LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013023\
Data File : VX033947.D
Acq On : 30 Jan 2023 15:28
Operator : JC/MD
Sample : 01356-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-J

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: VX033947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.373	205	211	222	rBV	14998	24768	1.65%	0.279%
2	2.788	271	279	288	rBV	14046	27532	1.83%	0.310%
3	4.715	586	595	609	rBV2	10330	30772	2.05%	0.347%
4	5.385	694	705	721	rBV2	81703	236747	15.76%	2.670%
5	5.550	721	732	746	rBV	147049	417436	27.79%	4.707%
6	5.952	787	798	813	rBV	81415	216200	14.39%	2.438%
7	6.336	852	861	880	rBV	60445	156856	10.44%	1.769%
8	6.763	916	931	944	rBV	214903	553748	36.86%	6.244%
9	7.635	1064	1074	1080	rBV	34888	68324	4.55%	0.770%
10	7.690	1080	1083	1093	rVB	10712	20293	1.35%	0.229%
11	7.793	1093	1100	1117	rBV	848021	1502353	100.00%	16.941%
12	8.549	1217	1224	1234	rBV	172911	286211	19.05%	3.227%
13	8.647	1234	1240	1256	rVB	438829	700315	46.61%	7.897%
14	8.952	1284	1290	1313	rBV	244559	368643	24.54%	4.157%
15	9.244	1332	1338	1345	rBV	249777	351322	23.38%	3.962%
16	9.305	1345	1348	1351	rVV	24148	36852	2.45%	0.416%
17	9.342	1351	1354	1356	rVV	37810	51944	3.46%	0.586%
18	9.378	1356	1360	1372	rVV	100728	163991	10.92%	1.849%
19	9.482	1372	1377	1388	rVV	434449	583595	38.85%	6.581%
20	9.579	1388	1393	1421	rVB	293304	410738	27.34%	4.632%
21	9.915	1442	1448	1463	rBV	742965	1009009	67.16%	11.378%
22	10.055	1463	1471	1477	rVV	435304	593164	39.48%	6.689%
23	10.506	1539	1545	1554	rBV2	10416	15231	1.01%	0.172%
24	10.640	1562	1567	1578	rBV	66596	86385	5.75%	0.974%
25	11.079	1634	1639	1656	rBV	340873	440135	29.30%	4.963%
26	12.024	1788	1794	1806	rBV	405130	515520	34.31%	5.813%

Sum of corrected areas: 8868084

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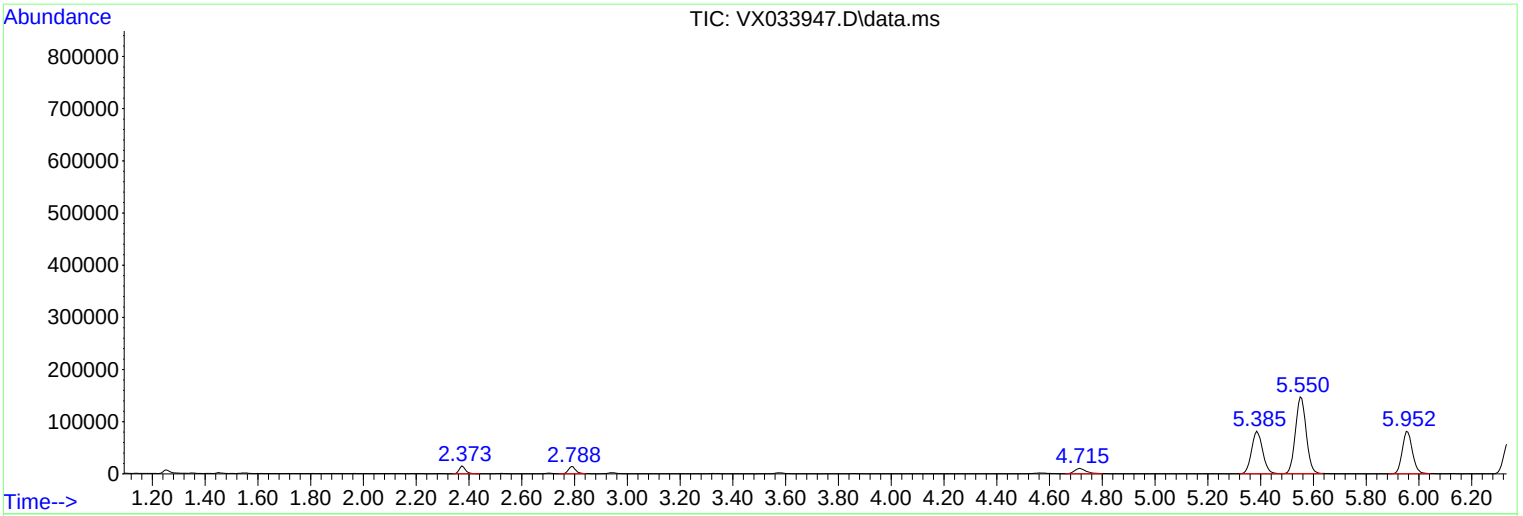
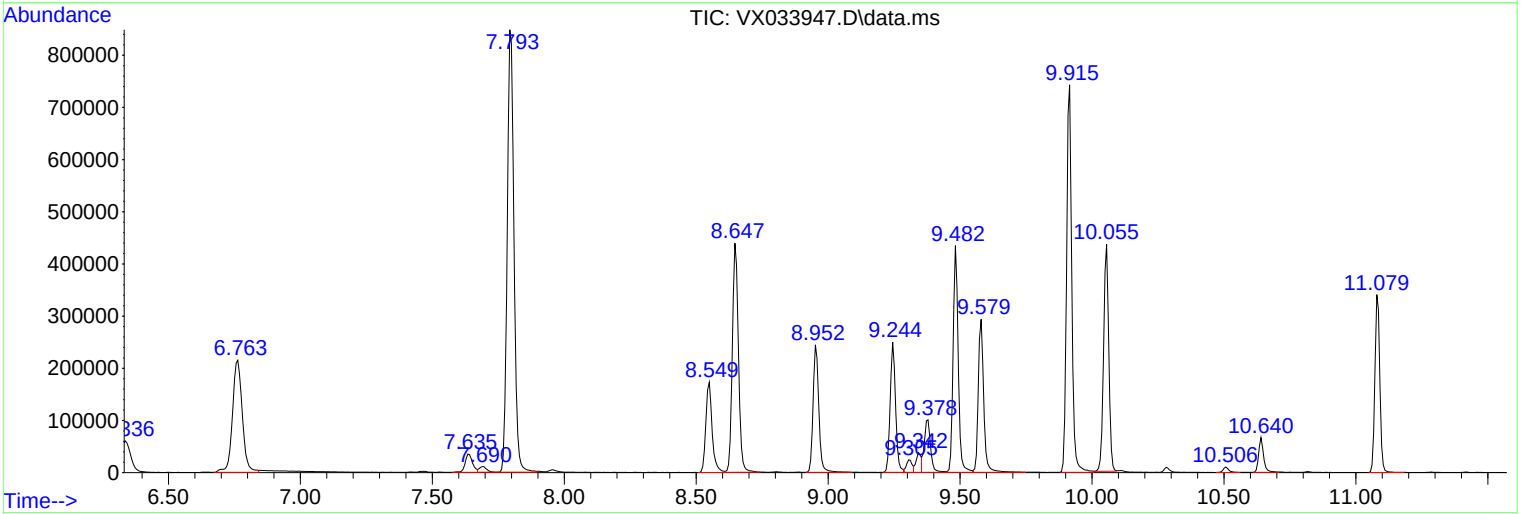
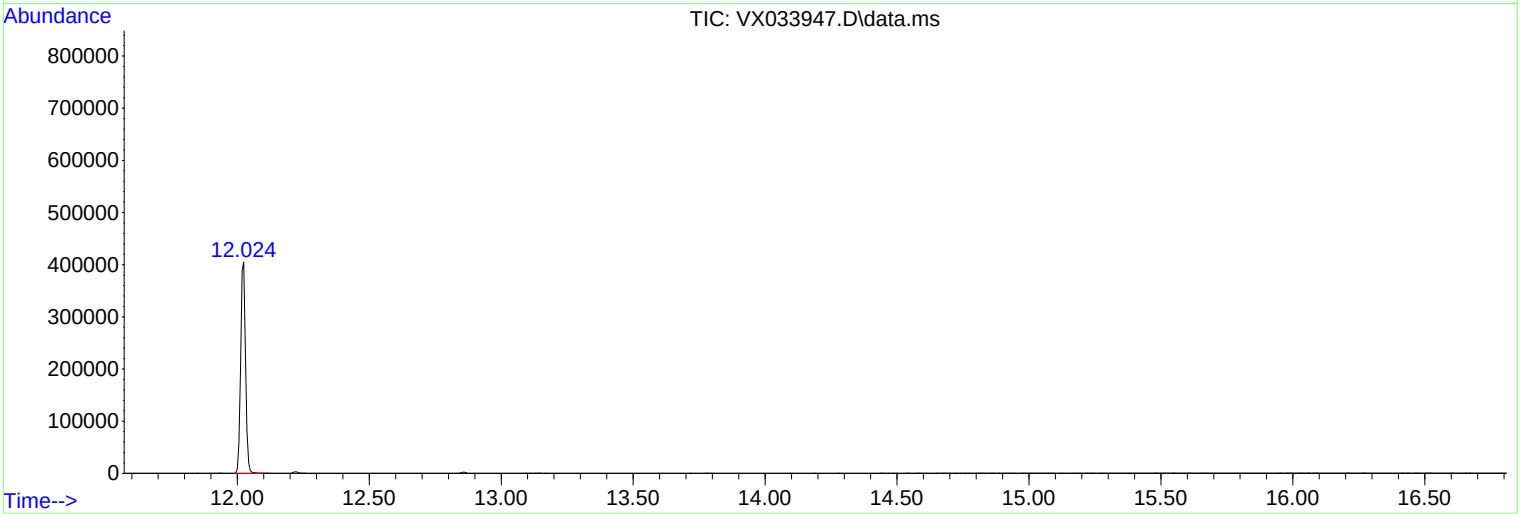
Instrument :
MSVOA_X
ClientSampleId :
TP-J

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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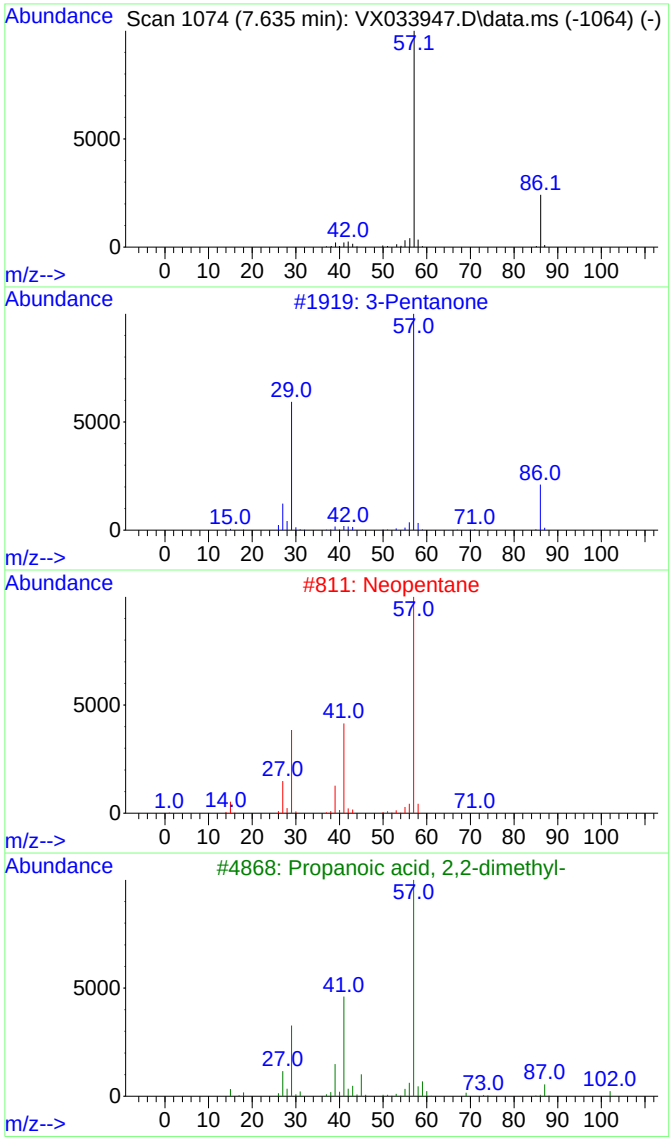
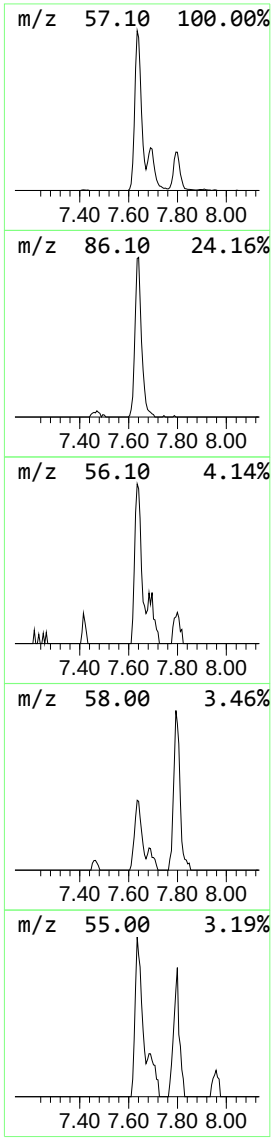
****
Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.635	6.17 ug/l	68324	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	25
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
4	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7
5	2-Hydroxybutanenitrile	85	C4H7NO	1000486-93-5	5





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Data File : VX033947.D
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-J

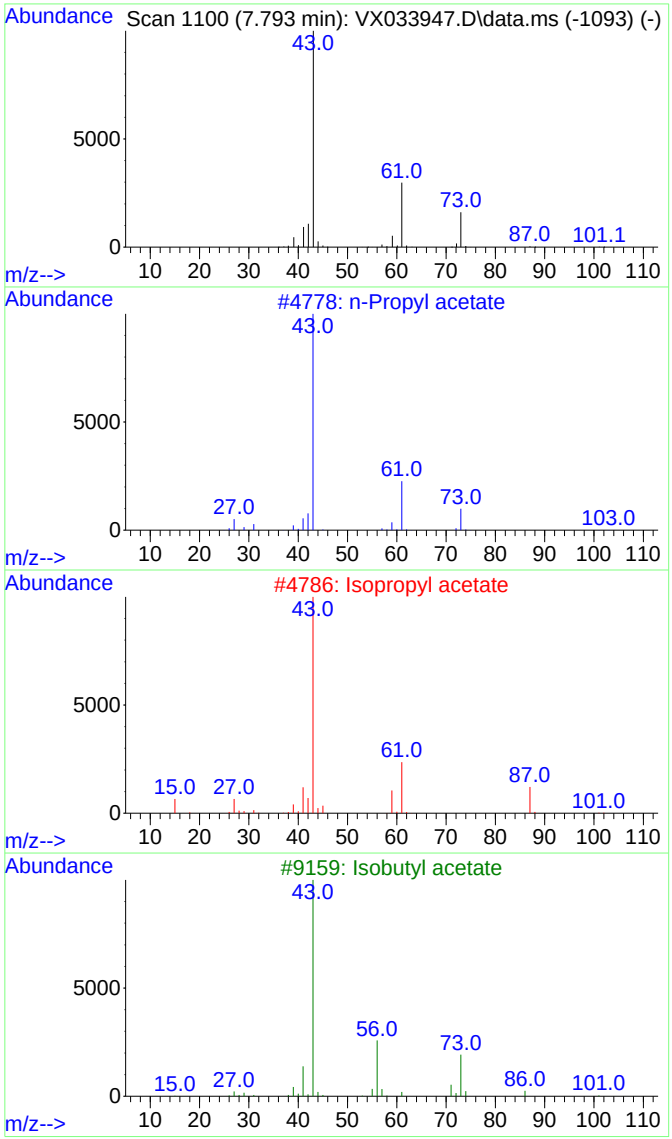
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

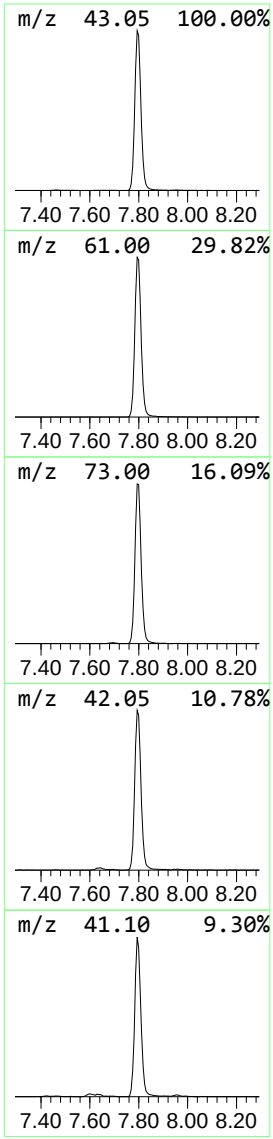
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.793	135.65 ug/l	1502350	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	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Instrument :
MSVOA_X
ClientSampleId :
TP-J

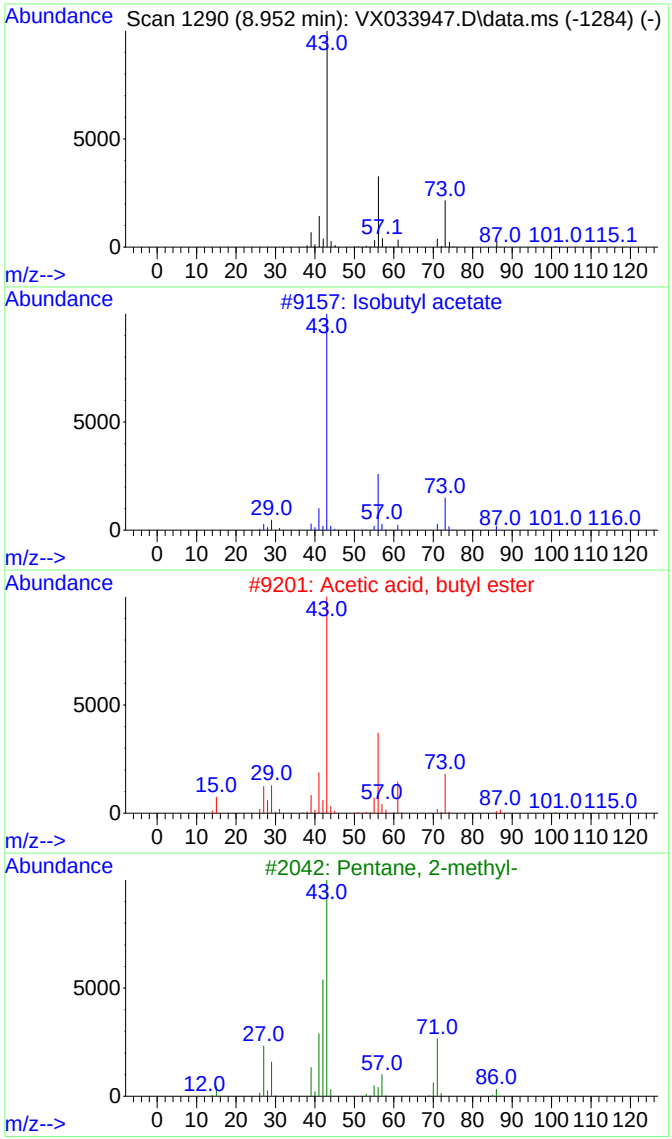
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

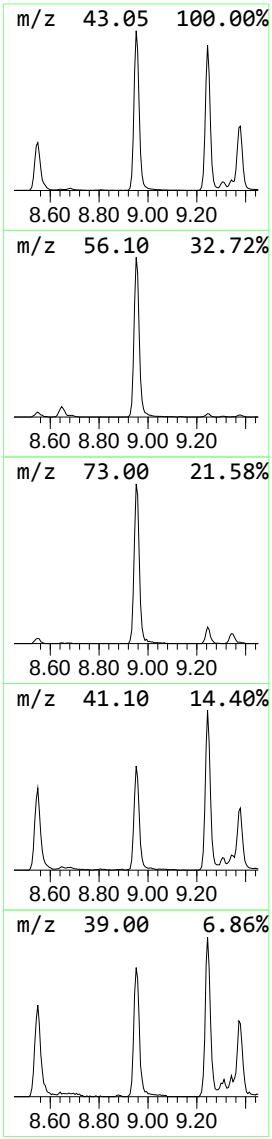
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	31.07 ug/l	368643	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	38
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9
5	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-J

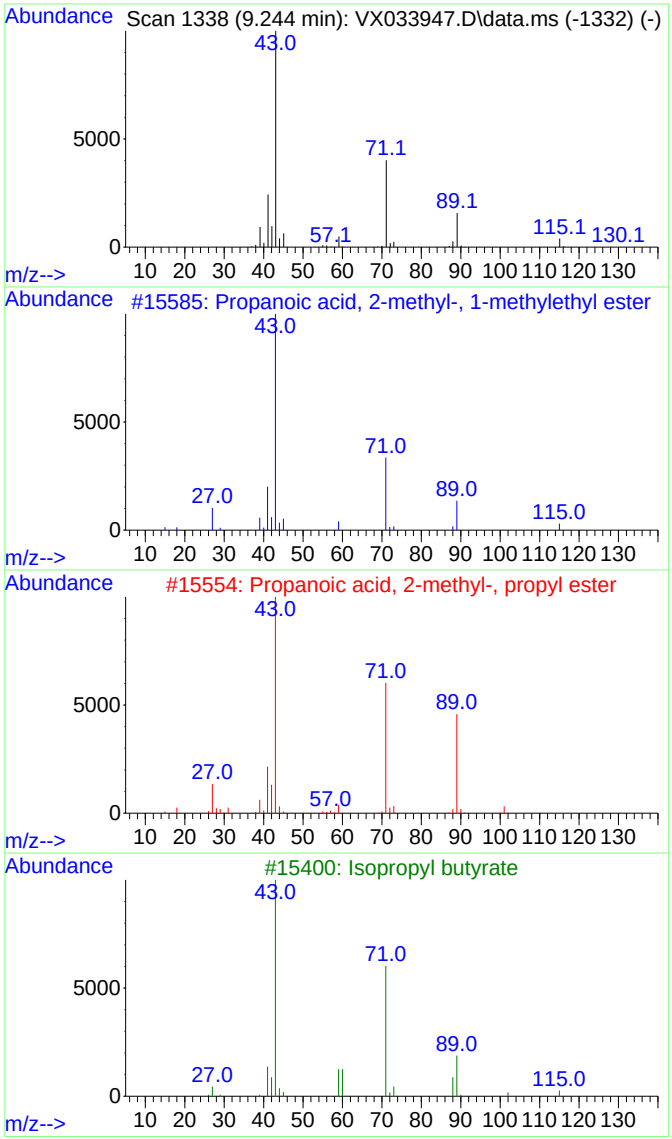
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

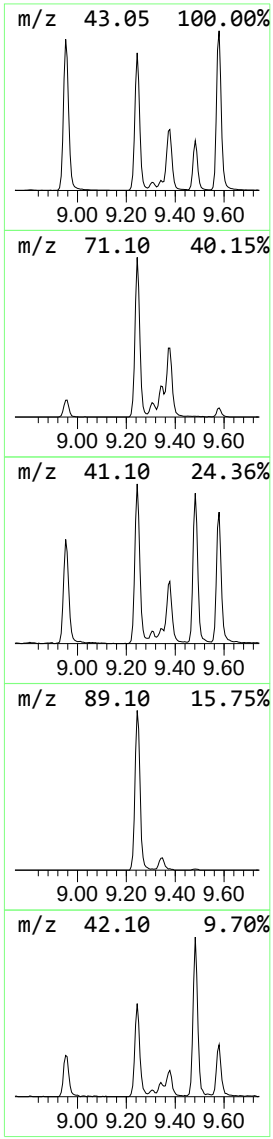
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	29.61 ug/l	351322	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	72
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013023\
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Operator : JC/MD
Sample : 01356-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-J

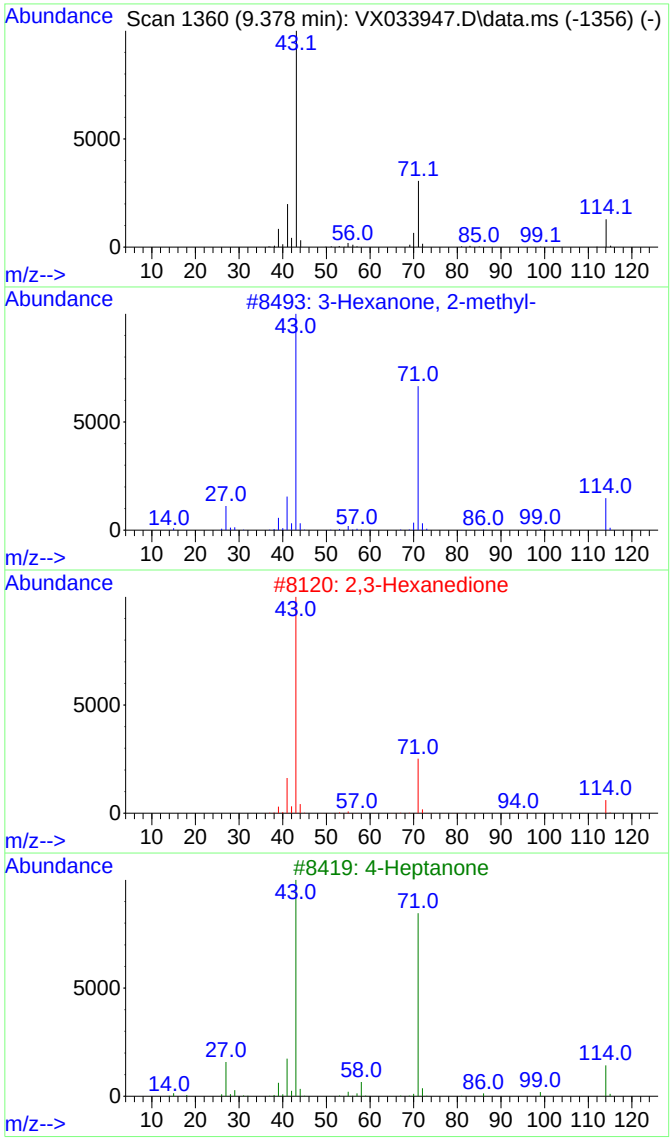
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

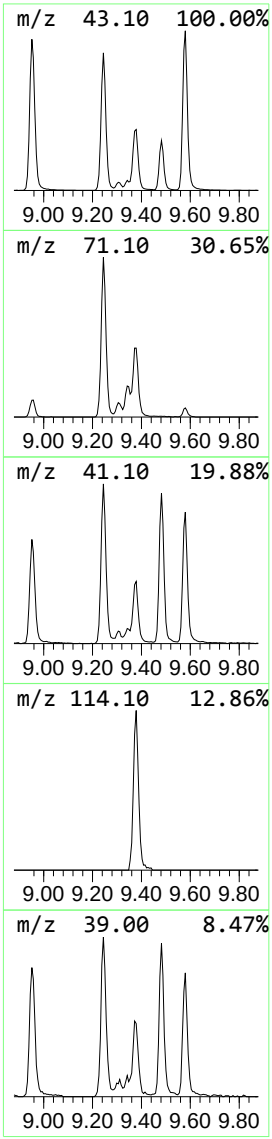
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Hexanone, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	13.82 ug/l	163991	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	4-Heptanone	114	C7H14O	000123-19-3	64
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	52
5	Butane, 2-(ethenyloxy)-2-methyl-	114	C7H14O	029281-39-8	39





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ALS Vial : 12 Sample Multiplier: 1

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

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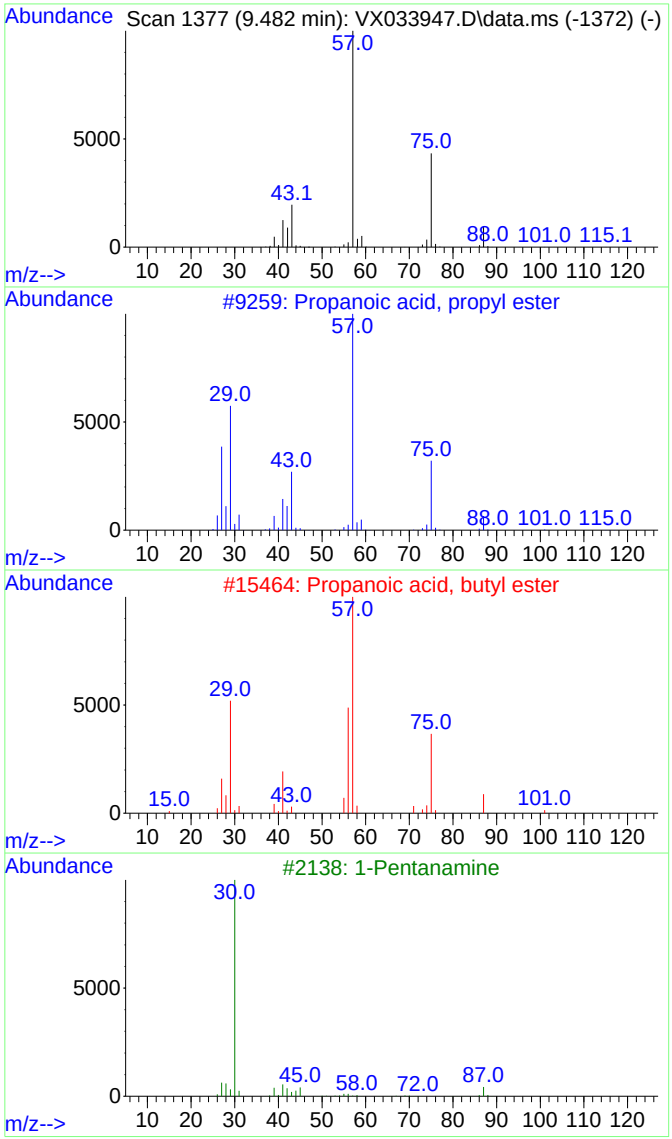
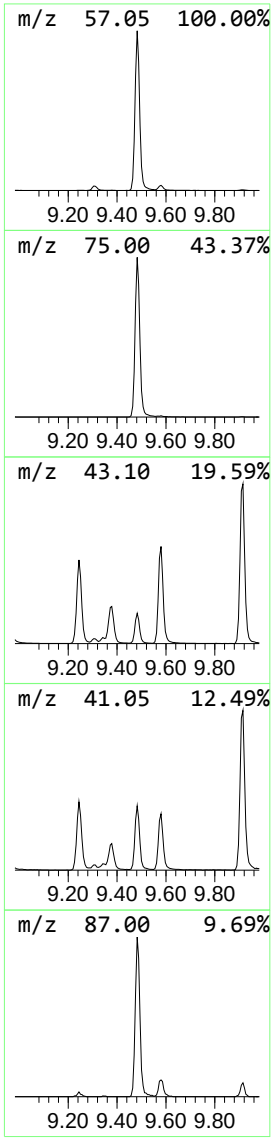
****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	49.19 ug/l	583595	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	39
3	1-Pentanamine	87	C5H13N	000110-58-7	10
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





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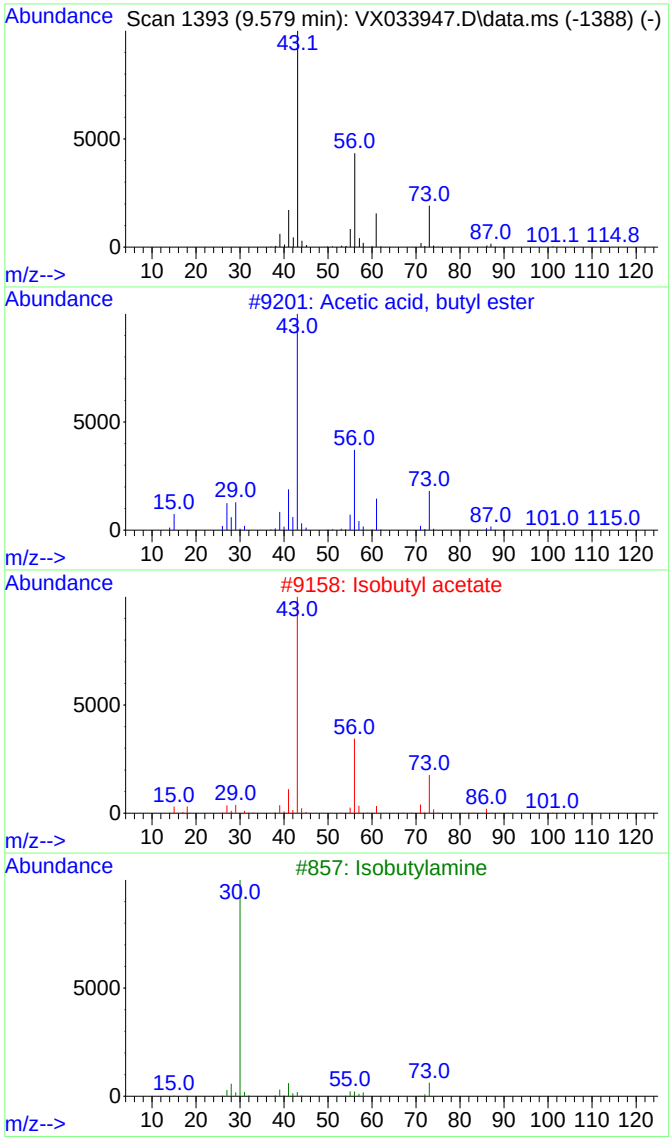
Quant Title : SW846 8260

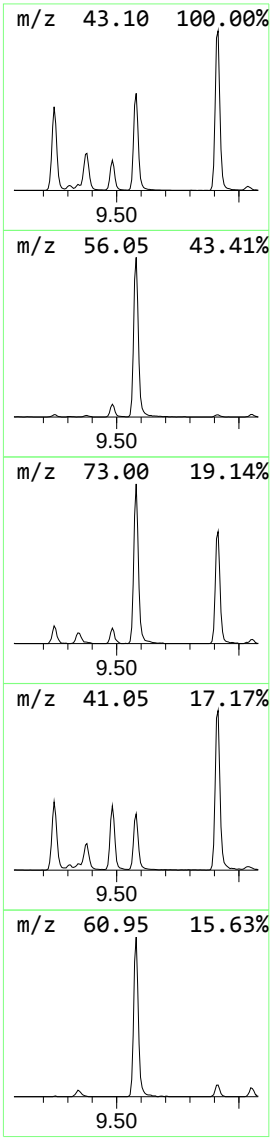
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	34.62 ug/l	410738	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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TIC Library : C:\Database\NIST20.L
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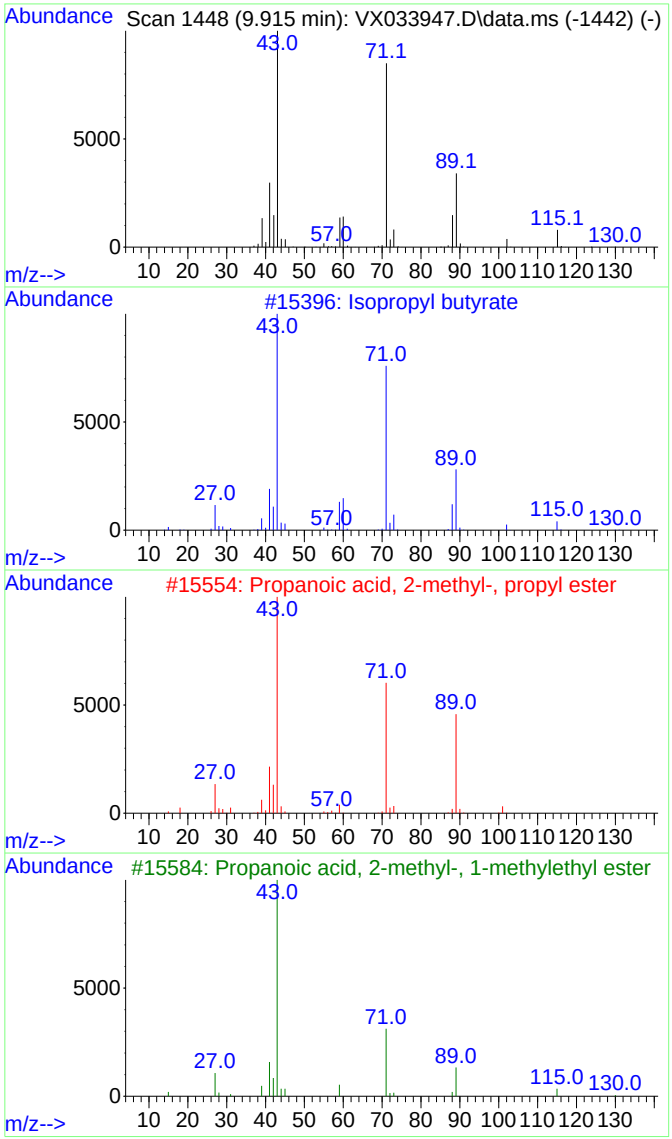
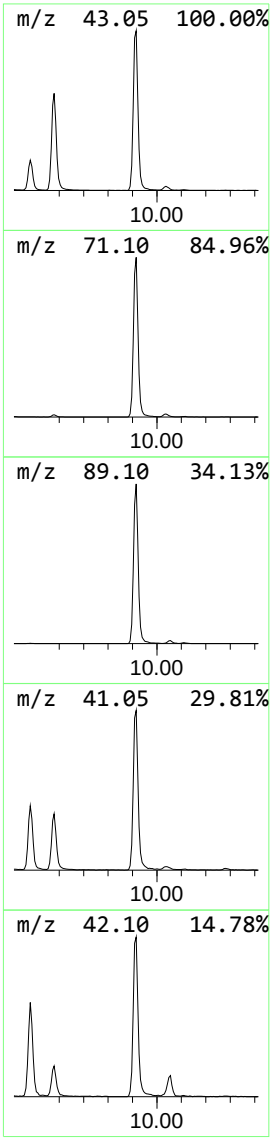
****
Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	85.05 ug/l	1009010	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	64





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-J

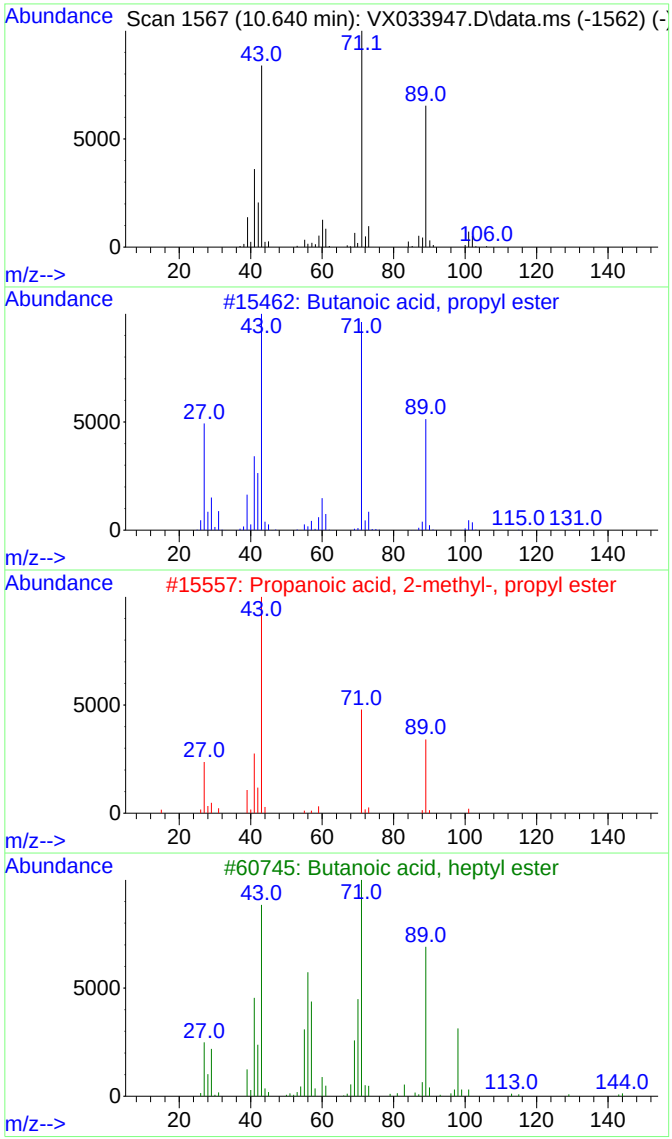
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

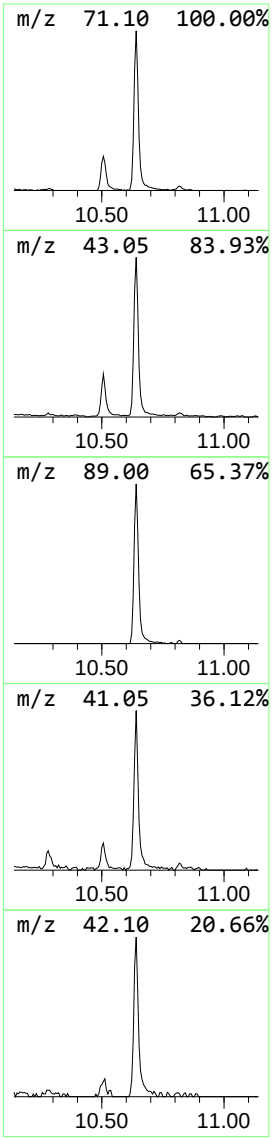
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.28 ug/l	86385	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, heptyl ester	186	C11H22O2	005870-93-9	72
4	Malic Acid	134	C4H6O5	006915-15-7	64
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013023\
Data File : VX033947.D
Acq On : 30 Jan 2023 15:28
Operator : JC/MD
Sample : 01356-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-J

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	7.635	6.2	ug/l	68324	2	6.763	553748	50.0
n-Propyl acetate	7.793	135.7	ug/l	1502350	2	6.763	553748	50.0
Isobutyl acetate	8.952	31.1	ug/l	368643	3	10.055	593164	50.0
Propanoic acid,...	9.244	29.6	ug/l	351322	3	10.055	593164	50.0
3-Hexanone, 2-m...	9.378	13.8	ug/l	163991	3	10.055	593164	50.0
Propanoic acid,...	9.482	49.2	ug/l	583595	3	10.055	593164	50.0
Acetic acid, bu...	9.579	34.6	ug/l	410738	3	10.055	593164	50.0
Isopropyl butyrate	9.915	85.1	ug/l	1009010	3	10.055	593164	50.0
Butanoic acid, ...	10.640	7.3	ug/l	86385	3	10.055	593164	50.0