LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033857.D
Acq On : 23 Jan 2023 18:15
Operator : JC/MD
Sample : 01252-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MH-9

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: VX033857.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.386	208	213	224	rVB	11899	22607	1.43%	0.244%
2	2.788	273	279	290	rVB	15258	28585	1.81%	0.308%
3	4.715	585	595	612	rBV2	10977	34304	2.17%	0.370%
4	5.385	693	705	721	rBV2	84575	246253	15.60%	2.657%
5	5.550	721	732	749	rVV	149472	423978	26.86%	4.574%
6	5.958	789	799	817	rBV	84153	225759	14.30%	2.436%
7	6.336	852	861	879	rBV	63948	167478	10.61%	1.807%
8	6.763	920	931	946	rBV	222308	568947	36.05%	6.138%
9	7.641	1064	1075	1080	rBV	33547	65004	4.12%	0.701%
10	7.690	1080	1083	1093	rVB	12041	21884	1.39%	0.236%
11	7.799	1093	1101	1122	rBV	888137	1578322	100.00%	17.029%
12	8.549	1217	1224	1234	rBV	190345	305496	19.36%	3.296%
13	8.647	1234	1240	1259	rVB	455226	722701	45.79%	7.797%
14	8.952	1284	1290	1307	rBV	265840	390088	24.72%	4.209%
15	9.244	1332	1338	1345	rBV	269750	379407	24.04%	4.093%
16	9.305	1345	1348	1351	rVV	23232	34479	2.18%	0.372%
17	9.342	1351	1354	1356	rVV	40640	55277	3.50%	0.596%
18	9.372	1356	1359	1370	rVV	105589	158513	10.04%	1.710%
19	9.482	1372	1377	1388	rVV	474089	612424	38.80%	6.608%
20	9.580	1388	1393	1406	rVB	314670	425033	26.93%	4.586%
21	9.915	1442	1448	1461	rBV	814846	1071795	67.91%	11.564%
22	10.055	1463	1471	1477	rBV	441109	617844	39.15%	6.666%
23	10.640	1561	1567	1584	rBV	71058	95636	6.06%	1.032%
24	11.079	1634	1639	1649	rBV	365367	464397	29.42%	5.010%
25	12.024	1788	1794	1803	rBV	430530	552359	35.00%	5.959%

Sum of corrected areas: 9268570

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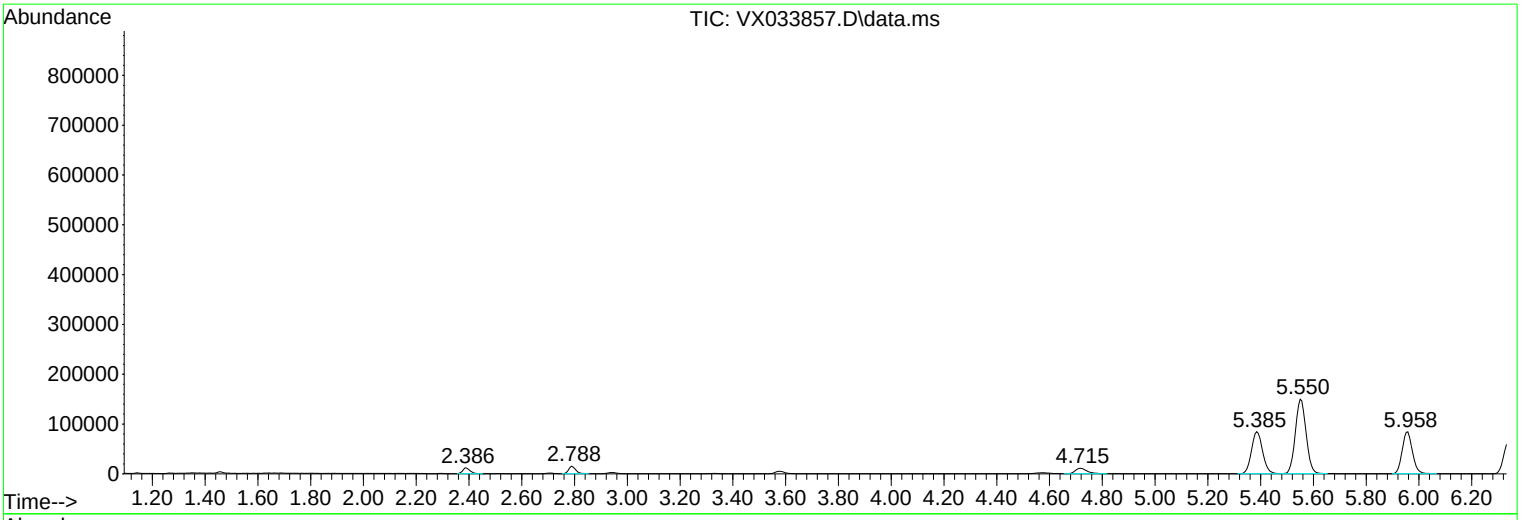
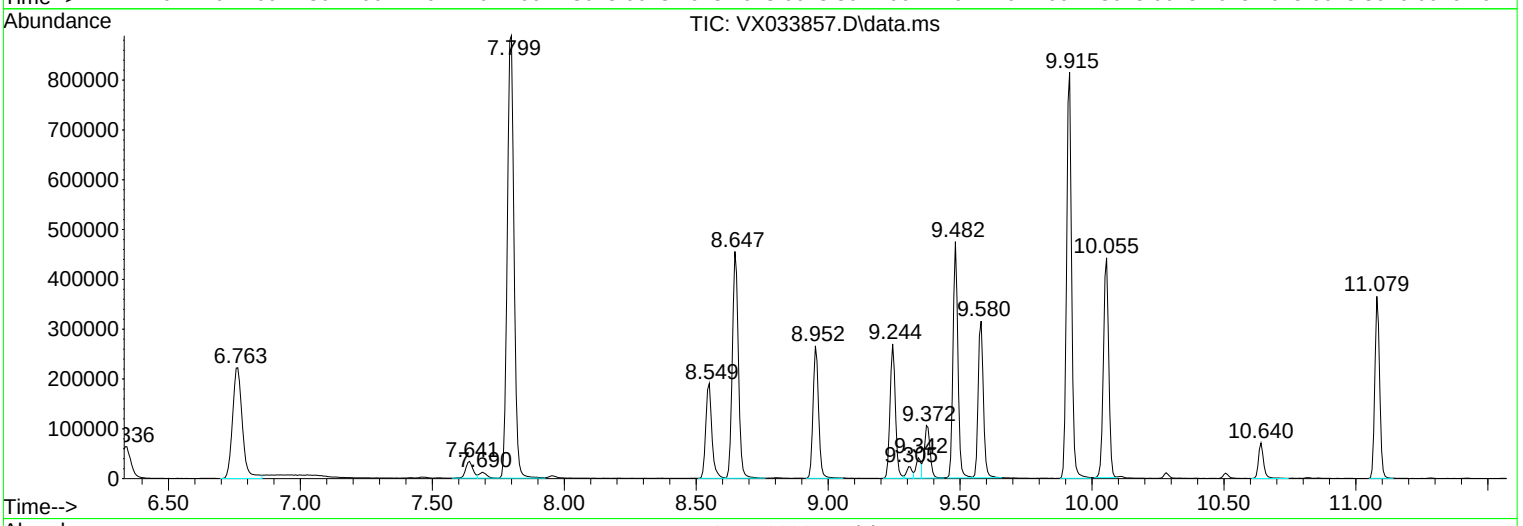
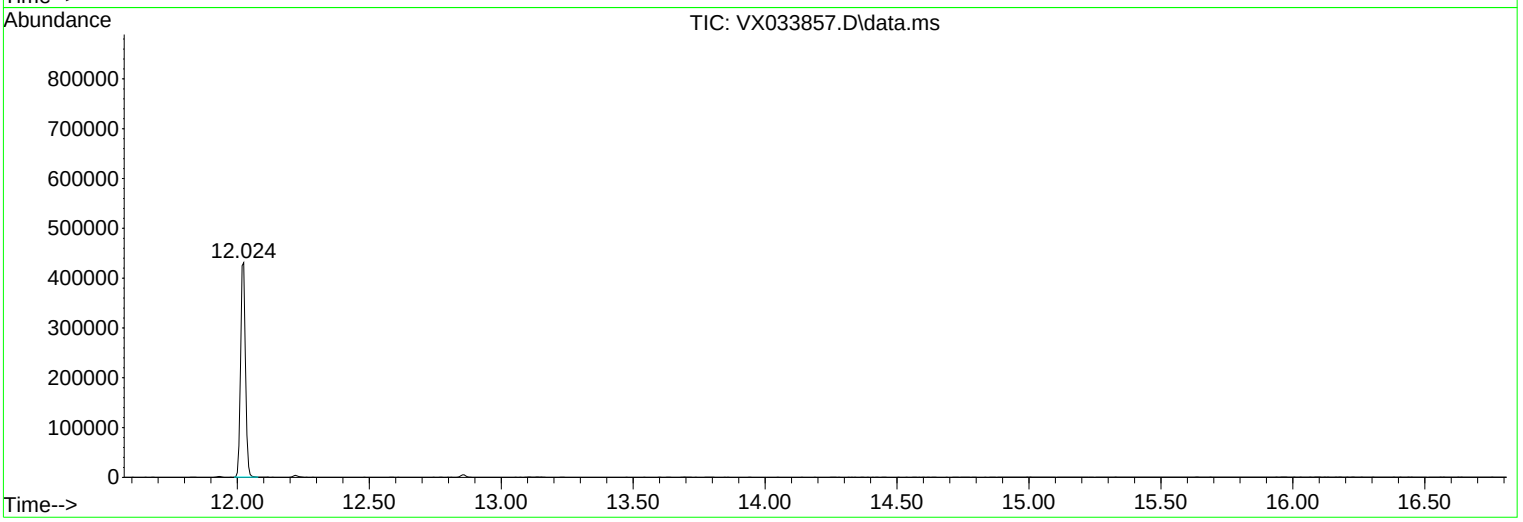
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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







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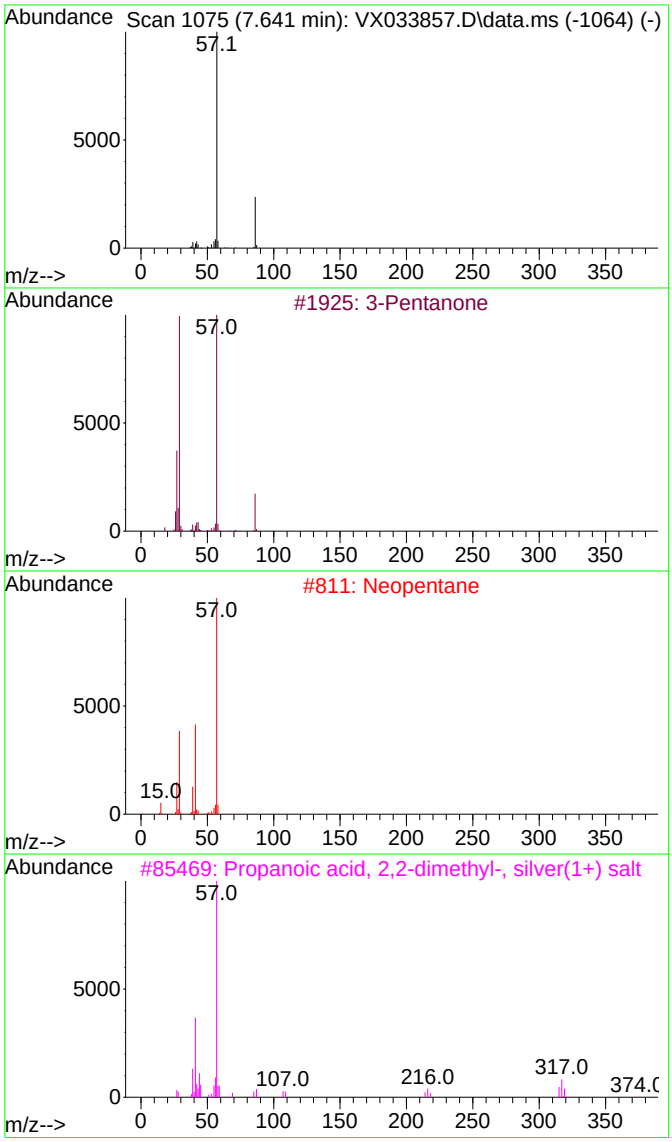
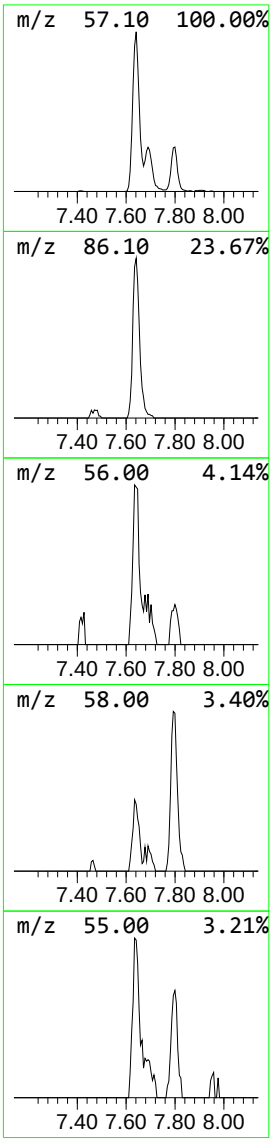
****

Peak Number 1 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	5.71 ug/l	65004	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	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
4	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7





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

TIC Library : C:\Database\NIST20.L
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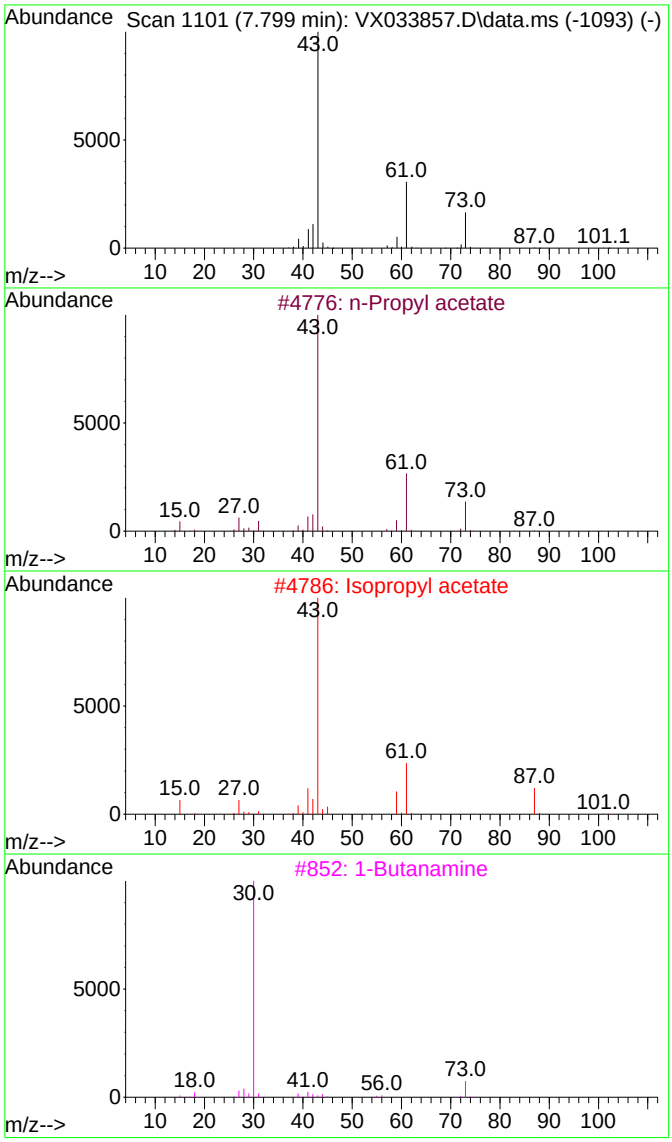
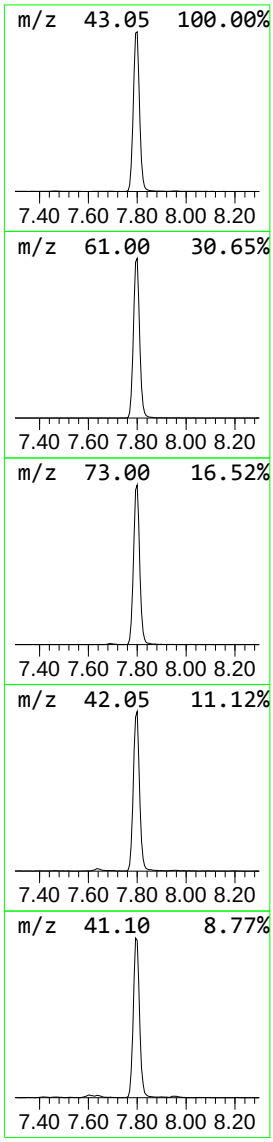
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	138.71 ug/l	1578320	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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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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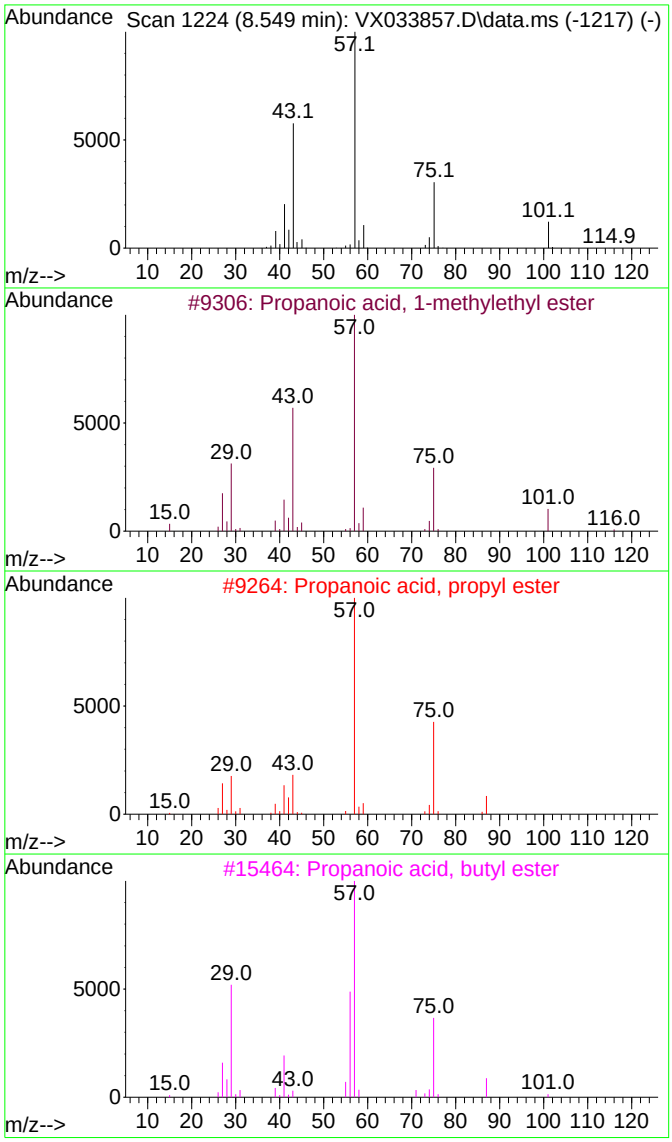
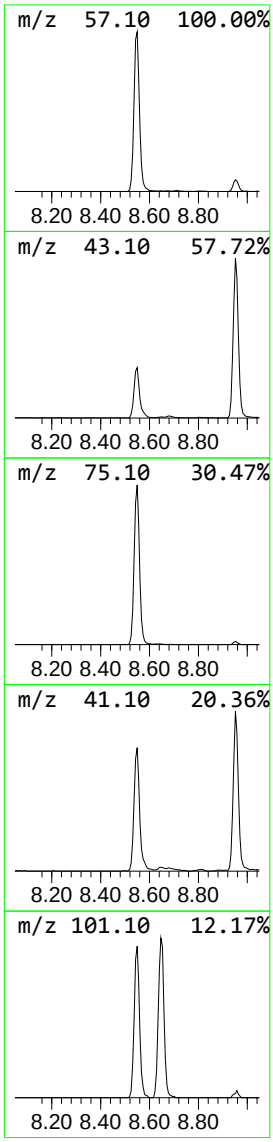
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	24.72 ug/l	305496	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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	14
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	10





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Instrument :
MSVOA_X
ClientSampleId :
MH-9

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

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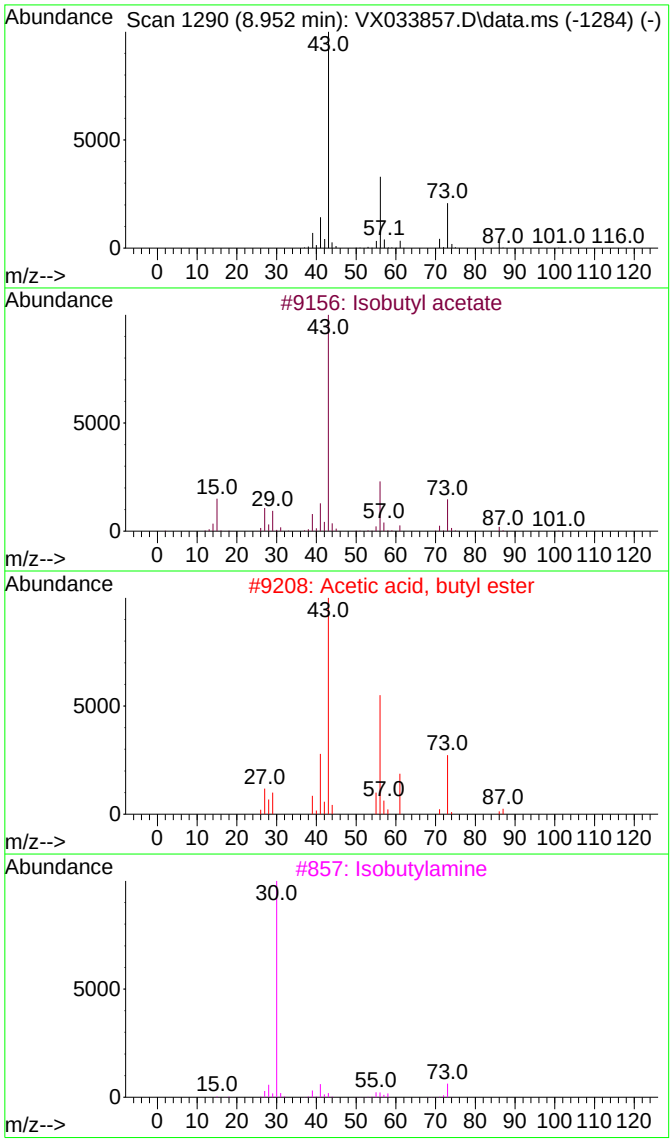
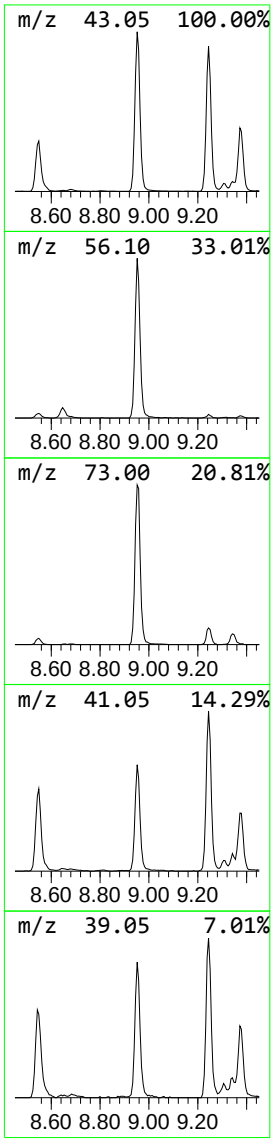
****

Peak Number 4 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	31.57 ug/l	390088	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	42
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
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TIC Library : C:\Database\NIST20.L
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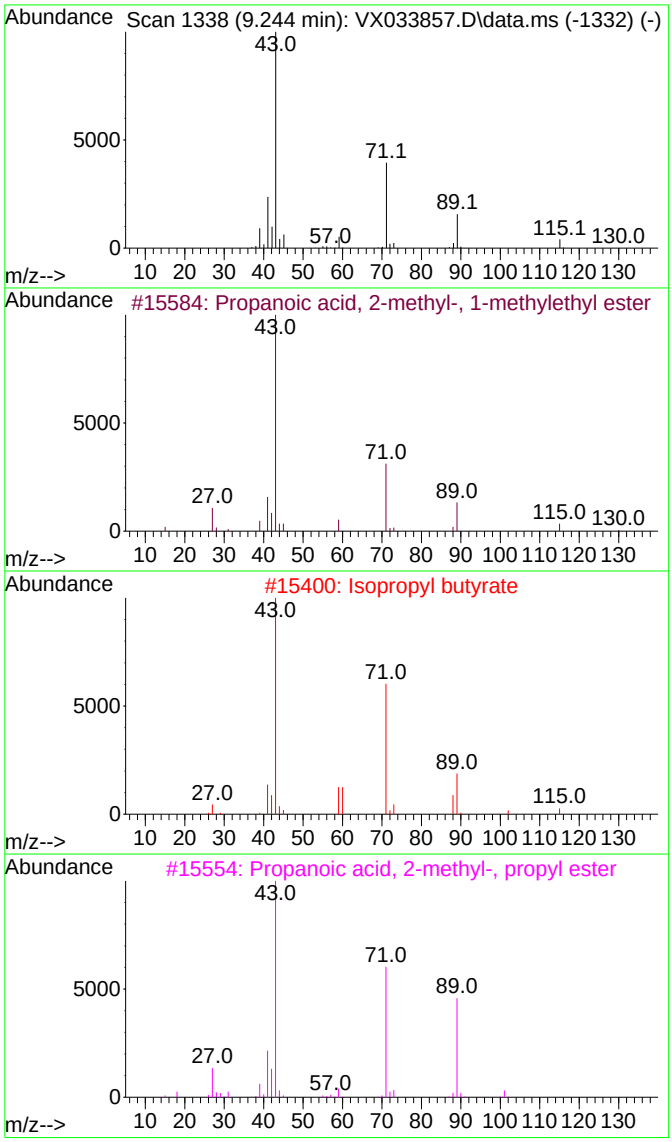
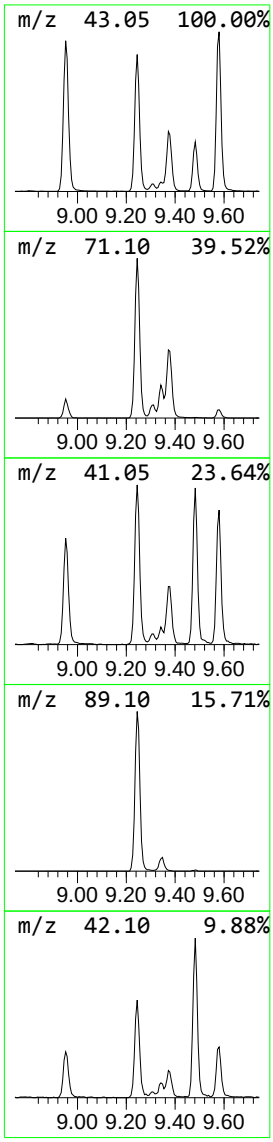
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	30.70 ug/l	379407	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	59
4	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	56
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	42





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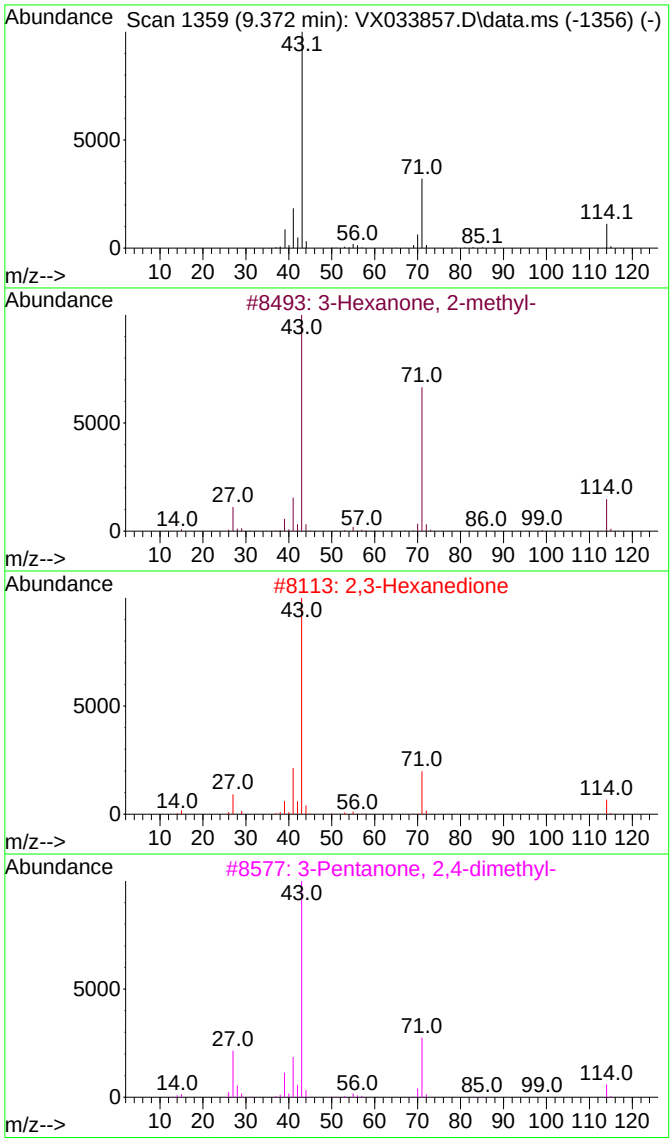
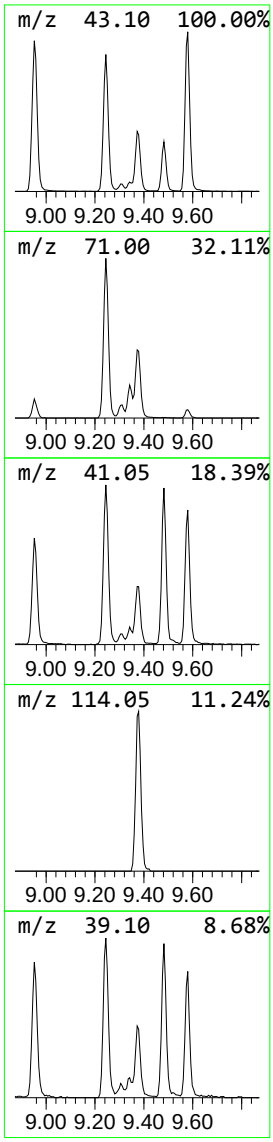
****
Peak Number 6 3-Hexanone, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.372	12.83 ug/l	158513	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	72
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
3	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	64
4	Pyrrolidine	71	C4H9N	000123-75-1	50
5	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50





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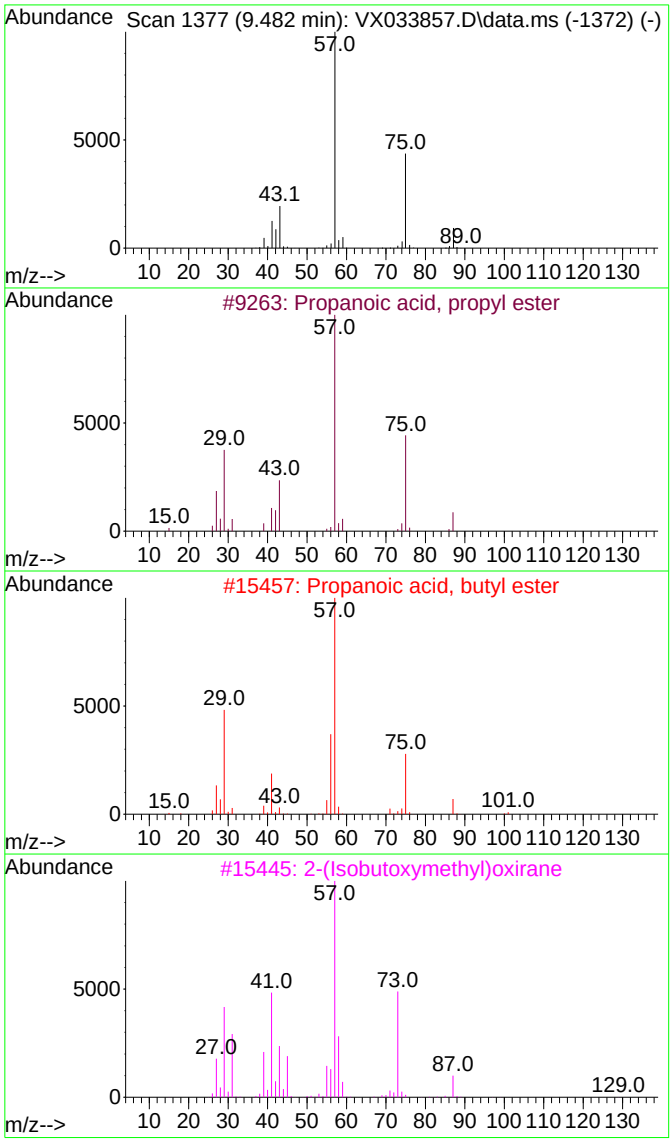
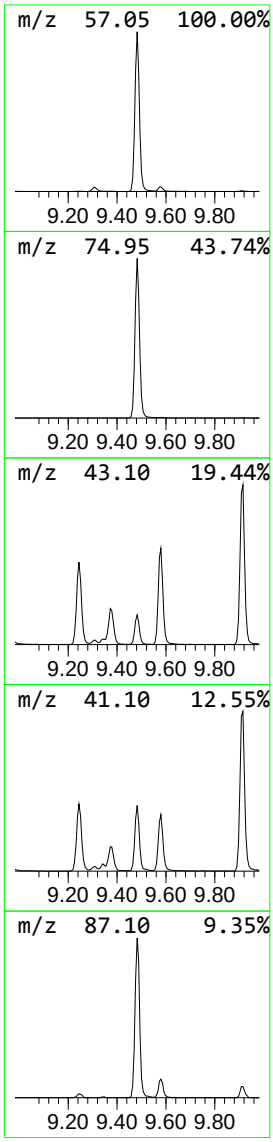
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	49.56 ug/l	612424	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	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	7





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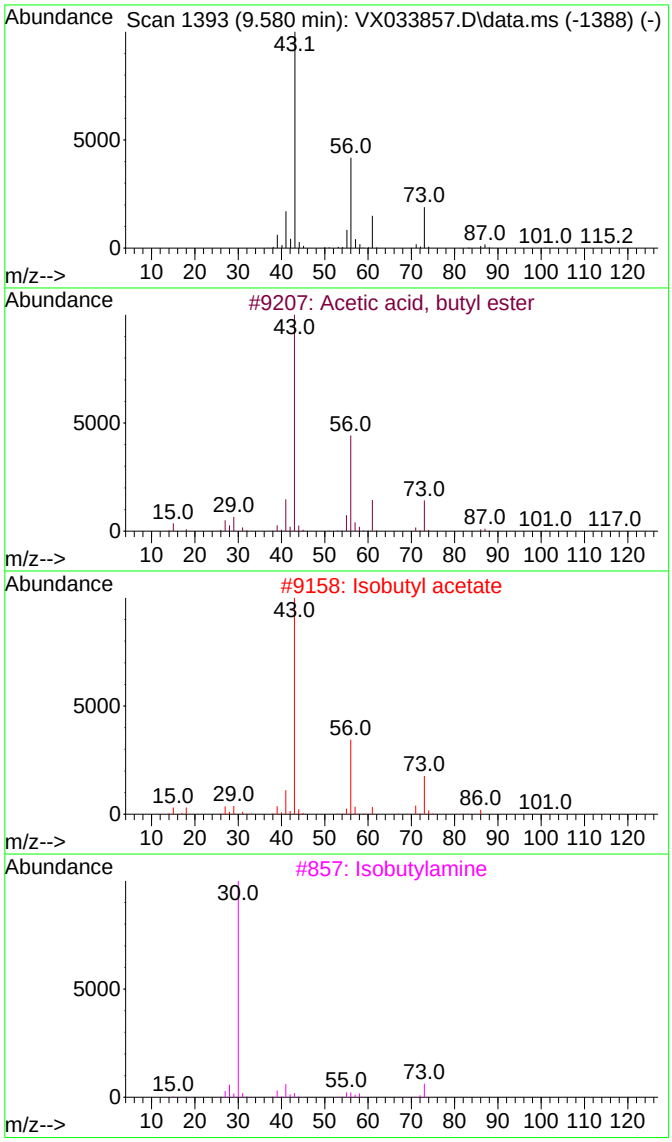
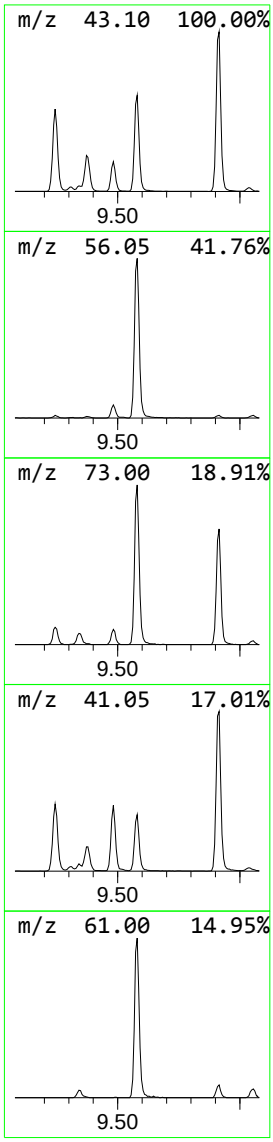
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	34.40 ug/l	425033	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	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9





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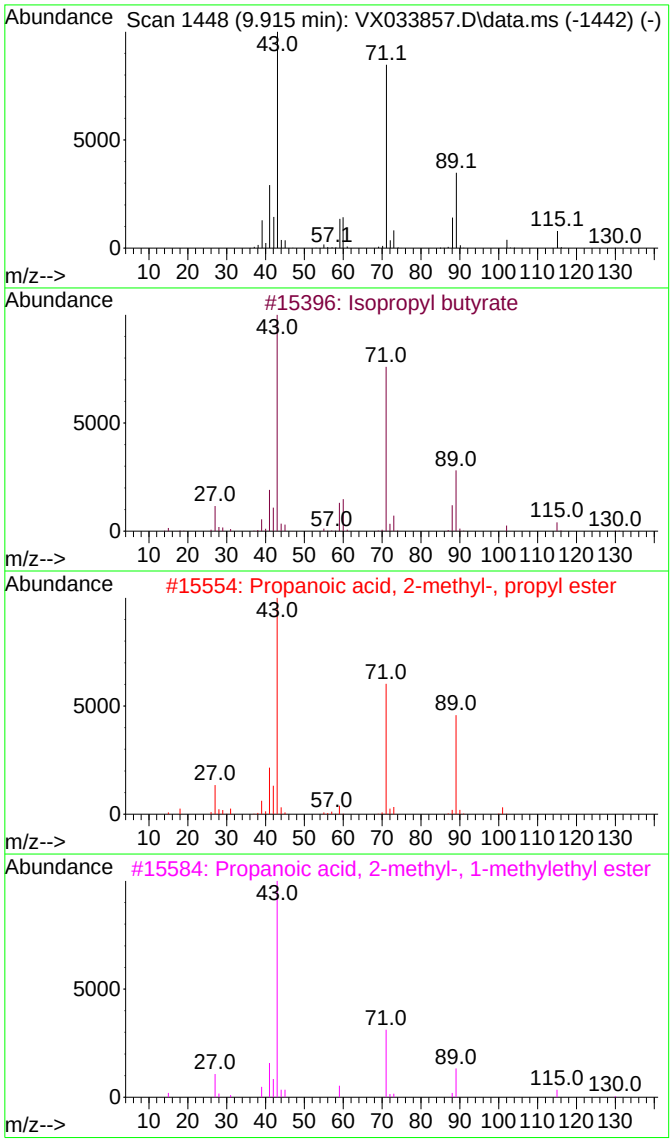
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

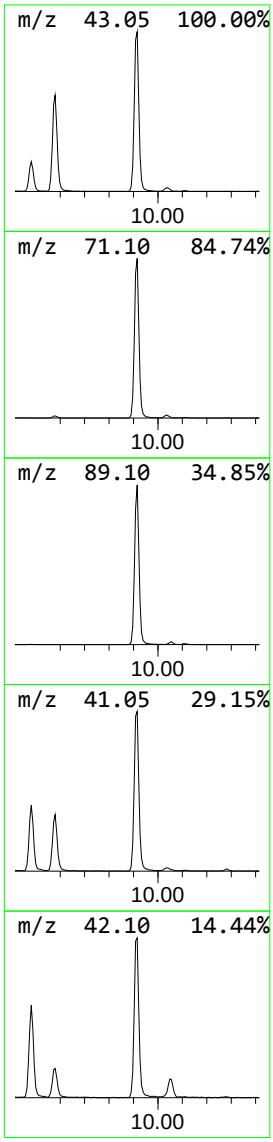
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	86.74 ug/l	1071800	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, pentyl ester	158	C9H18O2	000540-18-1	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





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MSVOA_X
ClientSampleId :
MH-9

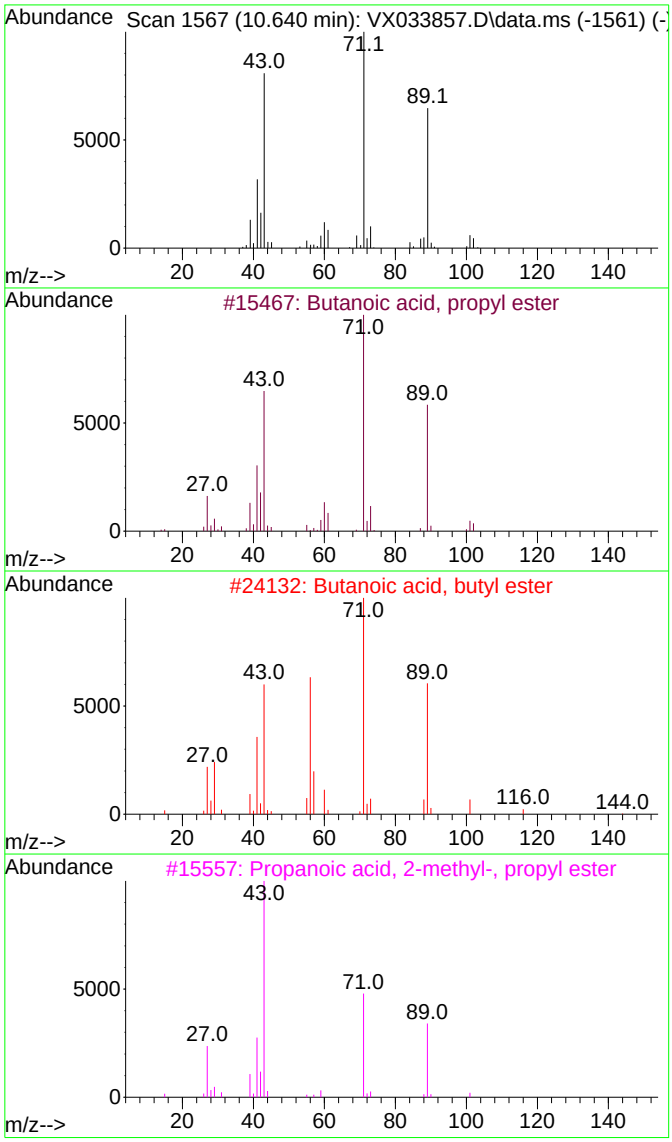
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

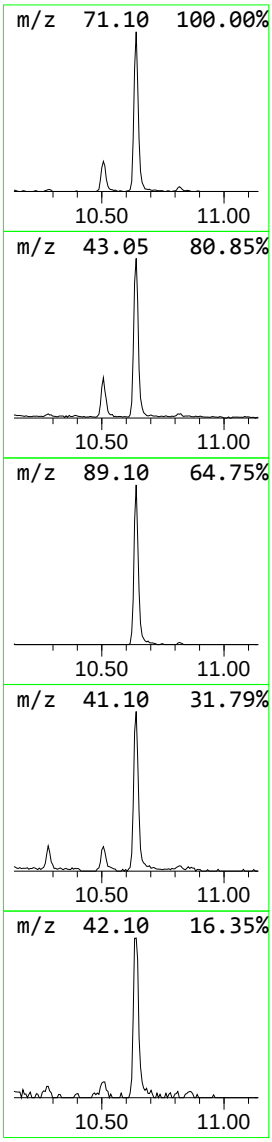
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.74 ug/l	95636	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	Malic Acid	134	C4H6O5	006915-15-7	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	56





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033857.D
Acq On : 23 Jan 2023 18:15
Operator : JC/MD
Sample : 01252-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MH-9

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	65004	2	6.763	568947	50.0
n-Propyl acetate	7.799	138.7	ug/l	1578320	2	6.763	568947	50.0
Propanoic acid,...	8.549	24.7	ug/l	305496	3	10.055	617844	50.0
Isobutyl acetate	8.952	31.6	ug/l	390088	3	10.055	617844	50.0
Propanoic acid,...	9.244	30.7	ug/l	379407	3	10.055	617844	50.0
3-Hexanone, 2-m...	9.372	12.8	ug/l	158513	3	10.055	617844	50.0
Propanoic acid,...	9.482	49.6	ug/l	612424	3	10.055	617844	50.0
Acetic acid, bu...	9.580	34.4	ug/l	425033	3	10.055	617844	50.0
Isopropyl butyrate	9.915	86.7	ug/l	1071800	3	10.055	617844	50.0
Butanoic acid, ...	10.640	7.7	ug/l	95636	3	10.055	617844	50.0