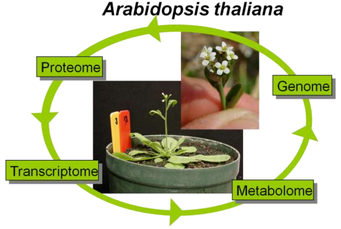
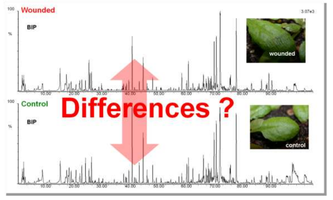
Metabolomics

The research and results presented in this poster are courtesy of Prof. J.-L. Wolfender, School of Pharmaceutical Sciences, University of Geneva, Switzerland

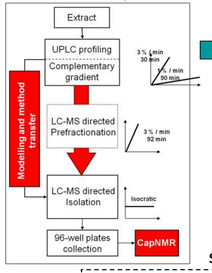


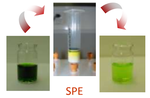


500 mg (analytical)
500 g (semi-prep)

500 µL (analytical)
1 L (semi-prep)

Multiple step MS-triggered micro isolation strategy for CapNMR





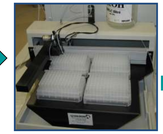
5 µL inj

500 mg inj

19x150mm 5µm

100 µL inj

44-well plates (pass 1)
8 mL, 1 min



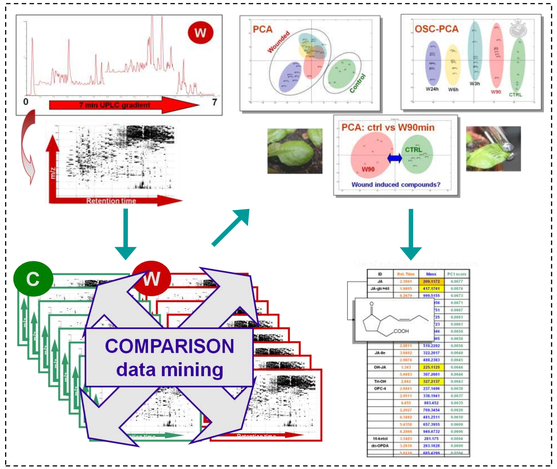
96-well plates (pass 2)
1 mL, 30 sec

10x250mm, 5µm 10x250mm, 5µm

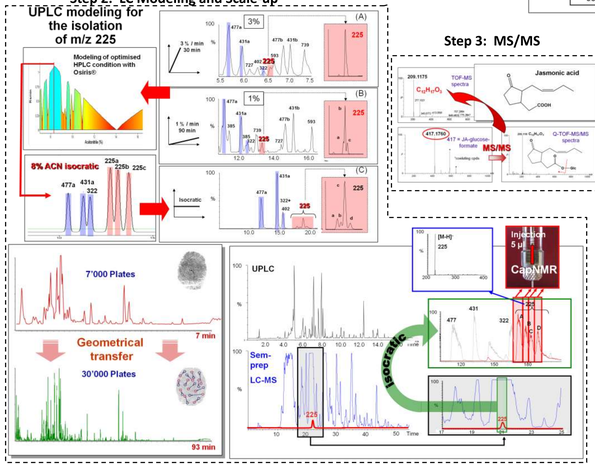
10s of ug

N_2 Dry

Step 1: Rapid UPLC Gradient + PCA

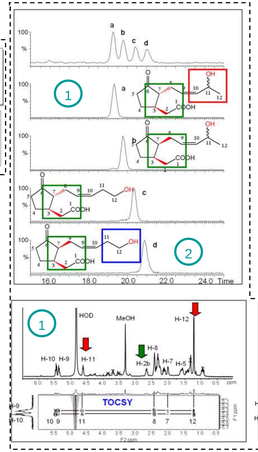


Step 2: LC Modeling and Scale-up

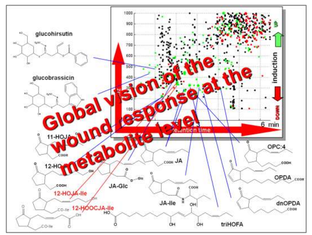


Step 3: MS/MS

Step 4: NMR



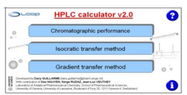
Ultimate Goal



Separation/ Purification	1	**Retsch Mixer Mill** MM200 **Waters UPLC-TOF-MS (Analytical)** Acquity BEH C18 150x2.1 **Varian HPLC-ESI-MS (Semi-prep)** Varian 9012 pump Xterra C18 150x19mm and Xbridge BEH C18 250x10
High Sensitivity Detection	2	**Micromass TOF MS (Analytical)** Model LCT orthogonal acc. reflectron TOF-MS **Thermo-Finnigan MS (Semi-prep)** TSQ-7000 Triple Quad MS Finnigan ESI Interface
Fraction Collection	3	**Gilson Fraction Collector** FC-204 **Ratiolab Wellplates** 44-well and 96-well formats
Sample Preparation	4	**Waters SPE** Sep-Pak Vac 1mL C18 **Nitrogen Drydown**
NMR	5	**Varian NMR** 500MHz Unity Inova **Protasis CapNMR** 5 uL g-ICG probe Manual Injection Module

Reporting 6

LC Modeling SW
Datalys Osiris
University of Geneva HPLC SW
Calc. Version 2.0, David Guillarme
Statistical Analysis Software



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