LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078029.D
Acq On : 02 Jun 2023 14:09
Operator : JC\MD
Sample : 03008-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-19-0A

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: VN078029.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	142	148	158	rVB4	30059	67397	1.29%	0.211%
2	4.448	414	424	436	rBV2	18237	57214	1.09%	0.179%
3	5.289	555	567	580	rBV	39951	116059	2.22%	0.363%
4	7.571	948	955	966	rVB2	48076	116010	2.21%	0.363%
5	8.177	1046	1058	1062	rBV	312503	720561	13.76%	2.254%
6	8.236	1062	1068	1082	rVB	501977	1160121	22.15%	3.629%
7	8.588	1117	1128	1135	rBV2	314137	719606	13.74%	2.251%
8	8.700	1135	1147	1154	rBV	400197	1236351	23.60%	3.868%
9	8.800	1159	1164	1182	rVB2	226481	743898	14.20%	2.327%
10	9.112	1206	1217	1232	rVB	773246	1632360	31.16%	5.107%
11	9.677	1305	1313	1318	rBV	134214	295822	5.65%	0.925%
12	9.747	1318	1325	1342	rVV	2813476	5238226	100.00%	16.387%
13	10.365	1421	1430	1440	rBV	658122	1124915	21.48%	3.519%
14	10.577	1457	1466	1478	rBV	1206597	2271100	43.36%	7.105%
15	10.735	1486	1493	1503	rVB	820050	1367824	26.11%	4.279%
16	10.994	1529	1537	1546	rBV	895113	1502146	28.68%	4.699%
17	11.088	1546	1553	1561	rVV3	166408	318602	6.08%	0.997%
18	11.212	1561	1574	1582	rVV2	1288459	2727989	52.08%	8.534%
19	11.294	1582	1588	1600	rVB	836324	1391346	26.56%	4.353%
20	11.606	1634	1641	1651	rBV	2537654	4064082	77.59%	12.714%
21	11.777	1664	1670	1679	rVB2	38105	71539	1.37%	0.224%
22	11.871	1679	1686	1697	rVV	1086190	1949024	37.21%	6.097%
23	11.965	1697	1702	1709	rVB	33446	54875	1.05%	0.172%
24	12.312	1754	1761	1769	rBV	190368	320234	6.11%	1.002%
25	12.859	1846	1854	1864	rBV	812024	1417467	27.06%	4.434%
26	13.800	2005	2014	2022	rBV	741526	1281411	24.46%	4.009%

Sum of corrected areas: 31966179

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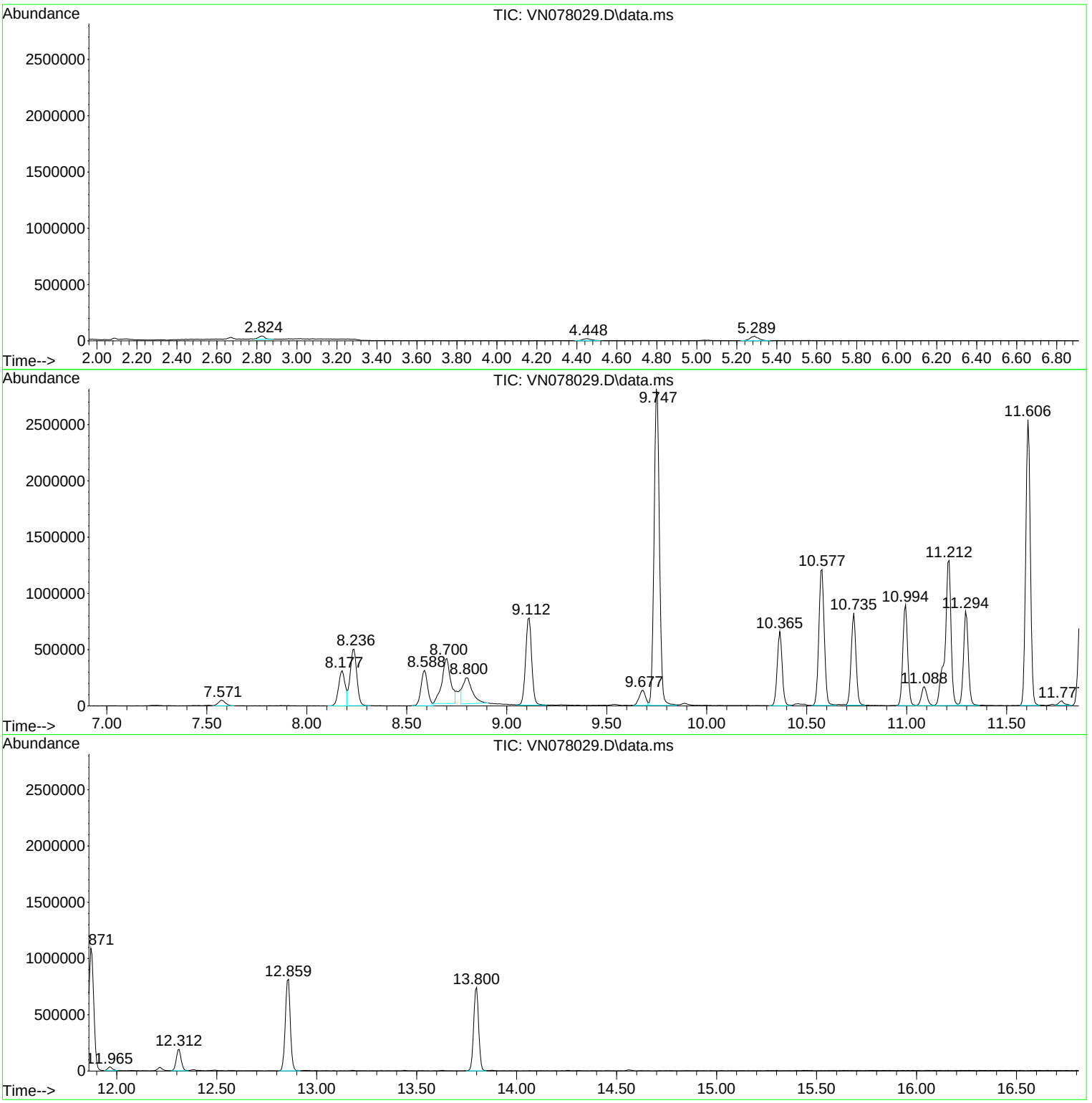
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



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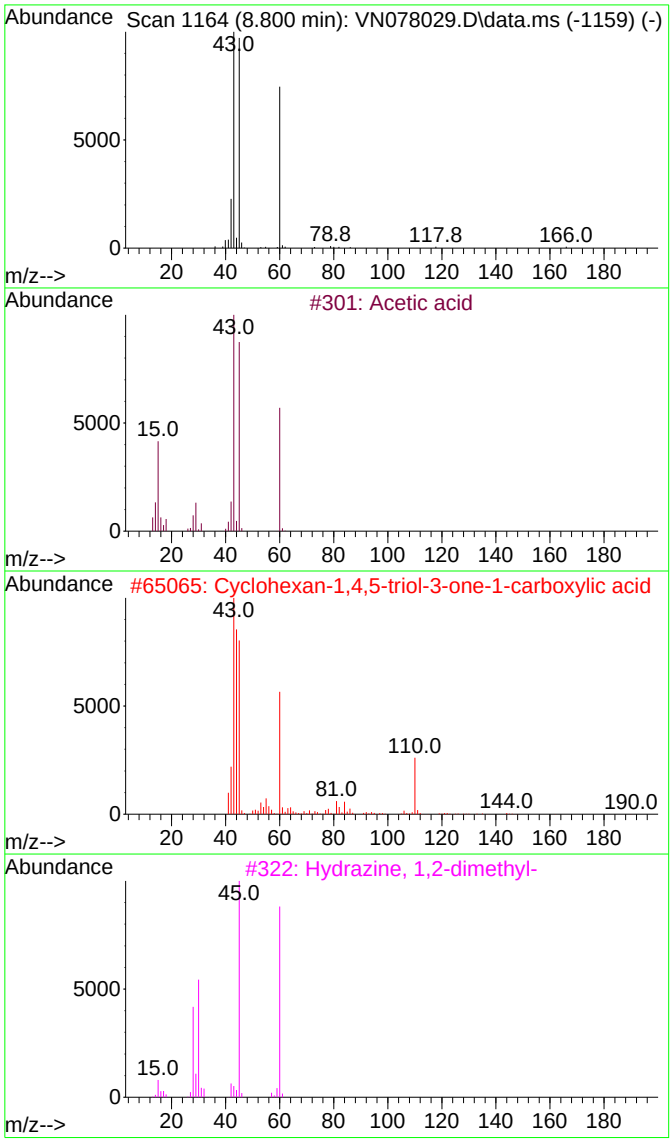
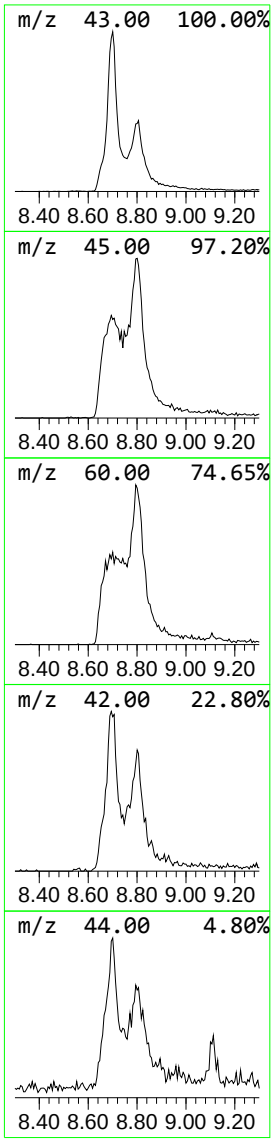
****

Peak Number 1 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.800	22.79 ug/l	743898	1,4-Difluorobenzene	9.112

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	86
2	Cyclohexan-1,4,5-triol-3-one-1-c...	190	C7H10O6	1000128-45-5	64
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	64
4	Thiirane	60	C2H4S	000420-12-2	38
5	Butanoic acid, 3-hydroxy-	104	C4H8O3	000300-85-6	9





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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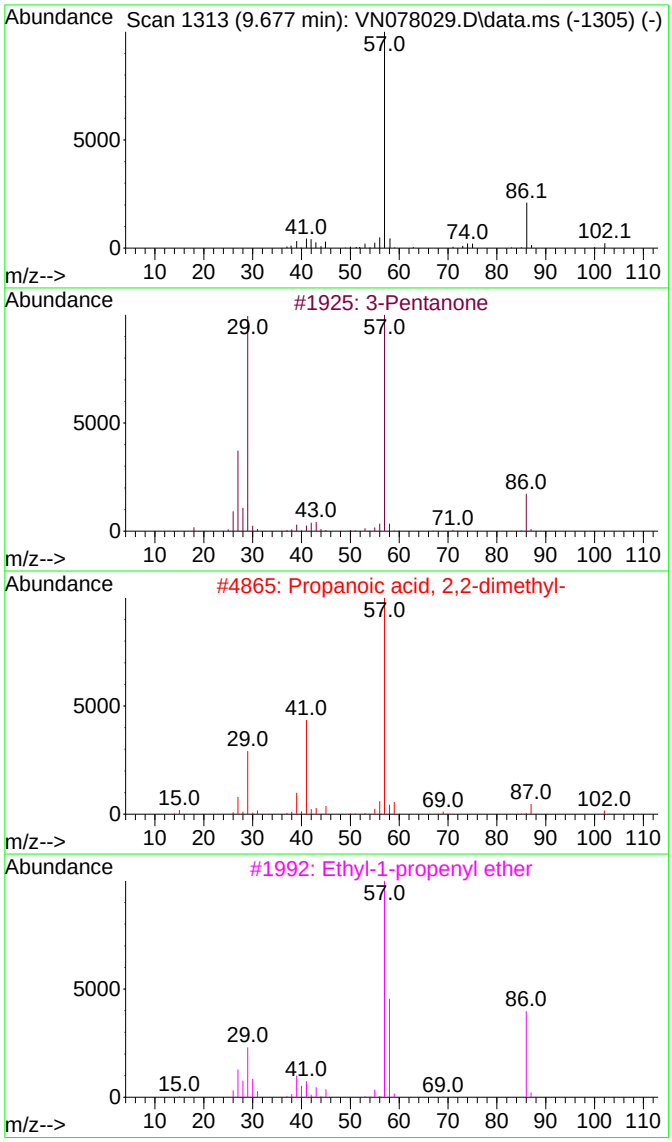
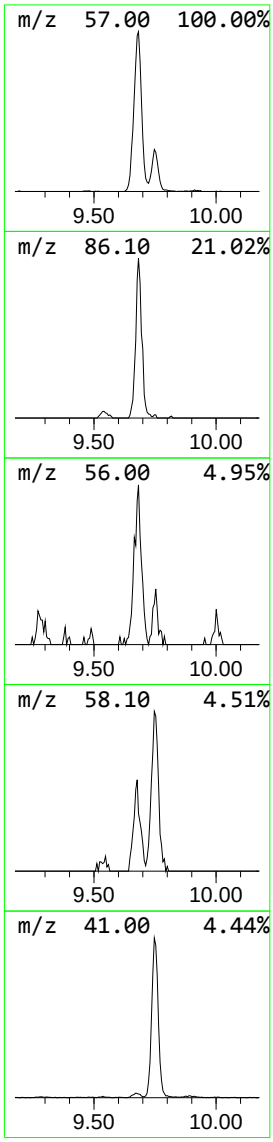
****
Peak Number 2 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	9.06 ug/l	295822	1,4-Difluorobenzene	9.112

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	38
3	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	35
4	1-Hydroxy-2-butanone	88	C4H8O2	005077-67-8	23
5	Isobutyl ether	130	C8H18O	000628-55-7	9





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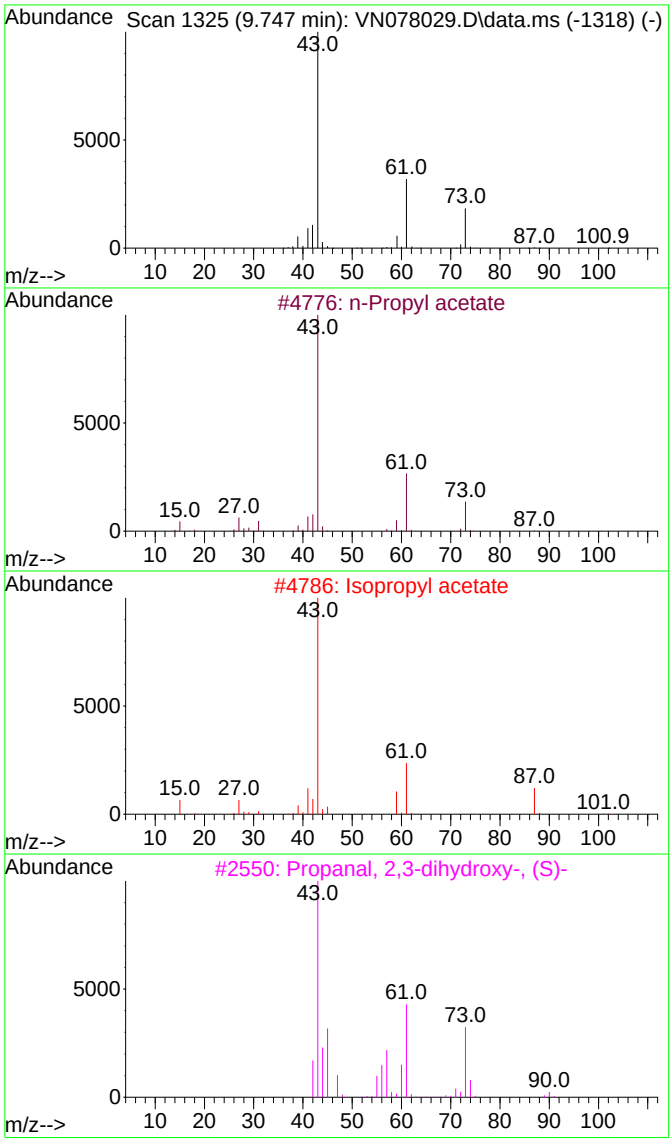
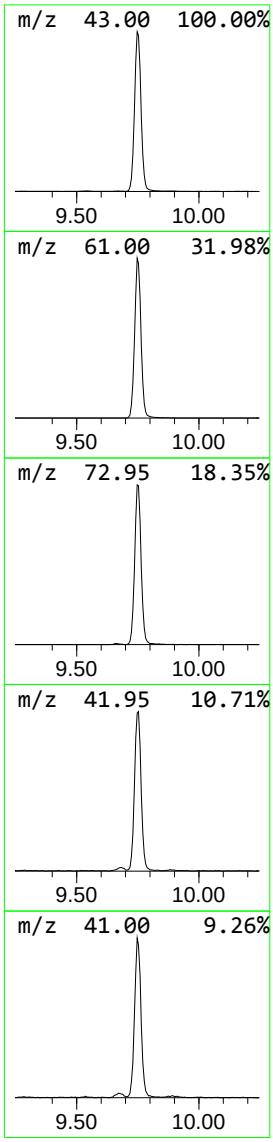
****

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	160.45 ug/l	5238230	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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





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

TIC Library : C:\Database\NIST20.L
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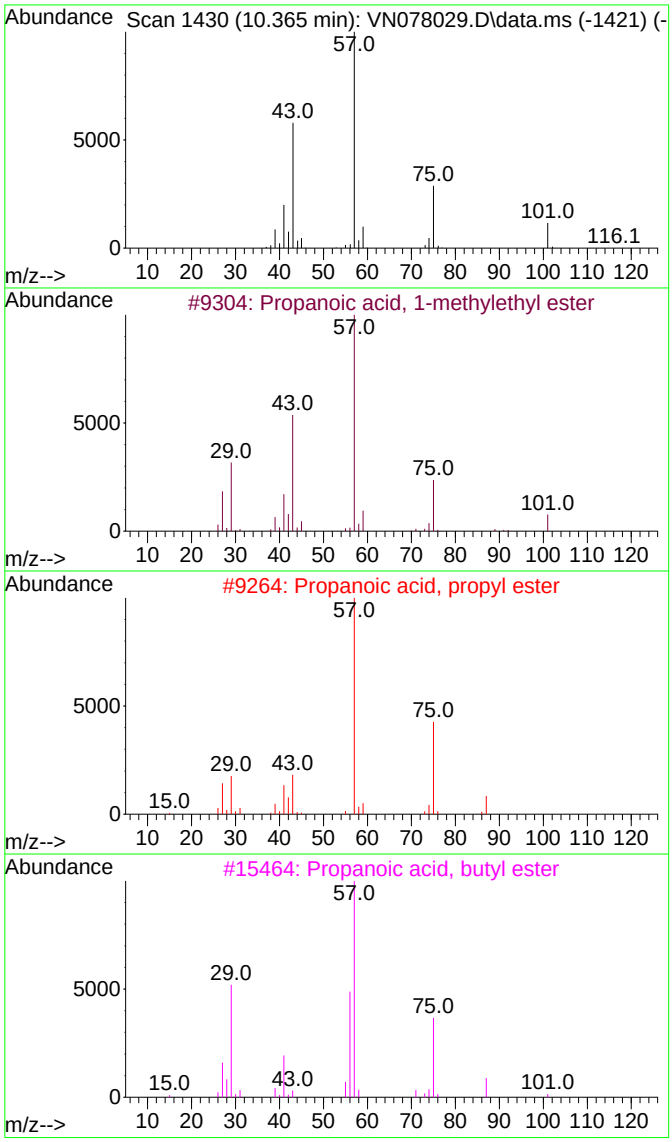
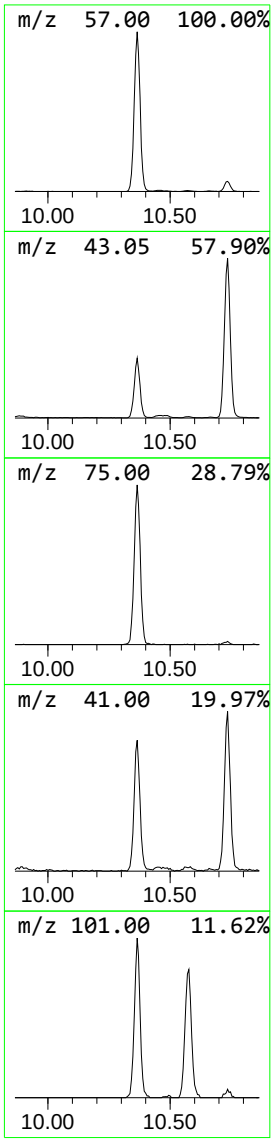
****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	34.46 ug/l	1124920	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	86
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	33
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	17
5	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9





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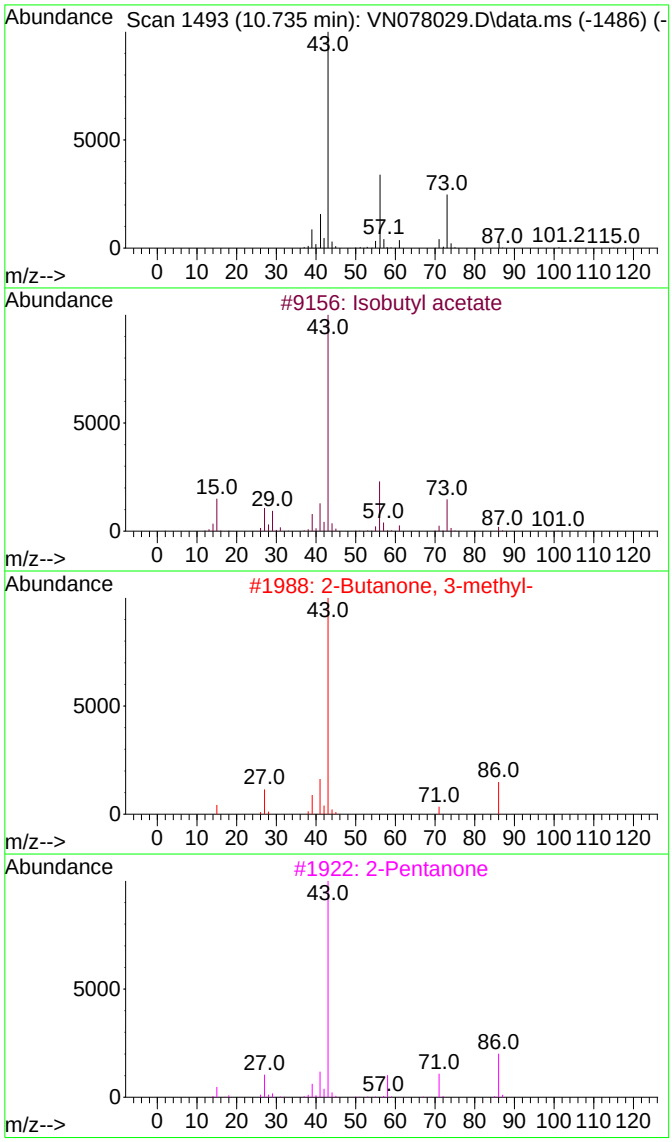
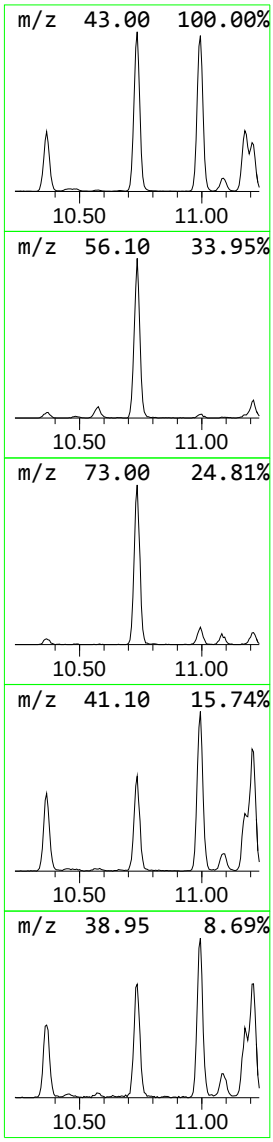
****

Peak Number 5 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	35.09 ug/l	1367820	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	2-Pentanone	86	C5H10O	000107-87-9	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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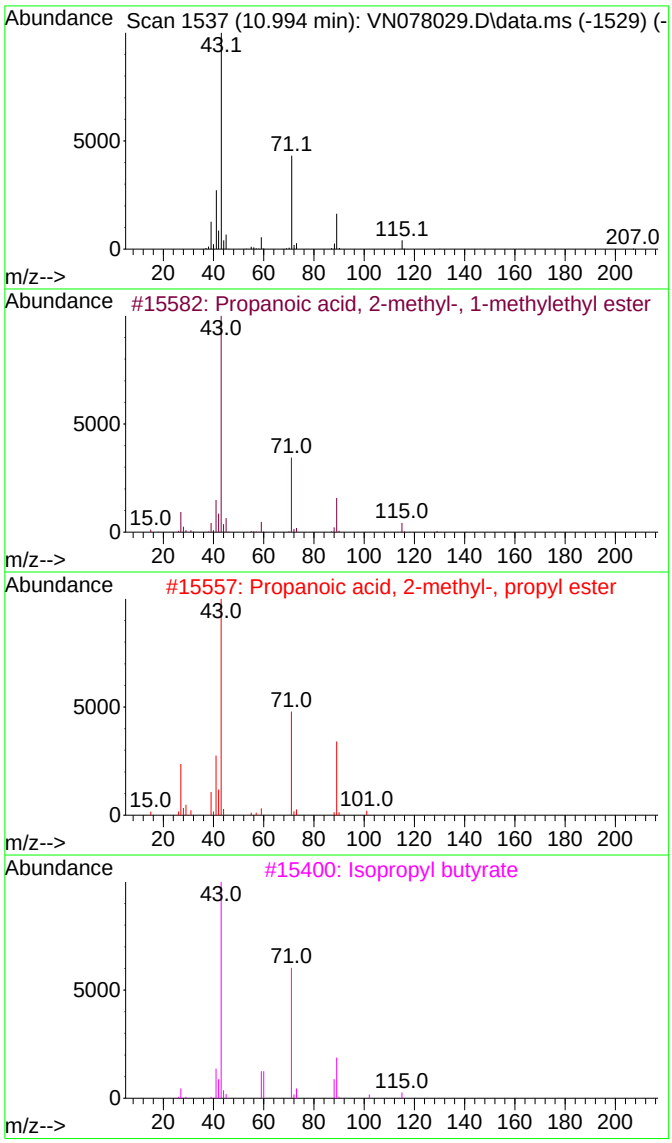
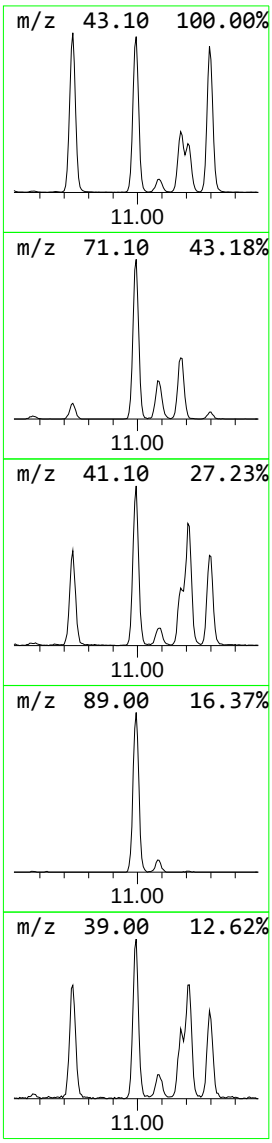
****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	38.54 ug/l	1502150	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	64
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	53
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	53





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Quant Title : SW846 8260

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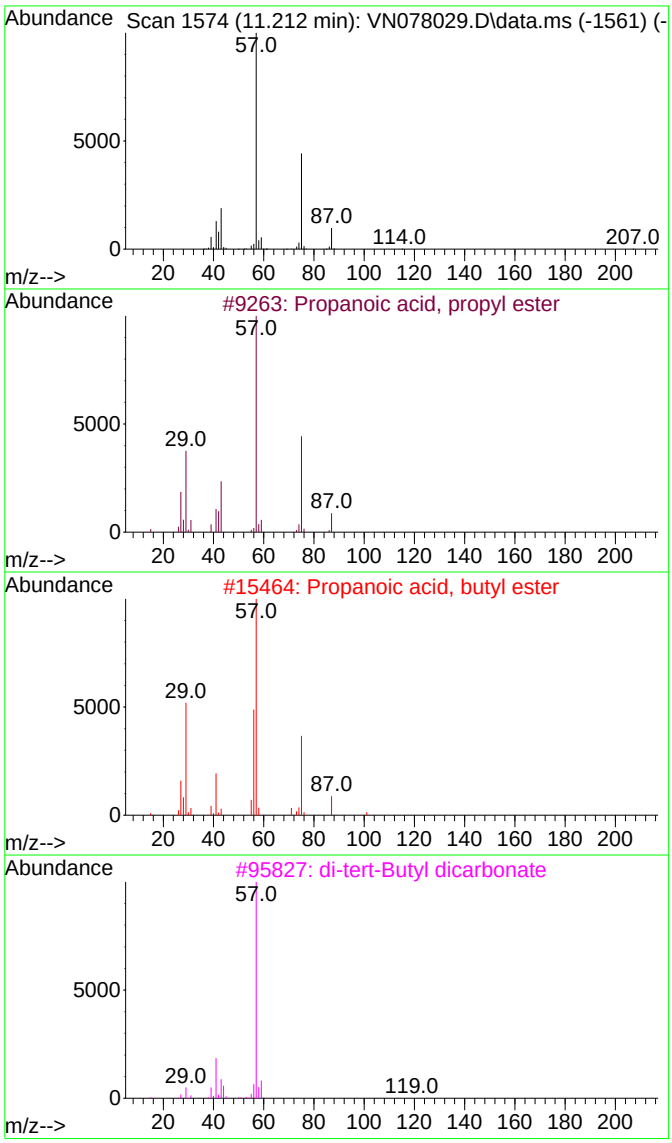
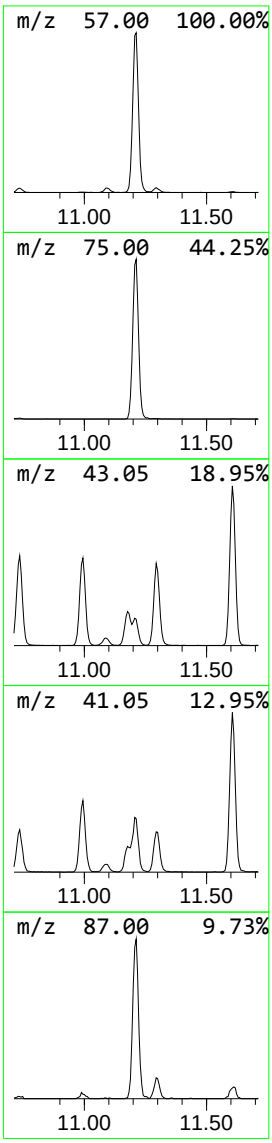
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.212	69.98 ug/l	2727990	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	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	10
4	Sulfone, 2-hydroxypropyl t-butyl	180	C7H16O3S	154619-05-3	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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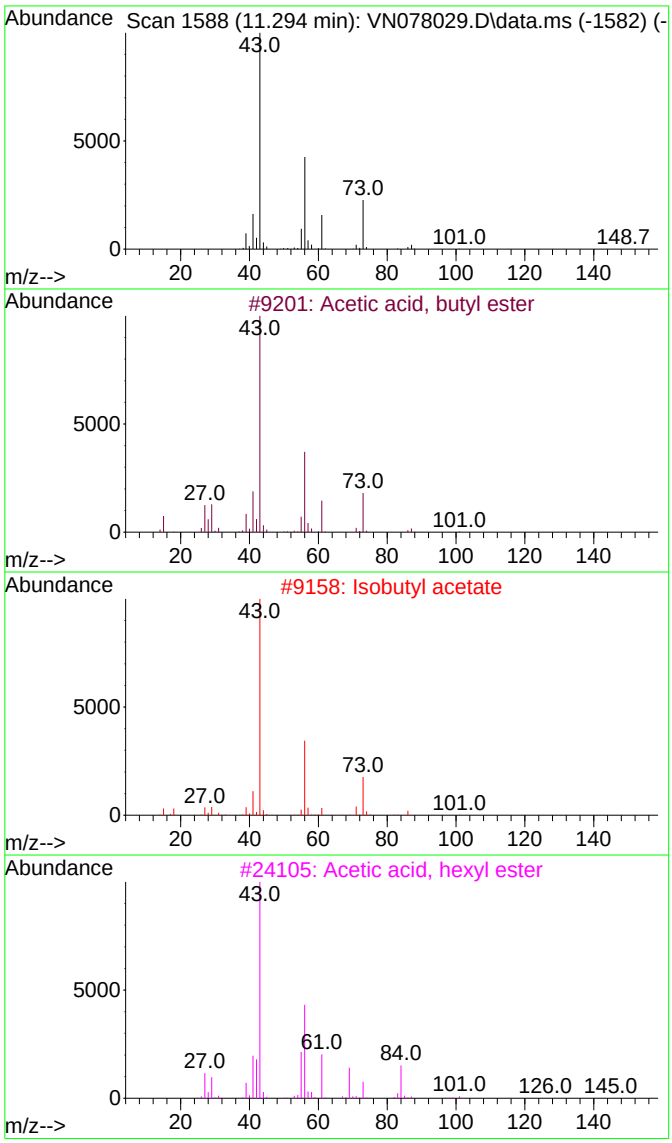
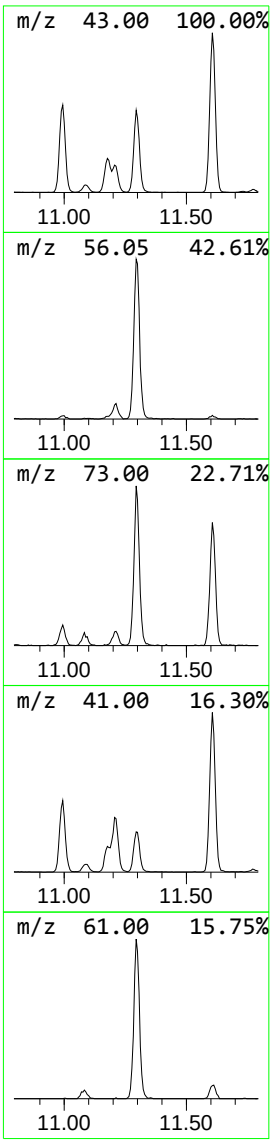
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	35.69 ug/l	1391350	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	Isobutyl acetate	116	C6H12O2	000110-19-0	39
3	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	10
5	Isobutylamine	73	C4H11N	000078-81-9	9





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Quant Title : SW846 8260

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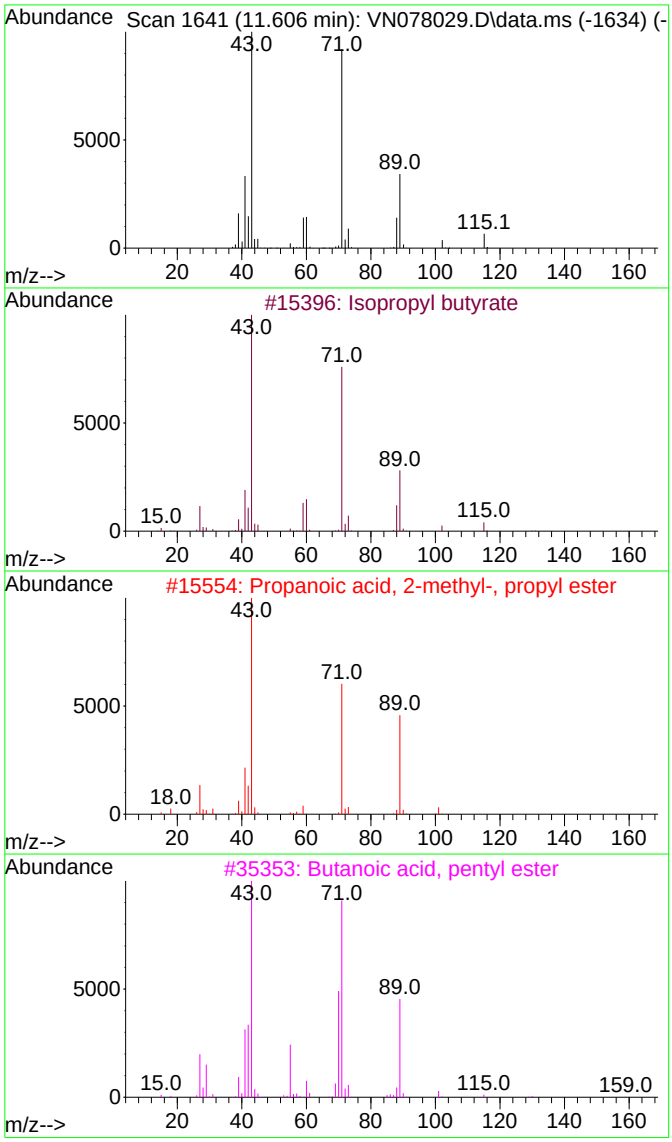
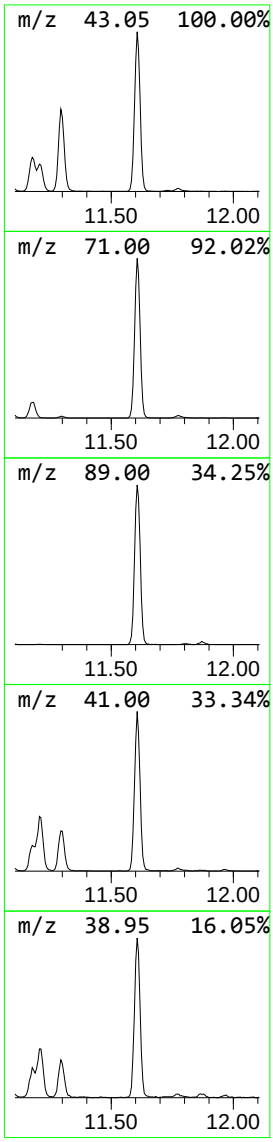
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	104.26 ug/l	4064080	Chlorobenzene-d5	11.871

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	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64





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TIC Integration Parameters: LSCINT.P

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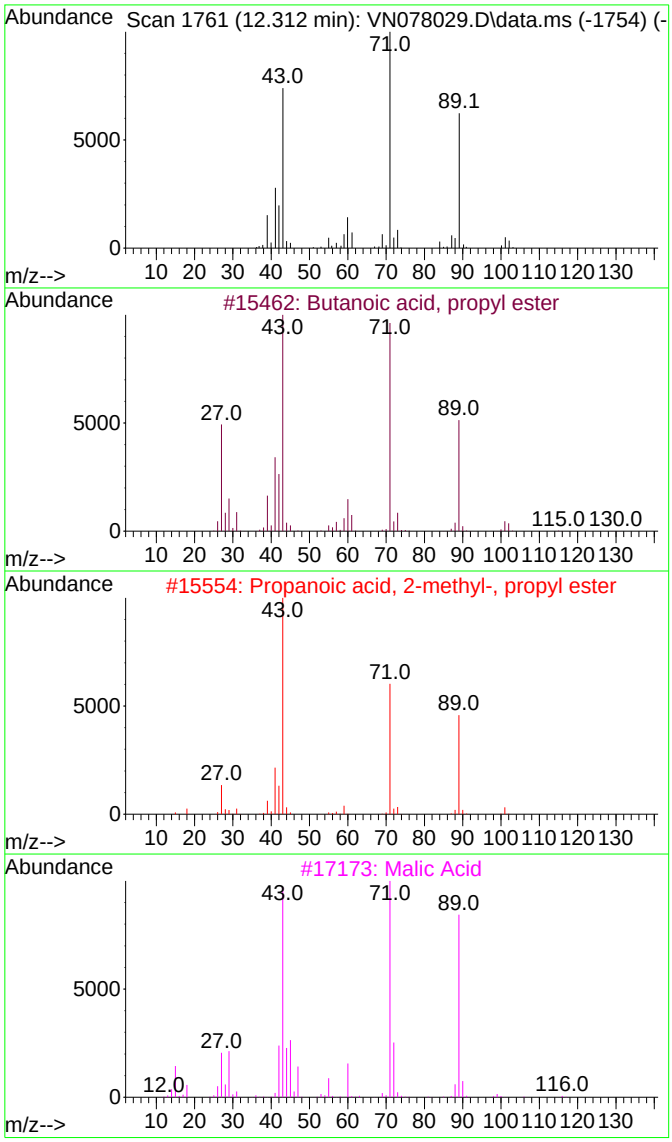
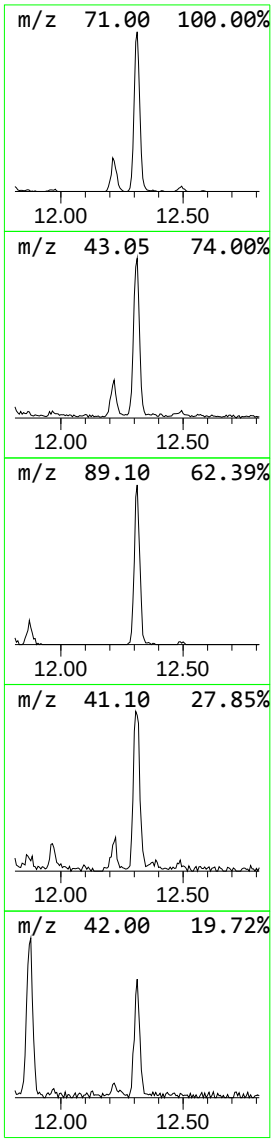
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.312	8.22 ug/l	320234	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	80
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Malic Acid	134	C4H6O5	006915-15-7	72
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	50
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078029.D
Acq On : 02 Jun 2023 14:09
Operator : JC\MD
Sample : 03008-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-19-0A

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
Acetic acid	8.800	22.8	ug/l	743898	2	9.112	1632360	50.0
3-Pentanone	9.677	9.1	ug/l	295822	2	9.112	1632360	50.0
n-Propyl acetate	9.747	160.4	ug/l	5238230	2	9.112	1632360	50.0
Propanoic acid,...	10.365	34.5	ug/l	1124920	2	9.112	1632360	50.0
Isobutyl acetate	10.735	35.1	ug/l	1367820	3	11.871	1949020	50.0
Propanoic acid,...	10.994	38.5	ug/l	1502150	3	11.871	1949020	50.0
Propanoic acid,...	11.212	70.0	ug/l	2727990	3	11.871	1949020	50.0
Acetic acid, bu...	11.294	35.7	ug/l	1391350	3	11.871	1949020	50.0
Isopropyl butyrate	11.606	104.3	ug/l	4064080	3	11.871	1949020	50.0
Butanoic acid, ...	12.312	8.2	ug/l	320234	3	11.871	1949020	50.0