Freie Universität Berlin

Computational Methods for High-Throughput Omics Data

General stuff …

- 1 proteomics OR 1 genomics paper
- Questionaire for audience
  - 5 to 10 questions for each talk
- Short summary [2-3 pages]

- Feedback sheet

- Camera [optional]

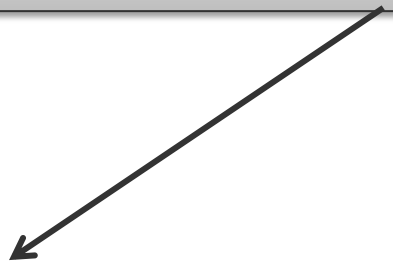
Grading & Attendance

- >= 80% (of 13)

- Final grade: average of talk & short summary

Proteomics

„Proteomics is defined as the study of the ensemble of proteins at a given point in time, especially their expression pattern, structure and function."



Quantitation

Identification

Proteomics

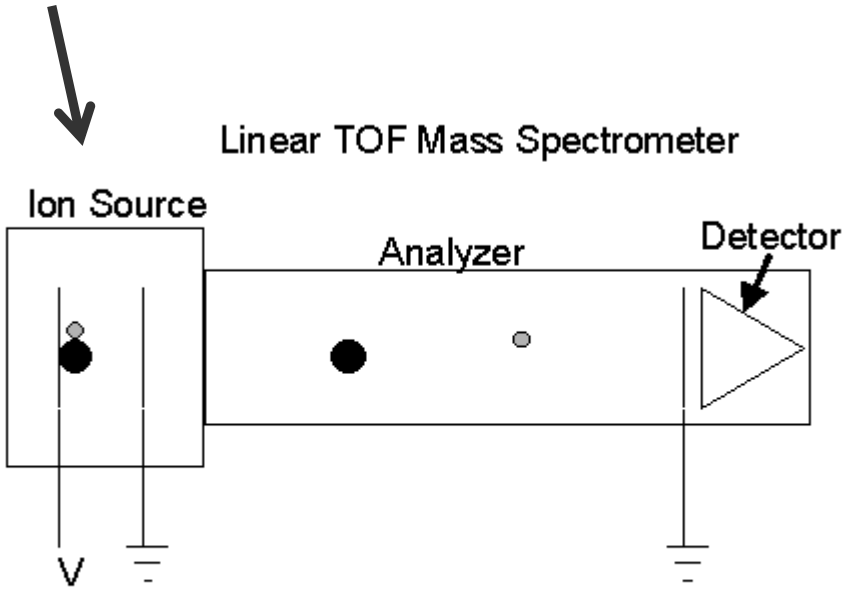
Identification & Quantitation methods:

- 2-D electrophoresis (isoelectric point + mass(SDS-PAGE)) + WesternBlot | Staining
- ELISA
- Liquid Chromatography (LC) (i.e., HPLC | CE)
- **Mass Spectrometry (MS)**

Basics

Basics

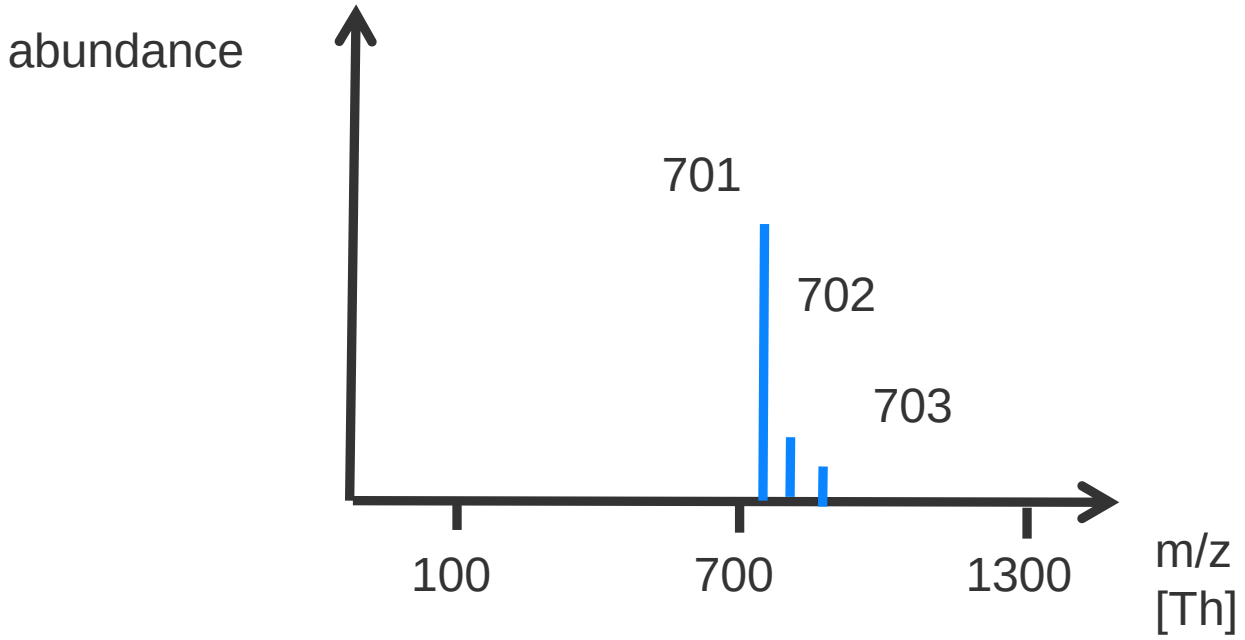
Protonation (H+)



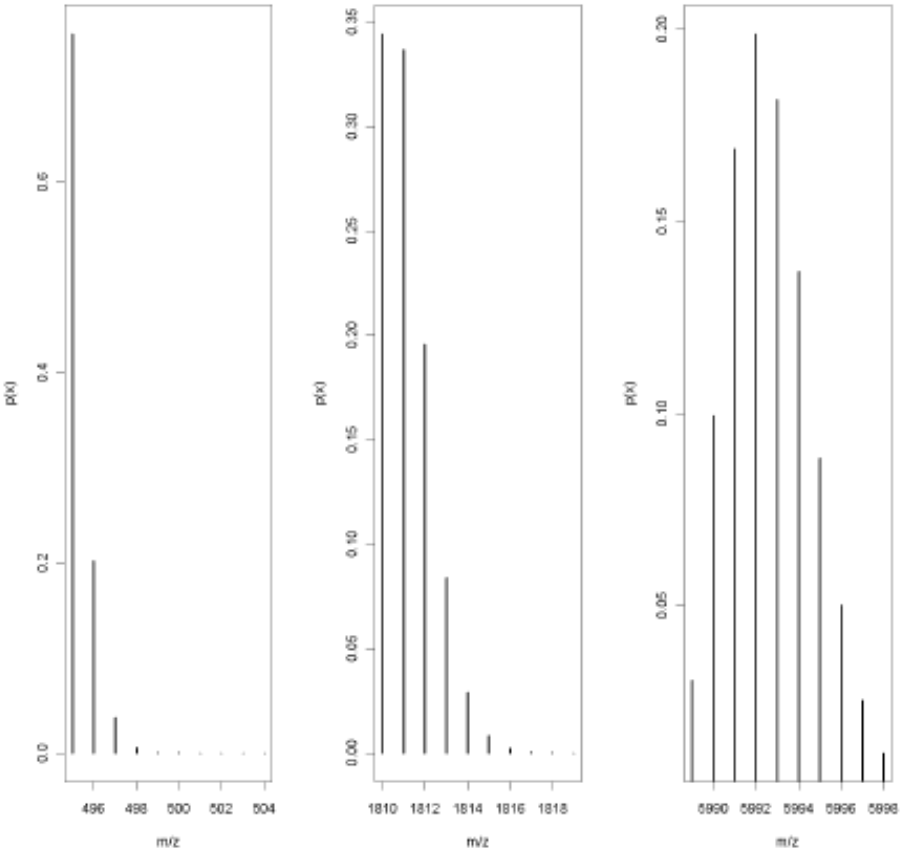
Basics

mass(„DPFINA“) = 700 Da = 700 u
charge = 1

SumFormula: $C_{31}H_{45}N_7O_{10}$
Isotopes: ^{12}C and ^{13}C



Basics

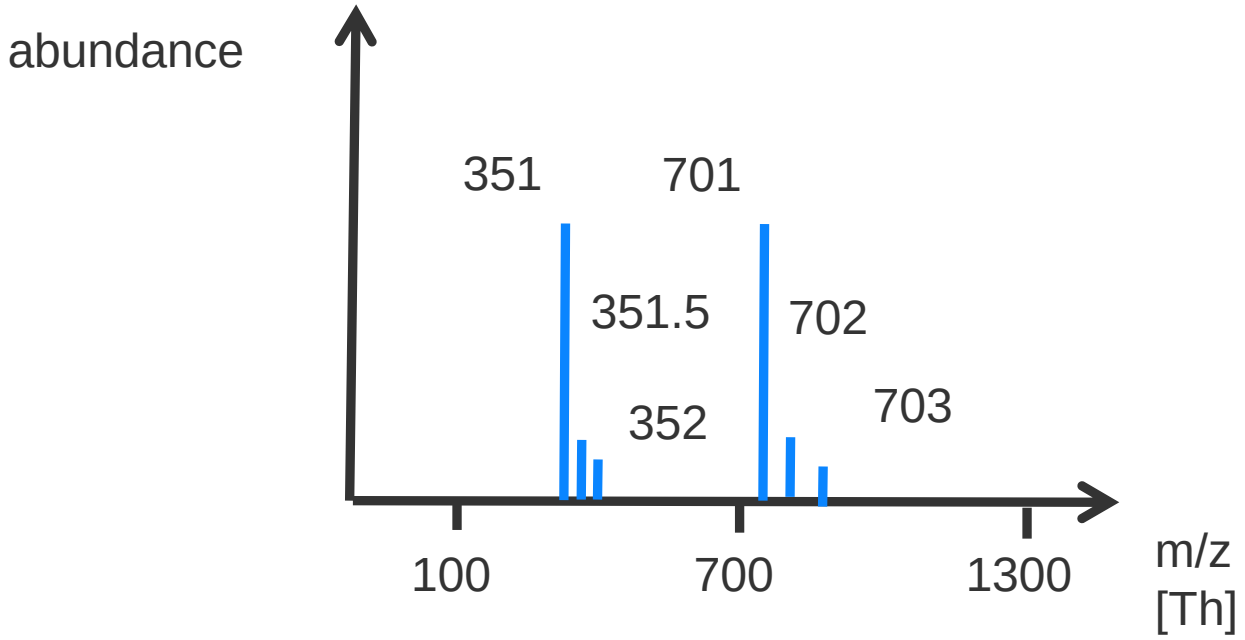


Mass (Da)	500	1800	6000

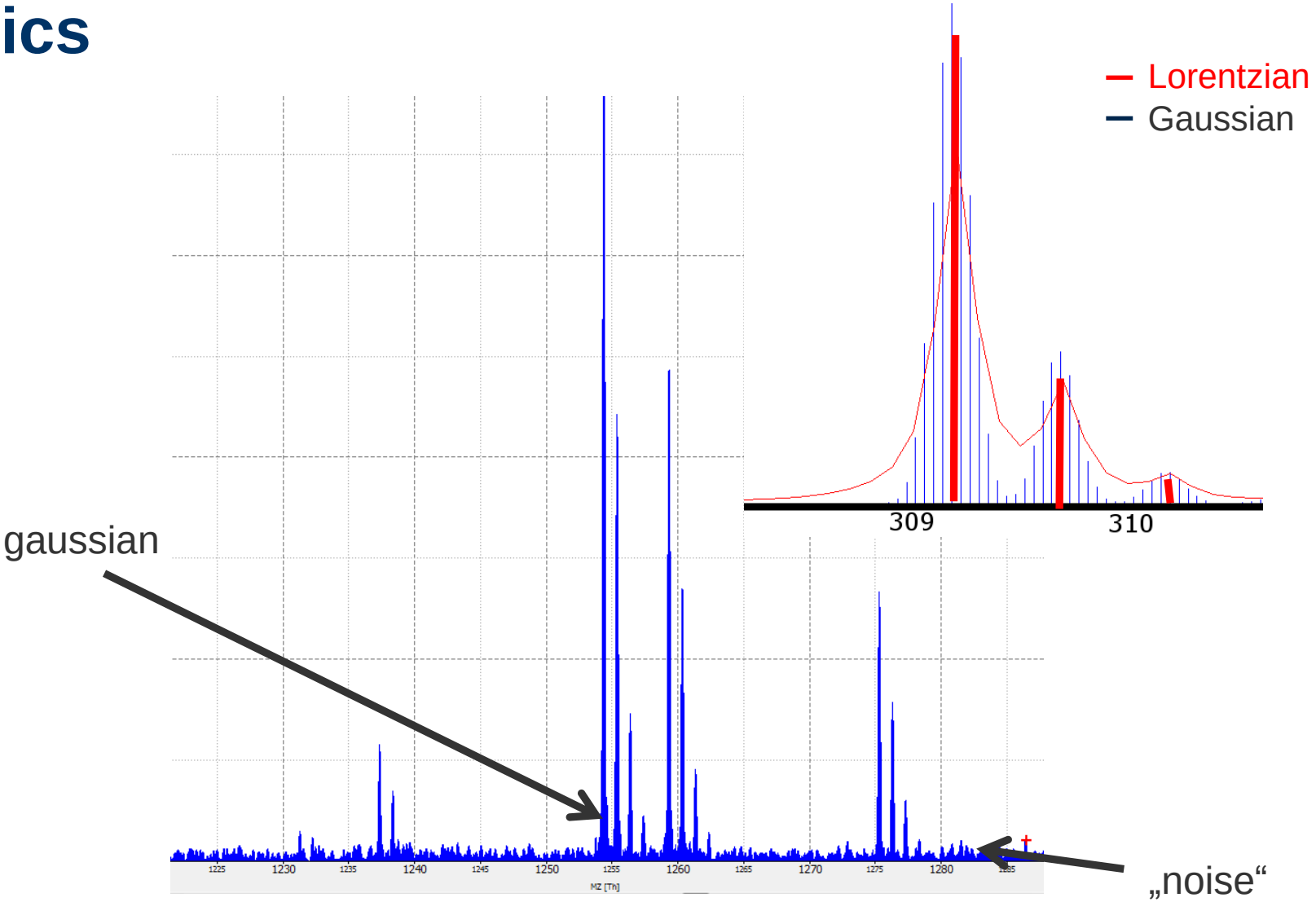
Basics

mass(„DPFINA“) = 700 Da = 700 u
charge = 2

SumFormula: $C_{31}H_{45}N_7O_{10}$
Isotopes: ^{12}C and ^{13}C



Basics


Lorentzian
Gaussian
309
310
gaussian
„noise“
1225
1230
1235
1240
1245
1250
1255
1260
1265
1270
1275
1280
m/z [Th]

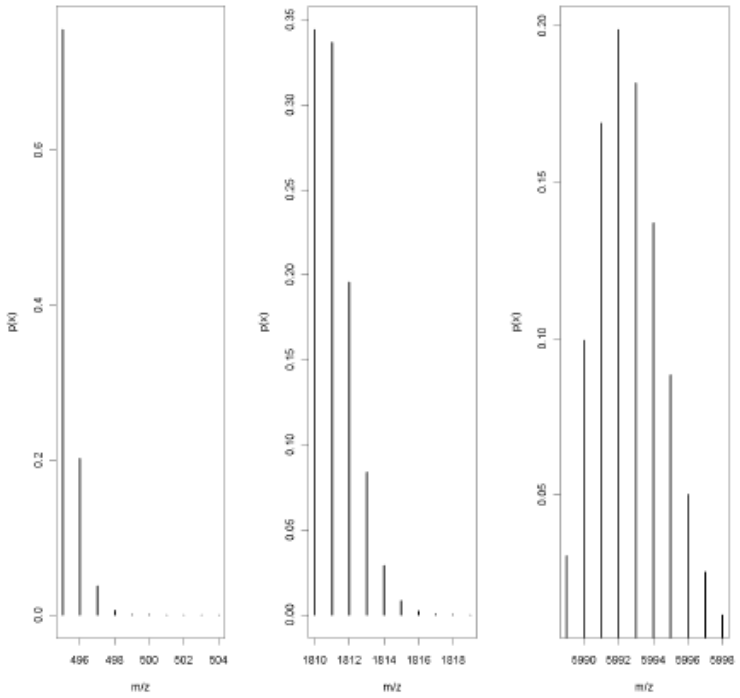
Talk: Isotope Distribution

Calculation of isotope distributions in mass spectrometry.
A trivial solution for a non-trivial problem

Hugo Kubinyi

Hauptlaboratorium, BASF AG, D-6700 Ludwigshafen (Germany)

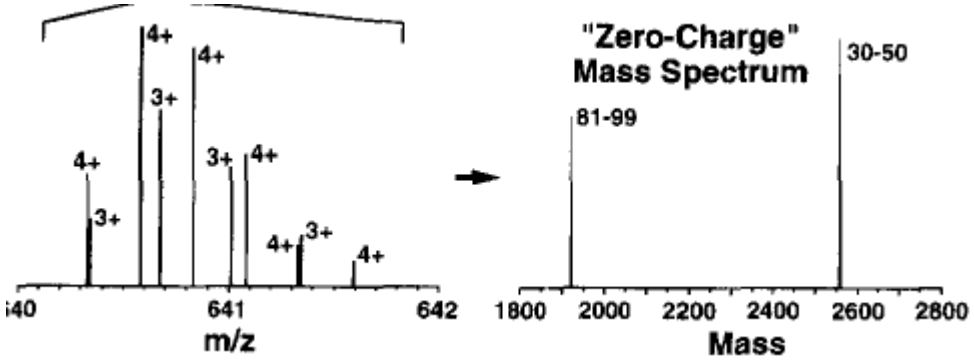
(Received 26th September 1990)



Talk: Decharging

A Universal Algorithm for Fast and Automated Charge State Deconvolution of Electrospray Mass-to-Charge Ratio Spectra

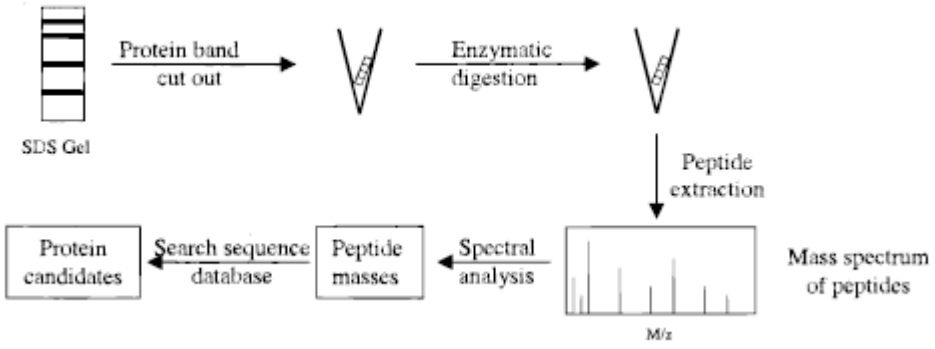
Zhongqi Zhang and Alan G. Marshall*
Center for Interdisciplinary Magnetic Resonance, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida, USA



Talk: Identification [PMF]

ProFound: An Expert System for Protein Identification Using Mass Spectrometric Peptide Mapping Information

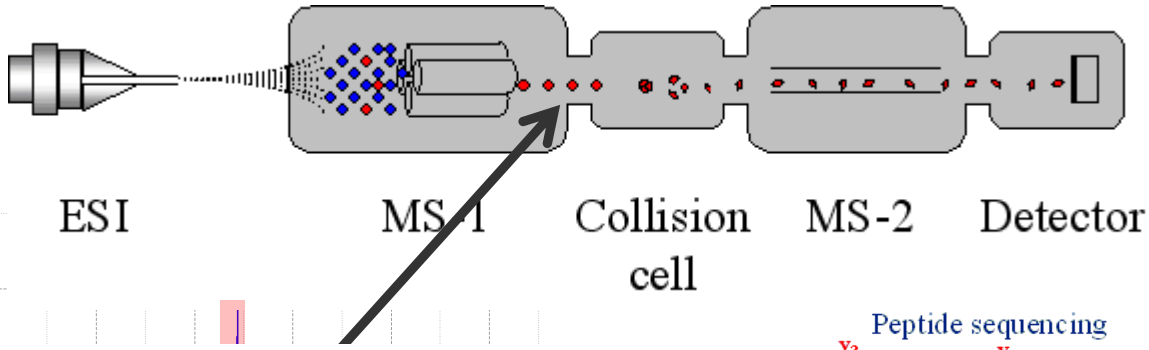
Wenzhu Zhang* and Brian T. Chait*

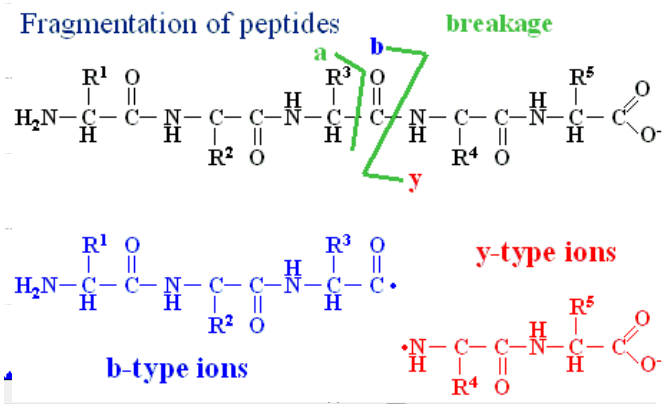


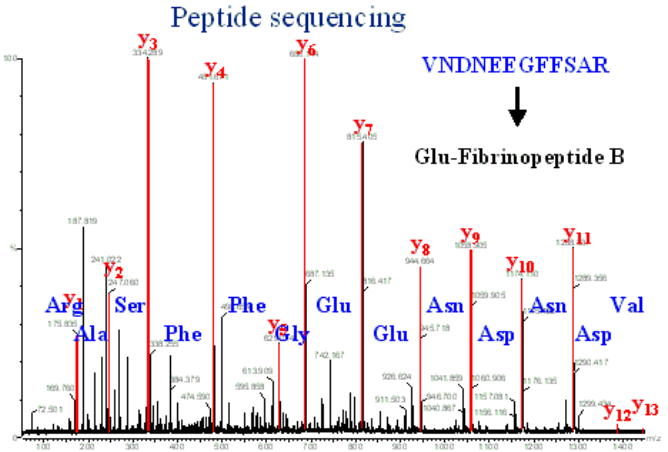
Talk: Identification

InsPecT: Identification of Posttranslationally Modified Peptides from Tandem Mass Spectra

Stephen Tanner,*,† Hongjun Shu,‡ Ari Frank,§ Ling-Chi Wang,|| Ebrahim Zandi,|| Marc Mumby,‡ Pavel A. Pevzner,§ and Vineet Bafna§

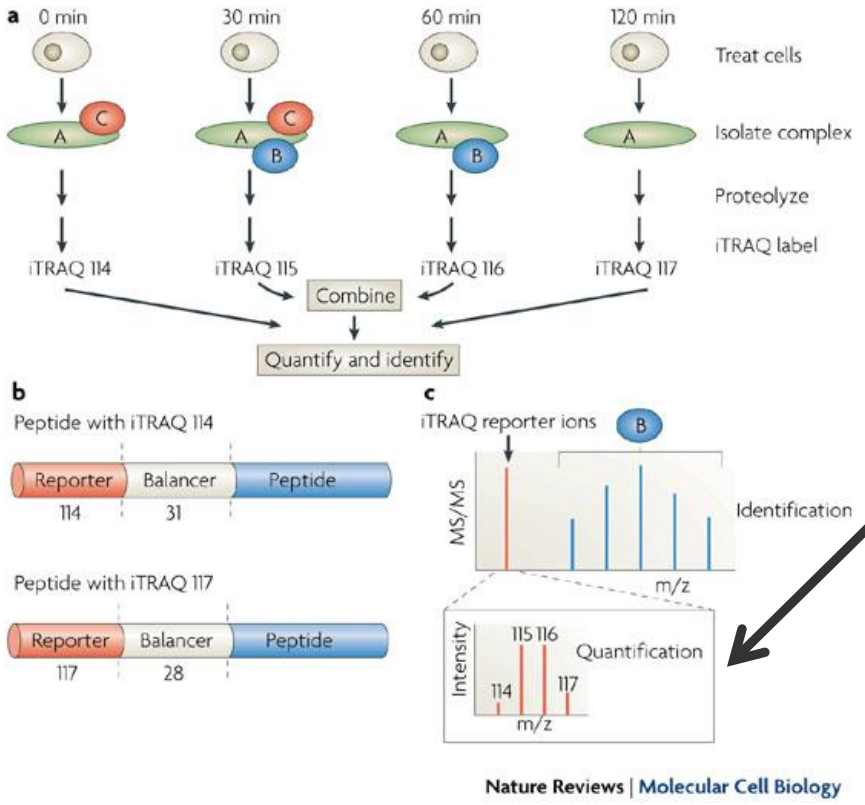






Talk: Multiplexing using iTRAQ

Isobaric tag for relative and absolute quantitation

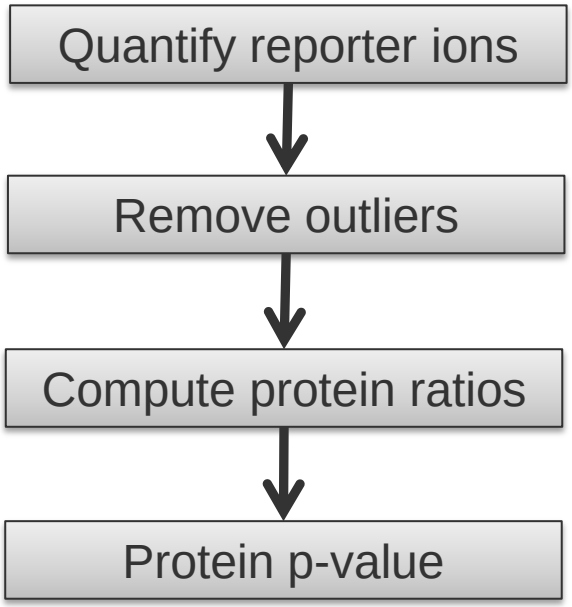


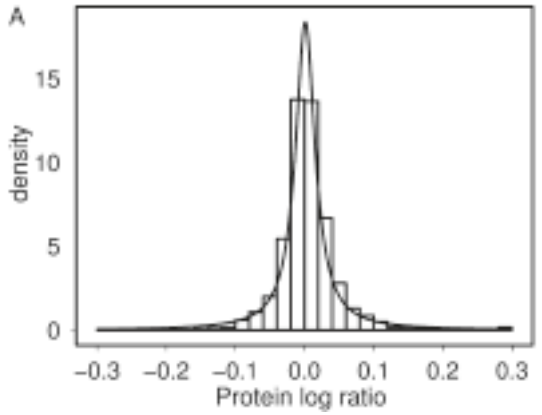
Peptides!

Talk: Multiplexing using iTRAQ

General Statistical Modeling of Data from Protein Relative Expression Isobaric Tags

Florian P. Breitwieser,[†] André Müller,[†] Loïc Dayon,[‡] Thomas Köcher,[¶] Alexandre Hainard,[‡] Peter Pichler,[§] Ursula Schmidt-Erfurth,[||] Giulio Superti-Furga,[†] Jean-Charles Sanchez,[‡] Karl Mechtler,[¶] Keiryn L. Bennett,[†] and Jacques Colinge*[,†]





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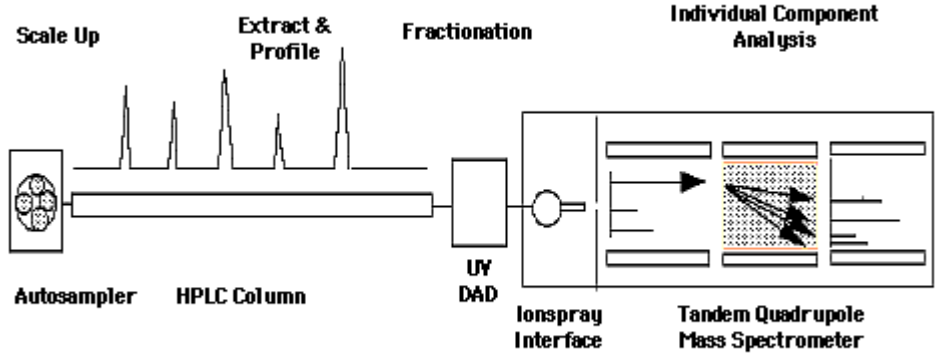

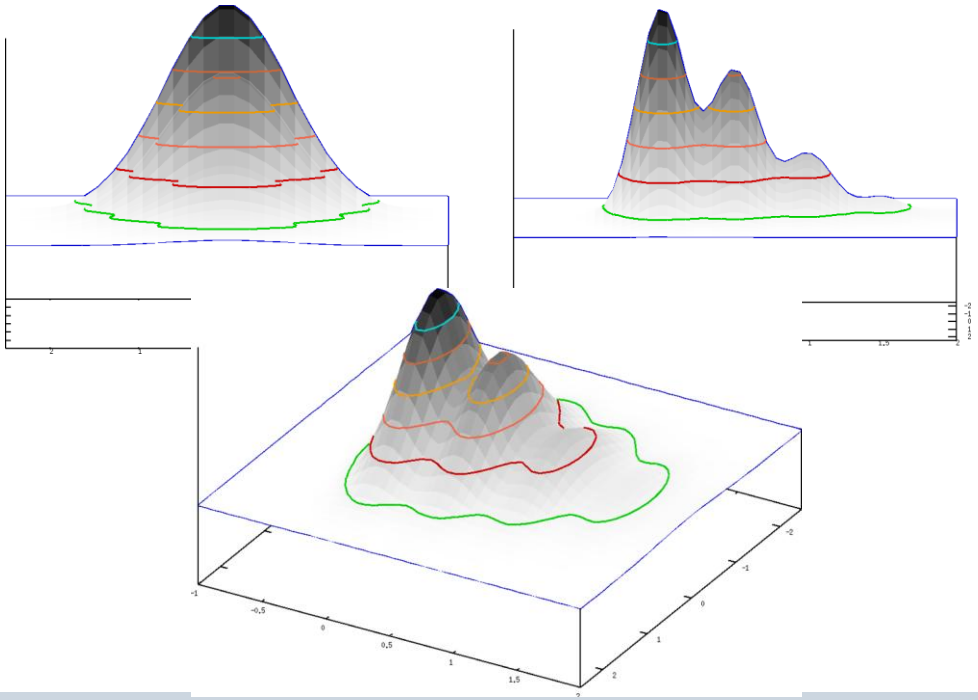

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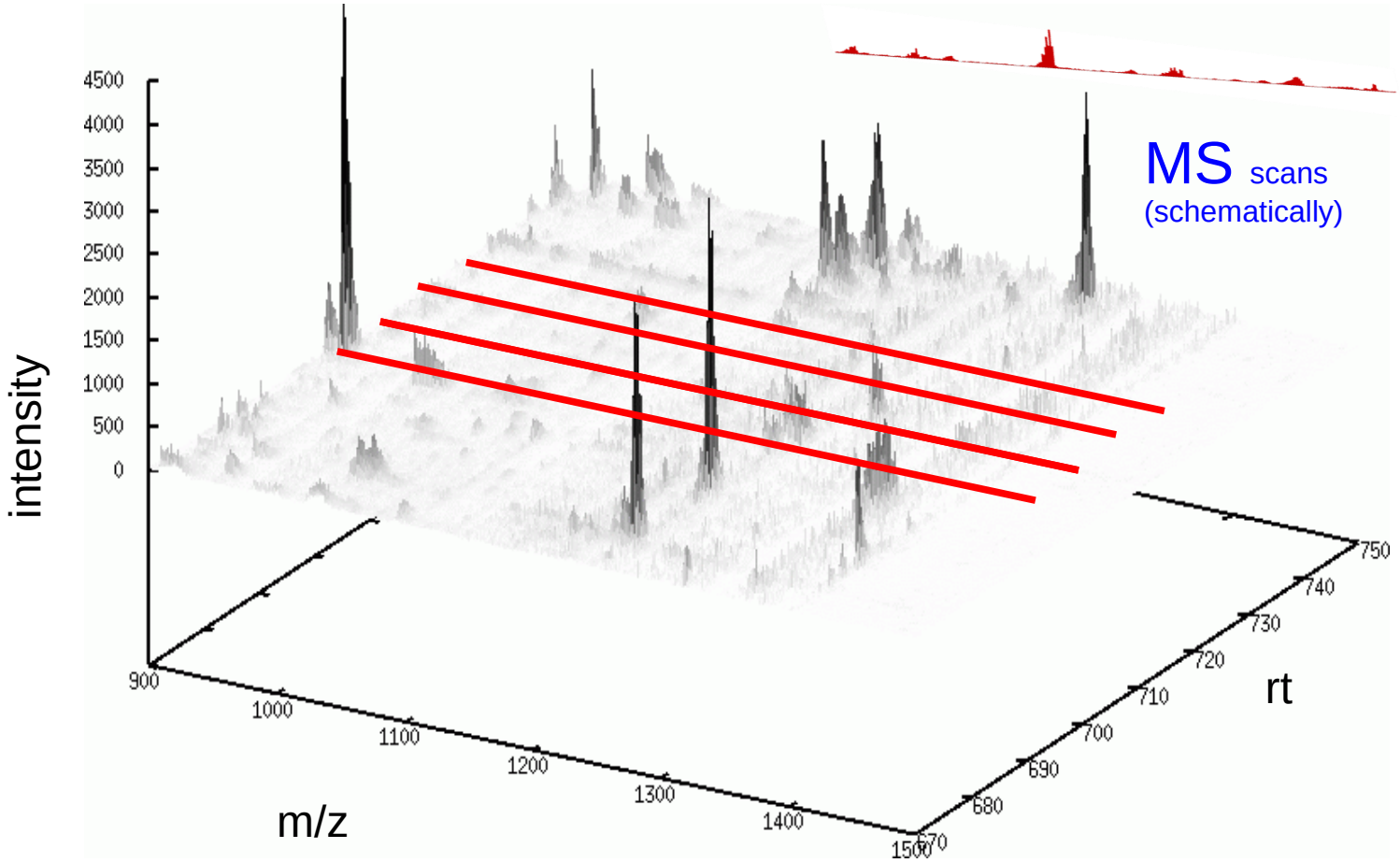
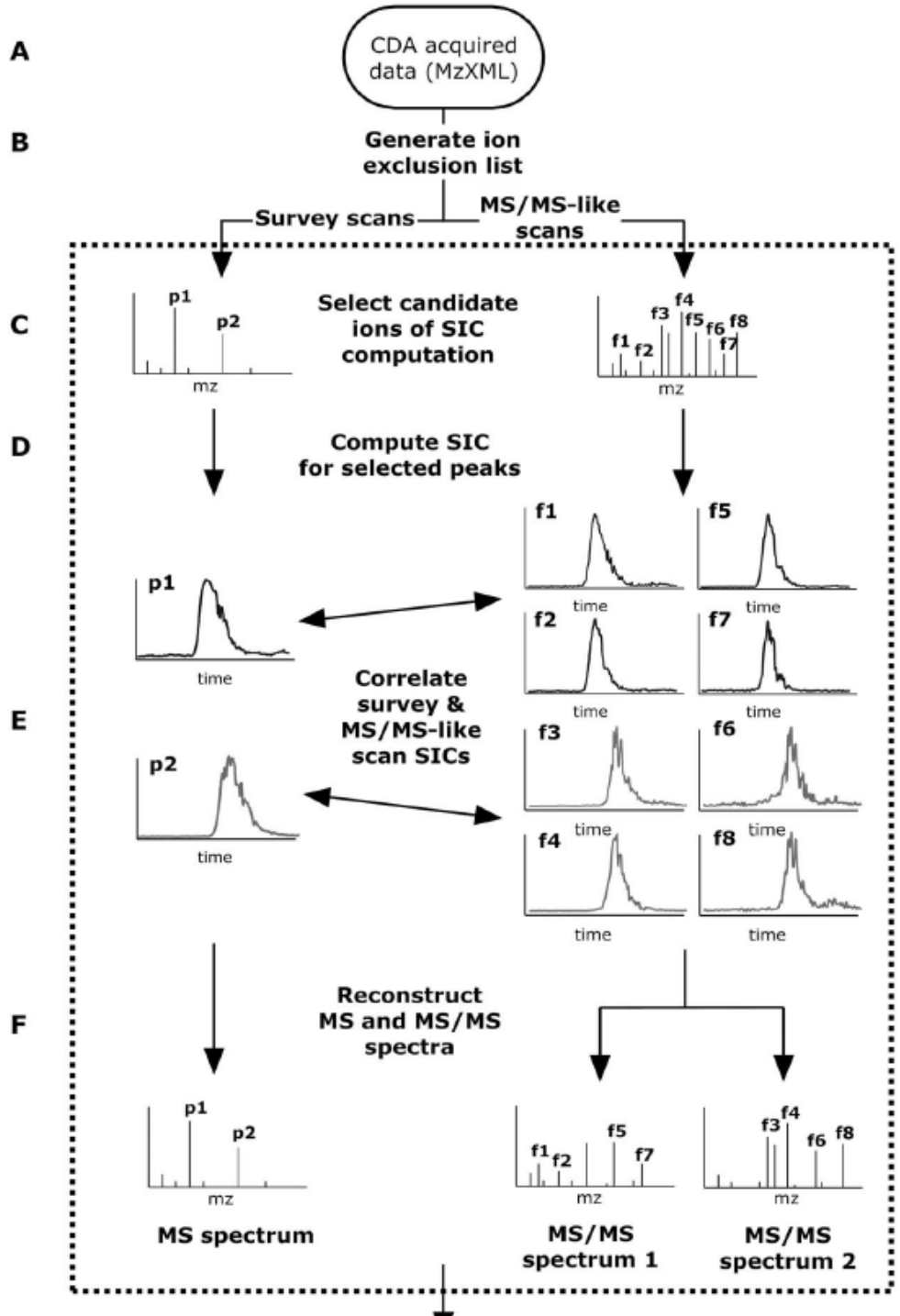
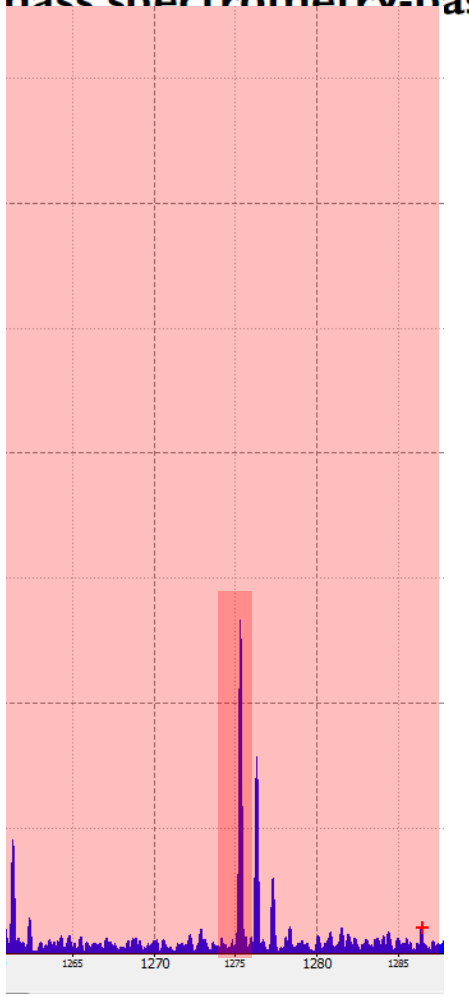




ıtion time ion sequencing
pass spectrometry-based



Talk: Experimental Design

Statistical Design of Quantitative Mass Spectrometry-Based Proteomic Experiments

Ann L. Oberg[†] and Olga Vitek[*,‡]

(a) Balanced Incomplete Block

Disease group	Replicate set 1 Block 1	Block 2	Block 3	Block 4	Block 5	Block 6	Block 7	Block 8	Block 9	Block 10	...
D_1	X_{L_1}	X_{L_2}	X_{L_1}	X_{L_2}							...
D_2	X_{L_2}				X_{L_1}	X_{L_2}	X_{L_1}				...
D_3		X_{L_1}			X_{L_2}			X_{L_1}	X_{L_2}		...
D_4			X_{L_2}			X_{L_1}		X_{L_2}		X_{L_1}	...
D_5				X_{L_1}			X_{L_2}		X_{L_1}	X_{L_2}	...

(b) Reference

Disease group	Replicate set 1 Block 1	Block 2	Block 3	Block 4	Block 5	...
R	R_{L_1}	R_{L_1}	R_{L_1}	R_{L_1}	R_{L_1}	...
D_1	X_{L_2}					...
D_2		X_{L_2}				...
D_3			X_{L_2}			...
D_4				X_{L_2}		...
D_5					X_{L_2}	...

(c) Loop

Disease group	Replicate set 1 Block 1	Block 2	Block 3	Block 4	Block 5	..
D_1	X_{L_1}				X_{L_2}	..
D_2	X_{L_2}	X_{L_1}				..
D_3		X_{L_2}	X_{L_1}			..
D_4			X_{L_2}	X_{L_1}		..
D_5				X_{L_2}	X_{L_1}	..