

ANALYTICAL AUTHENTICATION OF ORGANIC FOODS

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Organic vs. non-Organic



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Trace of pesticides?



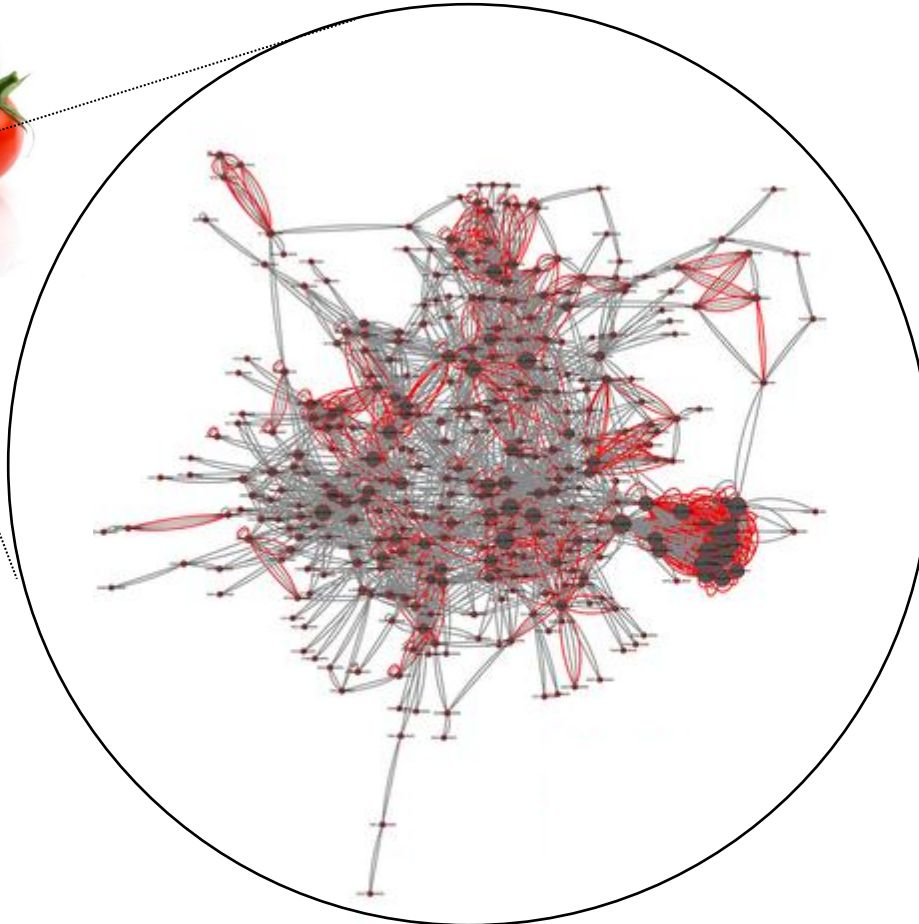
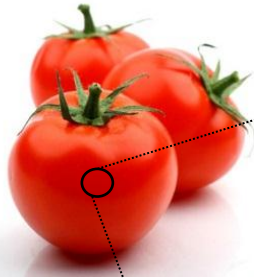
Price?



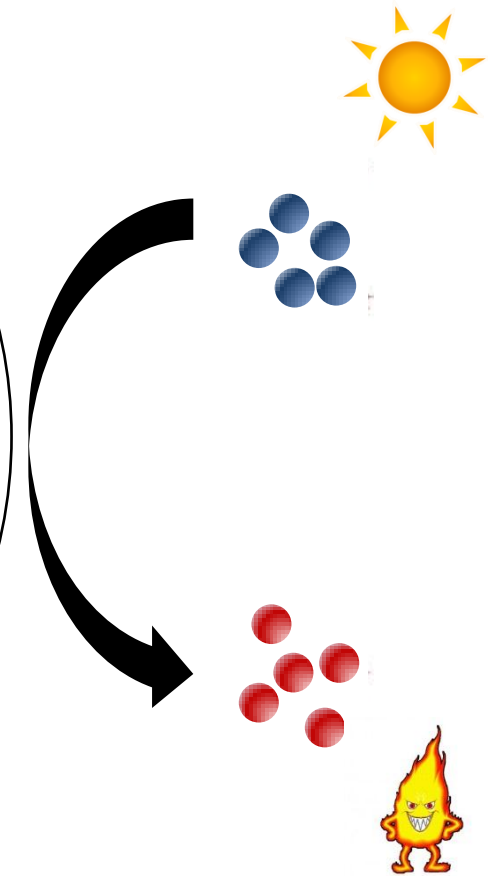
Chemical constituents?



Foods Are Complex Systems

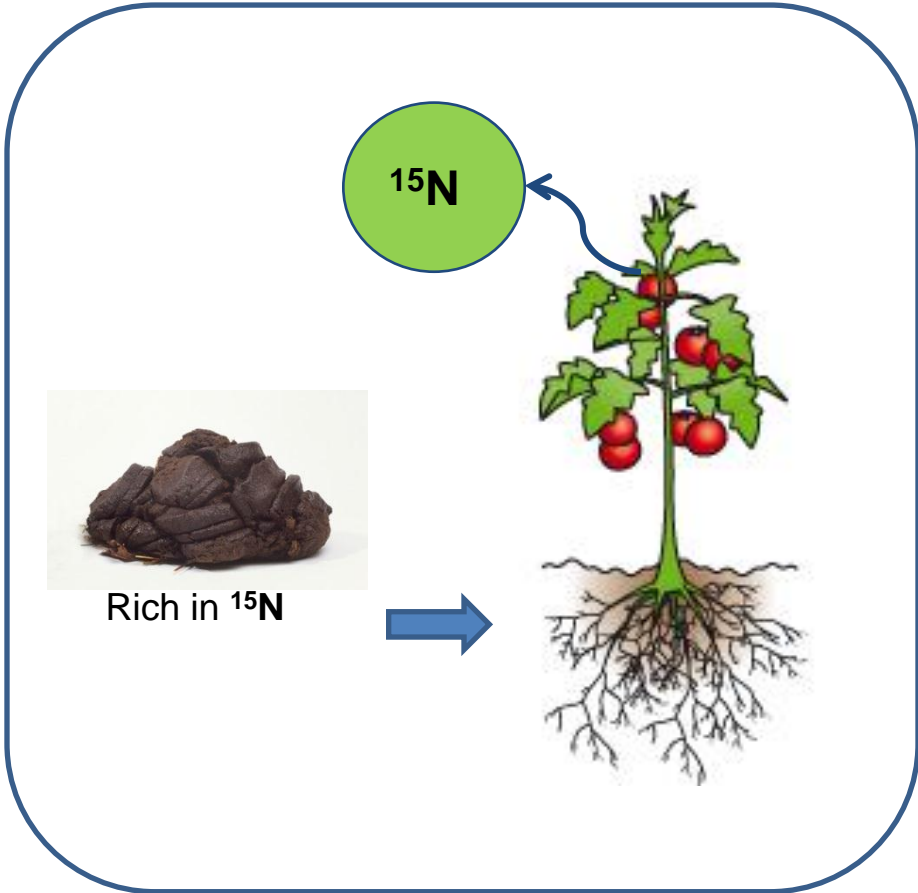


Biochemical networks

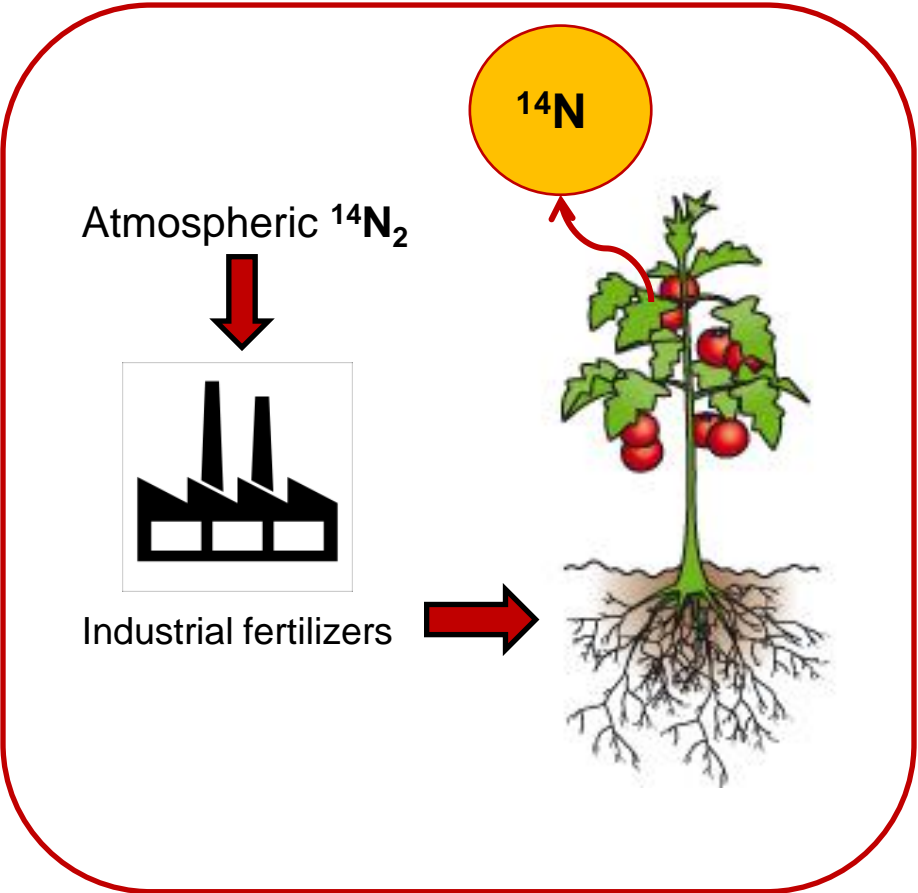


Exchange matter and energy with the environment.

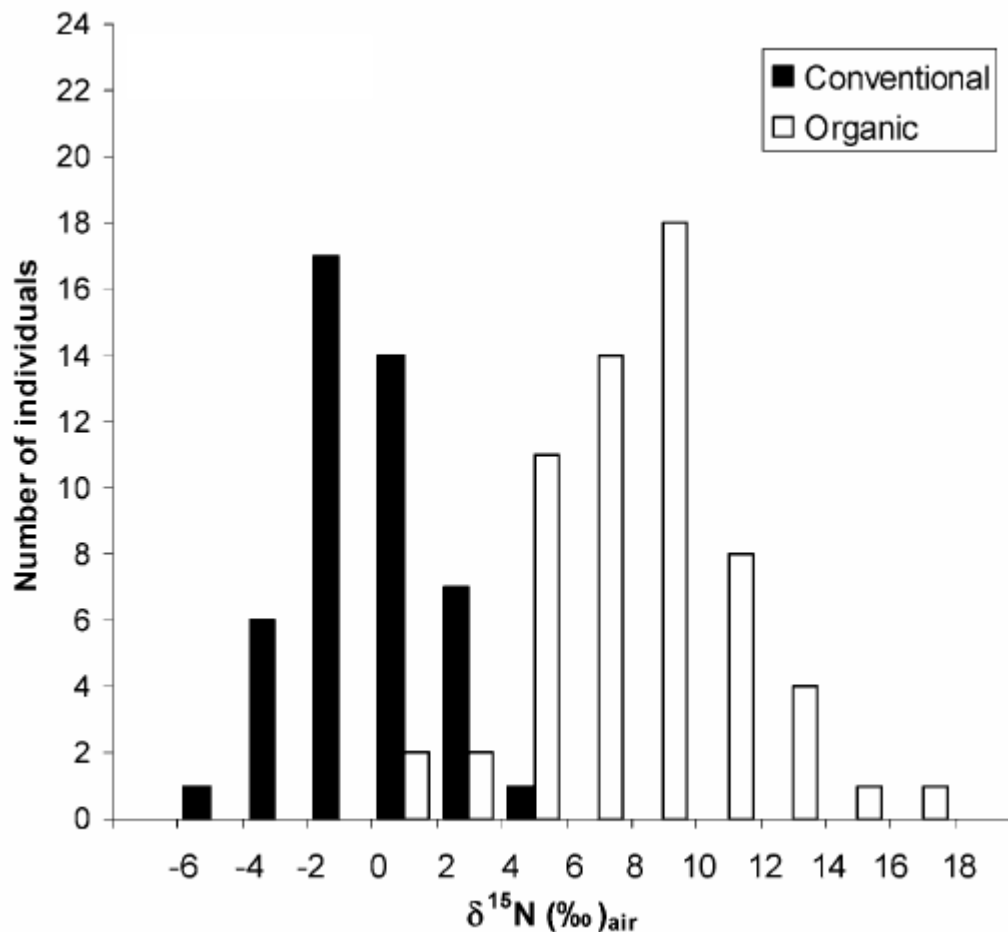
ORGANIC



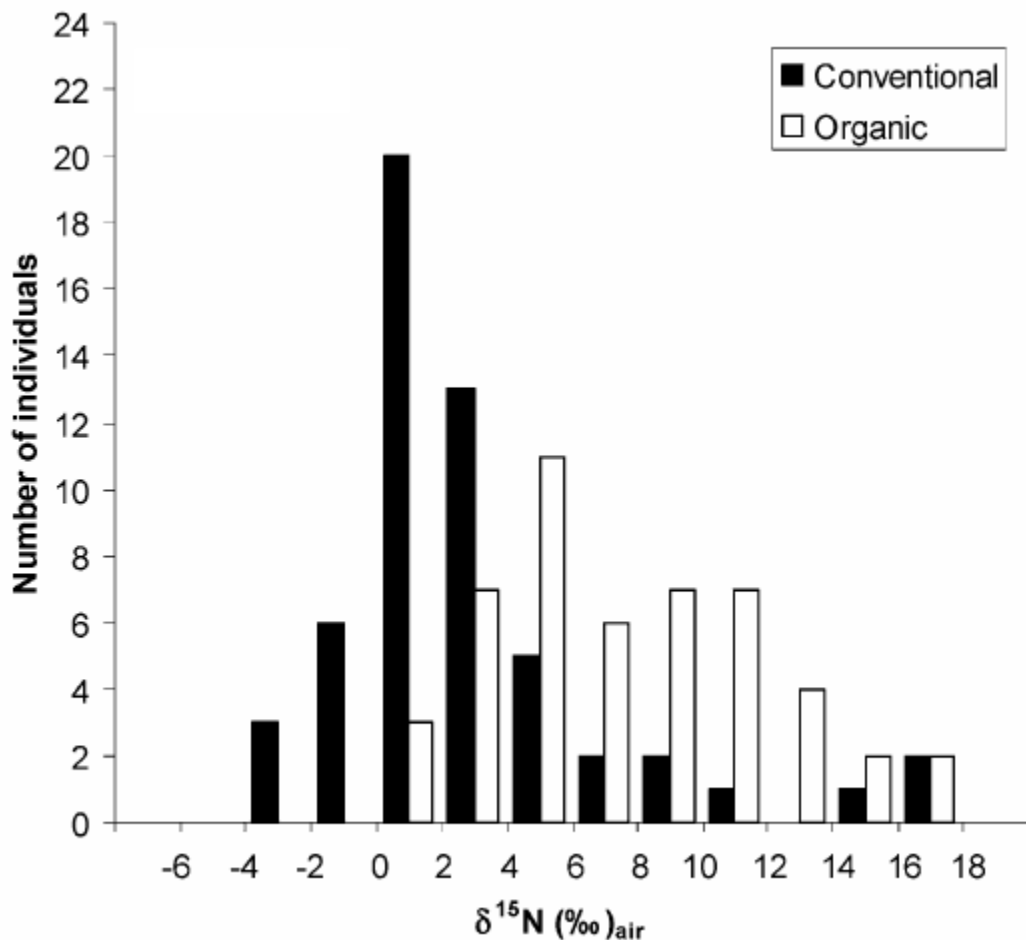
CONVENTIONAL



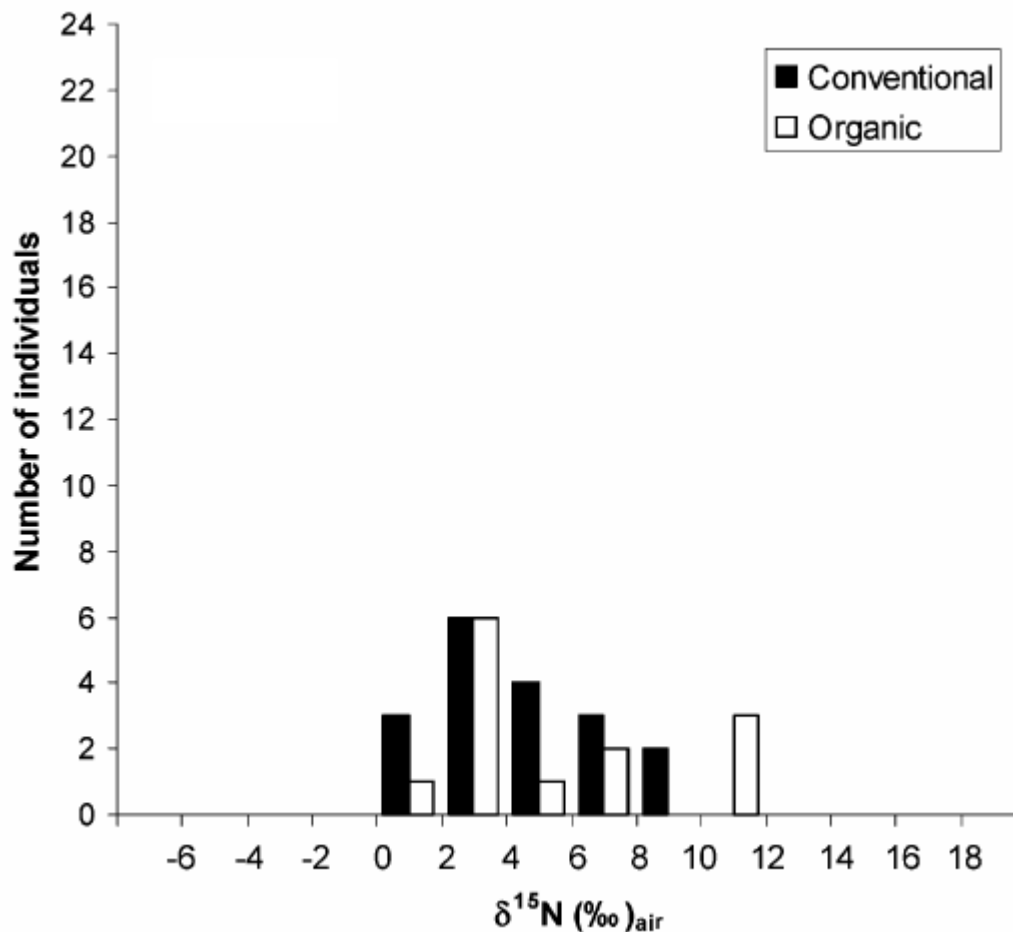
Higher concentration of ^{15}N in organic than in non-organic tomatoes



Overlapping concentrations of ^{15}N between organic and non-organic lettuce



Indistinguishable concentrations of ^{15}N between organic and non-organic carrots



Factors influencing the content of ^{15}N

Variability in fixation of atmospheric nitrogen

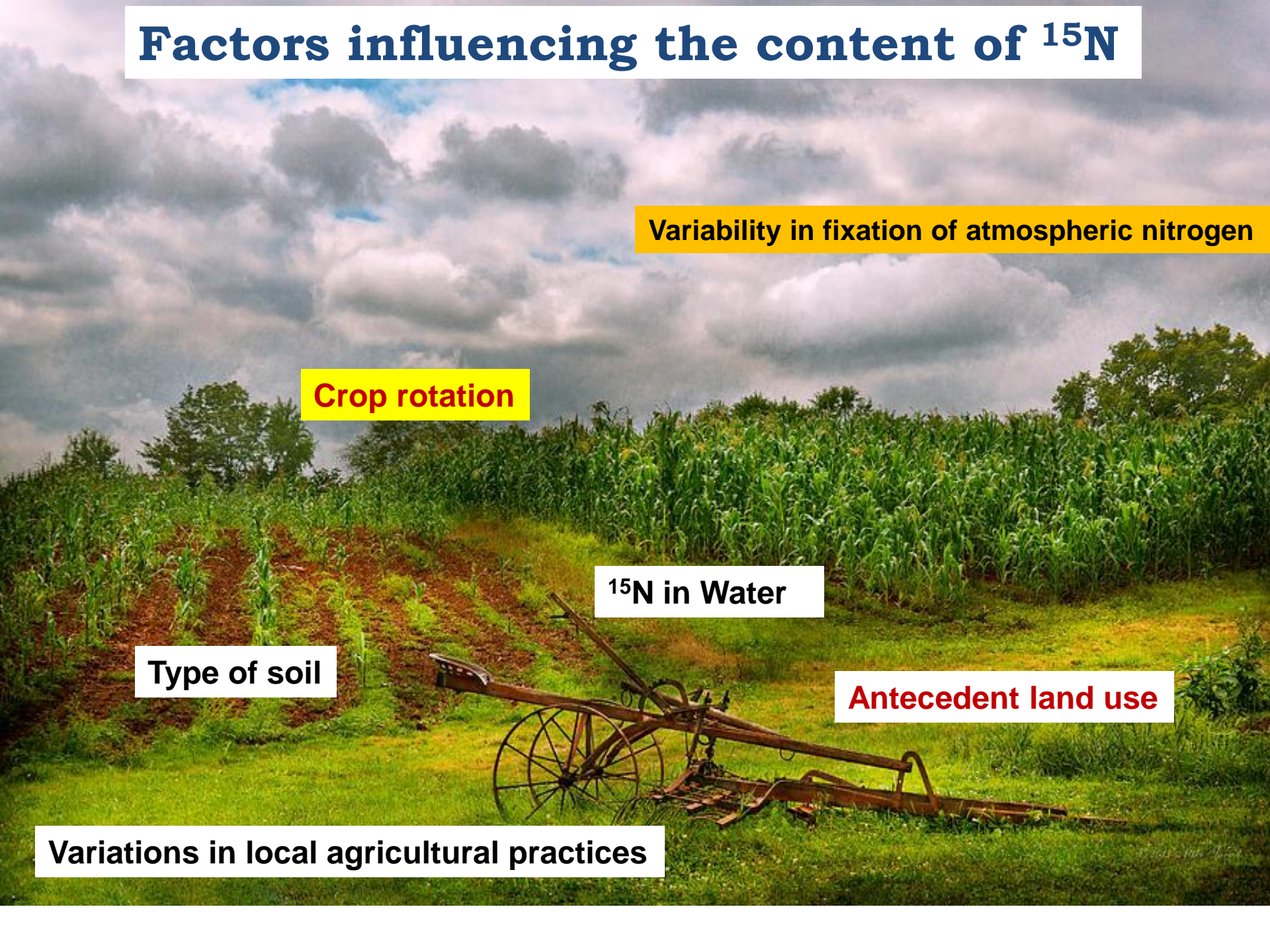
Crop rotation

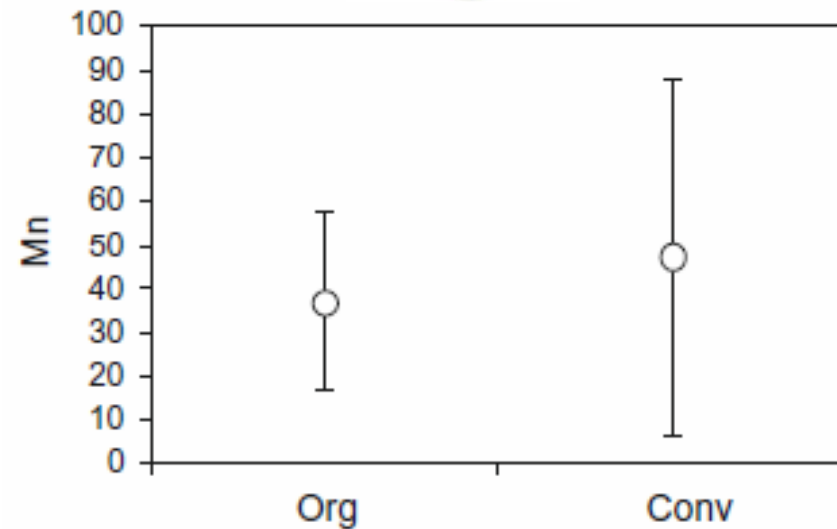
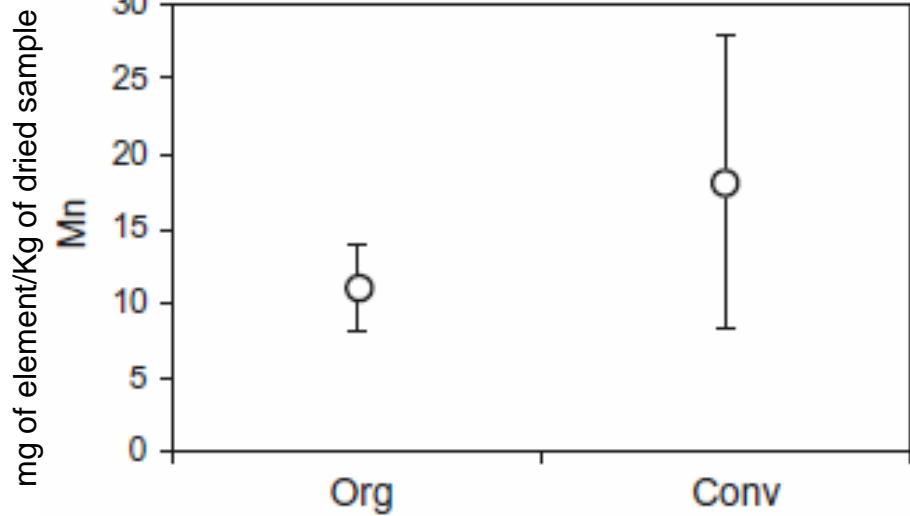
^{15}N in Water

Type of soil

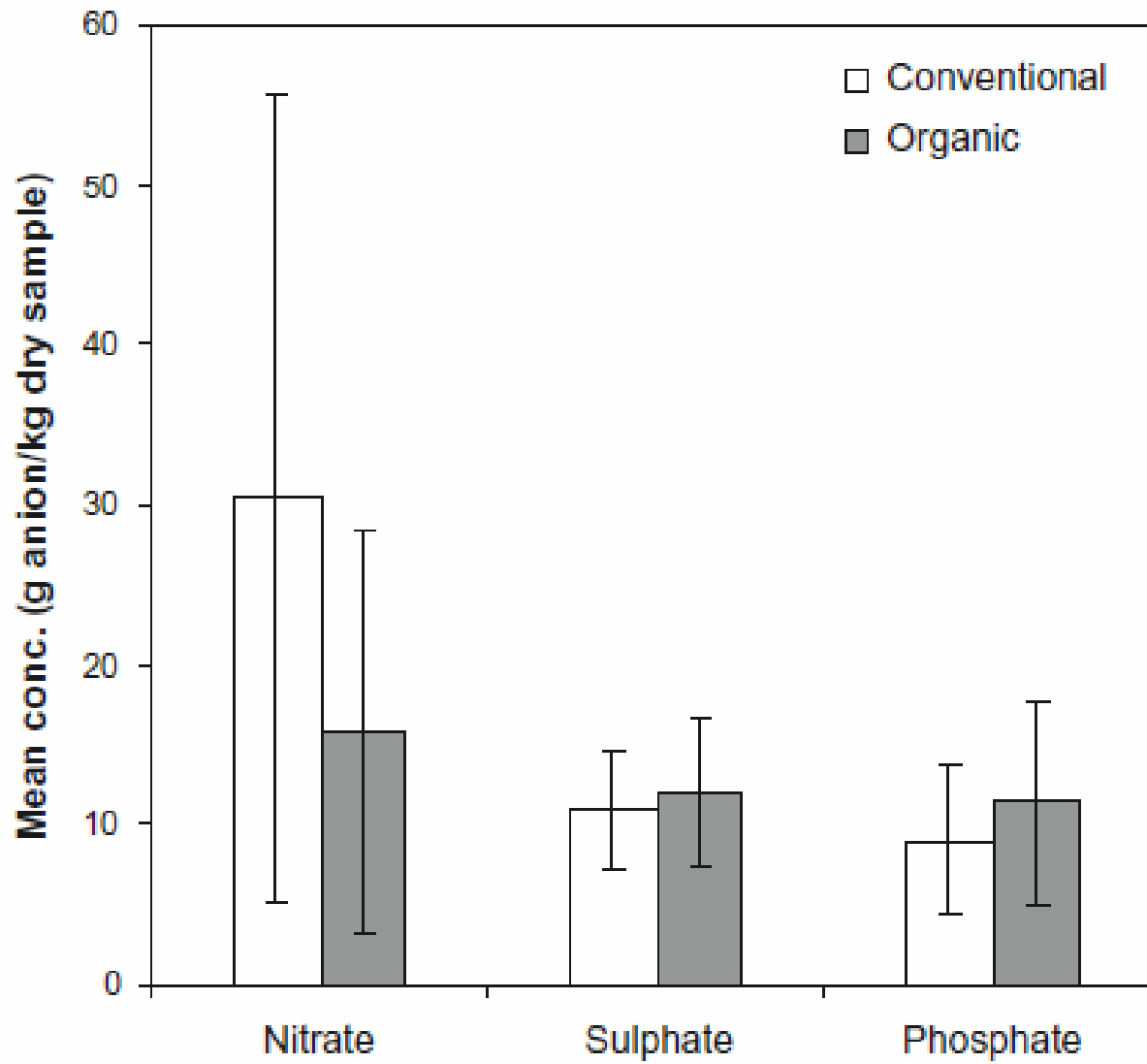
Antecedent land use

Variations in local agricultural practices

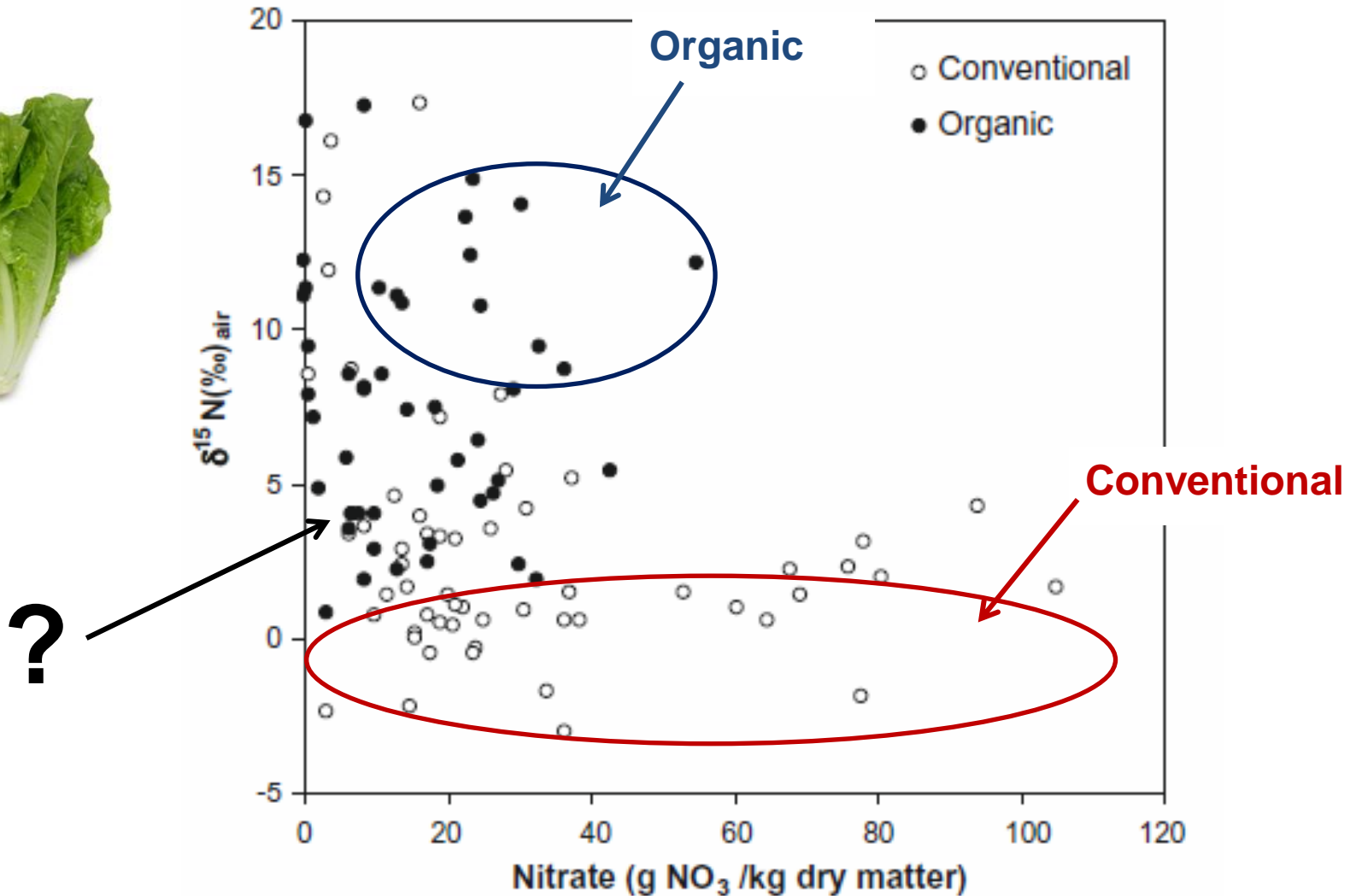




Comparing the concentrations of **Na, Fe, Ca, Rb, K, Cu, Mn** **did not** yield any **unambiguous** distinction between organic and conventional crops



Simultaneous analysis of two markers leads to (partial) classification of lettuce



Organic

vs.

non-Organic



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Organic

vs.

non-Organic



Caged

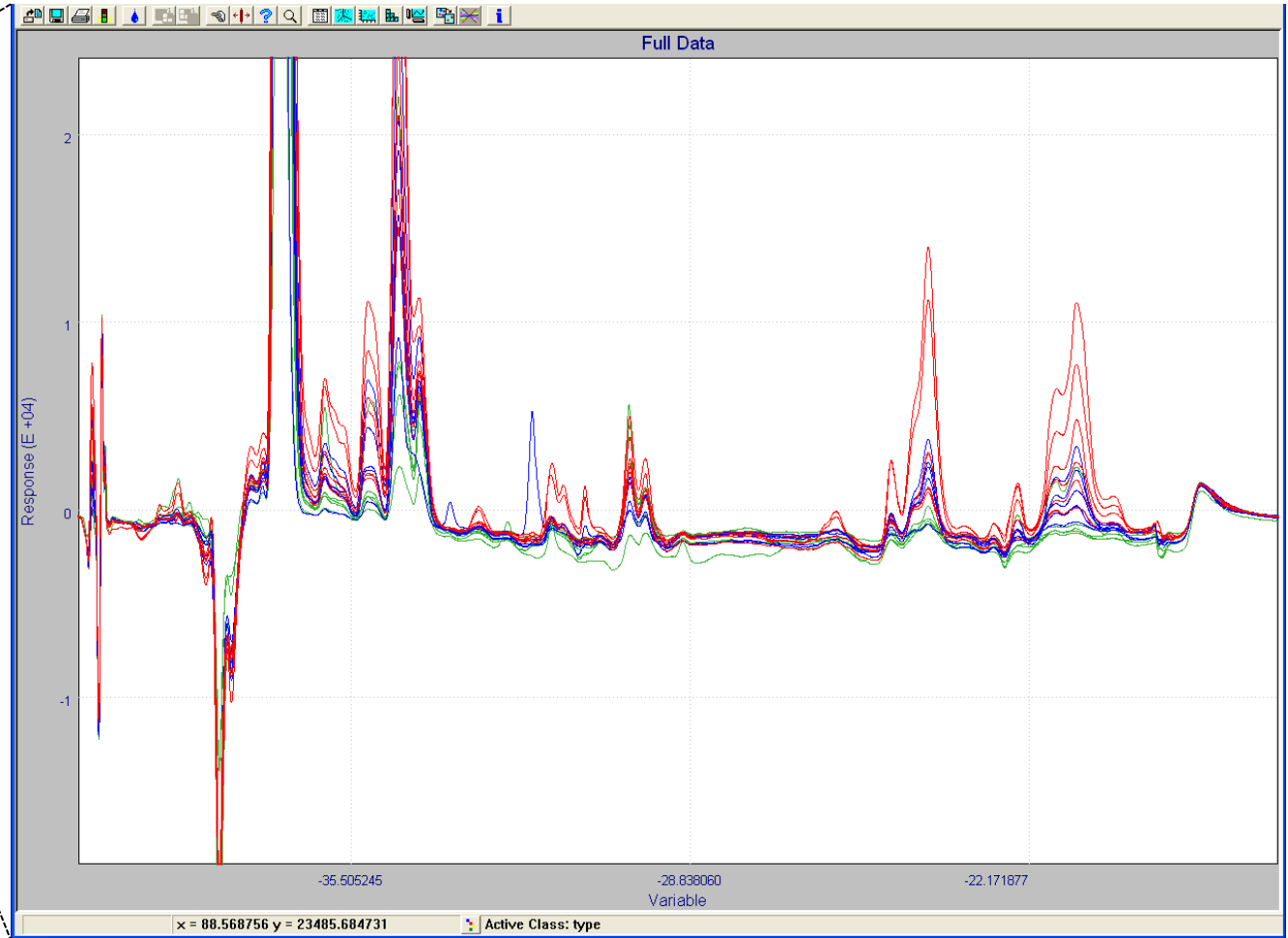
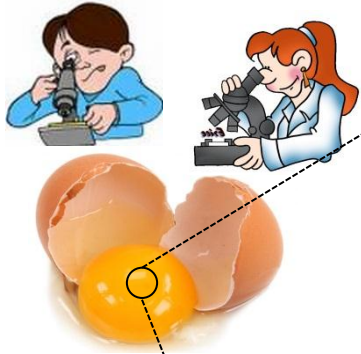


Barn



Free range

Analysis of yolks



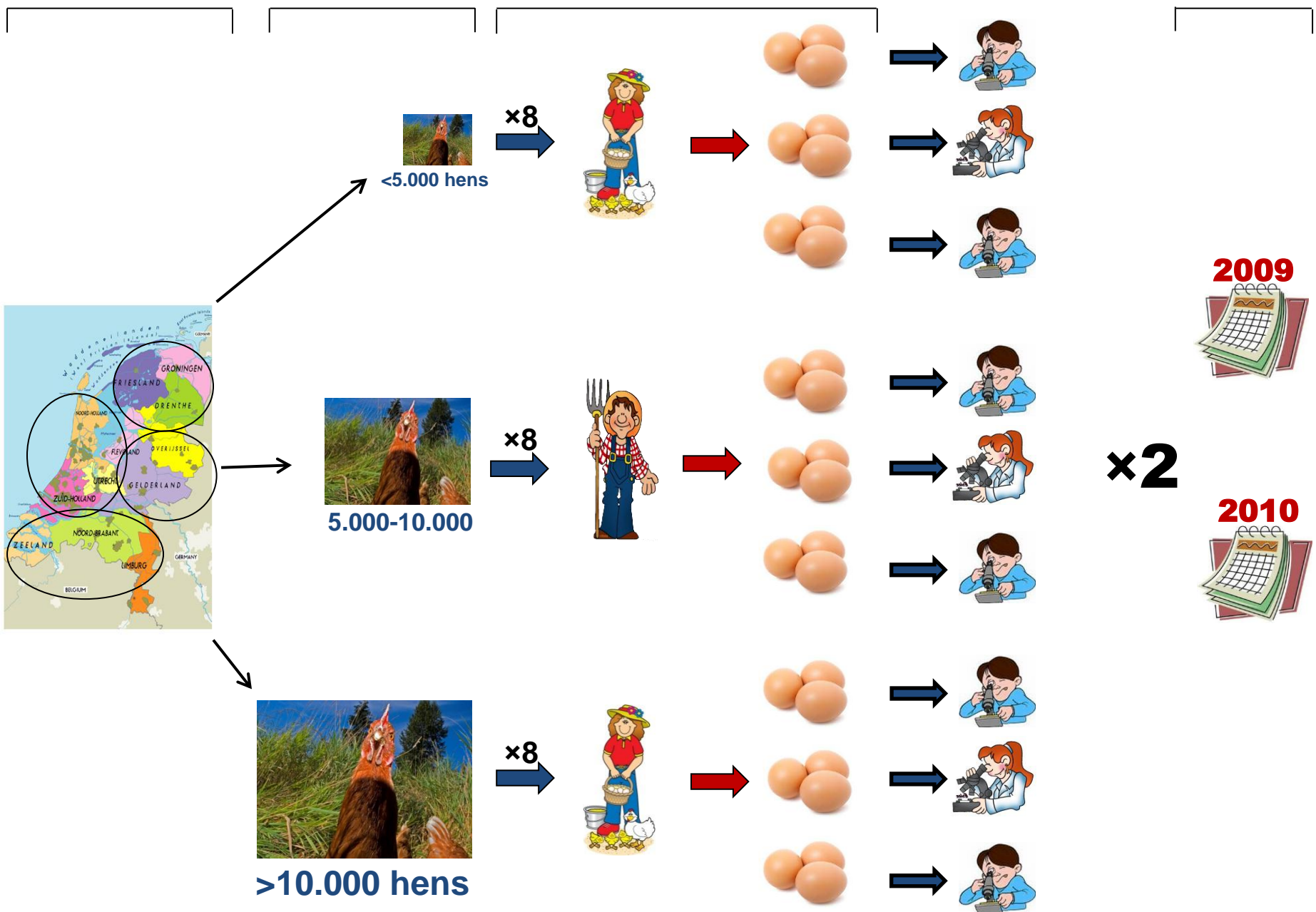
High Performance Liquid Chromatograms of yolks

Location

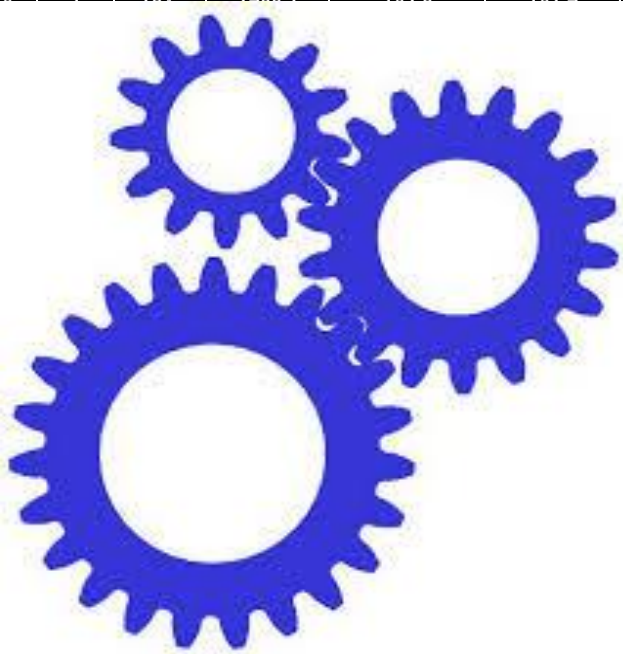
Size

Variability

Saison



Sample	Region	of ana	Class	g/non-r	Sample	Unknown 1	Canthaxanthin	Unknown 2	Unknown 3	Unknown 4	Unknown 5	β-apo-carotena	Unknown 6	Unknown 7	Unknown 8	B-Caroten
Barn3S	3	1	2	2	1A	665.6	45.7	27.4	0.00	0.00	0.00	0.00	11.81	9.98	0.00	0.0
FR2S	3	1	1	2	2A	624.9	294.5	16.2	0.00	0.00	0.00	0.00	14.61	12.27	0.00	0.0
FR2W	4	1	1	2	3A	624.3	64.0	34.4	8.03	0.00	0.00	0.00	10.31	13.09	0.00	0.0
FR2E	1	1	1	2	4A	668.9	364.2	25.1	0.00	0.00	0.00	0.00	15.63	16.01	148.10	0.0
Cage2N	2	1	3	2	5A	361.9	27.9	14.4	0.00	0.00	0.00	0.00	9.38	6.56	0.00	0.0
FR1E	1	1	1	2	6A	838.1	347.9	25.2	0.00	0.00	0.00	0.00	22.76	15.60	0.00	0.0
Bio2E	1	1	0	1	7A	1818.6	117.9	106.6	0.00	16.56	15.73	0.00	46.92	31.71	0.00	0.0
Bio1E	1	1	0	1	8A	981.7	63.9	57.5	0.00	0.00	0.00	0.00	24.58	22.15	0.00	0.0
FR2N	2	1	1	2	9A	582.3	368.2	18.7	0.00	0.00	0.00	0.00	19.12	17.32	225.07	0.0
Barn3N	2	1	2	2	10A1	722.4	330.7	24.9	0.00	0.00	0.00	0.00	21.15	9.15	0.00	0.0
Barn3N	2	1	2	2	10A2	694.7	335.4	28.0	0.00	0.00	0.00	0.00	24.00	16.01	0.00	0.0
Barn1N	2	1	2	2	11A	1002.6	71.2	41.7	0.00	0.00	0.00	0.00	27.49	19.81	0.00	0.0
Bio3N	2	1													0.00	0.0
Cage2E	1	1													0.00	0.0
Bio3W	4	1													0.00	0.0
FR3E	1	1													0.00	0.0
Bio2S	3	1													0.00	0.0
Barn3S	3	2													0.00	0.0
FR2S	3	2													0.00	0.0
FR2W	4	2													0.00	0.0
FR2E	1	2													209.25	0.0
FR2E	1	2													579.06	0.0
Cage2N	2	2													0.00	0.0
FR1E	1	2													0.00	0.0
Bio2E	1	2													0.00	0.0
Bio1E	1	2													0.00	0.0
FR2N	2	2													170.56	0.0
Barn3N	2	2													0.00	0.0
Barn1N	2	2													0.00	0.0
Bio3N	2	2													0.00	0.0
Cage2E	1	2													0.00	0.0
Bio3W	4	2													0.00	0.0
Bio3W	4	2													0.00	0.0
FR3E	1	2													0.00	0.0
Bio2S	3	2													0.00	0.0
Barn3S	3	8													0.00	0.0
FR2S	3	8													0.00	0.0
FR2W	4	8													0.00	0.0
FR2E	1	8													0.00	0.0
Cage2N	2	8	3	2	4C	639.2	436.2	36.0	0.00	0.00	0.00	0.00	36.15	24.07	239.66	0.0
FR1E	1	8	1	2	5C	498.1	32.5	23.4	0.00	0.00	0.00	0.00	16.17	10.92	0.00	0.0
FR1E	1	8	1	2	6C	1170.7	282.4	27.6	0.00	0.00	0.00	0.00	43.32	23.71	0.00	0.0
Bio2E	1	8	0	1	7C	2581.2	161.4	146.6	0.00	24.37	17.06	0.00	71.77	44.02	0.00	0.0
Bio1E	1	8	0	1	8C1	1542.9	81.1	74.1	0.00	0.00	0.00	0.00	44.78	41.35	0.00	0.0
Bio1E	1	8	0	1	8C2	1506.2	75.3	65.9	0.00	0.00	0.00	0.00	52.57	41.21	0.00	0.0
FR2N	2	8	1	2	9C	789.7	516.9	23.3	0.00	0.00	0.00	0.00	22.03	19.46	356.77	0.0
Barn3N	2	8	2	2	10C	919.3	426.6	27.7	0.00	0.00	0.00	0.00	23.64	12.23	0.00	0.0
Barn1N	2	8	2	2	11C	1384.7	74.4	100.1	0.00	0.00	0.00	0.00	32.55	23.91	0.00	0.0
Bio3N	2	8	0	1	12C	1948.9	99.5	112.7	0.00	17.72	10.58	0.00	75.67	57.49	0.00	0.0
Cage2E	1	8	3	2	13C	1109.1	56.0	79.7	0.00	0.00	0.00	0.00	47.67	35.99	0.00	0.0
Bio3W	4	8	0	1	14C	1574.4	81.5	97.6	0.00	27.40	12.63	0.00	143.71	124.76	0.00	0.0
FR3E	1	8	1	2	15C	1664.4	95.0	100.1	0.00	24.98	28.92	0.00	80.86	57.44	0.00	0.0
Bio2S	3	8	0	1	16C	1624.2	81.9	92.8	0.00	0.00	0.00	0.00	36.76	30.33	0.00	0.0
Bio3S	3	9	0	1	17A	1493.8	81.9	81.7	0.00	25.47	13.22	0.00	75.85	71.28	0.00	0.0
Cage2S	3	9	3	2	18A1	799.7	319.2	23.6	0.00	0.00	0.00	0.00	16.62	13.34	543.78	0.0
Cage2S	3	9	3	2	18A2	827.7	291.5	27.1	0.00	0.00	0.00	0.00	17.24	14.48	406.87	0.0



Big-data science:

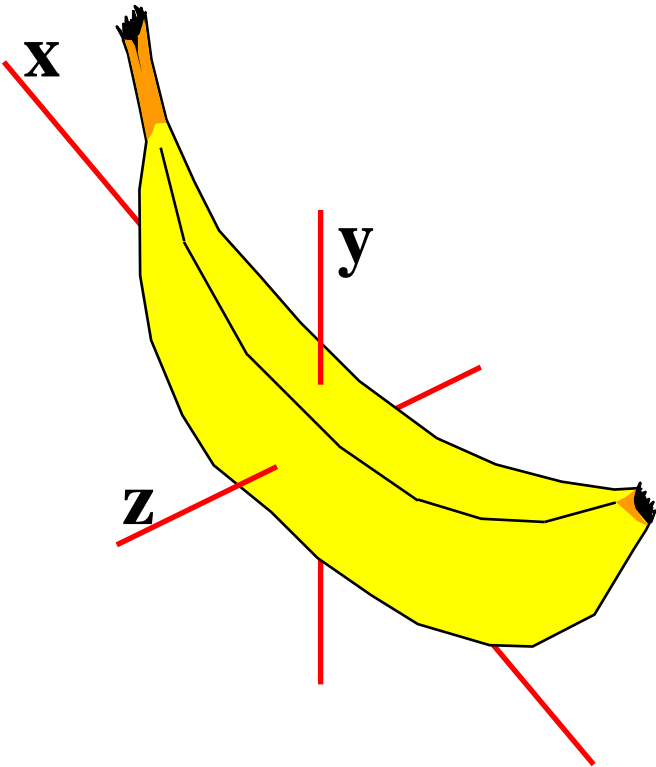
- Data mining;
- Machine learning.

Un-targeted analysis: “OMICS”

- Metabolomics;
- Proteomics;
- Genomics;
- Chemometrics.

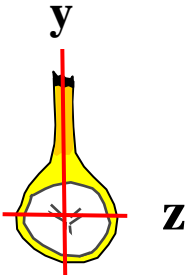
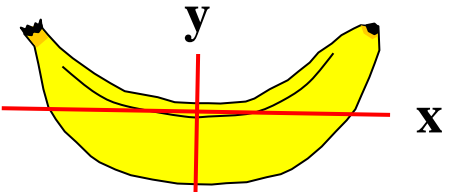
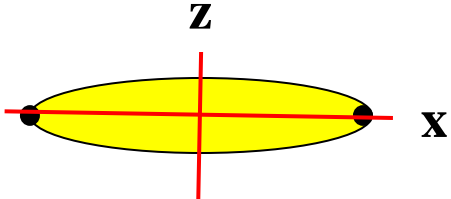
Chemometrics of a Banana

3D



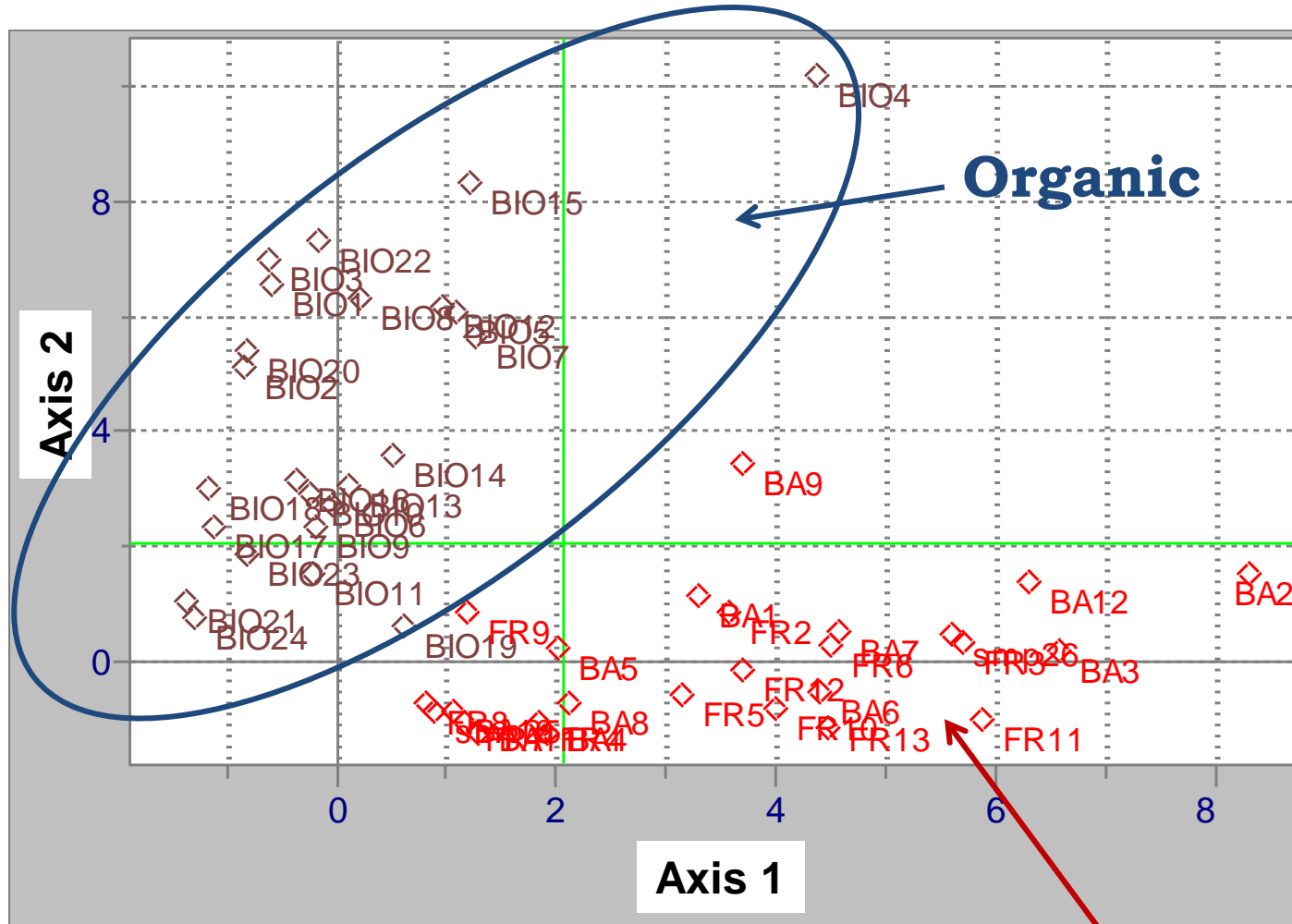
Reduction
of
dimensions

2D



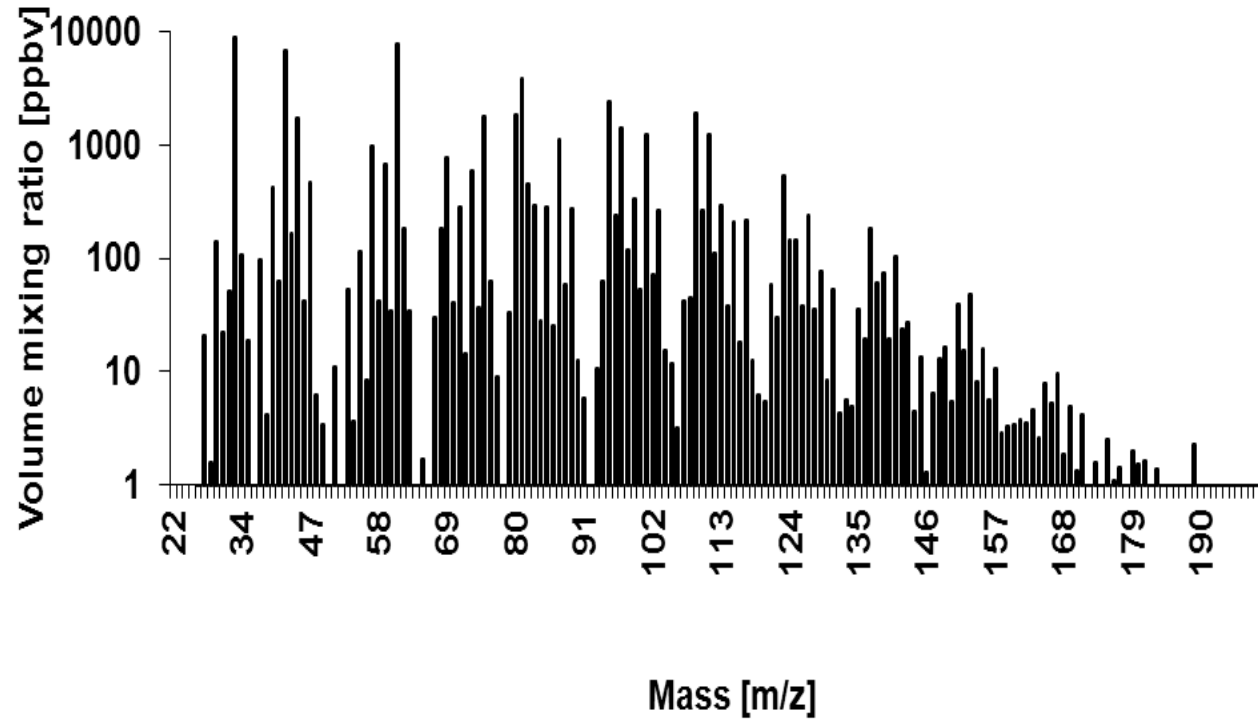
Sample	Region	of ana	Class	g/non-r	Sample	Unknown 1	Canthaxanthin	Unknown 2	Unknown 3	Unknown 4	Unknown 5	B-apo-carotena	Unknown 6	Unknown 7	Unknown 8	B-Carotene
Barn3S	3	1	2	2	1A	665.6	45.7	27.4	0.00	0.00	0.00	0.00	11.81	9.98	0.00	0.0
FR2S	3	1	1	2	2A	624.9	294.5	16.2	0.00	0.00	0.00	0.00	14.61	12.27	0.00	0.0
FR2W	4	1	1	2	3A	624.3	64.0	34.4	8.03	0.00	0.00	0.00	10.31	13.09	0.00	0.0
FR2E	1	1	1	2	4A	668.9	364.2	25.1	0.00	0.00	0.00	0.00	15.63	16.01	148.10	0.0
Cage2N	2	1	3	2	5A	361.9	27.9	14.4	0.00	0.00	0.00	0.00	9.38	6.56	0.00	0.0
FR1E	1	1	1	2	6A	838.1	347.9	25.2	0.00	0.00	0.00	0.00	22.76	15.60	0.00	0.0
Bio2E	1	1	0	1	7A	1818.6	117.9	106.6	0.00	16.56	15.73	0.00	46.92	31.71	0.00	0.0
Bio1E	1	1	0	1	8A	981.7	63.9	57.5	0.00	0.00	0.00	0.00	24.58	22.15	0.00	0.0
FR2N	2	1	1	2	9A	582.3	368.2	18.7	0.00	0.00	0.00	0.00	19.12	17.32	225.07	0.0
Barn3N	2	1	2	2	10A1	722.4	330.7	24.9	0.00	0.00	0.00	0.00	21.15	9.15	0.00	0.0
Barn3N	2	1	2	2	10A2	694.7	335.4	28.0	0.00	0.00	0.00	0.00	24.00	16.01	0.00	0.0
Barn1N	2	1	2	2	11A	1002.6	71.2	41.7	0.00	0.00	0.00	0.00	27.49	19.81	0.00	0.0
Bio3N	2	1	0	1	12A	1788.1	104.3	101.7	0.00	12.91	10.29	0.00	46.32	32.09	0.00	0.0
Cage2E	1	1	3	2	13A	932.1	68.6	42.6	0.00	0.00	0.00	0.00	23.07	21.37	0.00	0.0
Bio3W	4	1	0	1	14A	2625.1	174.0	161.8	0.00	15.15	16.42	0.00	55.31	47.53	0.00	0.0
FR3E	1	1	1	2	15A	1335.1	91.5	93.3	0.00	15.51	10.82	0.00	50.12	32.23	0.00	0.0
Bio2S	3	1	0	1	16A	990.3	59.7	60.5	0.00	0.00	0.00	0.00	18.50	31.13	0.00	0.0
Barn3S	3	2	2	2	1B	635.4	55.2	27.2	0.00	0.00	0.00	0.00	18.02	17.61	0.00	0.0
FR2S	3	2	1	2	2B	536.8	386.6	20.8	0.00	0.00	0.00	0.00	14.13	7.96	0.00	0.0
FR2W	4	2	1	2	3B	634.4	25.8	33.4	13.53	0.00	0.00	0.00	34.67	32.19	0.00	0.0
FR2E	1	2	1	2	4B1	808.9	470.4	29.2	0.00	0.00	0.00	0.00	23.28	14.64	209.25	0.0
FR2E	1	2	1	2	4B2	572.4	813.0	41.0	0.00	0.00	0.00	0.00	62.03	35.77	579.06	0.0
Cage2N	2	2	3	2	5B	441.2	33.4	22.6	0.00	0.00	0.00	0.00	13.79	6.39	0.00	0.0
FR1E	1	2	1	2	6B	980.9	425.4	29.7	0.00	0.00	0.00	0.00	25.77	14.33	0.00	0.0
Bio2E	1	2	0	1	7B	2109.3	126.8	131.1	0.00	20.07	8.38	0.00	43.58	26.90	0.00	0.0
Bio1E	1	2	0	1	8B	1280.8	73.7	67.7	0.00	0.00	0.00	0.00	36.46	36.35	0.00	0.0
FR2N	2	2	1	2	9B	701.3	341.4	23.4	0.00	0.00	0.00	0.00	21.26	17.15	170.56	0.0
Barn3N	2	2	2	2	10B	787.1	416.7	31.6	0.00	0.00	0.00	0.00	18.34	12.82	0.00	0.0
Barn1N	2	2	2	2	11B	1264.4	99.0	60.5	0.00	0.00	0.00	0.00	32.01	24.55	0.00	0.0
Bio3N	2	2	0	1	12B	1900.3	108.7	107.9	0.00	17.67	9.34	0.00	55.86	41.01	0.00	0.0
Cage2E	1	2	3	2	13B	1047.2	82.5	47.8	0.00	0.00	0.00	0.00	33.49	27.04	0.00	0.0
Bio3W	4	2	0	1	14B1	1445.5	93.3	103.9	0.00	27.08	14.06	0.00	120.60	113.38	0.00	0.0
Bio3W	4	2	0	1	14B2	1744.6	112.3	128.9	0.00	18.88	11.21	0.00	88.53	71.51	0.00	0.0
FR3E	1	2	1	2	15B	1811.8	94.4	100.9	0.00	18.10	6.93	0.00	68.75	38.66	0.00	0.0
Bio2S	3	2	0	1	16B	1386.4	79.4	80.6	0.00	17.53	11.23	0.00	48.41	30.66	0.00	0.0
Barn3S	3	8	2	2	1C	1076.1	92.6	50.6	0.00	0.00	0.00	0.00	34.73	27.45	0.00	0.0
FR2S	3	8	1	2	2C	753.3	443.0	18.5	0.00	0.00	0.00	0.00	19.78	12.64	0.00	0.0
FR2W	4	8	1	2	3C	1165.3	55.7	125.5	15.77	0.00	0.00	0.00	24.78	25.89	0.00	0.0
FR2E	1	8	1	2	4C	839.2	456.2	30.0	0.00	0.00	0.00	0.00	30.15	24.67	239.66	0.0
Cage2N	2	8	3	2	5C	498.1	32.5	23.4	0.00	0.00	0.00	0.00	16.17	10.92	0.00	0.0
FR1E	1	8	1	2	6C	1170.7	282.4	27.6	0.00	0.00	0.00	0.00	43.32	23.71	0.00	0.0
Bio2E	1	8	0	1	7C	2581.2	161.4	146.6	0.00	24.37	17.06	0.00	71.77	44.02	0.00	0.0
Bio1E	1	8	0	1	8C1	1542.9	81.1	74.1	0.00	0.00	0.00	0.00	44.78	41.35	0.00	0.0
Bio1E	1	8	0	1	8C2	1506.2	75.3	65.9	0.00	0.00	0.00	0.00	52.57	41.21	0.00	0.0
FR2N	2	8	1	2	9C	789.7	516.9	23.3	0.00	0.00	0.00	0.00	22.03	19.46	356.77	0.0
Barn3N	2	8	2	2	10C	919.3	426.6	27.7	0.00	0.00	0.00	0.00	23.64	12.23	0.00	0.0
Barn1N	2	8	2	2	11C	1384.7	74.4	100.1	0.00	0.00	0.00	0.00	32.55	23.91	0.00	0.0
Bio3N	2	8	0	1	12C	1948.9	99.5	112.7	0.00	17.72	10.58	0.00	75.67	57.49	0.00	0.0
Cage2E	1	8	3	2	13C	1109.1	56.0	79.7	0.00	0.00	0.00	0.00	47.67	35.99	0.00	0.0
Bio3W	4	8	0	1	14C	1574.4	81.5	97.6	0.00	27.40	12.63	0.00	143.71	124.76	0.00	0.0
FR3E	1	8	1	2	15C	1664.4	95.0	100.1	0.00	24.98	28.92	0.00	80.86	57.44	0.00	0.0
Bio2S	3	8	0	1	16C	1624.2	81.9	92.8	0.00	0.00	0.00	0.00	36.76	30.33	0.00	0.0
Bio3S	3	9	0	1	17A	1493.8	81.9	81.7	0.00	25.47	13.22	0.00	75.85	71.28	0.00	0.0
Cage2S	3	9	3	2	18A1	799.7	319.2	23.6	0.00	0.00	0.00	0.00	16.62	13.34	543.78	0.0
Cage2S	3	9	3	2	18A2	827.7	291.5	27.1	0.00	0.00	0.00	0.00	17.24	14.48	406.87	0.0

Graphical classification of eggs



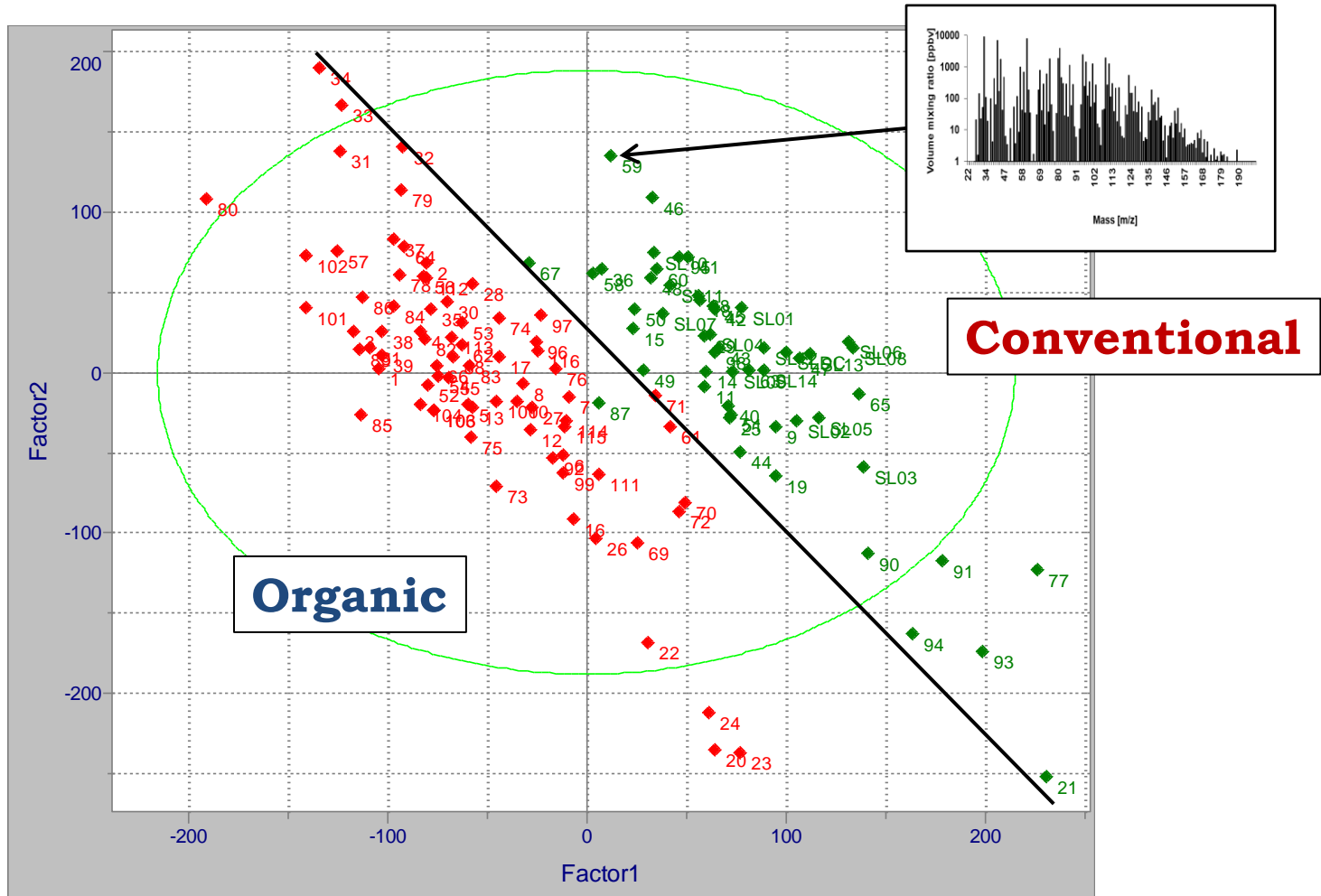
Conventional

Un-targeted analysis of coffee



Mass-spectra measure the mass of fragments

Graphical classification of types of coffee



Organic

vs.

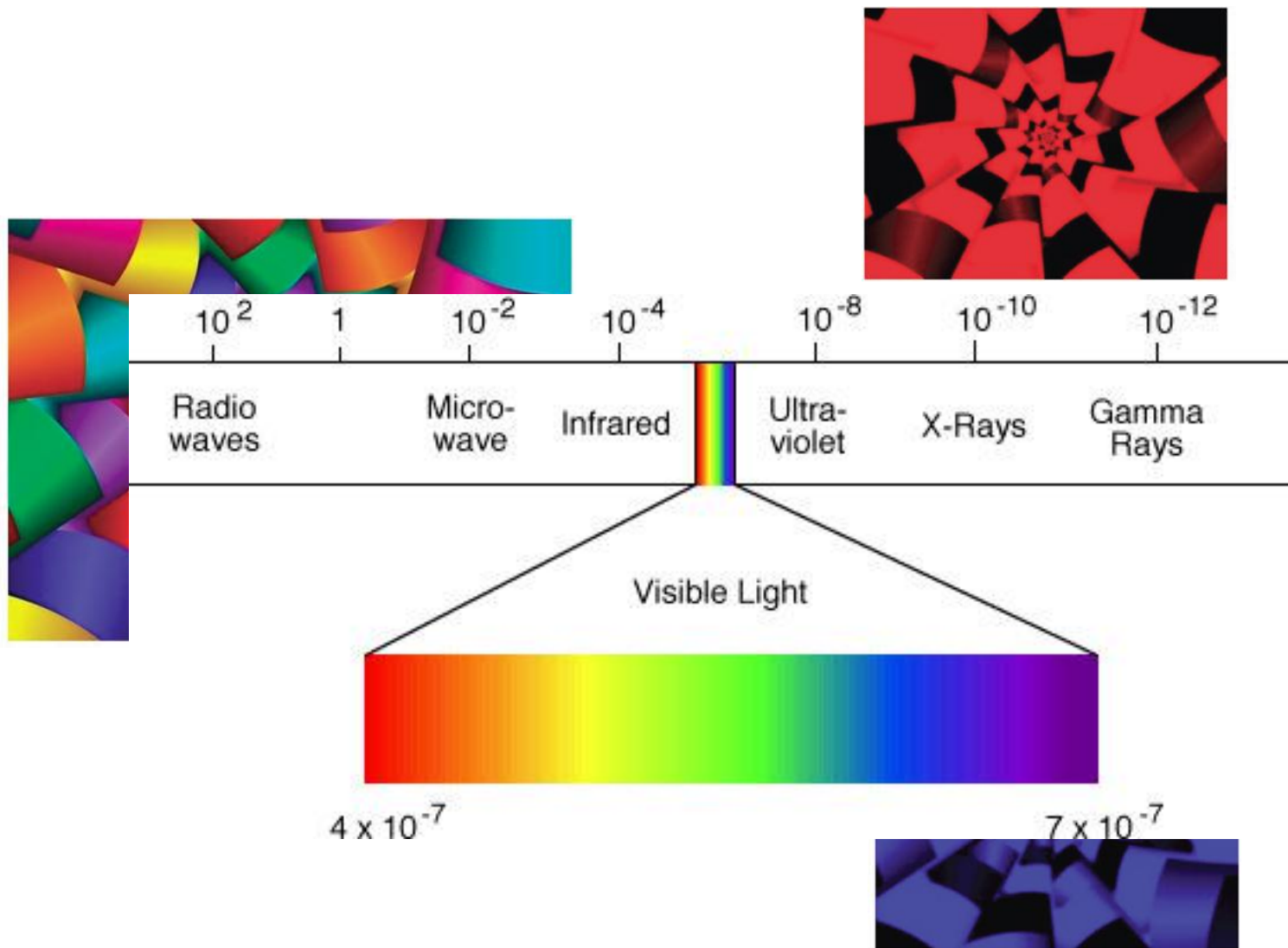
non-Organic

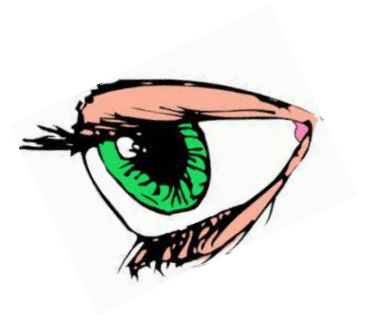
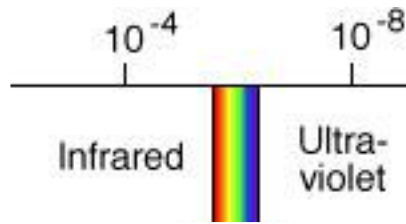
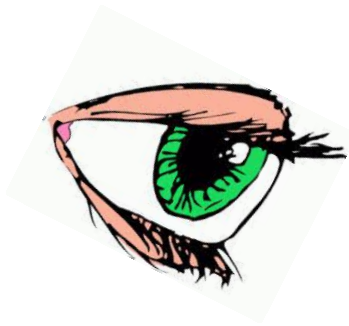


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Photography is Chemistry

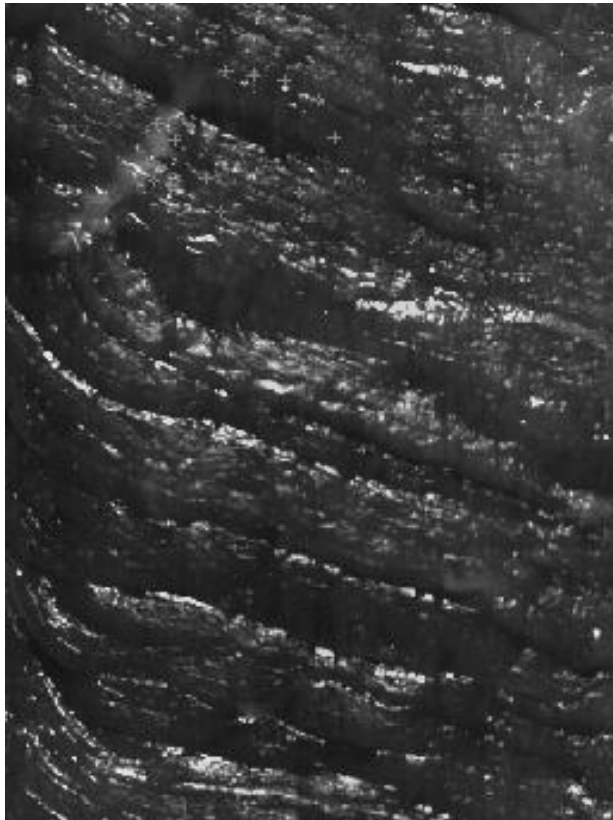




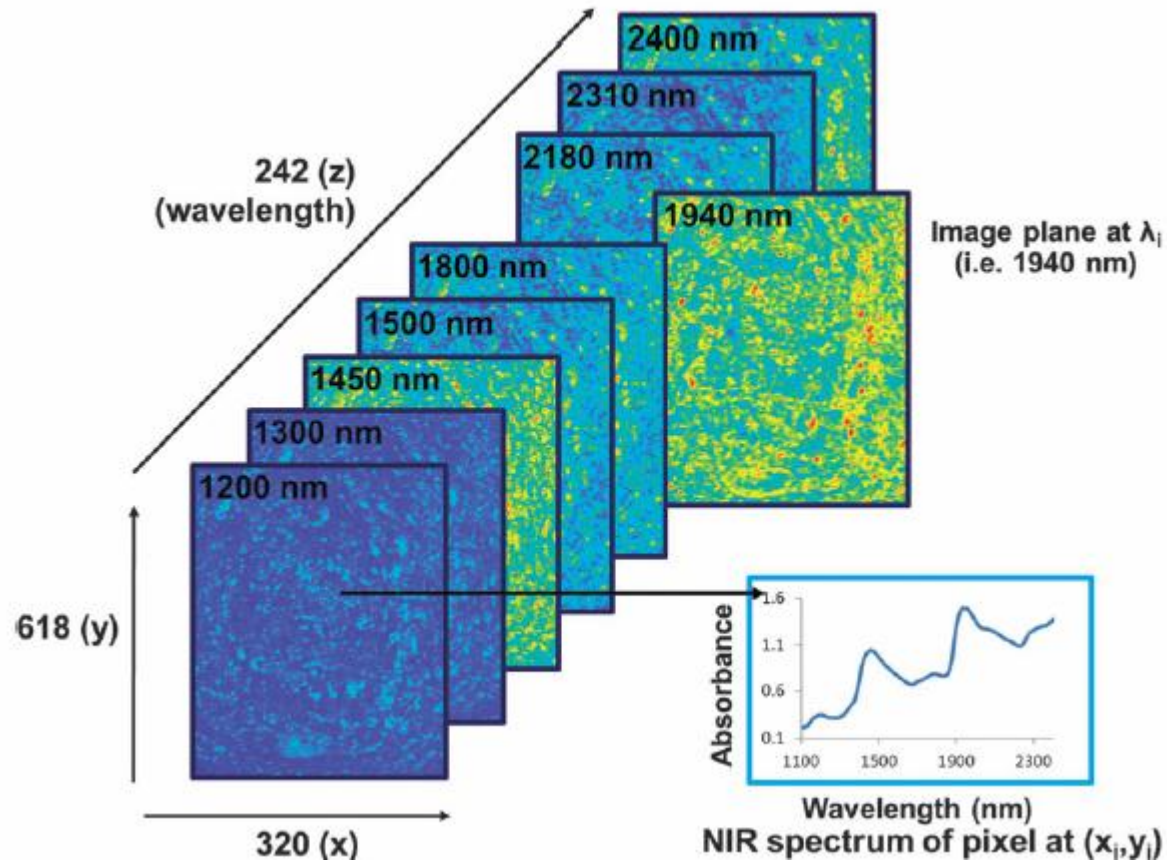
Organic

vs.

non-Organic



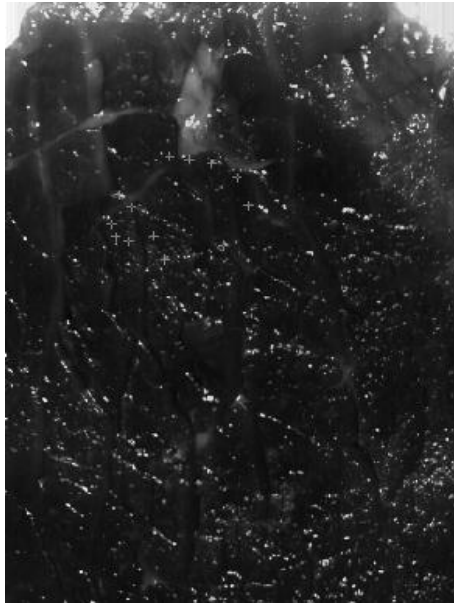
Hyperspectral imaging



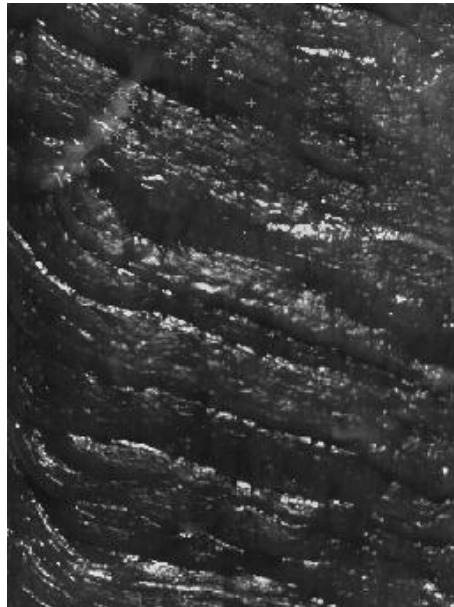
320 x 618 x 242 = ca 48.000.000 of data points

Invisible to the eye
(Near Infra Red photos)

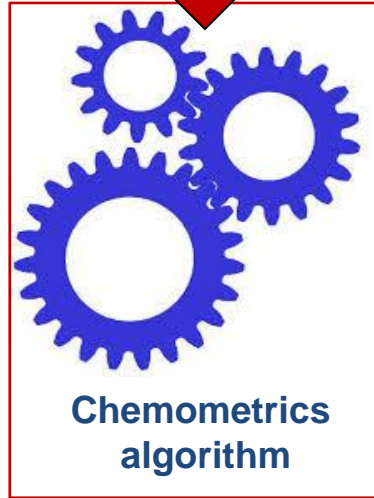
Regular beef



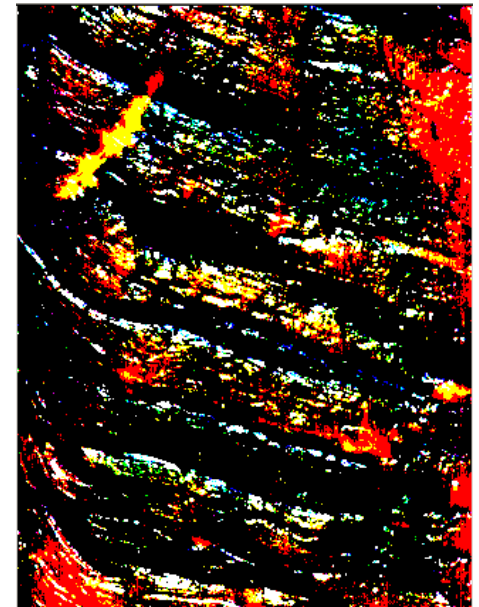
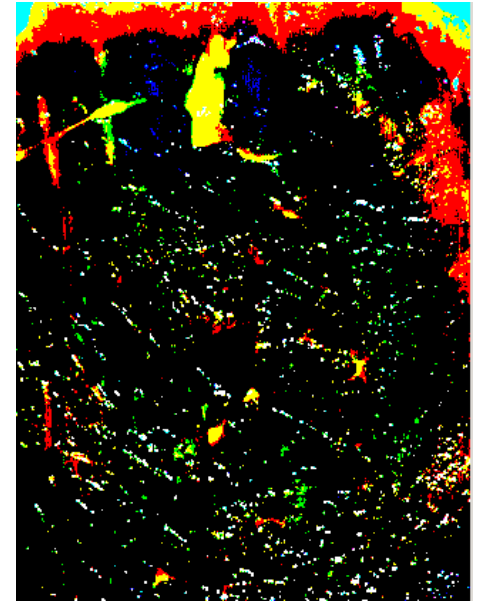
Organic beef



320 pixel x
425 pixel y
256 pixel λ

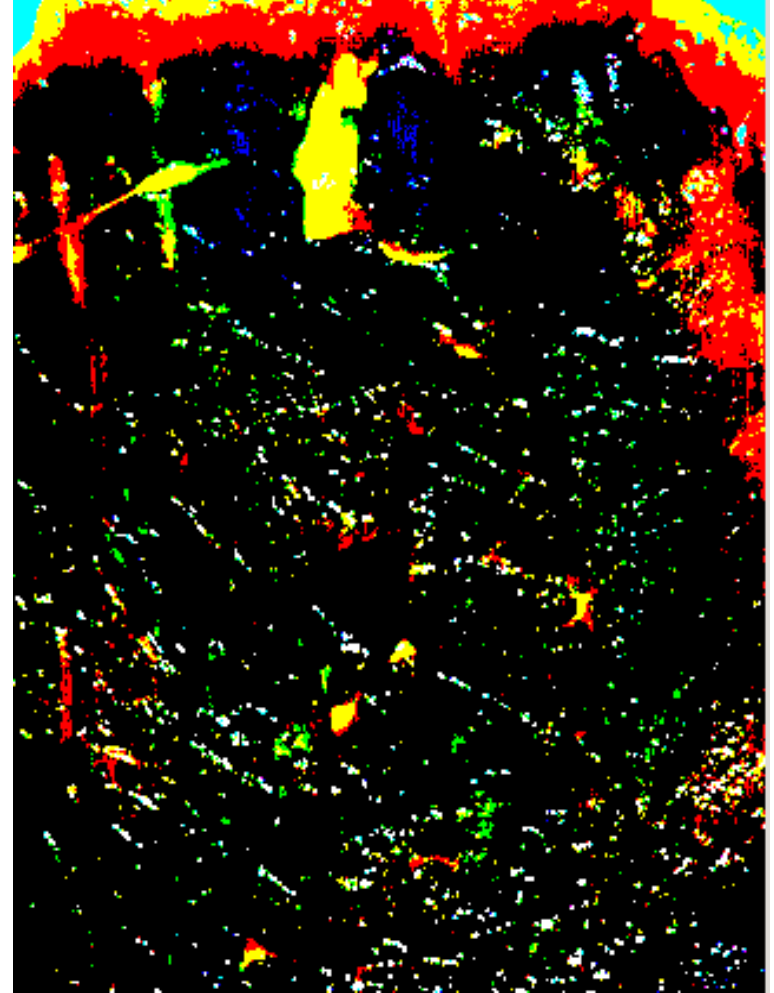
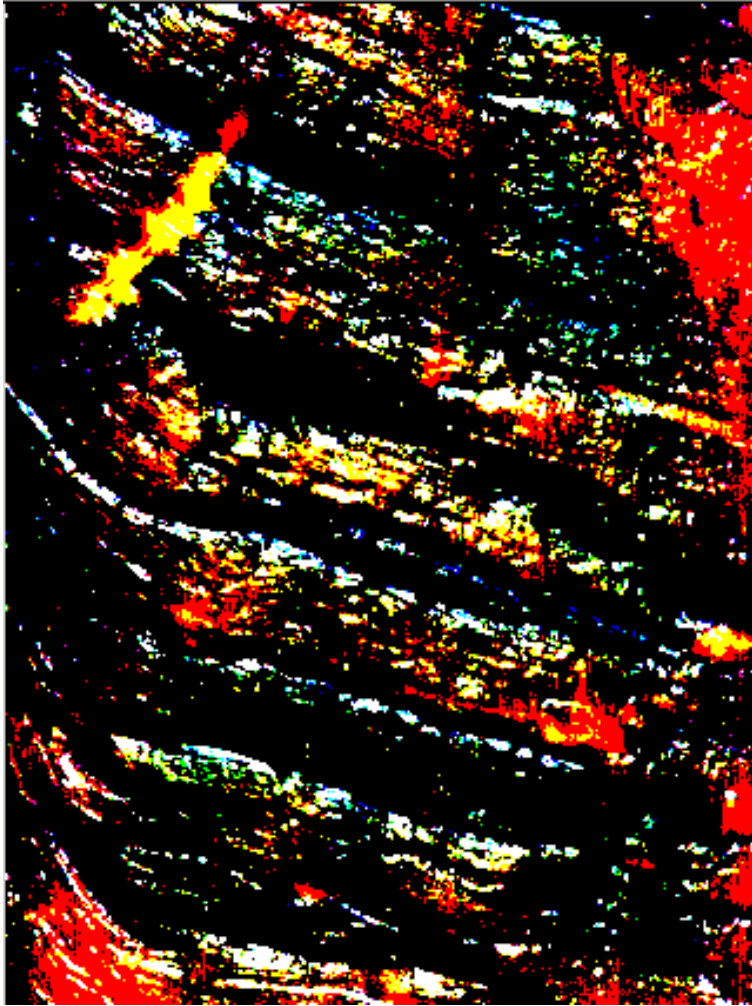


Visible
3 Channels pictures (RGB)

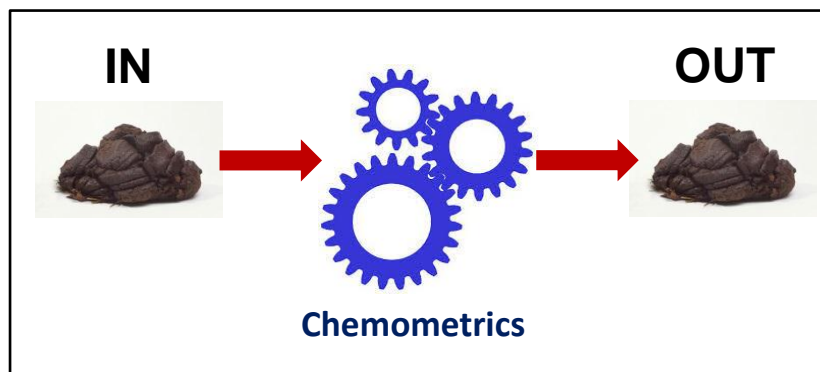


Organic

vs. non-Organic



Organic vs. non-Organic



**Untargeted analysis
prevents fraud.**





ANALYTICAL AUTHENTICATION OF ORGANIC FOODS

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ACKNOWLEDGEMENTS

- **Saskia van Ruth**
- **Martin Alewijn**
- **Yannick Weesepeel**
- **Annemieke Pustjens**
- **Valentina Acierno**
- **Erwin Cuijpers**



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