evropský sociální fond v ČR

EVROPSKÁ UNIE

MINISTERSTVO ŠKOLSTVÍ, MLÁDEŽE A TĚLOVÝCHOVY

OP Vzdělávání pro konkurenceschopnost

INVESTICE DO ROZVOJE VZDĚLÁVÁNÍ

Global Ecology Unit
CREAF-CSIC-CEAB
SeRMN

CREAF

SeRMN

DROUGHT STRESS: APPLICATION OF METABOLOMIC APPROACH

Albert Gargallo Garriga

Tato akce se koná v rámci projektu:
Vybudování vědeckého týmu environmentální metabolomiky a ekofyziologie a jeho zapojení do mezinárodních sítí (ENVIMET; r.č. **CZ.1.07/2.3.00/20.0246**) realizovaného v rámci Operačního programu Vzdělávání pro konkurenceschopnost.

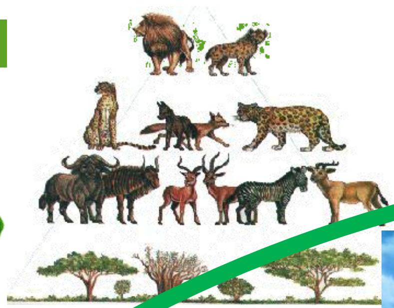
UAB
Universitat Autònoma de Barcelona

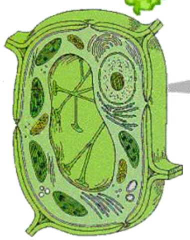
Brno, Czech Globe May 2014

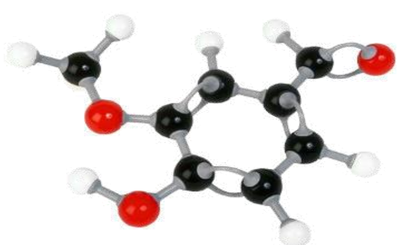
Ecometabolomics

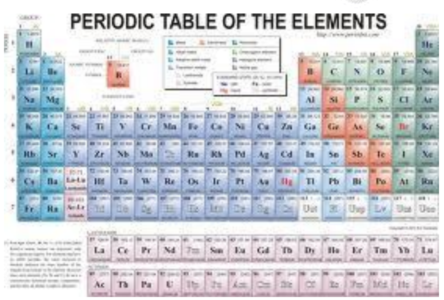
- Current cooperation and future challanges of cooperation between CREAF and CzechGlobe
- different methodological approaches
  - NMR x HPLC-MSn
- comparative ecological and ecophysiological studies
  - climatic and geographical gradients

Introduction



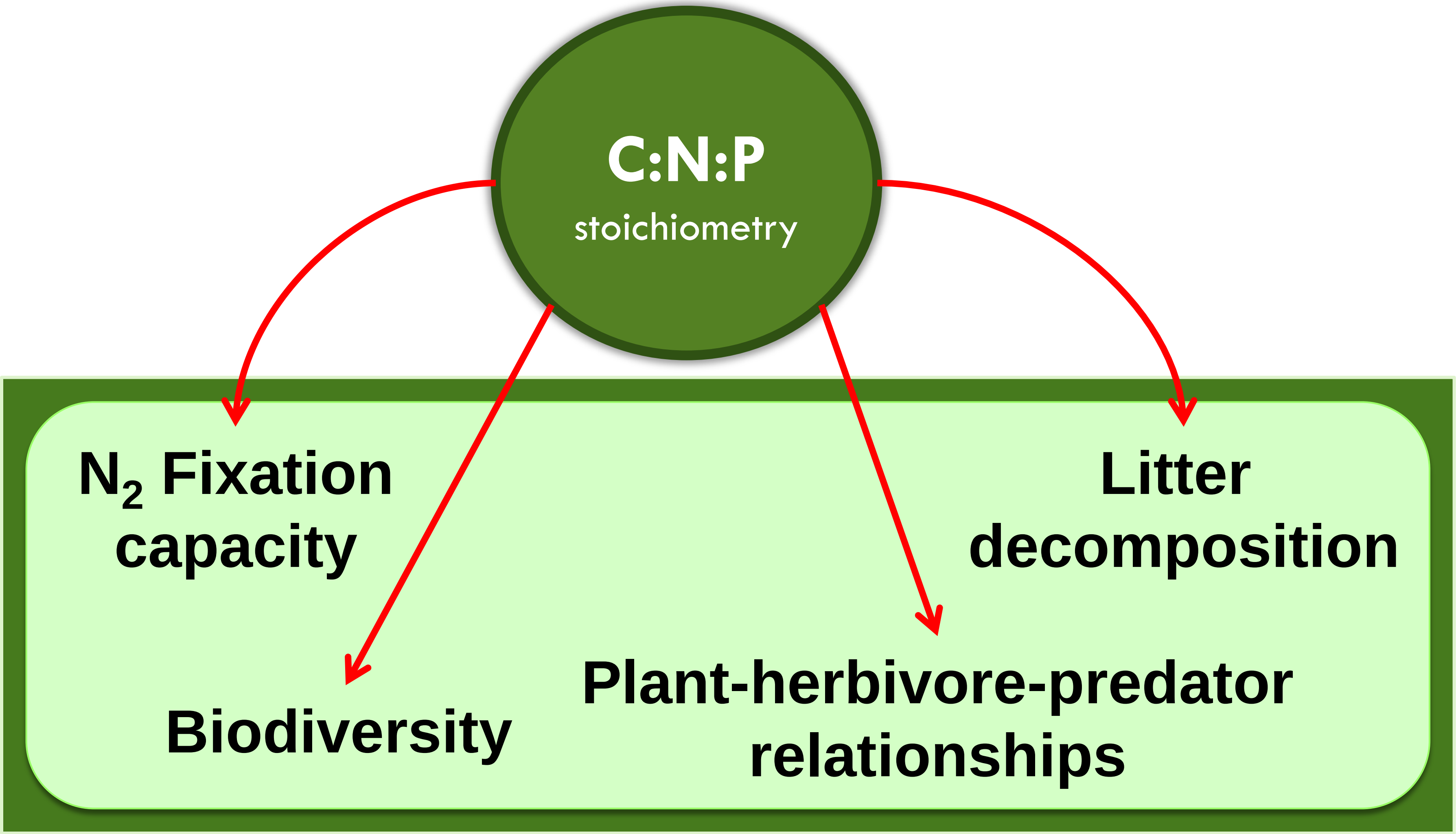






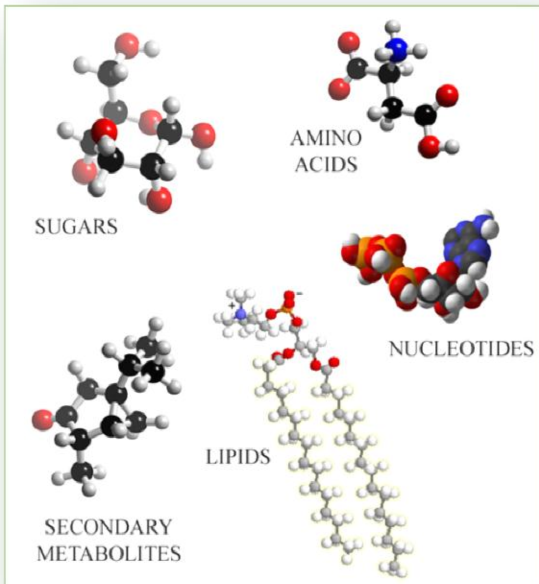
From elements to global scale

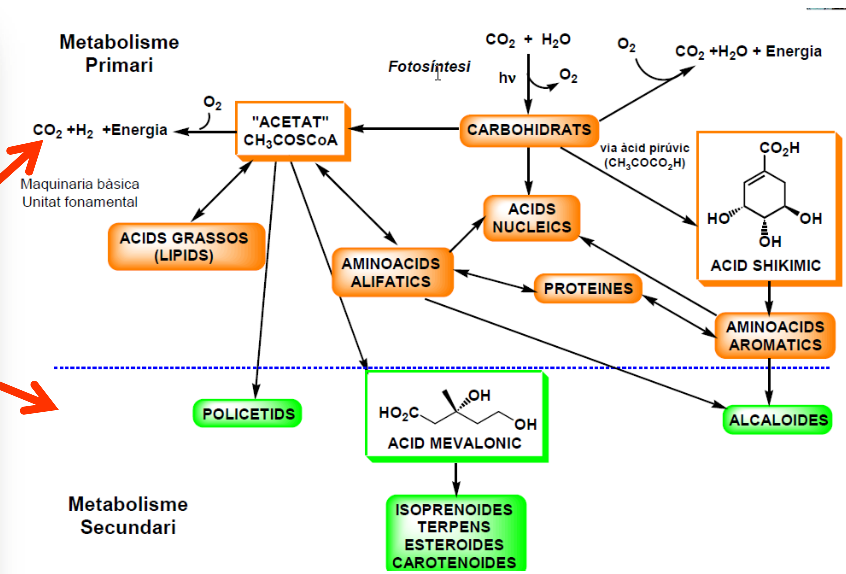
The ecological Stoichiometry



Metabolomica

C
K
N
P
Mg
Ca
P
S
Fe
Mn





Metabonomica

C
K
N
P
Mg
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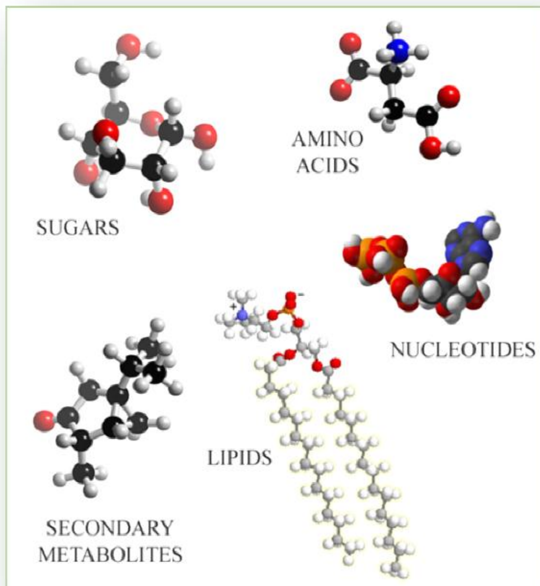
Fe
Mn



Primary

1. More abundants
2. Crucial in fisiologic
3. Directly in fotosinthesis

...

Secondary

1. Defense
2. Osmotic

METABOIOME

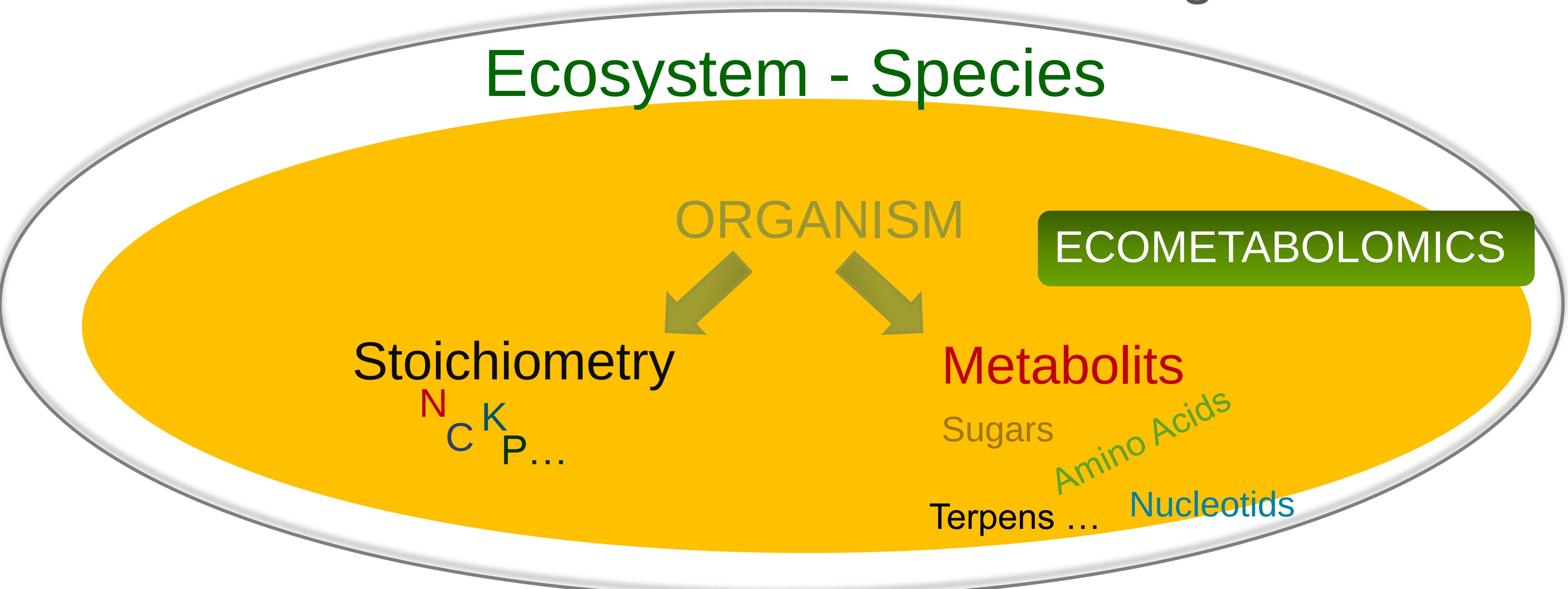
Ecometabolomics

Seasons (Ontogeny)

Plant-Herbivore interaction

Climate Change: Drought & Warming

Environmental Changes



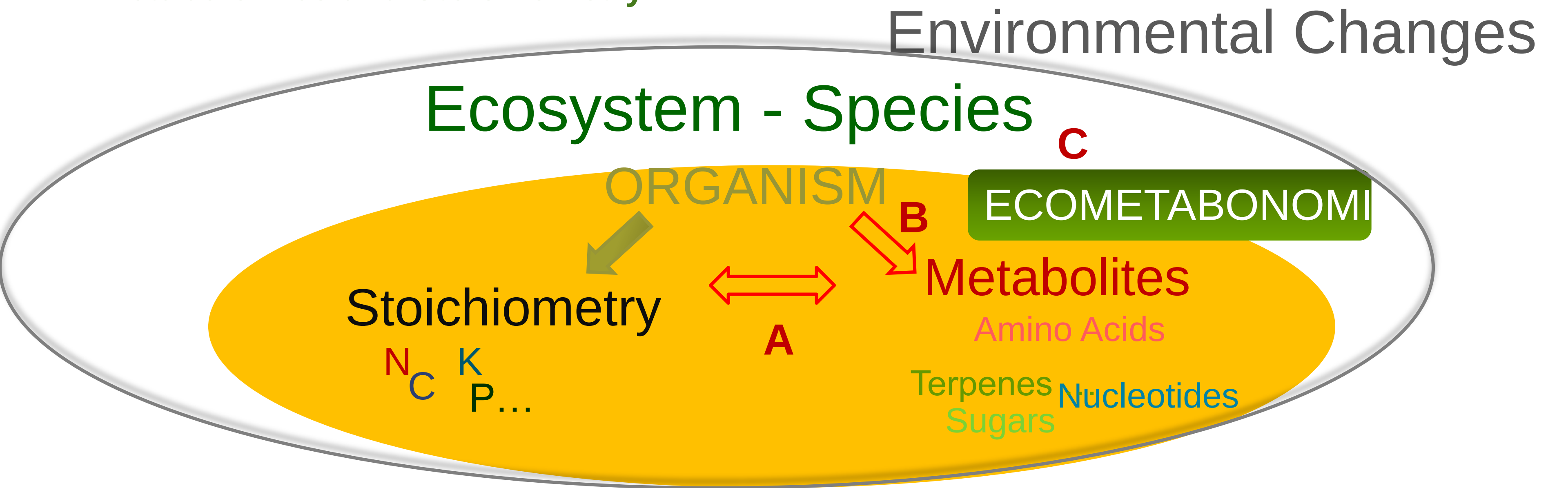
Objective

A. Understand the **Relationship between Metabolome and Stoichiometry**

B. Study the **Effects of Environmental changes on the Metabolome of a Species**

C. Study the **Structure & Function of the Ecosystem by Metabolomics and Stoichiometry.**

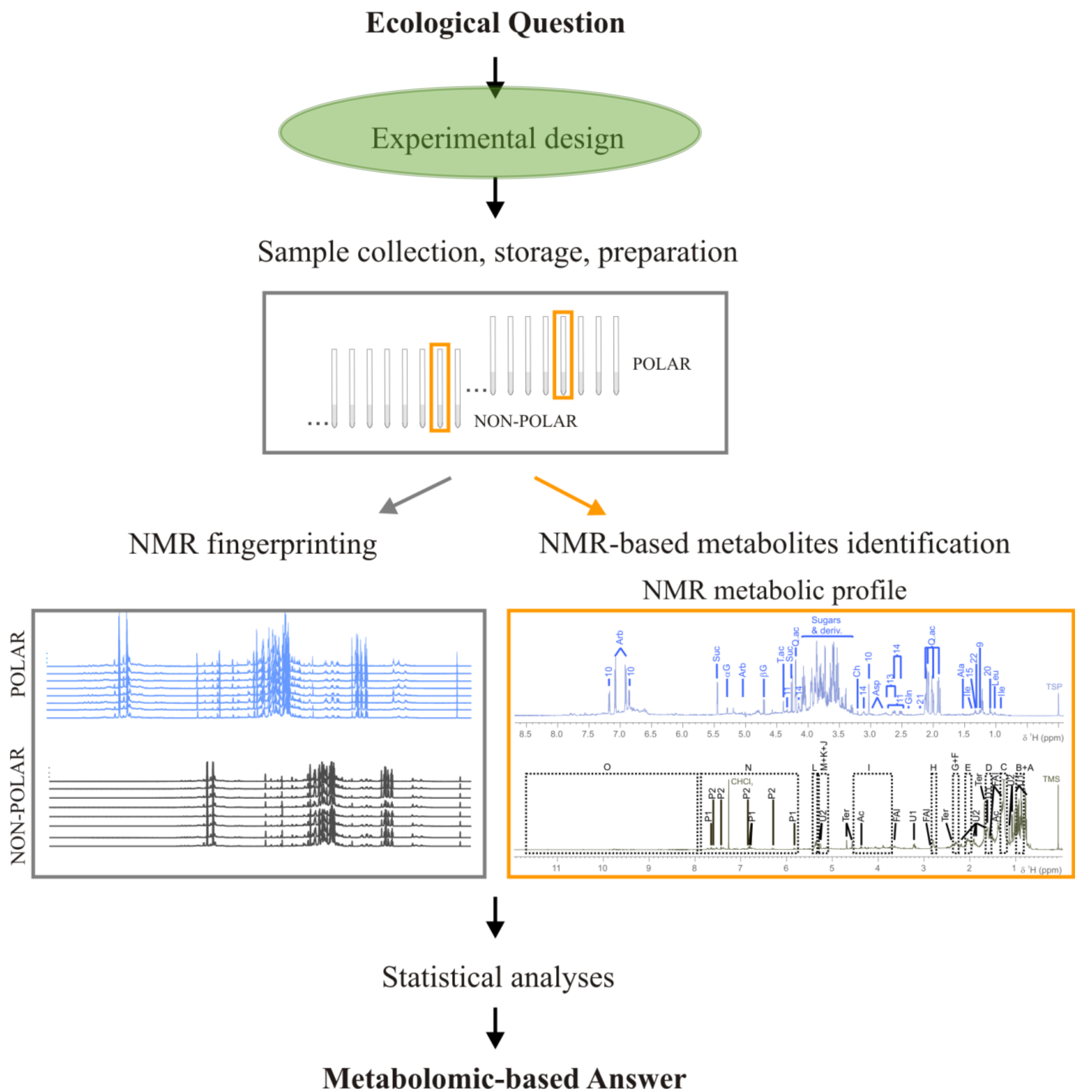
D. **Increase the Knowledge of the Ecosystem structure and fucntion by Metabolomics and Stoichiometry**



Ecological Question (first work)

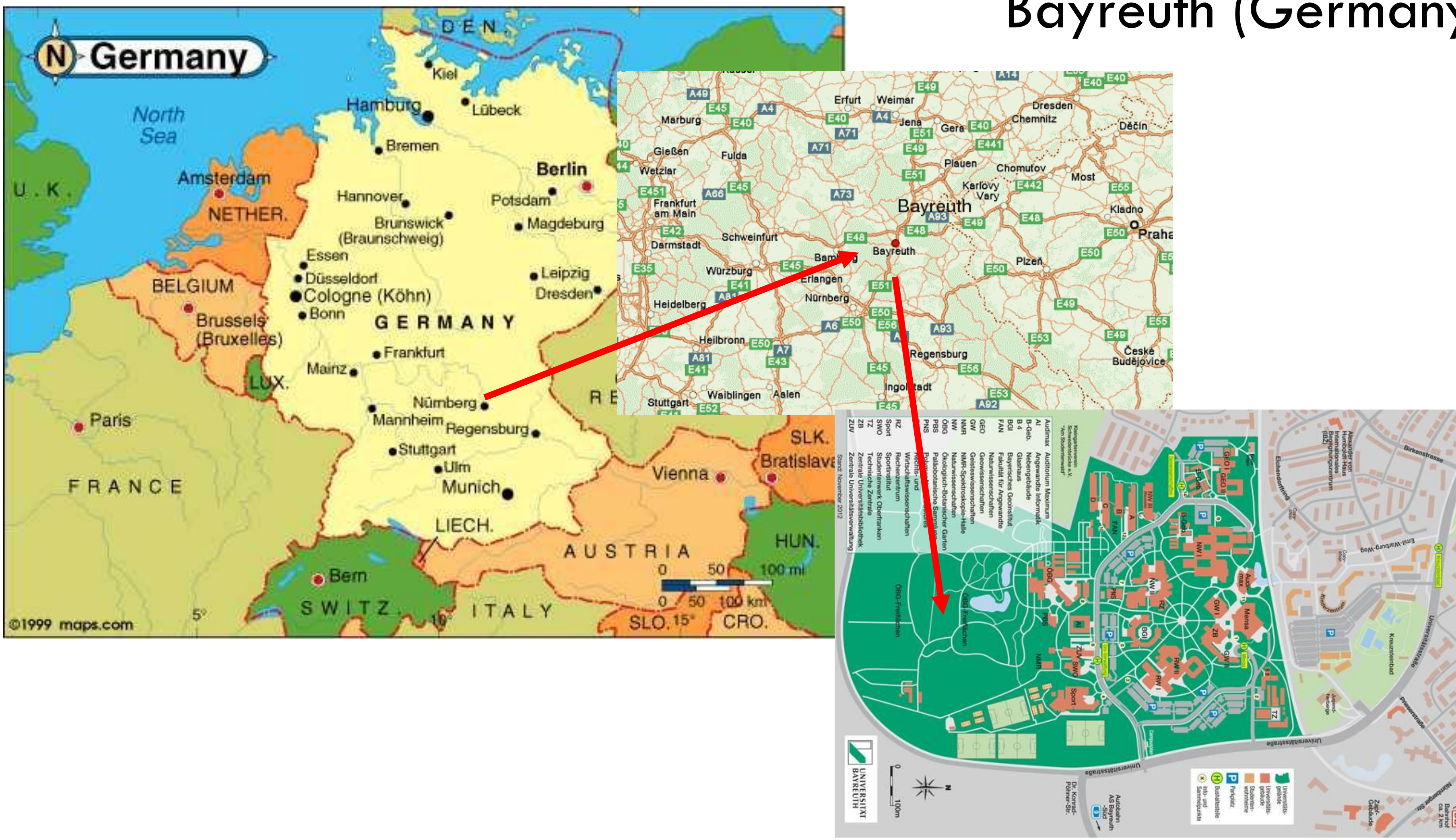
- Which are the metabolism of plants affected by:
  - Climate Change (Drought, warming, rainfall)
  - Phisiology (Structure & function)
  - Biodivesrtity or competition
  - Ontogeny

Experimental design



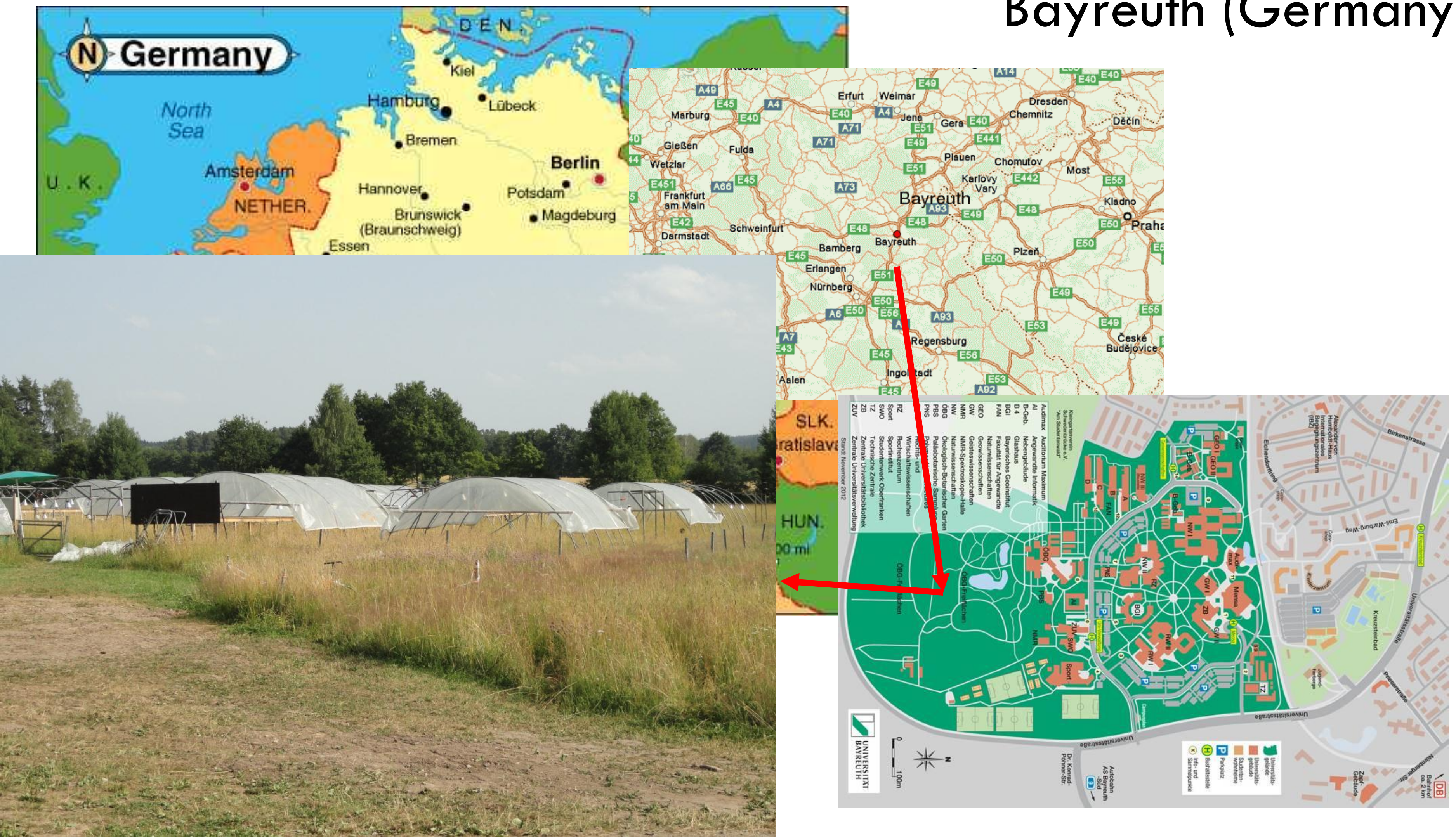
Experimental design

Bayreuth (Germany)

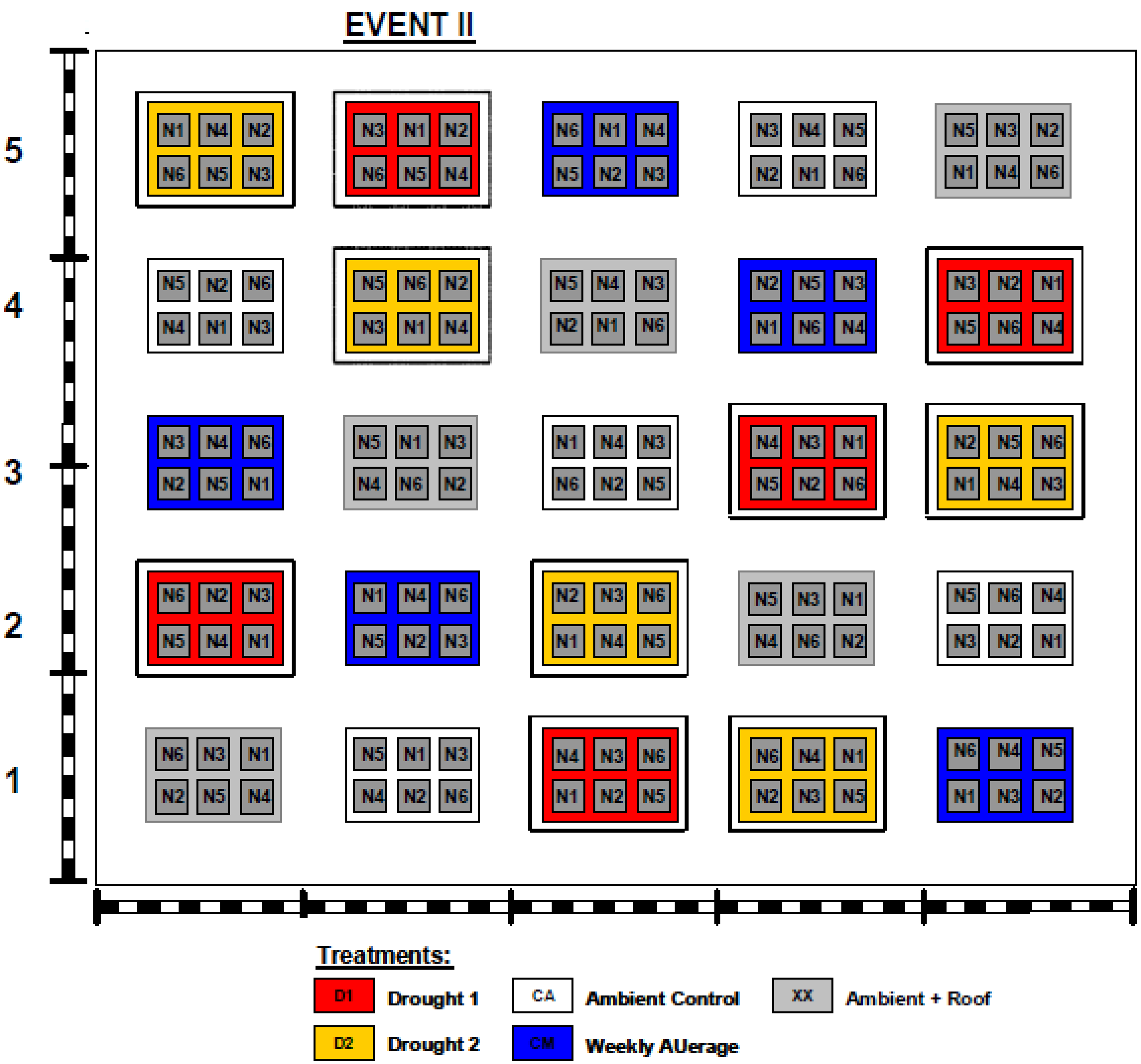


Experimental design

Bayreuth (Germany)



Experimental design

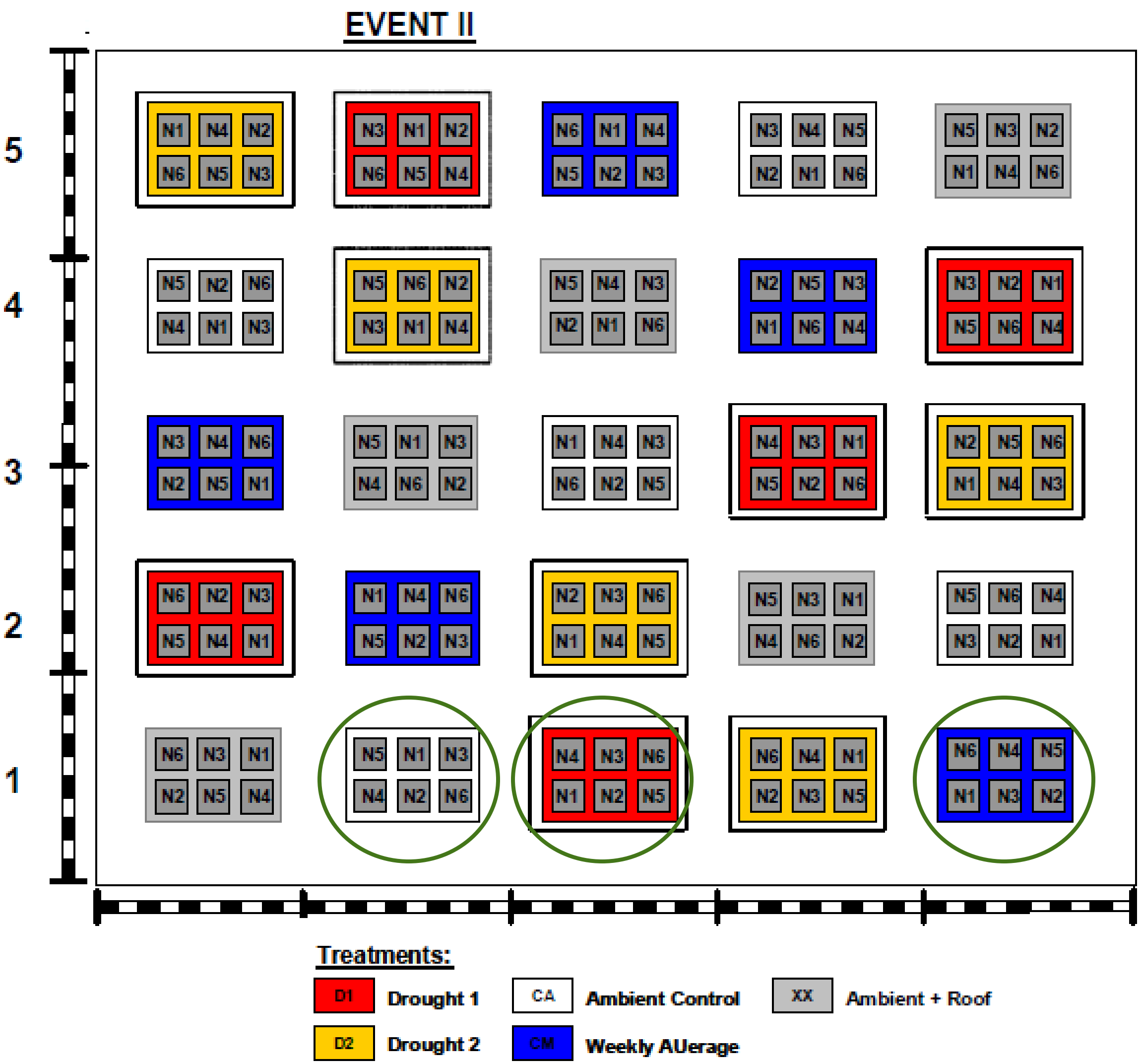


- **2 species (*Alopecurus pratensis* and *Holcus lanatus*)**

- **Five replications of five precipitation treatments.** Within each precipitation treatment six plots (1.5 m x 1.5 m size) receive different warming, winter rainfall and management manipulations (Figure 1).

- 2 time collect

Experimental design

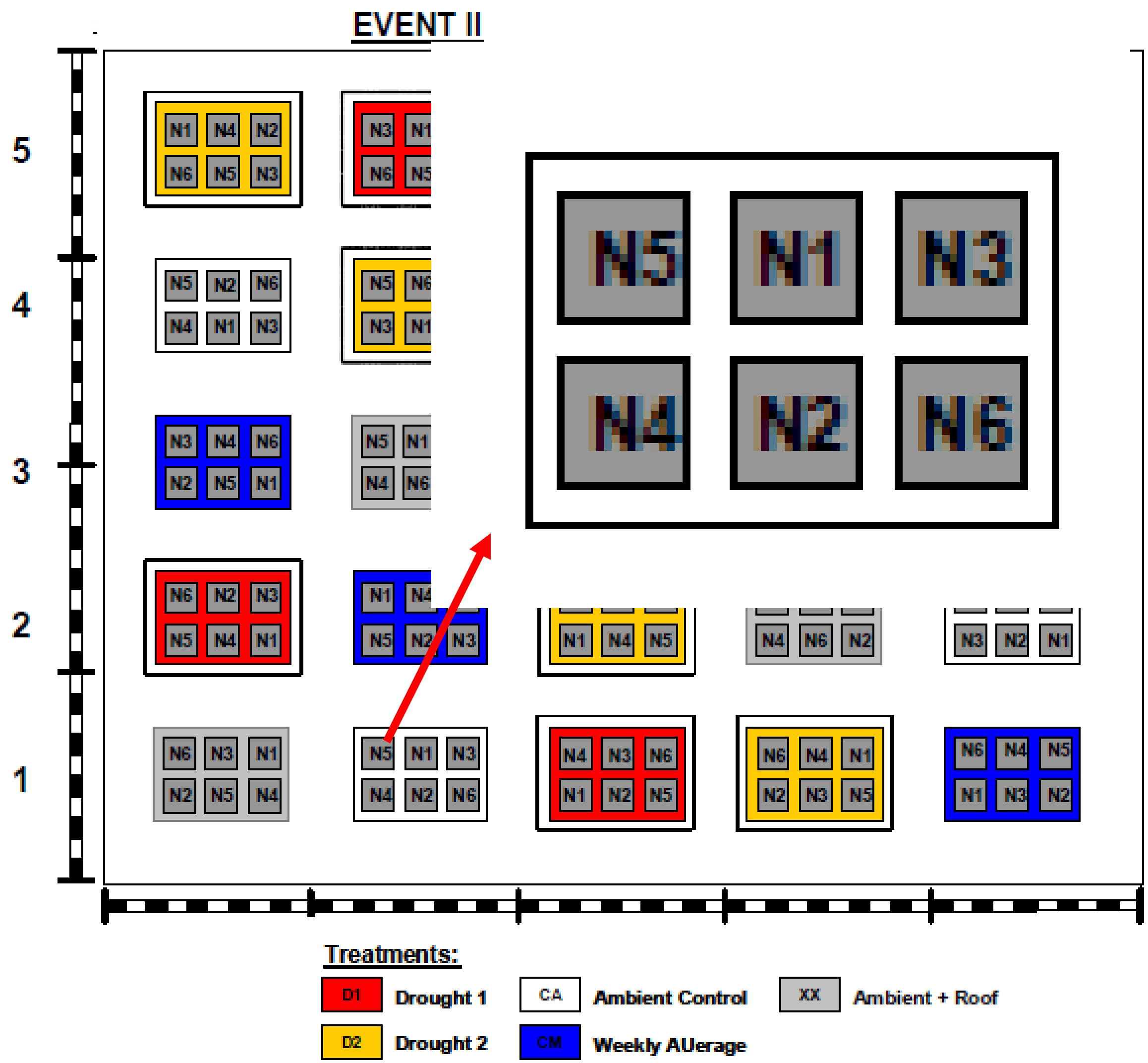


- **2 species (*Alopecurus pratensis* and *Holcus lanatus*)**

- **Five replications of five precipitation treatments. Within each** precipitation treatment six plots (1.5 m x 1.5 m size) receive different warming, winter rainfall and management manipulations (Figure 1).

- 2 time collect (July and September.

Experimental design

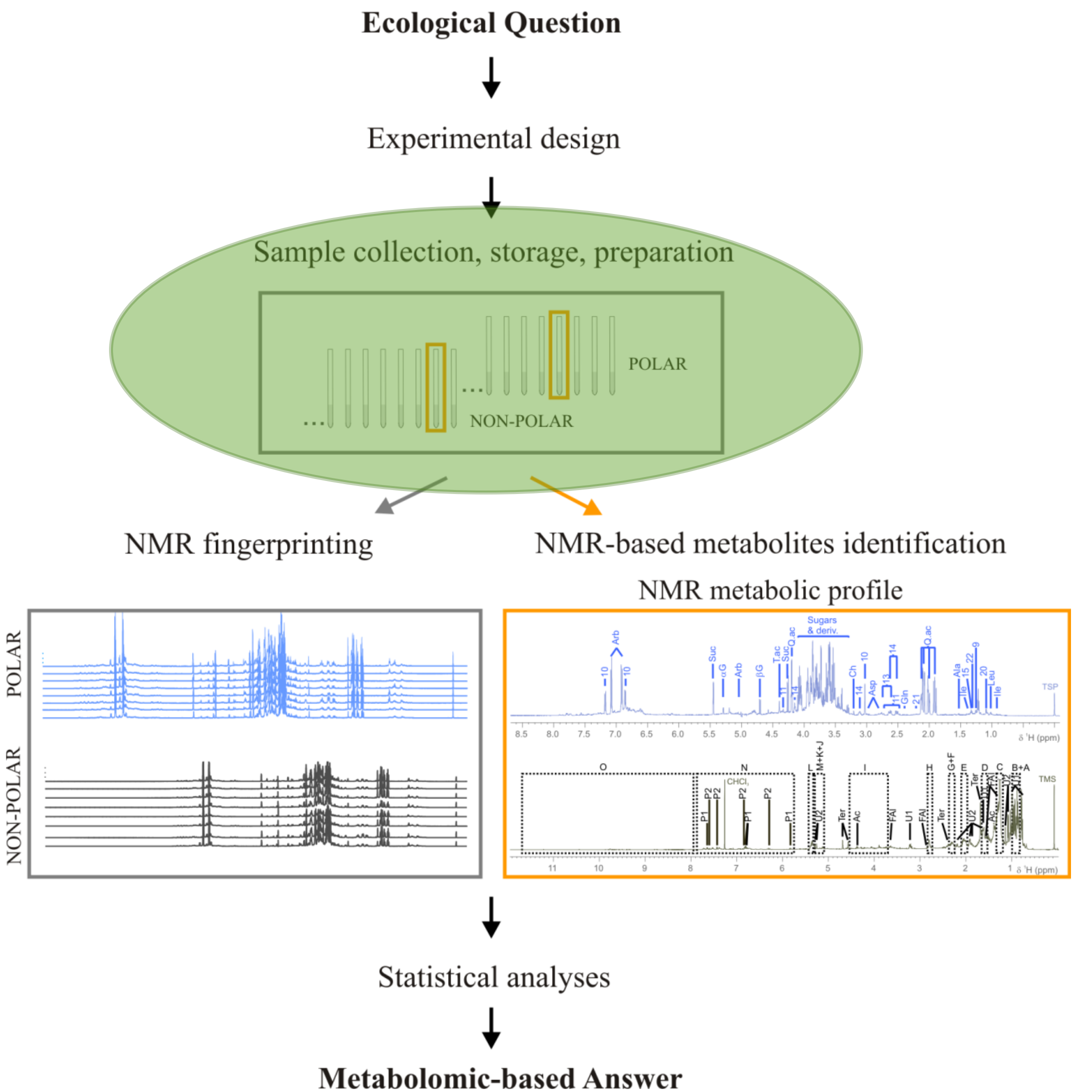


- **2 species (*Alopecurus pratensis* and *Holcus lanatus*)**

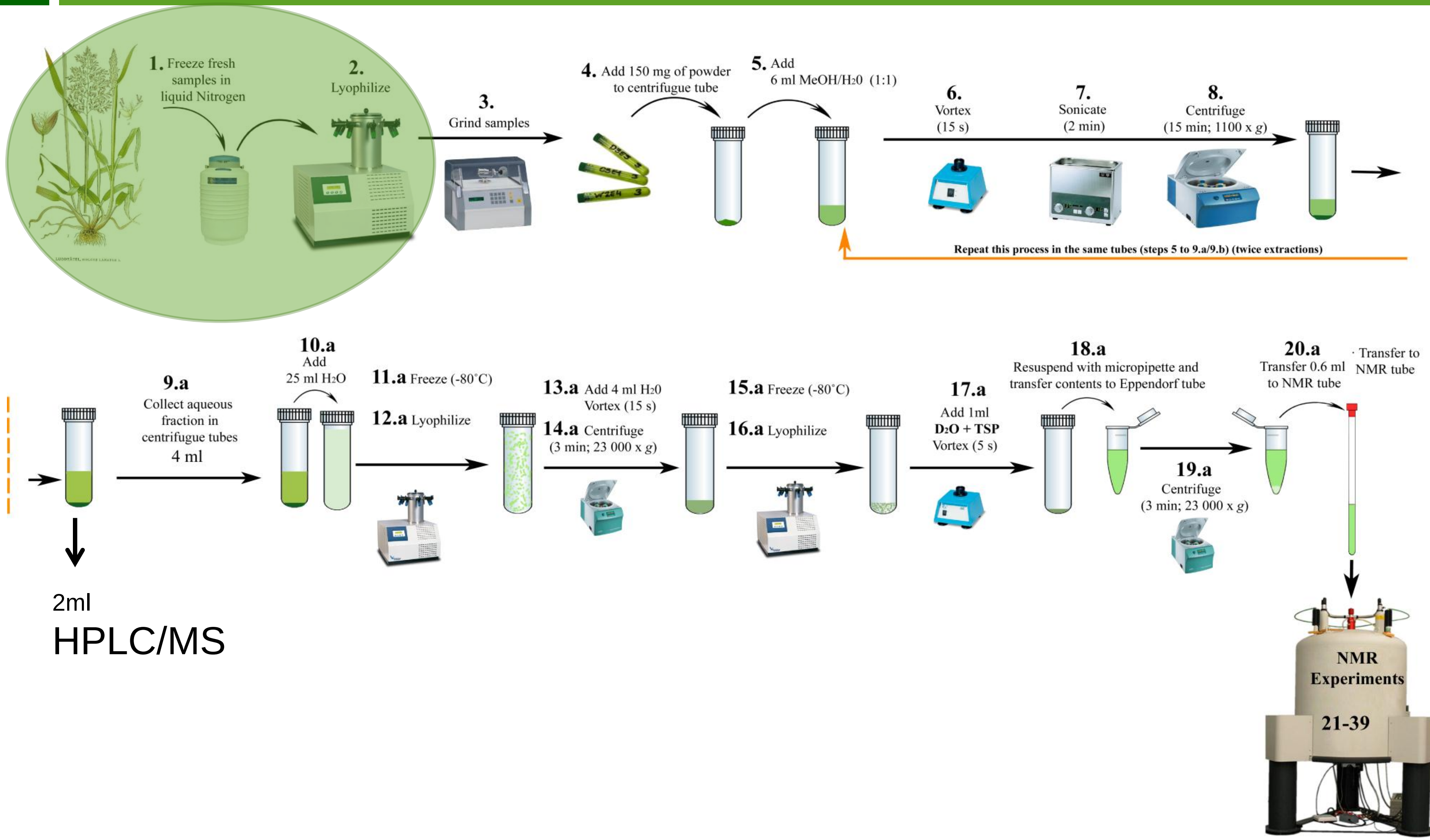
- **Five replications of five precipitation treatments. Within each** precipitation treatment six plots (1.5 m x 1.5 m size) receive different warming, winter rainfall and management manipulations (Figure 1).

- 400 samples

Sample collection

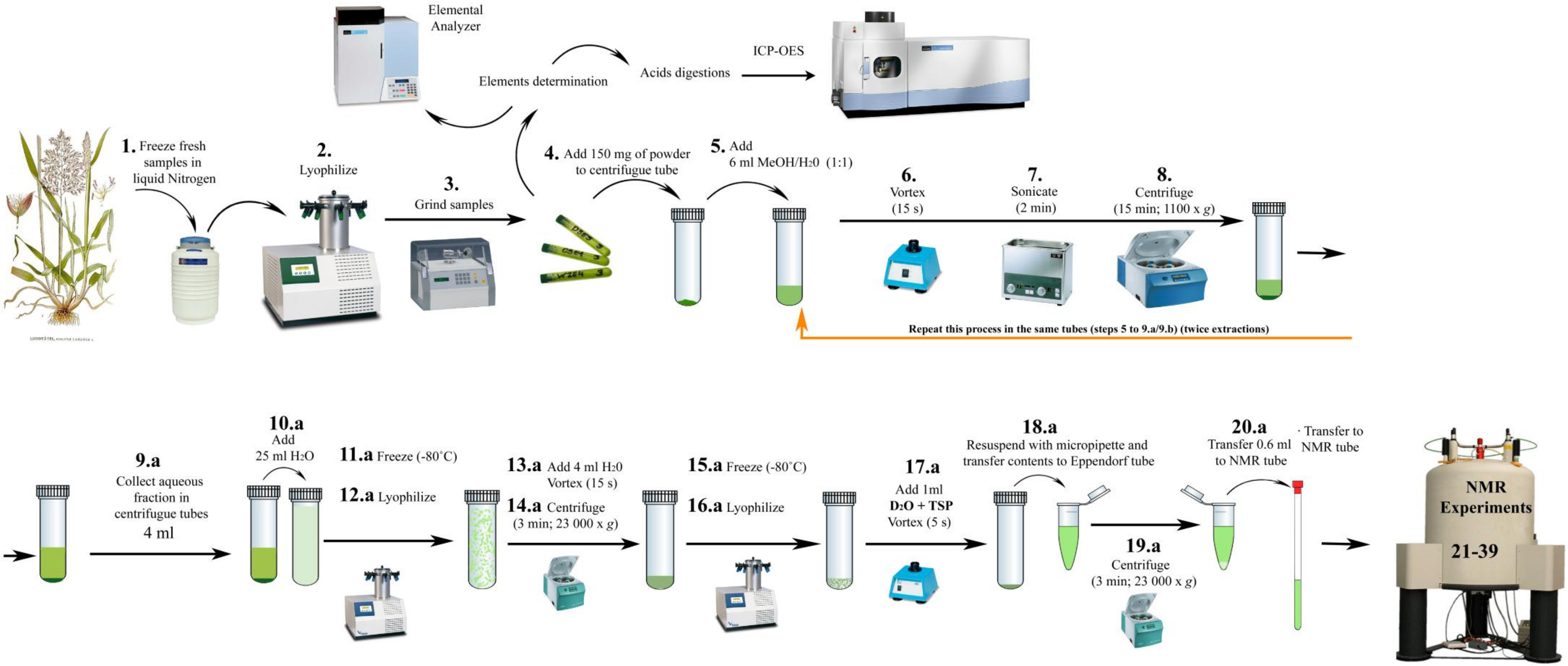


Sample collection

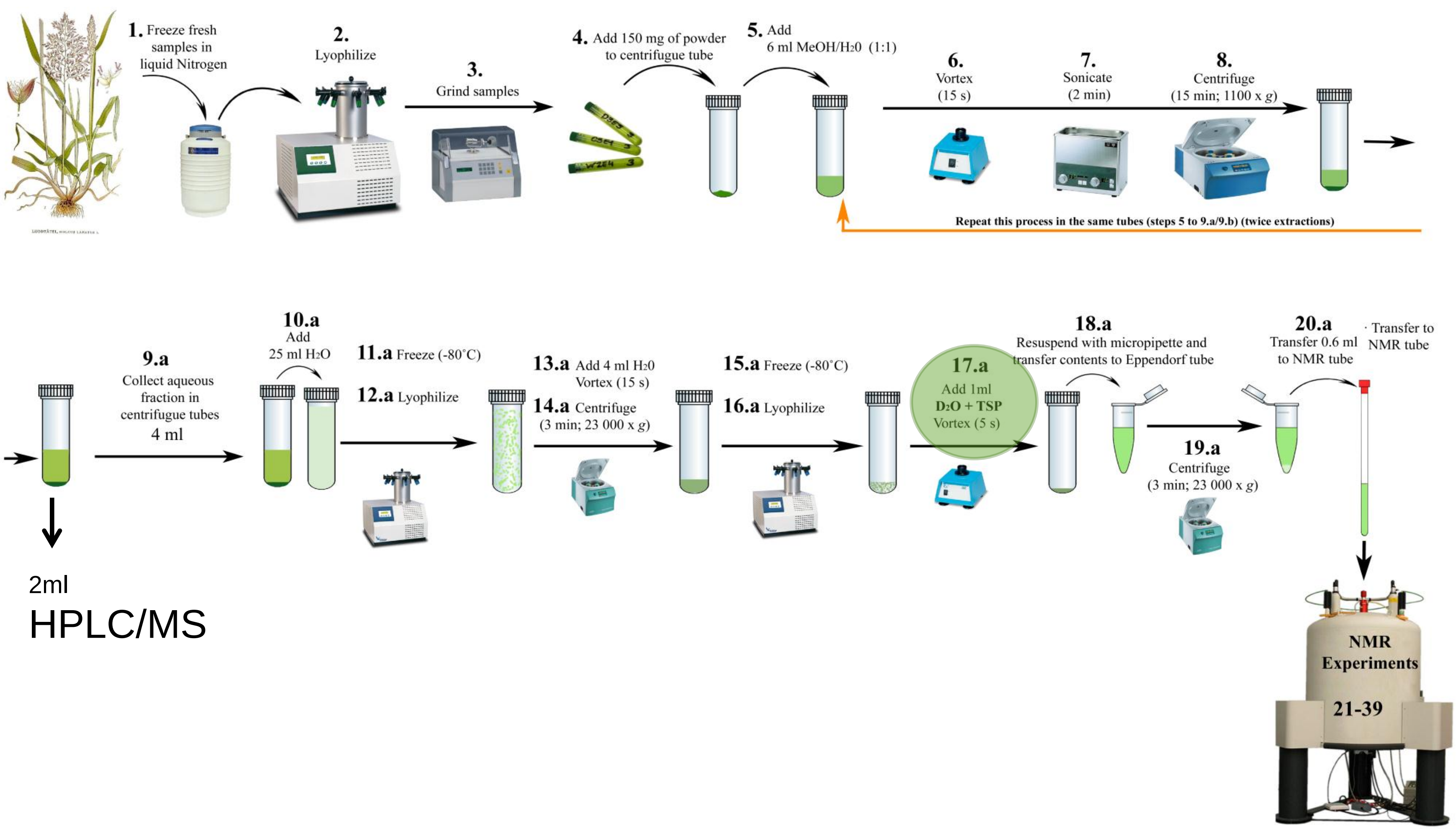


Sample collection

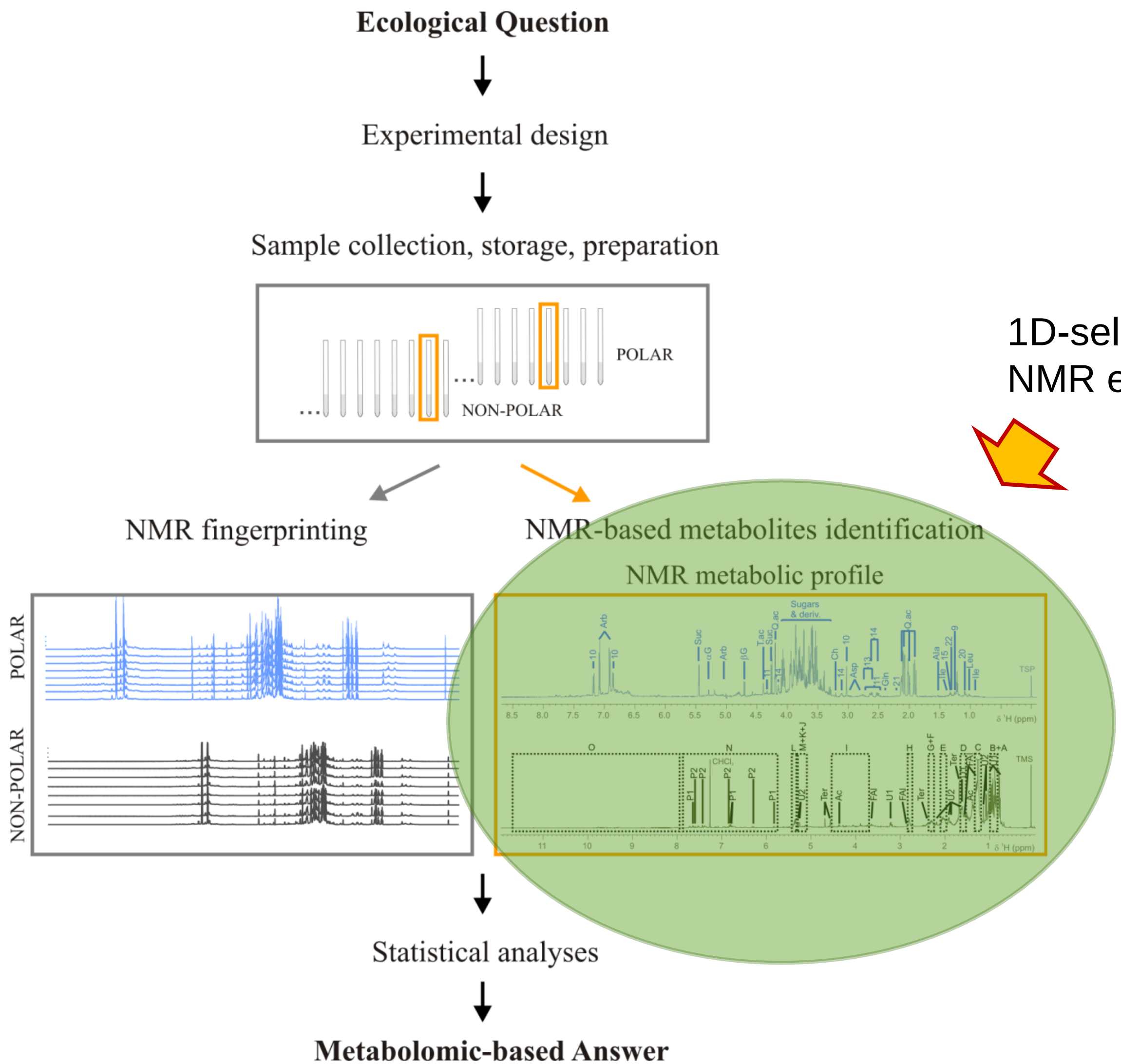
Sample collection



Sample collection

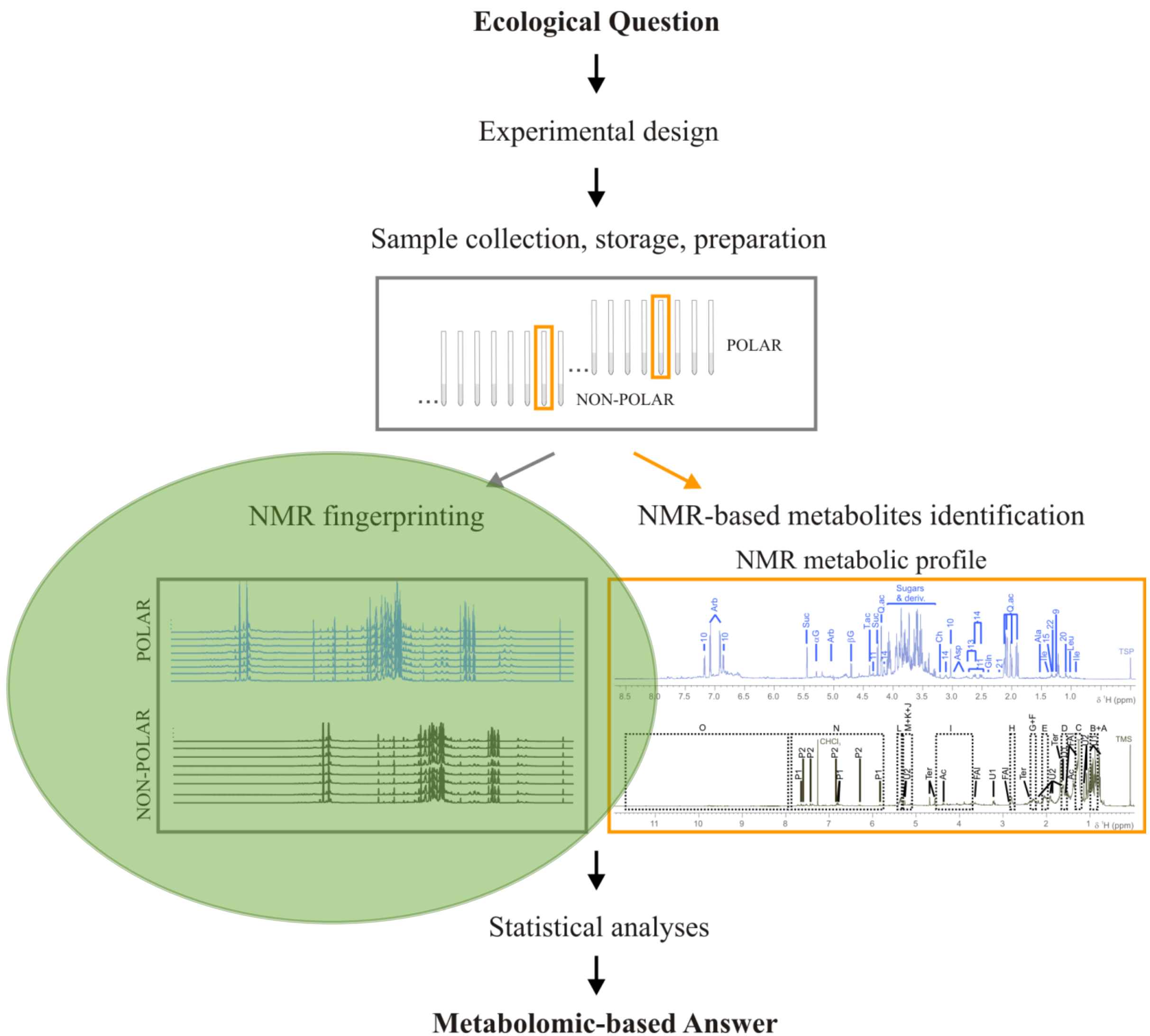


NMR-based metabolic profile



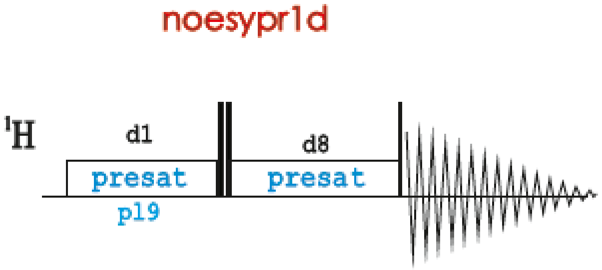
1D-selective & 2D NMR experiments

NMR-based metabolic profile



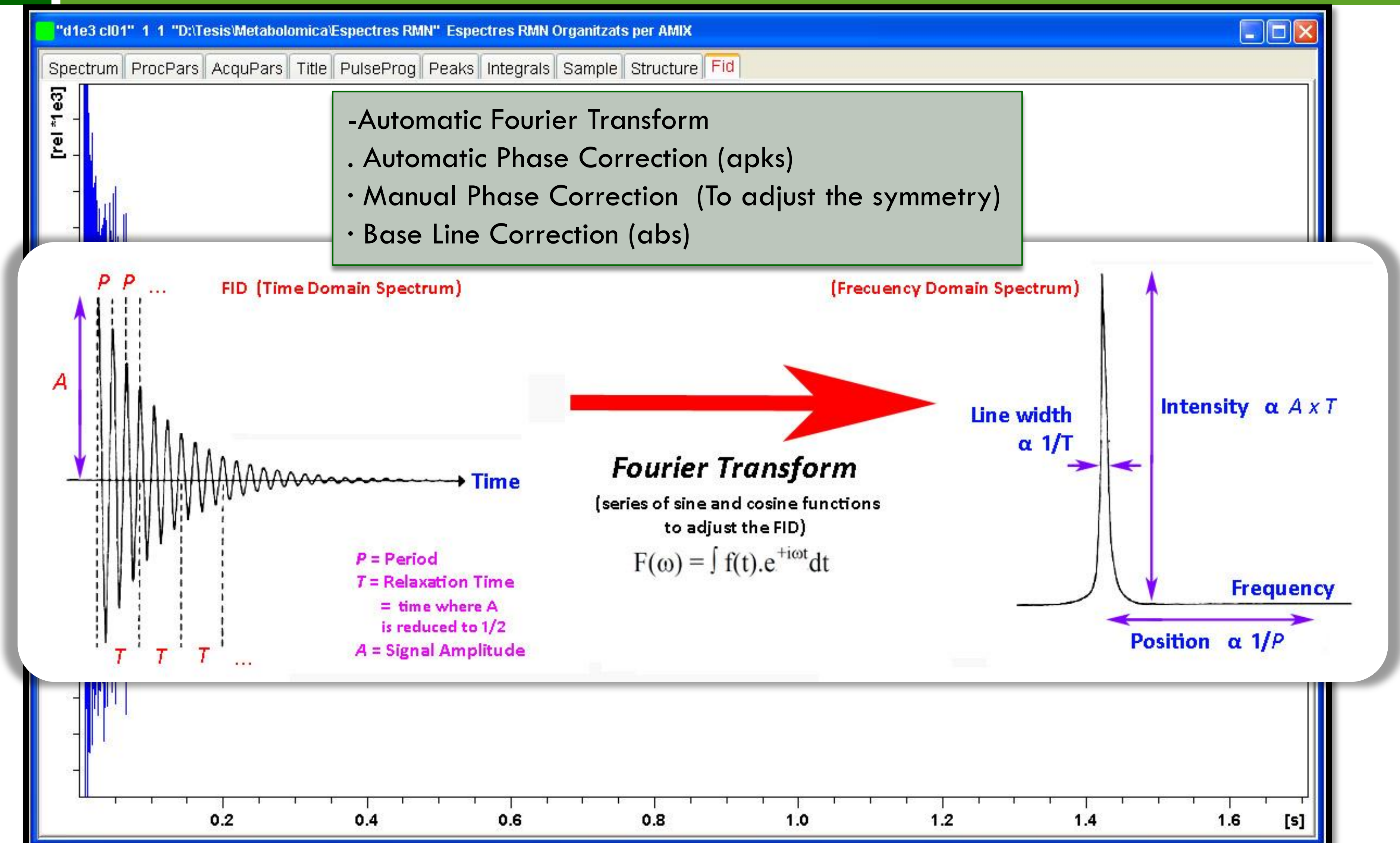
Fingerprinting (Adquisition)

- Automation
- All the samples doing with the same protocol and use the nmr-robot to doing the ^{1}H-spectrum.
- Reproducibility



NMR- Processing (Topspin & Amix software)

-Automatic Fourier Transform
- . Automatic Phase Correction (apks)
- · Manual Phase Correction (To adjust the symmetry)
- · Base Line Correction (abs)



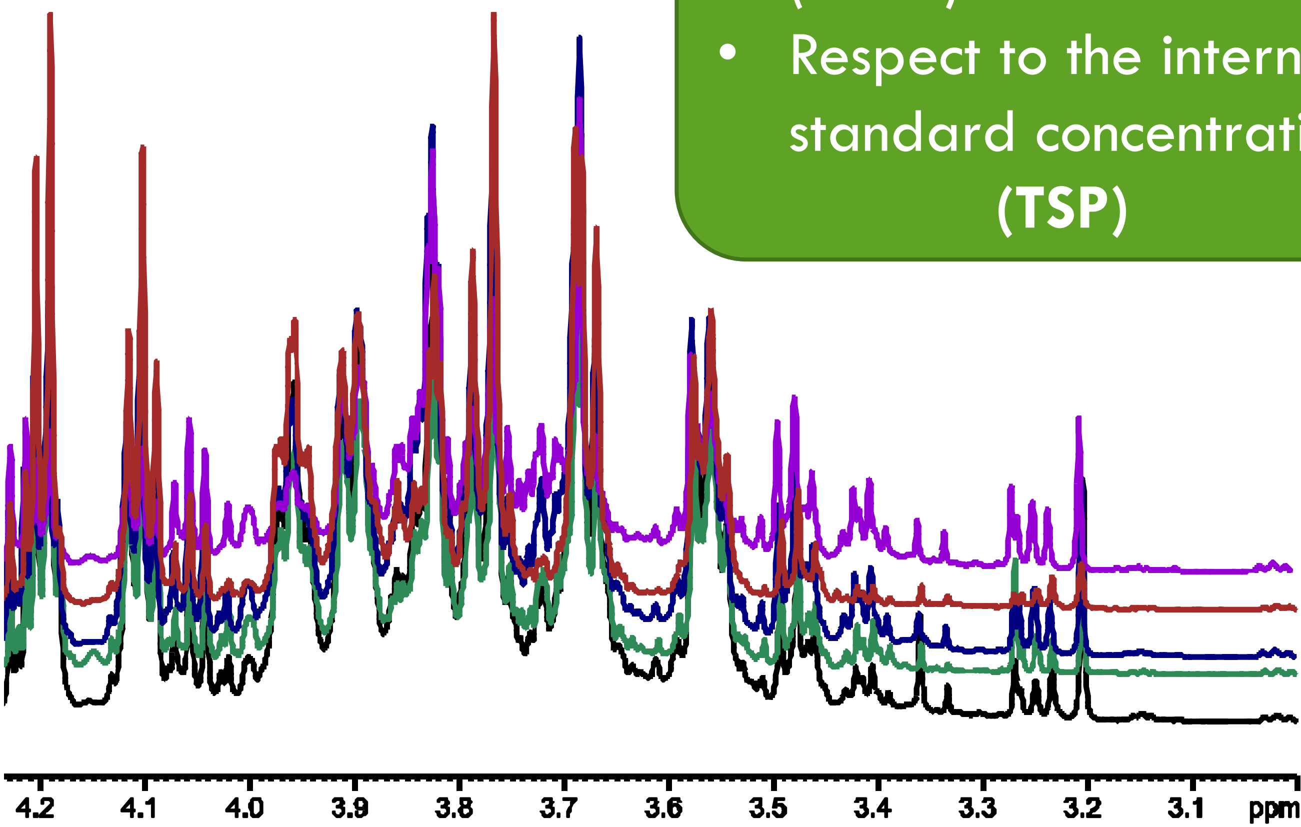
Post-Processing

integrals_192: Bloc de notas

Archivo Edición Formato Ver Ayuda

Number	Integrated Region		Integral
1	9.221	9.046	0.10323
2	8.956	8.723	0.15622
3	8.487	8.421	0.03722
4	8.120	8.038	0.13101
5	7.890	6.225	15.37703
6	6.128	5.921	0.54323
7	5.766	5.684	0.20155
8	5.587	5.536	0.15041
9	5.486	5.431	0.66421
10	5.435	5.400	7.94417
11	5.400	5.372	0.96177
12	5.373	5.314	0.49839
13	5.287	5.250	0.39146
14	5.249	5.220	0.76354
15	5.221	5.173	1.38018
16	5.171	5.118	0.58775
17	5.052	5.023	0.24556
18	5.023	4.960	0.52547
19	4.672	4.618	0.59628
20	4.466	4.426	0.75164
21	4.367	4.249	4.15057
22	4.249	4.151	45.30775
23	4.141	4.080	38.29610
24	4.080	4.035	12.02106
25	4.035	3.992	5.97331
26	3.992	3.932	42.94301
27	3.932	3.872	53.70915
28	3.872	3.849	12.62051
29	3.850	3.805	46.29956
30	3.805	3.732	64.96543
31	3.730	3.716	3.73860
32	3.713	3.628	68.43568
33	3.607	3.503	53.22546
34	3.503	3.447	15.73321
35	3.446	3.374	5.32279
36	3.374	3.349	1.88364
37	3.349	3.316	1.54200
38	3.287	3.223	6.56320
39	3.223	3.181	2.95495
40	3.168	3.122	0.70441
41	3.039	2.995	0.84750
42	2.991	2.962	0.63002
43	2.962	2.923	0.91779
44	2.897	2.870	0.82580
45	2.870	2.844	0.55973
46	2.844	2.821	0.37846
47	2.821	2.786	0.54277
48	2.721	2.649	2.09459
49	2.513	2.425	4.64855
50	2.425	2.383	1.35084
51	2.383	2.337	1.79870
52	2.334	2.268	1.09548
53	2.253	2.225	0.63043
54	2.200	2.103	6.24710
55	2.103	2.004	3.30611
56	2.004	1.969	1.47591
57	1.969	1.831	5.90750
58	1.788	1.700	2.46144
59	1.699	1.596	3.10153
60	1.592	1.523	1.10707
61	1.507	1.464	0.89044
62	1.352	1.317	1.96147
63	1.317	1.255	1.79880
64	1.196	1.157	0.88925
65	1.064	1.031	0.54831
66	1.031	1.007	0.36539
67	1.007	0.983	0.50861
68	0.983	0.920	1.13527

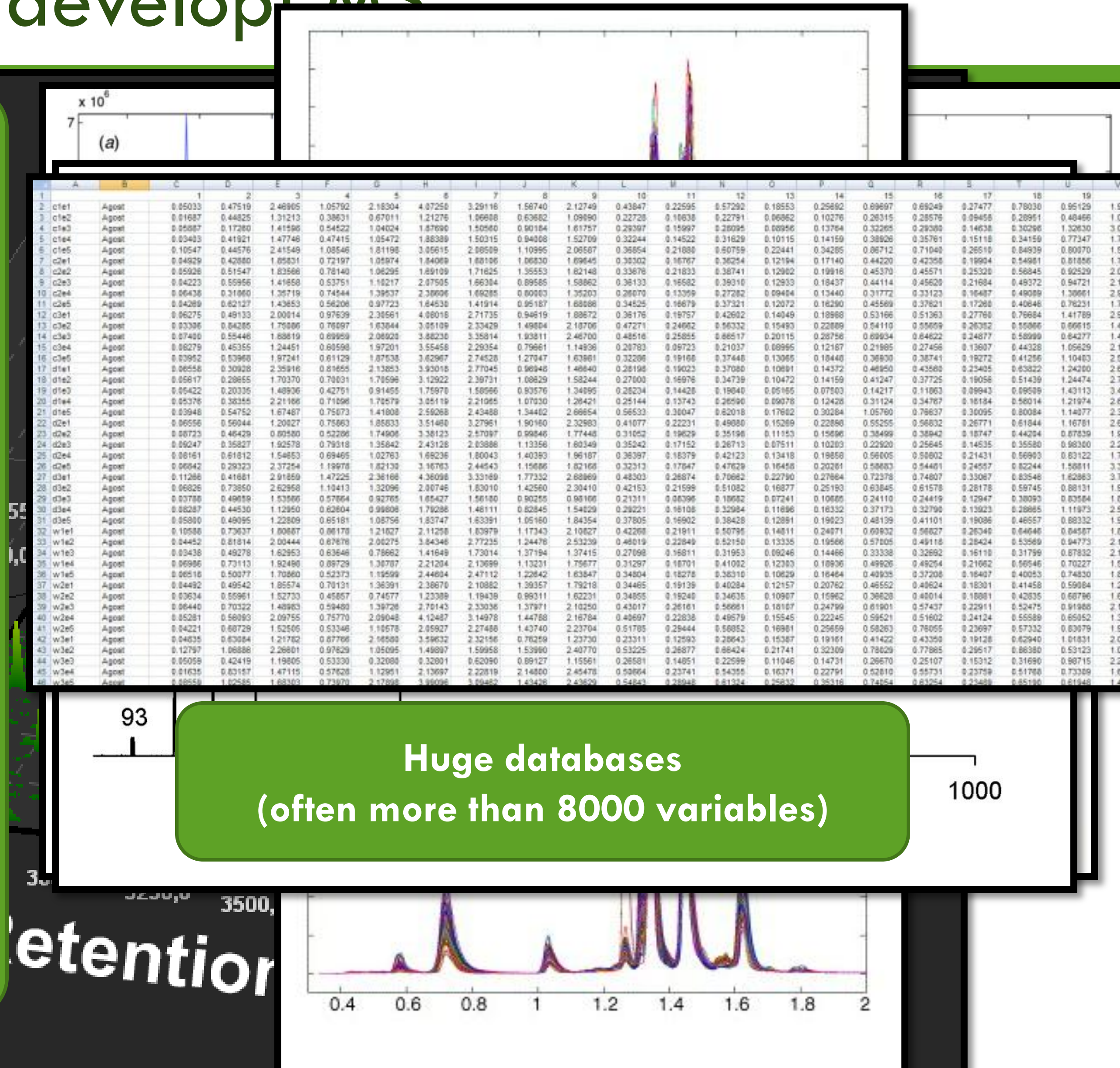
- Integrate all spectrum (AMIX)
- Respect to the internal standard concentration (TSP)



Methodology develop MS

MzMine

- Base Line Correction
- Mass Detection
- Chromarogram Builder
- Chromatogram Deconvolution
- Alignment
- Peak Finder
- Export



Huge databases
(often more than 8000 variables)

Methodology developt

NMR

ADVANTAGES

· High elucidation power

· Rapid H^1NMR spectra obtention

· High Reproducibility (even between labs and spectrometers)

· No destruction of samples

DISADVANTAGES

· Slow elucidation process

· Slow preparation of Extracts

· High overlapping signal

· Low sensitivity

LC-MS

ADVANTAGES

· High sensitivity

· Rapid preparation of Extracts

· Good compound separaton by chromatography

· Rapid metabolite assignation

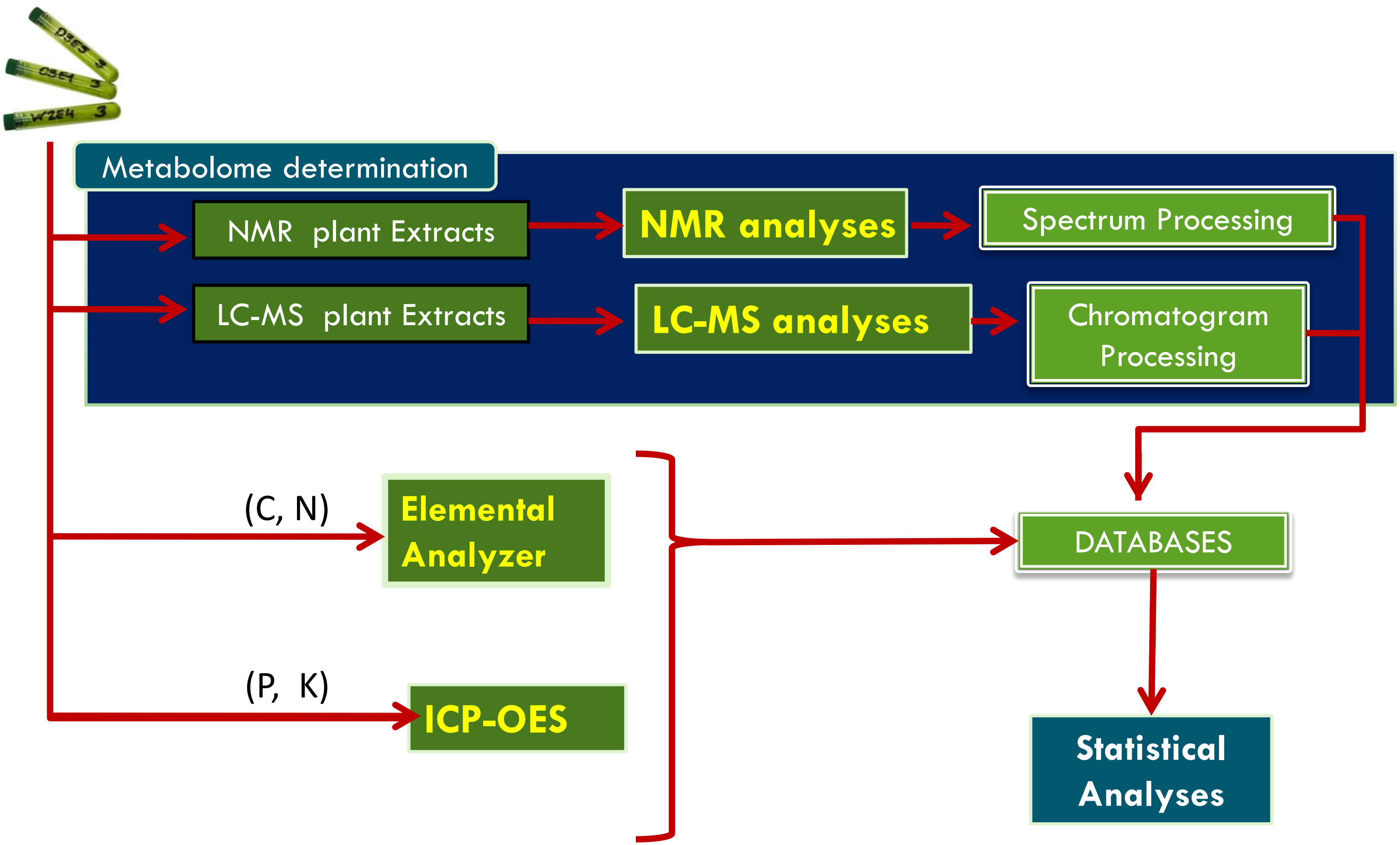
DISADVANTAGES

· Low elucidation power

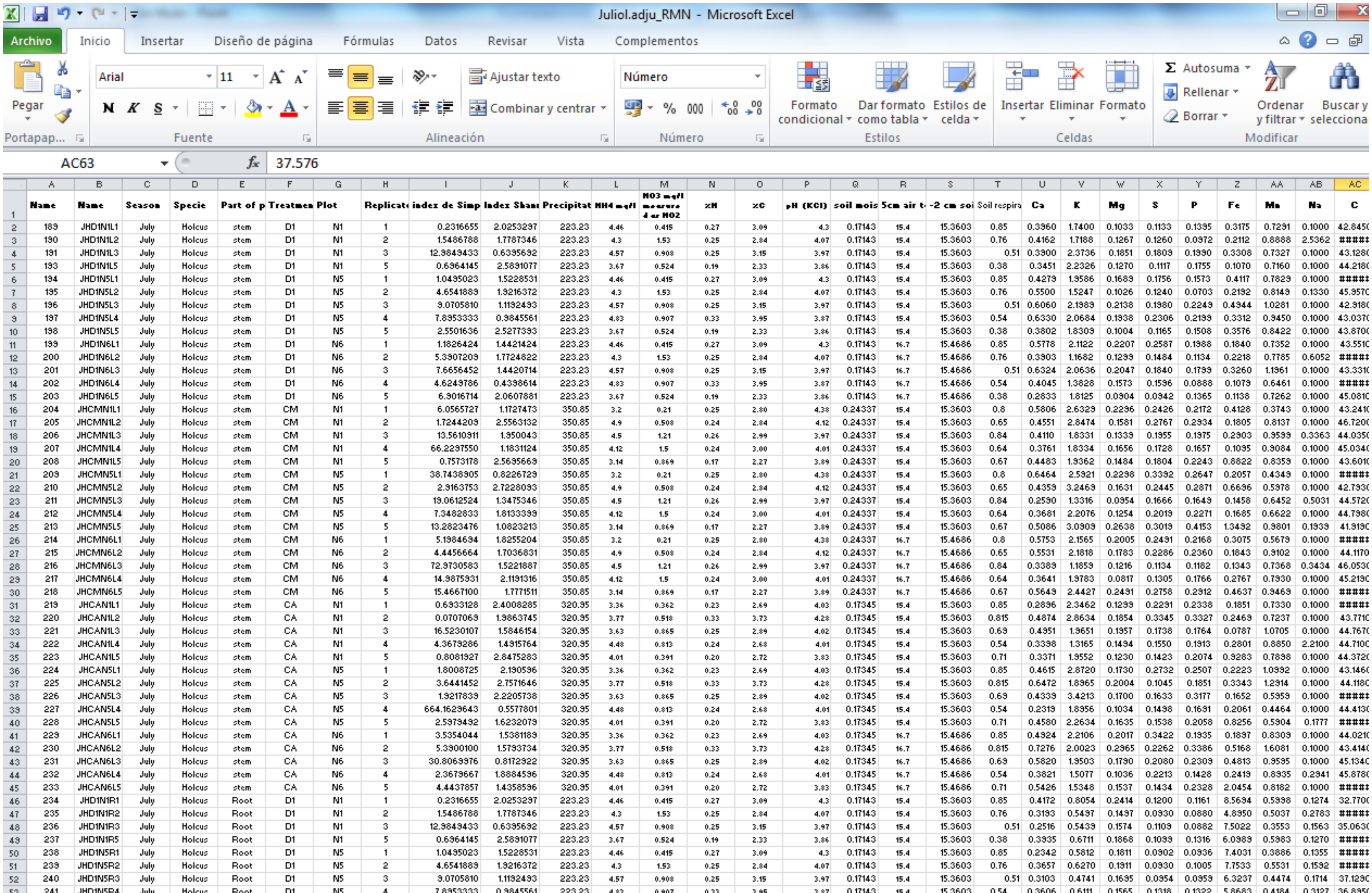
· Slow chromatographic separation

· Sample destruction

NMR-Ms-Stochiometry study



Pre-Processing statistical analysis

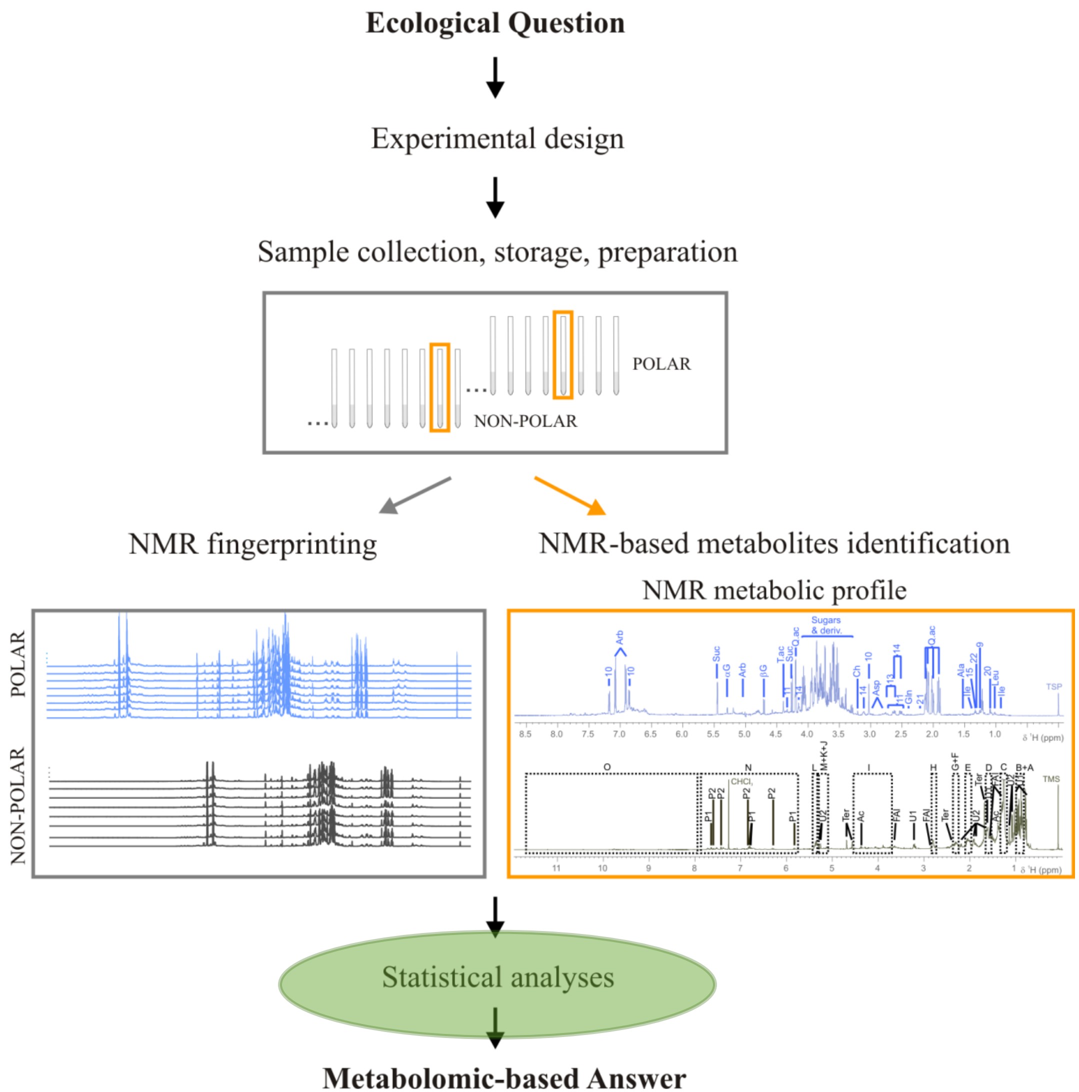


Juliol.adju_RMN - Microsoft Excel

AC63 | 37.576

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
1	Name	Name	Season	Specie	Part of p	Treatmen	Plot	Replicat	index de Simp	Index Shan	Precipitat	NH4 mg/l	NO3 mg/l measured ar NO2	xN	xC	pH (KCl)	soil mois	5cm air t	-2 cm soi	Soil respira	Ca	K	Mg	S	P	Fe	Mn	Na	C
2	189	JHD1N1L1	July	Holcus	stem	D1	N1	1	0.2316655	2.0253297	223.23	4.46	0.415	0.27	3.09	4.3	0.17143	15.4	15.3603	0.85	0.3960	1.7400	0.1033	0.1133	0.1395	0.3175	0.7291	0.1000	42.8450
3	190	JHD1N1L2	July	Holcus	stem	D1	N1	2	1.5486788	1.7787346	223.23	4.3	1.53	0.25	2.84	4.07	0.17143	15.4	15.3603	0.76	0.4162	1.7188	0.1267	0.1260	0.0972	0.2112	0.8888	2.5362	#####
4	191	JHD1N1L3	July	Holcus	stem	D1	N1	3	12.9849433	0.6395692	223.23	4.57	0.908	0.25	3.15	3.97	0.17143	15.4	15.3603	0.51	0.3900	2.3736	0.1851	0.1809	0.1990	0.3308	0.7327	0.1000	43.1280
5	193	JHD1N1L5	July	Holcus	stem	D1	N1	5	0.6964145	2.5891077	223.23	3.67	0.524	0.19	2.33	3.86	0.17143	15.4	15.3603	0.38	0.3451	2.2326	0.1270	0.1117	0.1755	0.1070	0.7160	0.1000	44.2180
6	194	JHD1N5L1	July	Holcus	stem	D1	N5	1	1.0495023	1.5228531	223.23	4.46	0.415	0.27	3.09	4.3	0.17143	15.4	15.3603	0.85	0.4279	1.9586	0.1689	0.1756	0.1573	0.4117	0.7829	0.1000	#####
7	195	JHD1N5L2	July	Holcus	stem	D1	N5	2	4.6541889	1.9216372	223.23	4.3	1.53	0.25	2.84	4.07	0.17143	15.4	15.3603	0.76	0.5500	1.5247	0.1026	0.1240	0.0703	0.2192	0.8149	0.1330	45.9570
8	196	JHD1N5L3	July	Holcus	stem	D1	N5	3	9.0705810	1.1192493	223.23	4.57	0.908	0.25	3.15	3.97	0.17143	15.4	15.3603	0.51	0.6060	2.1989	0.2138	0.1980	0.2249	0.4944	1.0281	0.1000	42.9180
9	197	JHD1N5L4	July	Holcus	stem	D1	N5	4	7.8953333	0.9845561	223.23	4.83	0.907	0.33	3.95	3.87	0.17143	15.4	15.3603	0.54	0.6330	2.0684	0.1938	0.2306	0.2199	0.3312	0.9450	0.1000	43.0370
10	198	JHD1N5L5	July	Holcus	stem	D1	N5	5	2.5501636	2.5277393	223.23	3.67	0.524	0.19	2.33	3.86	0.17143	15.4	15.3603	0.38	0.3802	1.8309	0.1004	0.1165	0.1508	0.3576	0.8422	0.1000	43.8700
11	199	JHD1N6L1	July	Holcus	stem	D1	N6	1	1.1826424	1.4421424	223.23	4.46	0.415	0.27	3.09	4.3	0.17143	16.7	15.4686	0.85	0.5778	2.1122	0.2207	0.2587	0.1988	0.1840	0.7352	0.1000	43.5510
12	200	JHD1N6L2	July	Holcus	stem	D1	N6	2	5.3907209	1.7724822	223.23	4.3	1.53	0.25	2.84	4.07	0.17143	16.7	15.4686	0.76	0.3903	1.1682	0.1299	0.1484	0.1134	0.2218	0.7785	0.6052	#####
13	201	JHD1N6L3	July	Holcus	stem	D1	N6	3	7.6656452	1.4420714	223.23	4.57	0.908	0.25	3.15	3.97	0.17143	16.7	15.4686	0.51	0.6324	2.0636	0.2047	0.1840	0.1799	0.3260	1.1961	0.1000	43.3310
14	202	JHD1N6L4	July	Holcus	stem	D1	N6	4	4.6249786	0.4398614	223.23	4.83	0.907	0.33	3.95	3.87	0.17143	16.7	15.4686	0.54	0.4045	1.3828	0.1573	0.1596	0.0888	0.1079	0.6461	0.1000	#####
15	203	JHD1N6L5	July	Holcus	stem	D1	N6	5	6.9016714	2.0607881	223.23	3.67	0.524	0.19	2.33	3.86	0.17143	16.7	15.4686	0.38	0.2833	1.8125	0.0904	0.0942	0.1365	0.1138	0.7262	0.1000	45.0810
16	204	JHCMN1L1	July	Holcus	stem	CM	N1	1	6.0565727	1.1727473	350.85	3.2	0.21	0.25	2.80	4.38	0.24337	15.4	15.3603	0.8	0.5806	2.6329	0.2296	0.2426	0.2172	0.4128	0.3743	0.1000	43.2410
17	205	JHCMN1L2	July	Holcus	stem	CM	N1	2	1.7244209	2.5563132	350.85	4.9	0.508	0.24	2.84	4.12	0.24337	15.4	15.3603	0.65	0.4551	2.8474	0.1581	0.2767	0.2934	0.1805	0.8137	0.1000	46.7200
18	206	JHCMN1L3	July	Holcus	stem	CM	N1	3	13.5610911	1.950043	350.85	4.5	1.21	0.26	2.99	3.97	0.24337	15.4	15.3603	0.84	0.4110	1.8331	0.1339	0.1955	0.1975	0.2903	0.9599	0.3363	44.0350
19	207	JHCMN1L4	July	Holcus	stem	CM	N1	4	66.2297550	1.1831124	350.85	4.12	1.5	0.24	3.00	4.01	0.24337	15.4	15.3603	0.64	0.3761	1.8334	0.1656	0.1728	0.1657	0.1095	0.9084	0.1000	45.0340
20	208	JHCMN1L5	July	Holcus	stem	CM	N1	5	0.7573178	2.5695669	350.85	3.14	0.869	0.17	2.27	3.89	0.24337	15.4	15.3603	0.67	0.4483	1.9362	0.1484	0.1804	0.2243	0.8822	0.8359	0.1000	43.6010
21	209	JHCMN5L1	July	Holcus	stem	CM	N5	1	38.7438905	0.8226729	350.85	3.2	0.21	0.25	2.80	4.38	0.24337	15.4	15.3603	0.8	0.6464	2.5921	0.2298	0.3392	0.2647	0.2057	0.4349	0.1000	#####
22	210	JHCMN5L2	July	Holcus	stem	CM	N5	2	2.9163753	2.7228093	350.85	4.9	0.508	0.24	2.84	4.12	0.24337	15.4	15.3603	0.65	0.4359	3.2469	0.1631	0.2445	0.2871	0.6696	0.5978	0.1000	42.7930
23	211	JHCMN5L3	July	Holcus	stem	CM	N5	3	19.0612524	1.3475346	350.85	4.5	1.21	0.26	2.99	3.97	0.24337	15.4	15.3603	0.84	0.2590	1.3316	0.0954	0.1666	0.1649	0.1458	0.6452	0.5031	44.5720
24	212	JHCMN5L4	July	Holcus	stem	CM	N5	4	7.3482833	1.8133399	350.85	4.12	1.5	0.24	3.00	4.01	0.24337	15.4	15.3603	0.64	0.3681	2.2076	0.1254	0.2019	0.2271	0.1685	0.6622	0.1000	44.7980
25	213	JHCMN5L5	July	Holcus	stem	CM	N5	5	13.2823476	1.0823213	350.85	3.14	0.869	0.17	2.27	3.89	0.24337	15.4	15.3603	0.67	0.5086	3.0909	0.2638	0.3019	0.4153	1.3492	0.9801	0.1939	41.9190
26	214	JHCMN6L1	July	Holcus	stem	CM	N6	1	5.1984694	1.8255204	350.85	3.2	0.21	0.25	2.80	4.38	0.24337	16.7	15.4686	0.8	0.5753	2.1565	0.2005	0.2491	0.2168	0.3075	0.5679	0.1000	#####
27	215	JHCMN6L2	July	Holcus	stem	CM	N6	2	4.4456664	1.7036831	350.85	4.9	0.508	0.24	2.84	4.12	0.24337	16.7	15.4686	0.65	0.5531	2.1818	0.1783	0.2286	0.2360	0.1843	0.9102	0.1000	44.1170
28	216	JHCMN6L3	July	Holcus	stem	CM	N6	3	72.9730583	1.5221887	350.85	4.5	1.21	0.26	2.99	3.97	0.24337	16.7	15.4686	0.84	0.3389	1.1859	0.1216	0.1134	0.1182	0.1343	0.7368	0.3434	46.0530
29	217	JHCMN6L4	July	Holcus	stem	CM	N6	4	14.9875931	2.1191316	350.85	4.12	1.5	0.24	3.00	4.01	0.24337	16.7	15.4686	0.64	0.3641	1.9783	0.0817	0.1305	0.1766	0.2767	0.7930	0.1000	45.2190
30	218	JHCMN6L5	July	Holcus	stem	CM	N6	5	15.4667100	1.7771511	350.85	3.14	0.869	0.17	2.27	3.89	0.24337	16.7	15.4686	0.67	0.5649	2.4427	0.2491	0.2758	0.2912	0.4637	0.9469	0.1000	#####
31	219	JHCAN1L1	July	Holcus	stem	CA	N1	1	0.6933128	2.4008285	320.95	3.36	0.362	0.23	2.69	4.03	0.17345	15.4	15.3603	0.85	0.2896	2.3462	0.1299	0.2291	0.2338	0.1851	0.7330	0.1000	#####
32	220	JHCAN1L2	July	Holcus	stem	CA	N1	2	0.0707069	1.9863745	320.95	3.77	0.518	0.33	3.73	4.28	0.17345	15.4	15.3603	0.815	0.4874	2.8634	0.1854	0.3345	0.3327	0.2469	0.7237	0.1000	43.7710
33	221	JHCAN1L3	July	Holcus	stem	CA	N1	3	16.5230107	1.5846154	320.95	3.63	0.865	0.25	2.89	4.02	0.17345	15.4	15.3603	0.69	0.4951	1.9651	0.1957	0.1738	0.1764	0.0787	1.0705	0.1000	44.7670
34	222	JHCAN1L4	July	Holcus	stem	CA	N1	4	4.3679286	1.4915764	320.95	4.48	0.813	0.24	2.68	4.01	0.17345	15.4	15.3603	0.54	0.3398	1.3165	0.1494	0.1550	0.1913	0.2801	0.8850	2.2100	44.7100
35	223	JHCAN1L5	July	Holcus	stem	CA	N1	5	0.8081927	2.8475283	320.95	4.01	0.391	0.20	2.72	3.83	0.17345	15.4	15.3603	0.71	0.3371	1.9552	0.1230	0.1423	0.2074	0.9283	0.7898	0.1000	44.3720
36	224	JHCAN5L1	July	Holcus	stem	CA	N5	1	1.8008725	2.190596	320.95	3.36	0.362	0.23	2.69	4.03	0.17345	15.4	15.3603	0.85	0.4615	2.8720	0.1730	0.2732	0.2507	0.2223	1.0992	0.1000	43.1460
37	225	JHCAN5L2	July	Holcus	stem	CA	N5	2	3.6441452	2.7571646	320.95	3.77	0.518	0.33	3.73	4.28	0.17345	15.4	15.3603	0.815	0.6472	1.8965	0.2004	0.1045	0.1851	0.3343	1.2914	0.1000	44.1180
38	226	JHCAN5L3	July	Holcus	stem	CA	N5	3	1.9217839	2.2205738	320.95	3.63	0.865	0.25	2.89	4.02	0.17345	15.4	15.3603	0.69	0.4339	3.4213	0.1700	0.1633	0.3177	0.1652	0.5959	0.1000	#####
39	227	JHCAN5L4	July	Holcus	stem	CA	N5	4	664.1629643	0.5577801	320.95	4.48	0.813	0.24	2.68	4.01	0.17345	15.4	15.3603	0.54	0.2319	1.8956	0.1034	0.1498	0.1691	0.2061	0.4464	0.1000	44.4130
40	228	JHCAN5L5	July	Holcus	stem	CA	N5	5	2.5979492	1.6232079	320.95	4.01	0.391	0.20	2.72	3.83	0.17345	15.4	15.3603	0.71	0.4580	2.2634	0.1635	0.1538	0.2058	0.8256	0.5904	0.1777	#####
41	229	JHCAN6L1	July	Holcus	stem	CA	N6	1	3.5354044	1.5381189	320.95	3.36	0.362	0.23	2.69	4.03	0.17345	16.7	15.4686	0.85	0.4924	2.2106	0.2017	0.3422	0.1935	0.1897	0.8309	0.1000	44.0210
42	230	JHCAN6L2	July	Holcus	stem	CA	N6	2	5.3900100	1.7036734	320.95	3.77	0.518	0.33	3.73	4.28	0.17345	16.7	15.4686	0.815	0.7276	2.0023	0.2262	0.2262	0.3386	0.5168	1.6081	0.1000	43.4140
43	231	JHCAN6L3	July	Holcus	stem	CA	N6	3	30.8069976	0.8172922	320.95	3.63	0.865	0.25	2.89	4.02	0.17345	16.7	15.4686	0.69	0.5820	1.9503	0.1790	0.2080	0.2309	0.4813	0.3595	0.1000	45.1340
44	232	JHCAN6L4	July	Holcus	stem	CA	N6	4	2.3679667	1.8884596	320.95	4.48	0.813	0.24	2.68	4.01	0.17345	16.7	15.4686	0.54	0.3821	1.5077	0.1036	0.2213	0.1428	0.2419	0.8935	0.2941	45.8780
45	233	JHCAN6L5	July	Holcus	stem	CA	N6	5	4.4437857	1.4358596	320.95	4.01	0.391	0.20	2.72	3.83	0.17345	16.7	15.4686	0.71	0.5426	1.5348	0.1537	0.1434	0.2328	2.0454	0.8182	0.1000	#####
46	234	JHD1N1R1	July	Holcus	Root	D1	N1	1	0.2316655	2.0253297	223.23	4.46	0.415	0.27	3.09	4.3	0.17143	15.4	15.3603	0.85	0.4172	0.8054	0.2414	0.1200	0.1161	8.5694	0.5998	0.1274	32.7700
47	235	JHD1N1R2	July	Holcus	Root	D1	N1	2	1.5486788	1.7787346	223.23	4.3	1.53	0.25	2.84	4.07	0.17143	15.4	15.3603	0.76	0.3193	0.5497	0.1497	0.0930	0.0880	4.8950	0.5037	0.2783	#####
48	236	JHD1N1R3	July	Holcus	Root	D1	N1	3	12.9849433	0.6395692	223.23	4.57	0.908	0.25	3.15	3.97	0.17143	15.4	15.3603	0.51	0.2516	0.5439	0.1574	0.1109	0.0882	7.5022	0.3553	0.1563	35.0630
49	237	JHD1N1R5	July	Holcus	Root	D1	N1	5	0.6964145	2.5891077	223.23	3.67	0.524	0.19	2.33	3.86	0.17143	15.4	15.3603	0.38	0.3935	0.6711	0.1868	0.1099	0.1316	6.0989	0.5983	0.1270	#####
50	238	JHD1N5R1	July	Holcus	Root	D1	N5	1	1.0495023	1.5228531	223.23	4.46	0.415	0.27	3.09	4.3	0.17143	15.4	15.3603	0.85	0.2342	0.5812	0.1811	0.0902	0.0936	7.4031	0.3886	0.1355	#####
51	239	JHD1N5R2	July	Holcus	Root	D1	N5	2	4.6541889	1.9216372	223.23	4.3	1.53	0.25	2.84	4.07	0.17143	15.4	15.3603	0.76	0.3657	0.6270	0.1911	0.0930	0.1005	7.7533	0.5531	0.1592	#####
52	240	JHD1N5R3	July	Holcus	Root	D1	N5	3	9.0705810	1.1192493	223.23	4.57	0.908	0.25	3.15	3.97	0.17143	15.4	15.3603	0.51	0.3103	0.4741	0.1695	0.0954	0.0959	6.3237	0.4474	0.1714	37.1290
53	241	JHD1N5R4	July	Holcus	Root	D1	N5	4	7.8953333	0.9845561	223.23	4.83	0.907	0.33	3.95	3.87	0.17143	15.4	15.3603	0.54	0.3606	0.6111	0.1565	0.1318	0.1322	5.8683	0.4184	0.3127	36.8950

Statistical analysis



Statistical analysis

1. PCA (multivariant ordenation)
   1. To help visualize the existence of groups in a or sample set variables.
   2. Reduce the number of variables without loss of information, thus allowing the application regression methods (ratio sample / regressors).
2. Anova and lineal regression (univariant)

Metabolomic-based Answer

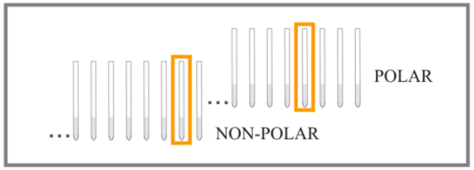
Ecological Question

↓

Experimental design

↓

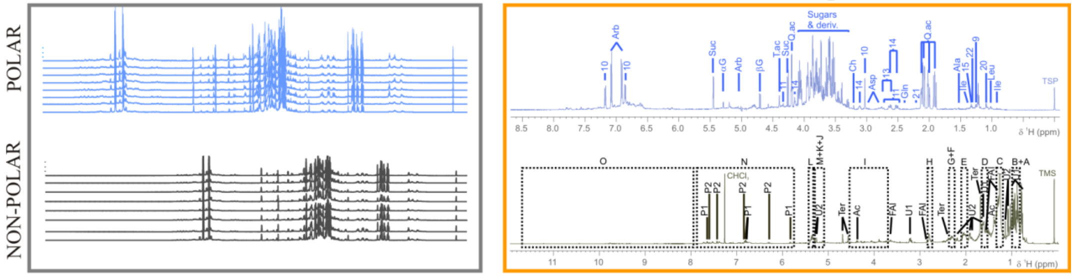
Sample collection, storage, preparation



NMR fingerprinting

NMR-based metabolites identification

NMR metabolic profile



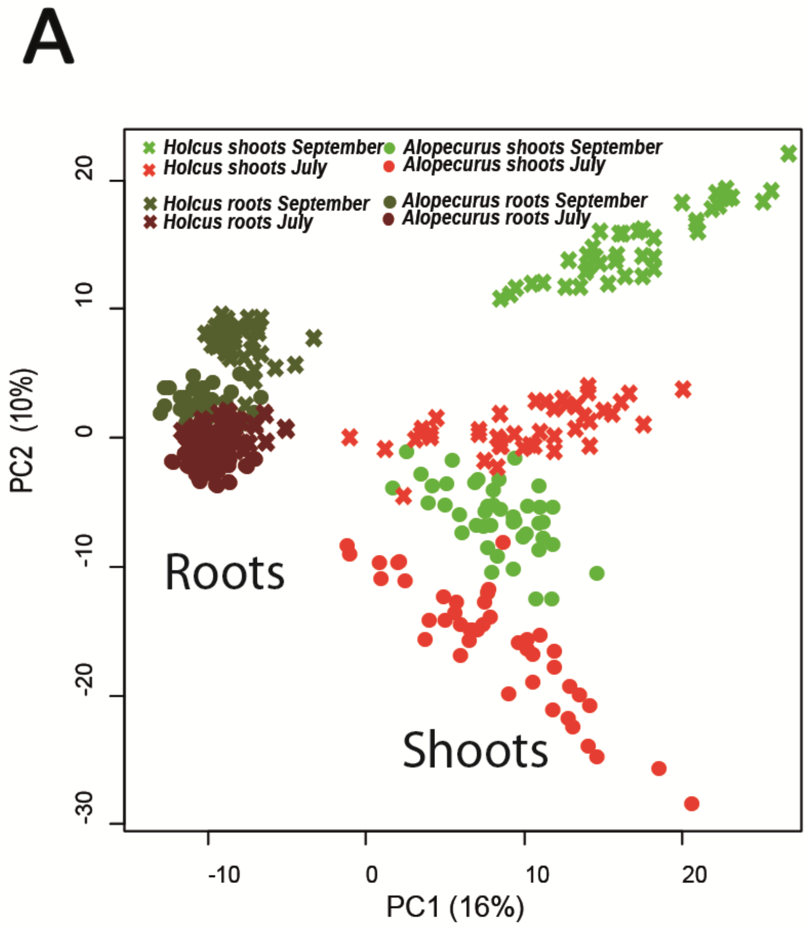
↓

Statistical analyses

↓

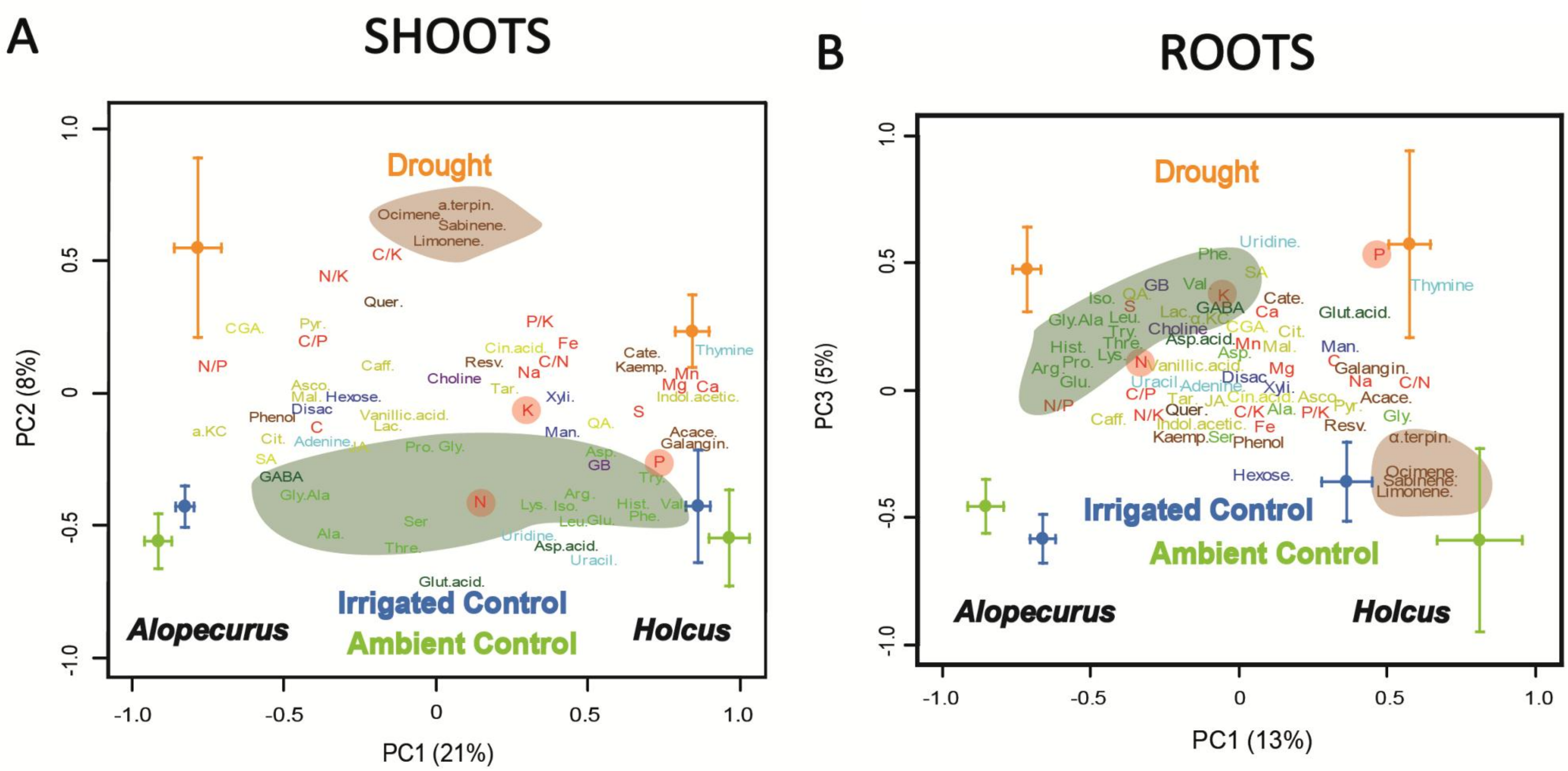
Metabolomic-based Answer

Metabolomic-based Answer



- Differences between the two species and between the two seasons of sampling
- Differences between shoots and roots at both the metabolic and elemental concentration levels
- PC2 scores show that the variability of the metabolome was lower in the root samples than in the shoot samples

Metabolomic-based Answer



- Shoots and roots of both plant species responded to drought in opposite ways

Conclusions

- Shoots and roots have different metabolomes and nutrient concentrations.
- Shoot metabolome is much more variable than the root
- Roots and shoots respond to drought with opposite metabolic changes

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ECOMETABOLOMICS

Thank you for your attention!

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