LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033856.D
Acq On : 23 Jan 2023 17:52
Operator : JC/MD
Sample : 01251-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

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: VX033856.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	208	214	228	rVB	10838	21587	1.44%	0.239%
2	2.794	273	280	296	rVB	16664	32271	2.16%	0.358%
3	4.714	586	595	607	rBV2	10946	31388	2.10%	0.348%
4	5.385	693	705	719	rBV	83696	244460	16.36%	2.709%
5	5.550	721	732	747	rVB	152082	424927	28.43%	4.709%
6	5.952	788	798	812	rBV2	83140	225598	15.10%	2.500%
7	6.336	849	861	876	rBV	62563	166508	11.14%	1.845%
8	6.763	921	931	945	rBV	222634	543597	36.37%	6.024%
9	7.641	1064	1075	1080	rBV2	32278	63760	4.27%	0.707%
10	7.690	1080	1083	1092	rVV	11877	22084	1.48%	0.245%
11	7.799	1093	1101	1121	rVV	842318	1494464	100.00%	16.561%
12	8.549	1216	1224	1234	rBV	189875	305918	20.47%	3.390%
13	8.647	1234	1240	1257	rVB	450786	724623	48.49%	8.030%
14	8.951	1284	1290	1302	rBV	248508	363281	24.31%	4.026%
15	9.244	1332	1338	1345	rBV	270105	381850	25.55%	4.231%
16	9.311	1345	1349	1351	rVV	21717	33371	2.23%	0.370%
17	9.342	1351	1354	1356	rVV	40794	54707	3.66%	0.606%
18	9.378	1356	1360	1368	rVV	101016	157060	10.51%	1.740%
19	9.482	1372	1377	1388	rVV	440569	590902	39.54%	6.548%
20	9.579	1388	1393	1410	rVB	278911	375806	25.15%	4.165%
21	9.915	1442	1448	1463	rBV	796486	1058736	70.84%	11.732%
22	10.055	1463	1471	1478	rBV	432924	614847	41.14%	6.813%
23	10.506	1539	1545	1555	rBV	10054	14999	1.00%	0.166%
24	10.640	1560	1567	1582	rBV	65897	87835	5.88%	0.973%
25	11.079	1634	1639	1654	rBV	355860	456514	30.55%	5.059%
26	12.024	1788	1794	1802	rBV	418253	532933	35.66%	5.906%

Sum of corrected areas: 9024026

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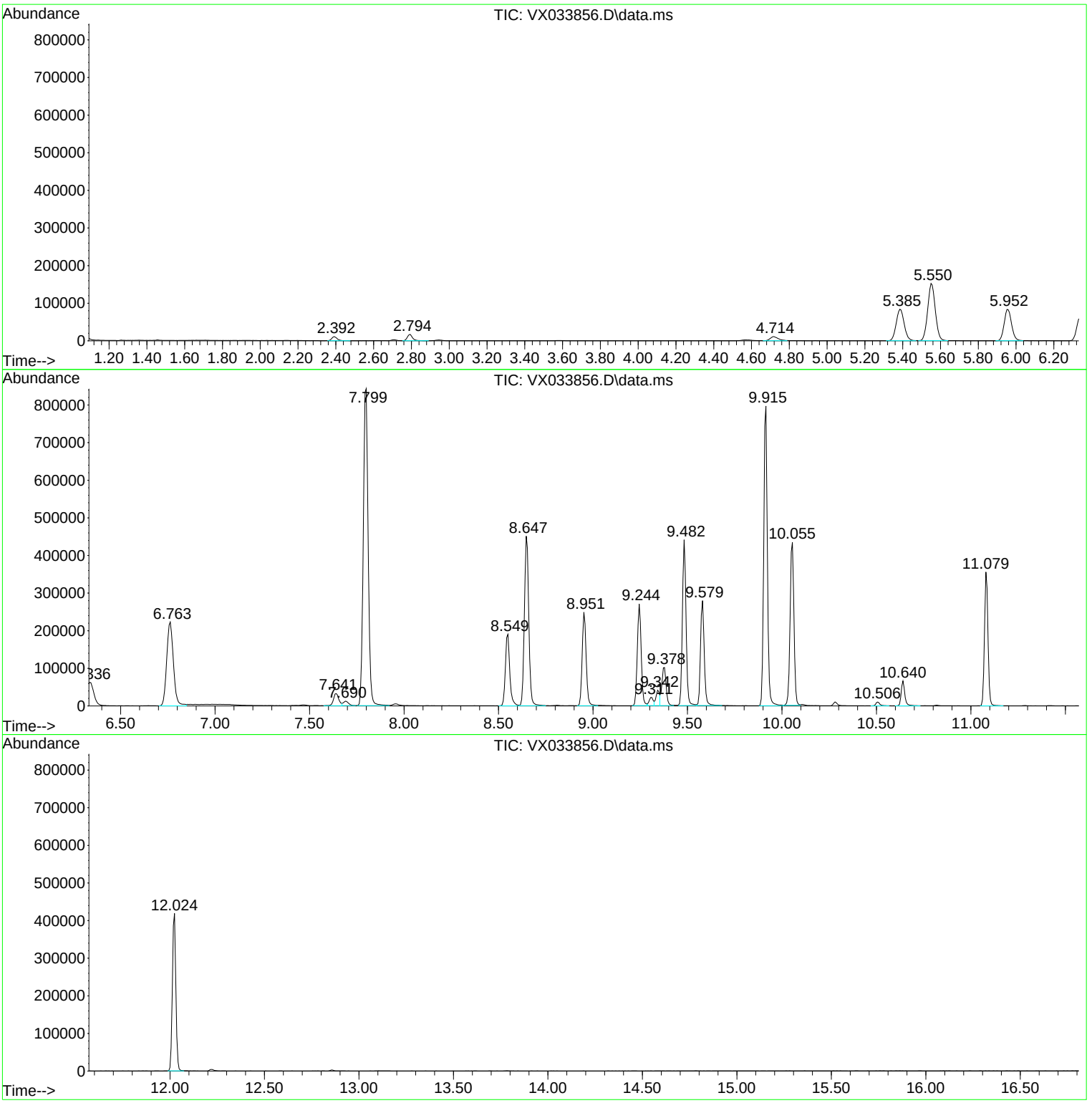
TCLP-2

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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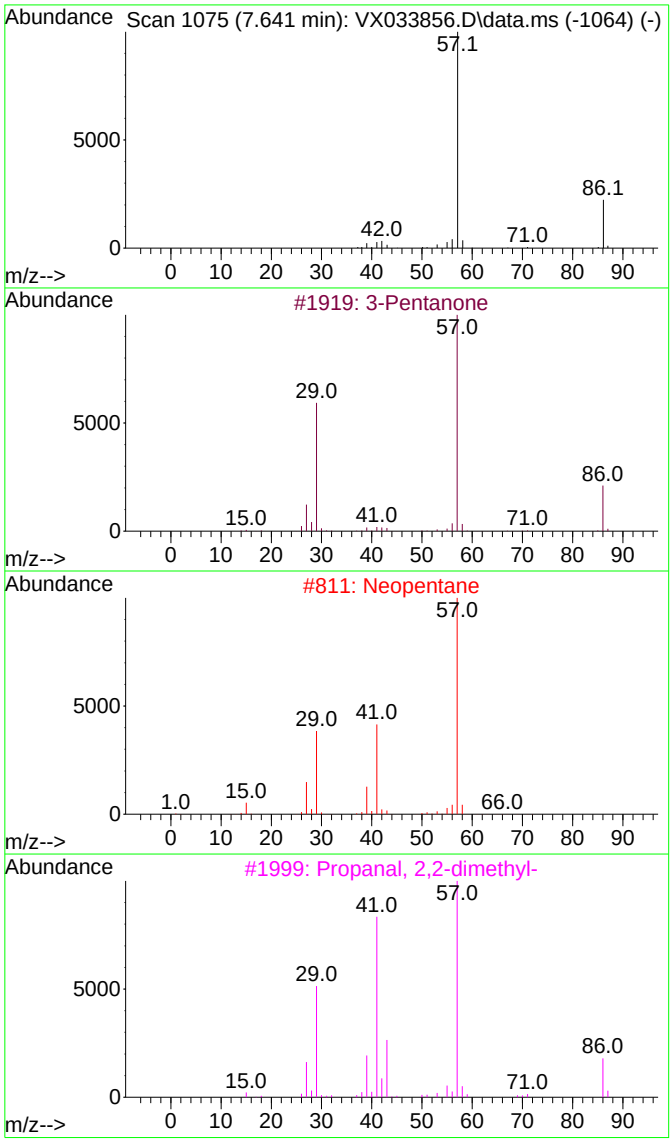
Quant Title : SW846 8260

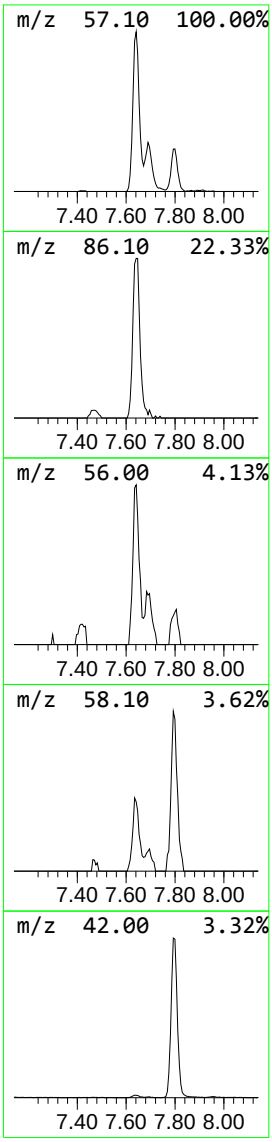
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	5.86 ug/l	63760	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	86
2	Neopentane	72	C5H12	000463-82-1	28
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7
4	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	5
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	4





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

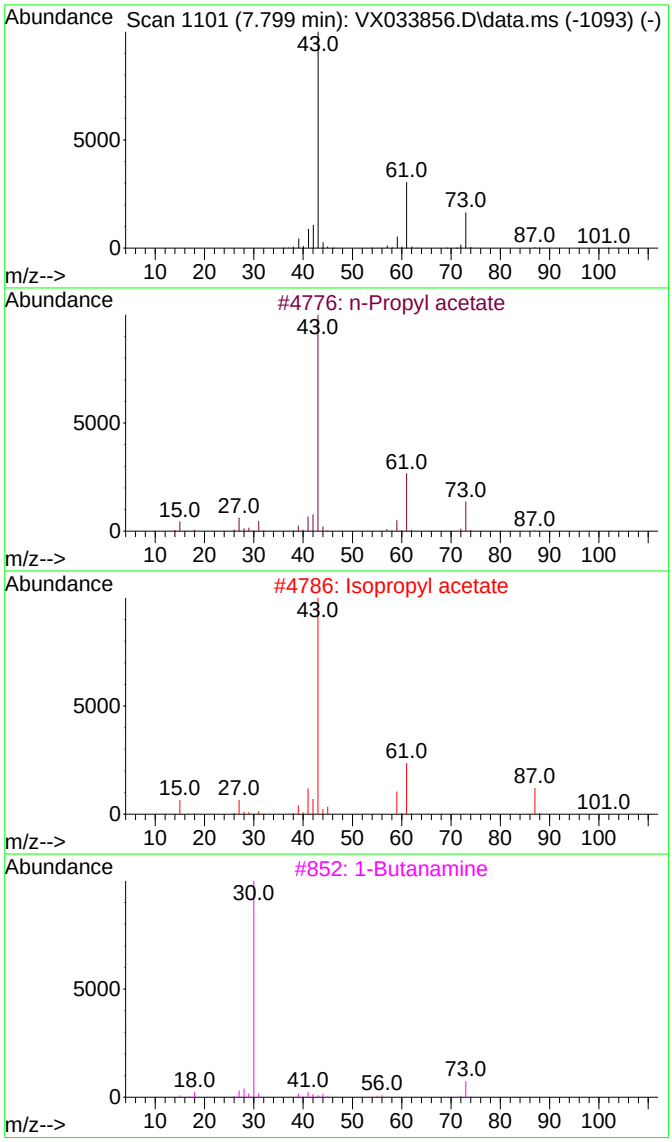
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

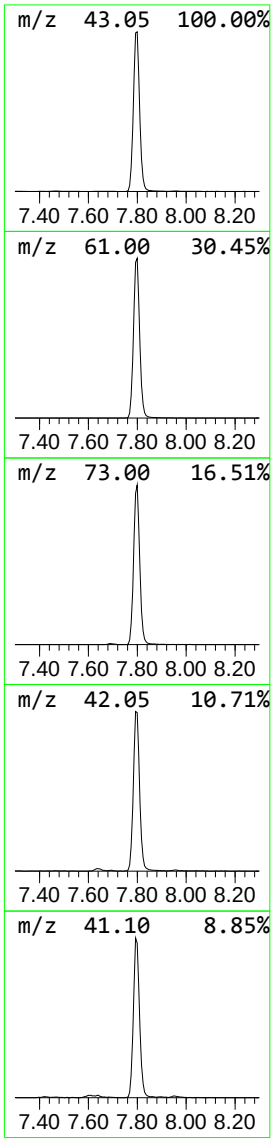
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	137.46 ug/l	1494460	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	4
5	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

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

TIC Library : C:\Database\NIST20.L
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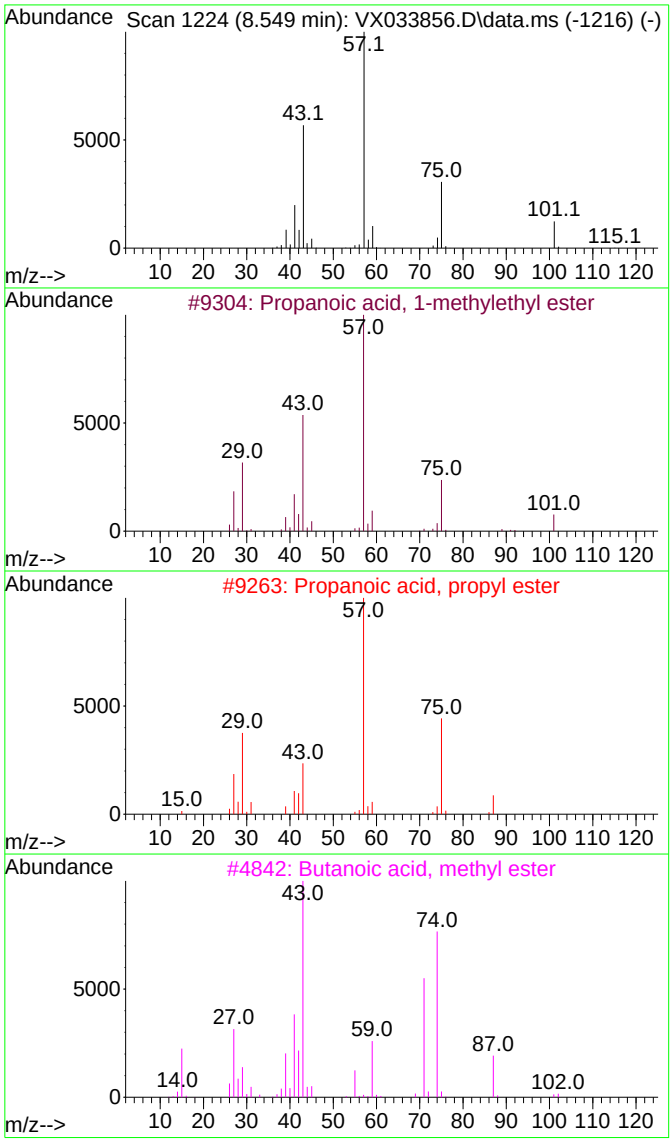
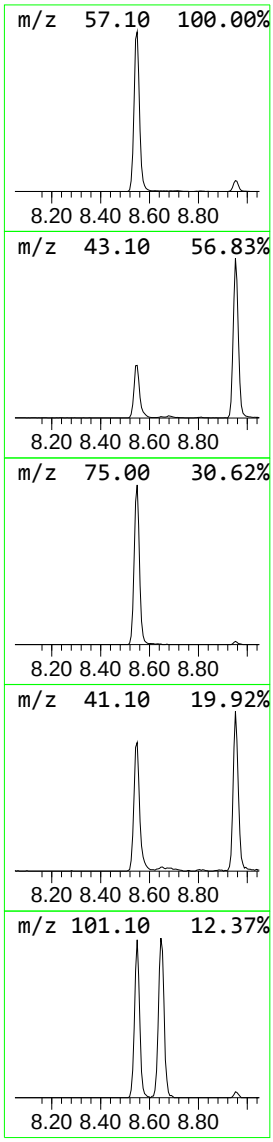
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	24.88 ug/l	305918	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	36
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
4	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

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

TIC Library : C:\Database\NIST20.L
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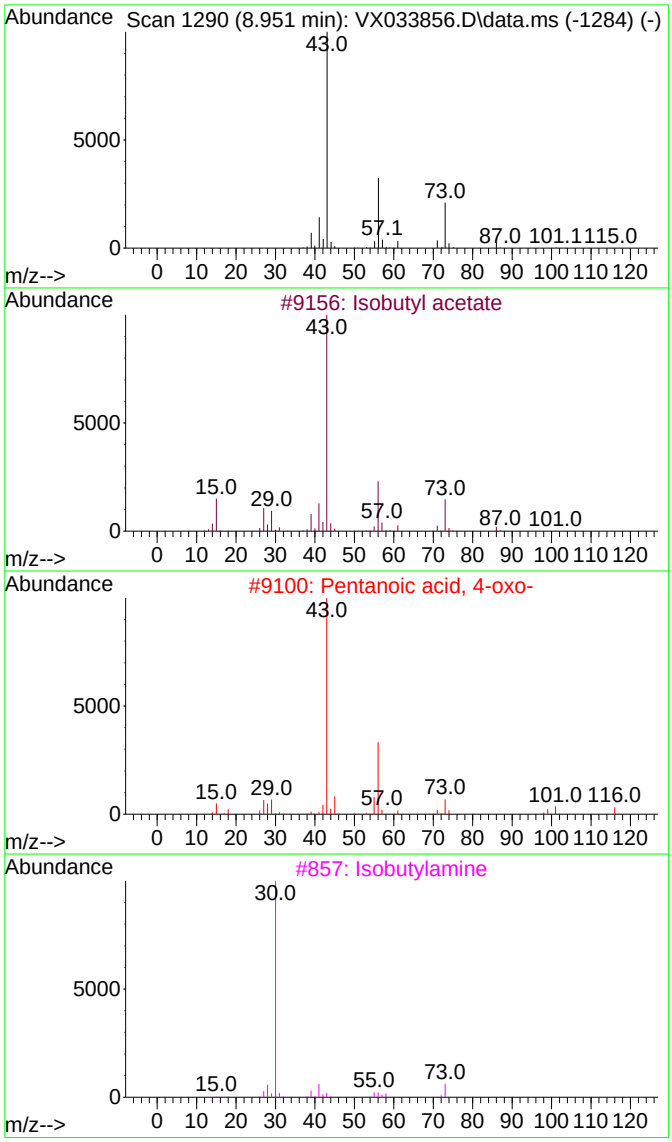
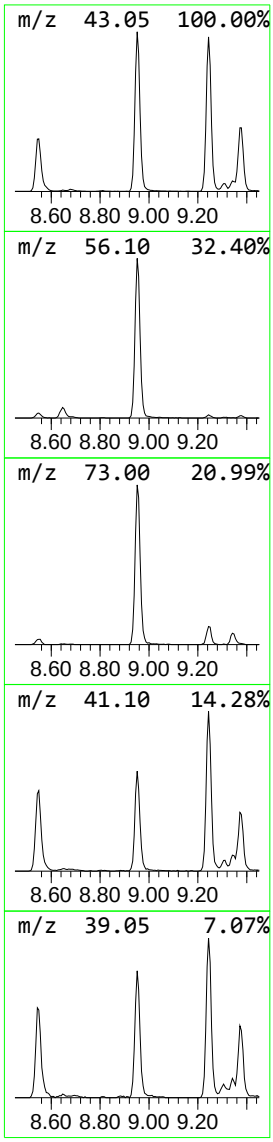
****

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.951	29.54 ug/l	363281	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	38
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

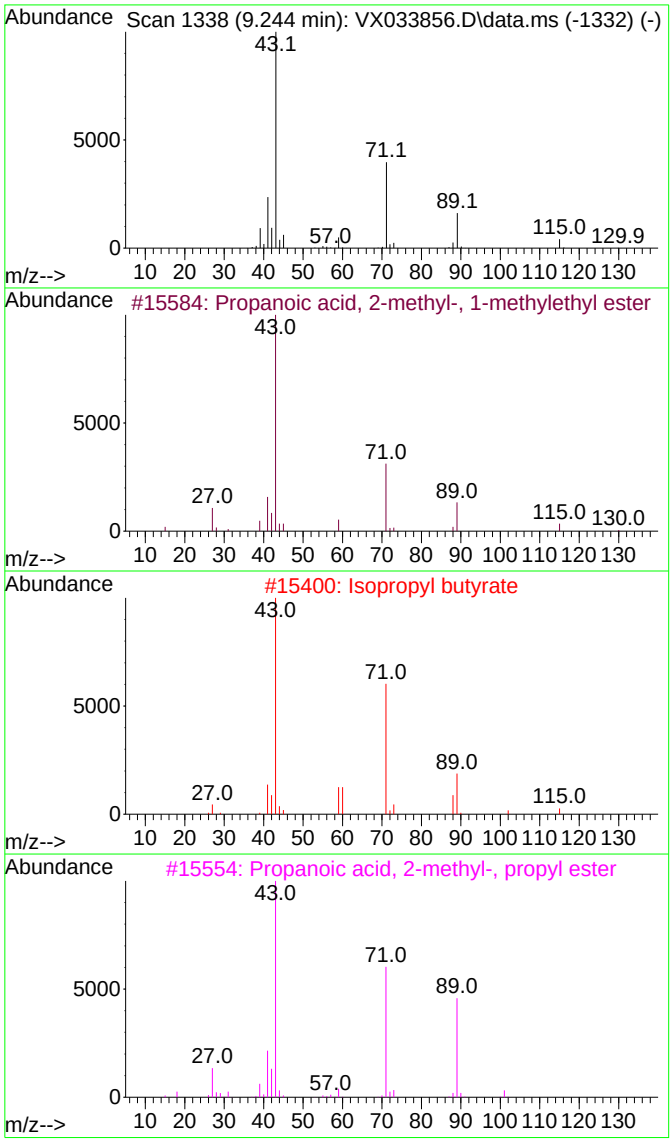
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

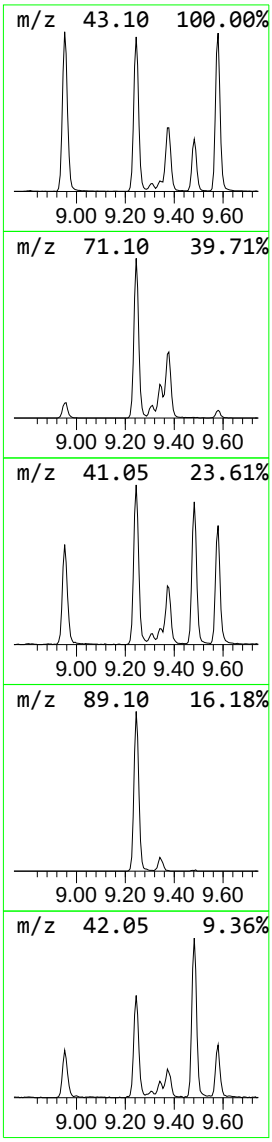
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	31.05 ug/l	381850	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	Isopropyl butyrate	130	C7H14O2	000638-11-9	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	53
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42





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Operator : JC/MD
Sample : 01251-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

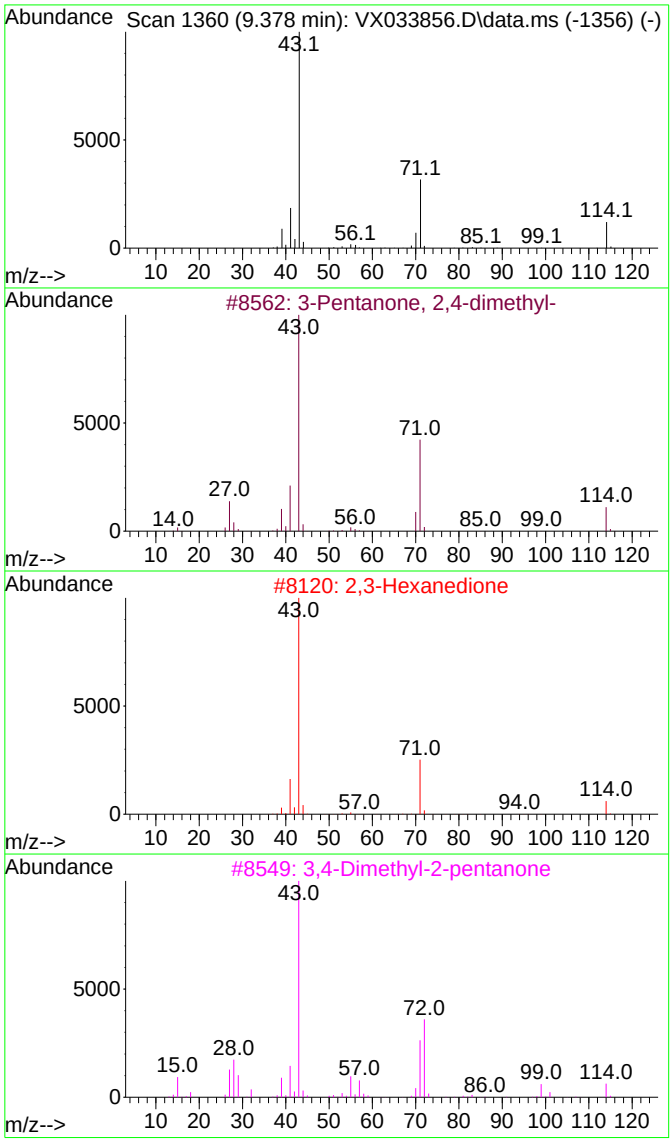
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

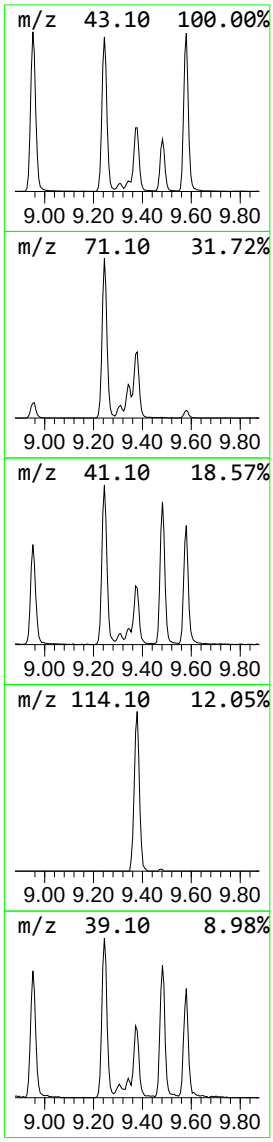
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	12.77 ug/l	157060	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	58
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	50
3	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50
4	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	45
5	4-Heptanone	114	C7H14O	000123-19-3	37





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

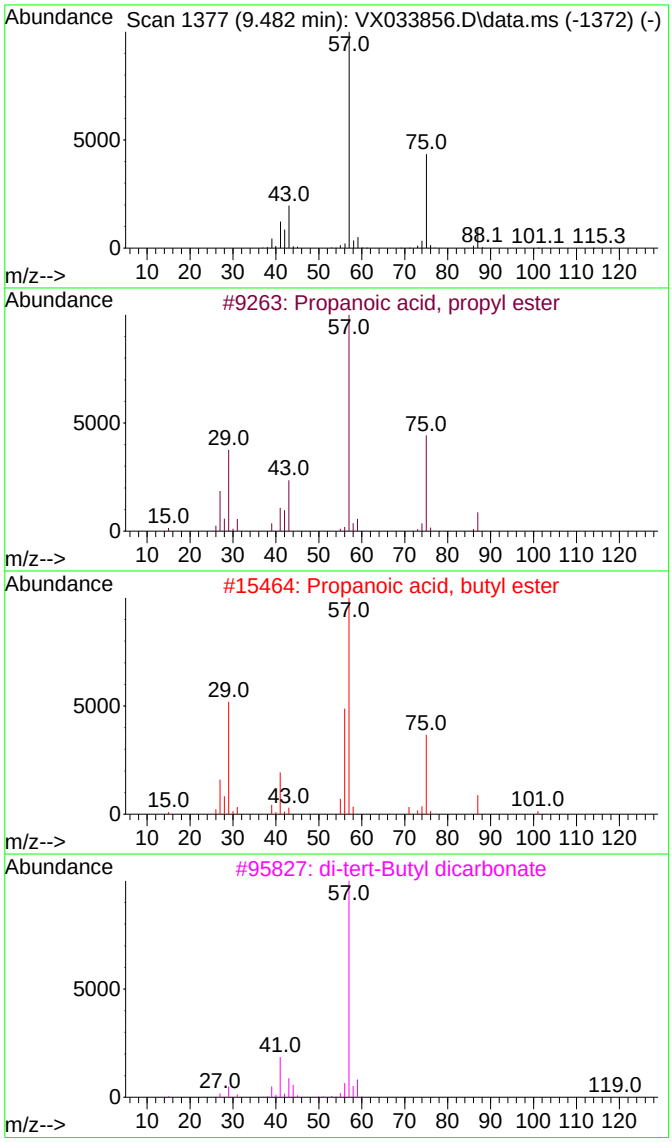
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

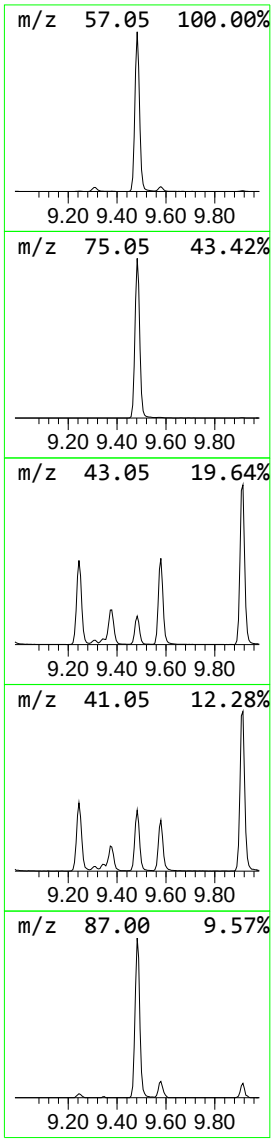
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	48.05 ug/l	590902	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	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Instrument :
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ClientSampleId :
TCLP-2

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

TIC Library : C:\Database\NIST20.L
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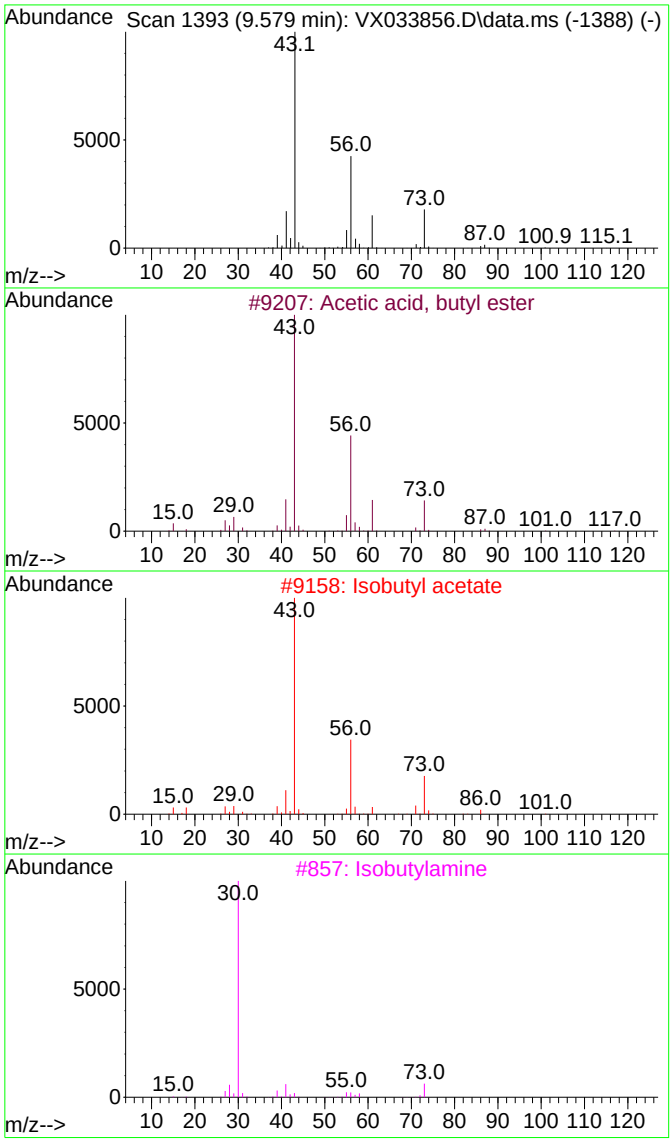
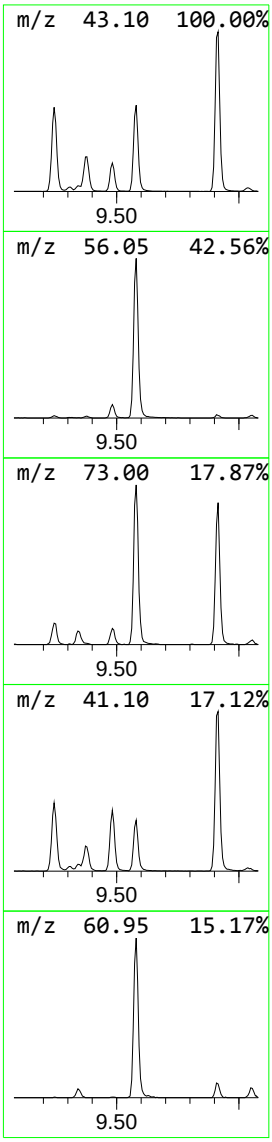
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	30.56 ug/l	375806	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	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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ClientSampleId :
TCLP-2

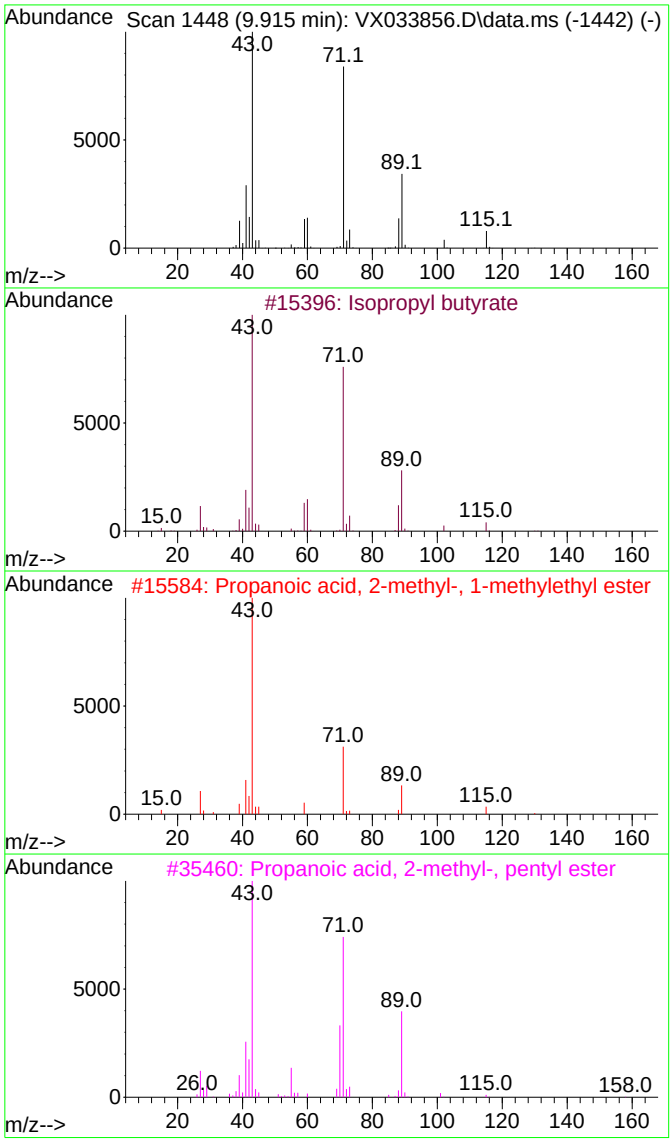
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

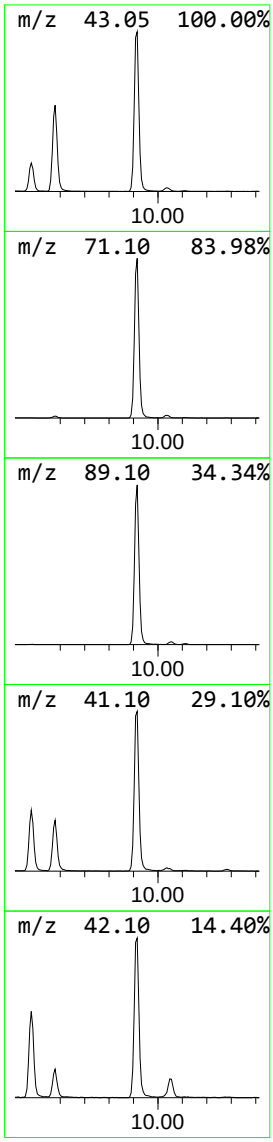
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	86.10 ug/l	1058740	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56





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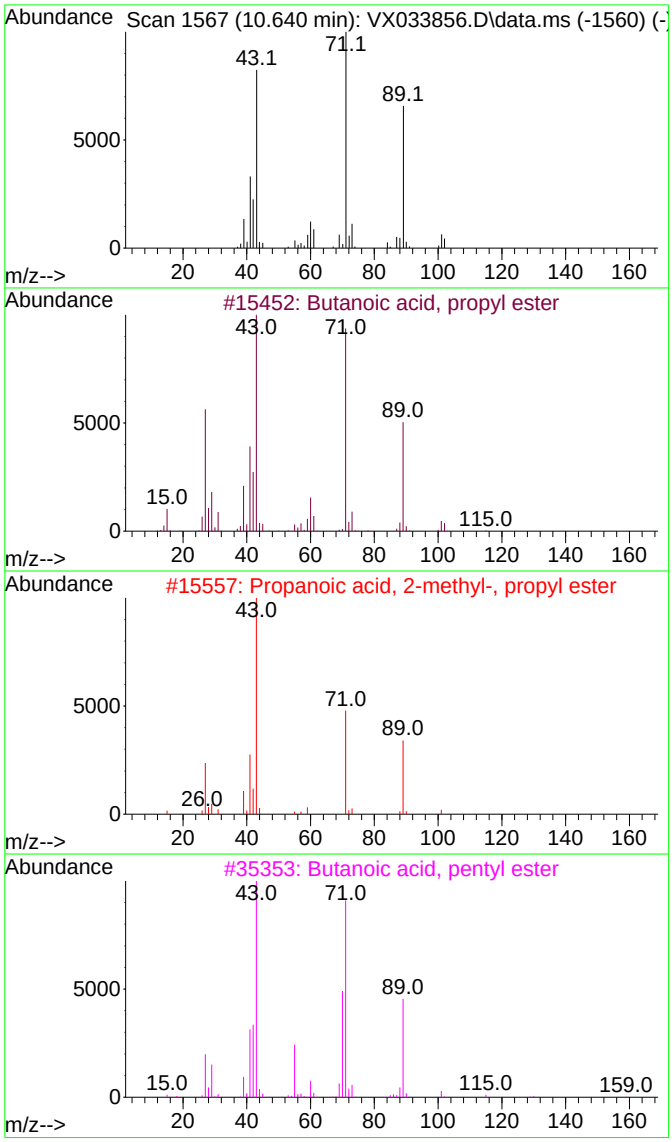
Quant Title : SW846 8260

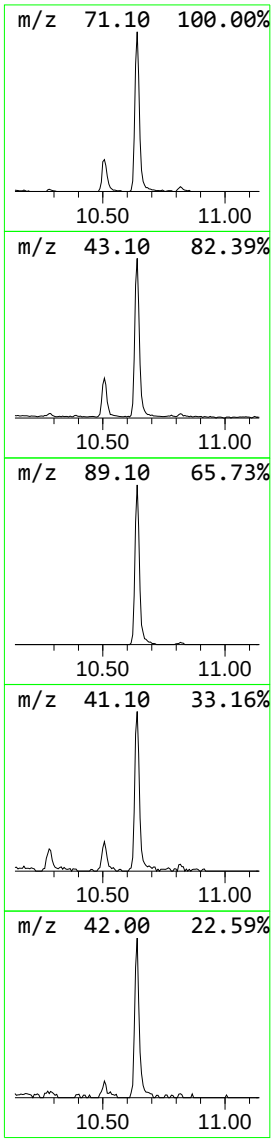
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.14 ug/l	87835	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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	78
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
5	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033856.D
Acq On : 23 Jan 2023 17:52
Operator : JC/MD
Sample : 01251-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TCLP-2

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	5.9	ug/l	63760	2	6.763	543597	50.0
n-Propyl acetate	7.799	137.5	ug/l	1494460	2	6.763	543597	50.0
Propanoic acid,...	8.549	24.9	ug/l	305918	3	10.055	614847	50.0
Isobutyl acetate	8.951	29.5	ug/l	363281	3	10.055	614847	50.0
Propanoic acid,...	9.244	31.1	ug/l	381850	3	10.055	614847	50.0
3-Pentanone, 2,...	9.378	12.8	ug/l	157060	3	10.055	614847	50.0
Propanoic acid,...	9.482	48.0	ug/l	590902	3	10.055	614847	50.0
Acetic acid, bu...	9.579	30.6	ug/l	375806	3	10.055	614847	50.0
Isopropyl butyrate	9.915	86.1	ug/l	1058740	3	10.055	614847	50.0
Butanoic acid, ...	10.640	7.1	ug/l	87835	3	10.055	614847	50.0