LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

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: VN078053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.830	141	149	154	rBV2	33217	80408	3.04%	0.427%
2	5.289	558	567	577	rVB4	13174	41886	1.58%	0.223%
3	7.571	948	955	966	rVB2	34900	84017	3.18%	0.446%
4	8.177	1046	1058	1062	rBV	324140	765363	28.95%	4.066%
5	8.235	1062	1068	1078	rVB	553217	1229642	46.51%	6.533%
6	8.588	1116	1128	1137	rBV	326094	743833	28.14%	3.952%
7	8.694	1137	1146	1162	rBV	228435	700284	26.49%	3.720%
8	9.106	1208	1216	1227	rBV	812520	1673082	63.29%	8.889%
9	9.676	1304	1313	1318	rBV	83662	182689	6.91%	0.971%
10	9.747	1318	1325	1344	rVV	1416891	2643622	100.00%	14.045%
11	10.365	1422	1430	1440	rBV	303804	540678	20.45%	2.872%
12	10.571	1457	1465	1476	rBV	1243019	2335439	88.34%	12.408%
13	10.735	1486	1493	1505	rVB	301127	527267	19.94%	2.801%
14	10.994	1528	1537	1546	rBV	279444	483236	18.28%	2.567%
15	11.088	1546	1553	1559	rVV3	52298	98594	3.73%	0.524%
16	11.176	1562	1568	1569	rVV	153077	208594	7.89%	1.108%
17	11.206	1569	1573	1582	rVV	338321	613601	23.21%	3.260%
18	11.294	1582	1588	1601	rVB2	164183	287549	10.88%	1.528%
19	11.606	1633	1641	1653	rBV	525076	843835	31.92%	4.483%
20	11.870	1678	1686	1697	rBV	1087303	1963520	74.27%	10.432%
21	12.306	1755	1760	1768	rBV3	19205	30722	1.16%	0.163%
22	12.853	1846	1853	1864	rVB	807730	1435416	54.30%	7.626%
23	13.800	2005	2014	2022	rBV	753037	1309312	49.53%	6.956%

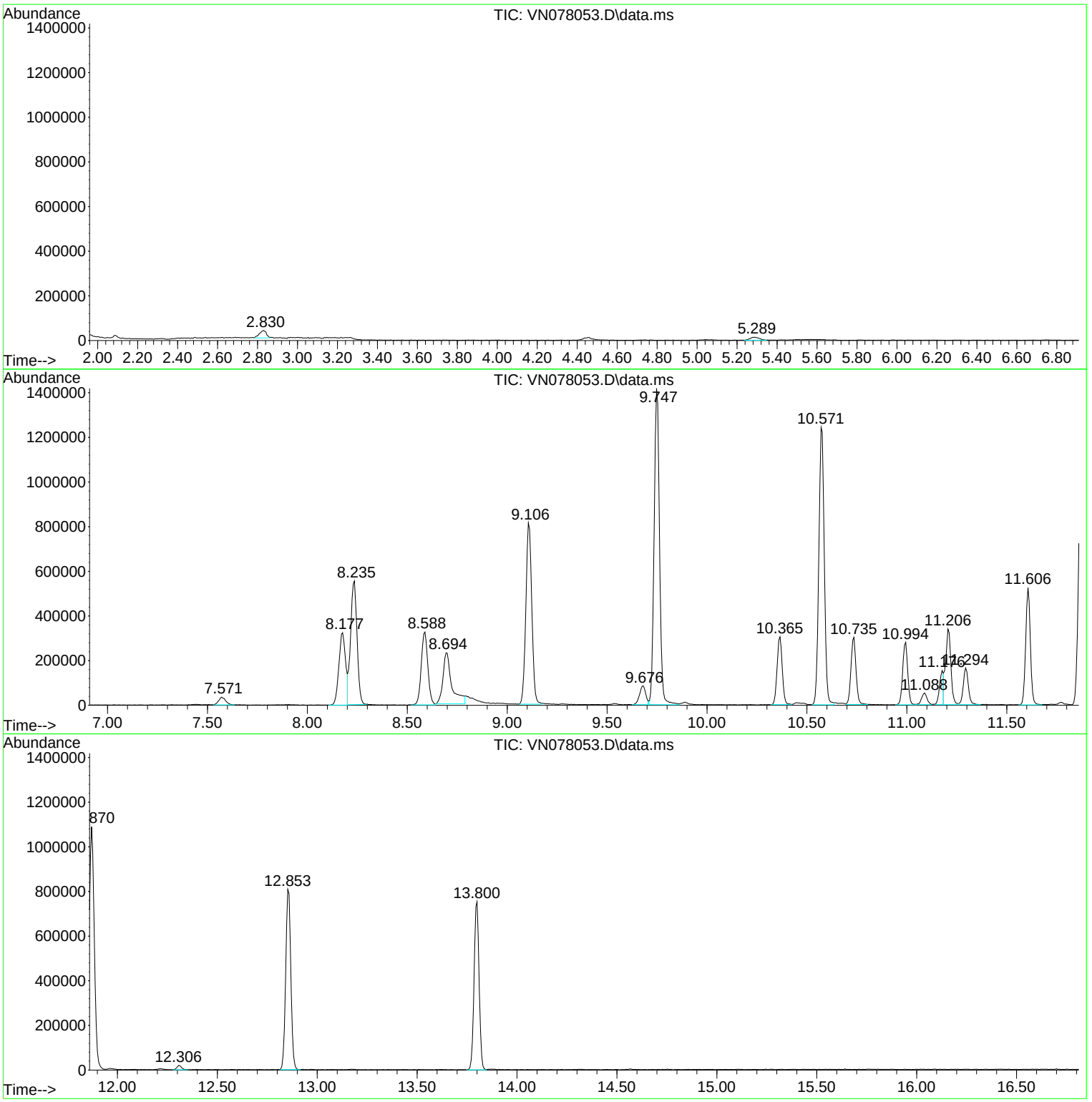
Sum of corrected areas: 18822589

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

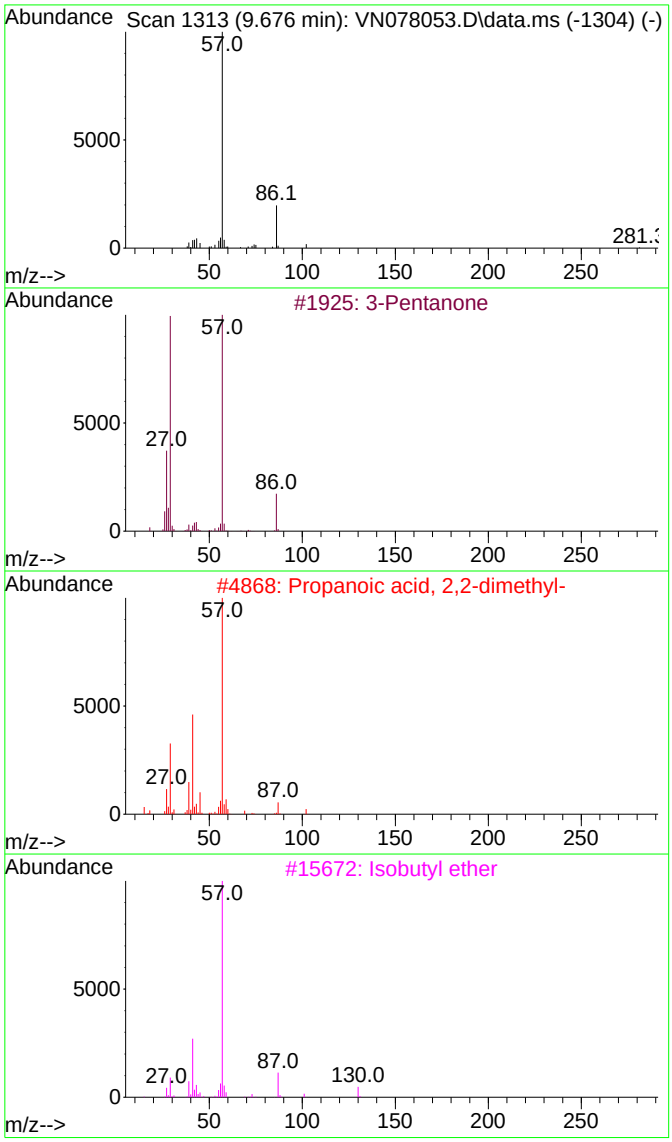
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

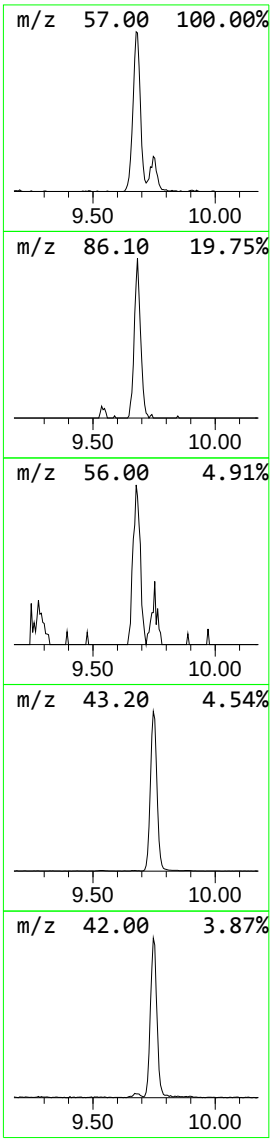
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.676	5.46 ug/l	182689	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	86
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	38
3	Isobutyl ether	130	C8H18O	000628-55-7	38
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	36
5	Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

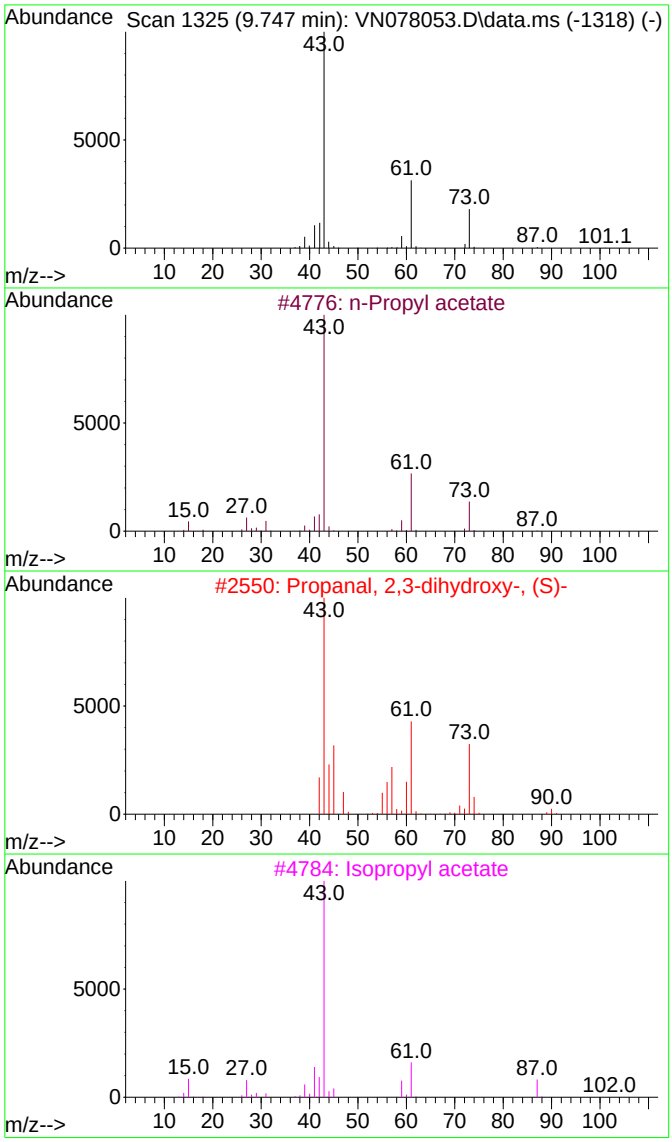
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

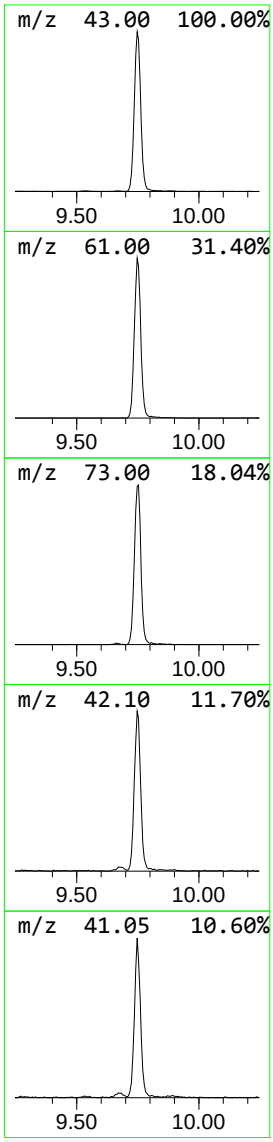
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	79.00 ug/l	2643620	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	36
3	Isopropyl acetate	102	C5H10O2	000108-21-4	9
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

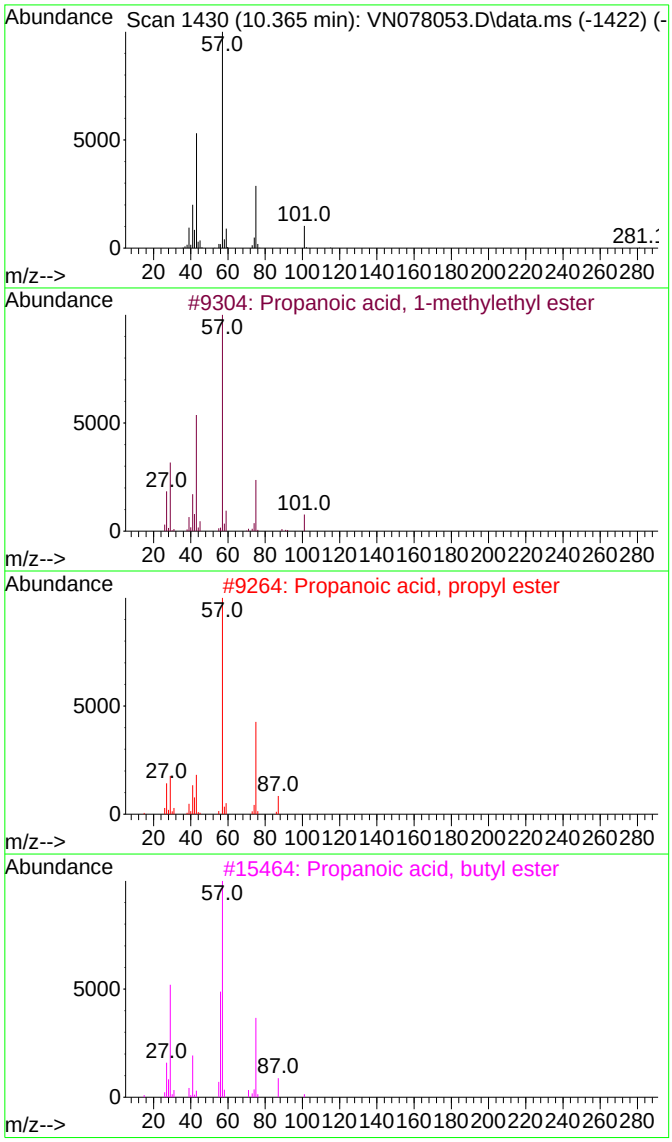
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

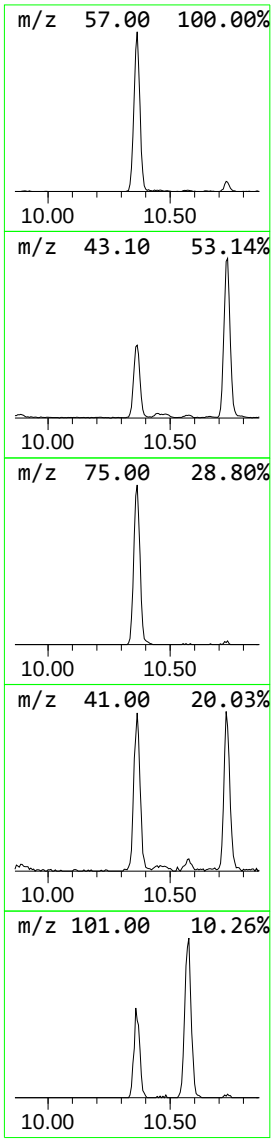
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	16.16 ug/l	540678	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	33
4	1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	9
5	2-Hydroxyguanidine	75	CH5N3O	1000489-19-8	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

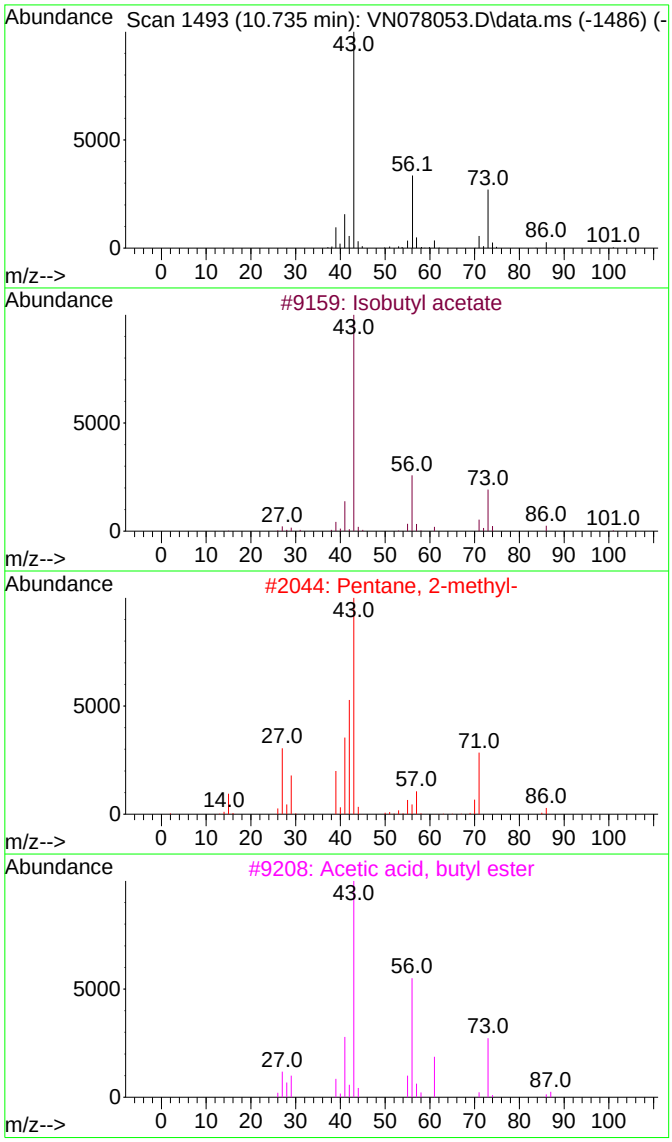
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

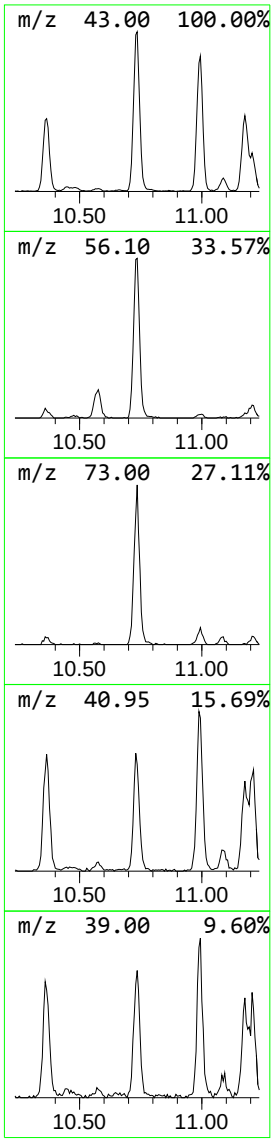
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	13.43 ug/l	527267	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
4	2-Pentanone	86	C5H10O	000107-87-9	9
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

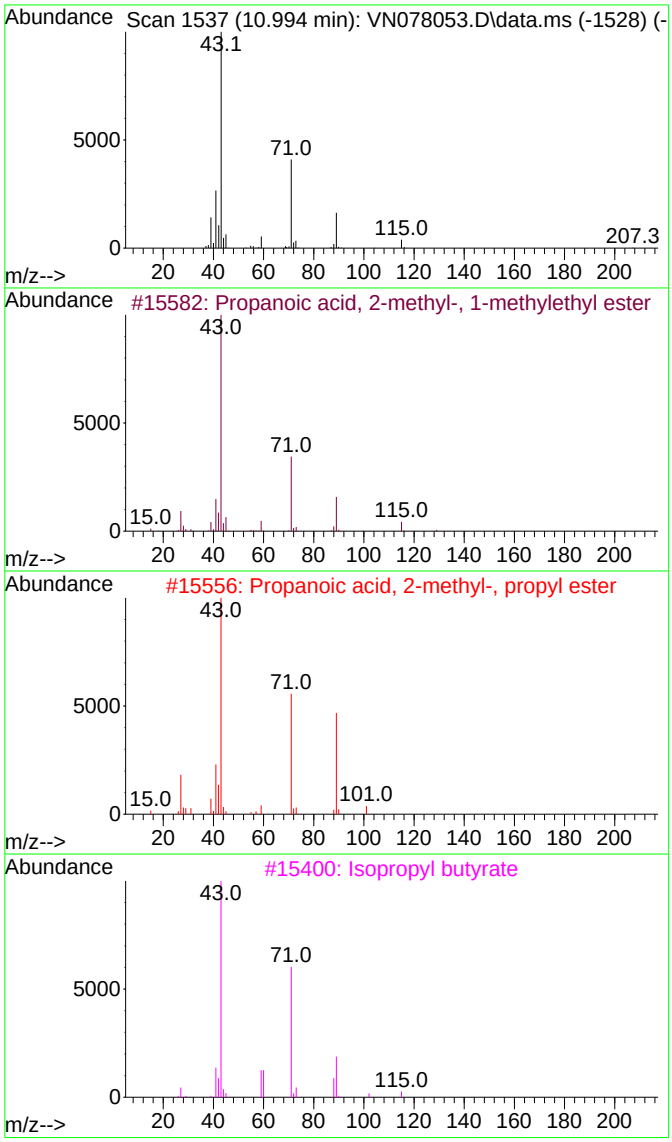
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

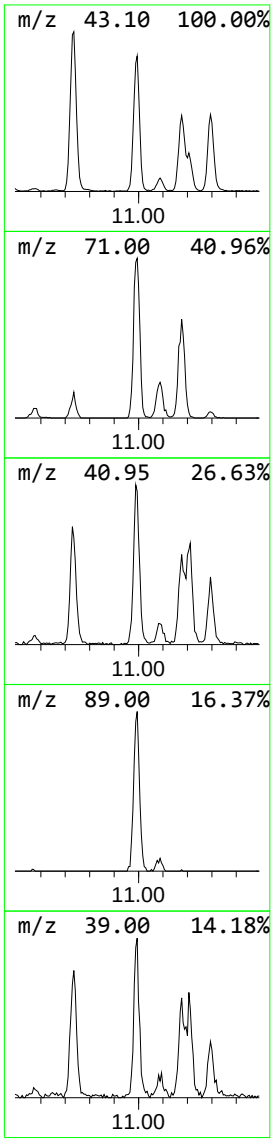
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	12.31 ug/l	483236	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	78
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4	2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	47
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

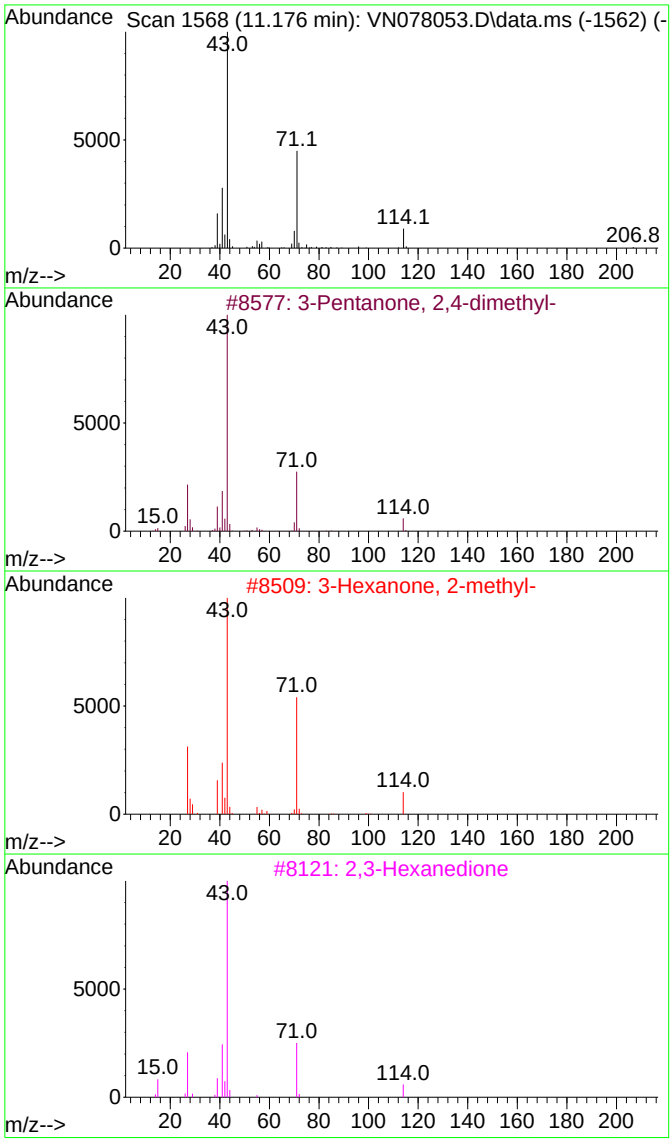
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

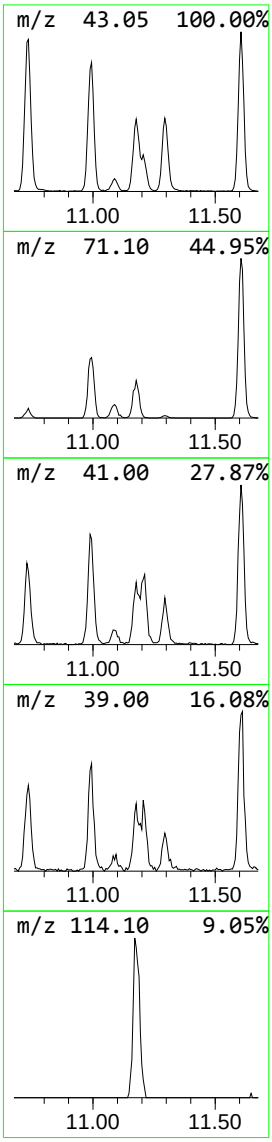
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.176	5.31 ug/l	208594	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	72
4	4-Heptanone	114	C7H14O	000123-19-3	64
5	Pyrrolidine	71	C4H9N	000123-75-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

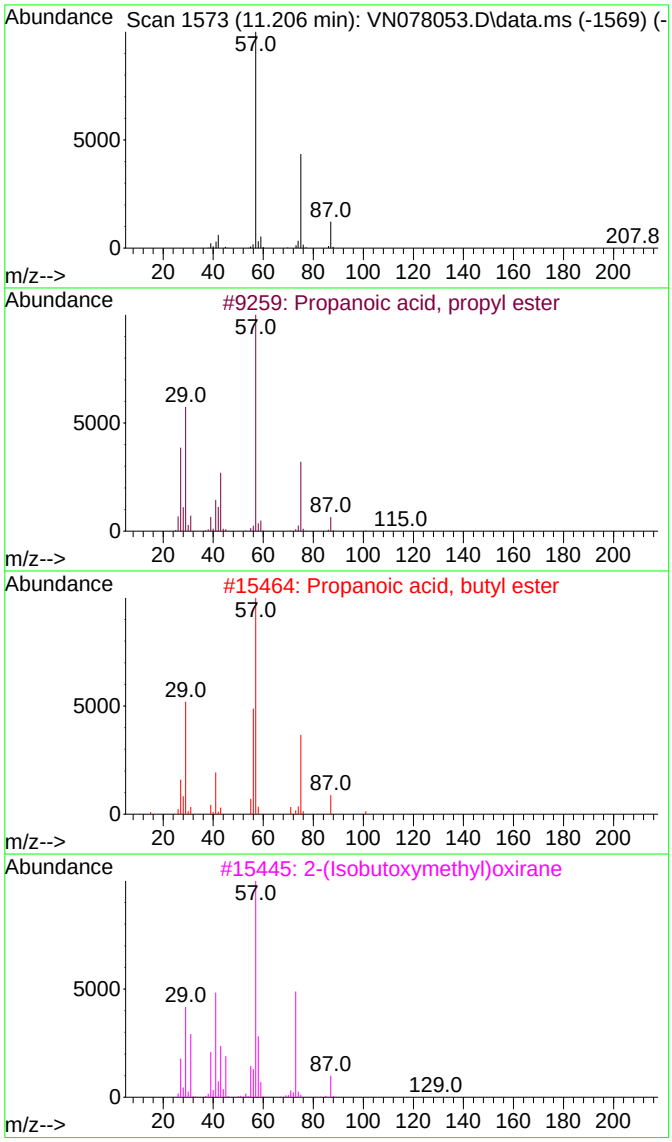
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

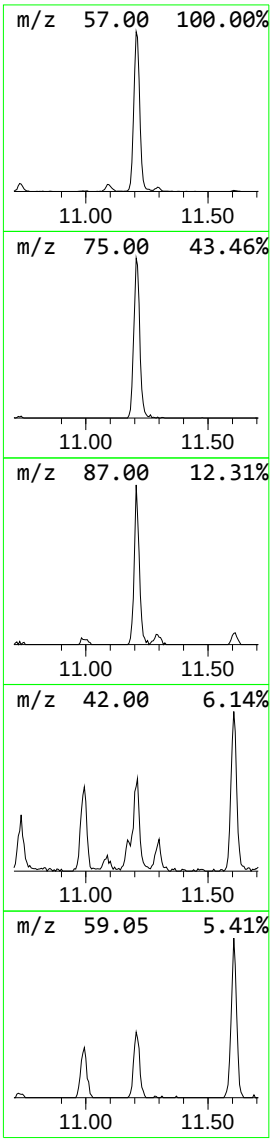
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	15.63 ug/l	613601	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	Morpholine	87	C4H9NO	000110-91-8	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

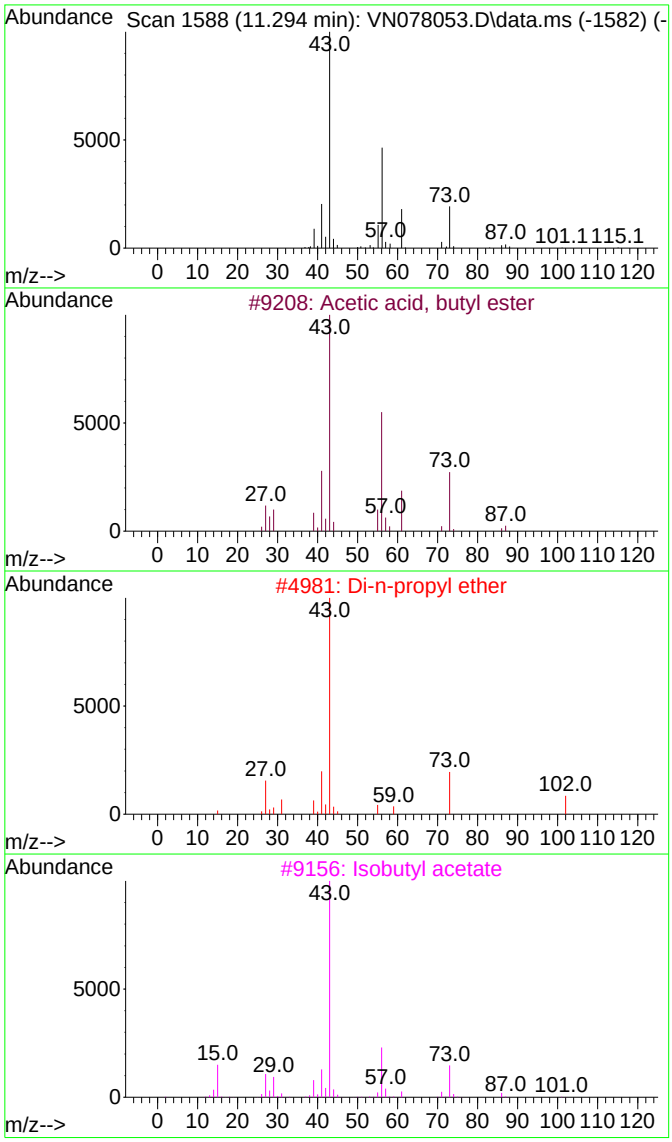
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

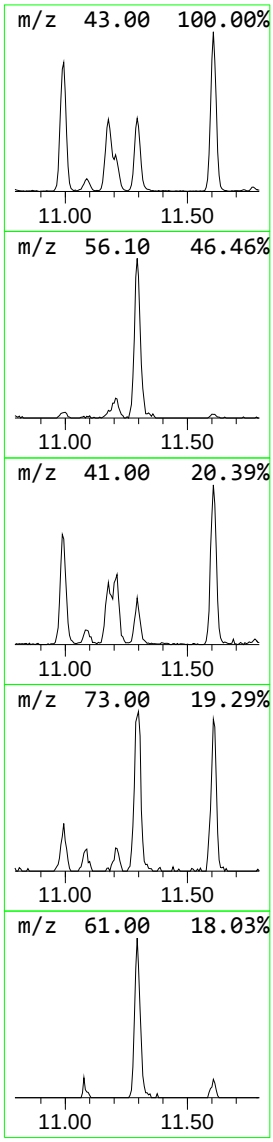
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	7.32 ug/l	287549	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	Di-n-propyl ether	102	C6H14O	000111-43-3	25
3	Isobutyl acetate	116	C6H12O2	000110-19-0	23
4	Ethane, diazo-	56	C2H4N2	001117-96-0	9
5	Isobutylamine	73	C4H11N	000078-81-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

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

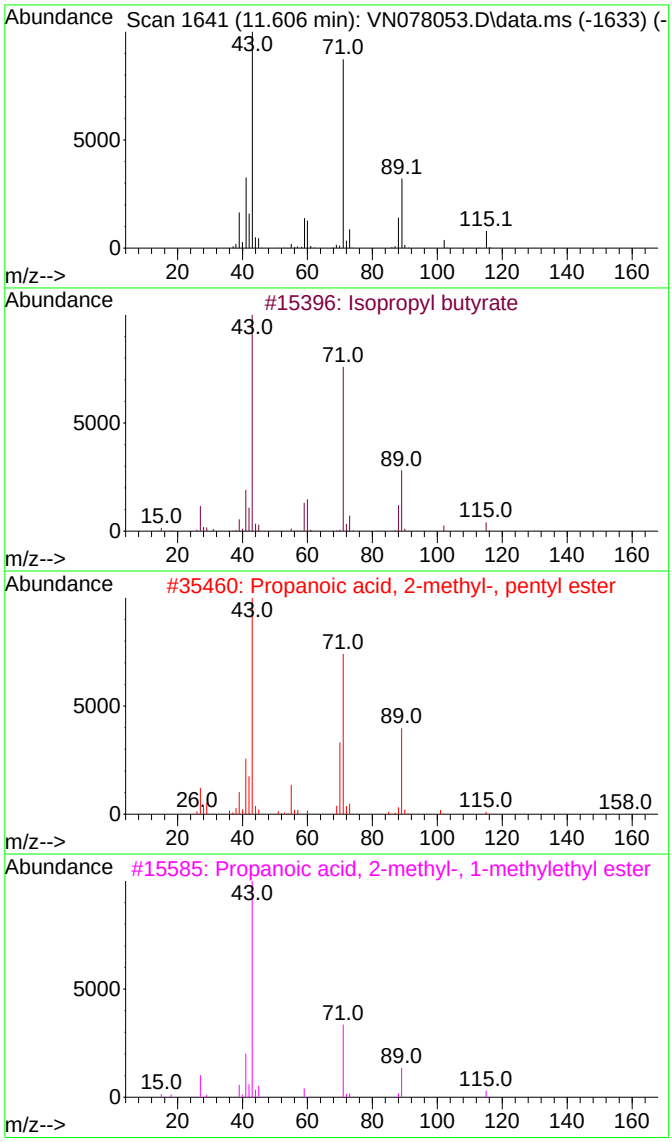
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

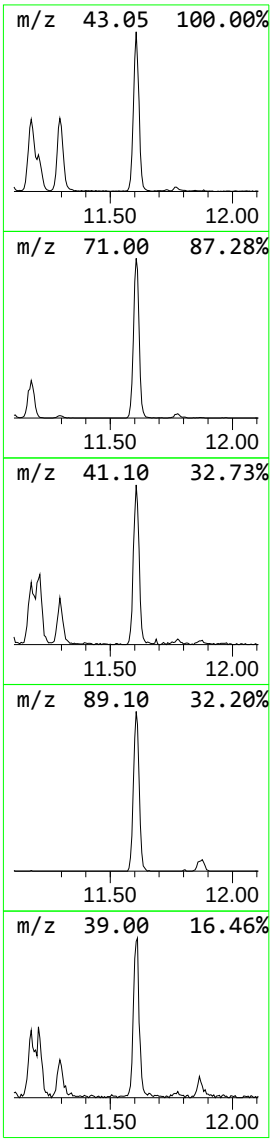
****

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	21.49 ug/l	843835	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-, penty...	158	C9H18O2	002445-72-9	64
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078053.D
Acq On : 05 Jun 2023 18:45
Operator : JC\MD
Sample : 03018-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
348

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	9.676	5.5	ug/l	182689	2	9.106	1673080	50.0
n-Propyl acetate	9.747	79.0	ug/l	2643620	2	9.106	1673080	50.0
Propanoic acid,...	10.365	16.2	ug/l	540678	2	9.106	1673080	50.0
Isobutyl acetate	10.735	13.4	ug/l	527267	3	11.871	1963520	50.0
Propanoic acid,...	10.994	12.3	ug/l	483236	3	11.871	1963520	50.0
3-Pentanone, 2,...	11.176	5.3	ug/l	208594	3	11.871	1963520	50.0
Propanoic acid,...	11.206	15.6	ug/l	613601	3	11.871	1963520	50.0
Acetic acid, bu...	11.294	7.3	ug/l	287549	3	11.871	1963520	50.0
Isopropyl butyrate	11.606	21.5	ug/l	843835	3	11.871	1963520	50.0