



The First Italian-Israeli Forum on Medicine

## Food and health: impact of computational and experimental studies

The Robert H Smith Faculty of Agriculture,  
Institute of Biochemistry, Food Science and Nutrition,  
The Hebrew University, Rehovot

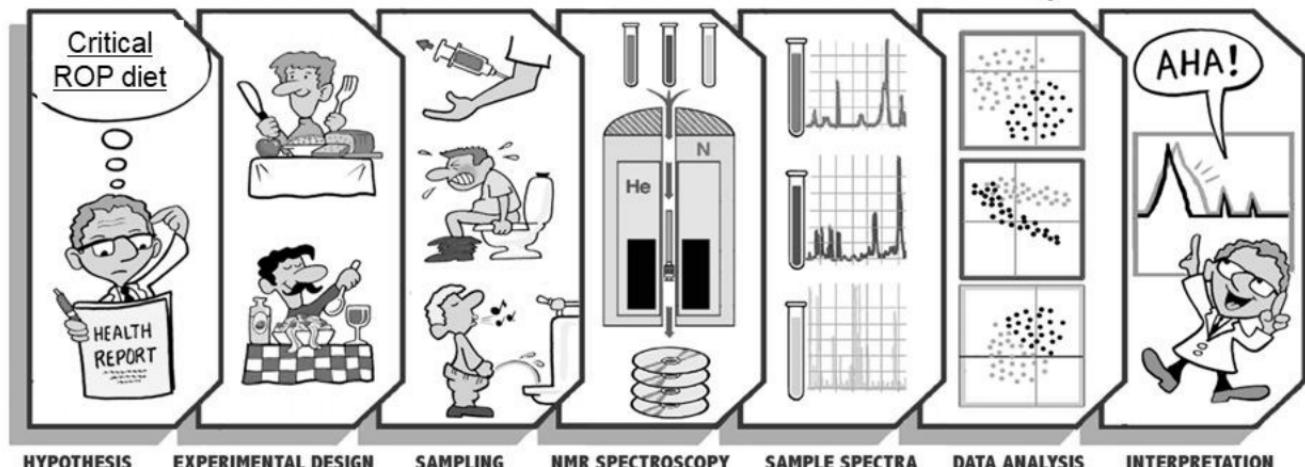
# Foodomics

*the right approach to discover the  
link between food and health*

Francesco Capozzi  
University of Bologna

# NUTRITIONAL METABOLOMICS

The workflow of a nutritional metabolomics study



Savorani F. et al. *Food Res. Int.* **54** (2013) 1131–1145

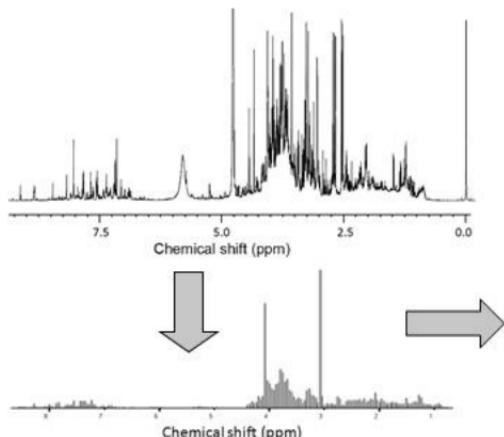
- Assessment of the metabolic consequences of critical diets for populations groups
- Helps to establish biomarkers for healthy or deleterious foods
- Potential to evaluate/develop stratified nutrition to different population groups



# SPECTRAL DATABASE

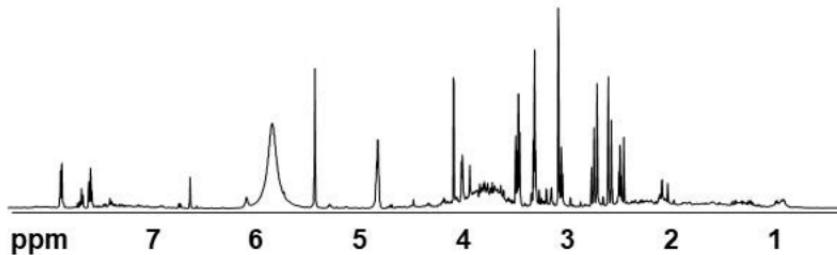
The metabolomic profile of each volunteer refers to the corresponding metadata (nutritional data and life style information).

The NMR database contains the whole binned spectra, each of them consisting of 600 buckets of 0.02 ppm width.

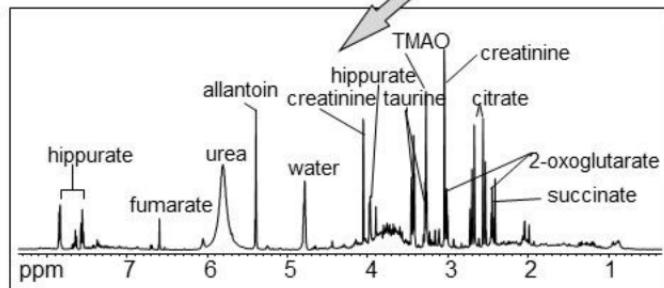


SPECTRUM NUMBER:														Printed on:	
A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	
3	W	C2	TOMEN	112089 9956	20710.71	32000.25	9600.71	10.00	0.00	10.00	10.00	10.00	10.00	10.00	
3	2	DM	Acetylaldehyde	300795.207	20000.87	575.0162	4010.1104	11000.254	27972.76	8648.1187	10905.213	7059.7503	10907.4710	—	—
4	3	DL	Malic acid	50893.0160	27204.064	20054.787	49349.718	34010.71	6844.0447	5710.0427	17971.115	921.06189	10504.935	—	—
5	4	C2	2-hydroxybutyrate	20015.0754	37134.648	2753.4037	34229.355	20000.925	42498.437	2365.3991	22743.072	22728.766	25249.404	—	—
6	5	DM	Acetone	24042.0000	20000.000	20000.000	20000.000	20000.000	20000.000	20000.000	20000.000	20000.000	20000.000	20000.000	
7	6	DM	2-hydroxypropanoate	154409.0023	20000.000	82745.1382	20071.403	78000.000	29557.079	50500.000	19500.000	19500.000	19500.000	19500.000	
8	7	DL	alpha,beta-dihydroxypropanoate	2803.7005	30000.000	82745.1382	20071.403	78000.000	29557.079	50500.000	19500.000	19500.000	19500.000	19500.000	
9	8	C2	2-hydroxybutyrate	47403.4230	30000.000	413000.000	20000.000	20000.000	100000.000	227500.000	100000.000	100000.000	100000.000	100000.000	
10	9	DM	alpha,beta-dihydroxypropanoate	50000.0000	30000.0000	100000.0000	20000.0000	20000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
11	10	DM	alpha,beta-dihydroxypropanoate	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	
12	11	DL	alpha,beta-dihydroxypropanoate	10000.0000	20000.0000	10000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	
13	12	DL	alpha,beta-dihydroxypropanoate	10000.0000	20000.0000	10000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	
14	13	DM	2-hydroxybutyrate	55313.5004	20244.1386	7493.2768	55490.000	27120.001	80513.054	20212.374	4430.431	34400.013	50500.000	264	
15	14	DM	2-hydroxybutyrate	55313.5004	20244.1386	7493.2768	55490.000	27120.001	80513.054	20212.374	4430.431	34400.013	50500.000	264	
16	15	DL	alpha,beta-dihydroxypropanoate	10000.0000	20000.0000	10000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	
17	16	DL	alpha,beta-dihydroxypropanoate	10000.0000	20000.0000	10000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	20000.0000	
18	17	DM	alpha,beta-dihydroxypropanoate	87184.9594	10570.000	44077.18	47610.153	24099.05	40952.025	20103.042	45001.002	35170.074	27422.000	30000.000	
19	18	DM	alpha,beta-dihydroxypropanoate	99705.6607	402000.000	300797.21	70000.000	40000.000	20000.000	22000.000	80000.000	30000.000	30000.000	30000.000	
20	19	DM	alpha,beta-dihydroxypropanoate	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
21	20	DL	alpha,beta-dihydroxypropanoate	74715.2709	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
22	21	DM	alpha,beta-dihydroxypropanoate	8637.5598	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
23	22	DL	alpha,beta-dihydroxypropanoate	8574.4577	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
24	23	DL	alpha,beta-dihydroxypropanoate	8574.4577	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
25	24	DL	alpha,beta-dihydroxypropanoate	8574.4577	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
26	25	DL	alpha,beta-dihydroxypropanoate	8574.4577	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
27	26	DM	alpha,beta-dihydroxypropanoate	200000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
28	27	DM	alpha,beta-dihydroxypropanoate	200000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
29	28	DM	alpha,beta-dihydroxypropanoate	200000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
30	29	DM	alpha,beta-dihydroxypropanoate	200000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	
31	30	DM	alpha,beta-dihydroxypropanoate	200000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	100000.0000	

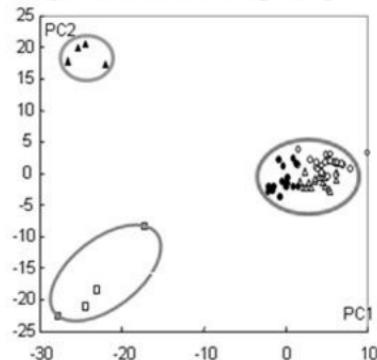
# TWO ROUTES TO METABOLOMICS



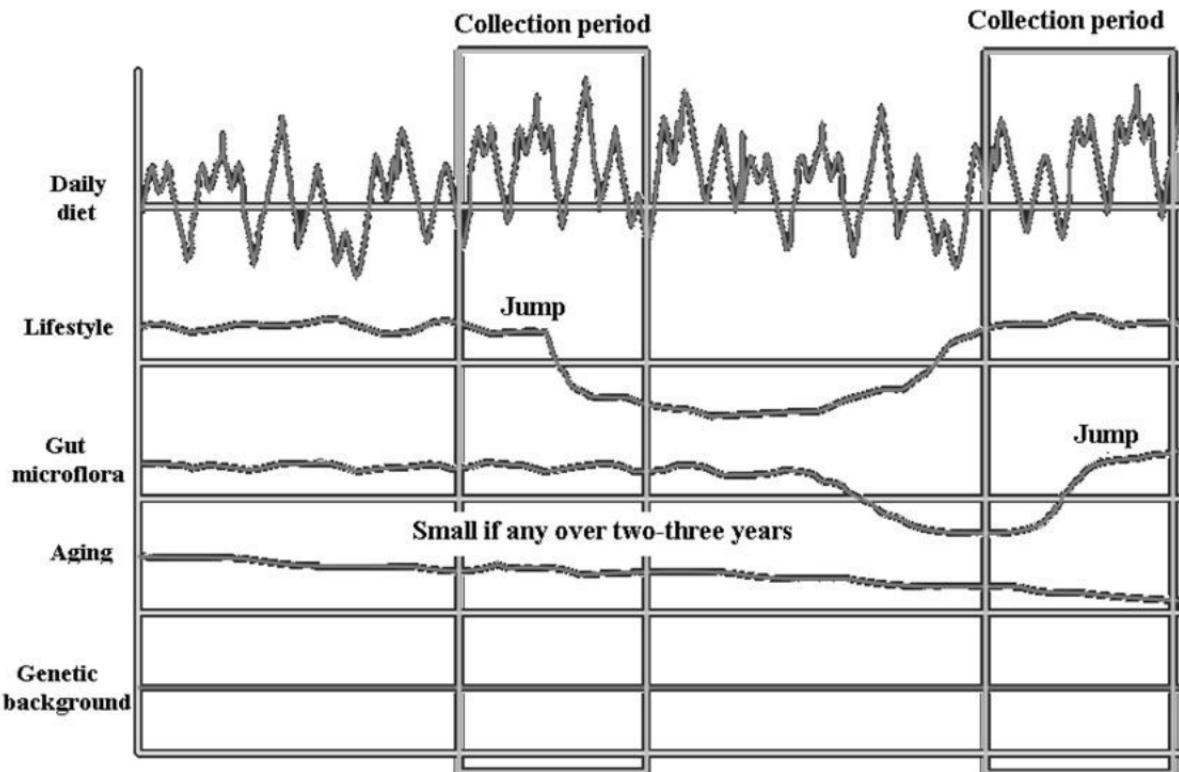
Quantitative Methods  
(Target Analysis)



Chemometric Methods  
(Pattern Analysis)

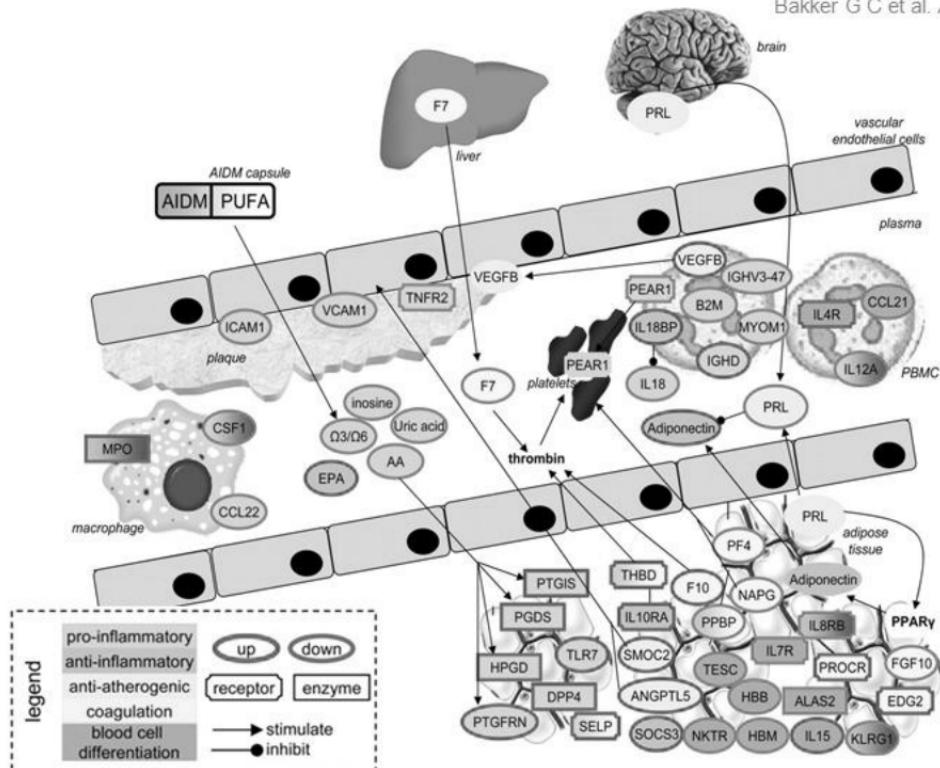


# TIME SERIAL DATA FOR METABOLOME



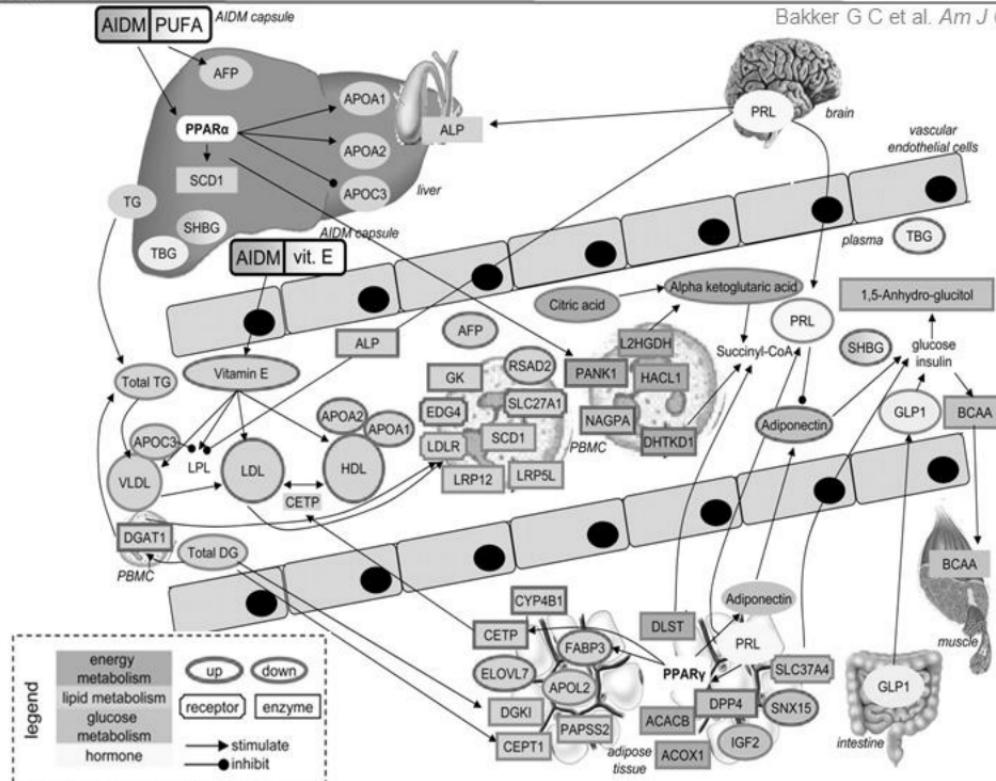
# MAIN EFFECTS OF THE AIDM DIET ON INFLAMMATION-RELATED PROCESSES

Bakker G C et al. Am J Clin Nutr 91 (2010)1044-1059

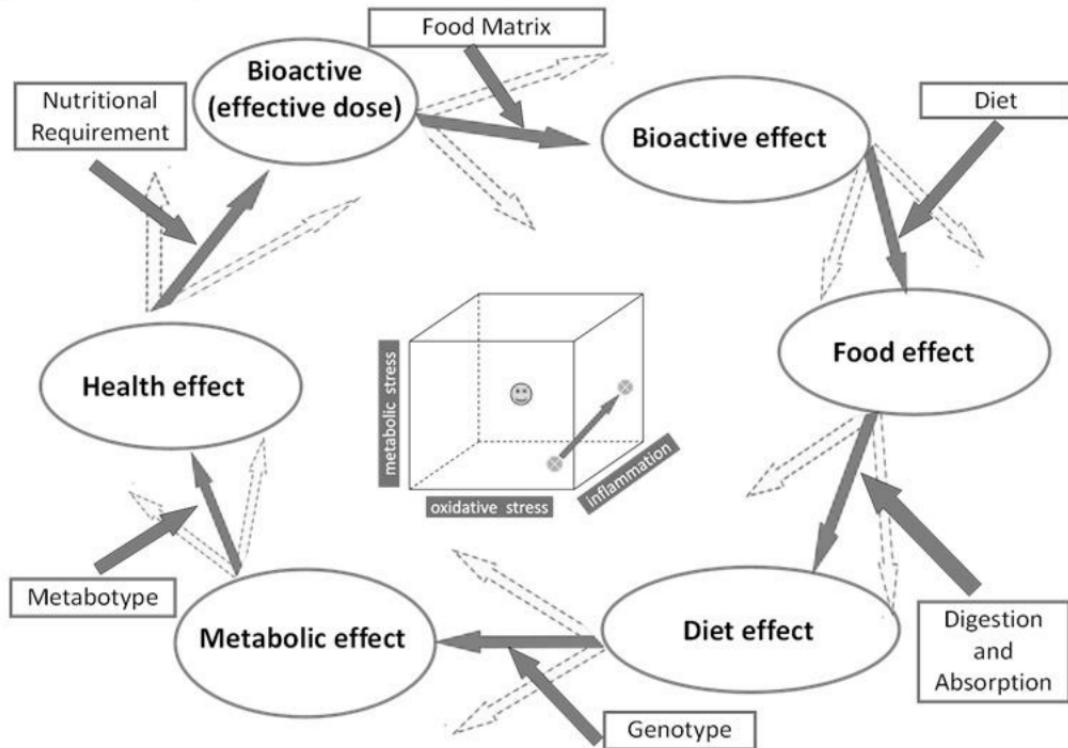


# MAIN EFFECTS OF THE AIDM DIET ON METABOLISM-RELATED PROCESSES

Bakker G C et al. Am J Clin Nutr 91 (2010)1044-1059



# FOOD MODULATION IN THE HEALTH SPACE





# CHALLENGES

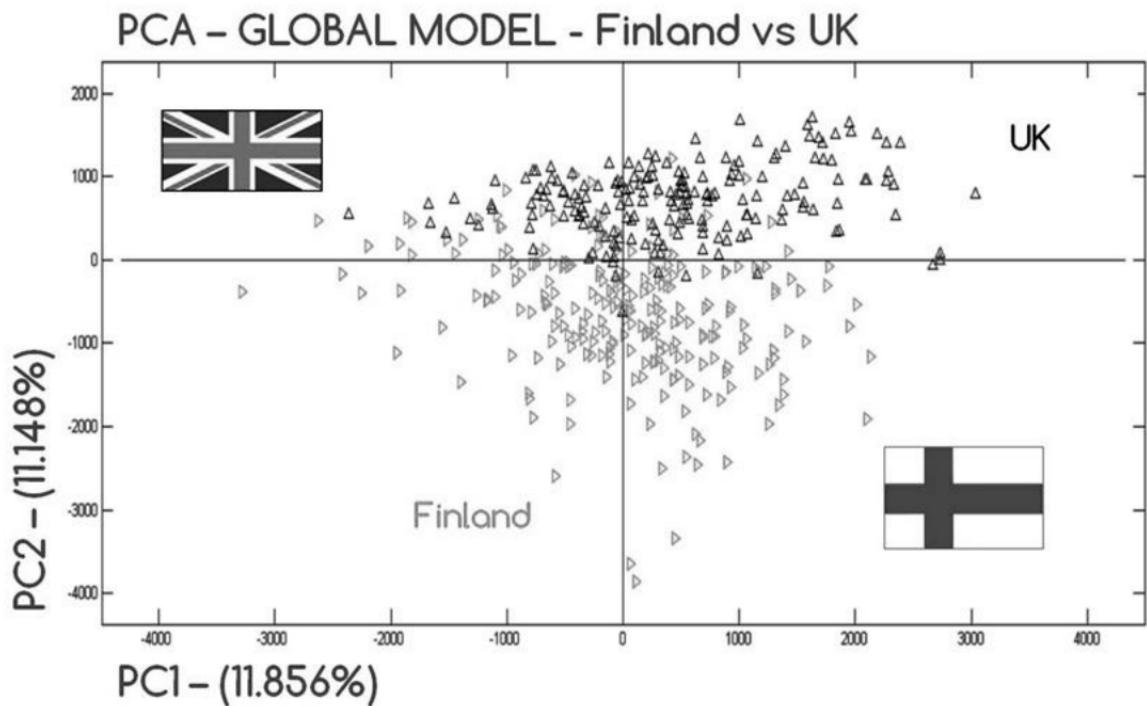
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***The scientific paradox: Difficult to define health in absence of disease: what to measure?***

***The genotype paradox: "One size does not fit all" – we are all genetically different in our response to diet and lifestyle – but dietary recommendations are targeted to populations***

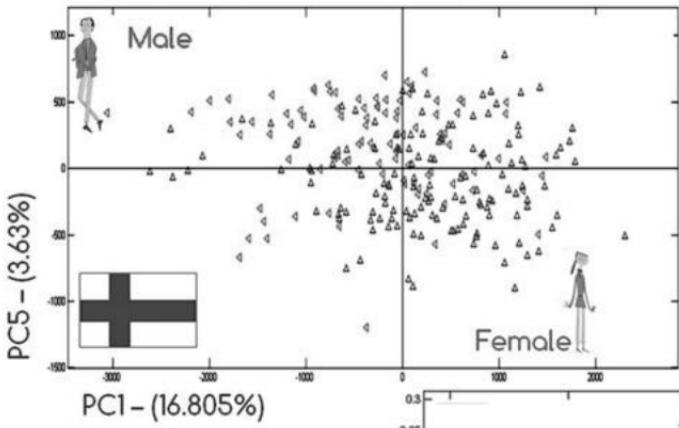
***The data paradox: Too much data too little information!***

## DIFFERENCES DUE TO POPULATION

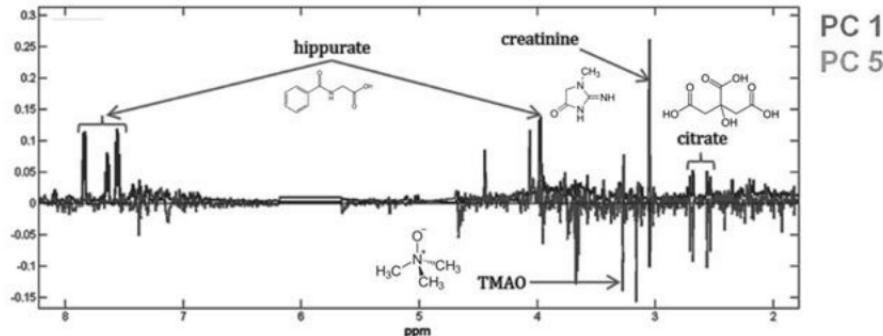
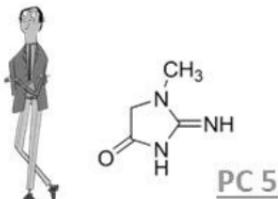
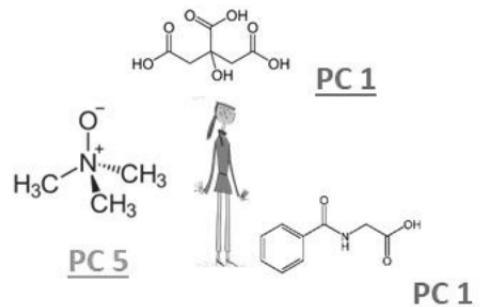


# DIFFERENCES DUE TO GENDER

PCA - FINNISH SAMPLES - Gender

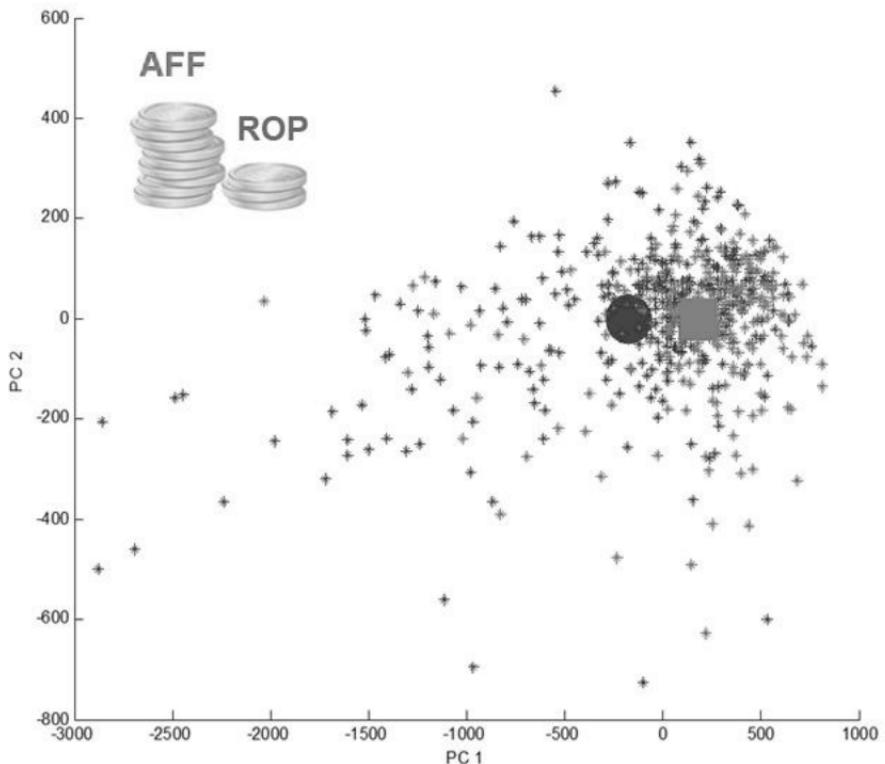


FINNISH SUBJECTS



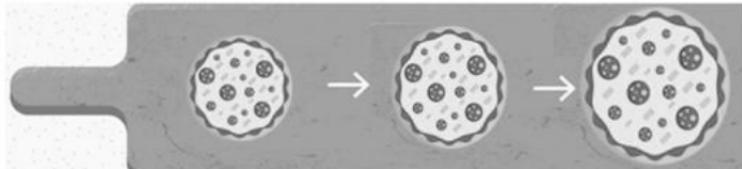
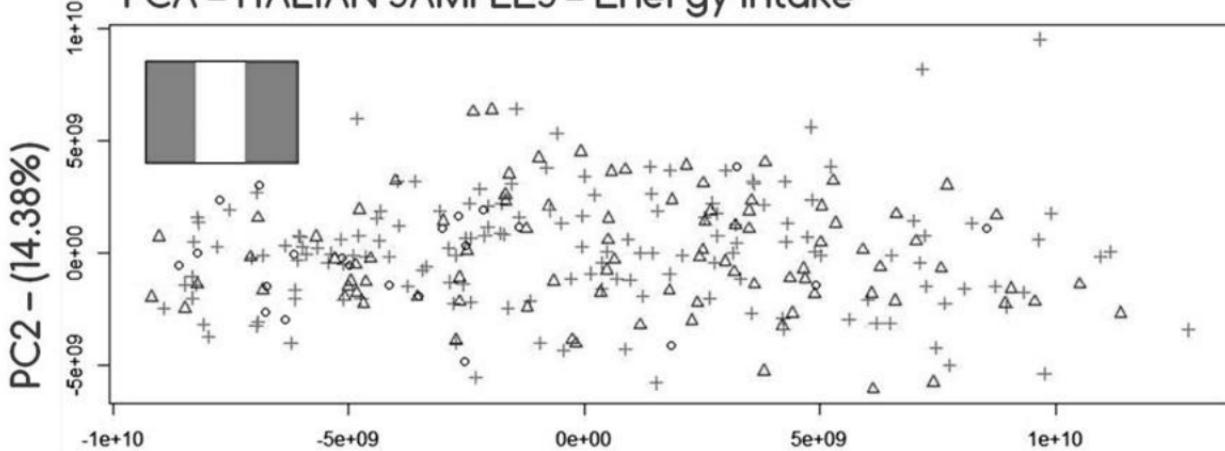


# ASCA ANALYSIS - PRELIMINARY RESULTS



# LOOKING FOR THE EFFECT OF DIET (DIFFERENT ENERGY INTAKE)

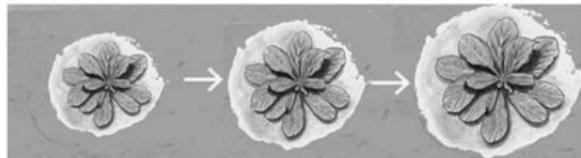
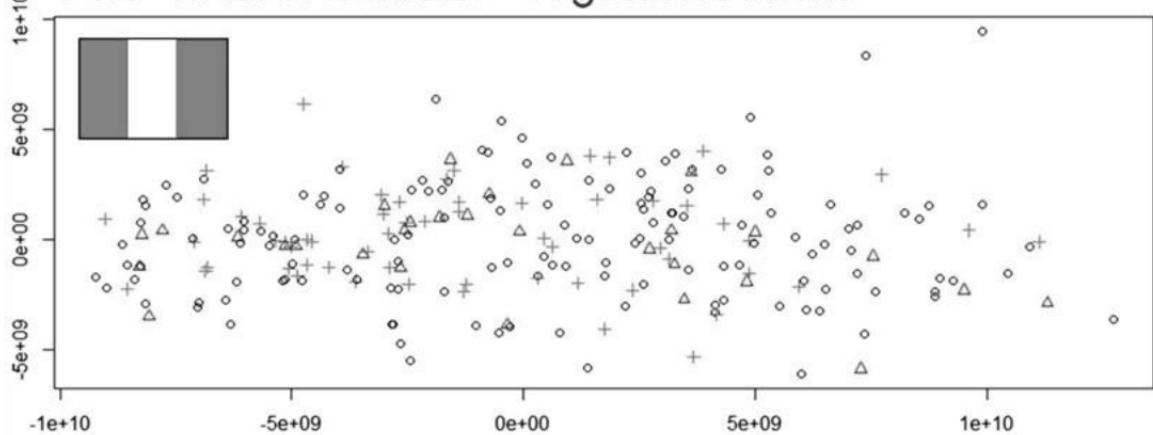
PCA - ITALIAN SAMPLES - Energy Intake



Chance

# LOOKING FOR THE EFFECT OF DIET (DIFFERENT VEGETABLES INTAKE)

PCA - ITALIAN SAMPLES - Vegetables Intake



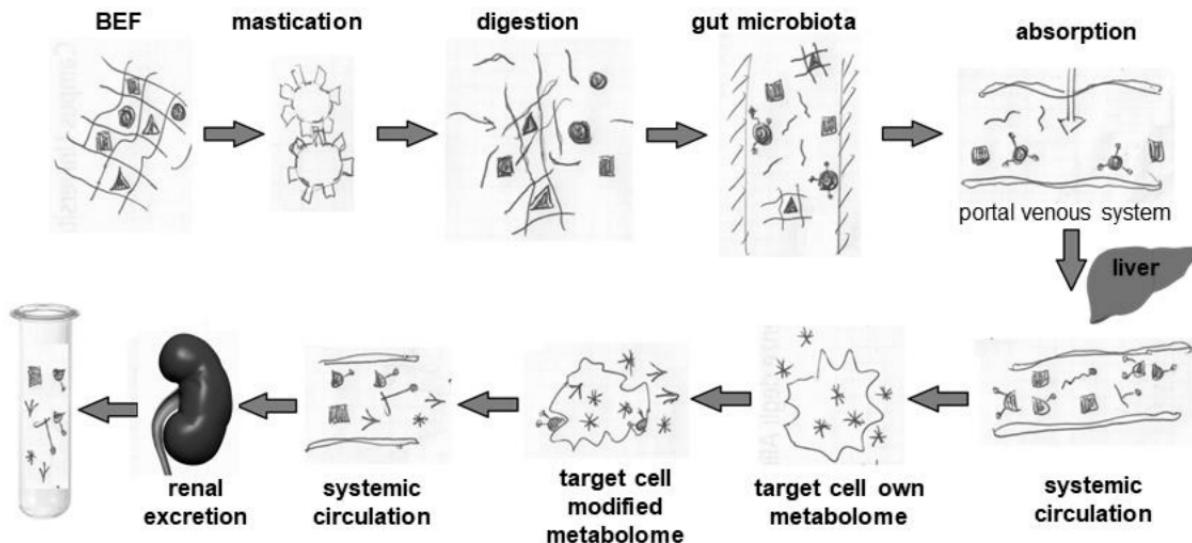
Chance

0 g

0-50 g

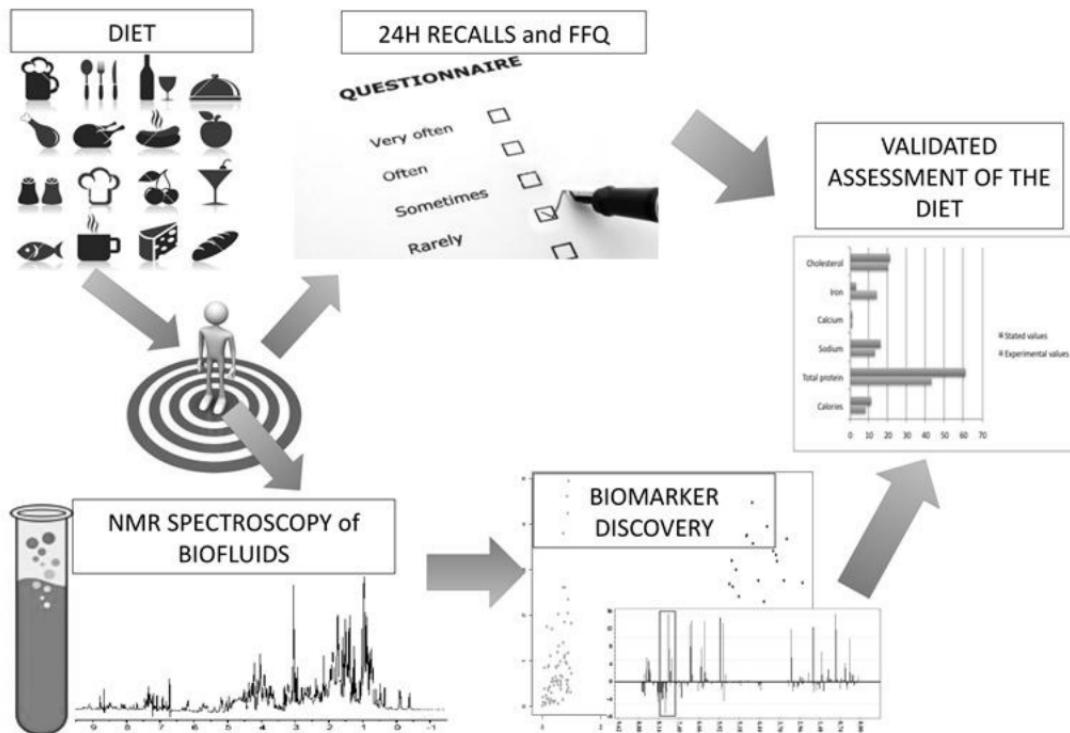
>50 g

# FROM BIOACCESSIBILITY TO EXCRETION

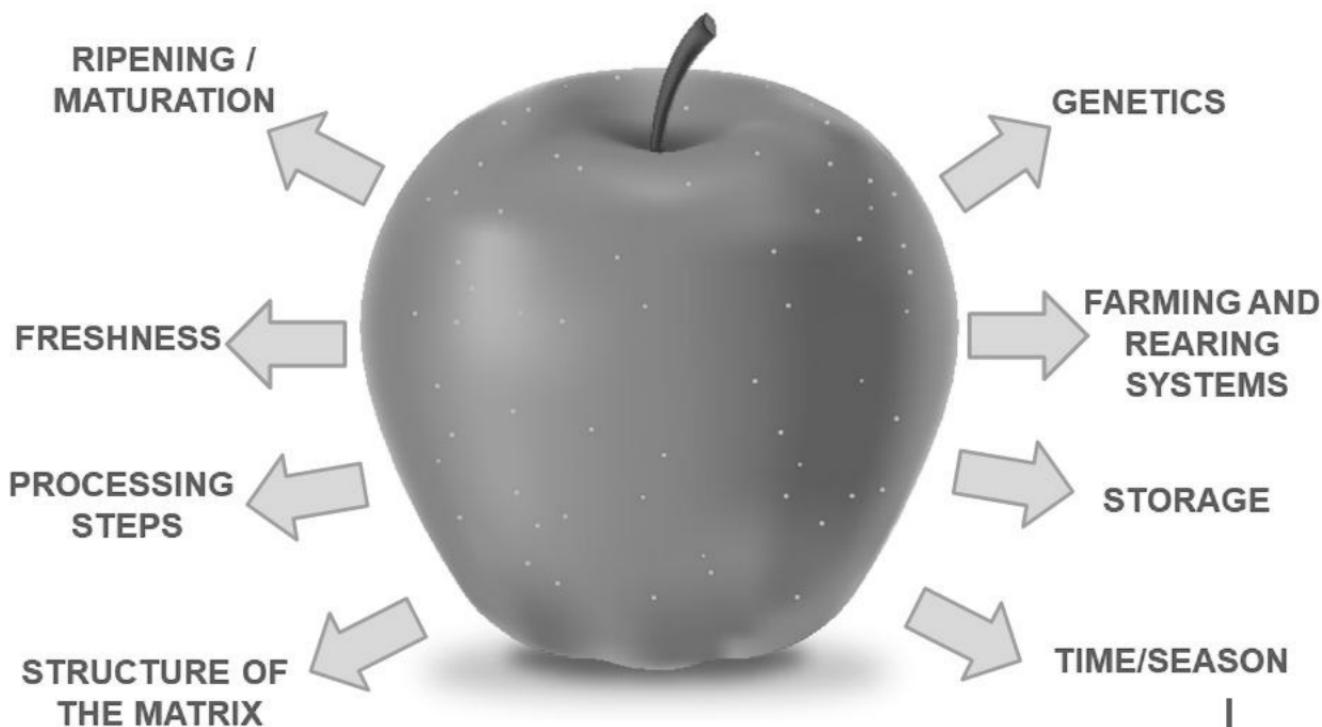




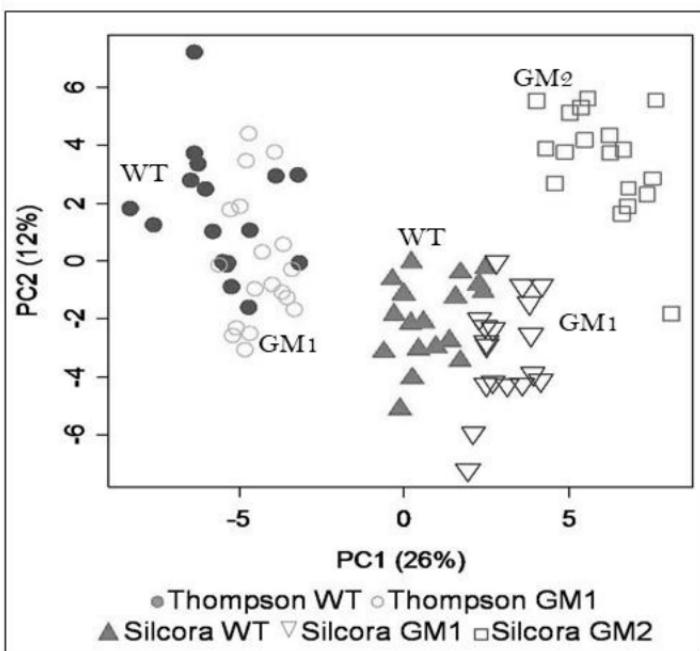
# LOOKING FOR VALIDATION OF THE DIETARY ASSESSMENT



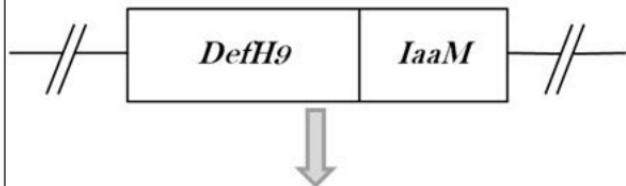
# FACTORS AFFECTING THE FOOD QUALITY



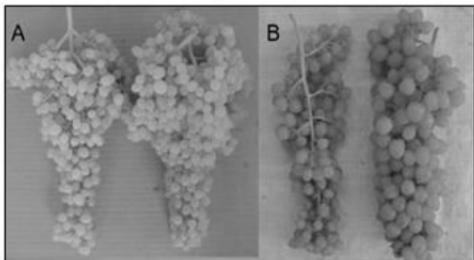
# GENETICS OF GRAPE BERRIES (GMOs)



The Genetically Modification  
The *DefH9-iaaM* gene  
(Mezzetti et al., 2004)

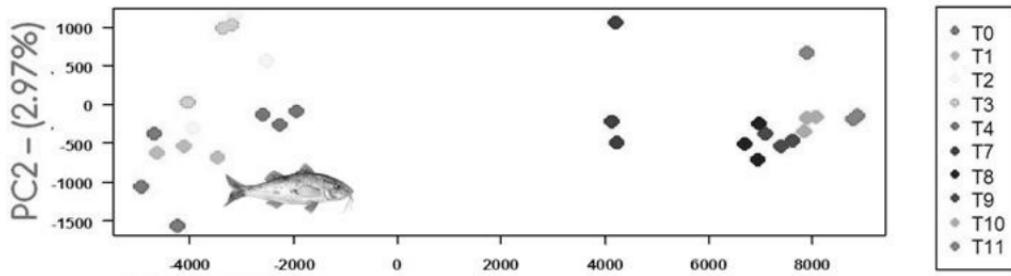


Increase the number of berries per bunch

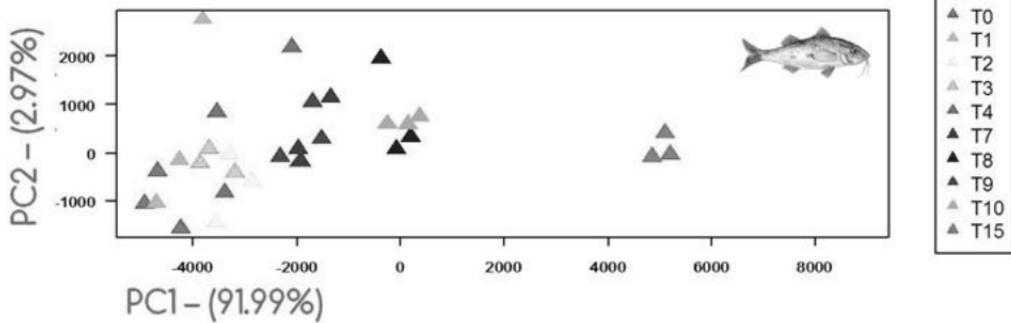


# EFFECT OF FRESHNESS ON MULLET

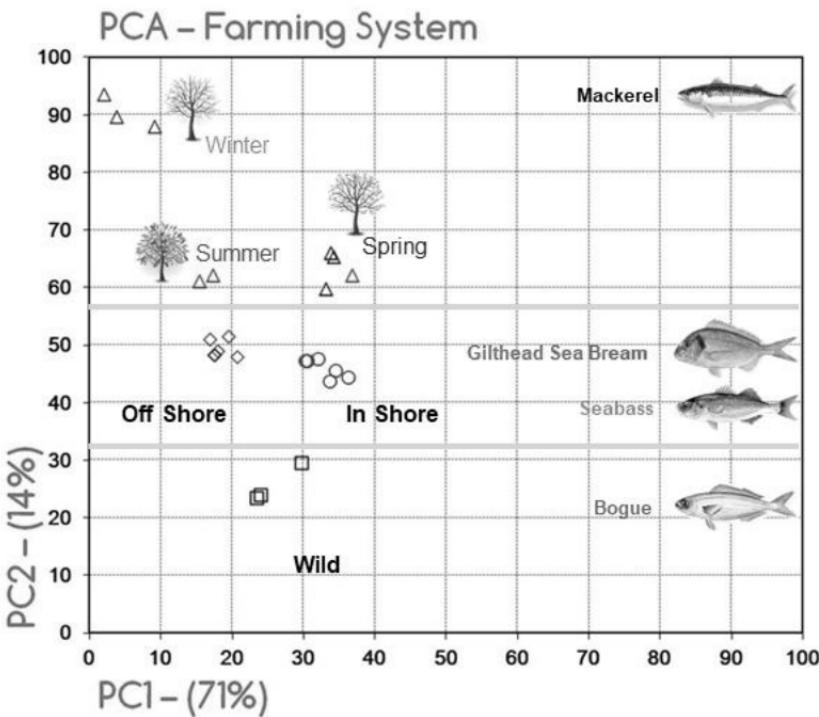
**4°C**



**0°C**



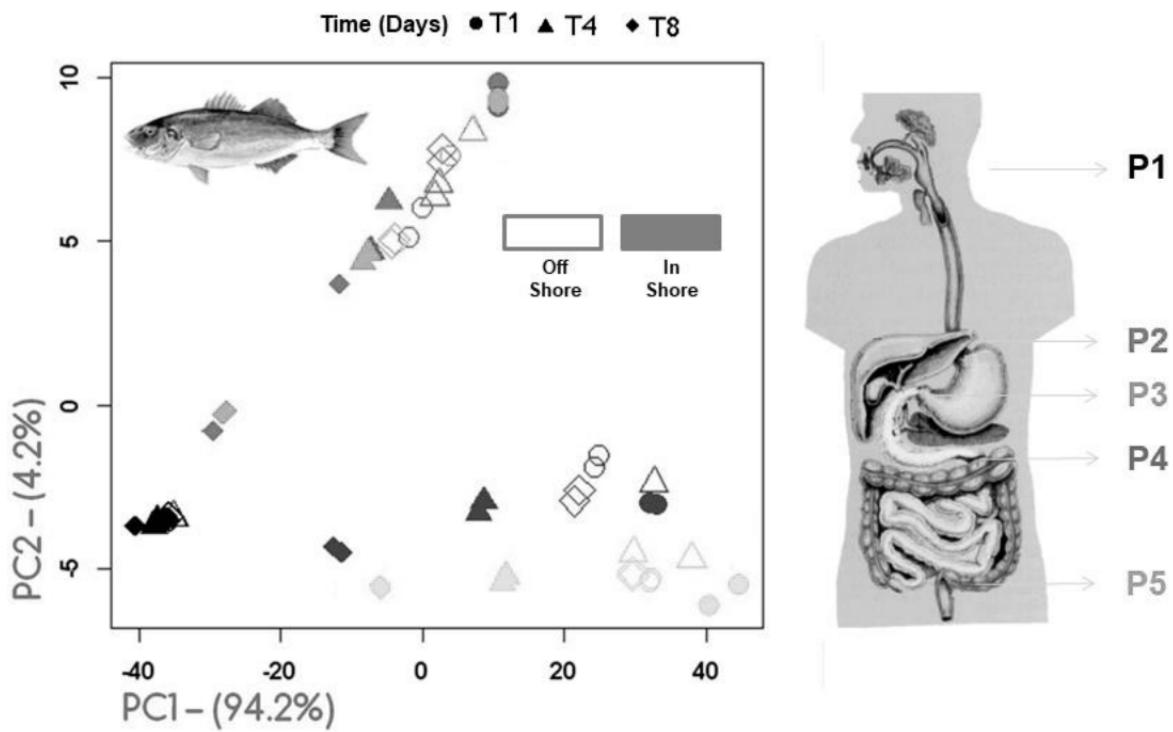
# EFFECTS OF SPECIES, SEASONS AND FARMING SYSTEM



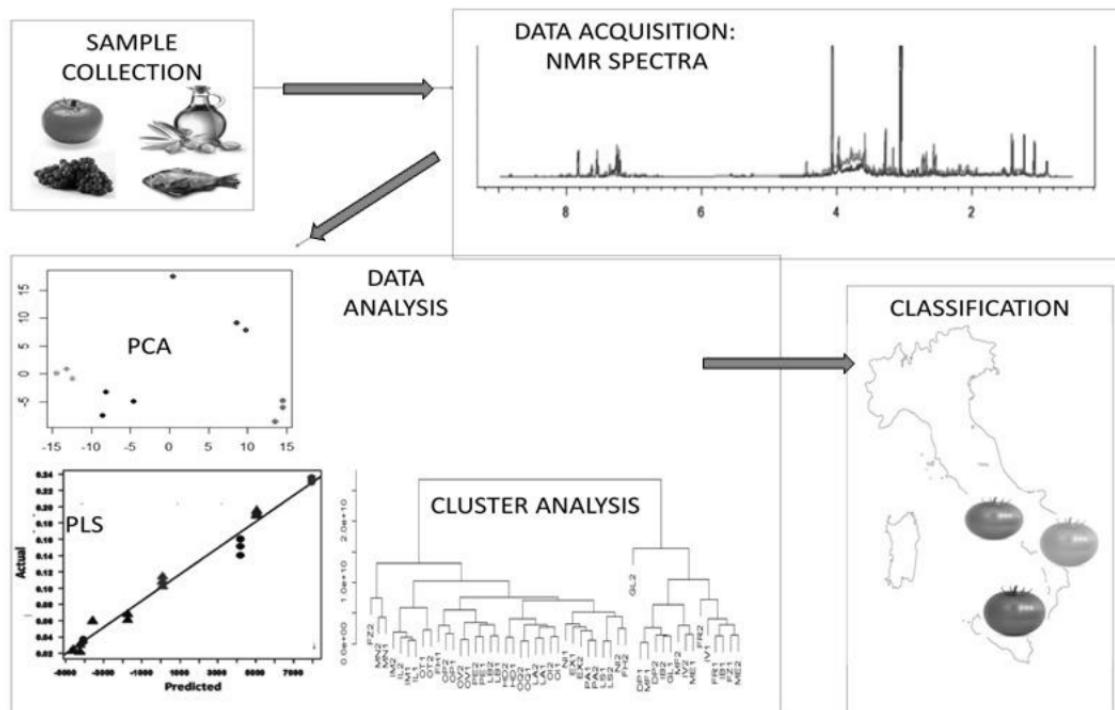
Seasons effects on Mackerel samples

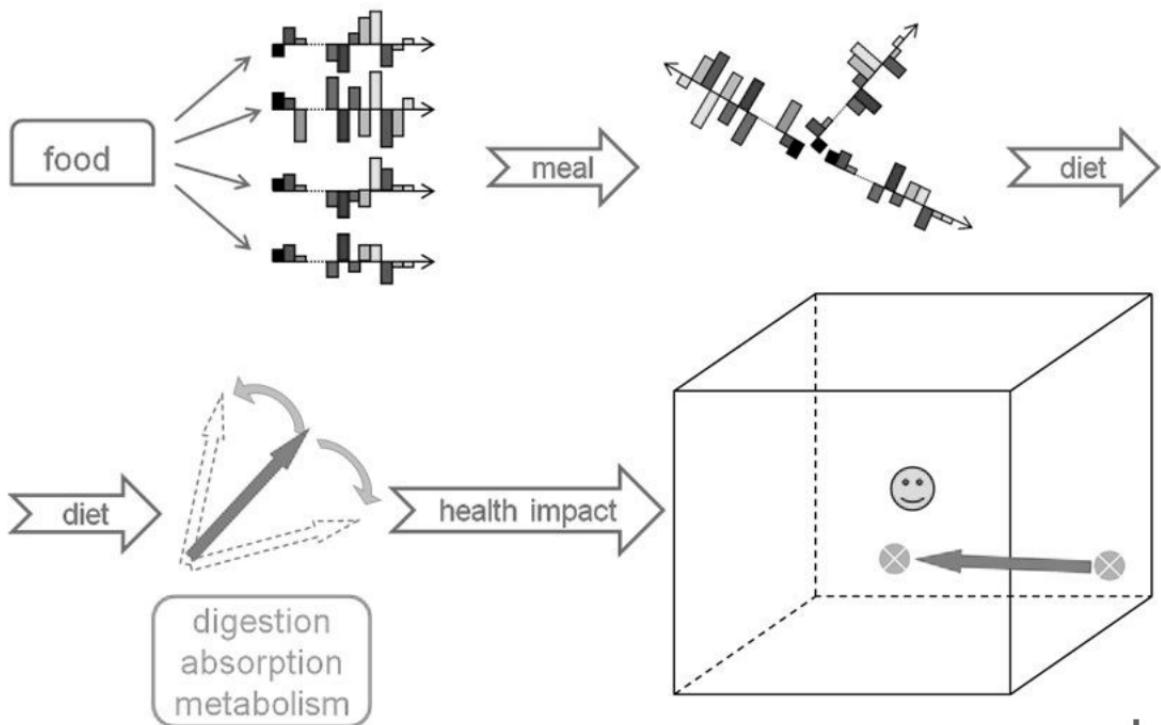
Farming effects on Bogue, Sea bass and Gilthead Sea Bream samples

# DIGESTION OF SEA BASS REARED IN DIFFERENT AQUACULTURE SYSTEMS



# DESCRIBING FOOD IN DETAIL







# DESCRIBING FOOD IN DETAIL



F. Capozzi, A. Trimigno  
**Using metabolomics to  
describe food in detail (Ch. 11)**

J. L. Sebedio, L. Brennan (Eds.)  
ISBN 978-1-78242-084-2



## Foodomics: the right approach to discover the link between food and health



# THANK YOU FOR YOUR KIND ATTENTION

### Bio-NMR

Luca Laghi  
Gianfranco Picone  
Alessandra Ciampa  
Elena Marcolini  
Alessia Trimigno

### Nutrition

Alessandra Bordoni  
Francesca Danesi  
Mattia Di Nunzio  
Veronica Valli

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