LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078287.D
Acq On : 19 Jun 2023 18:38
Operator : JC\MD
Sample : 03320-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-19

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\82N060623W.M
Title : SW846 8260

Signal : TIC: VN078287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.818	140	147	153	rBV2	19677	46150	1.00%	0.148%
2	5.283	556	566	577	rBV4	21303	66847	1.45%	0.215%
3	7.577	948	956	969	rVB3	41417	106751	2.32%	0.343%
4	8.177	1047	1058	1063	rBV2	406636	1020427	22.17%	3.280%
5	8.235	1063	1068	1083	rVB	652898	1401535	30.45%	4.504%
6	8.588	1113	1128	1139	rBV	403786	919075	19.97%	2.954%
7	8.700	1139	1147	1157	rBV	288605	675849	14.68%	2.172%
8	9.112	1206	1217	1232	rBV	953227	2016337	43.81%	6.480%
9	9.677	1304	1313	1319	rBV2	138605	304682	6.62%	0.979%
10	9.753	1319	1326	1345	rVV	2454258	4602524	100.00%	14.792%
11	10.365	1421	1430	1439	rBV	617717	1087458	23.63%	3.495%
12	10.576	1456	1466	1477	rBV	1413853	2668468	57.98%	8.576%
13	10.735	1486	1493	1504	rVB	654718	1141836	24.81%	3.670%
14	10.994	1528	1537	1546	rBV	884292	1463898	31.81%	4.705%
15	11.088	1546	1553	1561	rVV3	156942	296072	6.43%	0.952%
16	11.212	1569	1574	1582	rVB	1152324	2007615	43.62%	6.452%
17	11.294	1582	1588	1598	rVB	669677	1120529	24.35%	3.601%
18	11.606	1634	1641	1654	rBV	2441644	3949721	85.82%	12.694%
19	11.776	1665	1670	1678	rVB3	38755	73667	1.60%	0.237%
20	11.871	1678	1686	1697	rVV	1344339	2456806	53.38%	7.896%
21	11.965	1697	1702	1711	rVB2	32129	58718	1.28%	0.189%
22	12.218	1739	1745	1754	rVB2	27419	50368	1.09%	0.162%
23	12.312	1754	1761	1769	rBV	173733	286785	6.23%	0.922%
24	12.853	1844	1853	1864	rBV	955993	1688180	36.68%	5.426%
25	13.800	2007	2014	2023	rVB	942055	1604925	34.87%	5.158%

Sum of corrected areas: 31115223

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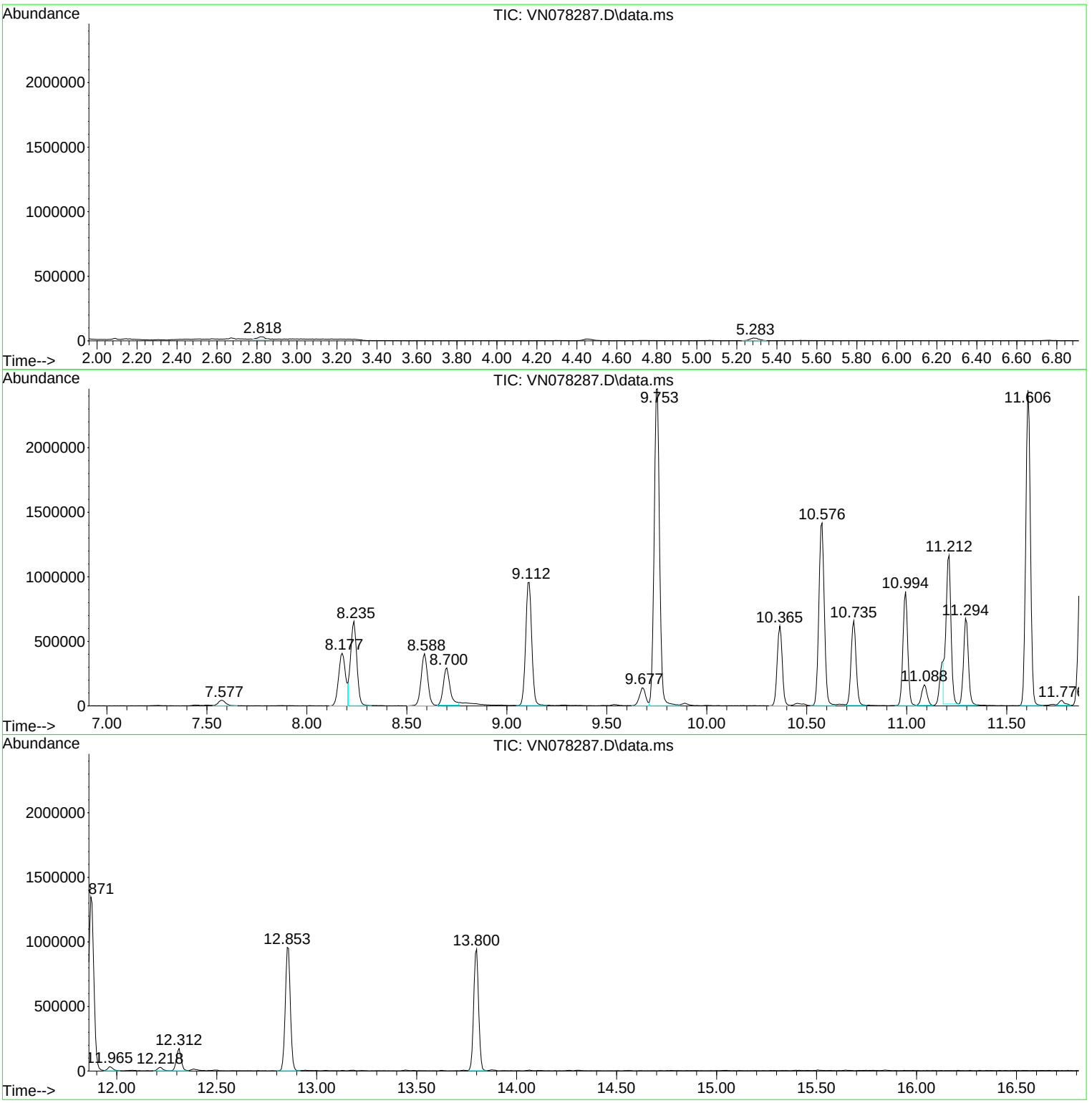
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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



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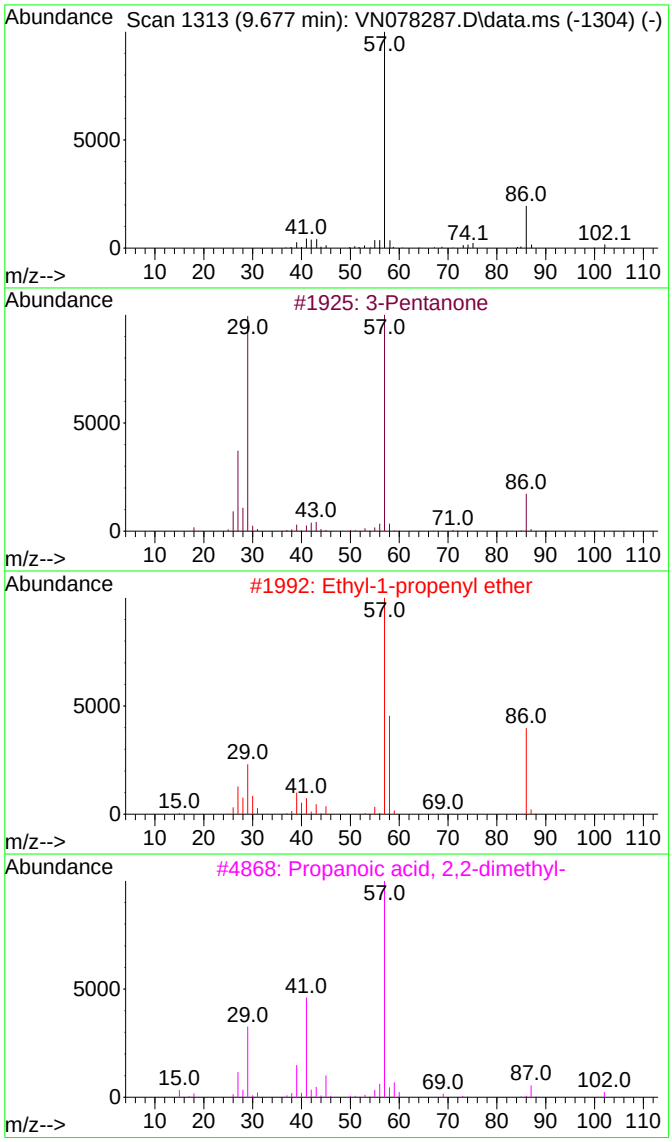
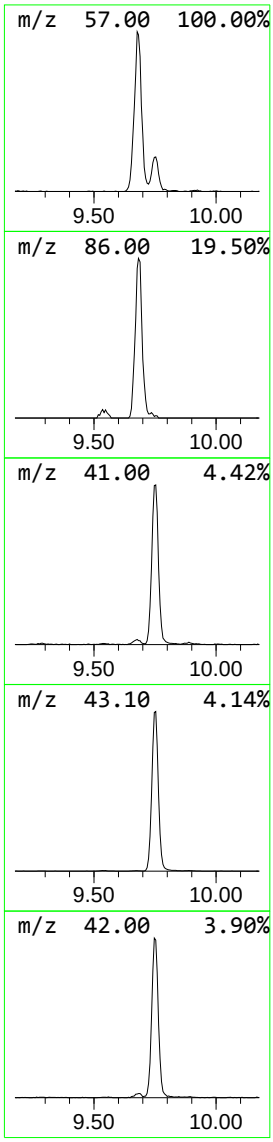
****

Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	7.56 ug/l	304682	1,4-Difluorobenzene	9.112

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	9
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	9





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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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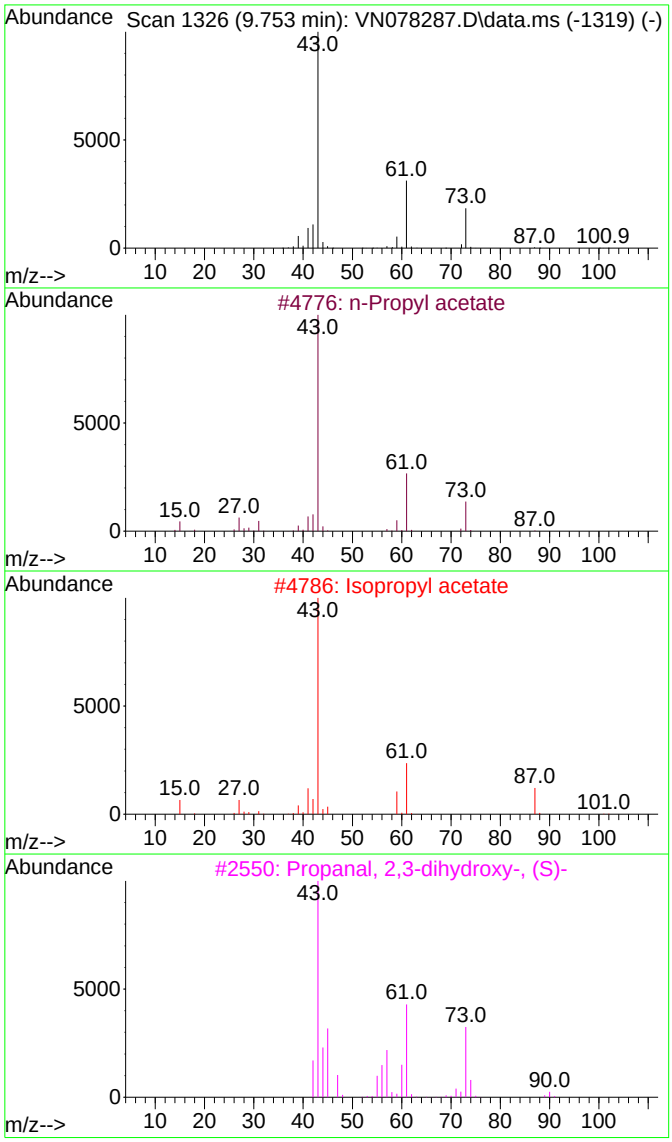
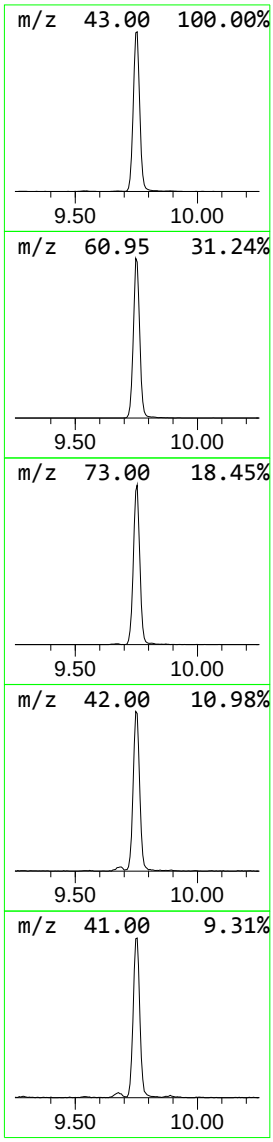
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.753	114.13 ug/l	4602520	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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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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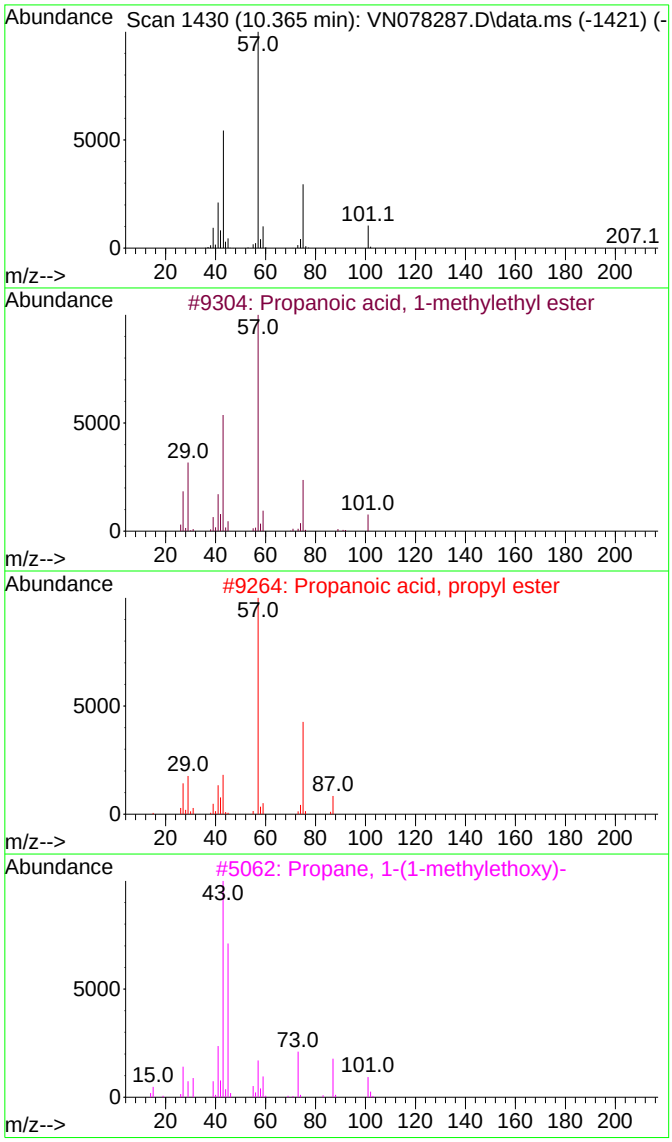
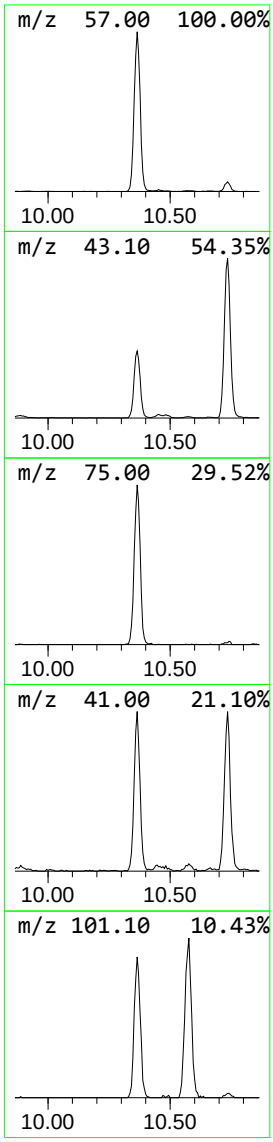
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	26.97 ug/l	1087460	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	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	Diethyl 2-(N-(tert-butoxycarbony...	275	C12H21NO6	102831-44-7	25
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	12





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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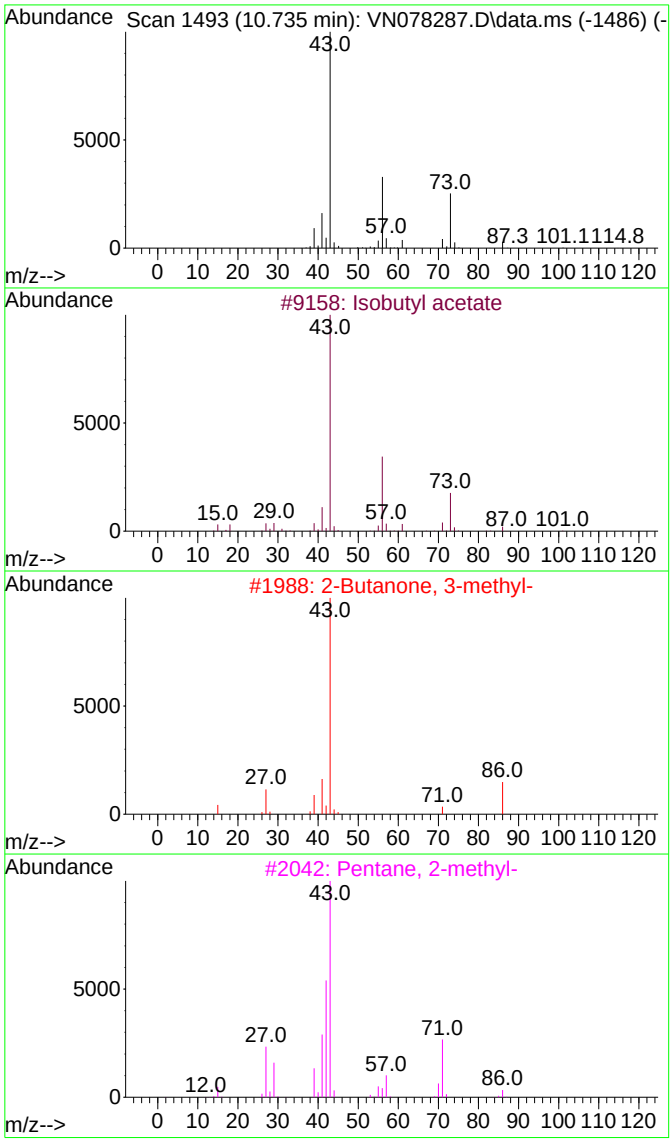
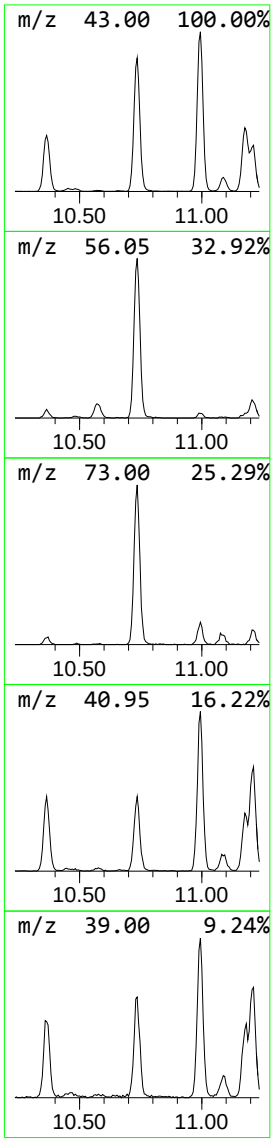
****
Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	23.24 ug/l	1141840	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	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





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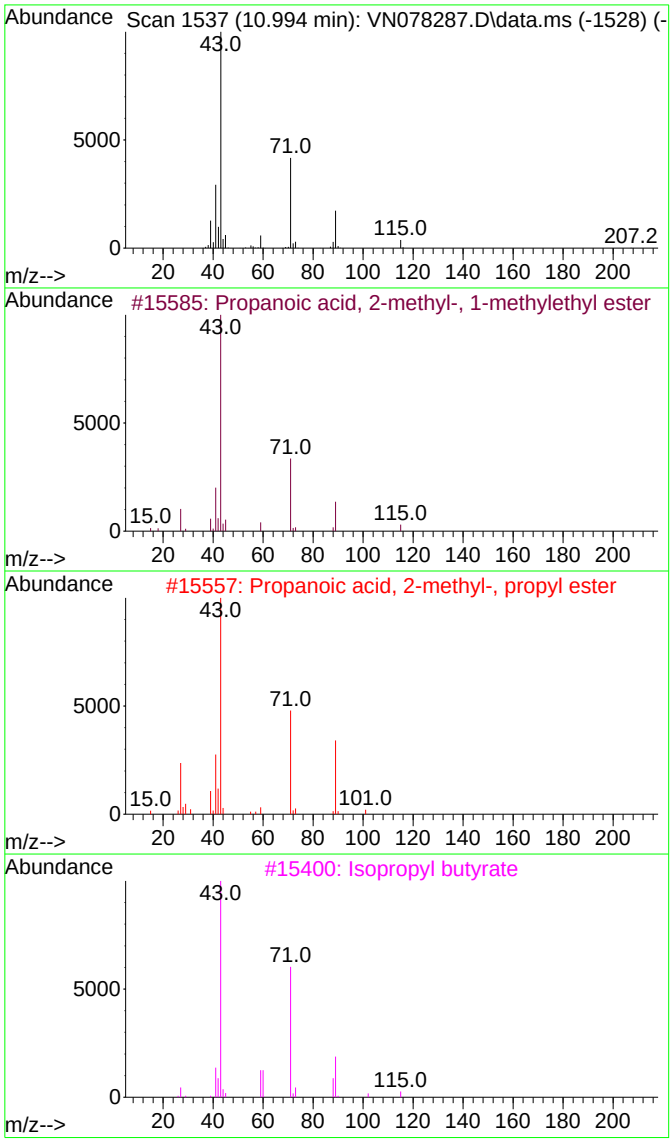
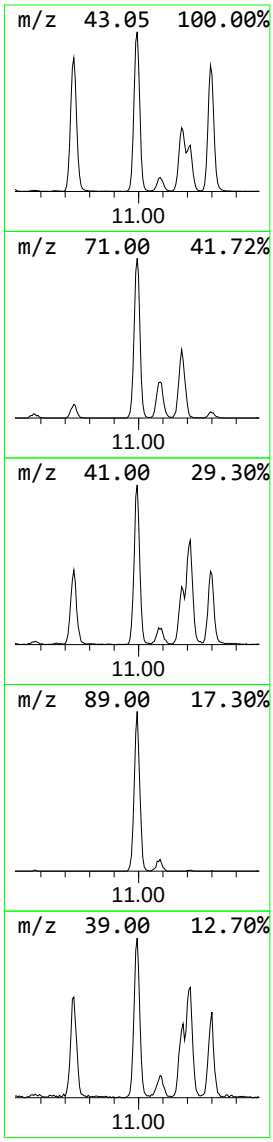
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	29.79 ug/l	1463900	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	2,3-Hexanedione	114	C6H10O2	003848-24-6	53
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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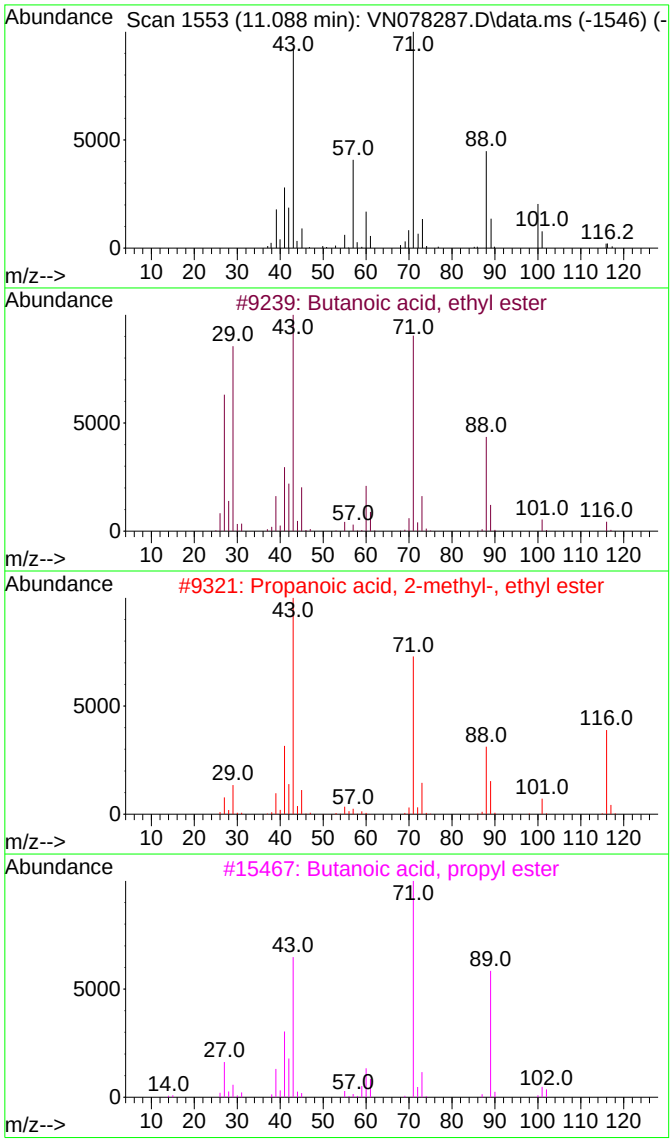
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

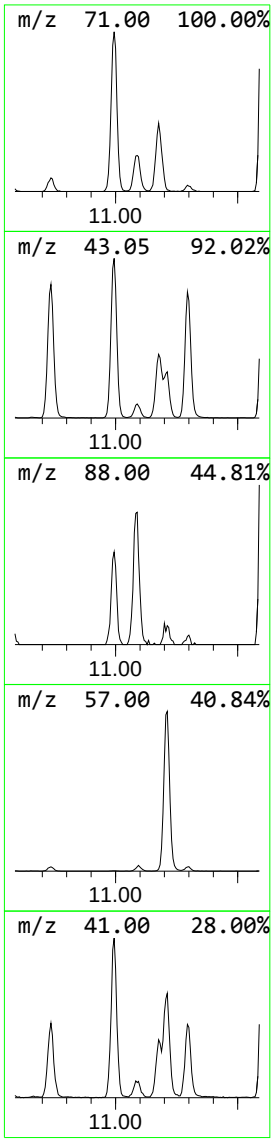
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	6.03 ug/l	296072	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	47
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45





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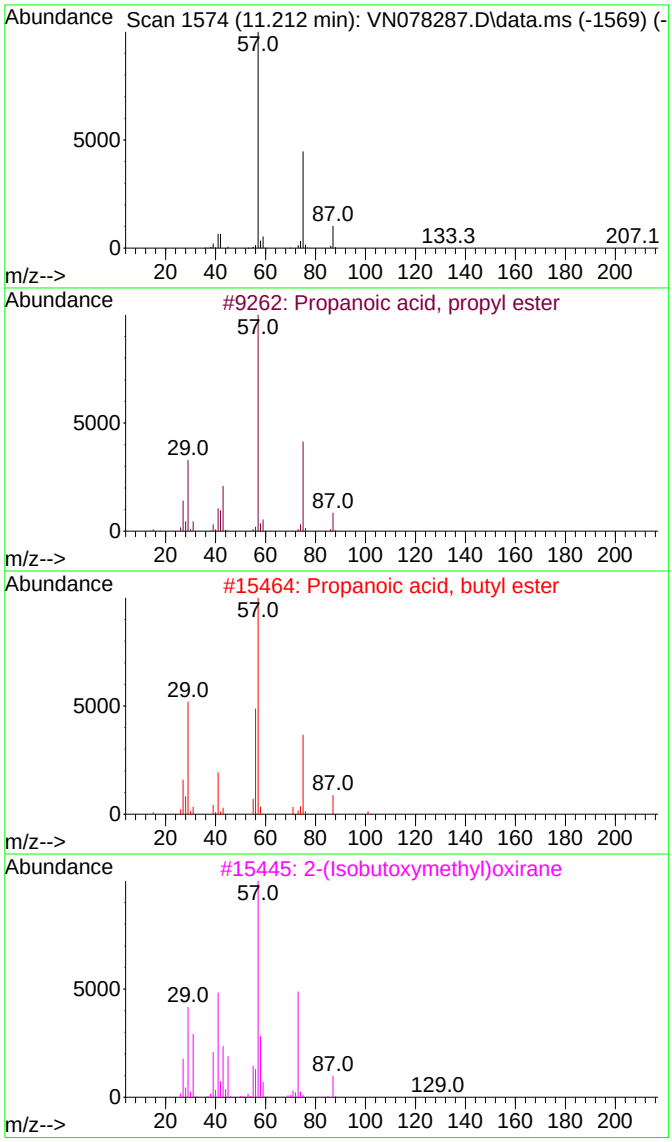
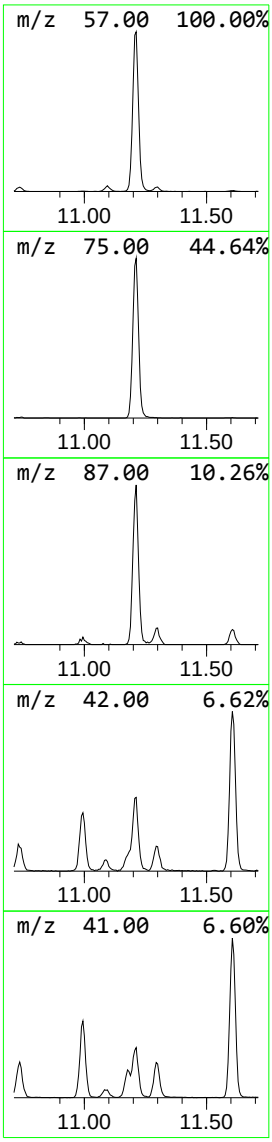
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.212	40.86 ug/l	2007620	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	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	1-Pentanamine	87	C5H13N	000110-58-7	7
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5





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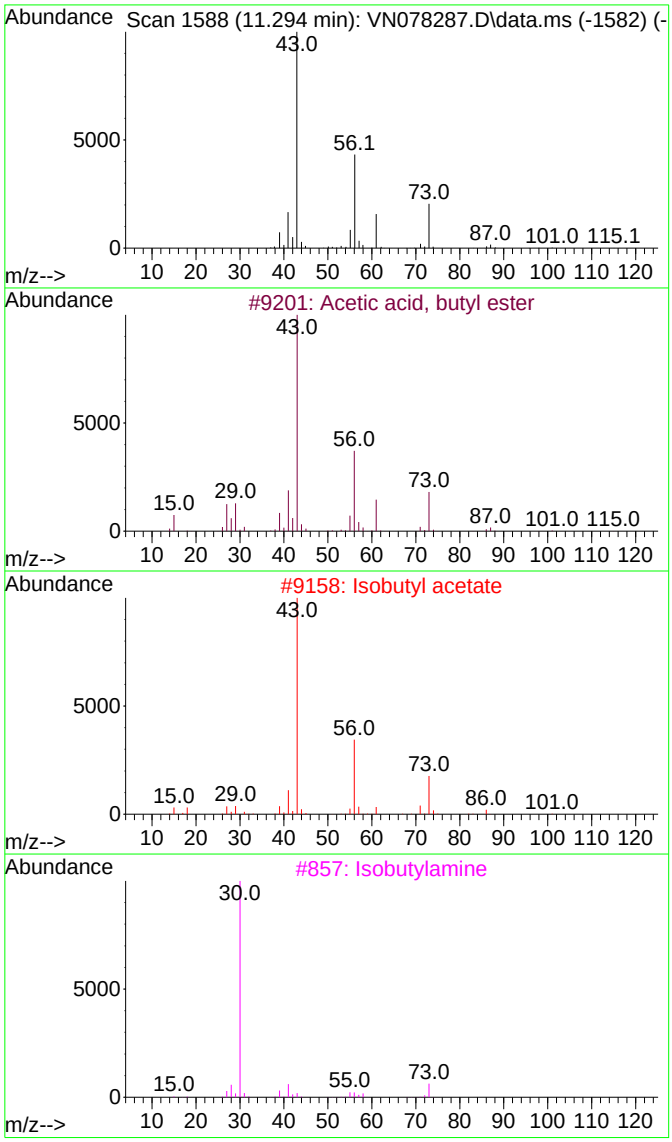
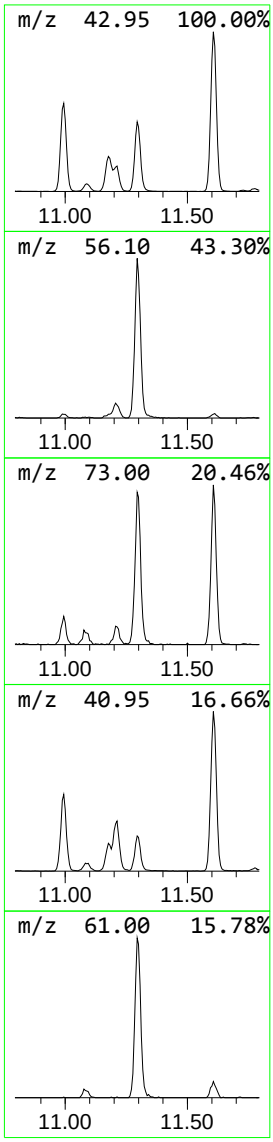
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	22.80 ug/l	1120530	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	40
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Ethane, diazo-	56	C2H4N2	001117-96-0	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





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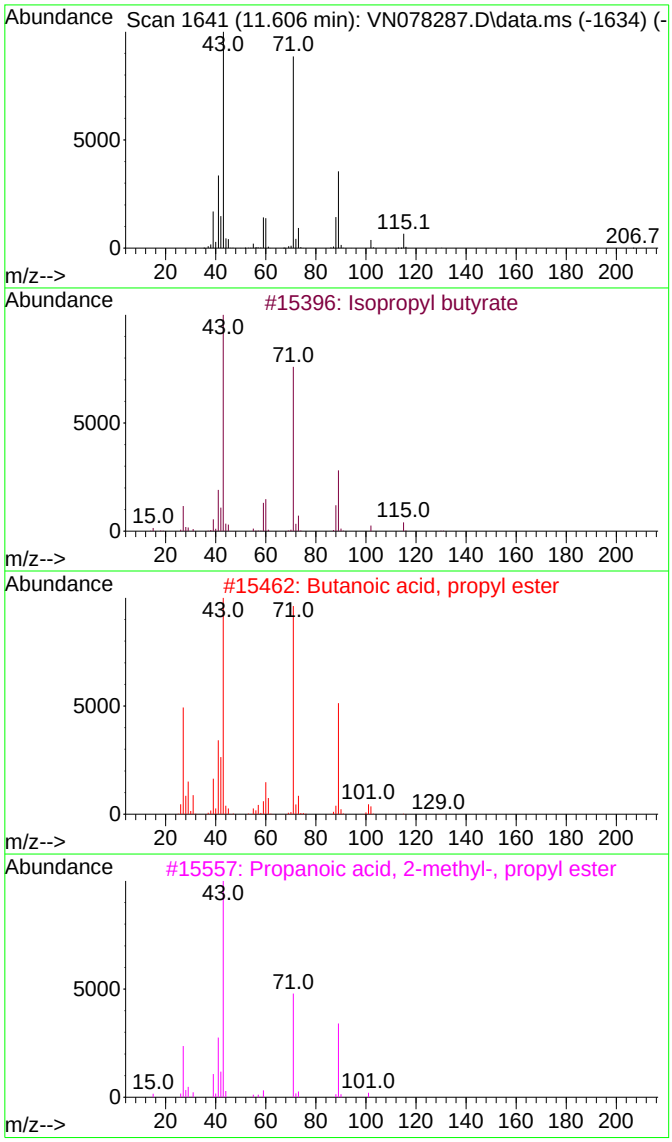
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

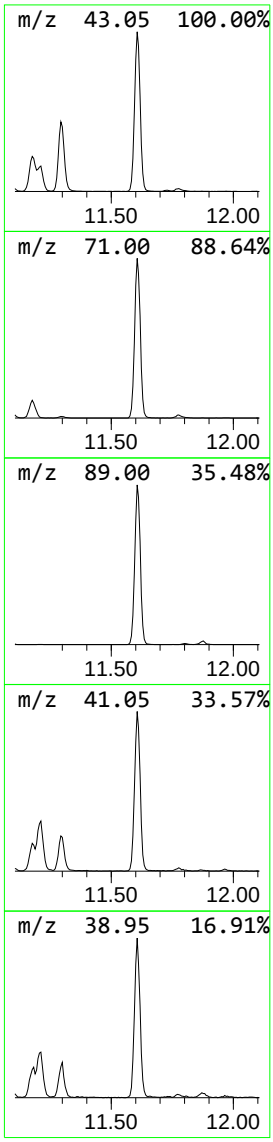
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	80.38 ug/l	3949720	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	94
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	50





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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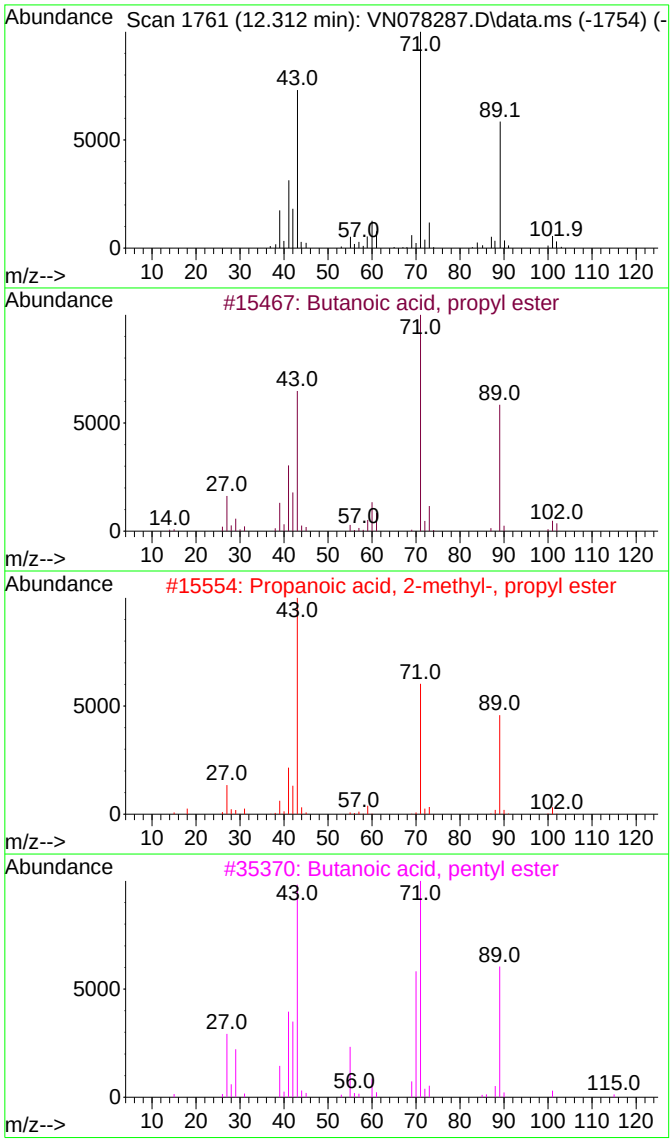
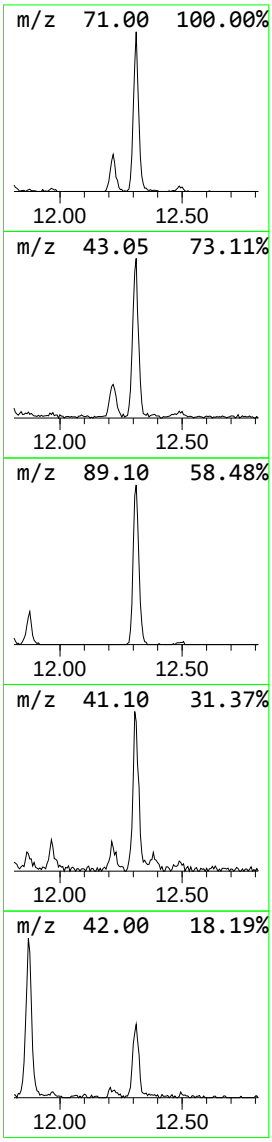
****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.312	5.84 ug/l	286785	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, pentyl ester	158	C9H18O2	000540-18-1	72
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
5	Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078287.D
Acq On : 19 Jun 2023 18:38
Operator : JC\MD
Sample : 03320-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-19

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.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	7.6	ug/l	304682	2	9.112	2016340	50.0
n-Propyl acetate	9.753	114.1	ug/l	4602520	2	9.112	2016340	50.0
Propanoic acid,...	10.365	27.0	ug/l	1087460	2	9.112	2016340	50.0
Isobutyl acetate	10.735	23.2	ug/l	1141840	3	11.871	2456810	50.0
Propanoic acid,...	10.994	29.8	ug/l	1463900	3	11.871	2456810	50.0
Butanoic acid, ...	11.088	6.0	ug/l	296072	3	11.871	2456810	50.0
Propanoic acid,...	11.212	40.9	ug/l	2007620	3	11.871	2456810	50.0
Acetic acid, bu...	11.294	22.8	ug/l	1120530	3	11.871	2456810	50.0
Isopropyl butyrate	11.606	80.4	ug/l	3949720	3	11.871	2456810	50.0
Butanoic acid, ...	12.312	5.8	ug/l	286785	3	11.871	2456810	50.0