LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033854.D
Acq On : 23 Jan 2023 17:06
Operator : JC/MD
Sample : 01251-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-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: VX033854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	205	214	224	rBV	11601	23655	1.51%	0.257%
2	2.788	273	279	291	rBV	21518	42860	2.74%	0.465%
3	4.721	586	596	608	rBV2	10670	32546	2.08%	0.353%
4	5.385	694	705	721	rBV2	84078	245031	15.65%	2.661%
5	5.550	721	732	746	rVV	149135	426487	27.23%	4.631%
6	5.952	788	798	814	rBV	82252	223866	14.30%	2.431%
7	6.336	849	861	877	rBV	63855	166930	10.66%	1.813%
8	6.763	921	931	946	rBV	222784	572221	36.54%	6.214%
9	7.641	1064	1075	1080	rBV	34292	65463	4.18%	0.711%
10	7.690	1080	1083	1093	rVV	11520	22221	1.42%	0.241%
11	7.793	1093	1100	1122	rVV	887419	1565992	100.00%	17.005%
12	8.549	1217	1224	1234	rBV	187783	302057	19.29%	3.280%
13	8.647	1234	1240	1256	rVB	465225	721017	46.04%	7.830%
14	8.952	1284	1290	1302	rBV	265236	383697	24.50%	4.167%
15	9.244	1332	1338	1345	rBV	272722	378077	24.14%	4.106%
16	9.305	1345	1348	1351	rVV	24391	34627	2.21%	0.376%
17	9.342	1351	1354	1356	rVV	42009	55247	3.53%	0.600%
18	9.372	1356	1359	1368	rVV	103852	158265	10.11%	1.719%
19	9.482	1372	1377	1388	rVV	467459	615228	39.29%	6.681%
20	9.580	1388	1393	1408	rVB	311766	417920	26.69%	4.538%
21	9.915	1442	1448	1463	rBV	812885	1072404	68.48%	11.645%
22	10.055	1463	1471	1477	rBV	444710	614903	39.27%	6.677%
23	10.640	1562	1567	1579	rBV	70881	93723	5.98%	1.018%
24	11.079	1634	1639	1647	rBV	356902	452227	28.88%	4.911%
25	12.018	1788	1793	1803	rBV	405913	522110	33.34%	5.670%

Sum of corrected areas: 9208774

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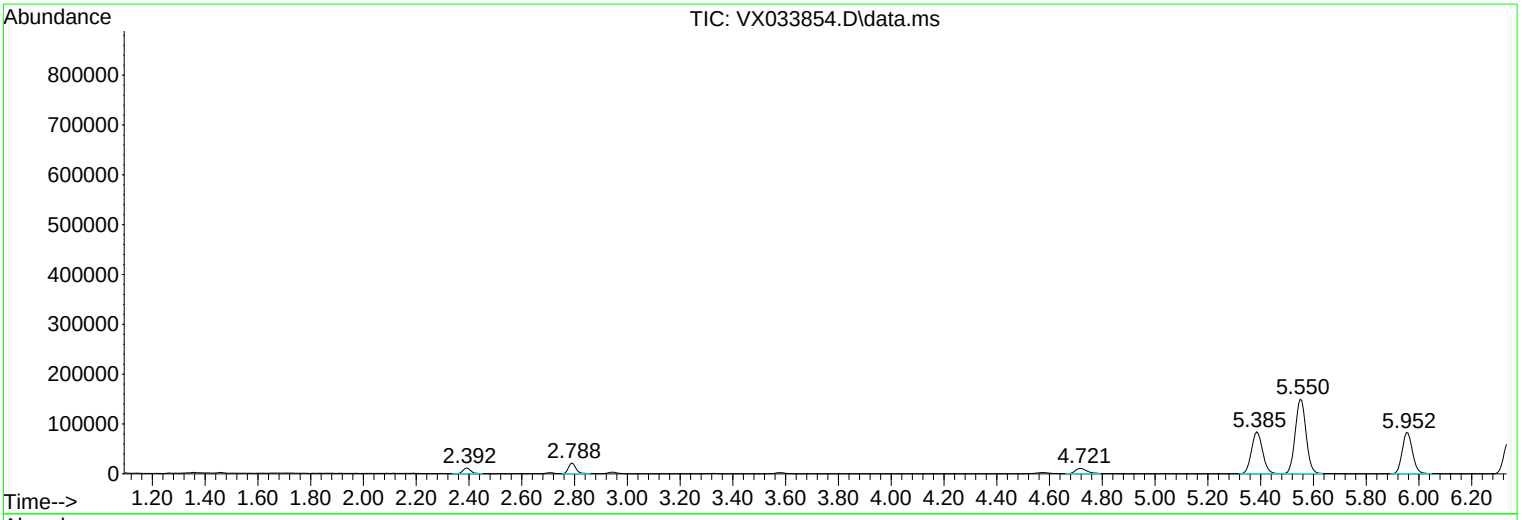
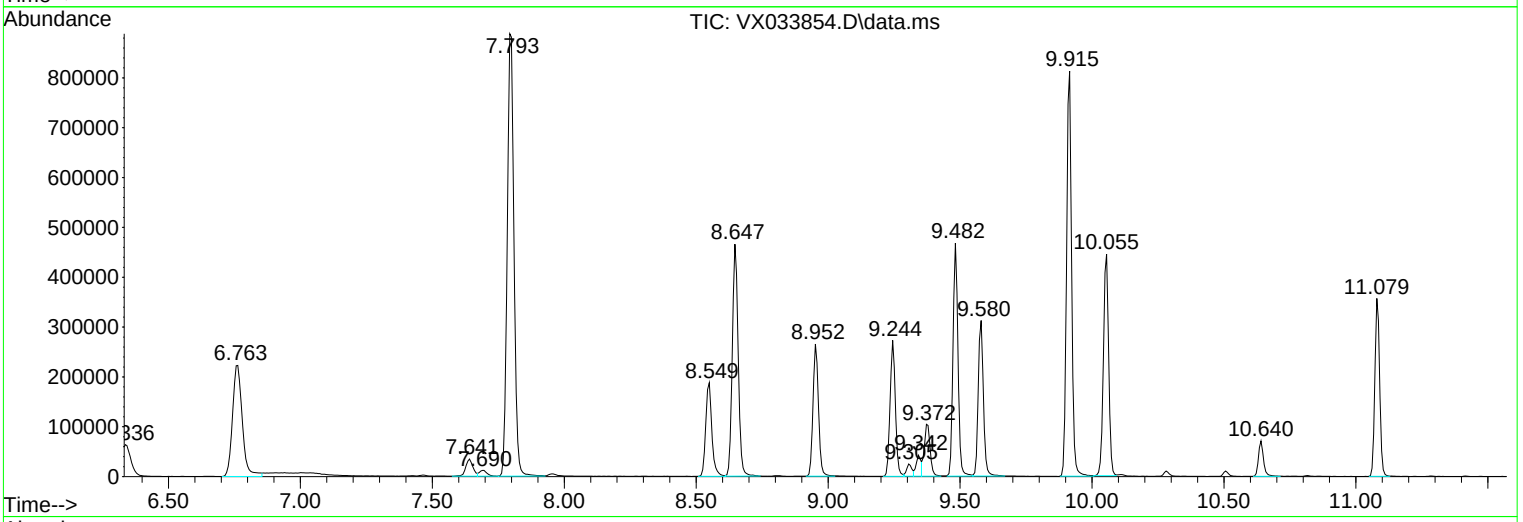
ALS Vial : 20 Sample Multiplier: 1

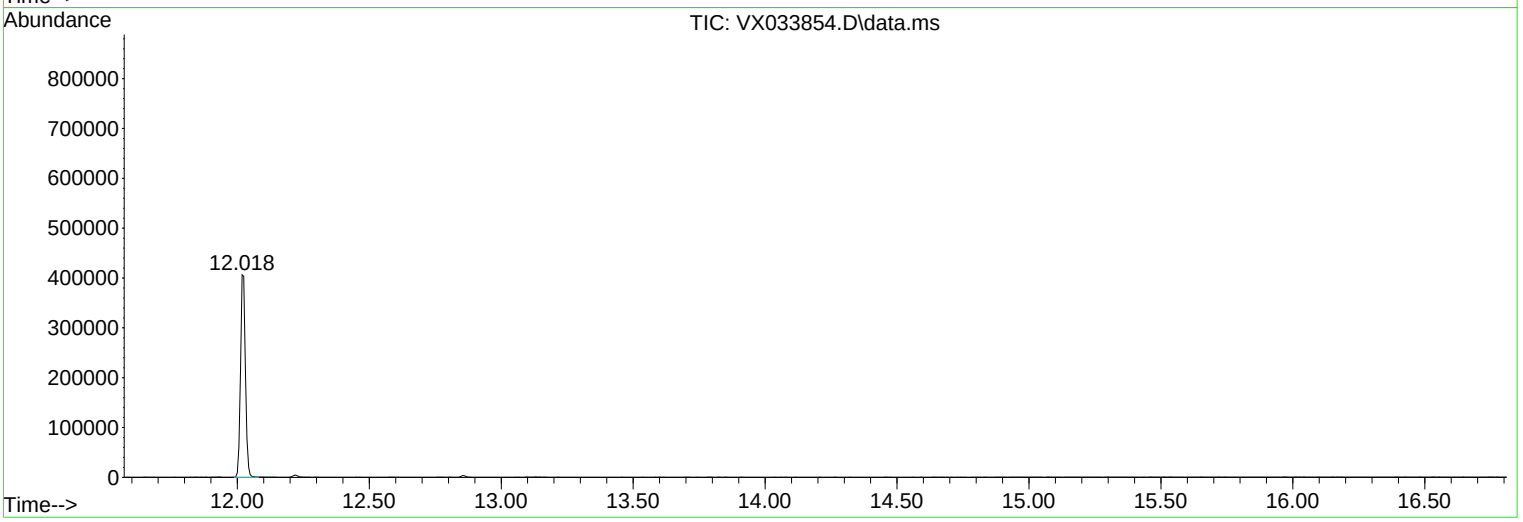
Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

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

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







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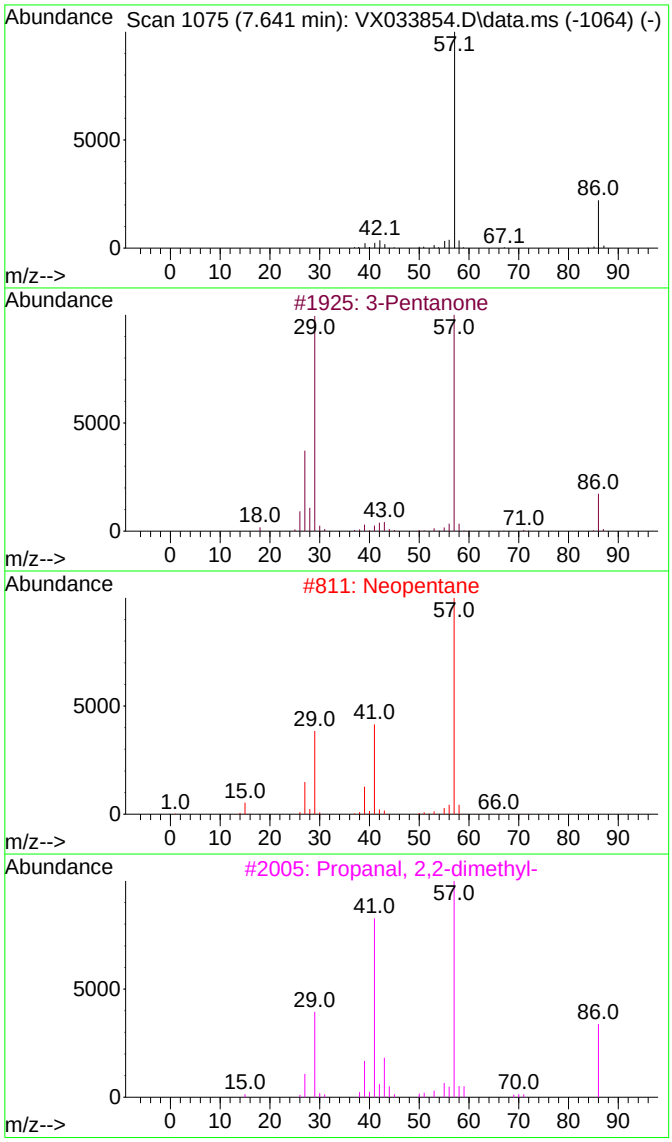
Quant Title : SW846 8260

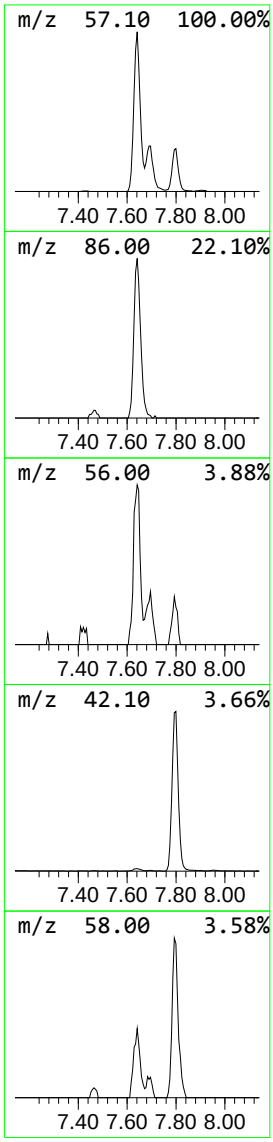
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	5.72 ug/l	65463	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	90
2	Neopentane	72	C5H12	000463-82-1	28
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
4	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9
5	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	4





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Data File : VX033854.D
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Operator : JC/MD
Sample : 01251-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

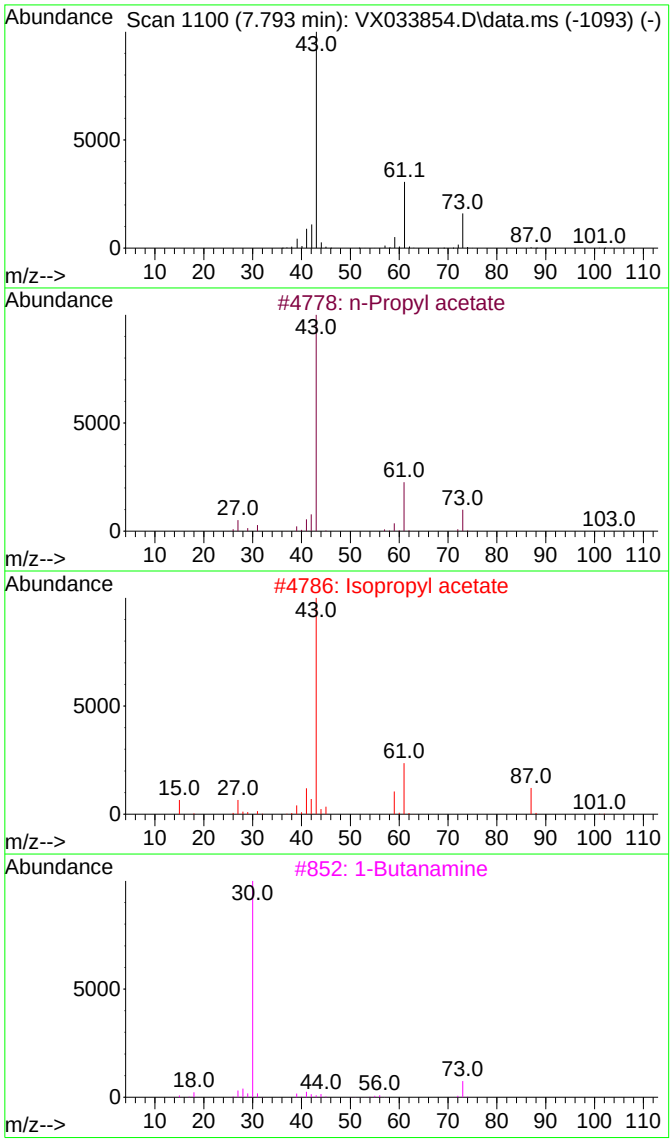
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

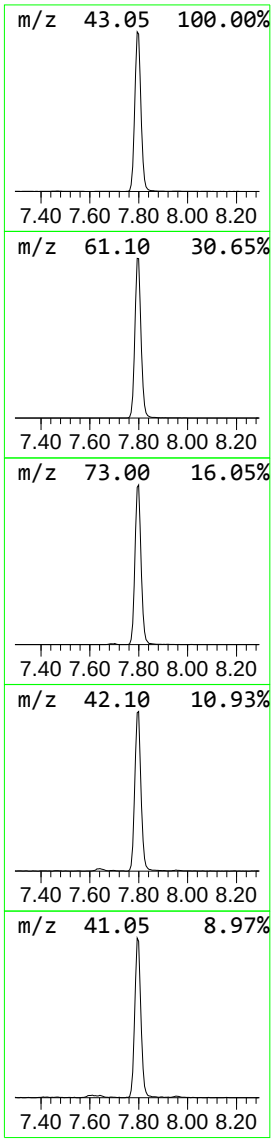
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.793	136.84 ug/l	1565990	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	Pentane	72	C5H12	000109-66-0	4





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

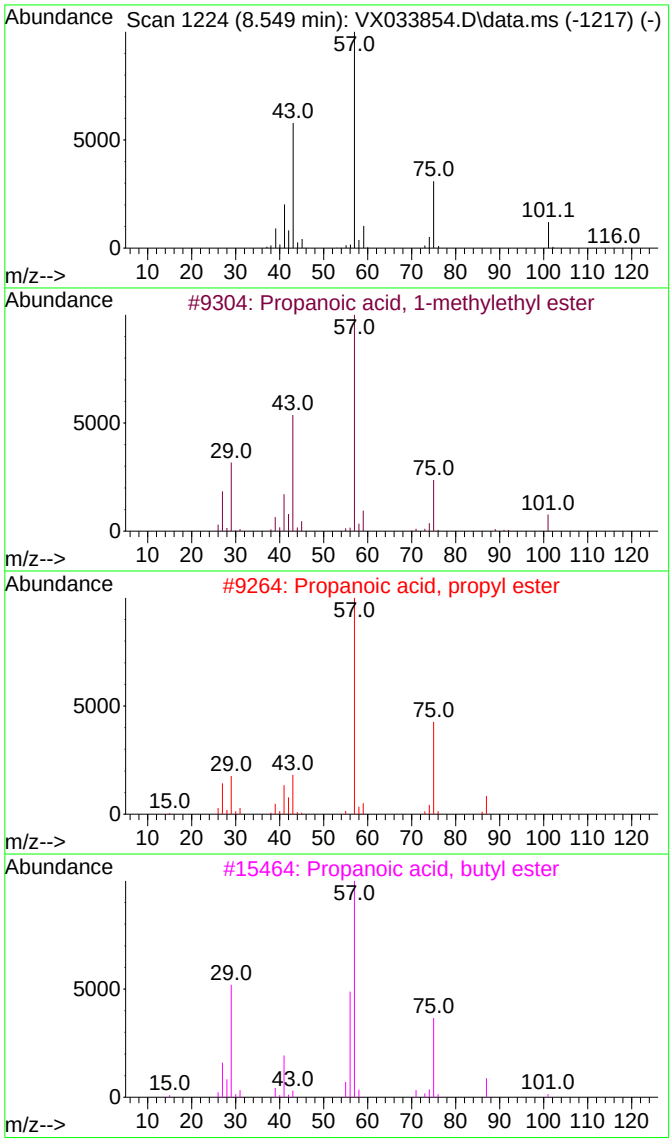
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

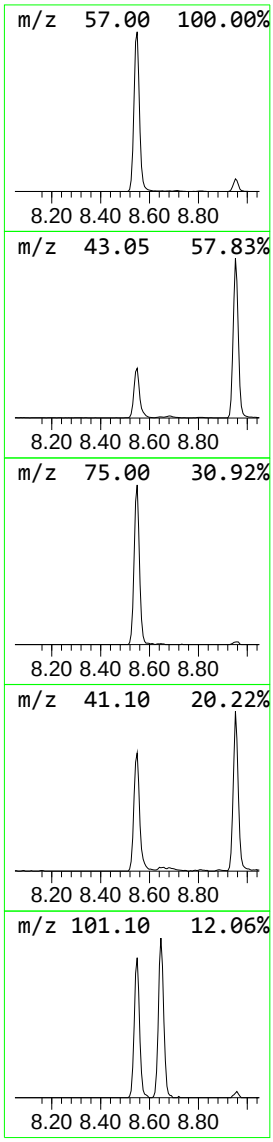
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	24.56 ug/l	302057	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	25
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
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Operator : JC/MD
Sample : 01251-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

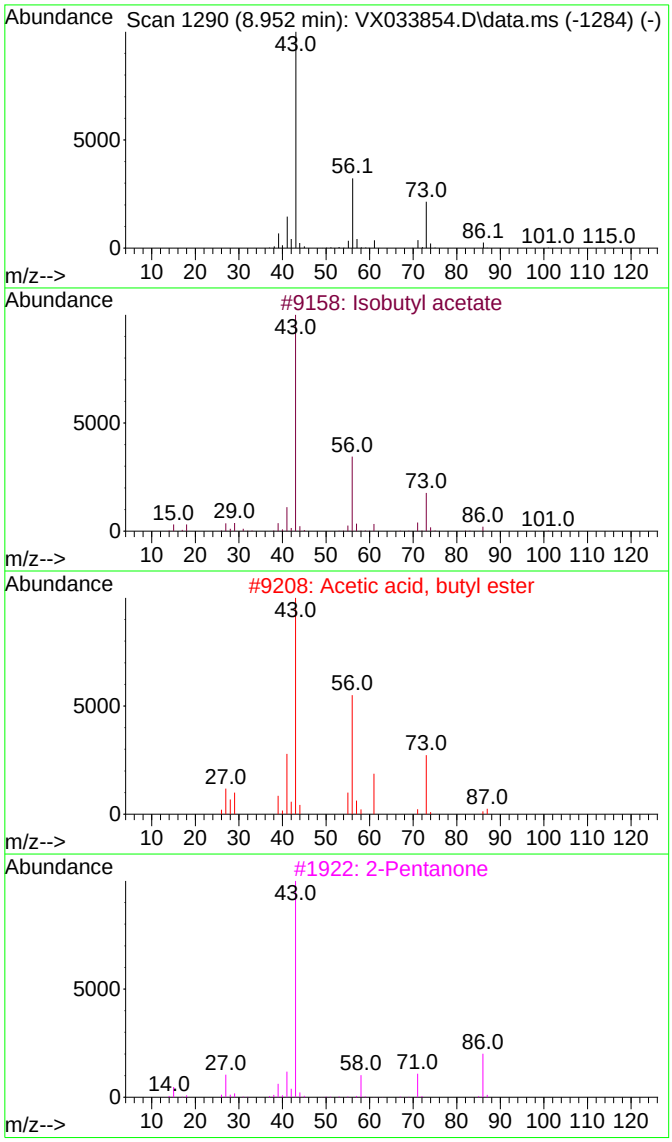
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

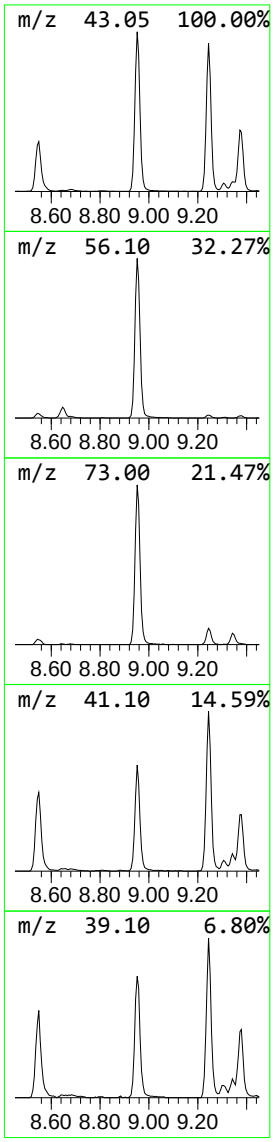
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	31.20 ug/l	383697	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
3	2-Pentanone	86	C5H10O	000107-87-9	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	Ethane, diazo-	56	C2H4N2	001117-96-0	7





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Operator : JC/MD
Sample : 01251-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

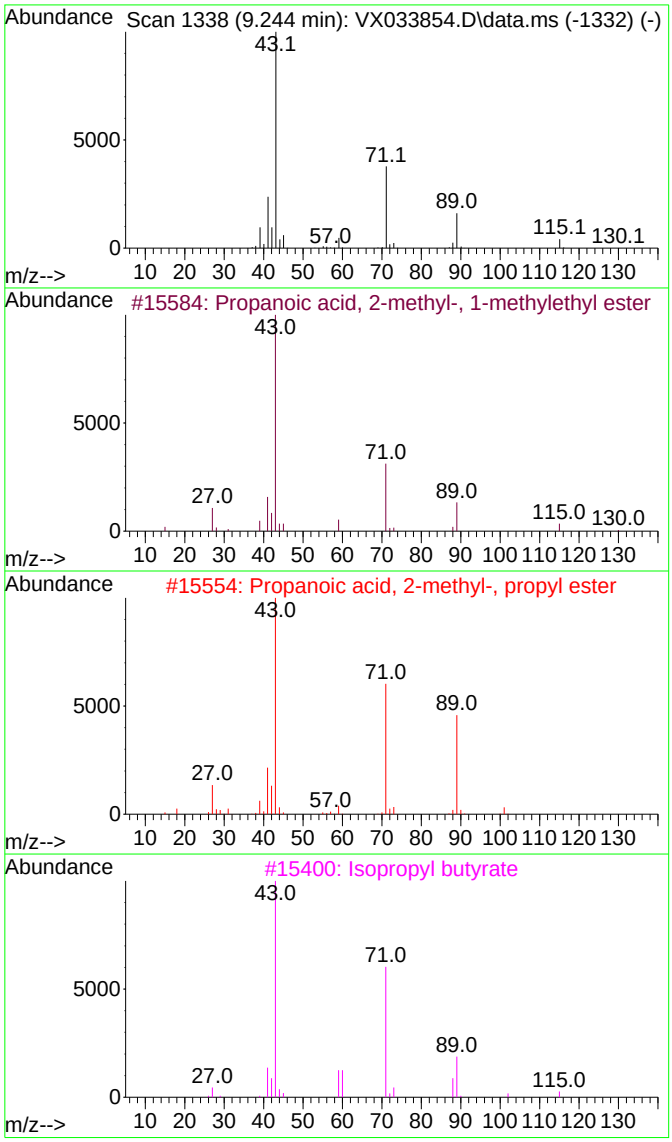
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

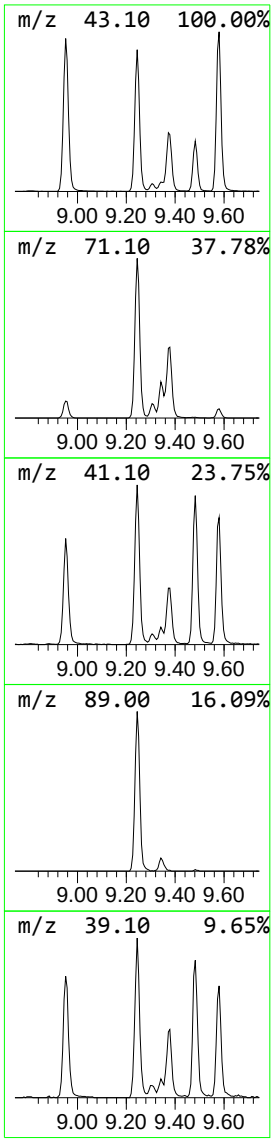
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	30.74 ug/l	378077	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	40
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	40
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

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

TIC Library : C:\Database\NIST20.L
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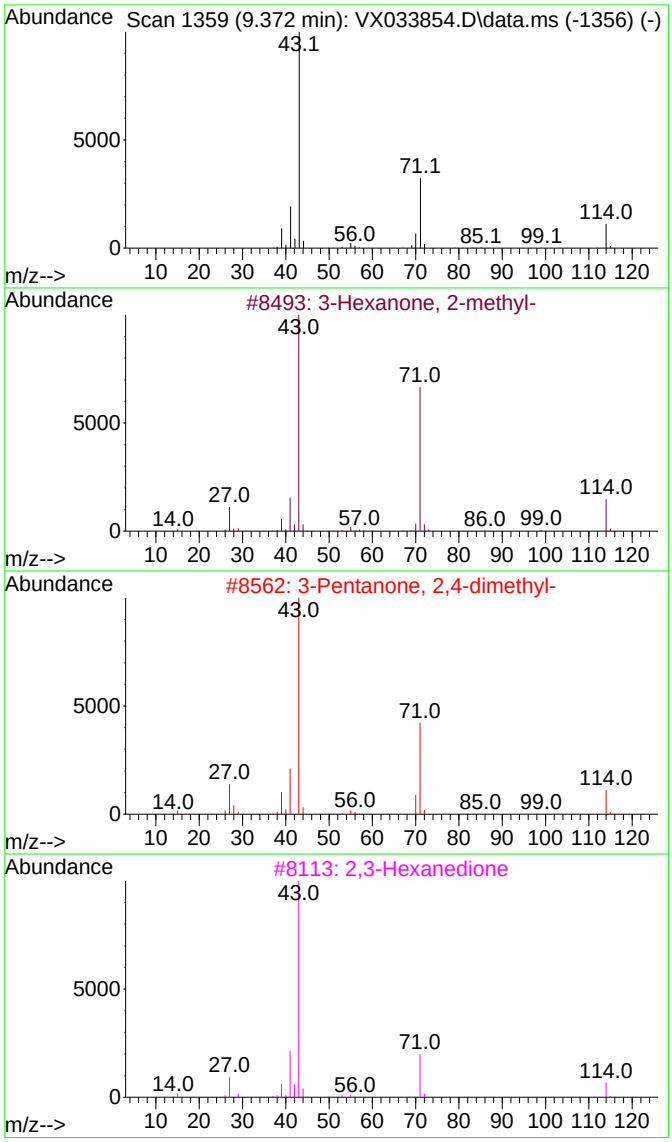
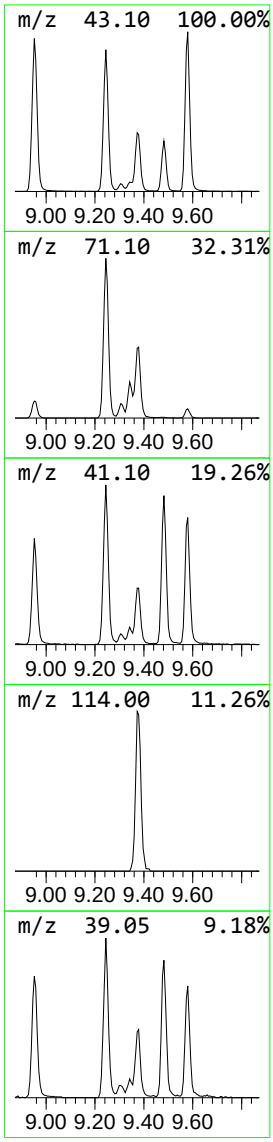
****
Peak Number 6 3-Hexanone, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.372	12.87 ug/l	158265	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78
2	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	72
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
4	Pyrrolidine	71	C4H9N	000123-75-1	50
5	2,5-Hexanedione	114	C6H10O2	000110-13-4	42





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

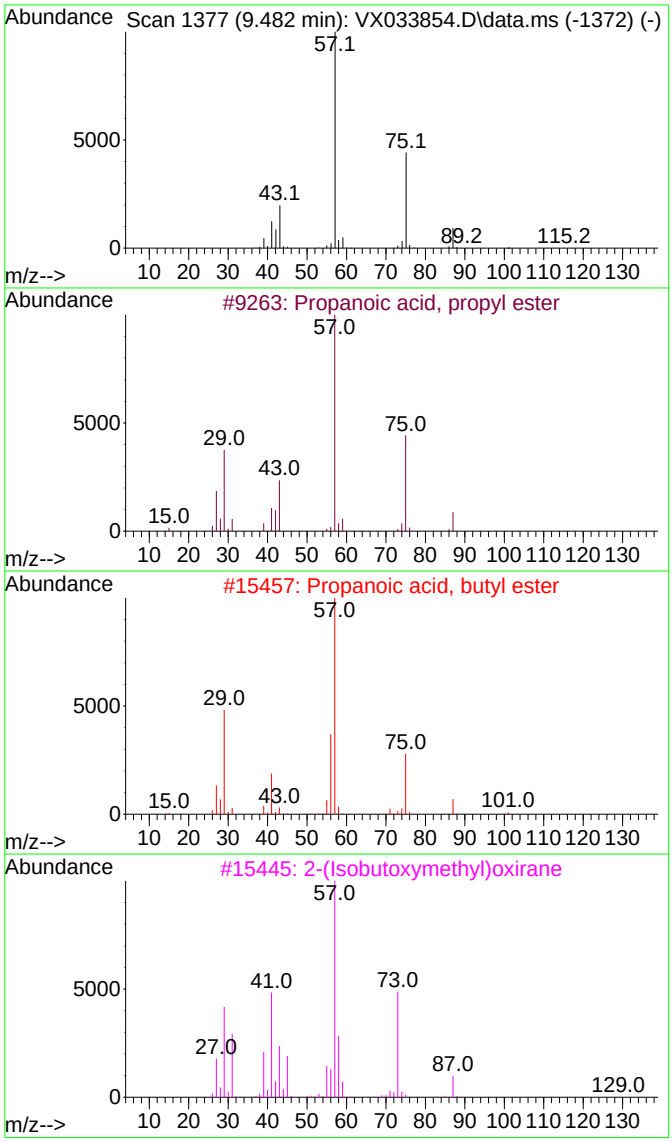
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

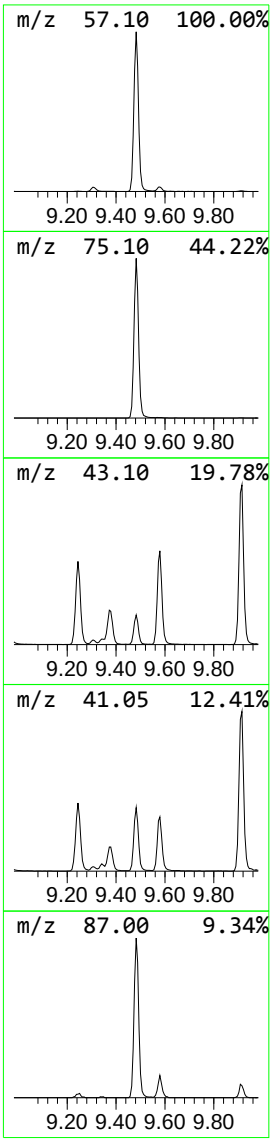
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	50.03 ug/l	615228	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	28
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

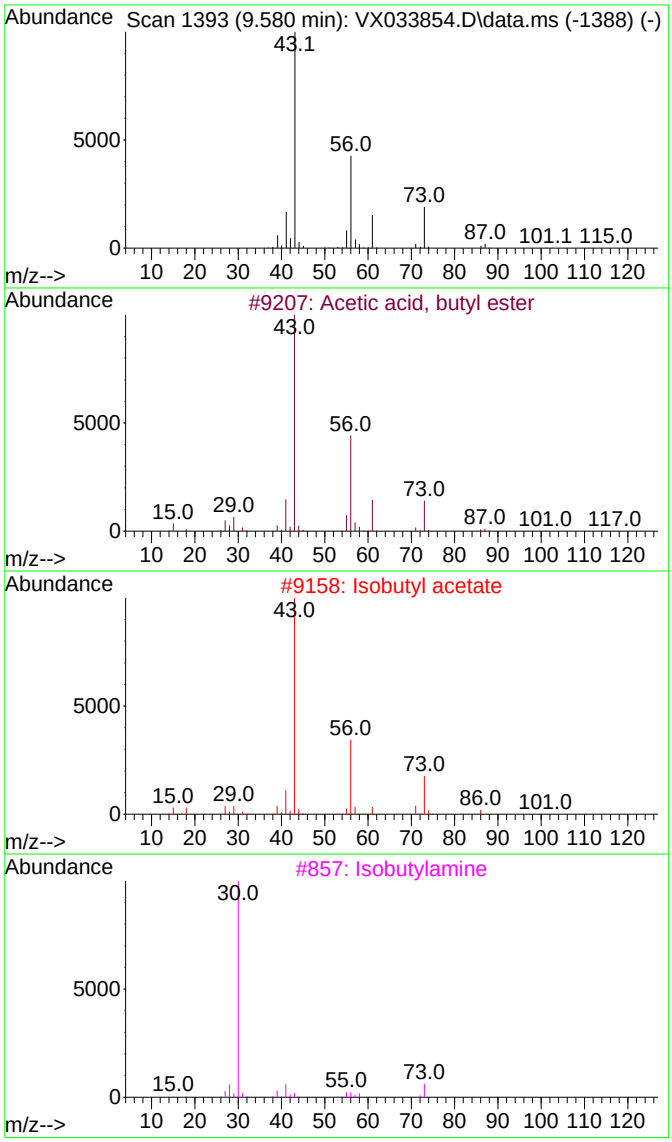
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

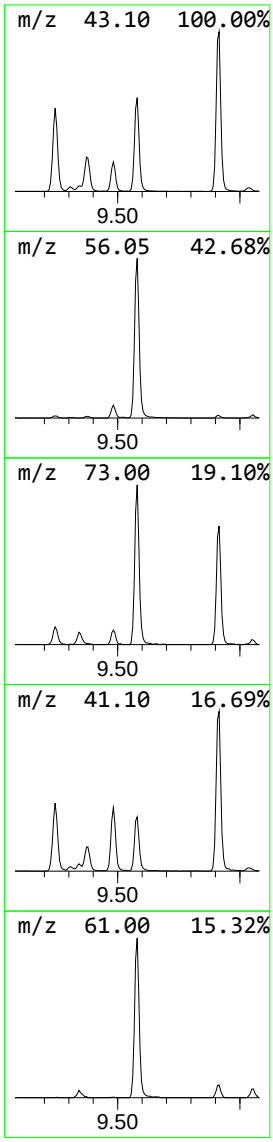
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	33.98 ug/l	417920	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	40
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





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

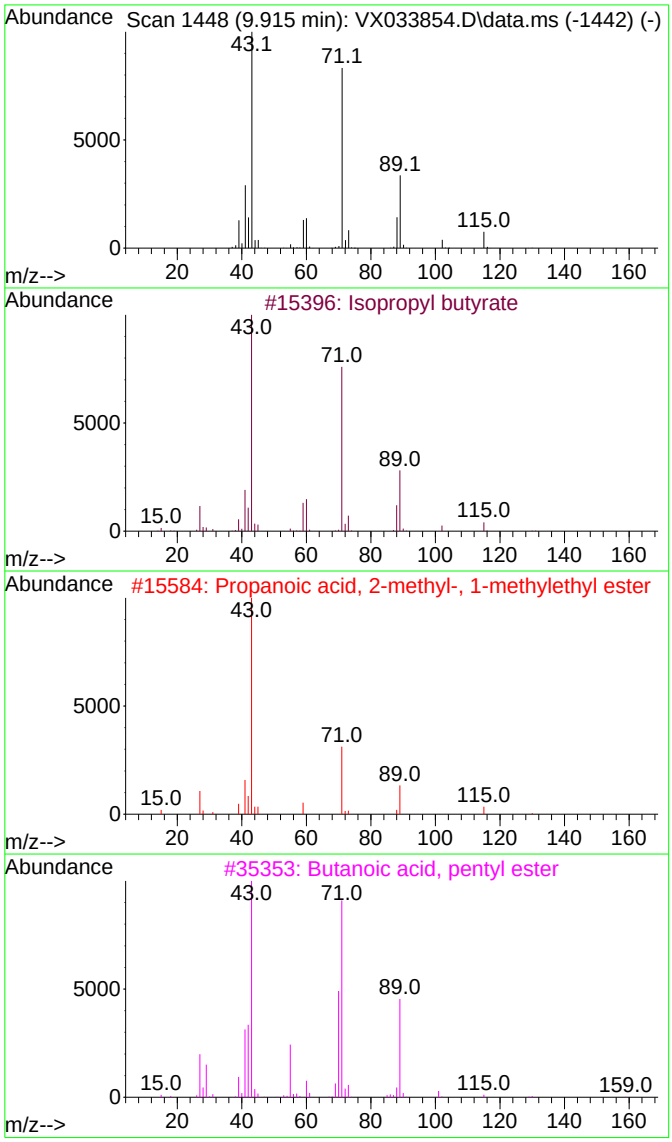
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

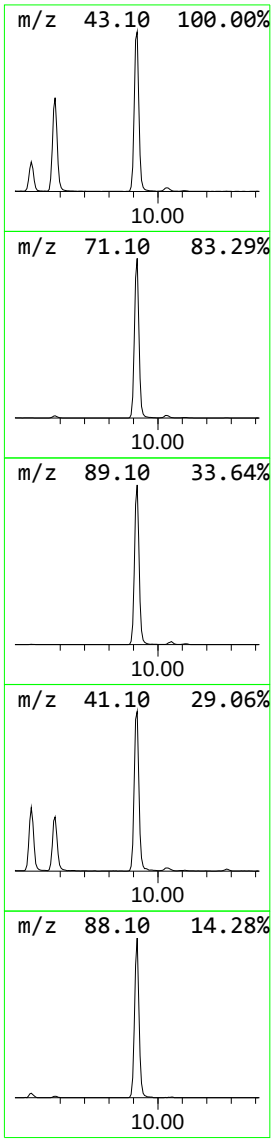
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	87.20 ug/l	1072400	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	94
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56





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Data File : VX033854.D
Acq On : 23 Jan 2023 17:06
Operator : JC/MD
Sample : 01251-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

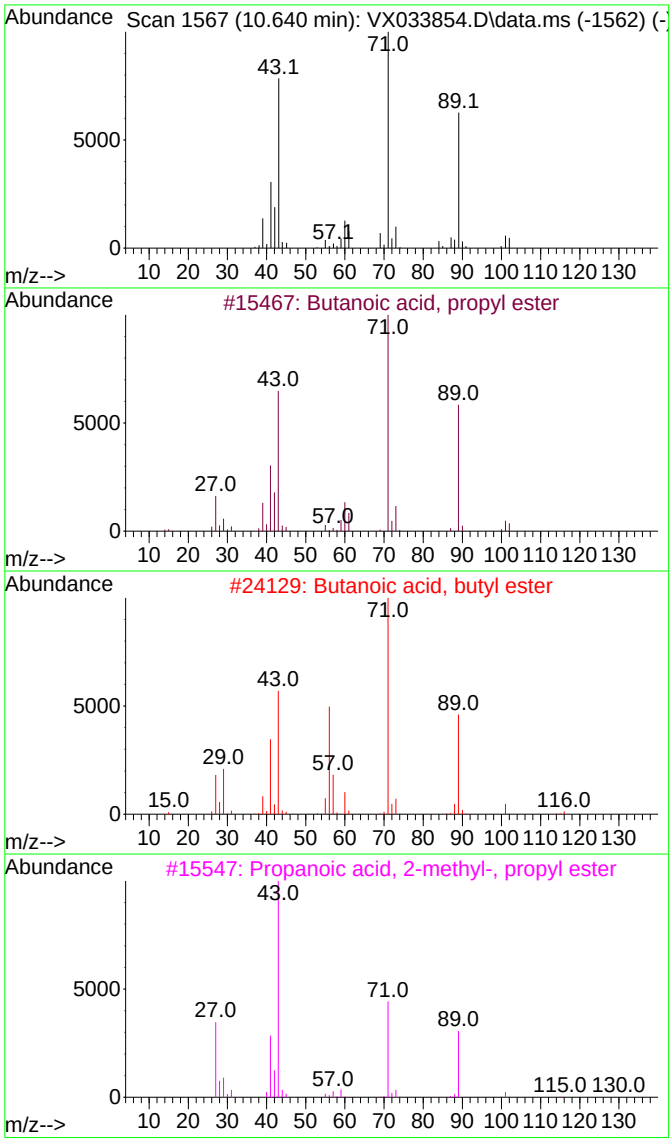
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

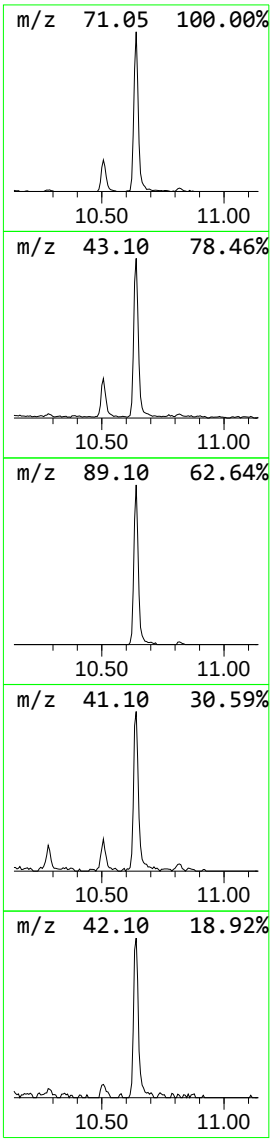
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.62 ug/l	93723	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033854.D
Acq On : 23 Jan 2023 17:06
Operator : JC/MD
Sample : 01251-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-1

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

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Pentanone	7.641	5.7	ug/l	65463	2	6.763	572221	50.0
n-Propyl acetate	7.793	136.8	ug/l	1565990	2	6.763	572221	50.0
Propanoic acid,...	8.549	24.6	ug/l	302057	3	10.055	614903	50.0
Isobutyl acetate	8.952	31.2	ug/l	383697	3	10.055	614903	50.0
Propanoic acid,...	9.244	30.7	ug/l	378077	3	10.055	614903	50.0
3-Hexanone, 2-m...	9.372	12.9	ug/l	158265	3	10.055	614903	50.0
Propanoic acid,...	9.482	50.0	ug/l	615228	3	10.055	614903	50.0
Acetic acid, bu...	9.580	34.0	ug/l	417920	3	10.055	614903	50.0
Isopropyl butyrate	9.915	87.2	ug/l	1072400	3	10.055	614903	50.0
Butanoic acid, ...	10.640	7.6	ug/l	93723	3	10.055	614903	50.0