LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122718\
Data File : VX006843.D
Acq On : 27 Dec 2018 15:35
Operator : JC/MD
Sample : J6579-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TN-122618-C

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_X\METHOD\82X121818W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.642	66	80	84	rVB5	48082	144869	3.58%	0.496%
2	2.446	206	212	218	rBV	55154	96607	2.38%	0.331%
3	2.861	272	280	294	rVV	517483	996061	24.59%	3.410%
4	5.501	700	713	727	rBV	361619	1039232	25.65%	3.558%
5	5.665	727	740	758	rVB	650857	1858433	45.87%	6.363%
6	6.068	795	806	825	rBV	378808	982177	24.24%	3.363%
7	6.458	859	870	881	rBV3	23152	64188	1.58%	0.220%
8	6.860	925	936	951	rBV	968353	2260768	55.80%	7.740%
9	7.549	1043	1049	1056	rBV2	22048	45864	1.13%	0.157%
10	7.878	1096	1103	1116	rBV	2422786	4051336	100.00%	13.871%
11	8.616	1218	1224	1233	rBV	487472	737279	18.20%	2.524%
12	8.713	1233	1240	1249	rBV	2046794	3153068	77.83%	10.796%
13	9.024	1284	1291	1296	rBV	47352	75093	1.85%	0.257%
14	9.305	1330	1337	1344	rBV	301979	432893	10.69%	1.482%
15	9.372	1344	1348	1350	rBV2	35677	47198	1.16%	0.162%
16	9.402	1350	1353	1357	rVV	118122	164347	4.06%	0.563%
17	9.439	1357	1359	1367	rVB	37959	49607	1.22%	0.170%
18	9.543	1371	1376	1383	rBV	2200527	2787332	68.80%	9.543%
19	9.640	1388	1392	1400	rVB	151330	191482	4.73%	0.656%
20	9.969	1440	1446	1459	rBV	1724225	2169170	53.54%	7.427%
21	10.110	1462	1469	1477	rBV	2018191	2780805	68.64%	9.521%
22	10.695	1560	1565	1571	rBV	108561	136270	3.36%	0.467%
23	11.134	1632	1637	1651	rBV	1717816	2227055	54.97%	7.625%
24	12.079	1786	1792	1800	rBV	2182110	2716093	67.04%	9.299%

Sum of corrected areas: 29207227

LSC Report - Integrated Chromatogram

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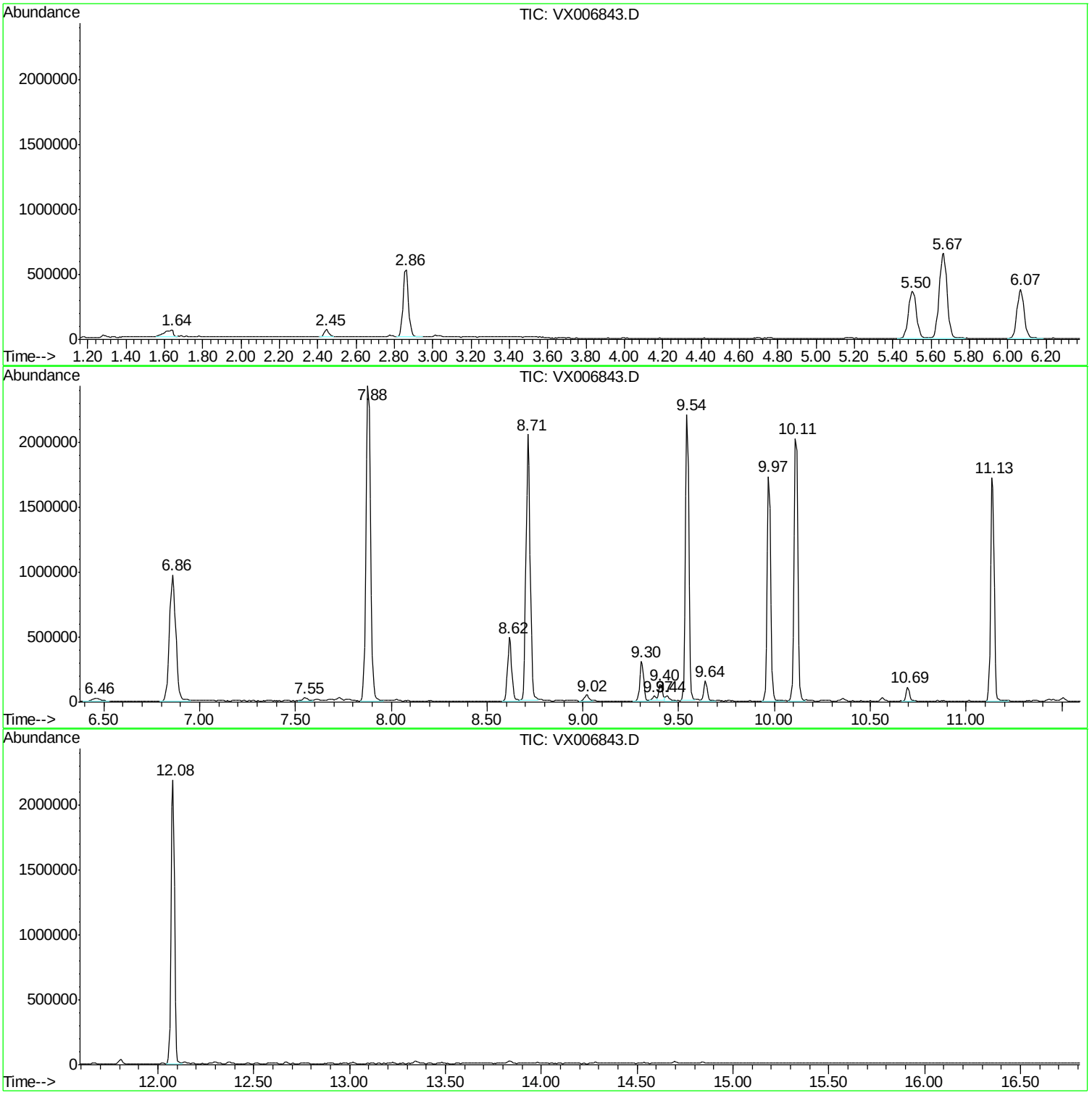
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TN-122618-C

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : VX006843.D
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Instrument : MSVOA_X
ClientSampleId : TN-122618-C

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

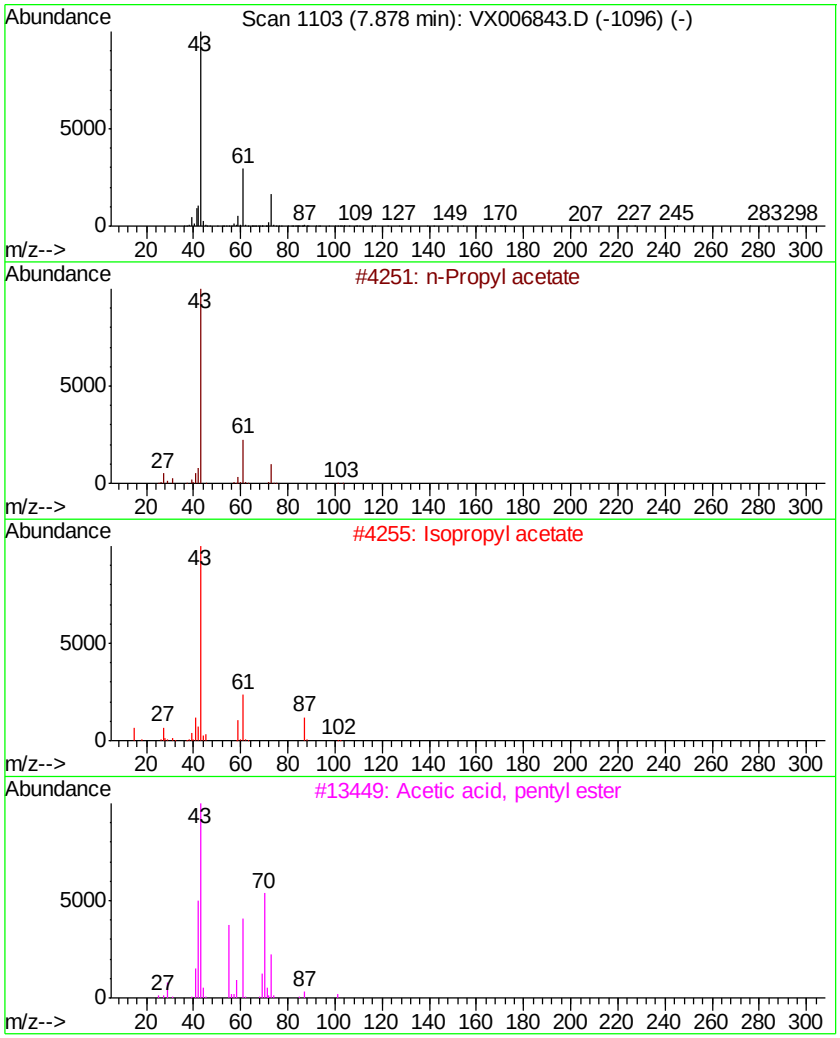
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

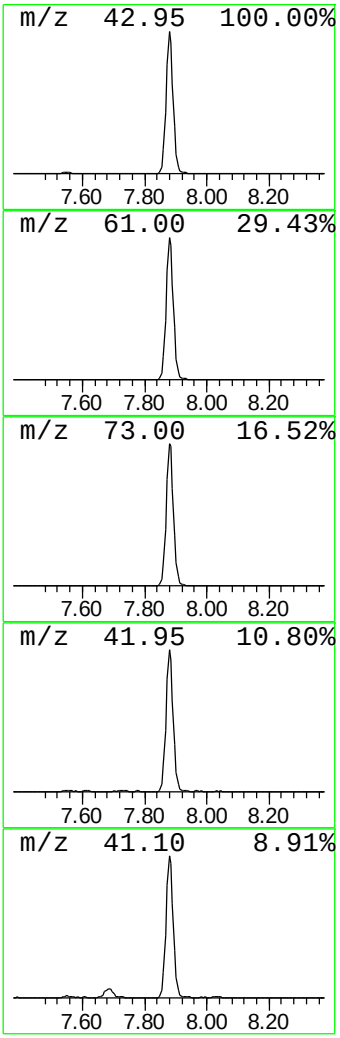
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	89.60 ug/l	4051340	1,4-Difluorobenzene	6.86

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	36
3	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122718\
Data File : VX006843.D
Acq On : 27 Dec 2018 15:35
Operator : JC/MD
Sample : J6579-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TN-122618-C

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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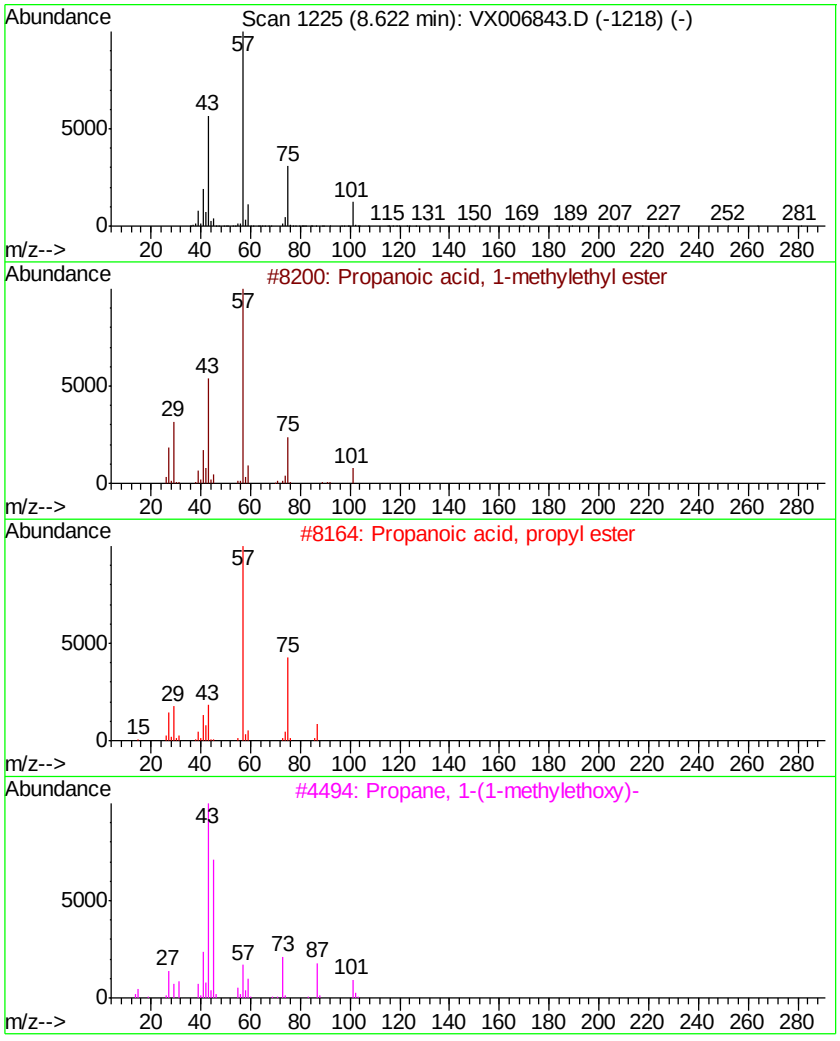
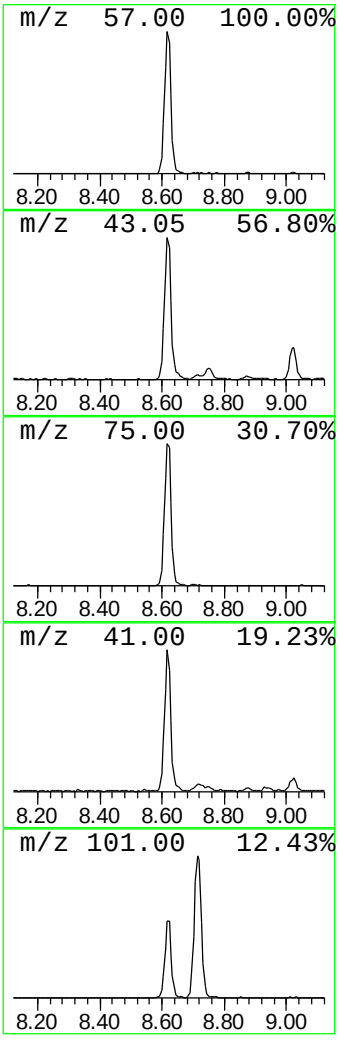
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	13.26 ug/l	737279	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	33
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TN-122618-C

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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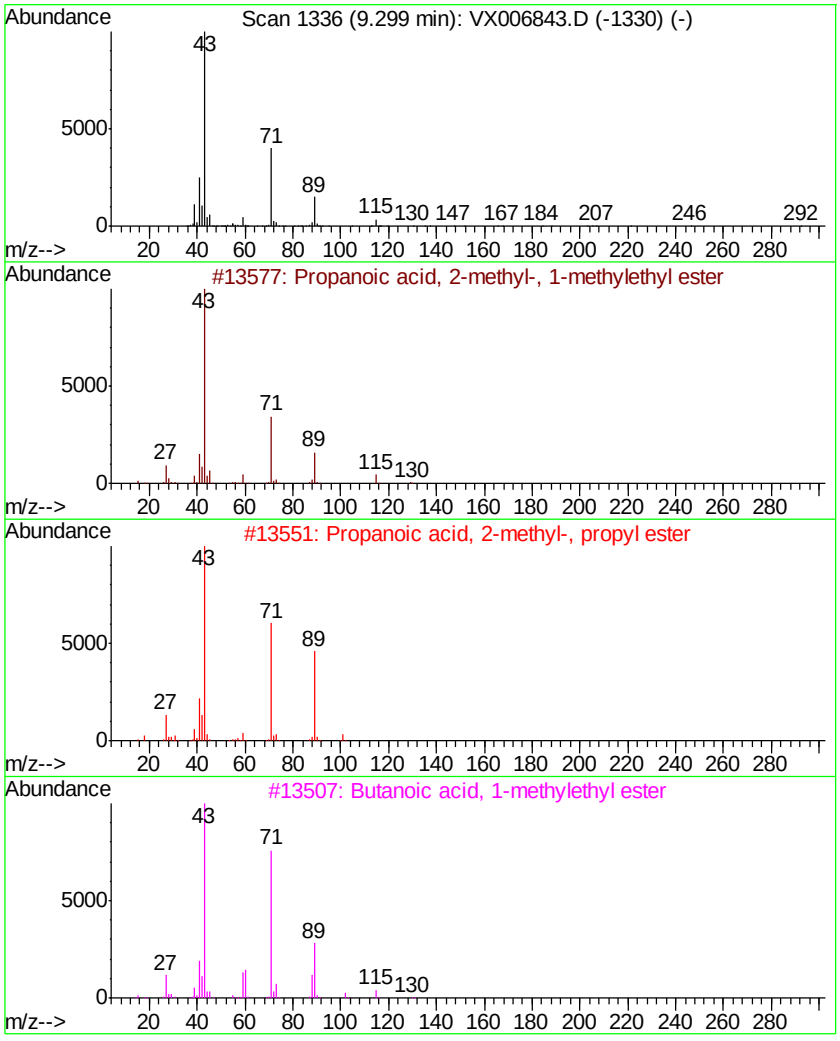
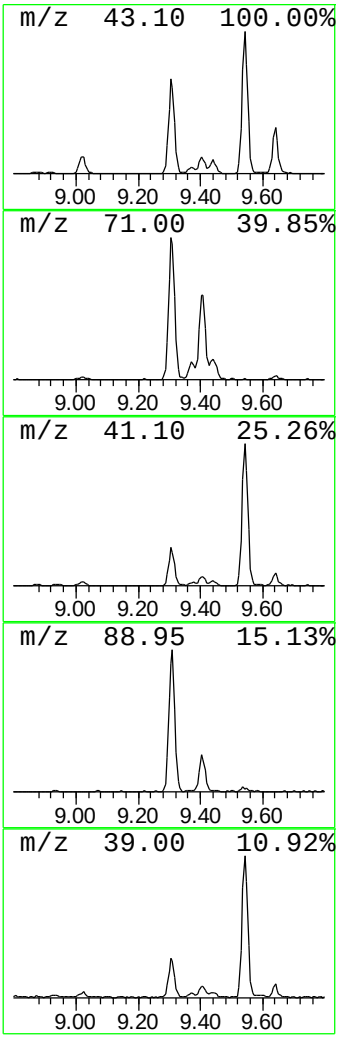
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.30	7.78 ug/l	432893	Chlorobenzene-d5	10.11

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	56
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	53
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	36





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TN-122618-C

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

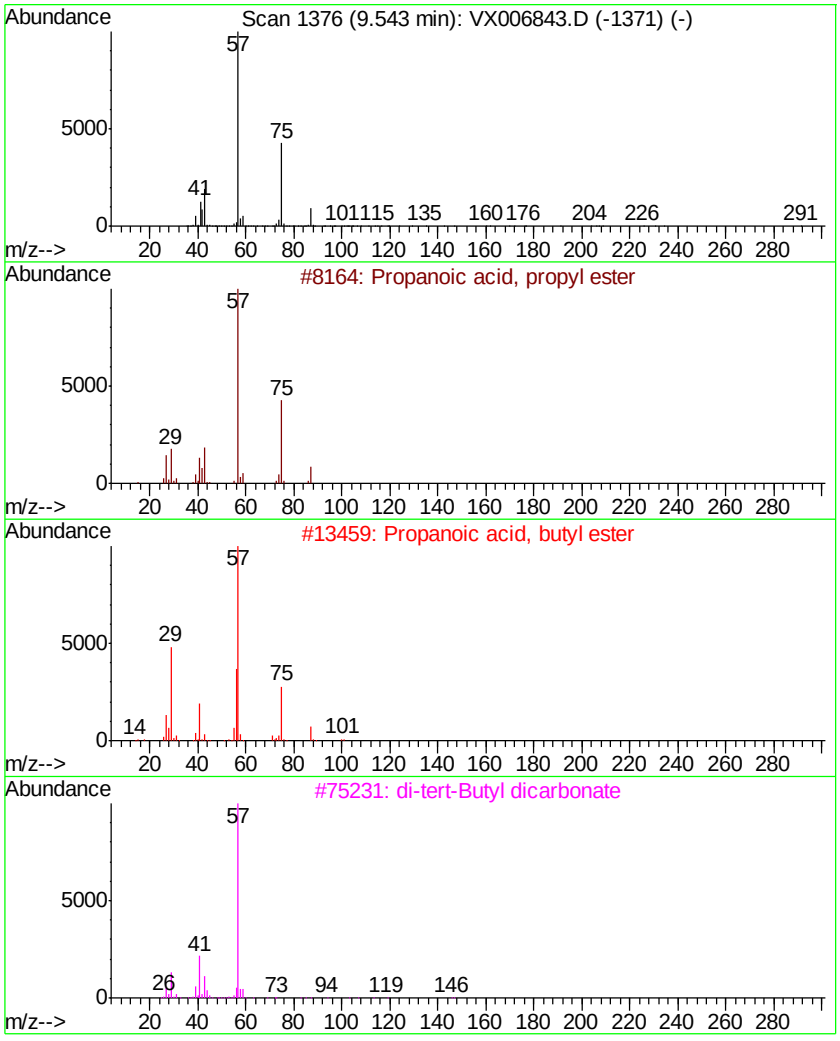
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

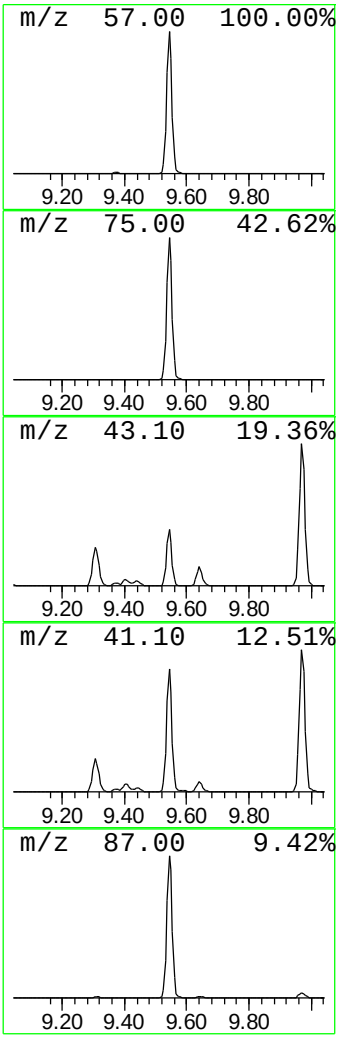
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	50.12 ug/l	2787330	Chlorobenzene-d5	10.11

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	28
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TN-122618-C

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

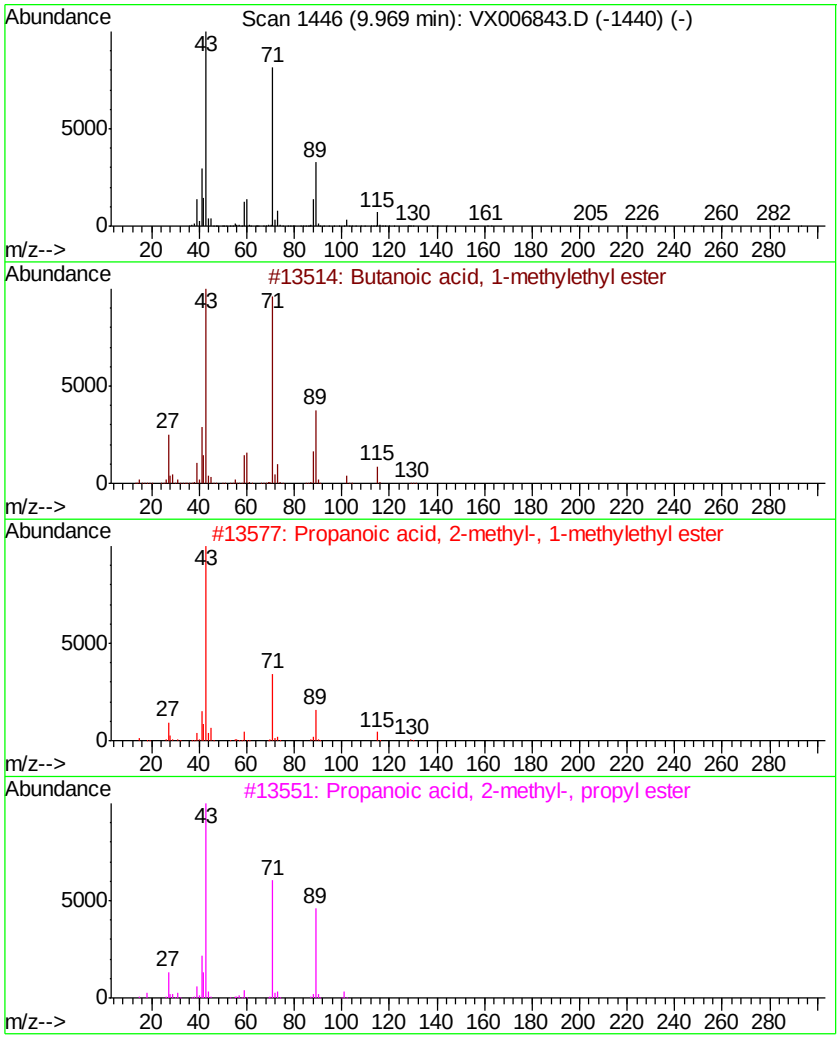
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

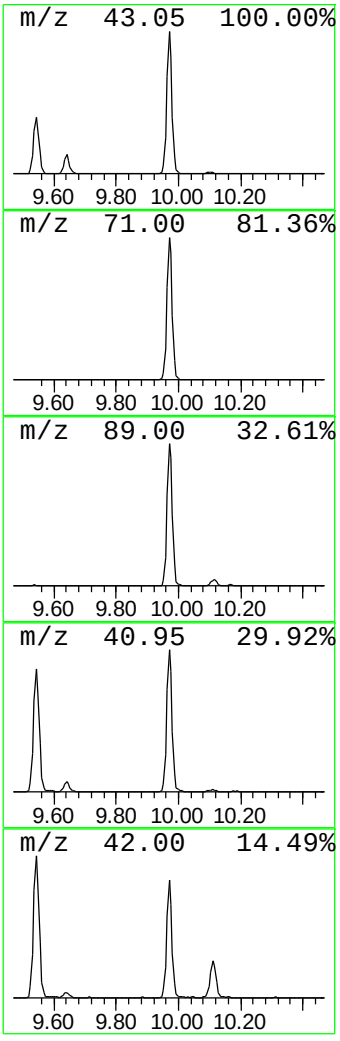
****

Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	39.00 ug/l	2169170	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50





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
n-Propyl acetate	7.88	89.6	ug/l	4051340	2	6.86	2260770	50.0
Propanoic acid, 1...	8.62	13.3	ug/l	737279	3	10.11	2780810	50.0
Propanoic acid, 2...	9.30	7.8	ug/l	432893	3	10.11	2780810	50.0
Propanoic acid, p...	9.54	50.1	ug/l	2787330	3	10.11	2780810	50.0
Butanoic acid, 1-...	9.97	39.0	ug/l	2169170	3	10.11	2780810	50.0