LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

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: VN078056.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	139	149	156	rBV2	37301	86167	3.28%	0.462%
2	5.289	557	567	576	rBV4	23036	69919	2.66%	0.375%
3	7.571	947	955	967	rVB2	33759	81166	3.09%	0.436%
4	8.177	1046	1058	1062	rBV2	310513	738431	28.08%	3.963%
5	8.230	1062	1067	1078	rVB	514864	1157767	44.02%	6.213%
6	8.588	1117	1128	1137	rBV	308522	702651	26.72%	3.771%
7	8.694	1137	1146	1154	rBV	233236	554457	21.08%	2.975%
8	9.106	1207	1216	1232	rVB	782442	1611448	61.27%	8.647%
9	9.677	1304	1313	1318	rBV	80861	180165	6.85%	0.967%
10	9.747	1318	1325	1341	rVV	1427168	2629890	100.00%	14.112%
11	10.365	1421	1430	1438	rBV	343382	590604	22.46%	3.169%
12	10.453	1440	1445	1457	rVB6	10986	31061	1.18%	0.167%
13	10.571	1457	1465	1475	rBV	1194746	2241085	85.22%	12.026%
14	10.735	1486	1493	1501	rVB	322534	540743	20.56%	2.902%
15	10.994	1529	1537	1544	rBV	336211	573614	21.81%	3.078%
16	11.088	1546	1553	1562	rVV4	53305	106003	4.03%	0.569%
17	11.176	1562	1568	1570	rVV	168617	286904	10.91%	1.540%
18	11.206	1570	1573	1582	rVV	364316	602967	22.93%	3.236%
19	11.294	1582	1588	1602	rVB	172383	299425	11.39%	1.607%
20	11.606	1634	1641	1653	rBV	632522	996773	37.90%	5.349%
21	11.871	1677	1686	1699	rBV	1049015	1914235	72.79%	10.272%
22	12.312	1754	1761	1768	rBV4	20075	34805	1.32%	0.187%
23	12.853	1842	1853	1865	rBV	764248	1364313	51.88%	7.321%
24	13.800	2007	2014	2021	rBV	718107	1240690	47.18%	6.658%

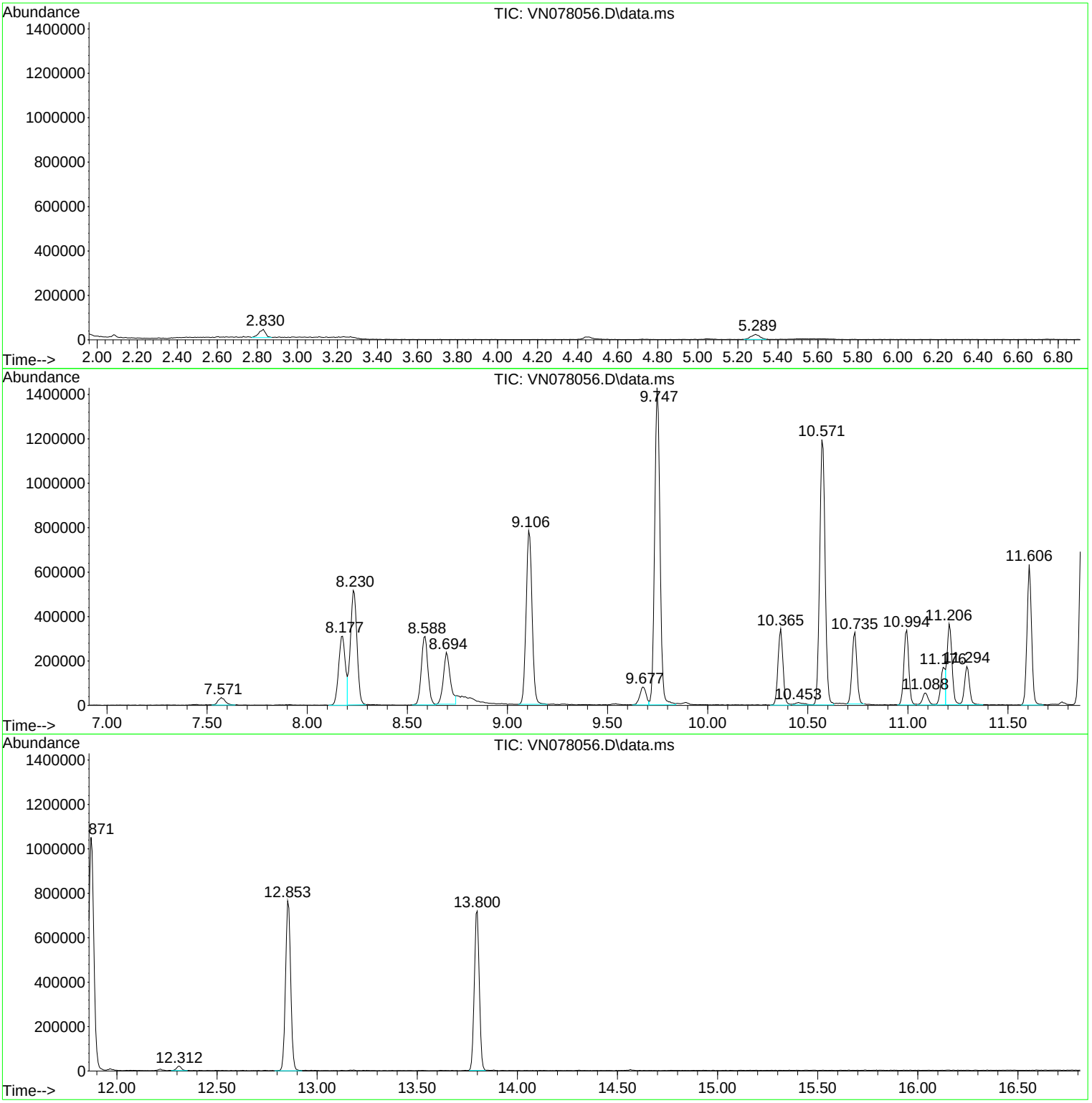
Sum of corrected areas: 18635283

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

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 : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

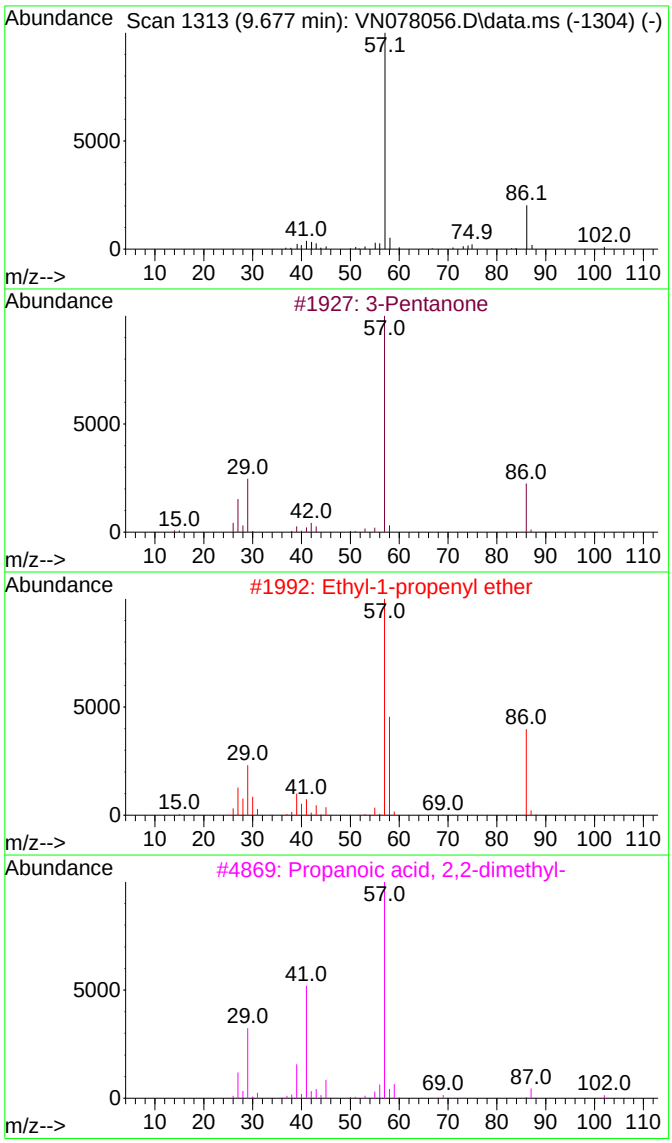
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

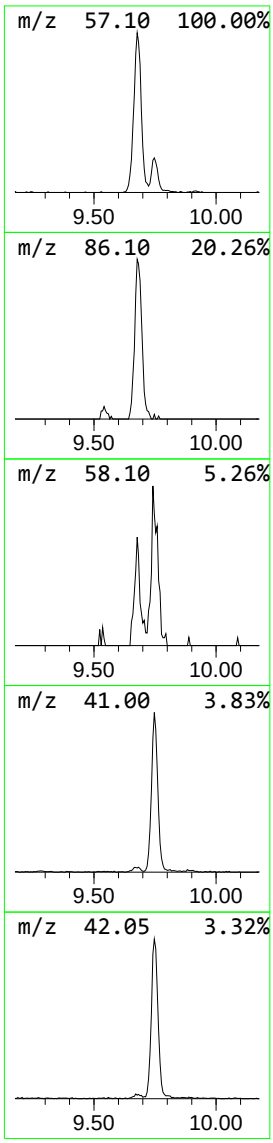
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	5.59 ug/l	180165	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	64
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	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

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

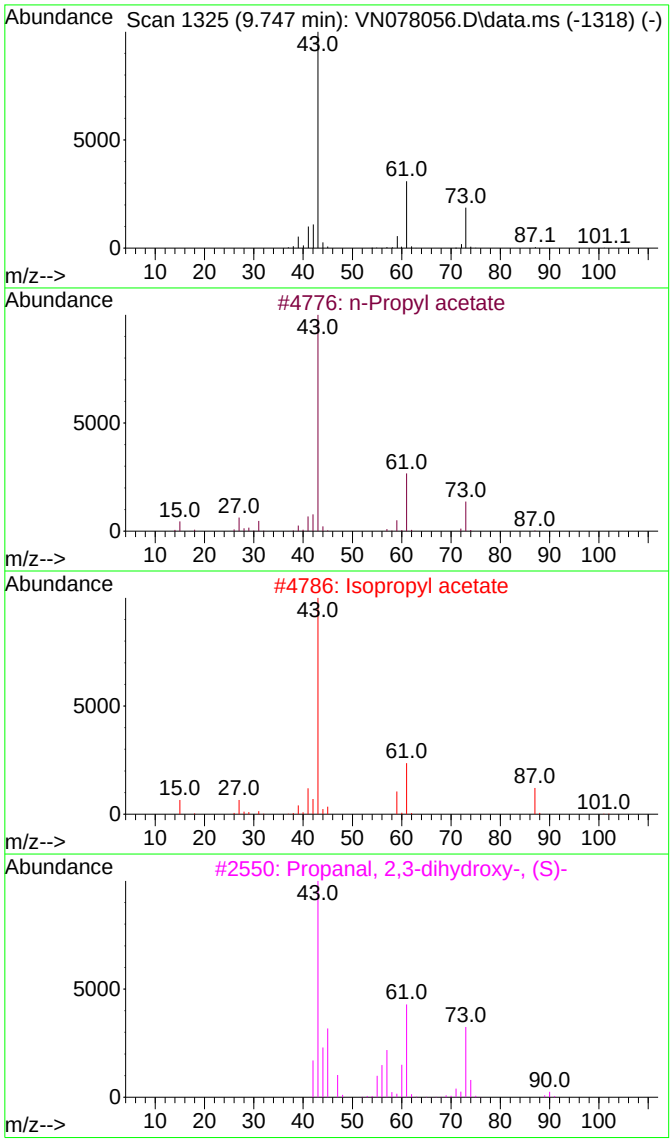
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

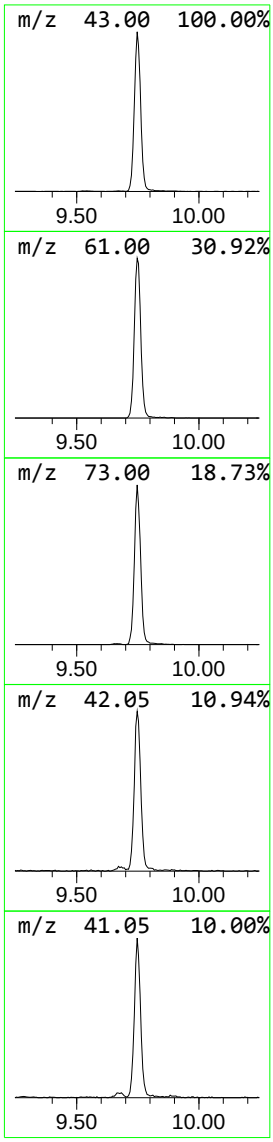
****

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	81.60 ug/l	2629890	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	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	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

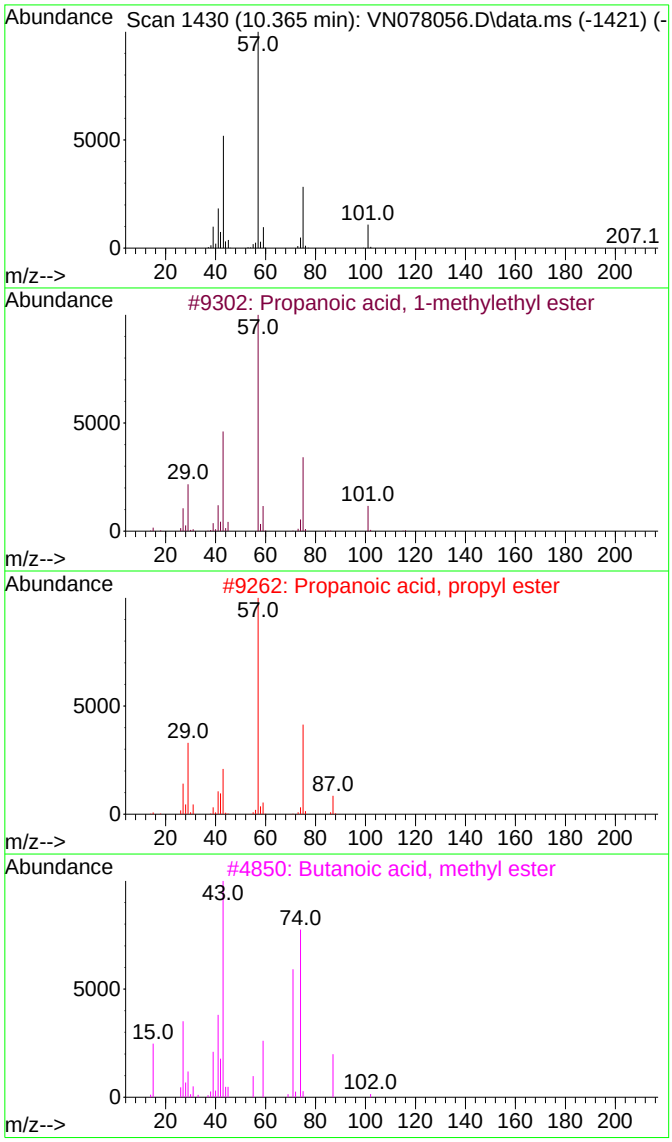
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

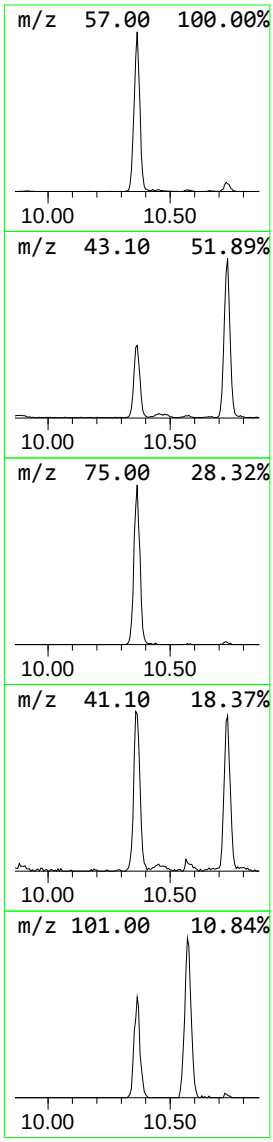
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	18.33 ug/l	590604	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	28
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	22
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

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

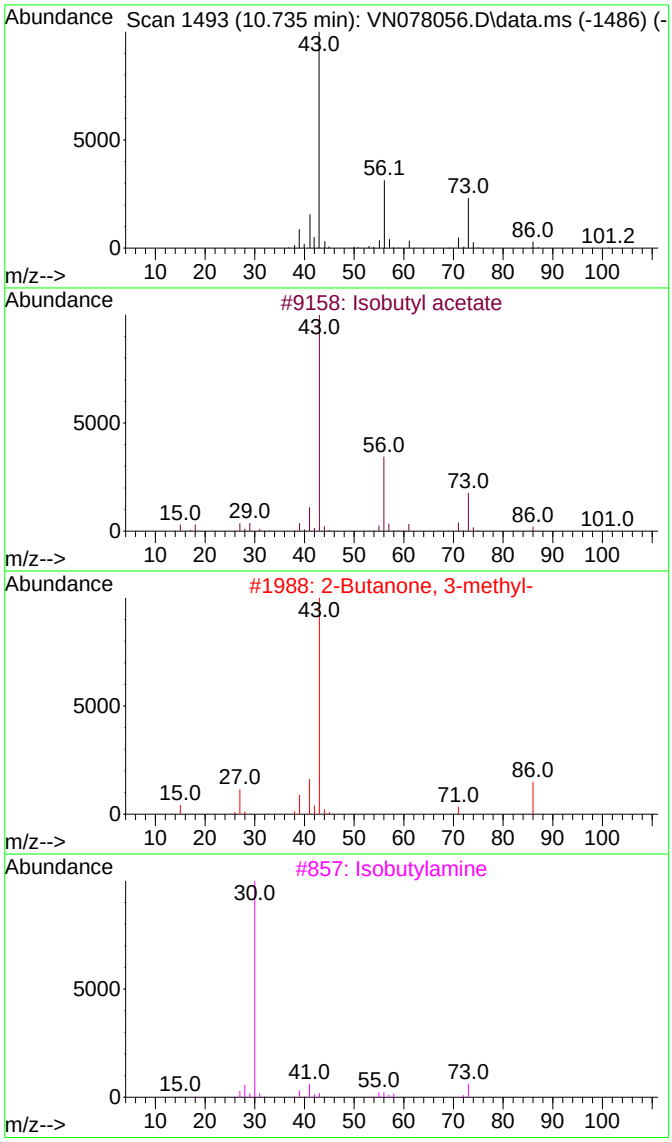
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

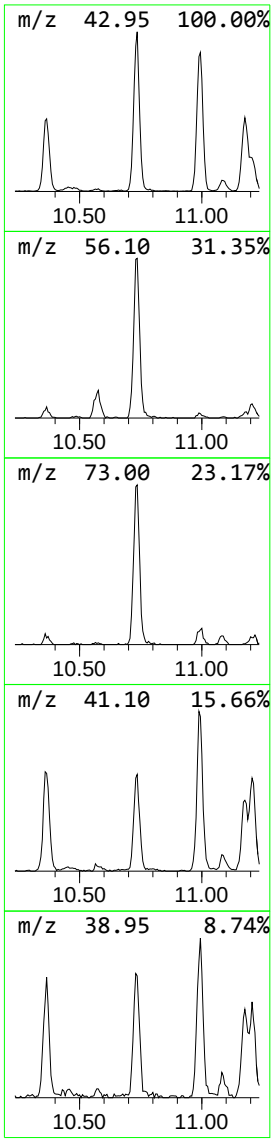
****

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	14.12 ug/l	540743	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	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

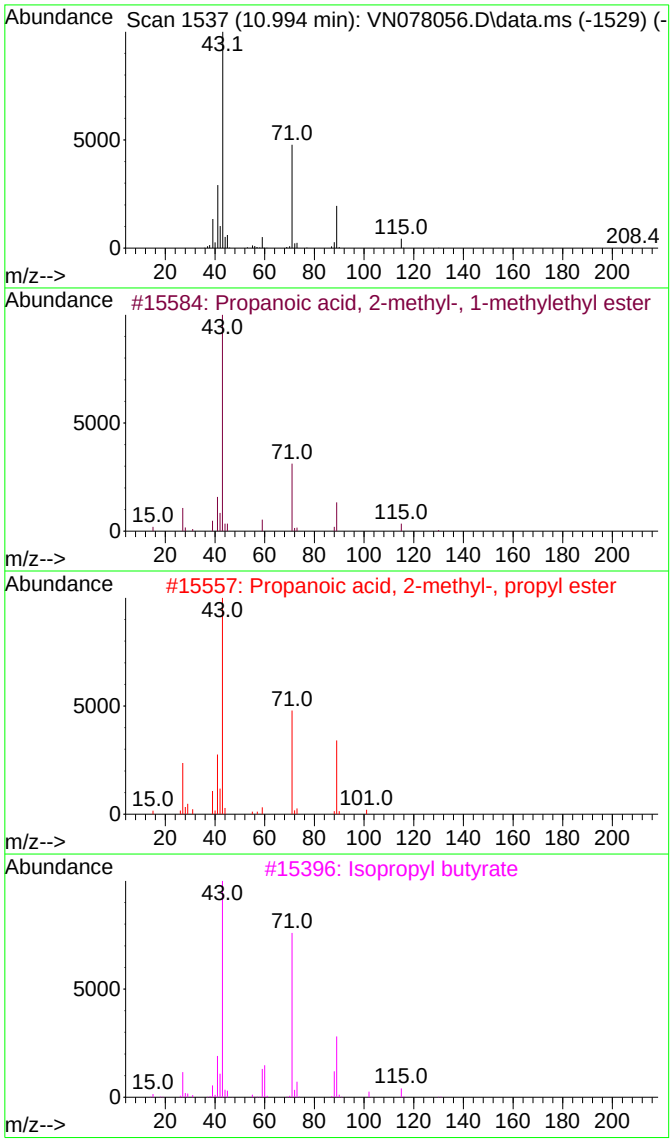
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

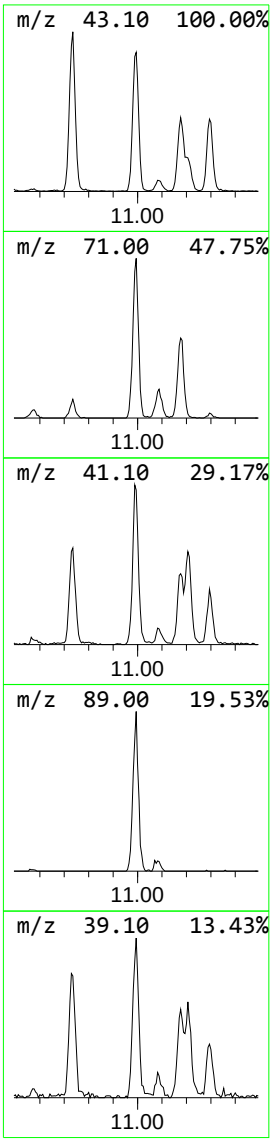
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	14.98 ug/l	573614	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	72
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	40
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

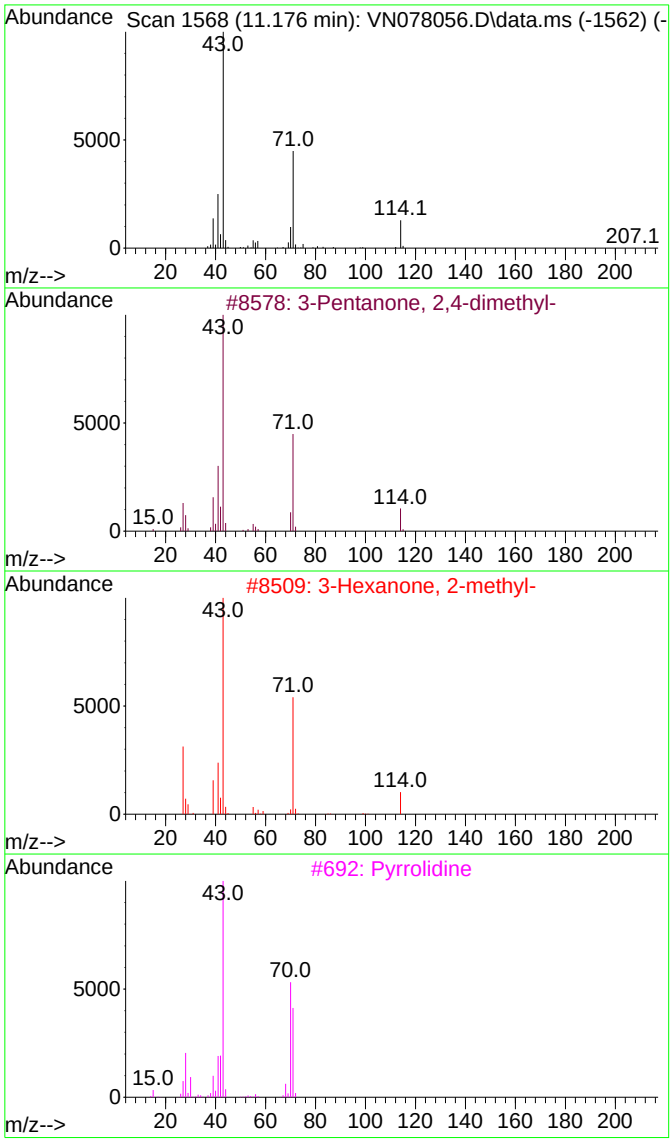
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

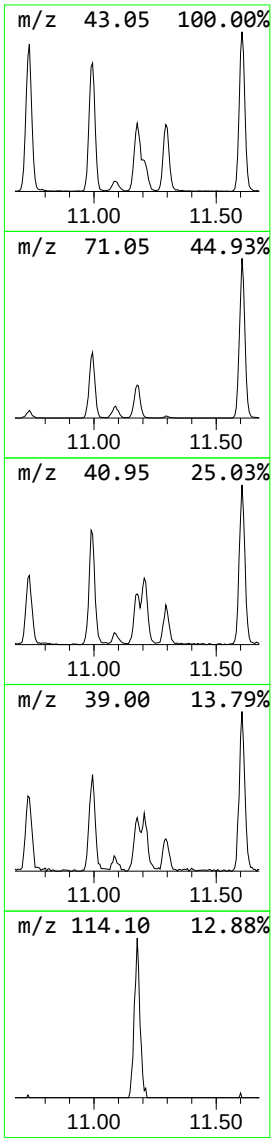
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.176	7.49 ug/l	286904	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
3	Pyrrolidine	71	C4H9N	000123-75-1	50
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	38
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

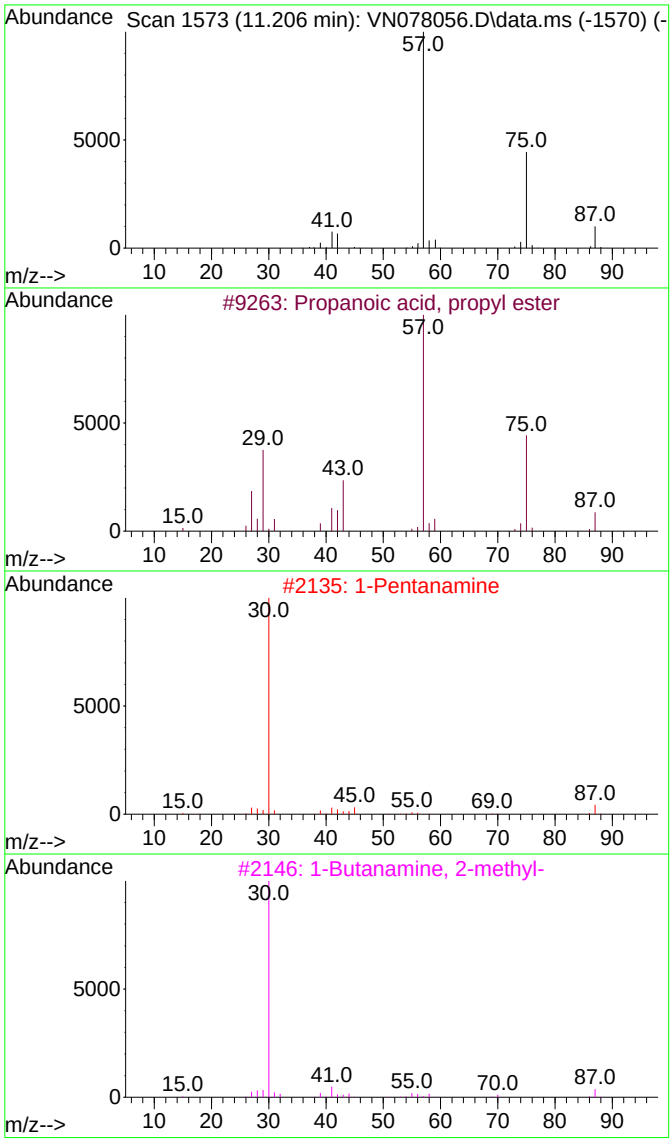
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

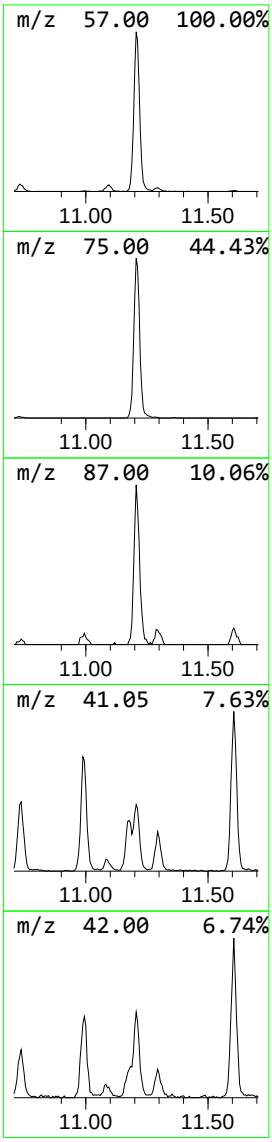
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	15.75 ug/l	602967	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	1-Pentanamine	87	C5H13N	000110-58-7	7
3	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

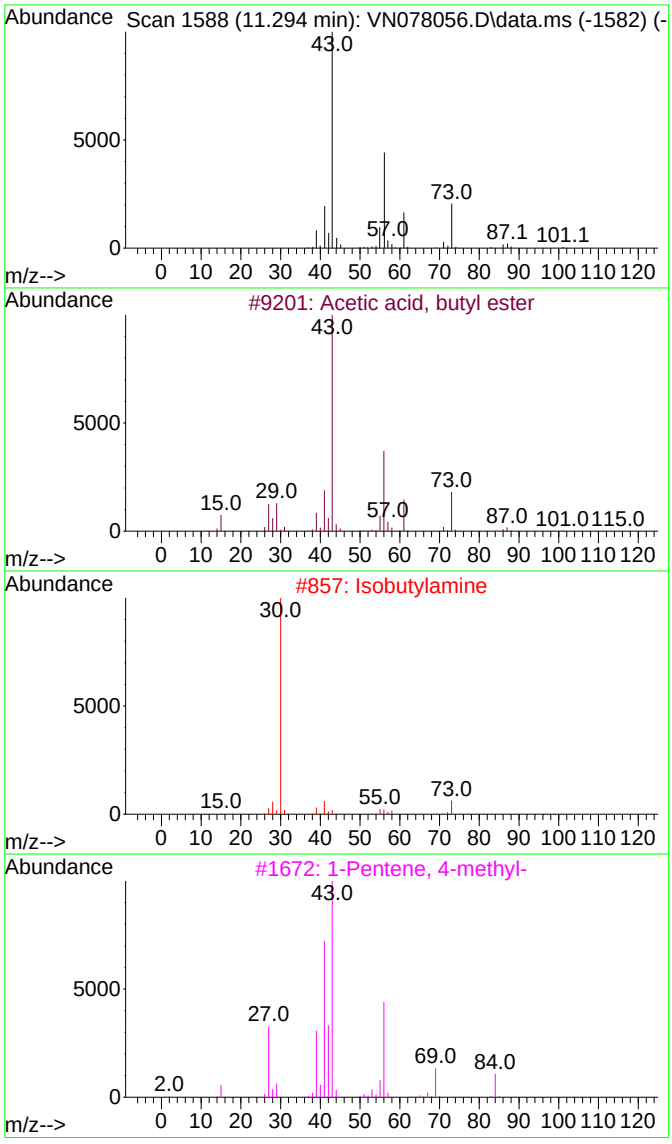
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

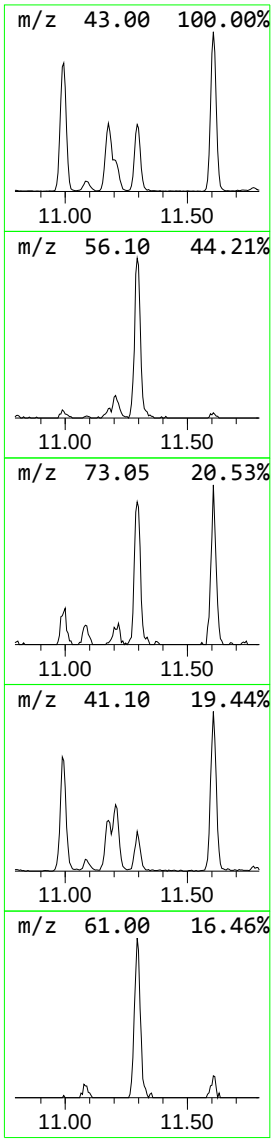
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	7.82 ug/l	299425	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	Isobutylamine	73	C4H11N	000078-81-9	9
3	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	9
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

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

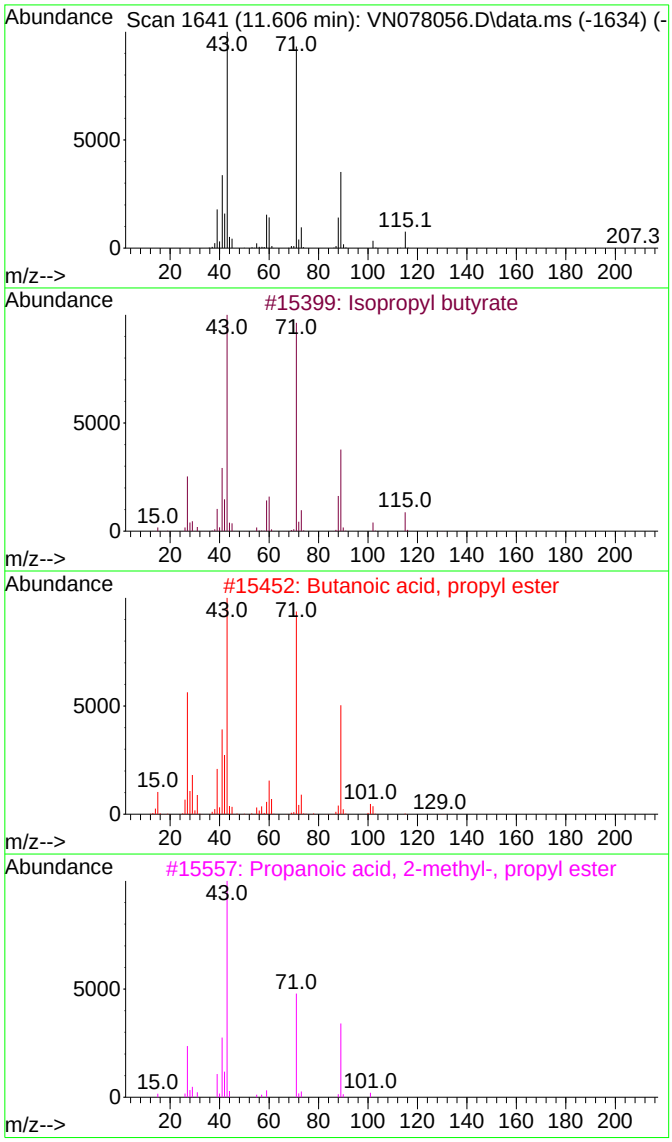
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

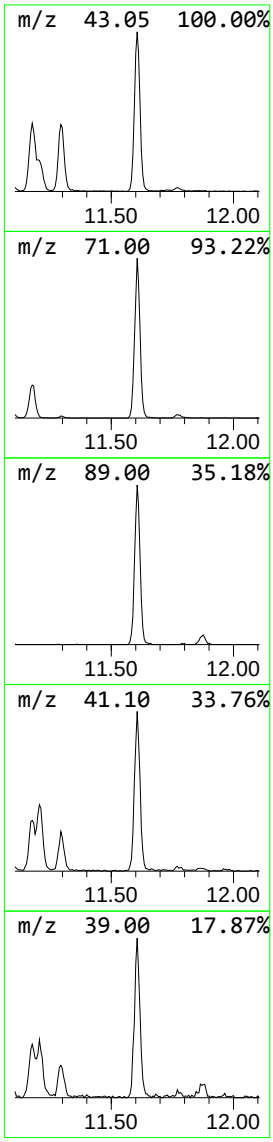
****

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	26.04 ug/l	996773	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	64
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078056.D
Acq On : 05 Jun 2023 19:57
Operator : JC\MD
Sample : 03018-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
278

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	5.6	ug/l	180165	2	9.106	1611450	50.0
n-Propyl acetate	9.747	81.6	ug/l	2629890	2	9.106	1611450	50.0
Propanoic acid,...	10.365	18.3	ug/l	590604	2	9.106	1611450	50.0
Isobutyl acetate	10.735	14.1	ug/l	540743	3	11.871	1914240	50.0
Propanoic acid,...	10.994	15.0	ug/l	573614	3	11.871	1914240	50.0
3-Pentanone, 2,...	11.176	7.5	ug/l	286904	3	11.871	1914240	50.0
Propanoic acid,...	11.206	15.8	ug/l	602967	3	11.871	1914240	50.0
Acetic acid, bu...	11.294	7.8	ug/l	299425	3	11.871	1914240	50.0
Isopropyl butyrate	11.606	26.0	ug/l	996773	3	11.871	1914240	50.0