LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051619\
Data File : VX009614.D
Acq On : 16 May 2019 17:55
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

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\82X042919W.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	2.446	204	212	222	rBV	27377	48284	2.22%	0.446%
2	2.855	271	279	295	rVB	437000	860388	39.60%	7.954%
3	3.666	404	412	422	rBV2	10349	26884	1.24%	0.249%
4	5.501	701	713	725	rBV	96812	279085	12.85%	2.580%
5	5.659	725	739	752	rVV	172406	490162	22.56%	4.531%
6	6.061	792	805	826	rBV	119986	320865	14.77%	2.966%
7	6.452	857	869	879	rBV2	9103	24622	1.13%	0.228%
8	6.860	922	936	953	rBV	289635	790745	36.40%	7.310%
9	7.171	983	987	1003	rVB2	7126	23002	1.06%	0.213%
10	7.543	1042	1048	1055	rBV2	13749	27952	1.29%	0.258%
11	7.872	1094	1102	1116	rBV	1293205	2172603	100.00%	20.085%
12	8.616	1217	1224	1233	rBV	228422	361422	16.64%	3.341%
13	8.713	1233	1240	1249	rBV	597935	940164	43.27%	8.692%
14	9.018	1284	1290	1296	rBV	28573	41991	1.93%	0.388%
15	9.305	1330	1337	1343	rBV	124873	176710	8.13%	1.634%
16	9.372	1343	1348	1350	rVV	16790	26827	1.23%	0.248%
17	9.402	1350	1353	1357	rVV	55042	75986	3.50%	0.702%
18	9.543	1370	1376	1382	rBV	961555	1239315	57.04%	11.457%
19	9.634	1387	1391	1399	rVB	67555	94542	4.35%	0.874%
20	9.969	1440	1446	1459	rBV	631485	787311	36.24%	7.279%
21	10.110	1462	1469	1477	rBV	555636	766166	35.26%	7.083%
22	10.695	1560	1565	1570	rBV	32843	39810	1.83%	0.368%
23	11.134	1631	1637	1648	rBV	430501	560128	25.78%	5.178%
24	12.079	1786	1792	1799	rBV	501532	641822	29.54%	5.934%

Sum of corrected areas: 10816786

LSC Report - Integrated Chromatogram

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Data File : VX009614.D
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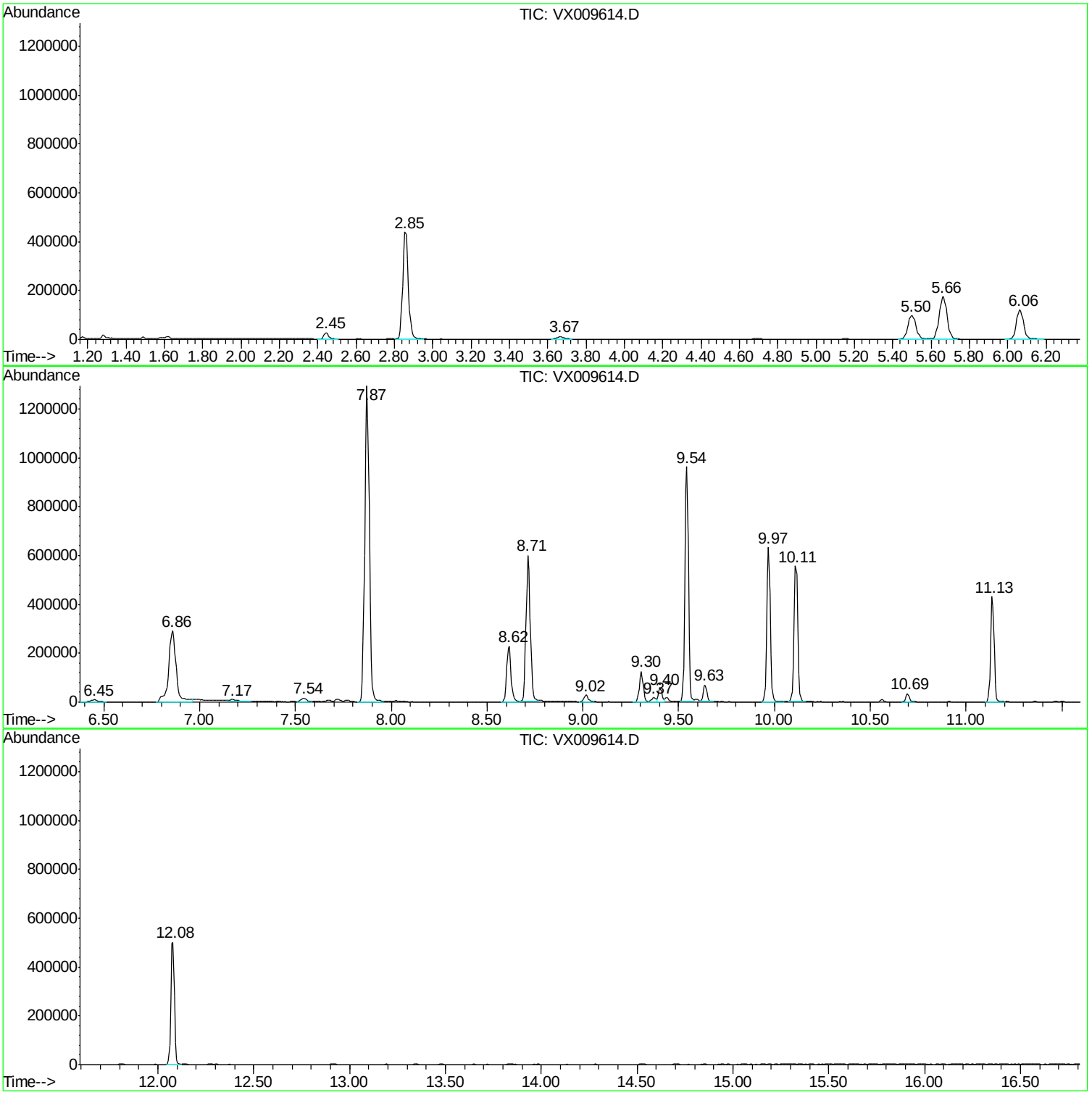
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051619\
Data File : VX009614.D
Acq On : 16 May 2019 17:55
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

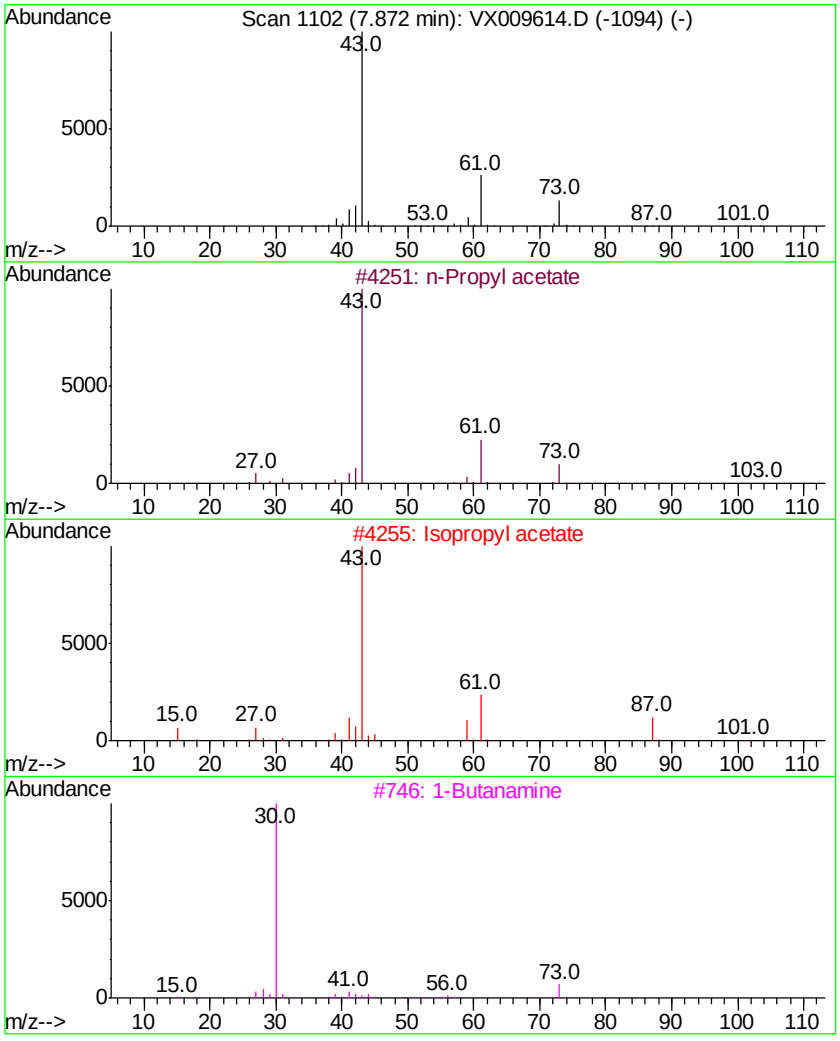
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

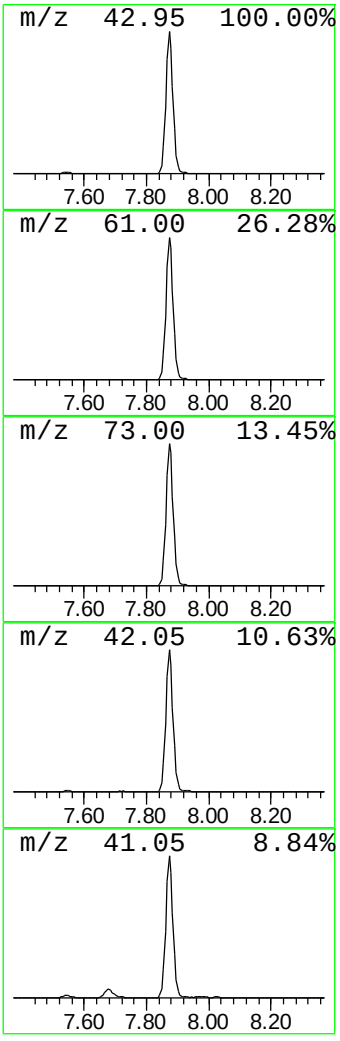
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.87	137.38 ug/l	2172600	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	45
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	5-Methyloxazolidine	87	C4H9NO	058328-22-6	4





Library Search Compound Report

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Data File : VX009614.D
Acq On : 16 May 2019 17:55
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

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

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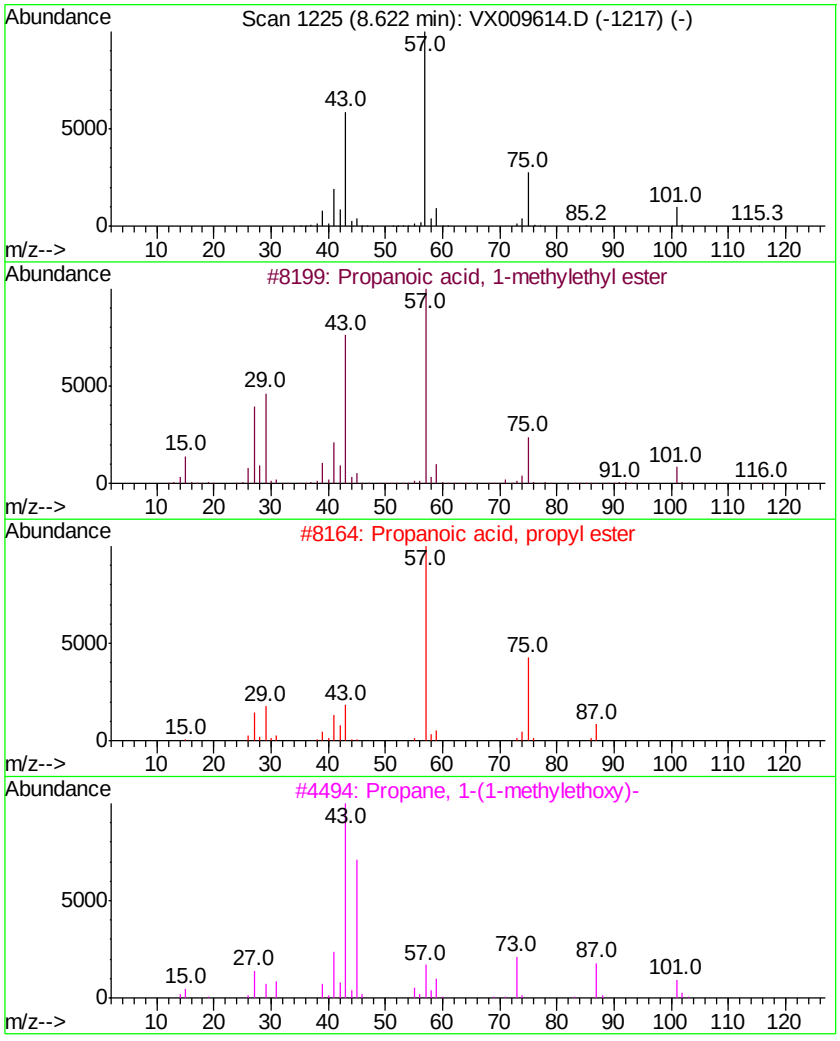
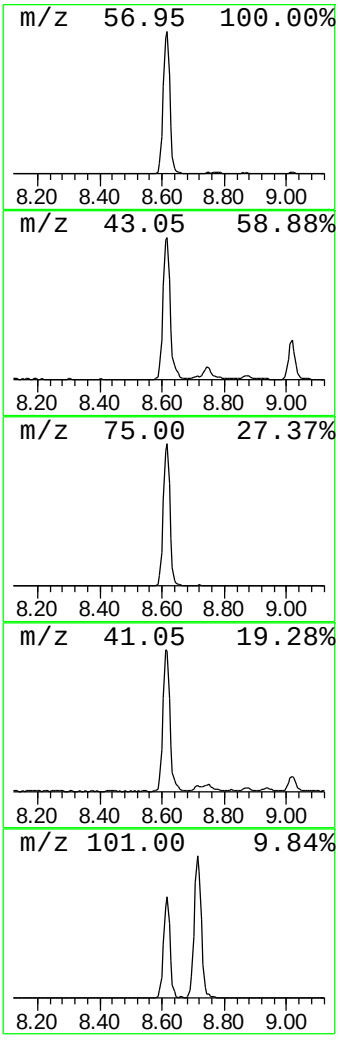
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	23.59 ug/l	361422	Chlorobenzene-d5	10.11

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	53
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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051619\
Data File : VX009614.D
Acq On : 16 May 2019 17:55
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

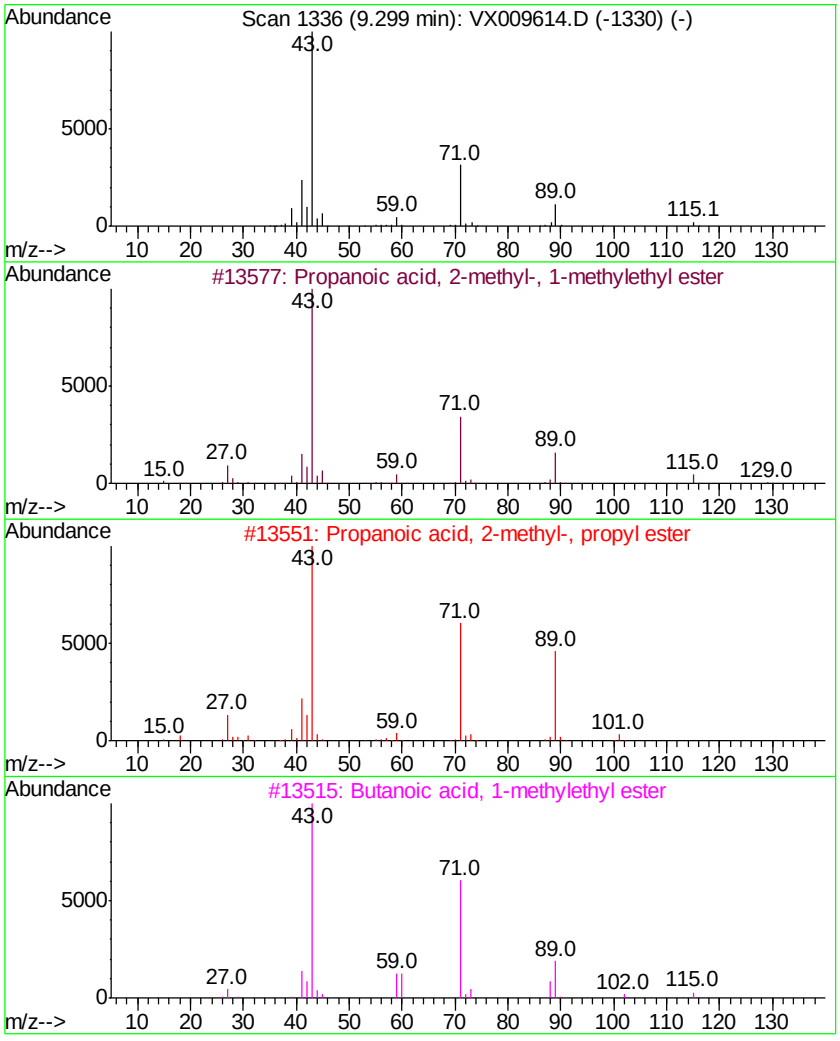
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

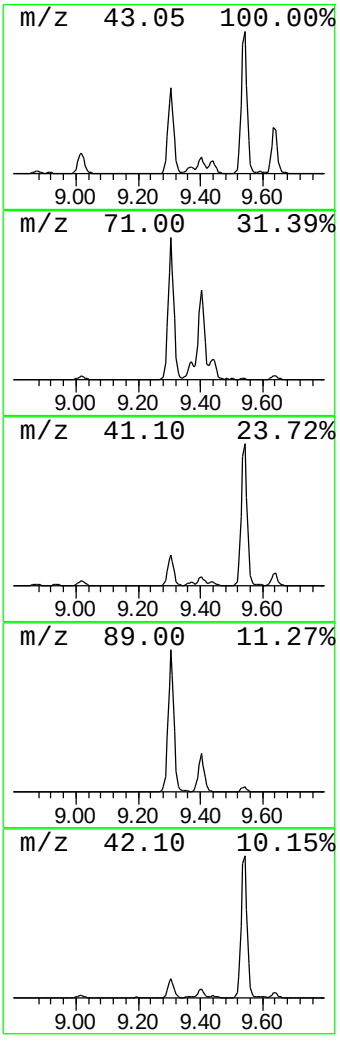
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.30	11.53 ug/l	176710	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	78
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	36
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051619\
Data File : VX009614.D
Acq On : 16 May 2019 17:55
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

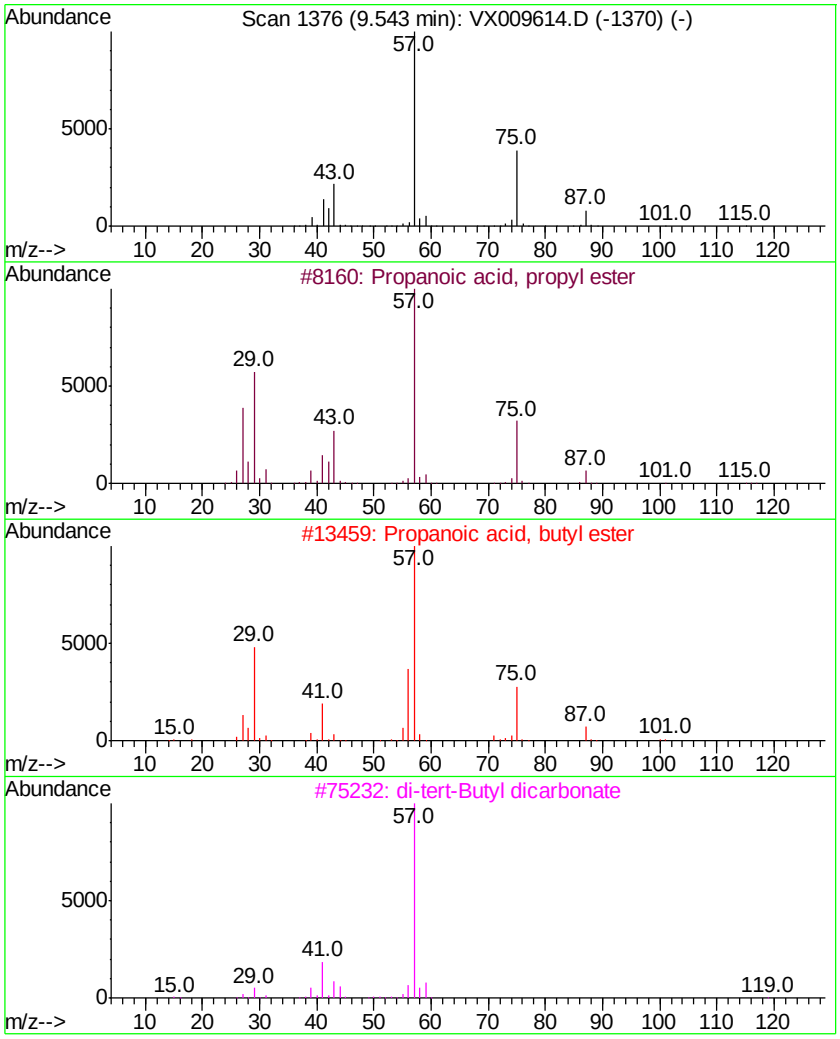
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

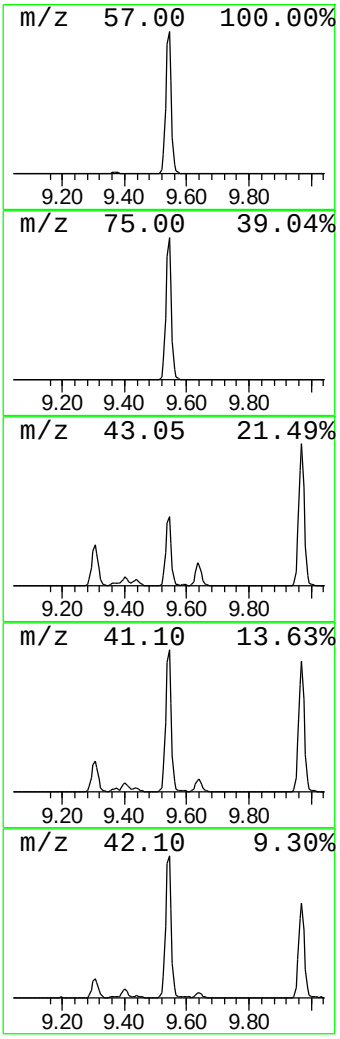
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	80.88 ug/l	1239320	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	25
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051619\
Data File : VX009614.D
Acq On : 16 May 2019 17:55
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

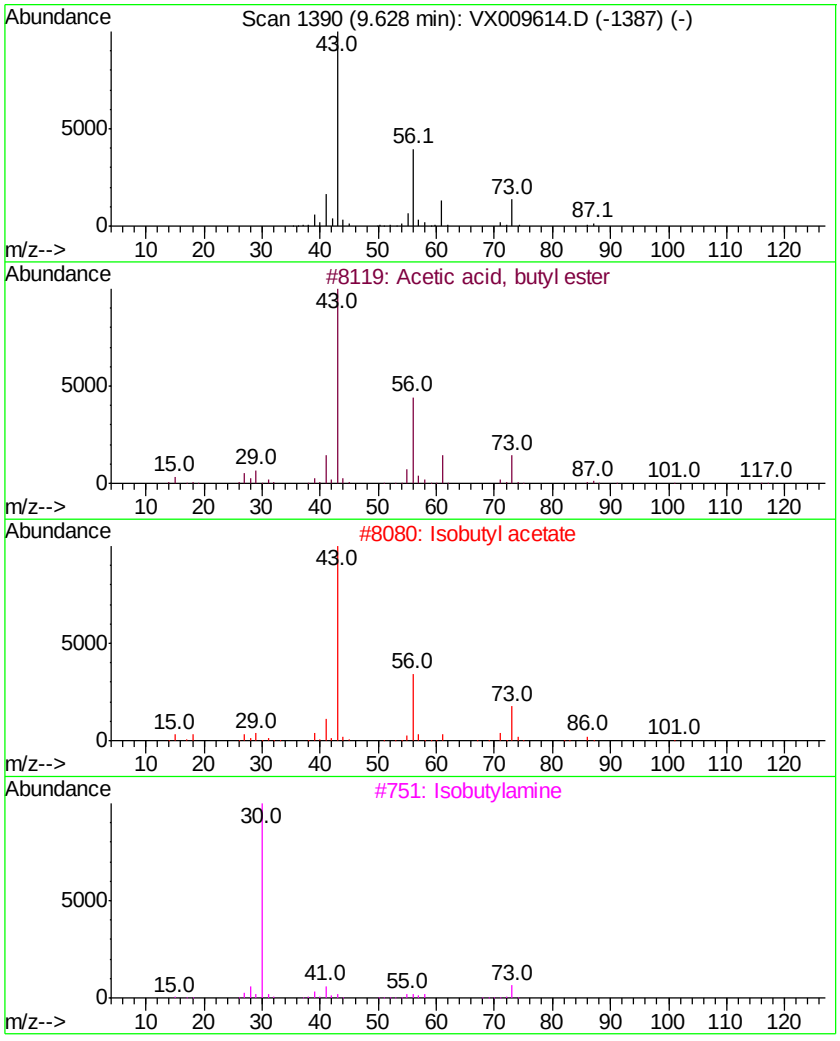
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

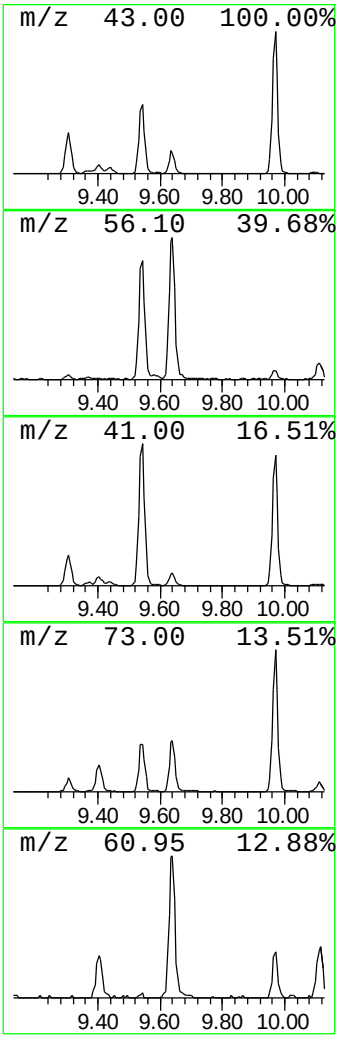
****

Peak Number 5 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	6.17 ug/l	94542	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Isobutyl acetate	116	C6H12O2	000110-19-0	38
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	2-Pentanone	86	C5H10O	000107-87-9	9





Library Search Compound Report

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Data File : VX009614.D
Acq On : 16 May 2019 17:55
Operator : JC/SP
Sample : K2866-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : TP-22-S

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X042919W.M
Quant Title : SW846 8260

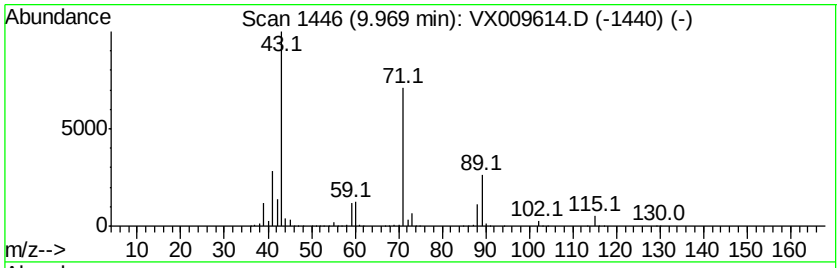
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

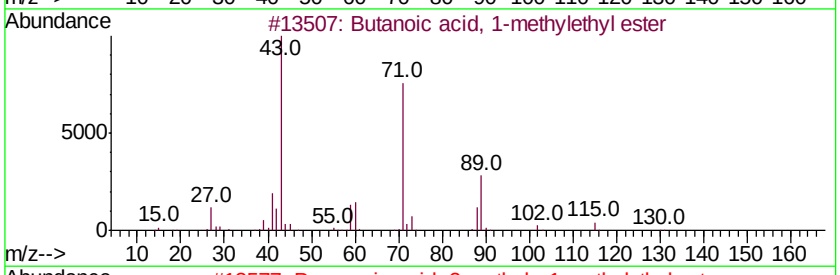
****

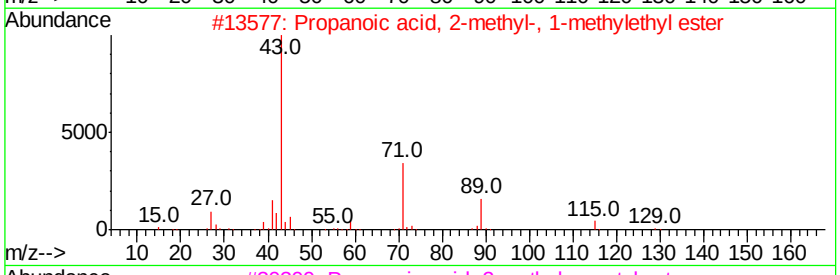
Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 3

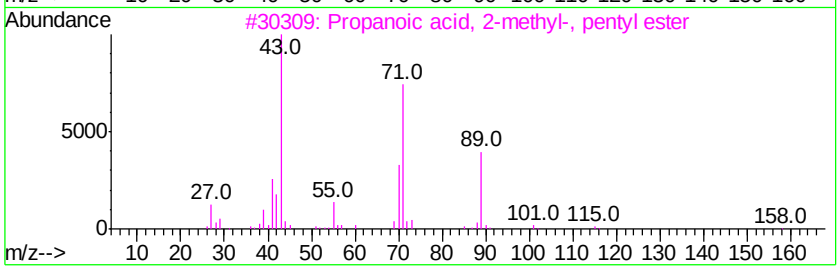
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	51.38 ug/l	787311	Chlorobenzene-d5	10.11

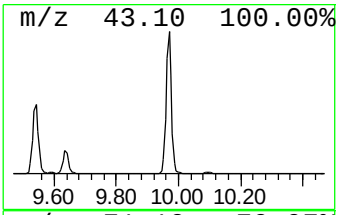
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	59
4	Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	45
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	43

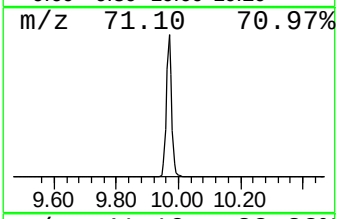


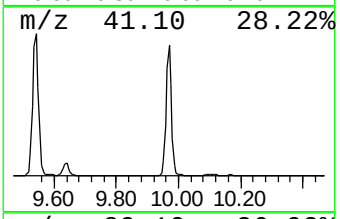


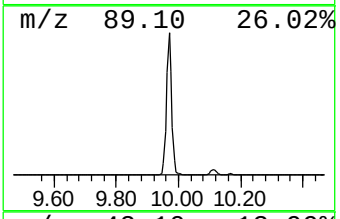


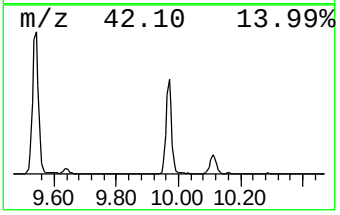












Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.87	137.4	ug/l	2172600	2	6.86	790745	50.0
Propanoic acid, 1...	8.62	23.6	ug/l	361422	3	10.11	766166	50.0
Propanoic acid, 2...	9.30	11.5	ug/l	176710	3	10.11	766166	50.0
Propanoic acid, p...	9.54	80.9	ug/l	1239320	3	10.11	766166	50.0
Acetic acid, buty...	9.63	6.2	ug/l	94542	3	10.11	766166	50.0
Butanoic acid, 1-...	9.97	51.4	ug/l	787311	3	10.11	766166	50.0