LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011123\
Data File : VN076201.D
Acq On : 11 Jan 2023 11:40
Operator : JC\MD
Sample : PB150155TB
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB150155TB

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_N\methods\82N121422W.M
Title : SW846 8260

Signal : TIC: VN076201.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.447	398	407	417	rBV	22533	65094	1.90%	0.296%
2	7.571	931	938	949	rVB2	27416	68738	2.01%	0.312%
3	8.177	1031	1041	1045	rBV	228292	554058	16.19%	2.517%
4	8.229	1045	1050	1064	rVB	450954	1004580	29.35%	4.564%
5	8.582	1099	1110	1121	rBV	227968	513252	14.99%	2.332%
6	8.694	1121	1129	1146	rBV	186522	431736	12.61%	1.962%
7	9.106	1190	1199	1214	rBV	599432	1235912	36.11%	5.615%
8	9.671	1287	1295	1301	rBV	86605	198456	5.80%	0.902%
9	9.747	1301	1308	1326	rVV	1826696	3423090	100.00%	15.552%
10	10.359	1405	1412	1421	rBV	428509	733847	21.44%	3.334%
11	10.447	1421	1427	1439	rVV4	18550	50212	1.47%	0.228%
12	10.570	1439	1448	1455	rVV	906160	1677924	49.02%	7.623%
13	10.729	1467	1475	1491	rVB	551009	940001	27.46%	4.271%
14	10.988	1510	1519	1529	rBV	604462	1021691	29.85%	4.642%
15	11.082	1529	1535	1543	rVV3	117586	220978	6.46%	1.004%
16	11.206	1543	1556	1564	rVV2	938219	1927907	56.32%	8.759%
17	11.288	1564	1570	1586	rVB	591580	986896	28.83%	4.484%
18	11.600	1615	1623	1638	rBV	1872851	3038287	88.76%	13.804%
19	11.770	1646	1652	1661	rVB3	25341	50858	1.49%	0.231%
20	11.865	1661	1668	1679	rVV	783768	1414101	41.31%	6.425%
21	11.965	1679	1685	1691	rVB	24287	39911	1.17%	0.181%
22	12.212	1718	1727	1734	rVB	20325	35475	1.04%	0.161%
23	12.306	1736	1743	1750	rBV	162001	258485	7.55%	1.174%
24	12.853	1828	1836	1845	rBV	586741	996803	29.12%	4.529%
25	13.794	1989	1996	2004	rVB	665540	1121879	32.77%	5.097%

Sum of corrected areas: 22010171

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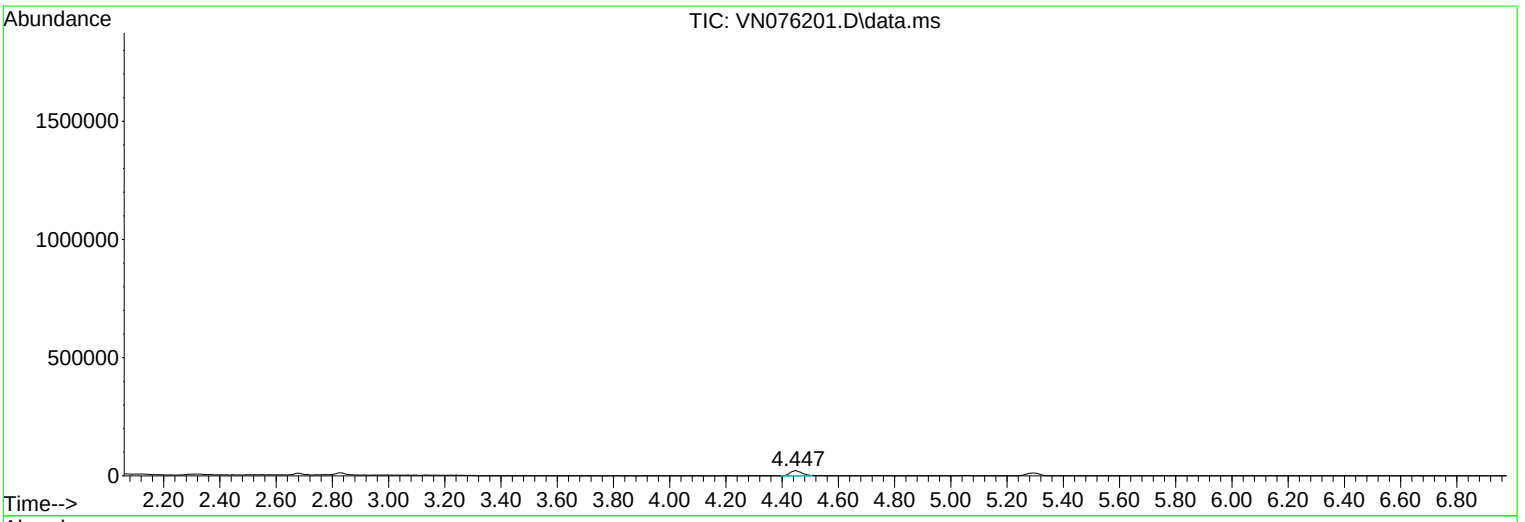
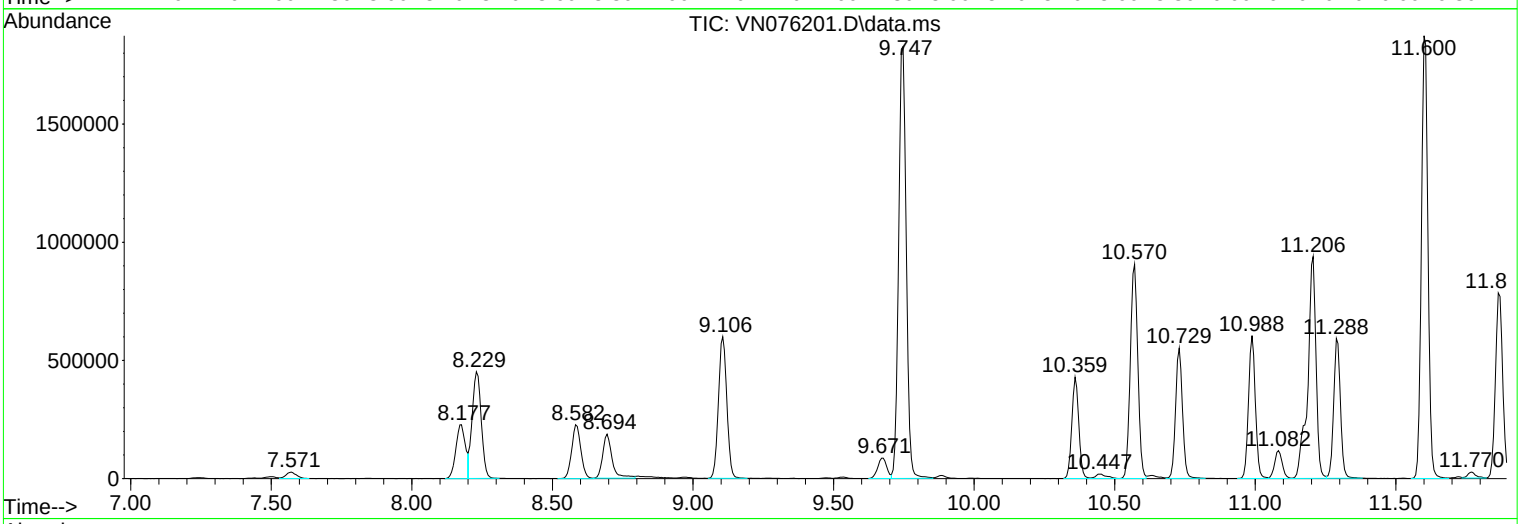
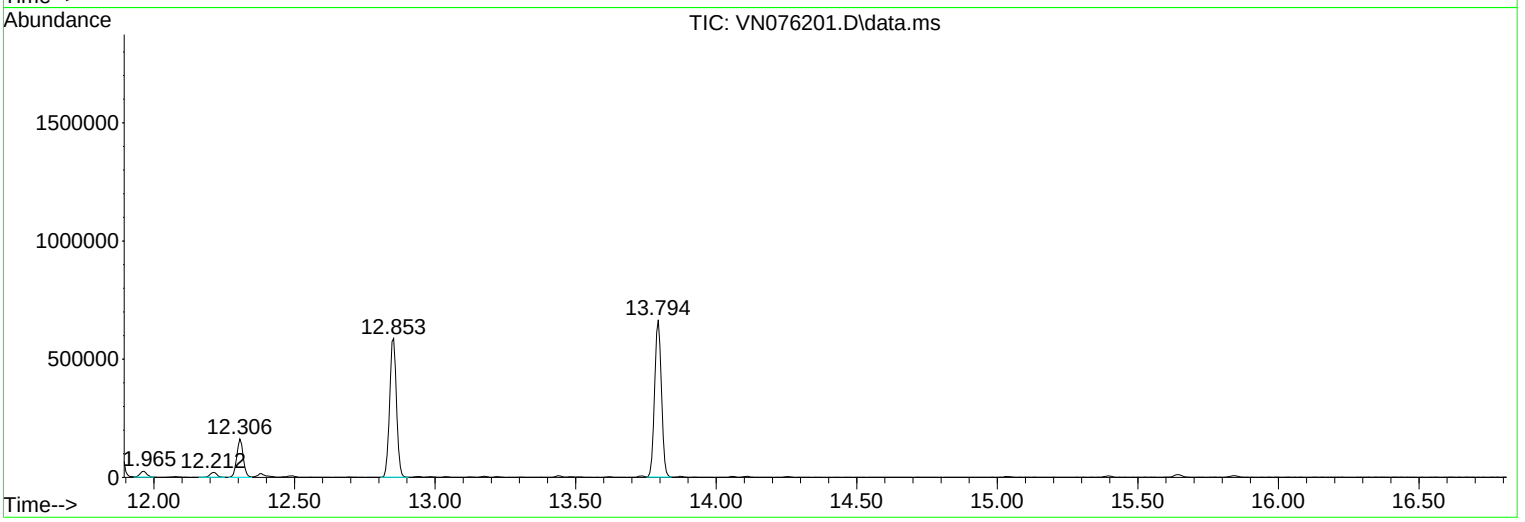
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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







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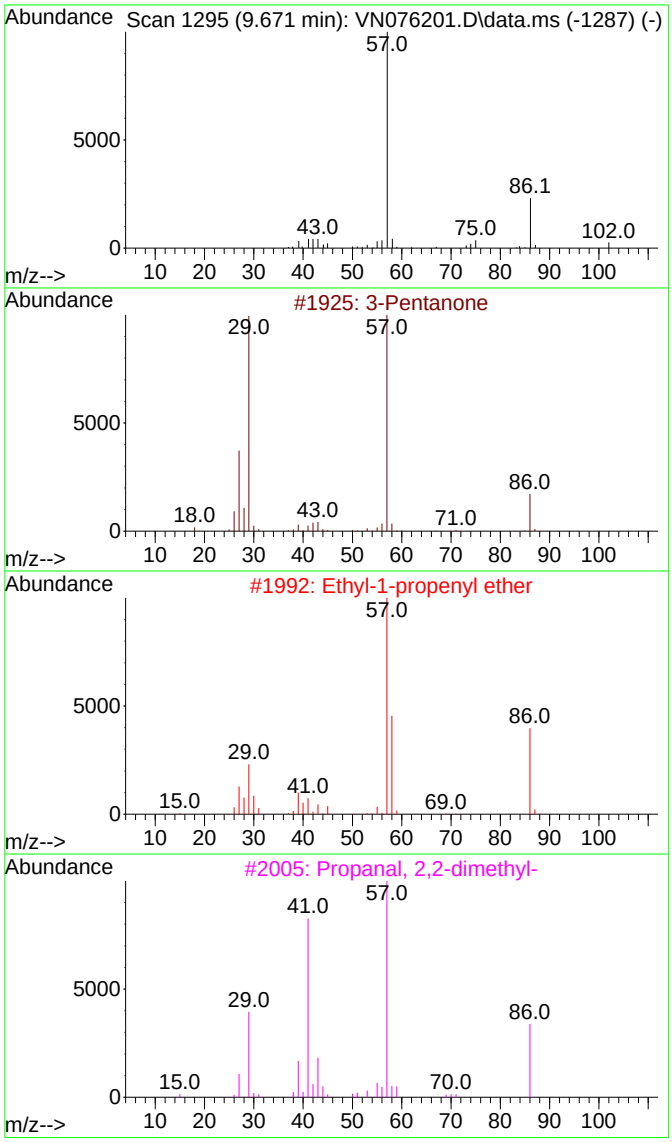
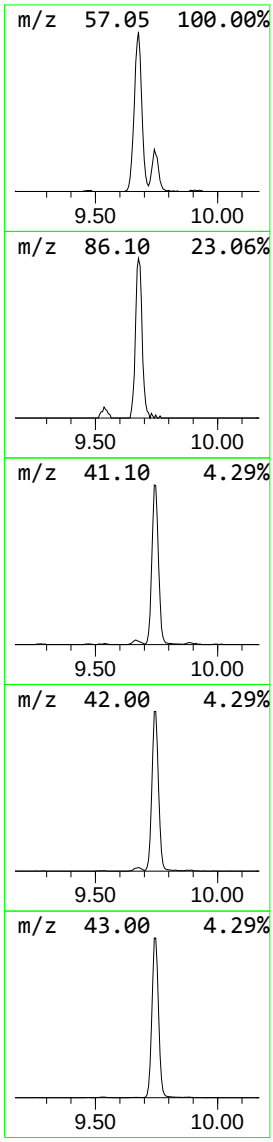
****

Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.671	8.03 ug/l	198456	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	47
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
4	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	25
5	Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	17





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Quant Title : SW846 8260

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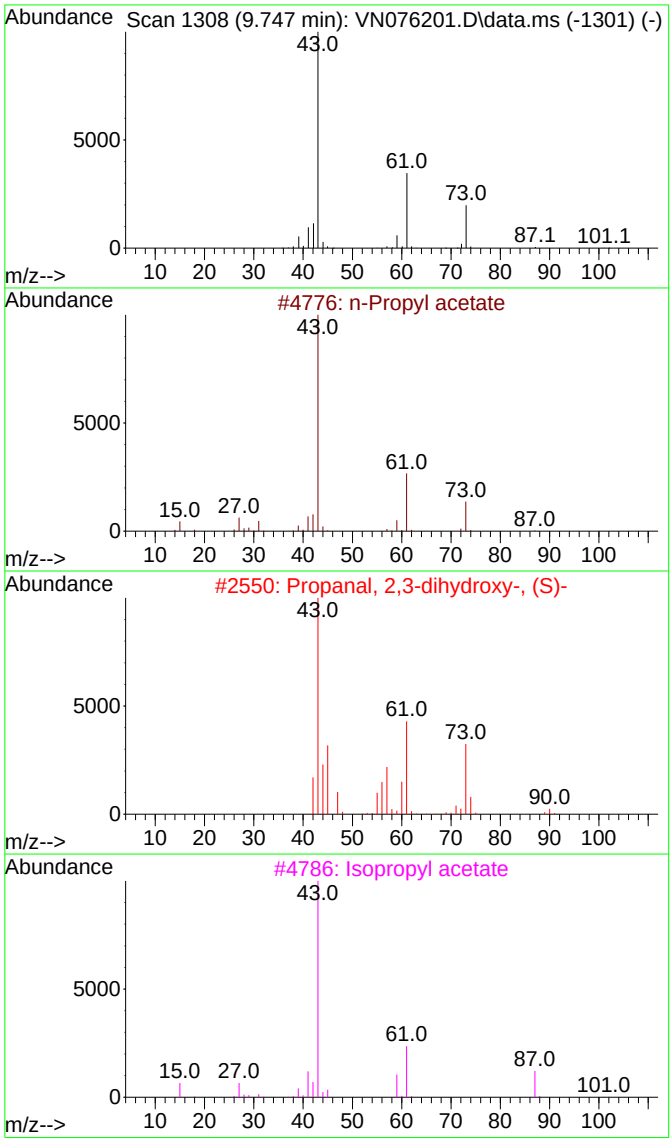
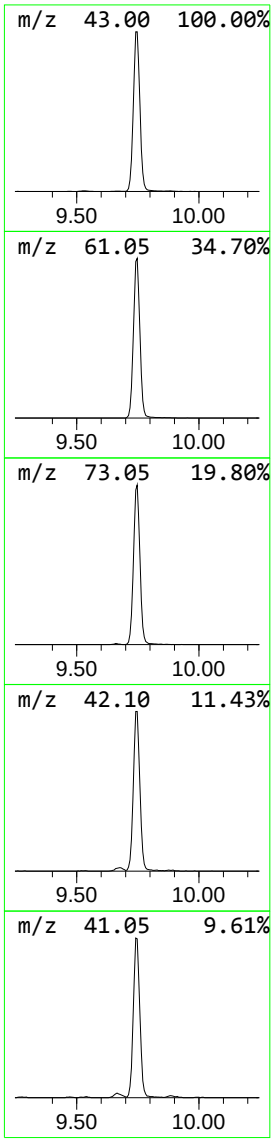
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	138.48 ug/l	3423090	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38
3	Isopropyl acetate	102	C5H10O2	000108-21-4	33
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





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PB150155TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
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TIC Library : C:\Database\NIST20.L
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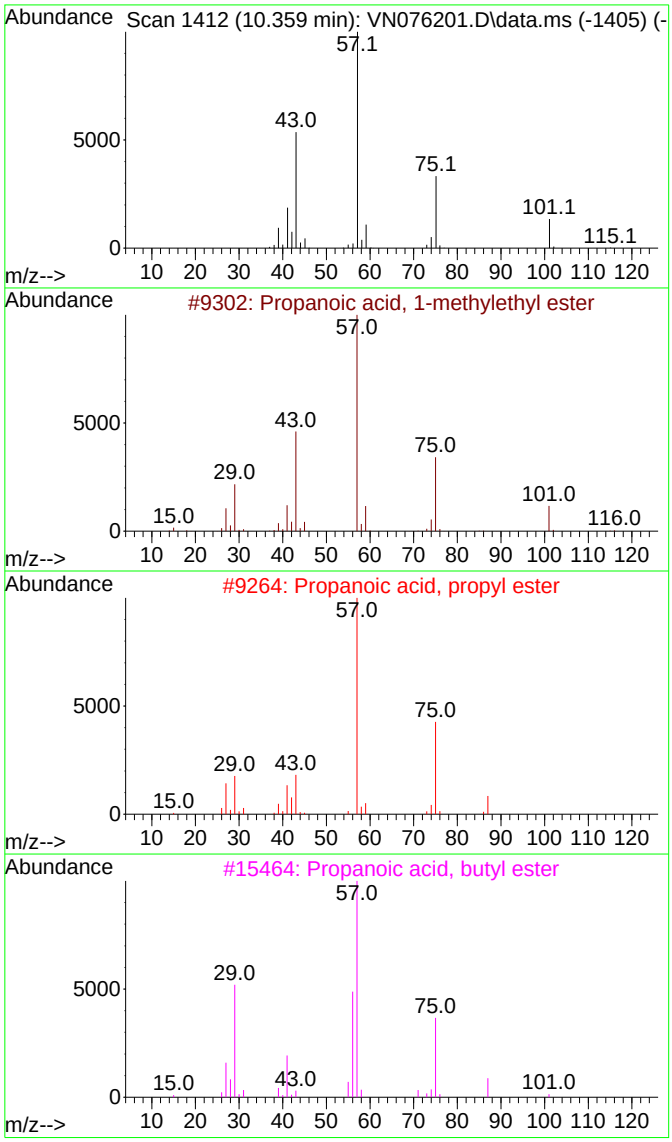
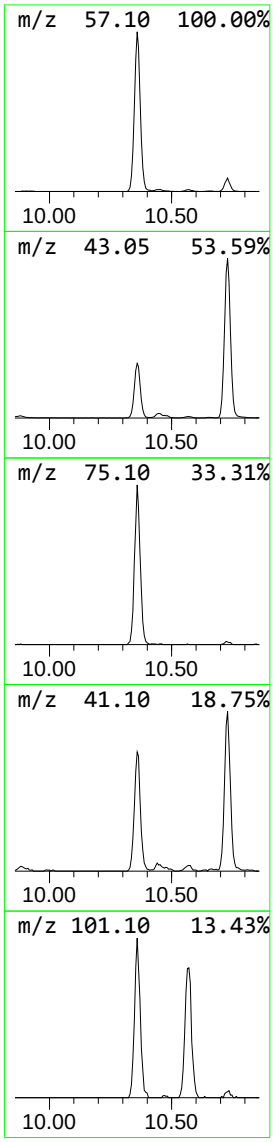
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.359	29.69 ug/l	733847	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	86
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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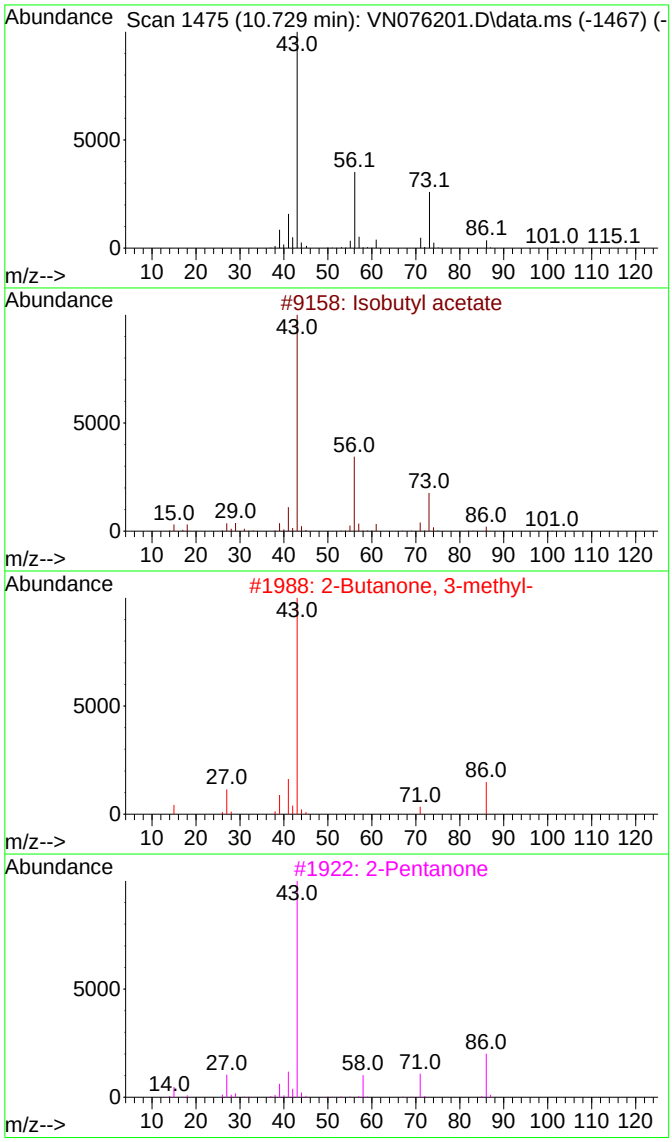
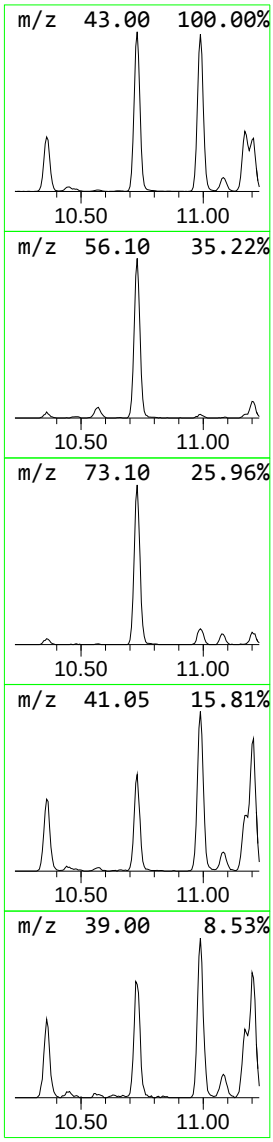
****

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.729	33.24 ug/l	940001	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
3	2-Pentanone	86	C5H10O	000107-87-9	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	Ethane, diazo-	56	C2H4N2	001117-96-0	7





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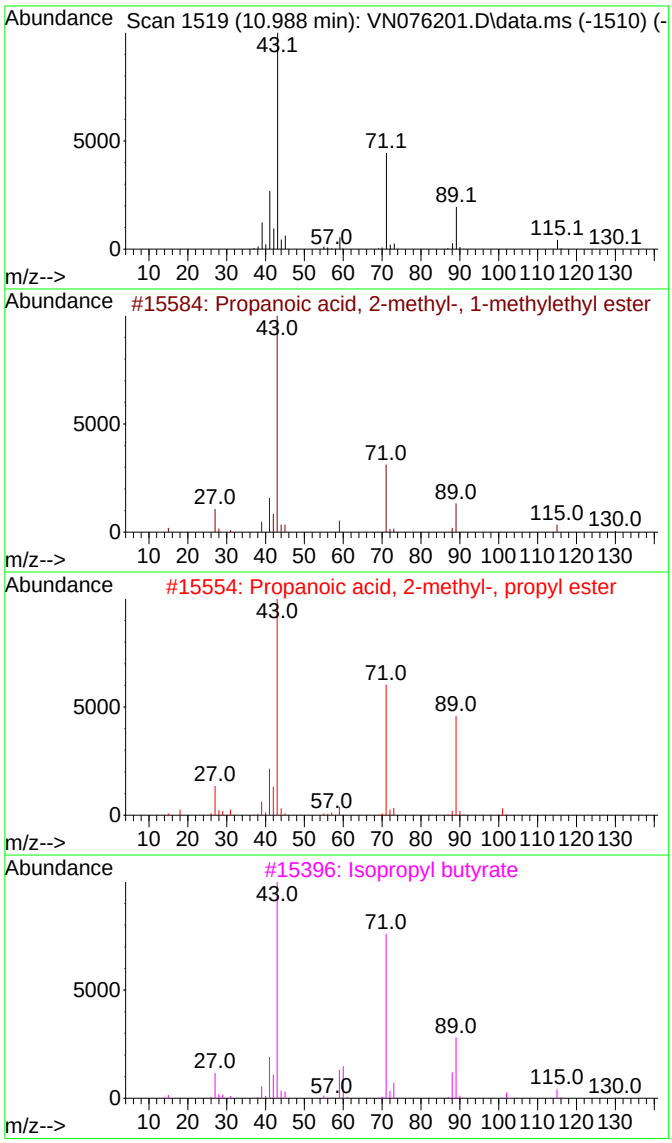
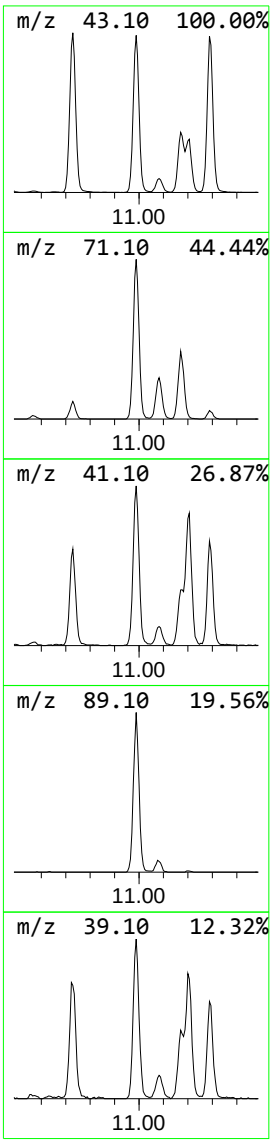
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	36.13 ug/l	1021690	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	90
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	59
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	50
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	45





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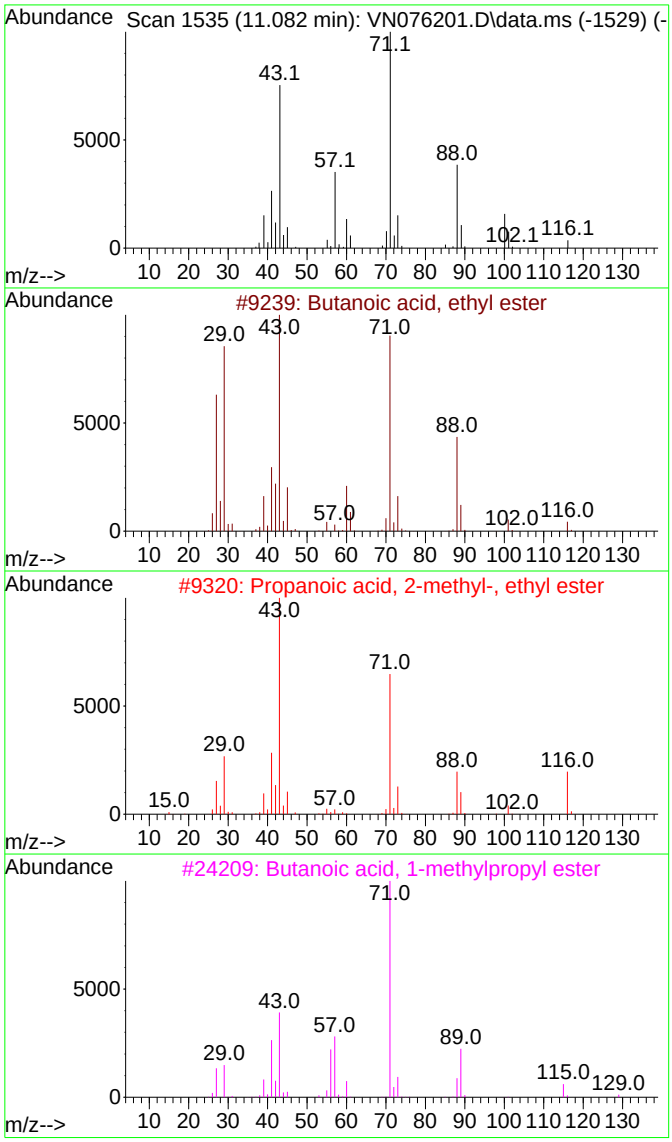
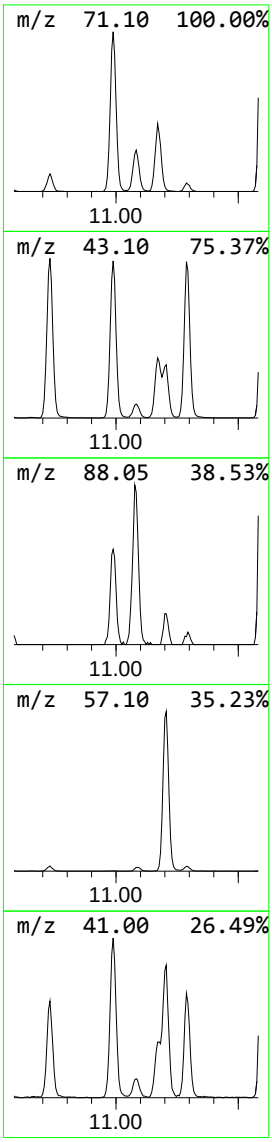
****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.082	7.81 ug/l	220978	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	72
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	62
3	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	50
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	47
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	43





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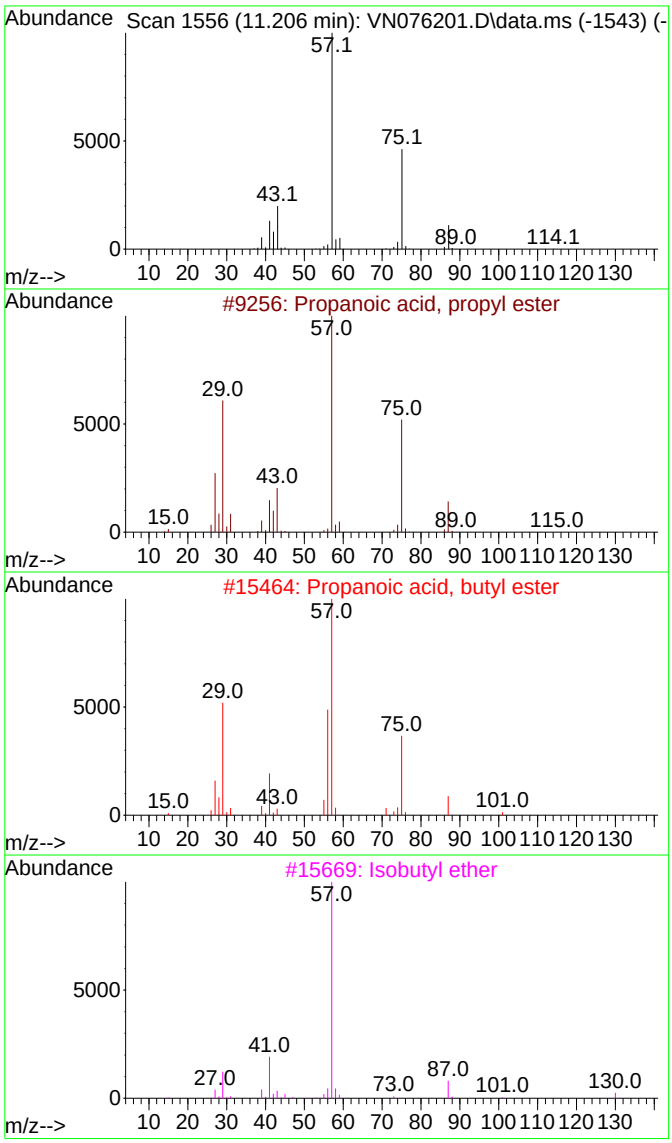
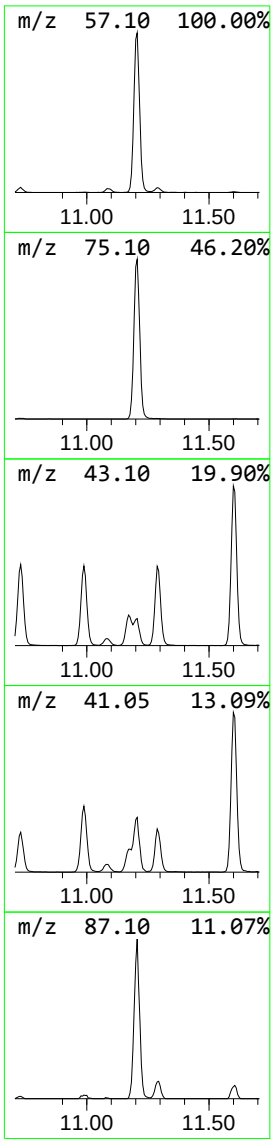
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	68.17 ug/l	1927910	Chlorobenzene-d5	11.865

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	Isobutyl ether	130	C8H18O	000628-55-7	17
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7





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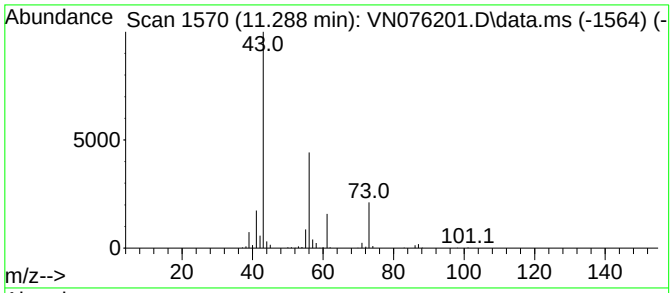
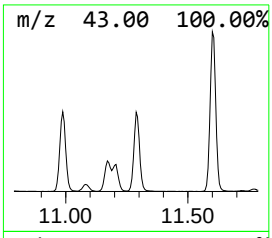
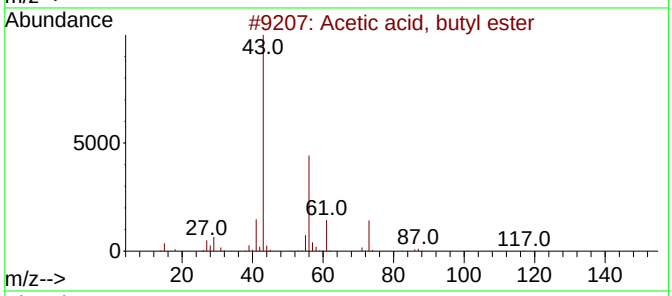
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

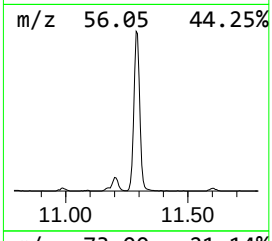
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.288	34.89 ug/l	986896	Chlorobenzene-d5	11.865

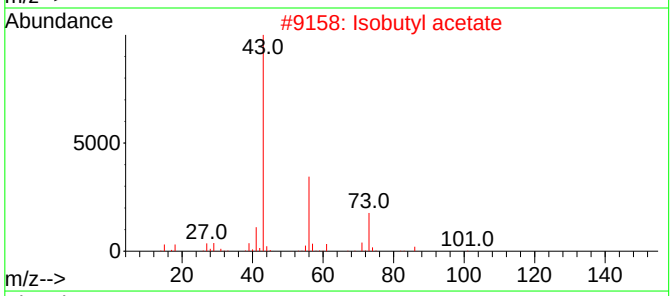
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
5	Isobutylamine	73	C4H11N	000078-81-9	9

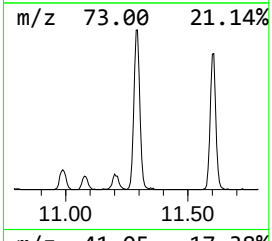


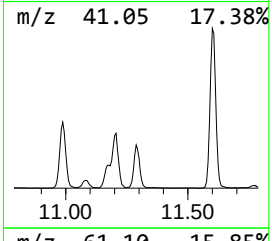


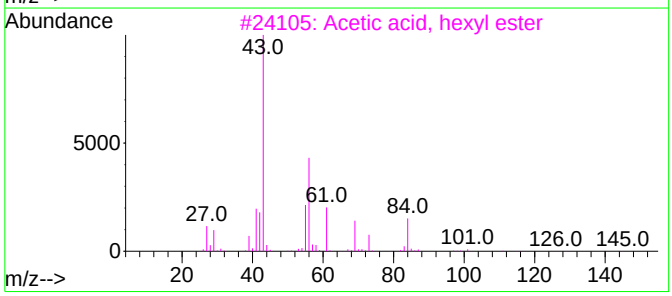


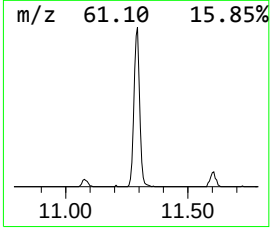












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011123\
Data File : VN076201.D
Acq On : 11 Jan 2023 11:40
Operator : JC\MD
Sample : PB150155TB
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB150155TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

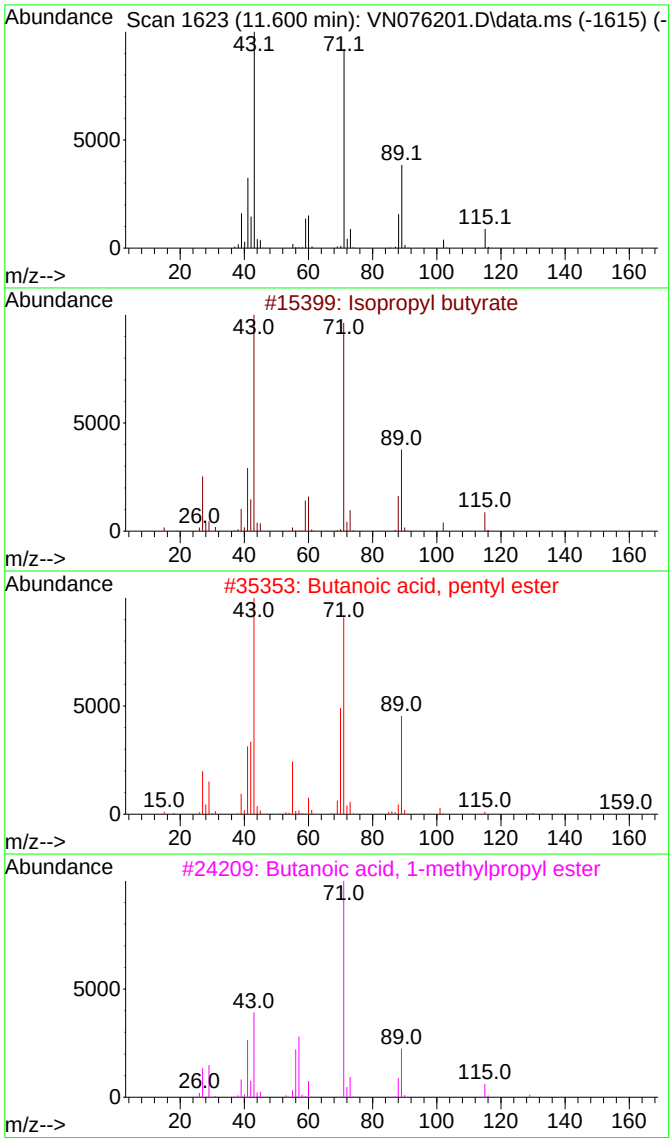
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

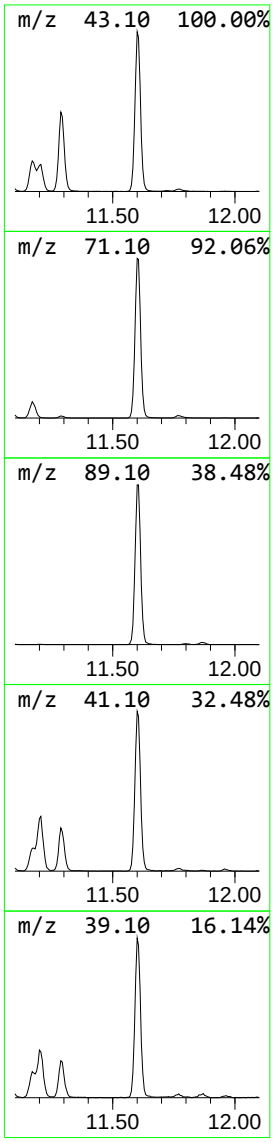
****

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.600	107.43 ug/l	3038290	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	72
3	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011123\
Data File : VN076201.D
Acq On : 11 Jan 2023 11:40
Operator : JC\MD
Sample : PB150155TB
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB150155TB

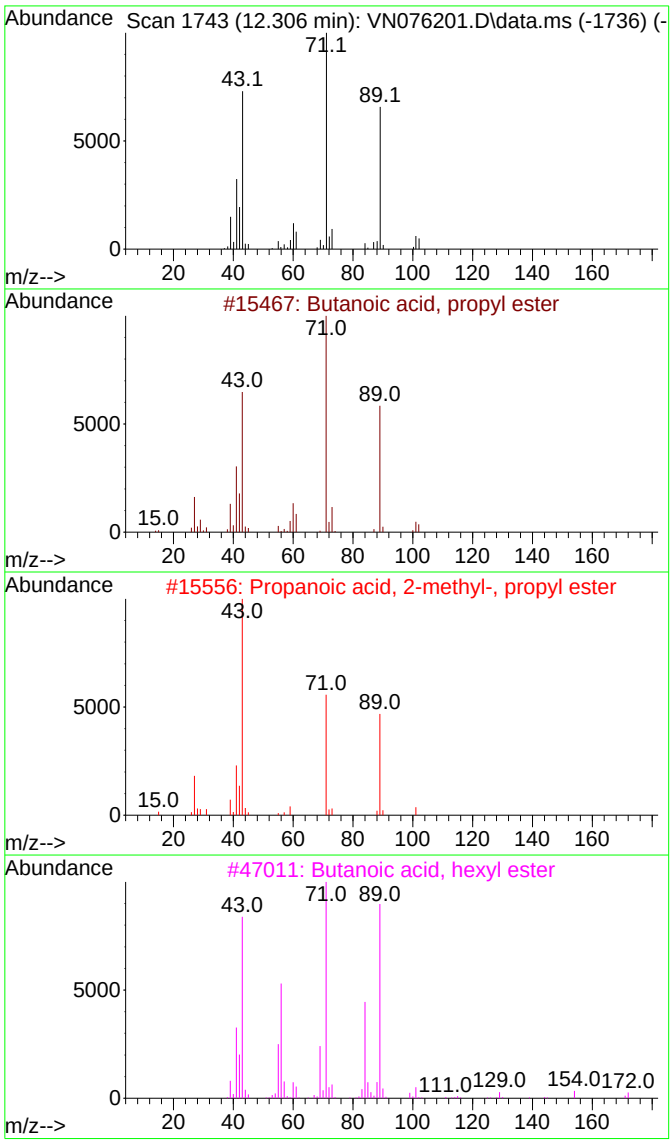
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

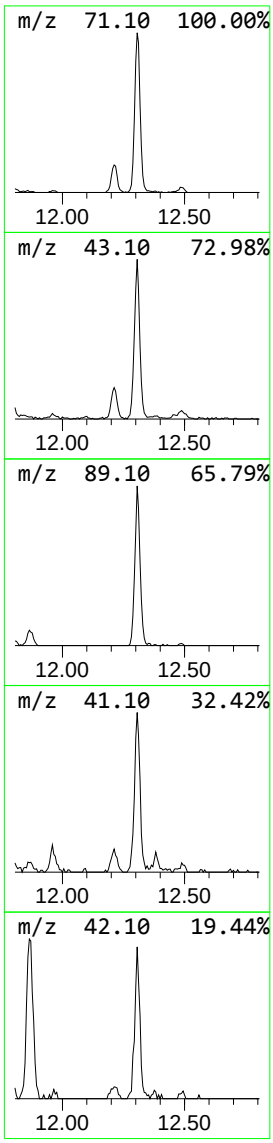
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.306	9.14 ug/l	258485	Chlorobenzene-d5	11.865

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, hexyl ester	172	C10H20O2	002639-63-6	64
4	Malic Acid	134	C4H6O5	006915-15-7	64
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011123\
Data File : VN076201.D
Acq On : 11 Jan 2023 11:40
Operator : JC\MD
Sample : PB150155TB
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB150155TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.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	9.671	8.0	ug/l	198456	2	9.106	1235910	50.0
n-Propyl acetate	9.747	138.5	ug/l	3423090	2	9.106	1235910	50.0
Propanoic acid,...	10.359	29.7	ug/l	733847	2	9.106	1235910	50.0
Isobutyl acetate	10.729	33.2	ug/l	940001	3	11.865	1414100	50.0
Propanoic acid,...	10.988	36.1	ug/l	1021690	3	11.865	1414100	50.0
Butanoic acid, ...	11.082	7.8	ug/l	220978	3	11.865	1414100	50.0
Propanoic acid,...	11.206	68.2	ug/l	1927910	3	11.865	1414100	50.0
Acetic acid, bu...	11.288	34.9	ug/l	986896	3	11.865	1414100	50.0
Isopropyl butyrate	11.600	107.4	ug/l	3038290	3	11.865	1414100	50.0
Butanoic acid, ...	12.306	9.1	ug/l	258485	3	11.865	1414100	50.0