LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033858.D
Acq On : 23 Jan 2023 18:39
Operator : JC/MD
Sample : 01255-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-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: VX033858.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	207	214	221	rBV	10051	20195	1.27%	0.220%
2	2.794	273	280	291	rVB	14465	27472	1.73%	0.299%
3	4.715	585	595	606	rBV	11471	32820	2.07%	0.357%
4	5.385	694	705	721	rBV	81285	236009	14.86%	2.566%
5	5.550	721	732	744	rBV	145483	410518	25.86%	4.464%
6	5.952	789	798	817	rBV	81132	220026	13.86%	2.393%
7	6.336	852	861	878	rBV	64627	169278	10.66%	1.841%
8	6.763	919	931	946	rBV	216323	556060	35.02%	6.047%
9	7.641	1068	1075	1080	rBV	32641	60690	3.82%	0.660%
10	7.690	1080	1083	1093	rVB2	11886	20867	1.31%	0.227%
11	7.793	1093	1100	1115	rBV	890361	1587713	100.00%	17.265%
12	8.549	1217	1224	1234	rBV	193729	308702	19.44%	3.357%
13	8.647	1234	1240	1255	rVB	433825	698739	44.01%	7.598%
14	8.952	1284	1290	1305	rBV	274316	399023	25.13%	4.339%
15	9.244	1332	1338	1345	rBV	271136	383173	24.13%	4.167%
16	9.305	1345	1348	1351	rVV	22639	33831	2.13%	0.368%
17	9.342	1351	1354	1356	rVV	41825	55421	3.49%	0.603%
18	9.378	1356	1360	1369	rVV	104581	160433	10.10%	1.745%
19	9.482	1371	1377	1388	rVV	477302	619768	39.04%	6.739%
20	9.580	1388	1393	1408	rVB	320219	422406	26.60%	4.593%
21	9.915	1442	1448	1463	rBV	809293	1085915	68.39%	11.808%
22	10.055	1463	1471	1478	rBV	427039	604902	38.10%	6.578%
23	10.640	1562	1567	1586	rVB	70959	94767	5.97%	1.030%
24	11.079	1634	1639	1647	rBV	359769	450189	28.35%	4.895%
25	12.024	1788	1794	1803	rBV	417814	537470	33.85%	5.844%

Sum of corrected areas: 9196387

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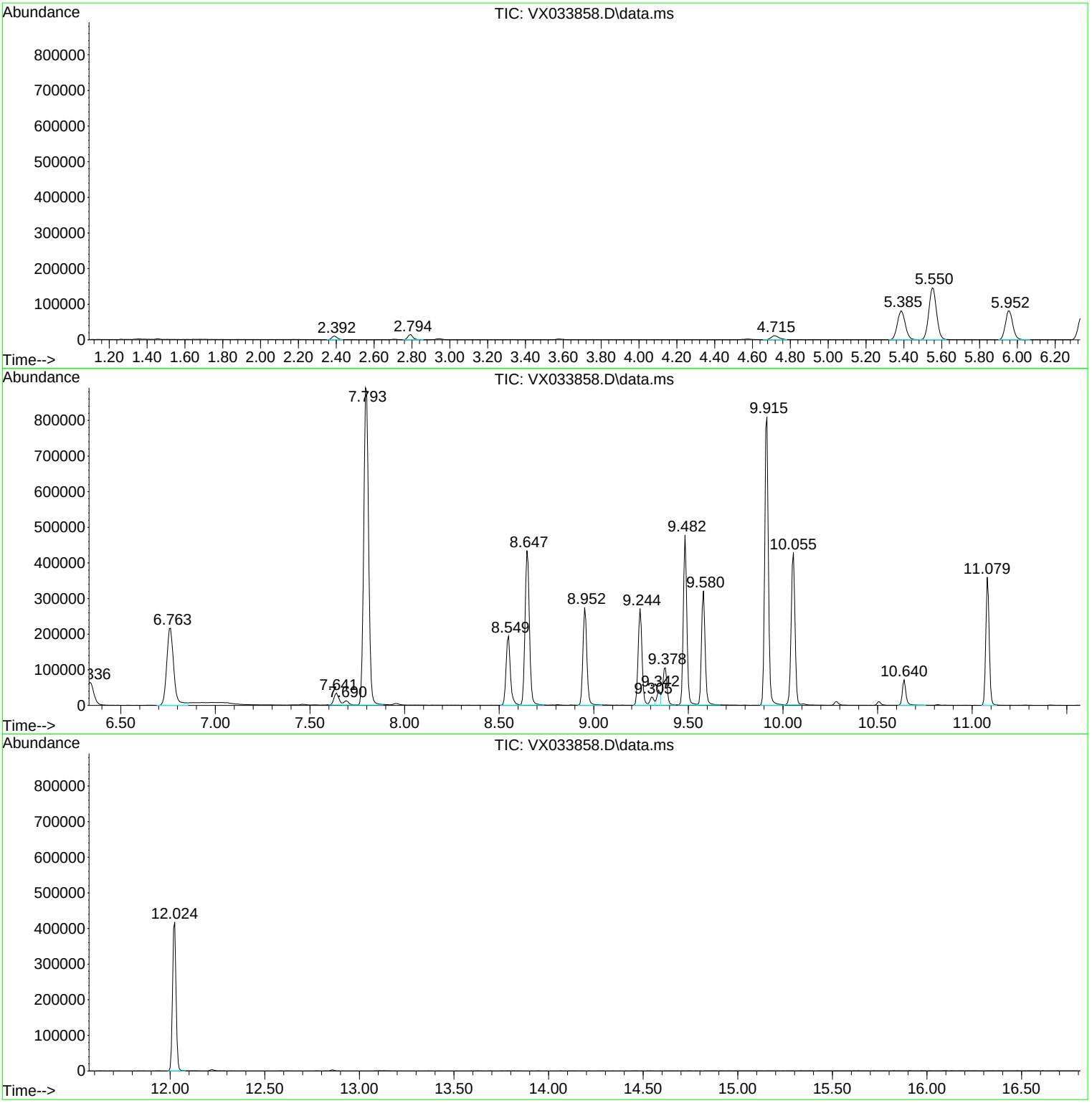
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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



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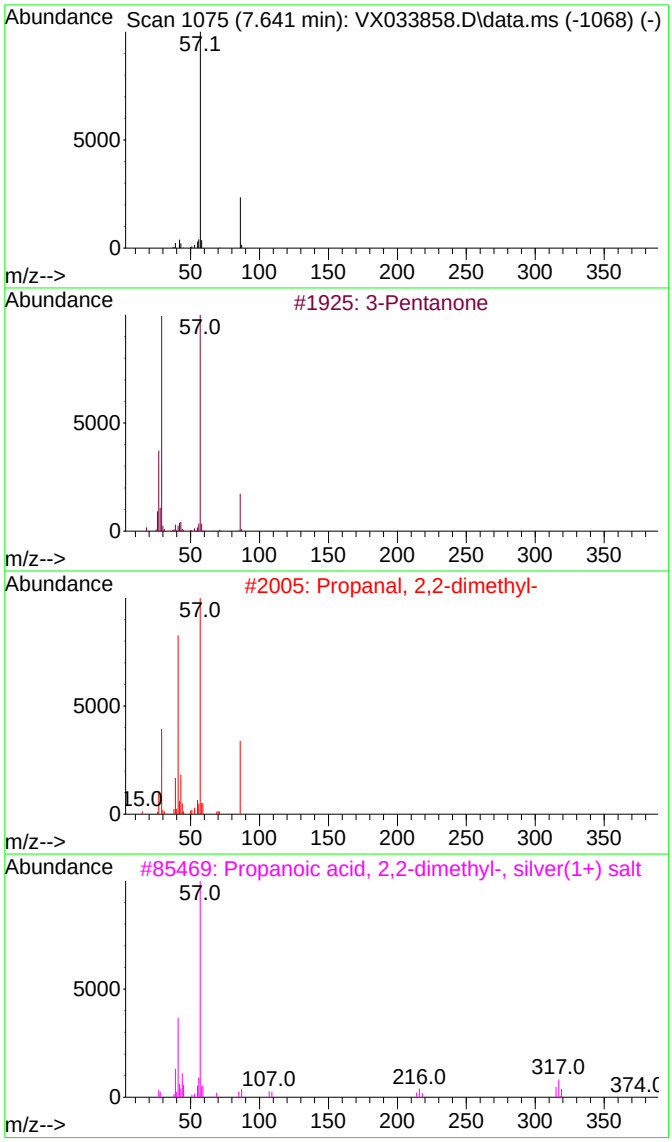
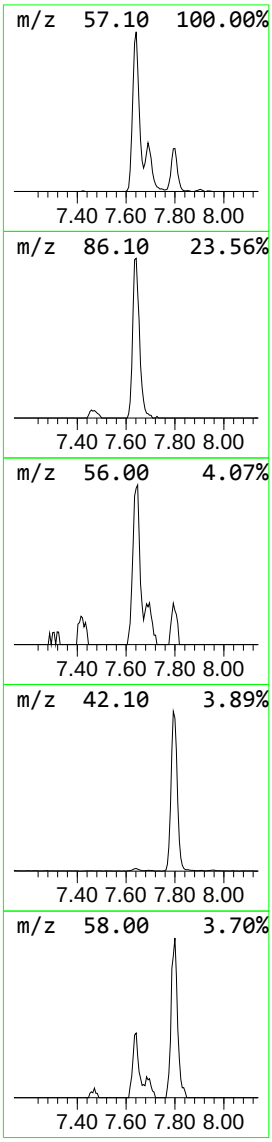
****

Peak Number 1 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	5.46 ug/l	60690	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	83
2	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
3	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
4	Neopentane	72	C5H12	000463-82-1	9
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9





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

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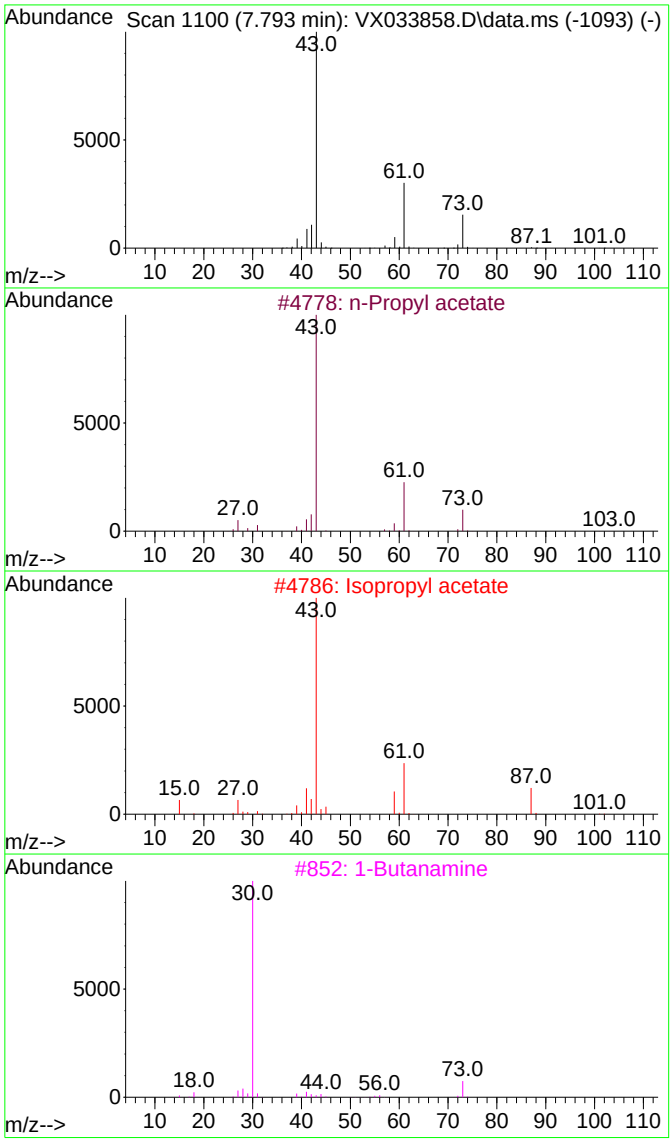
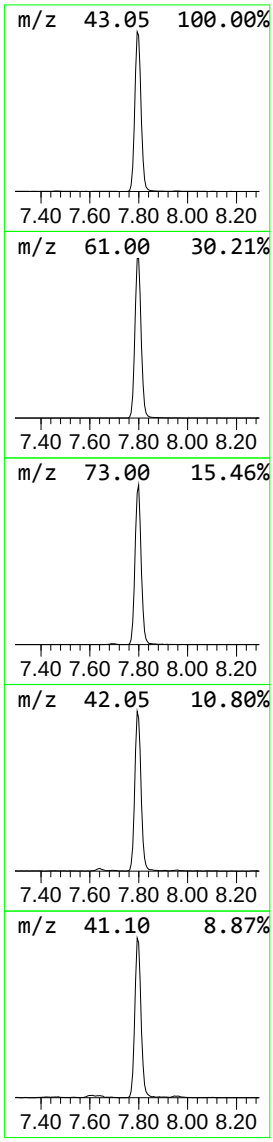
****

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.793	142.76 ug/l	1587710	1,4-Difluorobenzene	6.757

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	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	4





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
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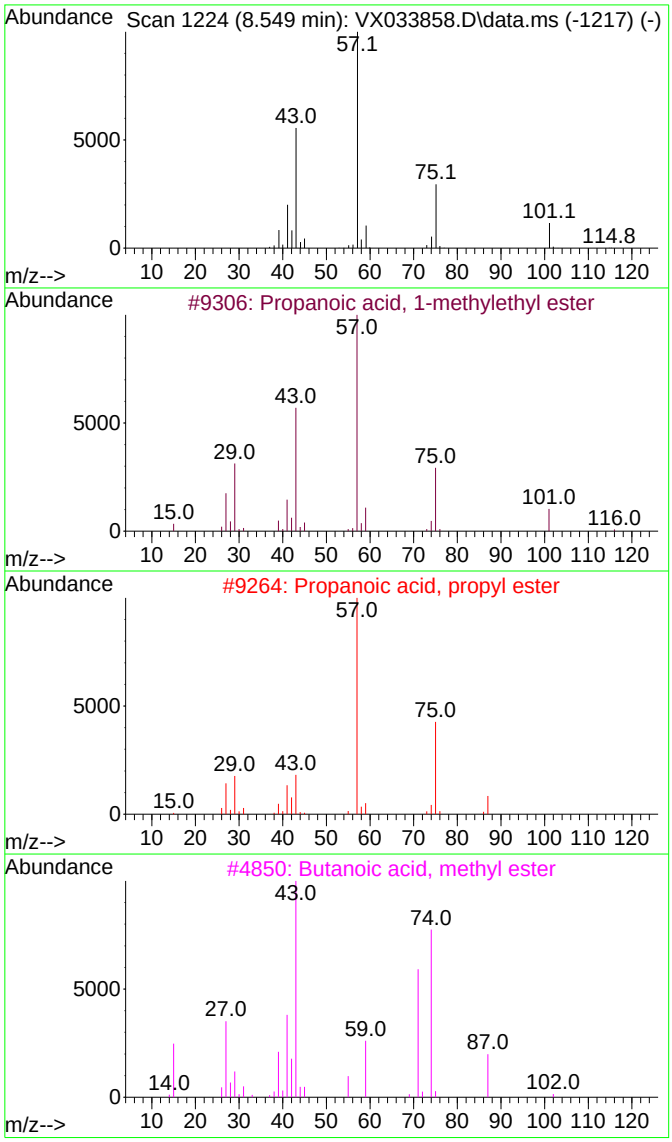
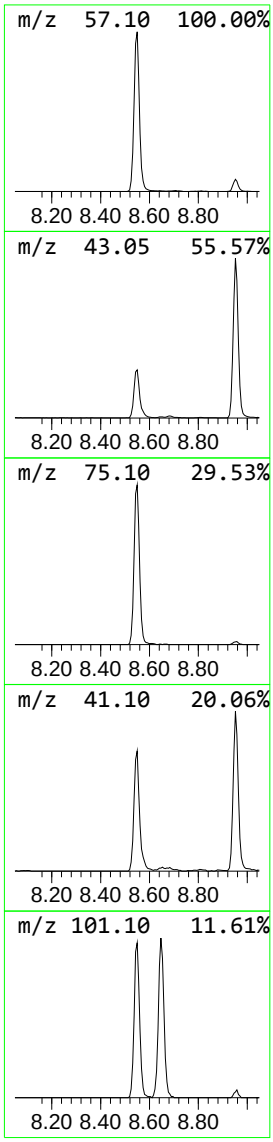
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	25.52 ug/l	308702	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	33
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
4	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument :
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ClientSampleId :
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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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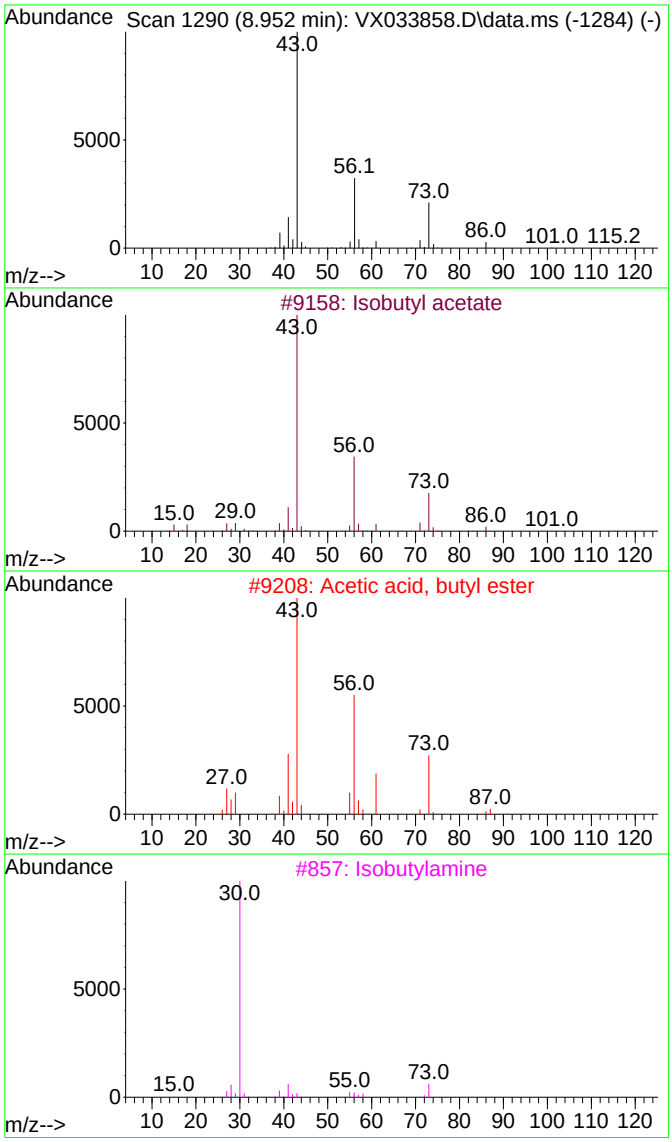
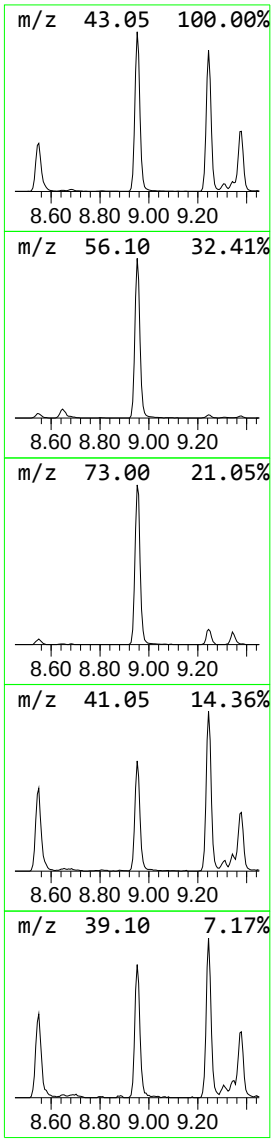
****

Peak Number 4 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	32.98 ug/l	399023	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	Ethane, diazo-	56	C2H4N2	001117-96-0	7





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Instrument :
MSVOA_X
ClientSampleId :
BORING-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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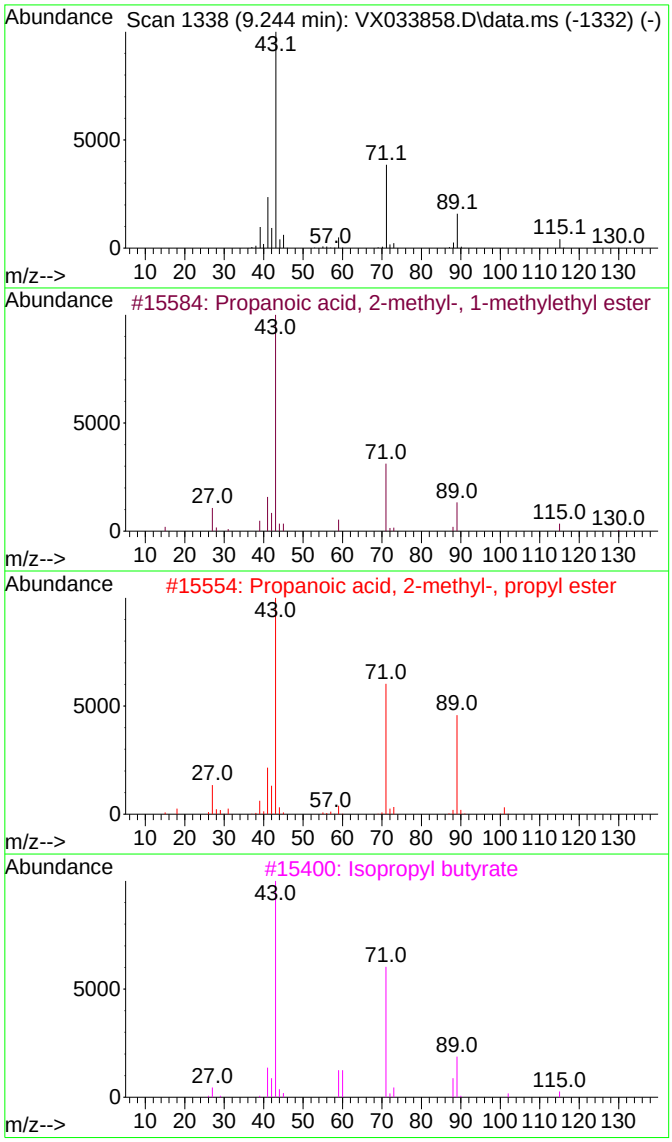
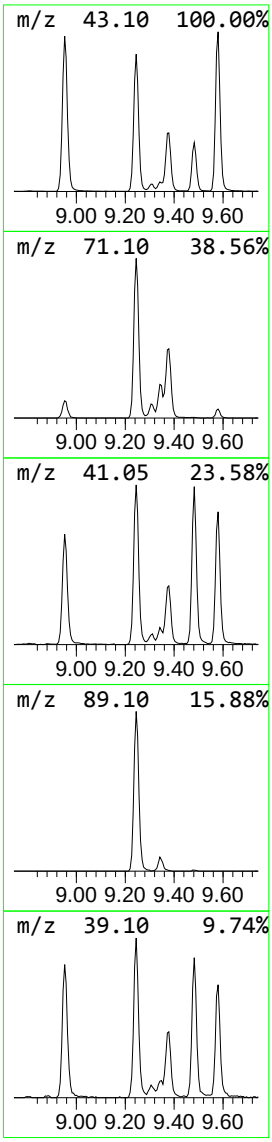
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	31.67 ug/l	383173	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	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	38





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-1

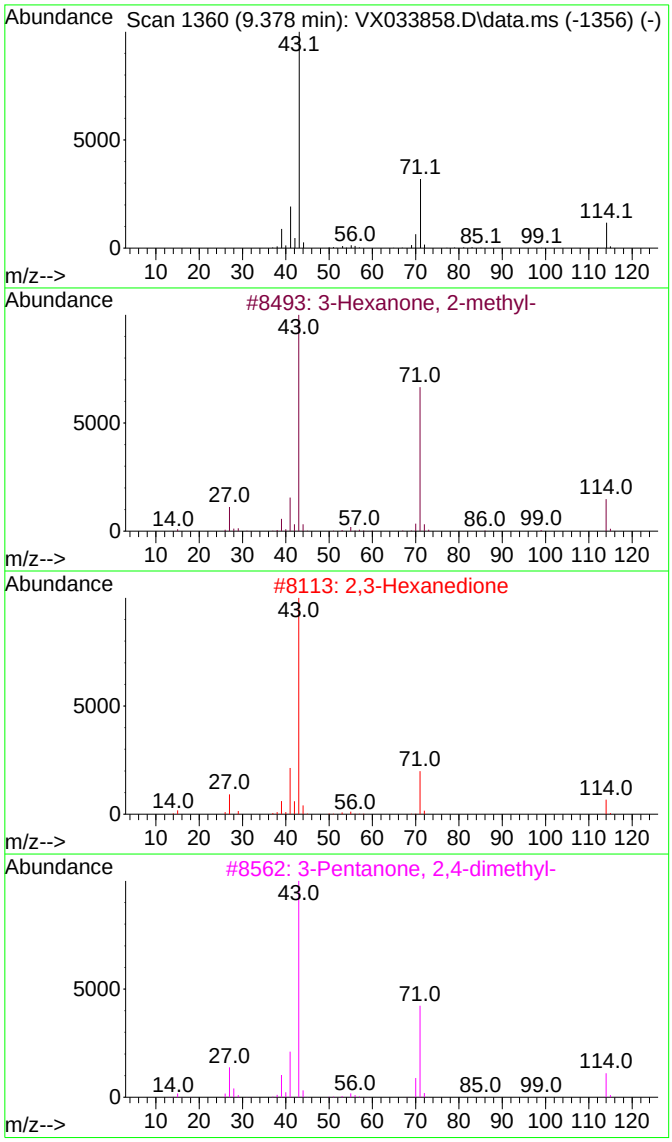
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

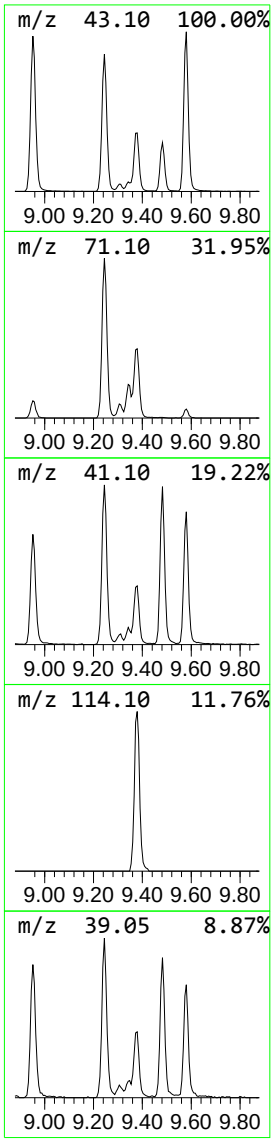
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	13.26 ug/l	160433	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	2,3-Hexanedione	114	C6H10O2	003848-24-6	58
3	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	58
4	4-Heptanone	114	C7H14O	000123-19-3	53
5	Pyrrolidine	71	C4H9N	000123-75-1	50





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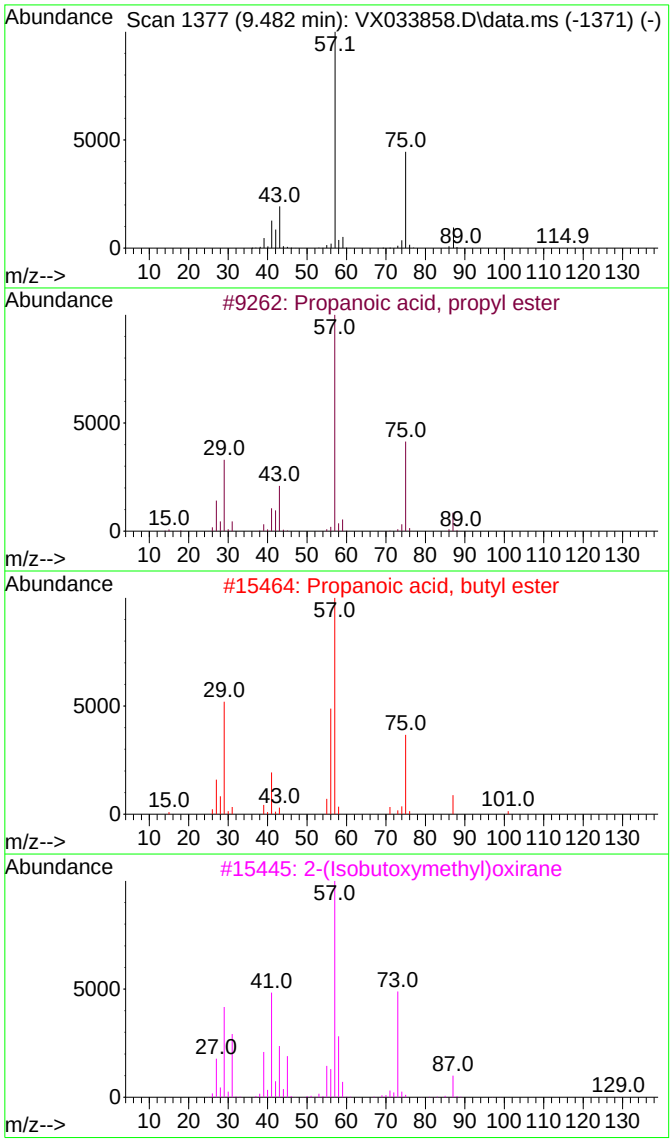
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

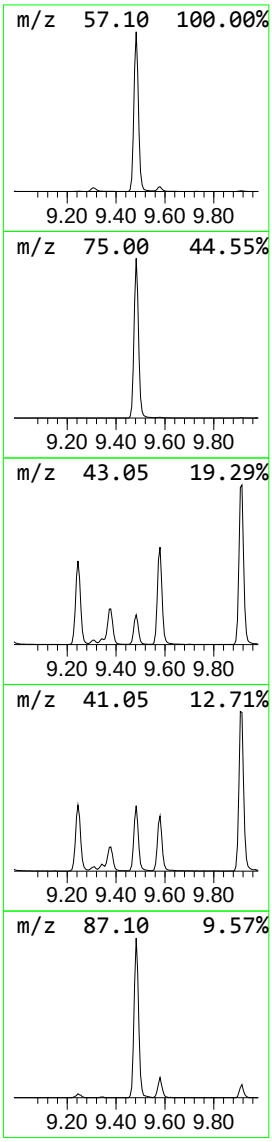
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	51.23 ug/l	619768	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	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	1-Penten-3-ol	86	C5H10O	000616-25-1	7
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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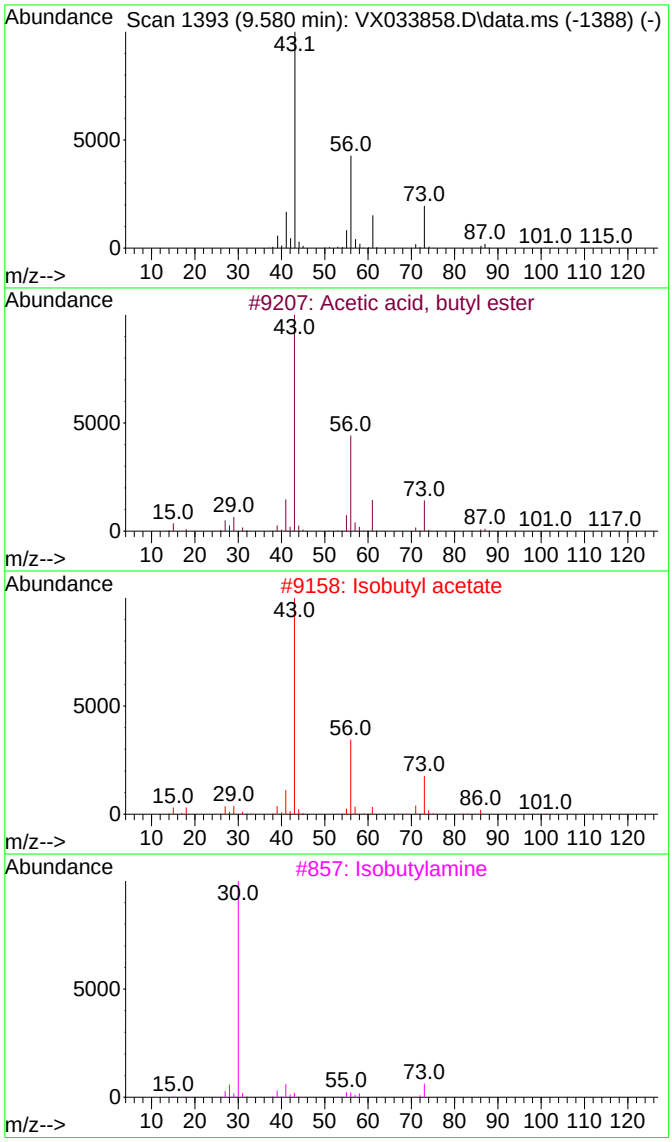
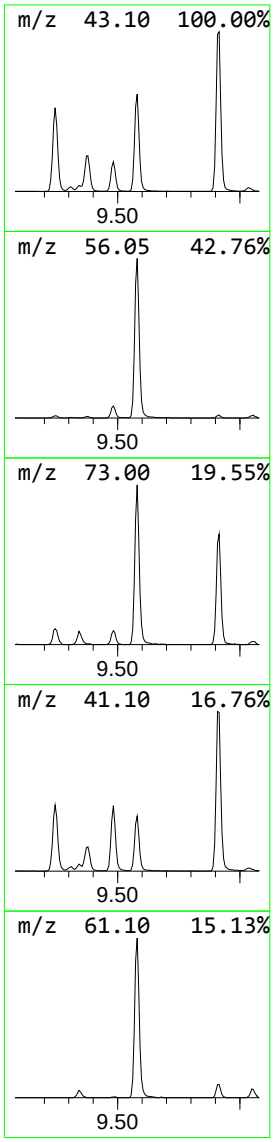
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	34.92 ug/l	422406	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	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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Quant Title : SW846 8260

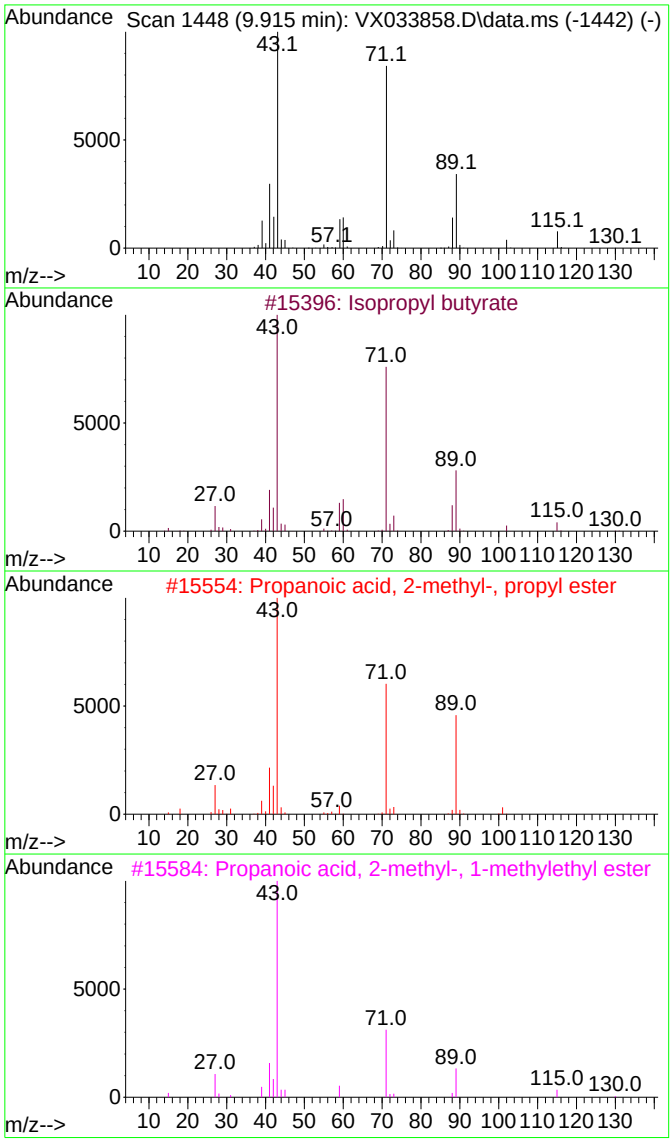
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

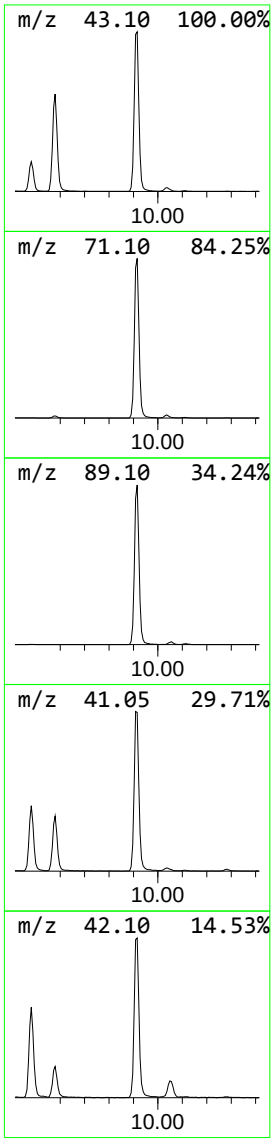
****

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	89.76 ug/l	1085920	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	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64





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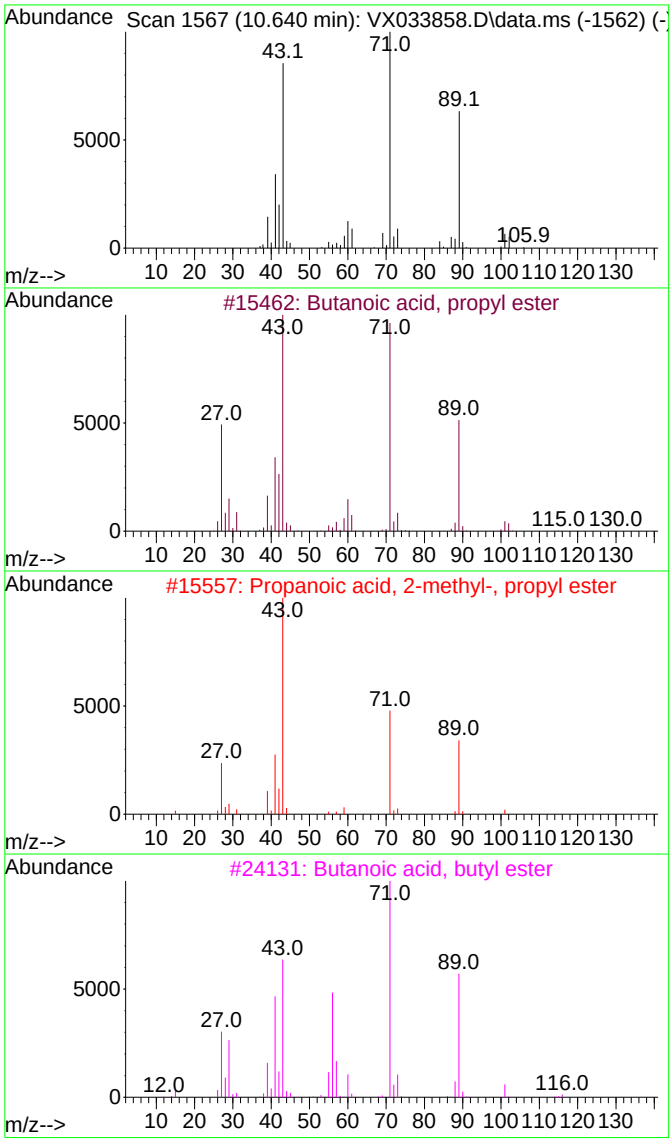
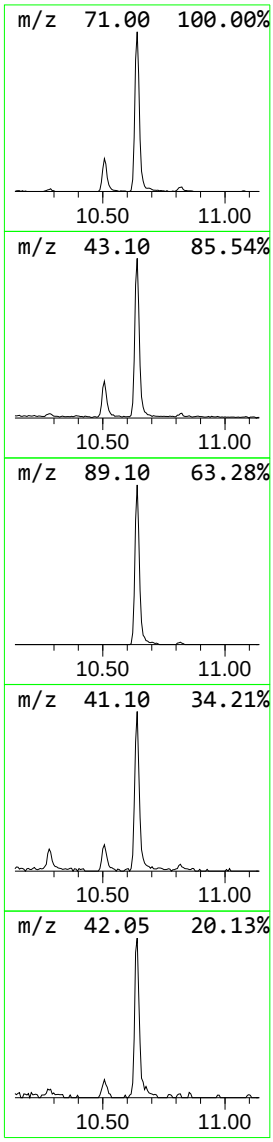
****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.83 ug/l	94767	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	64
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4	Malic Acid	134	C4H6O5	006915-15-7	64
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033858.D
Acq On : 23 Jan 2023 18:39
Operator : JC/MD
Sample : 01255-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-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	5.5	ug/l	60690	2	6.757	556060	50.0
n-Propyl acetate	7.793	142.8	ug/l	1587710	2	6.757	556060	50.0
Propanoic acid,...	8.549	25.5	ug/l	308702	3	10.055	604902	50.0
Isobutyl acetate	8.952	33.0	ug/l	399023	3	10.055	604902	50.0
Propanoic acid,...	9.244	31.7	ug/l	383173	3	10.055	604902	50.0
3-Hexanone, 2-m...	9.378	13.3	ug/l	160433	3	10.055	604902	50.0
Propanoic acid,...	9.482	51.2	ug/l	619768	3	10.055	604902	50.0
Acetic acid, bu...	9.580	34.9	ug/l	422406	3	10.055	604902	50.0
Isopropyl butyrate	9.915	89.8	ug/l	1085920	3	10.055	604902	50.0
Butanoic acid, ...	10.640	7.8	ug/l	94767	3	10.055	604902	50.0