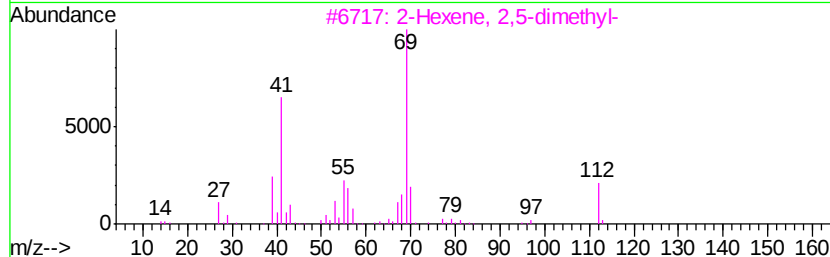
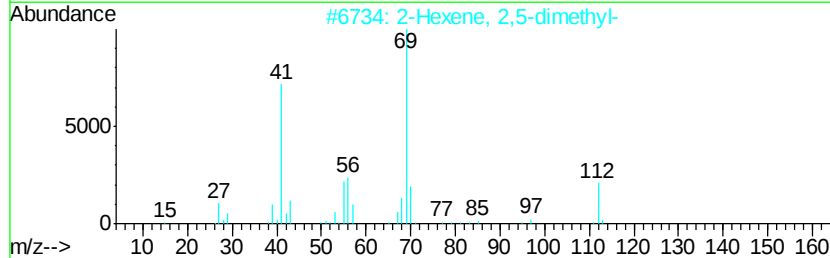
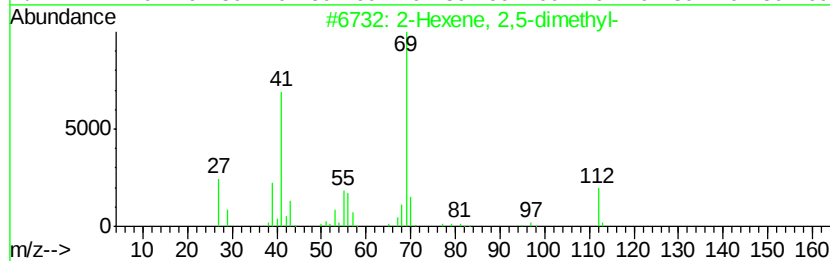
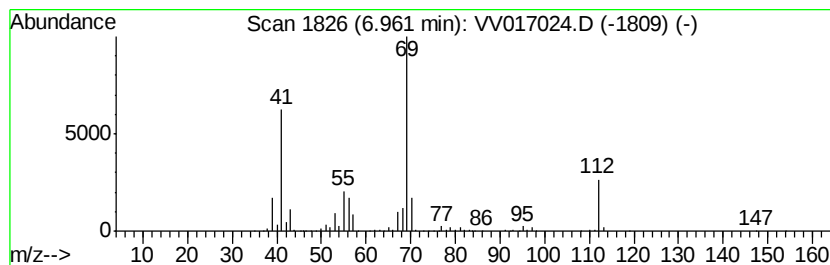
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	6.94 ug/L	650083	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	91
2		2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	91
3		2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	91
4		2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	91
5		3-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	80



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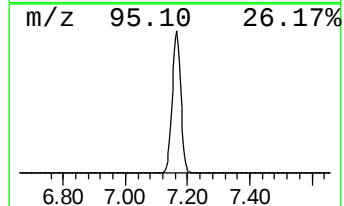
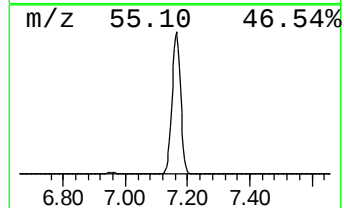
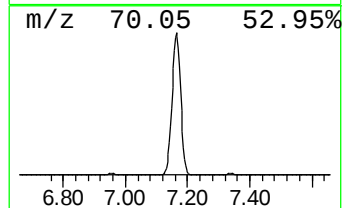
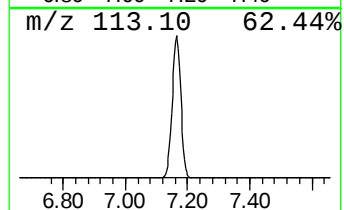
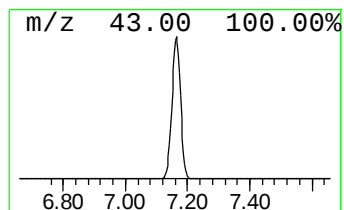
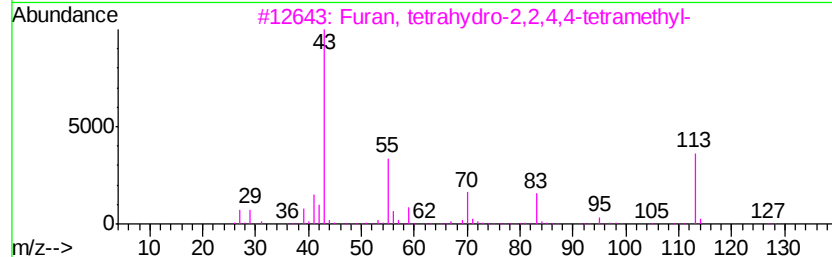
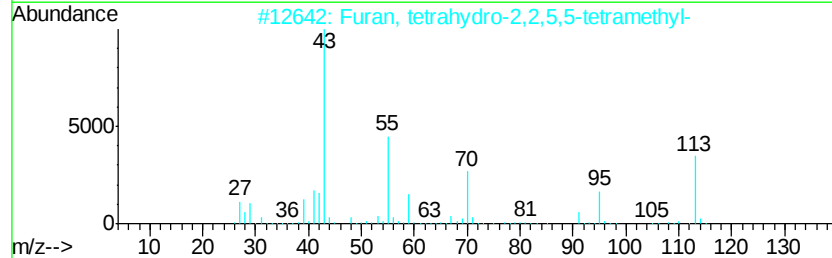
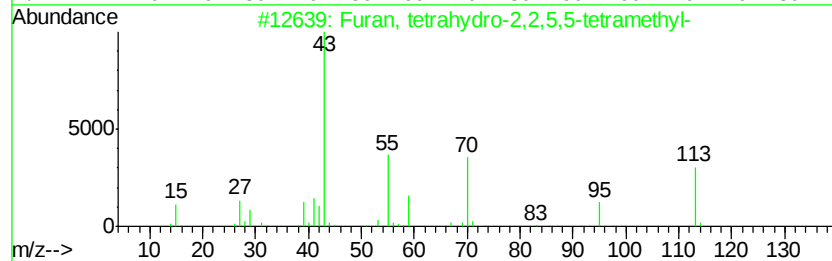
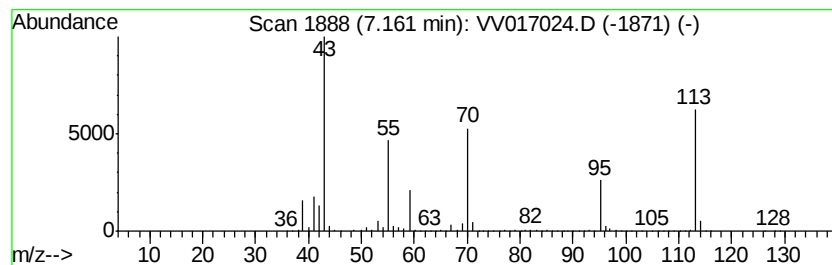
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	331.50 ug/L	31050700	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83		
2	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	56		
3	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53		
4	1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	47		
5	Propanone-1, 3-(4-methylpiperazi...	308	C20H24N2O	053756-76-6	43		



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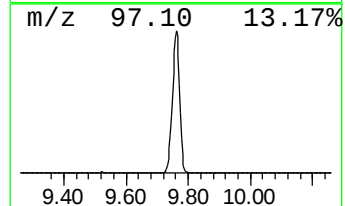
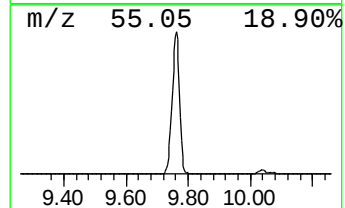
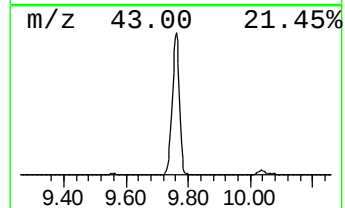
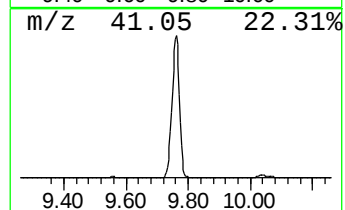
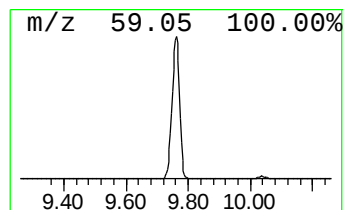
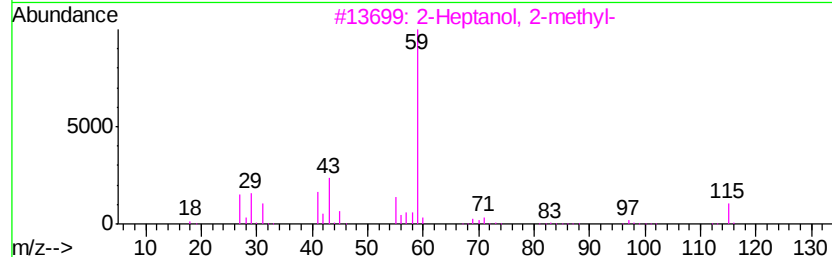
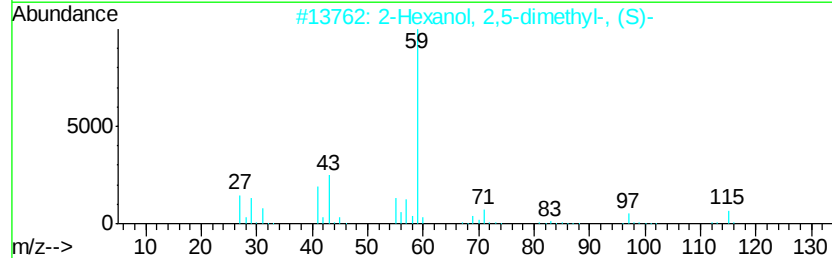
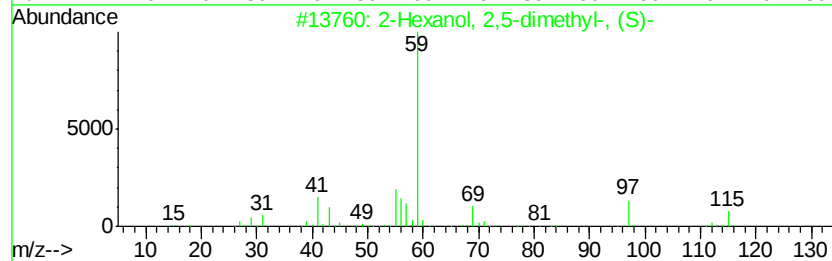
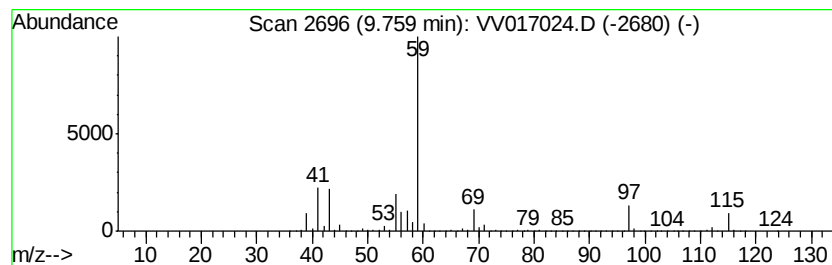
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	327.58 ug/L	32295200	Chlorobenzene-d5	8.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90	
2	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	78	
3	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	45	
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42	
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	42	



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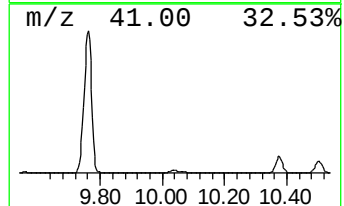
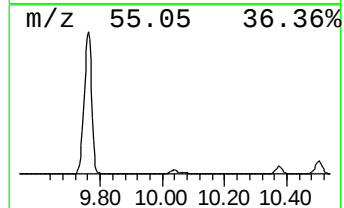
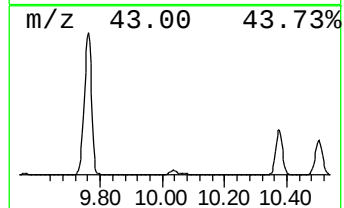
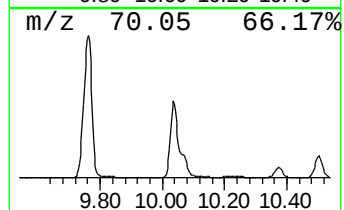
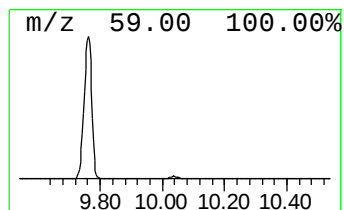
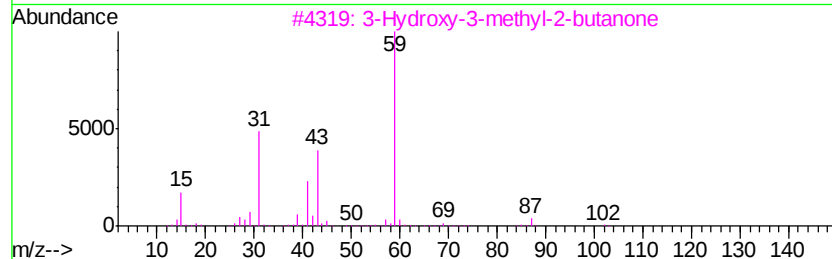
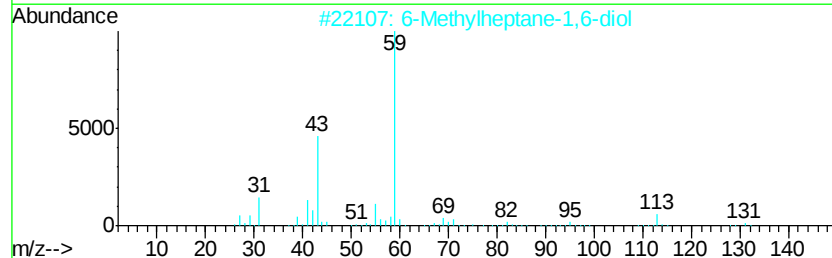
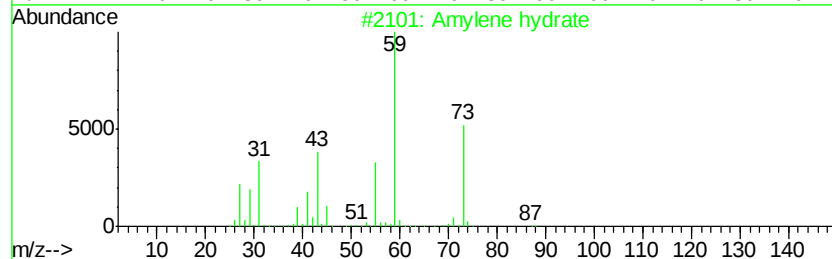
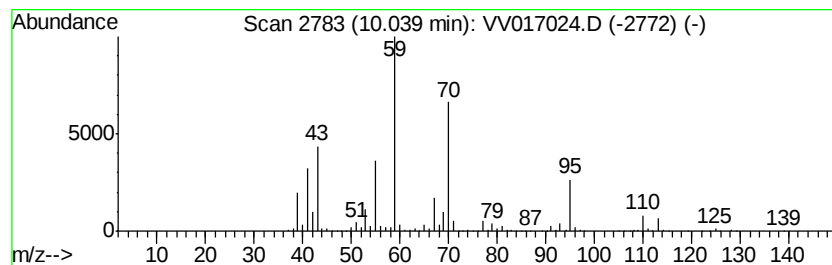
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.04	9.84 ug/L	970348	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Amylene hydrate	88	C5H12O	000075-85-4	25
2		6-Methylheptane-1,6-diol	146	C8H18O2	005392-57-4	25
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5		7-Octen-2-ol, 2-methyl-6-methylene-	154	C10H18O	000543-39-5	17



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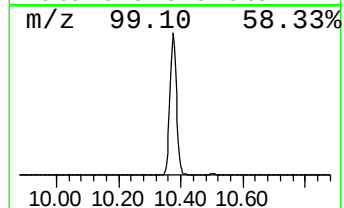
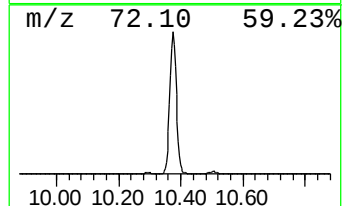
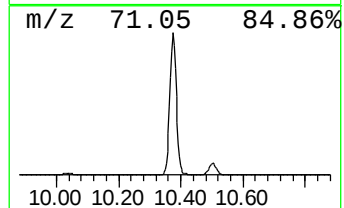
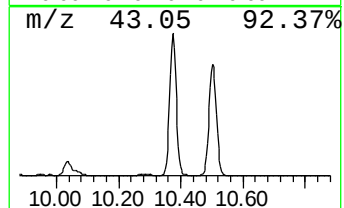
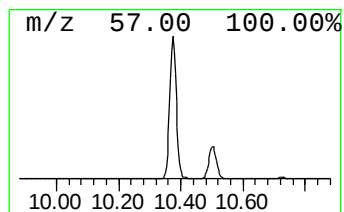
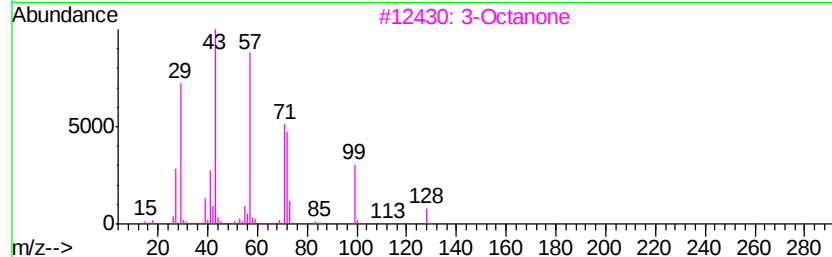
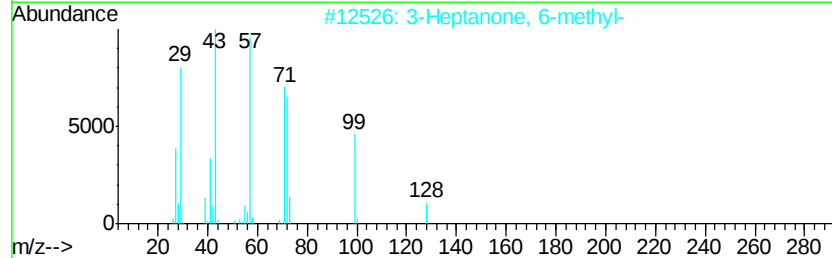
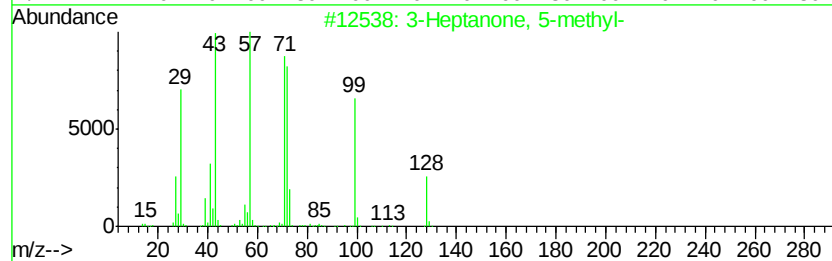
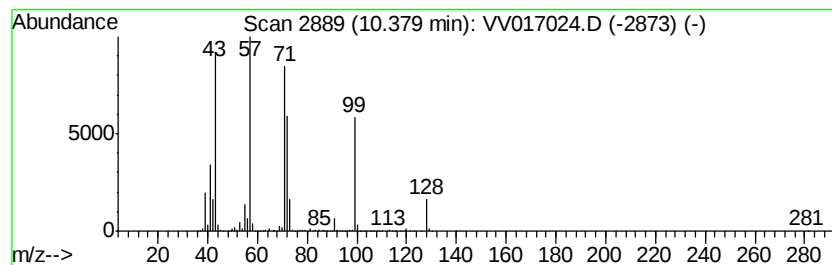
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 3-Heptanone, 5-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	40.58 ug/L	4470750	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	91
2		3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	90
3		3-Octanone	128	C8H16O	000106-68-3	86
4		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	81
5		3-Octanone	128	C8H16O	000106-68-3	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV062320\
Data File : VV017024.D
Acq On : 22 Jun 2020 18:10
Operator : SY/MD
Sample : L3067-03
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXG0

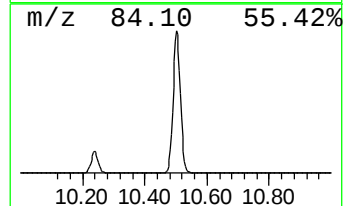
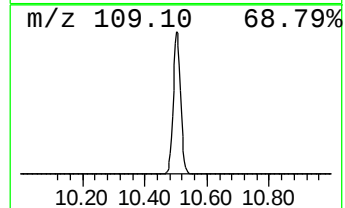
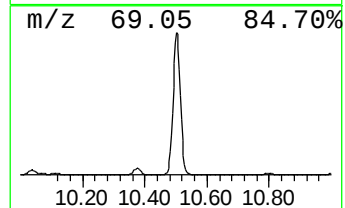
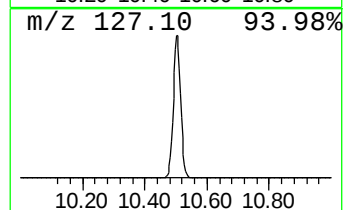
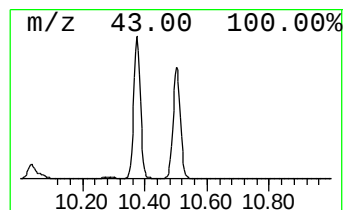
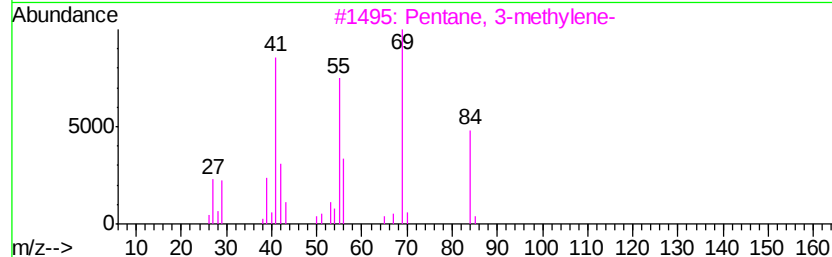
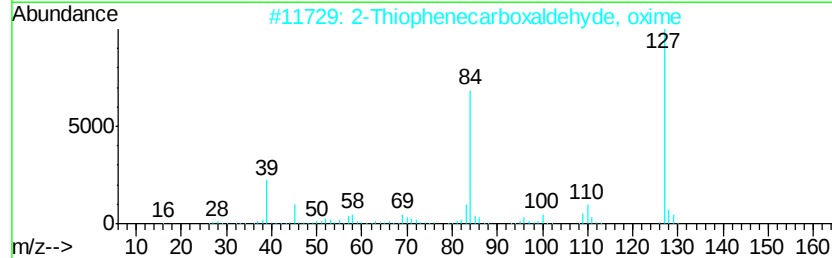
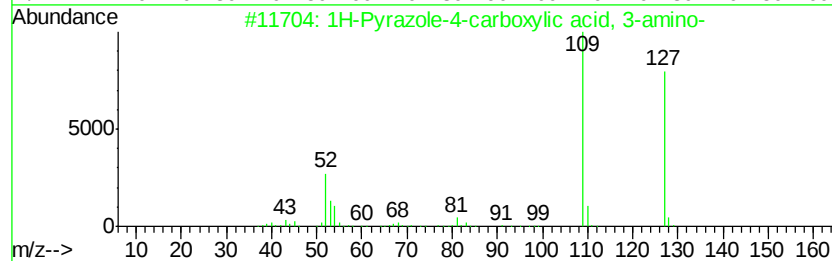
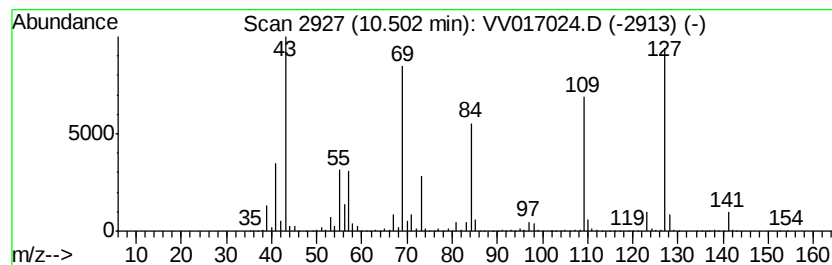
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	39.27 ug/L	4326160	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
2		2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
3		Pentane, 3-methylene-	84	C6H12	000760-21-4	27
4		2-Nonen-4-one	140	C9H16O	032064-72-5	27
5		Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV062320\
Data File : VV017024.D
Acq On : 22 Jun 2020 18:10
Operator : SY/MD
Sample : L3067-03
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXG0

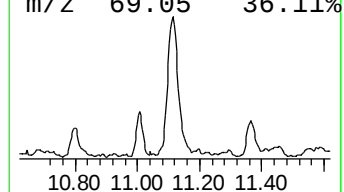
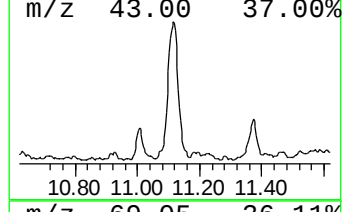
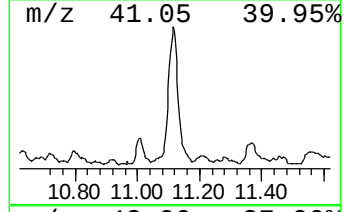
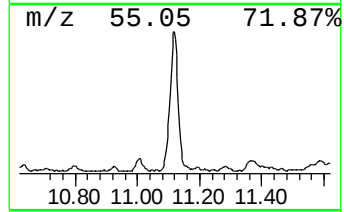
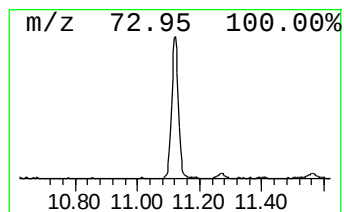
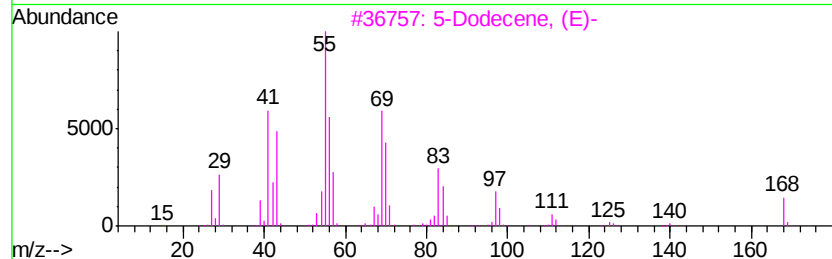
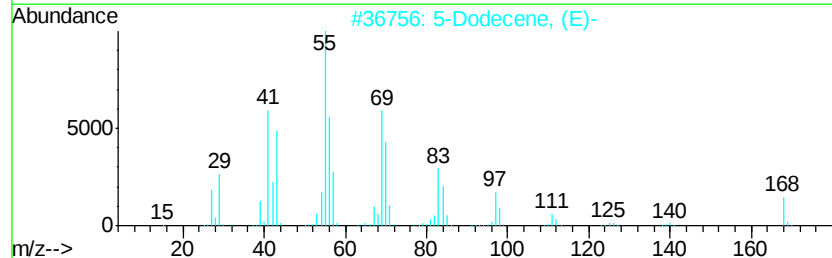
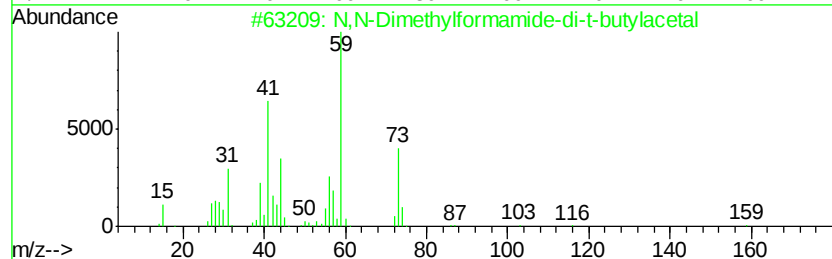
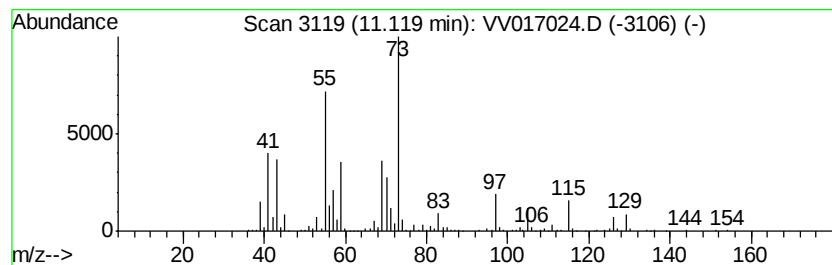
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 unknown-03 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	3.95 ug/L	435585	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N,N-Dimethylformamide-di-t-butyl...	203	C11H25NO2	036805-97-7	22
2		5-Dodecene, (E)-	168	C12H24	007206-16-8	22
3		5-Dodecene, (E)-	168	C12H24	007206-16-8	22
4		Trimethyl(n-pentyl)silane	144	C8H20Si	001641-49-2	16
5		4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	14



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV062320\
Data File : VV017024.D
Acq On : 22 Jun 2020 18:10
Operator : SY/MD
Sample : L3067-03
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
BFXG0

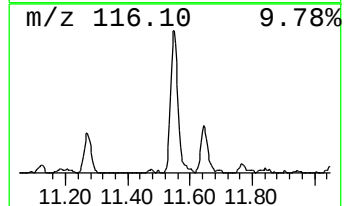
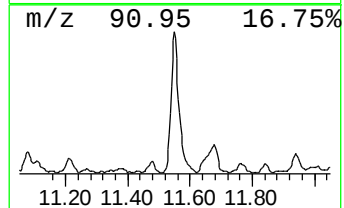
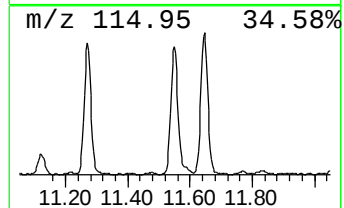
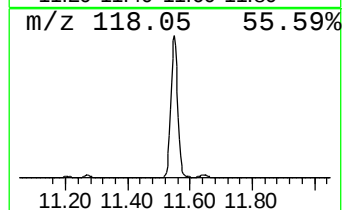
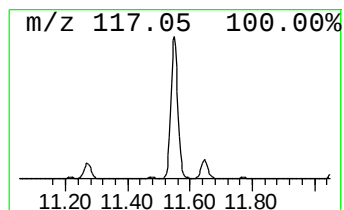
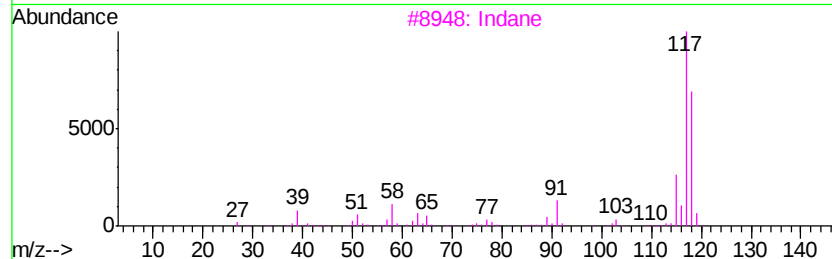
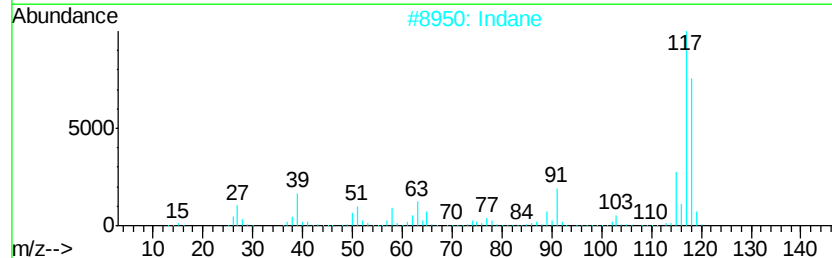
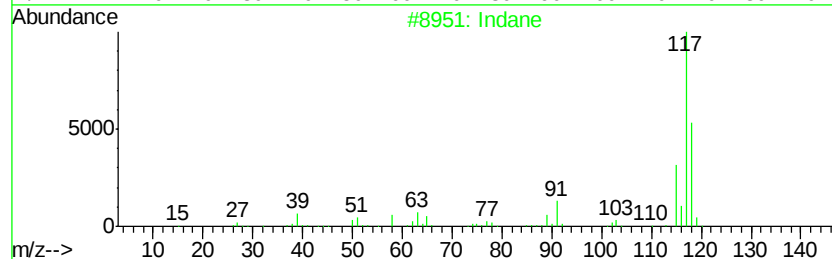
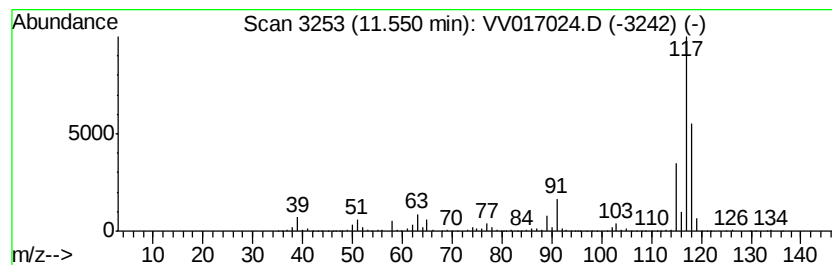
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	5.61 ug/L	618366	1,4-Dichlorobenzene-d4	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane		118	C9H10	000496-11-7	95
2	Indane		118	C9H10	000496-11-7	90
3	Indane		118	C9H10	000496-11-7	87
4	Benzene, 1-ethenyl-4-methyl-		118	C9H10	000622-97-9	83
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...		118	C9H10	1000191-13-7	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV062320\
Data File : VV017024.D
Acq On : 22 Jun 2020 18:10
Operator : SY/MD
Sample : L3067-03
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXG0

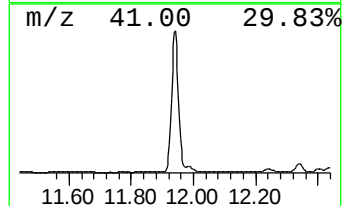
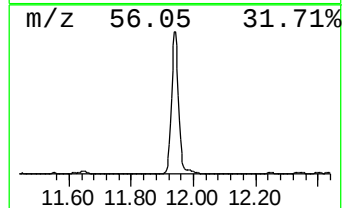
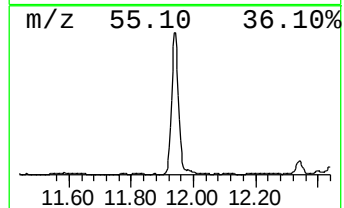
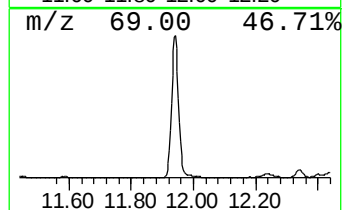
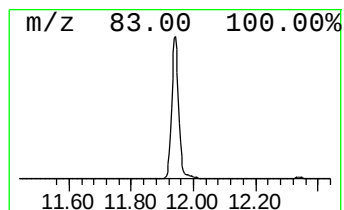
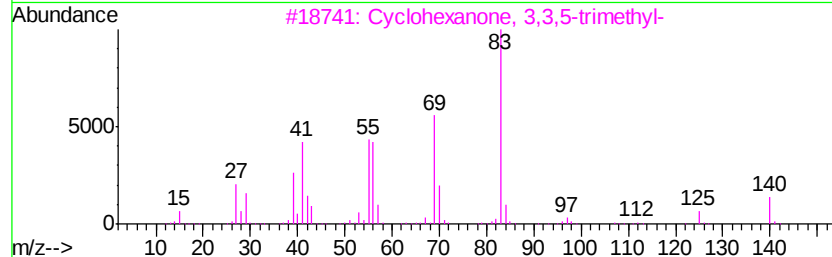
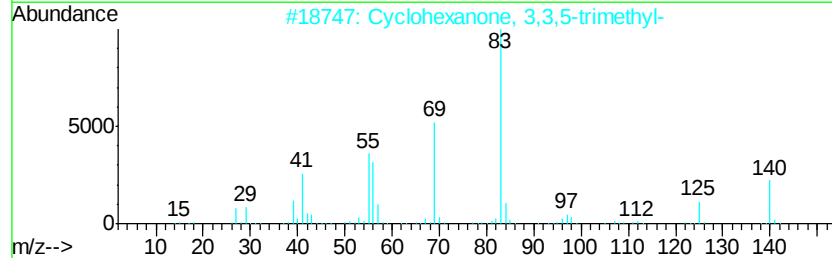
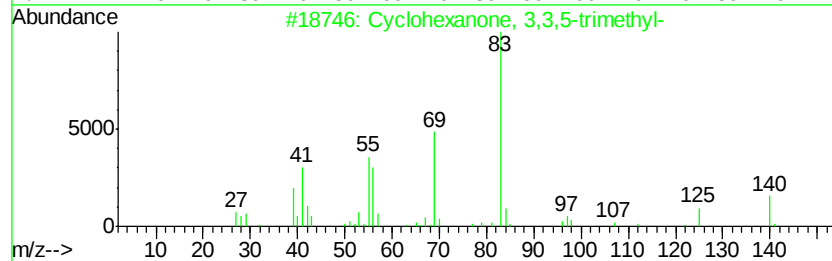
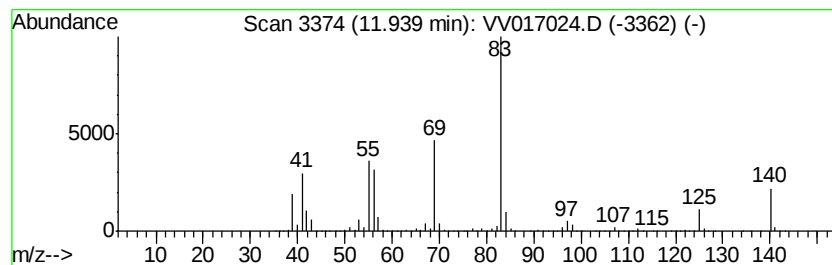
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Cyclohexanone, 3,3,5-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	26.24 ug/L	2890800	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	96
2		Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	96
3		Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
4		Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	86
5		1,3-Cyclohexanedione, 5,5-dimethyl-	140	C8H12O2	000126-81-8	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV062320\
 Data File : VV017024.D
 Acq On : 22 Jun 2020 18:10
 Operator : SY/MD
 Sample : L3067-03
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXG0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.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
2-Aminopyrimidine...	6.34	343.1	ug/L	32141100	1	5.64	468338	5.0
(DEL) Alkane: Str...	6.96	6.9	ug/L	650083	1	5.64	468338	5.0
Furan, tetrahydro...	7.16	331.5	ug/L	31050700	1	5.64	468338	5.0
2-Hexanol, 2,5-di...	9.76	327.6	ug/L	32295200	2	8.87	492942	5.0
unknown-01	10.04	9.8	ug/L	970348	2	8.87	492942	5.0
3-Heptanone, 5-me...	10.38	40.6	ug/L	4470750	3	11.27	550843	5.0
unknown-02	10.50	39.3	ug/L	4326160	3	11.27	550843	5.0
unknown-03	11.12	4.0	ug/L	435585	3	11.27	550843	5.0
Indane	11.55	5.6	ug/L	618366	3	11.27	550843	5.0
Cyclohexanone, 3,...	11.94	26.2	ug/L	2890800	3	11.27	550843	5.0