LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078059.D
Acq On : 05 Jun 2023 21:08
Operator : JC\MD
Sample : 03029-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-7

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\82N051523W.M
Title : SW846 8260

Signal : TIC: VN078059.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.824	141	148	156	rVB3	34976	77086	1.63%	0.264%
2	5.283	556	566	579	rBV2	20590	61784	1.30%	0.212%
3	7.577	947	956	967	rVB3	42417	112649	2.38%	0.386%
4	8.177	1048	1058	1062	rBV	313576	738091	15.57%	2.528%
5	8.235	1062	1068	1079	rVB	519758	1182576	24.94%	4.051%
6	8.588	1115	1128	1135	rBV	319219	716515	15.11%	2.454%
7	8.694	1135	1146	1160	rBV2	321809	1024105	21.60%	3.508%
8	9.106	1208	1216	1226	rBV	781241	1618252	34.13%	5.543%
9	9.677	1303	1313	1318	rBV	126994	275676	5.81%	0.944%
10	9.747	1318	1325	1341	rVV	2549011	4741637	100.00%	16.241%
11	10.365	1421	1430	1440	rBV	594960	1031255	21.75%	3.532%
12	10.571	1457	1465	1478	rBV	1209210	2309757	48.71%	7.912%
13	10.729	1486	1492	1503	rVB	681787	1186051	25.01%	4.063%
14	10.994	1528	1537	1545	rBV	793586	1345657	28.38%	4.609%
15	11.088	1546	1553	1560	rVV3	148650	280010	5.91%	0.959%
16	11.206	1561	1573	1582	rVV2	1192482	2504355	52.82%	8.578%
17	11.294	1582	1588	1602	rVB	725814	1211077	25.54%	4.148%
18	11.606	1631	1641	1652	rBV	2337832	3662029	77.23%	12.543%
19	11.771	1665	1669	1678	rVB2	35527	66204	1.40%	0.227%
20	11.871	1678	1686	1697	rVV	1105145	1987545	41.92%	6.808%
21	11.965	1697	1702	1711	rVB	28727	53621	1.13%	0.184%
22	12.312	1754	1761	1769	rVV	151816	253876	5.35%	0.870%
23	12.853	1844	1853	1864	rBV	823075	1433077	30.22%	4.909%
24	13.800	2006	2014	2025	rVB	748352	1321838	27.88%	4.528%

Sum of corrected areas: 29194723

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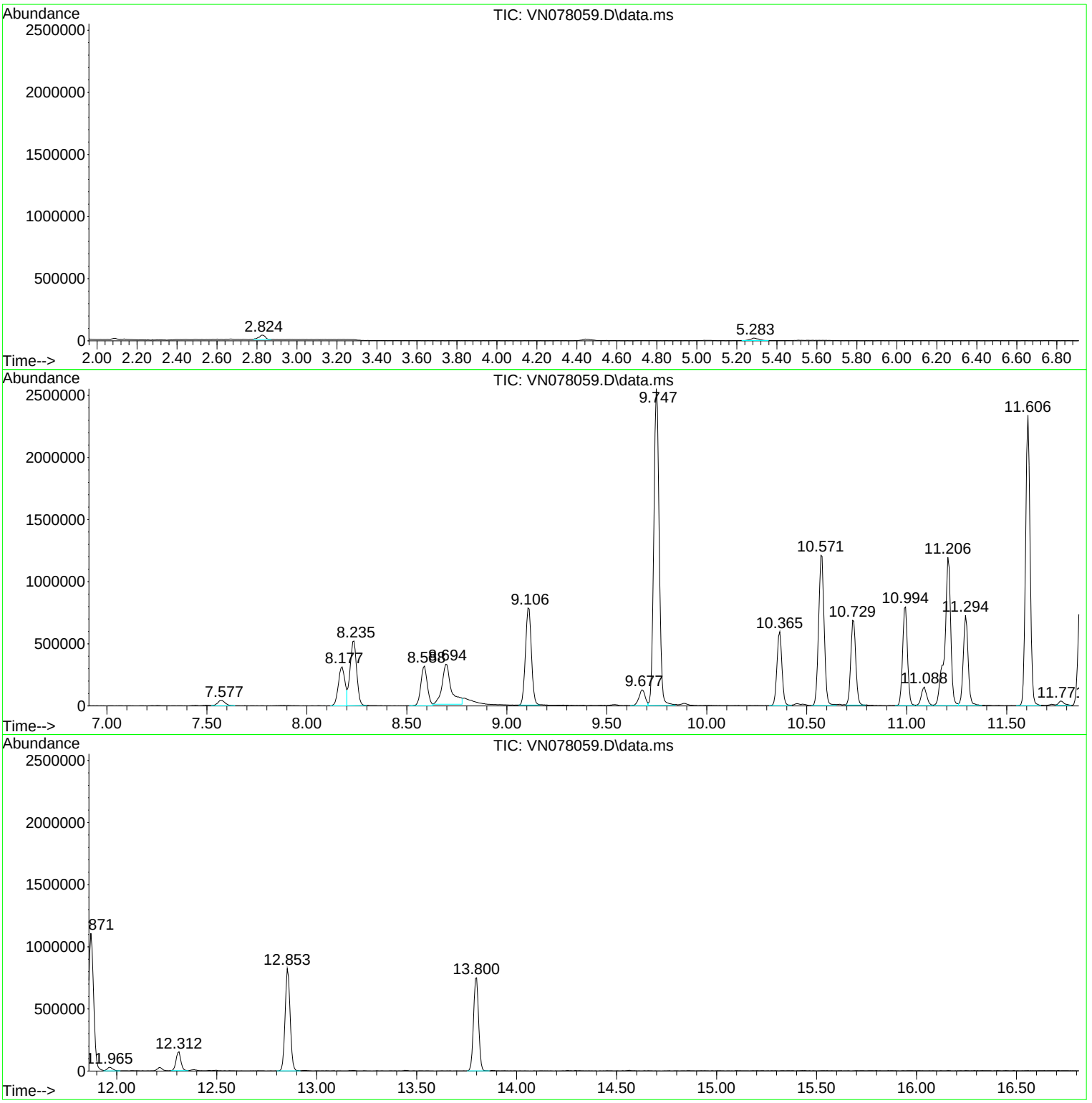
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



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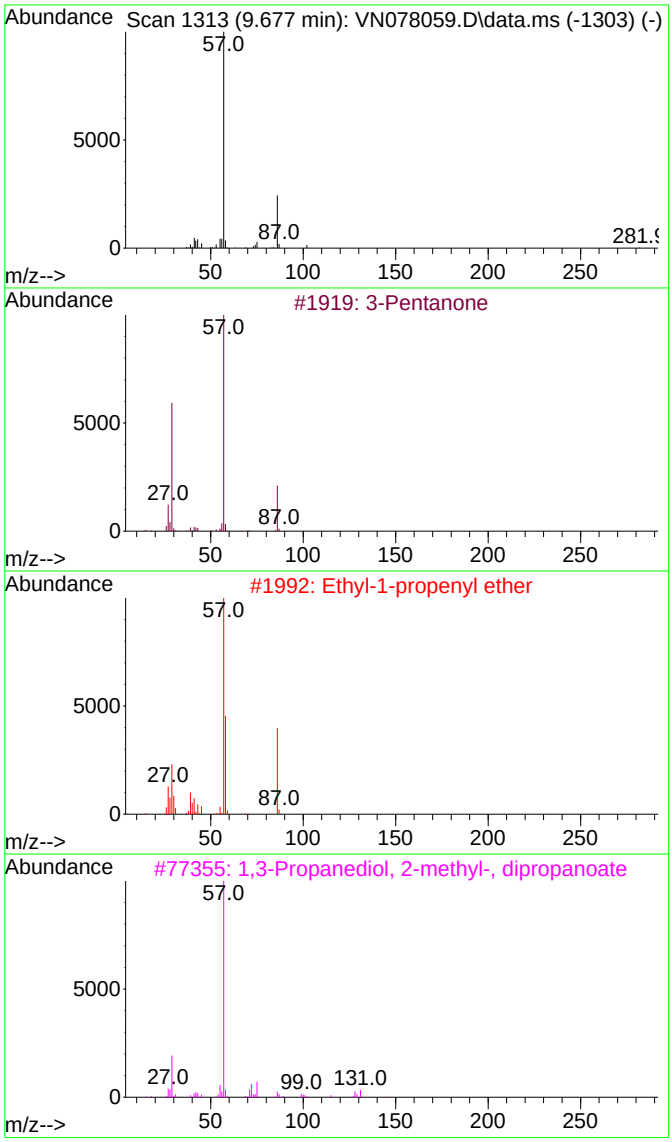
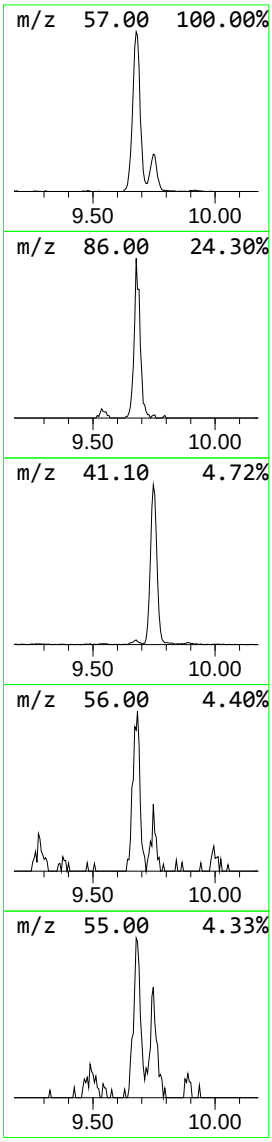
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	8.52 ug/l	275676	1,4-Difluorobenzene	9.112

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	72
2	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	40
3	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	25
4	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	23
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9





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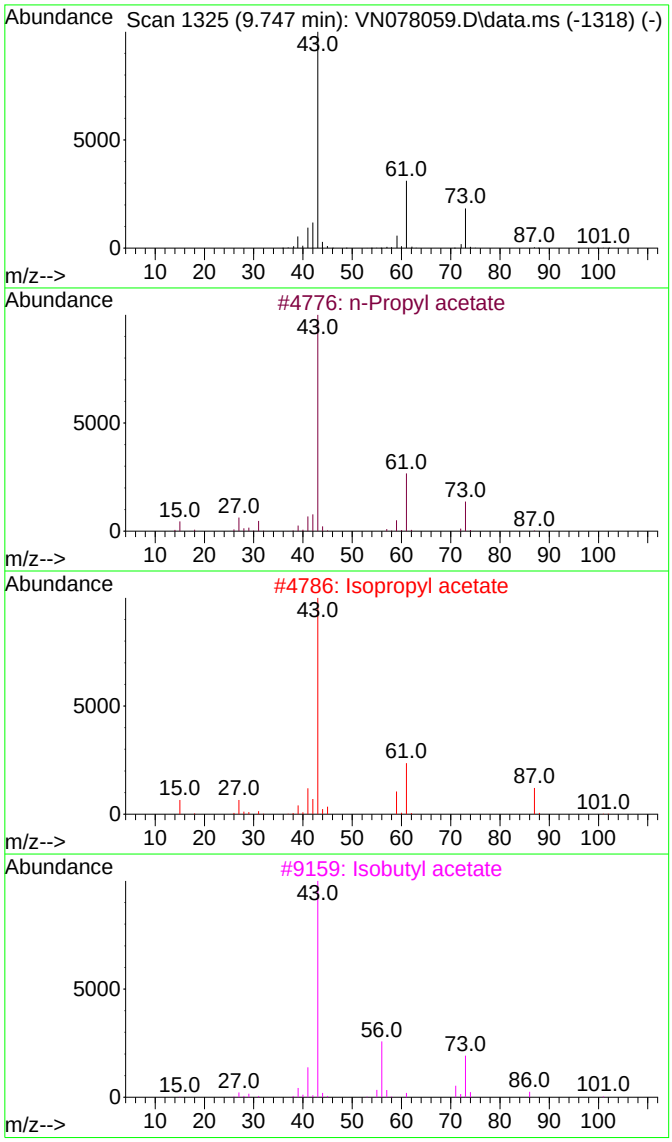
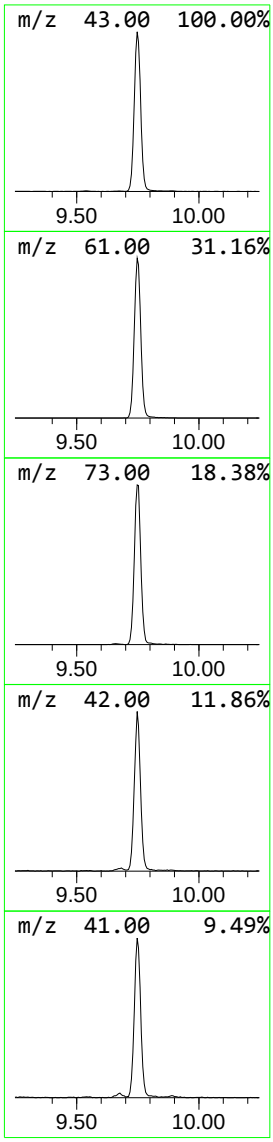
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	146.51 ug/l	4741640	1,4-Difluorobenzene	9.112

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	38
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





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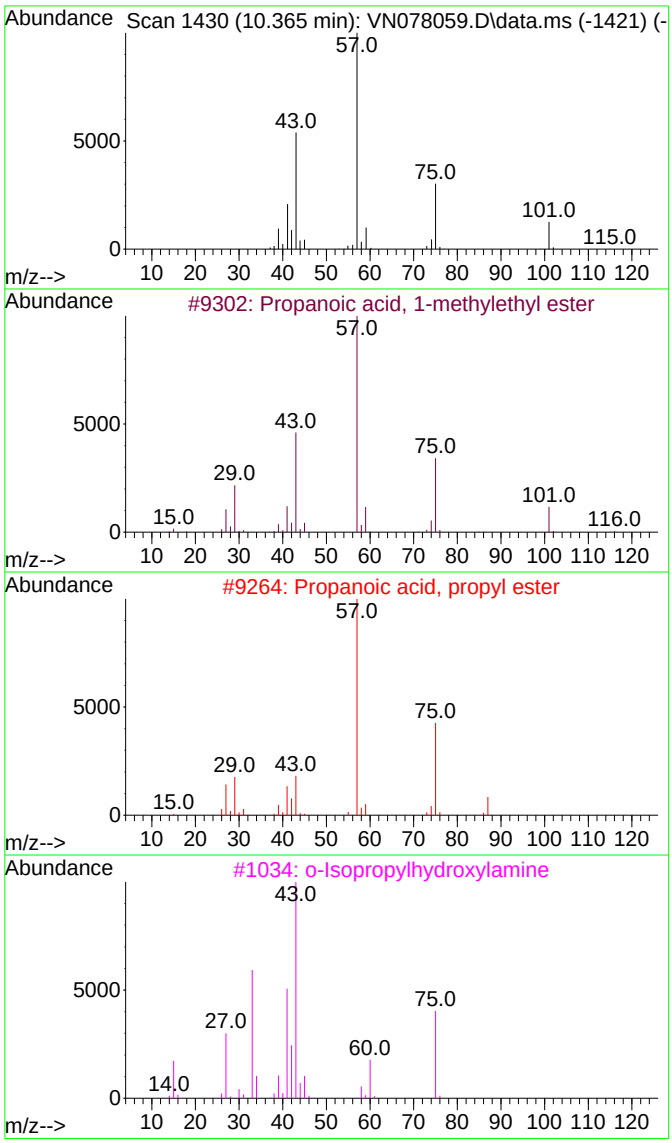
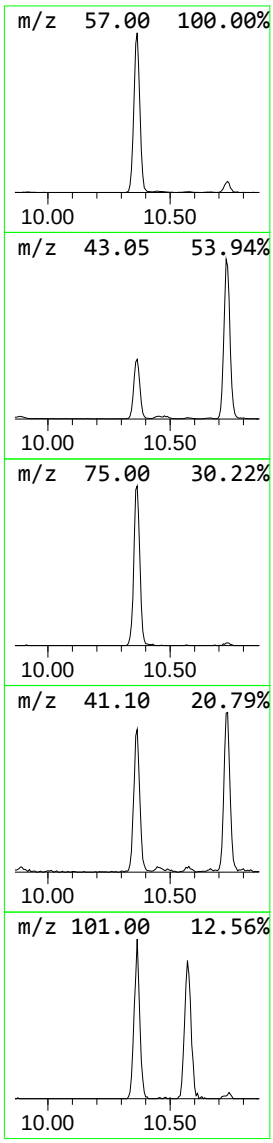
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	31.86 ug/l	1031260	1,4-Difluorobenzene	9.112

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	53
3	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	38
4	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	33
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9





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Quant Title : SW846 8260

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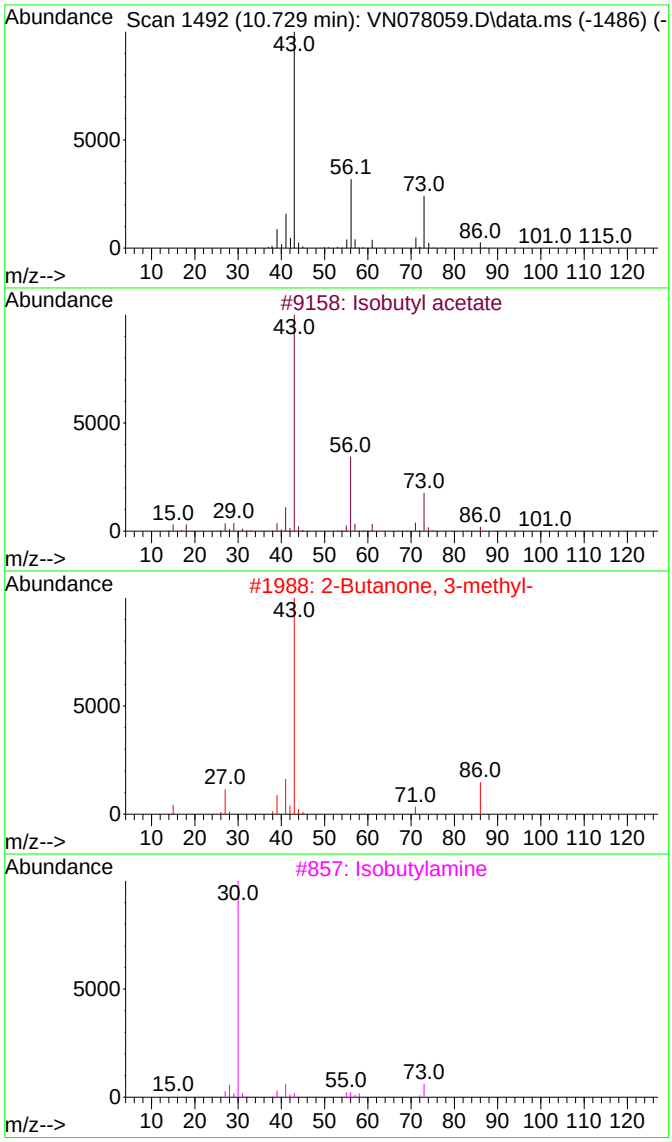
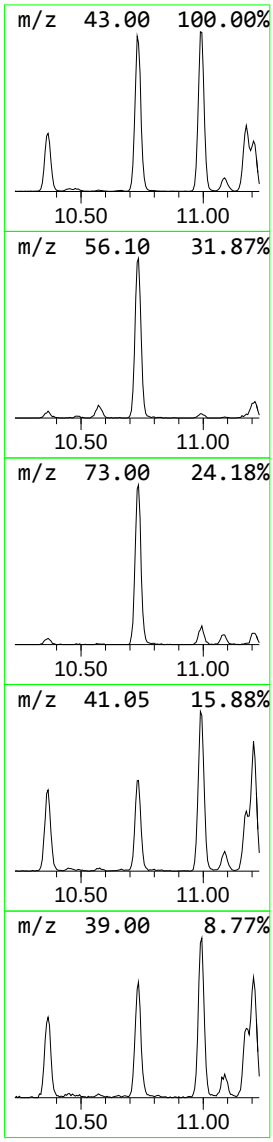
****
Peak Number 4 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.729	29.84 ug/l	1186050	Chlorobenzene-d5	11.871

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	Isobutylamine	73	C4H11N	000078-81-9	9
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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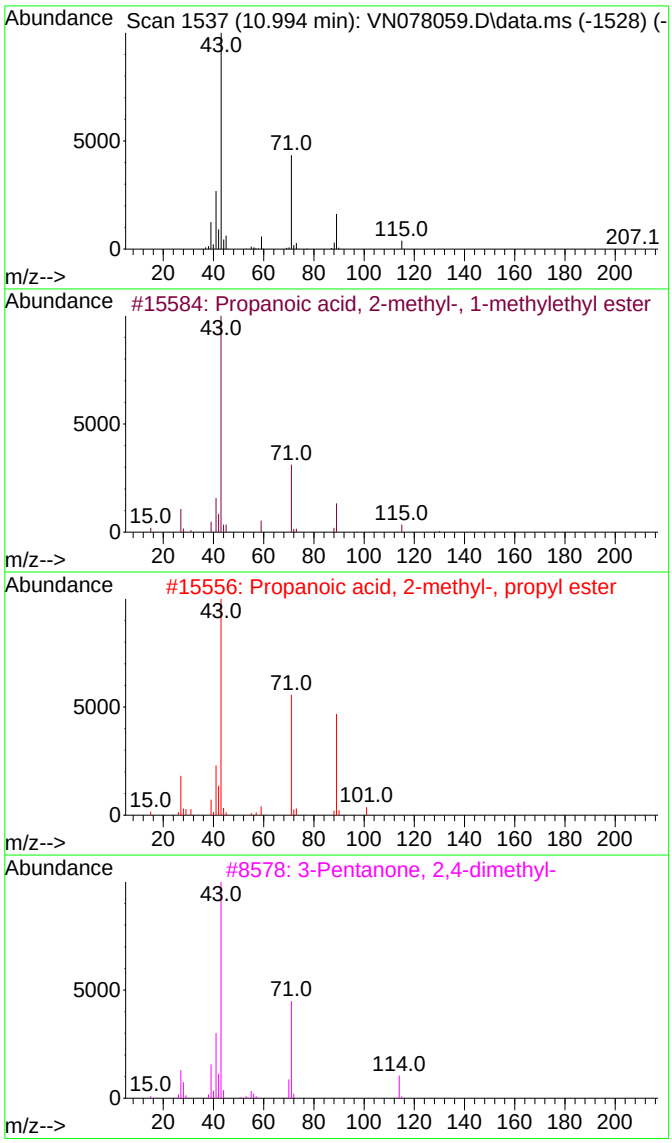
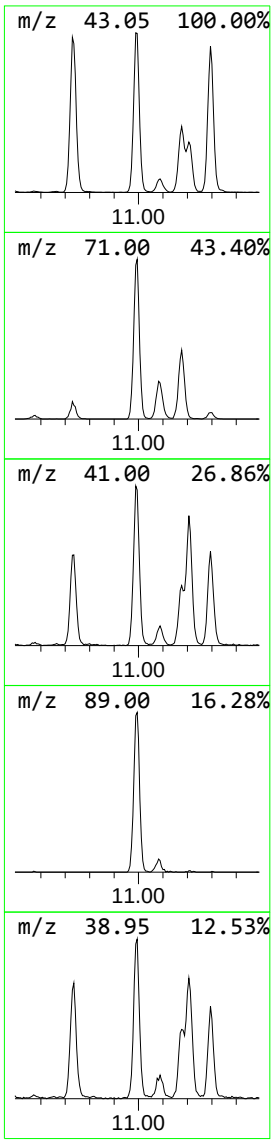
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	33.85 ug/l	1345660	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	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	53
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	45
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42





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TIC Library : C:\Database\NIST20.L
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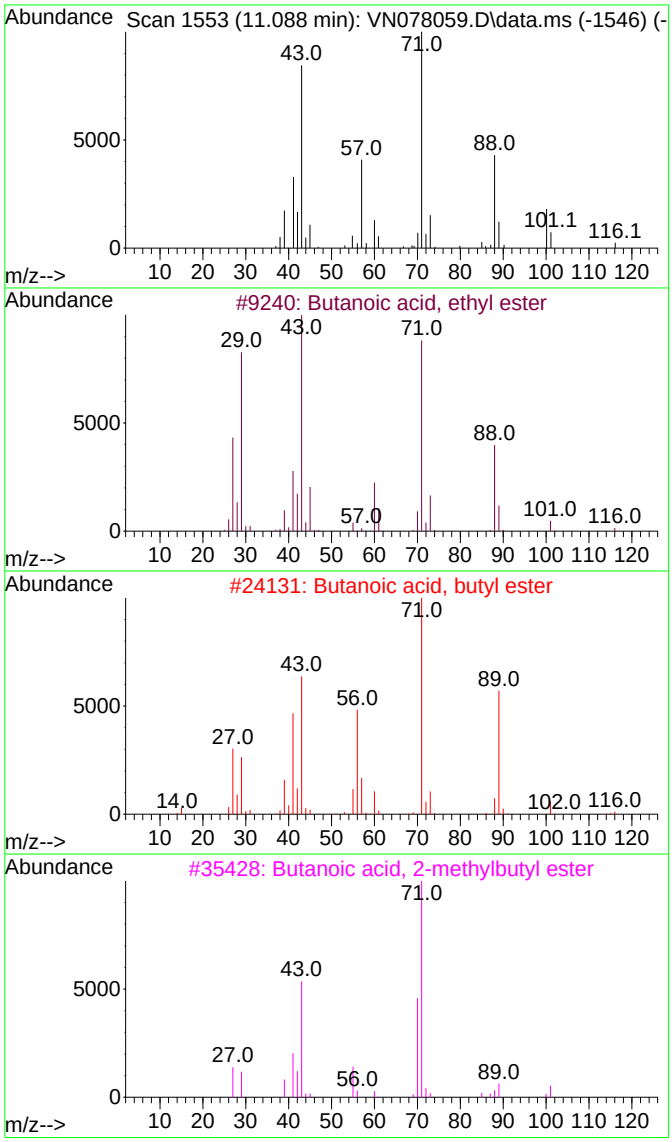
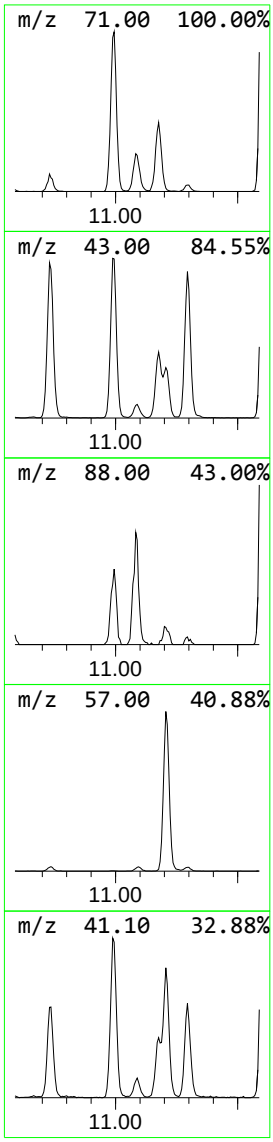
****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	7.04 ug/l	280010	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
2	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50
3	Butanoic acid, 2-methylbutyl ester	158	C9H18O2	051115-64-1	47
4	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	43
5	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	43





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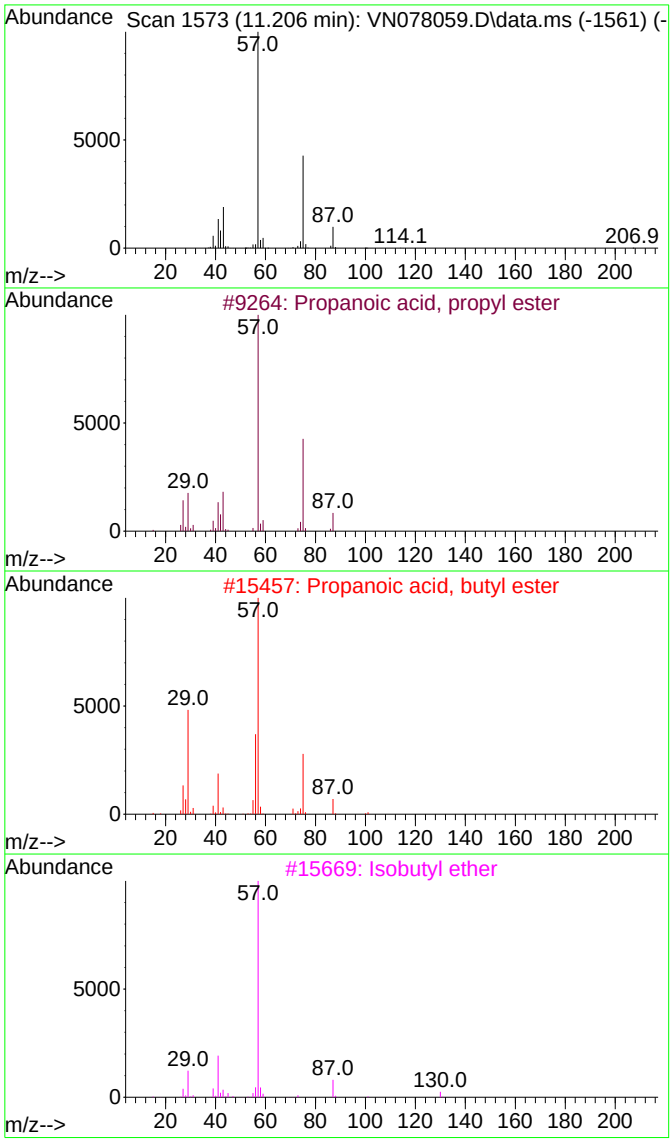
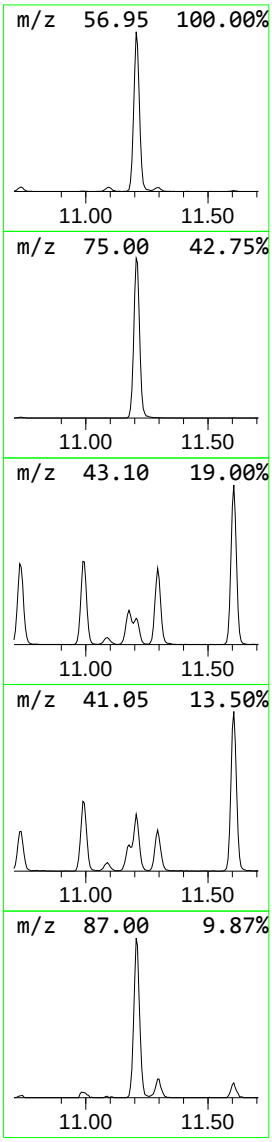
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	63.00 ug/l	2504360	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	28
3	Isobutyl ether	130	C8H18O	000628-55-7	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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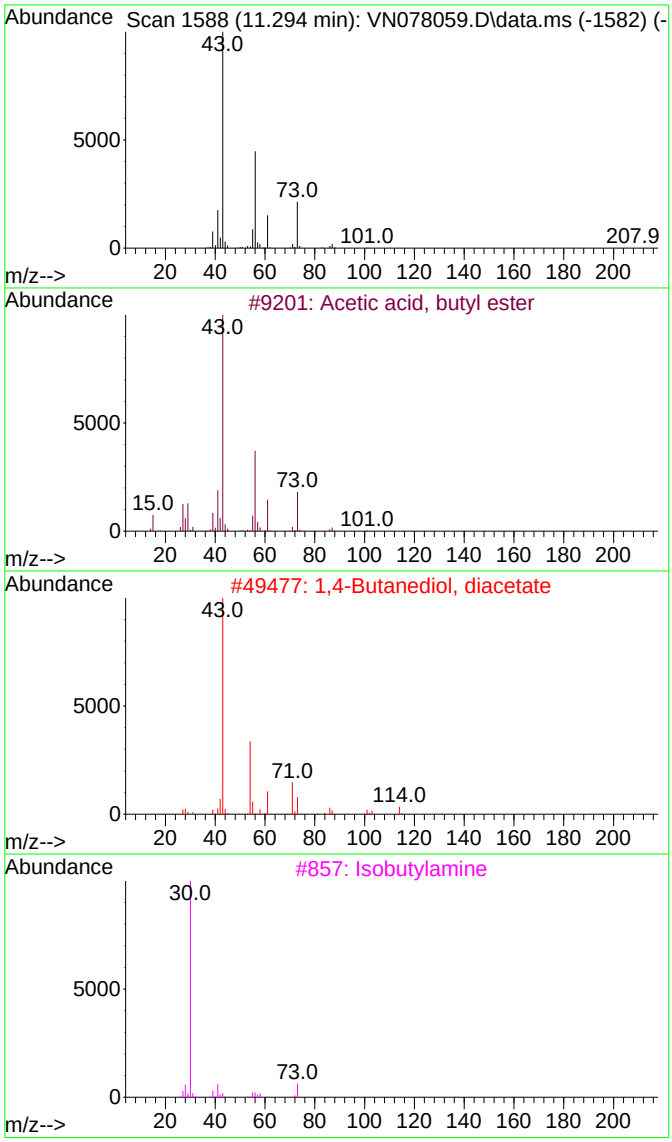
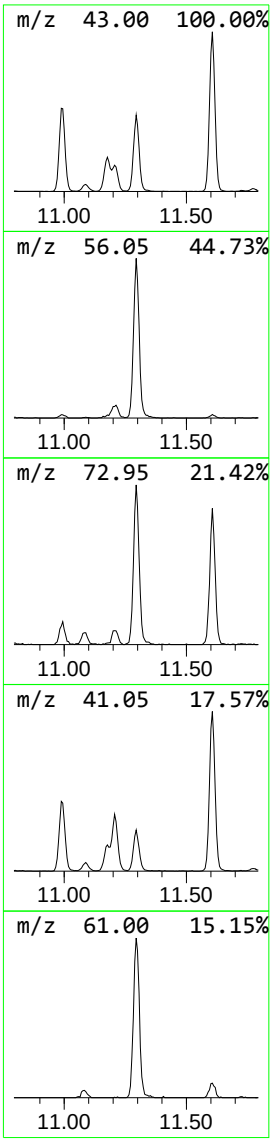
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	30.47 ug/l	1211080	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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TIC Library : C:\Database\NIST20.L
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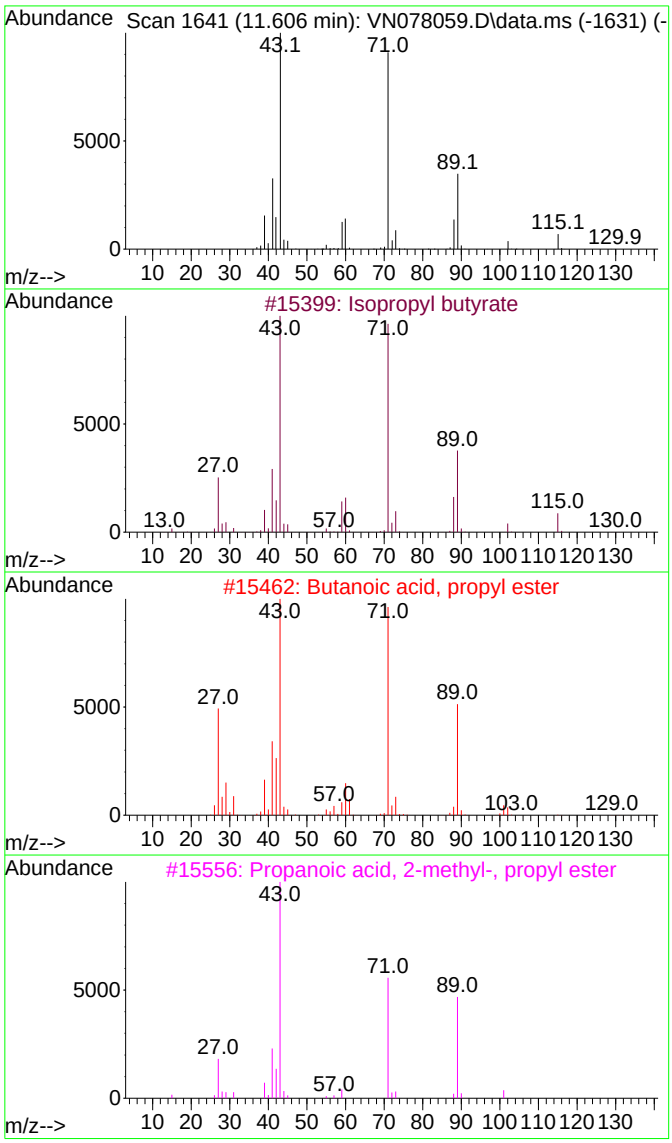
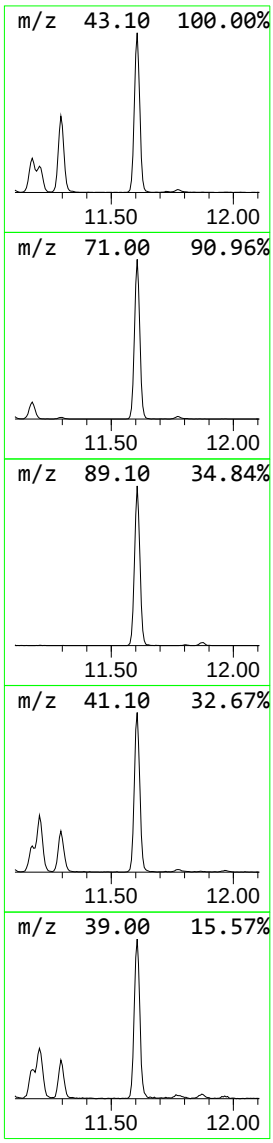
****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	92.12 ug/l	3662030	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64





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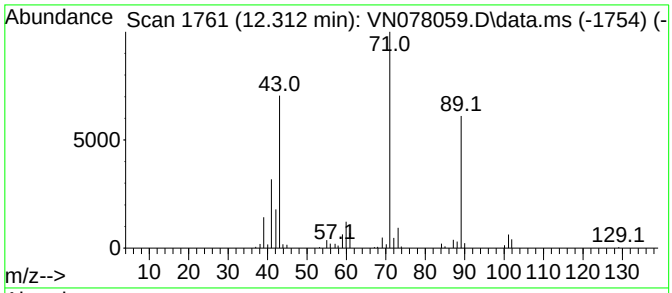
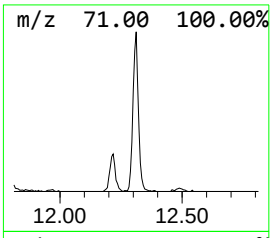
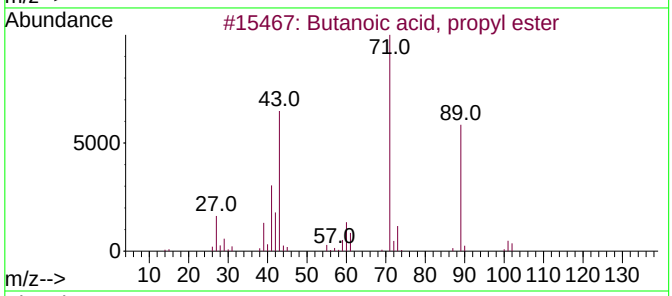
****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 10

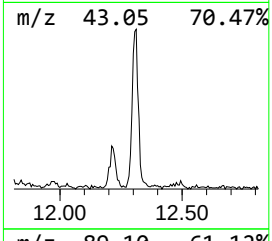
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.312	6.39 ug/l	253876	Chlorobenzene-d5	11.871

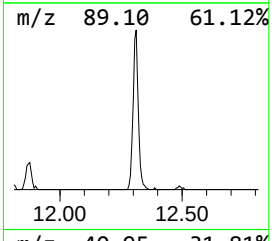
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50
5	Isopropyl butyrate	130	C7H14O2	000638-11-9	45

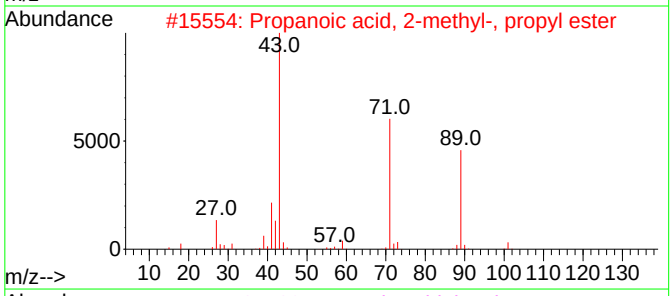


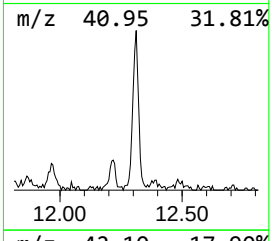


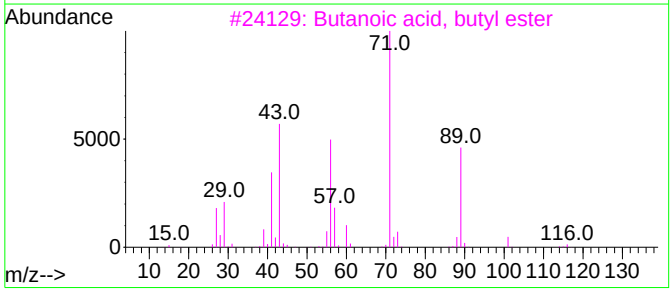


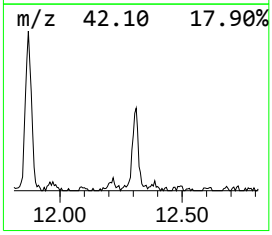












Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078059.D
Acq On : 05 Jun 2023 21:08
Operator : JC\MD
Sample : 03029-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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	9.677	8.5	ug/l	275676	2	9.112	1618250	50.0
n-Propyl acetate	9.747	146.5	ug/l	4741640	2	9.112	1618250	50.0
Propanoic acid,...	10.365	31.9	ug/l	1031260	2	9.112	1618250	50.0
Isobutyl acetate	10.729	29.8	ug/l	1186050	3	11.871	1987550	50.0
Propanoic acid,...	10.994	33.9	ug/l	1345660	3	11.871	1987550	50.0
Butanoic acid, ...	11.088	7.0	ug/l	280010	3	11.871	1987550	50.0
Propanoic acid,...	11.206	63.0	ug/l	2504360	3	11.871	1987550	50.0
Acetic acid, bu...	11.294	30.5	ug/l	1211080	3	11.871	1987550	50.0
Isopropyl butyrate	11.606	92.1	ug/l	3662030	3	11.871	1987550	50.0
Butanoic acid, ...	12.312	6.4	ug/l	253876	3	11.871	1987550	50.0