LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033852.D
Acq On : 23 Jan 2023 16:20
Operator : JC/MD
Sample : 01239-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

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: VX033852.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	206	214	224	rBV	10051	21412	1.35%	0.231%
2	2.788	273	279	292	rVB	10660	20951	1.32%	0.226%
3	4.715	586	595	608	rBV2	10579	32298	2.04%	0.349%
4	5.385	693	705	720	rBV	81775	239708	15.10%	2.589%
5	5.550	720	732	749	rVB	146119	416016	26.21%	4.493%
6	5.958	786	799	811	rBV	81244	220290	13.88%	2.379%
7	6.336	852	861	877	rBV	65988	168895	10.64%	1.824%
8	6.763	920	931	944	rBV	221402	557803	35.15%	6.024%
9	7.641	1068	1075	1080	rBV	33520	62374	3.93%	0.674%
10	7.690	1080	1083	1093	rVB	12018	21508	1.36%	0.232%
11	7.793	1093	1100	1114	rBV	903579	1587014	100.00%	17.139%
12	8.549	1217	1224	1234	rBV	189862	308822	19.46%	3.335%
13	8.647	1234	1240	1259	rVB	449484	708311	44.63%	7.650%
14	8.952	1284	1290	1311	rBV	271913	398281	25.10%	4.301%
15	9.244	1332	1338	1345	rBV	273755	386648	24.36%	4.176%
16	9.305	1345	1348	1351	rVV	24470	35000	2.21%	0.378%
17	9.342	1351	1354	1356	rVV	41853	56645	3.57%	0.612%
18	9.372	1356	1359	1368	rVV	105234	161765	10.19%	1.747%
19	9.482	1371	1377	1387	rVV	473624	624097	39.33%	6.740%
20	9.580	1388	1393	1409	rVB	318892	429684	27.07%	4.640%
21	9.915	1442	1448	1463	rBV	816923	1094733	68.98%	11.823%
22	10.055	1463	1471	1477	rBV	434477	607544	38.28%	6.561%
23	10.640	1562	1567	1580	rBV	73122	94289	5.94%	1.018%
24	11.079	1634	1639	1652	rBV	360759	459140	28.93%	4.959%
25	12.024	1788	1794	1802	rBV	413838	546319	34.42%	5.900%

Sum of corrected areas: 9259547

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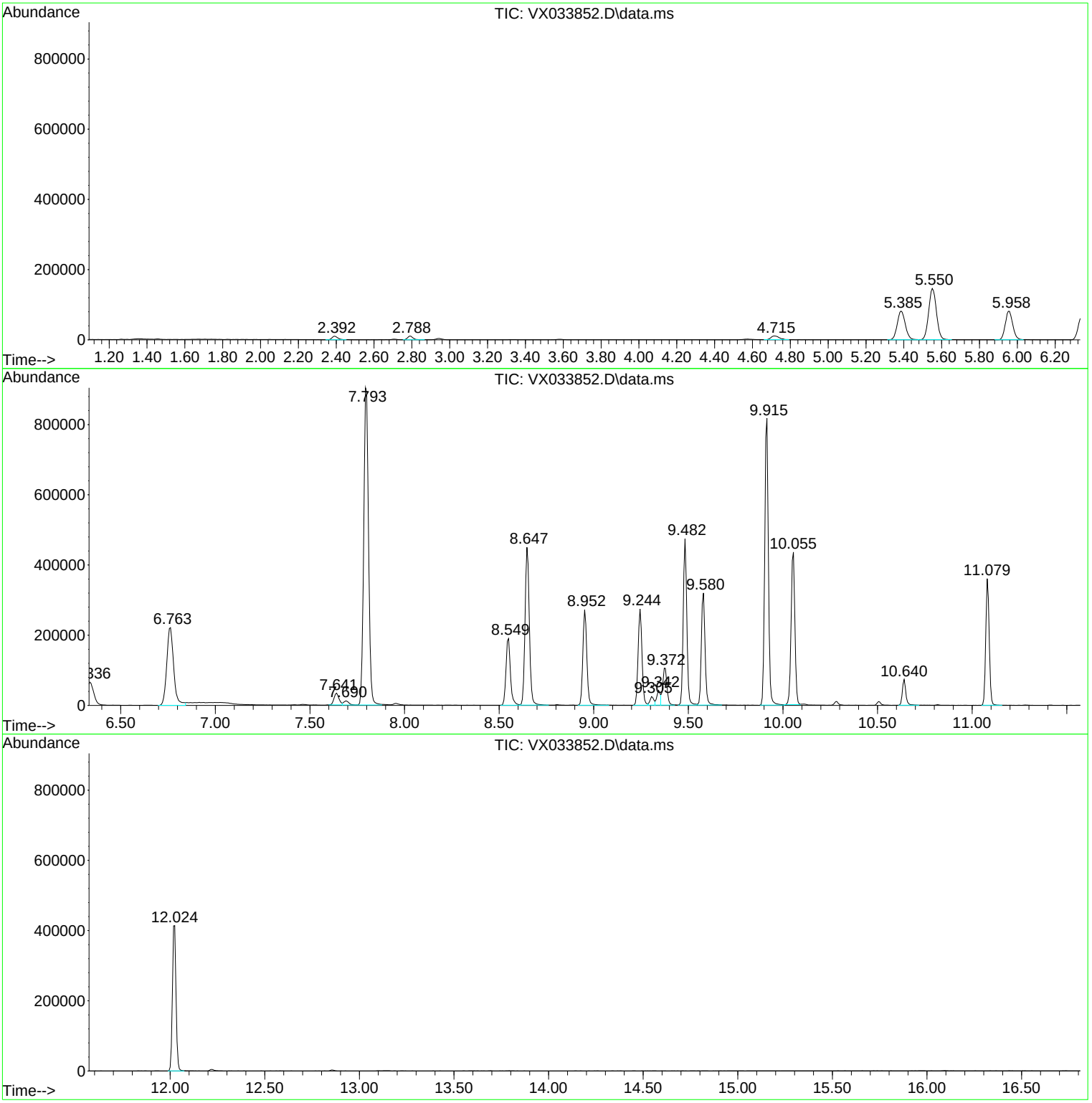
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

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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Data File : VX033852.D
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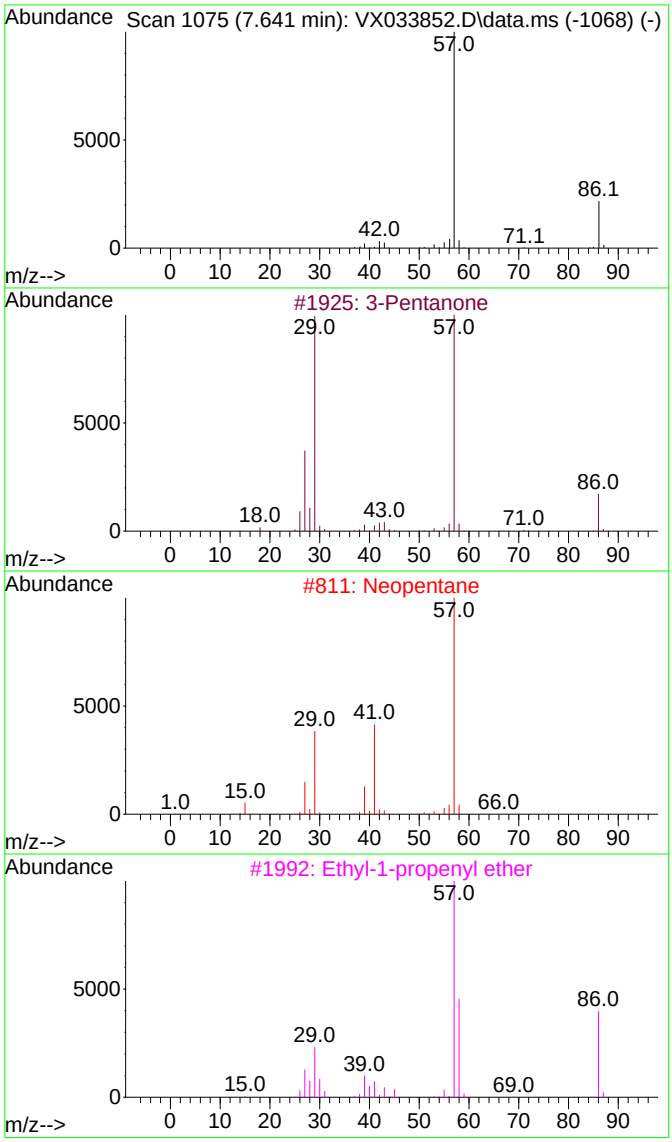
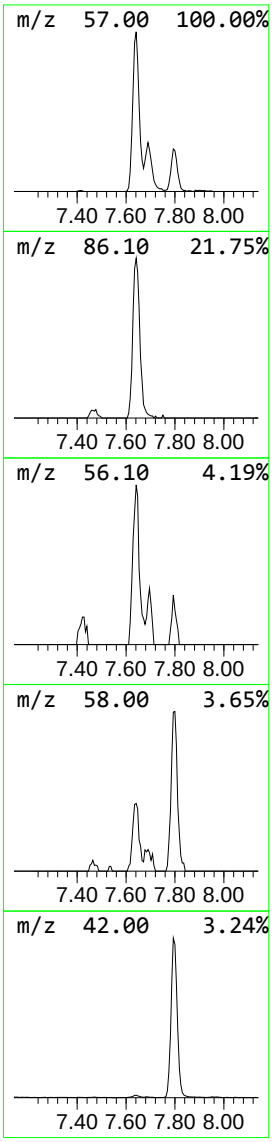
****
Peak Number 1 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	5.59 ug/l	62374	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	78
2	Neopentane	72	C5H12	000463-82-1	23
3	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
4	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
5	Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	9





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

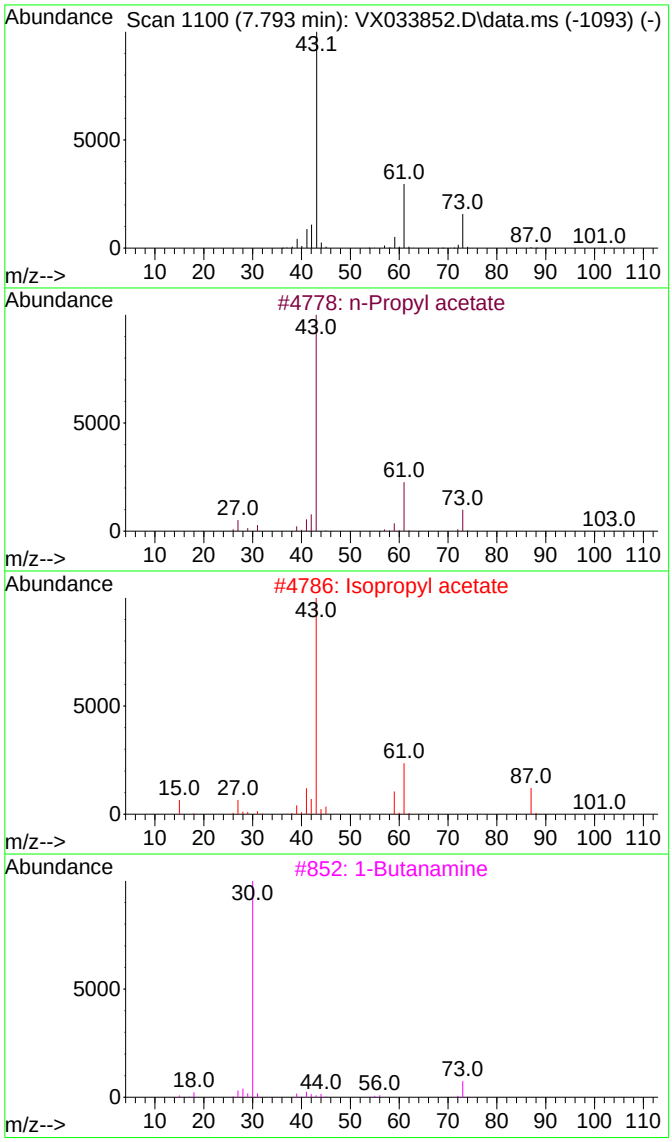
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

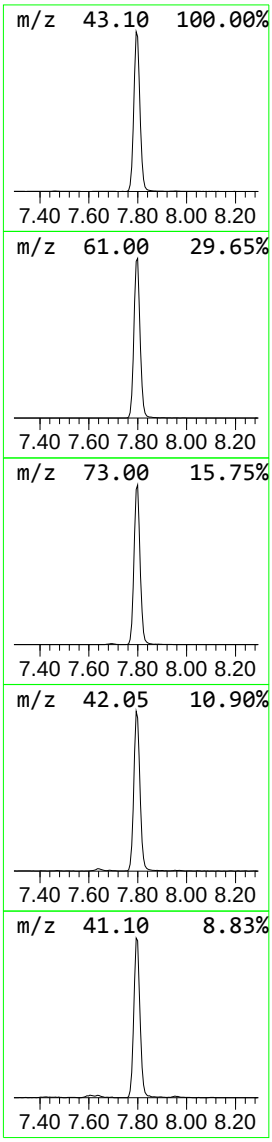
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.793	142.26 ug/l	1587010	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	5-Methyloxazolidine	87	C4H9NO	058328-22-6	4





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

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

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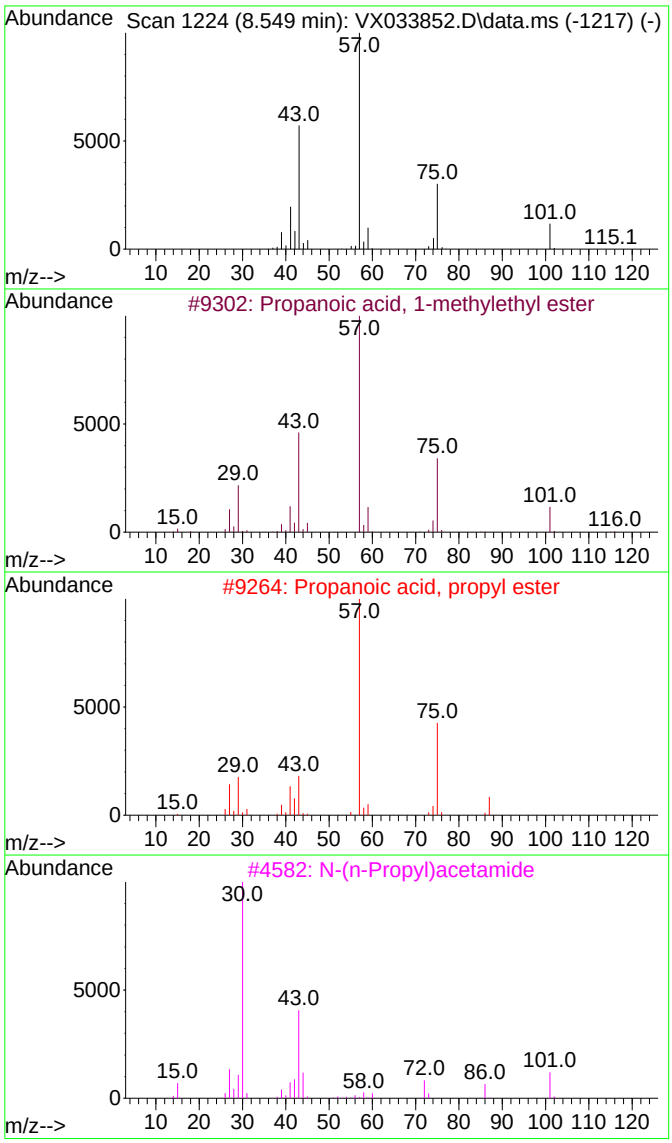
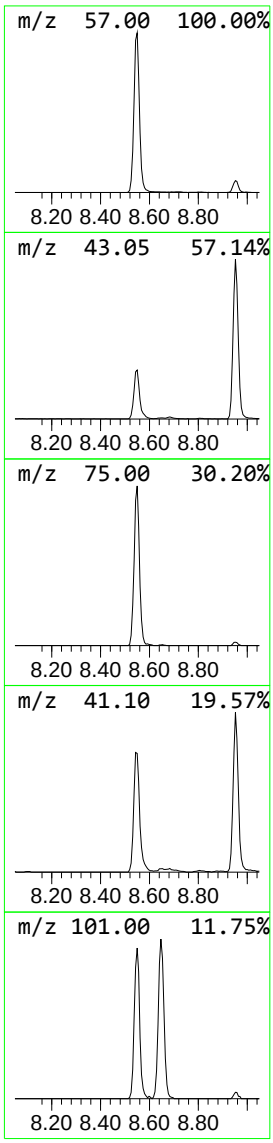
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	25.42 ug/l	308822	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	42
3	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : 01239-02
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

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

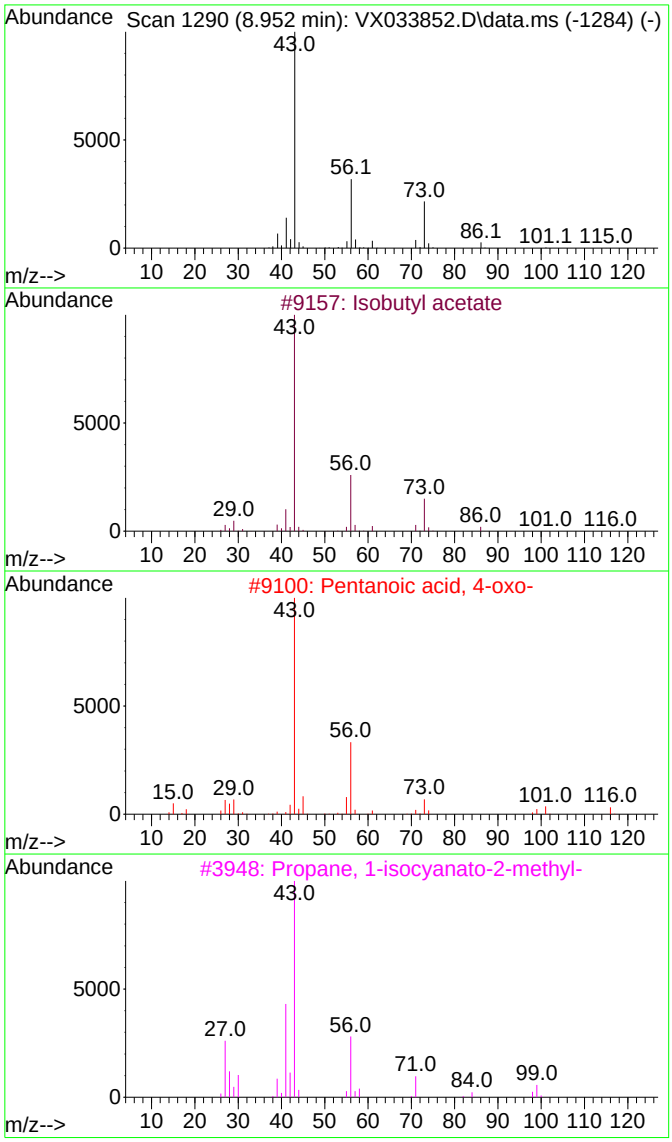
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

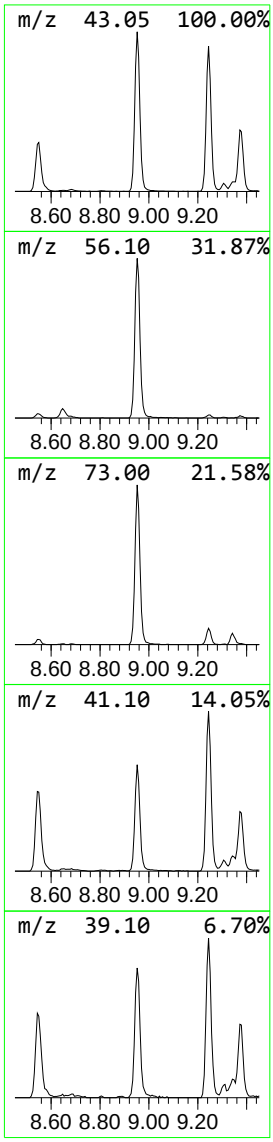
****

Peak Number 4 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	32.78 ug/l	398281	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	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

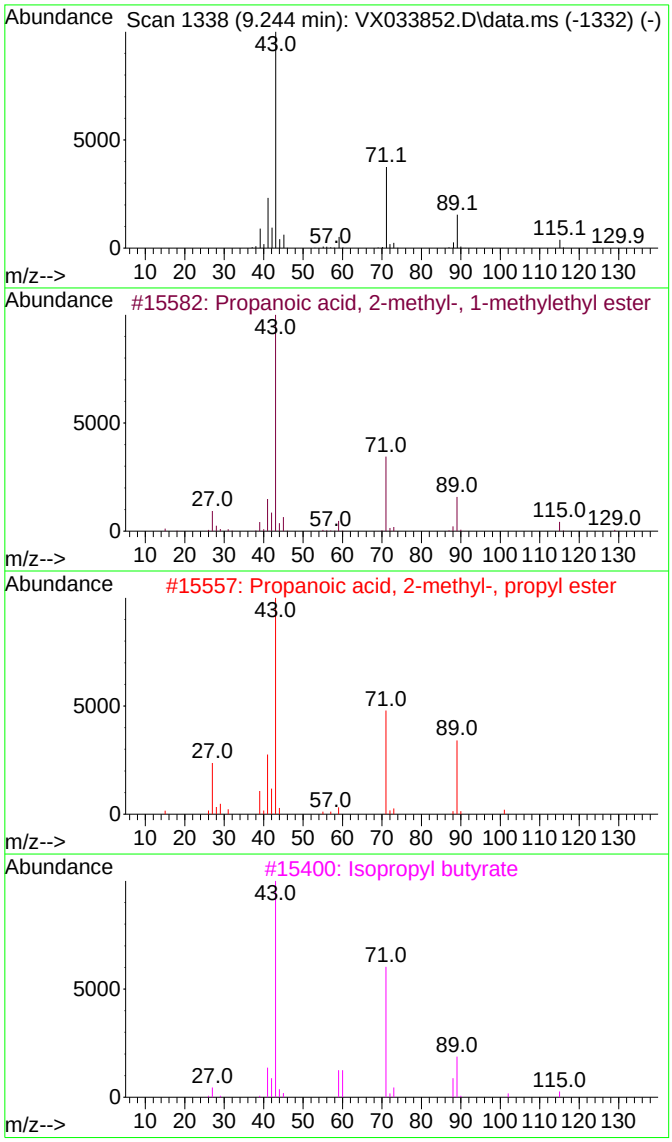
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

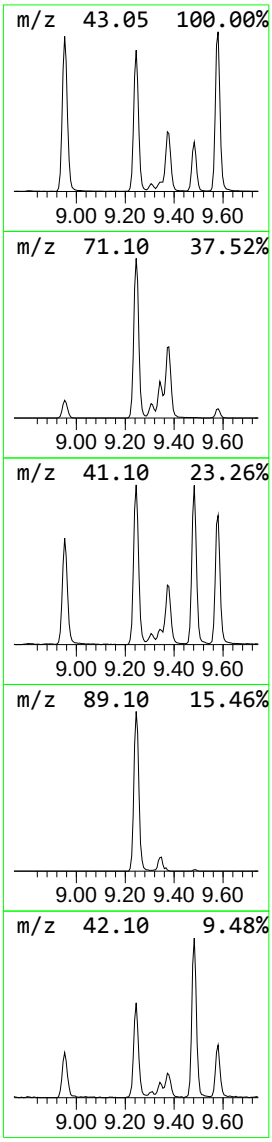
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	31.82 ug/l	386648	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	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38





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Operator : JC/MD
Sample : 01239-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

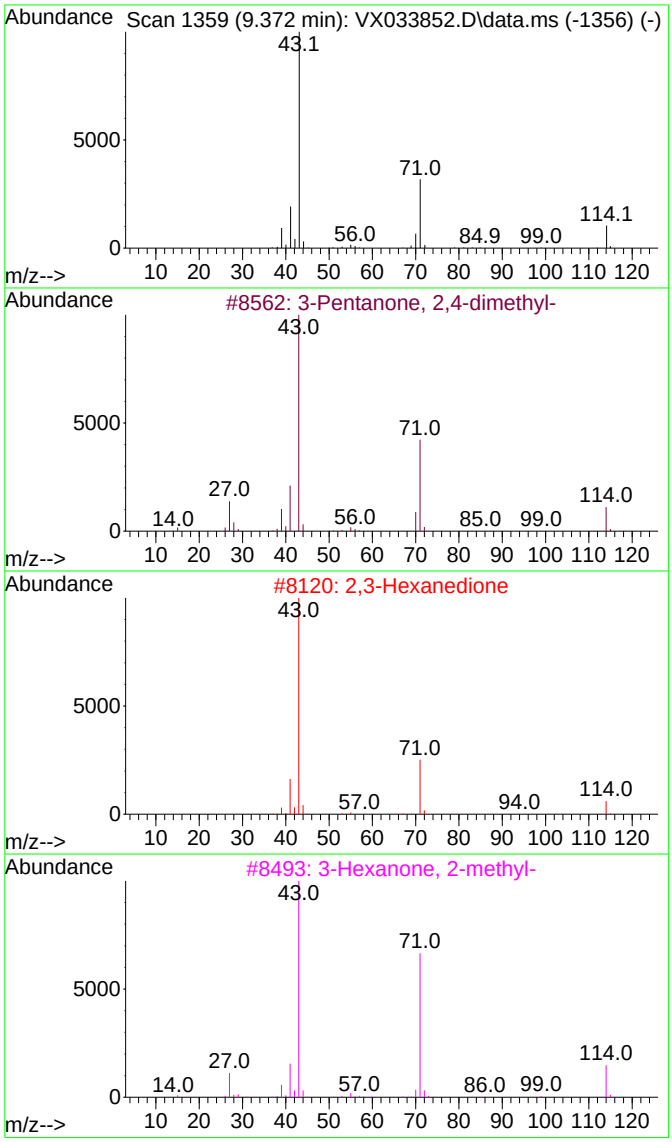
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

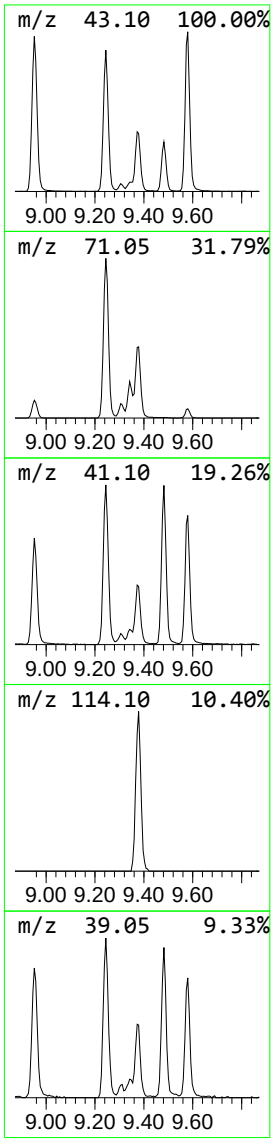
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.372	13.31 ug/l	161765	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
3	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	64
4	4-Heptanone	114	C7H14O	000123-19-3	53
5	Pyrrolidine	71	C4H9N	000123-75-1	53





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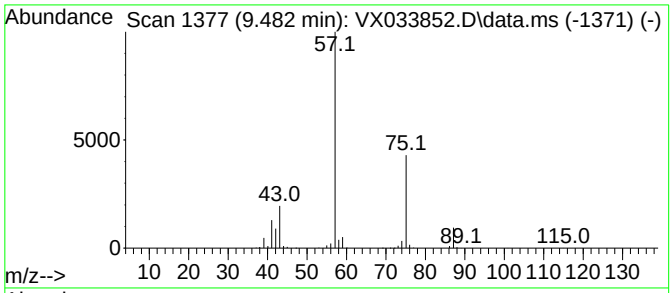
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

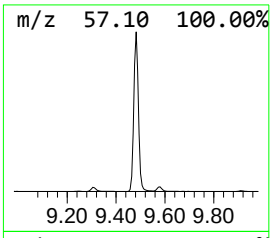
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

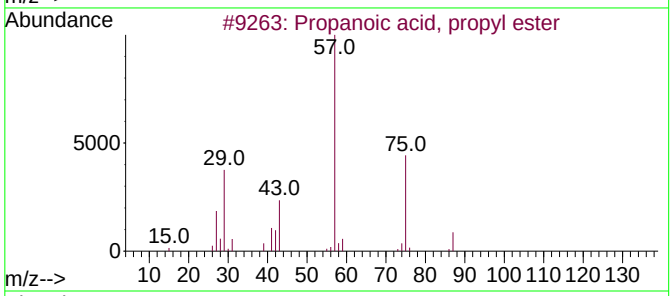
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

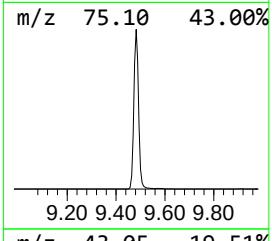
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	51.36 ug/l	624097	Chlorobenzene-d5	10.055

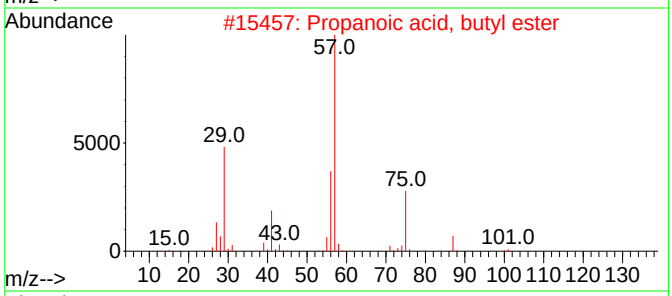
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7

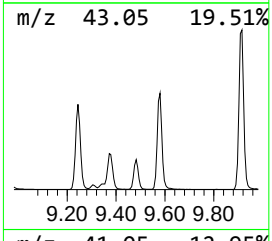


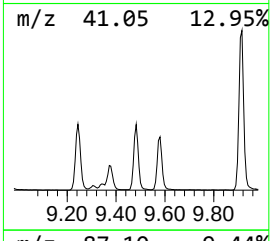


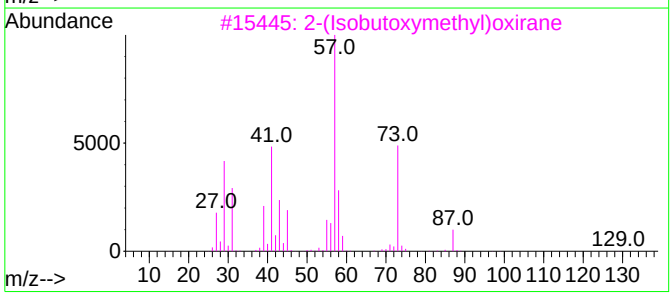


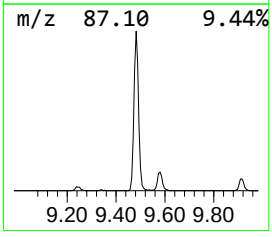












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ClientSampleId :
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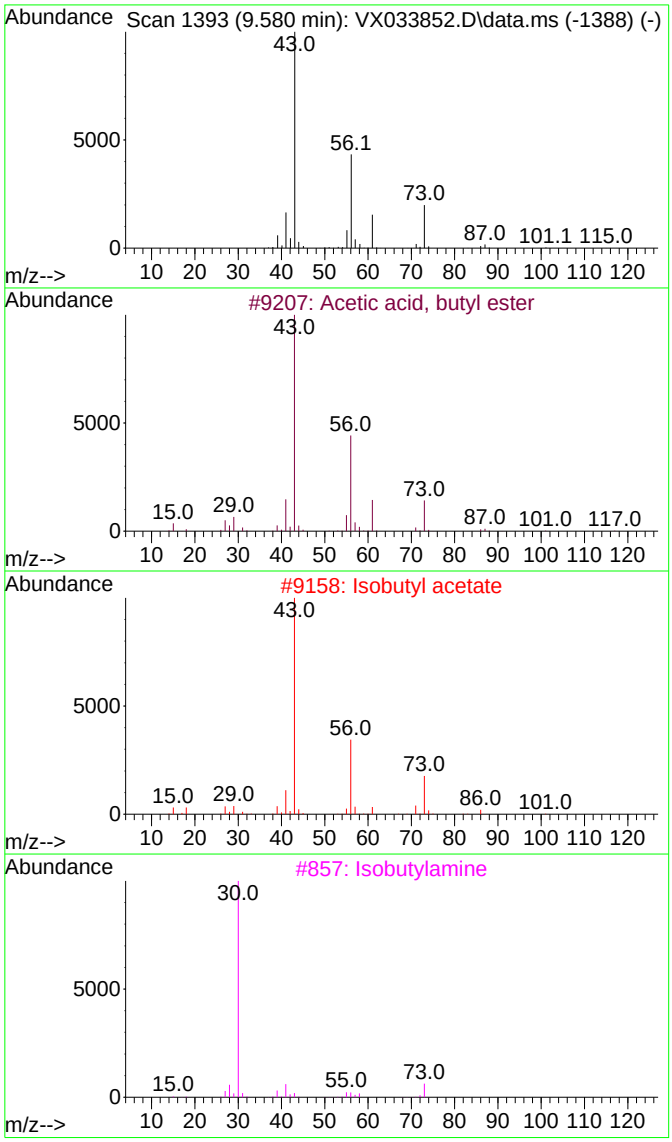
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

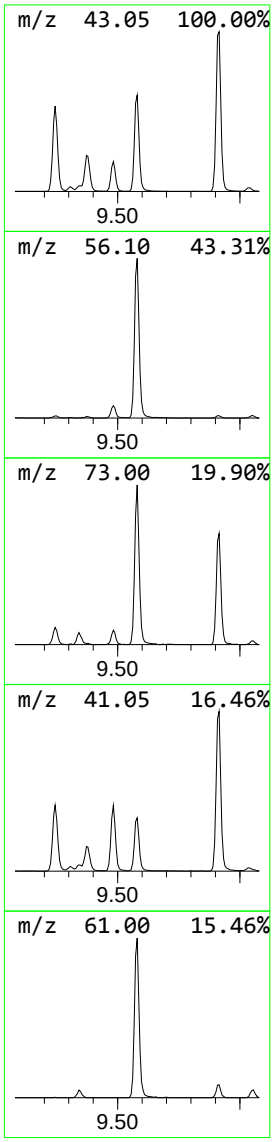
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	35.36 ug/l	429684	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	Isopropyl acetate	102	C5H10O2	000108-21-4	9





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ClientSampleId :
BORING-3

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

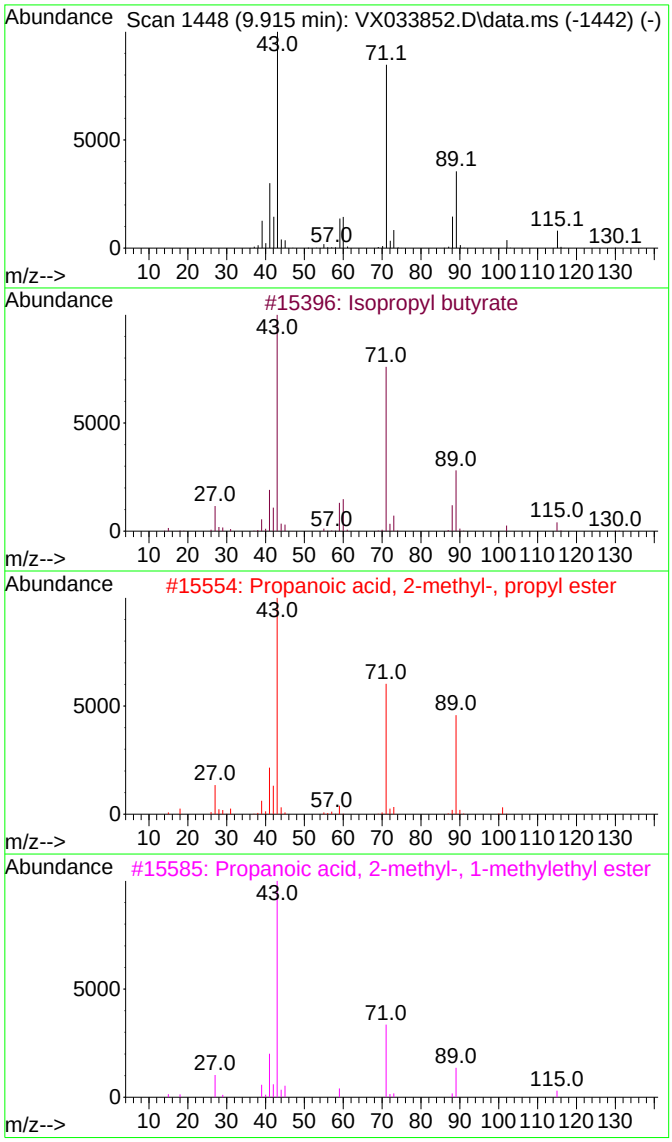
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

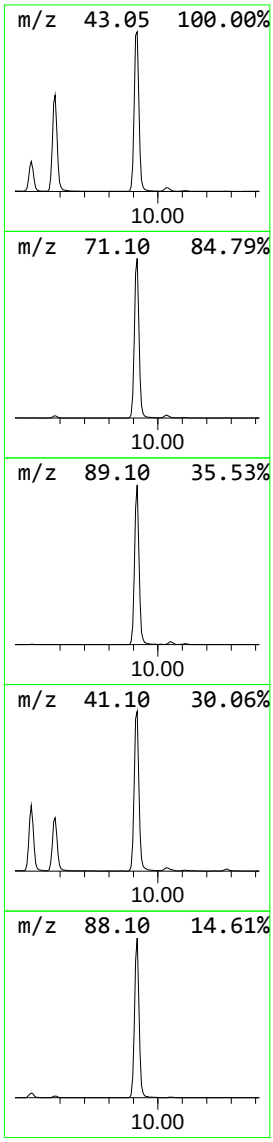
****

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	90.09 ug/l	1094730	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	59
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033852.D
Acq On : 23 Jan 2023 16:20
Operator : JC/MD
Sample : 01239-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

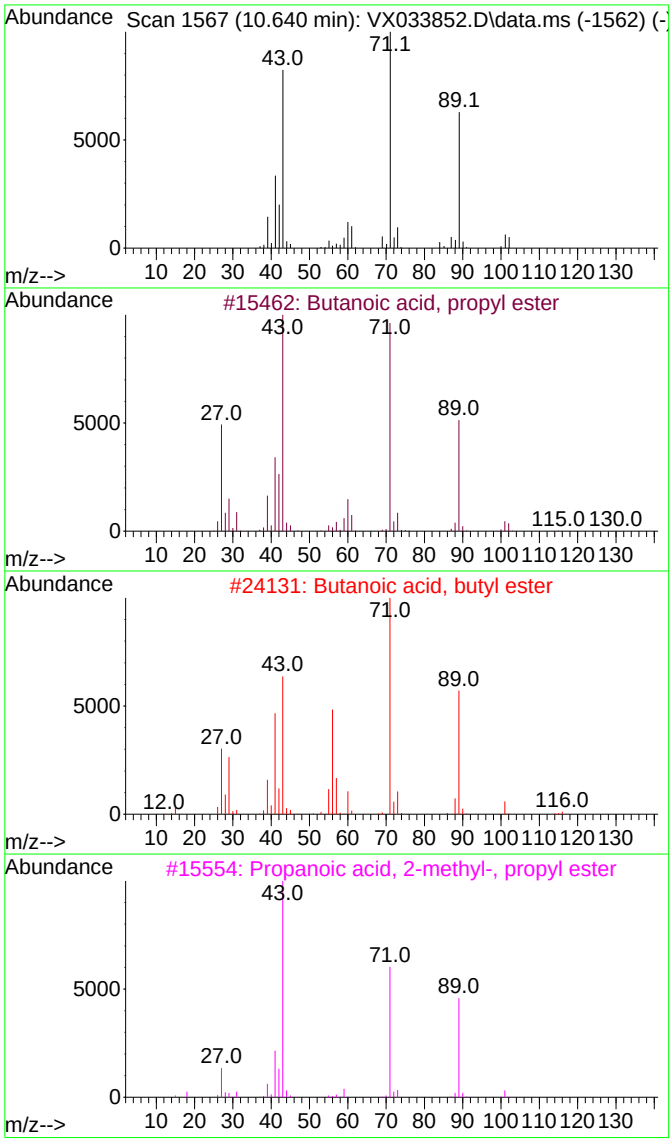
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

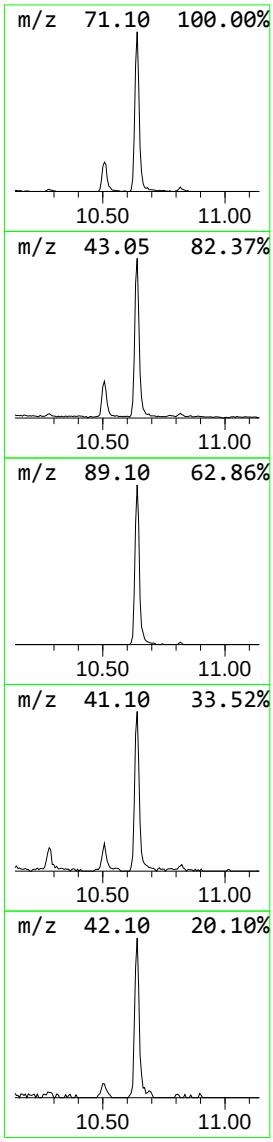
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	7.76 ug/l	94289	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	64
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	53
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033852.D
Acq On : 23 Jan 2023 16:20
Operator : JC/MD
Sample : 01239-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BORING-3

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	5.6	ug/l	62374	2	6.763	557803	50.0
n-Propyl acetate	7.793	142.3	ug/l	1587010	2	6.763	557803	50.0
Propanoic acid,...	8.549	25.4	ug/l	308822	3	10.055	607544	50.0
Isobutyl acetate	8.952	32.8	ug/l	398281	3	10.055	607544	50.0
Propanoic acid,...	9.244	31.8	ug/l	386648	3	10.055	607544	50.0
3-Pentanone, 2,...	9.372	13.3	ug/l	161765	3	10.055	607544	50.0
Propanoic acid,...	9.482	51.4	ug/l	624097	3	10.055	607544	50.0
Acetic acid, bu...	9.580	35.4	ug/l	429684	3	10.055	607544	50.0
Isopropyl butyrate	9.915	90.1	ug/l	1094730	3	10.055	607544	50.0
Butanoic acid, ...	10.640	7.8	ug/l	94289	3	10.055	607544	50.0