LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070588.D
Acq On : 12 Jan 2022 16:01
Operator : JC/MD
Sample : N1097-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-1D

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\82N122721W.M
Title : SW846 8260

Signal : TIC: VN070588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	81	91	101	rBV2	116730	250060	1.53%	0.366%
2	8.021	2226	2249	2260	rBV	563147	1351176	8.26%	1.977%
3	8.083	2260	2272	2300	rVB2	1078310	2492442	15.24%	3.647%
4	8.437	2383	2404	2432	rBV	700154	1611751	9.85%	2.358%
5	8.561	2434	2450	2465	rBV	100849	218402	1.34%	0.320%
6	8.705	2473	2504	2505	rBV	56138	183113	1.12%	0.268%
7	8.965	2582	2601	2627	rBV	1682791	3512389	21.47%	5.139%
8	9.547	2800	2818	2829	rBV3	109050	249829	1.53%	0.366%
9	9.623	2829	2846	2886	rVV	6579341	12271652	75.03%	17.956%
10	10.242	3060	3077	3099	rBV	996987	1774289	10.85%	2.596%
11	10.441	3133	3151	3172	rBV	2442207	4549145	27.81%	6.656%
12	10.612	3204	3215	3236	rVB2	112797	211104	1.29%	0.309%
13	10.872	3297	3312	3328	rBV2	268480	464175	2.84%	0.679%
14	10.964	3331	3346	3367	rVV2	621429	1087736	6.65%	1.592%
15	11.090	3370	3393	3413	rVV	9487642	16356417	100.00%	23.933%
16	11.175	3414	3425	3465	rVB	1024221	1921274	11.75%	2.811%
17	11.489	3525	3542	3576	rBV	5776483	9616685	58.79%	14.071%
18	11.741	3620	3636	3669	rVB	2232881	4052019	24.77%	5.929%
19	12.195	3792	3805	3824	rBV2	150814	261292	1.60%	0.382%
20	12.731	3986	4005	4036	rBV	1684183	3009000	18.40%	4.403%
21	13.672	4340	4356	4377	rBV	1610541	2898256	17.72%	4.241%

Sum of corrected areas: 68342206

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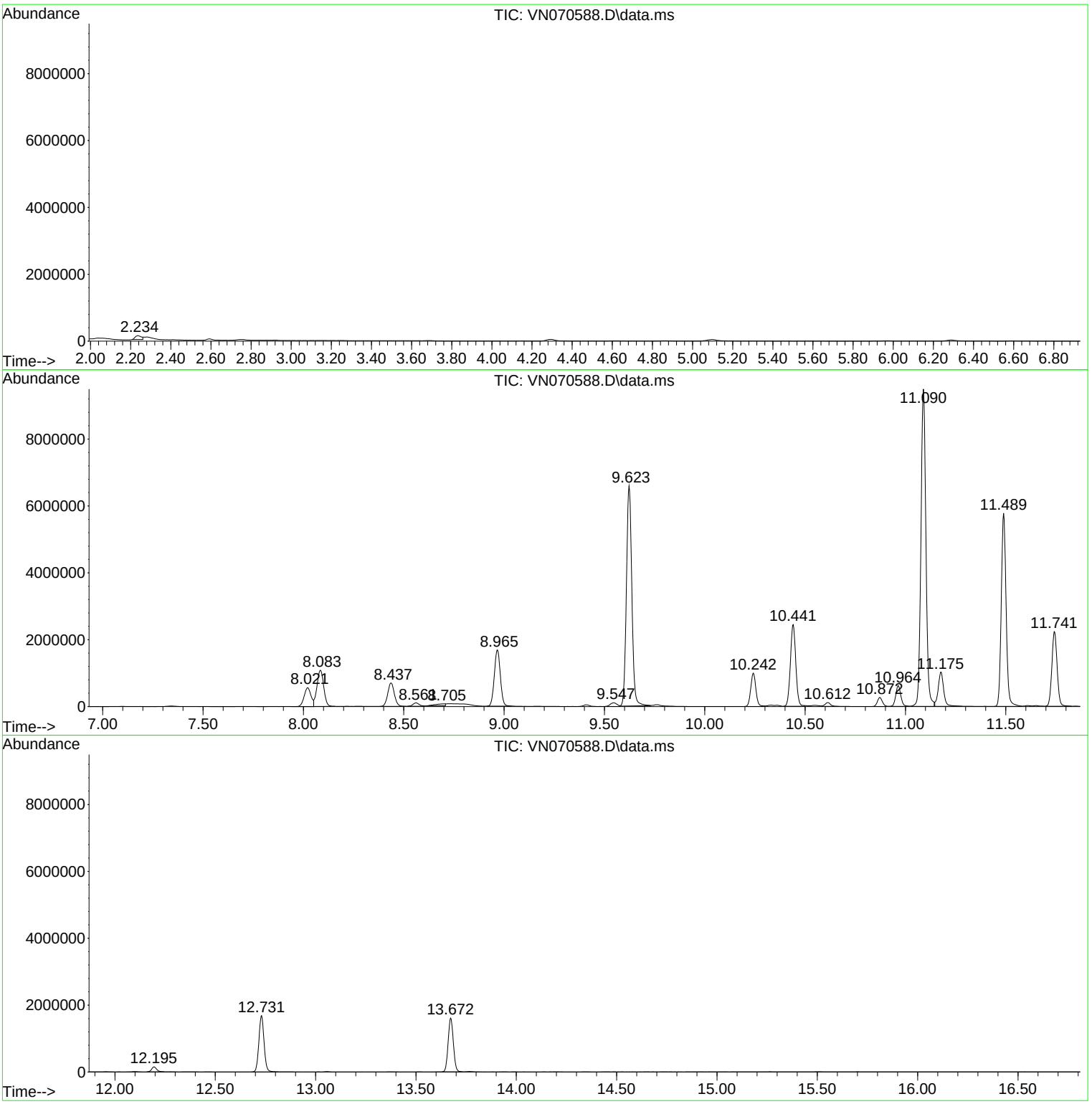
ClientSampleId :
TP-1D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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Data File : VN070588.D
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Quant Title : SW846 8260

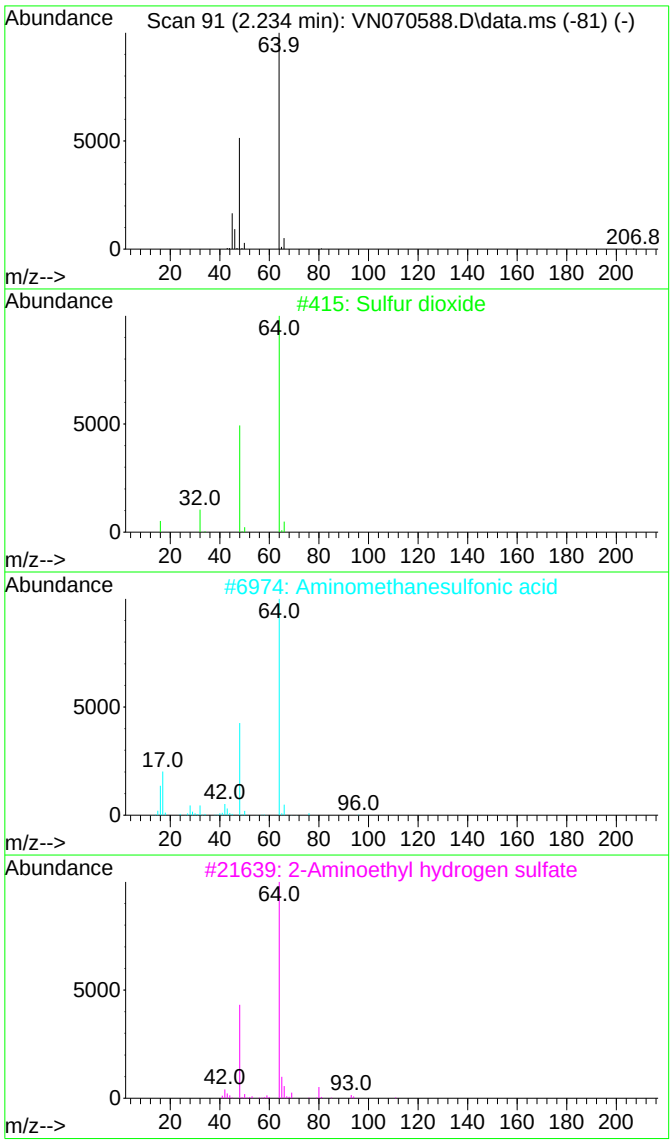
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

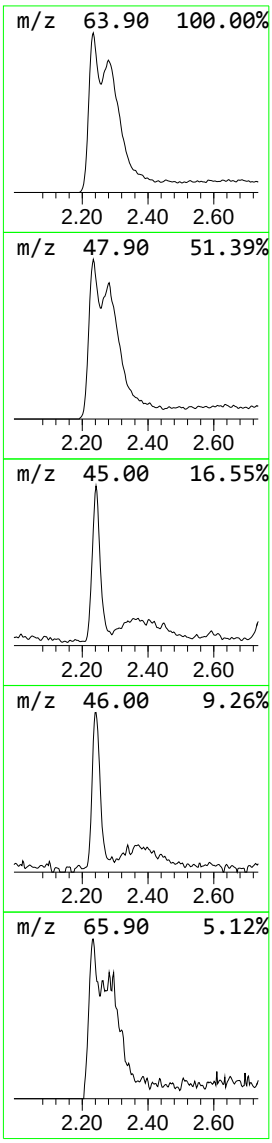
****

Peak Number 1 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	5.02 ug/l	250060	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	64
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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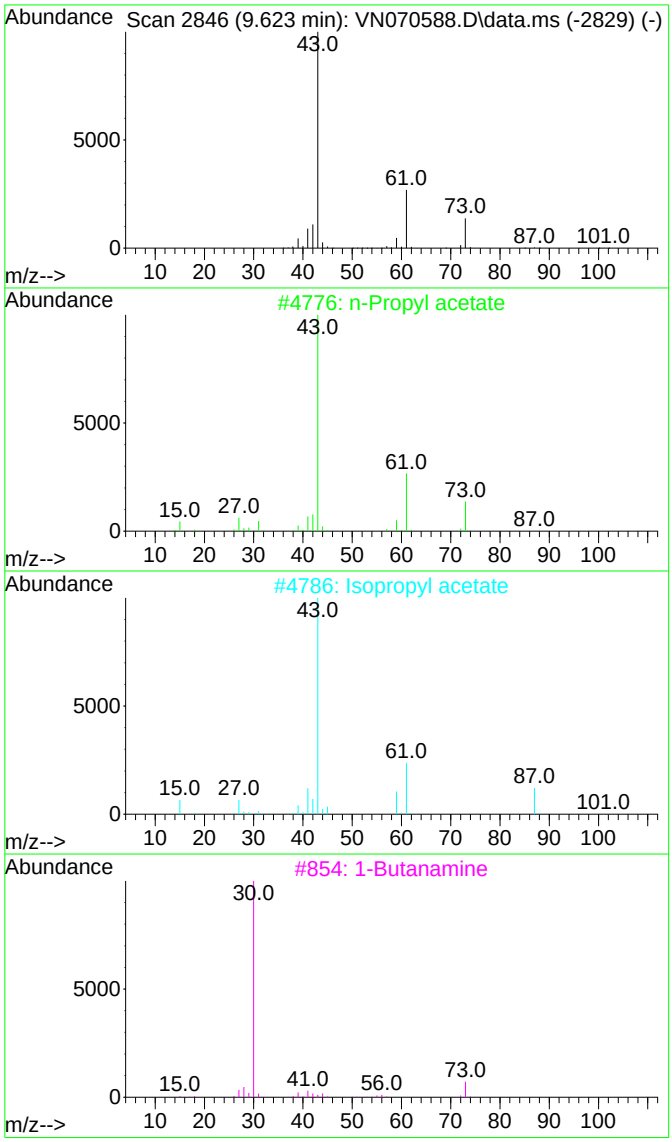
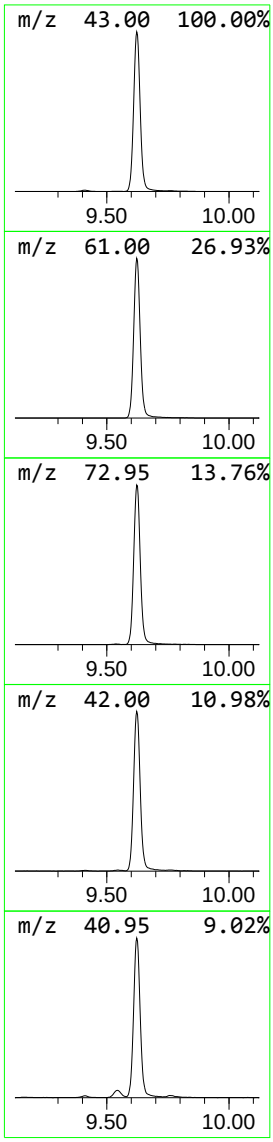
****
Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.623	174.69 ug/l	12271700	1,4-Difluorobenzene	8.968

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	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Hydrogen azide	43	HN3	007782-79-8	4





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Operator : JC/MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-1D

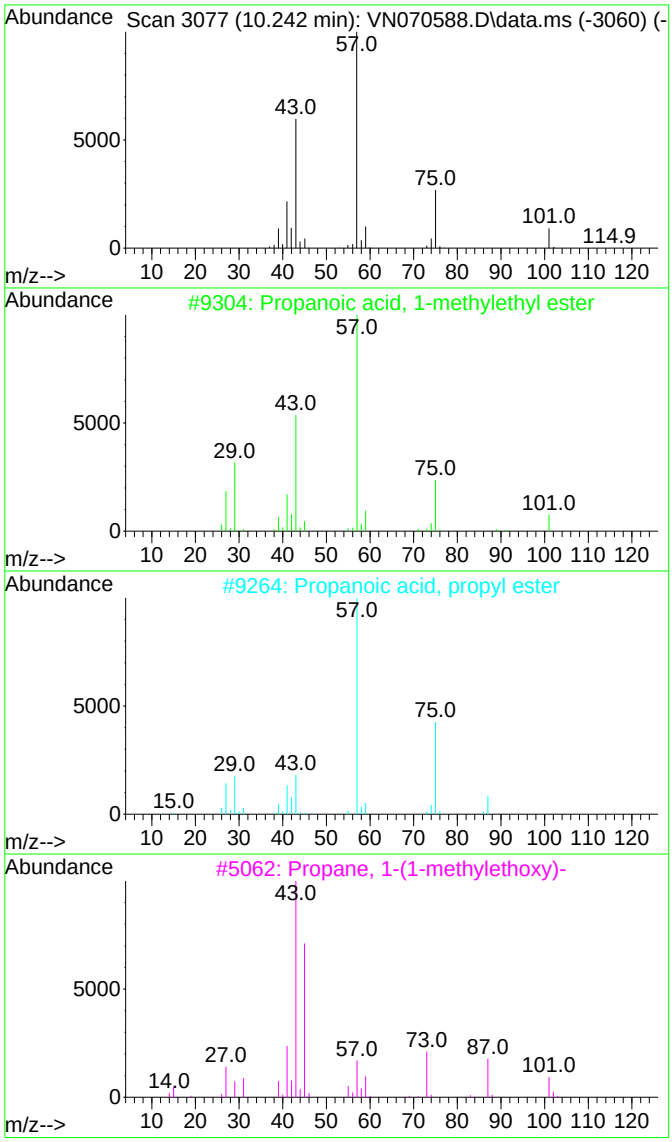
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

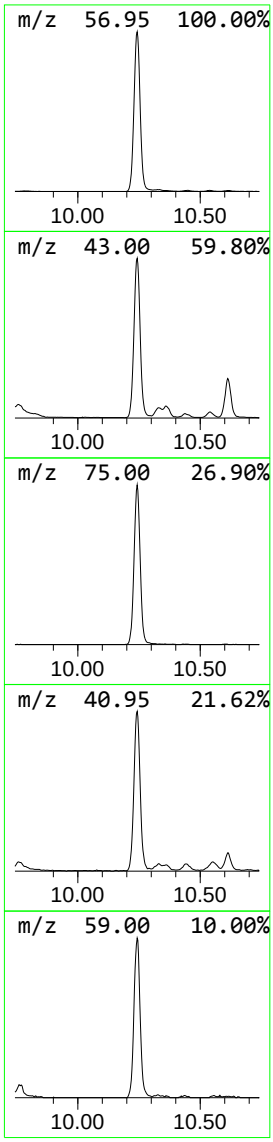
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.242	25.26 ug/l	1774290	1,4-Difluorobenzene	8.968

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	45
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	14
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-1D

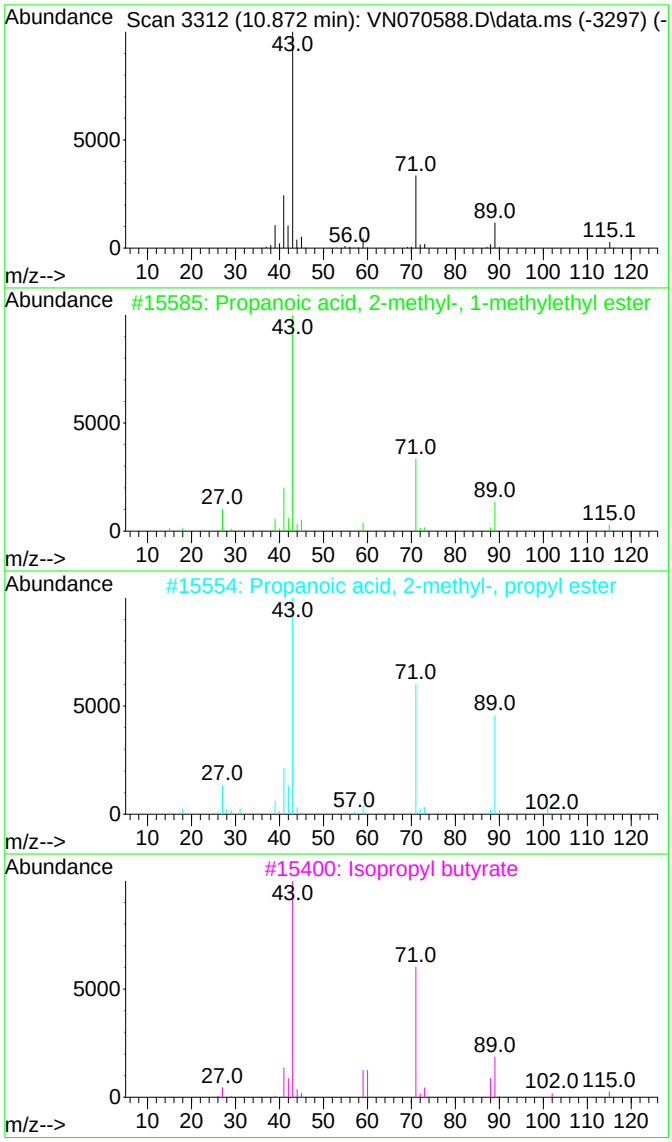
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

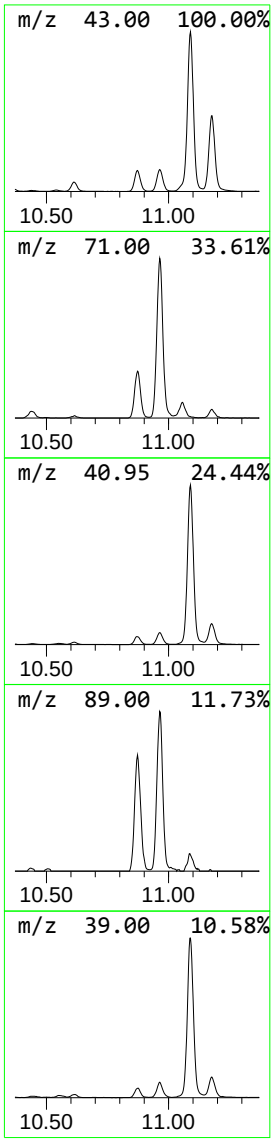
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.872	5.73 ug/l	464175	Chlorobenzene-d5	11.741

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	72
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 : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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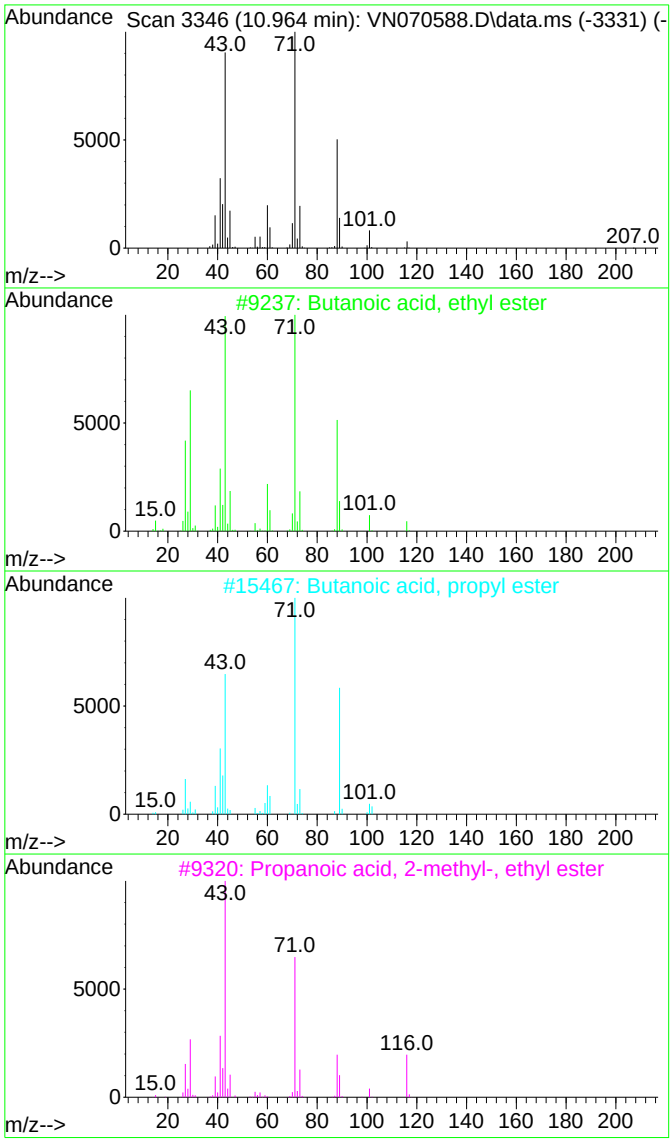
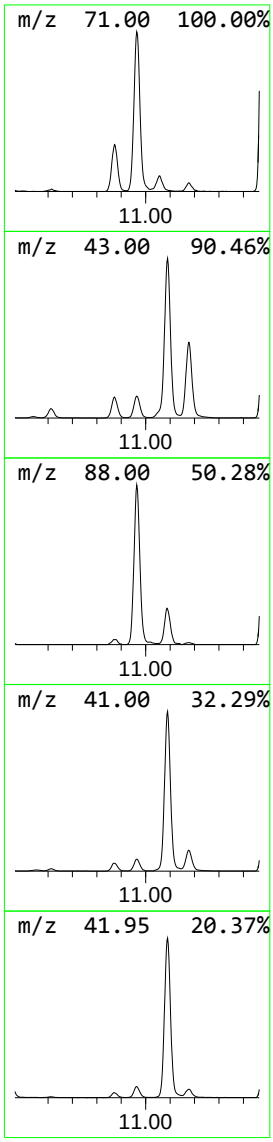
****
Peak Number 5 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.964	13.42 ug/l	1087740	Chlorobenzene-d5	11.741

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
3	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	50
4	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	43
5	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-1D

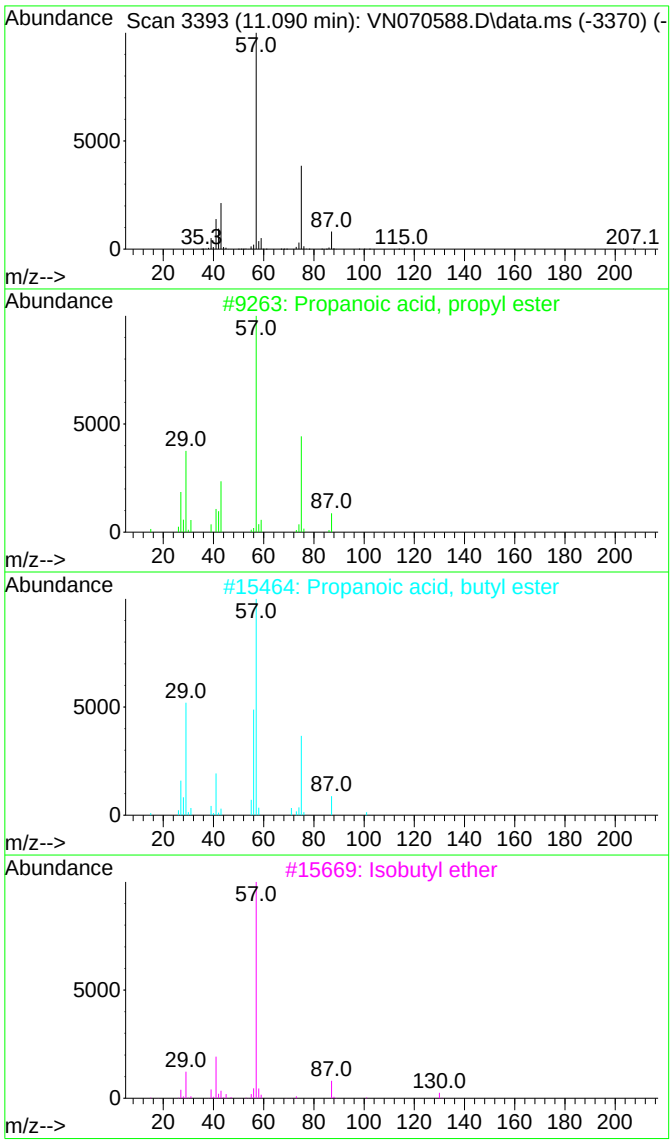
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

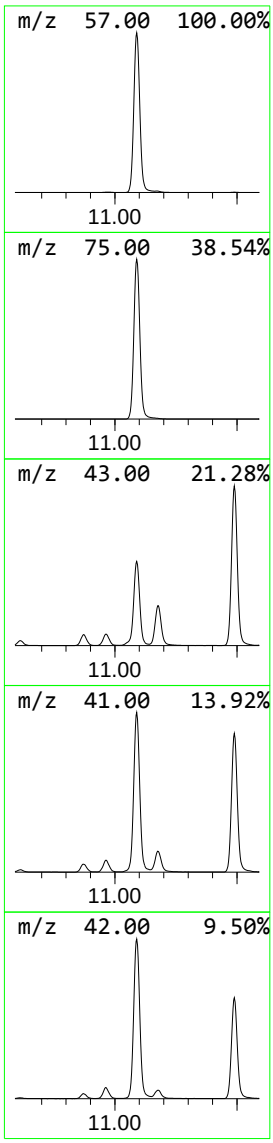
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.090	201.83 ug/l	16356400	Chlorobenzene-d5	11.741

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	38
3	Isobutyl ether	130	C8H18O	000628-55-7	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Instrument :
MSVOA_N
ClientSampleId :
TP-1D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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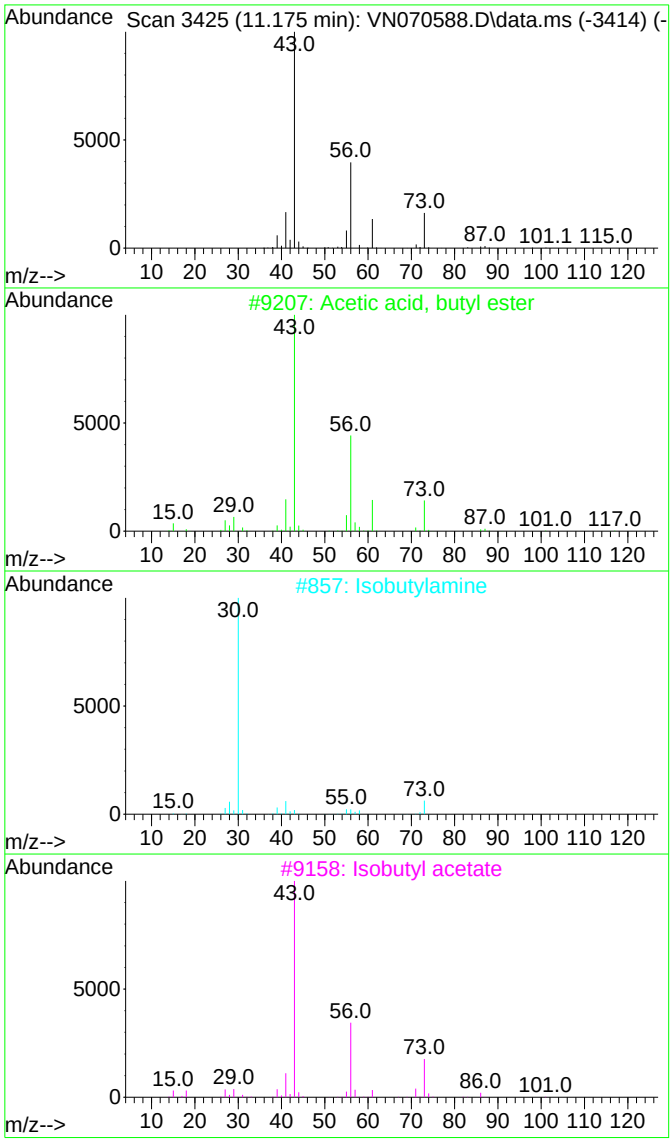
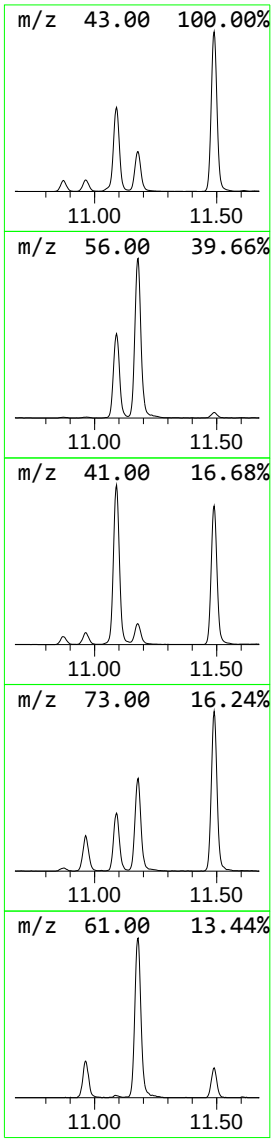
****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.175	23.71 ug/l	1921270	Chlorobenzene-d5	11.741

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	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
5	1-Butanamine	73	C4H11N	000109-73-9	5





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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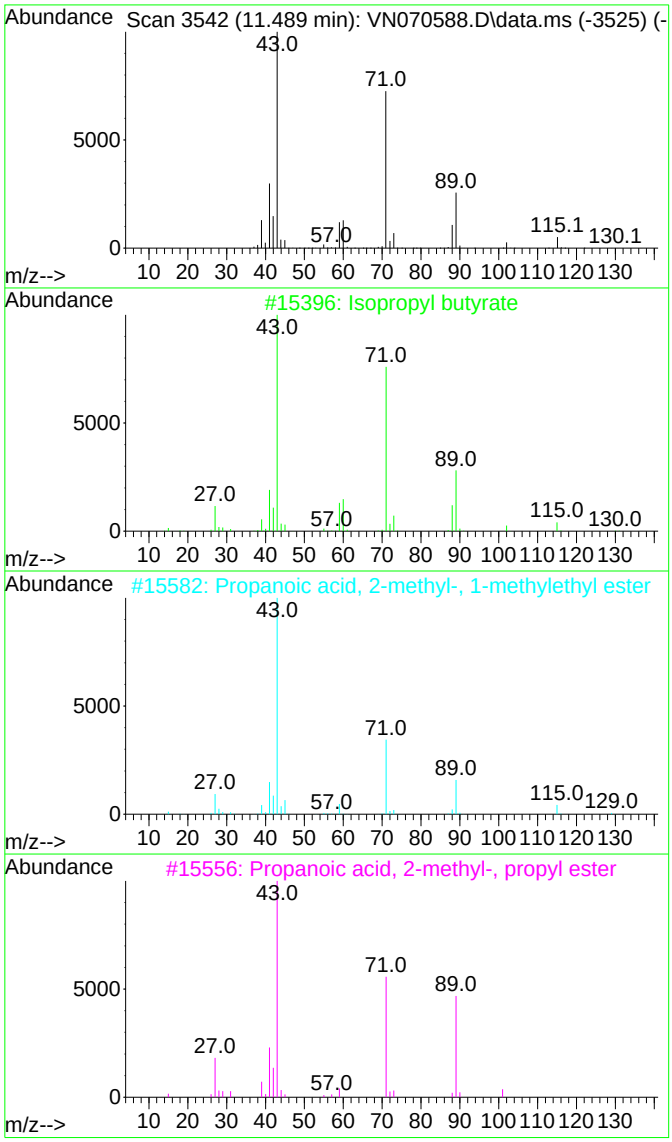
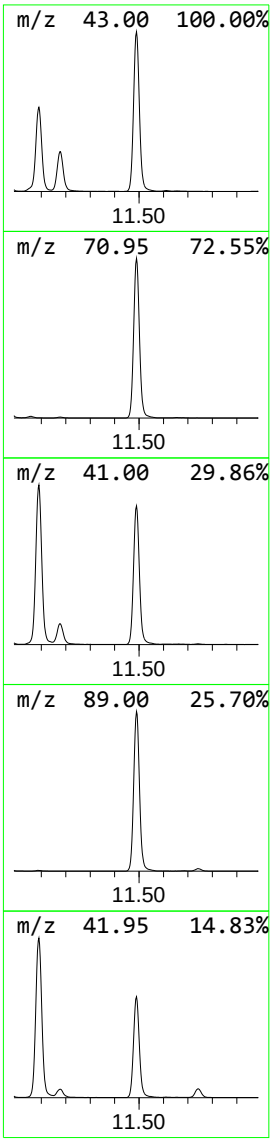
****
Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.489	118.67 ug/l	9616690	Chlorobenzene-d5	11.741

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	59
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	2.234	5.0	ug/l	250060	1	8.086	2492440	50.0
n-Propyl acetate	9.623	174.7	ug/l	12271700	2	8.968	3512390	50.0
Propanoic acid,...	10.242	25.3	ug/l	1774290	2	8.968	3512390	50.0
Propanoic acid,...	10.872	5.7	ug/l	464175	3	11.741	4052020	50.0
Butanoic acid, ...	10.964	13.4	ug/l	1087740	3	11.741	4052020	50.0
Propanoic acid,...	11.090	201.8	ug/l	16356400	3	11.741	4052020	50.0
Acetic acid, bu...	11.175	23.7	ug/l	1921270	3	11.741	4052020	50.0
Isopropyl butyrate	11.489	118.7	ug/l	9616690	3	11.741	4052020	50.0