

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
 Data File : VU042147.D
 Acq On : 21 Jan 2021 13:48
 Operator : SY/MD
 Sample : M1170-11
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFT92

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_U\METHOD\SOMUTR012021WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC: VU042147.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.356	3	5	20	rVB2	63349	54224	4.54%	0.713%
2	1.594	68	79	86	rVB2	58787	80268	6.72%	1.056%
3	1.716	107	117	142	rBV2	16952	41280	3.45%	0.543%
4	1.909	169	177	188	rVB	38718	48825	4.09%	0.642%
5	2.562	368	380	395	rBV	82470	133745	11.19%	1.760%
6	2.736	422	434	436	rBV9	8529	13985	1.17%	0.184%
7	3.600	695	703	718	rVB4	5994	14069	1.18%	0.185%
8	4.478	953	976	996	rBV4	14743	44534	3.73%	0.586%
9	4.723	1030	1052	1071	rBV2	39836	155277	12.99%	2.043%
10	5.070	1143	1160	1180	rBV	78888	171934	14.39%	2.262%
11	5.726	1342	1364	1390	rBV2	168481	403938	33.81%	5.315%
12	6.256	1516	1529	1548	rVB	151432	284604	23.82%	3.745%
13	6.546	1594	1619	1638	rBV	626069	1194906	100.00%	15.721%
14	6.700	1654	1667	1684	rVB	97511	185956	15.56%	2.447%
15	6.809	1690	1701	1716	rVB4	8348	16961	1.42%	0.223%
16	6.899	1717	1729	1743	rBV2	39214	77876	6.52%	1.025%
17	7.571	1923	1938	1960	rVB	57953	101999	8.54%	1.342%
18	7.816	2001	2014	2026	rBV2	8630	16621	1.39%	0.219%
19	7.903	2026	2041	2054	rVV	188745	323792	27.10%	4.260%
20	7.973	2054	2063	2073	rVB	25093	41695	3.49%	0.549%
21	8.186	2115	2129	2142	rBV3	43173	82859	6.93%	1.090%
22	8.272	2142	2156	2168	rVB5	6184	15634	1.31%	0.206%
23	8.558	2237	2245	2255	rVB3	10721	17970	1.50%	0.236%
24	8.652	2260	2274	2307	rBV	245267	474214	39.69%	6.239%
25	8.796	2307	2319	2346	rVB	263056	449633	37.63%	5.916%
26	9.423	2502	2514	2533	rBV	208621	336856	28.19%	4.432%
27	9.774	2611	2623	2641	rBV2	53936	97369	8.15%	1.281%
28	10.137	2720	2736	2747	rVB2	14813	29226	2.45%	0.385%
29	10.247	2758	2770	2782	rBV	17319	27552	2.31%	0.362%
30	10.353	2791	2803	2830	rVB	105512	169032	14.15%	2.224%
31	10.764	2919	2931	2943	rBV	73601	118862	9.95%	1.564%
32	11.054	3010	3021	3031	rBV2	24684	39944	3.34%	0.526%
33	11.121	3036	3042	3064	rVB	7829	14389	1.20%	0.189%
34	11.475	3145	3152	3167	rVB4	10179	16506	1.38%	0.217%
35	11.581	3175	3185	3195	rVB	10702	15684	1.31%	0.206%
36	11.697	3200	3221	3233	rBV	147114	221499	18.54%	2.914%

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Peak Location: TOP

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Title : TRACE VOA SOM01.0

37	11.819	3247	3259	3277	rVB	227486	354515	29.67%	4.664%
38	12.070	3324	3337	3365	rBV	193853	383365	32.08%	5.044%
39	12.201	3367	3378	3391	rVB	193862	310310	25.97%	4.083%
40	12.552	3478	3487	3504	rBV5	10790	22616	1.89%	0.298%
41	12.896	3581	3594	3609	rBV	375096	553347	46.31%	7.280%
42	13.217	3681	3694	3706	rBV	176429	259475	21.72%	3.414%
43	13.459	3759	3769	3779	rVB5	8813	14285	1.20%	0.188%
44	13.693	3834	3842	3855	rVB3	20324	31910	2.67%	0.420%
45	13.877	3891	3899	3909	rVB2	12818	19594	1.64%	0.258%
46	13.992	3927	3935	3950	rVB4	13264	21609	1.81%	0.284%
47	14.092	3952	3966	3977	rBV	18366	33995	2.84%	0.447%
48	14.742	4160	4168	4180	rVB7	8148	12844	1.07%	0.169%
49	15.237	4308	4322	4332	rBV5	7188	14977	1.25%	0.197%
50	15.407	4366	4375	4388	rVB5	8824	14897	1.25%	0.196%
51	15.532	4397	4414	4422	rBV2	11339	19116	1.60%	0.252%

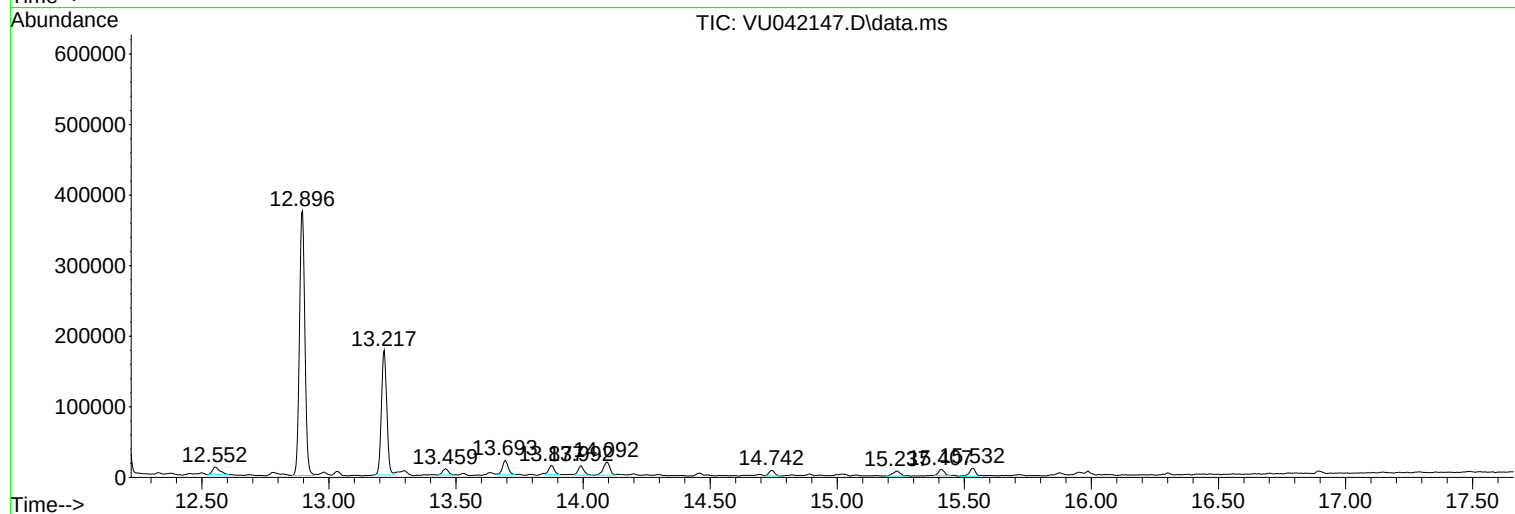
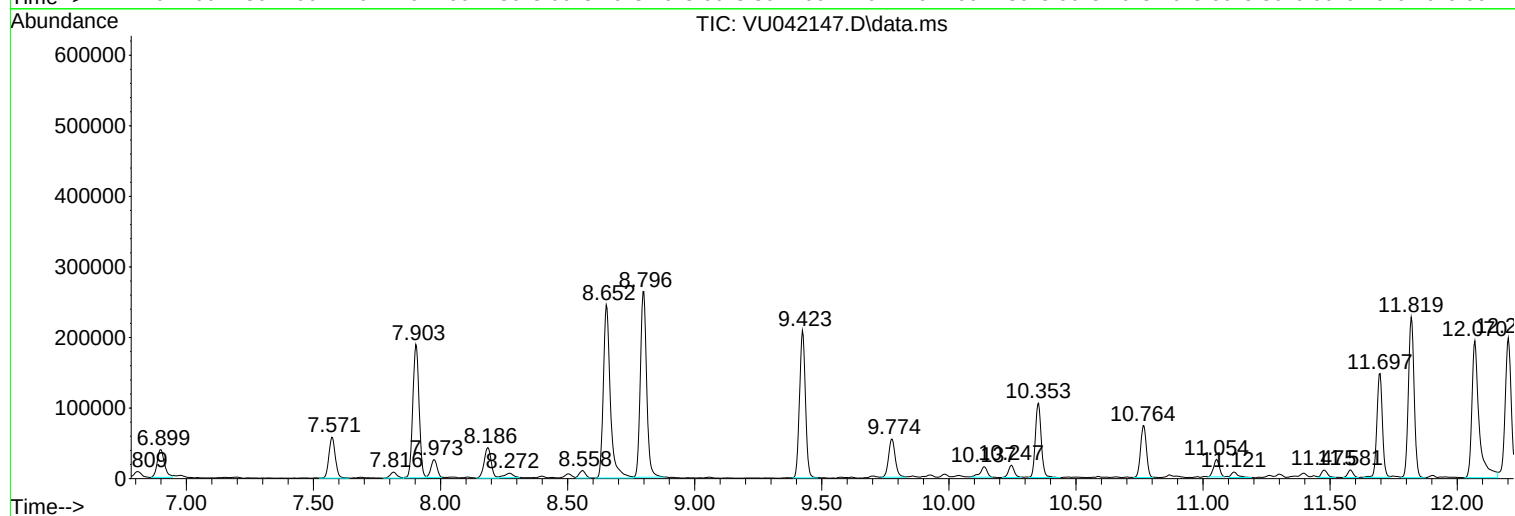
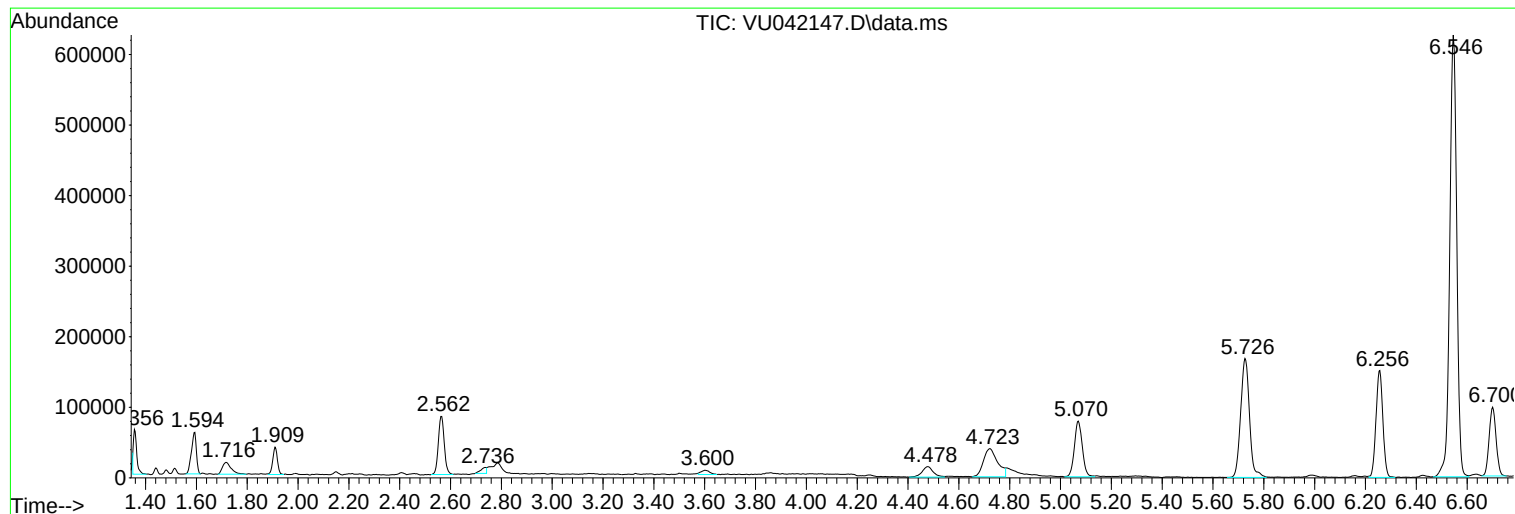
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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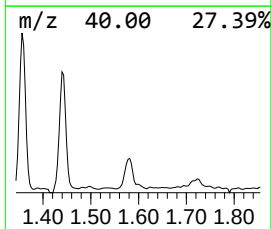
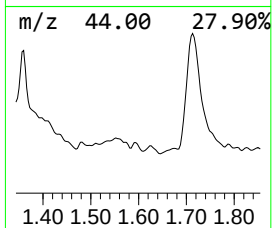
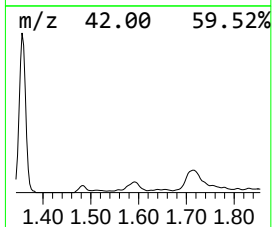
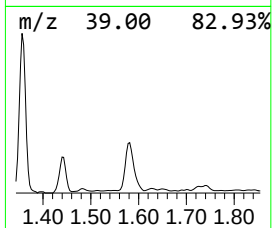
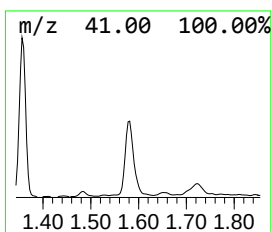
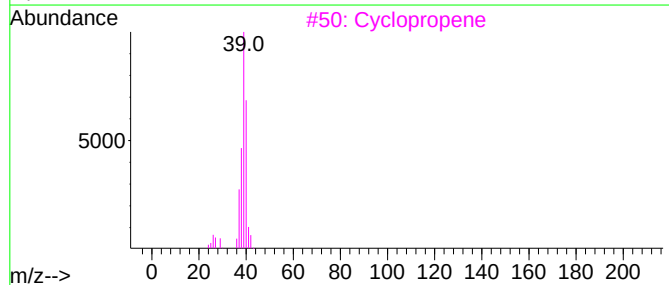
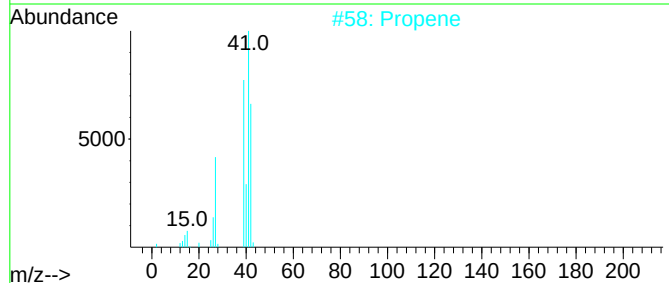
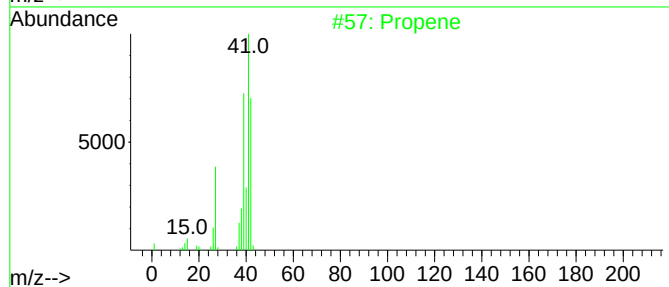
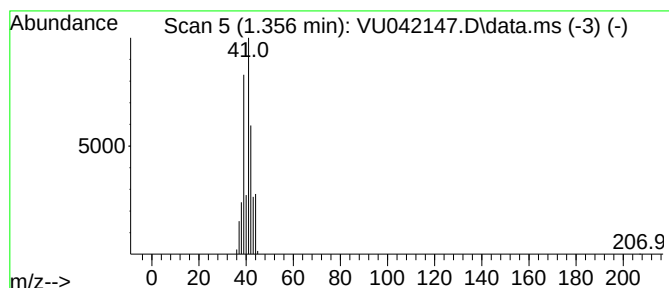
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.356	0.95 ug/L	54224	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	42
3			Cyclopropene	40	C3H4	002781-85-3	10
4			Cyclopropane	42	C3H6	000075-19-4	7
5			Cyclopropane	42	C3H6	000075-19-4	7



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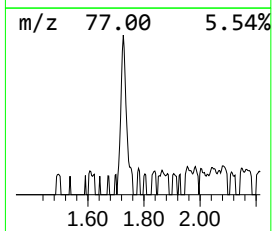
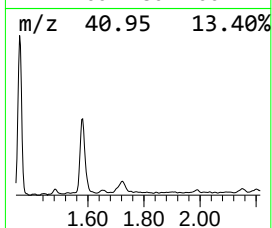
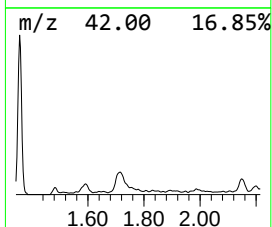
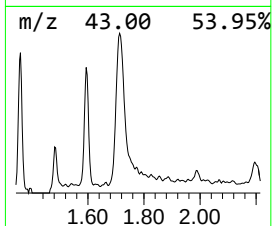
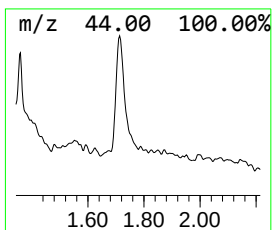
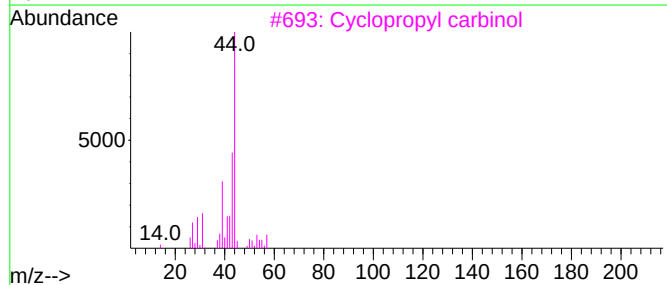
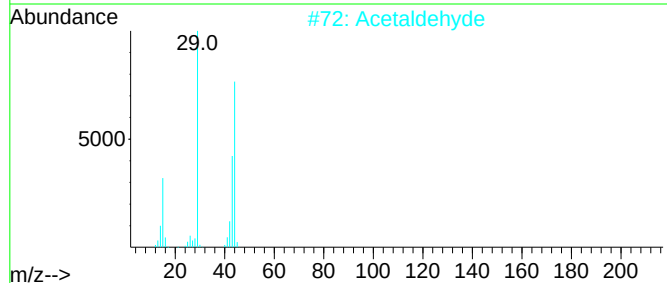
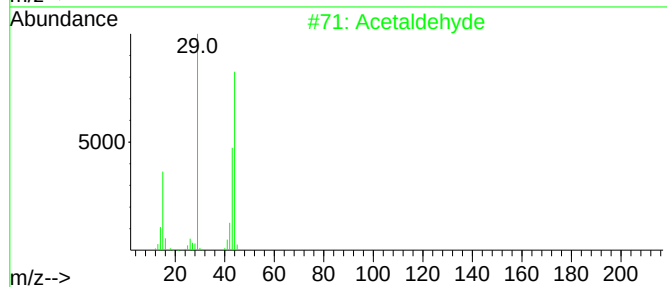
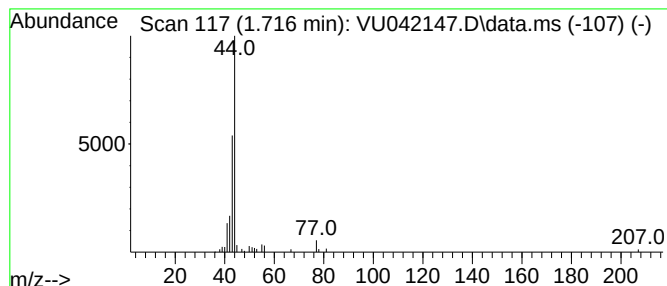
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 unknown-01 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.716	0.73 ug/L	41280	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	9
4			Phenethylamine, p,.alpha.-dimethyl-	149	C10H15N	000064-11-9	9
5			3-Hydroxy-N-methylphenethylamine	151	C9H13NO	1000335-06-7	9



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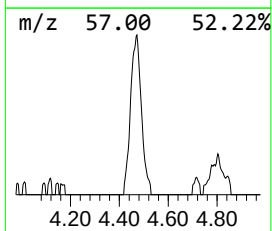
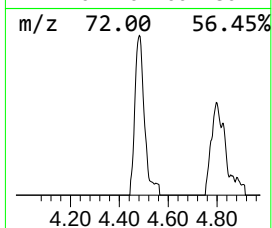
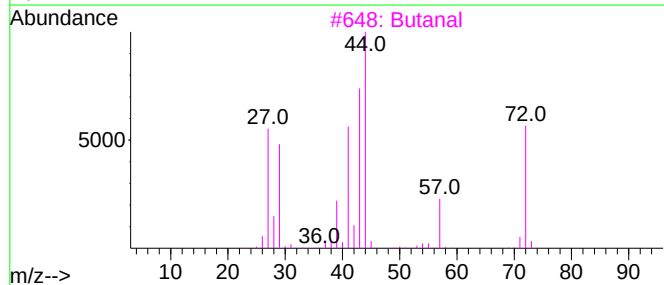
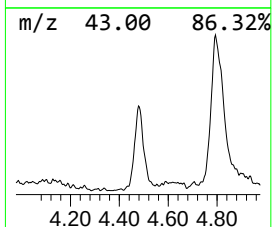
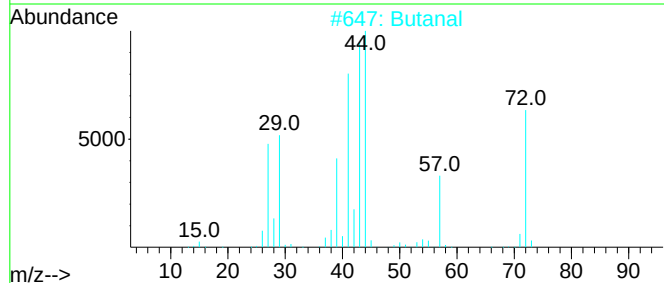
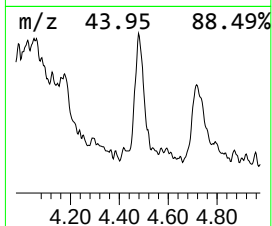
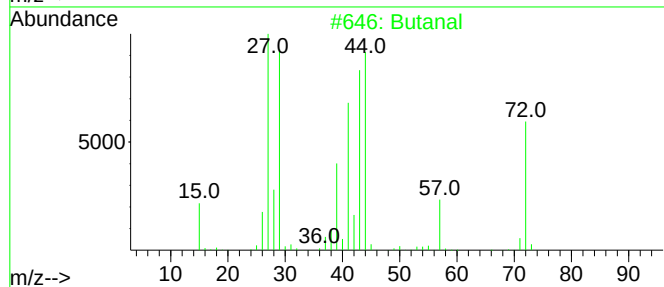
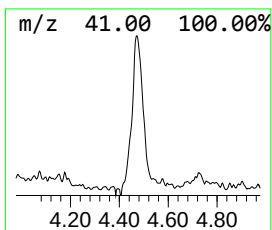
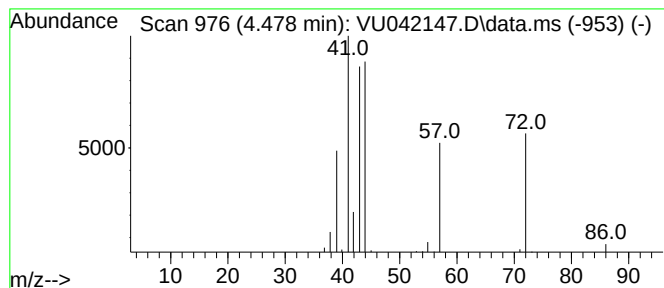
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Butanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.478	0.78 ug/L	44534	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	80
2			Butanal	72	C4H8O	000123-72-8	58
3			Butanal	72	C4H8O	000123-72-8	52
4			Butanal	72	C4H8O	000123-72-8	50
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38



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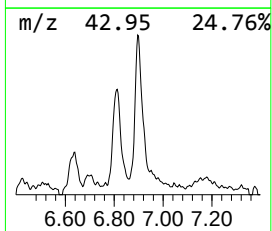
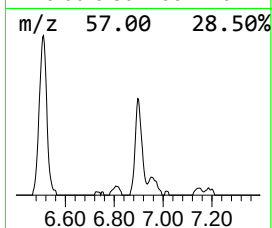
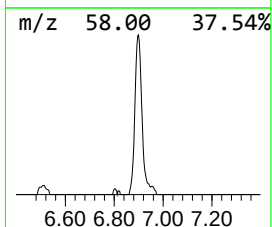
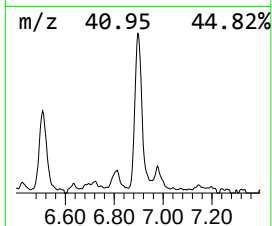
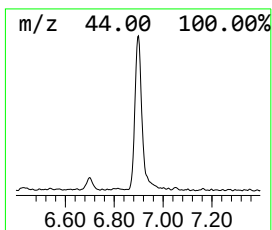
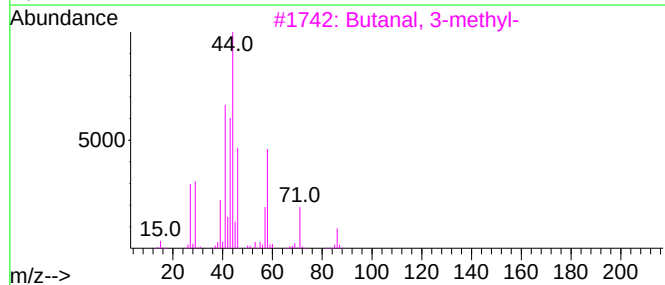
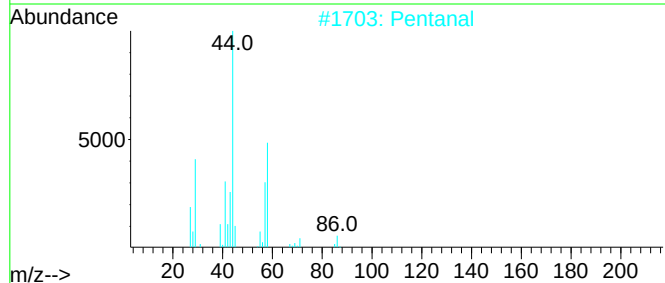
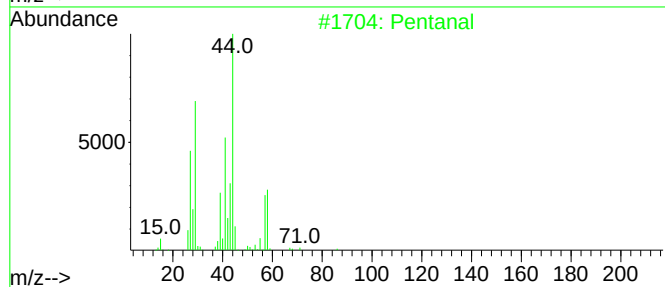
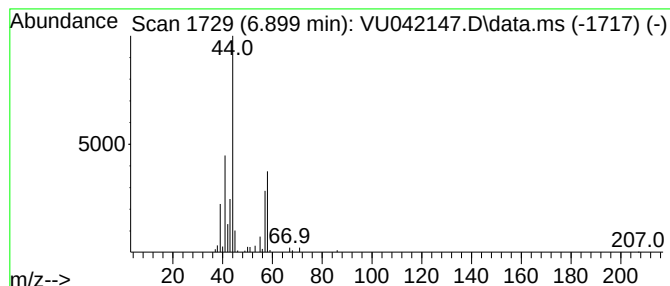
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.899	1.37 ug/L	77876	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	90
2	Pentanal			86	C5H10O	000110-62-3	78
3	Butanal, 3-methyl-			86	C5H10O	000590-86-3	74
4	Pentanal			86	C5H10O	000110-62-3	52
5	Butanal, 3-methyl-			86	C5H10O	000590-86-3	39



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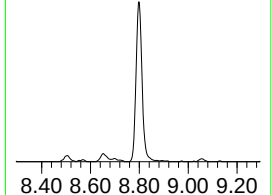
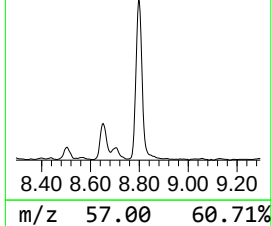
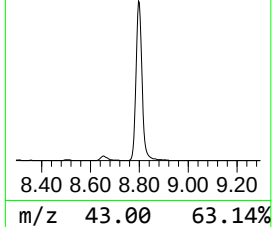
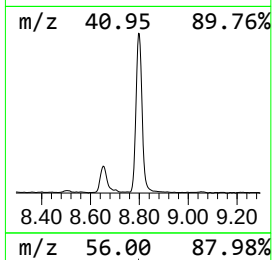
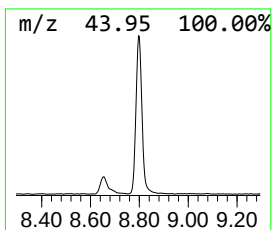
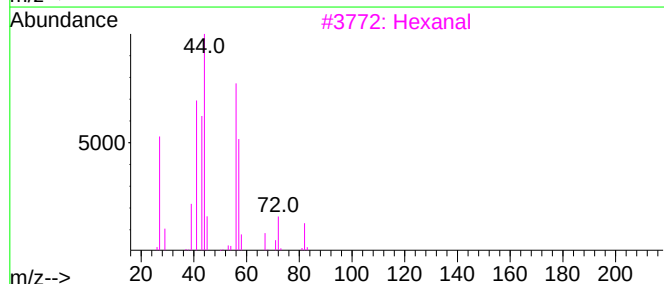
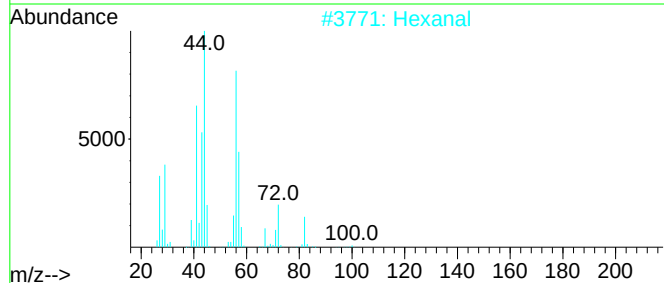
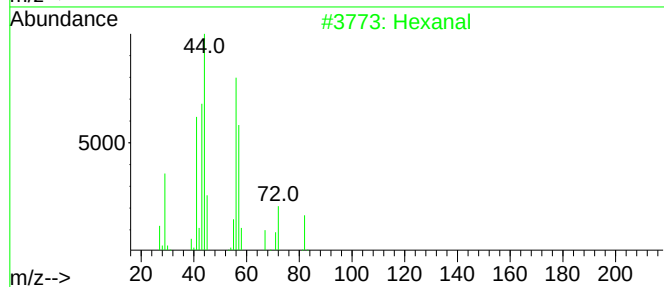
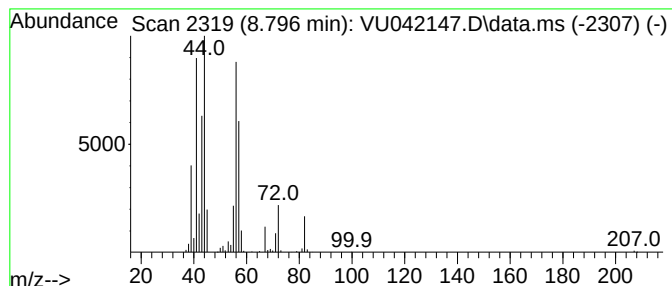
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.796	6.67 ug/L	449633	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	80
2	Hexanal			100	C6H12O	000066-25-1	80
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	72
5	Butanal			72	C4H8O	000123-72-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFT92

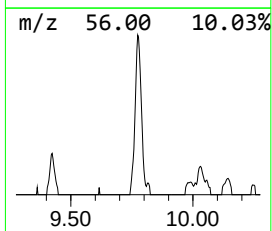
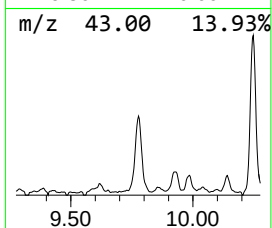
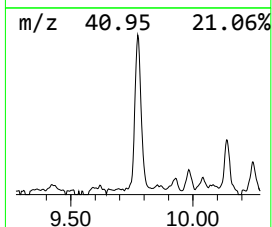
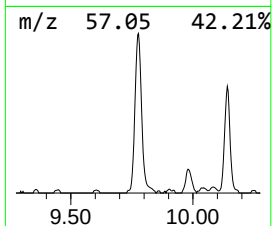
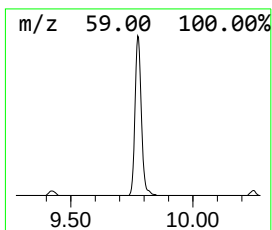
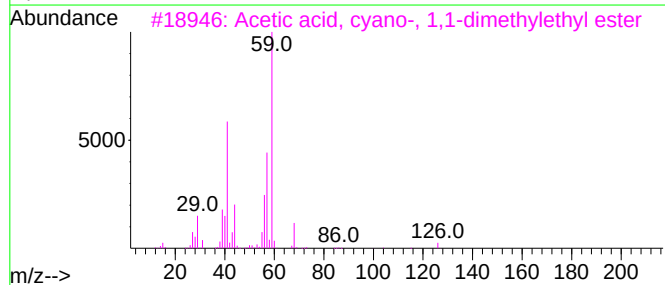
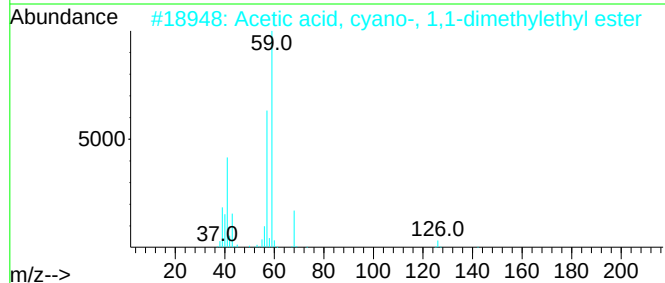
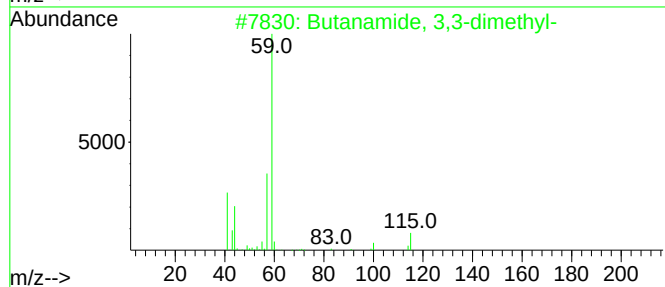
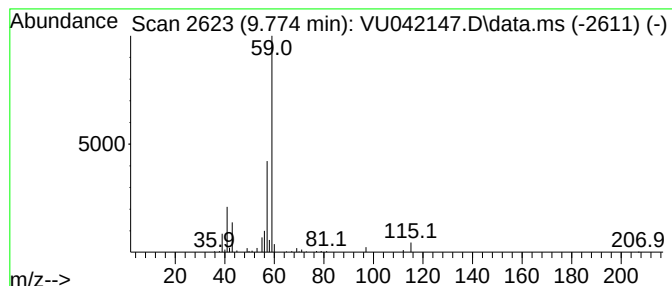
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Butanamide, 3,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.774	1.45 ug/L	97369	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	50
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	50
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
5			4-O-Acetyl-2,5-di-O-methyl-3,6-d...	215	C10H17NO4	1000101-80-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFT92

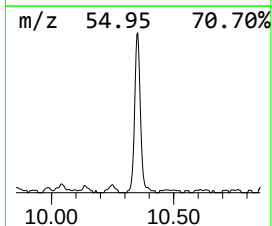
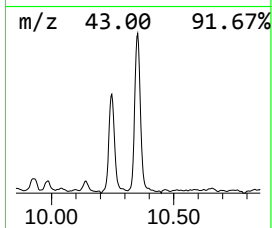
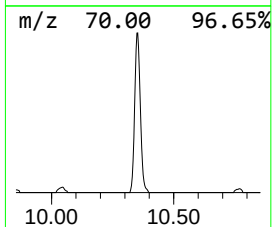
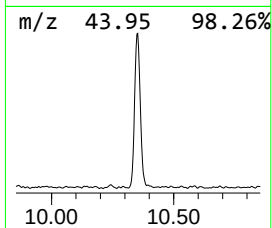
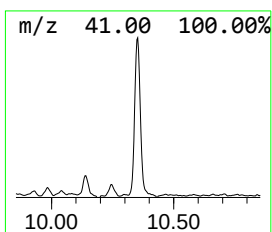
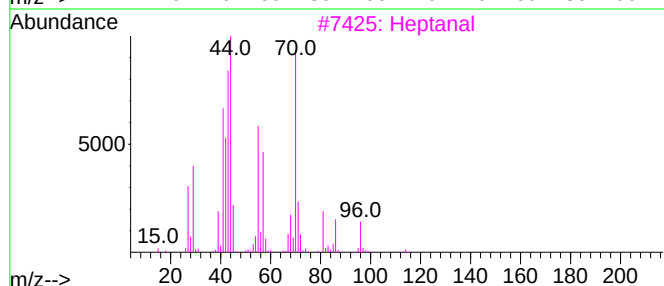
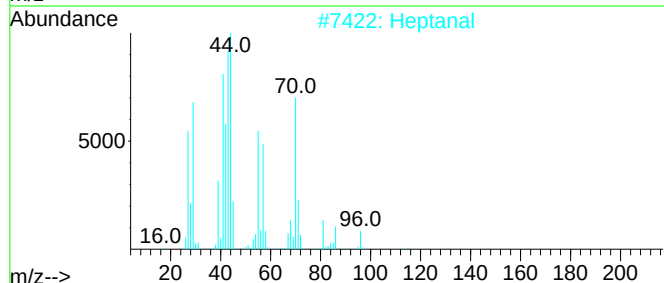
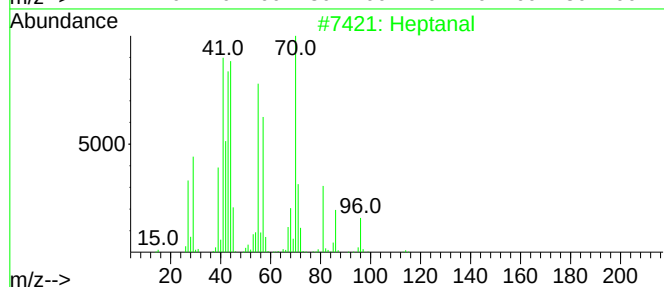
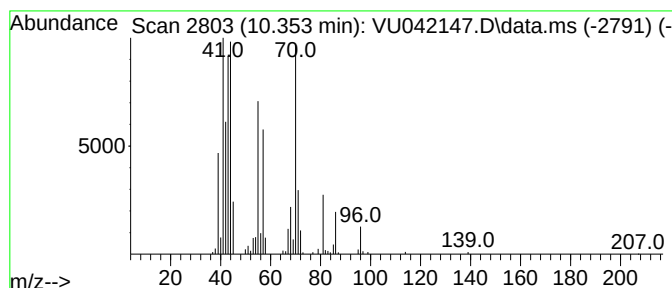
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.353	2.51 ug/L	169032	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	98
2	Heptanal			114	C7H14O	000111-71-7	93
3	Heptanal			114	C7H14O	000111-71-7	81
4	Heptanal			114	C7H14O	000111-71-7	81
5	Heptanal			114	C7H14O	000111-71-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFT92

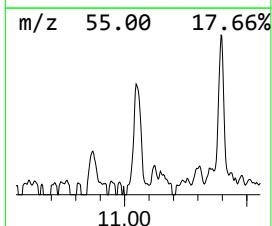
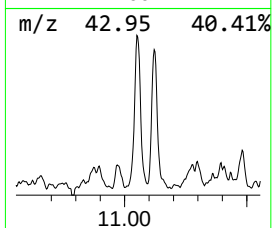
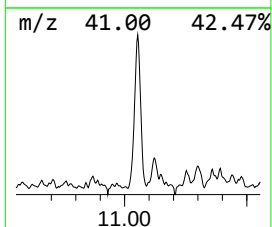
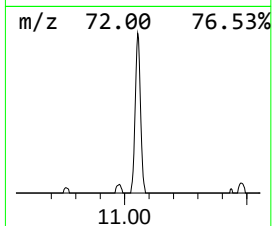
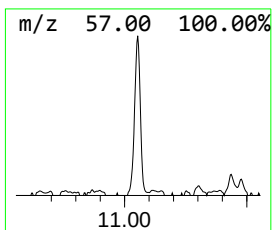
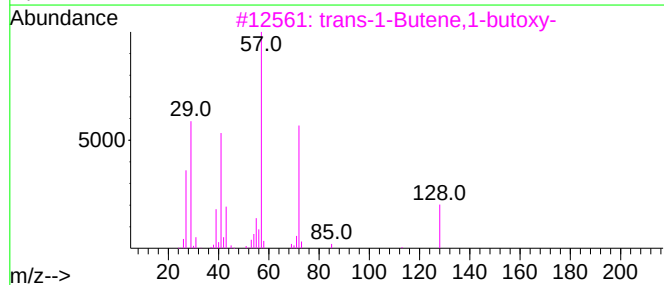
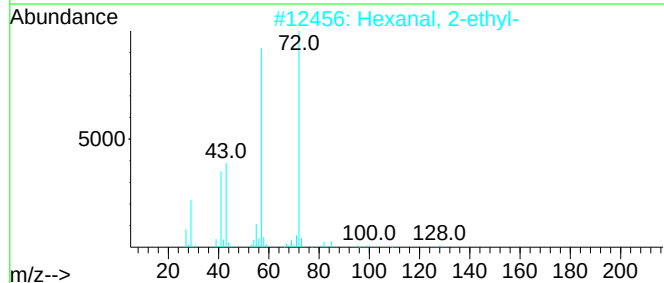
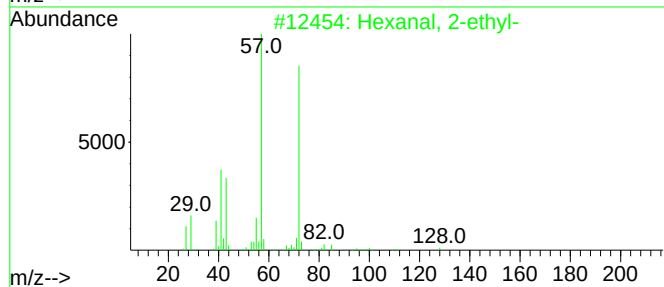
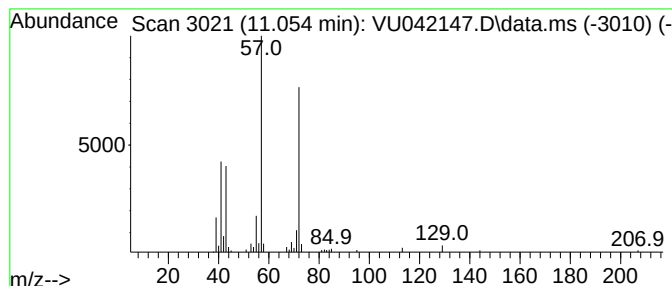
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Hexanal, 2-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.054	0.56 ug/L	39944	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	72
2			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	72
3			trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	72
4			Pentane, 1-(1-butenyloxy)-, (E)-	142	C9H18O	054004-25-0	64
5			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFT92

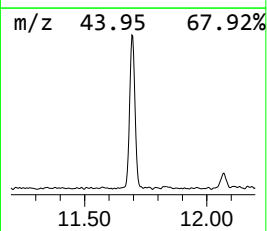
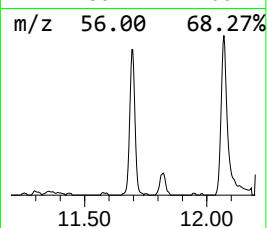
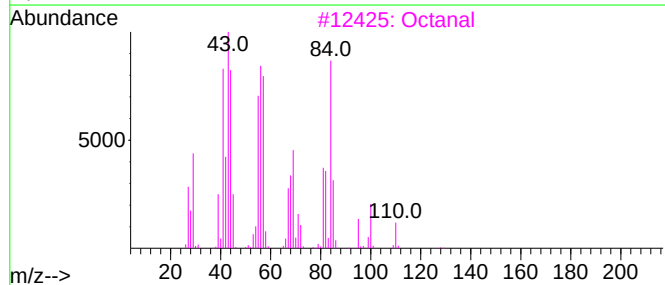
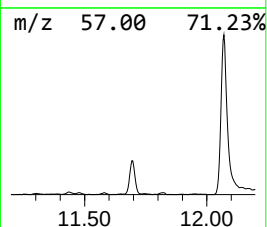
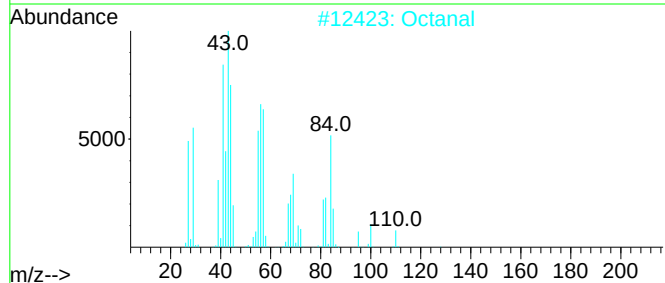
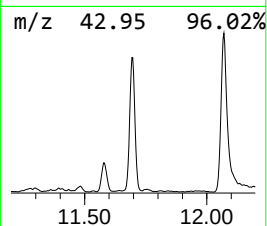
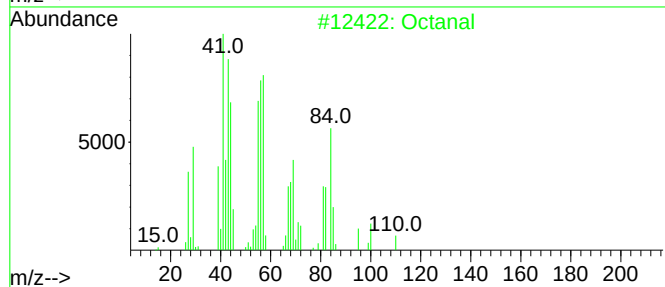
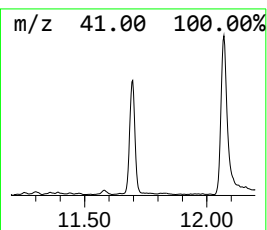
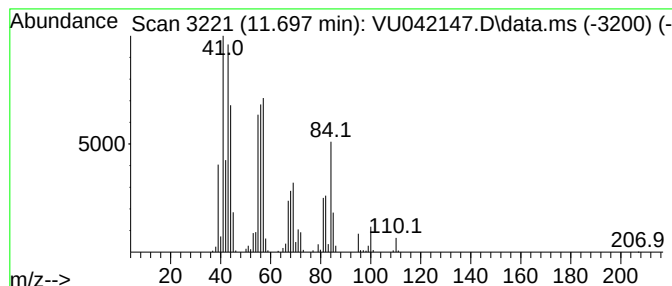
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Octanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.697	3.12 ug/L	221499	1,4-Dichlorobenzene-d4	11.819

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	91
4	Octanal			128	C8H16O	000124-13-0	87
5	Octanal			128	C8H16O	000124-13-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFT92

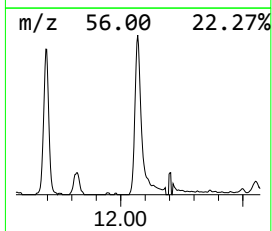
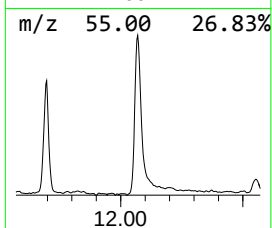
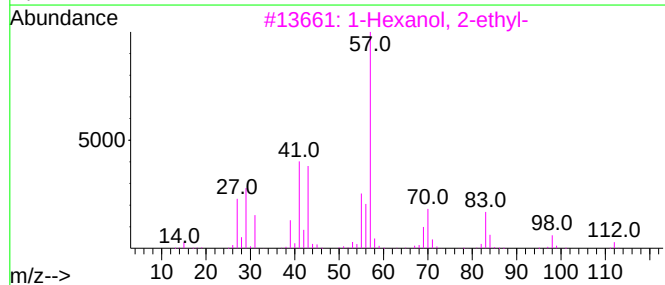
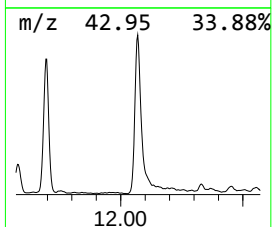
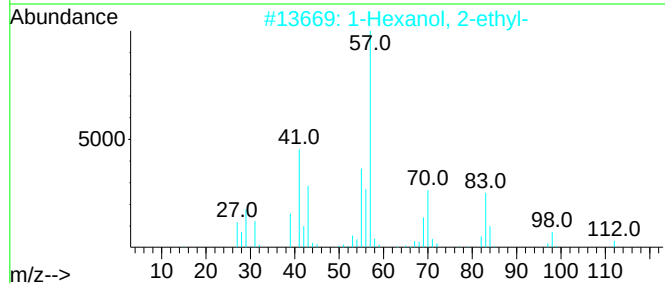
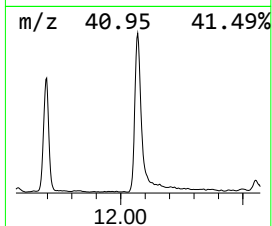
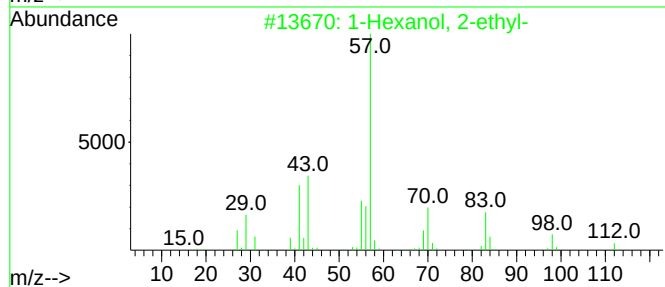
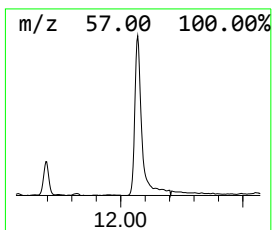
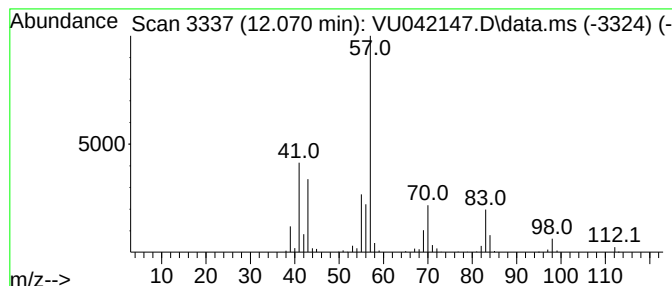
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	5.41 ug/L	383365	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
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ALS Vial : 11 Sample Multiplier: 1

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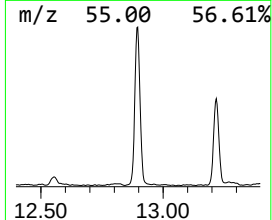
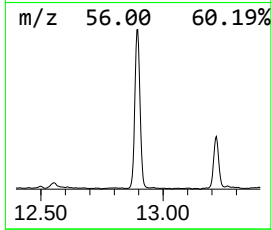
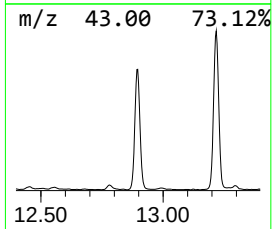
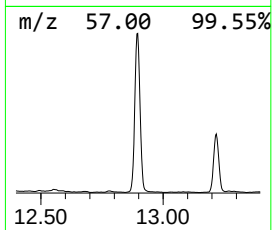
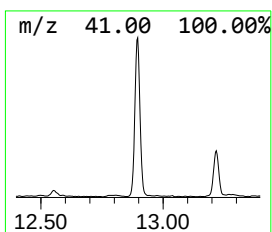
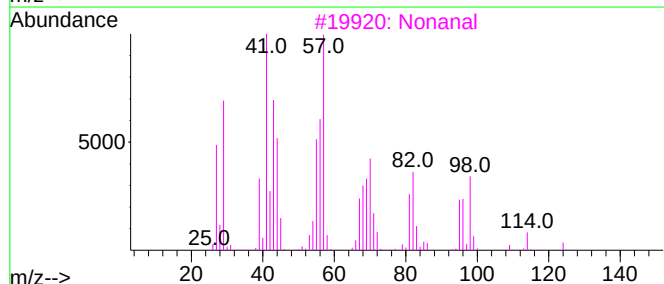
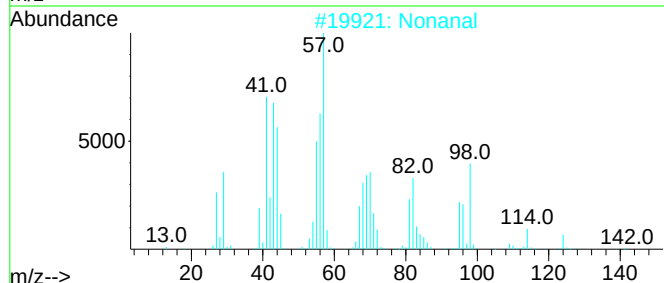
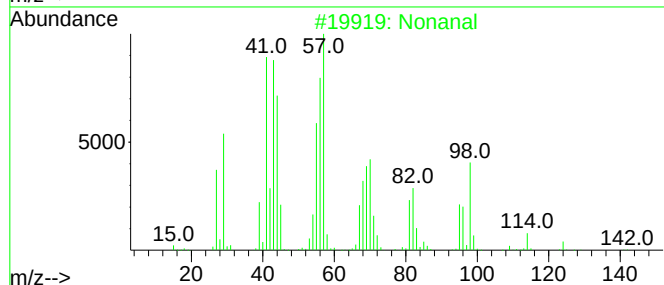
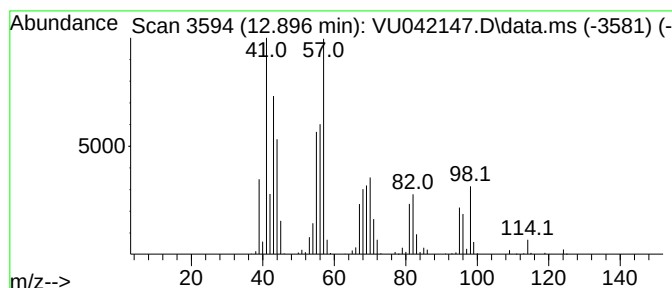
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 12 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.896	7.80 ug/L	553347	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal			142	C9H18O	000124-19-6	91
2	Nonanal			142	C9H18O	000124-19-6	90
3	Nonanal			142	C9H18O	000124-19-6	86
4	Nonanal			142	C9H18O	000124-19-6	80
5	Hexanal			100	C6H12O	000066-25-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

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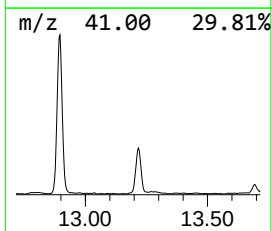
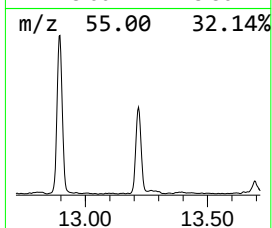
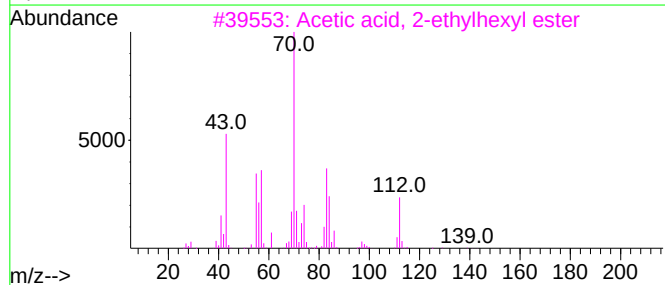
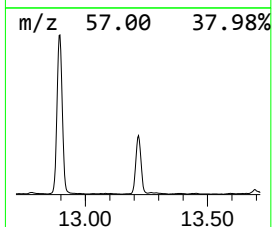
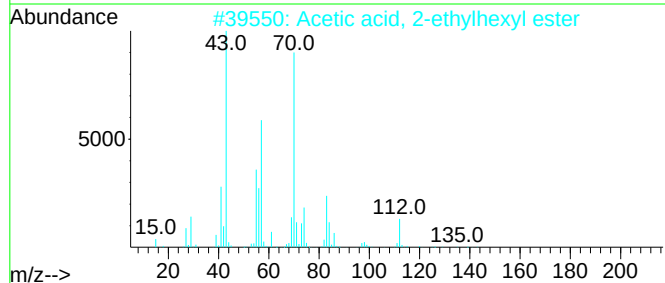
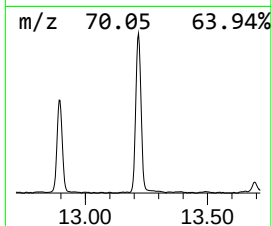
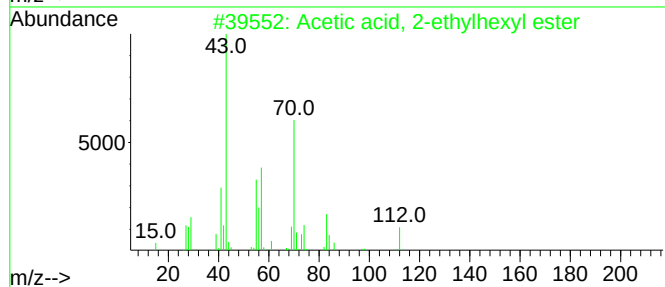
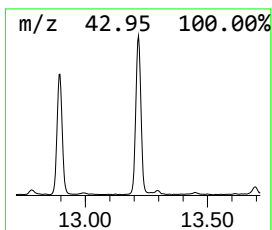
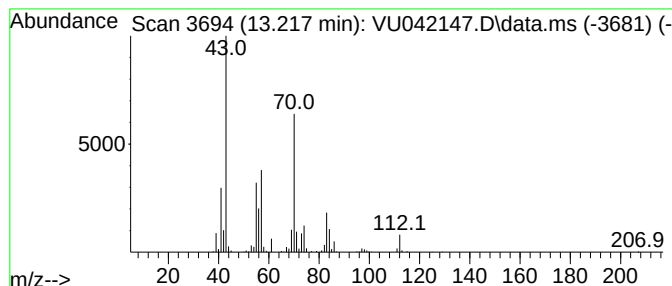
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 13 Acetic acid, 2-ethylhexyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.217	3.66 ug/L	259475	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	91
2			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	91
3			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	83
4			3-Methylheptyl acetate	172	C10H20O2	072218-58-7	78
5			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
Data File : VU042147.D
Acq On : 21 Jan 2021 13:48
Operator : SY/MD
Sample : M1170-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFT92

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.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
(DEL) Alkane: S...	1.356	0.9	ug/L	54224	1	6.256	284604	5.0
unknown-01	1.716	0.7	ug/L	41280	1	6.256	284604	5.0
Butanal	4.478	0.8	ug/L	44534	1	6.256	284604	5.0
Pentanal	6.899	1.4	ug/L	77876	1	6.256	284604	5.0
Hexanal	8.796	6.7	ug/L	449633	2	9.423	336856	5.0
Butanamide, 3,3...	9.774	1.5	ug/L	97369	2	9.423	336856	5.0
Heptanal	10.353	2.5	ug/L	169032	2	9.423	336856	5.0
Hexanal, 2-ethyl-	11.054	0.6	ug/L	39944	3	11.819	354515	5.0
Octanal	11.697	3.1	ug/L	221499	3	11.819	354515	5.0
1-Hexanol, 2-et...	12.070	5.4	ug/L	383365	3	11.819	354515	5.0
Nonanal	12.896	7.8	ug/L	553347	3	11.819	354515	5.0
Acetic acid, 2-...	13.217	3.7	ug/L	259475	3	11.819	354515	5.0