LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011222\
Data File : VN070587.D
Acq On : 12 Jan 2022 15:35
Operator : JC/MD
Sample : N1097-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-1S

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: VN070587.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	79	91	102	rBV2	107081	245111	1.66%	0.376%
2	8.021	2222	2249	2260	rBV2	625786	1520594	10.30%	2.330%
3	8.086	2260	2273	2299	rVB	1083608	2478095	16.79%	3.797%
4	8.437	2382	2404	2433	rBV	796456	1831170	12.40%	2.806%
5	8.560	2435	2450	2472	rVB2	96888	218775	1.48%	0.335%
6	8.965	2581	2601	2630	rBV	1679731	3486045	23.62%	5.341%
7	9.547	2798	2818	2829	rBV3	102644	241446	1.64%	0.370%
8	9.622	2829	2846	2887	rVV	5951428	11218723	76.00%	17.189%
9	10.242	3060	3077	3097	rBV	979953	1721331	11.66%	2.637%
10	10.440	3133	3151	3168	rBV	2748453	5122833	34.70%	7.849%
11	10.612	3204	3215	3233	rVB2	90324	169918	1.15%	0.260%
12	10.872	3295	3312	3328	rBV	260939	451939	3.06%	0.692%
13	10.963	3331	3346	3368	rVV2	542440	951124	6.44%	1.457%
14	11.089	3369	3393	3413	rBV	8628006	14761760	100.00%	22.618%
15	11.175	3415	3425	3448	rVB	779031	1398178	9.47%	2.142%
16	11.489	3524	3542	3577	rBV	5308290	9016525	61.08%	13.815%
17	11.741	3620	3636	3666	rVB	2212401	4028046	27.29%	6.172%
18	12.194	3790	3805	3825	rBV2	114713	203911	1.38%	0.312%
19	12.728	3987	4004	4029	rBV	1854801	3348006	22.68%	5.130%
20	13.672	4339	4356	4381	rBV	1606565	2852655	19.32%	4.371%

Sum of corrected areas: 65266185

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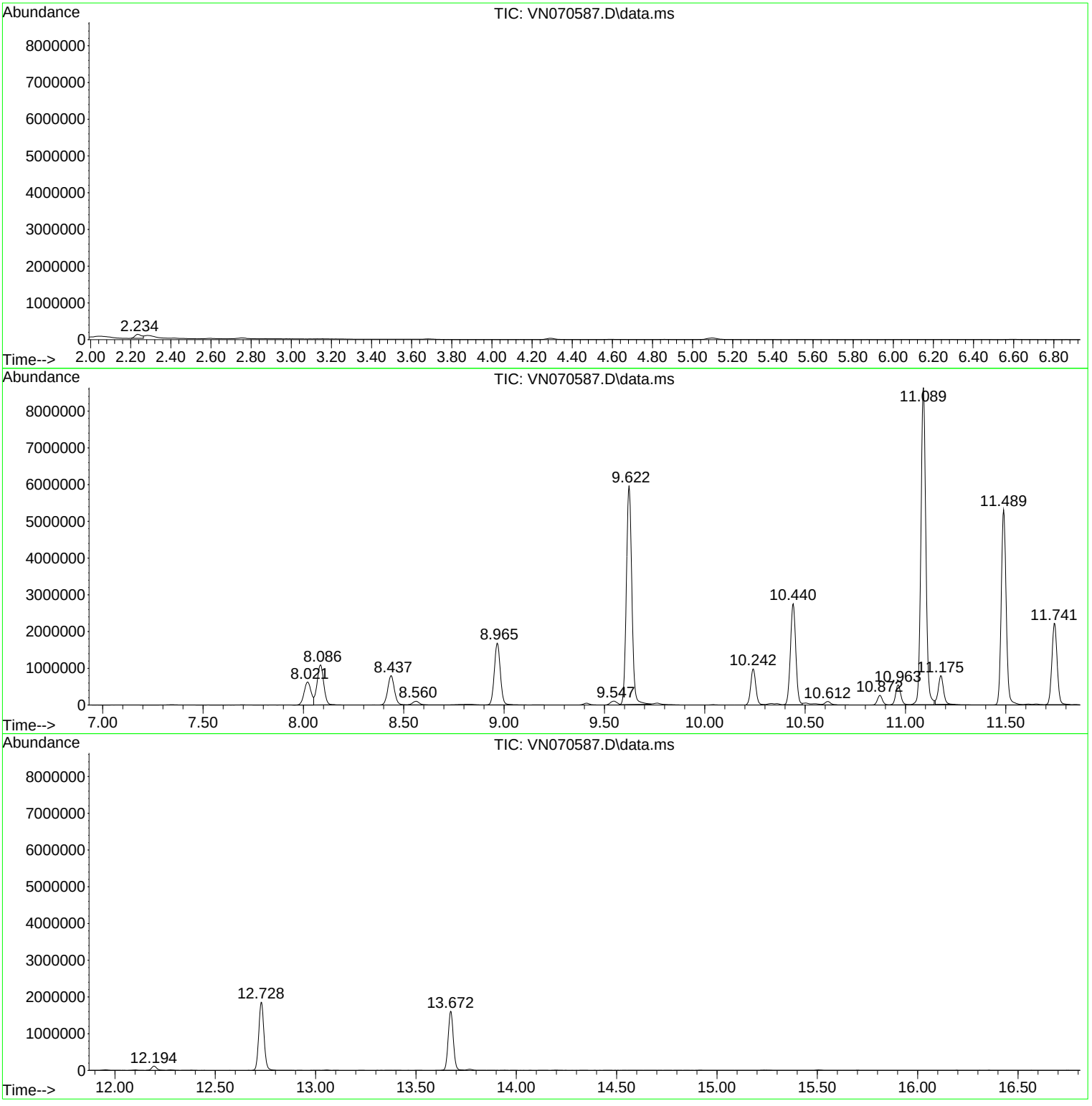
ClientSampleId :
TP-1S

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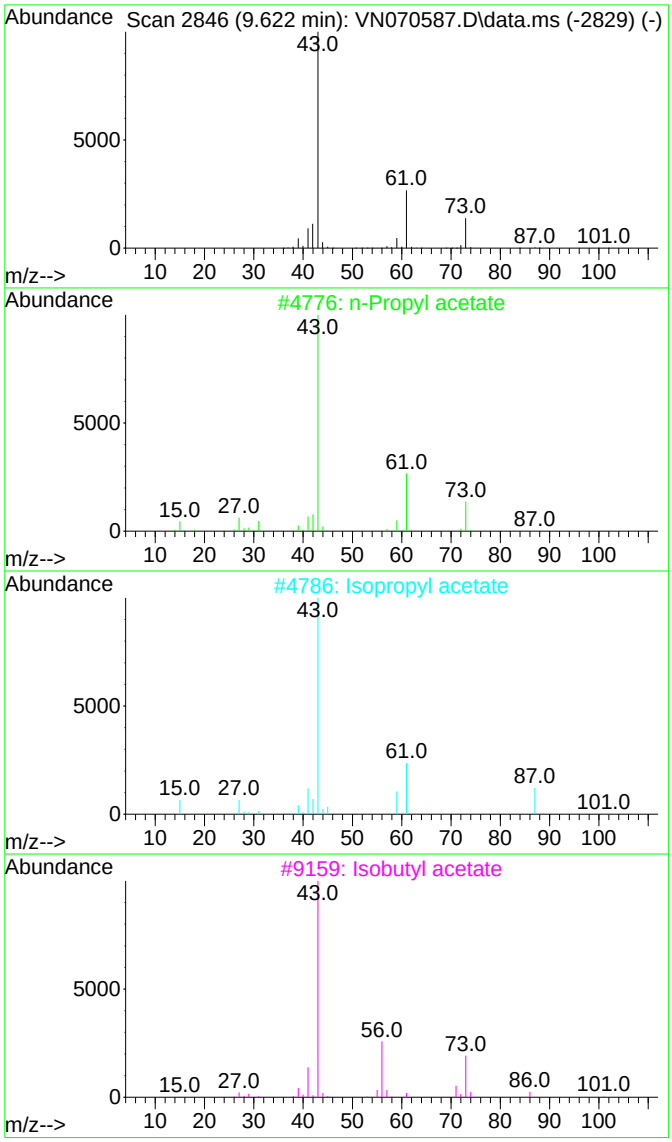
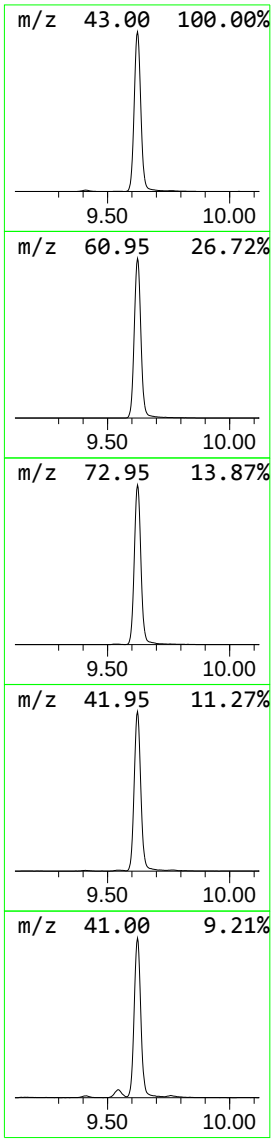
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.622	160.91 ug/l	11218700	1,4-Difluorobenzene	8.965

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	5





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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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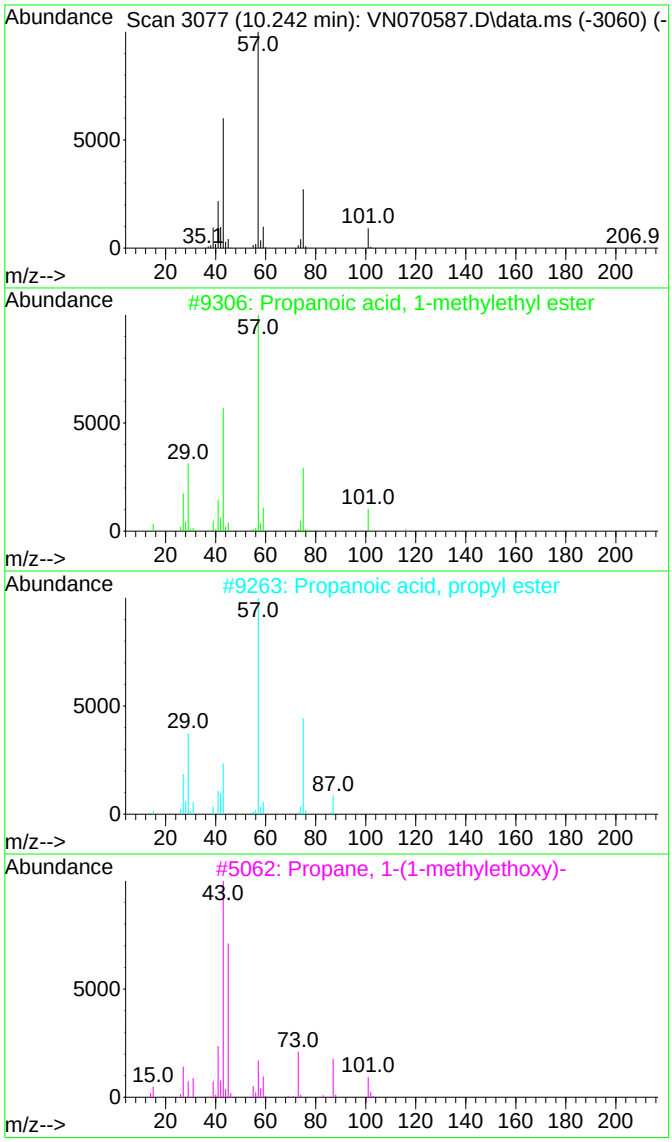
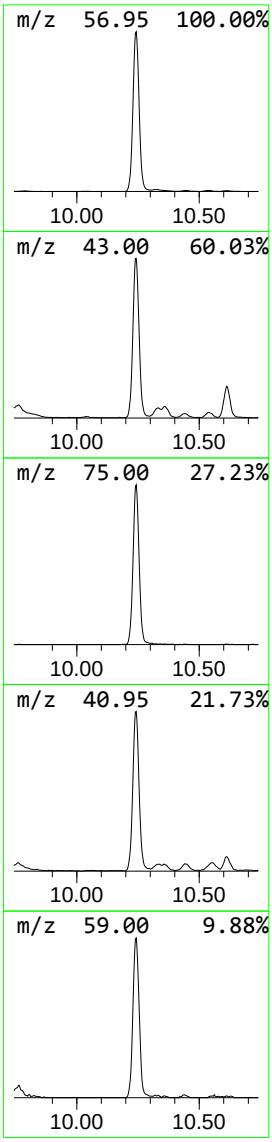
****
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.242	24.69 ug/l	1721330	1,4-Difluorobenzene	8.965

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	59
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	14
5	Azetidine	57	C3H7N	000503-29-7	12





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ALS Vial : 11 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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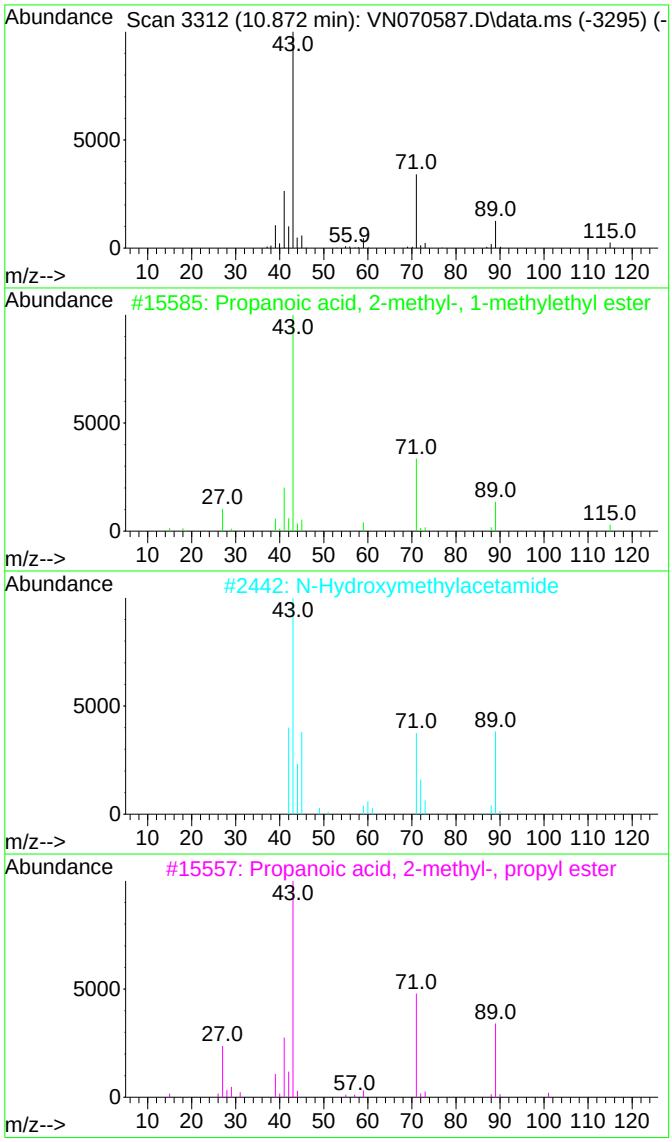
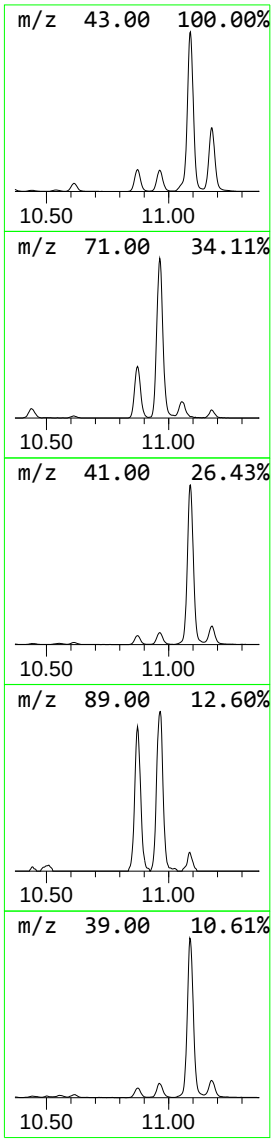
****
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.872	5.61 ug/l	451939	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	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	53
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	45
4	Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	42
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42





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Instrument :
MSVOA_N
ClientSampleId :
TP-1S

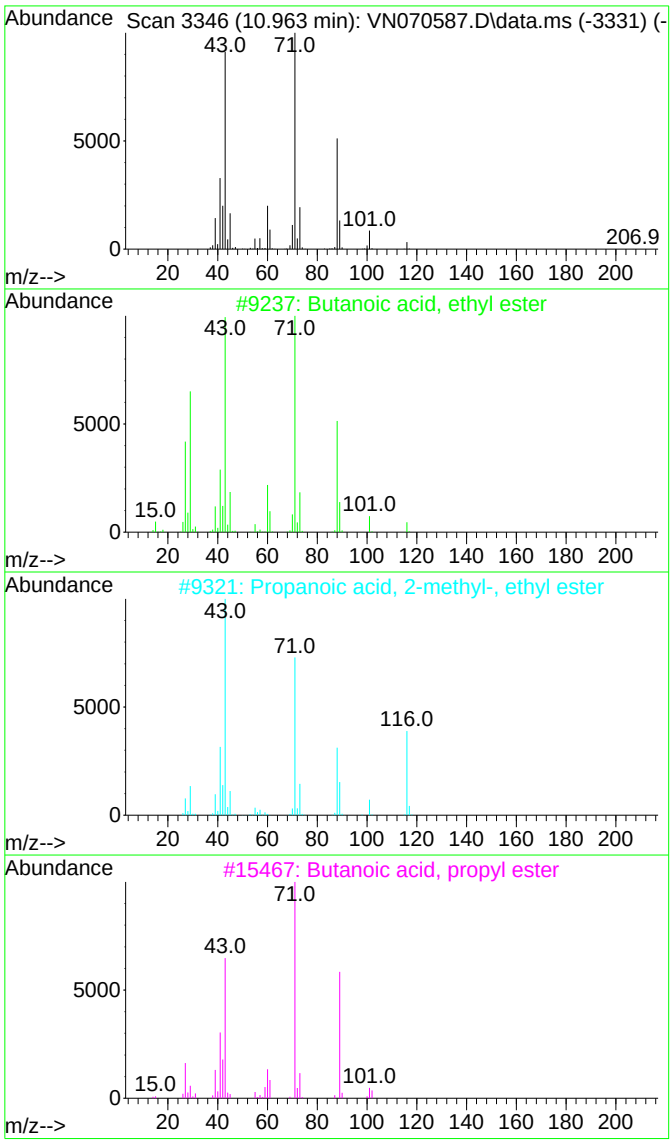
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

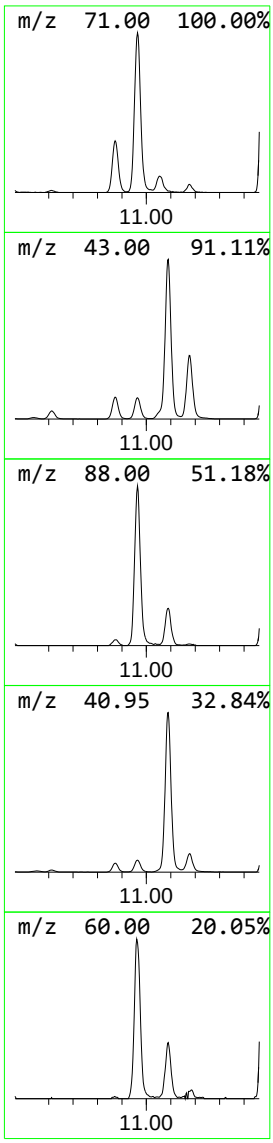
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.963	11.81 ug/l	951124	Chlorobenzene-d5	11.741

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	95
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	58
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
4	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	38





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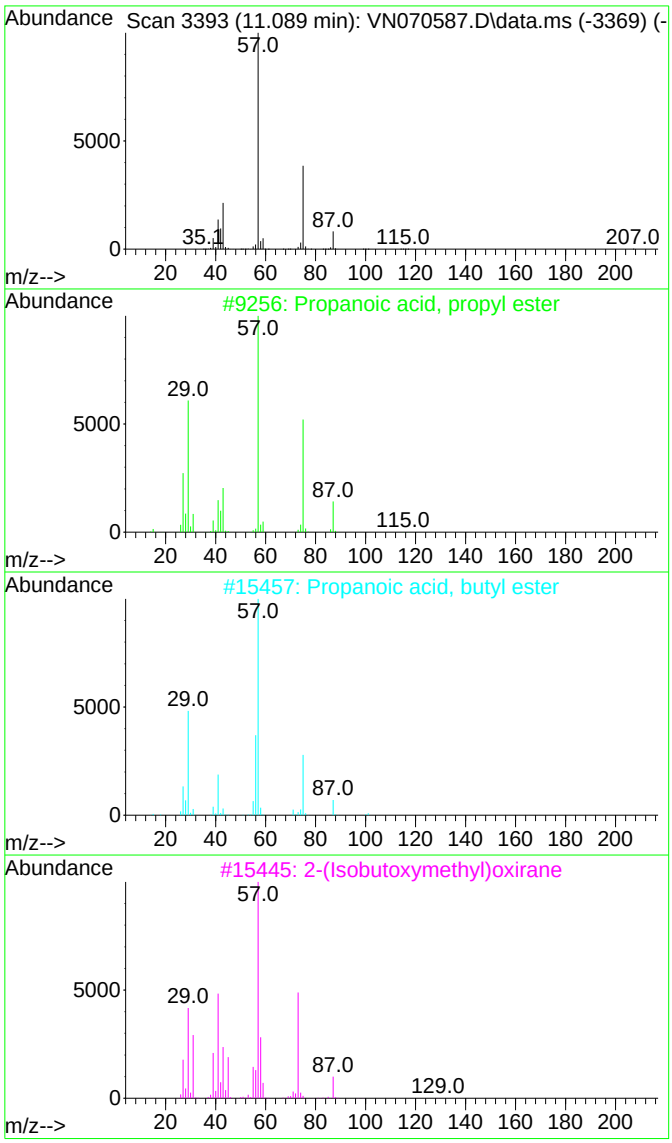
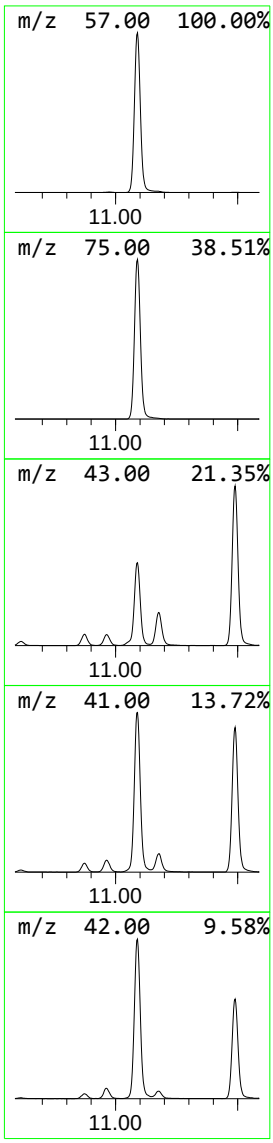
****
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.089	183.24 ug/l	14761800	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	25
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





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Quant Title : SW846 8260

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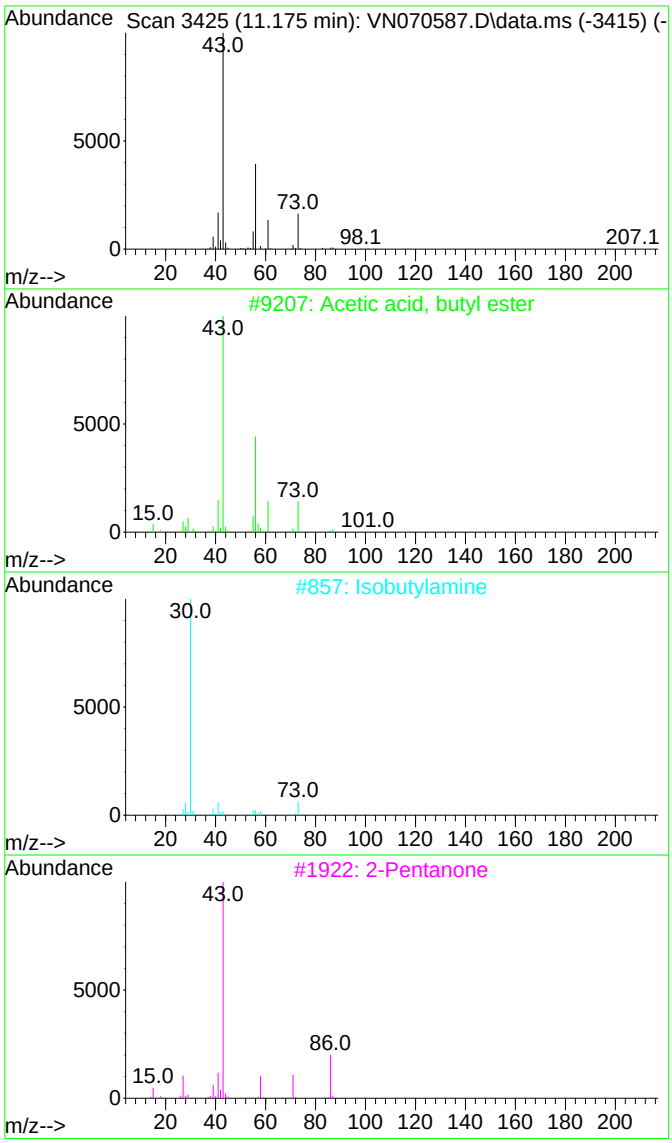
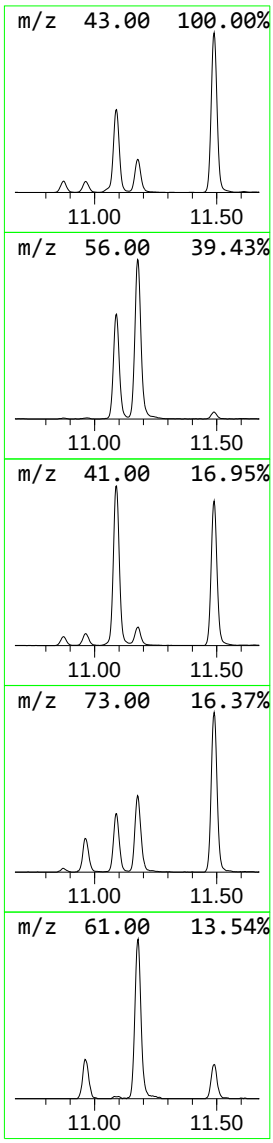
****
Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.175	17.36 ug/l	1398180	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	2-Pentanone	86	C5H10O	000107-87-9	9
4	Isobutyl acetate	116	C6H12O2	000110-19-0	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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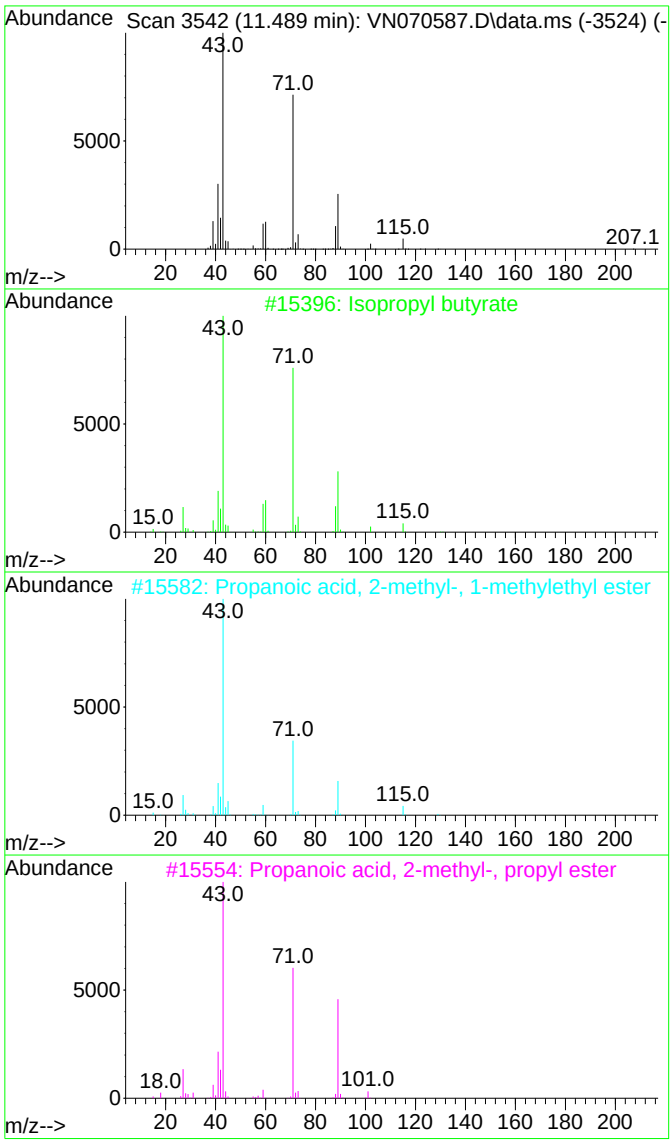
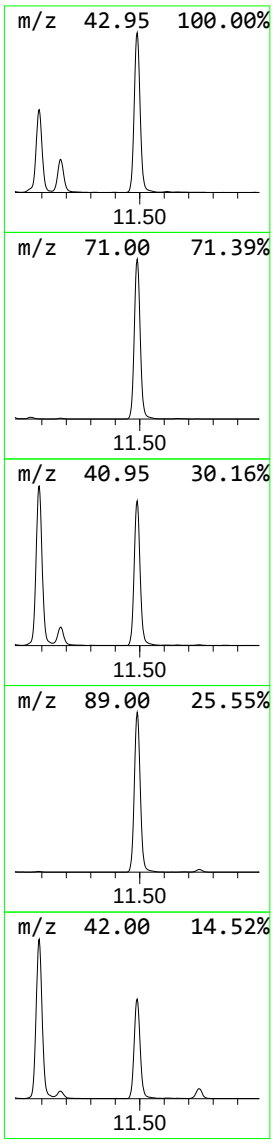
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.489	111.92 ug/l	9016530	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	59
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	59
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	53





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	9.622	160.9	ug/l	11218700	2	8.965	3486050	50.0
Propanoic acid,...	10.242	24.7	ug/l	1721330	2	8.965	3486050	50.0
Propanoic acid,...	10.872	5.6	ug/l	451939	3	11.741	4028050	50.0
Butanoic acid, ...	10.963	11.8	ug/l	951124	3	11.741	4028050	50.0
Propanoic acid,...	11.089	183.2	ug/l	14761800	3	11.741	4028050	50.0
Acetic acid, bu...	11.175	17.4	ug/l	1398180	3	11.741	4028050	50.0
Isopropyl butyrate	11.489	111.9	ug/l	9016530	3	11.741	4028050	50.0