LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

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: VN078028.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	142	149	157	rVB2	37302	84935	1.66%	0.269%
2	4.453	415	425	435	rBV2	22751	73222	1.43%	0.232%
3	5.289	556	567	576	rBV5	22602	72692	1.42%	0.230%
4	7.571	948	955	968	rVB2	46513	120339	2.35%	0.381%
5	8.177	1047	1058	1062	rBV	318134	732550	14.31%	2.321%
6	8.235	1062	1068	1080	rVB	522810	1184951	23.14%	3.755%
7	8.588	1118	1128	1134	rBV	320952	707049	13.81%	2.240%
8	8.700	1134	1147	1180	rVB2	416699	1880833	36.73%	5.960%
9	9.112	1207	1217	1230	rVB	778311	1628657	31.81%	5.161%
10	9.677	1305	1313	1318	rBV2	132033	296765	5.80%	0.940%
11	9.747	1318	1325	1344	rVV	2728794	5120285	100.00%	16.225%
12	10.365	1421	1430	1439	rBV	638425	1110108	21.68%	3.518%
13	10.576	1457	1466	1475	rBV	1221517	2277539	44.48%	7.217%
14	10.735	1486	1493	1512	rVB	771060	1319885	25.78%	4.182%
15	10.994	1529	1537	1546	rBV	888968	1483937	28.98%	4.702%
16	11.088	1546	1553	1561	rVV2	164178	306647	5.99%	0.972%
17	11.206	1561	1573	1582	rVV2	1243233	2646897	51.69%	8.387%
18	11.294	1582	1588	1600	rVB	817795	1332466	26.02%	4.222%
19	11.606	1633	1641	1653	rBV	2529783	4028248	78.67%	12.765%
20	11.771	1665	1669	1678	rVB3	36250	72789	1.42%	0.231%
21	11.871	1678	1686	1697	rVV	1058852	1956014	38.20%	6.198%
22	11.965	1697	1702	1710	rVB	34246	58253	1.14%	0.185%
23	12.312	1754	1761	1768	rBV	180189	304610	5.95%	0.965%
24	12.853	1846	1853	1861	rBV	810298	1440550	28.13%	4.565%
25	13.800	2005	2014	2022	rBV	764290	1317775	25.74%	4.176%

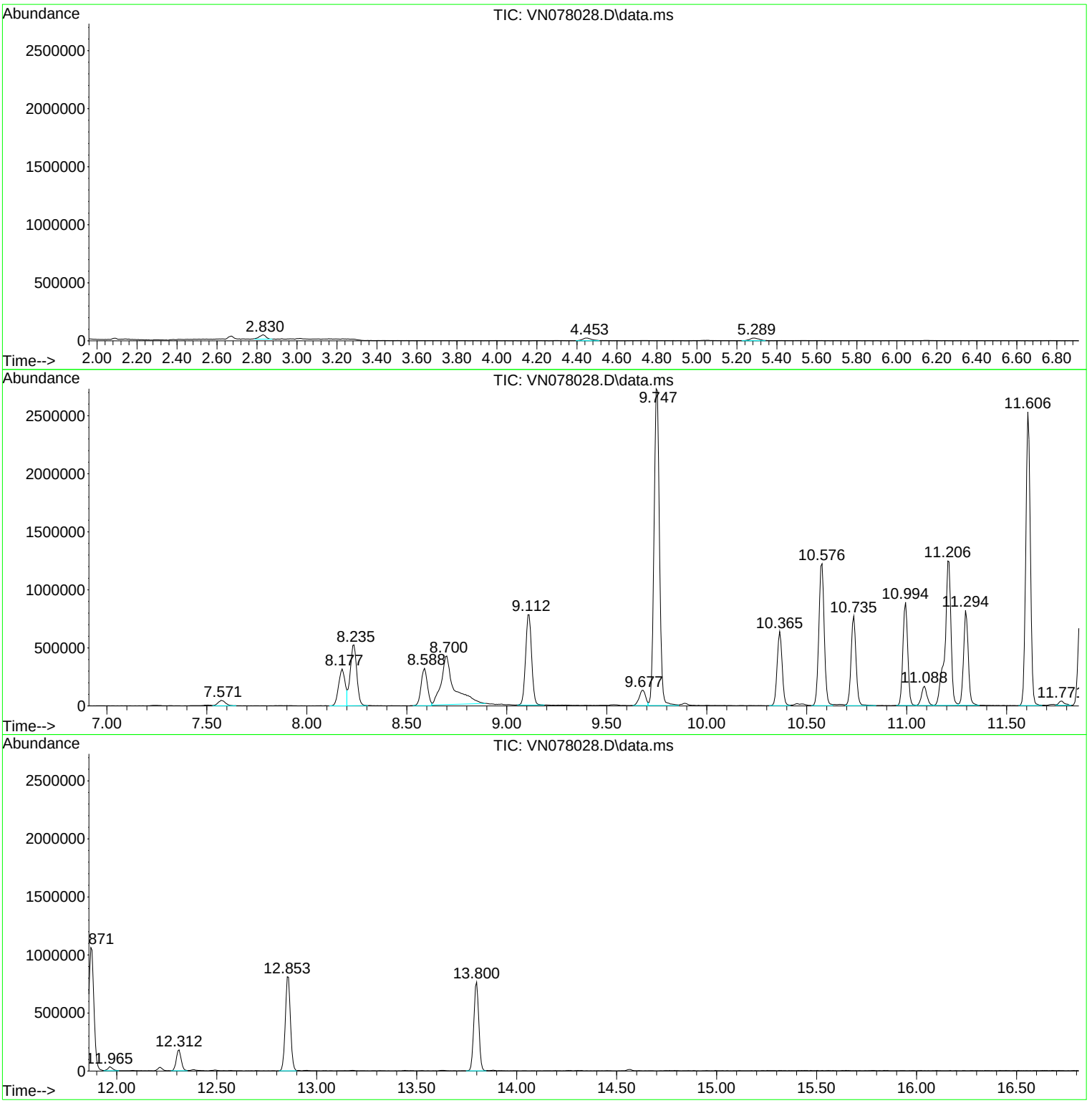
Sum of corrected areas: 31557996

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

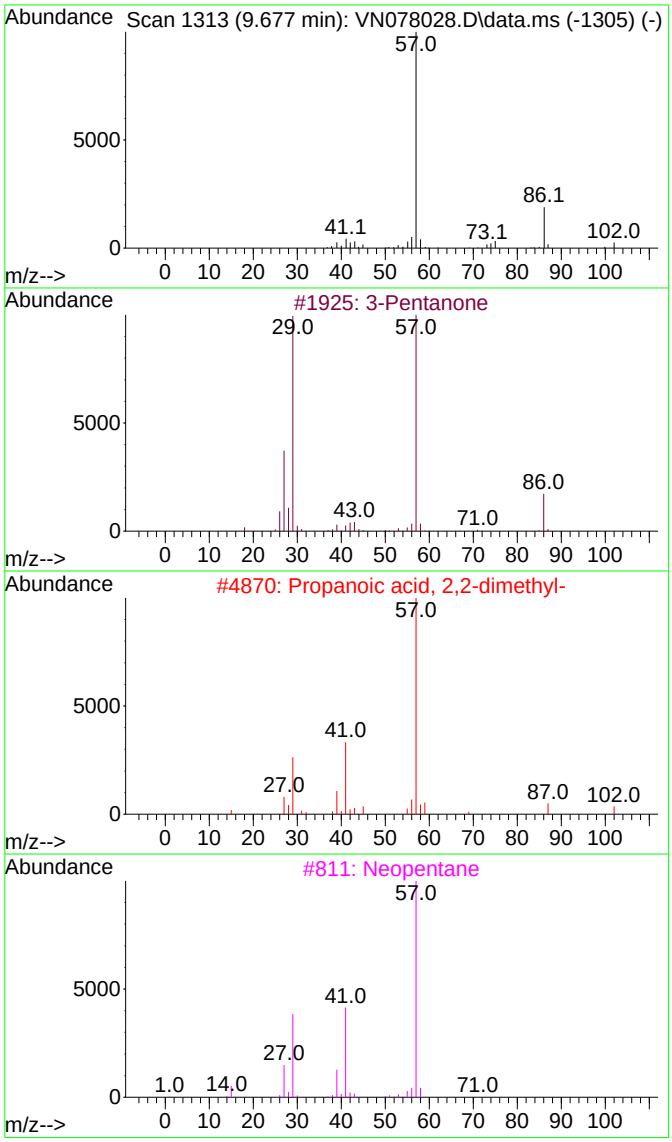
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

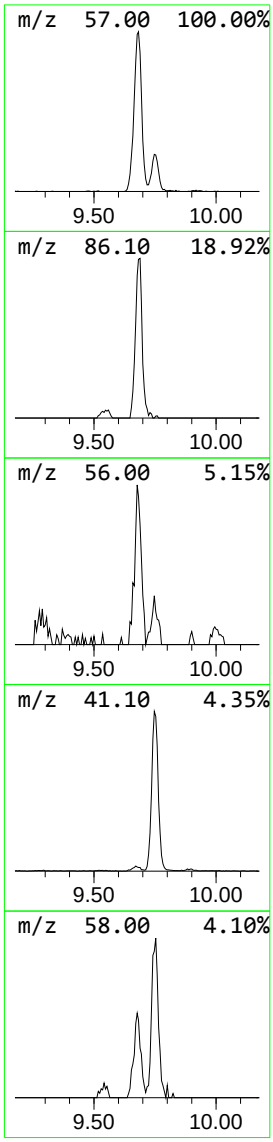
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	9.11 ug/l	296765	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	64
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	47
3	Neopentane	72	C5H12	000463-82-1	25
4	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

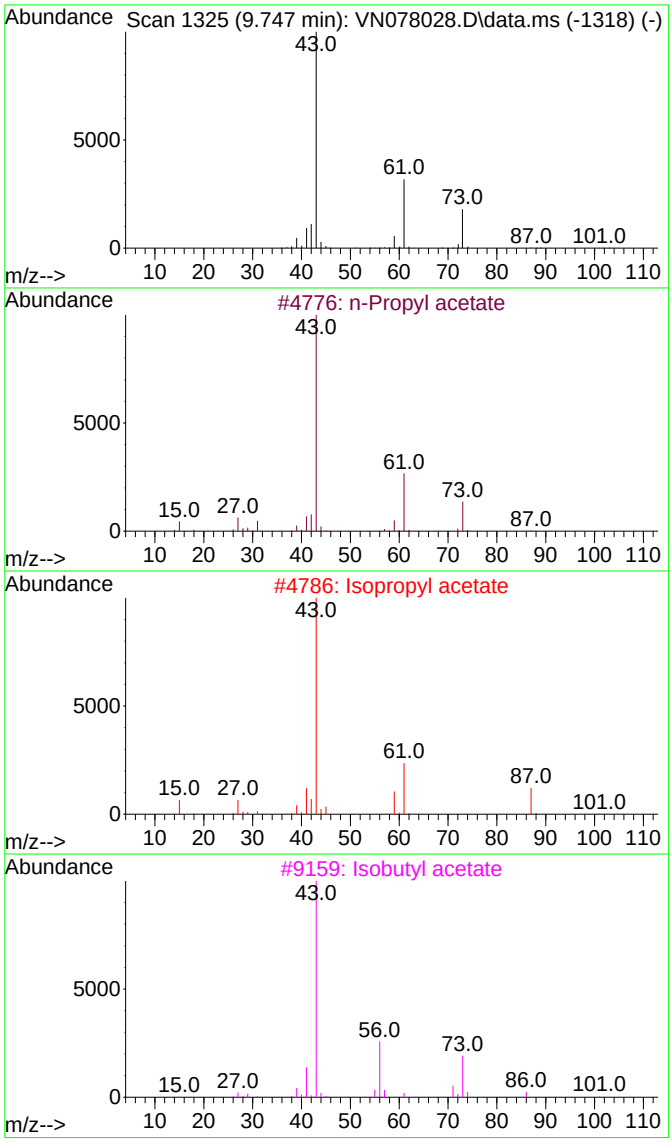
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

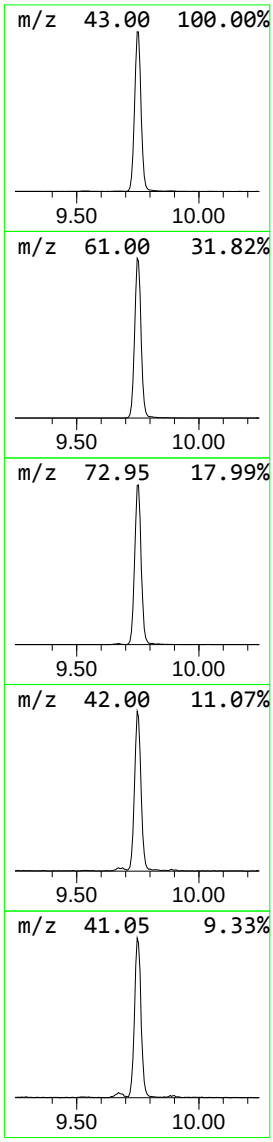
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	157.19 ug/l	5120290	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	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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

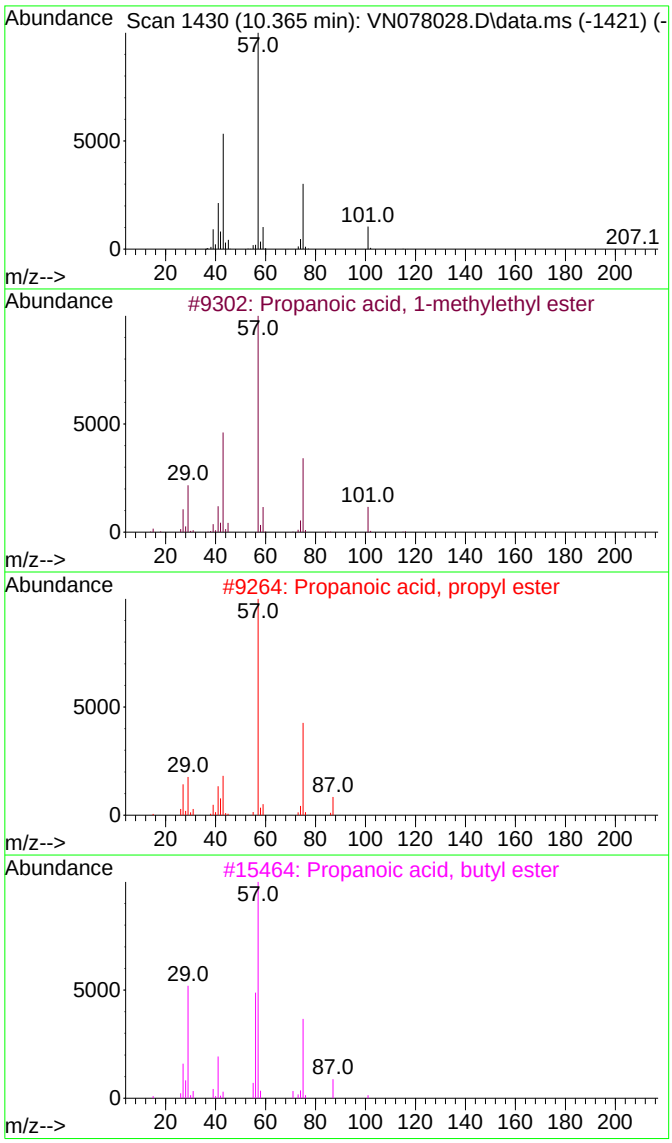
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

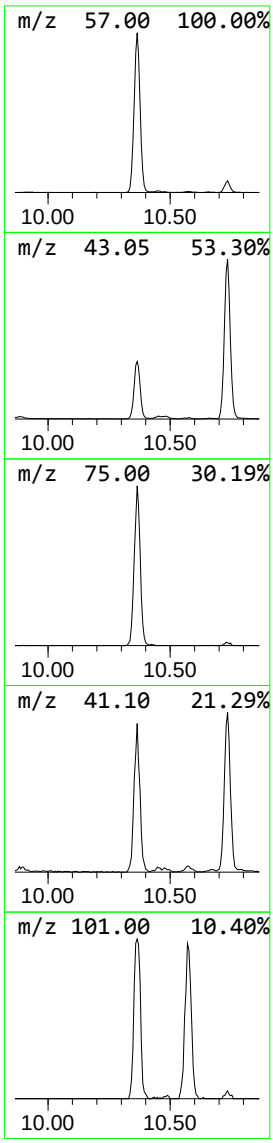
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	34.08 ug/l	1110110	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	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

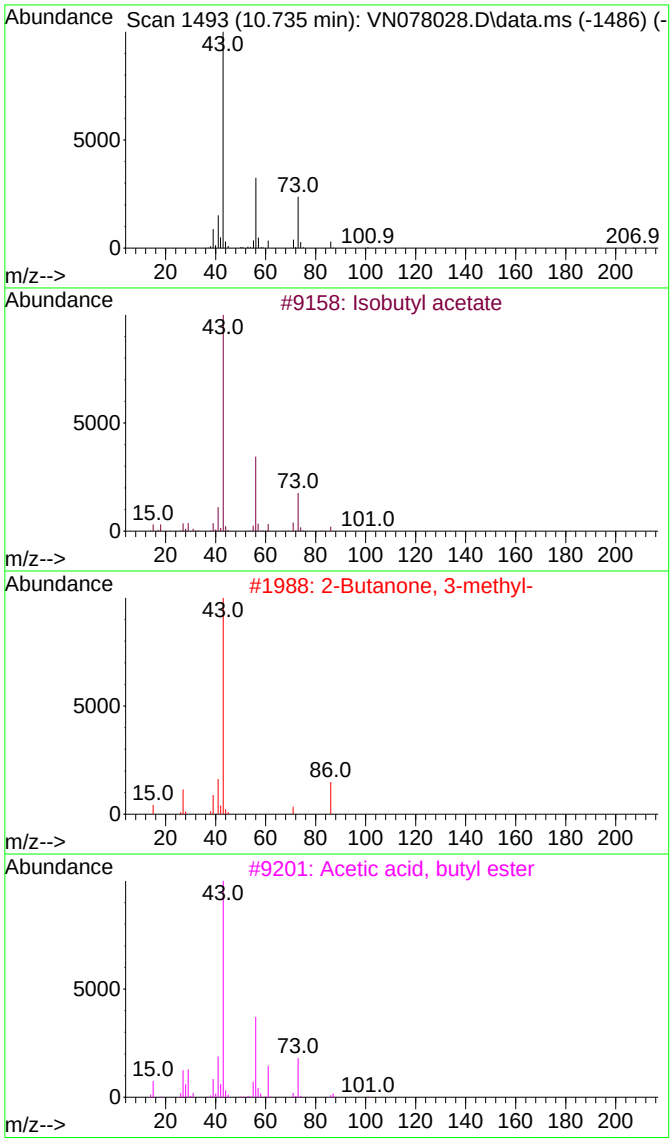
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

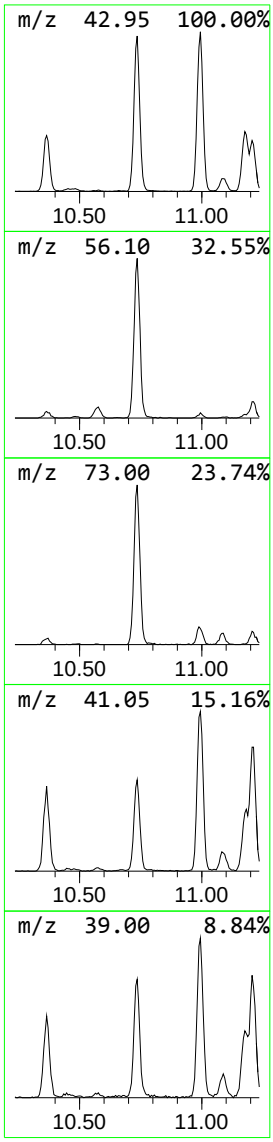
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	33.74 ug/l	1319890	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	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\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

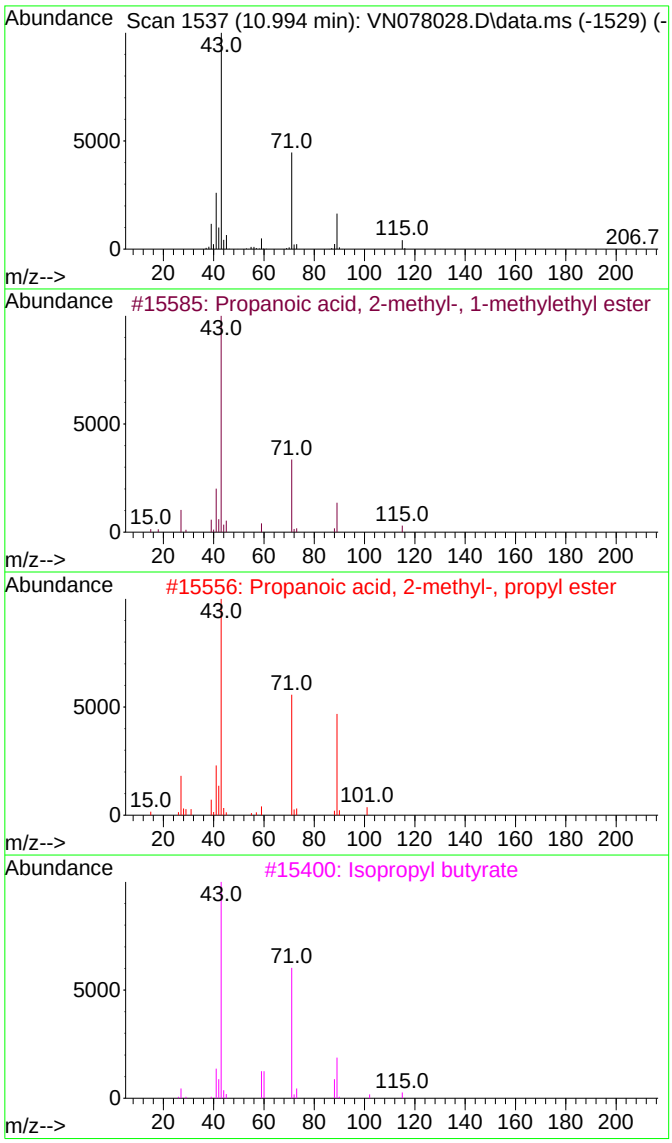
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

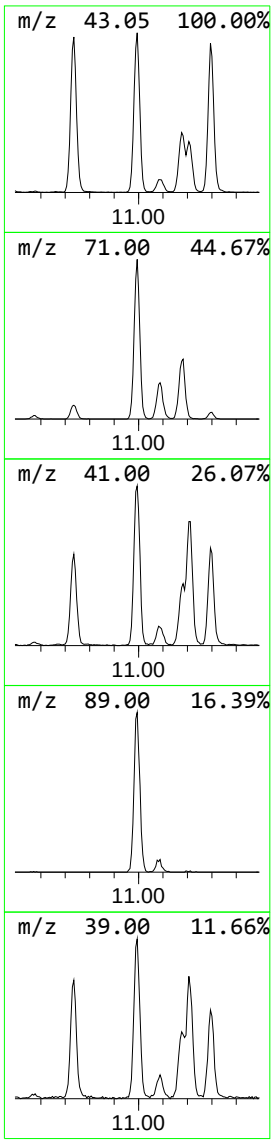
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	37.93 ug/l	1483940	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	56
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

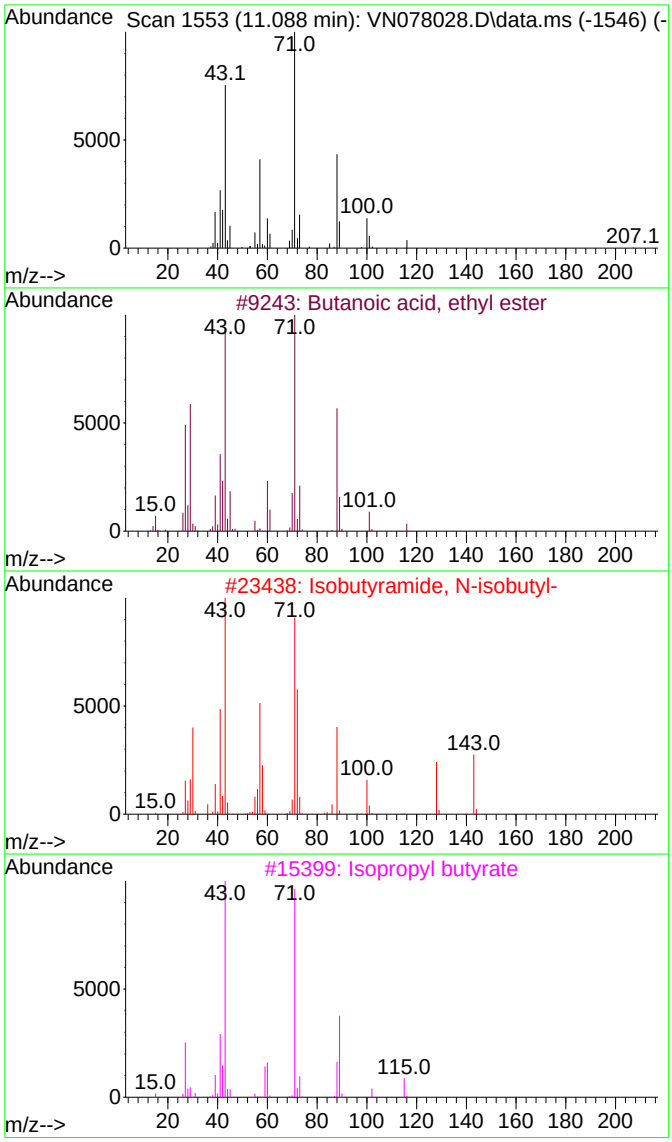
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

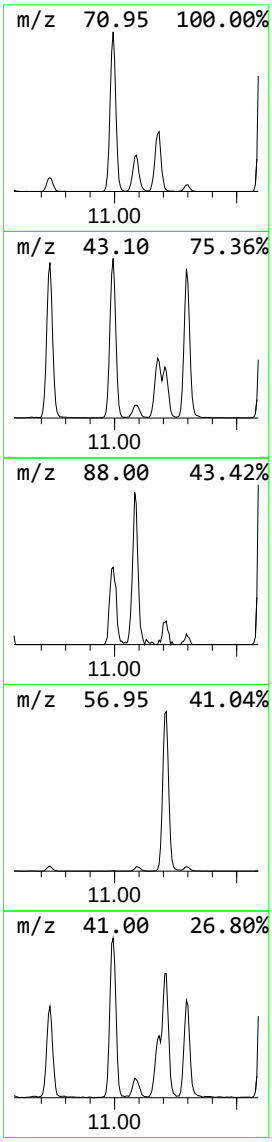
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	7.84 ug/l	306647	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	Isobutyramide, N-isobutyl-	143	C8H17NO	1000407-08-6	59
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	47
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
5	Butanoic acid, 2-methylbutyl ester	158	C9H18O2	051115-64-1	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

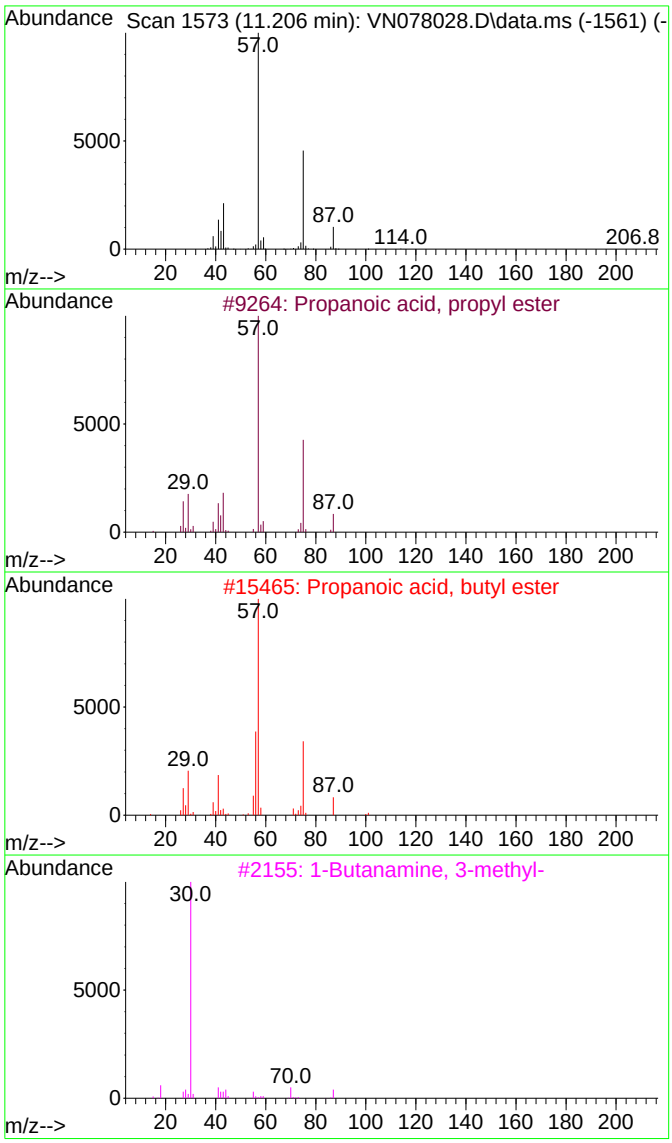
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

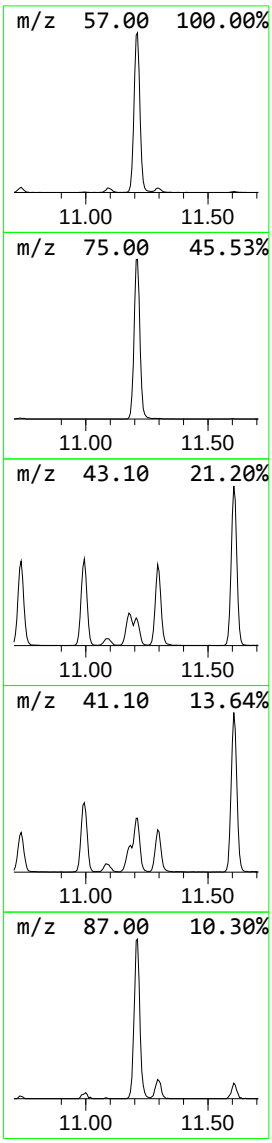
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	67.66 ug/l	2646900	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	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

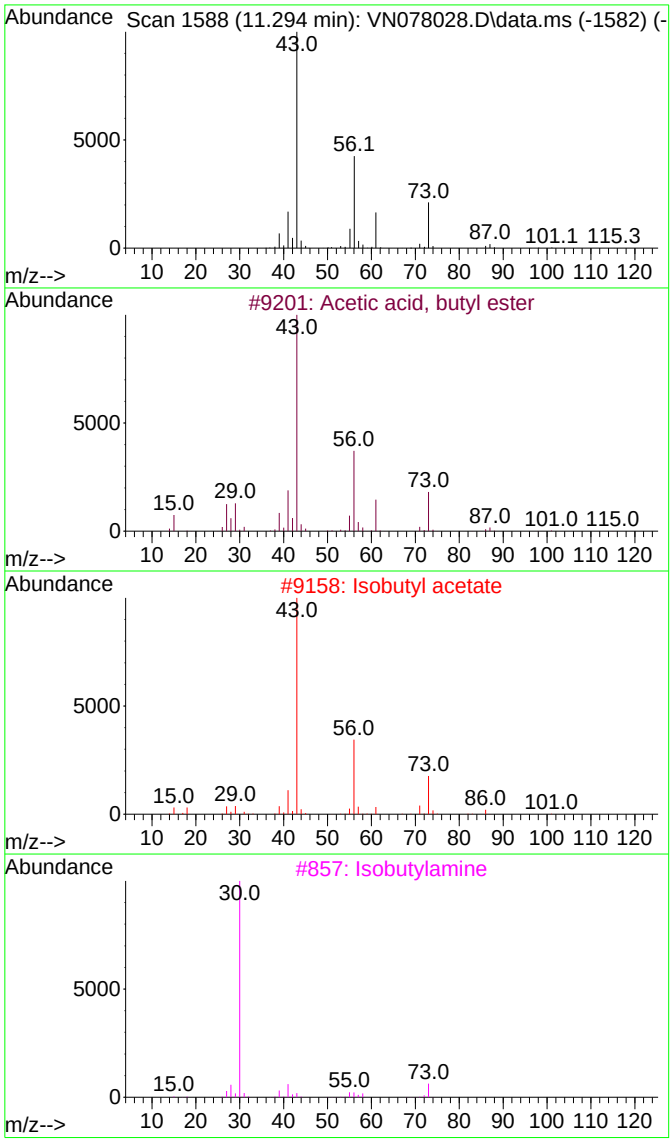
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

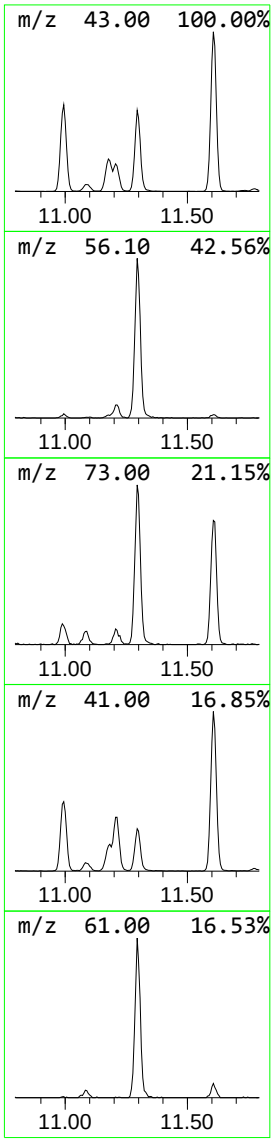
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	34.06 ug/l	1332470	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	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

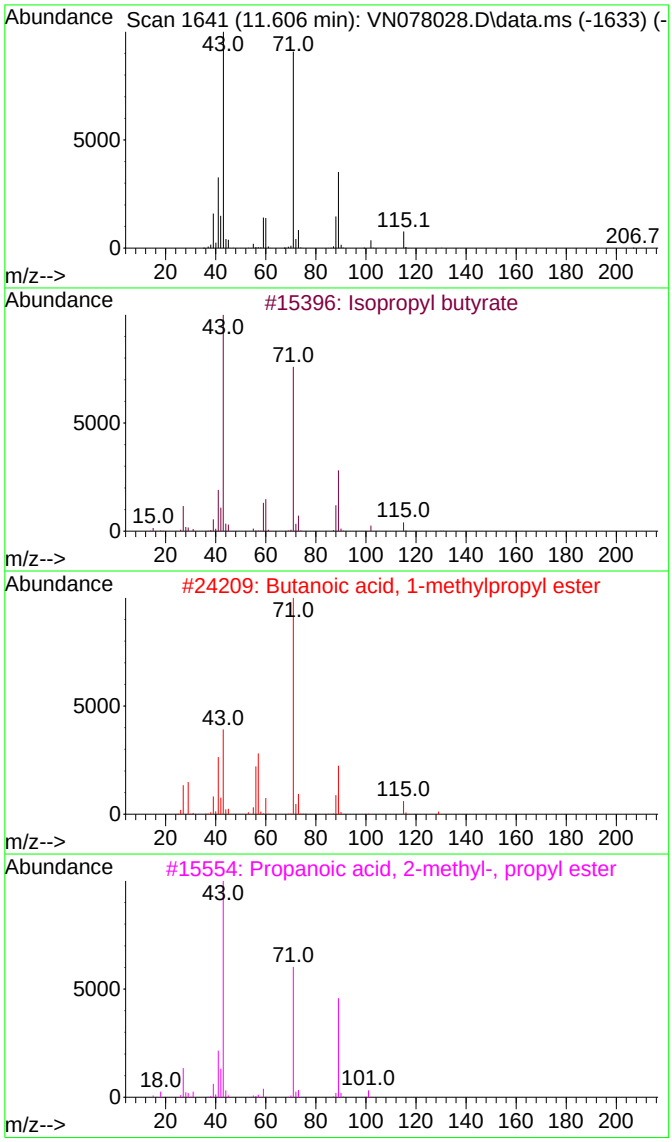
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

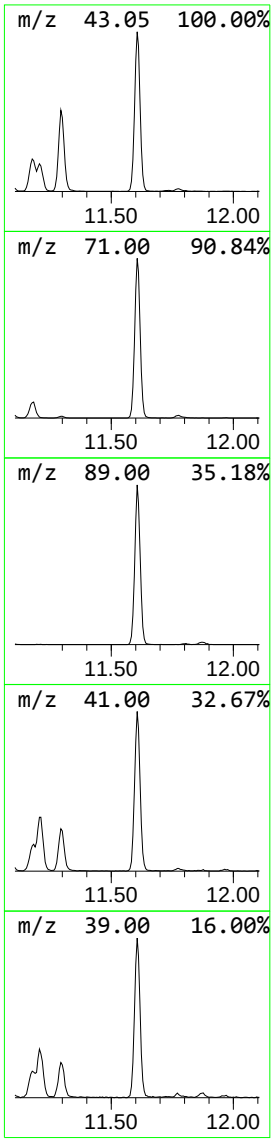
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	102.97 ug/l	4028250	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, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

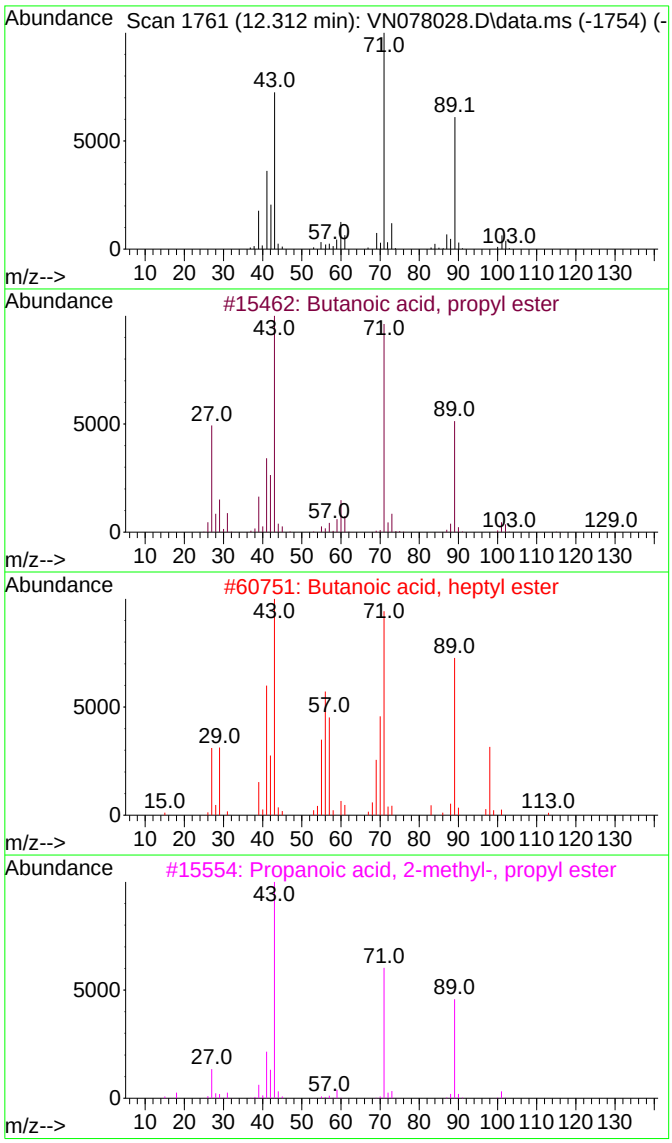
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

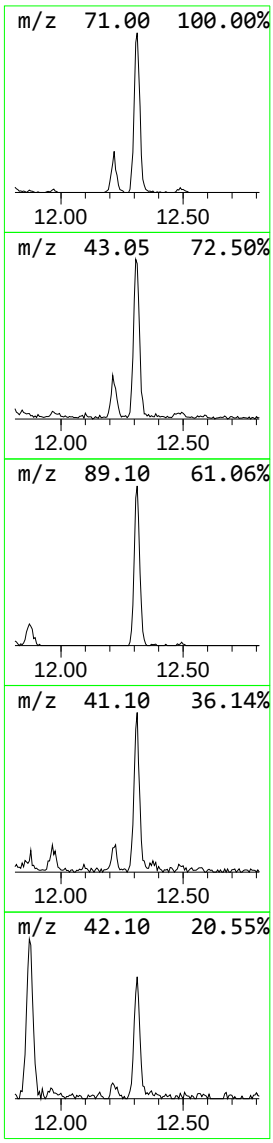
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.312	7.79 ug/l	304610	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	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5	Malic Acid	134	C4H6O5	006915-15-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078028.D
Acq On : 02 Jun 2023 13:45
Operator : JC\MD
Sample : 03008-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-18-0A

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
3-Pentanone	9.677	9.1	ug/l	296765	2	9.106	1628660	50.0
n-Propyl acetate	9.747	157.2	ug/l	5120290	2	9.106	1628660	50.0
Propanoic acid,...	10.365	34.1	ug/l	1110110	2	9.106	1628660	50.0
Isobutyl acetate	10.735	33.7	ug/l	1319890	3	11.871	1956010	50.0
Propanoic acid,...	10.994	37.9	ug/l	1483940	3	11.871	1956010	50.0
Butanoic acid, ...	11.088	7.8	ug/l	306647	3	11.871	1956010	50.0
Propanoic acid,...	11.206	67.7	ug/l	2646900	3	11.871	1956010	50.0
Acetic acid, bu...	11.294	34.1	ug/l	1332470	3	11.871	1956010	50.0
Isopropyl butyrate	11.606	103.0	ug/l	4028250	3	11.871	1956010	50.0
Butanoic acid, ...	12.312	7.8	ug/l	304610	3	11.871	1956010	50.0