LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006085.D
Acq On : 19 Nov 2018 12:34
Operator : JC/MD
Sample : J5991-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WS-RO-358

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\82X110718W.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	1.617	66	76	79	rBV5	3581	8164	1.20%	0.156%
2	2.446	207	212	220	rVB	4475	8071	1.19%	0.154%
3	2.861	272	280	297	rBV	223785	429883	63.36%	8.206%
4	5.507	702	714	727	rBV2	82073	226171	33.34%	4.317%
5	5.665	729	740	753	rBV2	140122	381298	56.20%	7.279%
6	6.074	796	807	828	rVB2	86616	225984	33.31%	4.314%
7	6.464	863	871	880	rBV2	5270	13703	2.02%	0.262%
8	6.860	926	936	948	rBV	206257	489991	72.22%	9.353%
9	7.555	1044	1050	1056	rBV	4027	7266	1.07%	0.139%
10	7.884	1096	1104	1120	rBV	396415	678457	100.00%	12.951%
11	8.622	1218	1225	1234	rBV	77461	120407	17.75%	2.298%
12	8.713	1234	1240	1259	rVB	354697	574105	84.62%	10.959%
13	9.018	1286	1290	1298	rBV	7374	10914	1.61%	0.208%
14	9.311	1332	1338	1344	rBV	45043	64364	9.49%	1.229%
15	9.372	1344	1348	1350	rVV	5384	7511	1.11%	0.143%
16	9.408	1350	1354	1357	rVV	13820	20705	3.05%	0.395%
17	9.445	1357	1360	1365	rVB	5914	8493	1.25%	0.162%
18	9.543	1371	1376	1388	rBV	250153	336055	49.53%	6.415%
19	9.640	1388	1392	1400	rVB	15629	20773	3.06%	0.397%
20	9.975	1441	1447	1463	rBV	199713	266050	39.21%	5.079%
21	10.116	1463	1470	1483	rVV	354137	493868	72.79%	9.427%
22	11.140	1632	1638	1653	rBV	291716	377047	55.57%	7.197%
23	12.079	1786	1792	1802	rBV	393204	469359	69.18%	8.960%

Sum of corrected areas: 5238639

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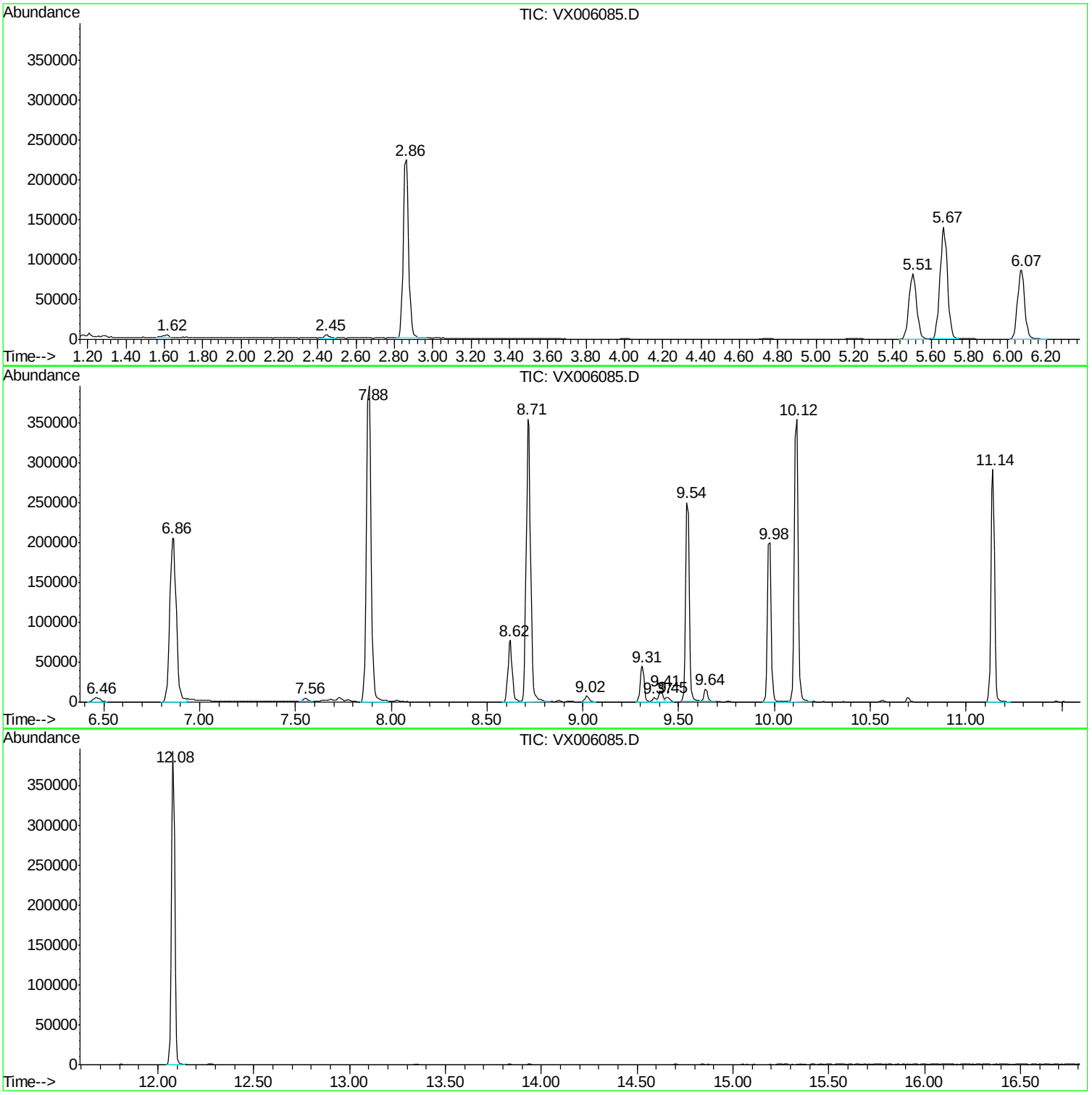
Instrument :
MSVOA_X
ClientSampleId :
WS-RO-358

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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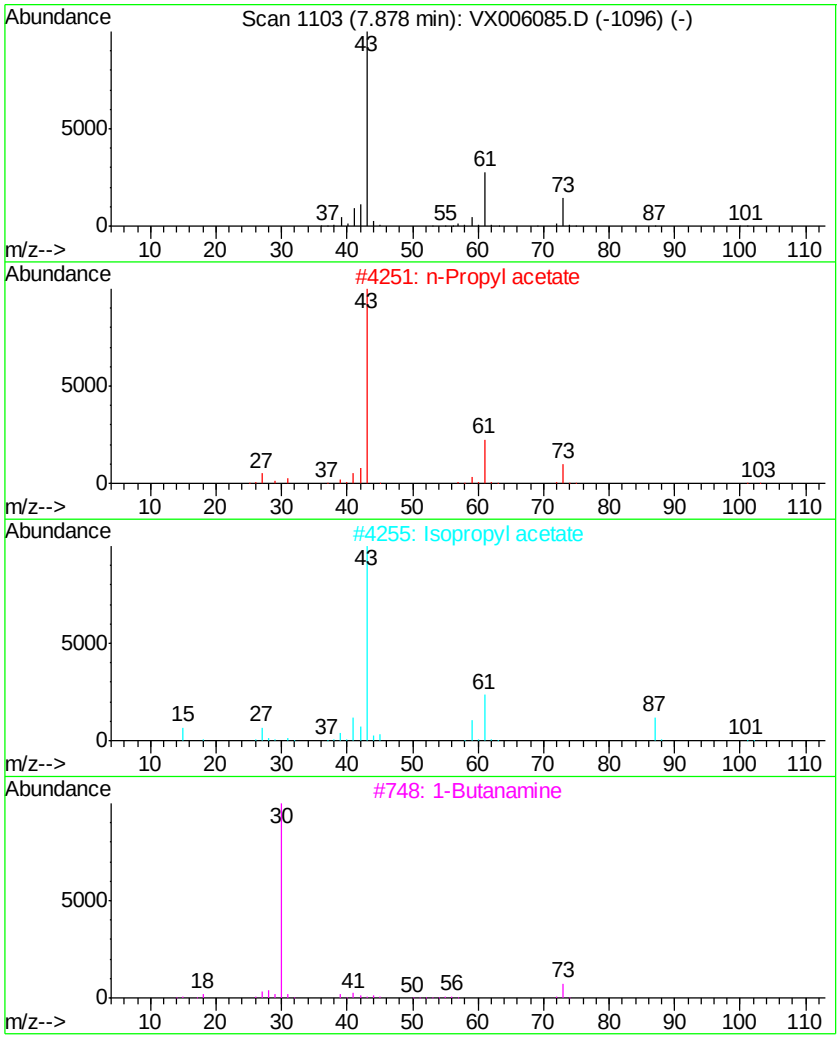
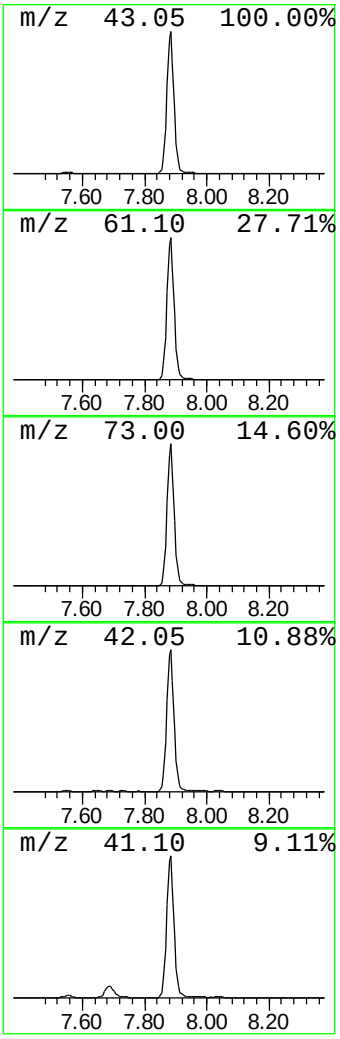
Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	69.23 ug/l	678457	1,4-Difluorobenzene	6.87

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	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	N-Acetylethylenediamine	102	C4H10N2O	001001-53-2	4





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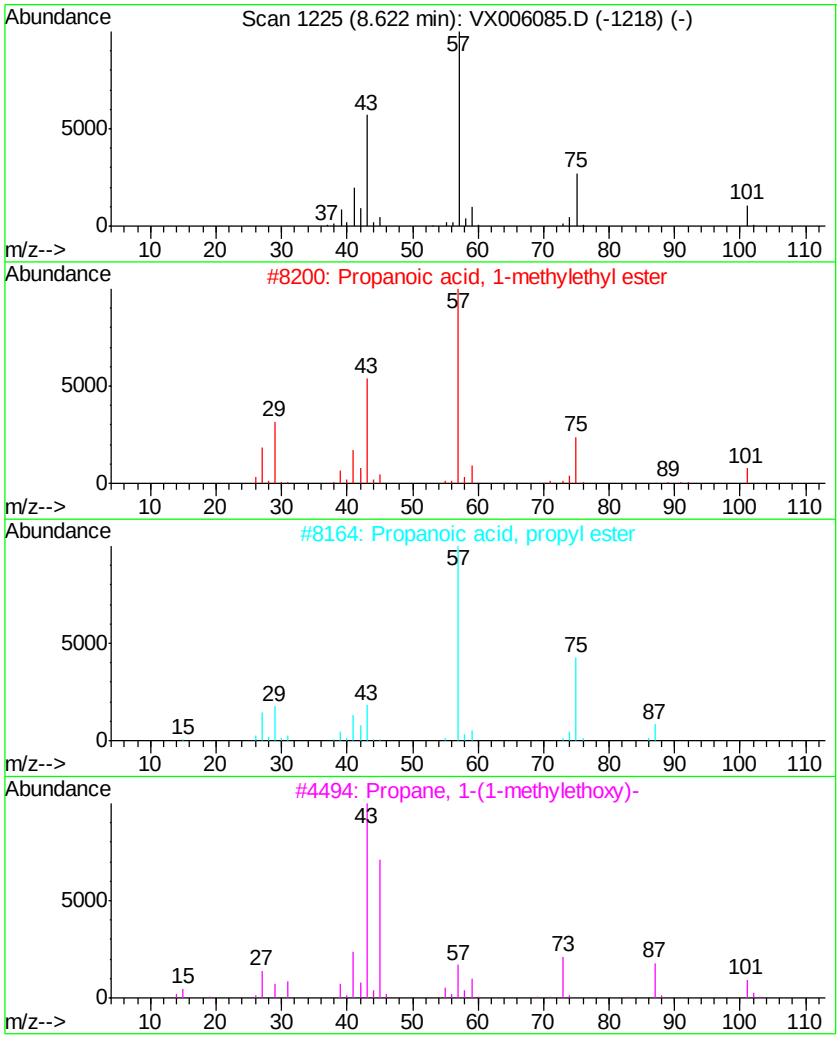
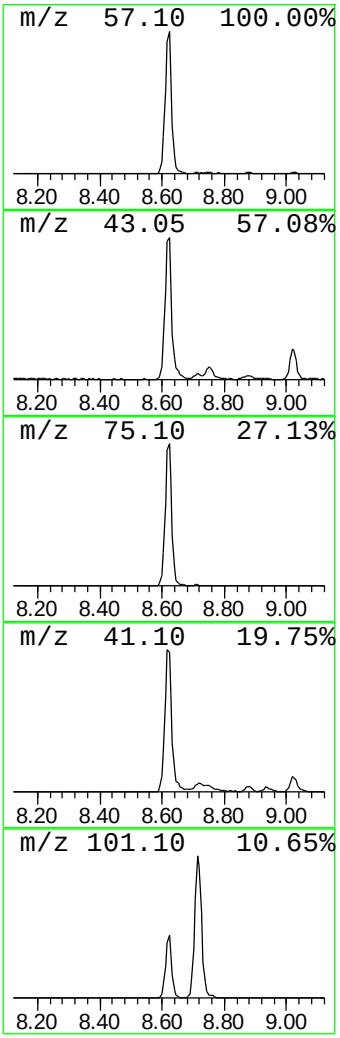
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	12.19 ug/l	120407	Chlorobenzene-d5	10.12

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	45
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	Azetidine	57	C3H7N	000503-29-7	12
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9





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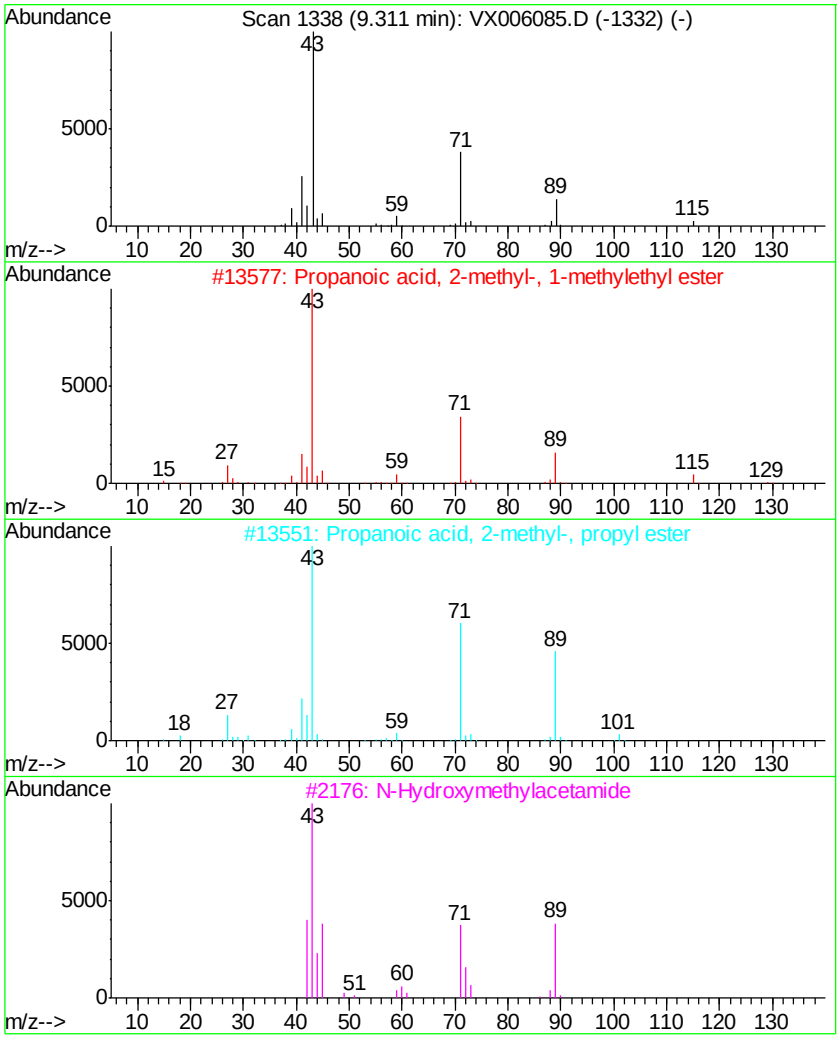
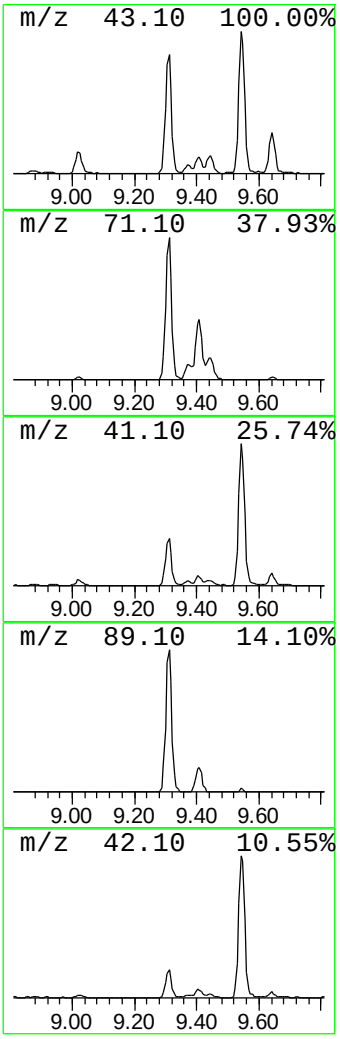
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.31	6.52 ug/l	64364	Chlorobenzene-d5	10.12

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	64
3	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	53
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	42
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42





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Quant Title : SW846 8260

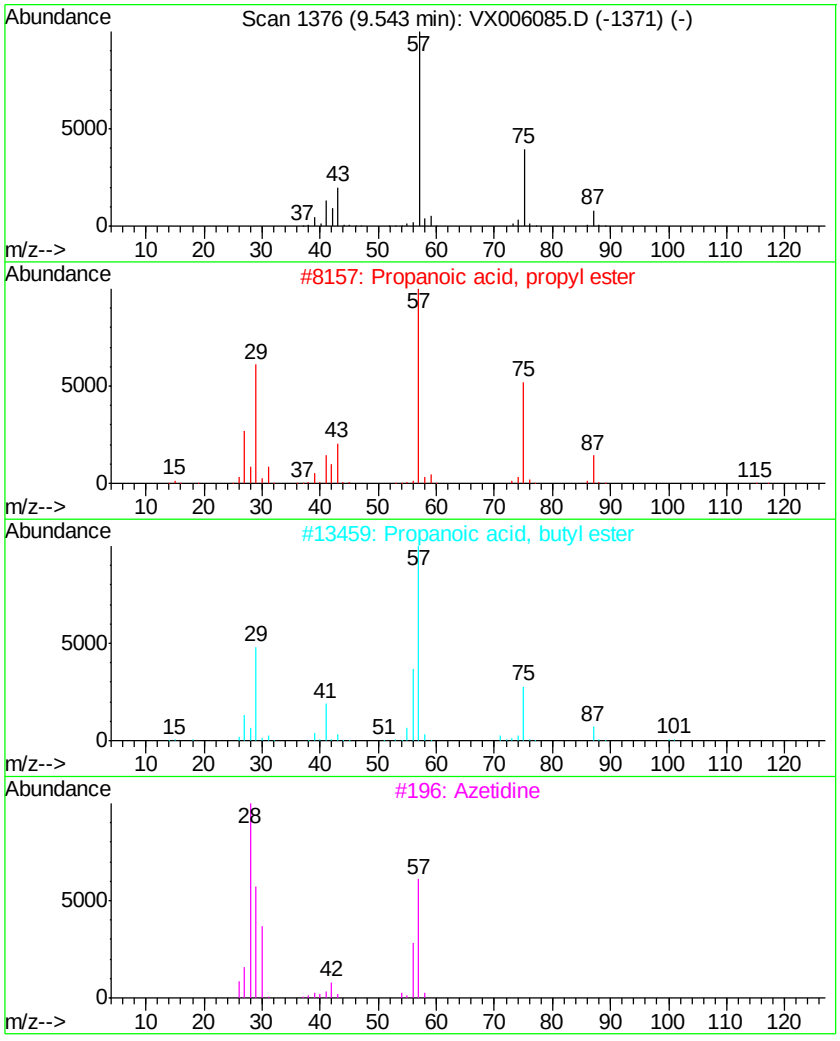
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

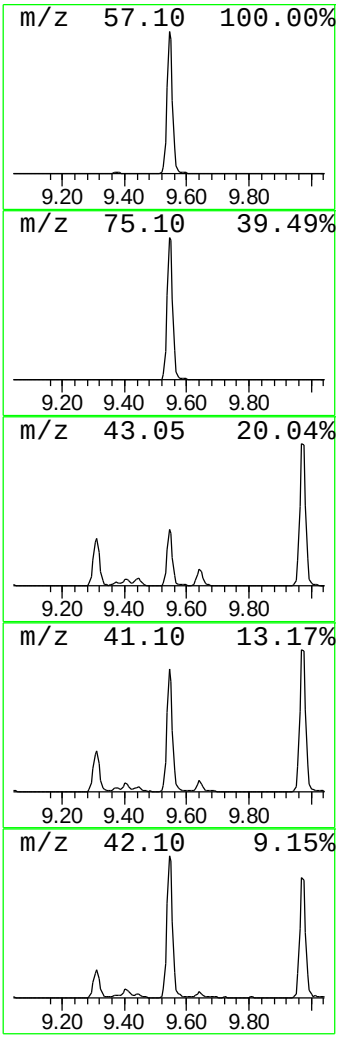
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	34.02 ug/l	336055	Chlorobenzene-d5	10.12

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	Azetidine	57	C3H7N	000503-29-7	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

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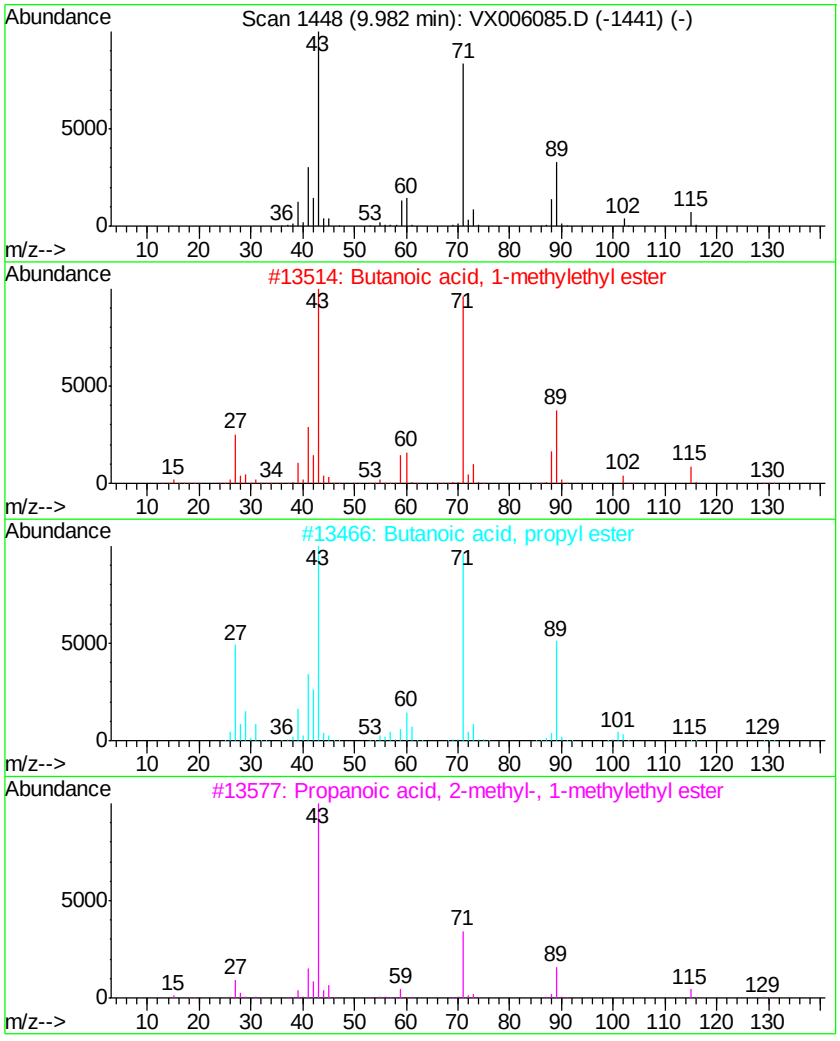
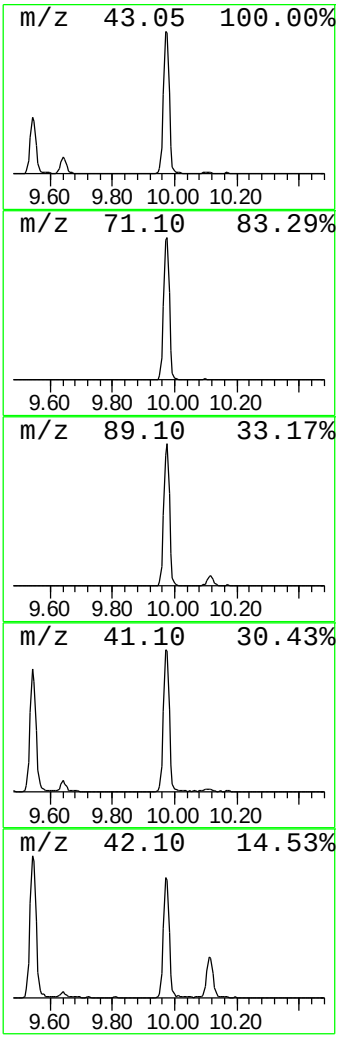
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.98	26.94 ug/l	266050	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.88	69.2	ug/l	678457	2	6.87	489991	50.0
Propanoic acid, 1...	8.62	12.2	ug/l	120407	3	10.12	493868	50.0
Propanoic acid, 2...	9.31	6.5	ug/l	64364	3	10.12	493868	50.0
Propanoic acid, p...	9.54	34.0	ug/l	336055	3	10.12	493868	50.0
Butanoic acid, 1-...	9.98	26.9	ug/l	266050	3	10.12	493868	50.0