LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011723\
Data File : VN076281.D
Acq On : 17 Jan 2023 15:36
Operator : JC\MD
Sample : 01172-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-F

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\82N011623W.M
Title : SW846 8260

Signal : TIC: VN076281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.453	398	408	417	rBV2	15309	46634	1.82%	0.246%
2	5.289	537	550	561	rBV5	14962	49570	1.94%	0.261%
3	7.571	931	938	947	rVB3	19119	47440	1.85%	0.250%
4	8.171	1029	1040	1045	rBV	230377	565458	22.11%	2.981%
5	8.230	1045	1050	1064	rVB	452051	981888	38.38%	5.176%
6	8.582	1098	1110	1118	rBV	229673	527060	20.60%	2.778%
7	8.694	1118	1129	1139	rBV2	178210	512423	20.03%	2.701%
8	9.106	1190	1199	1210	rBV	604074	1245995	48.71%	6.568%
9	9.671	1285	1295	1301	rBV2	68877	153122	5.99%	0.807%
10	9.747	1301	1308	1320	rVB	1411284	2558016	100.00%	13.484%
11	10.359	1401	1412	1422	rBV	336776	576915	22.55%	3.041%
12	10.447	1422	1427	1439	rVB4	13594	34934	1.37%	0.184%
13	10.571	1439	1448	1460	rBV	914656	1686690	65.94%	8.891%
14	10.729	1468	1475	1485	rVB	370877	632338	24.72%	3.333%
15	10.988	1512	1519	1528	rBV	478662	786871	30.76%	4.148%
16	11.082	1528	1535	1543	rVV3	83805	159323	6.23%	0.840%
17	11.206	1543	1556	1564	rVV2	700788	1432025	55.98%	7.548%
18	11.288	1564	1570	1583	rVB	409837	690287	26.99%	3.639%
19	11.600	1616	1623	1636	rBV	1411945	2267387	88.64%	11.952%
20	11.765	1647	1651	1661	rVB3	20173	40940	1.60%	0.216%
21	11.865	1661	1668	1679	rVV	796386	1454417	56.86%	7.667%
22	11.965	1679	1685	1692	rVB2	16182	29516	1.15%	0.156%
23	12.212	1720	1727	1736	rVB2	16153	26520	1.04%	0.140%
24	12.306	1736	1743	1752	rBV	98057	156860	6.13%	0.827%
25	12.853	1828	1836	1845	rBV	631311	1059761	41.43%	5.586%
26	13.794	1988	1996	2004	rBV	742765	1248636	48.81%	6.582%

Sum of corrected areas: 18971026

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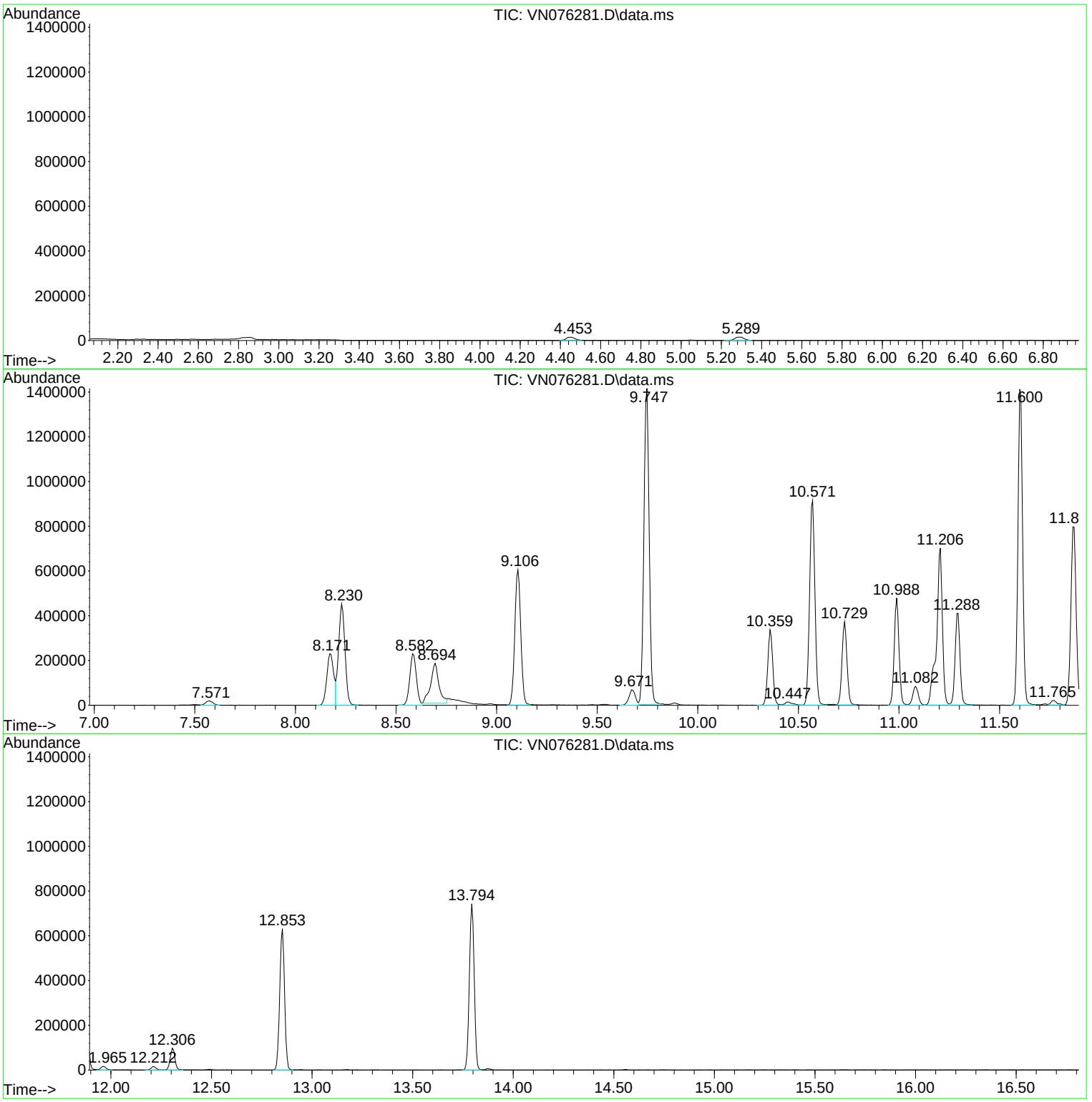
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

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



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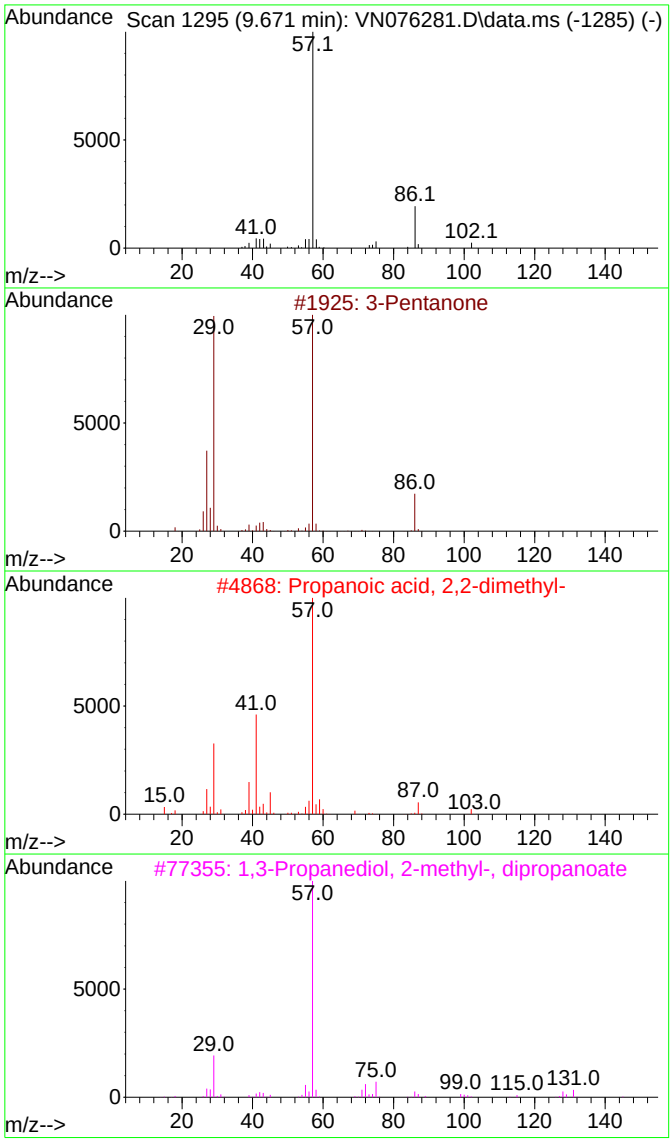
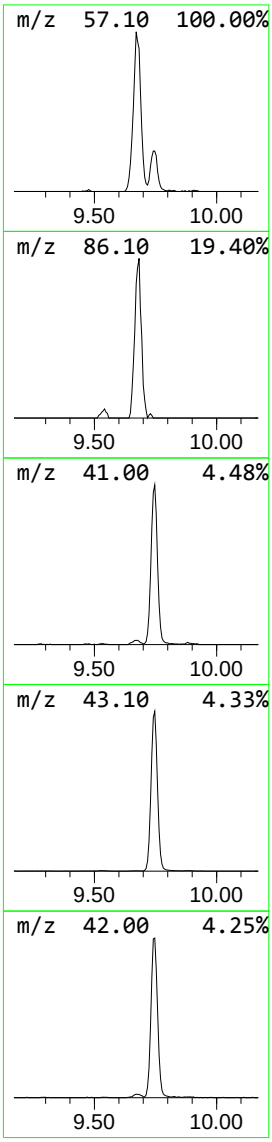
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.671	6.14 ug/l	153122	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	47
3	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	28
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
5	Neopentane	72	C5H12	000463-82-1	9





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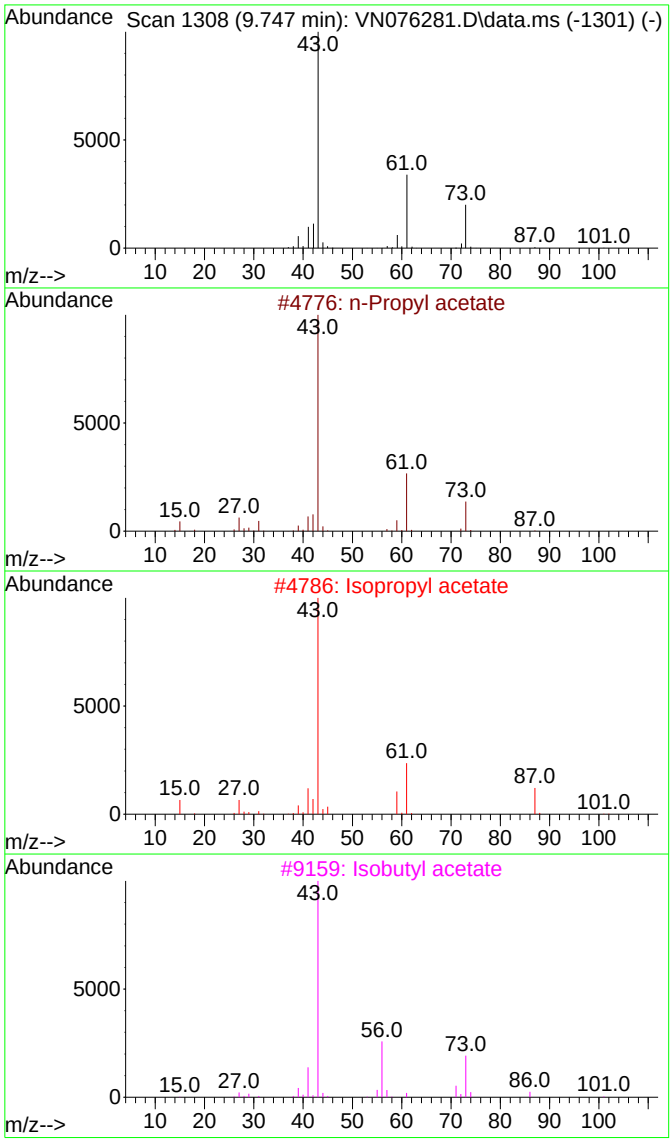
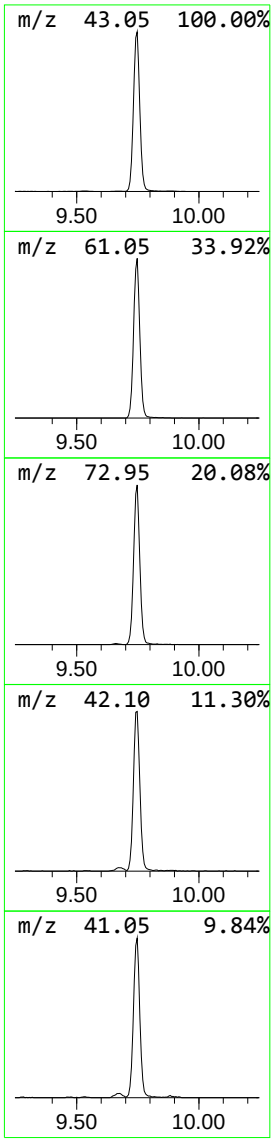
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	102.65 ug/l	2558020	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	Isopropyl acetate	102	C5H10O2	000108-21-4	33
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9
5	Methyl glyoxal	72	C3H4O2	000078-98-8	7





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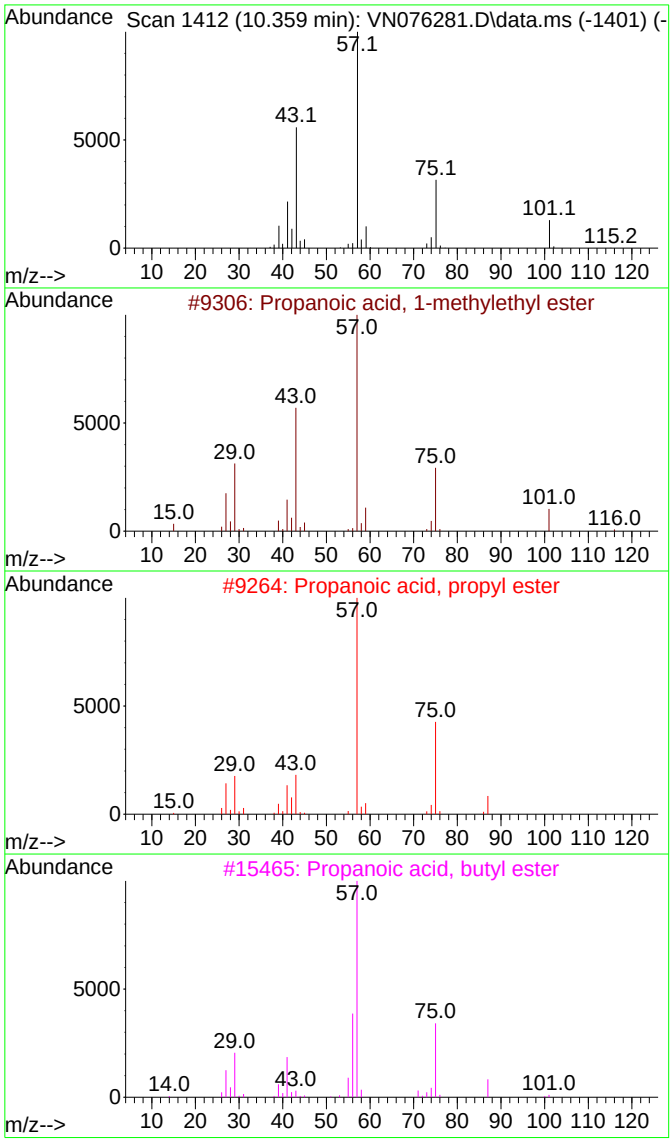
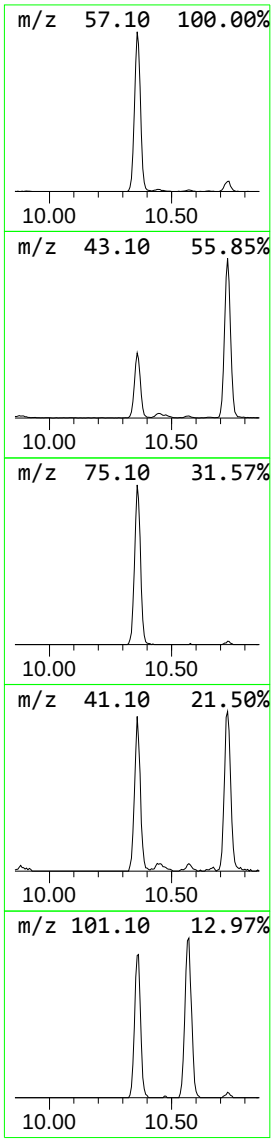
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.359	23.15 ug/l	576915	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	78
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	33
4	Azetidine	57	C3H7N	000503-29-7	10
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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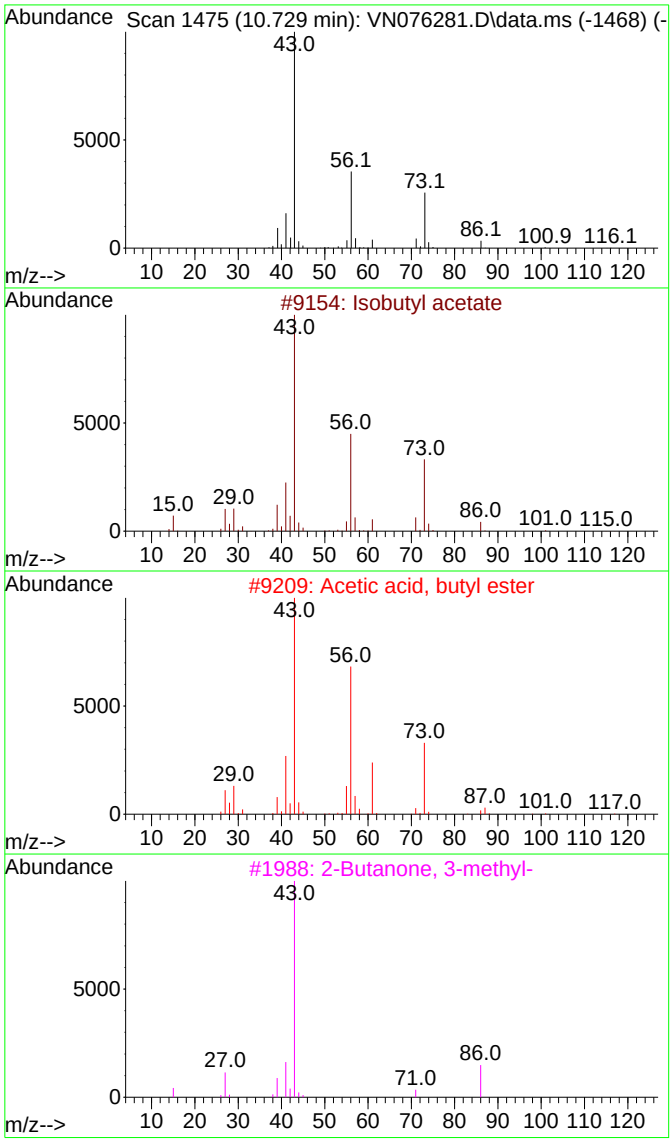
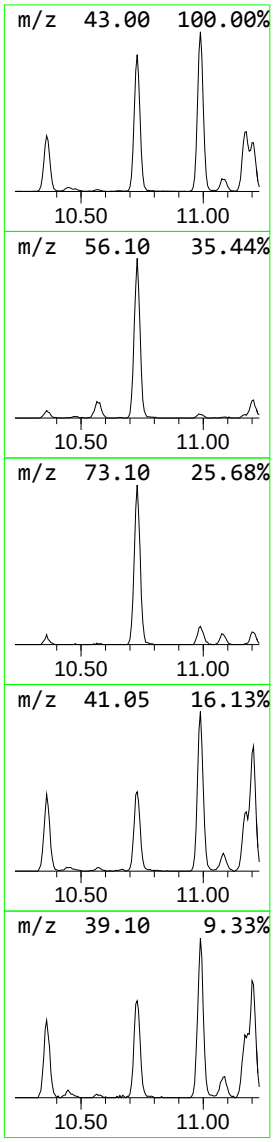
****
Peak Number 4 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.729	21.74 ug/l	632338	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	90
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	36
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
4	2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	9
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9





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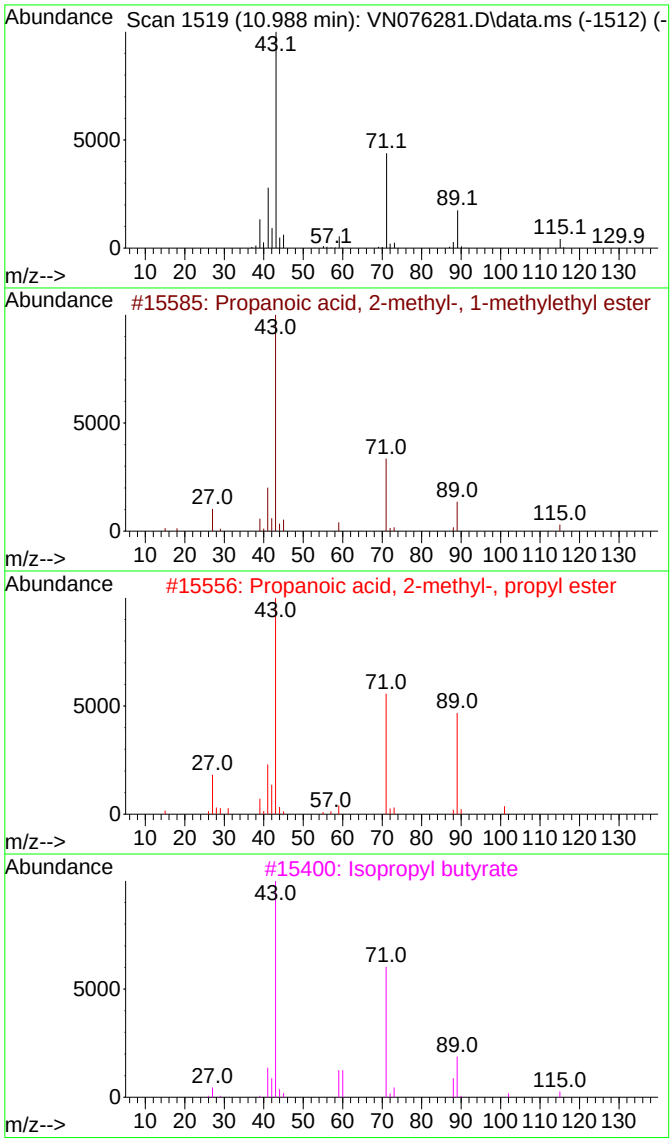
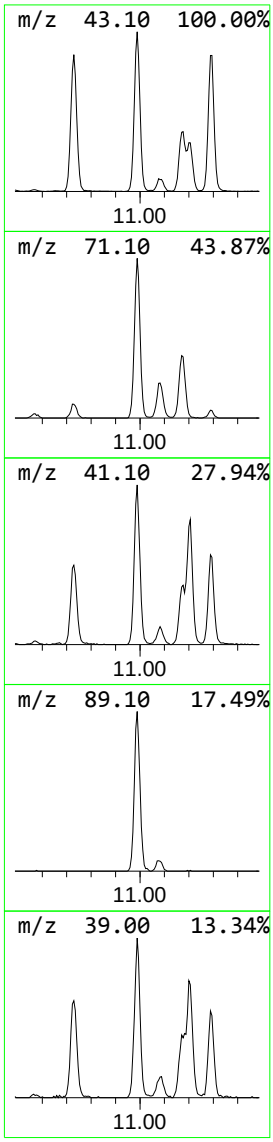
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	27.05 ug/l	786871	Chlorobenzene-d5	11.871

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	56
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	40





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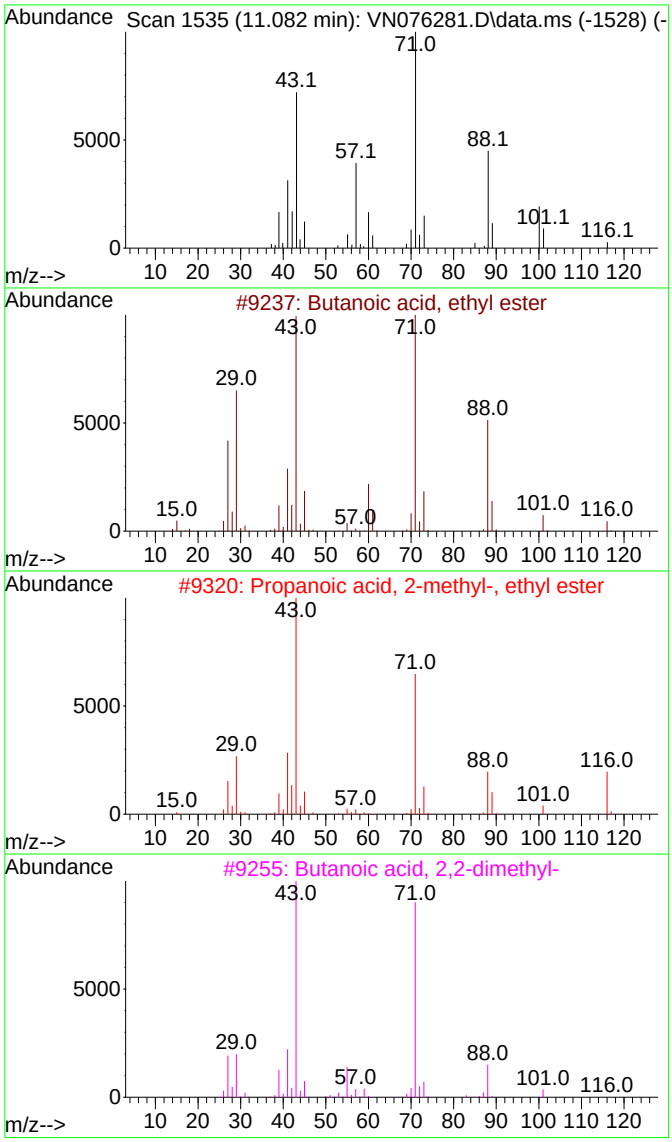
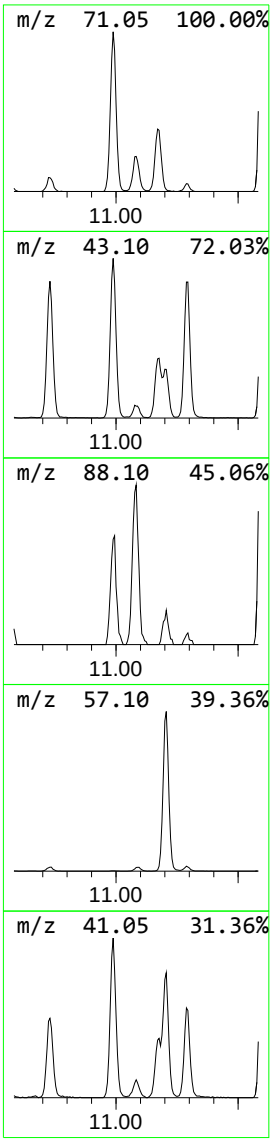
****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.082	5.48 ug/l	159323	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	60
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	47
3	Butanoic acid, 2,2-dimethyl-	116	C6H12O2	000595-37-9	43
4	Butanoic acid, 2-methylbutyl ester	158	C9H18O2	051115-64-1	43
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	38





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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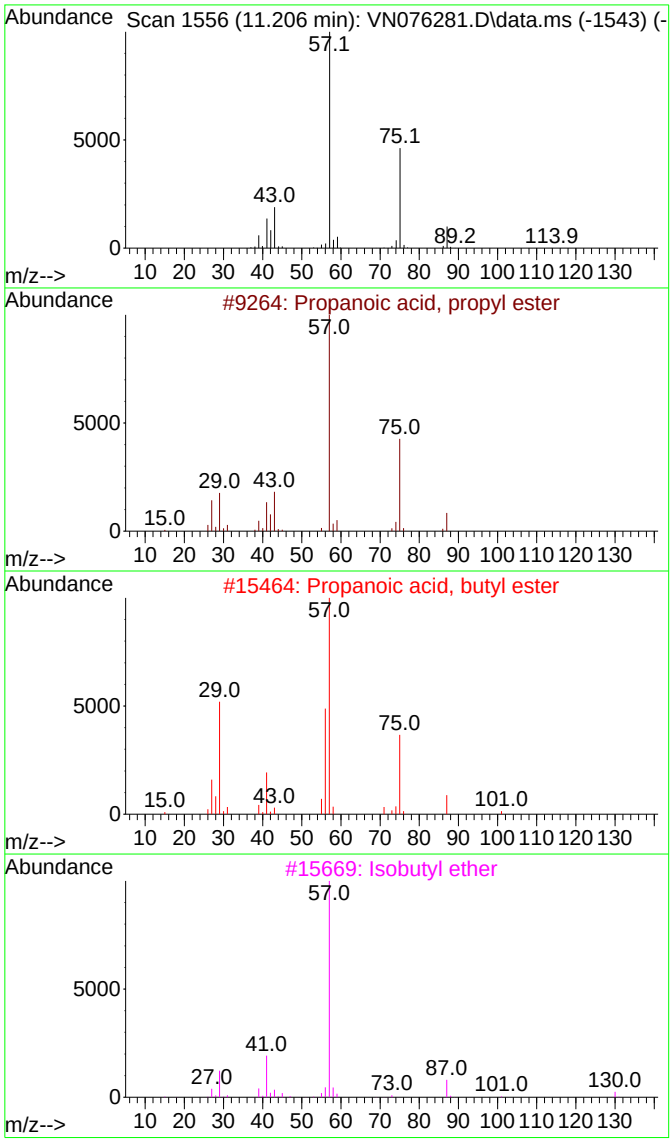
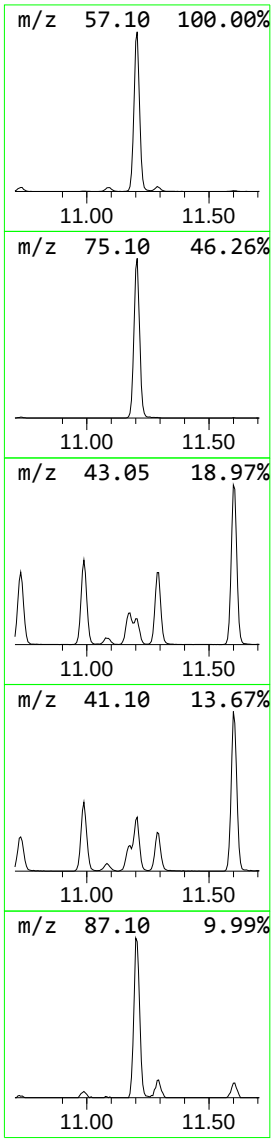
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	49.23 ug/l	1432030	Chlorobenzene-d5	11.871

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	12
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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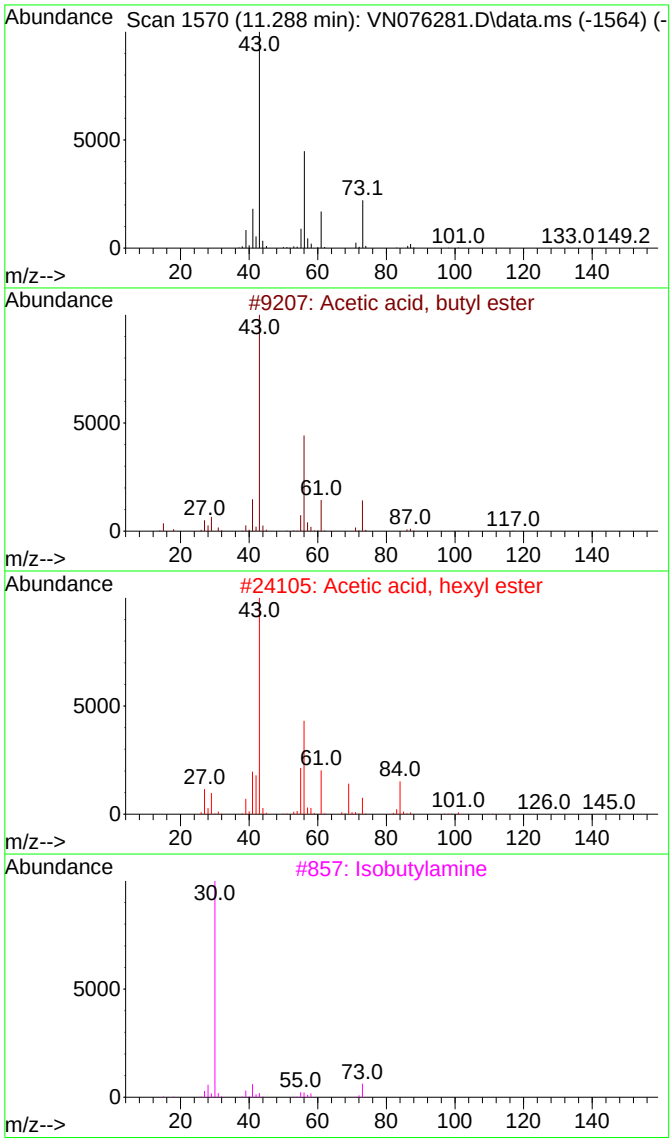
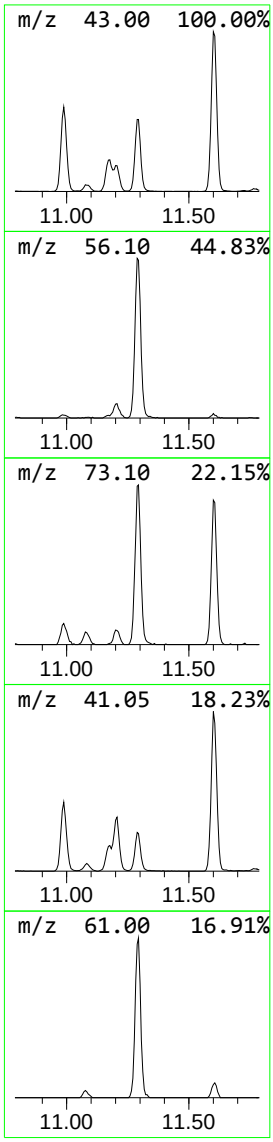
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.288	23.73 ug/l	690287	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
5	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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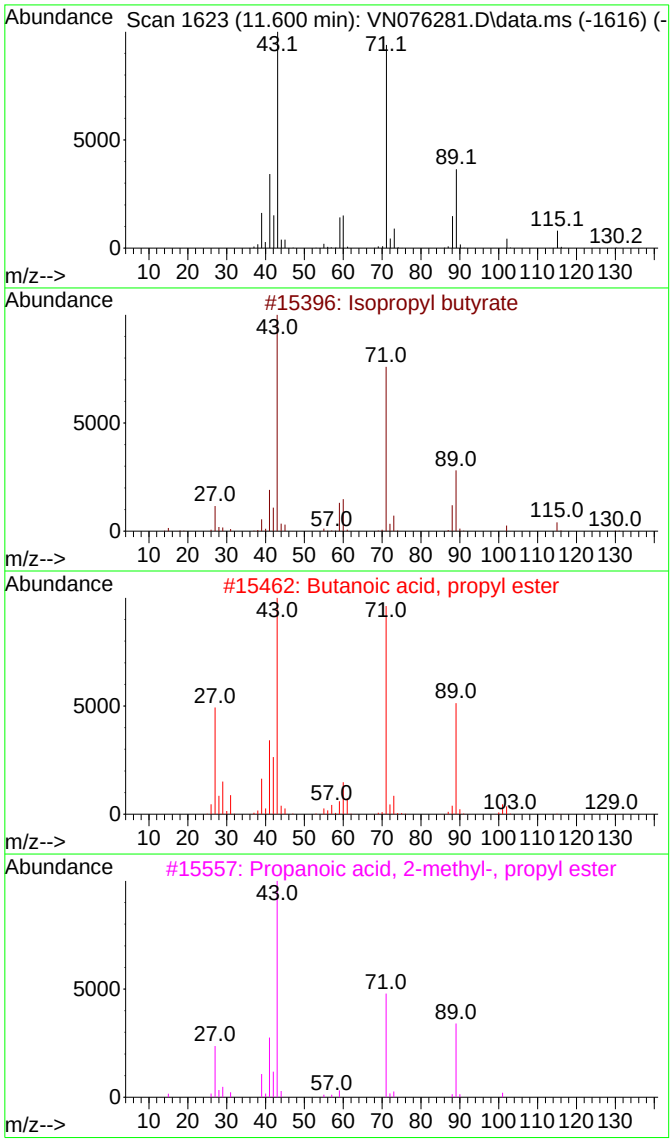
Quant Title : SW846 8260

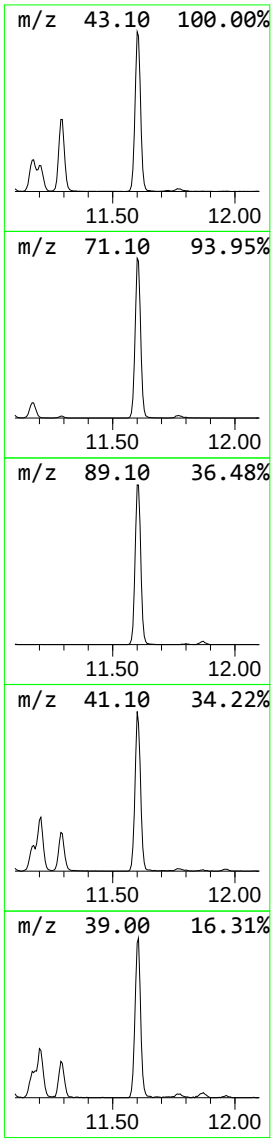
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.600	77.95 ug/l	2267390	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	97
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





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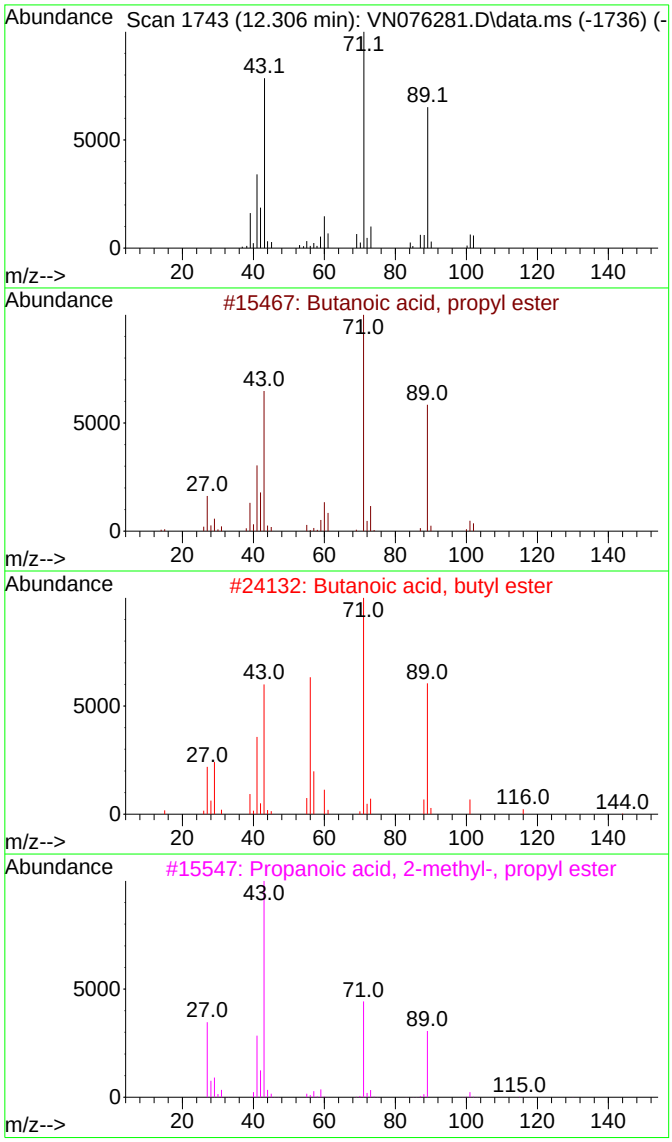
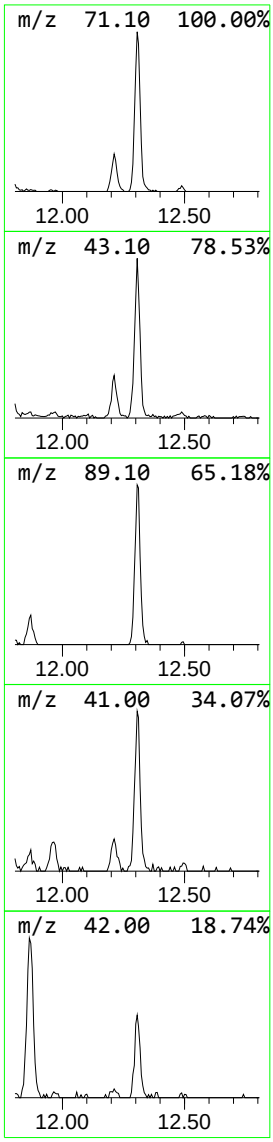
****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.306	5.39 ug/l	156860	Chlorobenzene-d5	11.871

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	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011723\
Data File : VN076281.D
Acq On : 17 Jan 2023 15:36
Operator : JC\MD
Sample : 01172-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-F

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.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	6.1	ug/l	153122	2	9.106	1246000	50.0
n-Propyl acetate	9.747	102.7	ug/l	2558020	2	9.106	1246000	50.0
Propanoic acid,...	10.359	23.1	ug/l	576915	2	9.106	1246000	50.0
Isobutyl acetate	10.729	21.7	ug/l	632338	3	11.871	1454420	50.0
Propanoic acid,...	10.988	27.1	ug/l	786871	3	11.871	1454420	50.0
Butanoic acid, ...	11.082	5.5	ug/l	159323	3	11.871	1454420	50.0
Propanoic acid,...	11.206	49.2	ug/l	1432030	3	11.871	1454420	50.0
Acetic acid, bu...	11.288	23.7	ug/l	690287	3	11.871	1454420	50.0
Isopropyl butyrate	11.600	78.0	ug/l	2267390	3	11.871	1454420	50.0
Butanoic acid, ...	12.306	5.4	ug/l	156860	3	11.871	1454420	50.0