

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
 Data File : VX033853.D
 Acq On : 23 Jan 2023 16:43
 Operator : JC/MD
 Sample : 01251-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-1

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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_X\Method\82X011123W.M
 Title : SW846 8260

Signal : TIC: VX033853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.788	271	279	314	rBV	6051774	13065472	100.00%	59.654%
2	5.385	693	705	720	rBV2	83524	245541	1.88%	1.121%
3	5.550	720	732	749	rVB	149035	429037	3.28%	1.959%
4	5.952	789	798	814	rBV	84932	225315	1.72%	1.029%
5	6.336	852	861	879	rBV2	61027	162754	1.25%	0.743%
6	6.763	921	931	944	rBV	226583	574774	4.40%	2.624%
7	7.799	1093	1101	1121	rBV	871893	1552922	11.89%	7.090%
8	8.549	1217	1224	1234	rBV	181614	294019	2.25%	1.342%
9	8.647	1234	1240	1256	rVB	455179	730048	5.59%	3.333%
10	8.952	1284	1290	1301	rBV	260309	377580	2.89%	1.724%
11	9.244	1332	1338	1345	rBV	251672	357092	2.73%	1.630%
12	9.372	1356	1359	1369	rVB	99107	150479	1.15%	0.687%
13	9.482	1372	1377	1388	rVV	477924	613181	4.69%	2.800%
14	9.580	1388	1393	1408	rVB	310241	417561	3.20%	1.906%
15	9.915	1442	1448	1463	rBV	790186	1059771	8.11%	4.839%
16	10.055	1463	1471	1478	rBV	446802	623416	4.77%	2.846%
17	11.079	1634	1639	1651	rBV	363656	468160	3.58%	2.138%
18	12.018	1788	1793	1806	rBV	421807	554937	4.25%	2.534%

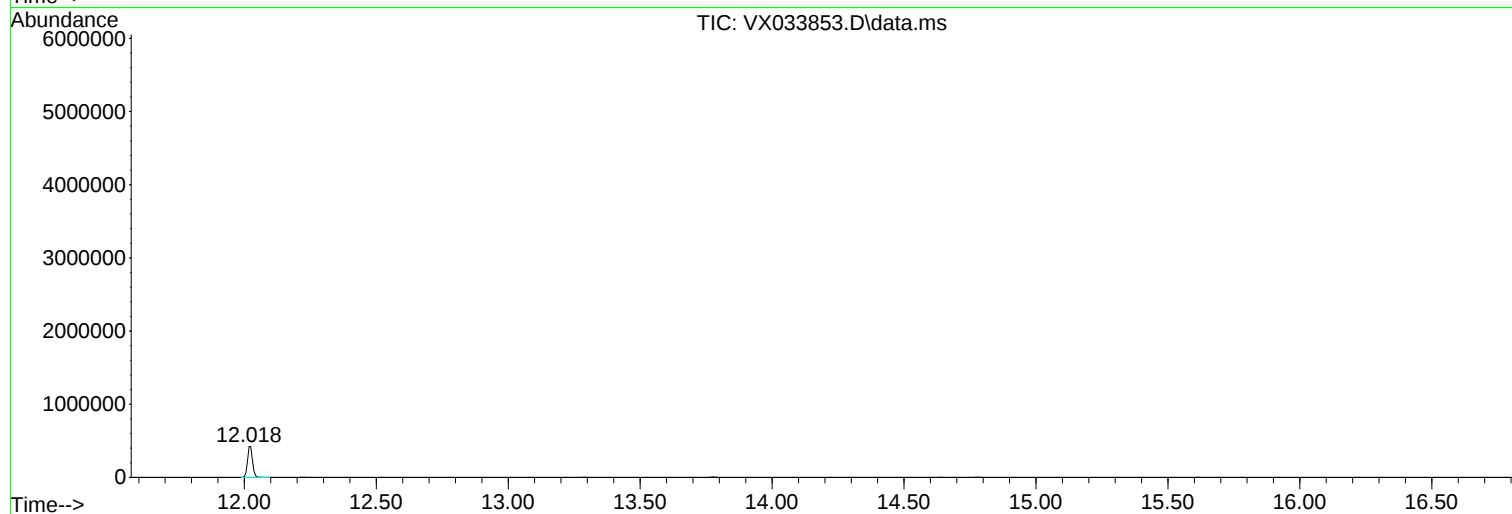
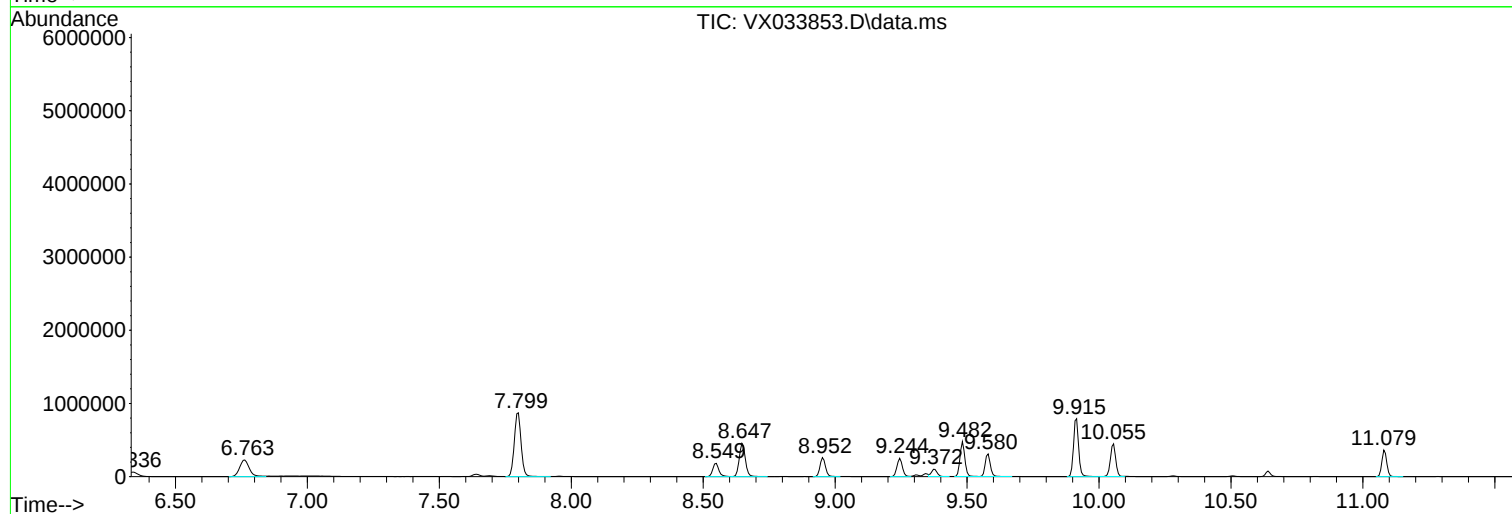
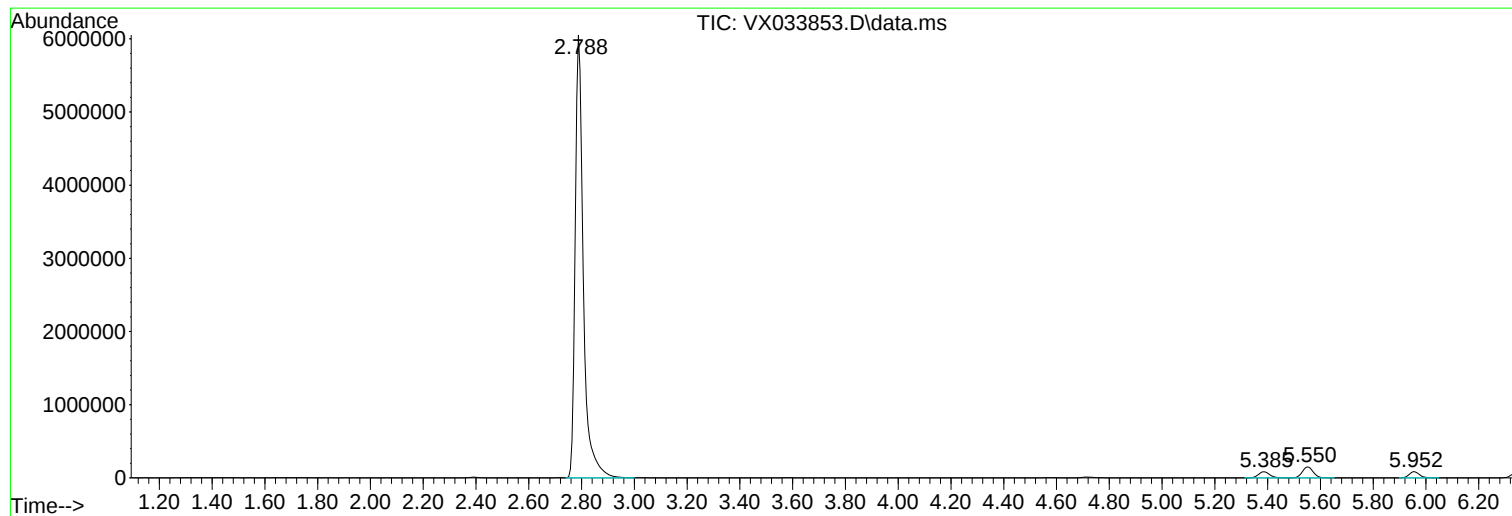
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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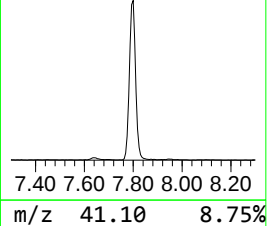
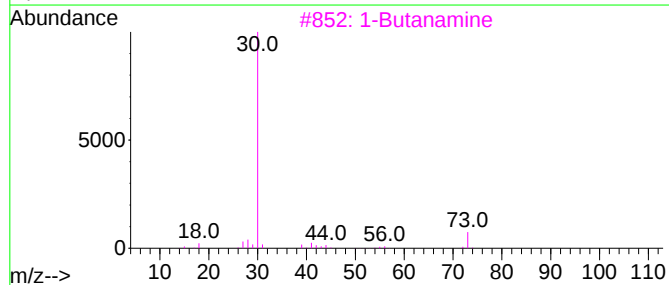
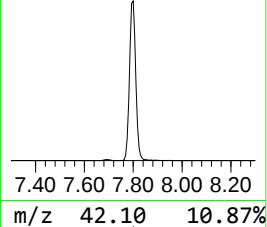
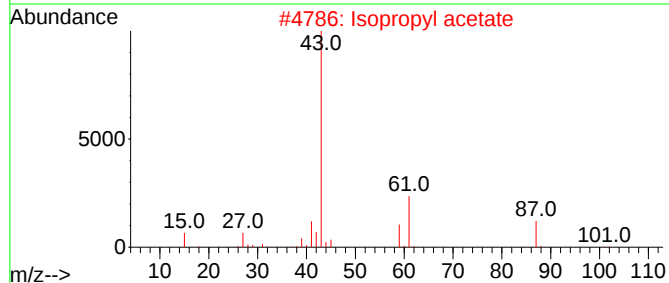
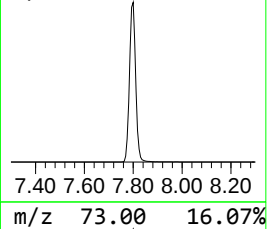
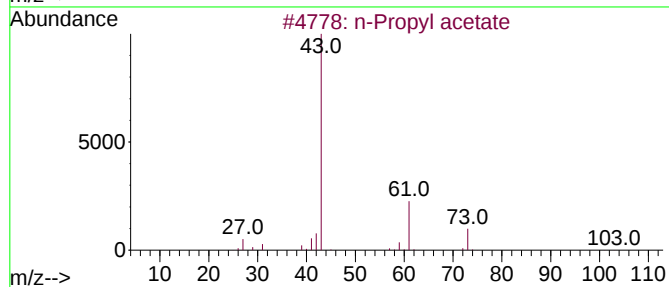
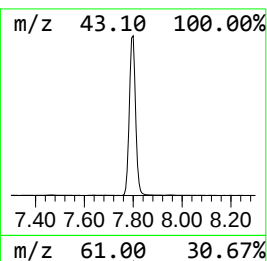
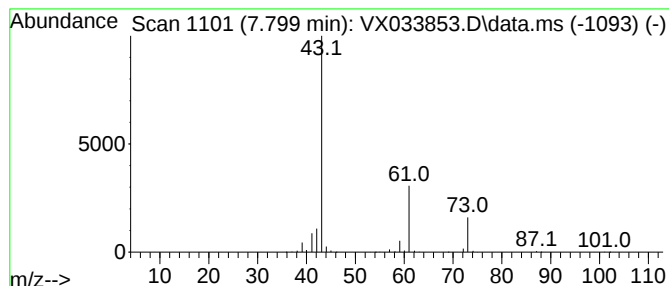
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	135.09 ug/l	1552920	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	36
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4



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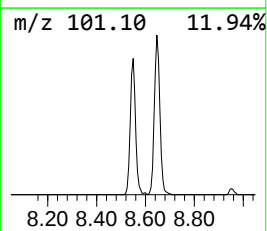
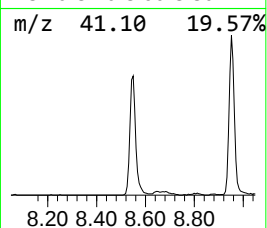
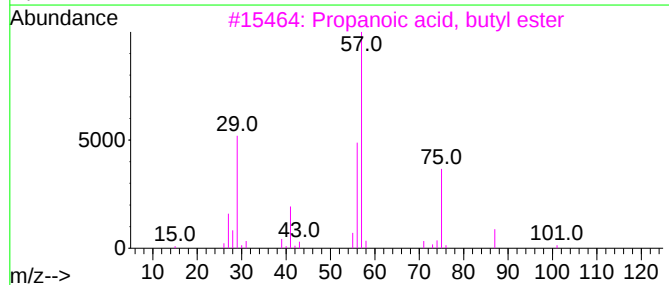
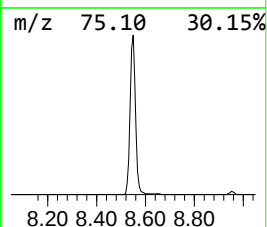
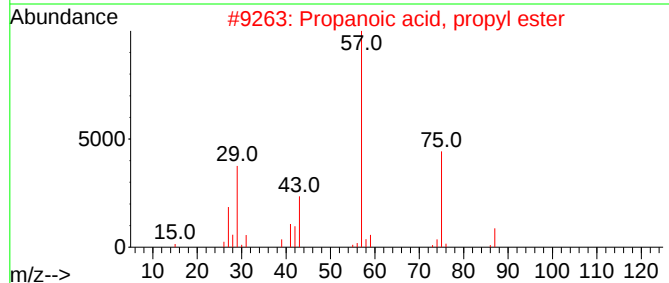
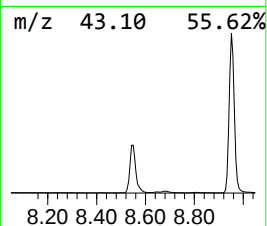
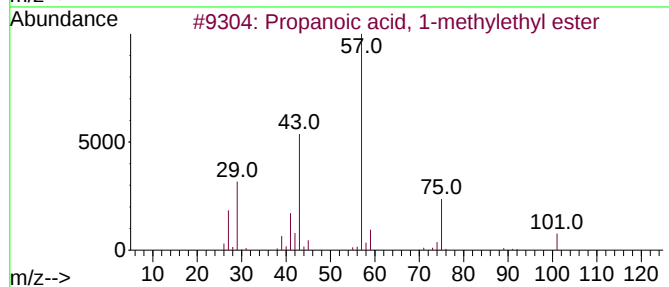
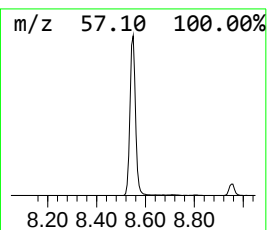
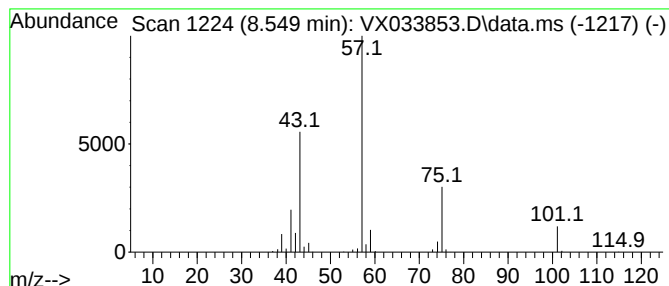
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Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	23.58 ug/l	294019	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	9



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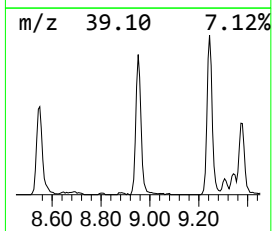
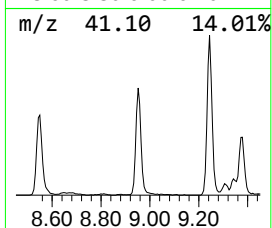
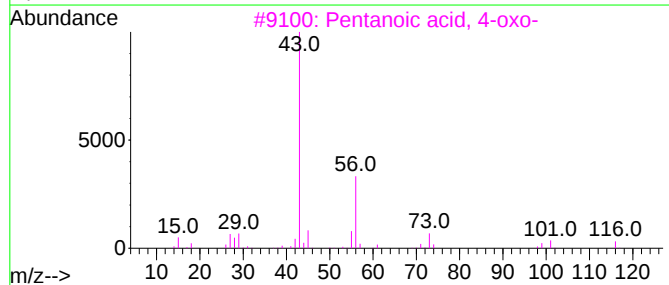
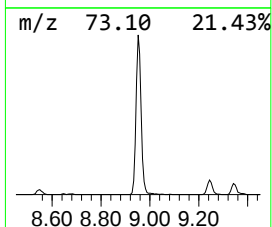
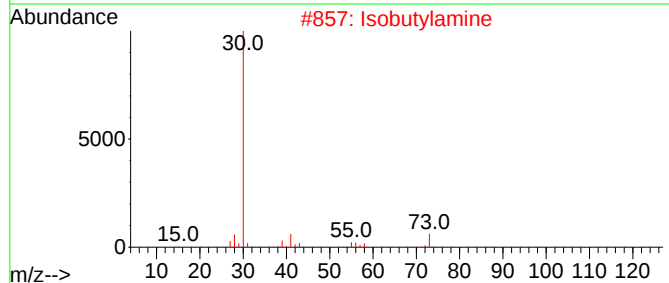
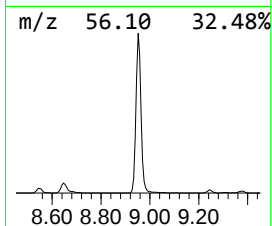
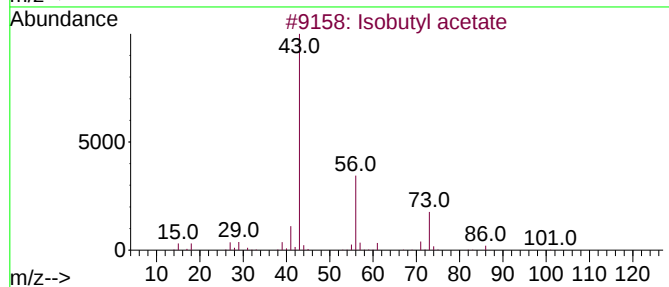
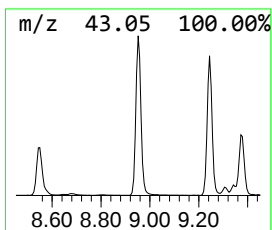
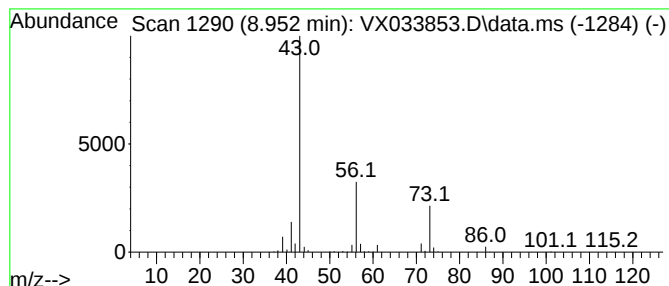
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Peak Number 3 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	30.28 ug/l	377580	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl acetate	116	C6H12O2	000110-19-0	83
2			Isobutylamine	73	C4H11N	000078-81-9	9
3			Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5			2-Pentanone	86	C5H10O	000107-87-9	9



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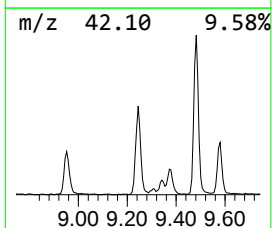
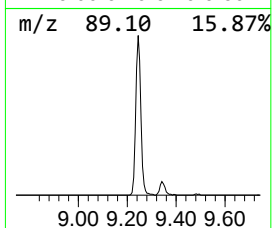
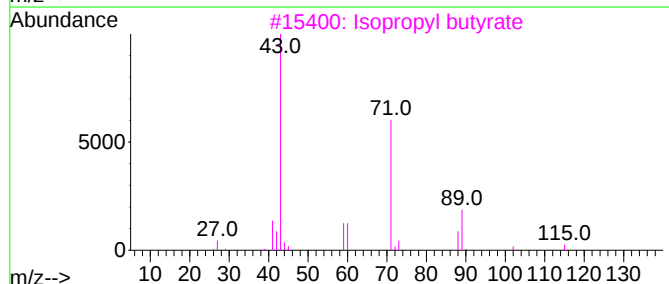
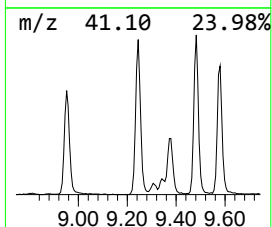
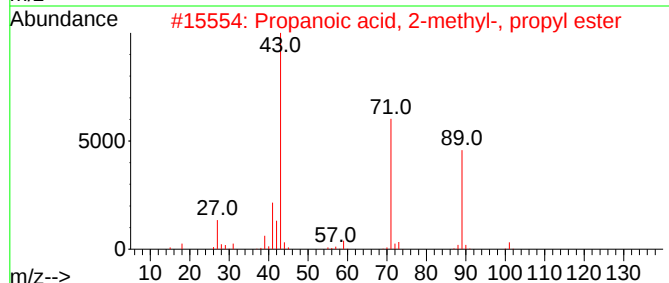
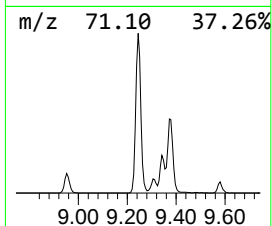
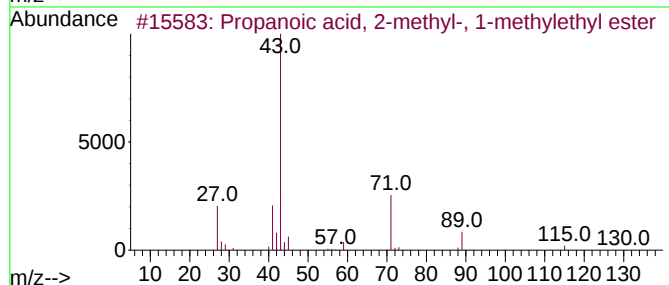
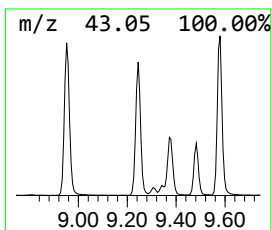
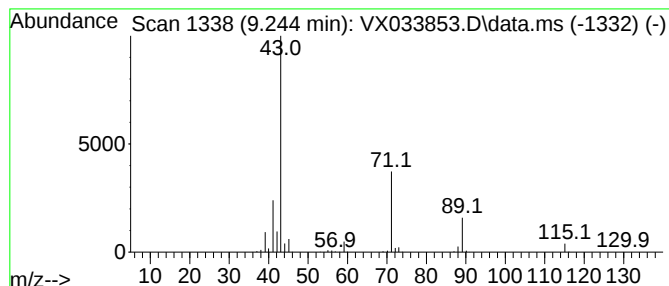
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	28.64 ug/l	357092	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	56
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	40
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38



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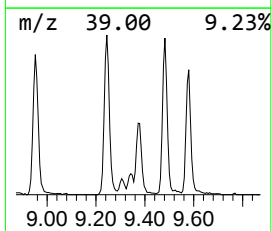
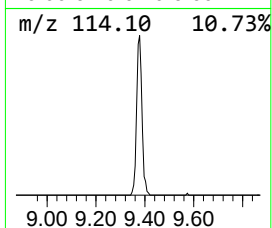
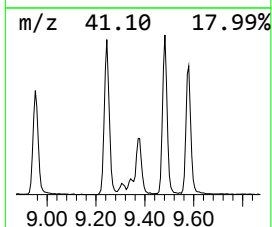
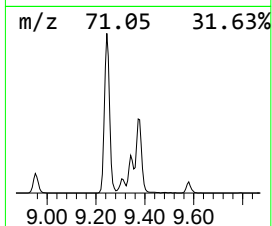
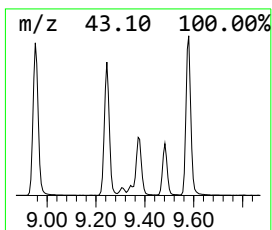
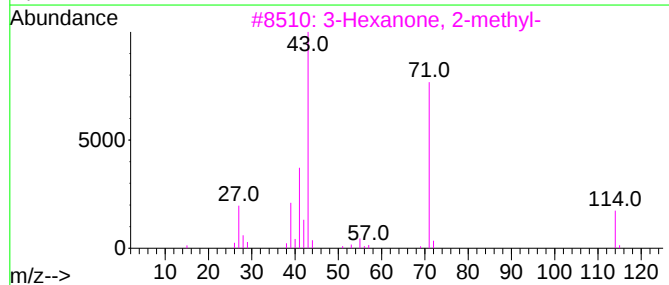
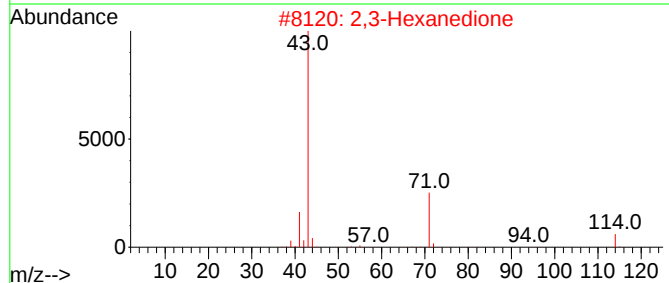
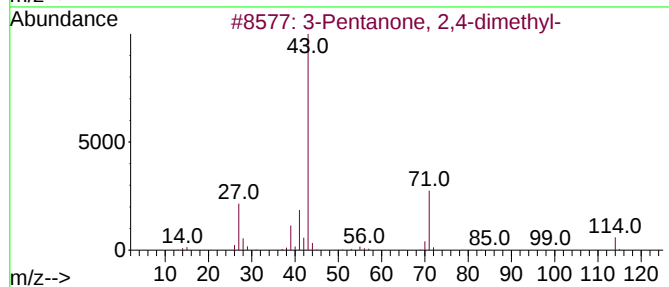
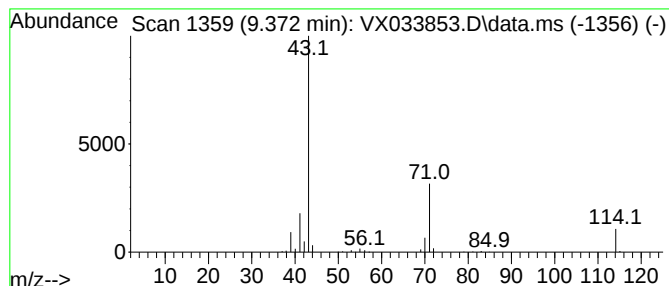
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Peak Number 5 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.372	12.07 ug/l	150479	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2			2,3-Hexanedione	114	C6H10O2	003848-24-6	72
3			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	50
4			4-Heptanone	114	C7H14O	000123-19-3	40
5			Butane, 2-(ethenyloxy)-2-methyl-	114	C7H14O	029281-39-8	39



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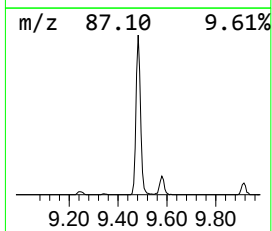
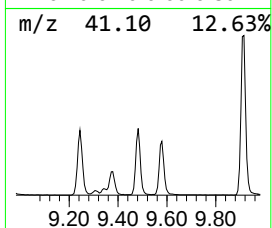
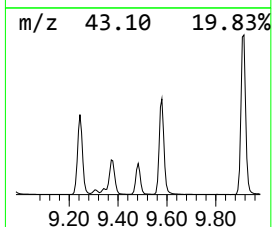
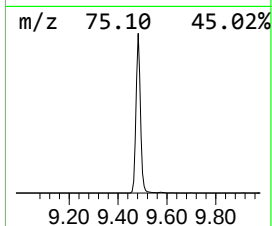
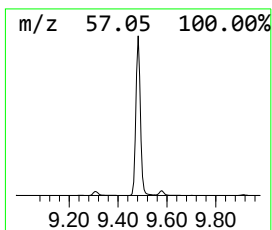
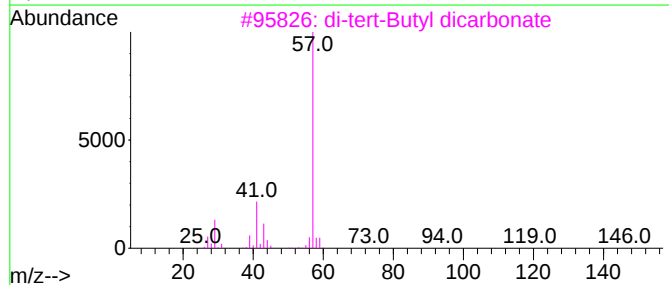
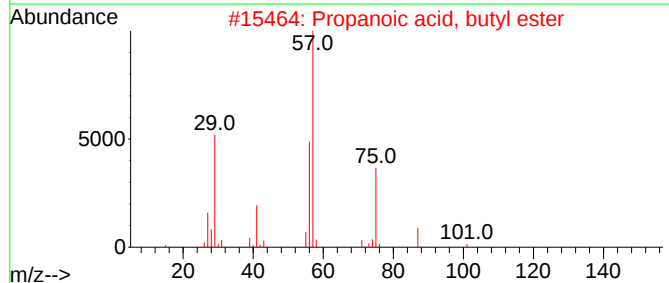
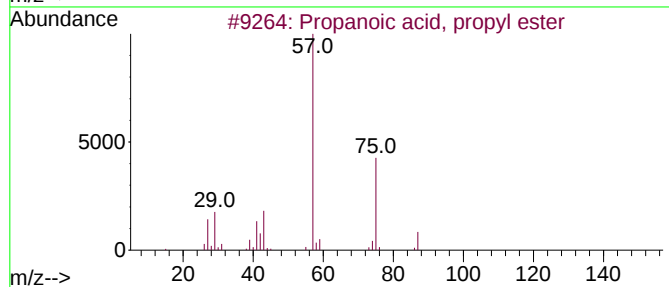
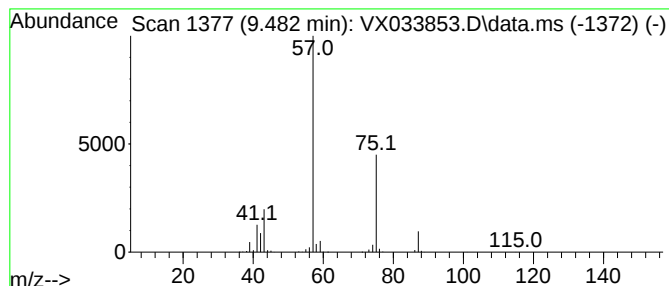
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	49.18 ug/l	613181	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5			S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033853.D
Acq On : 23 Jan 2023 16:43
Operator : JC/MD
Sample : 01251-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

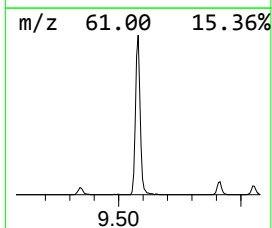
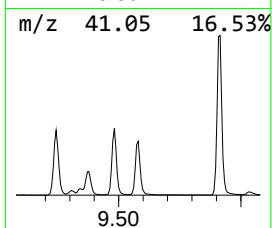
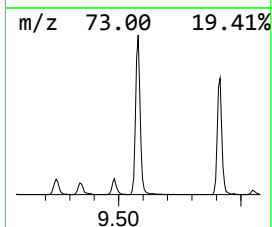
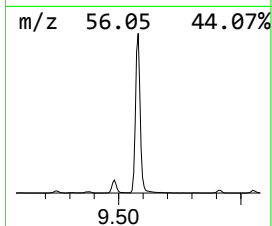
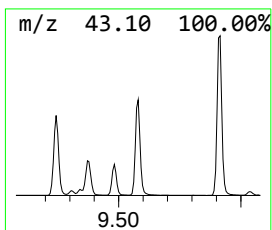
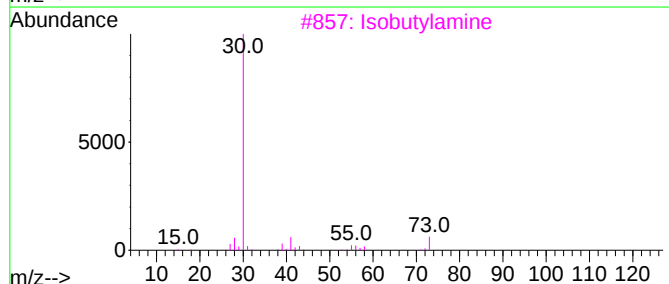
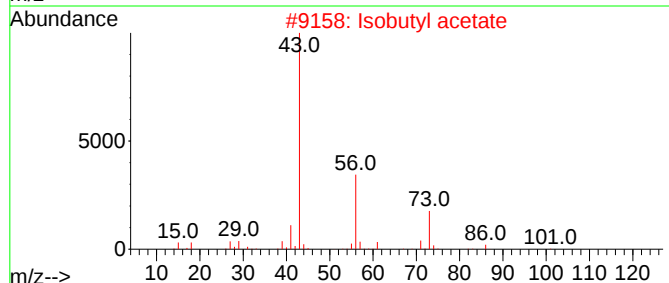
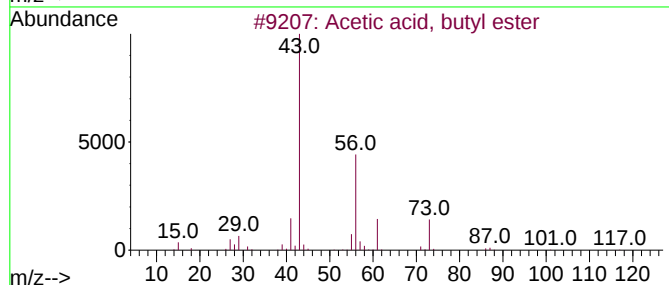
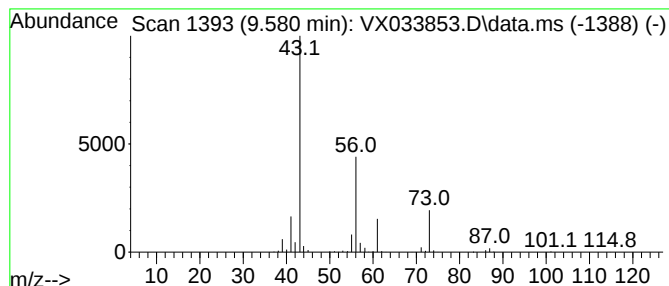
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	33.49 ug/l	417561	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	56
3			Isobutylamine	73	C4H11N	000078-81-9	9
4			Isopropyl acetate	102	C5H10O2	000108-21-4	9
5			Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033853.D
Acq On : 23 Jan 2023 16:43
Operator : JC/MD
Sample : 01251-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

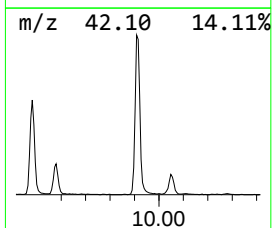
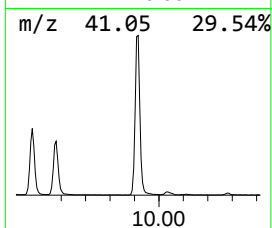
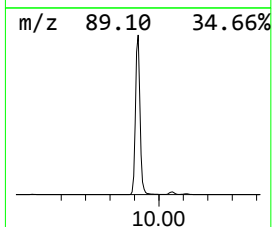
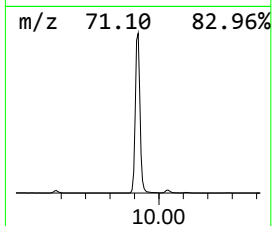
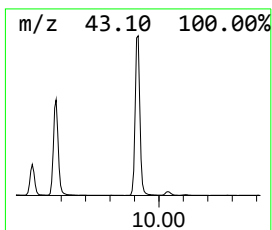
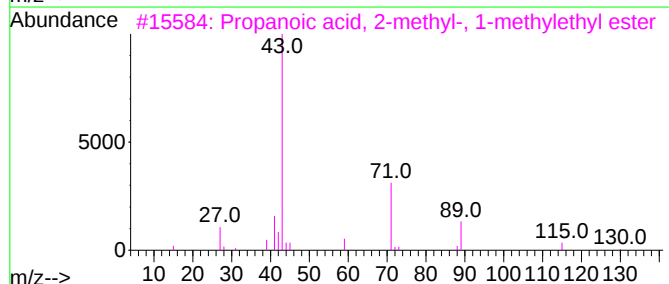
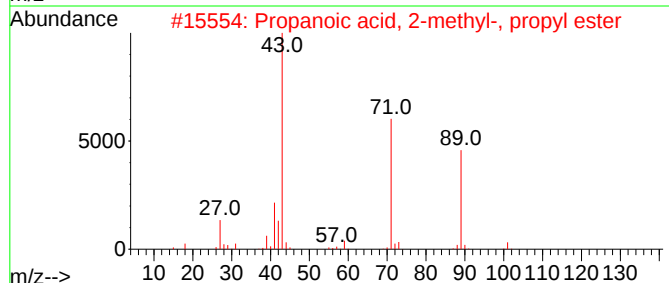
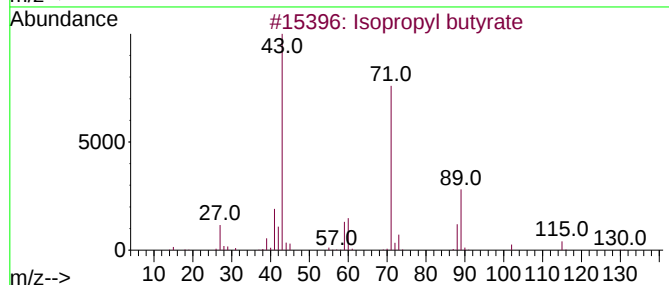
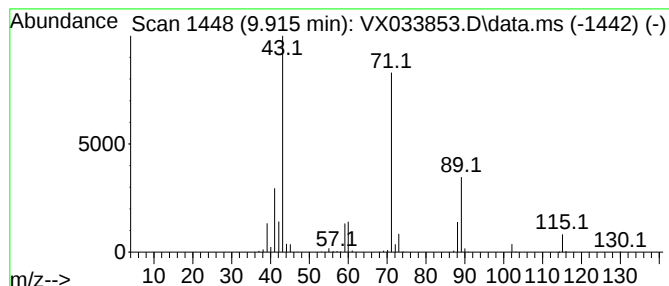
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	85.00 ug/l	1059770	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	97
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033853.D
Acq On : 23 Jan 2023 16:43
Operator : JC/MD
Sample : 01251-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.799	135.1	ug/l	1552920	2	6.763	574774	50.0
Propanoic acid,...	8.549	23.6	ug/l	294019	3	10.055	623416	50.0
Isobutyl acetate	8.952	30.3	ug/l	377580	3	10.055	623416	50.0
Propanoic acid,...	9.244	28.6	ug/l	357092	3	10.055	623416	50.0
3-Pentanone, 2,...	9.372	12.1	ug/l	150479	3	10.055	623416	50.0
Propanoic acid,...	9.482	49.2	ug/l	613181	3	10.055	623416	50.0
Acetic acid, bu...	9.580	33.5	ug/l	417561	3	10.055	623416	50.0
Isopropyl butyrate	9.915	85.0	ug/l	1059770	3	10.055	623416	50.0