

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV072820\
 Data File : VV017709.D
 Acq On : 28 Jul 2020 17:05
 Operator : SY/MD
 Sample : L3470-01
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 H0AE4

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\SOMVTR072320WMA.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	1.315	62	70	91	rVB	488073	502591	3.17%	2.057%
2	1.473	112	119	136	rBV	151614	263785	1.66%	1.080%
3	2.119	312	320	337	rVB3	111839	183446	1.16%	0.751%
4	3.933	865	884	948	rBV	6513633	15845526	100.00%	64.866%
5	4.373	1006	1021	1043	rBV	78878	188602	1.19%	0.772%
6	5.068	1220	1237	1260	rBV4	167840	406306	2.56%	1.663%
7	5.640	1402	1415	1437	rBV2	176193	350830	2.21%	1.436%
8	5.933	1492	1506	1532	rBV	911618	1762230	11.12%	7.214%
9	6.093	1543	1556	1581	rVB2	88449	184256	1.16%	0.754%
10	7.338	1931	1943	1958	rBV	192863	336706	2.12%	1.378%
11	8.119	2176	2186	2212	rBV2	128202	274025	1.73%	1.122%
12	8.260	2219	2230	2260	rBV	586116	1002625	6.33%	4.104%
13	8.871	2408	2420	2433	rBV	268310	448516	2.83%	1.836%
14	9.830	2705	2718	2744	rVB3	151192	271444	1.71%	1.111%
15	10.955	3060	3068	3082	rVB	204449	306455	1.93%	1.255%
16	11.058	3091	3100	3121	rVB3	96552	184041	1.16%	0.753%
17	11.170	3121	3135	3148	rBV3	184156	300564	1.90%	1.230%
18	11.270	3158	3166	3183	rVB	332280	512794	3.24%	2.099%
19	11.646	3268	3283	3295	rBV	229070	373980	2.36%	1.531%
20	12.026	3393	3401	3421	rBV2	95038	159851	1.01%	0.654%
21	12.392	3491	3515	3533	rVB	293484	569564	3.59%	2.332%

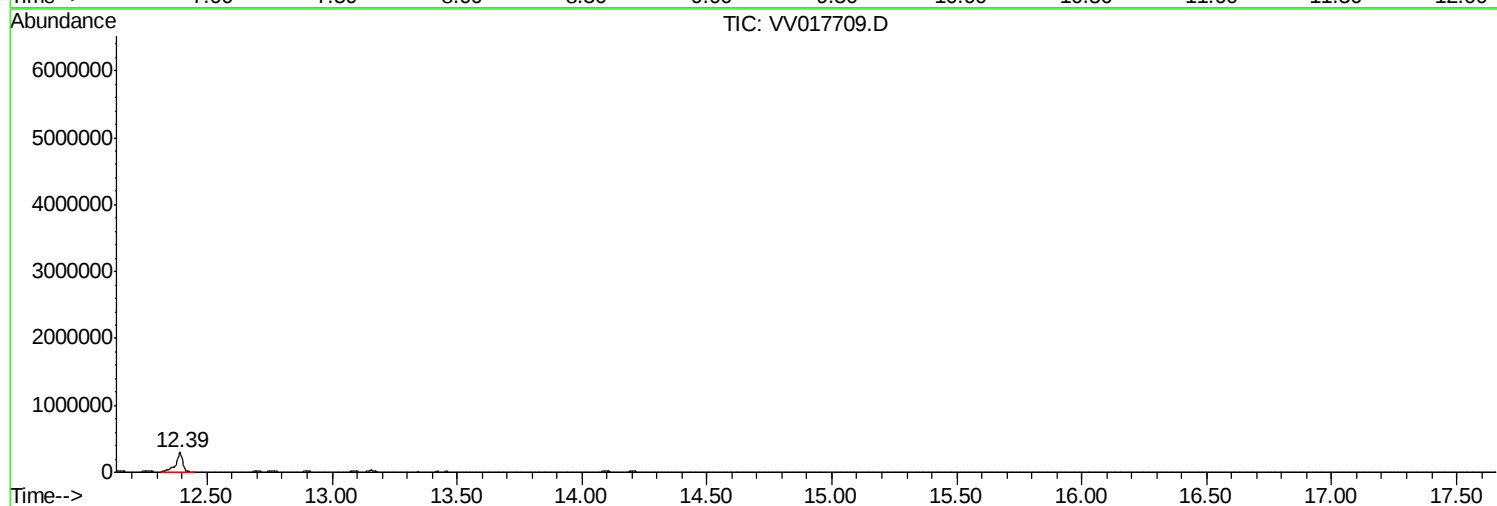
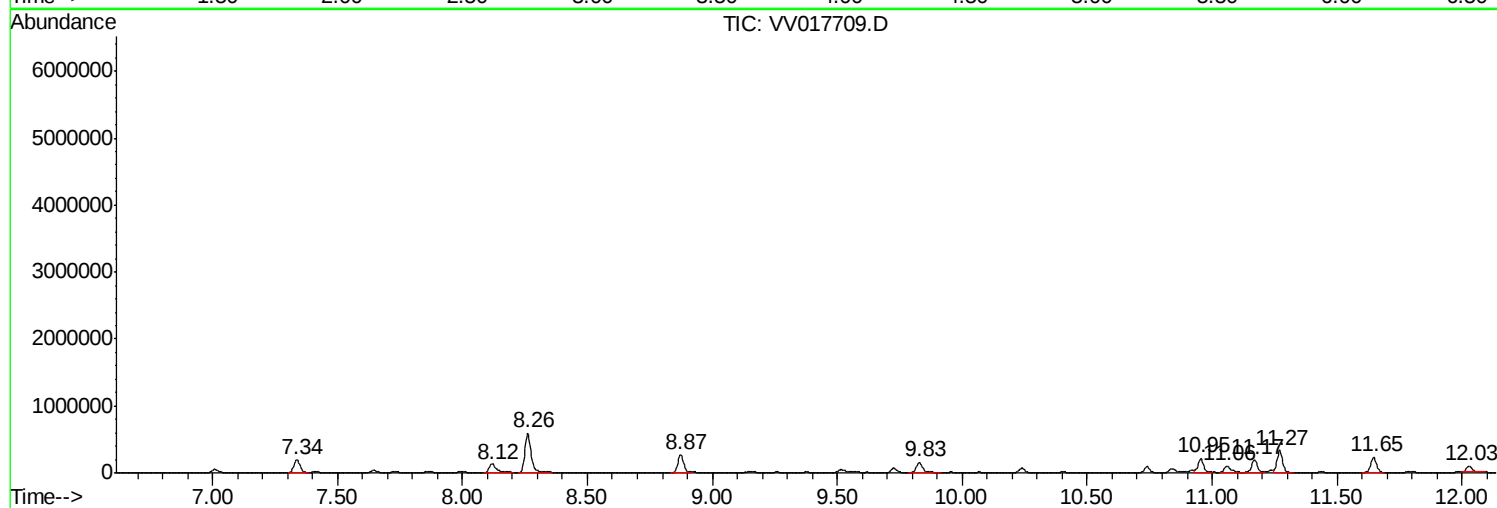
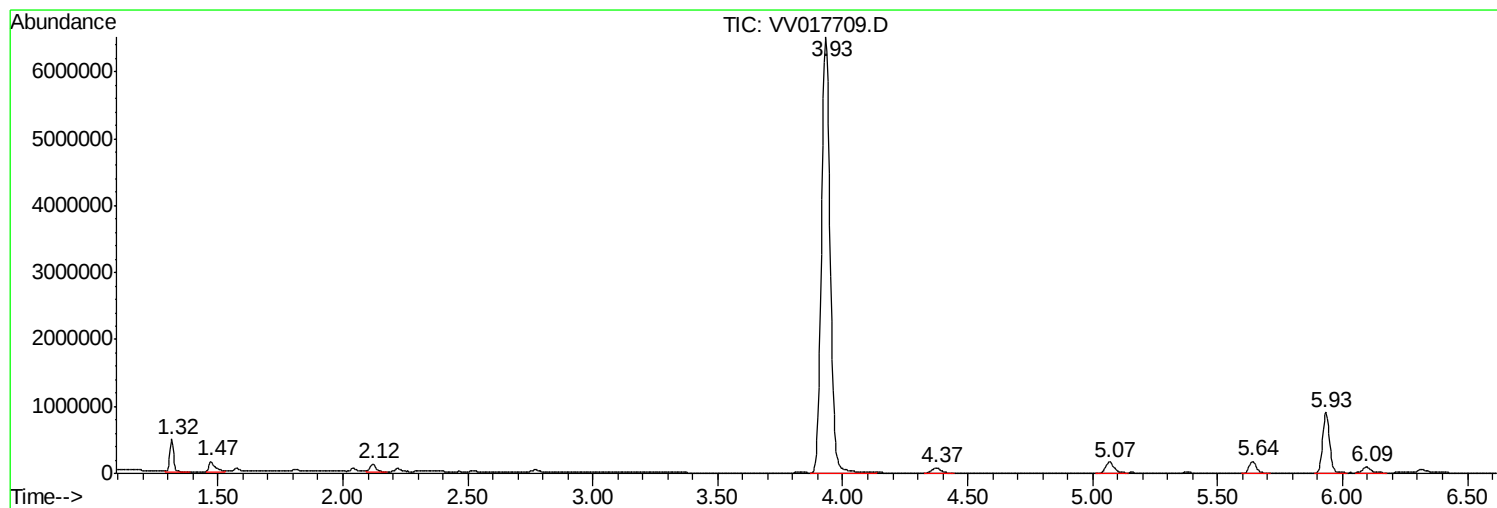
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Quant Title : TRACE VOA SOM01.0

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



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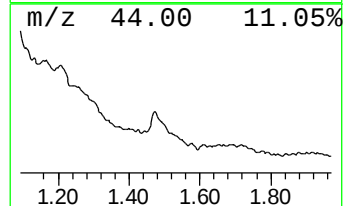
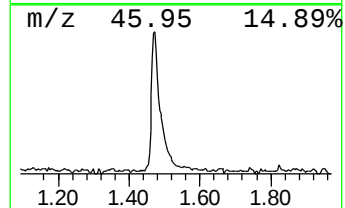
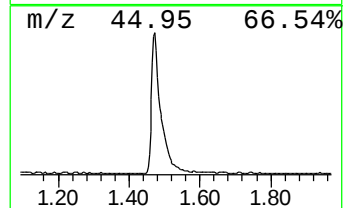
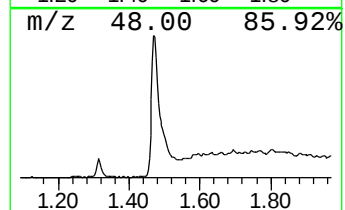
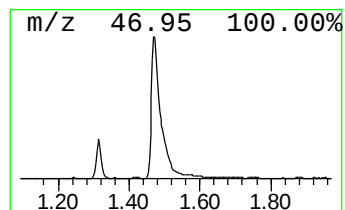
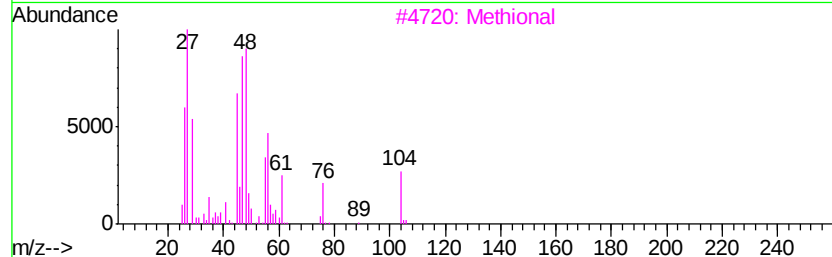
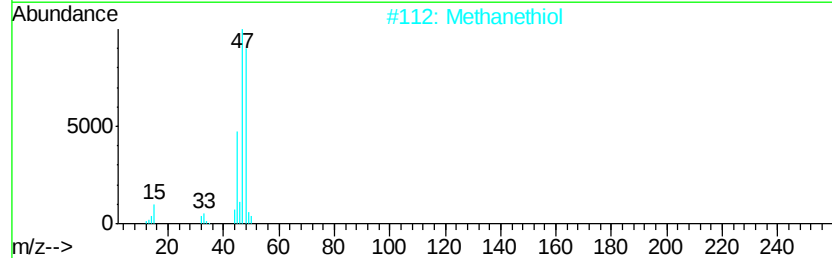
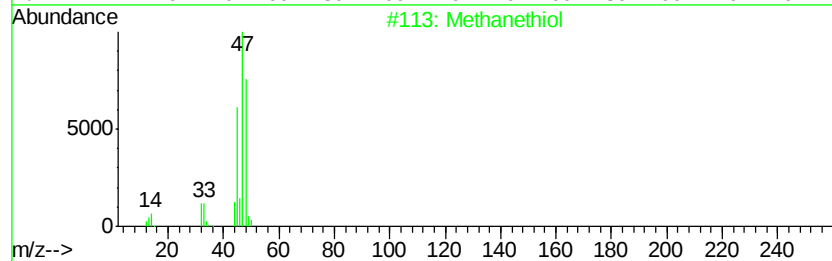
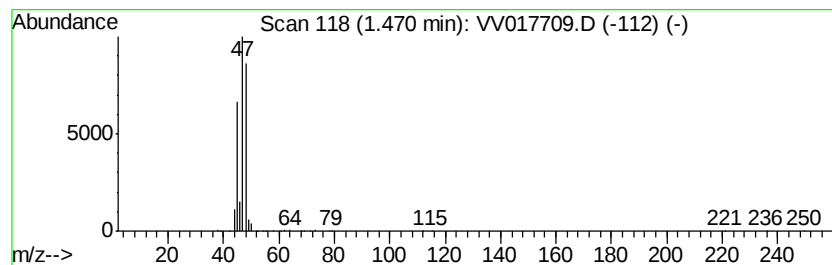
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	3.76 ug/L	263785	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	91
2		Methanethiol	48	CH4S	000074-93-1	90
3		Methional	104	C4H8OS	003268-49-3	56
4		Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
5		Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9



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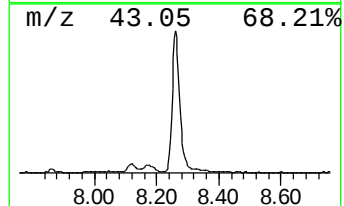
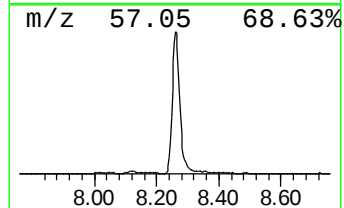
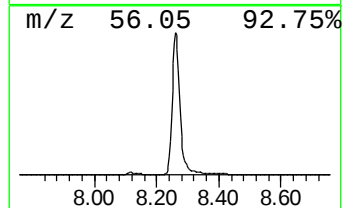
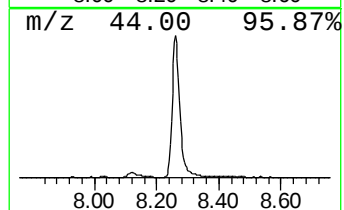
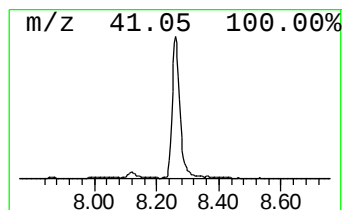
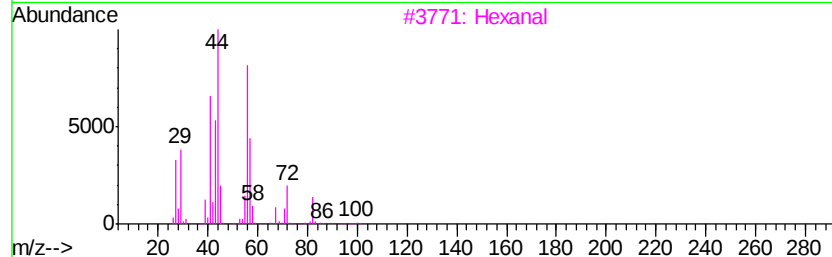
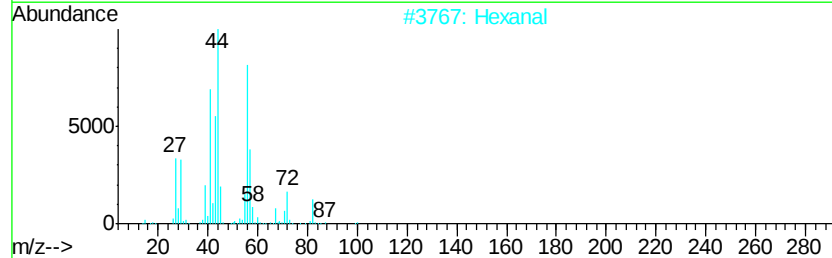
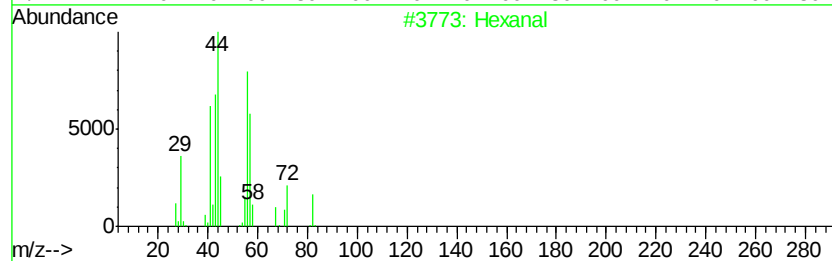
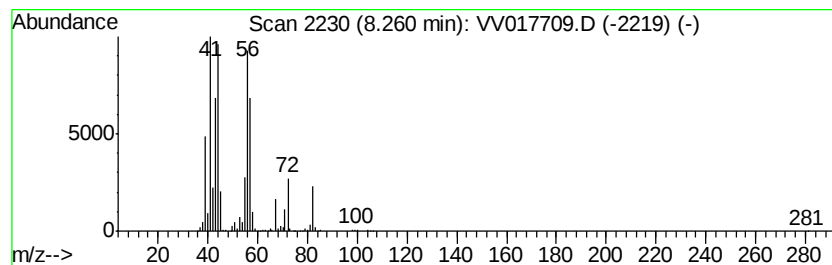
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 Quant Title : TRACE VOA SOM01.0

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

 Peak Number 2 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	11.18 ug/L	1002630	Chlorobenzene-d5	8.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal		100	C6H12O	000066-25-1	64
2	Hexanal		100	C6H12O	000066-25-1	64
3	Hexanal		100	C6H12O	000066-25-1	59
4	Hexanal		100	C6H12O	000066-25-1	53
5	2,2-Dimethyl-3-hydroxypropionald...		102	C5H10O2	000597-31-9	37



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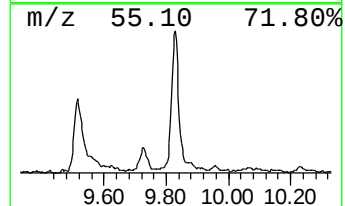
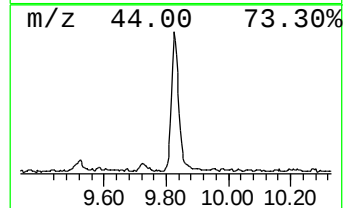
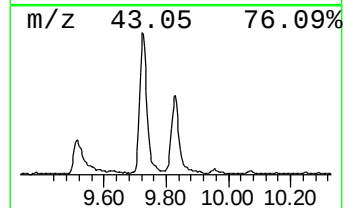
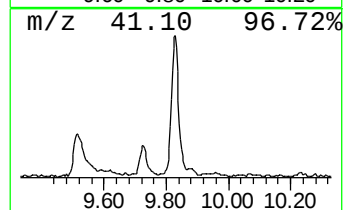
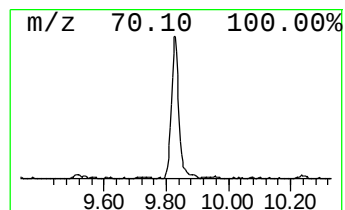
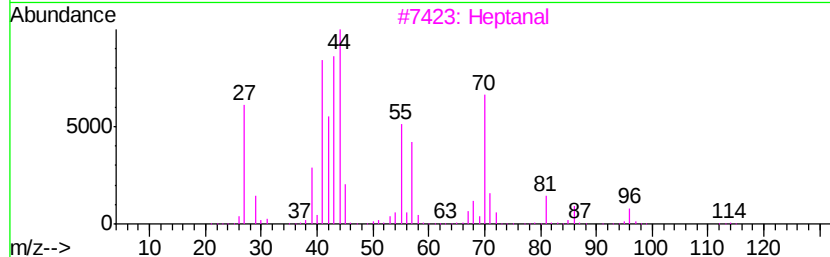
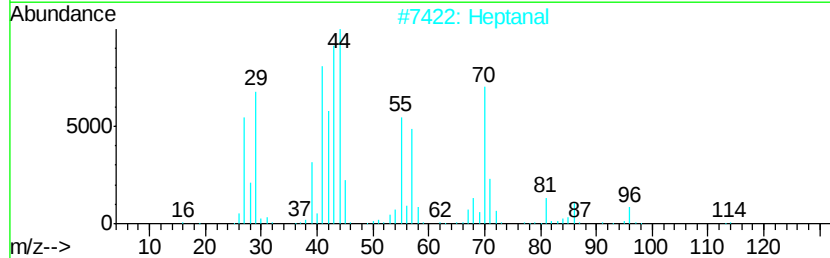
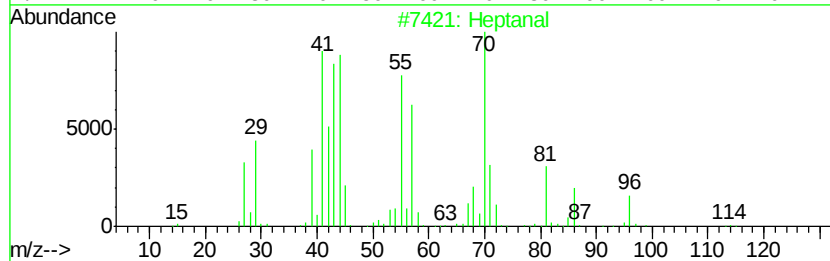
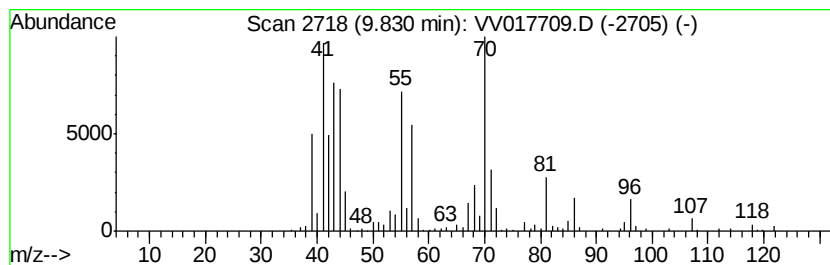
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	3.03 ug/L	271444	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanal	114	C7H14O	000111-71-7	96
2		Heptanal	114	C7H14O	000111-71-7	96
3		Heptanal	114	C7H14O	000111-71-7	95
4		Heptanal	114	C7H14O	000111-71-7	87
5		Heptanal	114	C7H14O	000111-71-7	43



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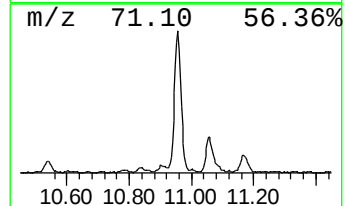
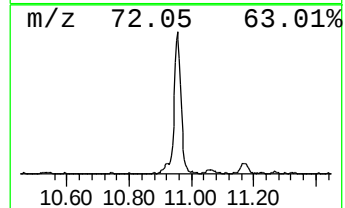
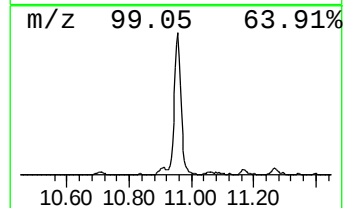
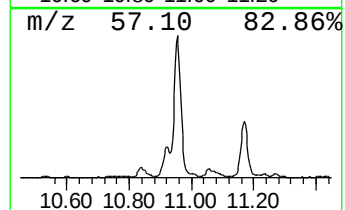
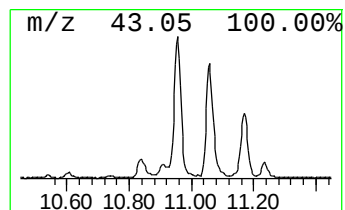
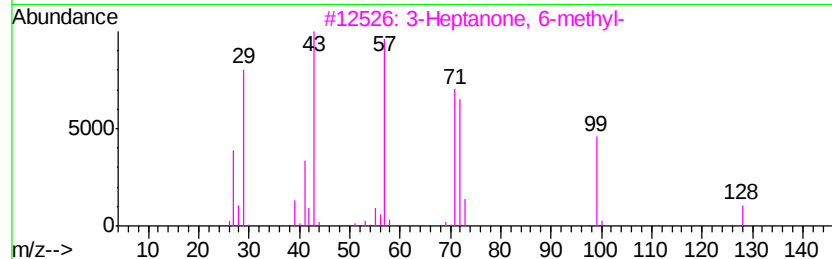
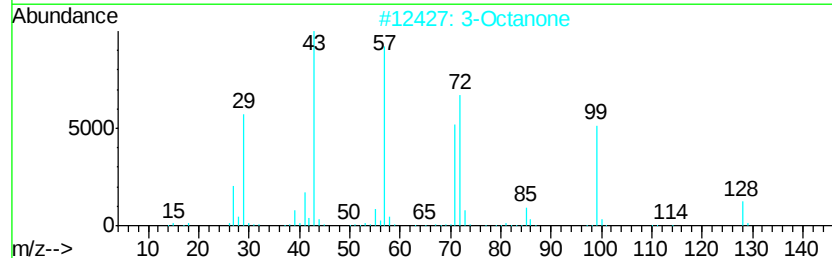
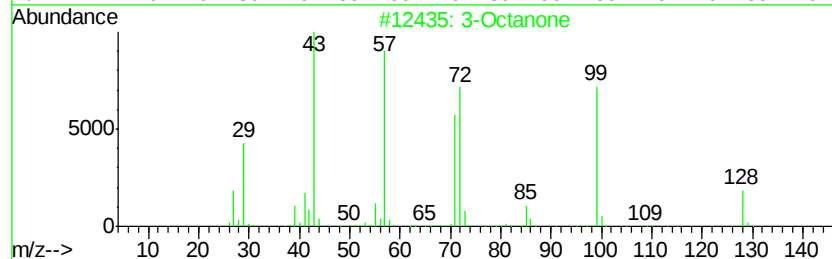
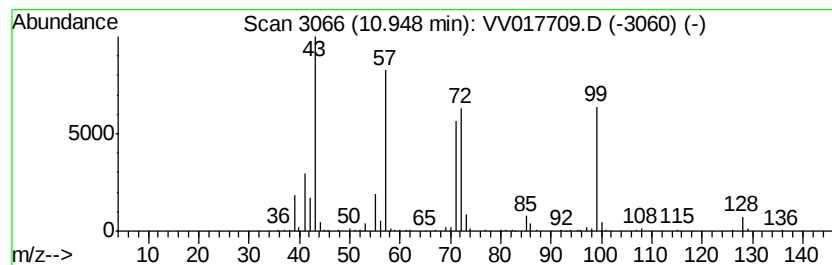
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.99 ug/L	306455	1,4-Dichlorobenzene-d4	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone		128	C8H16O	000106-68-3	90
2	3-Octanone		128	C8H16O	000106-68-3	74
3	3-Heptanone, 6-methyl-		128	C8H16O	000624-42-0	64
4	3-Octanone		128	C8H16O	000106-68-3	64
5	3-Heptanone, 6-methyl-		128	C8H16O	000624-42-0	50



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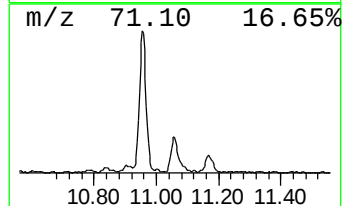
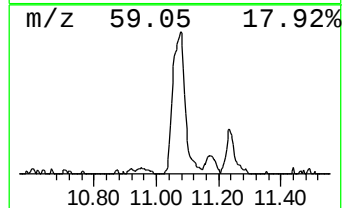
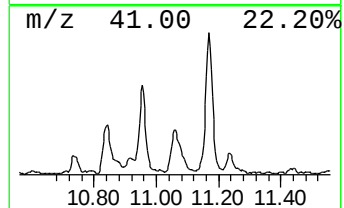
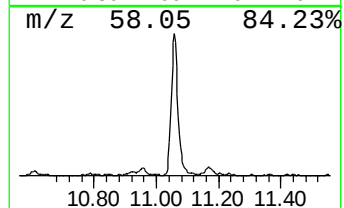
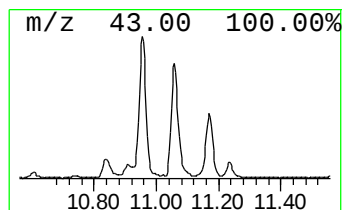
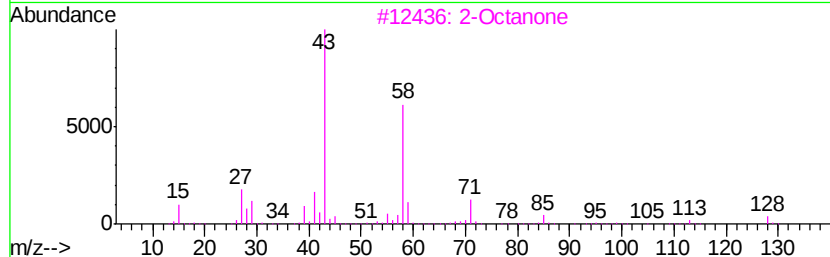
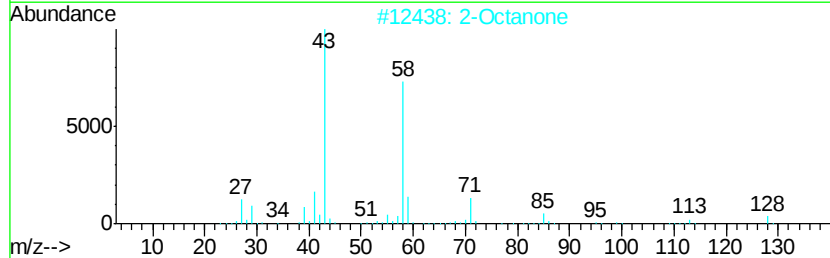
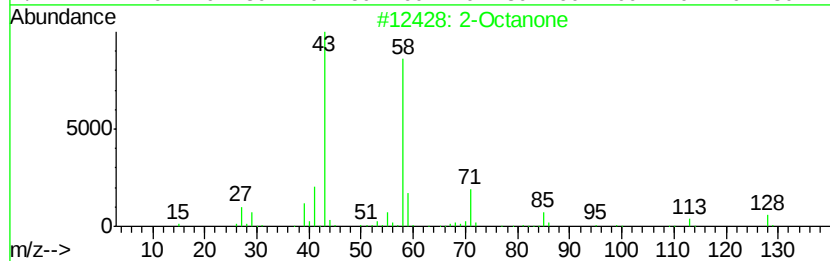
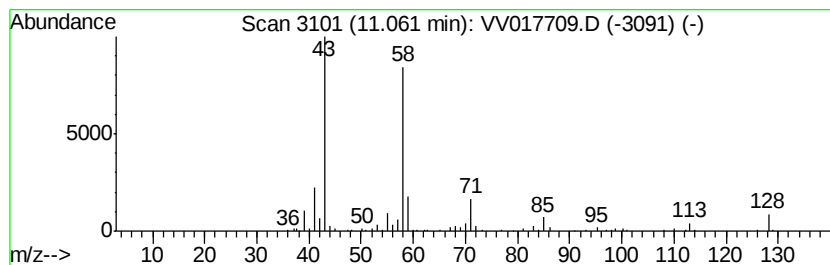
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Octanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	1.79 ug/L	184041	1,4-Dichlorobenzene-d4	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone		128	C8H16O	000111-13-7	94
2	2-Octanone		128	C8H16O	000111-13-7	94
3	2-Octanone		128	C8H16O	000111-13-7	91
4	2-Octanone		128	C8H16O	000111-13-7	91
5	2-Octanone		128	C8H16O	000111-13-7	81



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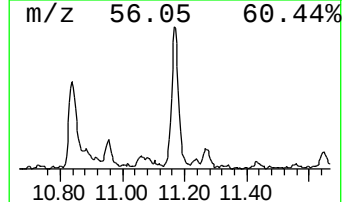
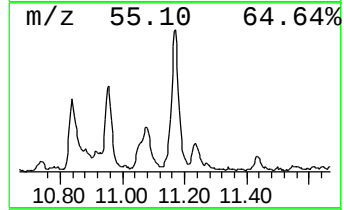
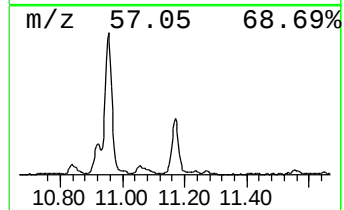
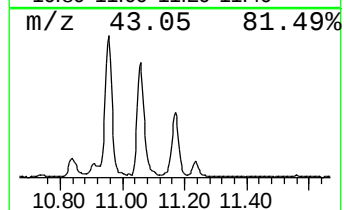
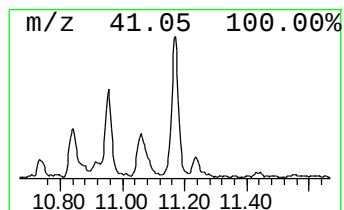
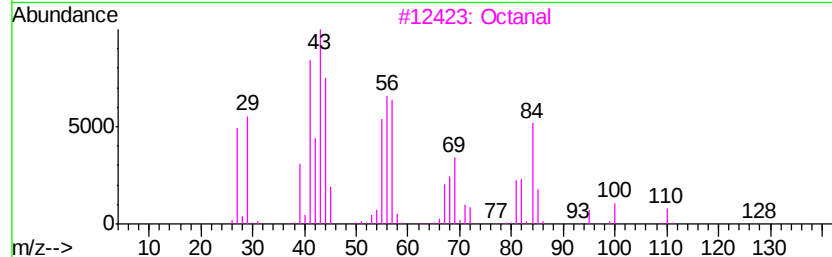
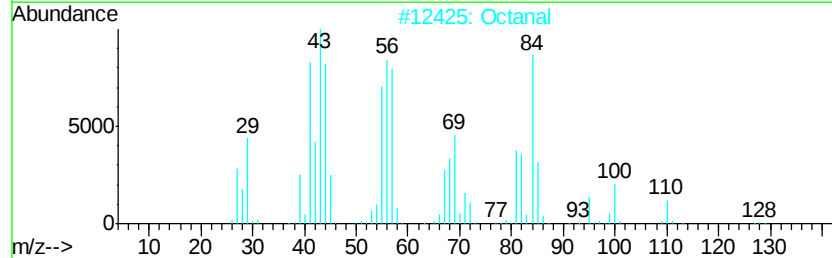
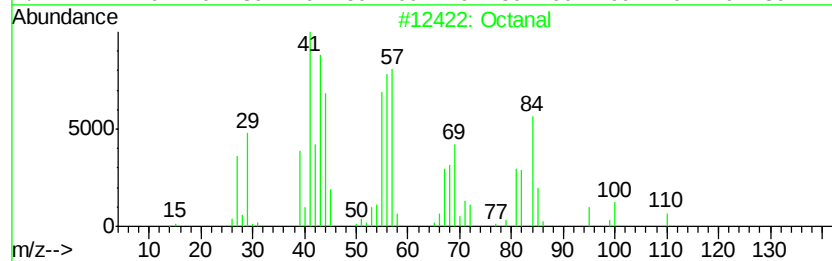
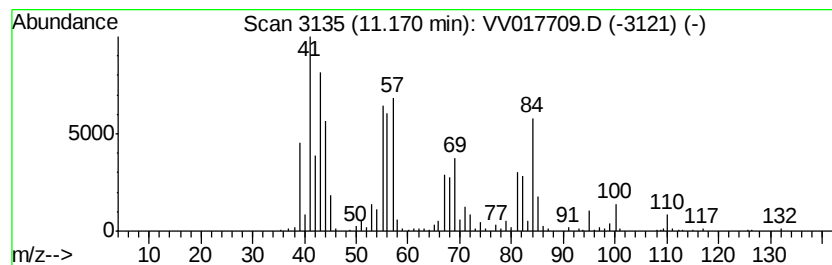
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Octanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	2.93 ug/L	300564	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanal	128	C8H16O	000124-13-0	91
2		Octanal	128	C8H16O	000124-13-0	80
3		Octanal	128	C8H16O	000124-13-0	80
4		Octanal	128	C8H16O	000124-13-0	72
5		Octanal	128	C8H16O	000124-13-0	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV072820\
Data File : VV017709.D
Acq On : 28 Jul 2020 17:05
Operator : SY/MD
Sample : L3470-01
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
H0AE4

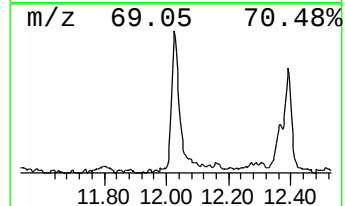
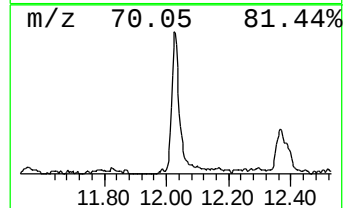
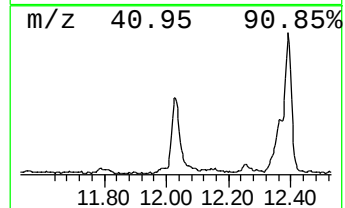
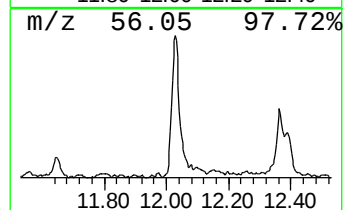
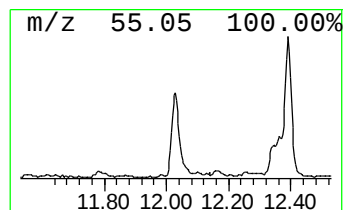
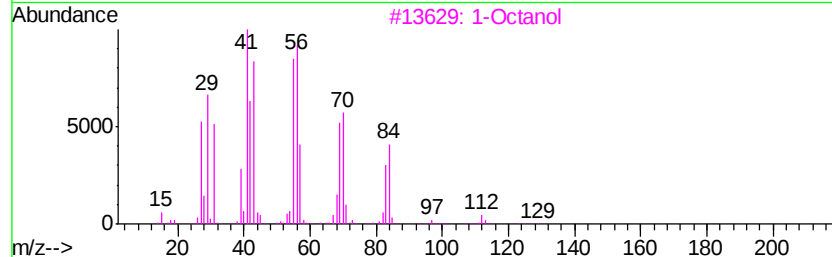
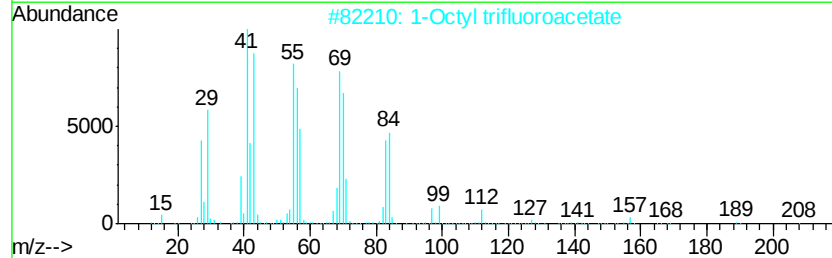
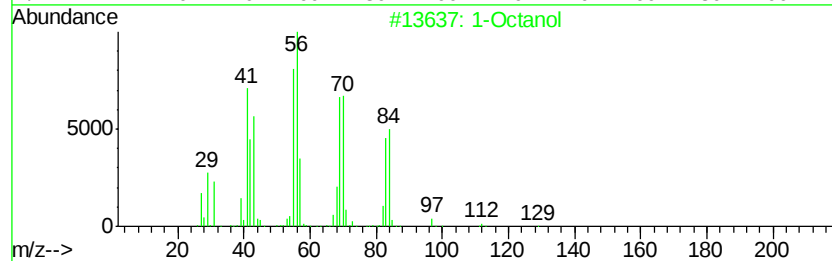
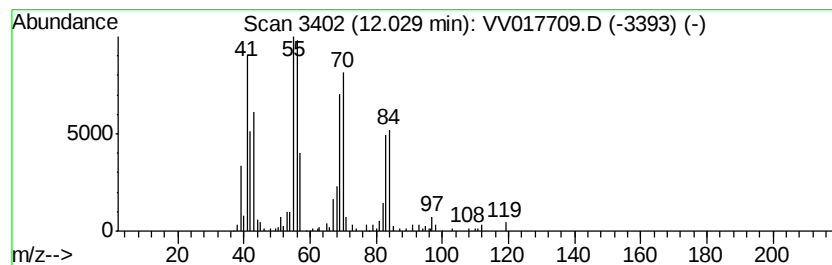
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 1-Octanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	1.56 ug/L	159851	1,4-Dichlorobenzene-d4	11.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	90
2			1-Octyl trifluoroacetate	226	C10H17F3O2	002561-21-9	83
3			1-Octanol	130	C8H18O	000111-87-5	83
4			1-Octanol	130	C8H18O	000111-87-5	80
5			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV072820\
Data File : VV017709.D
Acq On : 28 Jul 2020 17:05
Operator : SY/MD
Sample : L3470-01
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 20 Sample Multiplier: 1

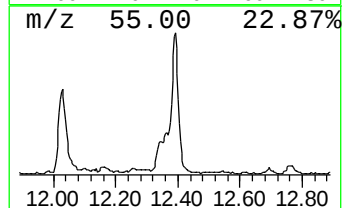
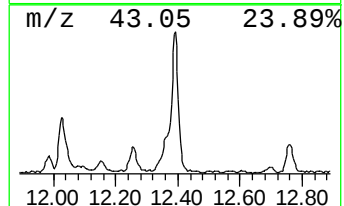
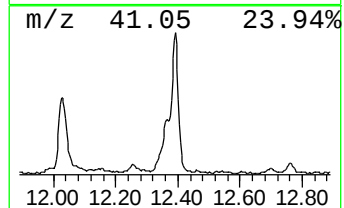
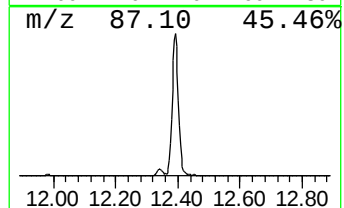
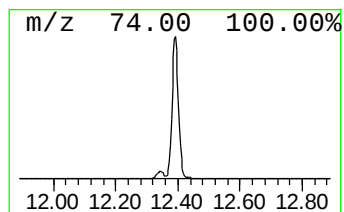
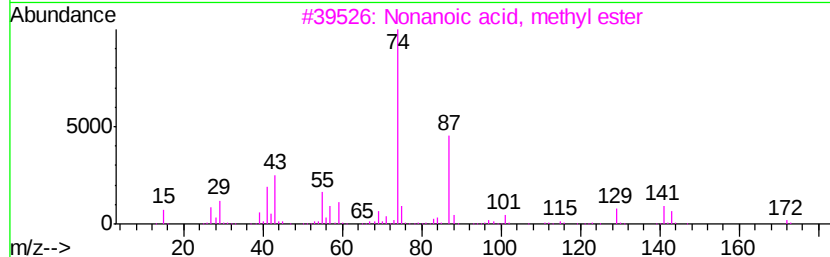
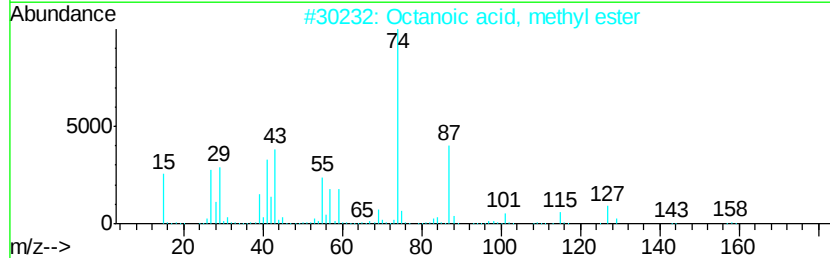
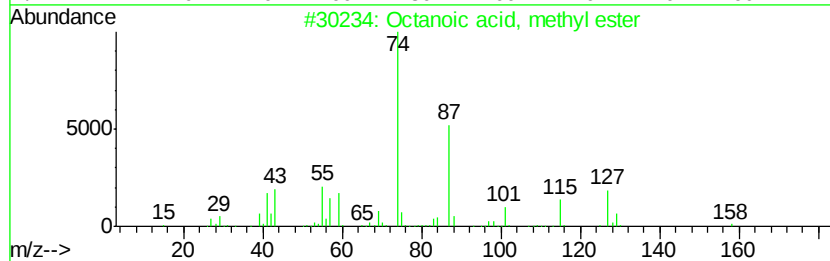
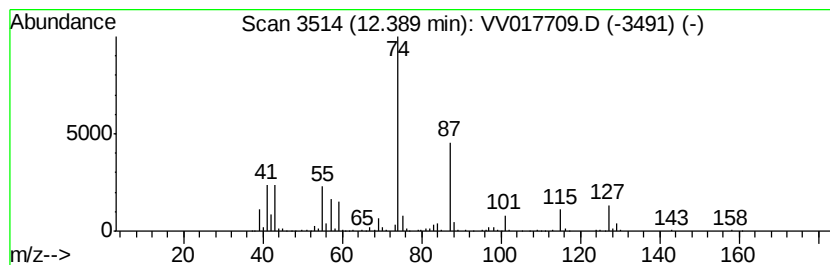
Instrument :
MSVOA_V
ClientSampled :
H0AE4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR072320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Octanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	5.55 ug/L	569564	1,4-Dichlorobenzene-d4	11.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octanoic acid, methyl ester	158 C9H18O2	000111-11-5	96
2	Octanoic acid, methyl ester	158 C9H18O2	000111-11-5	91
3	Nonanoic acid, methyl ester	172 C10H20O2	001731-84-6	72
4	Nonanoic acid, methyl ester	172 C10H20O2	001731-84-6	72
5	Nonanoic acid, methyl ester	172 C10H20O2	001731-84-6	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV072820\
Data File : VV017709.D
Acq On : 28 Jul 2020 17:05
Operator : SY/MD
Sample : L3470-01
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
H0AE4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR072320WMA.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
Methanethiol	1.47	3.8	ug/L	263785	1	5.64	350830	5.0
Hexanal	8.26	11.2	ug/L	1002630	2	8.87	448516	5.0
Heptanal	9.83	3.0	ug/L	271444	2	8.87	448516	5.0
3-Octanone	10.95	3.0	ug/L	306455	3	11.27	512794	5.0
2-Octanone	11.06	1.8	ug/L	184041	3	11.27	512794	5.0
Octanal	11.17	2.9	ug/L	300564	3	11.27	512794	5.0
1-Octanol	12.03	1.6	ug/L	159851	3	11.27	512794	5.0
Octanoic acid, me...	12.39	5.5	ug/L	569564	3	11.27	512794	5.0