LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033851.D
Acq On : 23 Jan 2023 15:56
Operator : JC/MD
Sample : 01237-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1-2-3A

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: VX033851.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	205	214	224	rBV	19854	38823	2.83%	0.443%
2	2.788	273	279	290	rVB	9759	19546	1.43%	0.223%
3	4.721	587	596	606	rBV3	9926	30128	2.20%	0.344%
4	5.385	694	705	721	rBV2	81293	240457	17.54%	2.746%
5	5.550	721	732	751	rVB	148292	417442	30.45%	4.768%
6	5.958	789	799	818	rBV	82274	221763	16.17%	2.533%
7	6.336	850	861	877	rBV	60632	157678	11.50%	1.801%
8	6.763	921	931	943	rBV	223908	565379	41.24%	6.457%
9	7.641	1065	1075	1080	rBV	33102	63720	4.65%	0.728%
10	7.690	1080	1083	1093	rVB	11685	21636	1.58%	0.247%
11	7.799	1093	1101	1121	rBV	766053	1371077	100.00%	15.659%
12	8.549	1217	1224	1234	rBV	184764	298064	21.74%	3.404%
13	8.647	1234	1240	1259	rVB	445676	708920	51.71%	8.096%
14	8.952	1284	1290	1303	rBV	215958	317402	23.15%	3.625%
15	9.244	1331	1338	1345	rBV	264661	376805	27.48%	4.303%
16	9.305	1345	1348	1351	rVV	22624	33938	2.48%	0.388%
17	9.342	1351	1354	1356	rVV	38868	51878	3.78%	0.592%
18	9.372	1356	1359	1371	rVV	105710	159314	11.62%	1.820%
19	9.482	1371	1377	1388	rVV	422506	558986	40.77%	6.384%
20	9.580	1388	1393	1410	rVB	249048	330373	24.10%	3.773%
21	9.915	1442	1448	1463	rBV	784610	1041156	75.94%	11.891%
22	10.055	1464	1471	1477	rBV	436326	611217	44.58%	6.981%
23	10.506	1540	1545	1551	rBV	10346	13813	1.01%	0.158%
24	10.640	1561	1567	1577	rBV	60241	79621	5.81%	0.909%
25	11.079	1634	1639	1650	rBV	352432	465785	33.97%	5.320%
26	12.018	1788	1793	1804	rBV	424291	560979	40.92%	6.407%

Sum of corrected areas: 8755900

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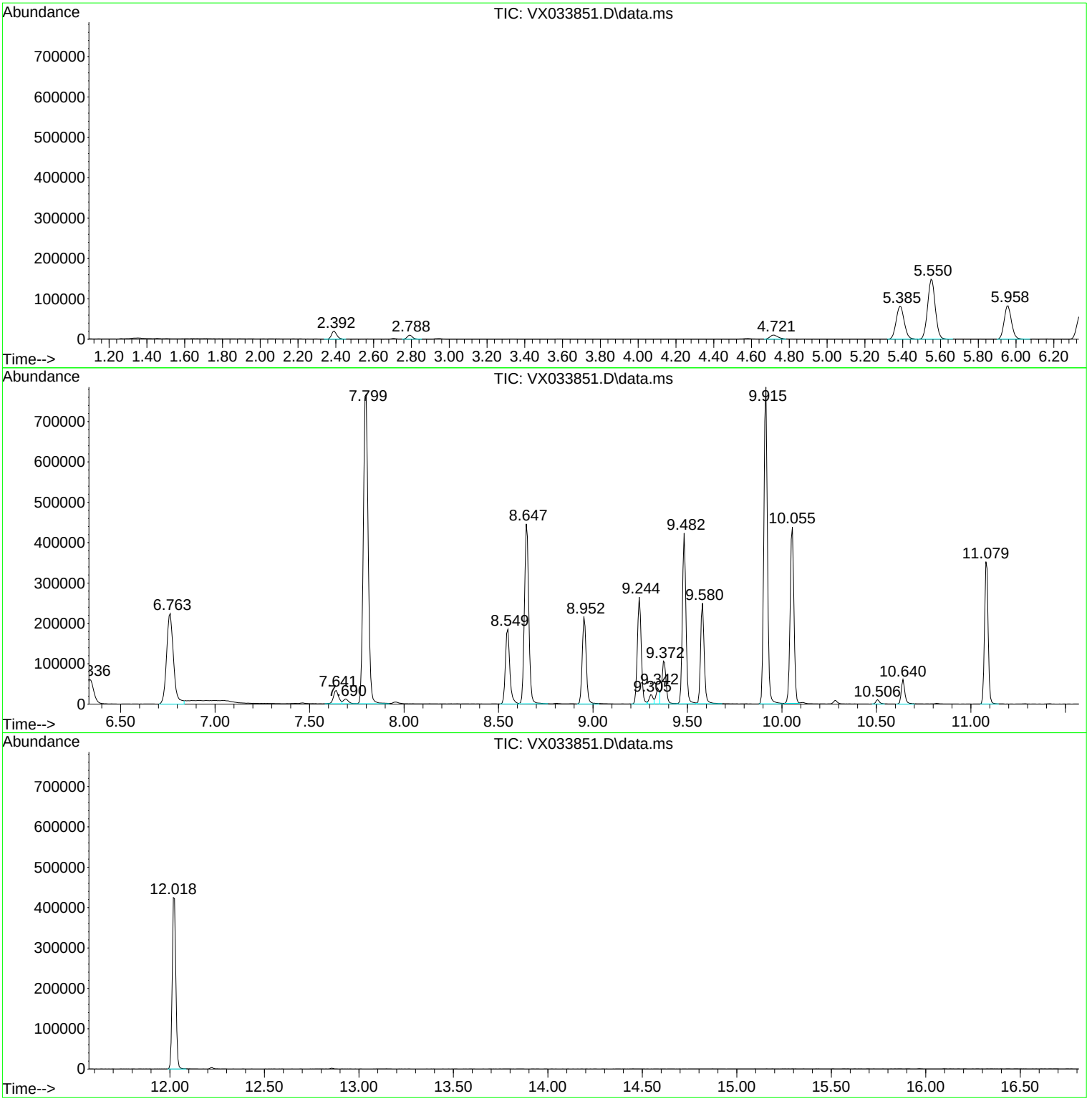
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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



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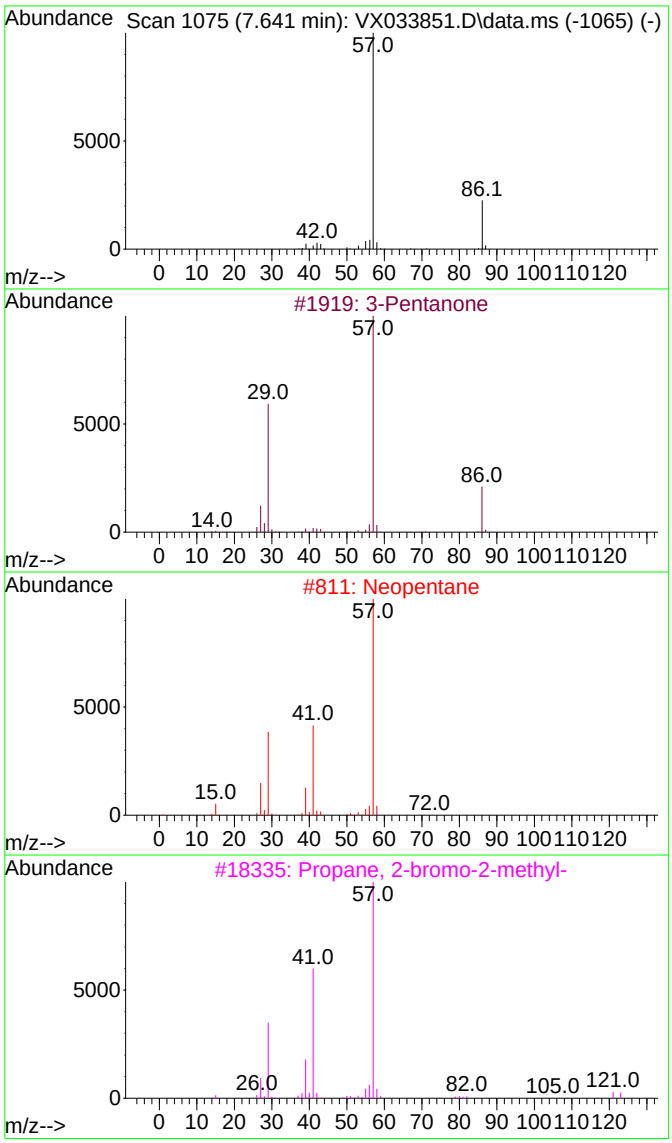
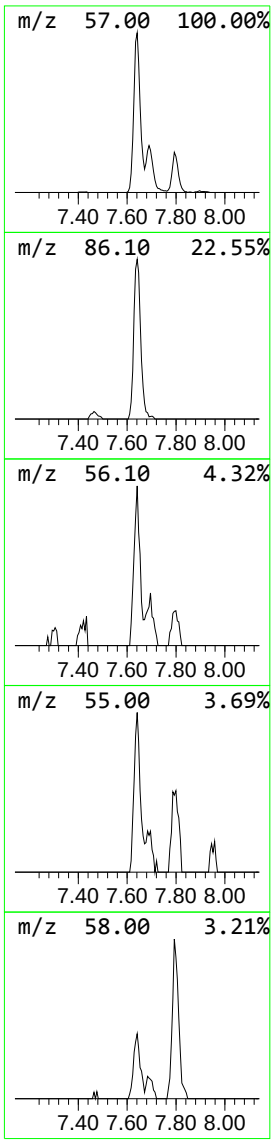
****
Peak Number 1 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	5.64 ug/l	63720	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Neopentane	72	C5H12	000463-82-1	25
3	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9
4	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
5	Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	9





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

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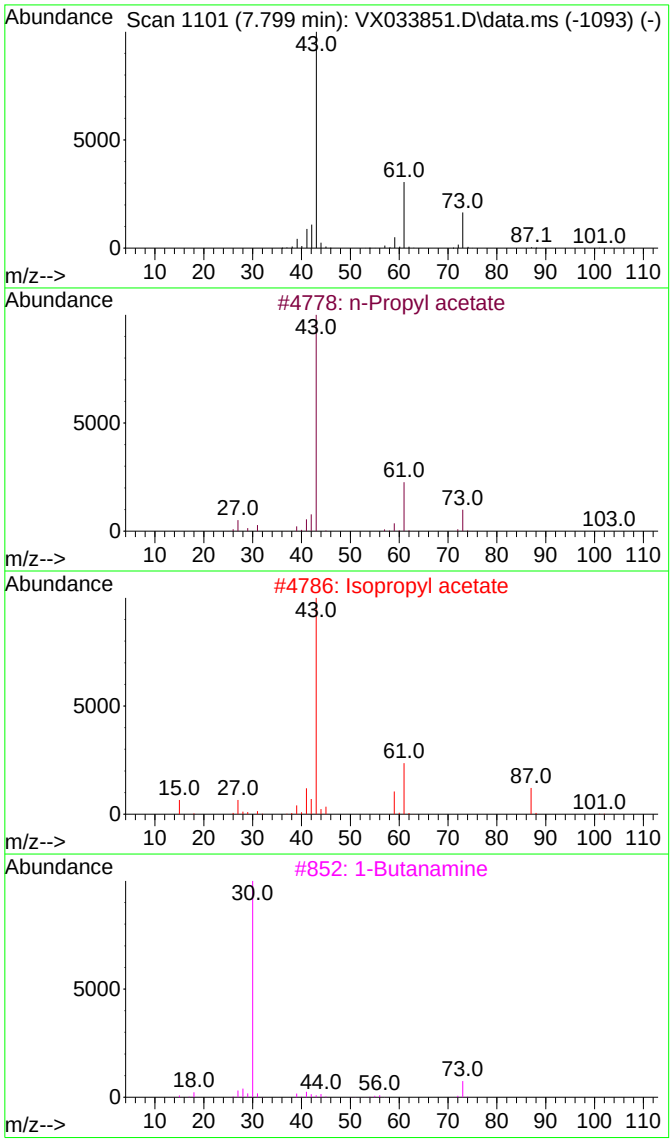
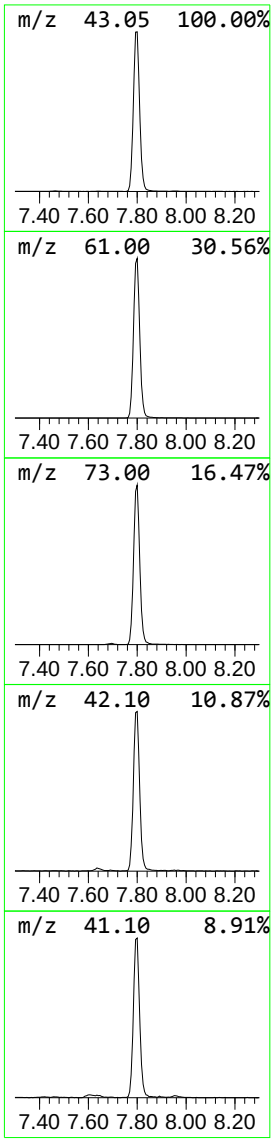
****

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	121.25 ug/l	1371080	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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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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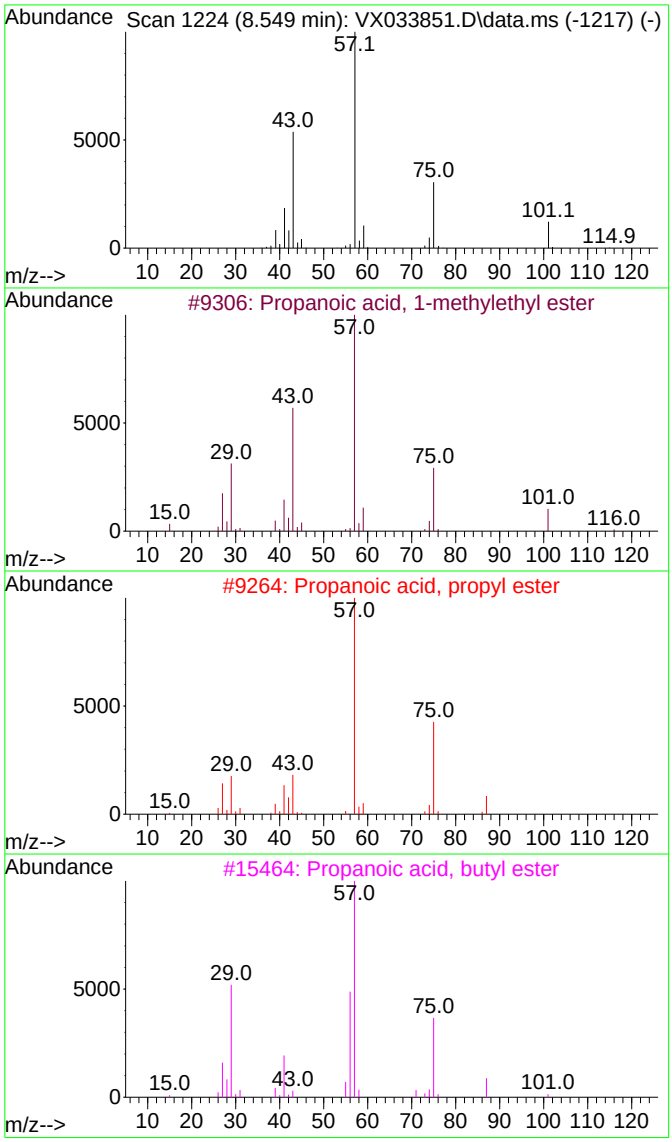
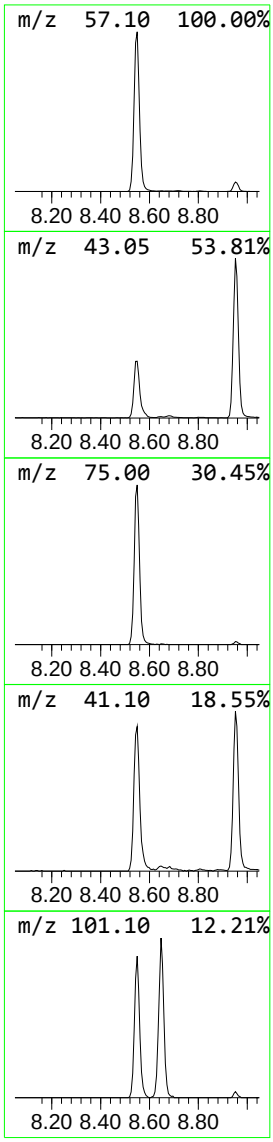
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	24.38 ug/l	298064	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	28
4	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	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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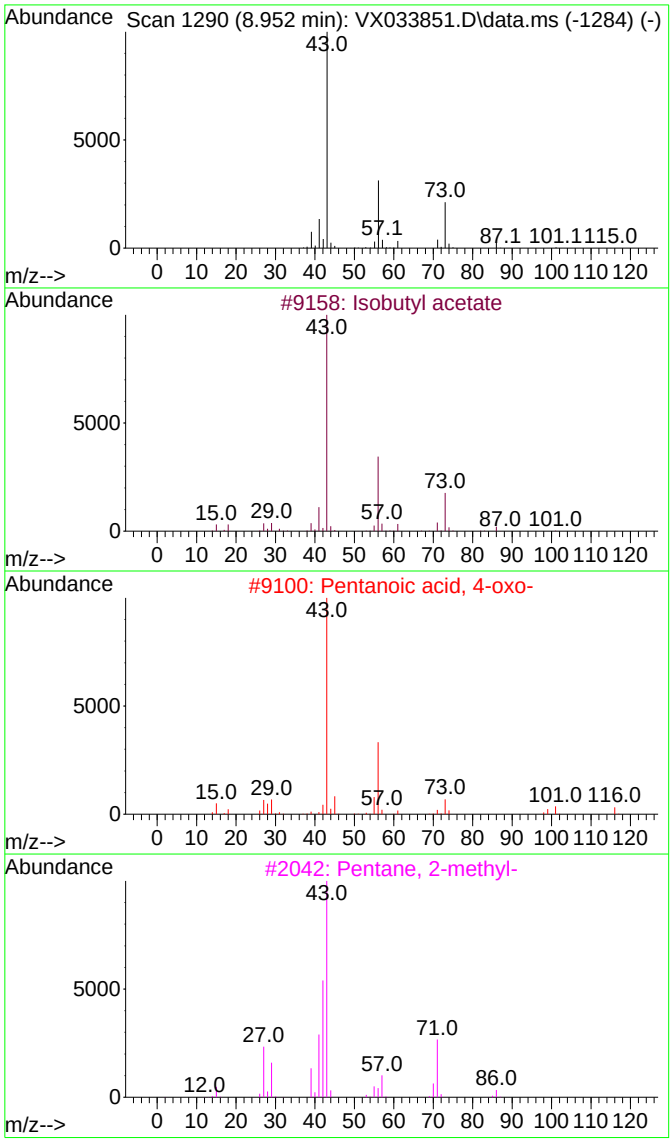
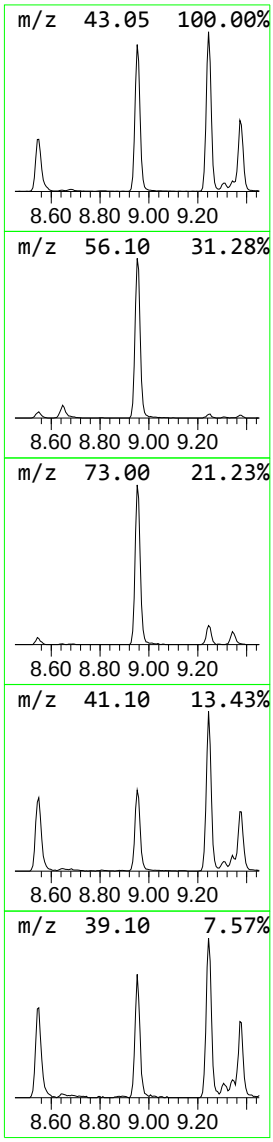
****
Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	25.96 ug/l	317402	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	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1-2-3A

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

TIC Library : C:\Database\NIST20.L
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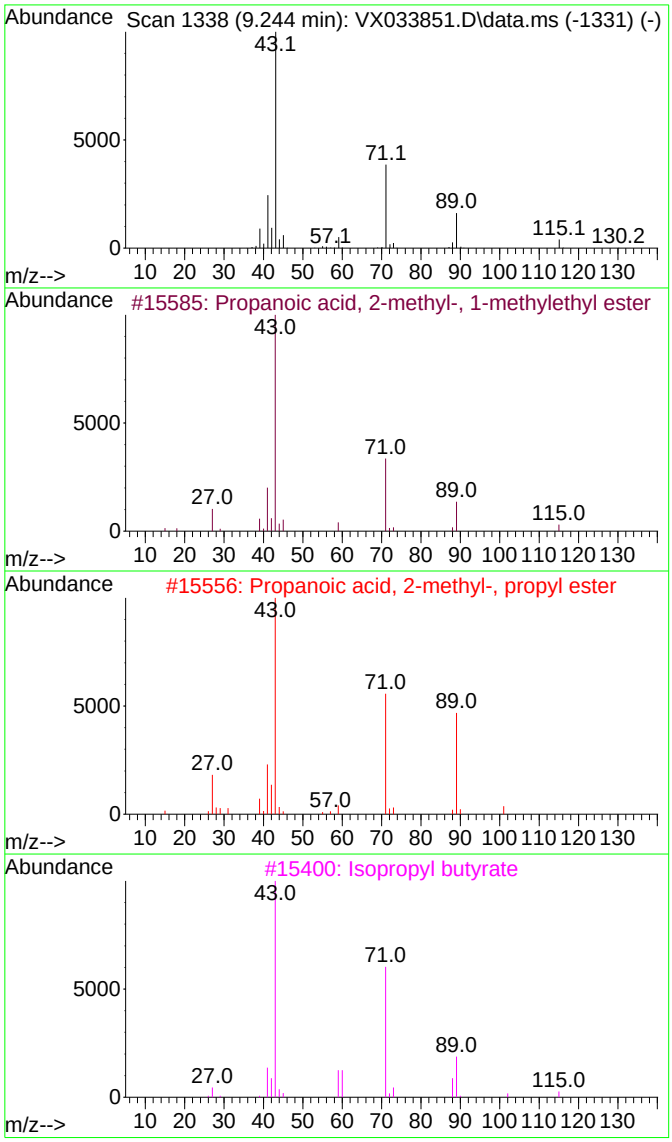
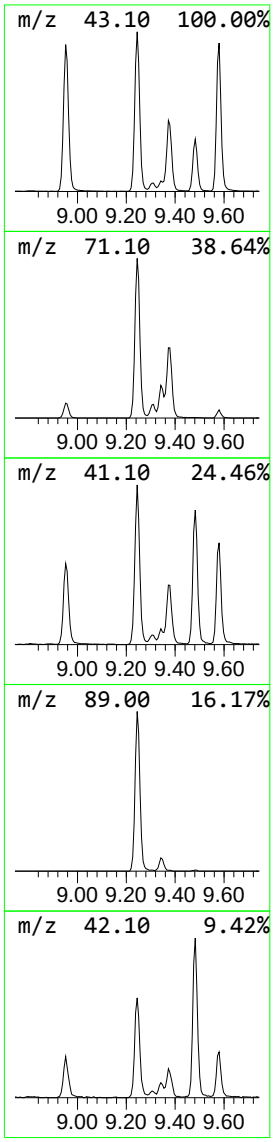
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	30.82 ug/l	376805	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	50
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	40





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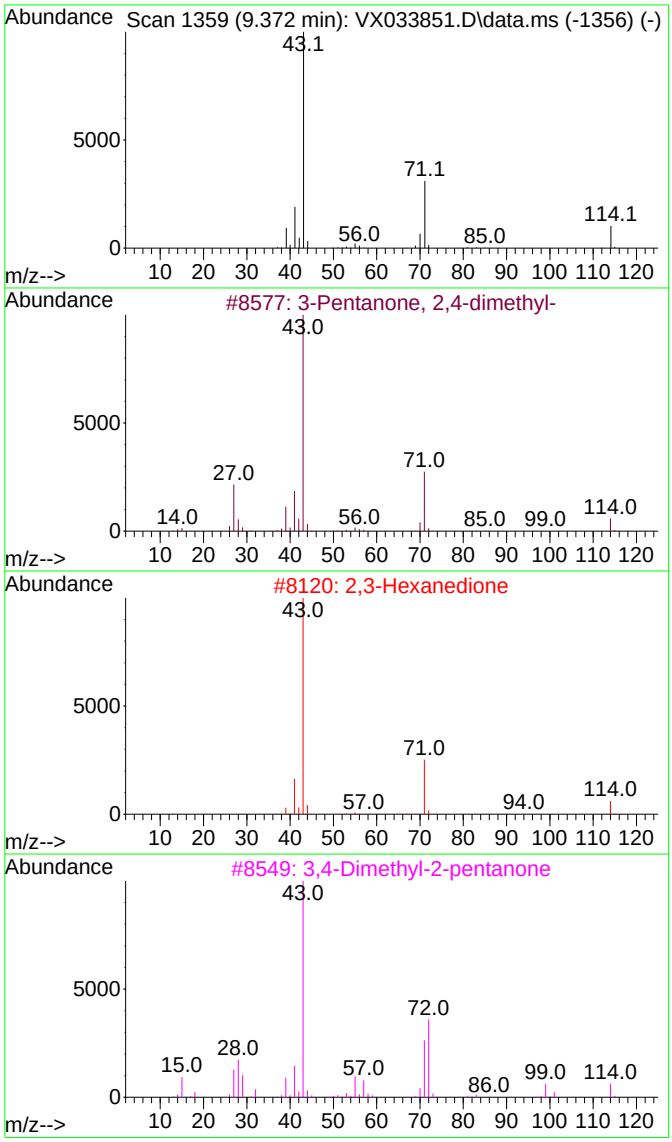
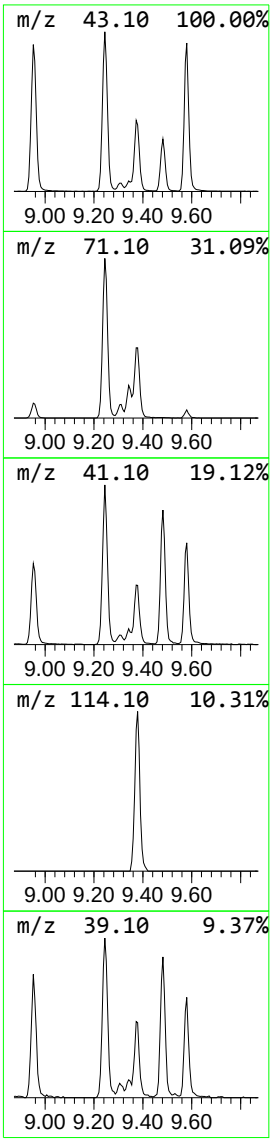
****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.372	13.03 ug/l	159314	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	59
3	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50
4	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	50
5	4-Heptanone	114	C7H14O	000123-19-3	40





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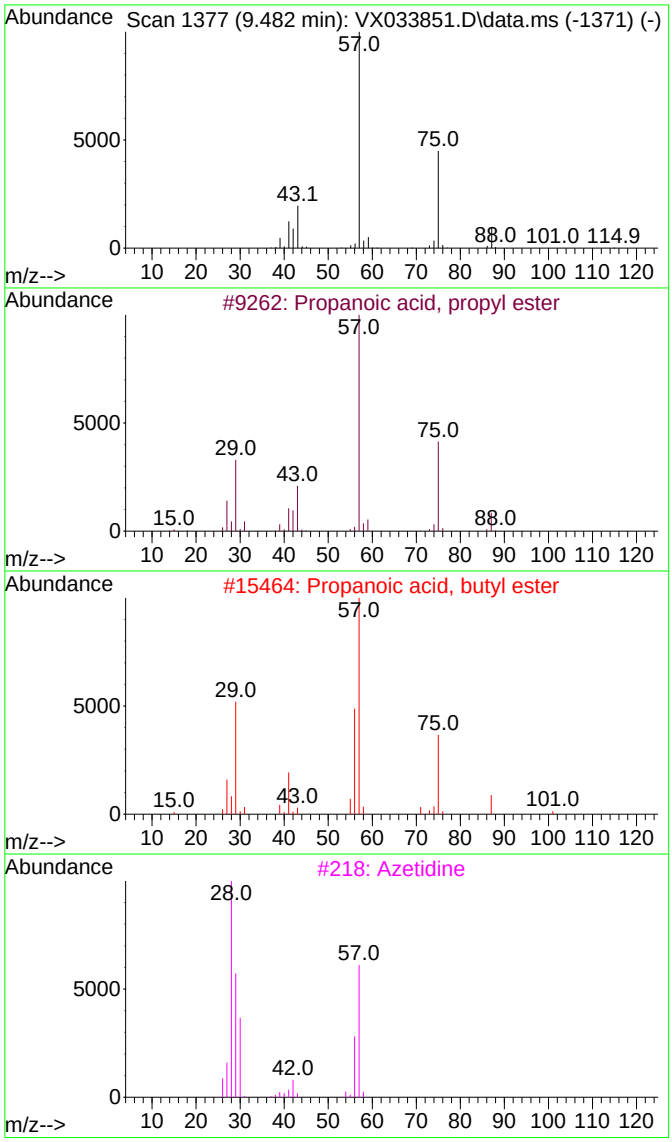
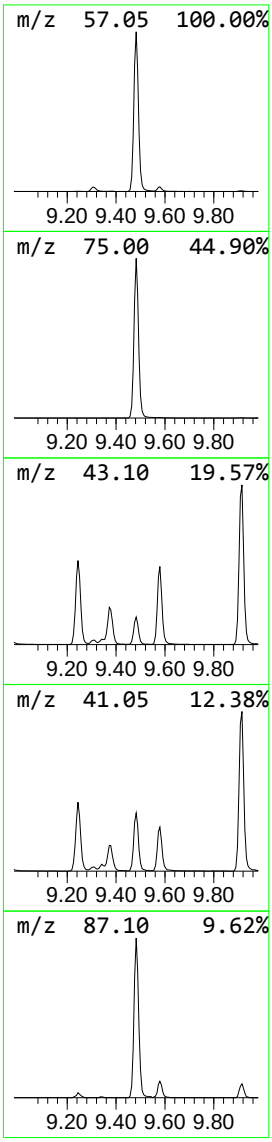
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	45.73 ug/l	558986	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	Azetidine	57	C3H7N	000503-29-7	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Pentanamine	87	C5H13N	000110-58-7	9





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ClientSampleId :
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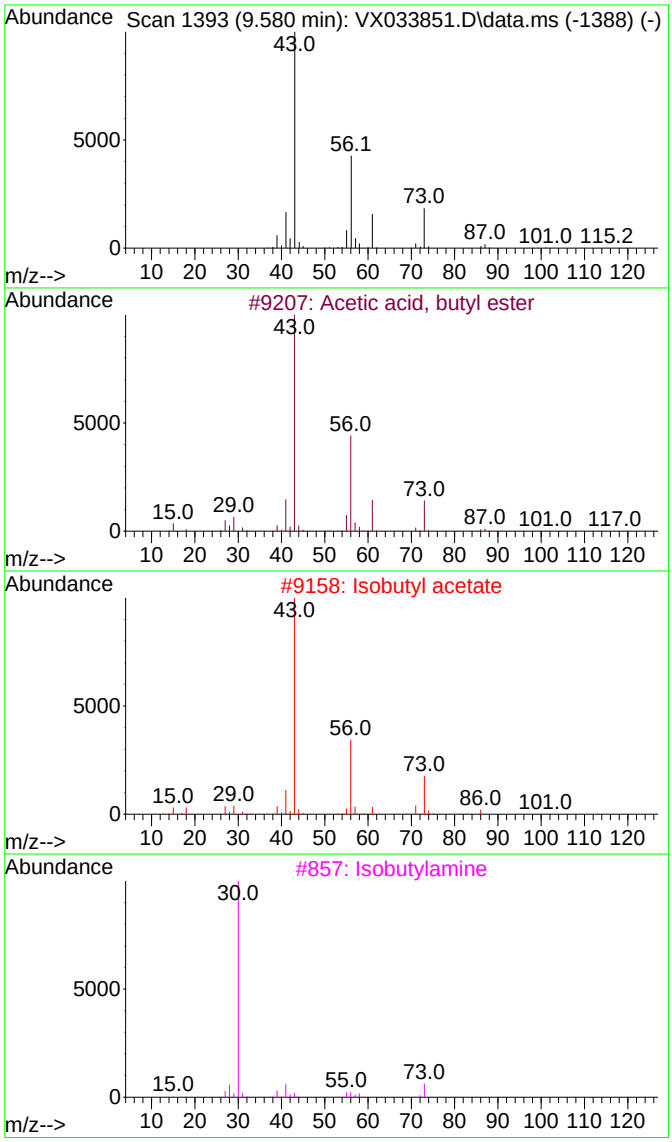
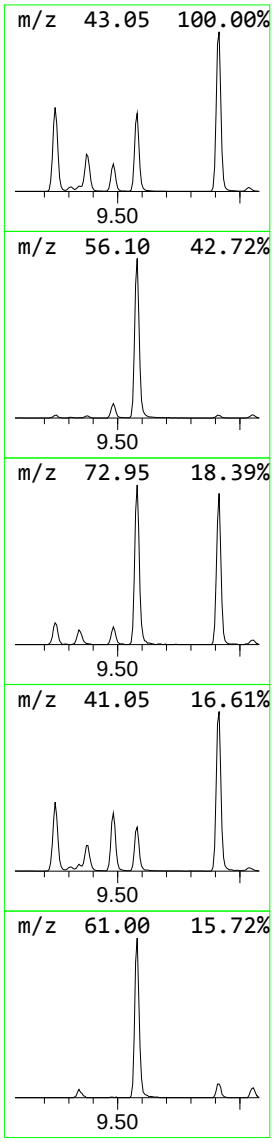
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	27.03 ug/l	330373	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	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
5	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9





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Quant Title : SW846 8260

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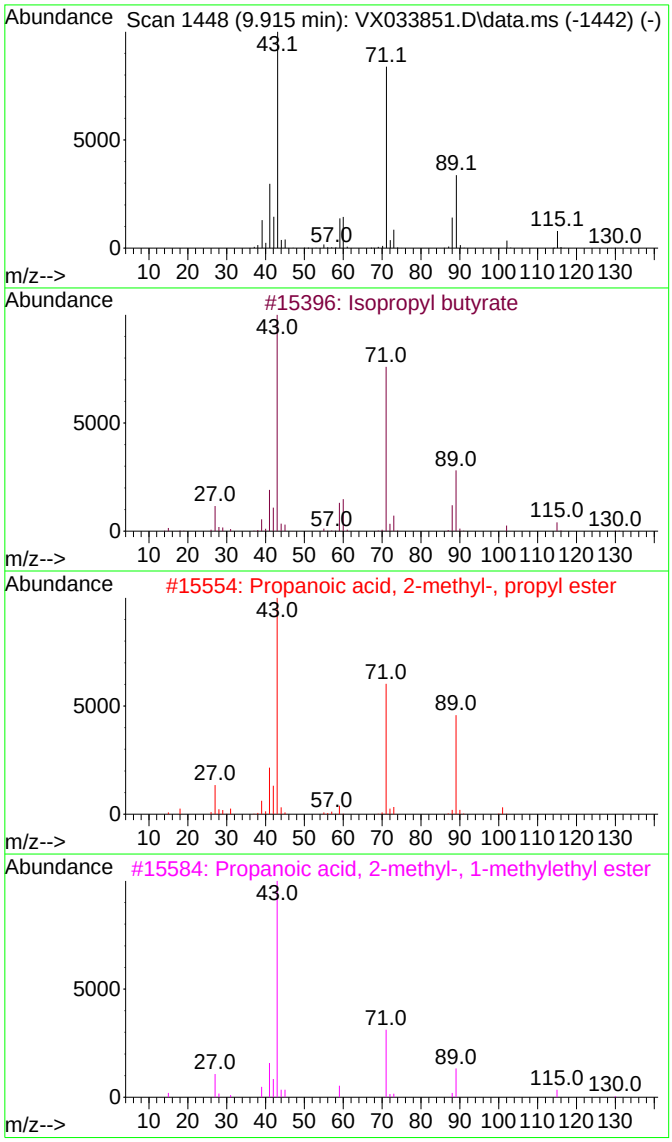
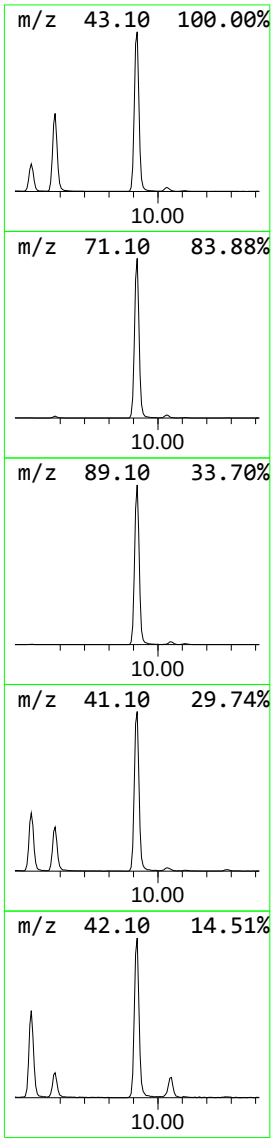
****

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	85.17 ug/l	1041160	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	94
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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





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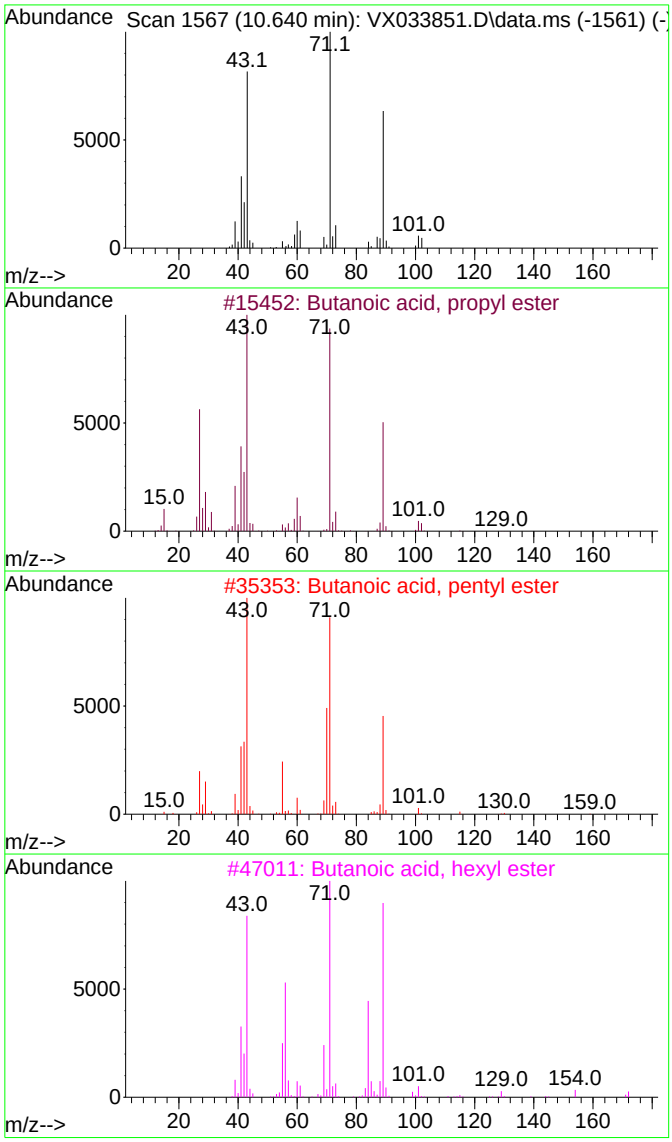
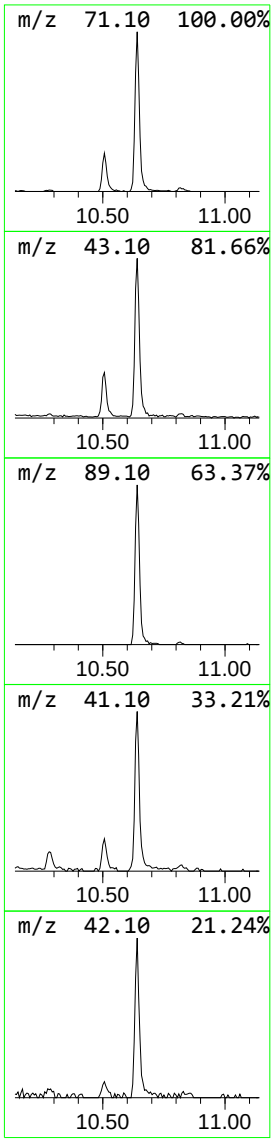
****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	6.51 ug/l	79621	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, pentyl ester	158	C9H18O2	000540-18-1	78
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033851.D
Acq On : 23 Jan 2023 15:56
Operator : JC/MD
Sample : 01237-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1-2-3A

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	63720	2	6.763	565379	50.0
n-Propyl acetate	7.799	121.3	ug/l	1371080	2	6.763	565379	50.0
Propanoic acid,...	8.549	24.4	ug/l	298064	3	10.055	611217	50.0
Isobutyl acetate	8.952	26.0	ug/l	317402	3	10.055	611217	50.0
Propanoic acid,...	9.244	30.8	ug/l	376805	3	10.055	611217	50.0
3-Pentanone, 2,...	9.372	13.0	ug/l	159314	3	10.055	611217	50.0
Propanoic acid,...	9.482	45.7	ug/l	558986	3	10.055	611217	50.0
Acetic acid, bu...	9.580	27.0	ug/l	330373	3	10.055	611217	50.0
Isopropyl butyrate	9.915	85.2	ug/l	1041160	3	10.055	611217	50.0
Butanoic acid, ...	10.640	6.5	ug/l	79621	3	10.055	611217	50.0