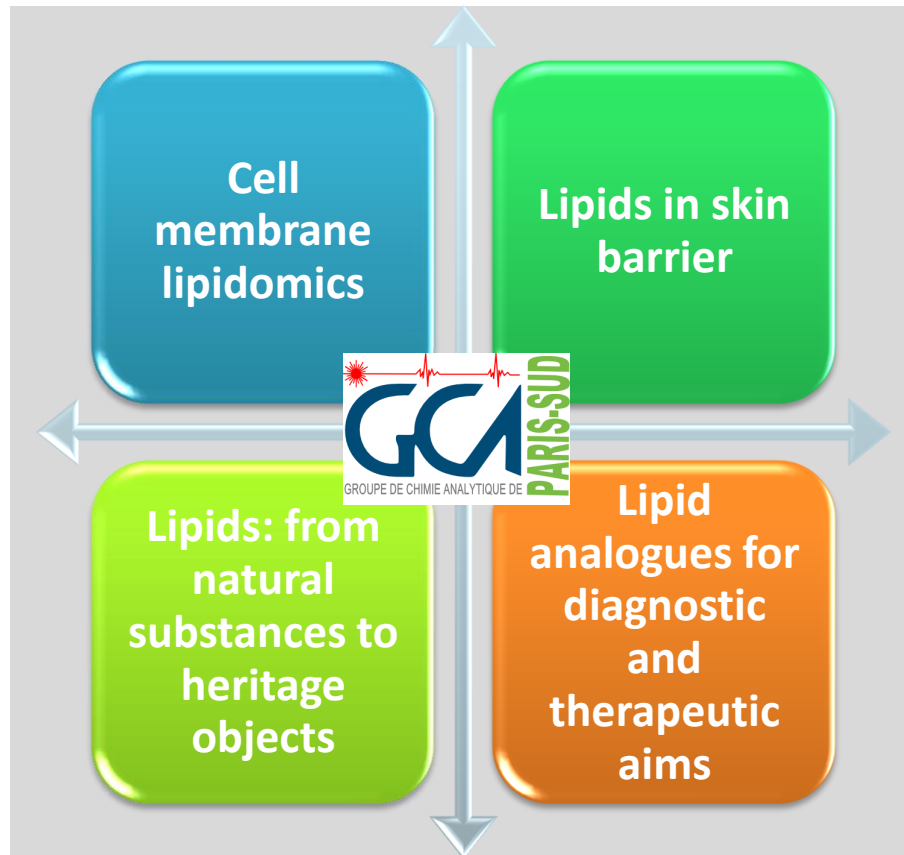


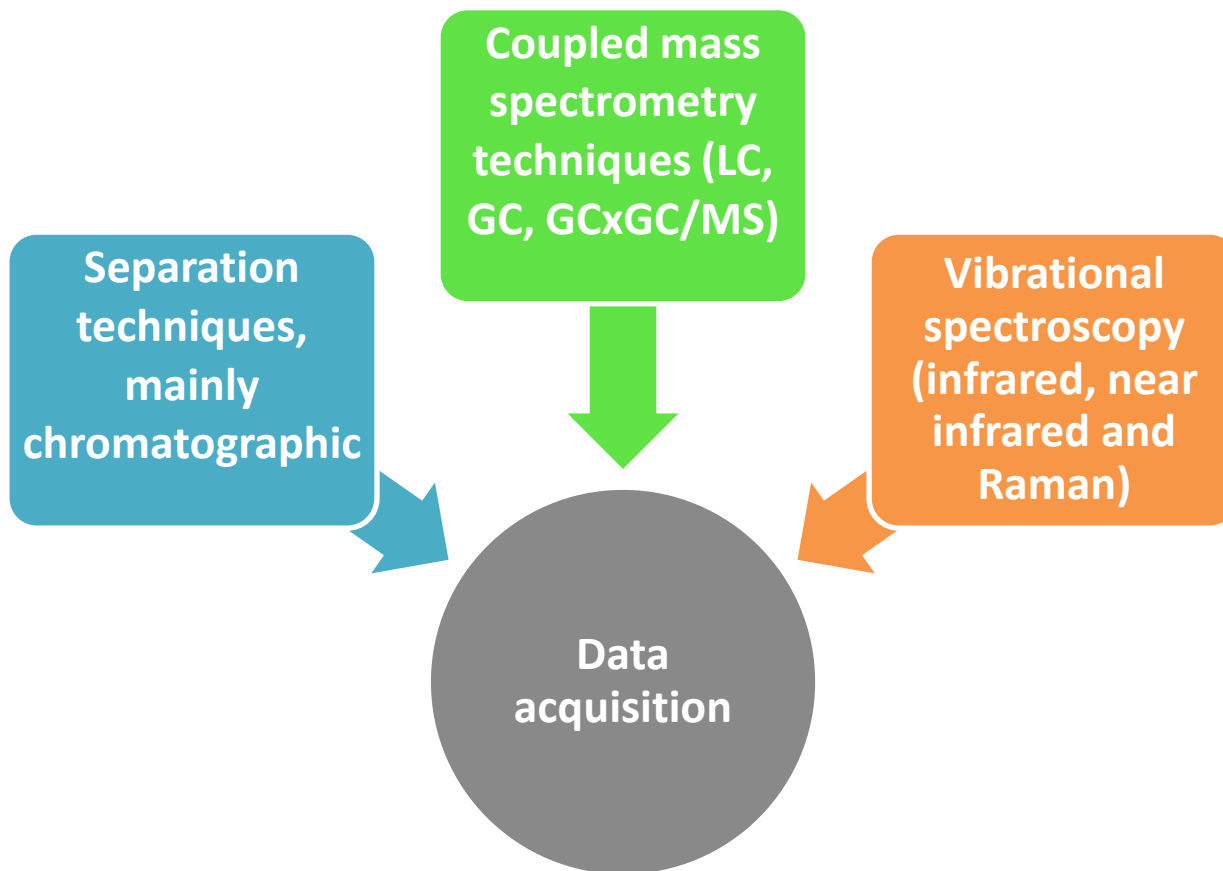
Analytical chemistry: from data (pre)-treatment optimization to data mining, data fusion and big data

EA4041, Groupe de Chimie Analytique de Paris-Sud 'GCAPS'

Four principle themes



Different analytical tools



Data (pre)-processing
Multivariate analysis
Chemometric techniques

Schedule

10h00-10h30:

«Analytical chemistry: cell membrane lipidomics and data analysis», Sana Tfali

10h30-11h00:

«Analytical chemistry and chemometrics: a tool for skin physiological and physiopathological characterization», Ali Tfayli

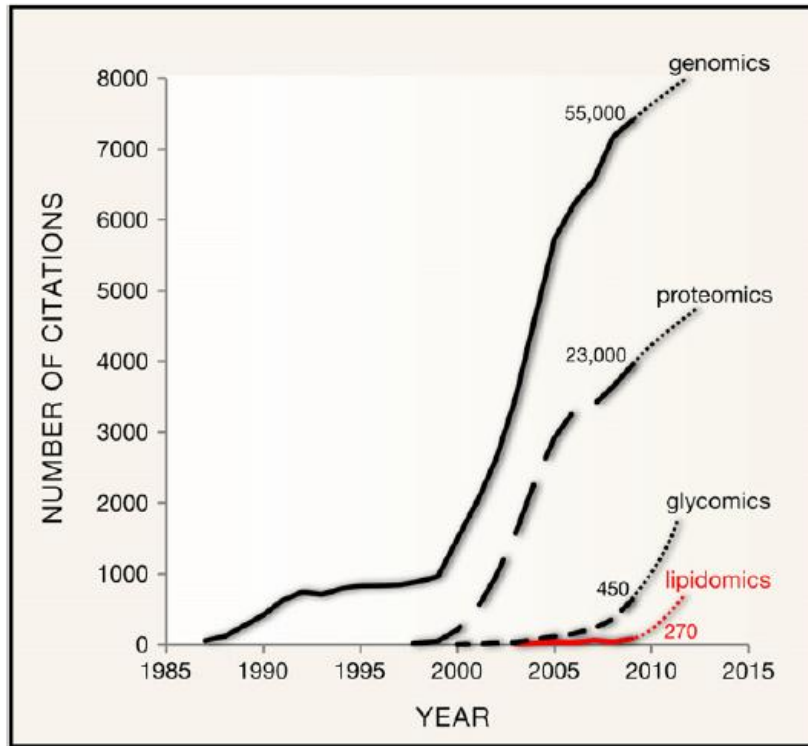
11h00-11h10:

«Analytical chemistry: from data (pre)-treatment optimization to data mining, data fusion and big data», S&A Tfai(y)li

Analytical chemistry: cell membrane lipidomics and data analysis

Sana Tfaili

Lipidomics



- Recent comparing to other omics
- Borrows heavily from metabolomics
- Specific analysis of lipids

Cell

Cell
PRESS

Volume 143, Issue 6, 10 December 2010, Pages 888–895

Primer

Lipidomics: New Tools and Applications

Markus R. Wenk^{1, 2}, , 

Analytical chemistry: cell membrane lipidomics and data analysis

Infectious diseases

- Leishmaniasis
- Impact of treatment on the lipid composition of membranes *Leishmania donovani*

Collaboration UMR BioCIS / Ph. Loiseau



Analytical chemistry: cell membrane lipidomics and data analysis

Hereditary diseases and RBCs

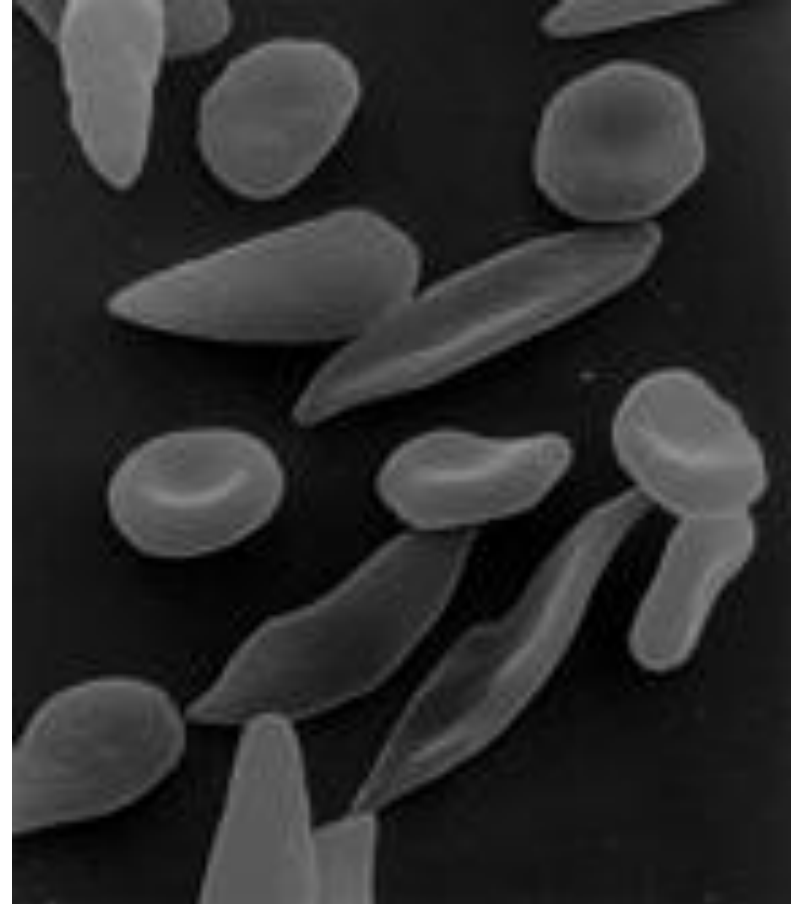
- Lipid composition and sickle cell disease

Olivier Blanc-Brude Paris Centre de Recherche Cardiovasculaire (PARCC)

- Lipid composition and Gaucher disease (LETIAM)

Institut National de Transfusion Sanguine
(Pr. Le Van Kim et Dr. M Franco)

Service de Neuro-Pédiatrie de l'Hôpital
Trousseau (Pr. T. Billette de Villemeur et Dr
C. Mignot)

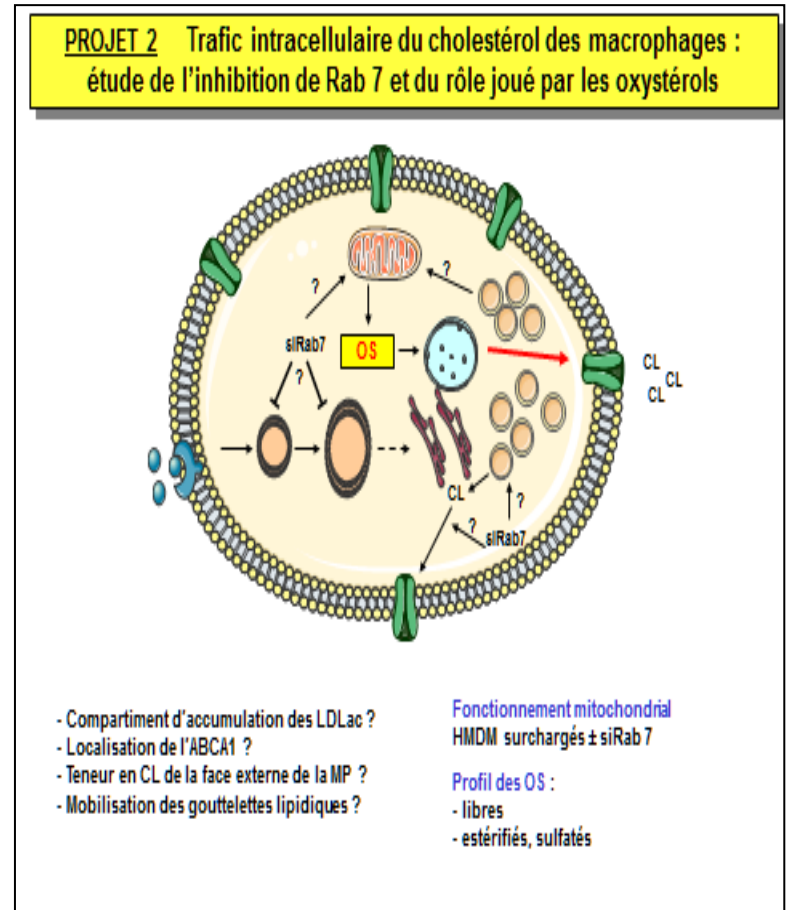


Analytical chemistry: cell membrane lipidomics and data analysis

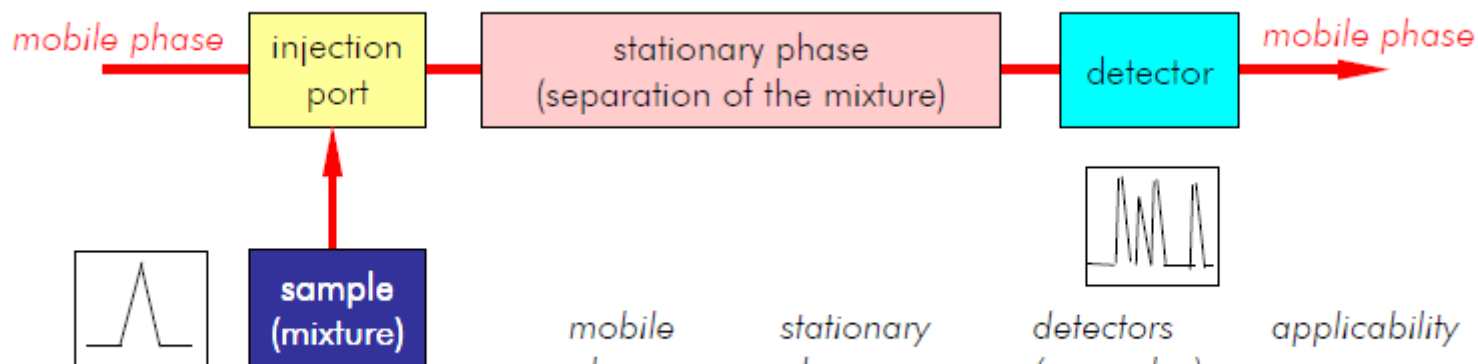
Lipidomics macrophages & Atherosclerosis

- Impact of membrane incorporation of ω 3 PUFA on cholesterol efflux from macrophages
- Intracellular trafficking of cholesterol from macrophages: study of the inhibition of Rab7 and the role of oxysterols

Collaboration EA4529 (cross-cutting theme in the future unit Lip (Sys) ²)

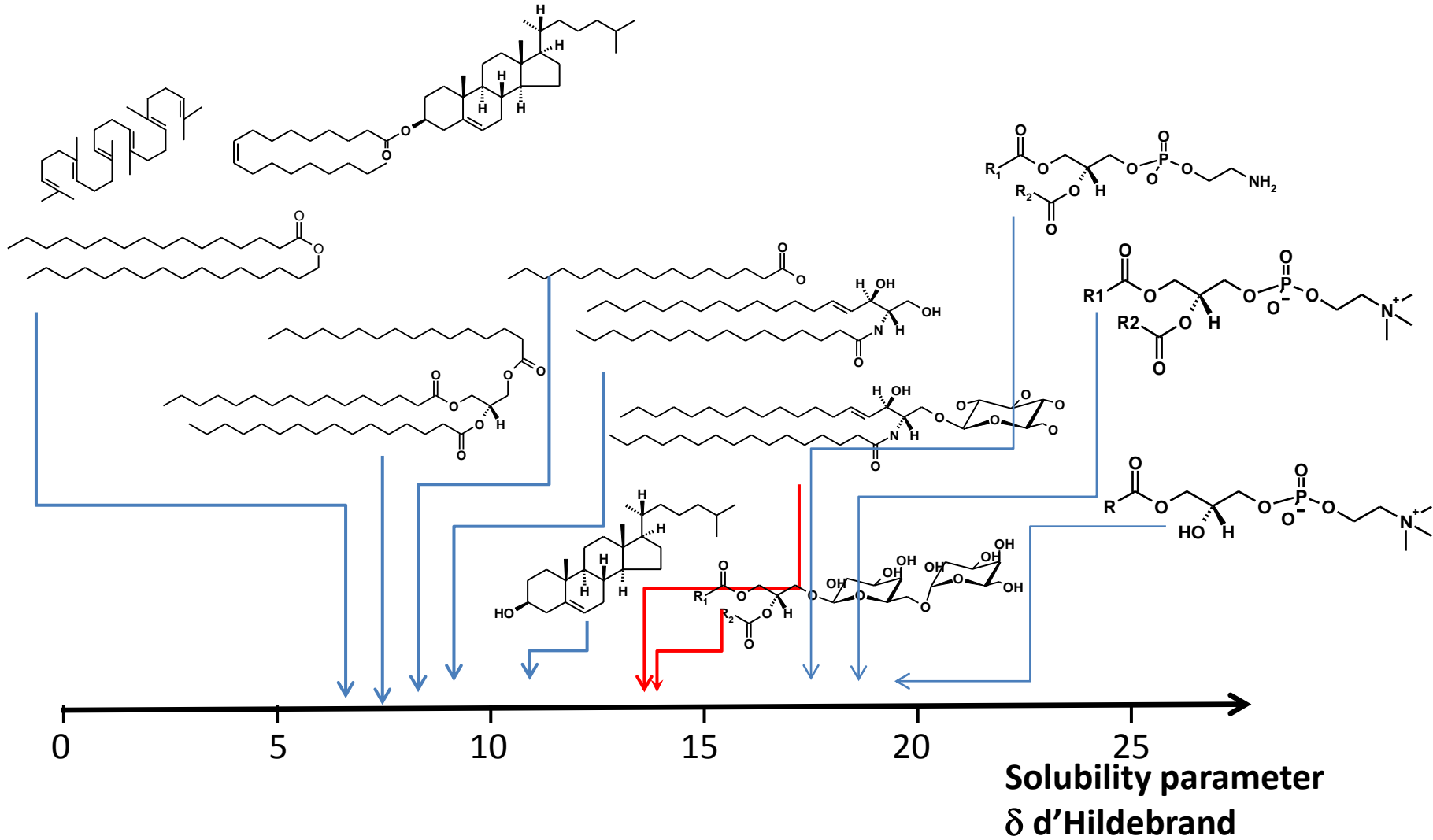


Chromatography



	<i>mobile phase</i>	<i>stationary phase</i>	<i>detectors (examples)</i>	<i>applicability</i>
Gas chromatography (GC):	gases (H ₂ , N ₂ , Ar, He)	capillary or packed columns with substituted siloxanes	TCD, FID, MSD	volatile organic compounds, permanent gases
High pressure liquid chromatography (HPLC):	H ₂ O, organic solvents	impregnated plates	UV-VIS, RI, MSD	organic compounds and inorganic salts
Thin layer chromatography (TLC):	vapor of organic solvents	impregnated plates	optical detection (UV-VIS, fluorescence)	organic compounds

Lipids and polarity

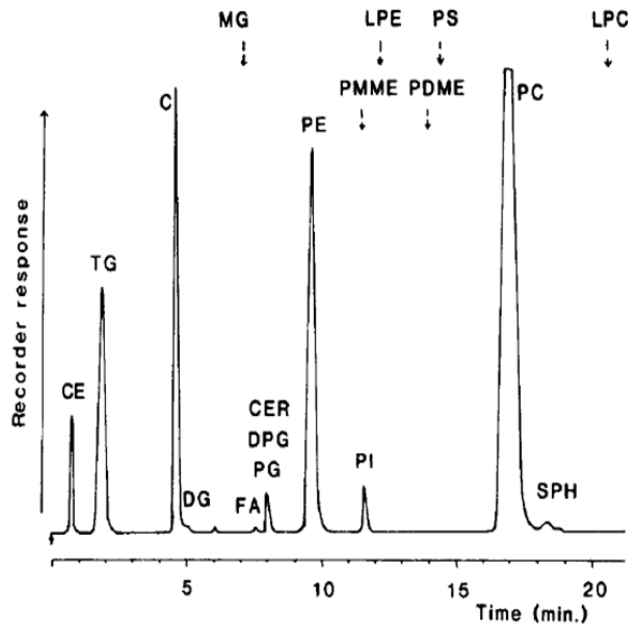


Normal Phase / Reversed Phase Liquid chromatography LC

Lipides de foie de rat

Colonne: Spherisorb 3µm 150x5mm

LIPID CLASSES ANALYSIS

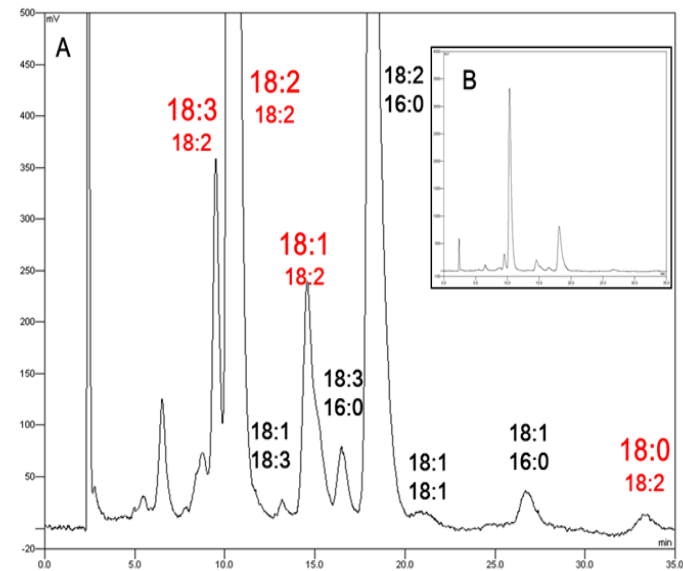


Rapid separation and quantification of lipid classes by high performance liquid chromatography and mass (light-scattering) detection. W W Christie, 1985 *The Journal of Lipid Research*, 26, 507-512.

Lipids are separated according to their polar moieties.

Digalactosyldiglycéride

Colonne Hypercarb®

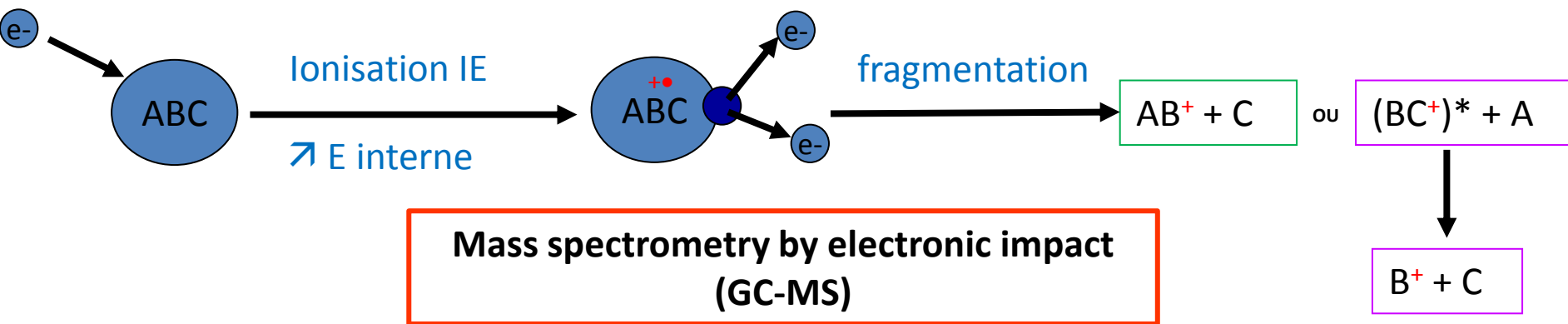
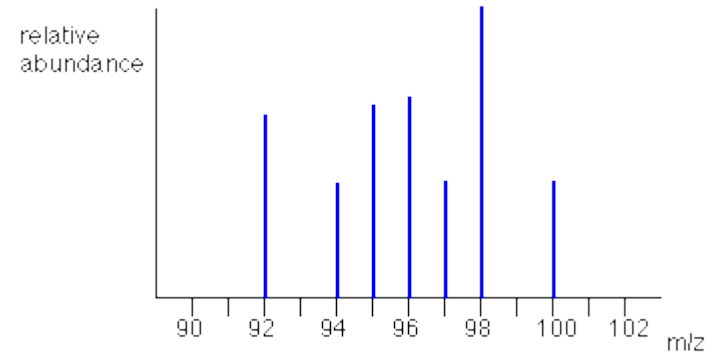
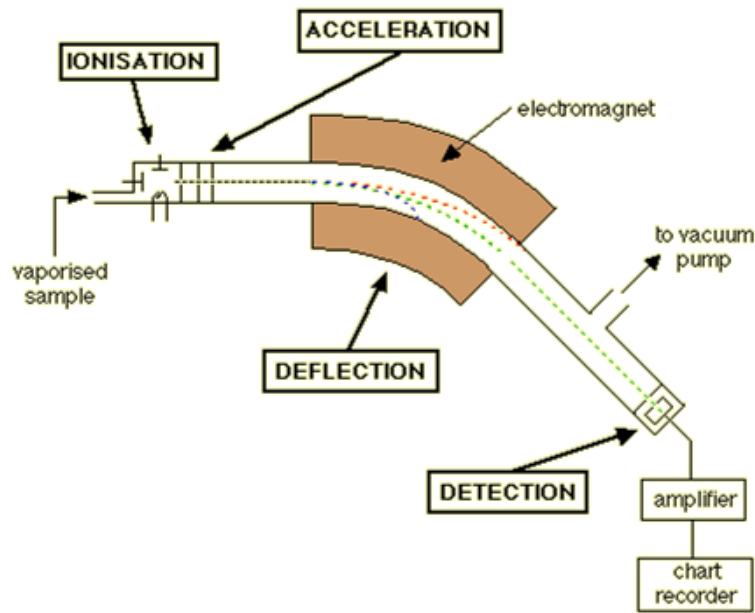


Deschamps F, Gaudin K, Baillet A & Chaminade P. Wheat digalactosyldiacylglycerol molecular species profiling using porous graphitic carbon stationary phase. *JOURNAL OF SEPARATION SCIENCE* (2004) 27: p. 1322.

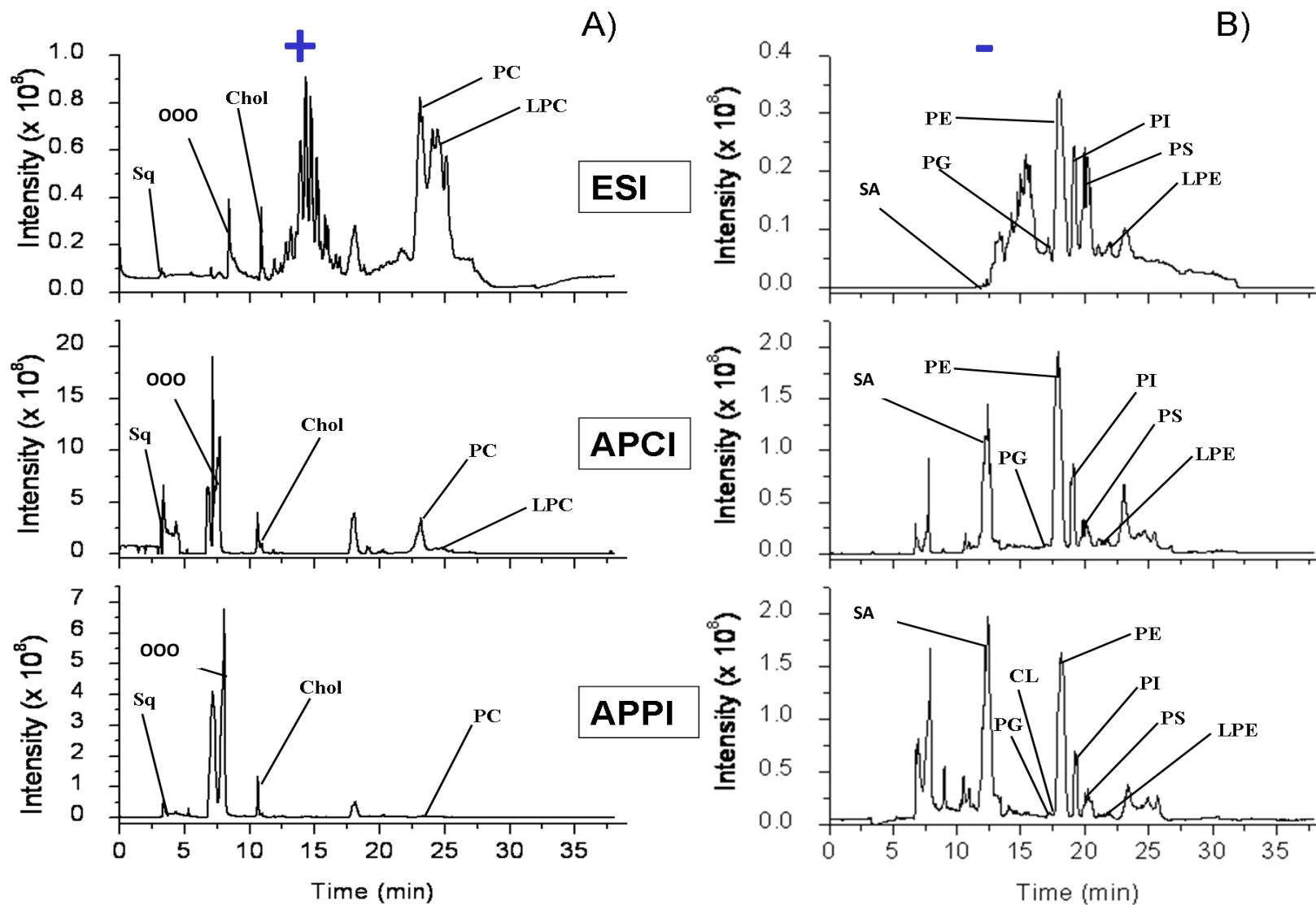
Lipids are separated according to their chain length & number and position of double bonds

LIPID MOLECULAR SPECIES ANALYSIS

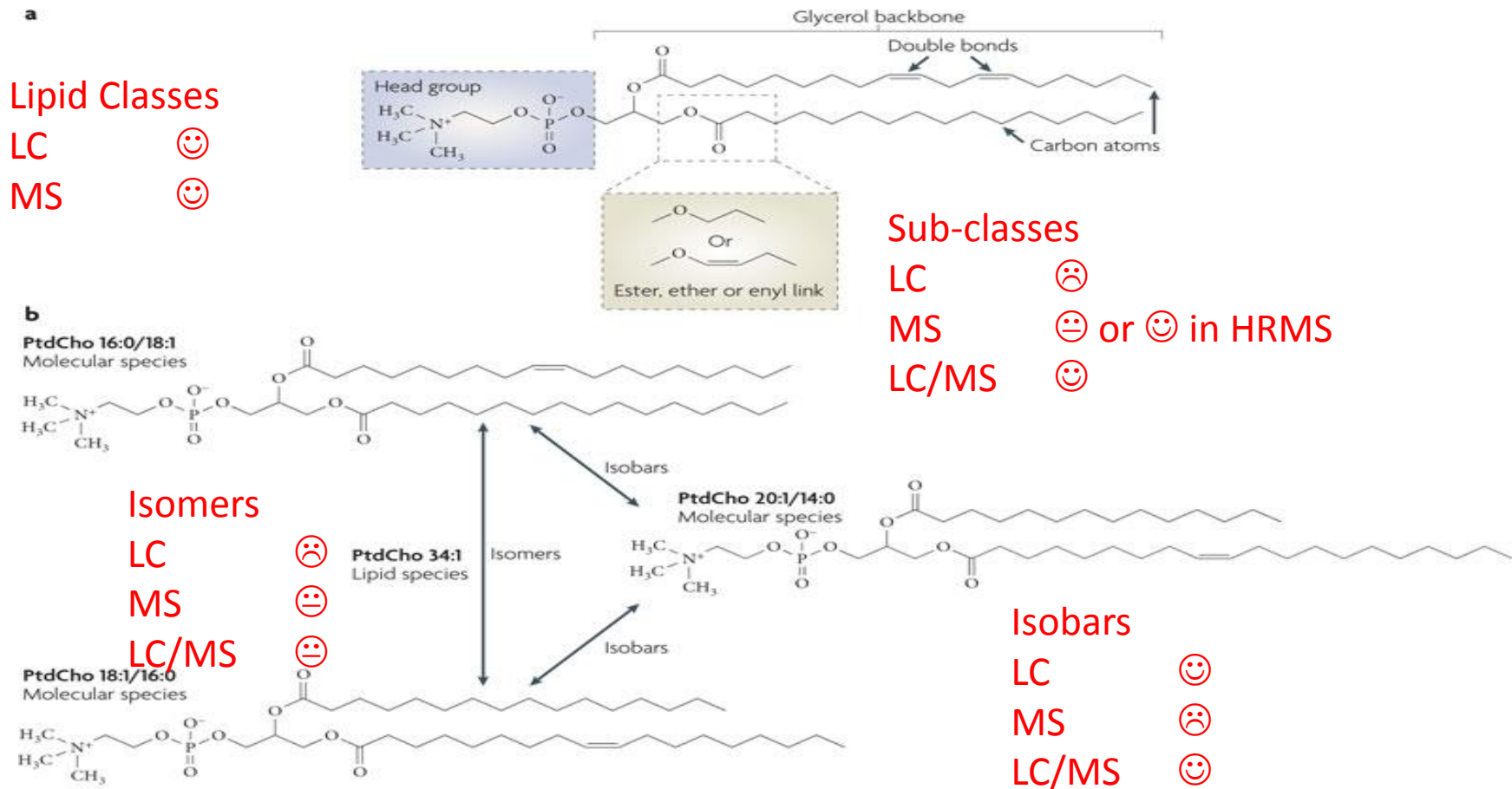
Mass spectrometry MS



LC-MS acquisitions: Different ionization modes



Lipid molecular species

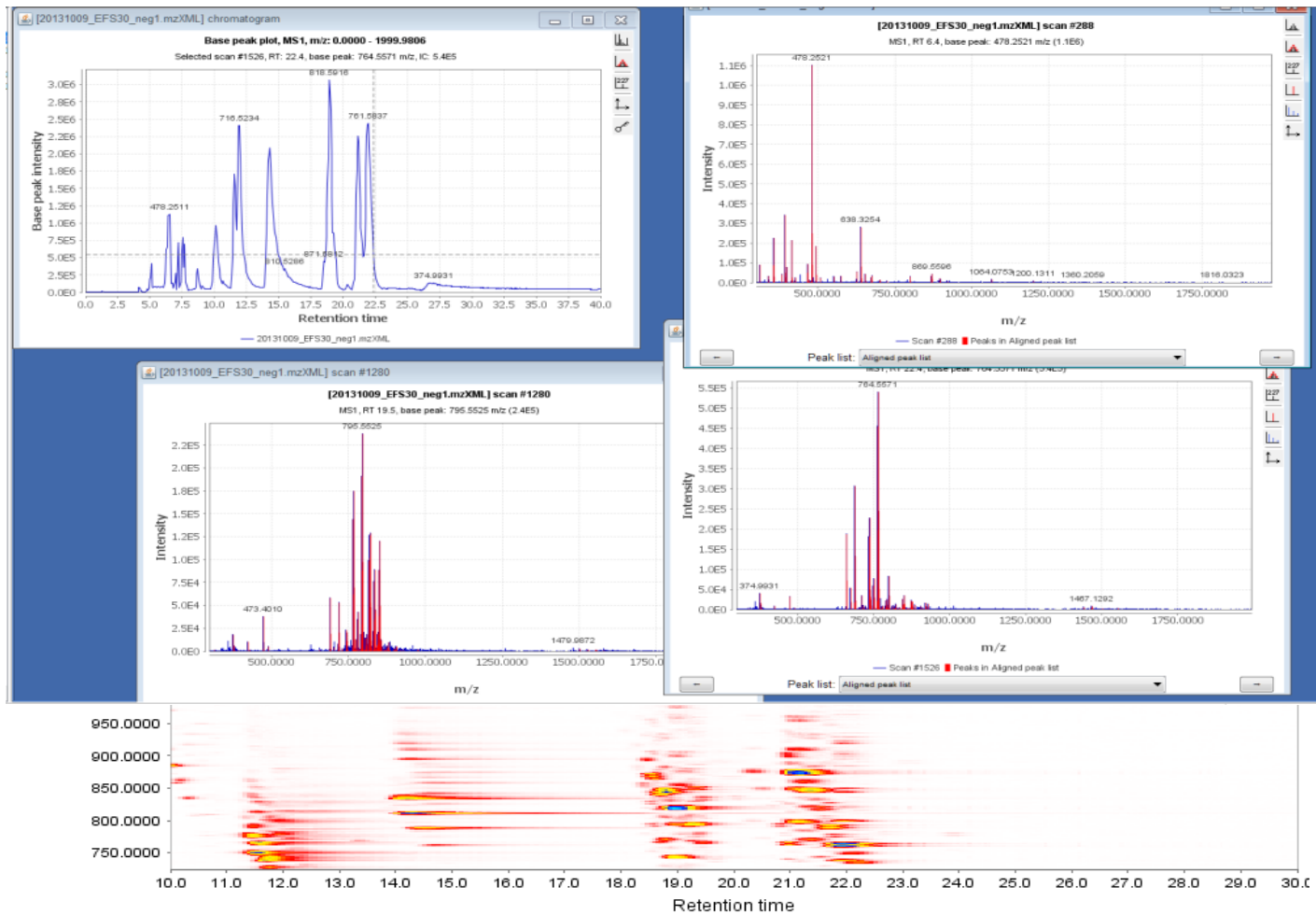


[Lipidomics: coming to grips with lipid diversity](#)

Andrej Shevchenko & Kai Simons

Nature Reviews Molecular Cell Biology 11, 593-598 (August 2010)

LC-MS data matrix



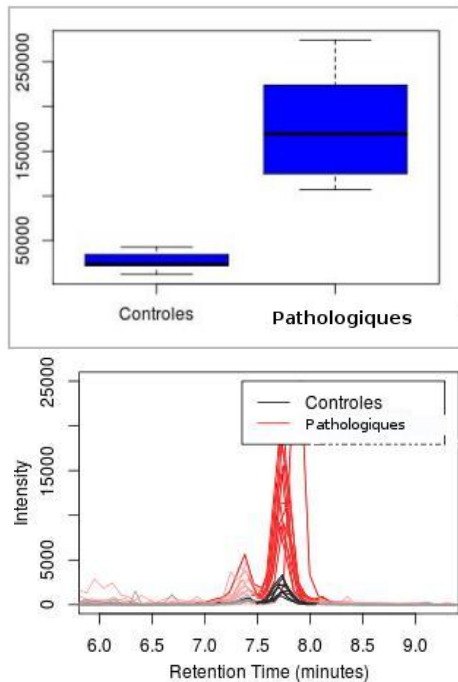
Data = 3D matrix
need to concatenate and "unfold" files
In the data matrix:
Objects (lines) = sample
Variables (columns) = couple (Tr, m/z)

LC-MS data matrix processing

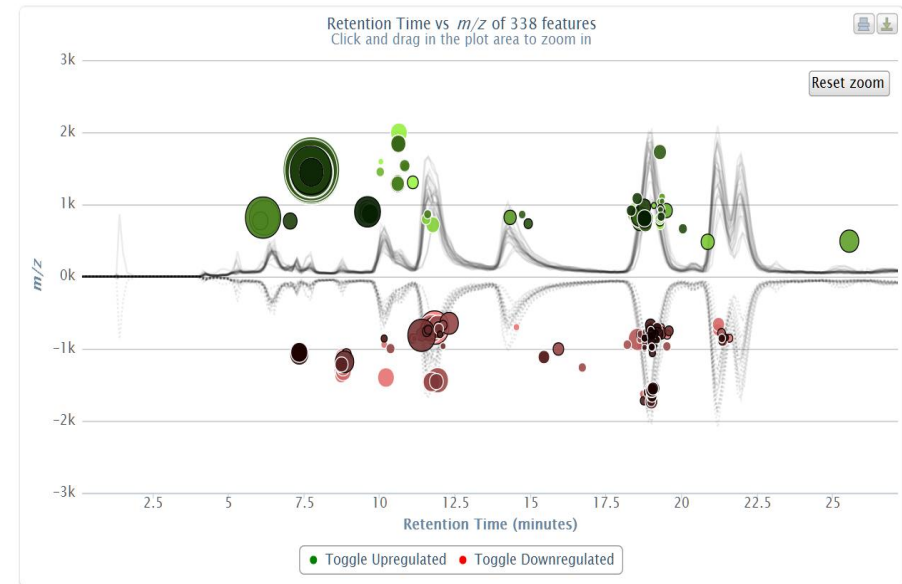
Univariate statistical analysis using XCMS online:

Paired Student t-test between the two groups of signals

Evident significant difference between the intensities of the ions.



m/z : 1447.969
retention time : 7.73 min
p-val : 0.006023
fold change : 6.635 (UP)
max intensity : 25008
2 matches found.
3 ppm [M-H] CL(18:2(9Z,12Z))/
3 ppm [M-H] CL(1'-[18:2(9Z,1



p-Value : 0-0.001 | fold change : 1.5 - 129.990 | *m/z* Range of 0 - 2197 | Retention Range of 1-42 | max intensity : 0-4444805.475 | Radius Scale : Fold Change

LC-MS data matrix processing

Alignment tools using MzMine

Raw data files

- 20131009_EFS30_neg1.mzXML
- 20131009_EFS32_neg1.mzXML

Peak lists

- 20131009_EFS30_neg1.mzXML
- 20131009_EFS32_neg1.mzXML
- Aligned peak list

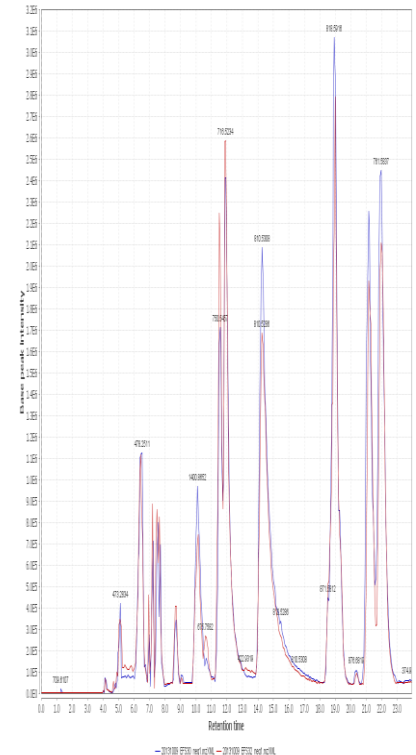
ID	Average		ID	Average		ID	Average		Ident...	Peak shape	20131009_EFS30_neg1.m...			20131009_EFS32_neg1.m...		
	m/z	Ret.time		m/z	Ret.time		m/z	Ret.time			Status	Height	...	Status	Height	...
178	747.5173	11.6	185	747.5163	11.6	175	746.5135	11.6			●	2.4E5	5...	●	4.5E5	1...
180	748.5299	11.6	187	748.5286	11.6	178	747.5168	11.6			●	9.6E4	2...	●	2.0E5	5...
182	749.5324	11.6	192	749.5306	11.6	180	748.5293	11.6			●	6.7E5	1...	●	9.4E5	2...
184	750.5454	11.6	207	764.5235	11.6	205	764.5214	11.6			●	6.5E5	1...	●	7.6E5	2...
185	751.5487	11.6	214	766.5391	11.6	213	766.5398	11.6			●	1.1E6	3...	●	9.5E5	2...
187	752.5584	11.6	218	767.5425	11.6	217	767.5431	11.6			●	4.9E5	1...	●	4.0E5	1...
205	764.5247	11.6	354	827.5175	11.6	700	1500.0829	11.6			●	5.0E4	1...	●	6.7E4	1...

Step 1: file by file, detection of ions (> threshold)
scan by scan

Step 2: ion chromatogram generation, file by file

Step 3: file by file, peak detection
table (ion; rt, intensity) (**data file**)

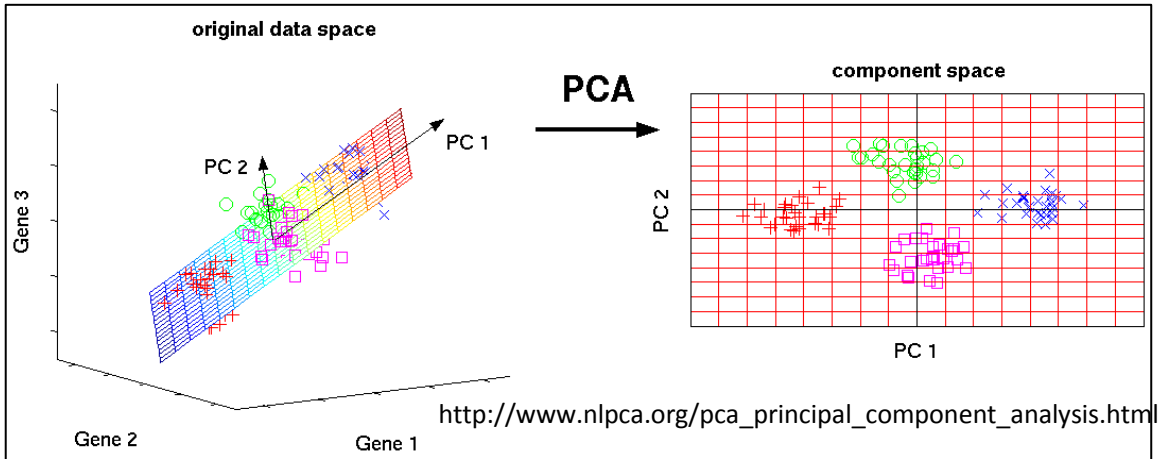
Step 4: Alignment: Setting a tolerance window (m/z, rt)
based in general on the first chromatogram. (**data set**)



LC-MS data matrix processing

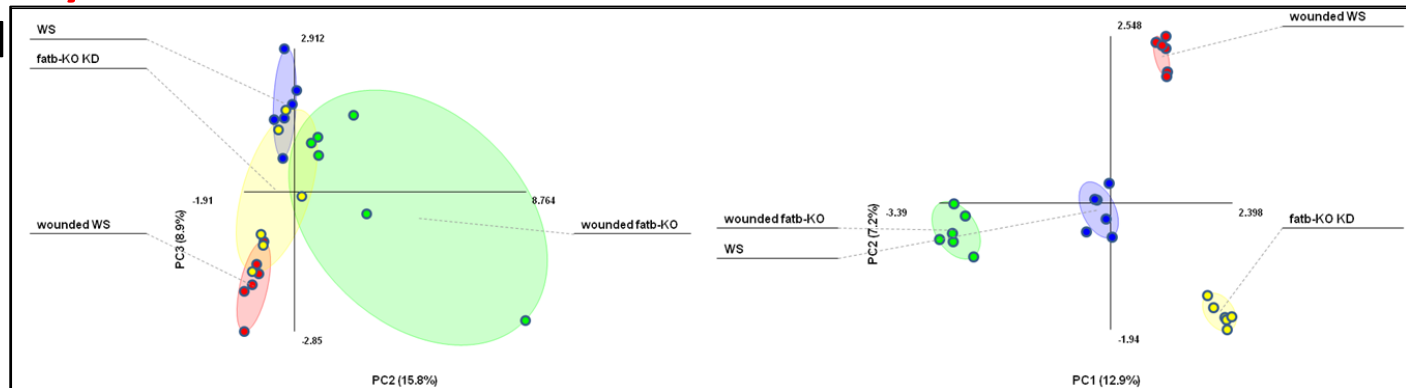
Principal component analysis

Unsupervised method
Data mining



PLS Discriminant analysis

Supervised method



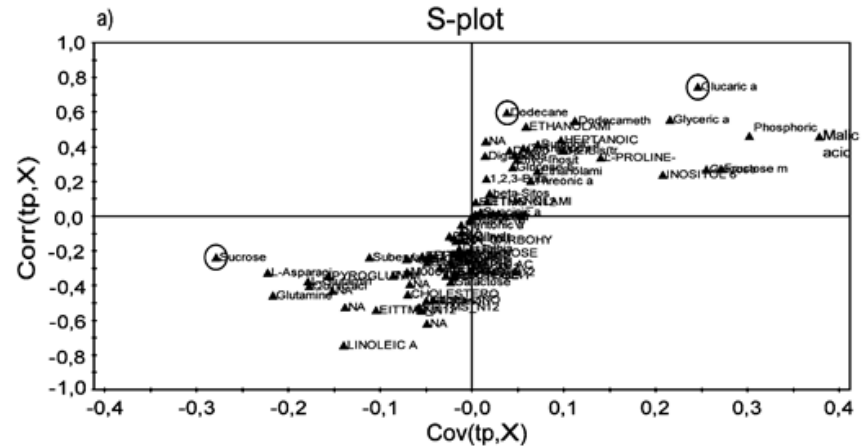
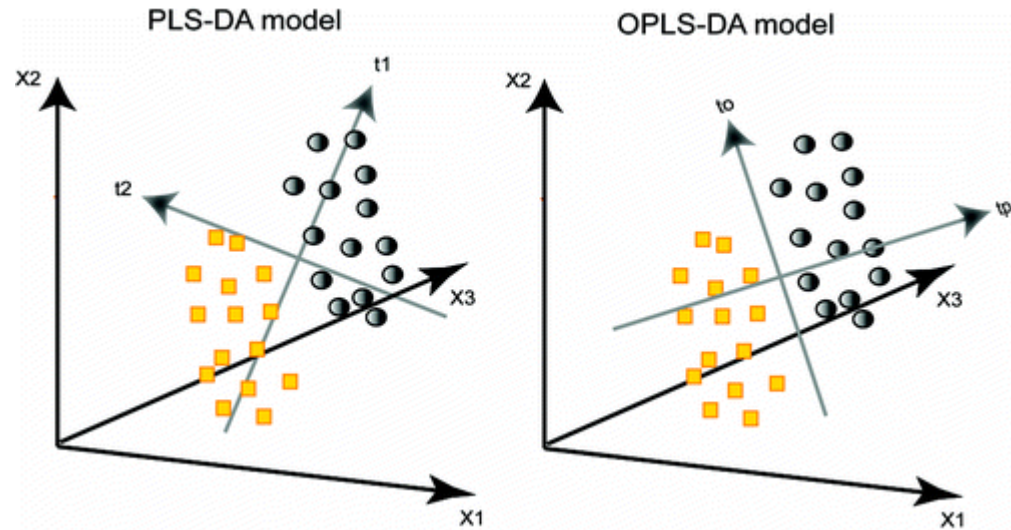
<http://fiehnlab.ucdavis.edu/staff/kind/Statistics/Concepts/OPLS-PLSDA>

LC-MS data matrix processing

Orthogonal PLS-DA (OPLS-DA)

Maximizes the discrimination between two classes in its first component

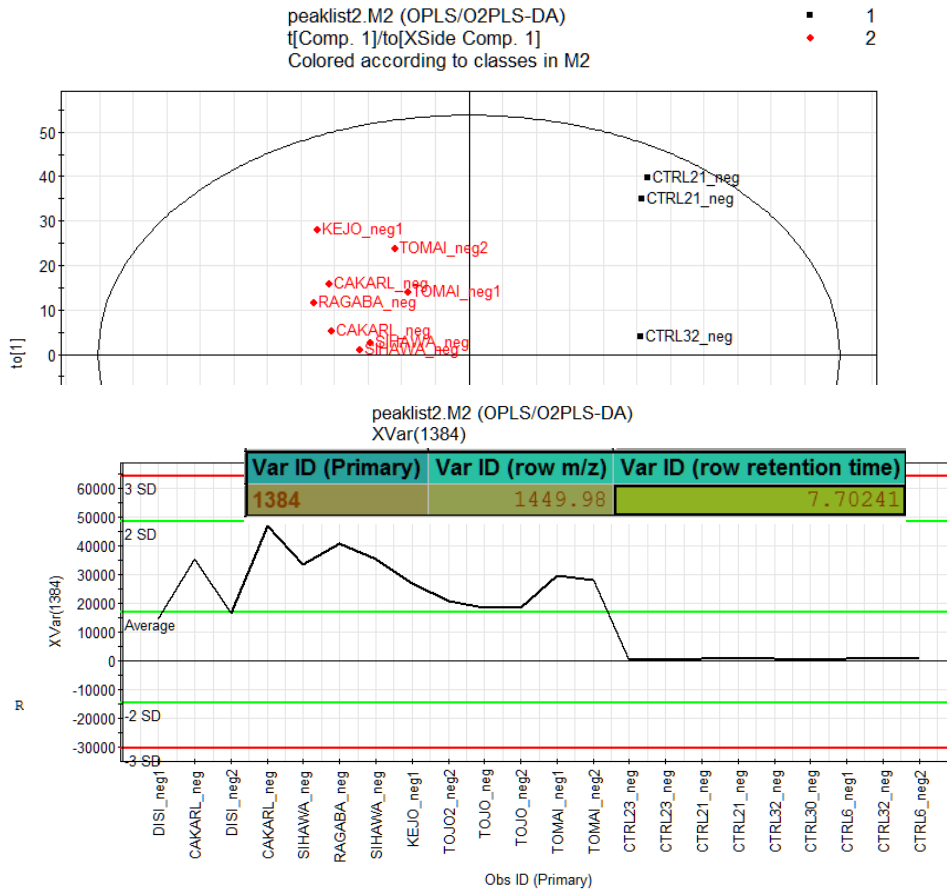
S-Plot expresses the relationship between the original variables (rt, m/z) and scores on the selected axis.



Published in: Susanne Wiklund; Erik Johansson; Lina Sjöström; Ewa J. Mellerowicz; Ulf Edlund; John P. Shockcor; Johan Gottfries; Thomas Moritz; Johan Trygg; Anal. Chem. 2008, 80, 115-122.

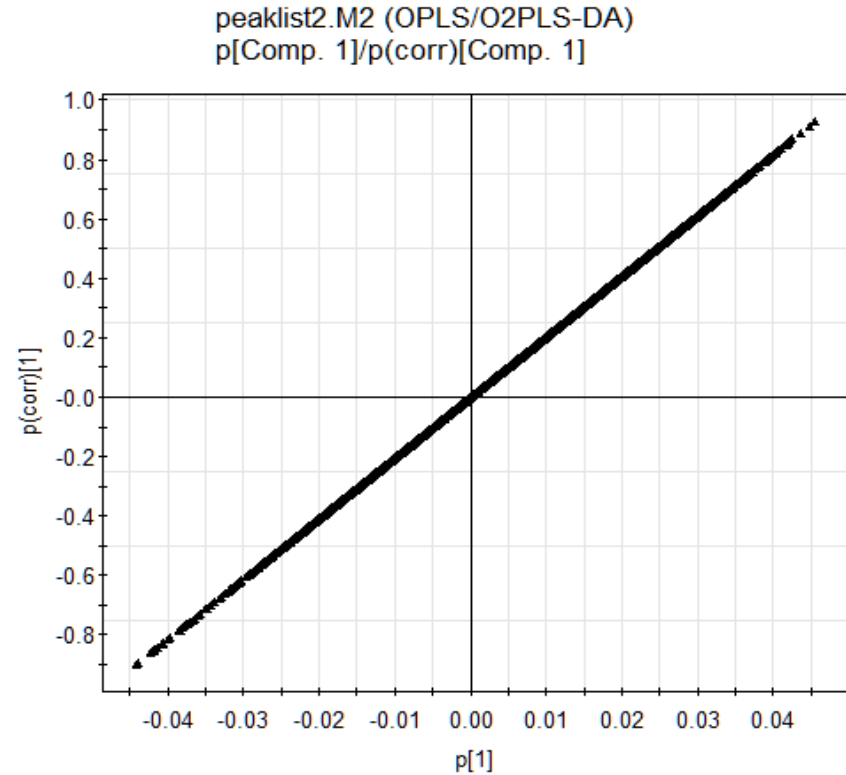
LC-MS data matrix processing

O-PLS and S-plot using SimcaP



-3 SD = -30237.3 -2 SD = -14489.3 Average = 17006.7 2 SD = 48502.7
3 SD = 64250.7

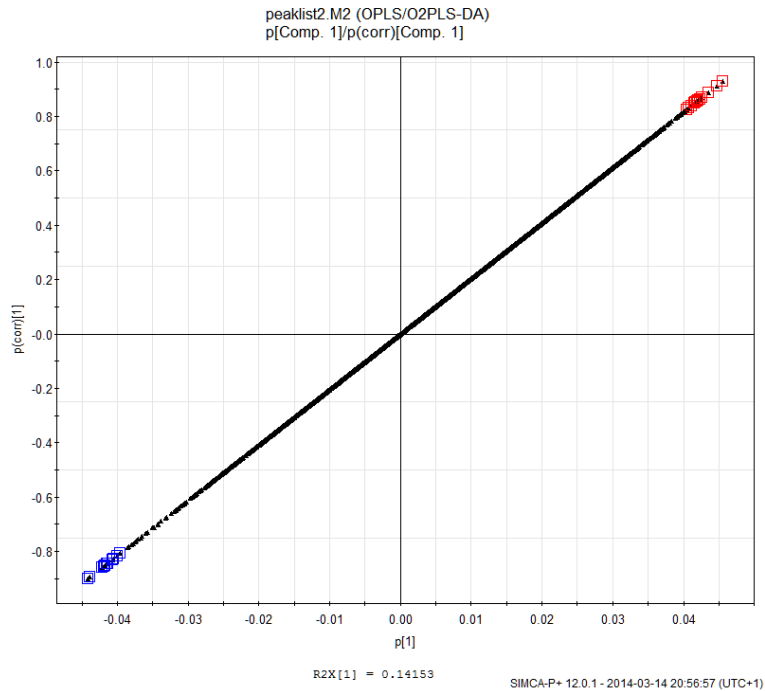
SIMCA-P+ 12.0.1 - 2014-03-14 20:48:10 (UTC+1)



R2X[1] = 0.14153
SIMCA-P+ 12.0.1 - 2014-03-14 20:45:48 (UTC+1)

LC-MS data matrix processing

S-plot / Selection of discriminate variables



General List [M2]

	1	2	3	4	5
1	Var ID (Primary)	Var ID (row m/z)	Var ID (row retention time)	M2.p[1]	M2.p[corr][1]
2	1280	1577.11	19.0169	0.0454953	0.927955
3	1561	1577.11	19.0146	0.0447281	0.912305
4	2475	720.497	11.7137	0.0423014	0.862809
5	2512	898.579	19.0235	0.0419978	0.856616
6	2661	1551.1	19.0404	0.0435393	0.888057
7	2683	814.561	18.9809	0.0421245	0.8592
8	2684	1550.1	19.0077	0.0425956	0.86881
9	2957	901.554	19.0197	0.0419536	0.855716

General List [M2]

	1	2	3	4	5
1	Var ID (Primary)	Var ID (row m/z)	Var ID (row retention time)	M2.p[1]	M2.p[corr][1]
2	294	807.588	18.7738	-0.0416959	-0.850459
3	305	804.61	18.7946	-0.0399648	-0.815149
4	838	830.627	18.6037	-0.0395783	-0.807266
5	1198	730.576	18.8086	-0.0407172	-0.830496
6	1302	834.608	18.6162	-0.0414102	-0.844632
7	1363	730.576	18.813	-0.0438618	-0.894635
8	1384	1449.98	7.70241	-0.0441028	-0.899551
9	1763	1452	7.71264	-0.0421506	-0.859734
10	1774	730.575	18.8107	-0.0406005	-0.828116
11	1830	780.567	18.8099	-0.0419063	-0.85475
12	2023	1449.98	7.70241	-0.0414215	-0.844861



Online databases

LIPID MAPS Tools : LIPID MAPS Lipid... x Identification of phospholipid specie... x Microsoft PowerPoint - EB_April_2013... x +

LIPID Metabolites and Pathways Strategy (LIPID MAPS)

Lipidomics Gateway

Search the Lipidomics Gateway ?

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Mass Spectrometry

Possible Cardiolipin Structures

Exact Mass: Mass Tolerance: [New Search](#)


C=Number of Carbons; DB=Number of double bonds; sn1('1),sn2...=MS/MS Product Ions (neutral loss)

Mass	C	DB	Abbreviation	sn1('1)	sn2('1)	sn1(2')	sn2(2')	Formula	Ion
1449.9806	72	7	18:1(9Z)/18:2(9Z,12Z)/18:2(9Z,12Z)/18:2(9Z,12Z)	1167.7248	1169.7404	1169.7404	1169.7404	C81H143O17P2	[M-H] ⁻
1449.9806	72	7	18:2(9Z,12Z)/18:2(9Z,12Z)/18:2(9Z,12Z)/18:1(9Z)	1169.7404	1169.7404	1169.7404	1167.7248	C81H143O17P2	[M-H] ⁻
1449.9806	72	7	18:2(9Z,12Z)/18:2(9Z,12Z)/18:1(9Z)/18:2(9Z,12Z)	1169.7404	1169.7404	1167.7248	1169.7404	C81H143O17P2	[M-H] ⁻
1449.9806	72	7	18:2(9Z,12Z)/18:1(9Z)/18:2(9Z,12Z)/18:2(9Z,12Z)	1169.7404	1167.7248	1169.7404	1169.7404	C81H143O17P2	[M-H] ⁻

Total of 4 Records

Online databases

Human Metabolome Database Version 3.5

Home Browse » Search » About » Downloads  Contact Us

Search HMDB for

MS Search [MS/MS Search](#) [GC/MS Search](#) [1D NMR Search](#) [2D NMR Search](#)

Mass Spectrum Search

Query Masses (Da)

Enter one mass per line (maximum 150 query masses per request)

Molecular Weight

Molecular Species

MS search for 1449.98 m/z $\Delta = \text{abs}(\text{query mass} - \text{adduct mass})$

Show 10 entries Search:

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB57086	CL(18:0/16:1(9Z))/22:5(7Z,10Z,13Z,16Z,19Z)/16:1(9Z))	M-H	1449.9806	1450.987876	0.0006
HMDB10246	CL(18:2(9Z,12Z))/18:2(9Z,12Z)/18:2(9Z,12Z)/18:1(11Z))	M-H	1449.9806	1450.987876	0.0006
HMDB57699	CL(16:1(9Z)/20:4(5Z,8Z,11Z,14Z))/18:1(9Z)/18:1(11Z))	M-H	1449.9806	1450.987876	0.0006
HMDB57636	CL(16:1(9Z)/18:1(9Z)/20:4(5Z,8Z,11Z,14Z)/18:1(11Z))	M-H	1449.9806	1450.987876	0.0006
HMDB56436	CL(16:0/16:0/18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	M-H	1449.9806	1450.987876	0.0006
HMDB57280	CL(18:0/22:5(4Z,7Z,10Z,13Z,16Z))/16:1(9Z)/16:1(9Z))	M-H	1449.9806	1450.987876	0.0006
HMDB57328	CL(18:0/22:5(7Z,10Z,13Z,16Z,19Z))/16:1(9Z)/16:1(9Z))	M-H	1449.9806	1450.987876	0.0006
HMDB56586	CL(16:0/18:1(11Z)/16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	M-H	1449.9806	1450.987876	0.0006
HMDB57998	CL(18:1(11Z)/18:1(11Z)/20:4(5Z,8Z,11Z,14Z)/16:1(9Z))	M-H	1449.9806	1450.987876	0.0006
HMDB58388	CL(18:1(9Z)/16:1(9Z)/18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	M-H	1449.9806	1450.987876	0.0006

Showing 1 to 10 of 125 entries ◀ Previous Next ▶

Online databases

MassBank | Statistics x Identification of phospholipid specie... x +

MassBank High Quality Mass Spectral Database

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Statistics

Publications

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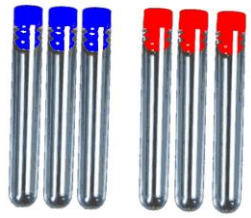
Statistics

Statistics

Last updated Mar 5, 2014 | Total Number of Spectra : *1 40,889 new

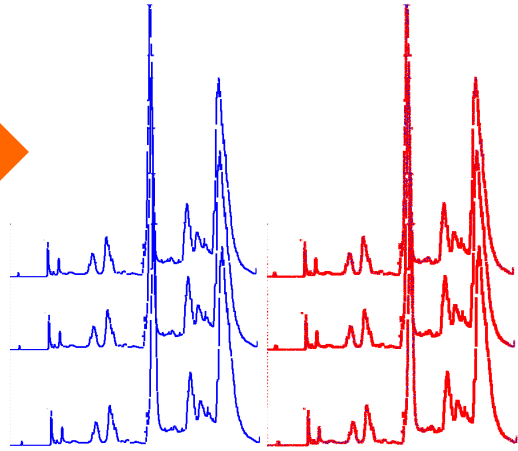
Research Groups (Contact Name)	Prefix of ID	Analysis Equipment (Analysis Method)	Number of Spectra	Number of Compounds
01. IAB, Keio U (Dr. Tomoyoshi Soga)	KOX	LC-ESI-QTOF (MS2)	※2 839	672
	KO	LC-ESI-QQ (MS2)	4,265	
		LC-ESI-IT (MS2,MS3,MS4)	515	
02. PSC, RIKEN (Dr. Masanori Arita)	PR	GC-EI-TOF (MS)	241	653
		LC-ESI-QTOF (MS,MS2)	1,371	
		LC-ESI-QQ (MS2)	87	
		CE-ESI-TOF (MS)	20	
03. Nihon Waters K.K. (Dr. Katsutoshi Nagase)	WA	LC-ESI-Q (MS)	2,719	575
		LC-ESI-QQ (MS2)	273	

Chemometric tools for LC-MS lipidomics profiles analysis.



Samples

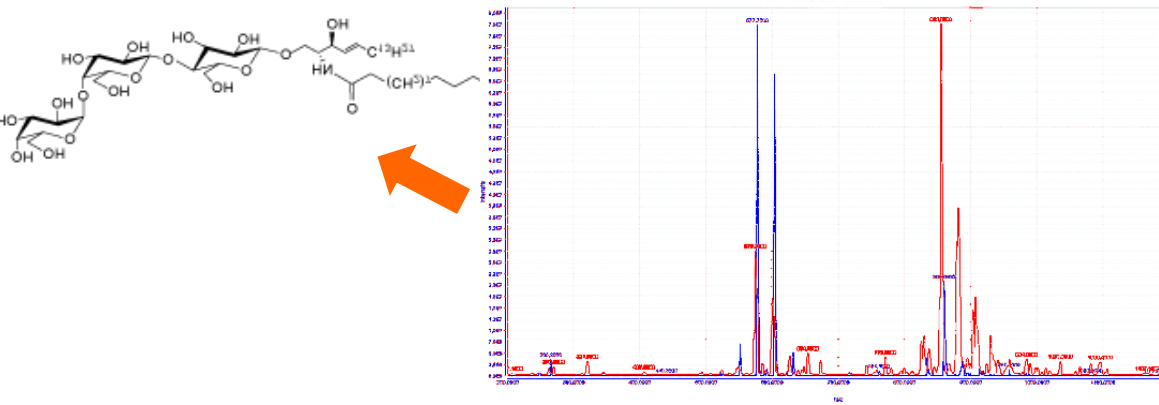
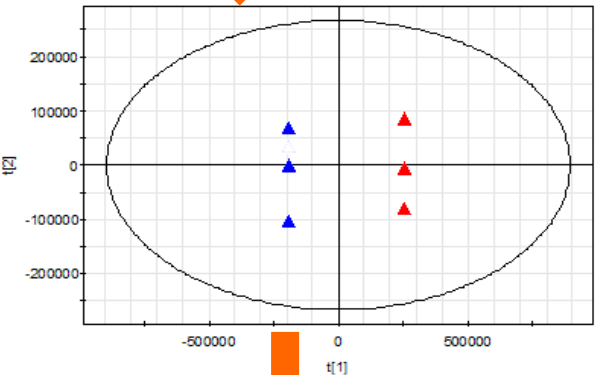
Biomarkers



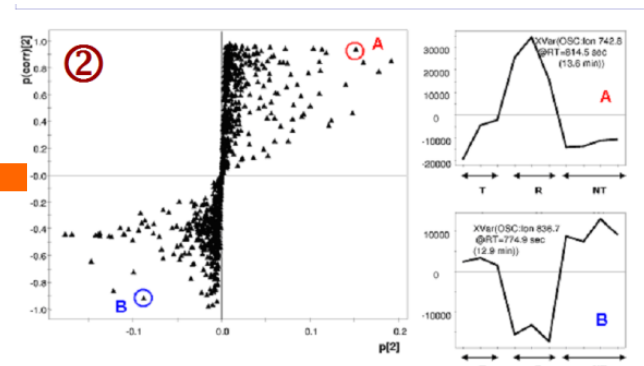
LC-MS profiles

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	
1	OSC Ion 936.8 @RT=777.7 sec (13.8 min)	OSC Ion 936.7 @RT=636.1 sec (10.5 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)	OSC Ion 936.8 @RT=596.5 sec (8.3 min)
2	L.Hight 1042.mzOM	-1071.6	-4.42712	16.7031	-15.9044	-3.64396	-0.042456	16.033	0.774109	-6.67197	14.5703	1.69574	126.106	7.93222	-191.75	2.97205	-6.16658	24	
3	L.Hight 7041.mzOM	-150.322	-0.942037	13.5884	56.2532	1.95332	-1.41082	63.8482	1.4683	11.0005	0.767114	2.79763	-65.7618	-8.25704	385.507	-2.92781	-6.03345	136	
4	L.Hight R043.mzOM	2911.37	37.8148	-4.91541	40.1657	4.70392	-0.202862	11.5938	0.00567	40.0367	0.07539	7.14327	13.1637	-25.4708	-162.331	-24.2411	-0.521931	1	
5	L.Hight R043.mzOM	-539.848	1.65627	-2.33228	-186.887	1.37889	1.91906	-12.7681	-0.629679	-6.10538	0.400546	16.8031	72.0138	12.1039	-153.584	0.125642	17.2003	-83	
6	L.Hight R043.mzOM	-1105.41	-116245	3.22223	-119.015	6.86708	0.590534	5.496066	-1.65335	-8.40432	-4.36631	16.232	-100.136	36.2501	112.331	36.7932	15.1197	-97	
7	L.Hight M723.mzOM	-552.861	3.09881	-5.19397	-186.536	-3.7493	2.04589	-43.5387	0.07204	-3.4576	7.88373	17.2895	231.889	7.21853	-541.645	-18.0388	17.8008	-54	
8	L.Hight M723.mzOM	227.295	-18.8198	-2.38703	-29.4264	-0.31058	-0.532031	3.89194	-3.48544	-0.77784	-0.88931	-16.2985	-87.2344	-24.0917	228.51	-21.4512	-14.7524	-46	
9	L.Hight M723.mzOM	-272.836	-3.51178	-0.59506	444.265	-0.04715	-0.768624	-5.23745	-1.44193	-0.912474	-10.9067	-13.745	-71.9327	-2.63401	316.423	4.1933	-5.34629	25	
10	L.Hight M723.mzOM	-164.626	-0.624453	-5.58369	107.481	2.57463	-1.37025	-26.4386	-2.03597	-5.49515	-6.23653	-18.0718	-70.564	-16.552	-28.0031	8.34209	-11.3442	-1	
11	L.Hight	863.34	-12.6162	-4.50268	-52.5967	0.897111	0.598333	-22.8508	-1.07442	-3.50372	-1.28334	-14.045	-107.305	13.5088	-18.4682	11.116	-3.7187	-10	

Statistical analysis



Highlighting specific MS signals of the 2 groups

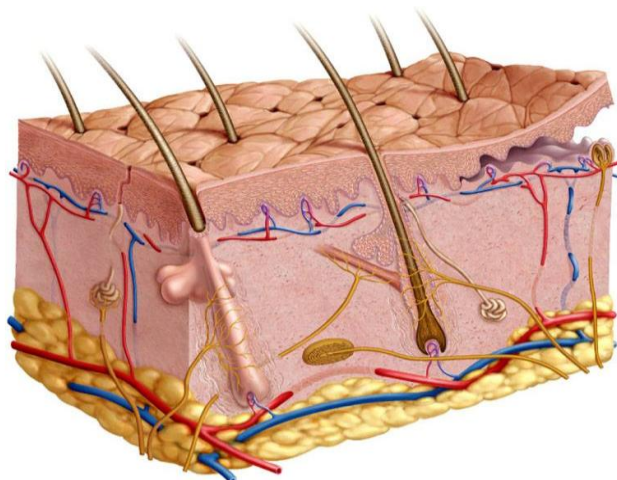


Analytical chemistry and chemometrics: a tool for skin physiological and physiopathological characterization

Ali Tfayli

Introduction

General structure of the skin



Largest organ in human body

Epidermis

- Stratum Basale
- Stratum Spinosum
- Stratum Granulosum
- **Stratum Corneum**

Dermis

- Superficial
- Deep

Barrier function

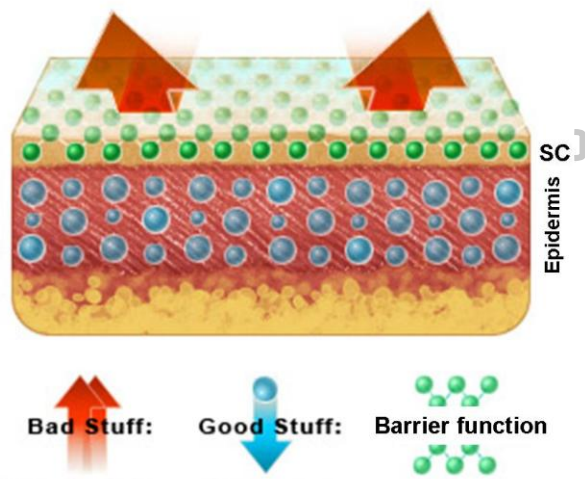
Sensation

Heat regulation

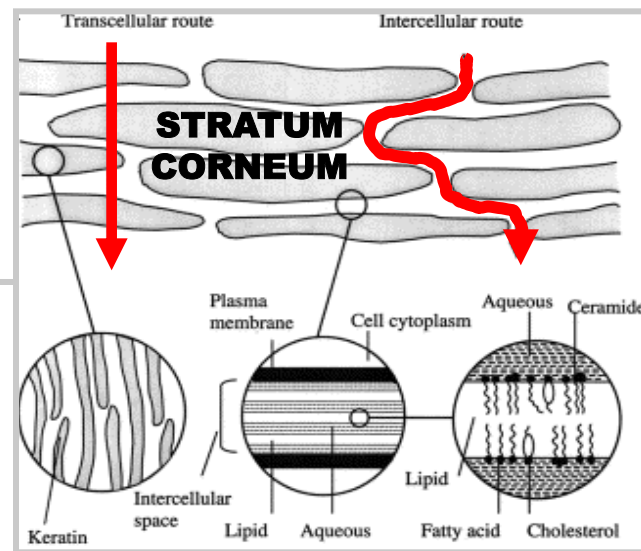
Secretion and excretion

Introduction

Skin Barrier function



SC structure



Barrier against

External insult

Water loss

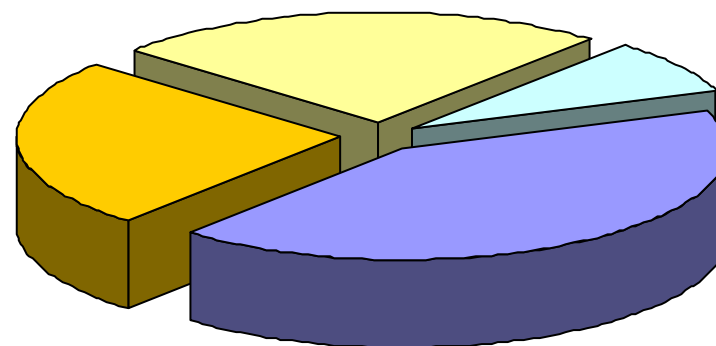
Keratin

Intercellular lipids

Introduction

Skin Barrier function

Composition of SC lipids

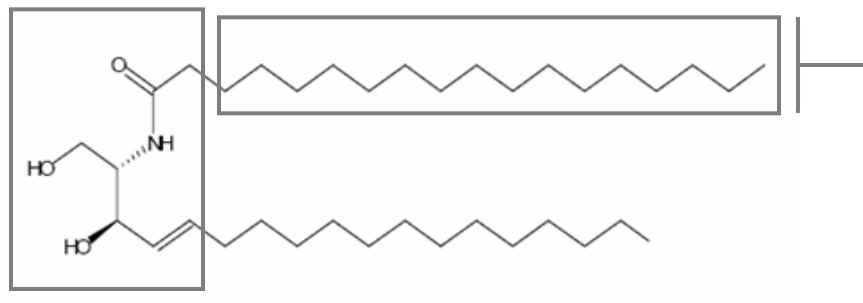


CERAMIDES

CHOLESTEROL

FATTY ACIDS

OTHERS



Structure of Ceramides

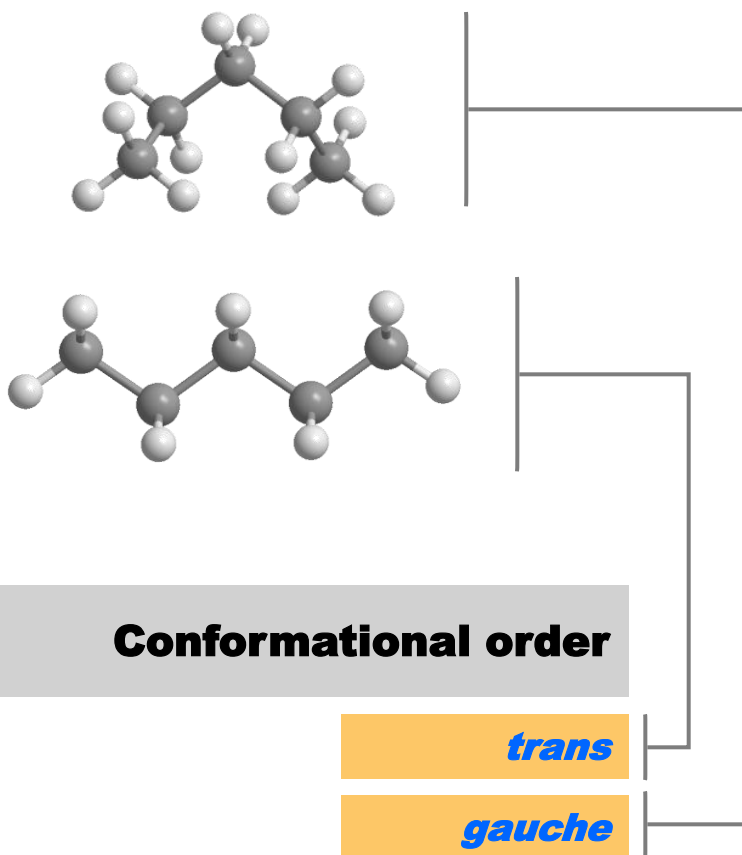
Different polar heads

Different chain lengths

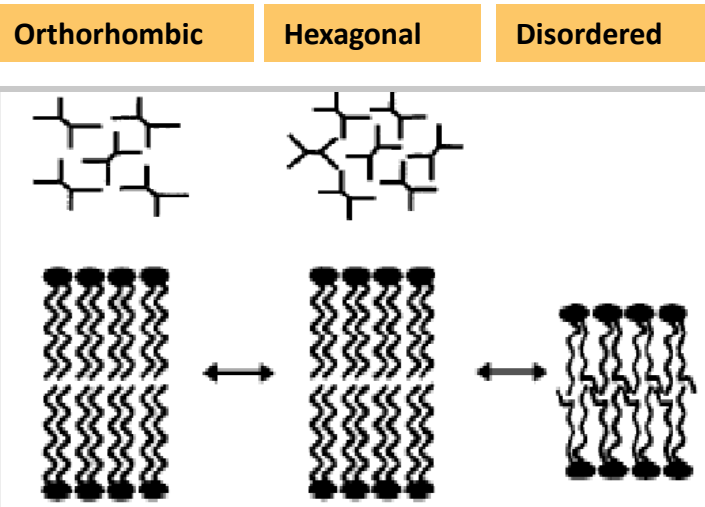
Presence of double bonds

Introduction

Skin Barrier function



Lateral packing of SC lipids

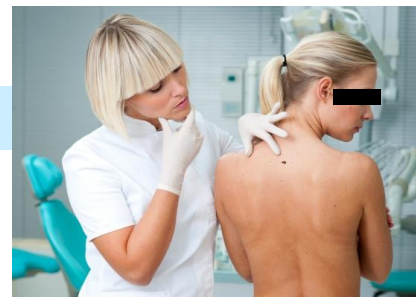


HIGHLY ORGANIZED



GOOD BARRIER PROPERTIES

Dermatology



Characterization of skin barrier

- Physiological status
- Physiopathological status

Skin aging

Skin hydration and dry skin diseases

Mechanical stress

Toxicology



Cosmetology

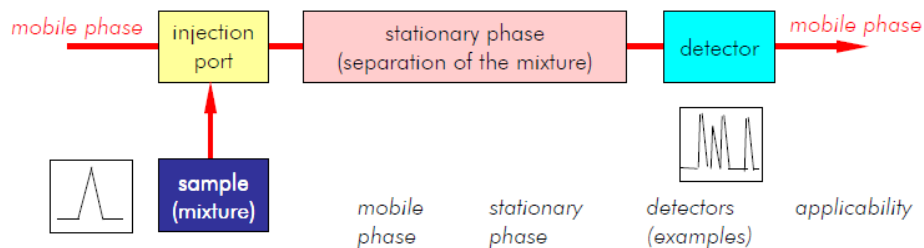


Analyses of skin barrier

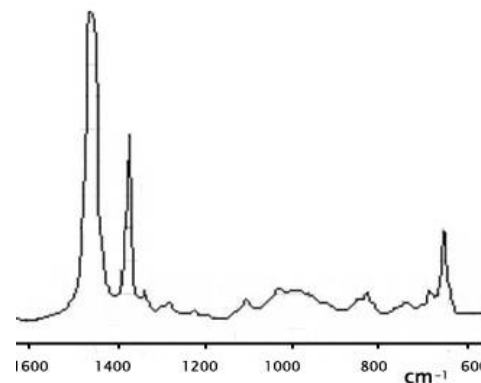
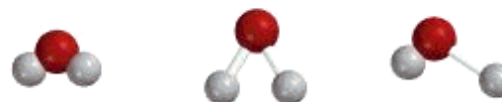
Organization, lateral packing

Composition and profiling

Separative techniques - mass



Vibrational spectroscopies:
 Infrared and Raman



Vibrational spectroscopies

INTERACTION

RAYONNEMENT - MATIERE

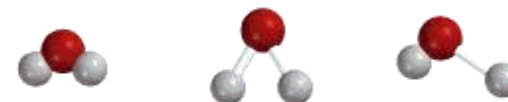


SPECTROSCOPIES OPTIQUES

ABSORPTION

EMISSION

DIFFUSION



$$\bar{\nu} = \frac{\nu}{C} = \frac{1}{2\pi C} \sqrt{\frac{k}{\mu}}$$

$\bar{\nu}$ = nombre d'onde, ν = fréquence, μ = masse réduite

$$\mu = \frac{m_A \cdot m_B}{m_A + m_B}$$

$$\mu_{\text{tot}} = \mu_{p(0)} + \sum_{n=1}^{3N-6} \left(\frac{d\mu_p}{dQ_n} \right) Q_0 \cos \nu_n t + \alpha_0 (\mathbf{E}_0 \cos \nu_0 t) + \frac{1}{2} \mathbf{E}_0 \sum_{n=1}^{3N-6} \left(\frac{d\alpha_0}{dQ_n} \right) Q_0 [\cos(\nu_0 - \nu_n)t + \cos(\nu_0 + \nu_n)t]$$

Vibrational spectroscopies

Jablonski diagram

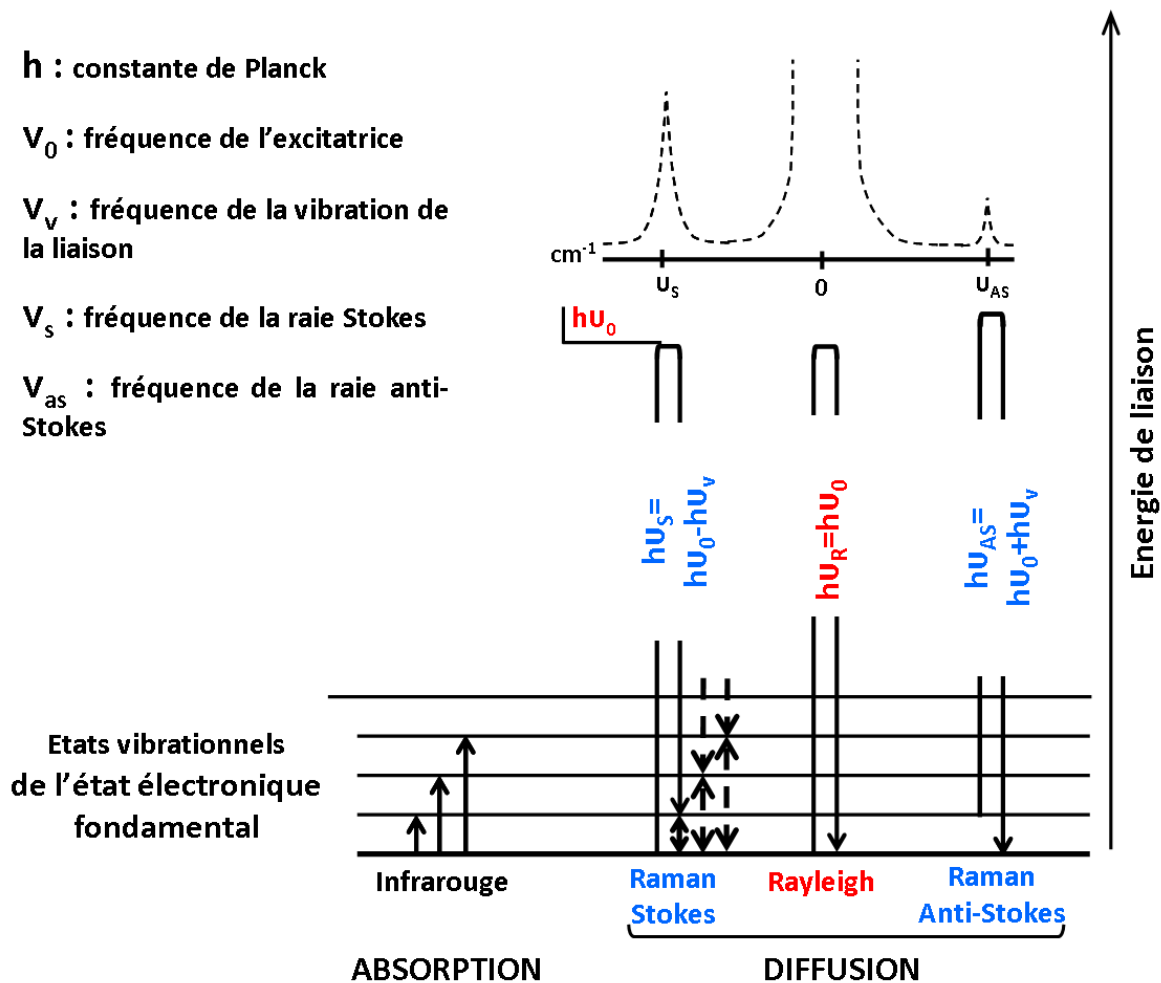
h : constante de Planck

ν_0 : fréquence de l'excitatrice

ν_v : fréquence de la vibration de la liaison

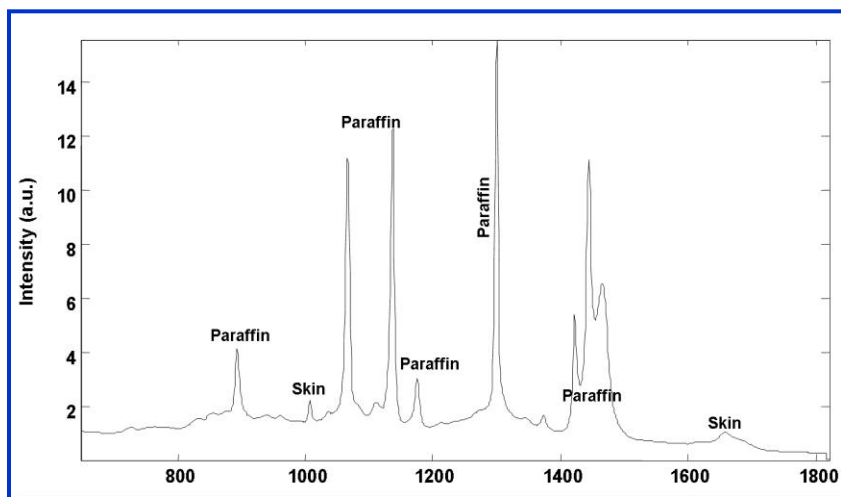
ν_s : fréquence de la raie Stokes

ν_{as} : fréquence de la raie anti-Stokes

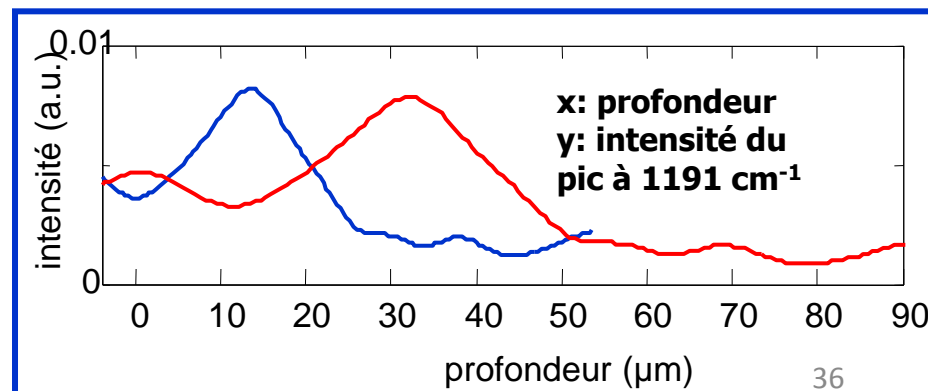
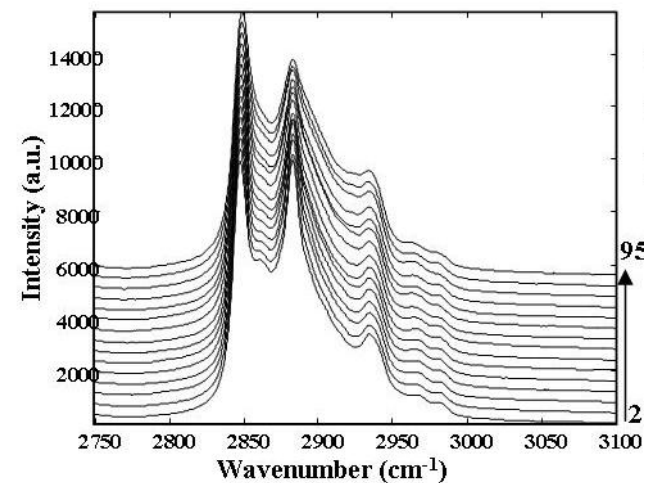
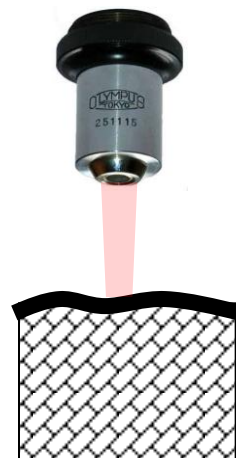


Vibrational signal collection

Individual spectral collection

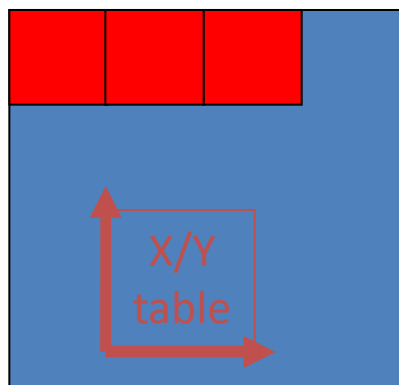


In depth spectral collection

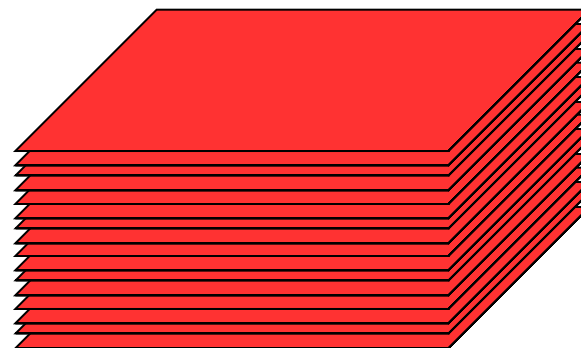


Vibrational signal collection

2D spectral mapping



3D spectral mapping



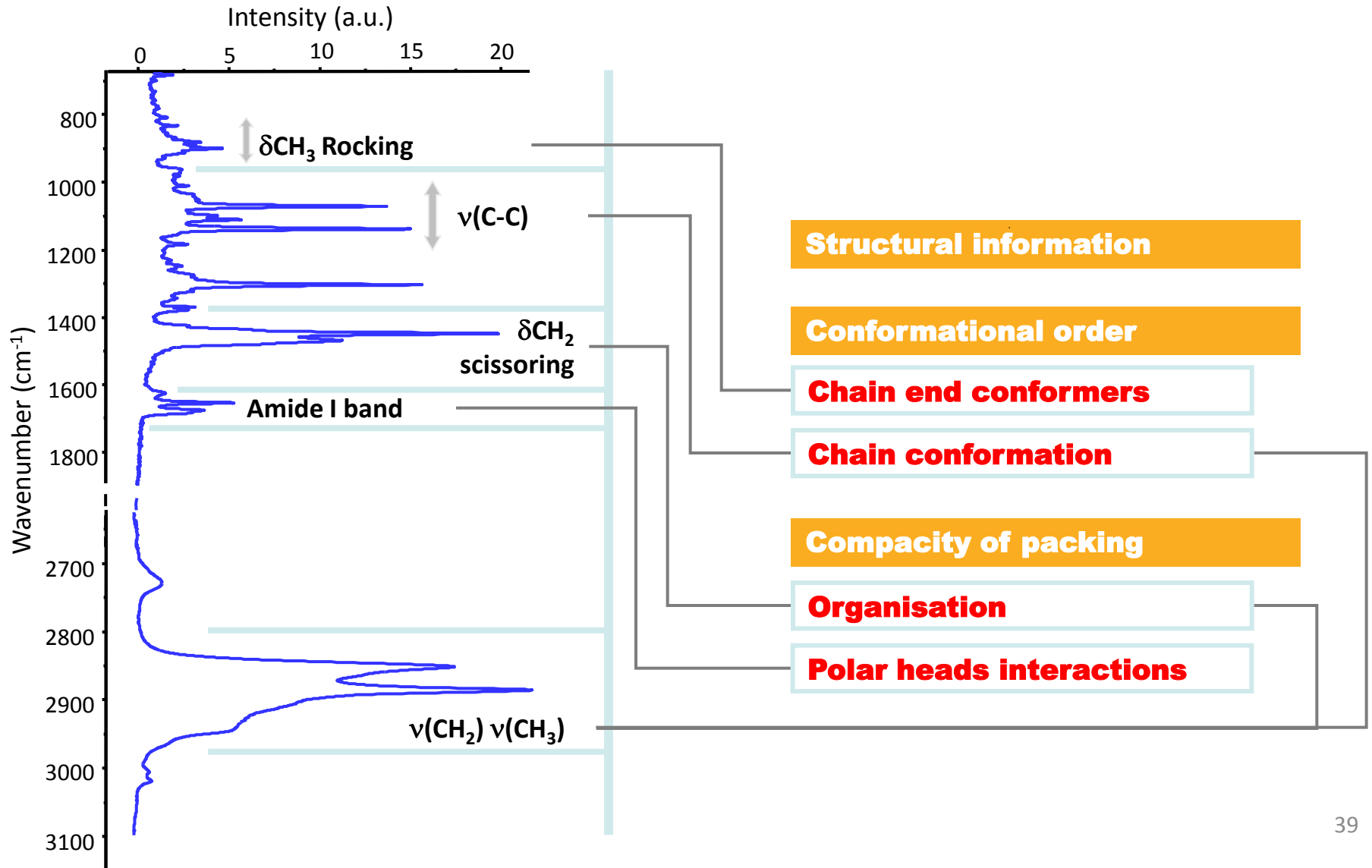
Data pre-processing

- Dark current
- CCD response correction
- Optical components contribution
- Smoothing
- Baseline correction
- Normalization

Vibrational spectroscopies VS barrier function

Physiological / Physiopathological status

Raman descriptors of SC barrier



Vibrational spectroscopies VS barrier function

Physiological / Physiopathological status

Skin aging

Ex vivo et in vivo

Volontaires

13 F & 7 M (22 à 64 ans)

Méthode

Surface nettoyée

1^{ère} acquisition *in vivo*

Extraction des lipides

2^{ème} acquisition *in vivo*

In vivo

Spectres *in vivo* avant l'extraction

–

Spectres *in vivo* après l'extraction

=

Signal *in vivo* des lipides

Ex vivo

Pas de séparation



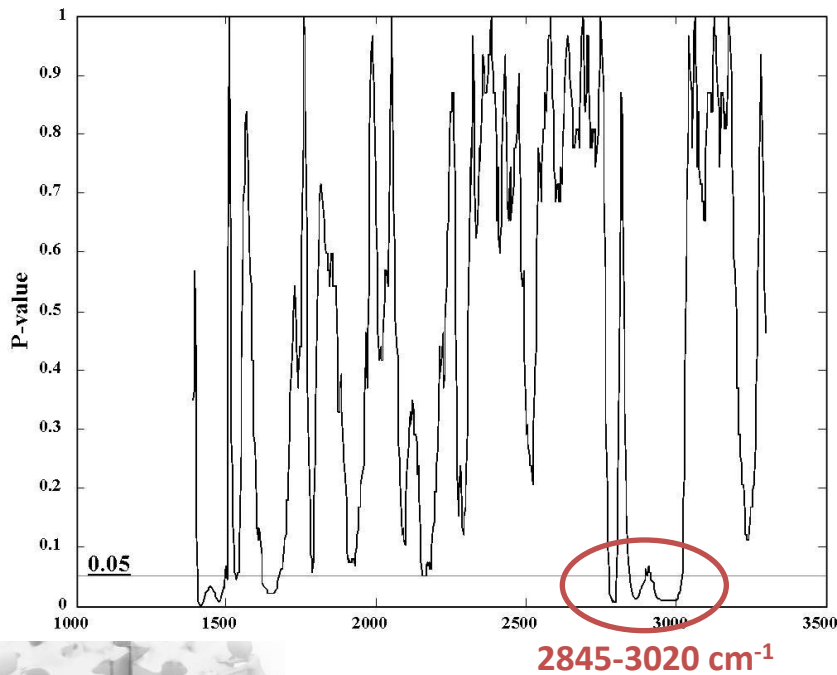
Vibrational spectroscopies VS barrier function

Physiological / Physiopathological status

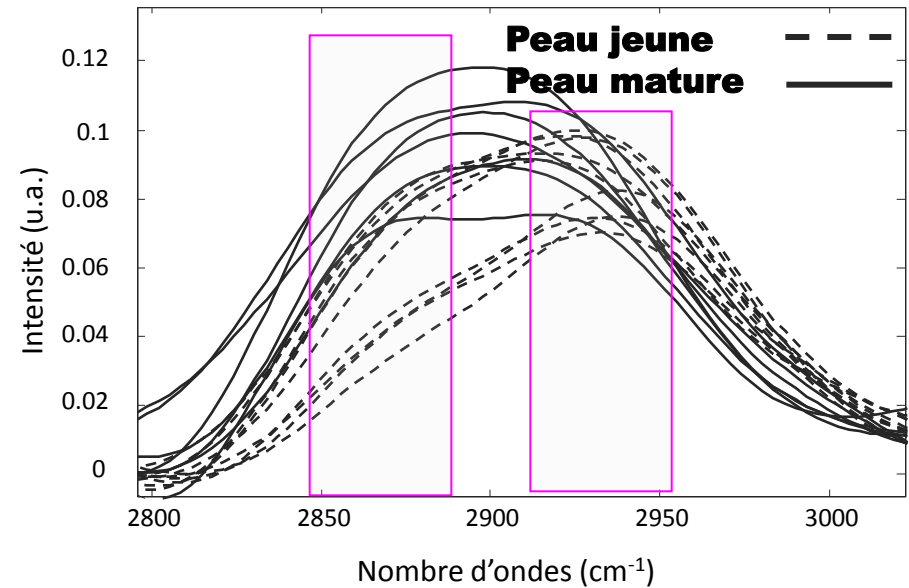
Skin aging

in vivo

kruskal Wallis



Observations directes



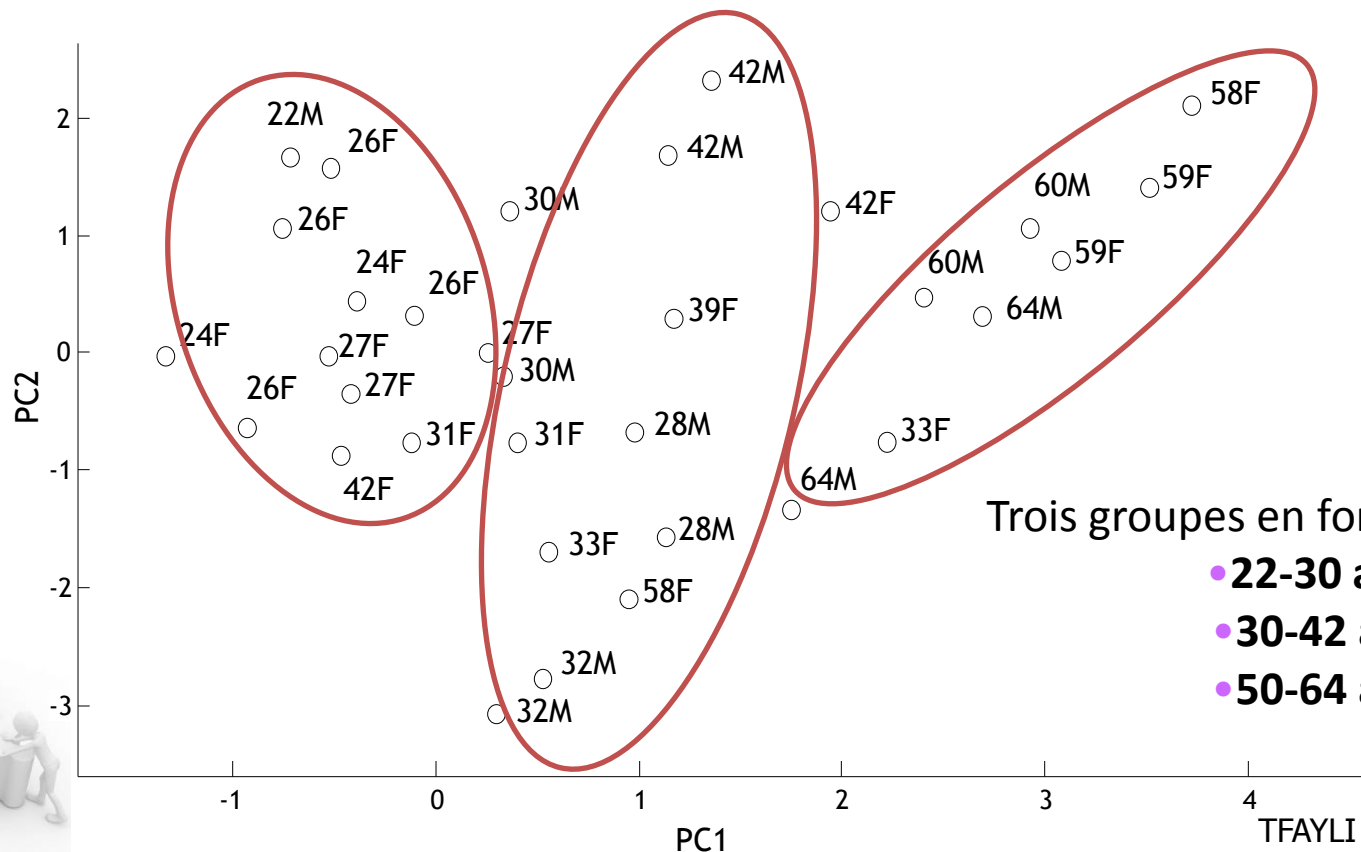
Vibrational spectroscopies VS barrier function

Physiological / Physiopathological status

Skin aging

in vivo

Analyse en composantes principales sur la gamme:
2845-3020 cm^{-1}



Vibrational spectroscopies VS barrier function

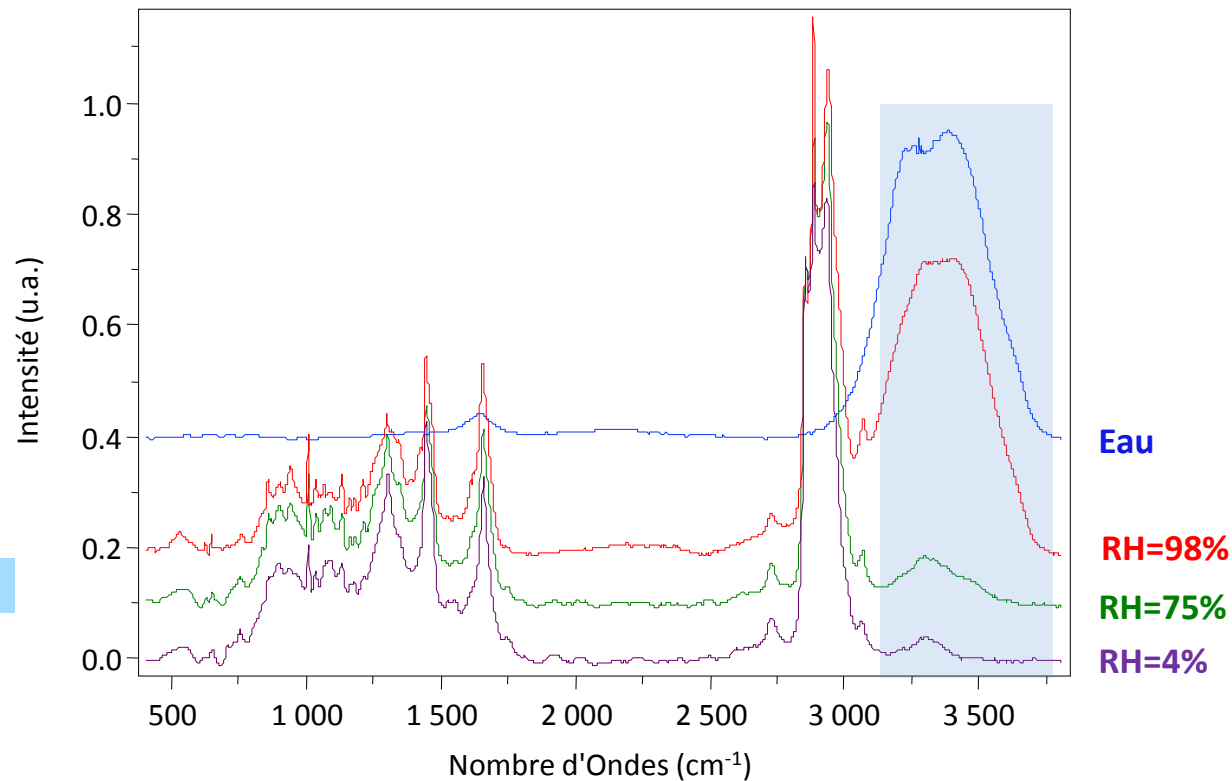
Physiological / Physiopathological status

Skin hydration / dry skin diseases



Ex vivo

Water structure



RH : 2.5% » 75%



Vibrational spectroscopies VS barrier function

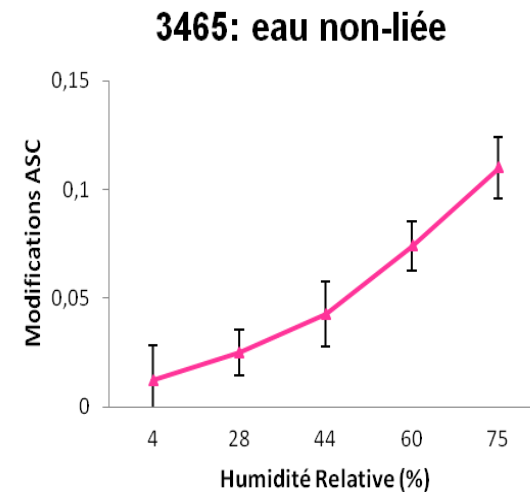
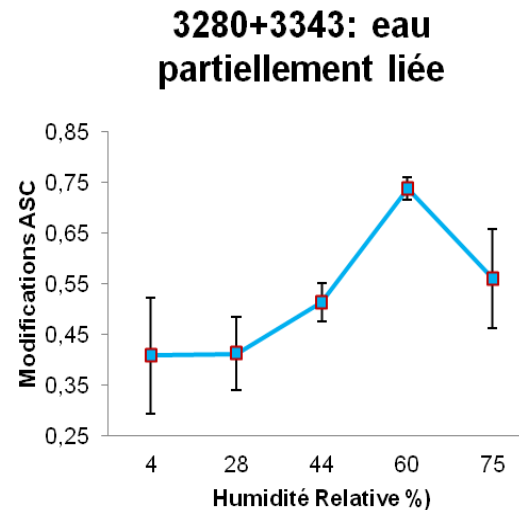
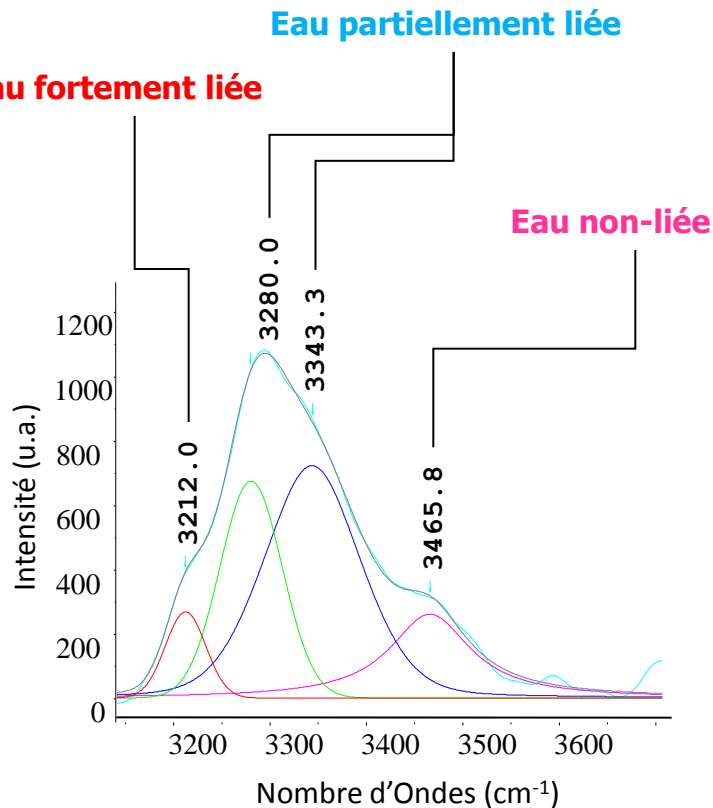
Physiological / Physiopathological status

Skin hydration / dry skin diseases



Ex vivo

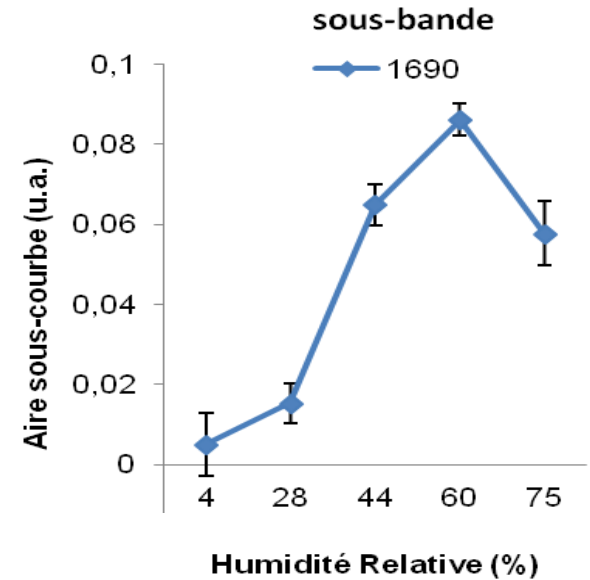
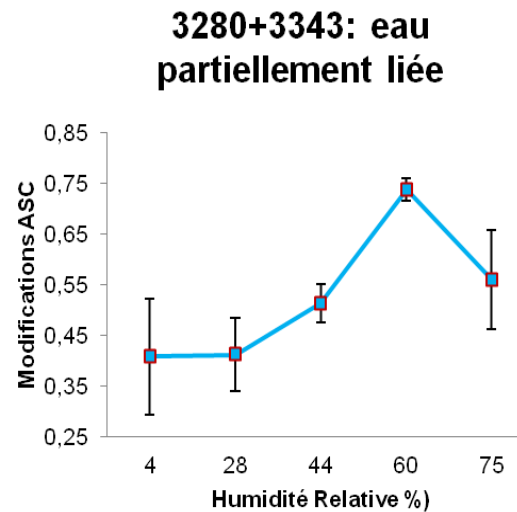
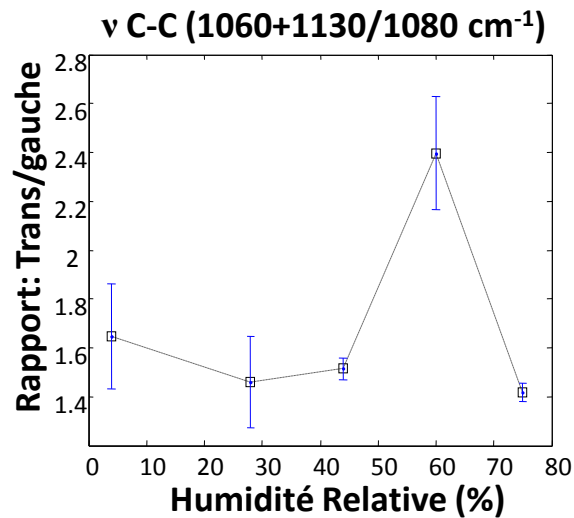
Water structure



Ex vivo

Conformation des chaînes lipidiques

Structure secondaire de la kératine: bande Amide I

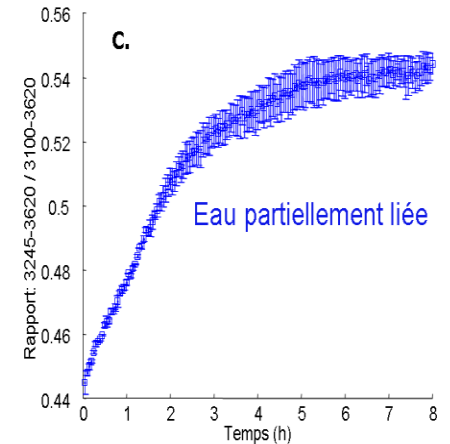
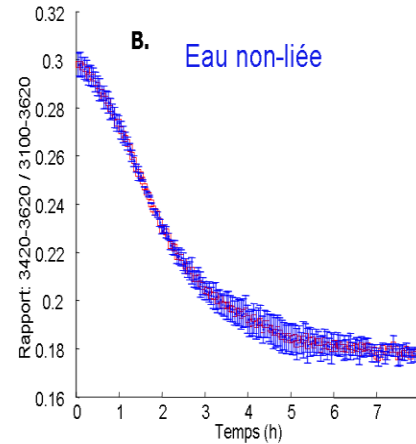
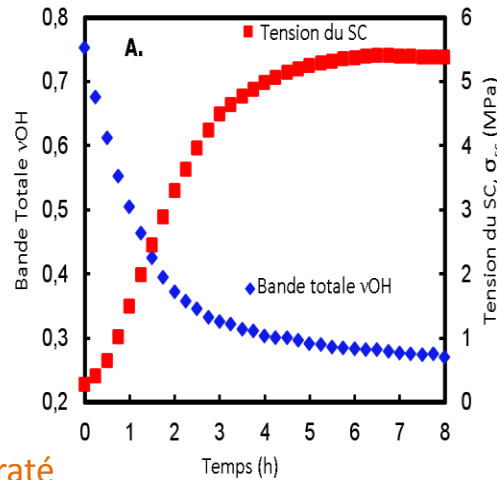
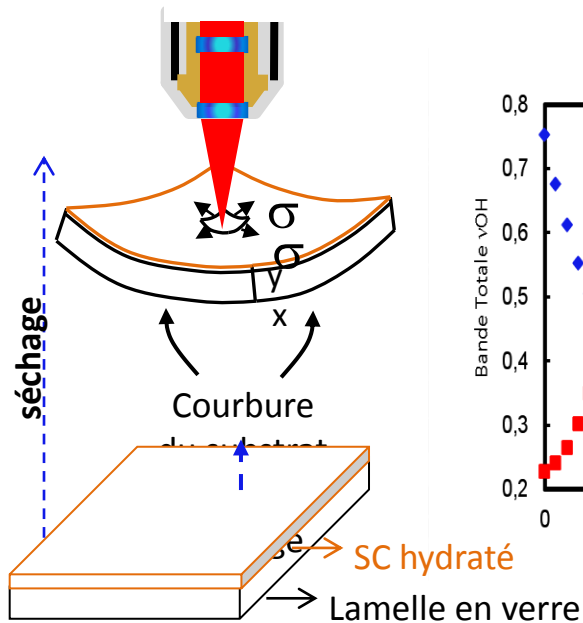


Vibrational spectroscopies VS barrier function

Physiological / Physiopathological status

Hydration and mechanical stress

Ex vivo



Tension mécanique du SC



Bande totale νOH



Vibrational spectroscopies VS barrier function

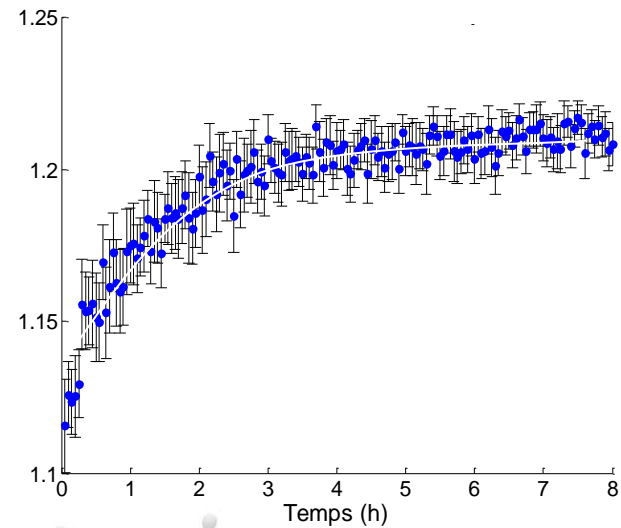
Physiological / Physiopathological status

Hydration and mechanical stress

Ex vivo

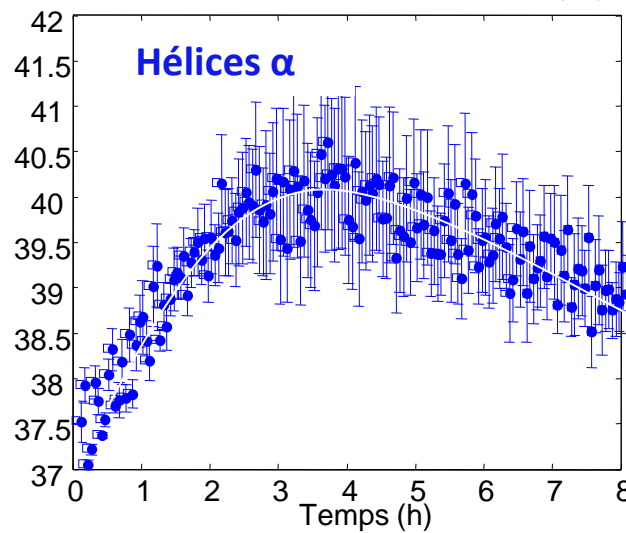
Conformation des lipides

Rapport : S1060 / S1080

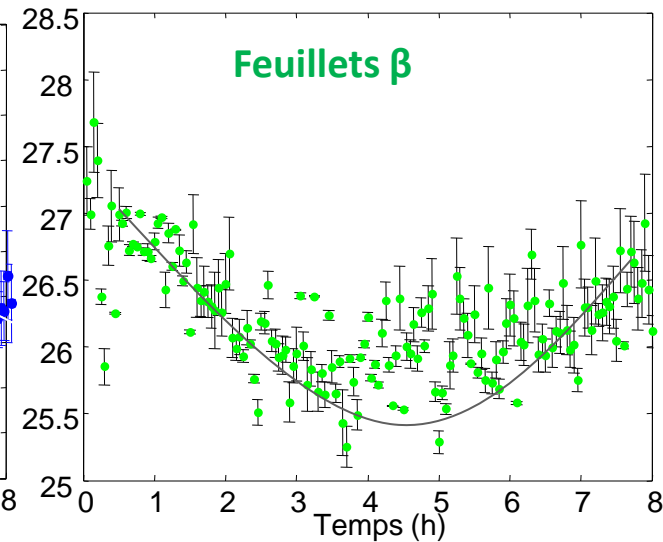


Structures secondaires des protéines

Aire Sous Courbe 1652 (%)

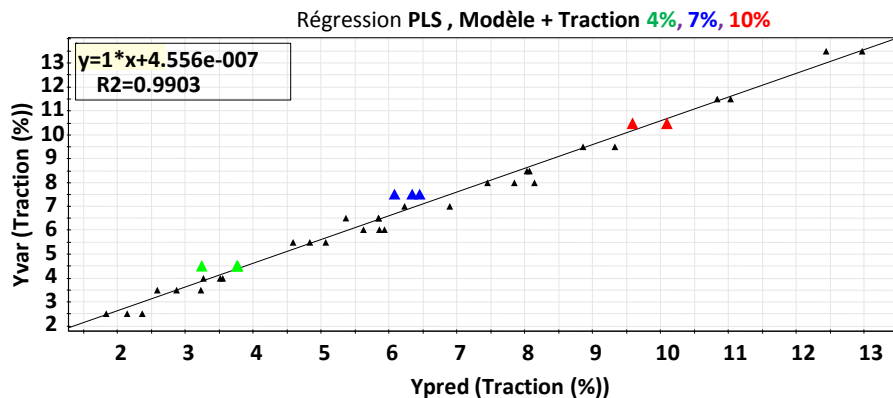


Aire Sous Courbe 1671 (%)



SC mechanical strains

Ex vivo



Analyse statistique multivariée



Pics discriminants



Interprétation structurale

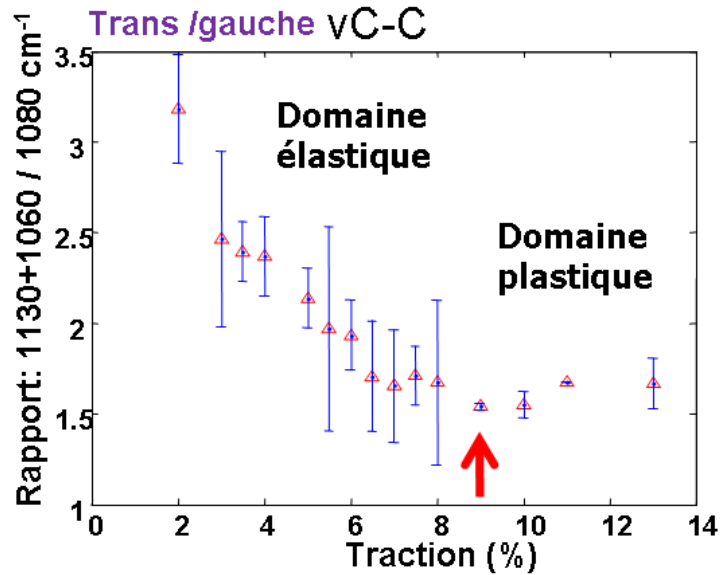


État moléculaire lié
au stress mécanique

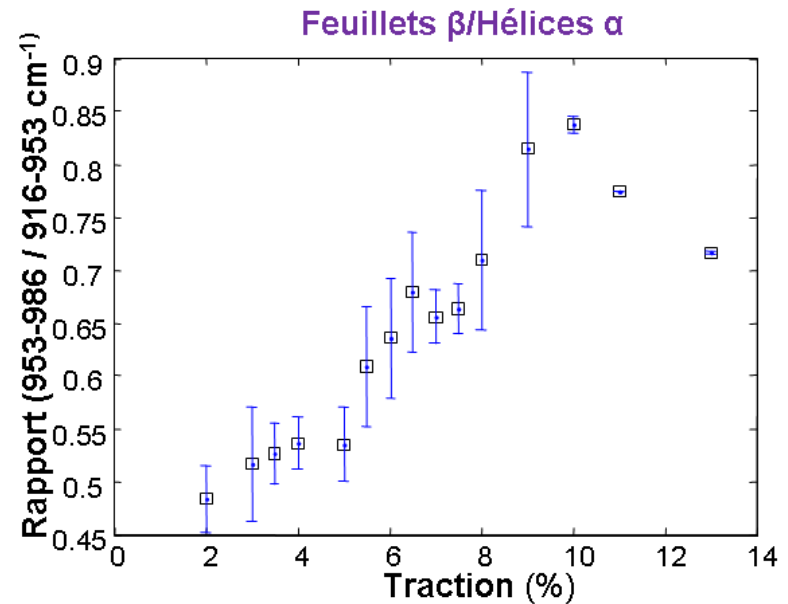


SC mechanical strains

Compacité des lipides



Structure secondaire des protéines



Deux domaines

zone élastique

zone plastique



Physiological status

“QR code” of the skin

Agence Nationale de la Recherche
ANR CARE

In vivo

Analyse multi-paramétrique du SC



Patients

pH	: pH mètre
PIE	: Tewl-mètre
Hydratation globale du SC	: Cornéomètre
Composition lipidique	: Chromatographies
Information moléculaire + profondeur:	Raman

**11 volontaires F sains
âgés de 57 à 62 ans**

**Analyse sur bras et
mollet**

- 1. Identification des relations entre les différents paramètres du Stratum Corneum**
- 2. Développement d'un outil multi-informationnel**

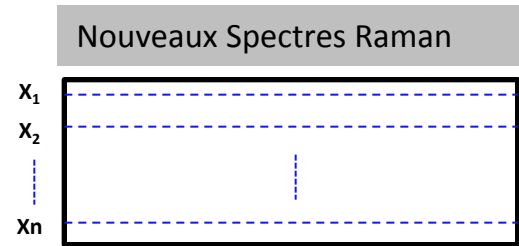
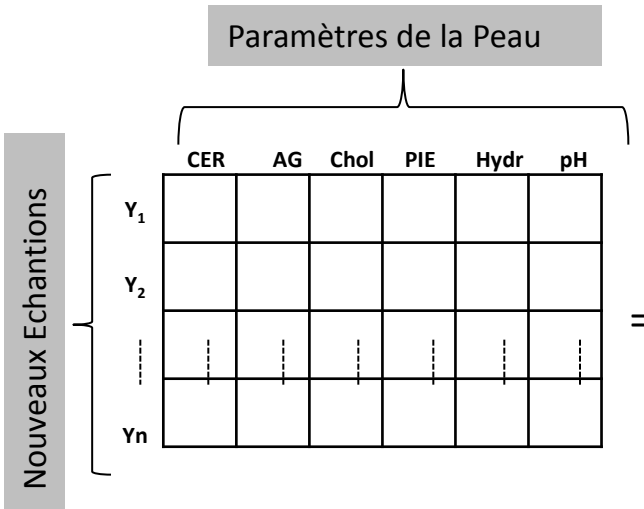


Physiological status

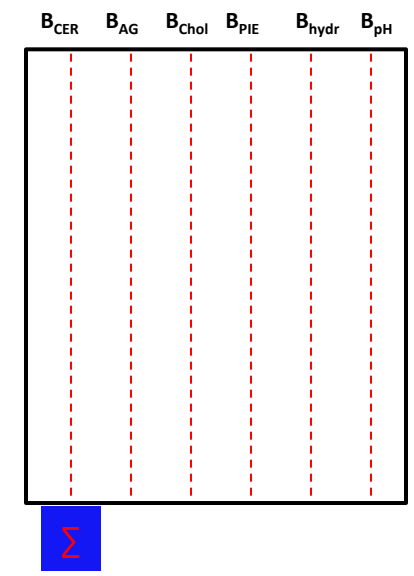
“QR code” of the skin



Modèle de prédiction



Coefficients de Régression (B)



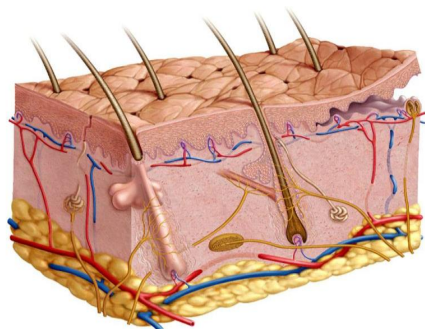
Données centrées-réduites; besoin de:

- X_m : spectre moyen
- X_{std} : écart-type des spectes
- Y_m : moyenne de Y
- Y_{std} : écart-type de Y

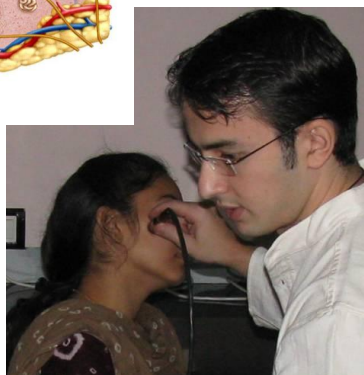


Raman et peau synthétique

Sources de peau



Peau humaine



Restriction

disponibilité

Manque de reproductibilité

Peau animale



Restriction

Interdiction

Peau synthétique



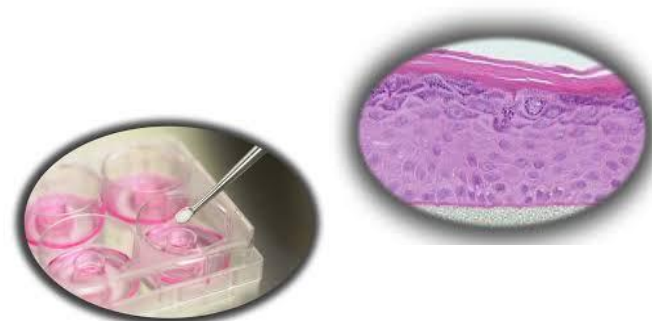
Culture de keratinocytes

Raman et peau synthétique

Evaluation des peaux

Validité en tant que substits

- Morphologie
- marqueurs biomécaniques
- Tests d'irritation
- Tests de phototoxicité
- Composition protéique
- Composition lipidique
- Perméabilité



**Les classes lipidiques majoritaires
sont présentes**

Perméabilité PLUS ÉLEVÉE

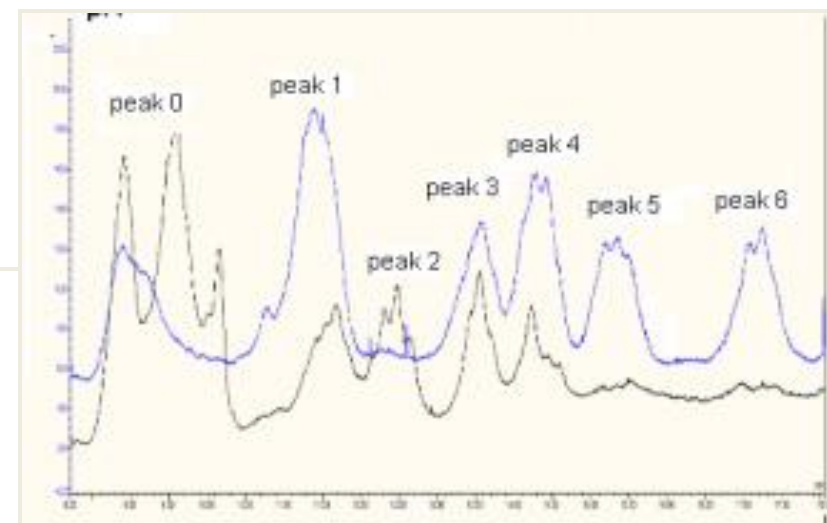
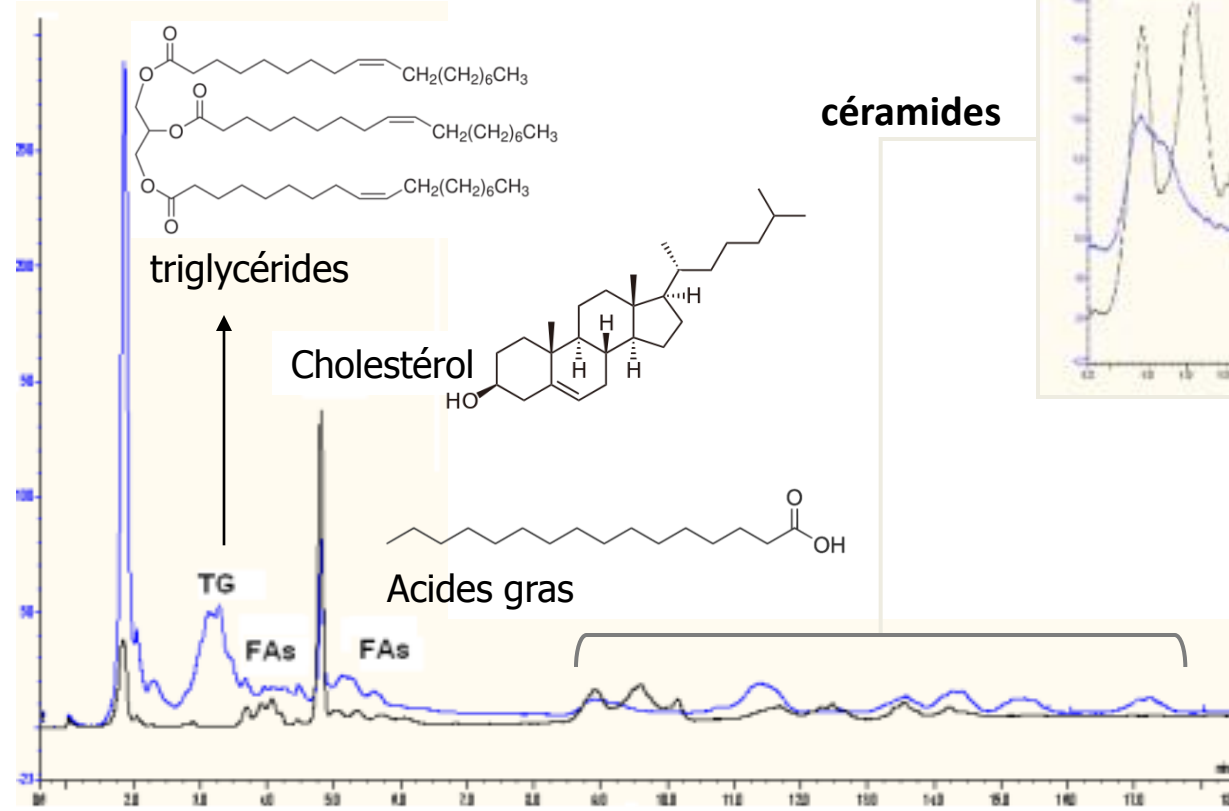
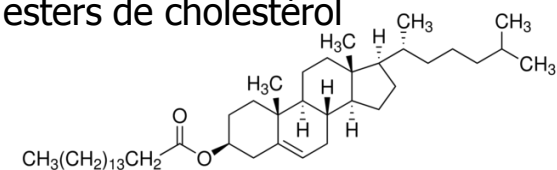
**Comparaison de la composition et de
l'organisation des lipides**

Raman et peau synthétique

Composition des lipides

Composition globale

esters de cholestérol



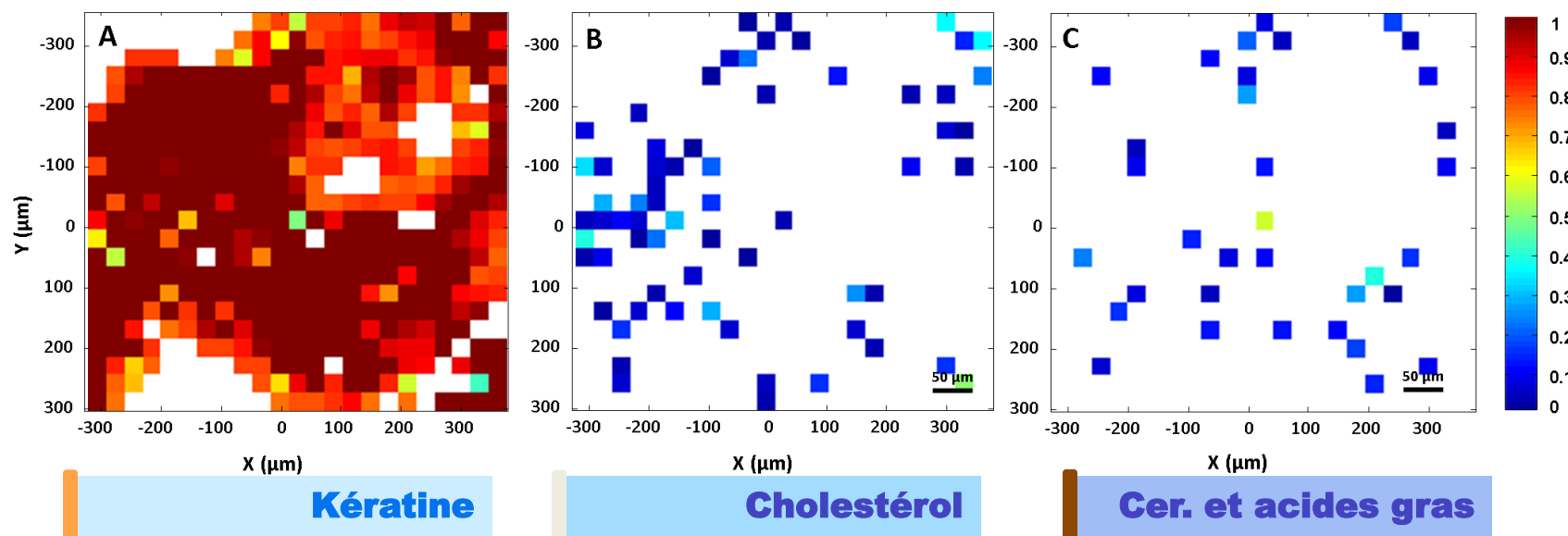
céramides

Peau humaine: bleu
Peau synthétique: noir

Raman et peau synthétique

Imagerie Raman + NCLS

Stratum corneum reconstruit



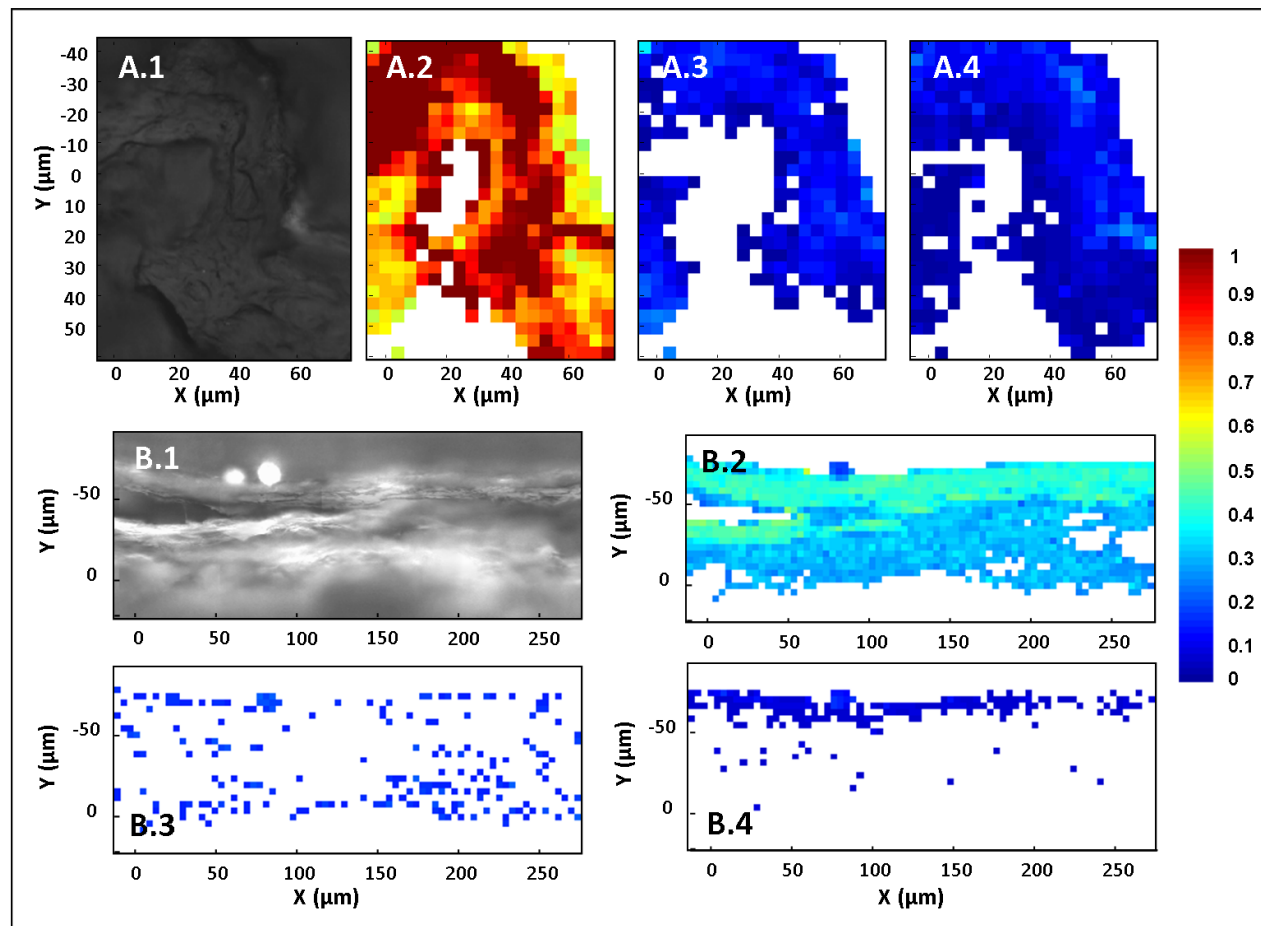
- Taille de l'image: $600 * 600 \mu\text{m}^2$
- Taille du pixel: $4 \mu\text{m}$
- Pas: $20 \mu\text{m}$

Distribution hétérogène des lipides

Raman et peau synthétique

Coupes de SC: imagerie Raman + NCLS

Stratum corneum humain



Stratum corneum synthétique

1. Lumière blanche

2. Kératine

3. Cholestérol

4. Cer. et acides gras



MERCI

DANKSCHEEN
 SPASSIBO
 SNACHALUNYA
 MARRH
 CHILTU
 YAQHANYELAY
 TASHAKKUR ATU
 MADEEJA MATYKA
 YPPAGALATIM
 TINGKI
GRACIAS
THANK
YOU
 SUKSAMA
 EKHMET
 ATTO
 SHUKURIA
 HERASTANBY
 SANGCO
 GOZAIMASHITA
 EFCHARISTO
 AGUYJK
 FAKAAIK
 KOMAPSUNNIDA
 LAI
 MAAKE
 GRAZIE
 MEHRBANI
 PALDIES
 BOLZIN
 MERCY
 BIYAN
 SHUKRIA
 GO RAIBH
 MAITH AGAT
 URAKOZE

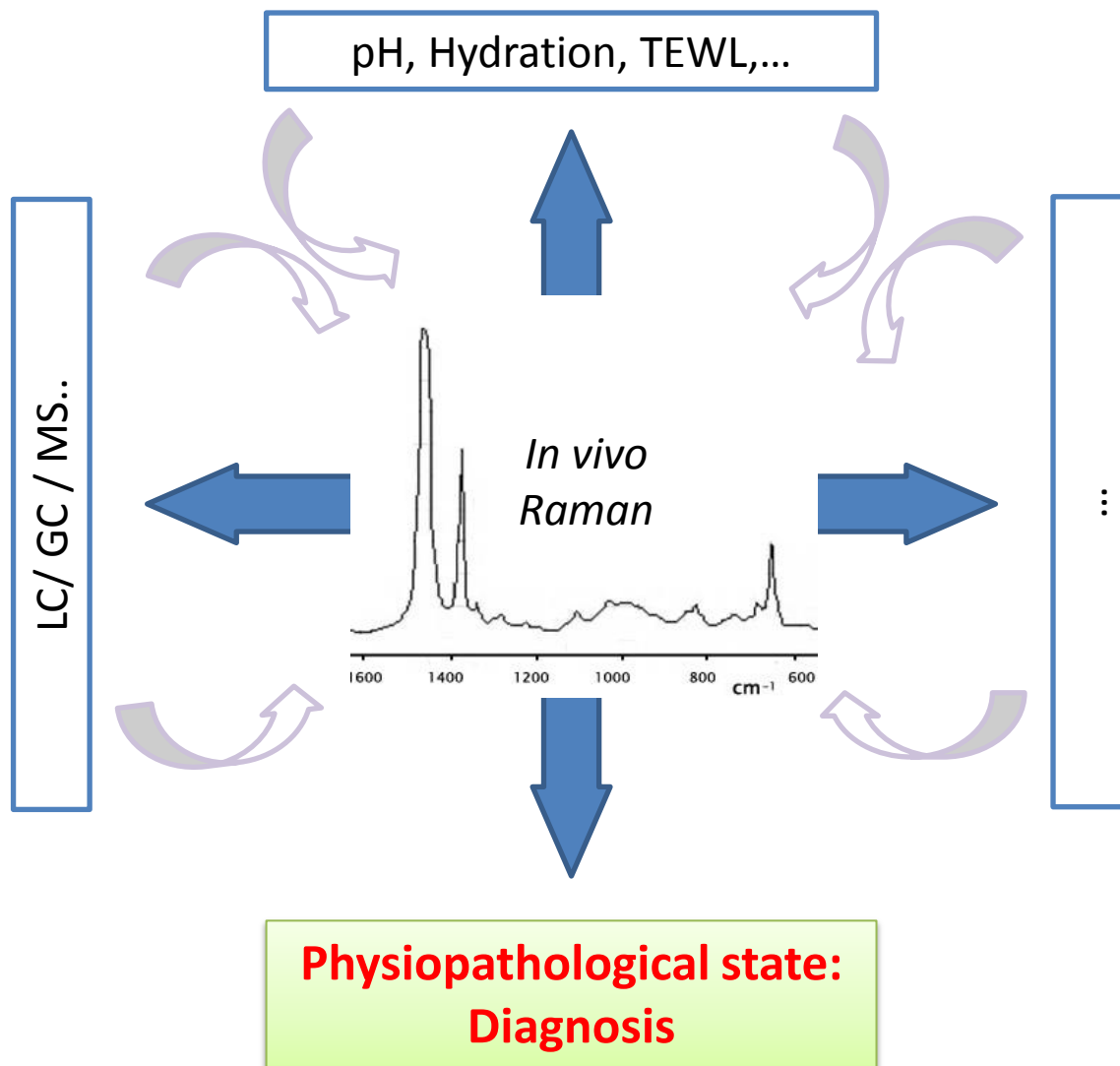
شكرا



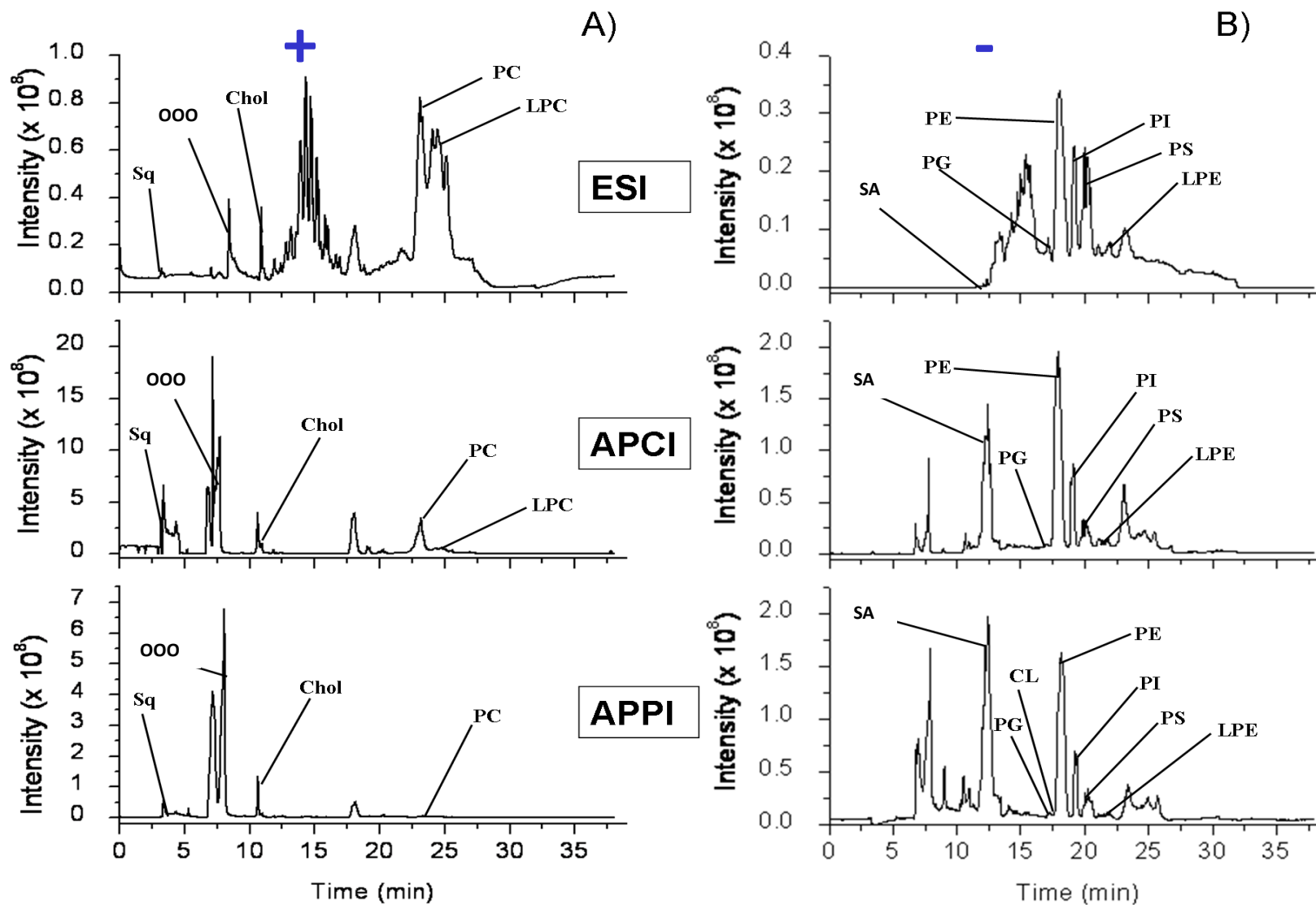
Analytical chemistry: from data (pre)-treatment optimization to data mining, data fusion and big data

Sana et Ali Tfai(y)li

Raman analyses: correlation with LC/GC/MS.., biometric data



LC-MS acquisitions: Different ionization modes (Data fusion?)



Data fusion and data mining

Perspectives:

Data fusion between:

- RPLC and NPLC in chromatography
- Different ionization modes in mass spectrometry
- Increase the separation dimensionality LCxLC MS... (new treatment approach)
- Between Separation techniques, coupled mass spectrometry
- Between several techniques: Raman, IR, separative techniques
- Multi-block analysis (specific algorithms for data processing and fusion)?

Additional analysis will increase the time for data processing: other approaches for data processing ?

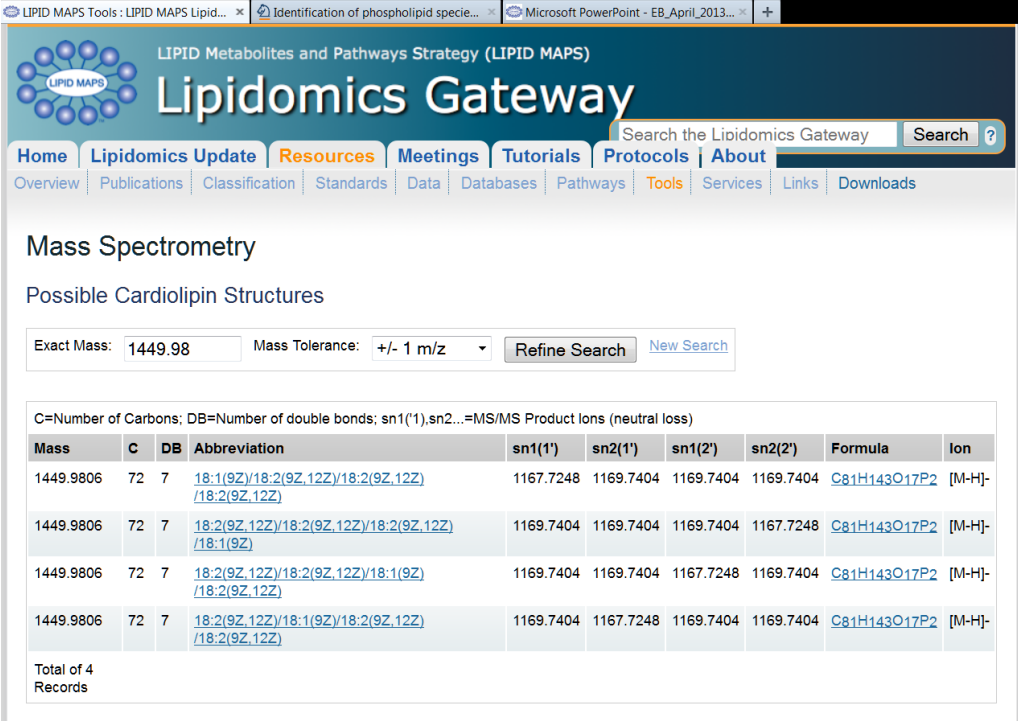
**Virtual data project (LAL): work on a cloud and save the image
Buy cores (possible demand through a project in process)**

Data storage

Perspectives:

DATA ARE NOT CENTRALIZED.

- centralize data
- Data storage and management
- Results storage and management
- Generate our own databases



The screenshot shows the Lipidomics Gateway website interface. The header includes the site logo and navigation tabs: Home, Lipidomics Update, Resources, Meetings, Tutorials, Protocols, and About. A search bar is present with the text "Search the Lipidomics Gateway". Below the header, there are sub-navigation tabs: Overview, Publications, Classification, Standards, Data, Databases, Pathways, Tools, Services, Links, and Downloads. The main content area is titled "Mass Spectrometry" and "Possible Cardiolipin Structures". It features a search form with "Exact Mass: 1449.98" and "Mass Tolerance: +/- 1 m/z". Below the search form is a table of results.

C=Number of Carbons; DB=Number of double bonds; sn1('),sn2...=MS/MS Product Ions (neutral loss)

Mass	C	DB	Abbreviation	sn1(')	sn2(')	sn1(2')	sn2(2')	Formula	Ion
1449.9806	72	7	18:1(9Z)/18:2(9Z,12Z)/18:2(9Z,12Z)/18:2(9Z,12Z)	1167.7248	1169.7404	1169.7404	1169.7404	C81H143O17P2	[M-H] ⁻
1449.9806	72	7	18:2(9Z,12Z)/18:2(9Z,12Z)/18:2(9Z,12Z)/18:1(9Z)	1169.7404	1169.7404	1169.7404	1167.7248	C81H143O17P2	[M-H] ⁻
1449.9806	72	7	18:2(9Z,12Z)/18:2(9Z,12Z)/18:1(9Z)/18:2(9Z,12Z)	1169.7404	1169.7404	1167.7248	1169.7404	C81H143O17P2	[M-H] ⁻
1449.9806	72	7	18:2(9Z,12Z)/18:1(9Z)/18:2(9Z,12Z)/18:2(9Z,12Z)	1169.7404	1167.7248	1169.7404	1169.7404	C81H143O17P2	[M-H] ⁻

Total of 4 Records