

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV073120\
 Data File : VV017770.D
 Acq On : 31 Jul 2020 13:10
 Operator : SY/MD
 Sample : L3486-10
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0Y33

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	1.113	3	7	14	rVB	54033	46000	3.03%	0.532%
2	1.312	60	69	82	rVB2	70349	96232	6.33%	1.112%
3	1.393	82	94	115	rBV	558877	736718	48.46%	8.514%
4	1.579	145	152	164	rVB	49453	58283	3.83%	0.674%
5	2.119	307	320	330	rBV2	121358	227154	14.94%	2.625%
6	2.196	330	344	375	rVB	576710	1520123	100.00%	17.567%
7	2.708	481	503	505	rBV4	11609	29566	1.94%	0.342%
8	3.724	801	819	839	rBV	85337	218174	14.35%	2.521%
9	3.926	868	882	892	rBV2	43094	121363	7.98%	1.403%
10	4.003	893	906	933	rVB	224864	661400	43.51%	7.643%
11	4.373	1003	1021	1040	rBV2	83637	201888	13.28%	2.333%
12	5.071	1222	1238	1259	rBV2	164520	401533	26.41%	4.640%
13	5.640	1400	1415	1434	rBV	188021	385889	25.39%	4.459%
14	6.093	1529	1556	1570	rBV2	91825	218376	14.37%	2.524%
15	6.203	1580	1590	1613	rVB	92408	186123	12.24%	2.151%
16	6.309	1613	1623	1631	rVV2	48297	85614	5.63%	0.989%
17	6.360	1631	1639	1654	rVB	49394	96622	6.36%	1.117%
18	7.010	1829	1841	1855	rBV2	49446	89697	5.90%	1.037%
19	7.338	1930	1943	1960	rBV	187086	336120	22.11%	3.884%
20	7.492	1980	1991	2003	rBV2	14822	30712	2.02%	0.355%
21	7.640	2029	2037	2049	rBV2	34424	59523	3.92%	0.688%
22	7.865	2096	2107	2116	rBV2	10520	18455	1.21%	0.213%
23	8.023	2144	2156	2172	rVB	44013	79726	5.24%	0.921%
24	8.109	2172	2183	2191	rBV	176221	301061	19.81%	3.479%
25	8.161	2191	2199	2217	rVV	219203	377201	24.81%	4.359%
26	8.261	2221	2230	2248	rVB2	65162	113720	7.48%	1.314%
27	8.871	2408	2420	2446	rBV	278881	478571	31.48%	5.531%
28	9.511	2605	2619	2630	rBV9	9472	21280	1.40%	0.246%
29	9.614	2643	2651	2670	rVB	103110	158041	10.40%	1.826%
30	9.720	2674	2684	2700	rBV	74836	117788	7.75%	1.361%
31	9.833	2712	2719	2732	rVB6	12074	19486	1.28%	0.225%
32	10.238	2833	2845	2858	rBV2	65937	104549	6.88%	1.208%
33	10.402	2883	2896	2905	rVB6	10425	22179	1.46%	0.256%
34	10.955	3059	3068	3081	rBV4	20596	31983	2.10%	0.370%

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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

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Title : TRACE VOA SOM01.0

35	11.058	3090	3100	3117	rBV	56291	92696	6.10%	1.071%
36	11.270	3154	3166	3186	rBV	321178	504150	33.17%	5.826%
37	11.585	3246	3264	3272	rBV	15021	33856	2.23%	0.391%
38	11.646	3273	3283	3305	rVB2	217577	355480	23.38%	4.108%
39	13.772	3933	3944	3955	rBV4	9593	15873	1.04%	0.183%

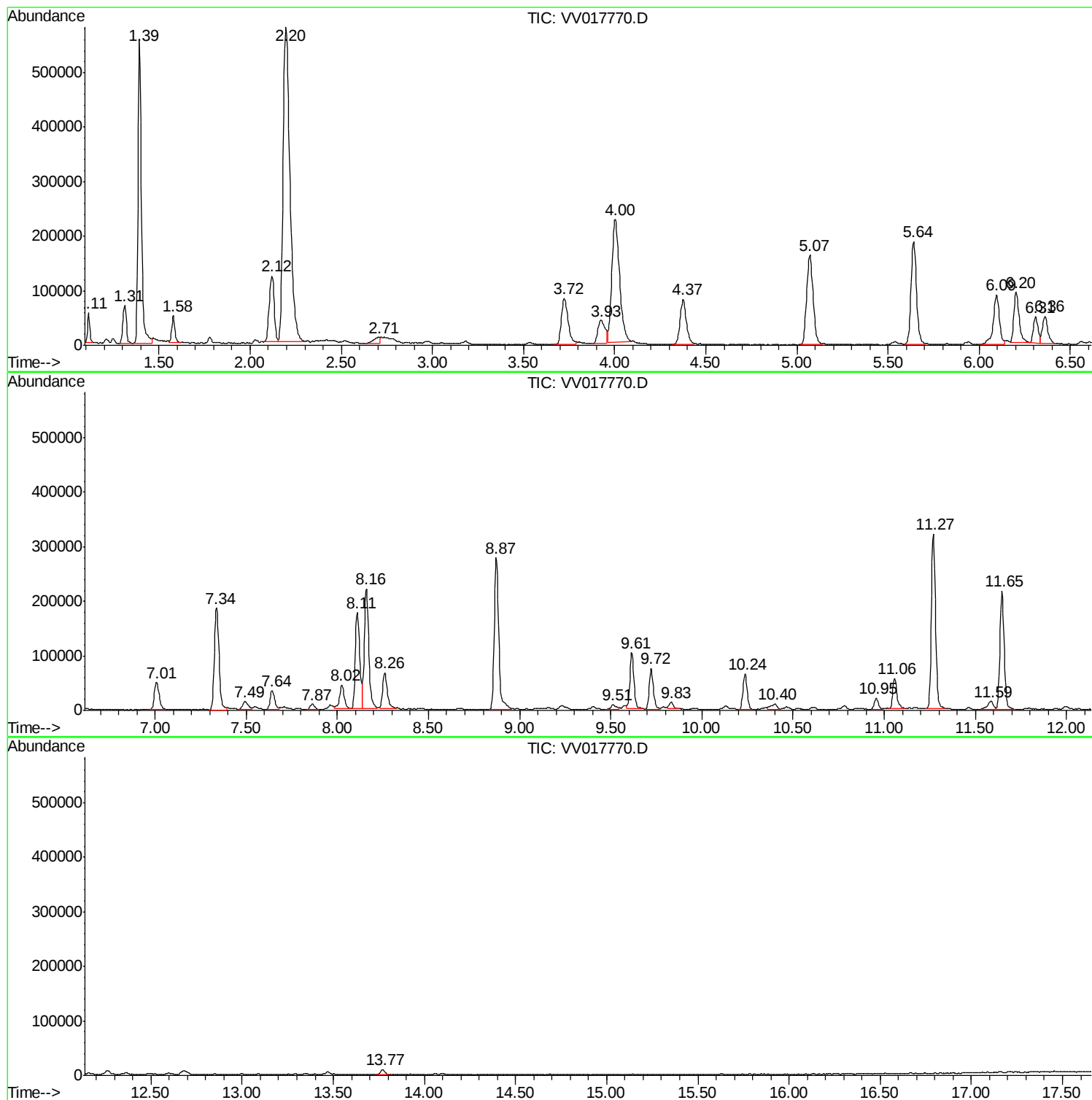
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Quant Title : TRACE VOA SOM01.0

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



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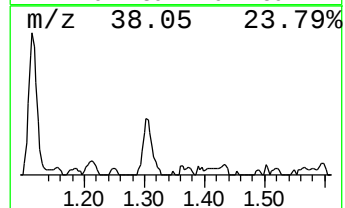
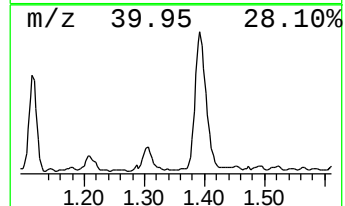
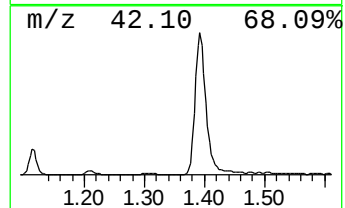
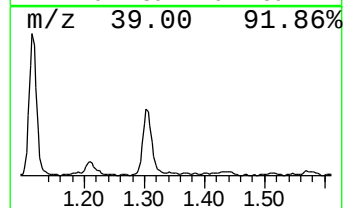
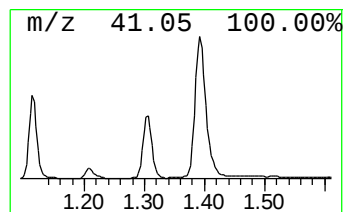
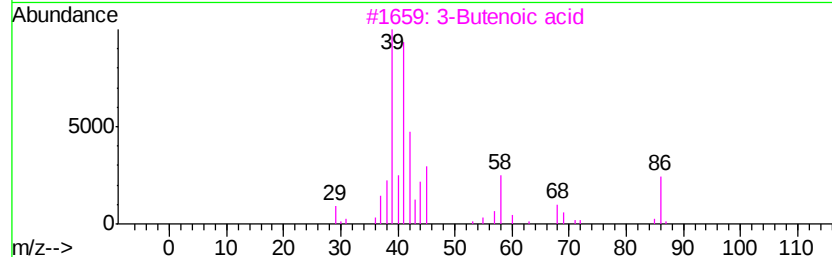
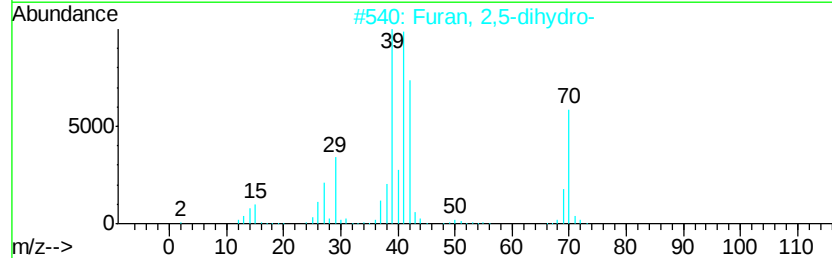
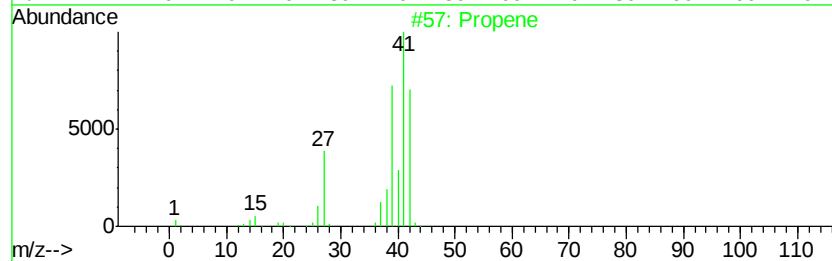
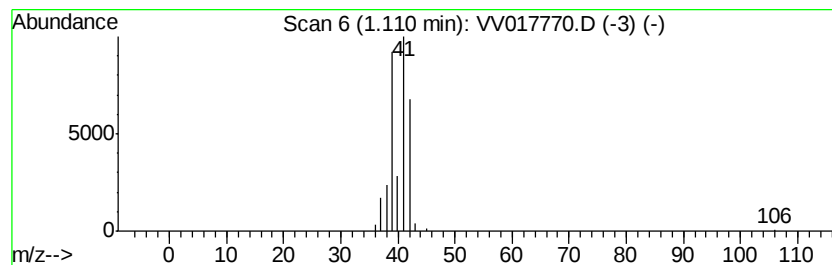
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR072320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.11	0.60 ug/L	46000	1,4-Difluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene		42	C3H6	000115-07-1	90
2	Furan, 2,5-dihydro-		70	C4H6O	001708-29-8	83
3	3-Butenoic acid		86	C4H6O2	000625-38-7	83
4	2-Butenal, (E)-		70	C4H6O	000123-73-9	83
5	N-Methyl-7-azabicyclo(2,2,1)hept...		109	C7H11N	055590-26-6	74



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Instrument :
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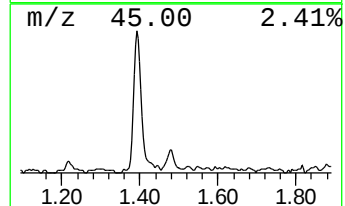
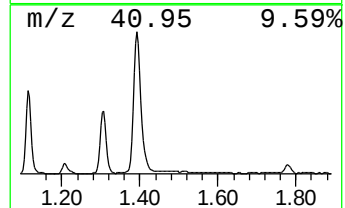
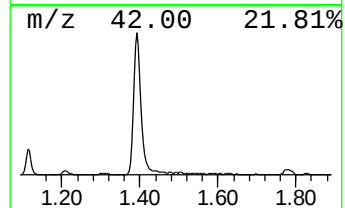
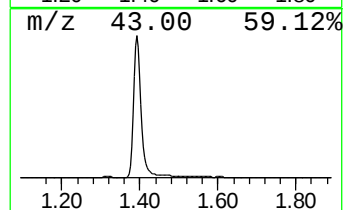
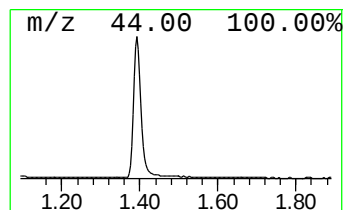
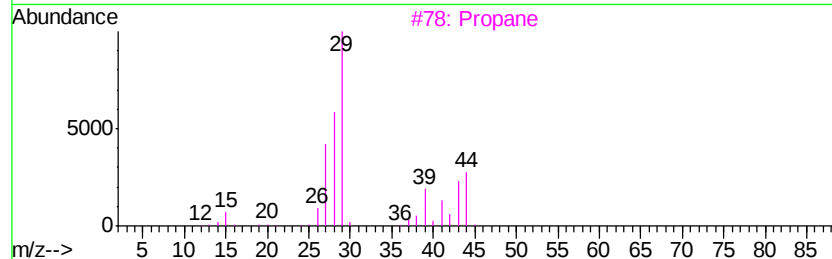
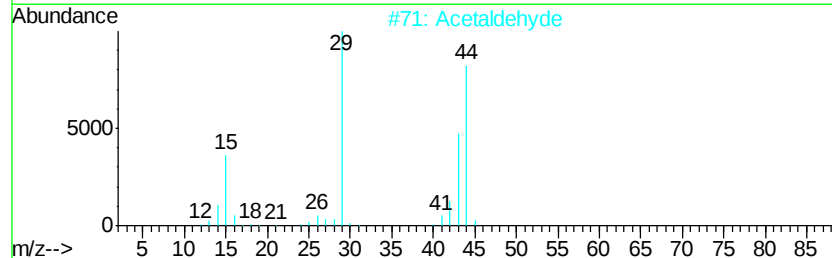
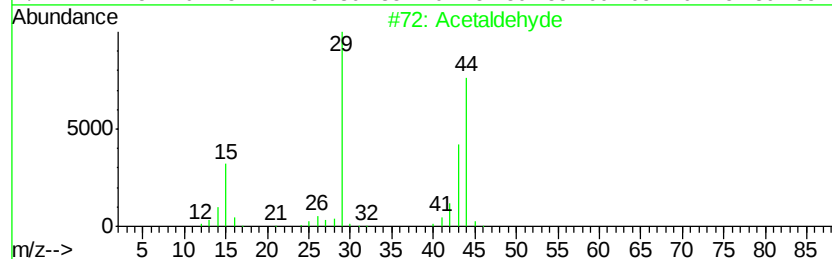
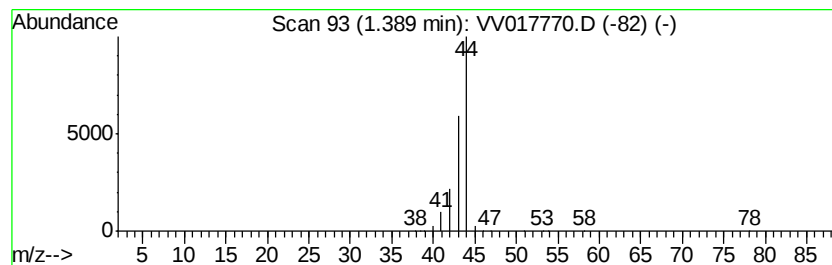
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.39	9.55 ug/L	736718	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehyde	44	C2H4O	000075-07-0	9
2		Acetaldehyde	44	C2H4O	000075-07-0	9
3		Propane	44	C3H8	000074-98-6	5
4		Ethylene oxide	44	C2H4O	000075-21-8	5
5		Ethylene oxide	44	C2H4O	000075-21-8	5



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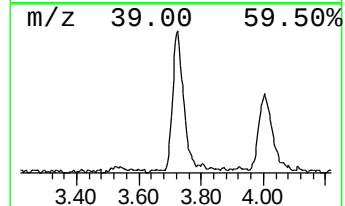
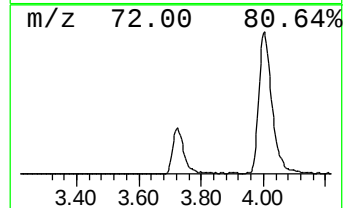
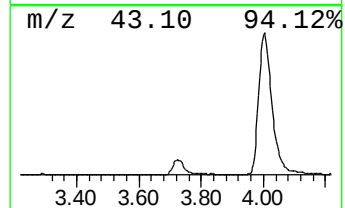
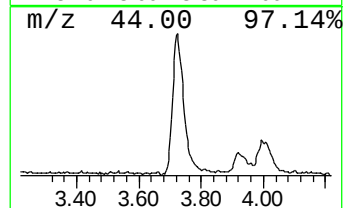
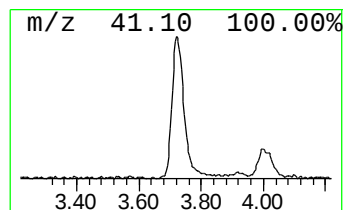
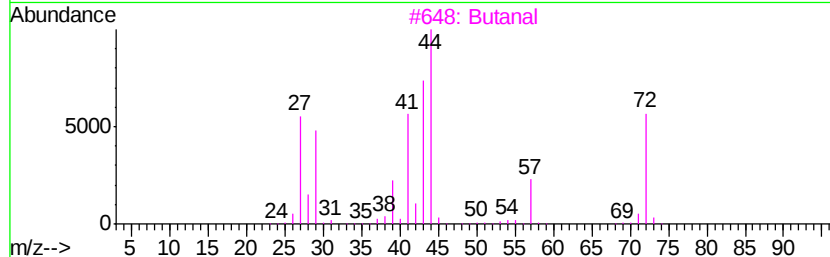
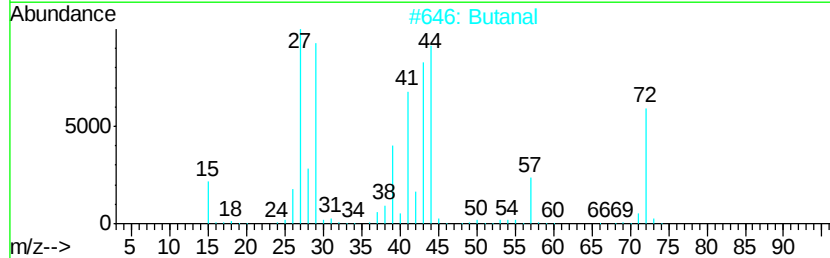
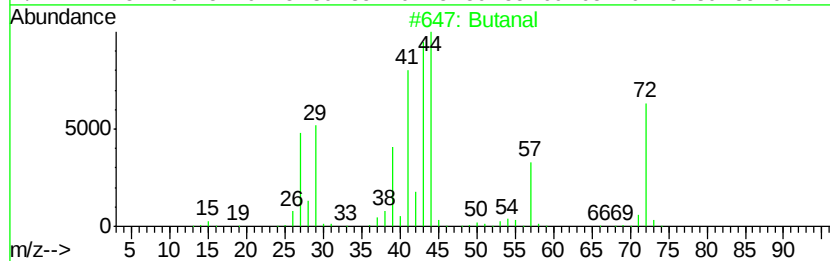
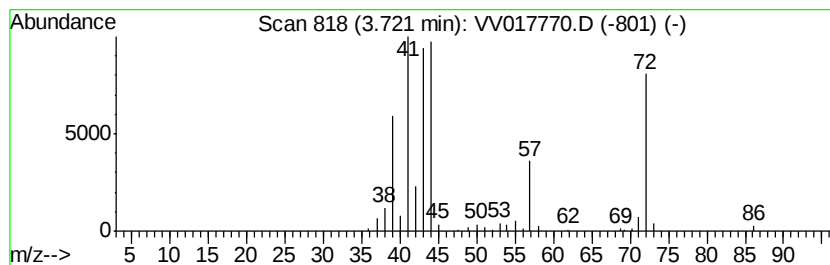
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	2.83 ug/L	218174	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	91
2		Butanal	72	C4H8O	000123-72-8	91
3		Butanal	72	C4H8O	000123-72-8	59
4		Butanal	72	C4H8O	000123-72-8	53
5		O-Methylisourea	74	C2H6N2O	002440-60-0	46



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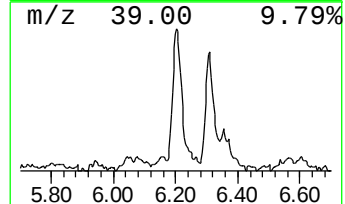
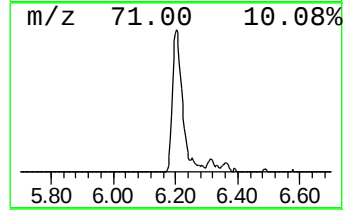
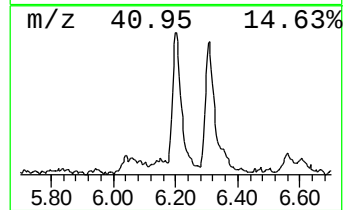
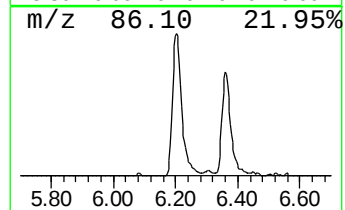
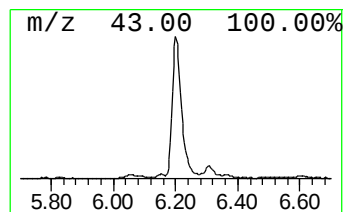
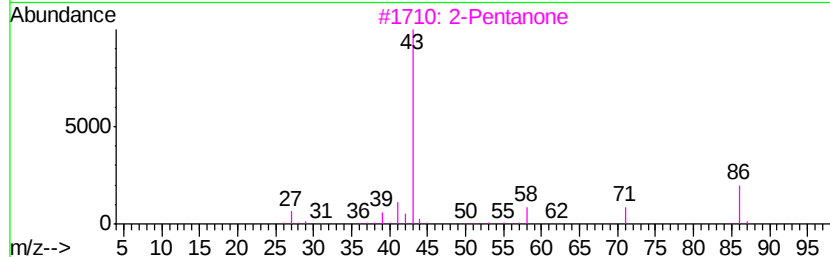
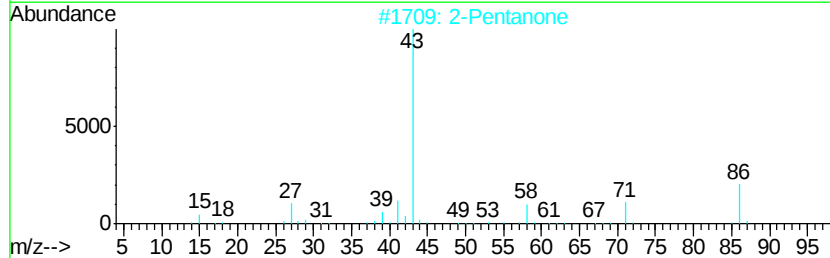
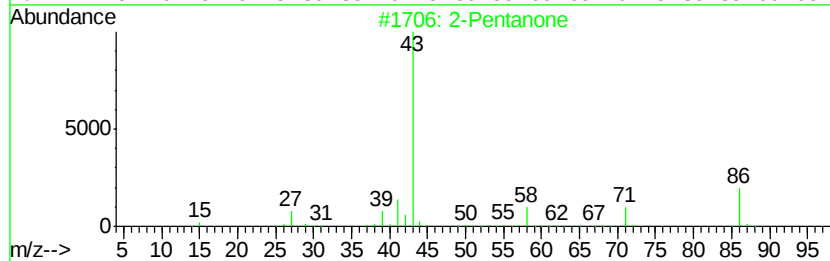
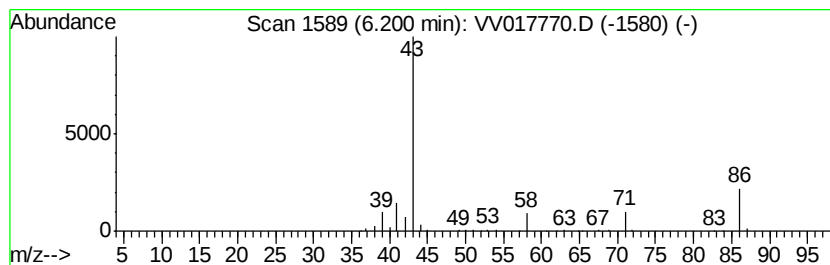
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 2-Pentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.20	2.41 ug/L	186123	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	87
2			2-Pentanone	86	C5H10O	000107-87-9	86
3			2-Pentanone	86	C5H10O	000107-87-9	80
4			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
5			2,3-Butanedione	86	C4H6O2	000431-03-8	50



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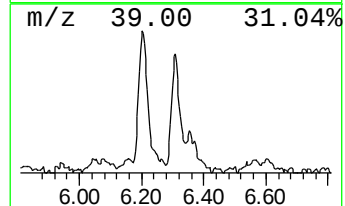
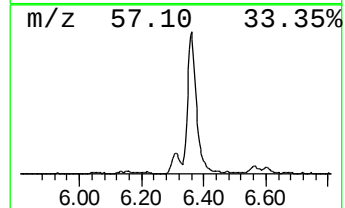
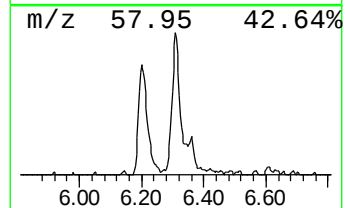
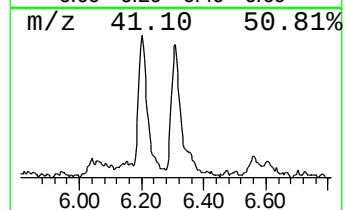
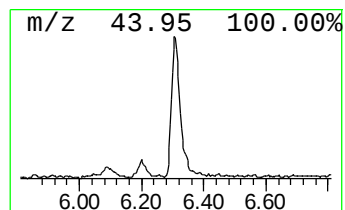
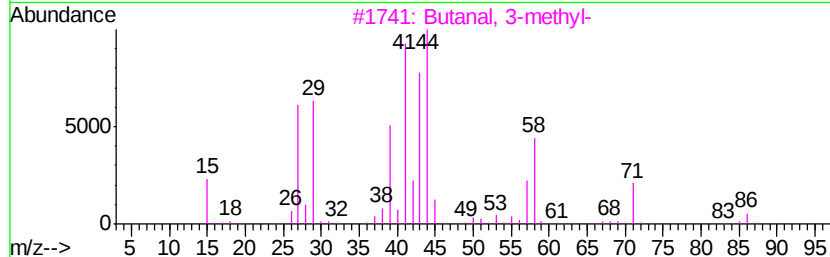
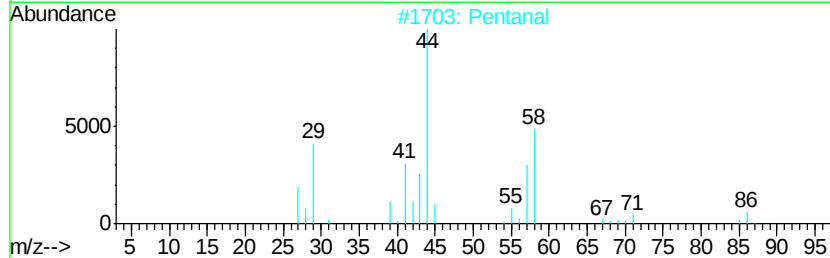
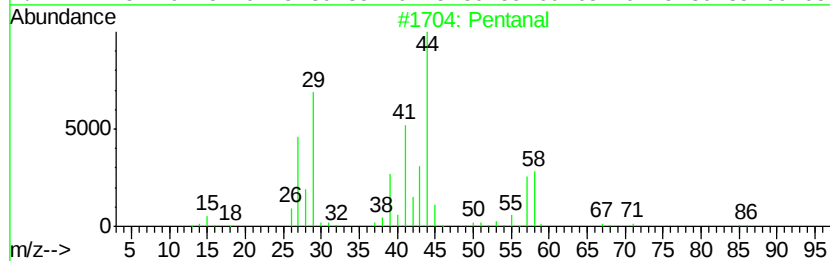
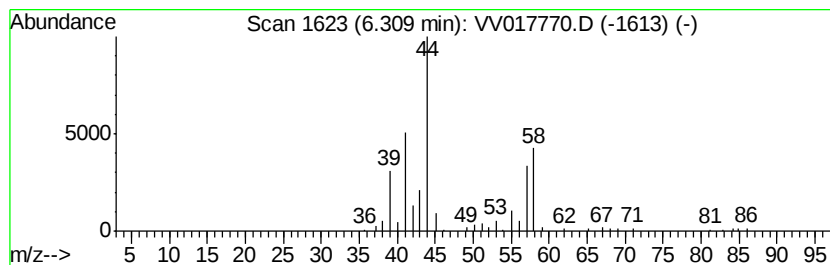
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	1.11 ug/L	85614	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	78
2		Pentanal	86	C5H10O	000110-62-3	64
3		Butanal, 3-methyl-	86	C5H10O	000590-86-3	50
4		Butanal, 3-methyl-	86	C5H10O	000590-86-3	43
5		1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV073120\
Data File : VV017770.D
Acq On : 31 Jul 2020 13:10
Operator : SY/MD
Sample : L3486-10
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0Y33

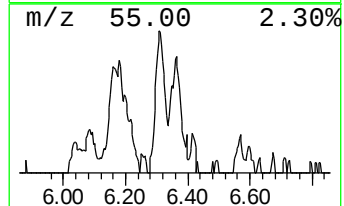
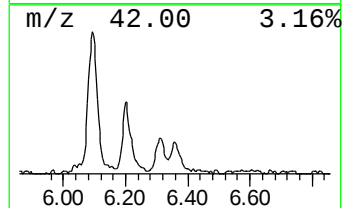
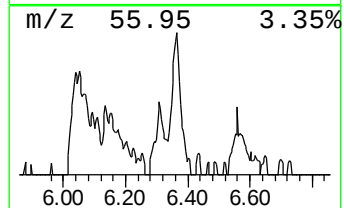
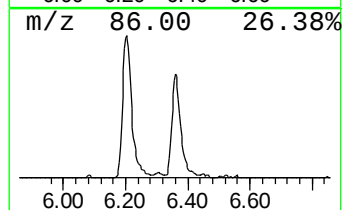
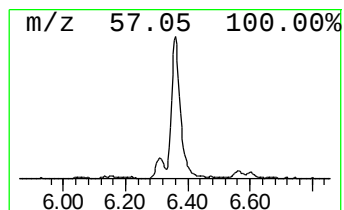
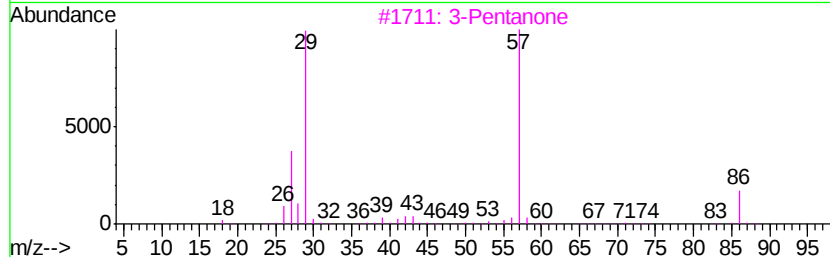
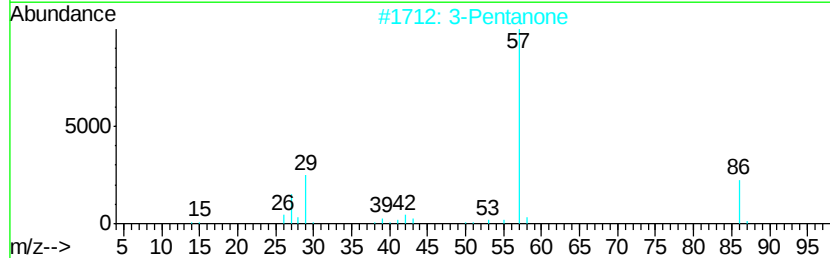
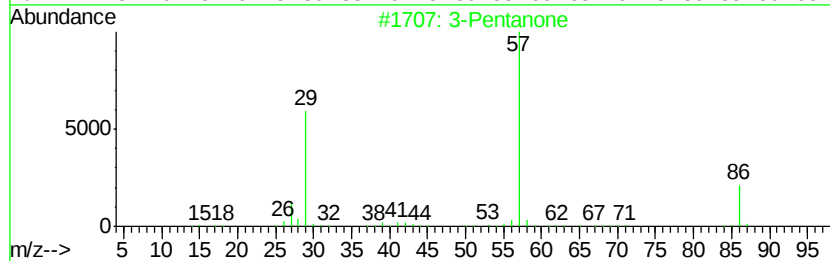
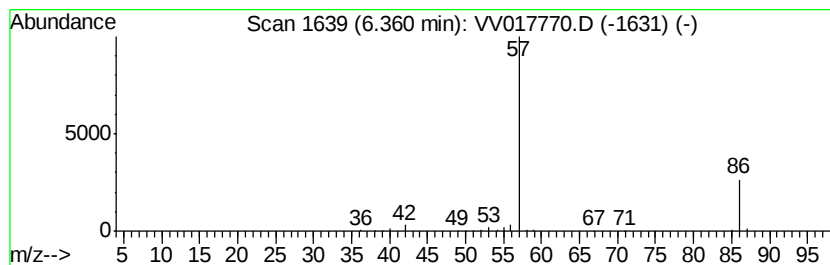
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 3-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	1.25 ug/L	96622	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone	86	C5H10O	000096-22-0	72
2		3-Pentanone	86	C5H10O	000096-22-0	9
3		3-Pentanone	86	C5H10O	000096-22-0	9
4		3-Pentanone	86	C5H10O	000096-22-0	5
5		1,4-Dioxin, 2,3-dihydro-	86	C4H6O2	000543-75-9	5



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV073120\
Data File : VV017770.D
Acq On : 31 Jul 2020 13:10
Operator : SY/MD
Sample : L3486-10
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0Y33

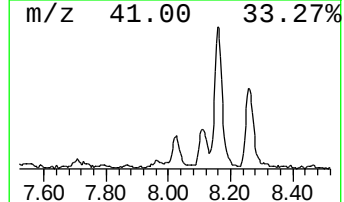
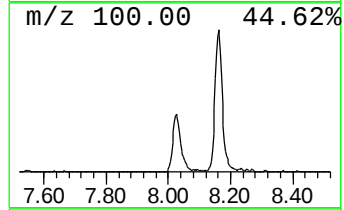
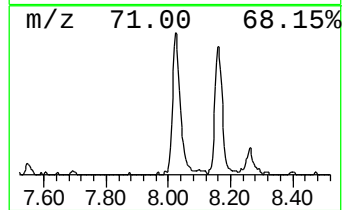
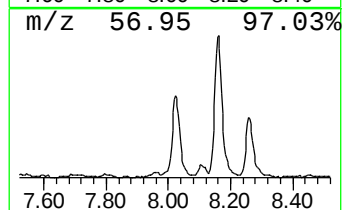
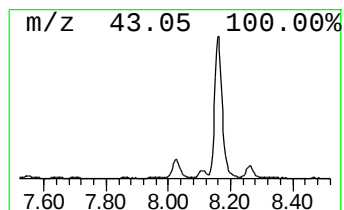
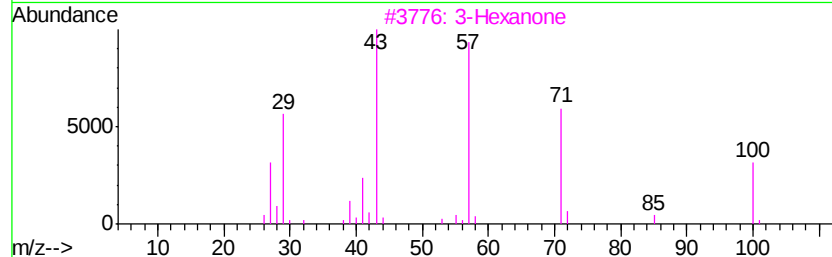
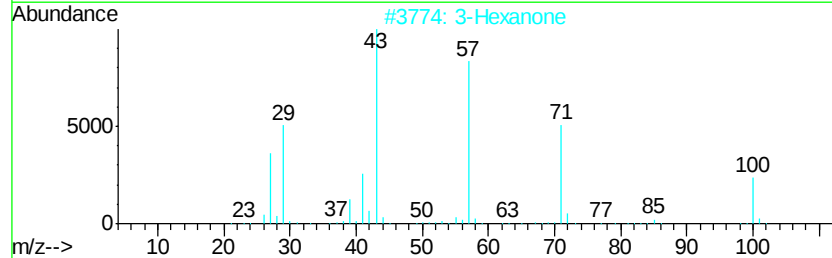
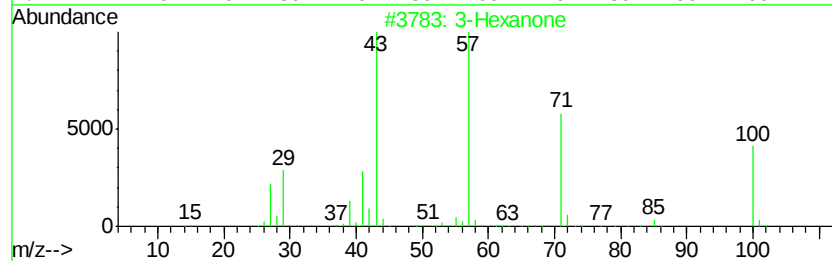
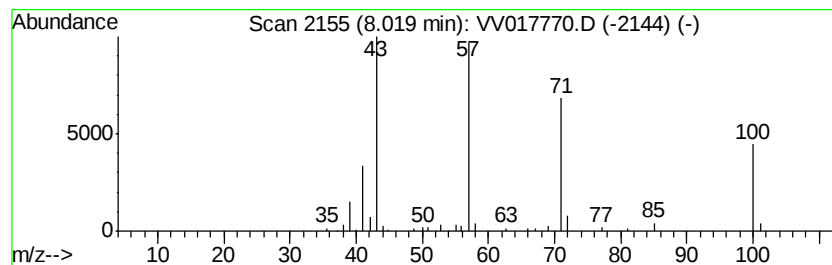
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 3-Hexanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.02	0.83 ug/L	79726	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanone	100	C6H12O	000589-38-8	91
2			3-Hexanone	100	C6H12O	000589-38-8	90
3			3-Hexanone	100	C6H12O	000589-38-8	78
4			3-Hexanone	100	C6H12O	000589-38-8	72
5			3-Hexanone	100	C6H12O	000589-38-8	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV073120\
Data File : VV017770.D
Acq On : 31 Jul 2020 13:10
Operator : SY/MD
Sample : L3486-10
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0Y33

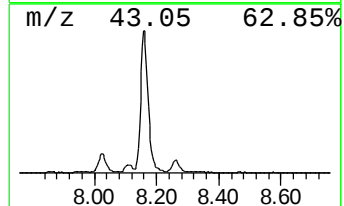
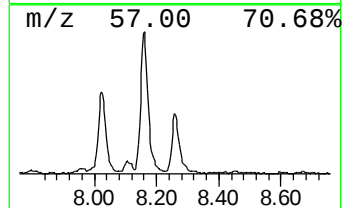
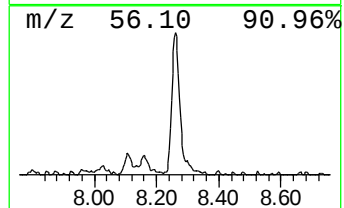
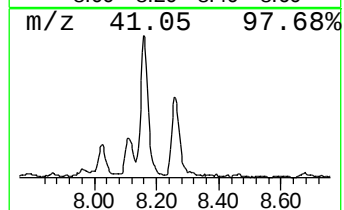
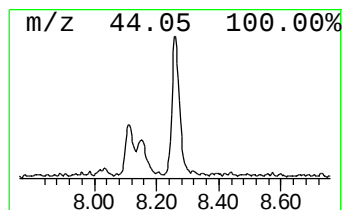
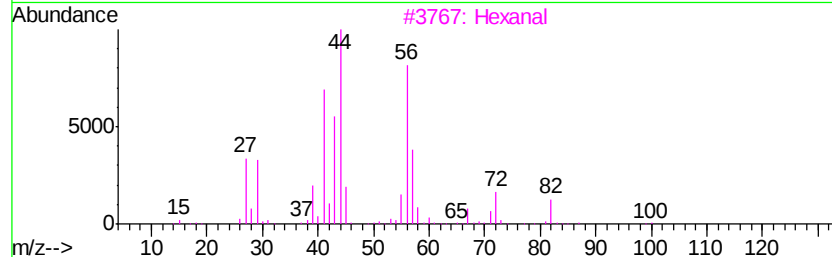
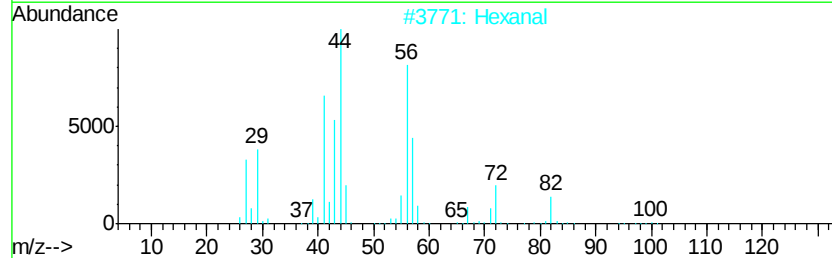
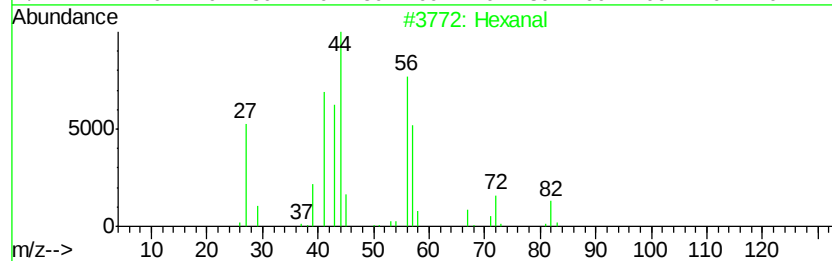
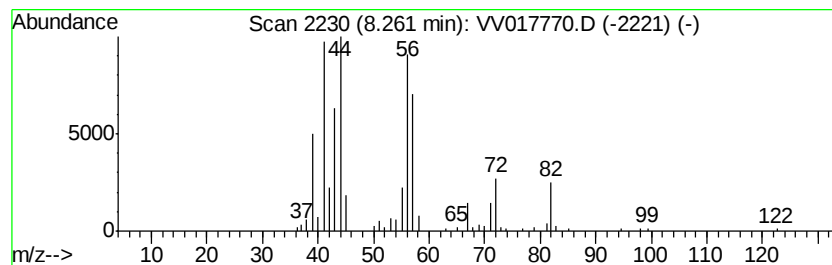
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Hexanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	1.19 ug/L	113720	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	53
2		Hexanal	100	C6H12O	000066-25-1	53
3		Hexanal	100	C6H12O	000066-25-1	53
4		Hexanal	100	C6H12O	000066-25-1	45
5		Butanal, 3-methyl-	86	C5H10O	000590-86-3	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV073120\
Data File : VV017770.D
Acq On : 31 Jul 2020 13:10
Operator : SY/MD
Sample : L3486-10
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0Y33

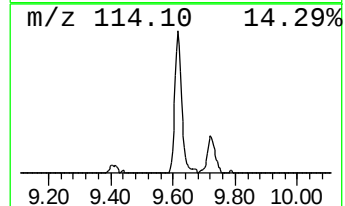
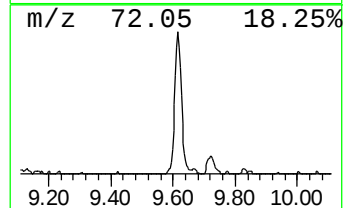
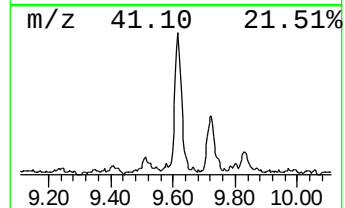
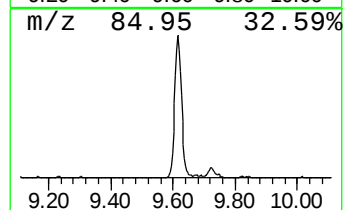
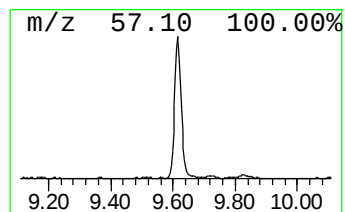
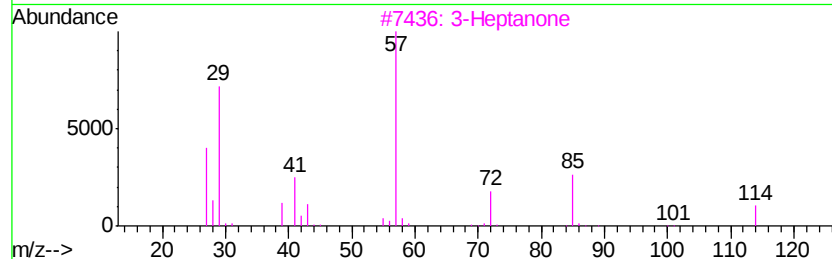
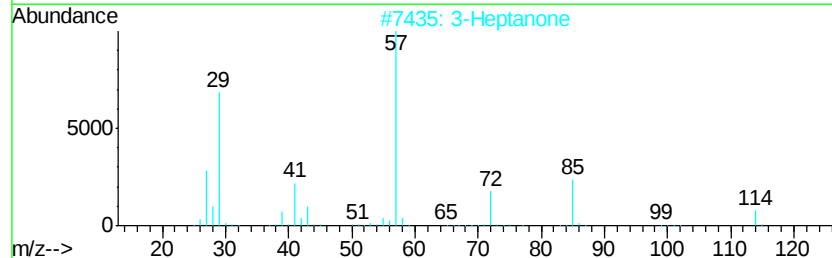
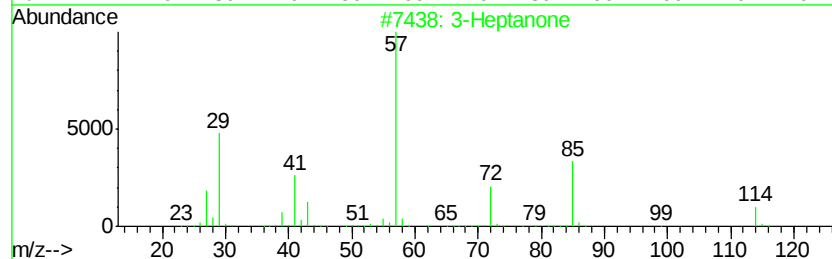
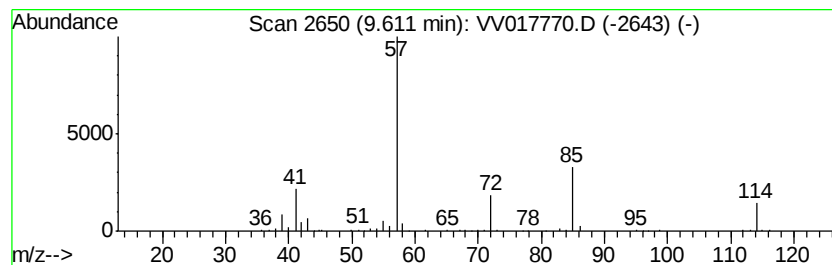
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 3-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.61	1.65 ug/L	158041	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone	114	C7H14O	000106-35-4	90
2			3-Heptanone	114	C7H14O	000106-35-4	87
3			3-Heptanone	114	C7H14O	000106-35-4	86
4			3,5-Octanedione, 2,2,4,7-tetrame...	198	C12H22O2	1000161-72-3	78
5			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV073120\
Data File : VV017770.D
Acq On : 31 Jul 2020 13:10
Operator : SY/MD
Sample : L3486-10
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0Y33

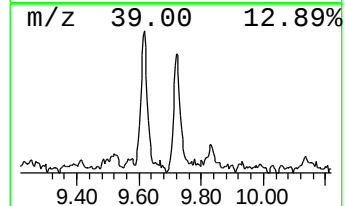
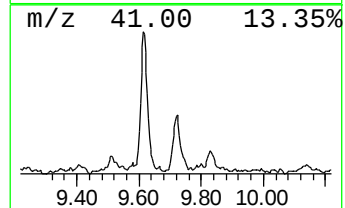
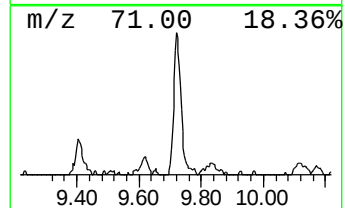
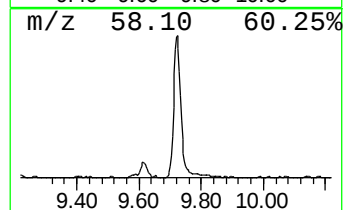
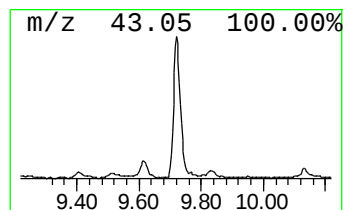
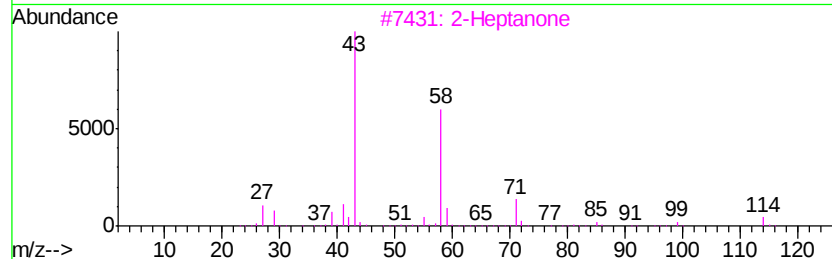
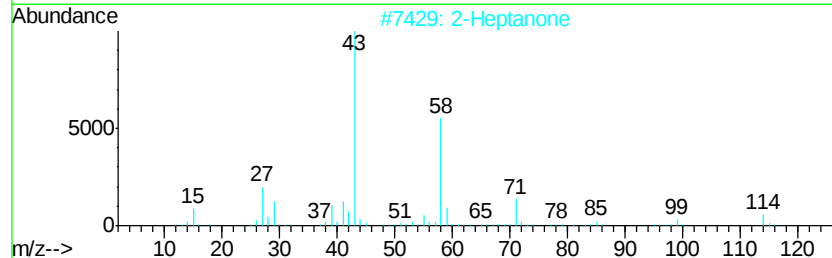
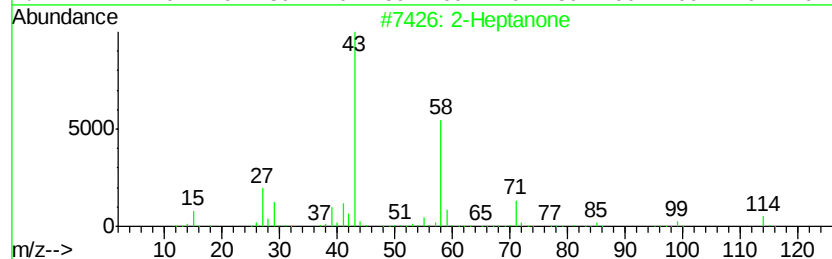
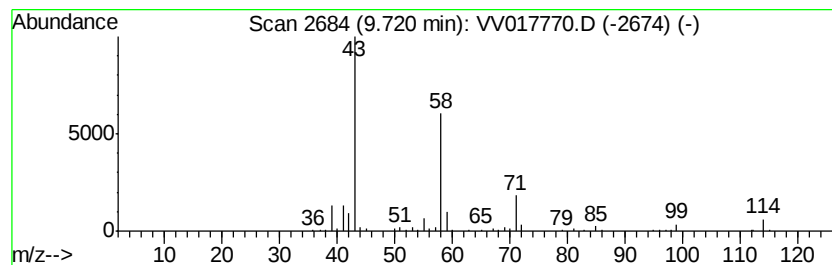
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.72	1.23 ug/L	117788	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Heptanone	114	C7H14O	000110-43-0	91
3			2-Heptanone	114	C7H14O	000110-43-0	87
4			2-Heptanone	114	C7H14O	000110-43-0	81
5			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV073120\
Data File : VV017770.D
Acq On : 31 Jul 2020 13:10
Operator : SY/MD
Sample : L3486-10
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0Y33

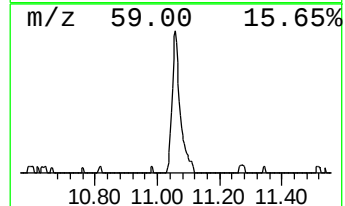
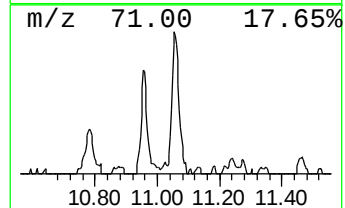
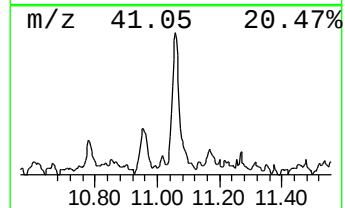
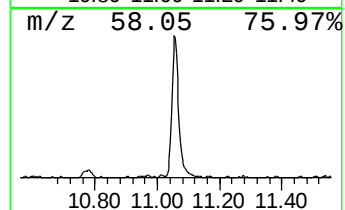
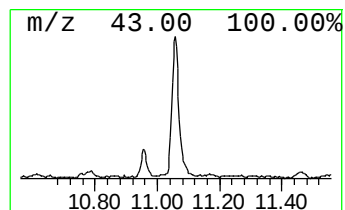
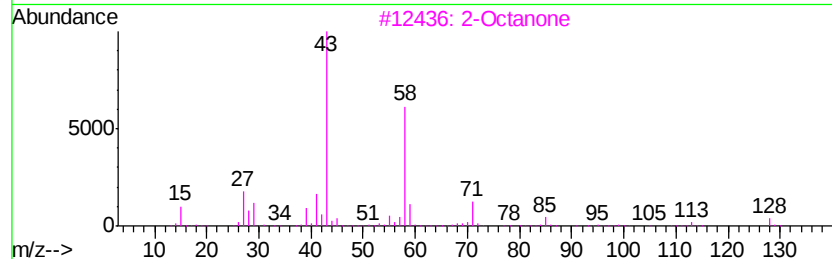
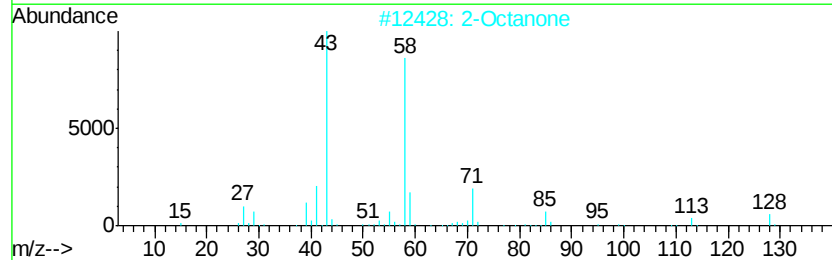
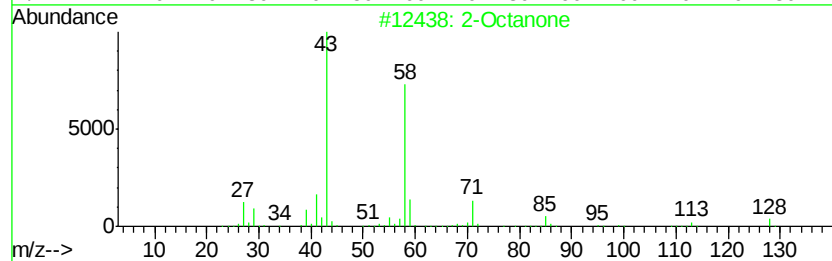
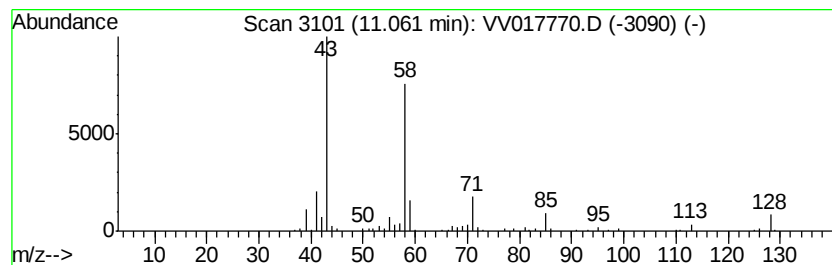
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 12 2-Octanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	0.92 ug/L	92696	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	91
3			2-Octanone	128	C8H16O	000111-13-7	91
4			2-Octanone	128	C8H16O	000111-13-7	90
5			2-Octanone	128	C8H16O	000111-13-7	80



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV073120\
Data File : VV017770.D
Acq On : 31 Jul 2020 13:10
Operator : SY/MD
Sample : L3486-10
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0Y33

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
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unknown-01	1.39	9.6	ug/L	736718	1	5.64	385889	5.0
Butanal	3.72	2.8	ug/L	218174	1	5.64	385889	5.0
2-Pentanone	6.20	2.4	ug/L	186123	1	5.64	385889	5.0
Pentanal	6.31	1.1	ug/L	85614	1	5.64	385889	5.0
3-Pentanone	6.36	1.3	ug/L	96622	1	5.64	385889	5.0
3-Hexanone	8.02	0.8	ug/L	79726	2	8.87	478571	5.0
Hexanal	8.26	1.2	ug/L	113720	2	8.87	478571	5.0
3-Heptanone	9.61	1.6	ug/L	158041	2	8.87	478571	5.0
2-Heptanone	9.72	1.2	ug/L	117788	2	8.87	478571	5.0
2-Octanone	11.06	0.9	ug/L	92696	3	11.27	504150	5.0