CROPS in a changing climate

PANOMICS meets Germplasm

Understanding intraspecific crop plant variation

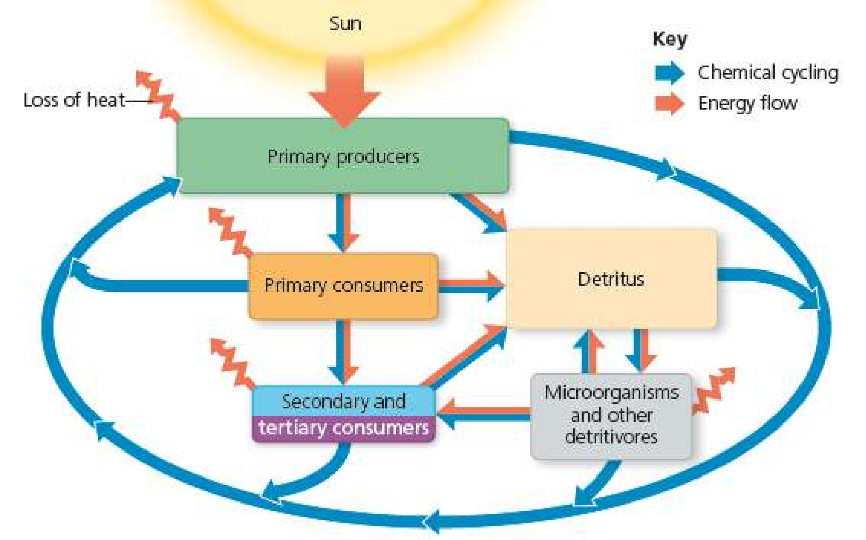
Wolfram Weckwerth

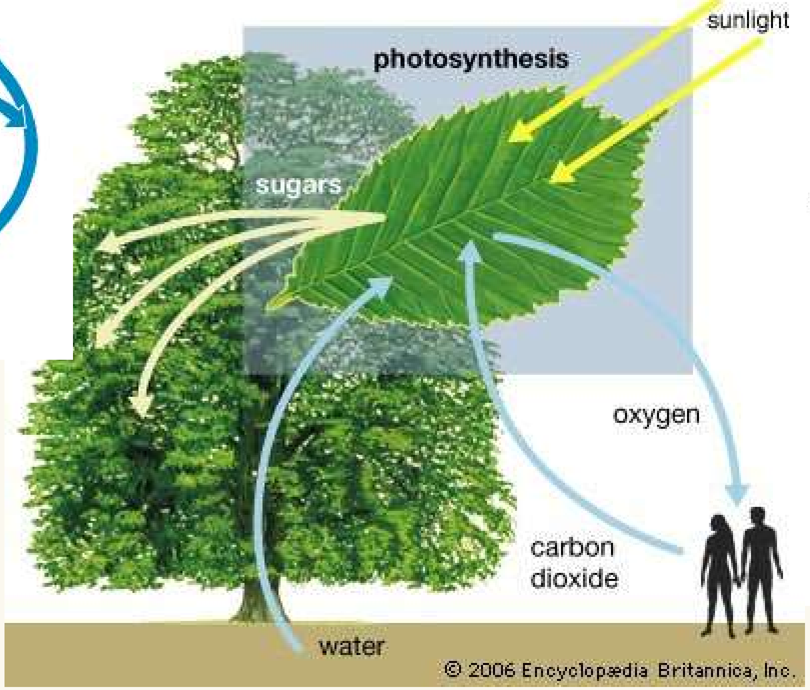
Head of Molecular Systems Biology (MOSYS)
Director of the Vienna Metabolomics Center (VIME)

ViMe
Vienna Metabolomics Center

MoSys
universität wien

Net primary production – the perfect balance on earth





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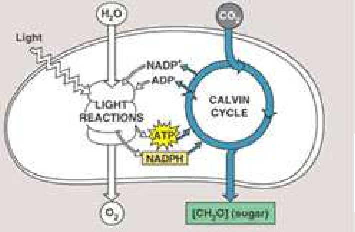
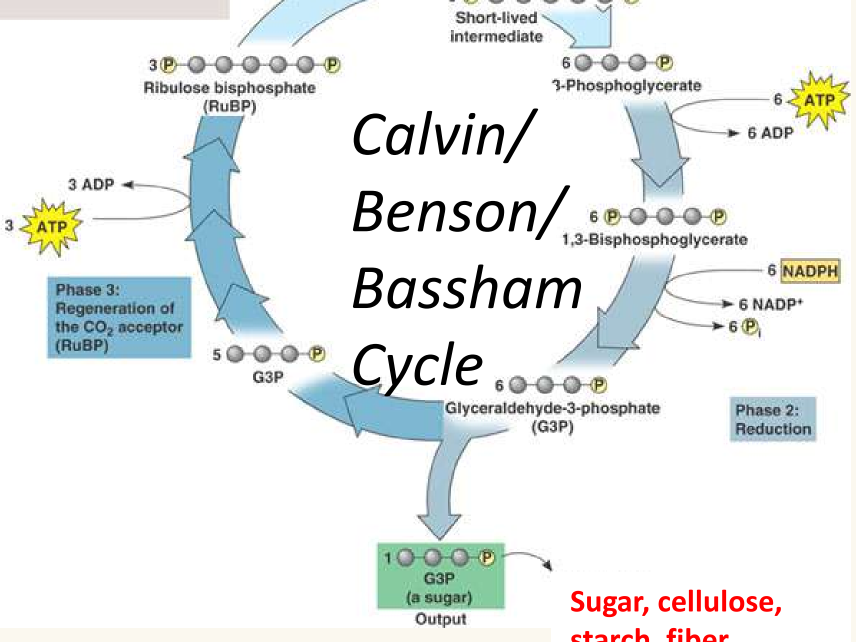


CO_2

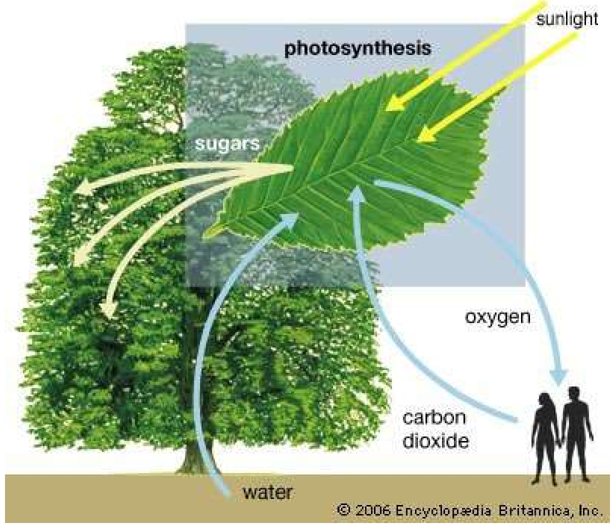
RUBISCO



Calvin/ Benson/ Bassham Cycle

Sugar, cellulose, starch, fiber, natural products, vitamins, etc.

NUTRITION, ENERGY


photosynthesis
sunlight
sugars
oxygen
carbon dioxide
water
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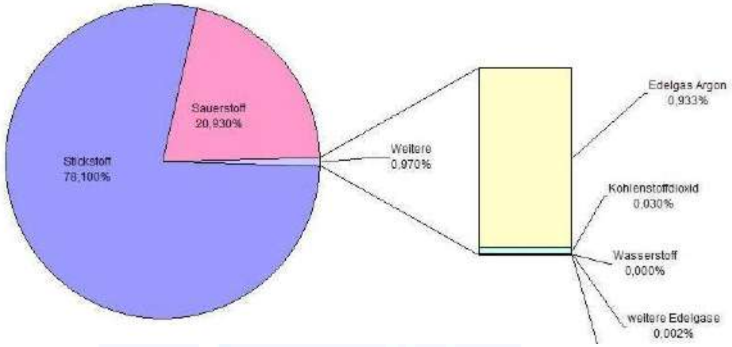
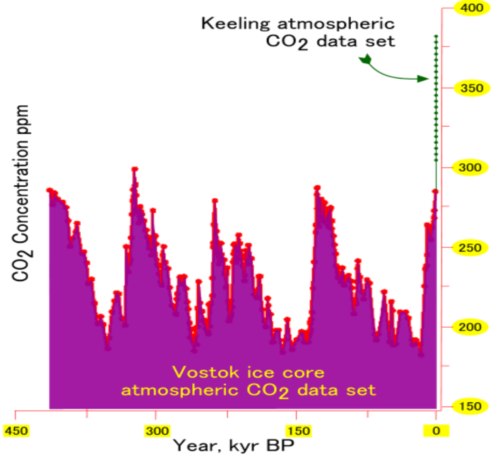
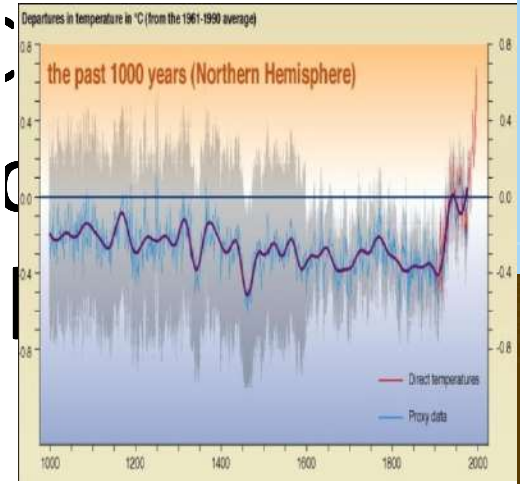
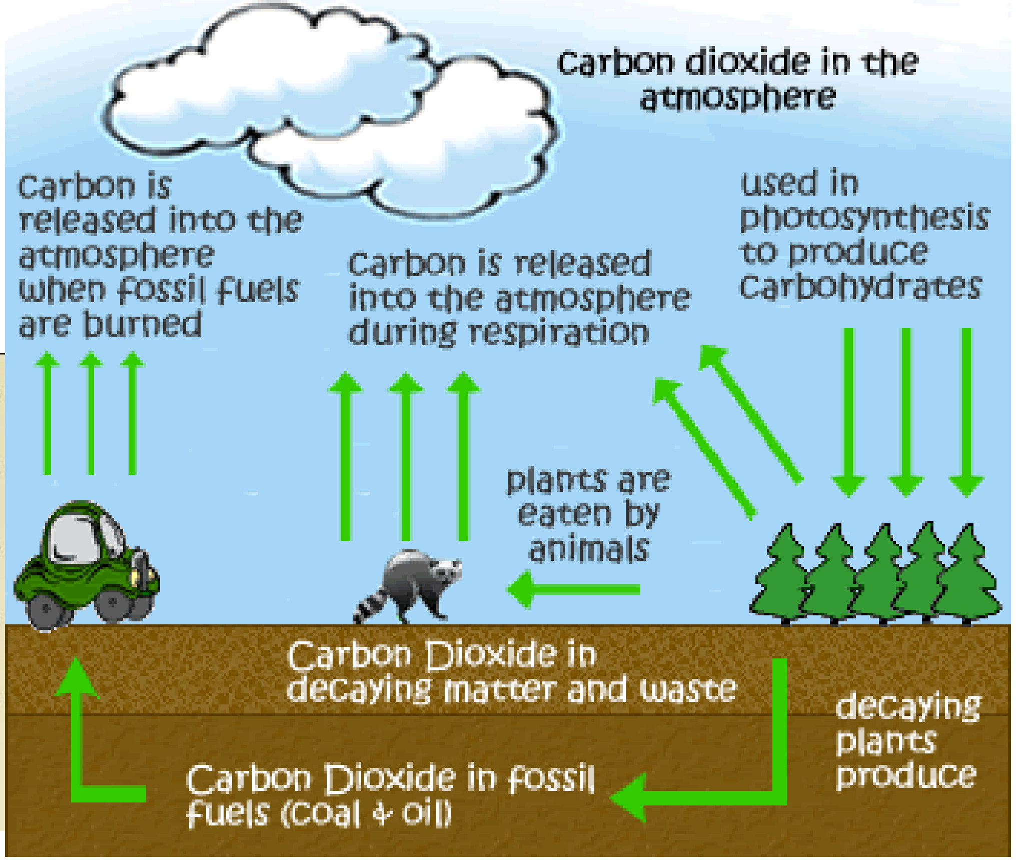

Sauerstoff 20,930%
Stickstoff 78,100%
Weitere 0,970%
Edelgas Argon 0,933%
Kohlenstoffdioxid 0,030%
Wasserstoff 0,000%
weitere Edelgase 0,002%


Keeling atmospheric CO2 data set
CO2 Concentration ppm
400
350
300
250
200
150
Vostok ice core atmospheric CO2 data set
450
300
150
0
Year, kyr BP

→ Renewal


Departures in temperature in °C (from the 1961-1990 average)
the past 1000 years (Northern Hemisphere)
0.8
0.4
0.0
-0.4
-0.8
Direct temperatures
Proxy data
1000
1200
1400
1600
1800
2000

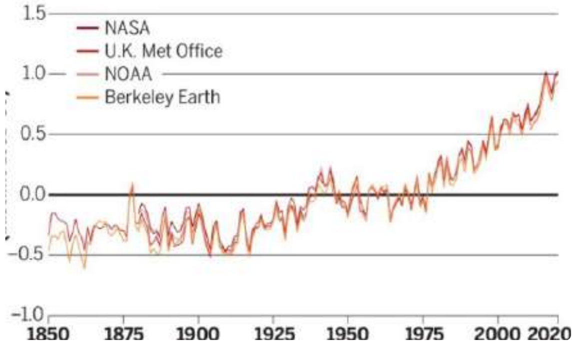

Carbon dioxide in the atmosphere
Carbon is released into the atmosphere when fossil fuels are burned
Carbon is released into the atmosphere during respiration
used in photosynthesis to produce carbohydrates
plants are eaten by animals
Carbon Dioxide in decaying matter and waste
decaying plants produce
Carbon Dioxide in fossil fuels (coal & oil)

Global climate crisis

Science AAAS

January 2021

2020 hottest year ever



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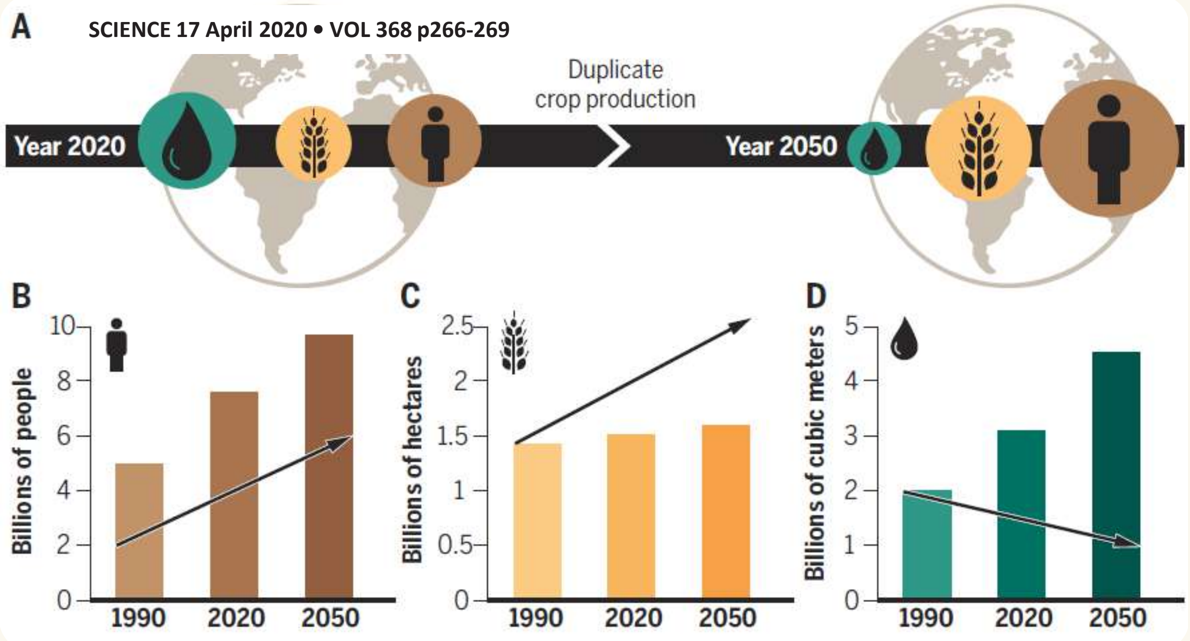
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How one error muddles the cancer genome pp. 240 & 282

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Science

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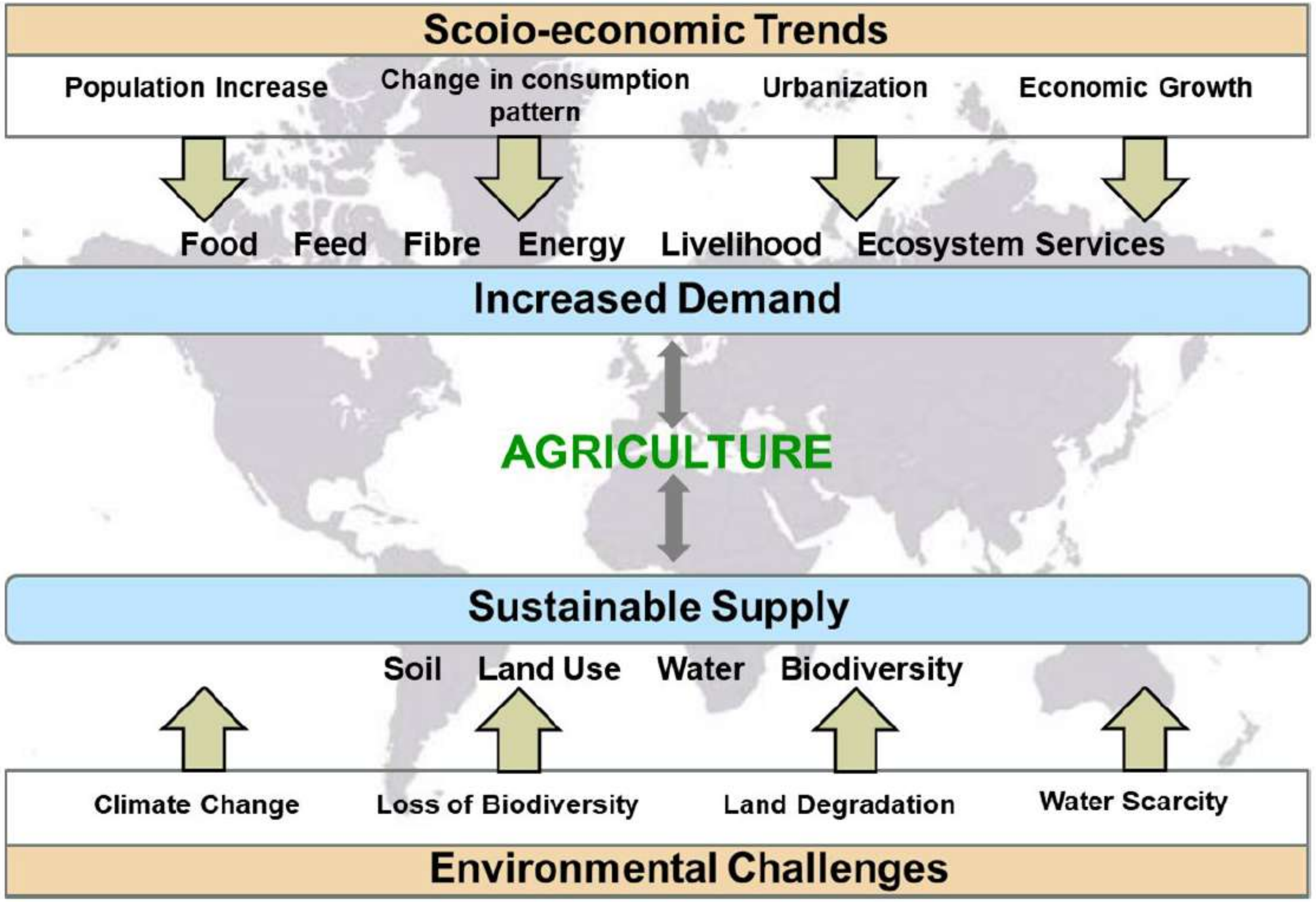
AAAS

DROUGHT

Pressures on Agriculture – Megatrends Food, Feed, Fibre



Scoio-economic Trends

Population Increase

Change in consumption pattern

Urbanization

Economic Growth

Food Feed Fibre Energy Livelihood Ecosystem Services

Increased Demand

AGRICULTURE

Sustainable Supply

Soil Land Use Water Biodiversity

Climate Change

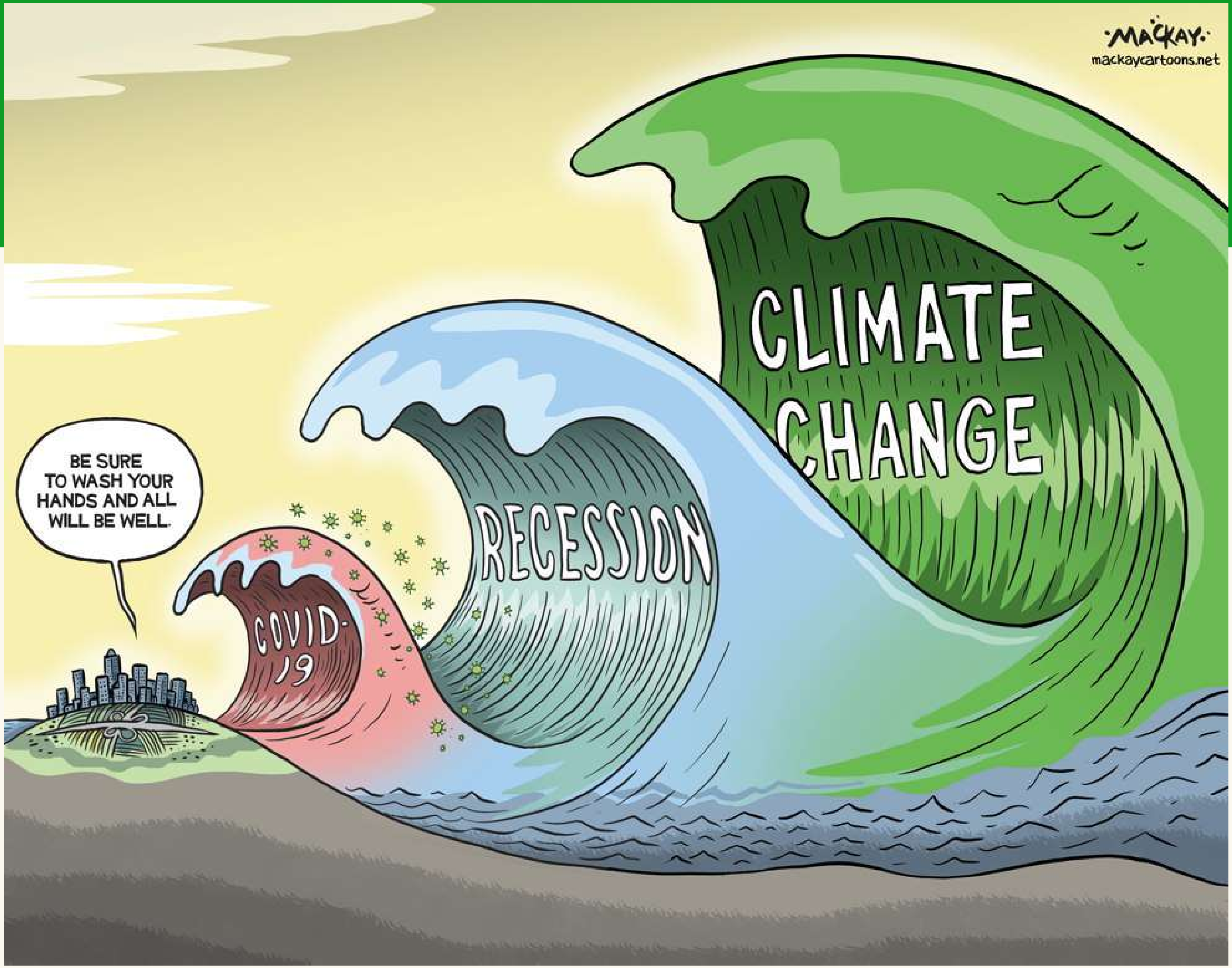
Loss of Biodiversity

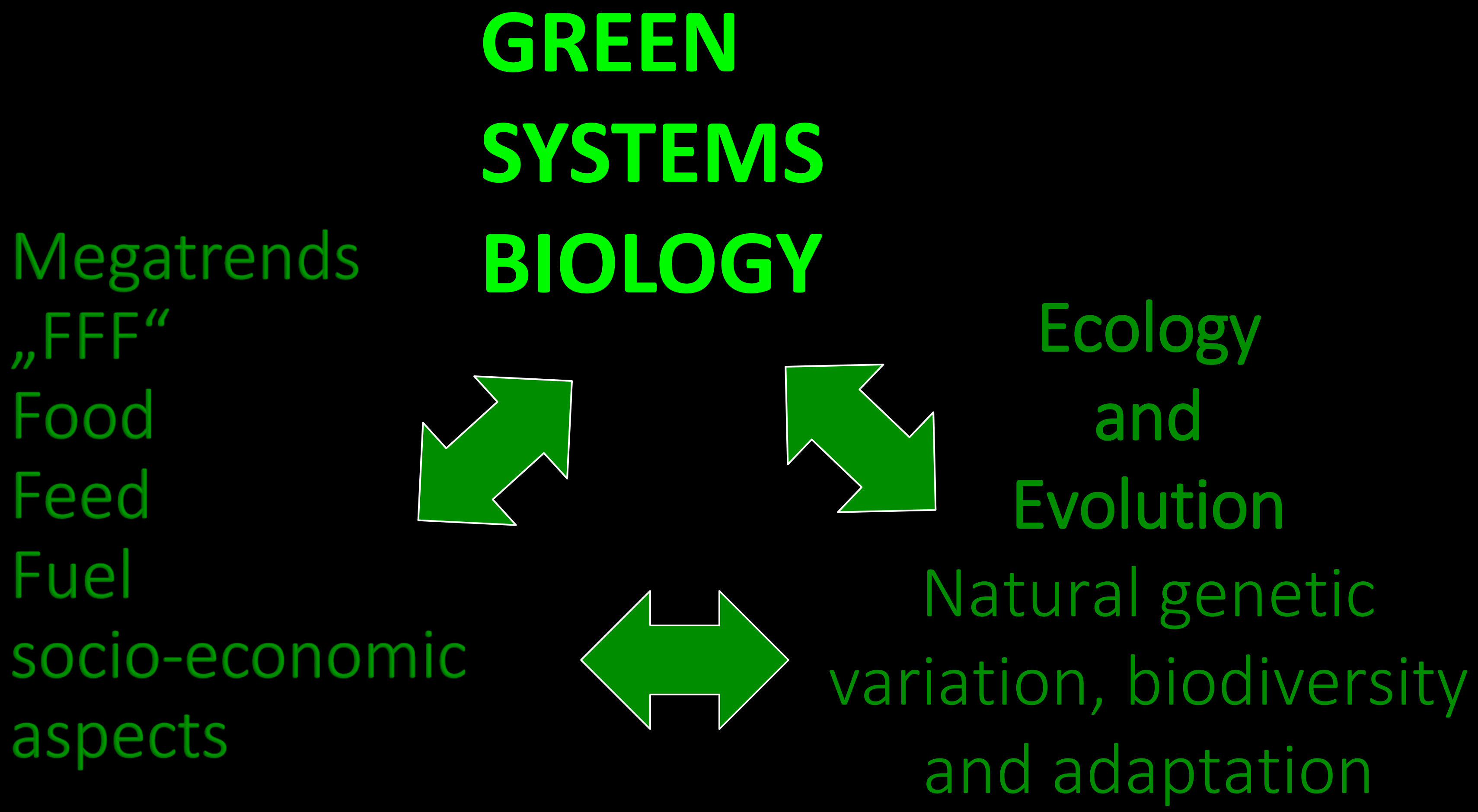
Land Degradation

Water Scarcity

Environmental Challenges

Source: FAO 2009


MACKAY
mackaycartoons.net
BE SURE TO WASH YOUR HANDS AND ALL WILL BE WELL.
COVID-19
RECESSION
CLIMATE CHANGE

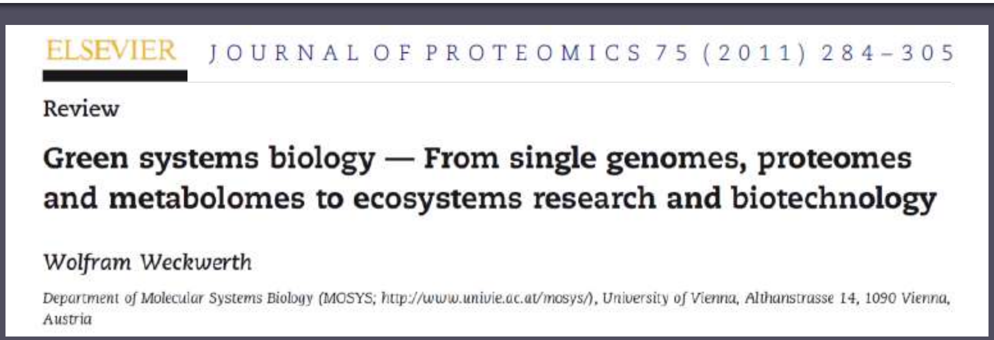


GREEN SYSTEMS BIOLOGY

Megatrends
„FFF“
Food
Feed
Fuel
socio-economic aspects

Ecology
and
Evolution

Natural genetic variation, biodiversity and adaptation



ELSEVIER JOURNAL OF PROTEOMICS 75 (2011) 284–305

Review

Green systems biology — From single genomes, proteomes and metabolomes to ecosystems research and biotechnology

Wolfram Weckwerth

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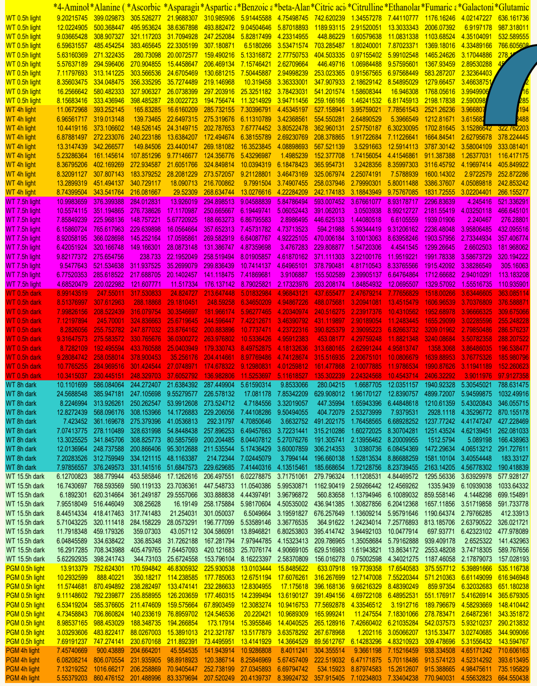
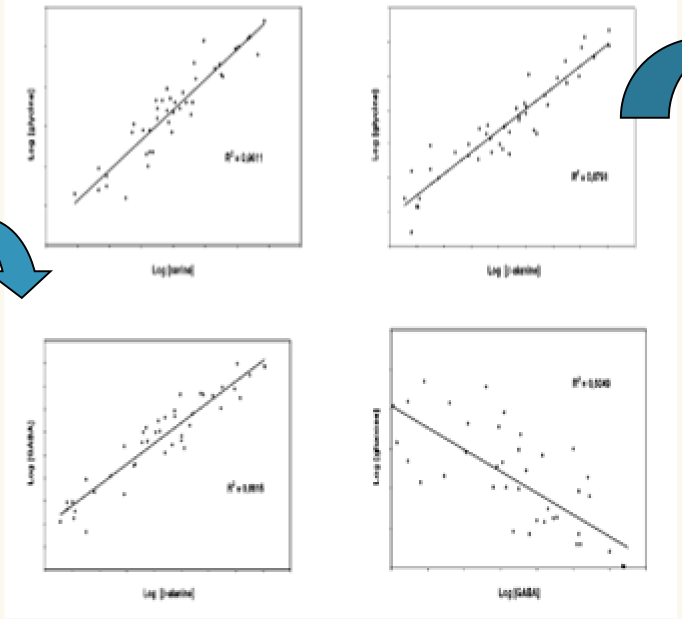
Green Systems Biology – a genotype-phenotype equation

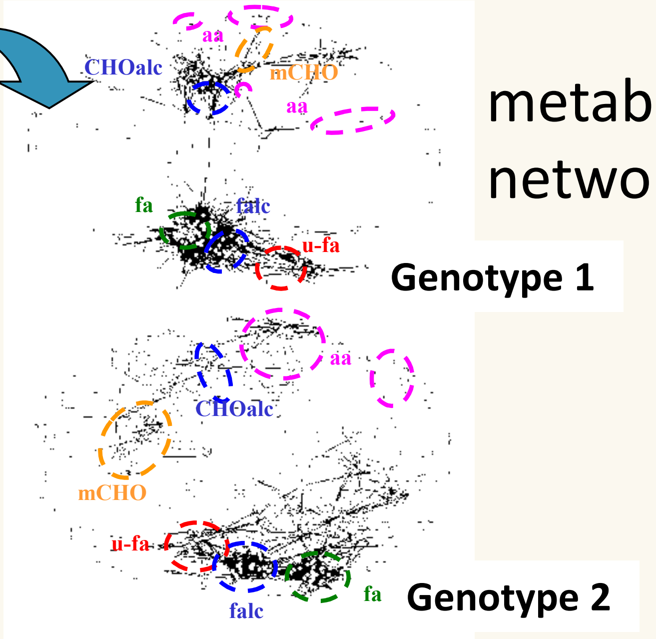
Metabolomics Correlation and Network Analysis

Data matrix
Samples, Metabolites

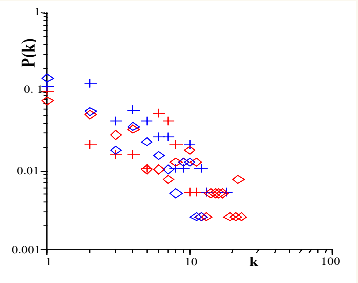


	*4-Aminol	*Alanine (	*Ascorbic	*Asparagi	*Aspartic a	*Benzoic a	*beta-Alan	*Citric aci	*Citrulline	*Ethanolar	*Fumaric a	*Galactoni	*Glutamic
WT 0.5h light	9.20215745	399.029873	305.526277	21.9688307	310.985906	5.91445588	4.75498745	742.620239	1.34557278	7.44110777	1176.16246	4.02147227	636.161736
WT 0.5h light	12.0224905	500.368447	495.953624	38.6367898	493.882472	9.04504646	5.87018893	1189.93115	2.91520051	13.3033343	2006.07392	6.9197178	987.318011
WT 0.5h light	9.03665428	308.907327	321.117203	31.7094928	247.252084	5.82817499	4.23314955	448.86229	1.60579638	11.0831338	1103.68524	4.35104091	532.589555
WT 0.5h light	6.59631557	485.454254	383.465645	22.3305199	307.180871	6.5180266	3.53471574	703.285487	1.80240001	7.87023371	1369.18016	4.33489166	766.605608
WT 0.5h light	5.63160369	271.322435	280.73098	20.0072577	159.490216	5.13316872	2.77750753	404.503335	0.97155402	5.99102548	1465.24626	3.17044886	[illegible]
WT 0.5h light	5.57637189	294.596406	270.904855	15.4458647	206.469134	7.15746421	2.62709664	446.49716	1.06984488	9.57595601	1367.93459	2.89530288	[illegible]
WT 0.5h light	7.11797693	313.141225	303.566536	24.6705469	130.681215	7.50445887	2.94998239	253.023365	0.91567565	6.97568449	583.287207	2.32364403	[illegible]
WT 0.5h light	8.35603475	334.048475	356.335295	35.7274489	219.146968	10.319458	3.36333001	347.907933	2.18629142	8.54895029	1279.66457	3.46638751	[illegible]
WT 0.5h light	16.2566642	580.482333	327.906327	26.0738399	297.203916	25.3251182	3.78423031	541.201574	1.58608344	16.946308	1768.05616	[illegible]	[illegible]
WT 0.5h light	8.15683416	333.436946	398.485287	28.0022723	194.756474	11.3214929	3.94711456	259.166166	1.46241532	6.81745913	2198.17838	[illegible]	[illegible]
WT 4h light	11.0672968	393.252145	165.83285	16.6160209	285.732155	7.30396791	4.45345197	527.158941	3.95759021	7.78561543	2521.26236	[illegible]	[illegible]
WT 4h light	6.96561717	319.013148	139.73465	22.6497315	275.319676	6.11310789	3.42368561	554.550281	2.64890529	5.3966549	1212.81671	[illegible]	[illegible]
WT 4h light	10.4419116	373.106602	149.526145	24.3149715	202.787653	7.67774452	3.80522478	362.960131	2.57750187	6.30230095	1702.81645	3.15286642	322.762203
WT 4h light	6.87881497	272.233076	240.223186	13.6384207	172.494674	6.38155789	2.69230769	208.378865	1.91722684	7.11226641	1664.84541	2.62795678	378.224445
WT 4h light	13.3147439	342.266577	149.84506	23.4400147	269.181082	16.3523845	4.08898693	567.521139	3.5291663	12.5914113	3787.30142	3.58004109	333.081401
WT 4h light	5.23286364	161.145614	107.851296	9.77146677	124.356776	5.43296987	1.4985239	152.377708	1.74156054	4.41546861	911.387388	1.26377031	116.417175
WT 4h light	8.36795206	402.169269	272.934587	21.6051766	324.849814	10.0394319	6.18478423	365.954731	3.2428356	8.35997303	3116.45792	4.19697414	405.849922
WT 4h light	8.32091127	307.807143	183.379252	28.2081229	273.572057	9.21128801	3.46473169	325.067974	2.25074191	7.5788939	1600.14302	2.9722579	252.872286
WT 4h light	13.2899319	451.494137	340.729117	18.090713	216.700862	9.7991504	3.74907455	258.037946	2.79990301	5.80011488	3386.37607	4.05089818	242.853242
WT 4h light	8.74399504	343.541764	216.081667	29.52309	268.634744	13.0276616	4.22284209	242.174183	3.18843949	9.75767085	1831.72555	3.02204401	266.155277
WT 7.5h light	10.9983659	376.399388	284.012831	13.926019	294.898513	9.04588839	5.84786494	593.007452	3.67661077	8.93178717	2296.83639	4.245416	521.336291
WT 7.5h light	10.5574115	351.194865	276.738626	17.1170987	250.665667	6.19449741	5.06052443	391.062013	3.0503938	8.99212727	2181.55419	4.03250118	466.645101
WT 7.5h light	7.85849239	225.968136	148.757221	5.67720925	188.663273	6.86795583	2.8986495	446.625133	1.44080518	6.6105559	1939.01906	2.240467	276.28801
WT 7.5h light	6.15860724	765.617963	229.639898	16.0564664	357.652313	7.45731782	4.73713523	594.21988	5.39344419	9.31206162	2236.48048	3.95806485	432.095516
WT 7.5h light	8.92058195	366.028698	145.252164	17.0595861	269.582919	6.64087767	4.92225105	470.006184	3.10013063	8.63958246	1903.57956	2.73344934	357.406774
WT 7.5h light	6.42051924	320.166748	149.166301	28.0873148	131.386747	4.87359698	3.4767283	229.808877	1.54720306	4.4541545	1299.26645	2.6602503	181.968062
WT 7.5h light	9.82177372	275.654756	238.733	22.1952049	258.519494	8.01905857	4.61870162	371.111303	3.22100176	11.9519221	1991.78338	3.58673729	320.194222
WT 7.5h light	9.5477643	521.534638	311.937525	35.2699079	299.836439	10.7414137	4.64965101	378.790481	4.81710543	8.33765566	1915.42092	3.38286549	305.16063
WT 7.5h light	6.77520353	285.618522	217.688705	20.1402457	141.118475	7.41869681	3.9106887	155.502589	2.39905137	6.64764864	1712.66682	2.94010291	113.183208
WT 7.5h light	4.68520479	220.022982	121.607771	11.517334	176.137142	8.79025821	2.17323976	203.208174	1.84854932	12.0695507	1329.57092	1.55516735	110.935901
WT 0.5h dark	8.99143519	247.55011	317.530833	24.824727	213.647448	5.01832984	4.96843121	437.655477	2.47679214	7.77656829	1518.00266	3.63446605	363.085114
WT 0.5h dark	8.51376997	307.612963	288.18868	29.1810451	248.59258	6.34650209	4.94867226	488.075681	3.20941081	13.4515479	1606.96539	3.70376809	376.588871
WT 0.5h dark	7.99826156	208.522439	316.079754	30.3546697	181.966174	5.96277465	4.20340974	240.516275	2.23917376	10.4310562	1952.68978	3.96666325	309.675066
WT 0.5h dark	7.12197894	245.70001	324.836663	25.6719645	244.596447	7.42212671	3.46390792	431.119897	2.90189054	11.2483445	1655.29099	3.02285596	255.248228
WT 0.5h dark	8.2826056	255.752782	247.877032	23.8764162	200.883896	10.7737471	4.23722316	390.825379	2.39095223	6.82663732	3209.01962	2.79850486	286.576237
WT 0.5h dark	9.31647573	275.583572	330.765676	36.0300272	263.976802	10.5336426	4.95912383	453.08177	4.29759248	11.8821348	3240.08684	3.50782358	288.207522
WT 0.5h dark	8.7282109	192.495594	433.760588	25.0403949	179.330743	8.49752875	4.18132636	313.680165	2.62991244	4.95813747	1358.3068	3.86486035	196.538477
WT 0.5h dark	9.28084742	258.058014	378.900453	35.256176	204.414661	8.97769486	4.74128674	315.516935	2.20675101	10.0806679	1639.88953	3.76775326	185.980796
WT 0.5h dark	10.7765255	284.969516	301.424544	27.0748971	174.678322	9.12980831	4.01259812	161.477868	2.10077885	11.9786534	1990.87626	3.11941189	152.260623
WT 0.5h dark	10.3415037	230.445151	248.329703	37.6052792	136.982806	11.5253697	5.11618527	135.302239	2.24324568	10.4543714	2406.32292	3.9011976	97.9127358
WT 8h dark	10.1101699	586.084064	244.272407	21.6384392	287.449904	5.61590314	9.8533066	280.04215	1.6687705	12.0351157	1940.92328	5.30545021	788.631475
WT 8h dark	24.5688548	385.947181	247.105698	9.55279577	226.578132	17.081178	7.85342209	629.908012	1.96170127	12.8390757	4899.72007	5.94599875	1032.49916
WT 8h dark	8.2246994	313.926261	250.262547	53.9912608	273.524712	4.7184556	3.32019057	447.35994	1.65943396	6.44848618	1210.61359	5.43020843	346.055715
WT 8h dark	12.8272439	568.096176	308.153966	14.1726883	229.206056	7.44108286	9.50494055	404.72079	2.53273999	7.9379531	2928.1118	4.35296772	870.155178
WT 8h dark	7.423452	361.169678	275.379396	41.0536813	292.31797	4.70850646	3.6632752	491.202175	1.76458565	6.68928252	1237.77242	4.41747247	427.228469
WT 8h dark	7.07413775	278.110489	328.631998	54.8448438	257.896253	6.49457663	3.72231441	315.210286	1.60272025	8.30704281	1251.43524	4.62139451	262.081033
WT 8h dark	13.3025525	341.845706	308.825773	80.5857569	200.204485	8.04407812	5.27076276	191.305741	2.13956462	8.20009955	1512.5794	5.089198	166.438963
WT 8h dark	12.0136964	248.737588	200.866406	95.3012688	211.535544	5.17436429	3.60007859	306.214353	3.0380736	6.08454369	1472.29634	4.06513212	291.727611
WT 8h dark	7.20283526	312.759949	334.121115	48.1163387	214.72344	7.02445079	3.7994144	196.660138	1.52813534	8.86688259	1581.10104	3.40554448	183.33127
WT 8h dark	7.97856557	376.249573	331.141516	51.6847573	229.629685	7.41440316	4.13515461	185.668654	1.72128756	8.23739455	2163.14205	4.56778302	190.418839
WT 15.5h dark	6.12700823	388.779944	453.585846	17.1262616	206.497551	6.02278875	3.71751061	279.796324	1.11208531	4.84469572	1295.56336	3.63929978	577.928127
WT 15.5h dark	16.7430697	768.593569	590.119133	23.7036361	447.548733	11.0540386	5.99530871	1162.90419	2.59266442	12.4569262	1335.9439	6.10939038	1033.64332
WT 15.5h dark	6.1892301	620.314664	361.249187	29.5557066	303.888838	4.44397491	3.96796872	560.83658	1.13794946	6.10089032	859.558146	4.1448298	699.154891
WT 15.5h dark	7.95518049	516.446049	308.25628	16.19149	258.175884	5.98170604	4.50535002	436.941385	1.30827856	6.20412368	1657.11856	3.51719858	591.733778
WT 15.5h dark	8.44514334	418.417463	317.741483	21.254031	301.050037	6.5049664	3.19591827	676.257649	1.13609214	5.95791646	1190.64374	2.79766285	412.33913
WT 15.5h dark	5.71043225	320.111418	284.158229	28.0573291	196.777099	5.53589146	3.36776535	364.91622	1.24234014	7.25776893	813.185706	2.63790522	326.021721
WT 15.5h dark	11.7918348	459.179326	359.07303	43.057112	304.586091	13.8946821	6.80253803	395.414742	3.94492103	10.0477914	697.93771	6.42323102	477.978089
WT 15.5h dark	6.04845589	334.638422	336.85348	31.7262188	167.281794	7.97944785	4.15323413	209.786965	1.35058684	5.79162888	939.409178	2.6525322	141.432963
WT 15.5h dark	16.2917285	708.343988	405.479765	7.64457093	420.121683	25.7076174	4.90669105	629.516983	1.61943821	13.8634172	2553.48208	3.74718305	589.767656
WT 15.5h dark	5.62292935	398.241743	344.73103	25.6724558	153.796104	8.16223397	2.58370809	156.016278	0.75002598	4.34021275	1187.46058	2.17879073	157.028193
PGM 0.5h light	13.913379	752.624301	170.594842	46.8305932	225.930538	13.0103444	15.8485622	633.07918	19.7739358	17.6540583	375.557712	5.39891666	535.116738
PGM 0.5h light	10.2932599	888.40221	350.18217	114.238585	177.785063	12.6751194	17.6076261	316.267699	12.7147008	7.55220344	571.210363	6.61149099	616.946948
PGM 0.5h light	11.5744681	870.494892	238.282497	133.474141	232.286633	12.8304955	17.175618	396.168136	9.66216329	8.48390249	859.97354	6.32032683	651.180238
PGM 0.5h light	9.11148602	792.239877	235.858955	126.203659	177.460315	14.2399494	13.6190127	391.494156	4.69722108	6.48952531	551.176917	5.41626914	365.679305
PGM 0.5h light	6.53419204	585.376605	211.474609	159.575664	67.8903459	12.3083274	10.9416753	77.5692878	4.33546512	3.1912716	189.796679	4.58293669	148.410442
PGM 0.5h light	4.73458843	706.860824	140.233619	76.8959702	124.546536	20.220421	10.9689309	165.999241	11.247554	7.18301066	278.783471	2.64872361	343.351872
PGM 0.5h light	8.98537165	988.453029	188.348735	194.266854	173.17914	15.3955846	14.4040525	265.128916	7.42660402	6.21035284	542.037573	5.93210237	290.213832
PGM 0.5h light	3.03293606	483.822417	88.0267003	15.3891013	212.321787	13.5177879	3.63578292	267.678968	1.202116	3.05066207	1315.33477	3.02740685	344.909066
PGM 0.5h light	7.69191237	747.274141	230.670168	211.892391	73.4495951	13.4141929	14.3664529	89.5612767	6.14283296	4.83210923	309.478696	5.31556432	143.594767
PGM 4h light	7.45740669	900.43889	204.664201	45.554535	141.943914	10.9286808	8.4011241	304.355514	9.3661198	7.15216459	938.334508	4.65171242	710.606163
PGM 4h light	6.08208214	806.070554	231.935905	98.8918923	120.386714	8.25846969	5.67457409	222.519032	6.47171875	5.70118486	913.574123	4.52314292	393.613495
PGM 4h light	7.13219252	1016.66217	206.258869	70.9405447	252.738199	27.0345893	6.69794742	534.15923	8.87974583	15.2612607	915.388665	4.98475611	735.195829
PGM 4h light	5.55379203	860.476152	201.488996	83.3379694	207.520249	20.4139737	8.39924732	357.915405	7.10234803	7.33404238	770.940031	4.55632823	664.550438





metabolite
network



Weckwerth et al. (2001) ASMS
Weckwerth (2003) Annual Review of Plant Biology.
Weckwerth et al. (2004) PNAS
Weckwerth et al. (2004) Proteomics

1. Stochastic Model of metabolism
2. Network topology

Fundamental relation between network dynamics (statistics) and GENOME SEQUENCE

stochas
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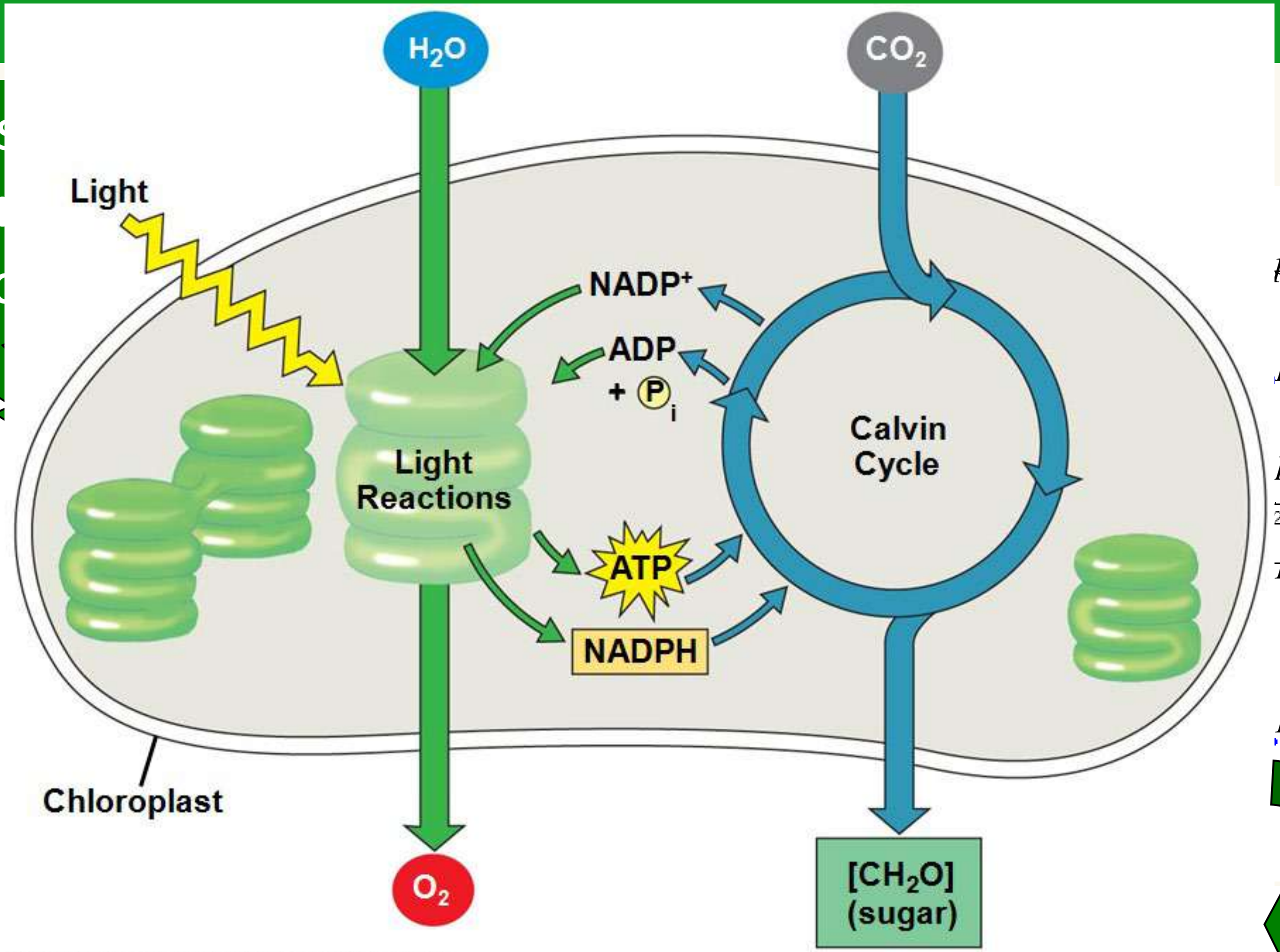
equati

Steuer et al. (2003) Bioinformatics
Weckwerth (2003) Annual Review of Plant Biology
Morgenthal et al. (2006) Biosystems
Müller-Linow et al. (2007) BMC Systems Biology
Weckwerth (2010) Bioanalysis
Weckwerth (2011) Analytical and Bioanalytical Chemistry
Weckwerth (2011) Proteomics
Weckwerth (2019) Frontiers Applied Math and Statistics
…



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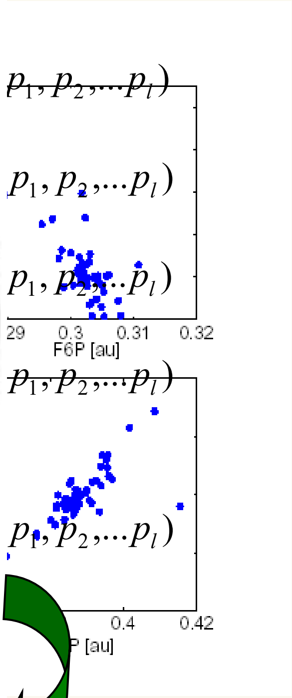
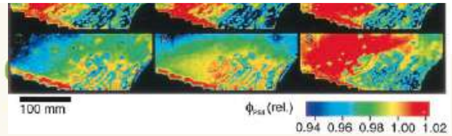




iance matrix

Fundamental relation between network dynamics (statistics/correlation/covariance/network) and GENOME SEQUENCE

Weckwerth (2019) Frontiers Applied Mathematics and Statistics 5, 29

Jacobian entries are the Elasticities of the **enzymatic Reactions** dependent on metabolite concentration changes

$$\frac{\partial f}{\partial M}$$

→ Change in reaction rate ∂f_i

→ Change in metabolite concentrations ∂M_i

$$\frac{dM_1}{dt} = f_1(M_1, M_2, ...M_n)$$
$$\frac{dM_2}{dt} = f_2(M_1, M_2, ...M_n)$$
$$\frac{dM_3}{dt} = f_3(M_1, M_2, ...M_n)$$
$$\frac{dM_4}{dt} = f_4(M_1, M_2, ...M_n)$$
$$.....$$
$$\frac{dM_n}{dt} = f_n(M_1, M_2, ...M_n)$$

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial M_1} & \frac{\partial f_1}{\partial M_2} & \cdots & \frac{\partial f_1}{\partial M_n} \\ \frac{\partial f_2}{\partial M_1} & \frac{\partial f_2}{\partial M_2} & \cdots & \frac{\partial f_2}{\partial M_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial M_1} & \frac{\partial f_n}{\partial M_2} & \cdots & \frac{\partial f_n}{\partial M_n} \end{pmatrix}_{n \times n}$$

J = N*∂f/ ∂M

- ➢ J: Jacobian matrix
- ➢N: stoichiometric Matrix

=> GENOME SEQUENCE

- ➢v: Reaction rate;

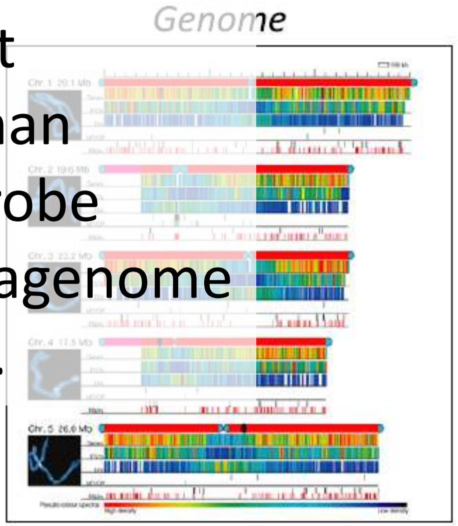
M: metabolite

Genome-scale metabolic reconstruction

Weckwerth (2019) Frontiers Applied Mathematics and Statistics 5, 29

Genome-scale metabolic reconstruction

- Plant
- Human
- Microbe
- Metagenome
- etc…



namic phenotypic plasticity

Fundamental relation between network dynamics (statistics/correlation/covariance/network) and GENOME SEQUENCE

Weckwerth (2019) Frontiers Applied Mathematics and Statistics 5, 29

Jacobian entries are the Elasticities of the **enzymatic Reactions** dependent on metabolite concentration changes

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$$\ldots\ldots$$
$$\frac{dM_n}{dt} = f_n(M_1, M_2, \ldots M_n)$$

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial M_1} & \frac{\partial f_1}{\partial M_2} & \cdots & \frac{\partial f_1}{\partial M_n} \\ \frac{\partial f_2}{\partial M_1} & \frac{\partial f_2}{\partial M_2} & \cdots & \frac{\partial f_2}{\partial M_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial M_1} & \frac{\partial f_n}{\partial M_2} & \cdots & \frac{\partial f_n}{\partial M_n} \end{pmatrix}_{n \times n}$$

$$\underline{J = N * \partial f / \partial M}$$

- J: Jacobian matrix
- N: stoichiometric Matrix

=> GENOME SEQUENCE

- v: Reaction rate;

M: metabolite

A genotype-phenotype-equation

Weckwerth (2019) Frontiers Applied Mathematics and Statistics 5, 29

Genome sequence

↕

Data derived dynamic model of the phenotype

Structure of the Jacobi is defined by the stoichiometric Matrix derived from the genome

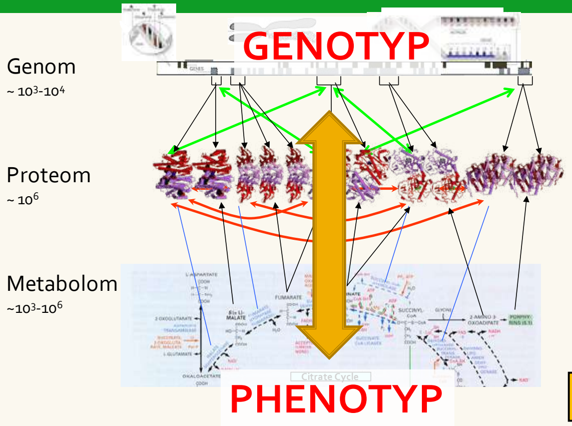
Environmentally driven stochastic Diffusionmatrix

$$JC + CJ^T = -2D$$

Covariance Matrix (dynamic network of the metabolic system)

A systematic relation

Weckwerth (2011) *Unpredictability of Metabolism*
Weckwerth (2011) *Green Systems Biology*
Weckwerth (2019) *Unification of system theory in Biology and Ecology*

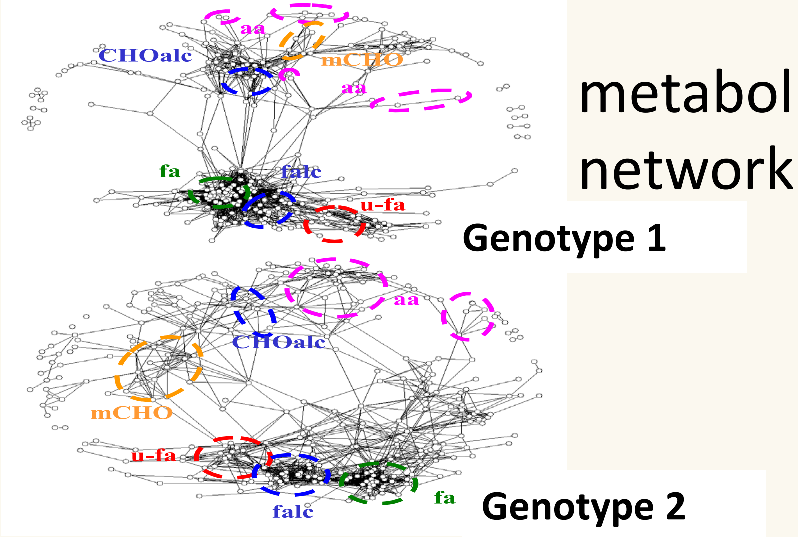


$$\begin{array}{c|cccccc} & M1 & M2 & M3 & \dots & Mn \\ \hline S1 & q_{1,1} & q_{1,2} & q_{1,3} & \dots & q_{1,n} \\ S2 & q_{2,1} & q_{2,2} & q_{2,3} & \dots & q_{2,n} \\ S3 & q_{3,1} & q_{3,2} & q_{3,3} & \dots & q_{3,n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ Sm & q_{m,1} & q_{m,2} & q_{m,3} & & q_{m,n} \end{array}$$

n-dimensional Data matrix

$$\frac{dM_1}{dt} = f(M_1, M_2, \dots M_n)$$
$$\frac{dM_2}{dt} = f(M_1, M_2, \dots M_n)$$
.....
$$\frac{dM_n}{dt} = f(M_1, M_2, \dots M_n)$$

Systems equations



metabolite network

PHENOTYPE C

Systems theory J

$$\boxed{JC + CJ^T = -2D}$$

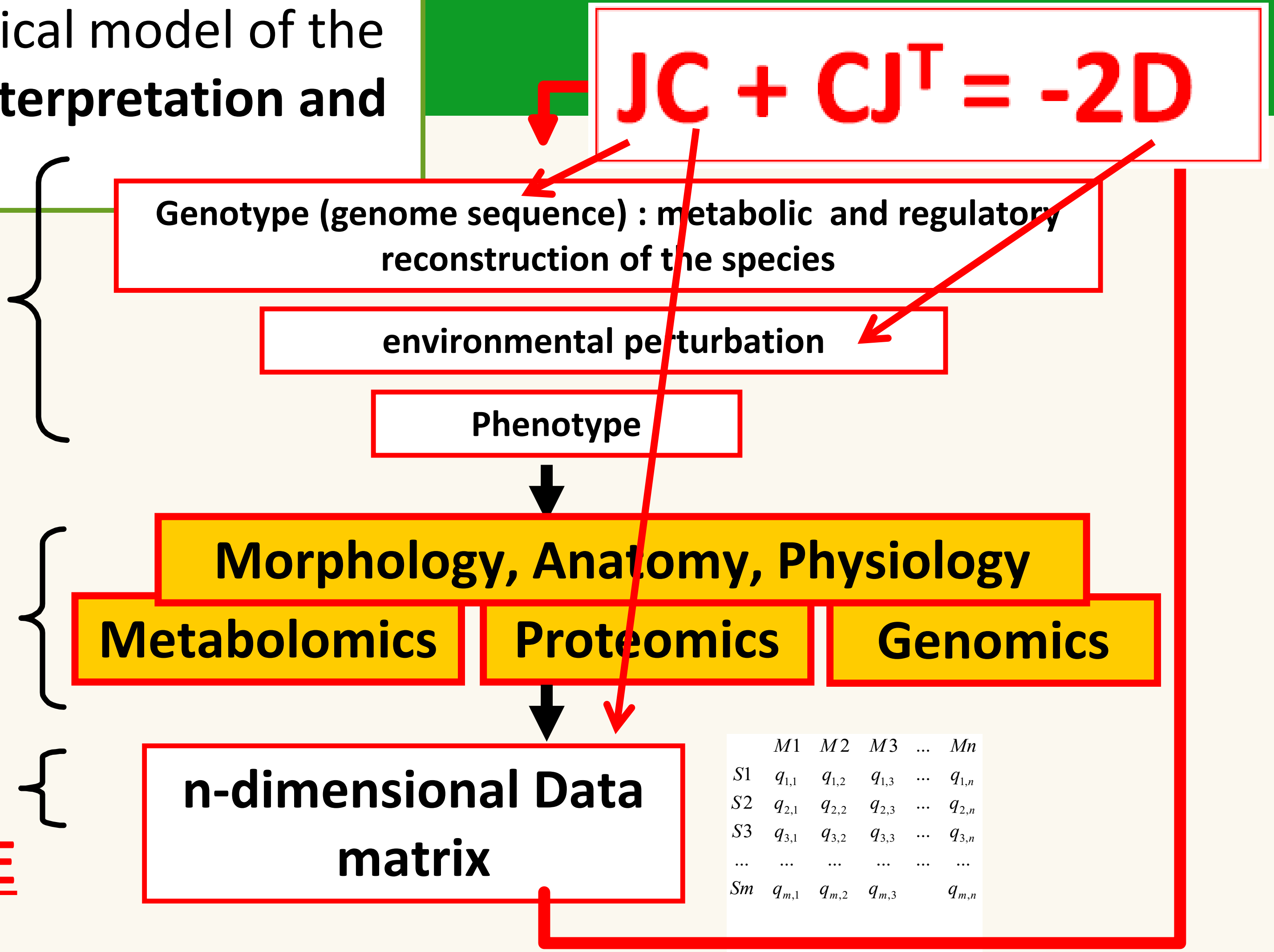
Multivariate
Statistics
Trajectories

Genome
sequence
GENOTYPE N

Linking OMICS and Modelling Platform MoSys

Weckwerth (2011) Green Systems Biology

Data driven mathematical model of the system – **Functional interpretation and Prediction**



$$JC + CJ^T = -2D$$

Genotype-Phenotype - relationship

Genotype (genome sequence) : metabolic and regulatory reconstruction of the species

environmental perturbation

Phenotype

“READOUT”

Morphology, Anatomy, Physiology

Metabolomics

Proteomics

Genomics

in vivo

Dynamics - PHENOTYPE

n-dimensional Data matrix

$$\begin{array}{c|ccccc} & M1 & M2 & M3 & \dots & Mn \\ S1 & q_{1,1} & q_{1,2} & q_{1,3} & \dots & q_{1,n} \\ S2 & q_{2,1} & q_{2,2} & q_{2,3} & \dots & q_{2,n} \\ S3 & q_{3,1} & q_{3,2} & q_{3,3} & \dots & q_{3,n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ Sm & q_{m,1} & q_{m,2} & q_{m,3} & & q_{m,n} \end{array}$$

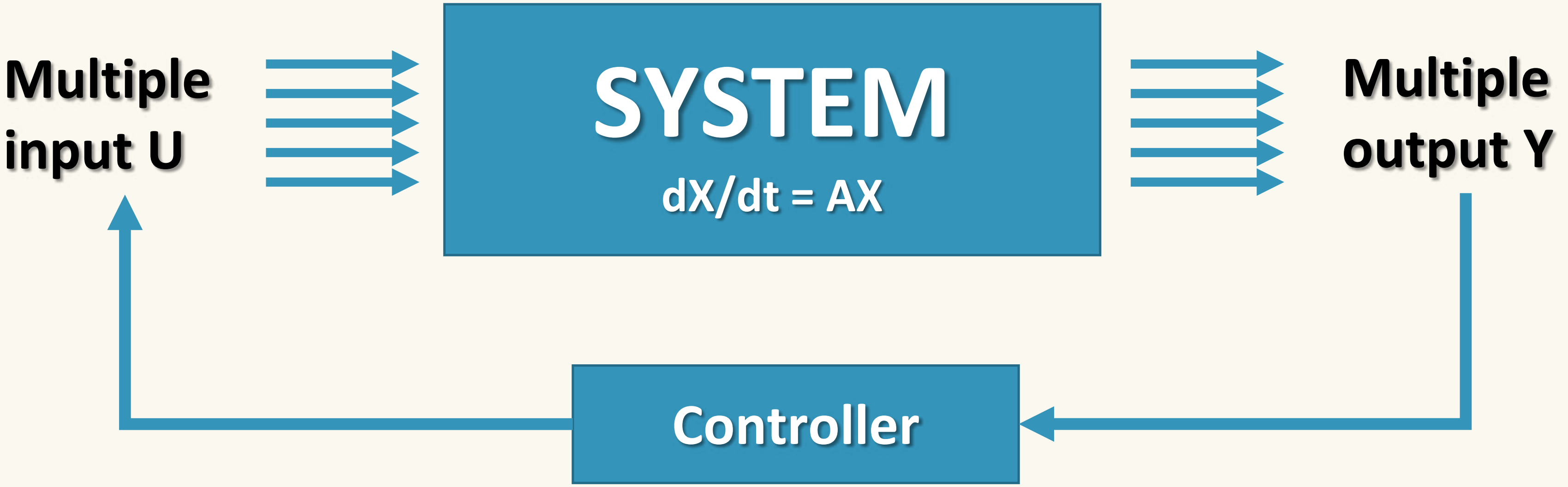
Lyapunov matrix equation in ecology/population dynamics – Richard Levins and Robert May

Weckwerth (2019) Frontiers Applied Mathematics and Statistics 5, 29

- Introduction of the Population Community Matrix which is equivalent with the Jacobi matrix
- Introduction of the Lyapunov matrix equation for stochastic systems $A^TP + P\,A + Q = O$
- Applications to population dynamics
- May Hypothesis: increasing diversity destabilizes the ecosystem measured by the eigenvalues of the Jacobian but….
- no random structure of the community matrix

Lyapunov matrix equation is a central approach in artificial intelligence and bioinspired control theory

MIMO



Multiple input U

SYSTEM

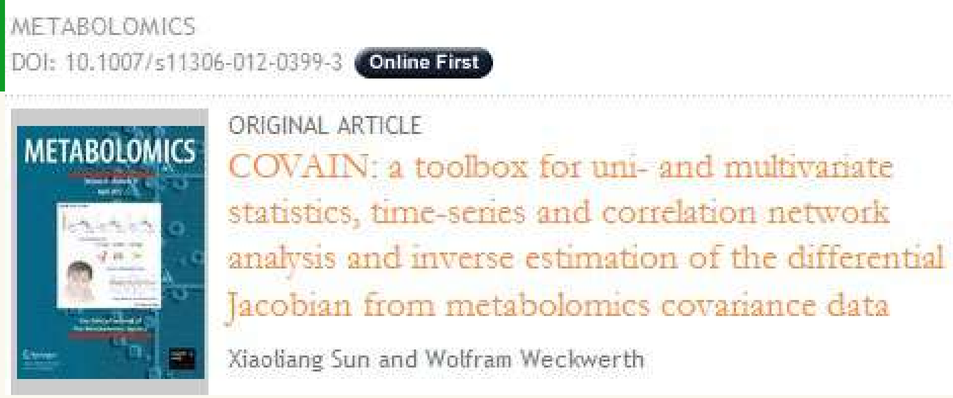
$dX/dt = AX$

Multiple output Y

Controller

Weckwerth (2019) Towards a unification of **system-theoretical** concepts in biology and ecology – the stochastic Lyapunov matrix equation and its inverse application. Frontiers Applied Mathematics and Statistics 5,29

COVAIN – *COVA*riance *IN*verse: toolbox for data integration and mining



METABOLOMICS
DOI: 10.1007/s11306-012-0399-3 Online First

ORIGINAL ARTICLE

COVAIN: a toolbox for uni- and multivariate statistics, time-series and correlation network analysis and inverse estimation of the differential Jacobian from metabolomics covariance data

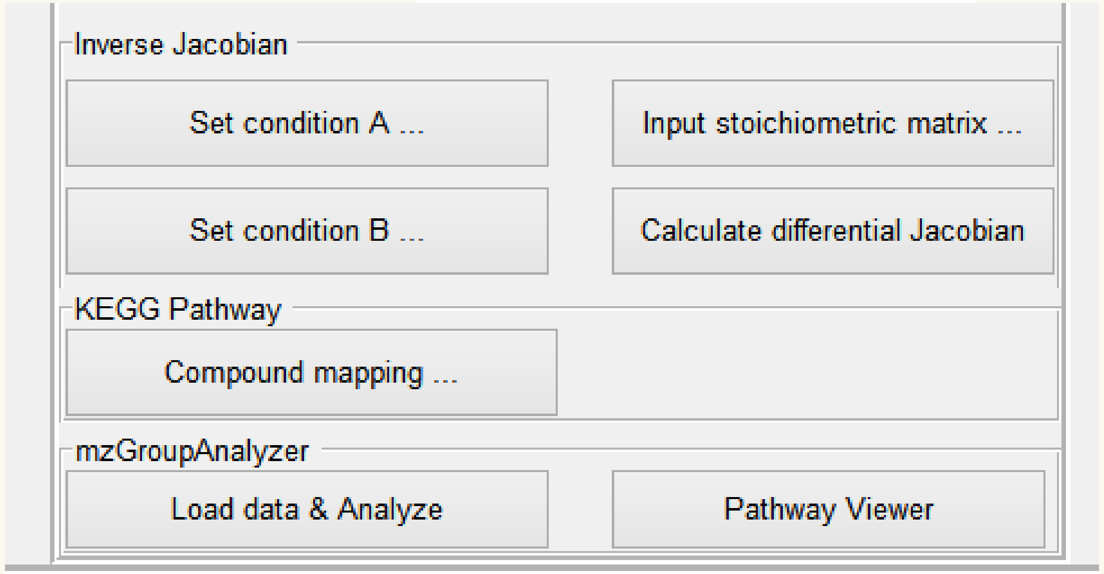
Xiaoliang Sun and Wolfram Weckwerth

- PCA, ICA, HCA, etc.
- GRANGER CAUSALITY
- data integration
- data transformation
- data normalization
- metabolic modelling
- metabolomics
- proteomics
- transcriptomics
- other data

Sun & Weckwerth
2012 Metabolomics

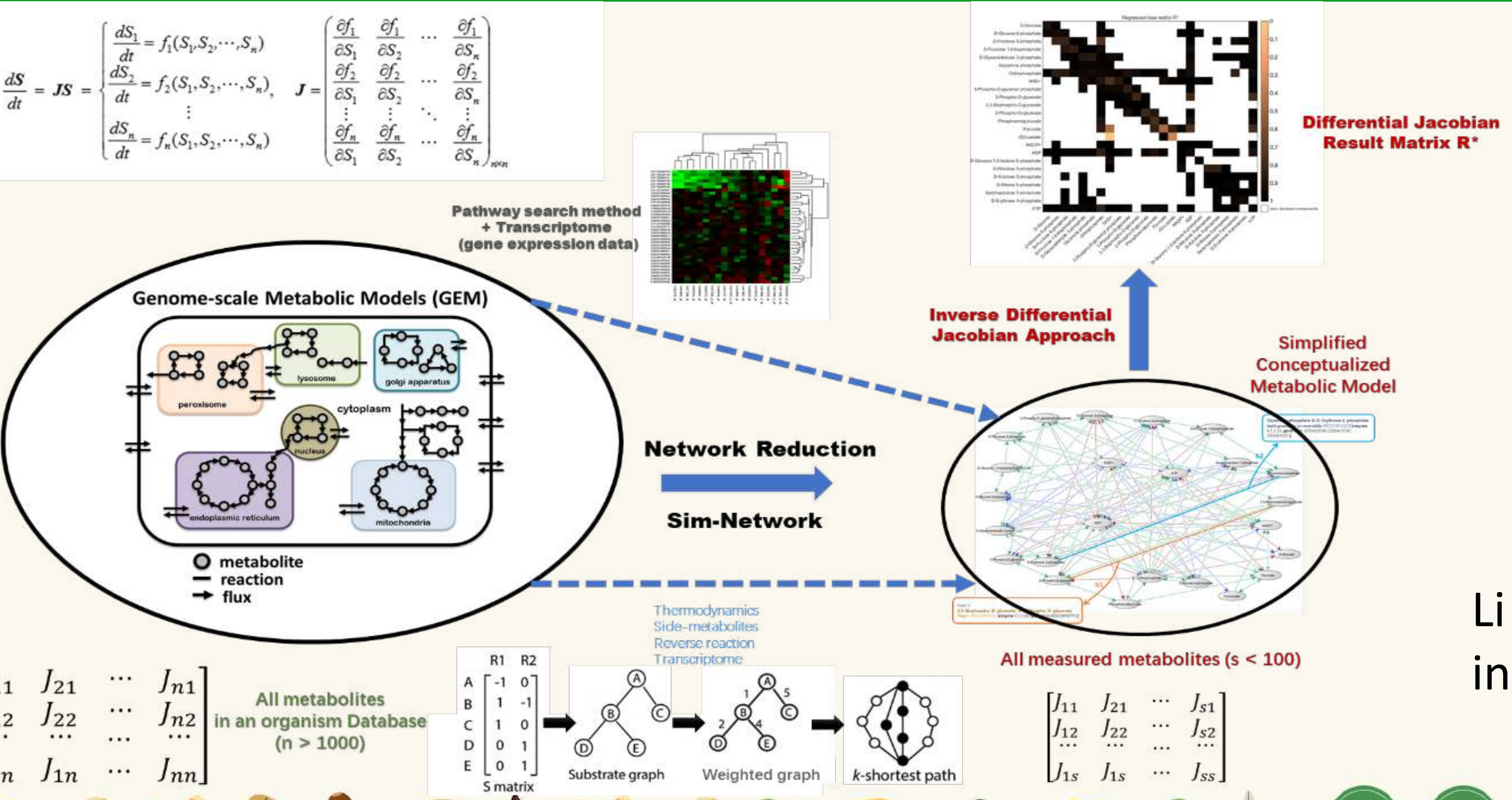
$$\boxed{JC + CJ^T = -2D}$$

COVAIN GUI Matlab



COVRECON: Combining Genome-scale Metabolic Network Reconstruction and Data-driven Inverse Modeling

$$\frac{d\mathbf{S}}{dt} = \mathbf{JS} = \begin{cases} \frac{dS_1}{dt} = f_1(S_1, S_2, \cdots, S_n) \\ \frac{dS_2}{dt} = f_2(S_1, S_2, \cdots, S_n), \\ \vdots \\ \frac{dS_n}{dt} = f_n(S_1, S_2, \cdots, S_n) \end{cases} \quad \mathbf{J} = \begin{pmatrix} \frac{\partial f_1}{\partial S_1} & \frac{\partial f_1}{\partial S_2} & \cdots & \frac{\partial f_1}{\partial S_n} \\ \frac{\partial f_2}{\partial S_1} & \frac{\partial f_2}{\partial S_2} & \cdots & \frac{\partial f_2}{\partial S_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial S_1} & \frac{\partial f_n}{\partial S_2} & \cdots & \frac{\partial f_n}{\partial S_n} \end{pmatrix}_{n\times n}$$



$$\begin{bmatrix} J_{11} & J_{21} & \cdots & J_{n1} \\ J_{12} & J_{22} & \cdots & J_{n2} \\ \cdots & \cdots & \cdots & \cdots \\ J_{1n} & J_{1n} & \cdots & J_{nn} \end{bmatrix}$$

$$\begin{array}{c|cc} & R1 & R2 \\ \hline A & -1 & 0 \\ B & 1 & -1 \\ C & 1 & 0 \\ D & 0 & 1 \\ E & 0 & 1 \end{array}$$

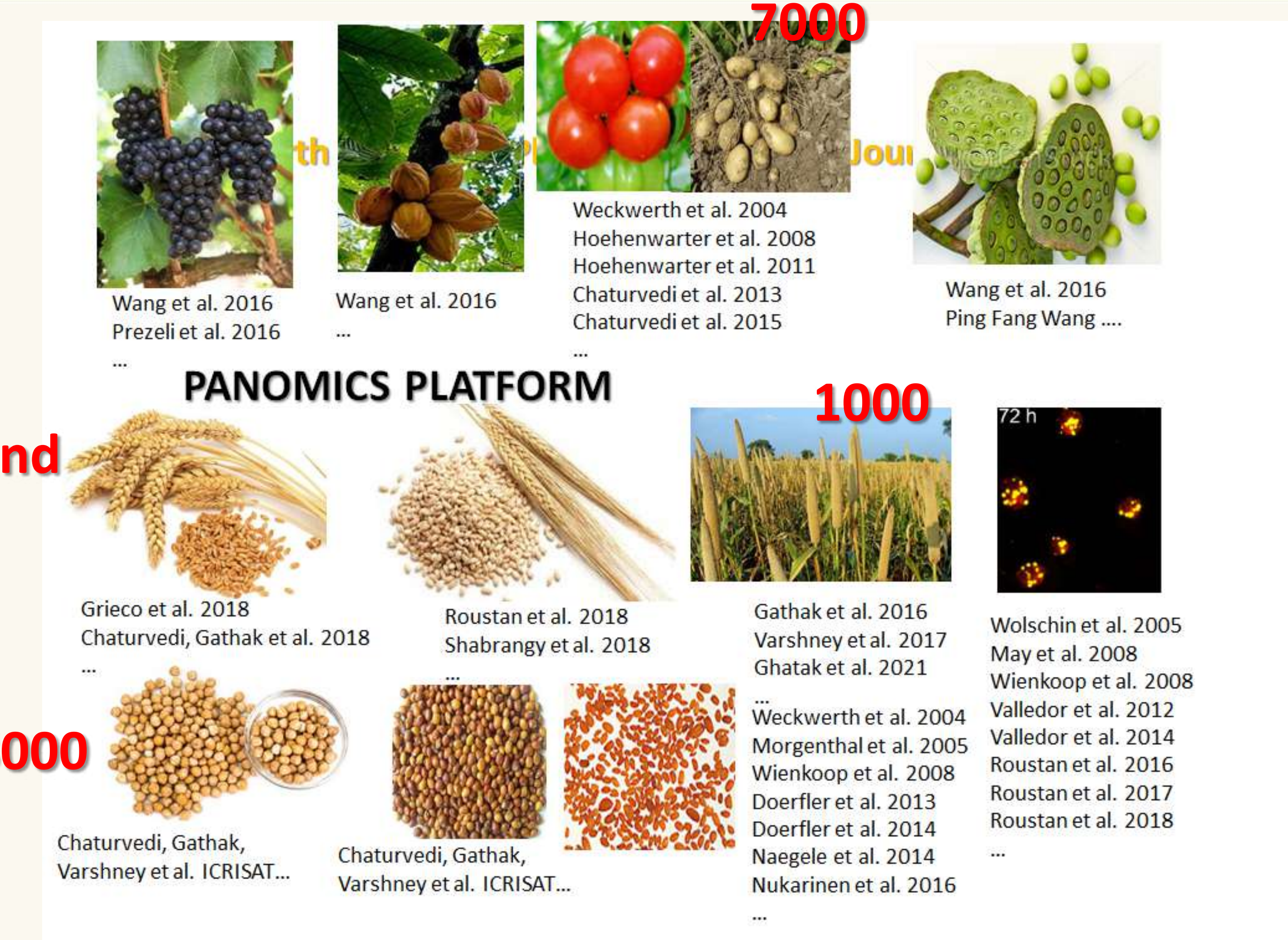
$$\begin{bmatrix} J_{11} & J_{21} & \cdots & J_{s1} \\ J_{12} & J_{22} & \cdots & J_{s2} \\ \cdots & \cdots & \cdots & \cdots \\ J_{1s} & J_{1s} & \cdots & J_{ss} \end{bmatrix}$$

Jiahang Li

Li et al. 2022
in preparation

Panomics meets Germplasm

Weckwerth et al 2020 Plant Biotechnology Journal



7000

Wang et al. 2016
Prezeli et al. 2016
...

Wang et al. 2016
...

Weckwerth et al. 2004
Hoehenwarter et al. 2008
Hoehenwarter et al. 2011
Chaturvedi et al. 2013
Chaturvedi et al. 2015
...

Wang et al. 2016
Ping Fang Wang ....

PANOMICS PLATFORM

1001 and more?

1000

Grieco et al. 2018
Chaturvedi, Gathak et al. 2018
...

Roustan et al. 2018
Shabrangy et al. 2018
...

Gathak et al. 2016
Varshney et al. 2017
Ghatak et al. 2021
...

Wolschin et al. 2005
May et al. 2008
Wienkoop et al. 2008
Valledor et al. 2012
Valledor et al. 2014
Roustan et al. 2016
Roustan et al. 2017
Roustan et al. 2018
...

3000

Chaturvedi, Gathak,
Varshney et al. ICRISAT...

Chaturvedi, Gathak,
Varshney et al. ICRISAT...

Weckwerth et al. 2004
Morgenthal et al. 2005
Wienkoop et al. 2008
Doerfler et al. 2013
Doerfler et al. 2014
Naegele et al. 2014
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...

From Farm to Table to Health - Panomics

Weckwerth et al. PANOMICS meets germplasm. *Plant Biotechnology Journal* ***18, 1507-1525 (2020).***

Zhang et al. Spatial distribution of proteins and metabolites in developing wheat grain and their differential regulatory response during the grain filling process. *The Plant Journal* ***107, 669-687 (2021).***

Atanasov et al. Natural products in drug discovery: advances and opportunities. *Nature Reviews Drug Discovery* ***20, 200-216 (2021).***

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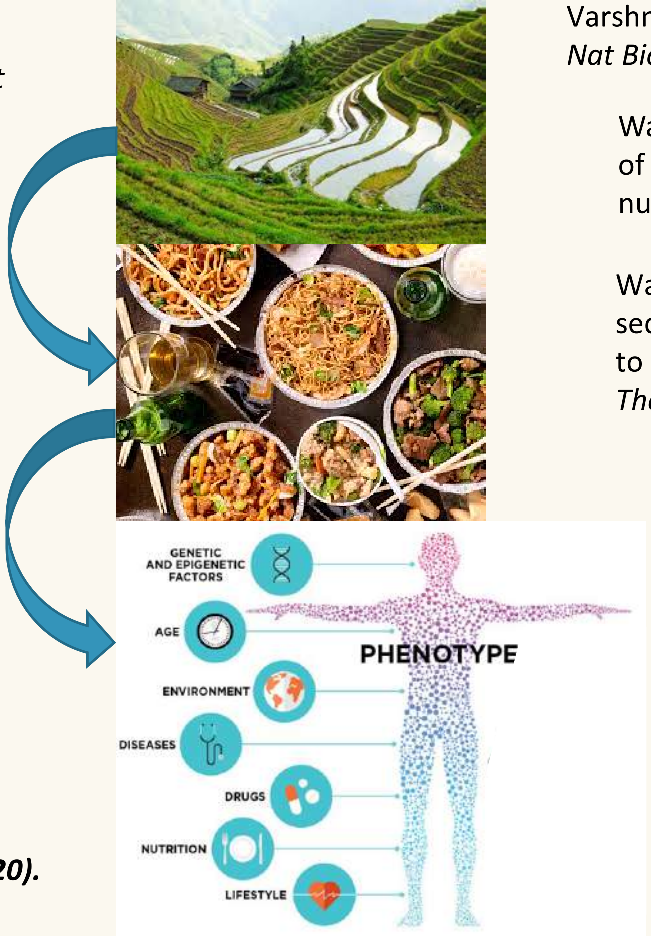
Wilson et al. Inverse data-driven modeling and multiomics analysis reveals phgdh as a metabolic checkpoint of macrophage polarization and proliferation. *Cell Reports* ***30, 1542-1552. e1547 (2020).***



Varshney et al. Rapid delivery systems for future food security. *Nat Biotechnol* ***39, 1179-1181 (2021).***

Wang et al. Metabolomic and proteomic profiles reveal the dynamics of primary metabolism during seed development of lotus (Nelumbo nucifera). *Frontiers in plant science* ***7, 750 (2016).***

Wang et al. System level analysis of cacao seed ripening reveals a sequential interplay of primary and secondary metabolism leading to polyphenol accumulation and preparation of stress resistance. *The Plant Journal* ***87, 318-332 (2016).***

Wang et al. System-level and granger network analysis of integrated proteomic and metabolomic dynamics identifies key points of grape berry development at the interface of primary and secondary metabolism. *Frontiers in plant science* ***8, 1066 (2017).***

Bässler et al. Evidence for novel tomato seed allergens: IgE-reactive legumin and vicilin proteins identified by multidimensional protein fractionation− mass spectrometry and in silico epitope modeling. ***J Proteome Res 8, 1111-1122 (2009).***

Leitner et al. Combined metabolomic analysis of plasma and urine reveals AHBA, tryptophan and serotonin metabolism as potential risk factors in gestational diabetes mellitus (GDM). *Frontiers in Molecular Biosciences* ***4, 84 (2017).***

Check for updates

correspondence

Rapid delivery systems for future food security

To the Editor — The current world population of 7.8 billion is predicted to reach 10 billion by 2057 (https://www.worldometers.info/world-population/#pastfuture). Future access to affordable and healthy food will be challenging, with malnutrition already affecting one in three people worldwide. The agricultural sector currently provides livelihoods for 1.1 billion people and accounts for 26.7% of global employment (https://data.worldbank.org/indicator/SL.AGR.EMPL.ZS). However, our reliance on a small number of crop species for agricultural calorie production and depletion of land, soil, water and genetic resources, combined with extreme weather events and changing disease/pest dynamics, are already jeopardizing future food security[1]. Climate change–induced reductions in the global yield of major crops (for example, rice, wheat, maize and soybean) are more pronounced in low-latitude regions and thus affect farmers in developing countries[2]. As is evident from temperate cereal crops, a robust seed system that delivers improved cultivars to replace old cultivars is a plausible approach to adapting agriculture to climate change[3]. Here we provide an overview of how seed input supply systems and new production and harvesting technologies can generate increased incomes for developing world farmers and deliver better products

required to realize higher crop yields and income for smallholder farmers and deliver enhanced agricultural outputs (Fig. 1). The integration of planting good-quality seeds of elite crop varieties with improved decision support tools, mechanical harvesting and post-harvest management will increase production gains. Electronic trading portals (for example, Wefarm (https://about.wefarm.com/), eNAM (https://www.enam.gov.in/web/) and Digital Mandi (https://www.iitk.ac.in/MLAsia/digimandi.htm)) and support from farmer associations should help farmers market their produce directly for fairer prices. Further processing and addition of value can also deliver improved products to consumers and increase farmer's income (Fig. 1).

Seed is the single entry point for crop resilience and productivity. The sustainability of crop production is vitally dependent on the timely supply of improved seed and other inputs. In developing countries, formal seed supply systems generally do not meet farmers' demands, such that smallholder farmers source more than 80% of their seed from informal seed systems. Some South Asian countries, such as Nepal, ensure seed supply through community-based seed banks[9], but most of the seed is not from elite varieties, which limits productivity and reduces environmental resilience. Promoting elite

protect the environment[11]. Seeding rate and planting time are critical components of crop production packages, but they vary between locations. For instance, in China over-seeding of wheat reduced potential yield by 6.3% and under-seeding of maize reduced potential yields by 20.6%; meanwhile, timely sowing increased yields by 6.3% for wheat and 15% for maize. Timely irrigation and fertilizer application reduced wheat yield losses by 6.2%, whereas maize yield increased by 7.5% and wheat by 11.6% following recommended fertilizer regimes[10]. Integrated nutrient management incorporates optimal nutrients from various resources and synchronizes crop demand and supply. Using innovative nutrient-specific strategies such as urease inhibitors, fertilizer incorporation at depth and coated urea could improve nutrient use efficiency and crop productivity. Integrated pest management involving innovative ecological pest management strategies could help manage agricultural pests. Under rain-fed conditions, the use of mulch (for example, crop straw, plastic or gravel sand) can preserve soil moisture and increase moisture availability to crops. In China, ridge–furrow plastic mulching of maize increased water-use efficiency by 70% and improved nitrogen-uptake efficiency by 45%, relative to flat irrigation[12].

Nature Biotechnology 2021

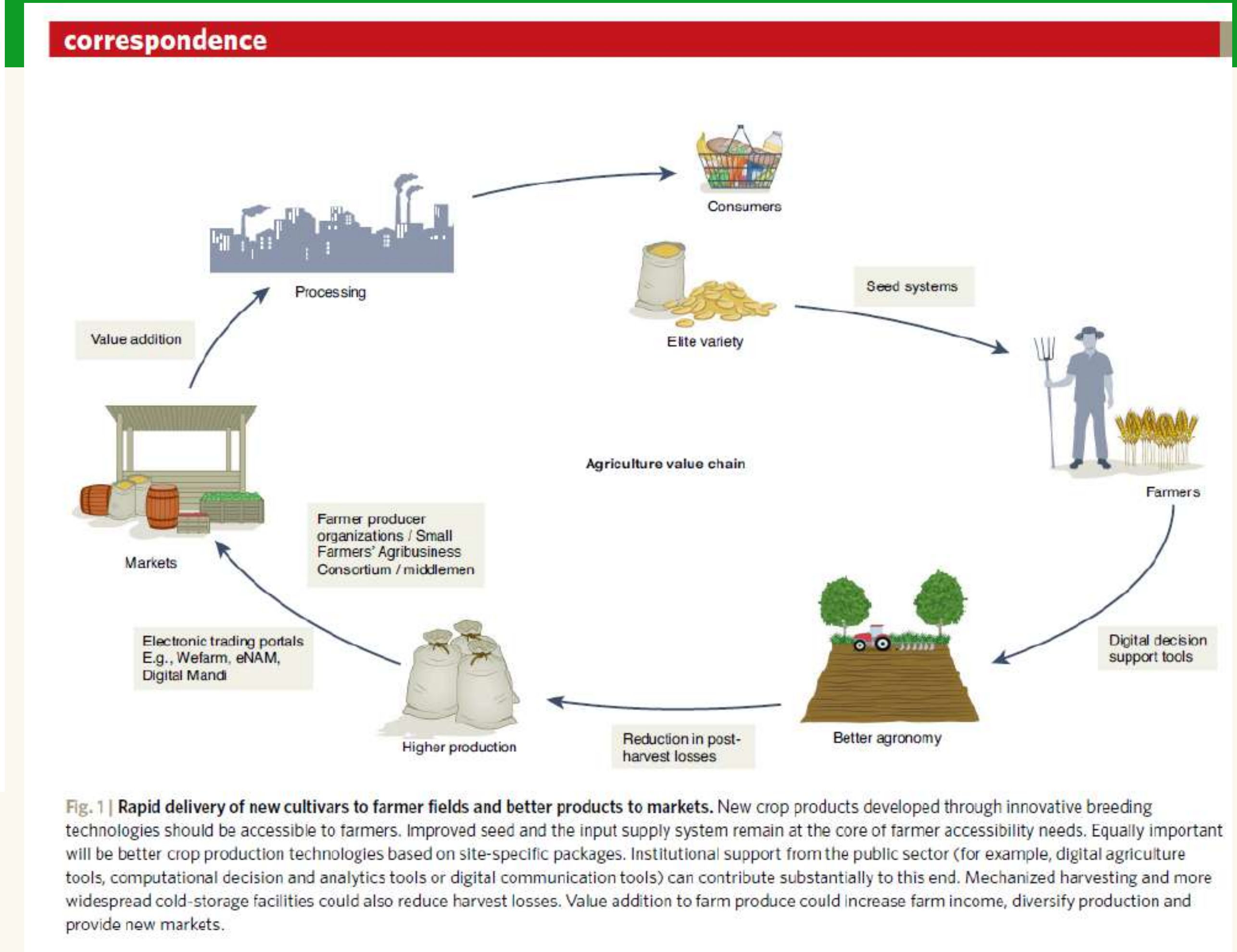


Fig. 1 | **Rapid delivery of new cultivars to farmer fields and better products to markets.** New crop products developed through innovative breeding technologies should be accessible to farmers. Improved seed and the input supply system remain at the core of farmer accessibility needs. Equally important will be better crop production technologies based on site-specific packages. Institutional support from the public sector (for example, digital agriculture tools, computational decision and analytics tools or digital communication tools) can contribute substantially to this end. Mechanized harvesting and more widespread cold-storage facilities could also reduce harvest losses. Value addition to farm produce could increase farm income, diversify production and provide new markets.

CROPS in a changing climate

PANOMICS meets Germplasm

Understanding intraspecific crop plant adaptation in the climate crisis for climate change mitigation

ViMe
Vienna Metabolomics Center

MoSys
universität wien

HYPOTHESIS

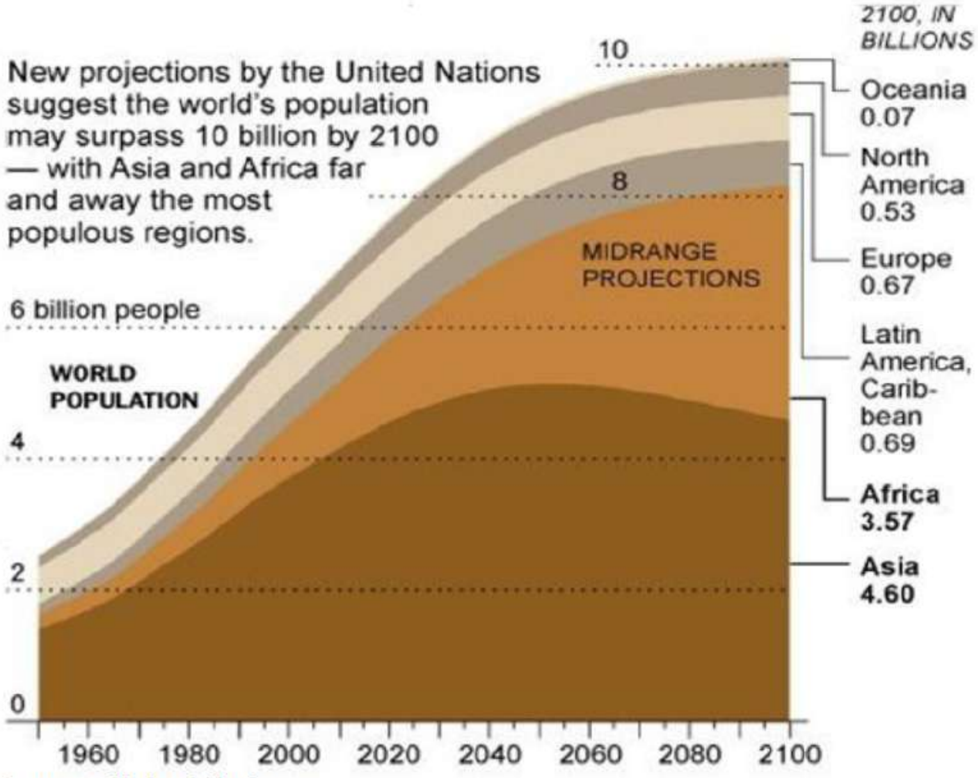
Agriculture contributes to the mitigation of climate change due to its nature as carbon sequestration process - photosynthesis and CO_2 -fixation

versus current state:

1. Harsh climate reduces plant growth and productivity leading to inefficient CO_2-neutral biomass and food production
2. High demand on industrial nitrogen fertilizer for productivity but low nitrogen use efficiency (NUE) due to losses (50-70%) in the soil – nitrification processes and GHG emissions (N_2O)
3. Food production – industrial processes

Net GHG emission instead of sequestration

Transformation of Agriculture



Towards 10 Billion

New projections by the United Nations suggest the world's population may surpass 10 billion by 2100 — with Asia and Africa far and away the most populous regions.

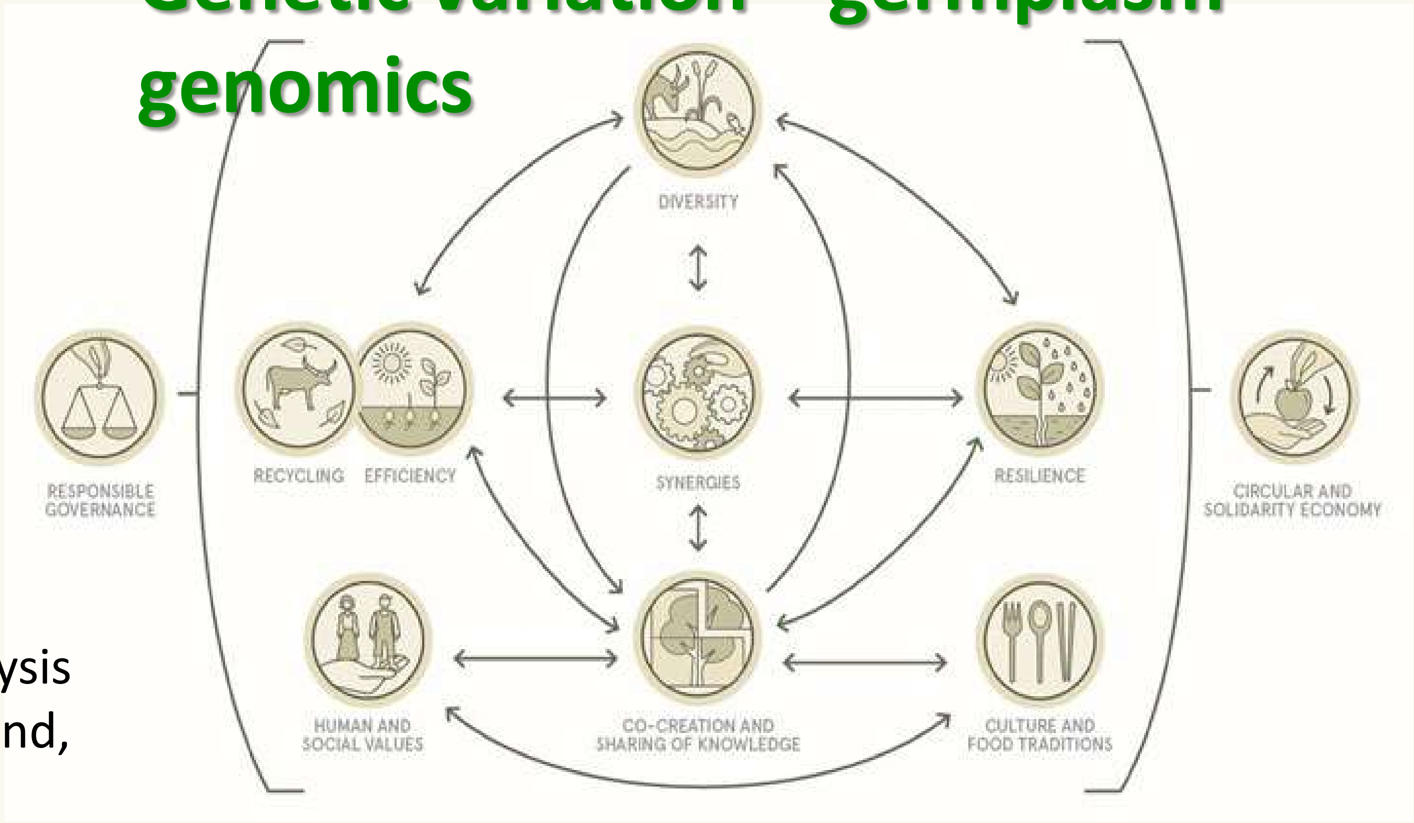
Source: United Nations

- **World population will reach 9 billion by 2050**
- **FAO estimates that agricultural production will have to increase by 60% by then**
- **Agriculture should undergo a significant transformation to feed the growing global population**
- **Climate change adds extra challenges in reaching this goal – esp. developing countries where food insecurity and poverty are prevalent**

Agroecology: Key to agricultural resilience and ecosystem recovery

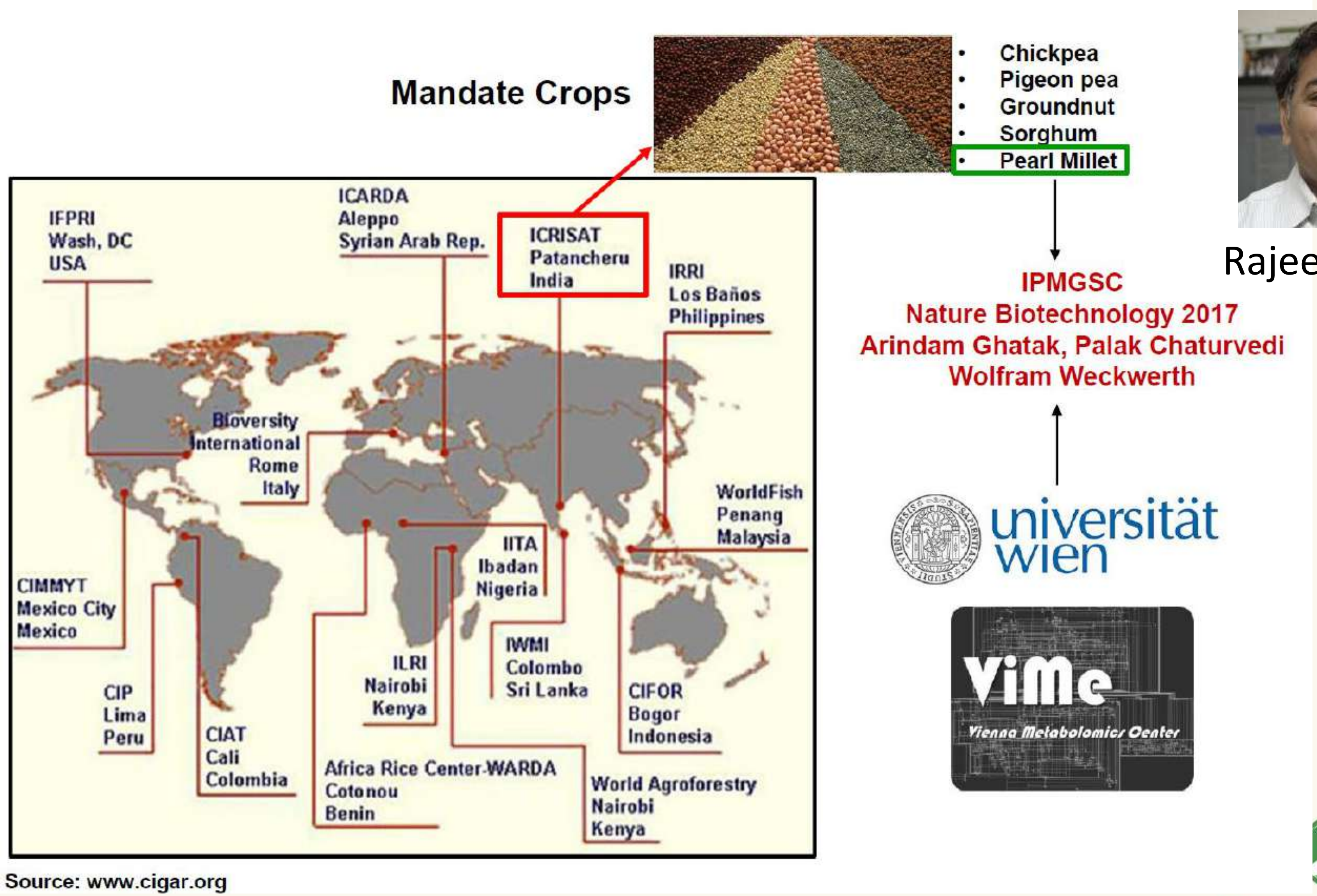
- Four major themes of agroecosystems (Conway 1983):
  - Productivity
  - Stability
  - Sustainability
  - Equability
- Fundamental properties of any complex system and derived from **SYSTEM THEORY**
- Agroecology and agroecosystems analysis is intimately bound to system theory and, thus, to systems biology

Genetic variation – germplasm genomics



http://www.fao.org/agroecology/knowledge/science/en/

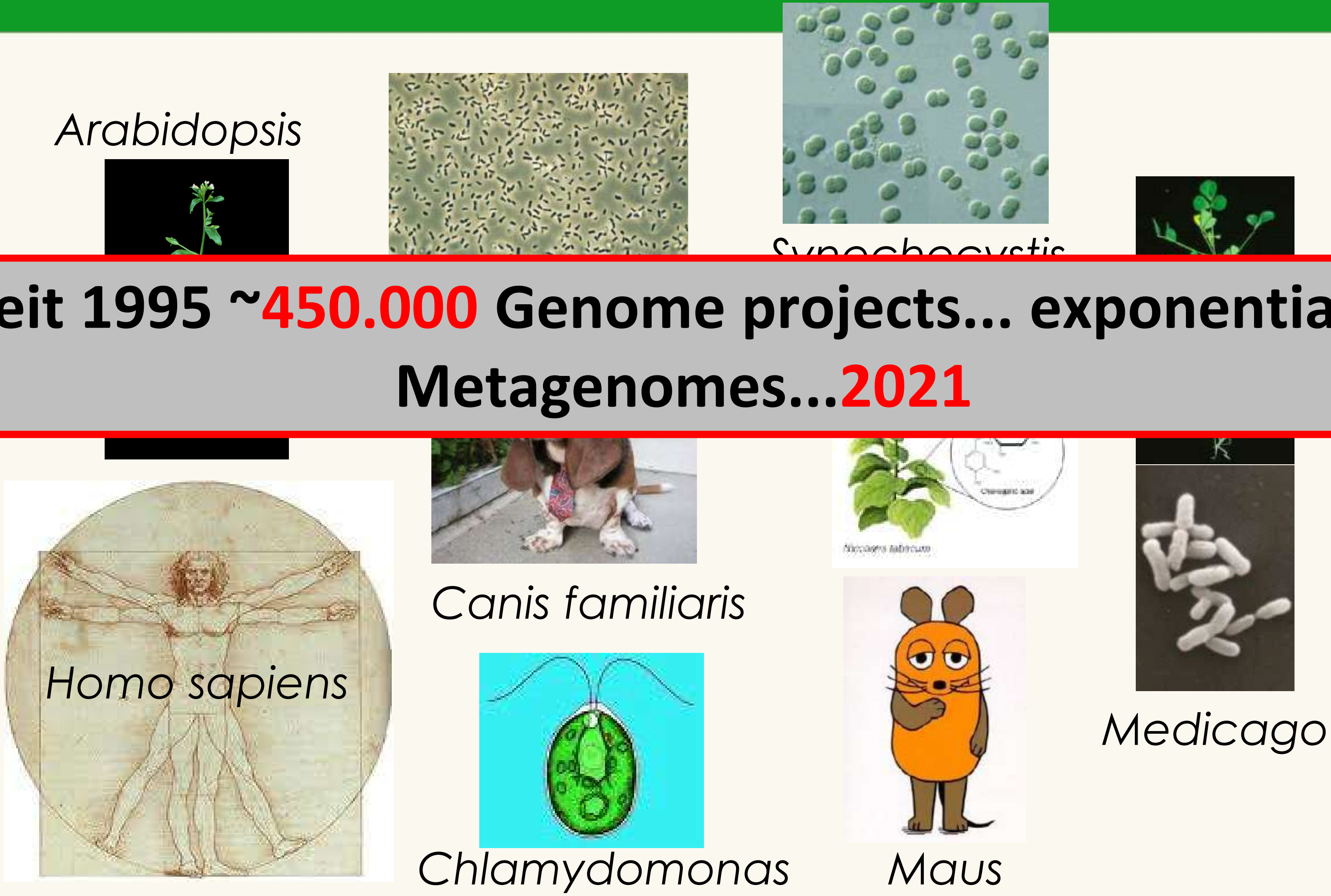
Consultative Group on International Agriculture Research (CGIAR)



Source: www.cigar.org

Rajeev Varshney

Next generation sequencing...


Arabidopsis

Synechocystis

Canis familiaris

Homo sapiens

Chlamydomonas

Maus

Medicago

Seit 1995 ~450.000 Genome projects... exponential...
Metagenomes...2021

Plant Genomes

Oryza sativa

2002

Populus trichocarpa

2006

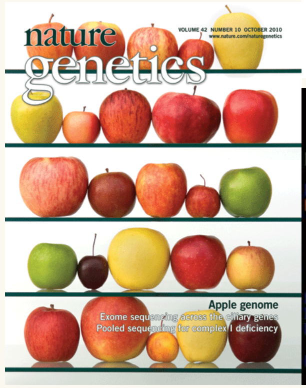
Vitis vinifera

2007

Zea mays

2009

Malus × domestica Borkh.



2009

Medicago truncatula

2011

Ricinus communis

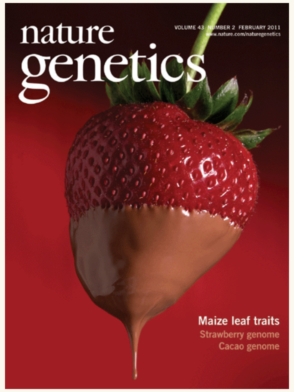
2010

Solanum tuberosum

7000

2011

Fragaria vesca
Theobroma cacao

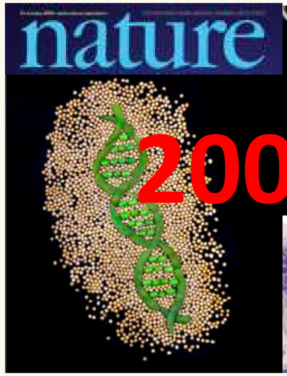


2011

Solanum lycopersicum

2012

Glycine max

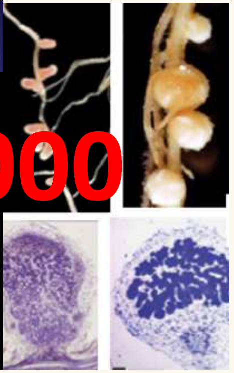


20000

Photo: Roy Kaltschmidt, LBNL

2010

Rhizobium leguminosarum

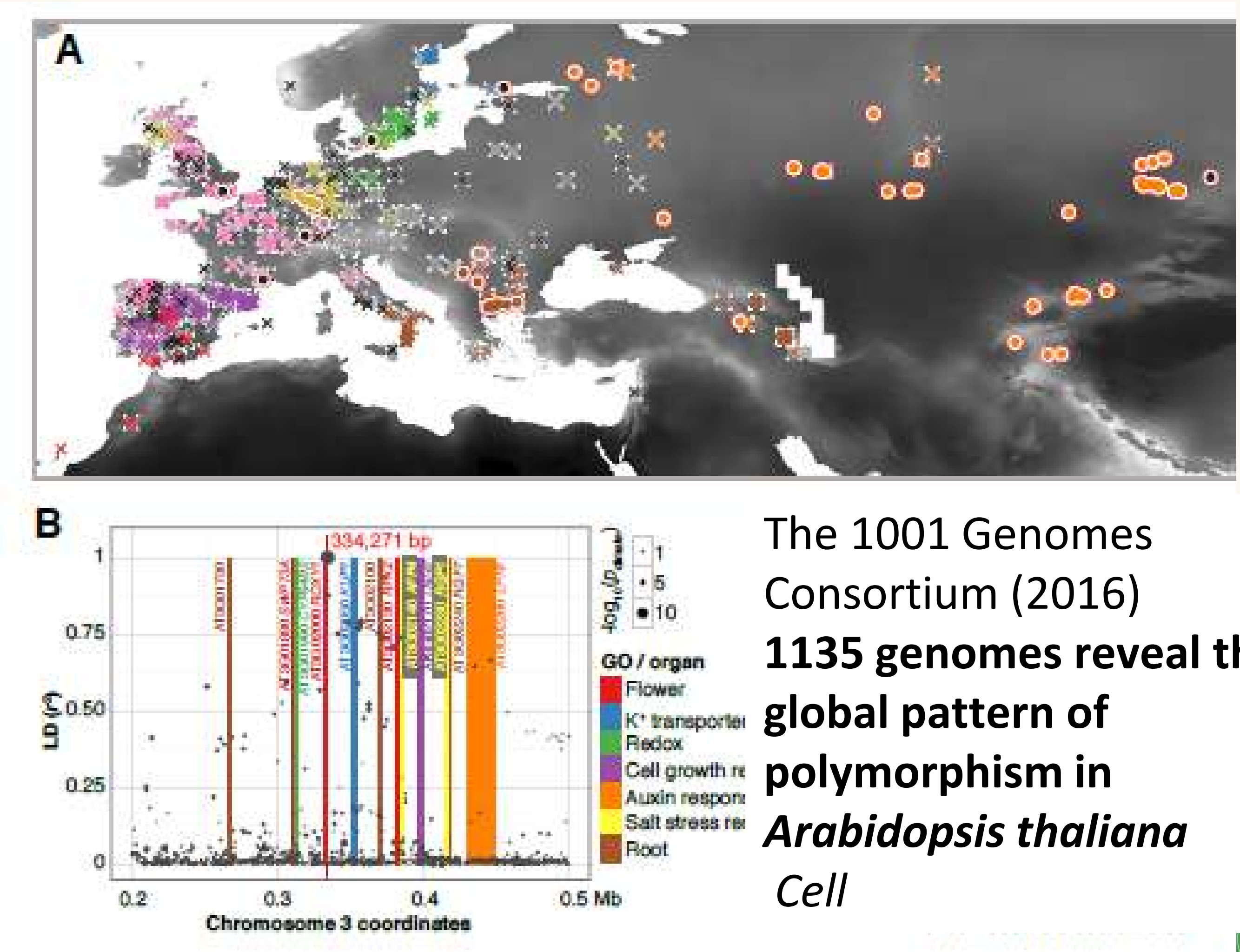


2006

• • •

Germplasm genomics intraspecific variation

Polymorphism involved in climate adaption

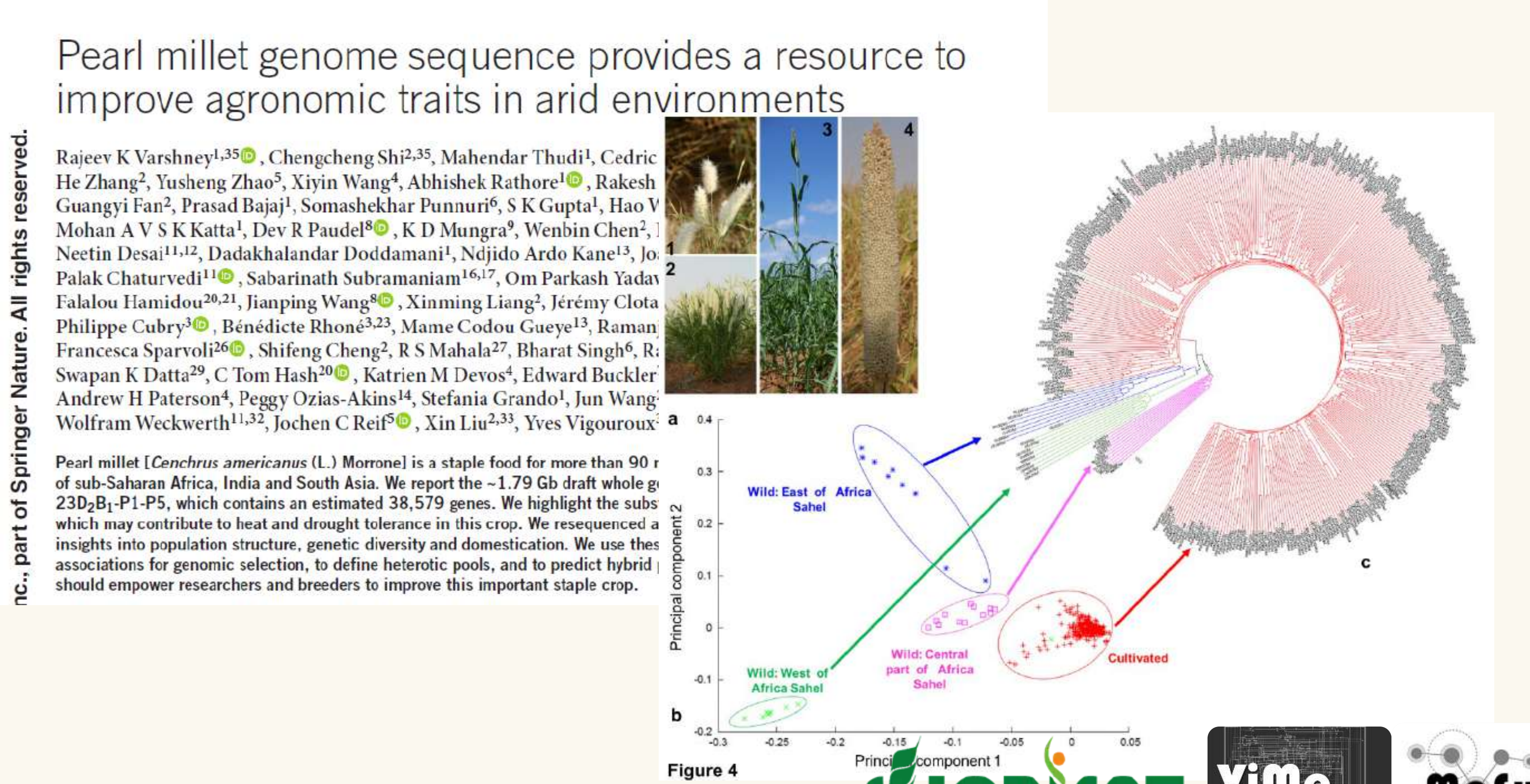


The 1001 Genomes Consortium (2016)

1135 genomes reveal the global pattern of polymorphism in *Arabidopsis thaliana*

Cell

Germplasm genomics
Pearl Millet



Pearl millet genome sequence provides a resource to improve agronomic traits in arid environments

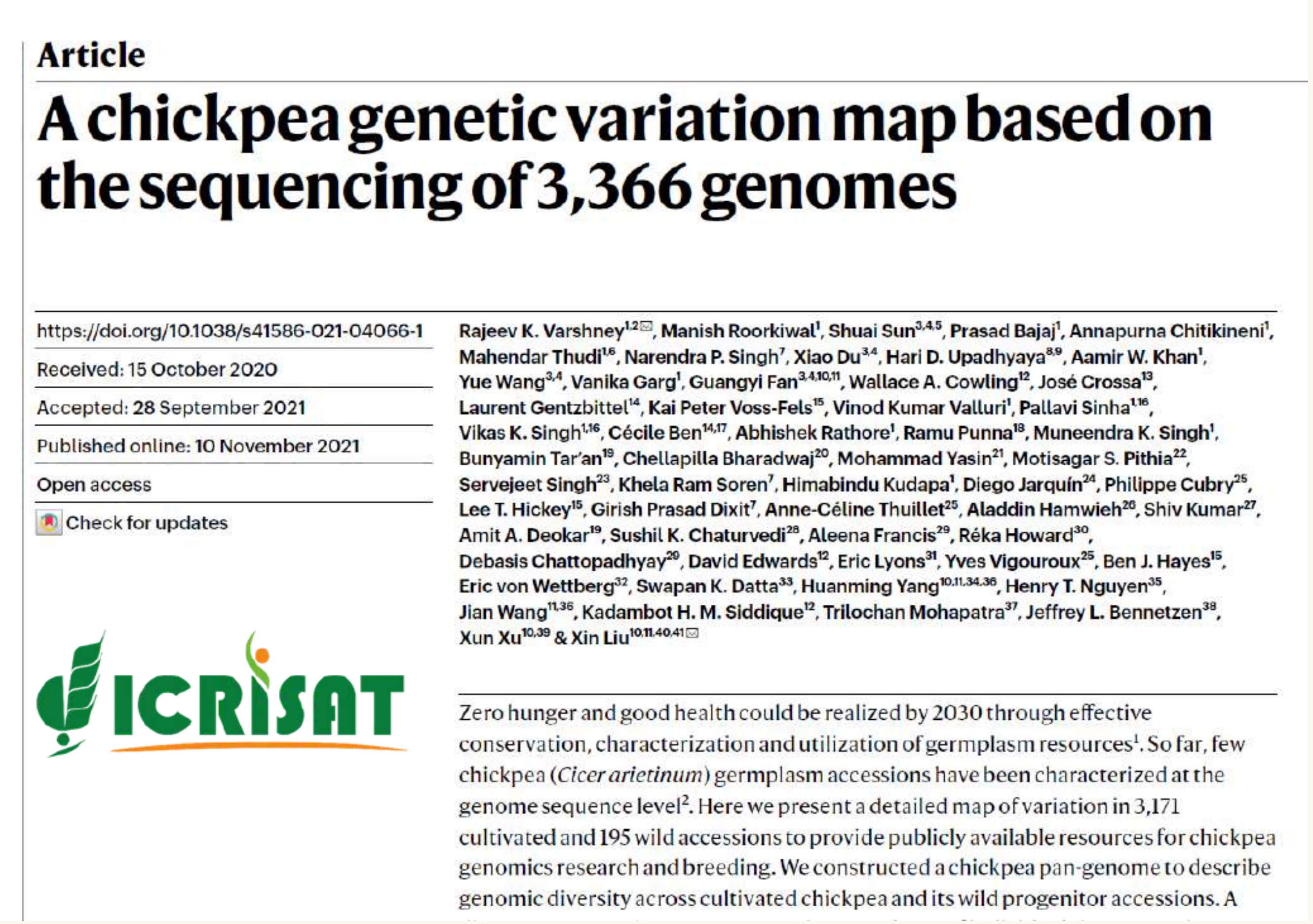
Rajeev K Varshney[1,35], Chengcheng Shi[2,35], Mahendar Thudi[1], Cedric
He Zhang[2], Yusheng Zhao[5], Xiyin Wang[4], Abhishek Rathore[1], Rakesh
Guangyi Fan[2], Prasad Bajaj[1], Somashekhar Punnuri[6], S K Gupta[1], Hao
Mohan A V S K Katta[1], Dev R Paudel[8], K D Mungra[9], Wenbin Chen[2],
Neetin Desai[11,12], Dadakhalandar Doddamani[1], Ndjido Ardo Kane[13],
Palak Chaturvedi[11], Sabarinath Subramaniam[16,17], Om Parkash
Falalou Hamidou[20,21], Jianping Wang[8], Xinming Liang[2], Jérémy Clota
Philippe Cubry[3], Bénédicte Rhoné[3,23], Mame Codou Gueye[13],
Francesca Sparvoli[26], Shifeng Cheng[2], R S Mahala[27], Bharat Singh[6],
Swapan K Datta[29], C Tom Hash[20], Katrien M Devos[4], Edward Buckler
Andrew H Paterson[4], Peggy Ozias-Akins[14], Stefania Grando[1], Jun
Wolfram Weckwerth[11,32], Jochen C Reif[5], Xin Liu[2,33], Yves Vigouroux

Pearl millet [*Cenchrus americanus* (L.) Morrone] is a staple food for more than 90
of sub-Saharan Africa, India and South Asia. We report the ~1.79 Gb draft whole
$23D_2B_1$-P1-P5, which contains an estimated 38,579 genes. We highlight the
which may contribute to heat and drought tolerance in this crop. We resequenced
insights into population structure, genetic diversity and domestication. We use
associations for genomic selection, to define heterotic pools, and to predict hybrid
should empower researchers and breeders to improve this important staple crop.

Figure 4

Nature Biotechnology 2017

Germplasm genomics:
Chickpea



Article

A chickpea genetic variation map based on the sequencing of 3,366 genomes

https://doi.org/10.1038/s41586-021-04066-1
Received: 15 October 2020
Accepted: 28 September 2021

Rajeev K. Varshney[1,2]✉, **Manish Roorkiwal**[1], **Shuai Sun**[3,4,5], **Prasad Bajaj**[1], **Annapurna Chitikineni**[1], **Mahendar Thudi**[1,6], **Narendra P. Singh**[7], **Xiao Du**[3,4], **Hari D. Upadhyaya**[8,9], **Aamir W. Khan**[1], **Yue Wang**[3,4], **Vanika Garg**[1], **Guangyi Fan**[3,4,10,11], **Wallace A. Cowling**[12], **José Crossa**[13], **Laurent Gentzbittel**[14], **Kai Peter Voss-Fels**[15], **Vinod Kumar Valluri**[1], **Pallavi Sinha**[1,16], **Vikas K. Singh**[1,16], **Cécile Ben**[14,17], **Abhishek Rathore**[1], **Ramu Punna**[18], **Muneendra K. Singh**[1], **Bunyamin Tar'an**[19], **Chellapilla Bharadwaj**[20], **Mohammad Yasin**[21], **Motisagar S. Pithia**[22], **Servejeet Singh**[23], **Khela Ram Soren**[7], **Himabindu Kudapa**[1], **Diego Jarquín**[24], **Philippe Cubry**[25], **Lee T. Hickey**[15], **Girish Prasad Dixit**[7], **Anne-Céline Thuillet**[25], **Aladdin Hamwieh**[26], **Shiv Kumar**[27], **Amit A. Deokar**[19], **Sushil K. Chaturvedi**[28], **Aleena Francis**[29], **Réka Howard**[30], **Debasis Chattopadhyay**[29], **David Edwards**[12], **Eric Lyons**[31], **Yves Vigouroux**[25], **Ben J. Hayes**[15], **Eric von Wettberg**[32], **Swapan K. Datta**[33], **Huanming Yang**[10,11,34,36], **Henry T. Nguyen**[35], **Jian Wang**[11,36], **Kadambot H. M. Siddique**[12], **Trilochan Mohapatra**[37], **Jeffrey L. Bennetzen**[38], **Xun Xu**[10,39] & **Xin Liu**[10,11,40,41]✉

Zero hunger and good health could be realized by 2030 through effective conservation, characterization and utilization of germplasm resources[1]. So far, few chickpea (*Cicer arietinum*) germplasm accessions have been characterized at the genome sequence level[2]. Here we present a detailed map of variation in 3,171 cultivated and 195 wild accessions to provide publicly available resources for chickpea genomics research and breeding. We constructed a chickpea pan-genome to describe genomic diversity across cultivated chickpea and its wild progenitor accessions. A

ICRISAT

Chickpea 3000 project

ViMe
Vienna Metabolomics Center

MoSys

Question:

From all these data

….can we predict metabolite dynamics and/or protein dynamics or transcript dynamics?

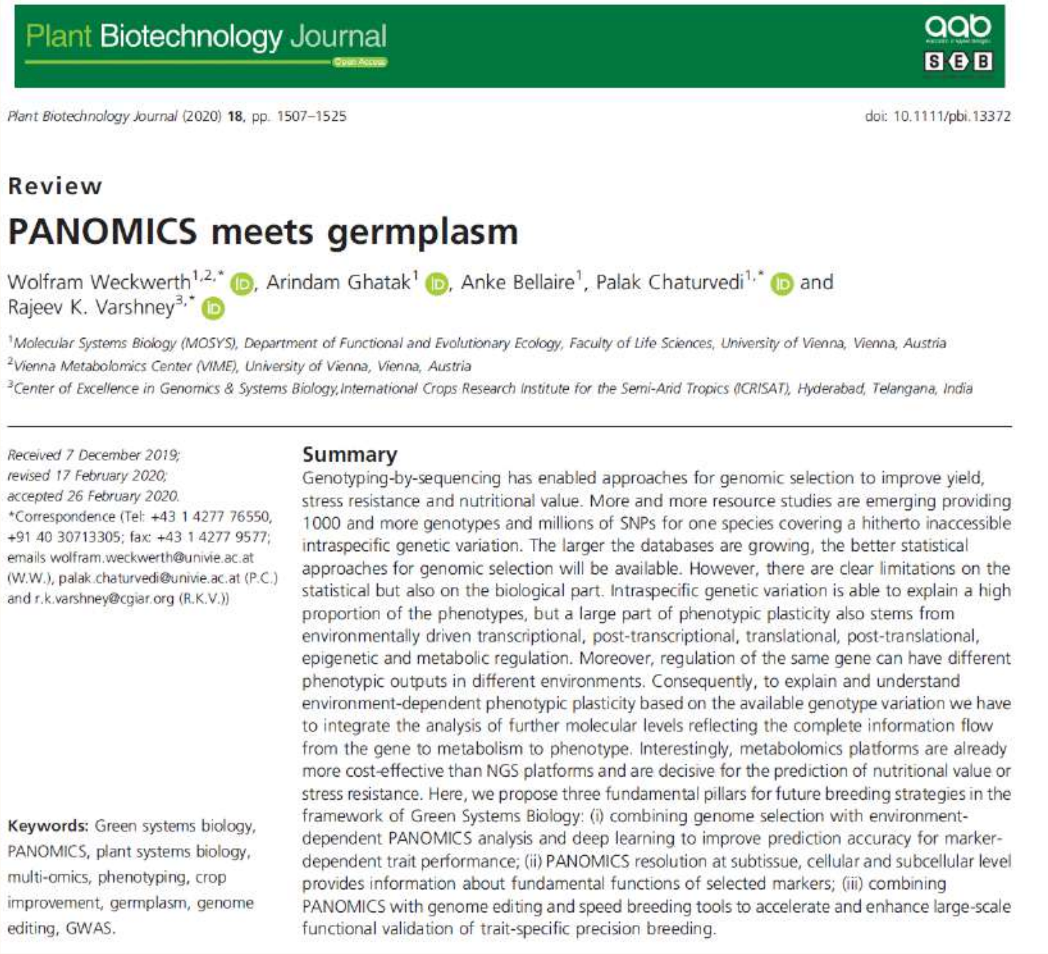
Regulation? Growth? Physiology?

Morphotyp? Stress phenotype? Yield?

Quality? Adaptation to climate change?

Panomics meets Germplasm

Weckwerth et al 2020 Plant Biotechnolgy Journal



Plant Biotechnology Journal

Plant Biotechnology Journal (2020) **18**, pp. 1507–1525

doi: 10.1111/pbi.13372

Review

PANOMICS meets germplasm

Wolfram Weckwerth[1,2,*], Arindam Ghatak[1], Anke Bellaire[1], Palak Chaturvedi[1,*] and Rajeev K. Varshney[3,*]

[1] *Molecular Systems Biology (MOSYS), Department of Functional and Evolutionary Ecology, Faculty of Life Sciences, University of Vienna, Vienna, Austria*
[2] *Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria*
[3] *Center of Excellence in Genomics & Systems Biology, International Crops Research Institute for the Semi-Arid Tropics (ICRISAT), Hyderabad, Telangana, India*

Received 7 December 2019;
revised 17 February 2020;
accepted 26 February 2020.

*Correspondence (Tel: +43 1 4277 76550, +91 40 30713305; fax: +43 1 4277 9577; emails wolfram.weckwerth@univie.ac.at (W.W.), palak.chaturvedi@univie.ac.at (P.C.) and r.k.varshney@cgiar.org (R.K.V.))

Keywords: Green systems biology, PANOMICS, plant systems biology, multi-omics, phenotyping, crop improvement, germplasm, genome editing, GWAS.

Summary

Genotyping-by-sequencing has enabled approaches for genomic selection to improve yield, stress resistance and nutritional value. More and more resource studies are emerging providing 1000 and more genotypes and millions of SNPs for one species covering a hitherto inaccessible intraspecific genetic variation. The larger the databases are growing, the better statistical approaches for genomic selection will be available. However, there are clear limitations on the statistical but also on the biological part. Intraspecific genetic variation is able to explain a high proportion of the phenotypes, but a large part of phenotypic plasticity also stems from environmentally driven transcriptional, post-transcriptional, translational, post-translational, epigenetic and metabolic regulation. Moreover, regulation of the same gene can have different phenotypic outputs in different environments. Consequently, to explain and understand environment-dependent phenotypic plasticity based on the available genotype variation we have to integrate the analysis of further molecular levels reflecting the complete information flow from the gene to metabolism to phenotype. Interestingly, metabolomics platforms are already more cost-effective than NGS platforms and are decisive for the prediction of nutritional value or stress resistance. Here, we propose three fundamental pillars for future breeding strategies in the framework of Green Systems Biology: (i) combining genome selection with environment-dependent PANOMICS analysis and deep learning to improve prediction accuracy for marker-dependent trait performance; (ii) PANOMICS resolution at subtissue, cellular and subcellular level provides information about fundamental functions of selected markers; (iii) combining PANOMICS with genome editing and speed breeding tools to accelerate and enhance large-scale functional validation of trait-specific precision breeding.

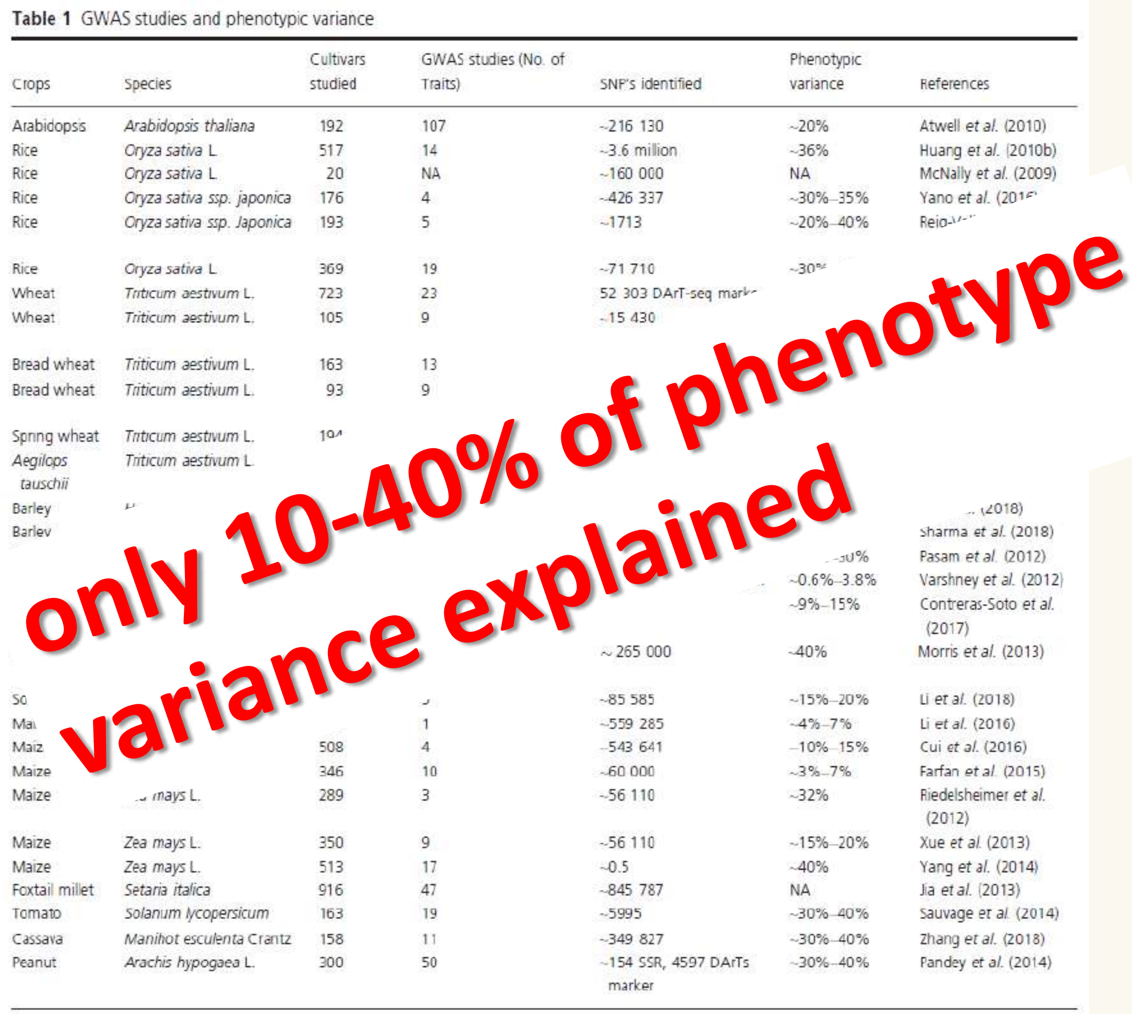
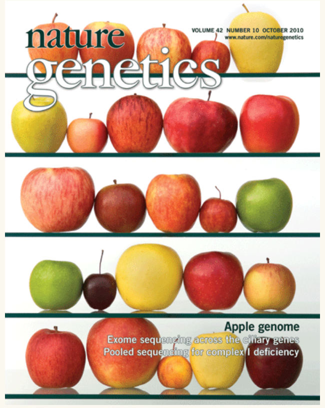


Table 1 GWAS studies and phenotypic variance

Crops	Species	Cultivars studied	GWAS studies (No. of Traits)	SNP's identified	Phenotypic variance	References
Arabidopsis	*Arabidopsis thaliana*	192	107	~216 130	~20%	Atwell *et al.* (2010)
Rice	*Oryza sativa* L.	517	14	~3.6 million	~36%	Huang *et al.* (2010b)
Rice	*Oryza sativa* L.	20	NA	~160 000	NA	McNally *et al.* (2009)
Rice	*Oryza sativa ssp. japonica*	176	4	~426 337	~30%–35%	Yano *et al.* (201
Rice	*Oryza sativa ssp. Japonica*	193	5	~1713	~20%–40%	Reio-
Rice	*Oryza sativa* L.	369	19	~71 710	~30	
Wheat	*Triticum aestivum* L.	723	23	52 303 DArT-seq mark		
Wheat	*Triticum aestivum* L.	105	9	~15 430		
Bread wheat	*Triticum aestivum* L.	163	13			
Bread wheat	*Triticum aestivum* L.	93	9			
Spring wheat	*Triticum aestivum* L.	19				
Aegilops tauschii	*Triticum aestivum* L.					
Barley	H					(2018)
Barley						Sharma *et al.* (2018)
					30%	Pasam *et al.* (2012)
					~0.6%–3.8%	Varshney *et al.* (2012)
					~9%–15%	Contreras-Soto *et al.* (2017)
				~265 000	~40%	Morris *et al.* (2013)
So				~85 585	~15%–20%	Li *et al.* (2018)
Ma			1	~559 285	~4%–7%	Li *et al.* (2016)
Maiz		508	4	~543 641	~10%–15%	Cui *et al.* (2016)
Maize		346	10	~60 000	~3%–7%	Farfan *et al.* (2015)
Maize	*mays* L.	289	3	~56 110	~32%	Riedelsheimer *et al.* (2012)
Maize	*Zea mays* L.	350	9	~56 110	~15%–20%	Xue *et al.* (2013)
Maize	*Zea mays* L.	513	17	~0.5	~40%	Yang *et al.* (2014)
Foxtail millet	*Setaria italica*	916	47	~845 787	NA	Jia *et al.* (2013)
Tomato	*Solanum lycopersicum*	163	19	~5995	~30%–40%	Sauvage *et al.* (2014)
Cassava	*Manihot esculenta* Crantz	158	11	~349 827	~30%–40%	Zhang *et al.* (2018)
Peanut	*Arachis hypogaea* L.	300	50	~154 SSR, 4597 DArTs marker	~30%–40%	Pandey *et al.* (2014)

only 10-40% of phenotype variance explained

How is complexity encoded?



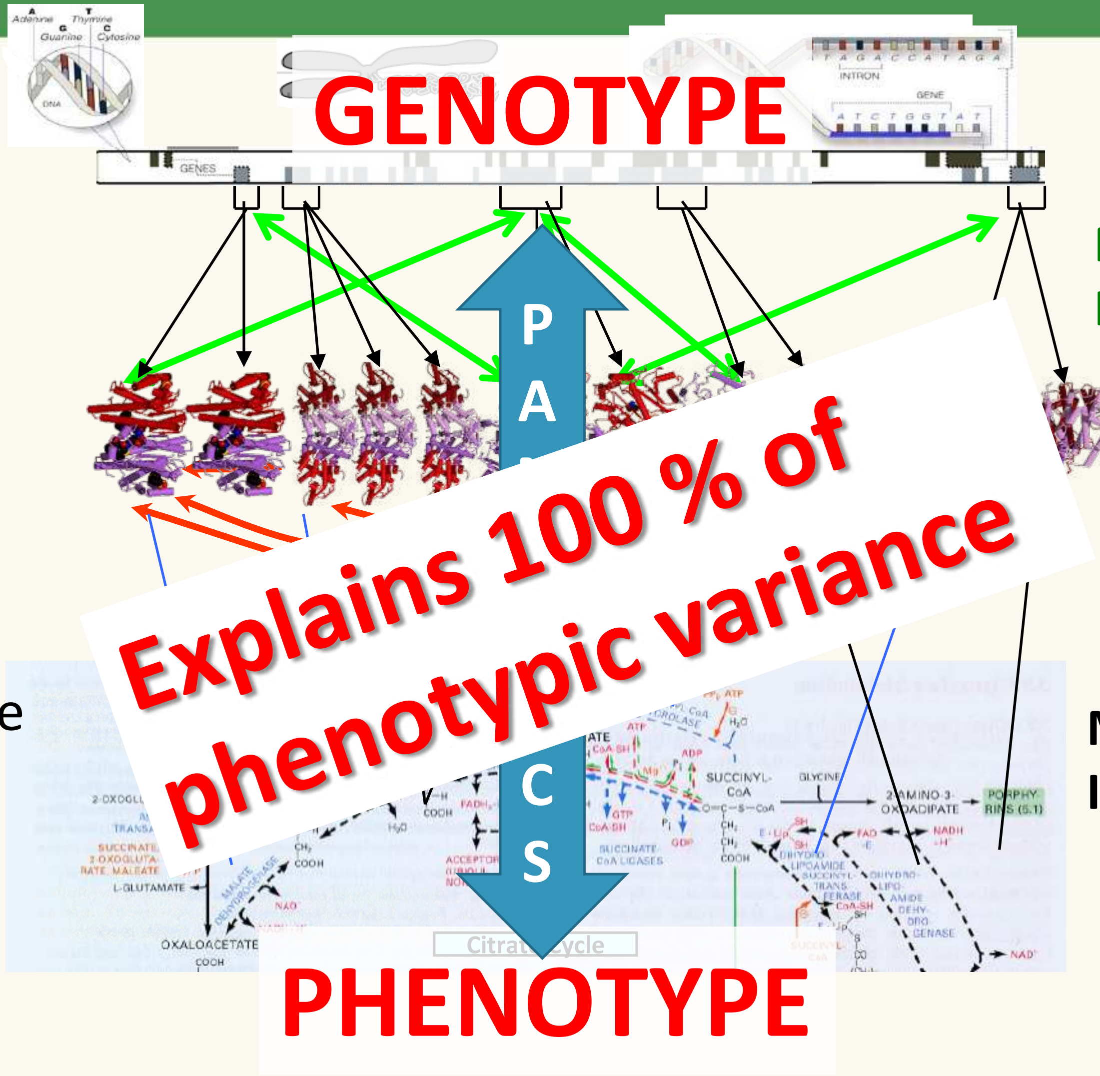
Genome
~ 10^3-10^5

Proteome
~ 10^6

PTM
~ 10^{6-7}

Metabolome
~10^5-10^6

“OMICS”



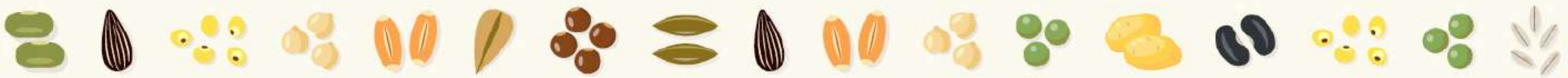
Explains 100 % of phenotypic variance

Protein-Gene Interactions

Protein-Protein Interactions

Metabolite-Protein Interactions

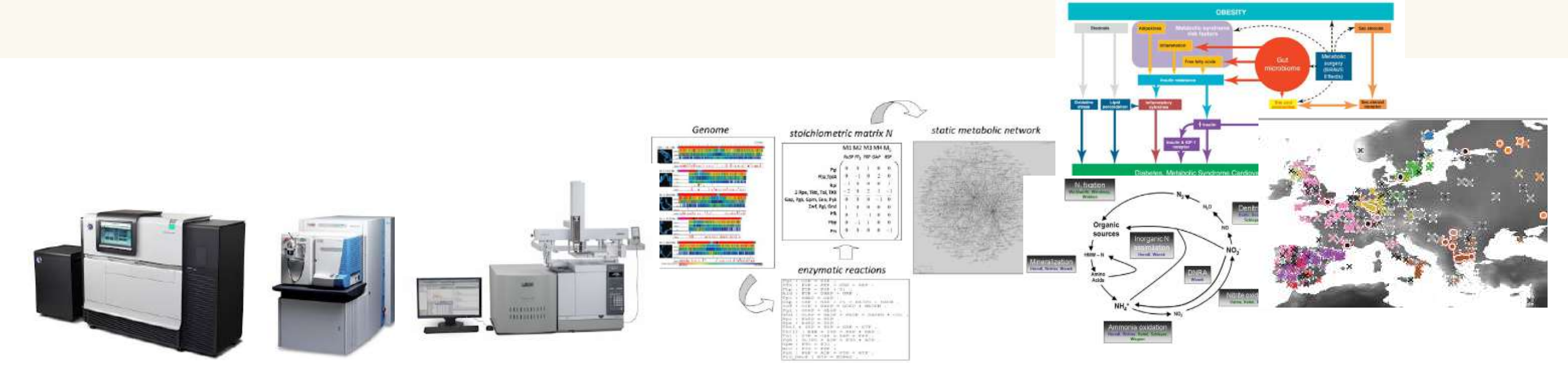
“OMICS”



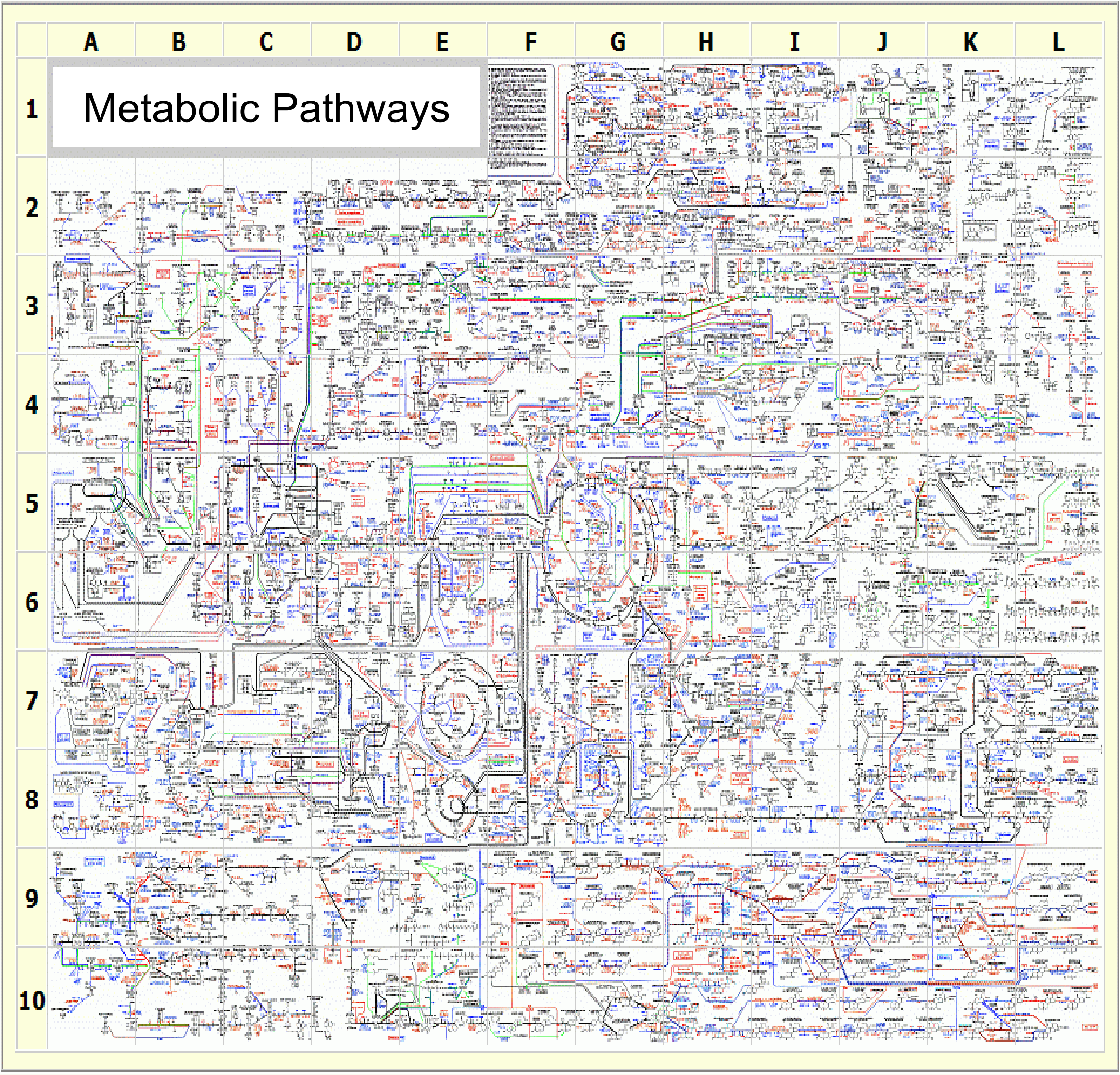
Panomics meets Germplasm

Weckwerth et al 2020 Plant Biotechnology Journal

- **From Model Organisms to Ecosystems**
- **Genomics, Transcriptomics, Proteomics, Metabolomics, Physiology, Phenotype** Weckwerth 2011 Green Systems Biology



NGS Proteomics Metabolomics Genome-scale modelling Ecosystems analysis



Metabolomics

-non-targeted metabolite analysis

- integrative part of systems biology

Weckwerth (2003)
Metabolomics in Systems Biology.
Annual Review of Plant Biology

Vienna Metabolomics Center

ViMe

Vienna Metabolomics Center

- **Research Platform University of Vienna (**http://metabolomics.univie.ac.at**)**
- **Coordinator: Univ.-Prof. Dr. Wolfram Weckwerth**
- **Faculties of Life Sciences and Chemistry, CMESS and Medical University**

universität wien

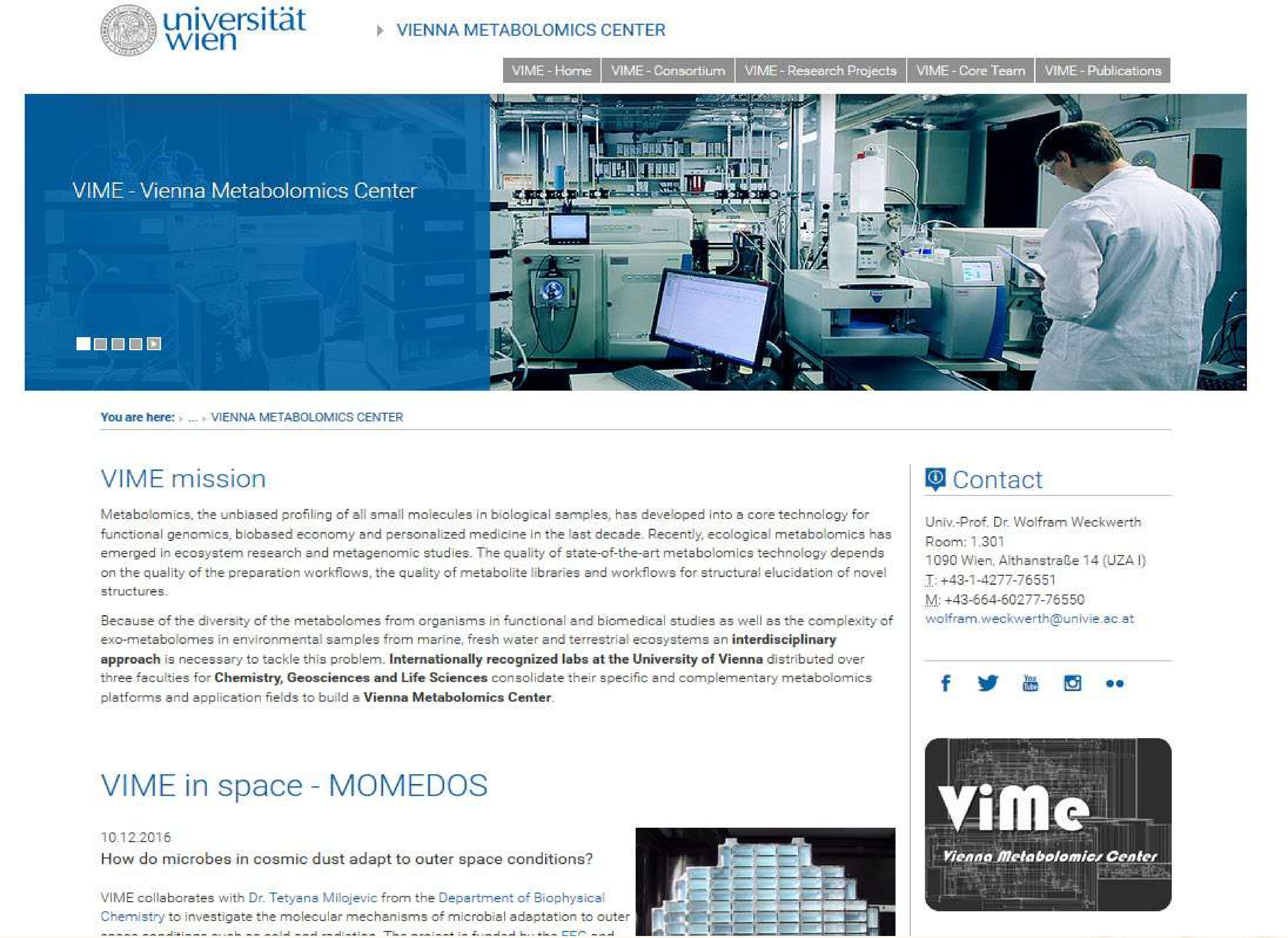
Vienna Metabolomics Center

- **ViMe – Vienna Metabolomics Center – is an open research platform for national and international scientific collaborations**
- **Provides a full suite for metabolomic profiling combining GC-MS, LC-MS, structural elucidation, databases, multivariate statistics, data integration and metabolic modelling**
- **Provides a full suite for proteomic/phosphoproteomic profiling**
- **More than 120 publications including Cell, PNAS, Nature Biotechnology, Nature Immunology, Cancer Cell, Plant Cell, Plant Physiology, Plant Journal, and many more**
- **Contact: wolfram.weckwerth@univie.ac.at**

http://metabolomics.univie.ac.at/

VIM

n Green
d Industries



universität wien

VIENNA METABOLOMICS CENTER

VIME - Vienna Metabolomics Center

You are here: » ... » VIENNA METABOLOMICS CENTER

VIME mission

Metabolomics, the unbiased profiling of all small molecules in biological samples, has developed into a core technology for functional genomics, biobased economy and personalized medicine in the last decade. Recently, ecological metabolomics has emerged in ecosystem research and metagenomic studies. The quality of state-of-the-art metabolomics technology depends on the quality of the preparation workflows, the quality of metabolite libraries and workflows for structural elucidation of novel structures.

Because of the diversity of the metabolomes from organisms in functional and biomedical studies as well as the complexity of exo-metabolomes in environmental samples from marine, fresh water and terrestrial ecosystems an **interdisciplinary approach** is necessary to tackle this problem. **Internationally recognized labs at the University of Vienna** distributed over three faculties for **Chemistry, Geosciences and Life Sciences** consolidate their specific and complementary metabolomics platforms and application fields to build a **Vienna Metabolomics Center**.

VIME in space - MOMEDOS

10.12.2016

How do microbes in cosmic dust adapt to outer space conditions?

VIME collaborates with Dr. Tetyana Milojevic from the Department of Biophysical Chemistry to investigate the molecular mechanisms of microbial adaptation to outer

Contact

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wolfram.weckwerth@univie.ac.at

Integrative Multiomics protocol

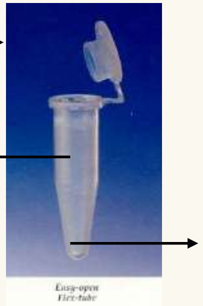
ViMe
Vienna Metabolomics Center

Tissue, Cells, Fluids

+ 1mL pre-chilled (-20°C) extraction mixture of MeOH : CHCl3 : H2O (2 : 1 : 1, v/v/v)
+ 10µL Internal Standard (2mg/mL)

Shake for 10 min at 4°c

Centrifuge at 14.000 rpm for 5min



Plant, Microbes, environmental samples, Human, Animal

Supernatant, contains soluble metabolites

Methanol/H_2O

Methoxyamine/MSTFA

GC/MS

AA, sugars, organic acids, etc.

Chloroform

TMSH

FAME

Pellet, contains insoluble metabolites, cell walls, RNA, DNA and Proteins

Shotgun proteomics
Shotgun phosphoproteomics
RNAseq
DNA/Cell wall

Weckwerth et al. 2004 Proteomics
Valledor et al. 2014 protocol extended to microbes
Linke et al. 2017 Nature Immunology
Wilson et al. 2020 Cell reports

Workflow Metabolomics

Weckwerth 2011 Unpredictability of Metabolism.ABC

GC-MS
↓
postprocessing
↓
GC-PA

(extraction of RI, mass spectra, relative fragment intensities, sample versus variable alignment)

nanoLC-MS
↓
mzXML
↓
mzFun

(extraction of accurate precursor m/z, spectral count, sample versus variable alignment)

Data Matrix

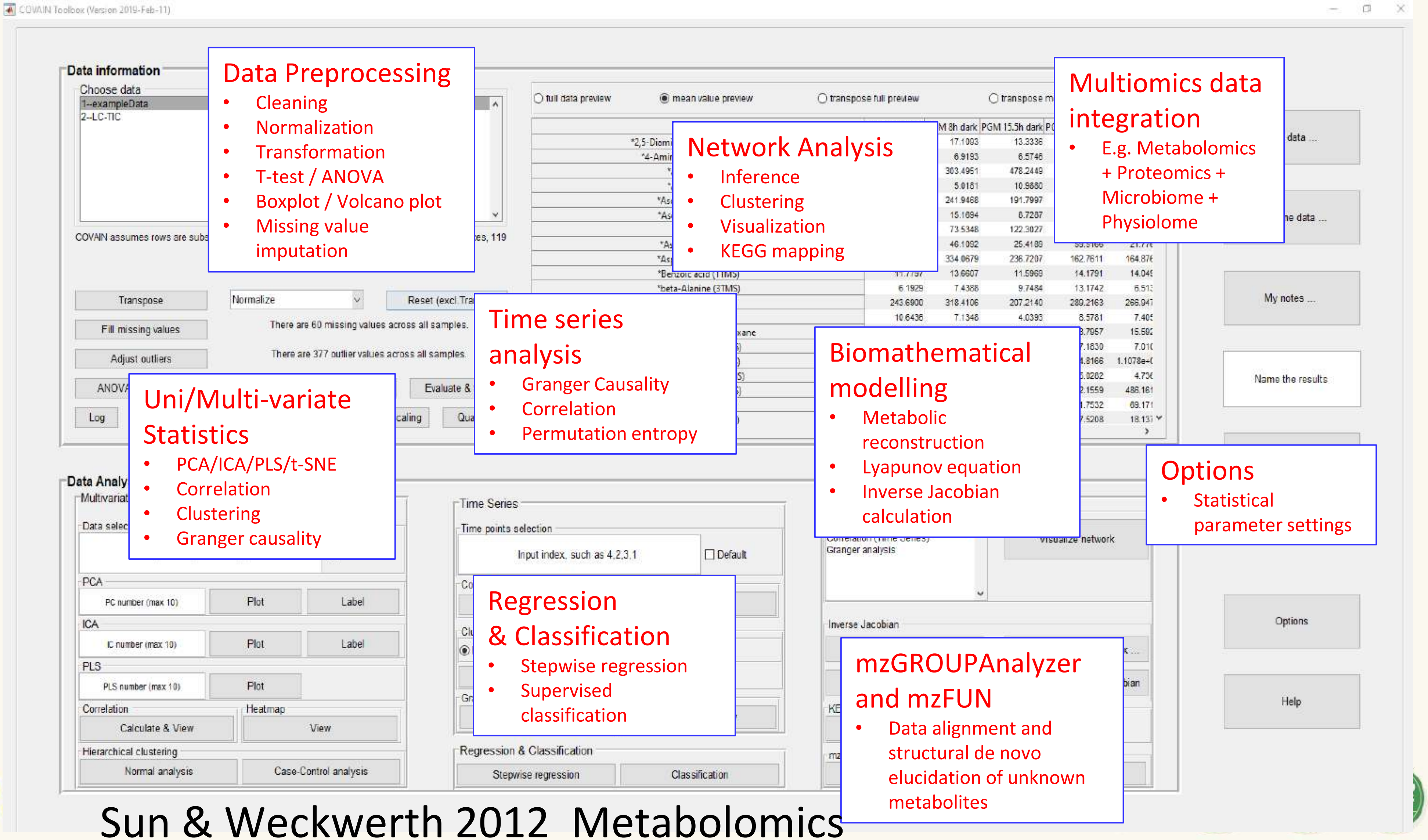
VIME
(metabolite database)

VIME
(metabolite database)

COVAIN/Machine learning
Sun & Weckwerth 2012 Metabolomics

sample pattern recognition/biological interpretation

COVAIN (*COVA*riance *IN*verse) – a toolbox for OMICS data processing, statistics and machine learning, data integration, inverse data modelling, and *de novo* structural elucidation



COVAIN assumes rows are subs

There are 60 missing values across all samples.

There are 377 outlier values across all samples.

Data Preprocessing

- Cleaning
- Normalization
- Transformation
- T-test / ANOVA
- Boxplot / Volcano plot
- Missing value imputation

Network Analysis

- Inference
- Clustering
- Visualization
- KEGG mapping

Multiomics data integration

- E.g. Metabolomics + Proteomics + Microbiome + Physiolome

Time series analysis

- Granger Causality
- Correlation
- Permutation entropy

Biomathematical modelling

- Metabolic reconstruction
- Lyapunov equation
- Inverse Jacobian calculation

Uni/Multi-variate Statistics

- PCA/ICA/PLS/t-SNE
- Correlation
- Clustering
- Granger causality

Options

- Statistical parameter settings

Regression & Classification

- Stepwise regression
- Supervised classification

mzGROUPAnalyzer and mzFUN

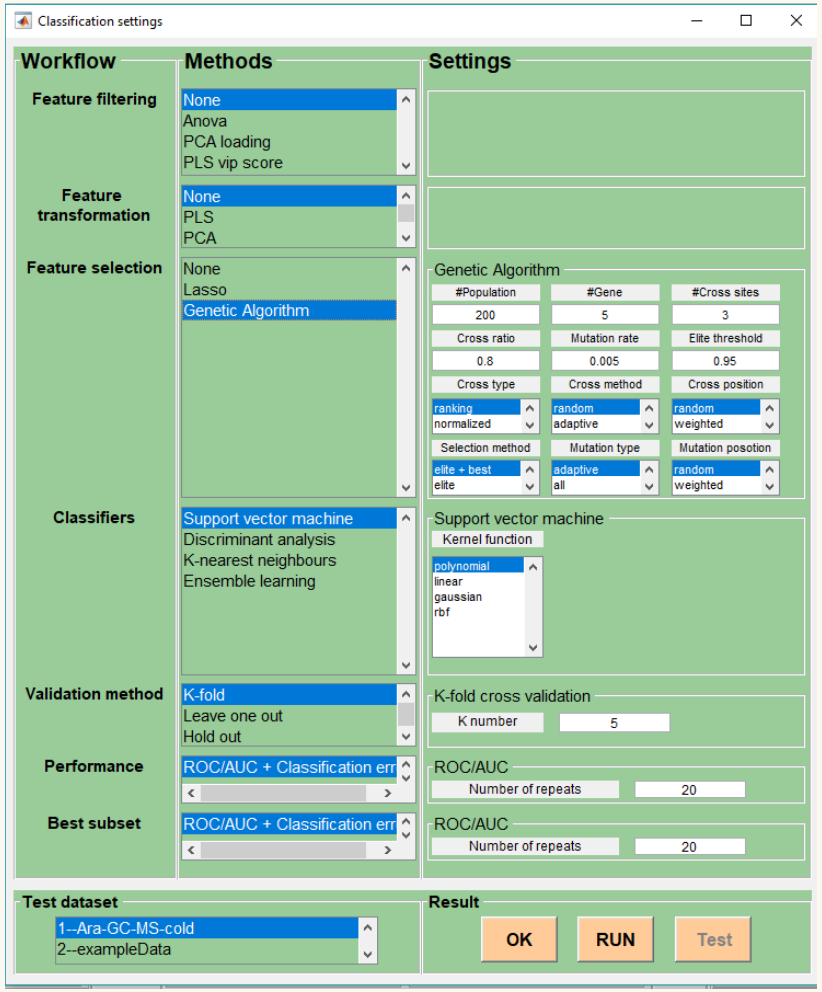
- Data alignment and structural de novo elucidation of unknown metabolites

Sun & Weckwerth 2012 Metabolomics

Machine learning workflow and methods in COVAIN

- Feature filtering
- Feature transformation(engineering)
- **Feature selection**
- Classification /Regression
- Validation
- Model evaluation (performance)
- Best feature subset

Leitner et al. 2017



Feature filtering: None

Feature transformation: None

Feature selection: Genetic Algorithm

Genetic Algorithm

#Population	#Gene	#Cross sites
200	5	3
Cross ratio	Mutation rate	Elite threshold
0.8	0.005	0.95
Cross type	Cross method	Cross position
ranking	random	random
Selection method	Mutation type	Mutation posotion
elite + best	adaptive	random

Classifiers: Support vector machine

Support vector machine
Kernel function: polynomial

Validation method: K-fold

K-fold cross validation
K number: 5

Performance: ROC/AUC + Classification err

ROC/AUC
Number of repeats: 20

Best subset: ROC/AUC + Classification err

ROC/AUC
Number of repeats: 20

Test dataset: 1--Ara-GC-MS-cold

Integration of proteome/metabolome and machine learning techniques in the field - FIELDOMICS

Potato germplasm collection

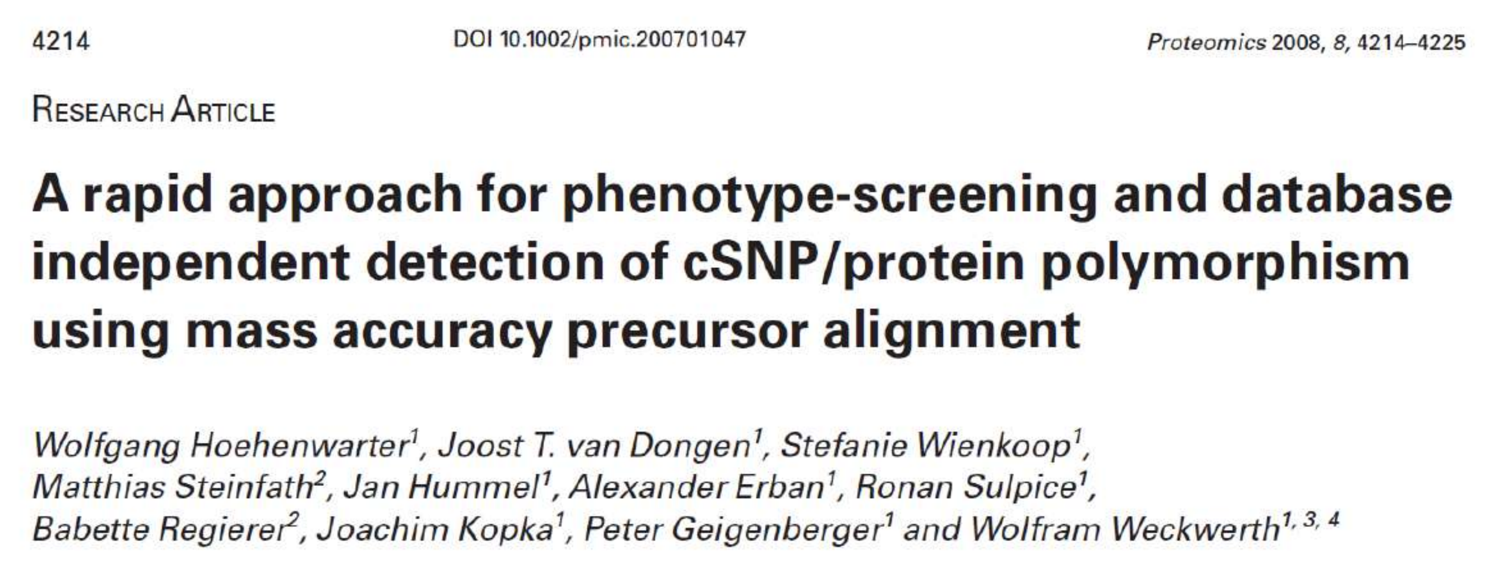
- Mature tubers of tetraploid cultivars of *Solanum tuberosum*:
    - Ag, Agria¸Al, Alliance; Ar, Arnika; F, Festien; G, Goldika; K, Kuras; LC, Lady Claire; Ma, Marabel; Mi, Milva; O, Omega; RF, Red Fantasy; T, Topas
- Grown on 3 plots each on 2 geographically separated fields in Germany
- 4 to 6 tubers of each cultivar were analyzed each three times = more than 500 shotgun proteomics analyses

Hoehenwarter et al. 2008 Proteomics

Wolfgang Hoehenwarter

MAPA

Mass ***A***ccuracy ***P***recursor ***A***lignment



4214 DOI 10.1002/pmic.200701047 *Proteomics* 2008, *8*, 4214–4225

RESEARCH ARTICLE

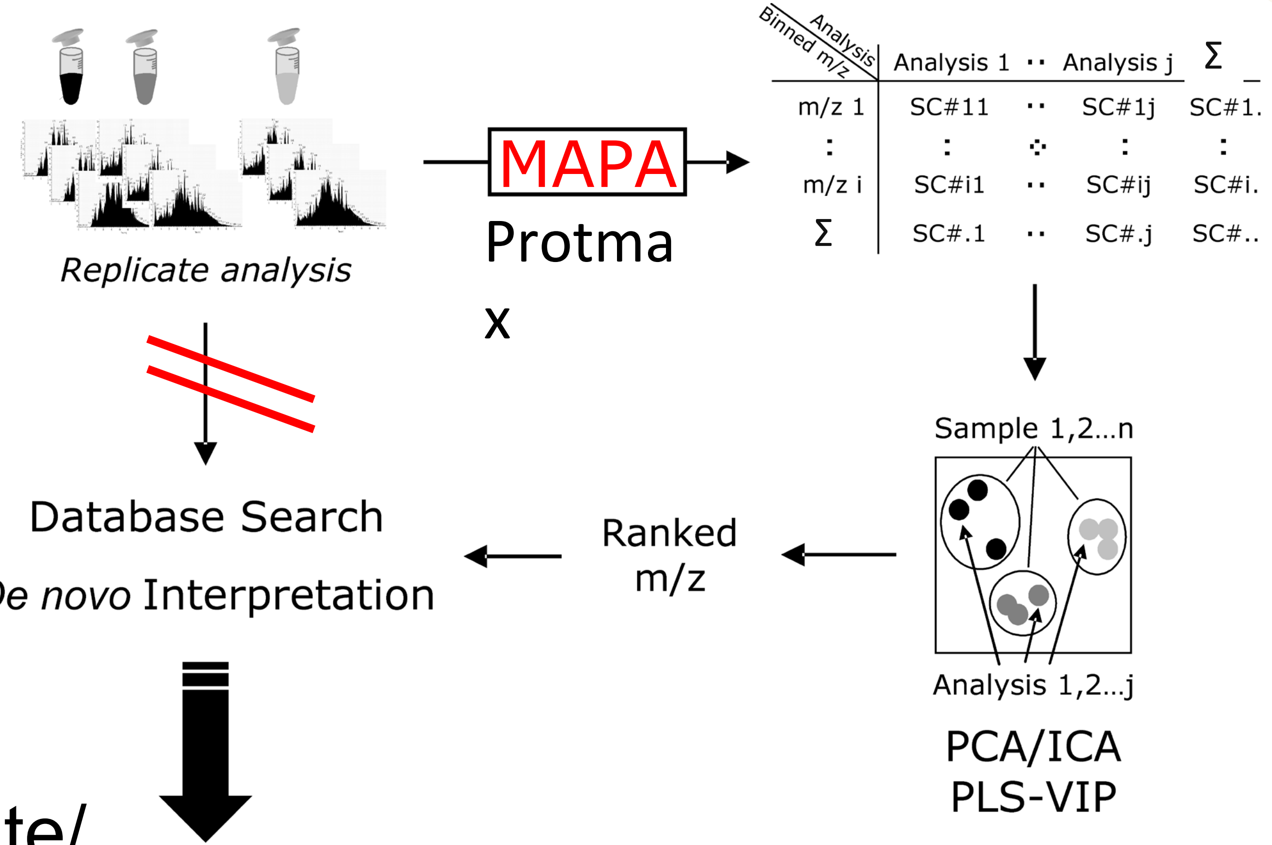
A rapid approach for phenotype-screening and database independent detection of cSNP/protein polymorphism using mass accuracy precursor alignment

Wolfgang Hoehenwarter[1], Joost T. van Dongen[1], Stefanie Wienkoop[1], Matthias Steinfath[2], Jan Hummel[1], Alexander Erban[1], Ronan Sulpice[1], Babette Regierer[2], Joachim Kopka[1], Peter Geigenberger[1] and Wolfram Weckwerth[1, 3, 4]

MAPA – Proteomics/Metabolomics

Sample 1,2…n

Analysis 1,2…j



Replicate analysis

MAPA

Protmax

Binned m/z \ Analysis	Analysis 1	··	Analysis j	Σ
m/z 1	SC#11	··	SC#1j	SC#1.
:	:	⁘	:	:
m/z i	SC#i1	··	SC#ij	SC#i.
Σ	SC#.1	··	SC#.j	SC#..

PCA/ICA
PLS-VIP

Ranked m/z

Database Search

De novo Interpretation

Metabolite/
Protein Marker Identification

Hoehenwarter et al. 2008 Proteomics
Doerfler et al. 2013 Metabolomics

Machine learning/classification

4 splitting rules X 500 training/test sets each

- 5-fold cross validation
- Leave one out cross validation
- Bootstrap sampling
- Monte Carlo cross validation

2000 training/test sets

123 predictors

4 classification methods

- LDA
- KNNC
- SVM
- Random Forest (RF)

500 training/test sets each

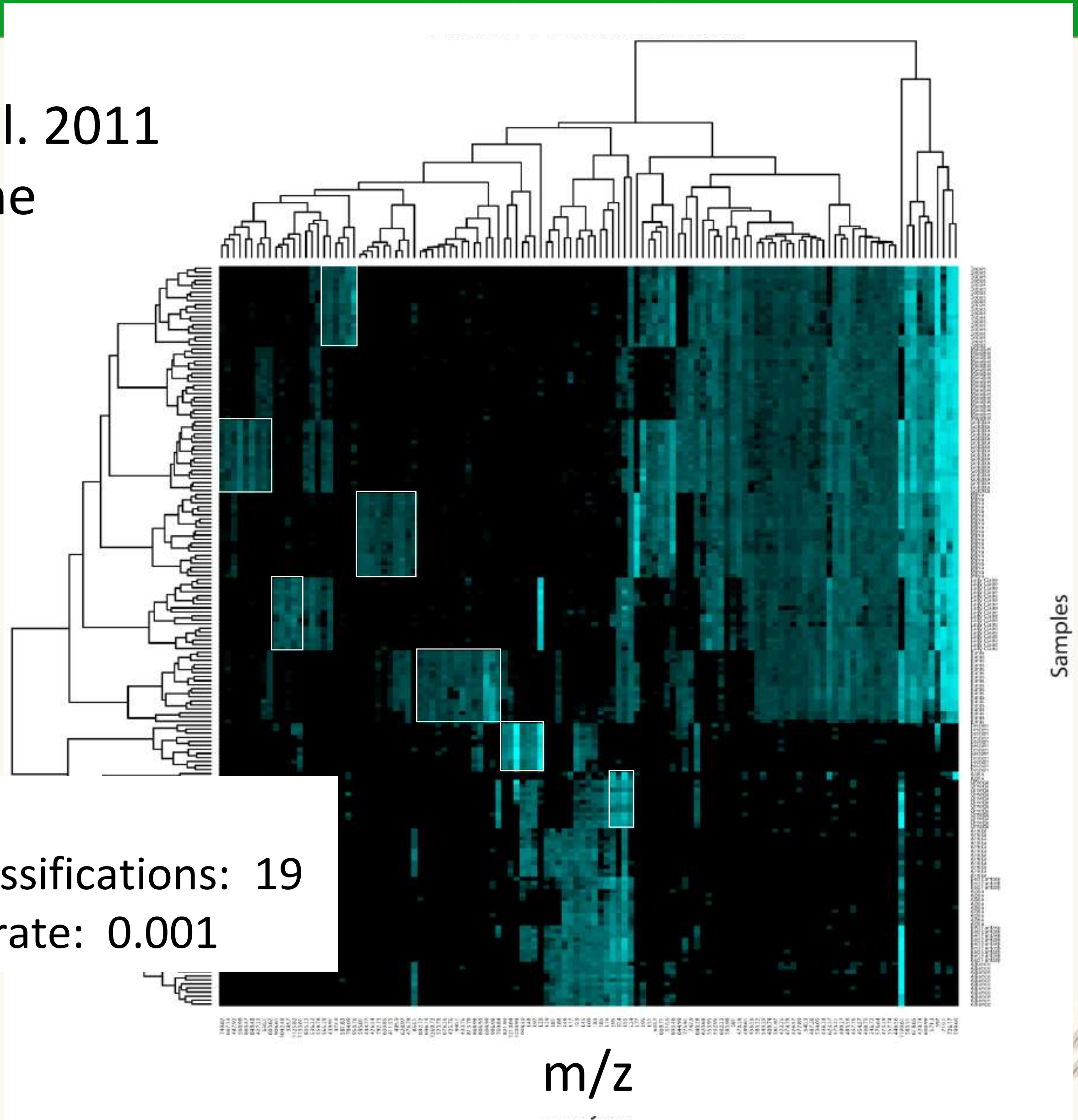
- 5-fold cross validation

18300 predictions each

Hoehenwarter et al. 2011
Journal of Proteome Research

Machine learning of shotgun proteomics data identifies highly specific cultivar markers

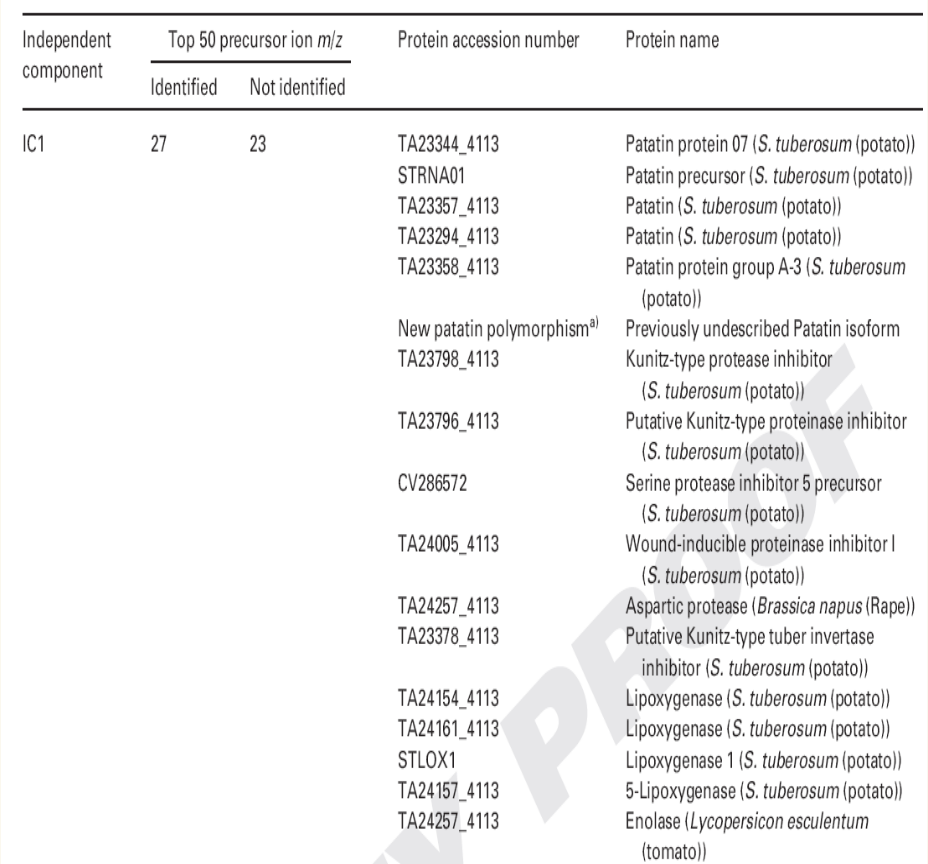
Hoehenwarter et al. 2011
Journal of Proteome
Research



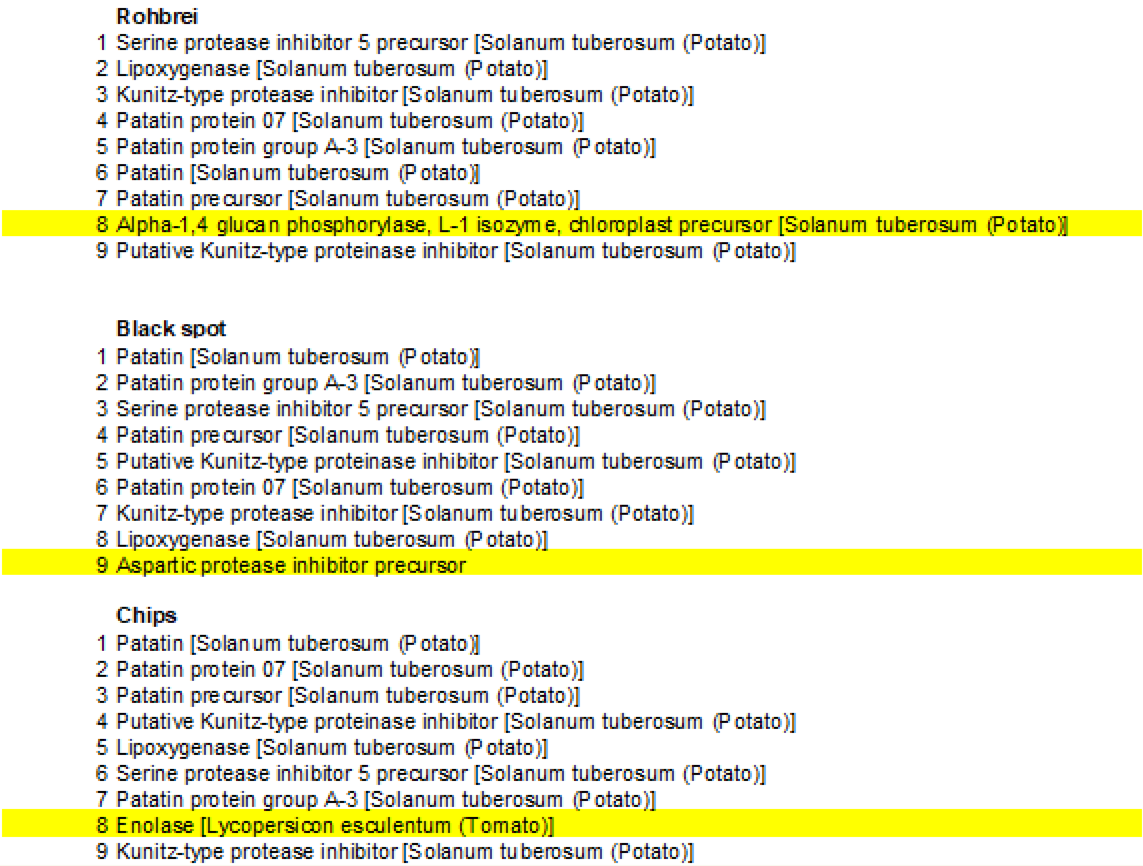
Topas
Marabel
Goldika
Milva
Lady Claire
Kuras
Festien
Omega
Arnika
Agria
Red Fantasy
Alliance

18300 predictions
number of missclassifications: 19
missclassification rate: 0.001

Protein Marker? VIP versus ICA



Independent component	Top 50 precursor ion *m/z*		Protein accession number	Protein name
	Identified	Not identified		
IC1	27	23	TA23344_4113	Patatin protein 07 (*S. tuberosum* (potato))
			STRNA01	Patatin precursor (*S. tuberosum* (potato))
			TA23357_4113	Patatin (*S. tuberosum* (potato))
			TA23294_4113	Patatin (*S. tuberosum* (potato))
			TA23358_4113	Patatin protein group A-3 (*S. tuberosum* (potato))
			New patatin polymorphism[a]	Previously undescribed Patatin isoform
			TA23798_4113	Kunitz-type protease inhibitor (*S. tuberosum* (potato))
			TA23796_4113	Putative Kunitz-type proteinase inhibitor (*S. tuberosum* (potato))
			CV286572	Serine protease inhibitor 5 precursor (*S. tuberosum* (potato))
			TA24005_4113	Wound-inducible proteinase inhibitor I (*S. tuberosum* (potato))
			TA24257_4113	Aspartic protease (*Brassica napus* (Rape))
			TA23378_4113	Putative Kunitz-type tuber invertase inhibitor (*S. tuberosum* (potato))
			TA24154_4113	Lipoxygenase (*S. tuberosum* (potato))
			TA24161_4113	Lipoxygenase (*S. tuberosum* (potato))
			STLOX1	Lipoxygenase 1 (*S. tuberosum* (potato))
			TA24157_4113	5-Lipoxygenase (*S. tuberosum* (potato))
			TA24257_4113	Enolase (*Lycopersicon esculentum* (tomato))



Rohbrei

1 Serine protease inhibitor 5 precursor [Solanum tuberosum (Potato)]
2 Lipoxygenase [Solanum tuberosum (Potato)]
3 Kunitz-type protease inhibitor [Solanum tuberosum (Potato)]
4 Patatin protein 07 [Solanum tuberosum (Potato)]
5 Patatin protein group A-3 [Solanum tuberosum (Potato)]
6 Patatin [Solanum tuberosum (Potato)]
7 Patatin precursor [Solanum tuberosum (Potato)]
8 Alpha-1,4 glucan phosphorylase, L-1 isozyme, chloroplast precursor [Solanum tuberosum (Potato)]
9 Putative Kunitz-type proteinase inhibitor [Solanum tuberosum (Potato)]

Black spot

1 Patatin [Solanum tuberosum (Potato)]
2 Patatin protein group A-3 [Solanum tuberosum (Potato)]
3 Serine protease inhibitor 5 precursor [Solanum tuberosum (Potato)]
4 Patatin precursor [Solanum tuberosum (Potato)]
5 Putative Kunitz-type proteinase inhibitor [Solanum tuberosum (Potato)]
6 Patatin protein 07 [Solanum tuberosum (Potato)]
7 Kunitz-type protease inhibitor [Solanum tuberosum (Potato)]
8 Lipoxygenase [Solanum tuberosum (Potato)]
9 Aspartic protease inhibitor precursor

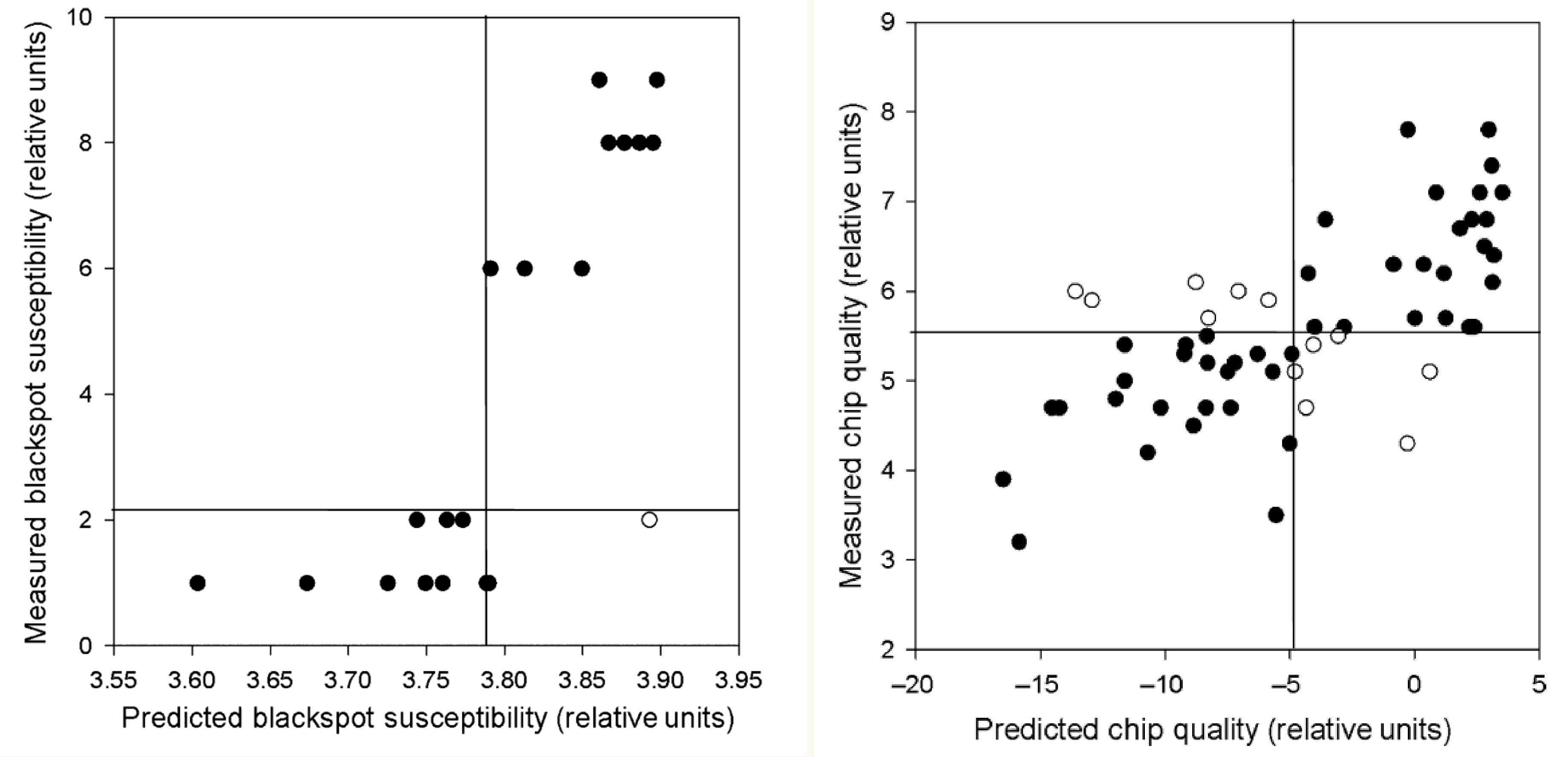
Chips

1 Patatin [Solanum tuberosum (Potato)]
2 Patatin protein 07 [Solanum tuberosum (Potato)]
3 Patatin precursor [Solanum tuberosum (Potato)]
4 Putative Kunitz-type proteinase inhibitor [Solanum tuberosum (Potato)]
5 Lipoxygenase [Solanum tuberosum (Potato)]
6 Serine protease inhibitor 5 precursor [Solanum tuberosum (Potato)]
7 Patatin protein group A-3 [Solanum tuberosum (Potato)]
8 Enolase [Lycopersicon esculentum (Tomato)]
9 Kunitz-type protease inhibitor [Solanum tuberosum (Potato)]

Hoehenwarter et al. 2008 Proteomics

MoSys
universität wien

Metabolite marker for prediction



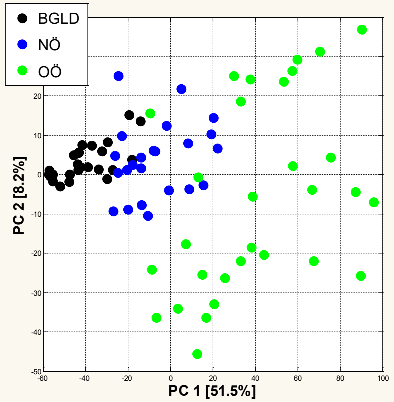
Steinfath et al. 2010 Plant Biotechn.

Metabolomics, genetic variation and *in situ* modelling

Eco-Metabolomics and *in situ* metabolic modelling Nagler et al. 2018 Frontiers Plant Science

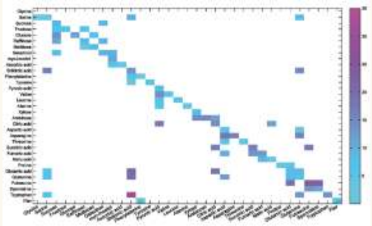
Arabidopsis thaliana natural populations

variance



variance

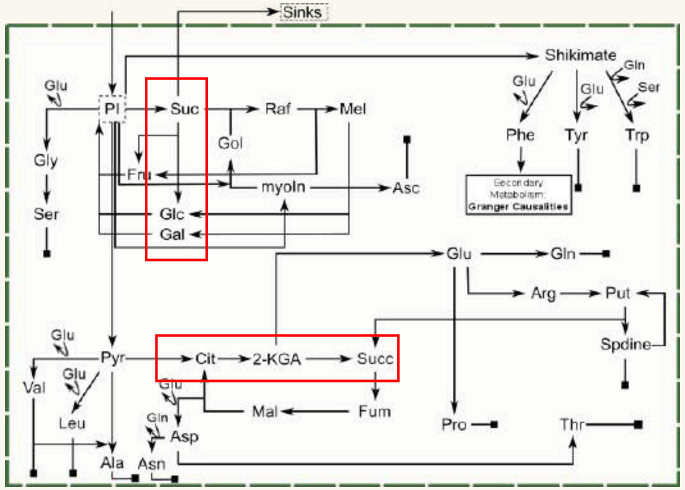
Stoichiometric matrix N (Genotype)



Differential Jacobian

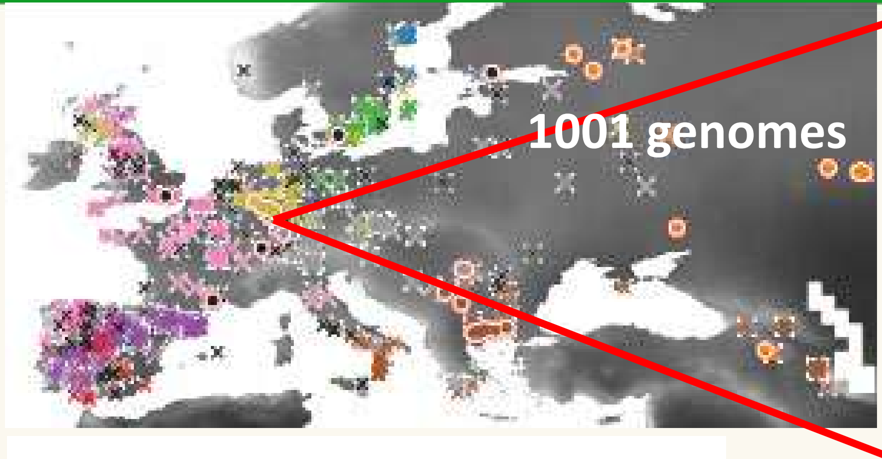
$$\frac{\partial f}{\partial M}$$

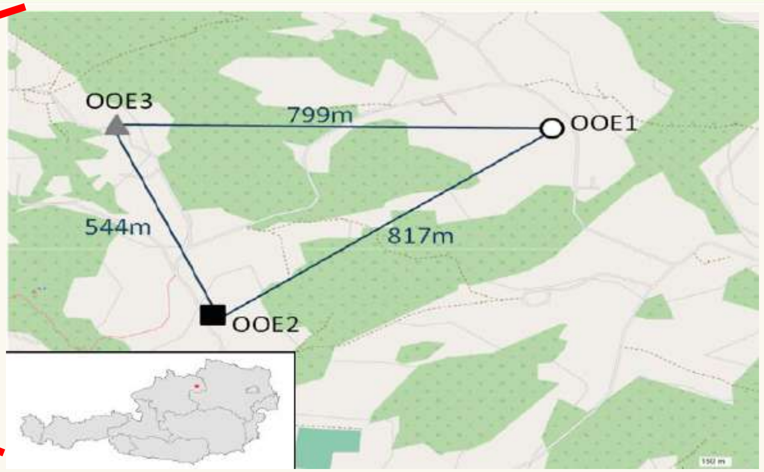
Reaction rate elasticities



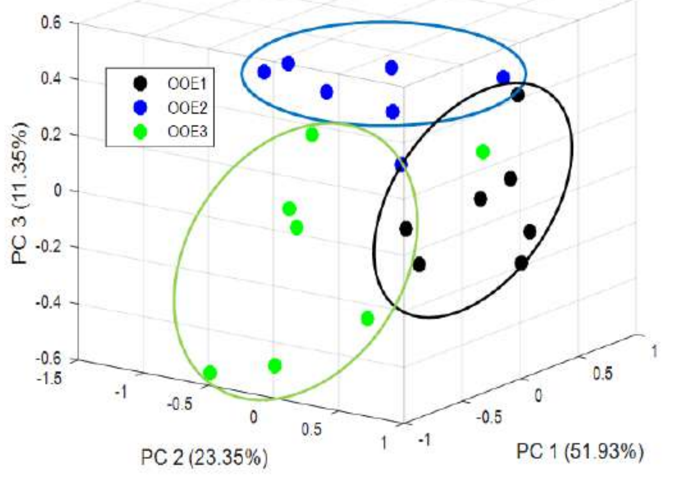
Physiology

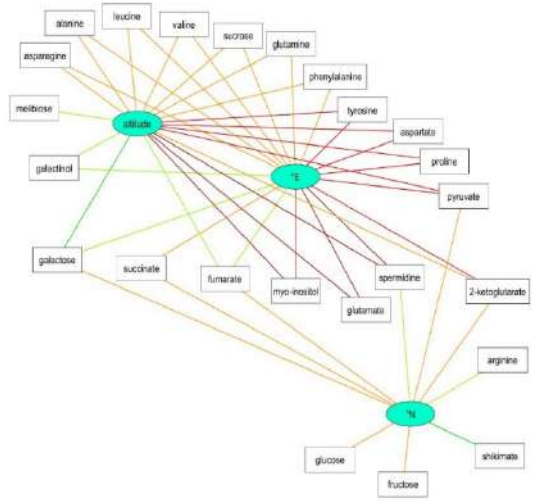
Eco-Metabolomics and *in situ* metabolic modelling Nagler et al. 2018 Frontiers Plant Science





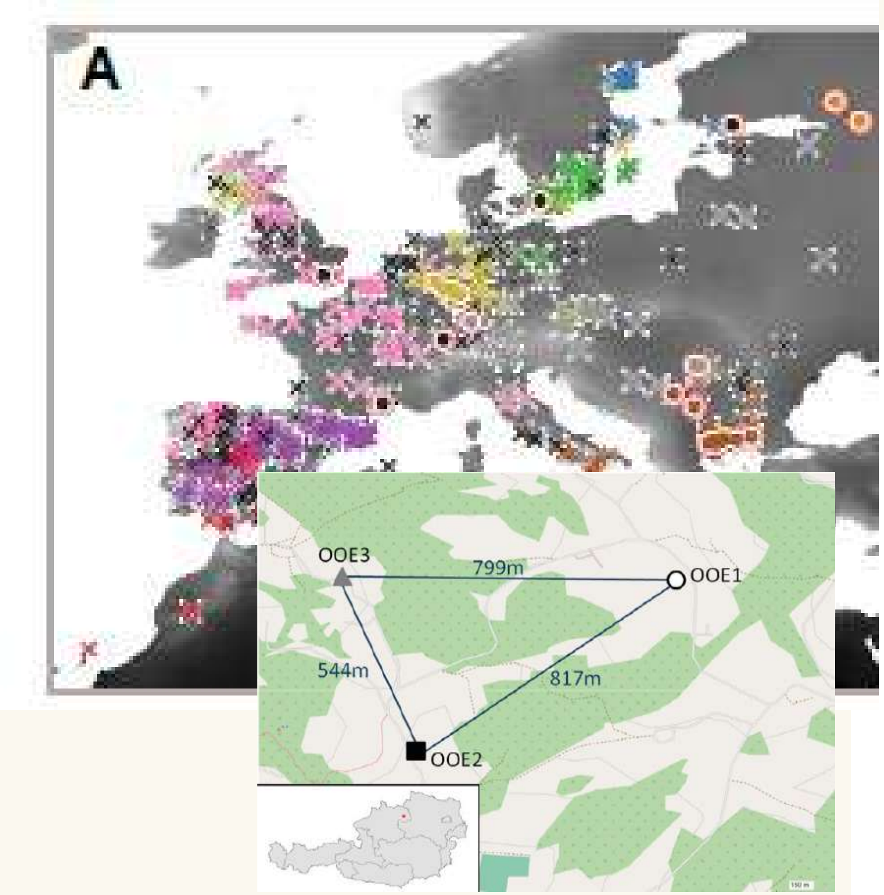
GC-MS/LC-MS Metabolomics

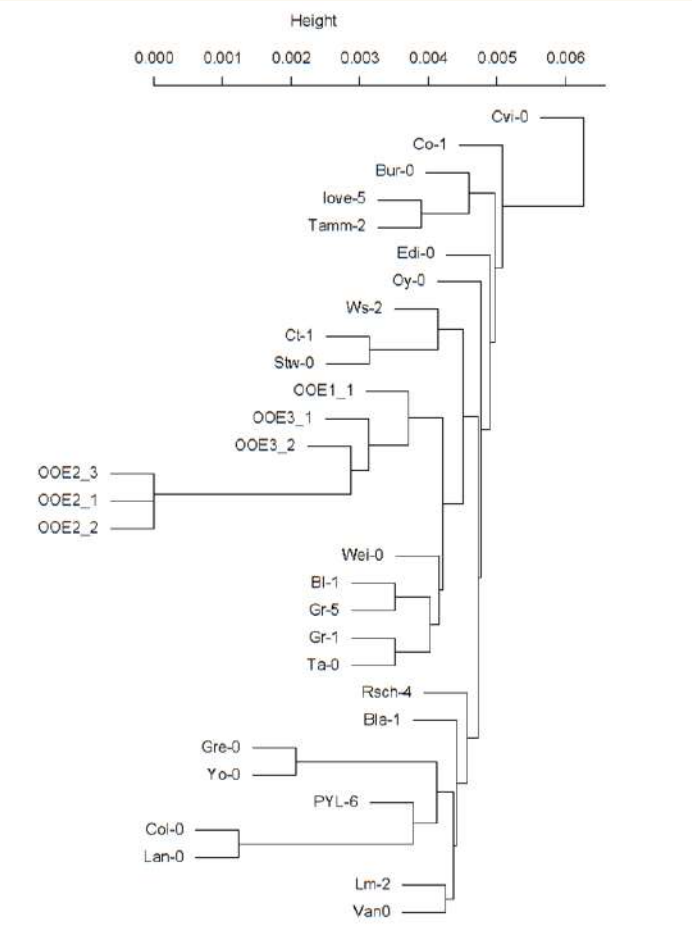




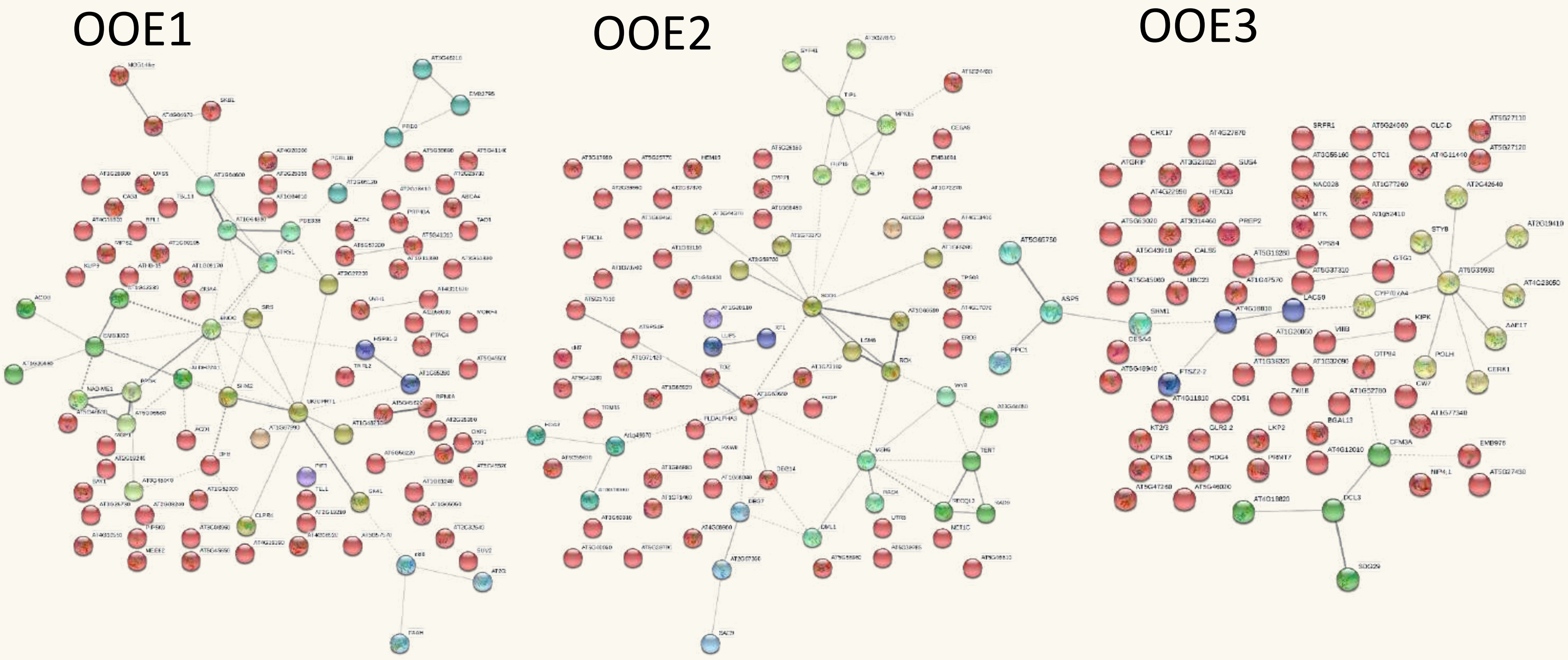
Strong GPS-metabolite correlations

Eco-Metabolomics and *in situ* metabolic modelling Nagler et al. 2018 Frontiers Plant Science





Eco-Metabolomics and *in situ* metabolic modelling Nagler et al. 2018 Frontiers Plant Science


OOE1

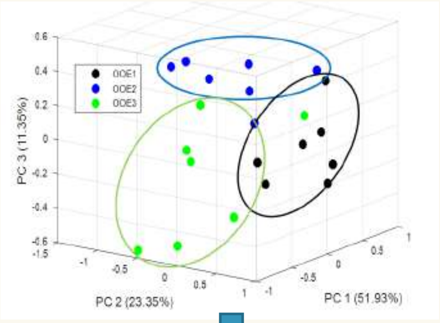
OOE2

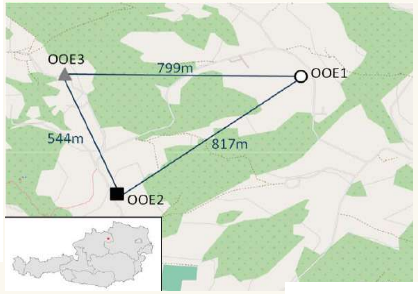
OOE3

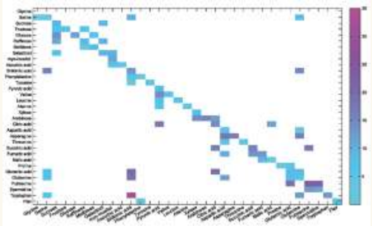
Population specific protein-interaction networks of SNP enriched genes

SNP enrichments of different genotypes correlate with biochemical prediction

GC-MS/LC-MS Metabolomics



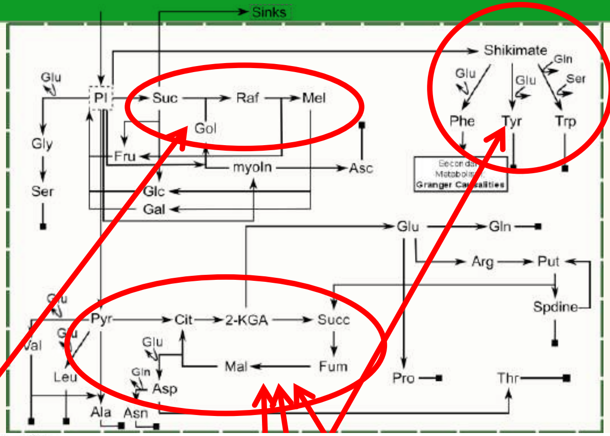


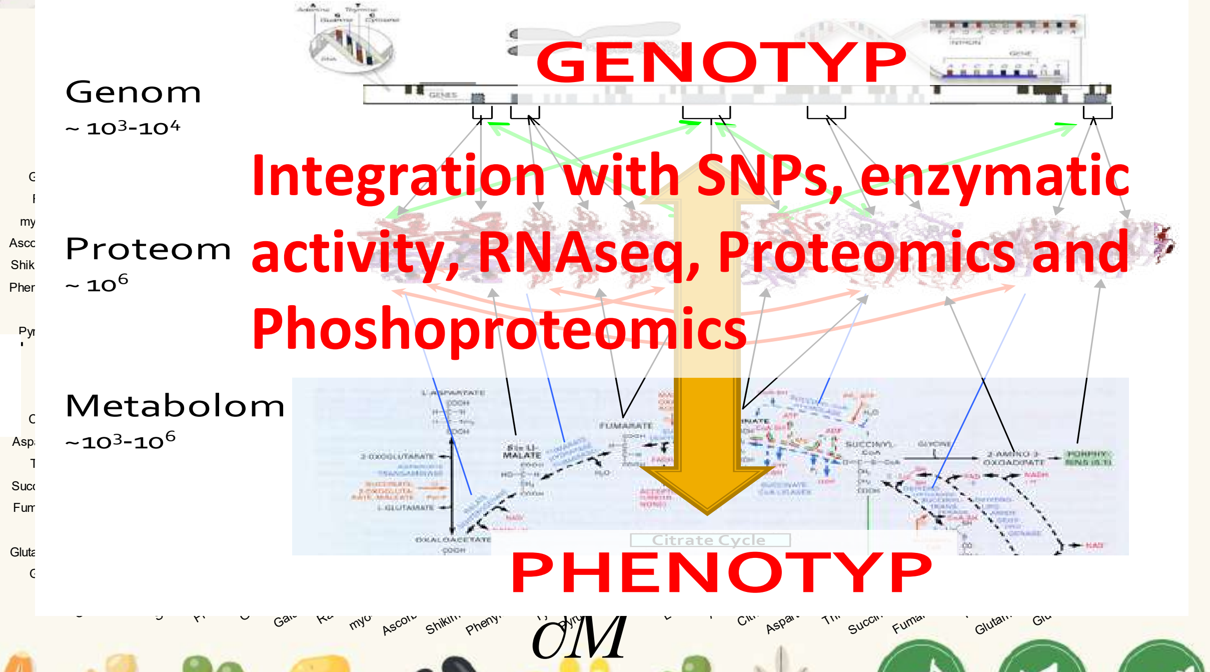


Differential Jacobian

$$\frac{\partial f}{\partial M}$$

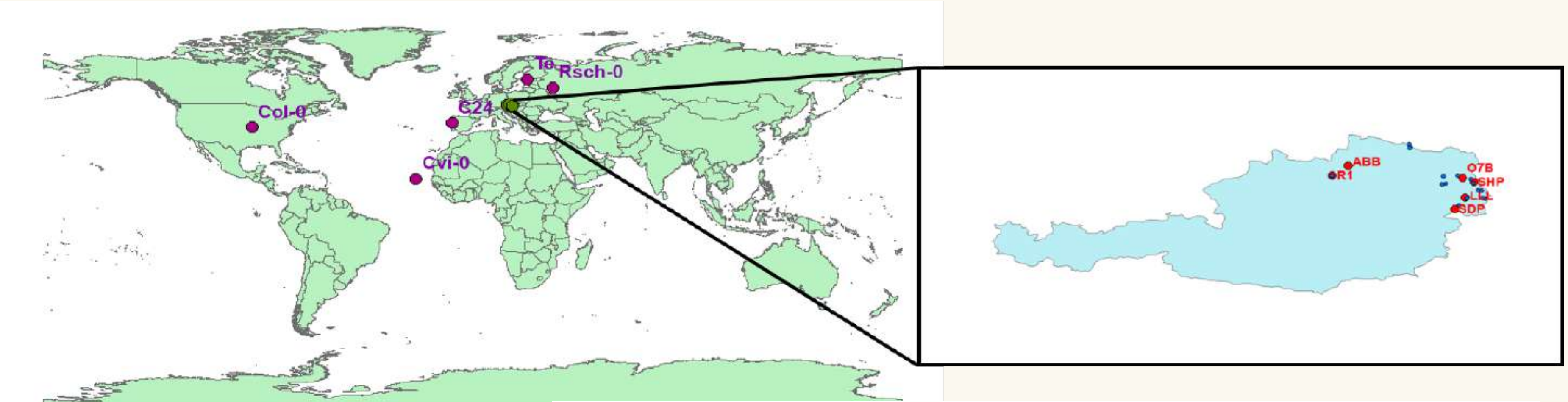
Prediction of changed proteins



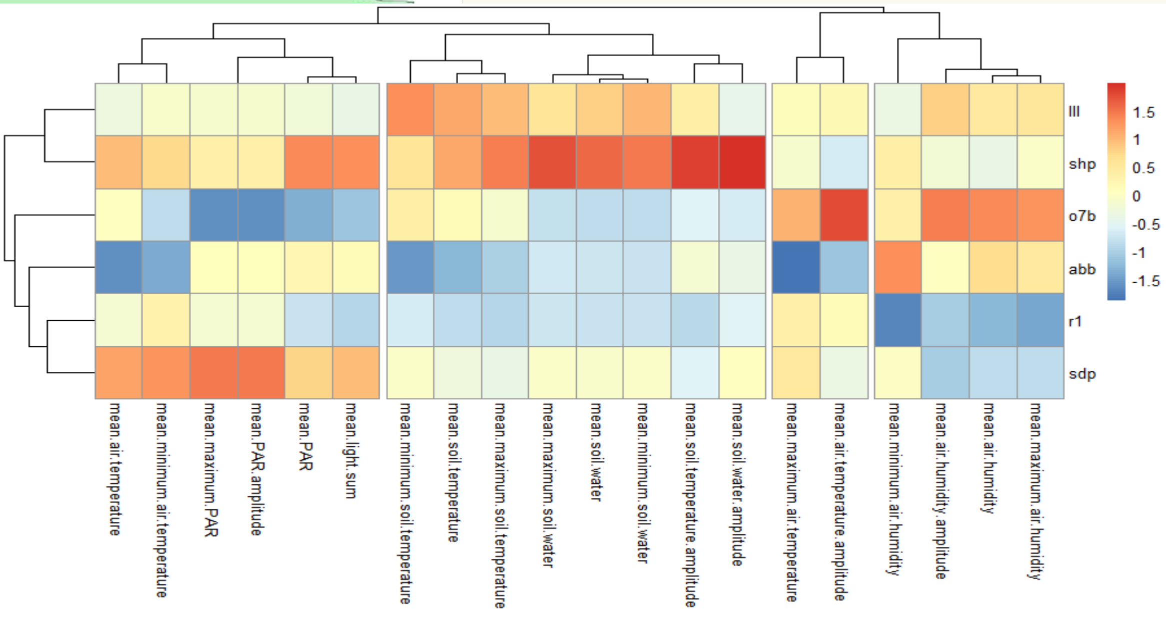


Integration with SNPs, enzymatic activity, RNAseq, Proteomics and Phoshoproteomics

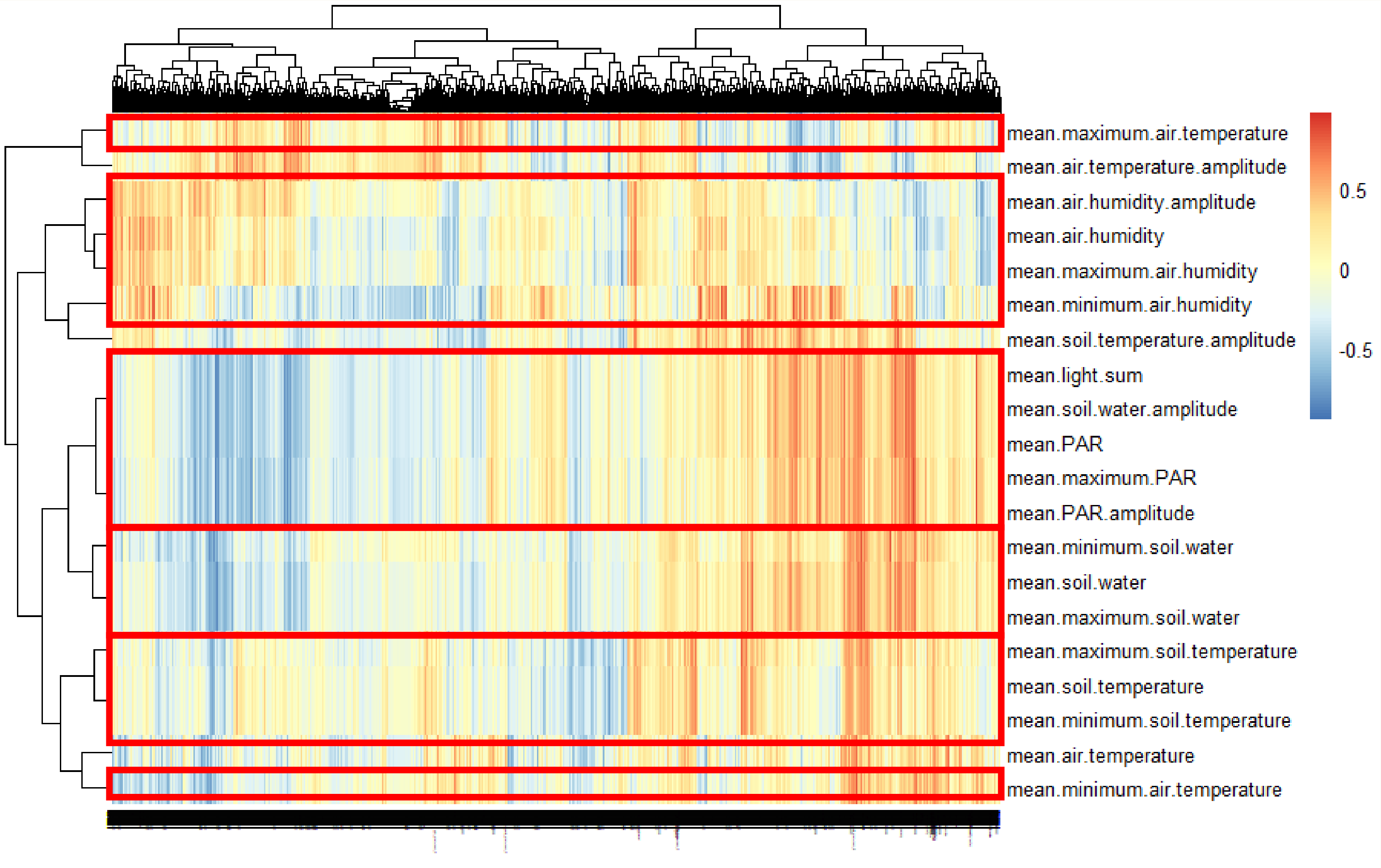
Multiomics analysis of *in situ* Arabidopsis populations



Data logger:
Temp, PAR,
humidity, soil
water, etc

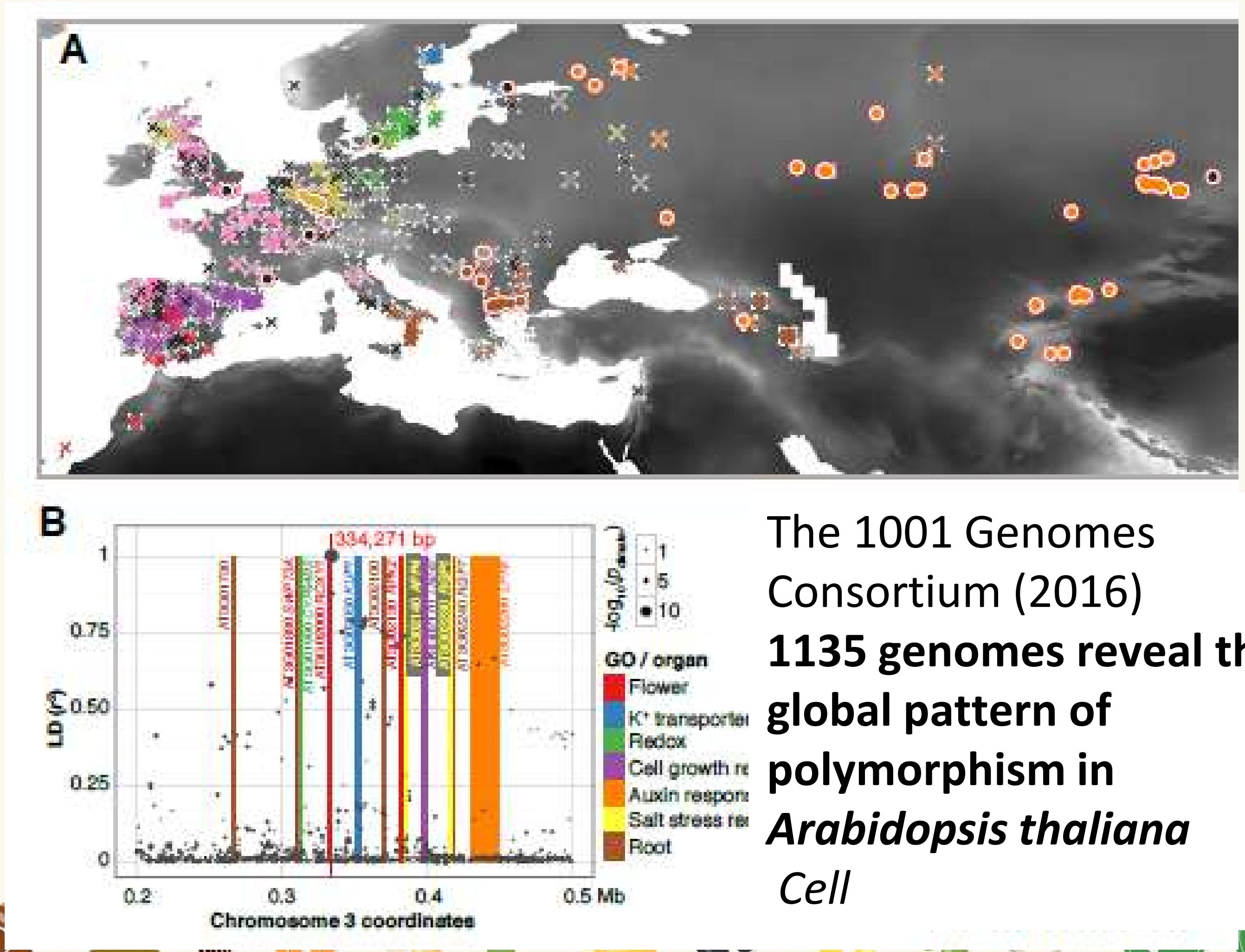


Multiomics analysis of *in situ* Arabidopsis populations – correlation with environmental data



Metabolic genome wide association studies mGWAS

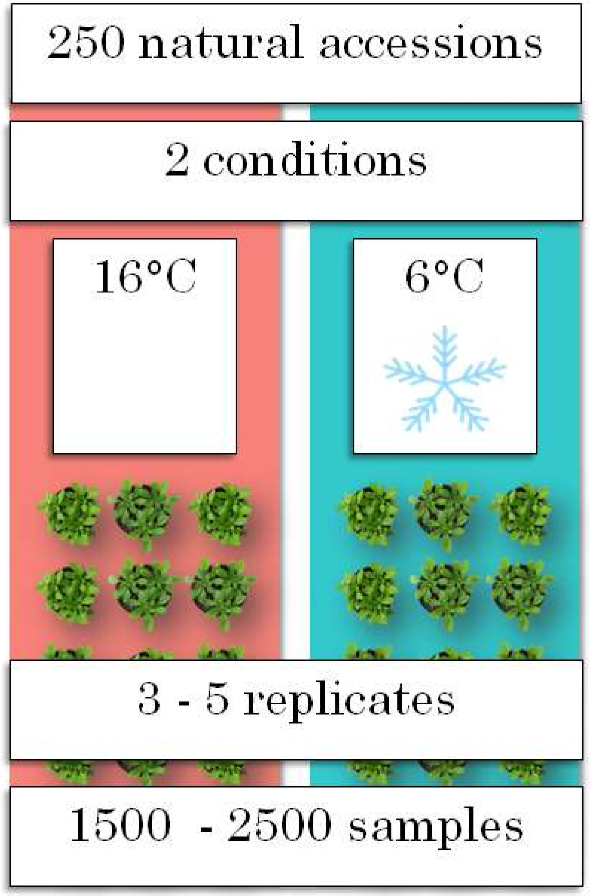
Germplasm genomics intraspecific variation



Polymorphism involved in climate adaption

The 1001 Genomes Consortium (2016)
1135 genomes reveal the global pattern of polymorphism in *Arabidopsis thaliana*
Cell

250 Arabidopsis genotypes in control and cold stress



250 natural accessions

2 conditions

16°C

6°C

3 - 5 replicates

1500 - 2500 samples

automatic phenotyping

SNP sequencing

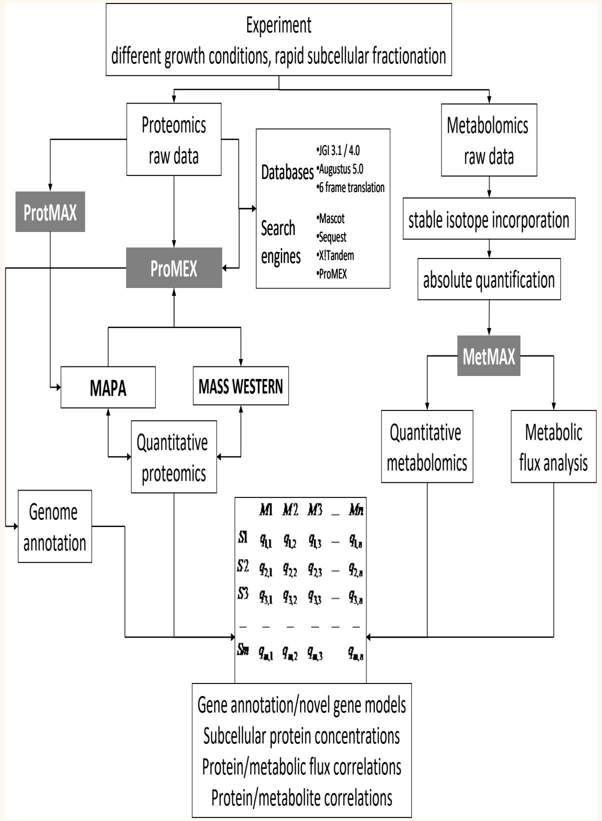
RNA-seq

metabolomics

metabolic modelling

Weiszmann et al. 2020

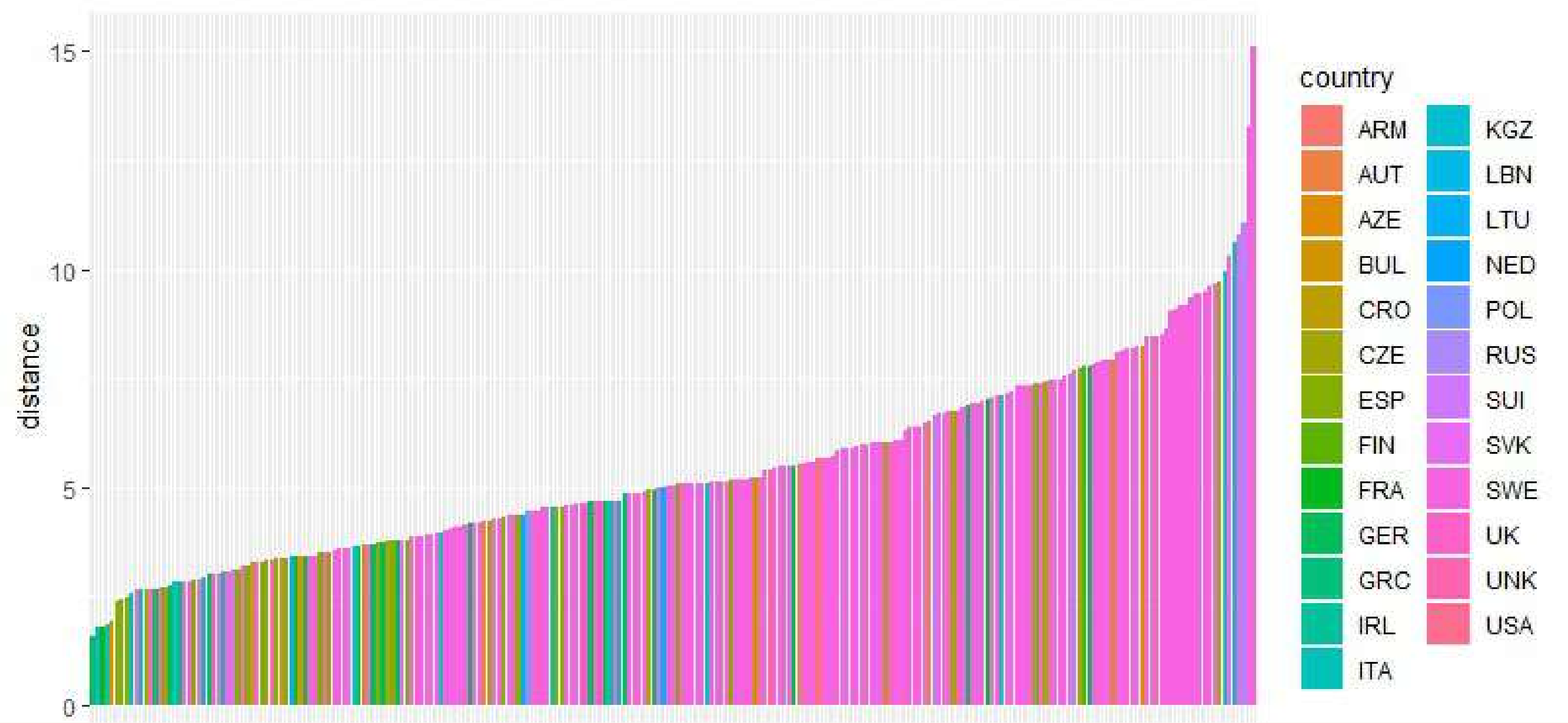
Some 3000 samples later…



Metabolic distance of stress adaptation

Genotype-dependent metabolic distance of stress adaptation

Weiszmann et al. 2020



Natural metabolic variation is predicted by early spring time temperature of the natural habitate

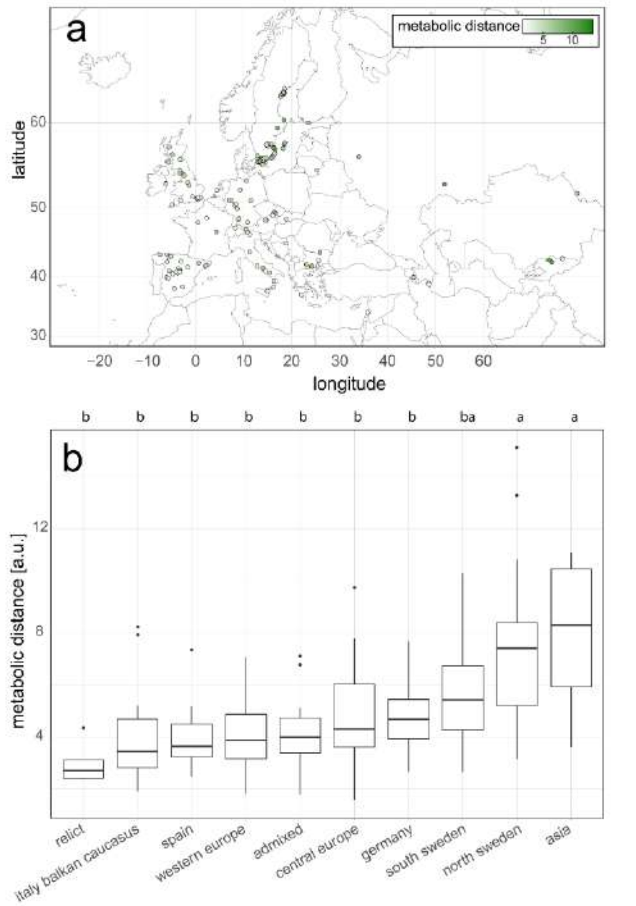
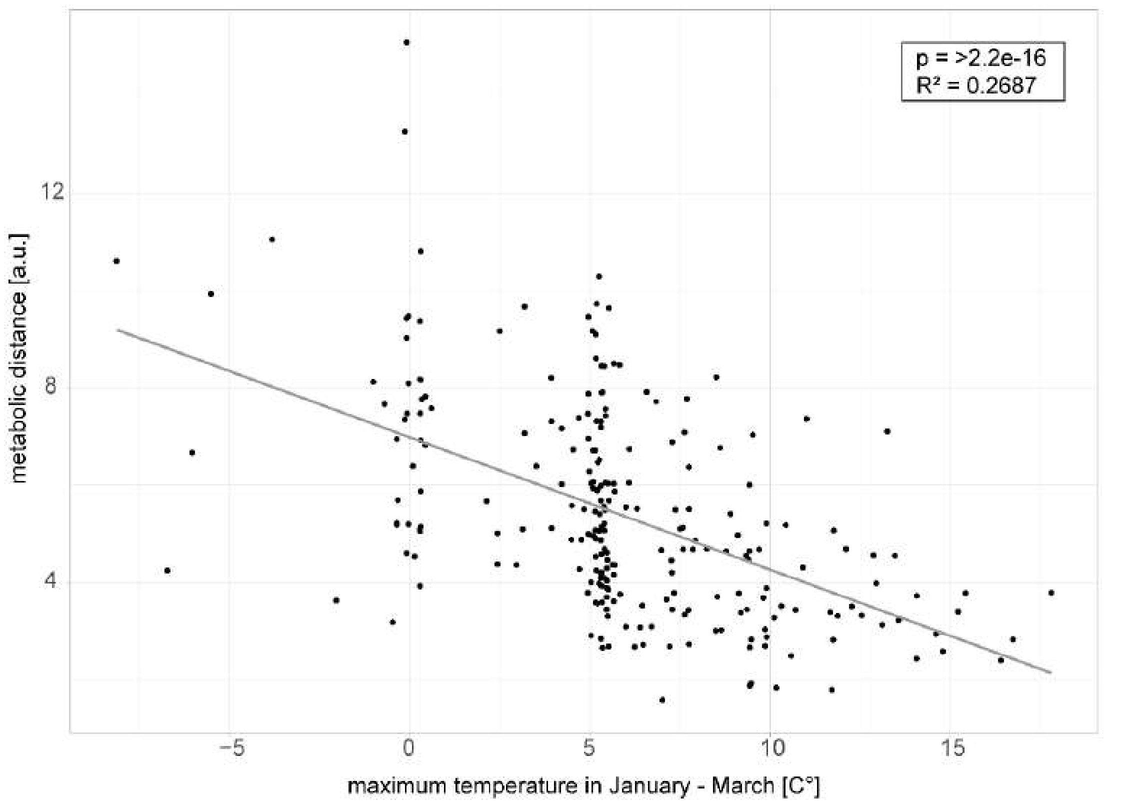
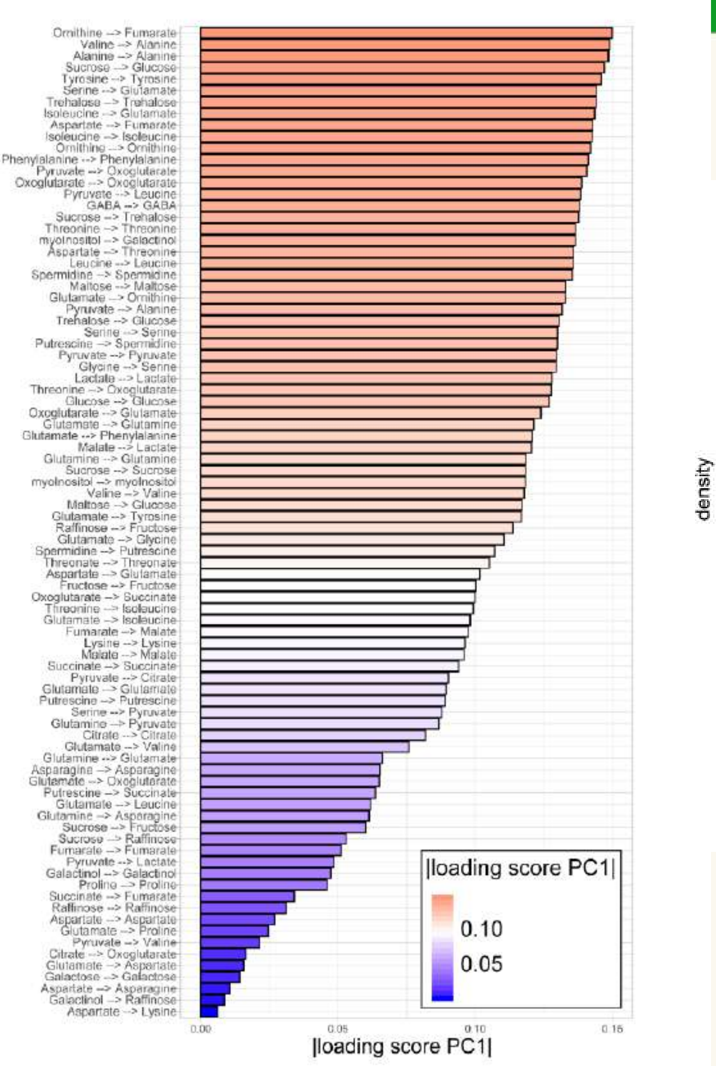


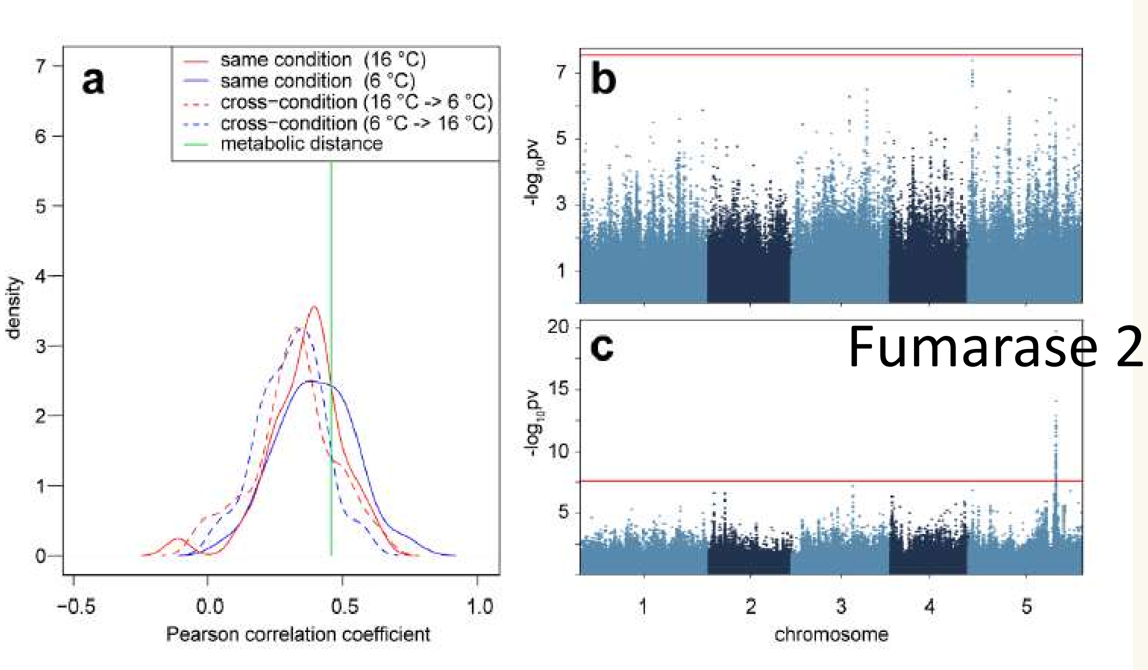
Figure 4 a – Map of included natural Arabidopsis accessions, colour corresponds to metabolic distance between 16 °C and 6 °C growth condition (4 Asian accessions not shown). b - Metabolic distances of Arabidopsis natural accessions, grouped by genetic admixture group. Letters denote significance groups according to ANOVA with a Tukey- HSD post-hoc test.



Weiszmann et al. 2020

Allelic variation correlates with metabolic prediction





Fumarase 2

Weiszmann et al. 2020

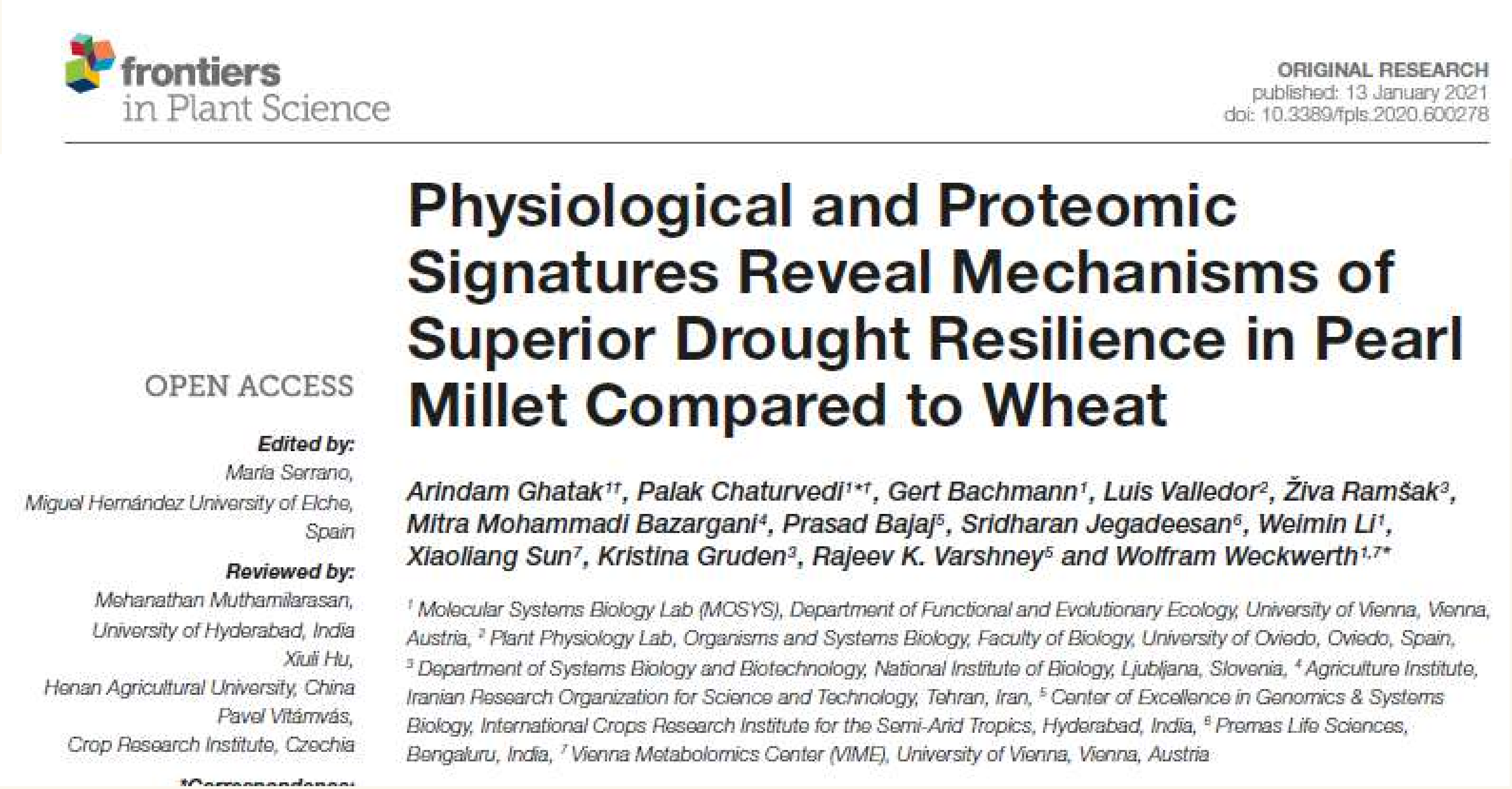
Conclusion

Every location and microhabitat creates a unique phenotype. This suggests that locally selected and developed cultivars may be superior to seed stocks produced and distributed globally.

Comment in social media

Germplasm collections offer „climate smart crops“

Germplasm collections offer „climate smart crops“ – stress resilience



frontiers
in Plant Science

ORIGINAL RESEARCH
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Physiological and Proteomic Signatures Reveal Mechanisms of Superior Drought Resilience in Pearl Millet Compared to Wheat

Arindam Ghatak[1†], Palak Chaturvedi[1†], Gert Bachmann[1], Luis Valledor[2], Živa Ramšak[3], Mitra Mohammadi Bazargani[4], Prasad Bajaj[5], Sridharan Jegadeesan[6], Weimin Li[1], Xiaoliang Sun[7], Kristina Gruden[3], Rajeev K. Varshney[5] and Wolfram Weckwerth[1,7*]*

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Ghatak et al. 2021
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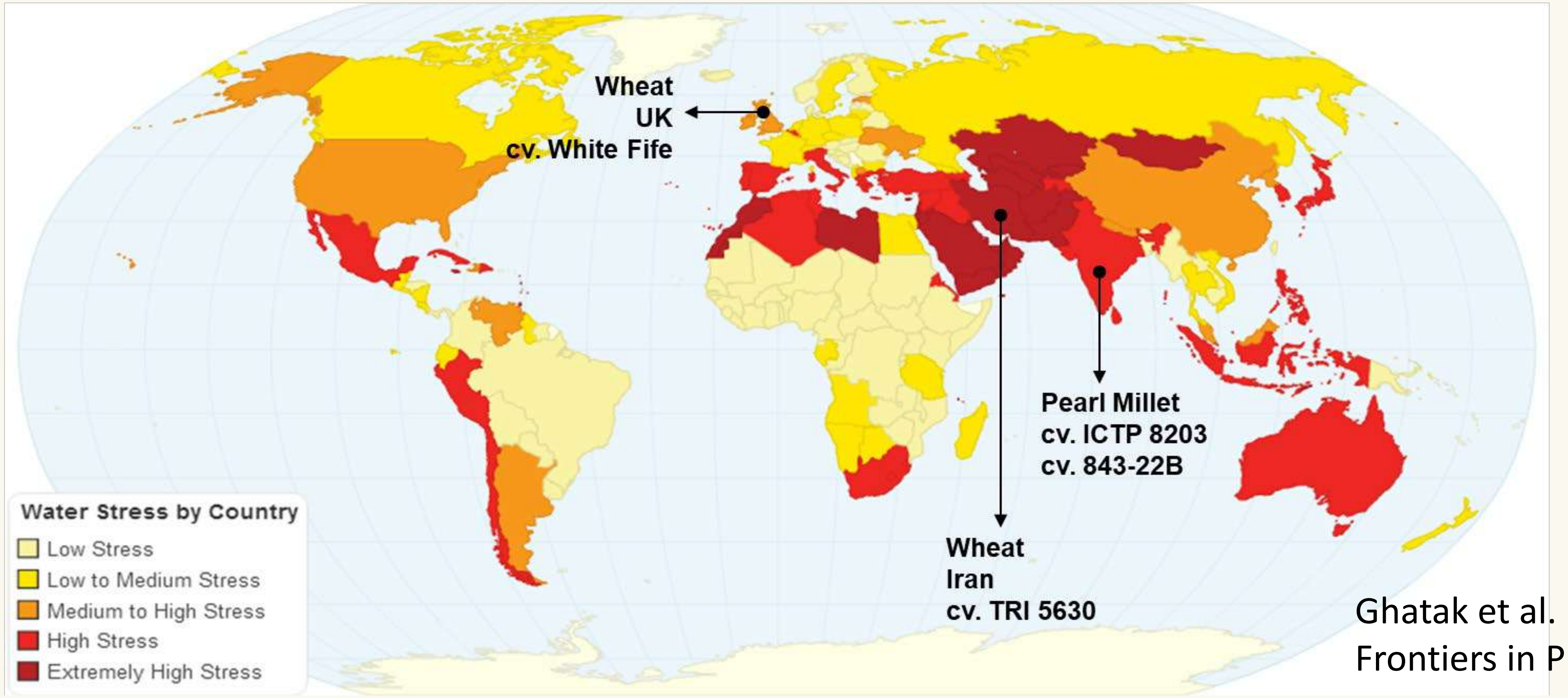
Coping strategies under drought stress: Integrated physiological and multiomic analysis of roots, leaves and seeds in Pearl millet and Wheat



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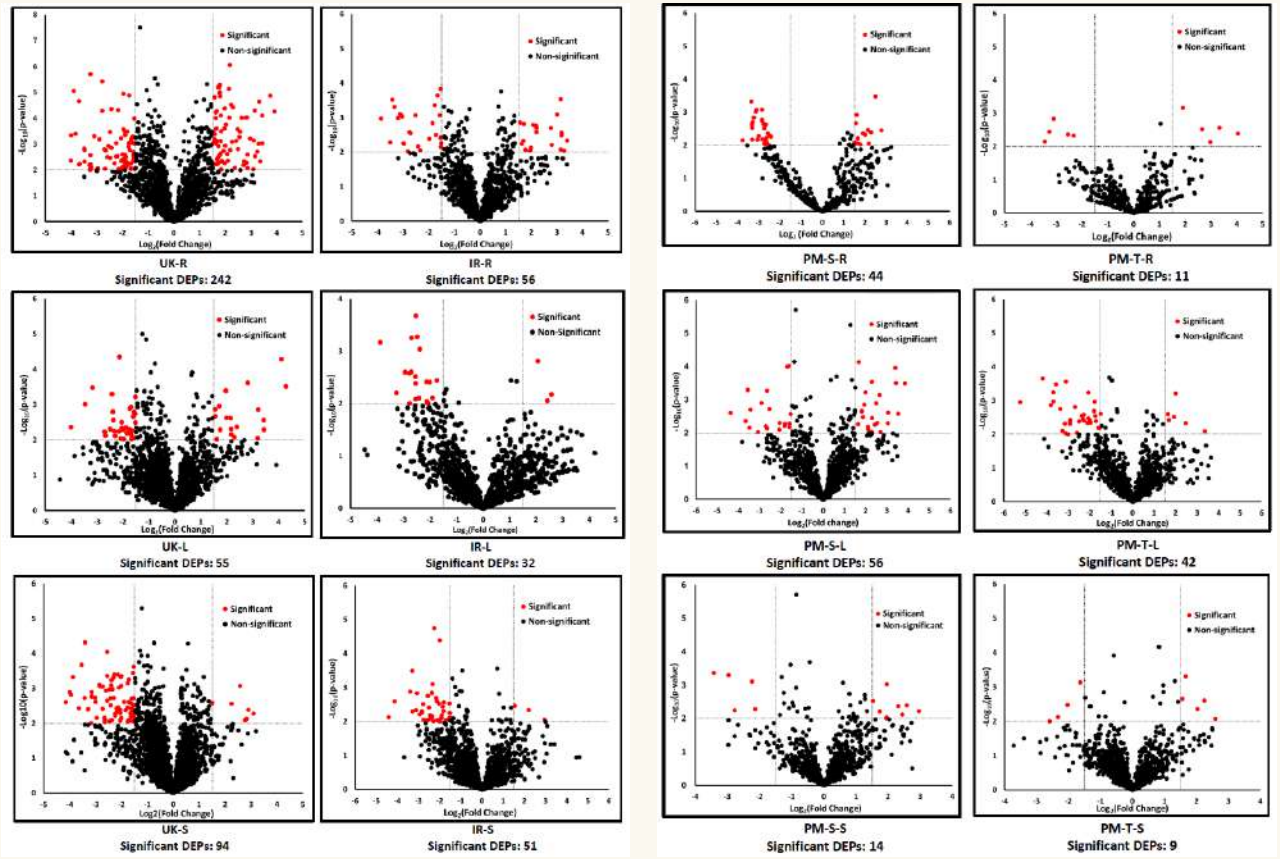
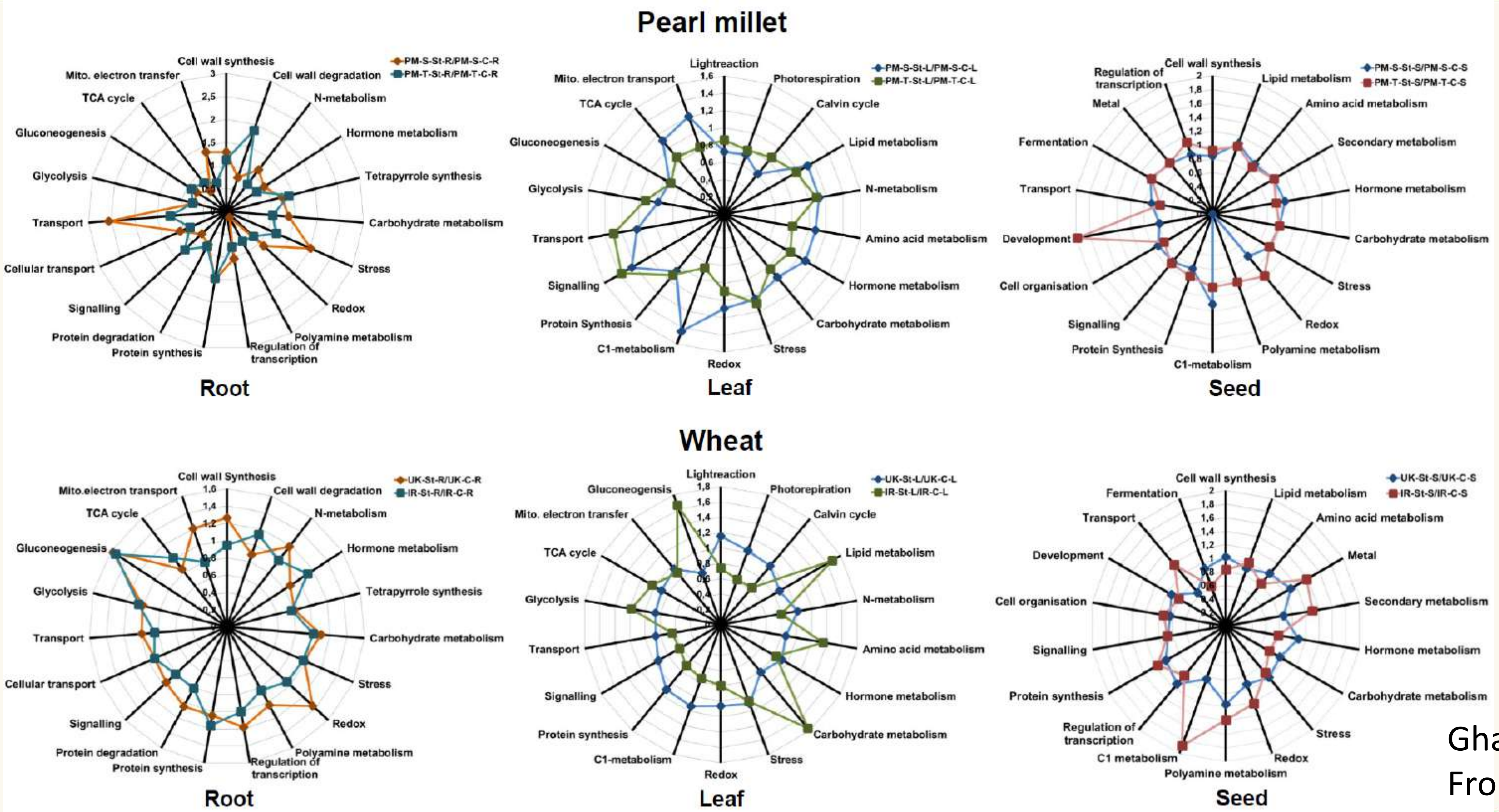
http://chartsbin.com/view/30647

Proteome plasticity of resistant and susceptible wheat and pearl millet genotypes under drought stress



Ghatak et al. 2021
Frontiers in Plant Science

Proteome plasticity of resistant and susceptible wheat and pearl millet genotypes under drought stress



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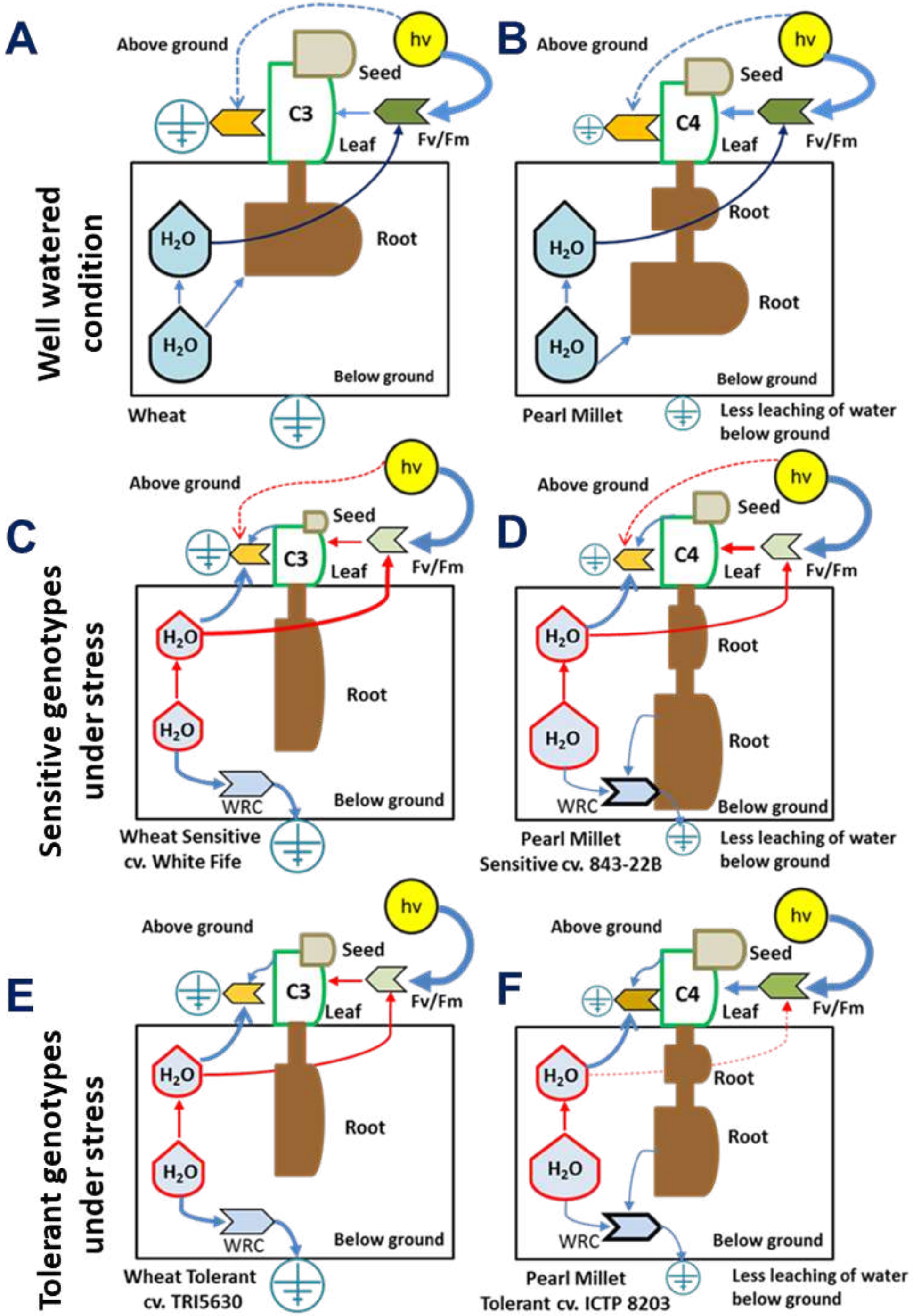
Molecular-physiological models of drought resistant and susceptible Pearl millet and Wheat genotypes



- ▭ Leaf FM
- ▭ Seed Weight
- ▬ Root length
- ◀ Regulation of Stomata Opening
- ◀ Regulation of light harvesting
- ○ Soil Water
- hv Light Energy
- ⊕ Loss of Water
- ▶ Water retention capacity

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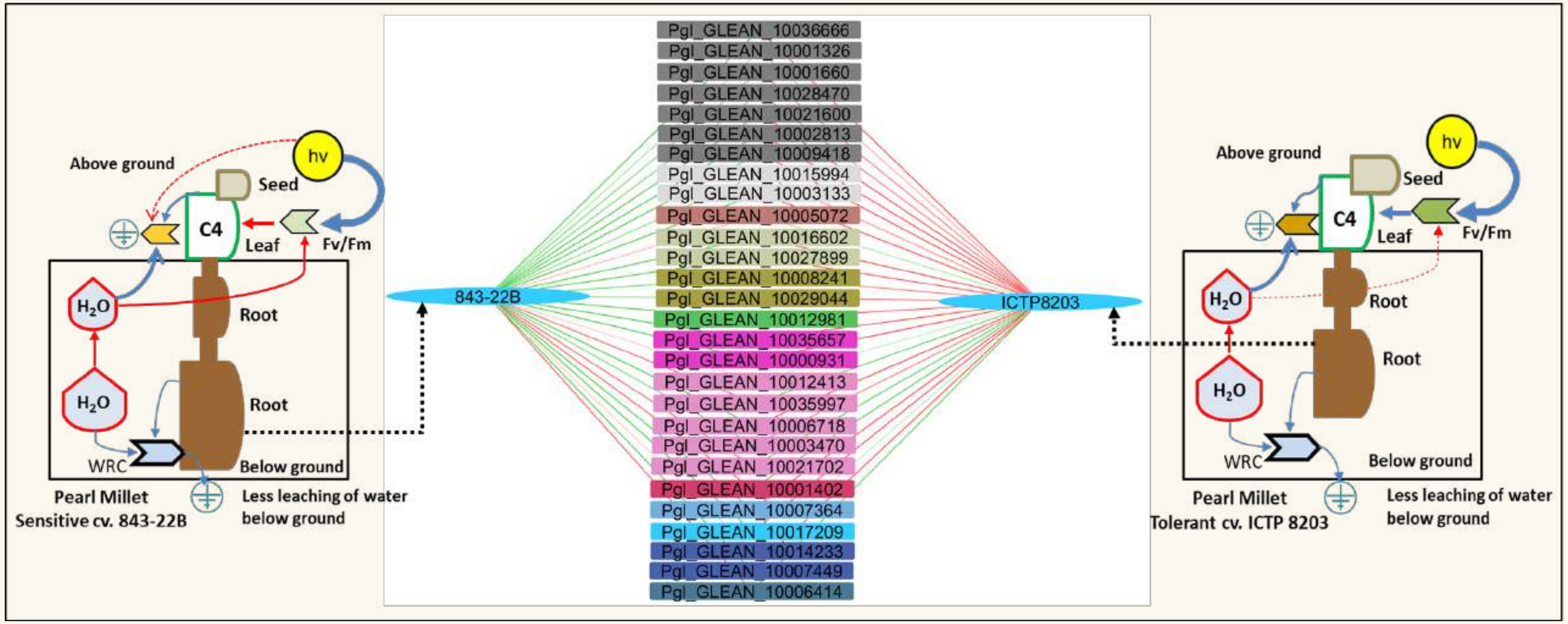
Proteome plasticity of resistant and susceptible wheat and pearl millet genotypes under drought stress

Sparse Partial Least Square analysis: **Predictors for root physiology in pearl millet**



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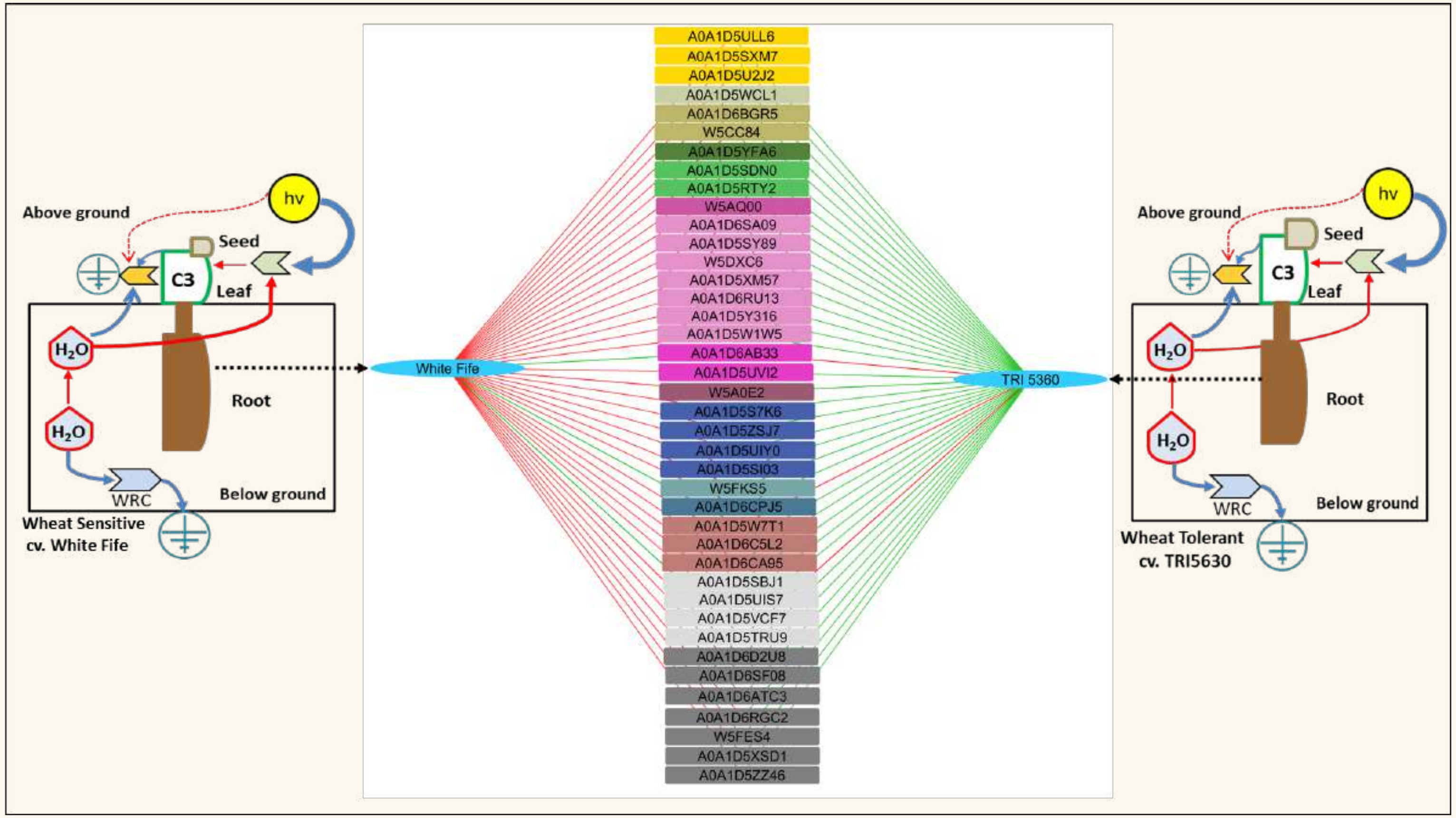
Ghatak , Chaturvedi et al.

Proteome plasticity of resistant and susceptible wheat and pearl millet genotypes under drought stress

Sparse Partial Least Square analysis: **Predictors for root physiology in wheat**



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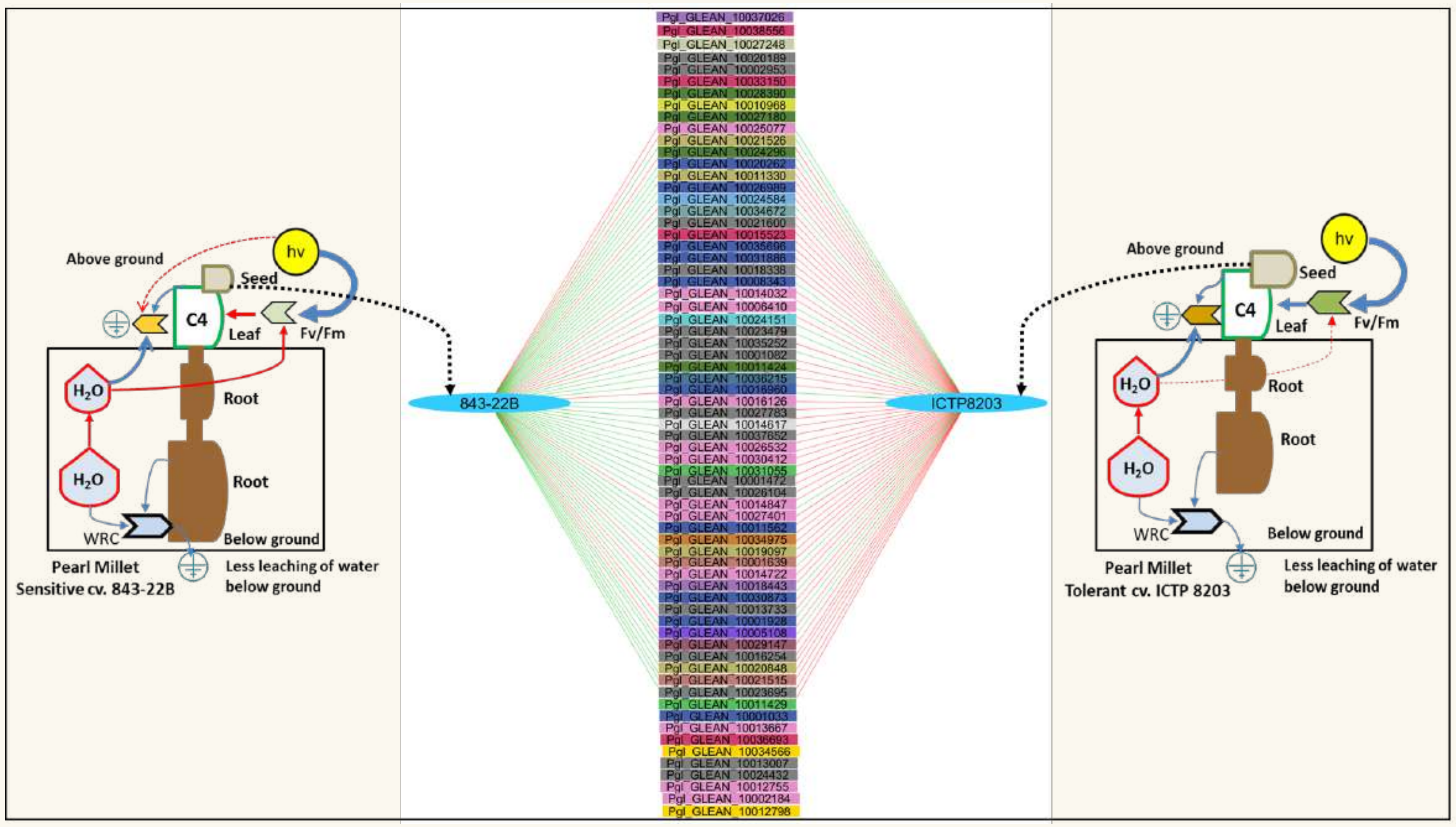
Frontiers in Plant Science

Ghatak , Chaturvedi et al.

Proteome plasticity of resistant and susceptible wheat and pearl millet genotypes under drought stress

Sparse Partial Least Square analysis: **Predictors for seed yield in Pearl millet**



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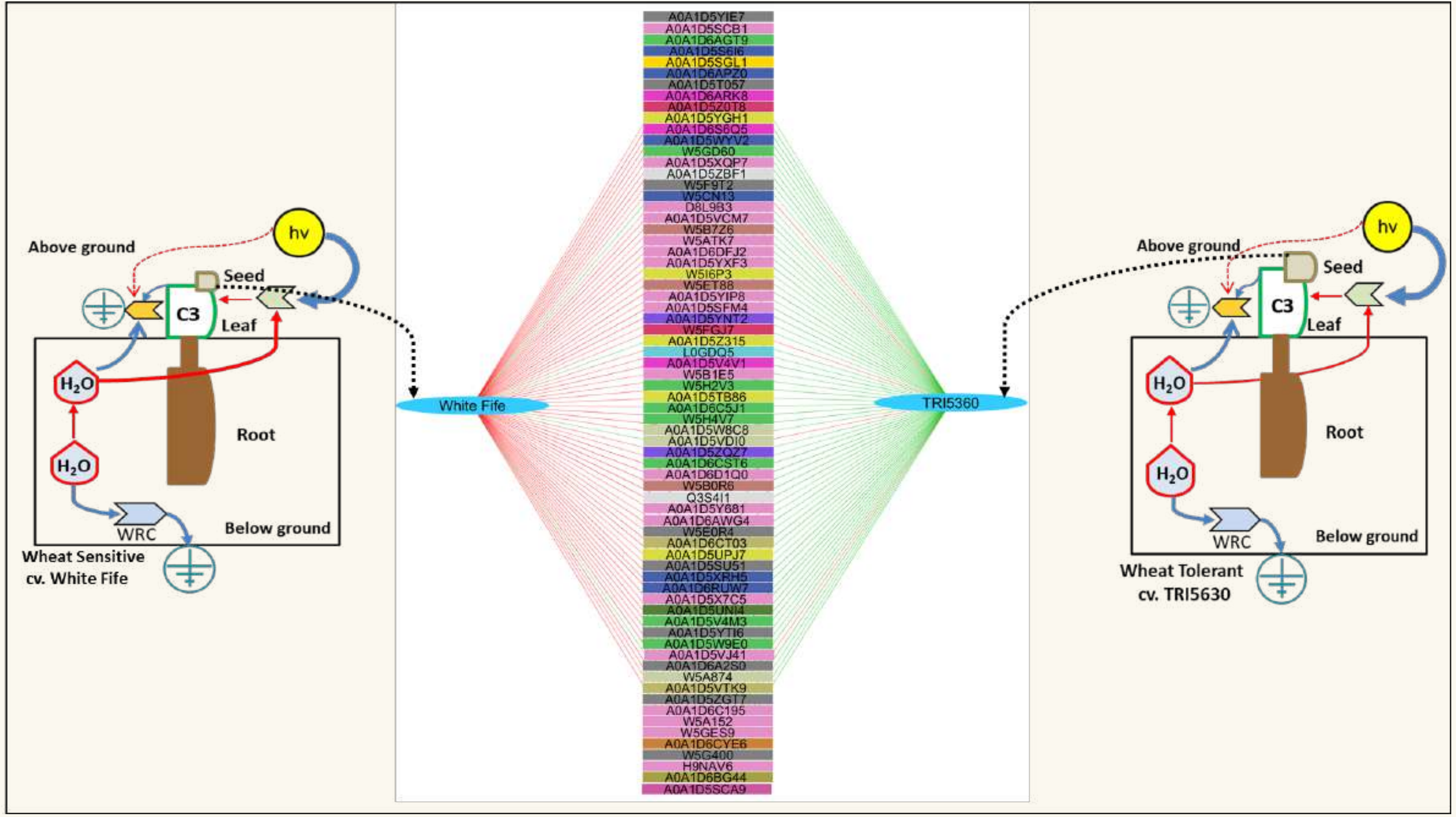
Ghatak , Chaturvedi et al.

Proteome plasticity of resistant and susceptible wheat and pearl millet genotypes under drought stress

Sparse Partial Least Square analysis: **Predictors for seed yield in wheat**



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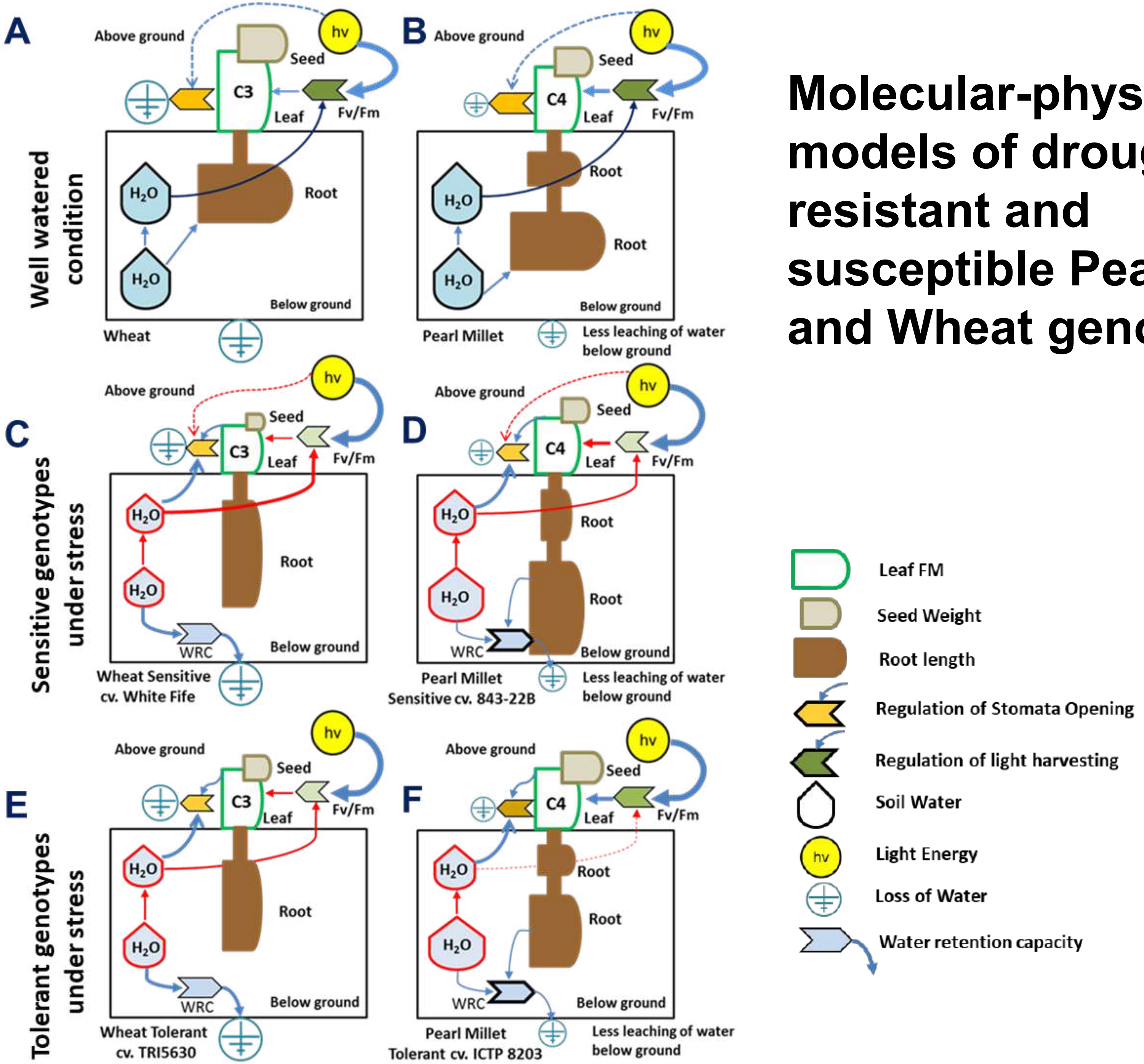
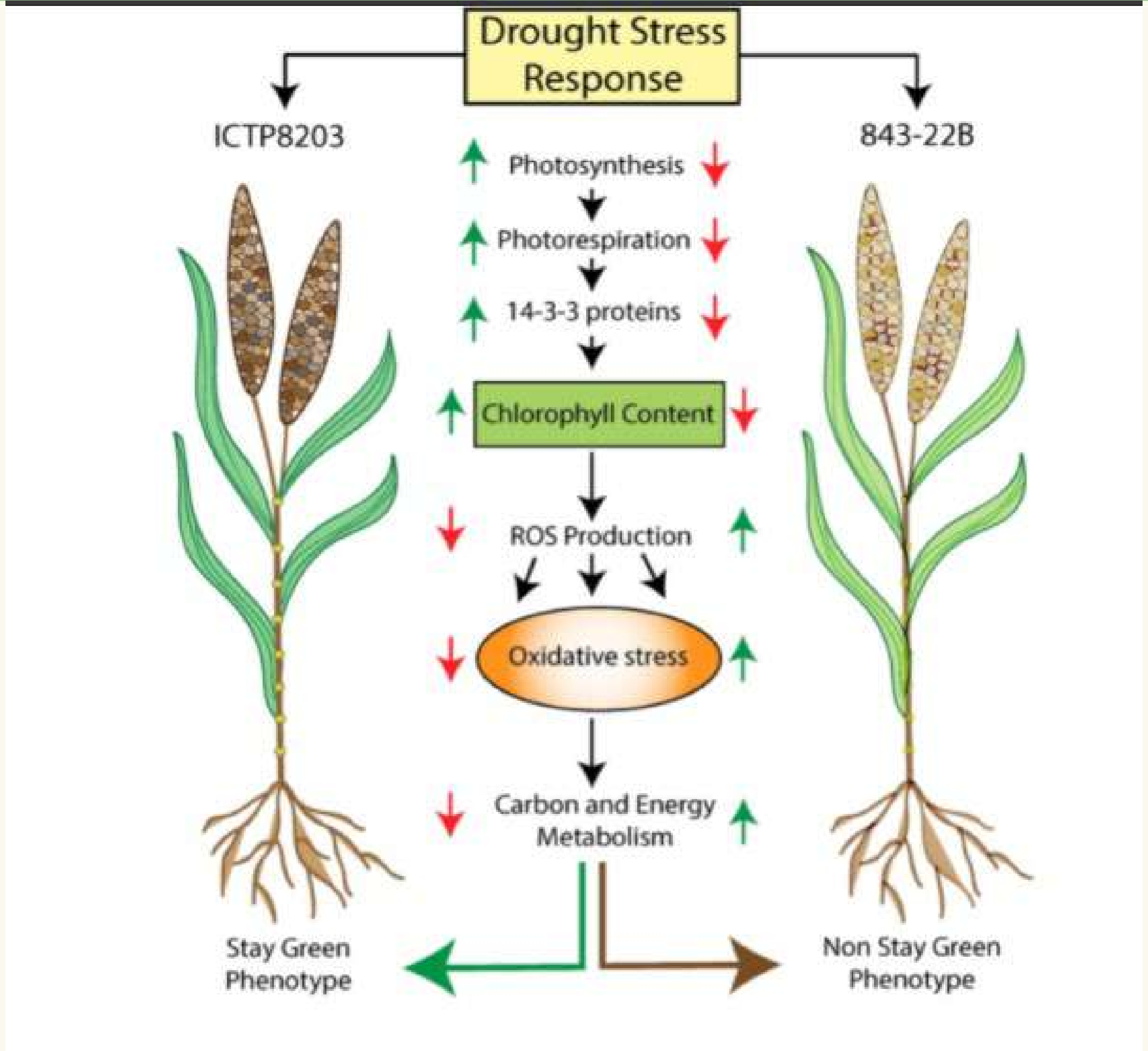
Molecular-physiological models of drought resistant and susceptible Pearl millet and Wheat genotypes



Ghatak et al. 2021
Frontiers in Plant Science

Germplasm collections offer „climate smart crops“ – stress resilience



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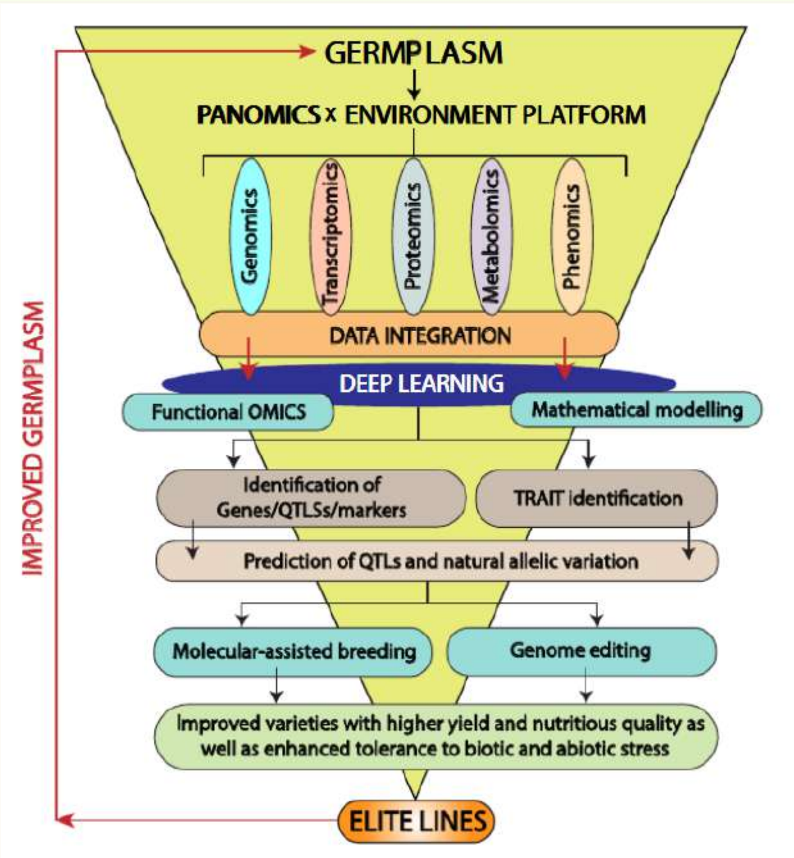
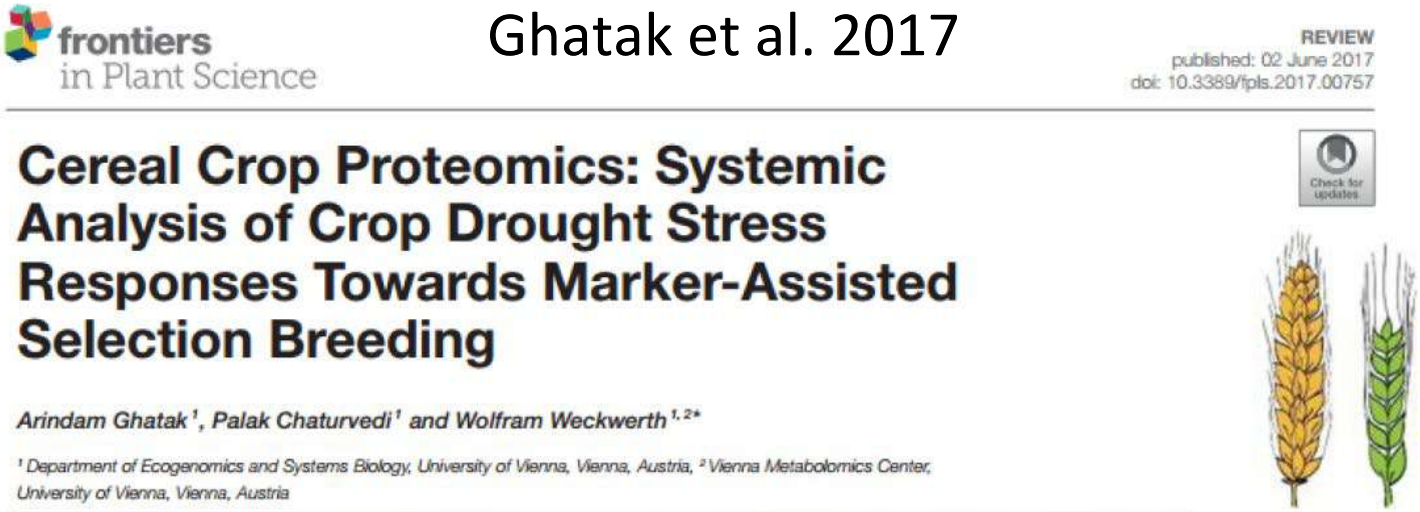
Frontiers in Plant Science



Weckwerth et al. 2020
Plant Biotechnology

Ghatak et al. 2017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REVIEW
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Cereal Crop Proteomics: Systemic Analysis of Crop Drought Stress Responses Towards Marker-Assisted Selection Breeding

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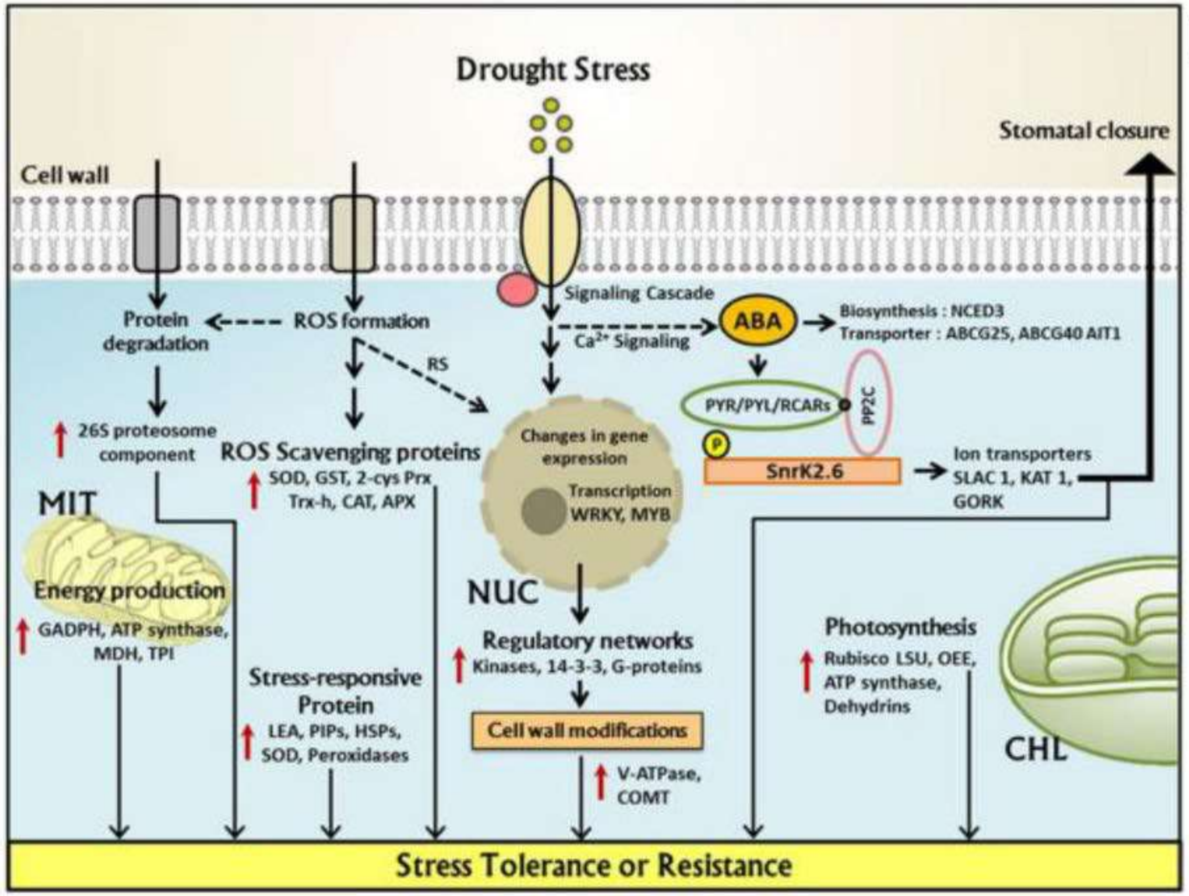
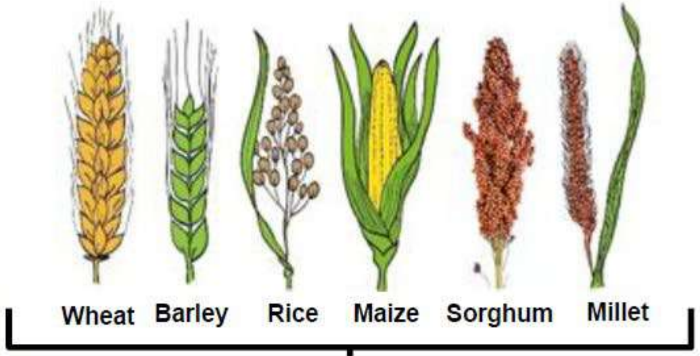




WHEAT, RICE, BARLEY, MAIZE, SORGHUM, PEARL MILLET

Comparative summary of more than 200 publications and biomarker selection

HYPOTHESIS

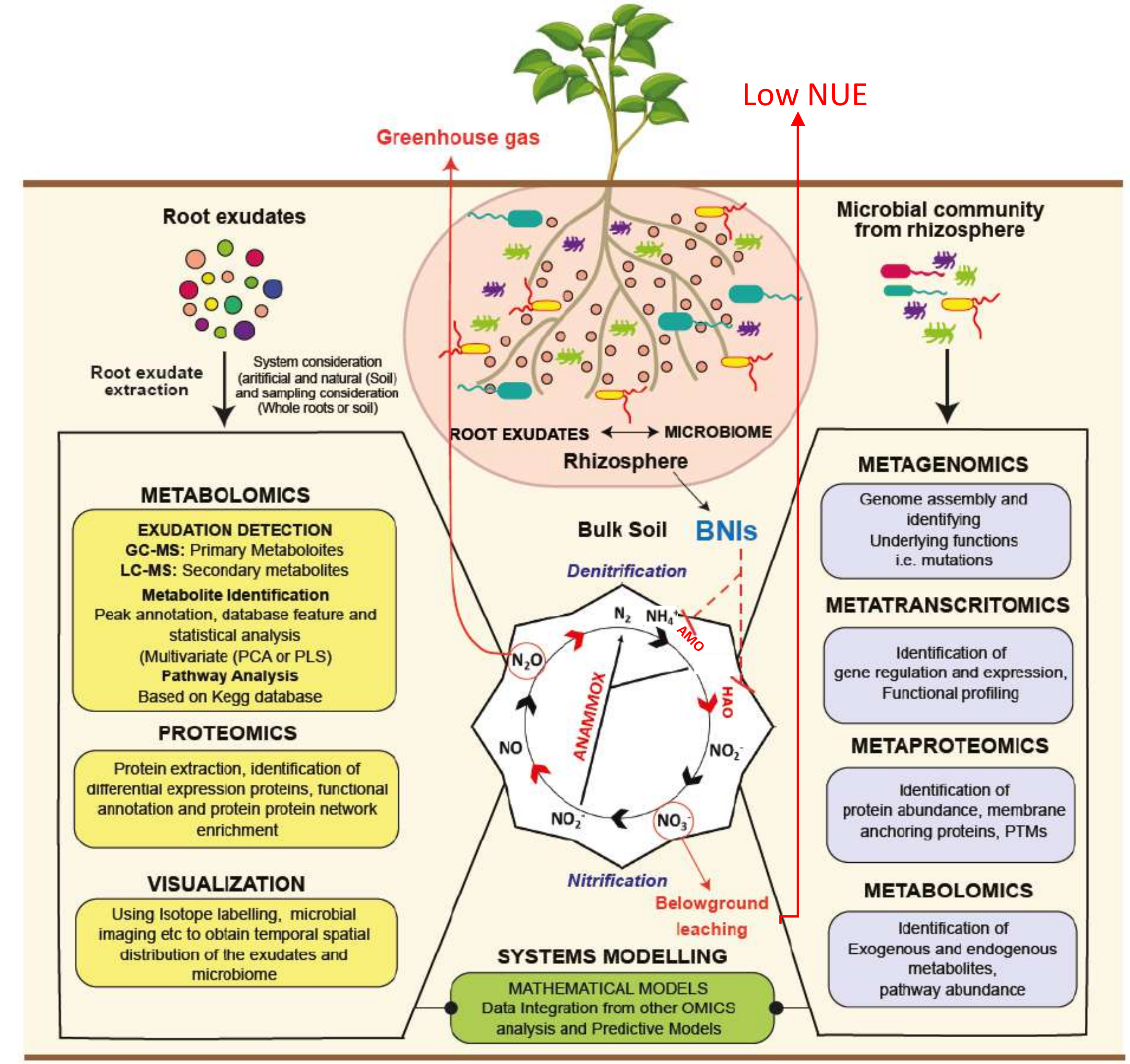
Agriculture contributes to the mitigation of climate change due to its nature as carbon sequestration process - photosynthesis and CO_2 -fixation

versus current state:

1. Harsh climate reduces plant growth and productivity leading to inefficient CO_2-neutral biomass and food production
2. High demand on industrial nitrogen fertilizer for productivity but low nitrogen use efficiency (NUE) due to losses (50-70%) in the soil – nitrification processes and GHG emissions (N_2O)
3. Food production – industrial processes

Net GHG emission instead of sequestration

Germplasm collections offer climate smart crops – Biological nitrification inhibition (BNI)



Ghatak et al. PANOMICS meets root soil microbiome under review

Germplasm collections offer climate smart crops – Biological nitrification inhibition (BNI)

Biology and Fertility of Soils
https://doi.org/10.1007/s00374-021-01578-w

ORIGINAL PAPER

Root exudation of contrasting drought-stressed pearl millet genotypes conveys varying biological nitrification inhibition (BNI) activity

Arindam Ghatak[1] · Florian Schindler[1] · Gert Bachmann[1] · Doris Engelmeier[1] · Prasad Bajaj[2] · Martin Brenner[1,3] · Lena Fragner[1,3] · Rajeev K. Varshney[2,4] · Guntur Venkata Subbarao[5] · Palak Chaturvedi[1] · Wolfram Weckwerth[1,3]

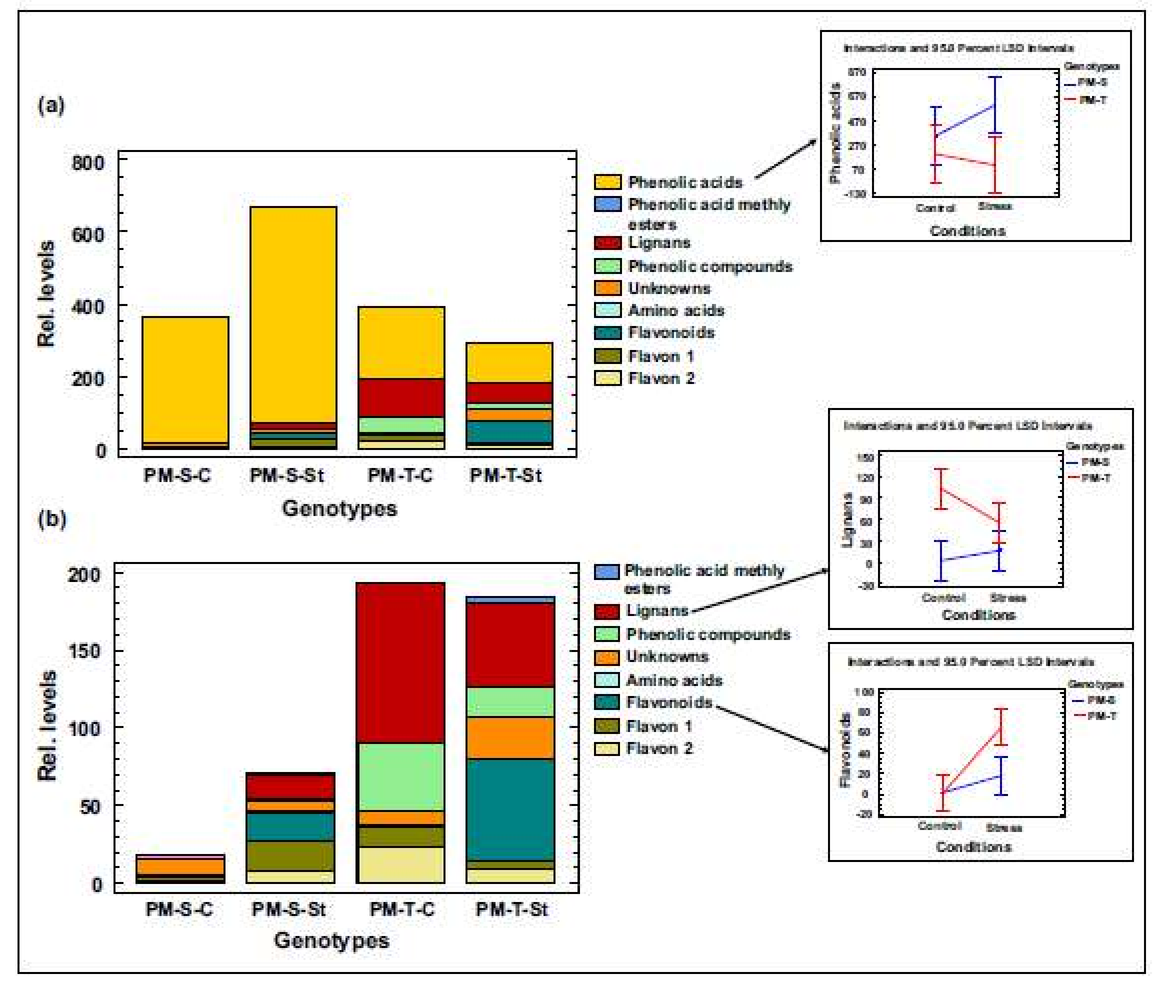
Received: 30 July 2020 / Revised: 10 June 2021 / Accepted: 12 June 2021

Abstract
Roots secrete a vast array of low molecular weight compounds into the soil broadly referred to as root exudates. It is a key mechanism by which plants and soil microbes interact in the rhizosphere. The effect of drought stress on the exudation process and composition is rarely studied, especially in cereal crops. This study focuses on comparative metabolic profiling of the exudates from sensitive and tolerant genotypes of pearl millet after a period of drought stress. We employed a combined platform of gas and liquid chromatography coupled to mass spectrometry to cover both primary and secondary metabolites. The results obtained demonstrate that both genotype and drought stress have a significant impact on the concentration and composition of root exudates. The complexity and function of these differential root exudates are discussed. To reveal the potential effect of root exudates on the soil microbial community after a period of drought stress, we also tested for biological nitrification inhibition (BNI) activity. The analysis revealed a genotype-dependent enhancement of BNI activity after a defined period of drought stress. In parallel, we observed a genotype-specific relation of elongated root growth and root exudation under drought stress. These data suggest that the drought stress-dependent change in root exudation can manipulate the microbial soil communities to adapt and survive under harsh conditions.

Root exudate metabolomics

Ghatak et al. 2021
Biology and Fertility of Soils

Germplasm collections offer climate smart crops – Biological nitrification inhibition (BNI)



ViMe
Vienna Metabolomics Center

Root exudate metabolomics

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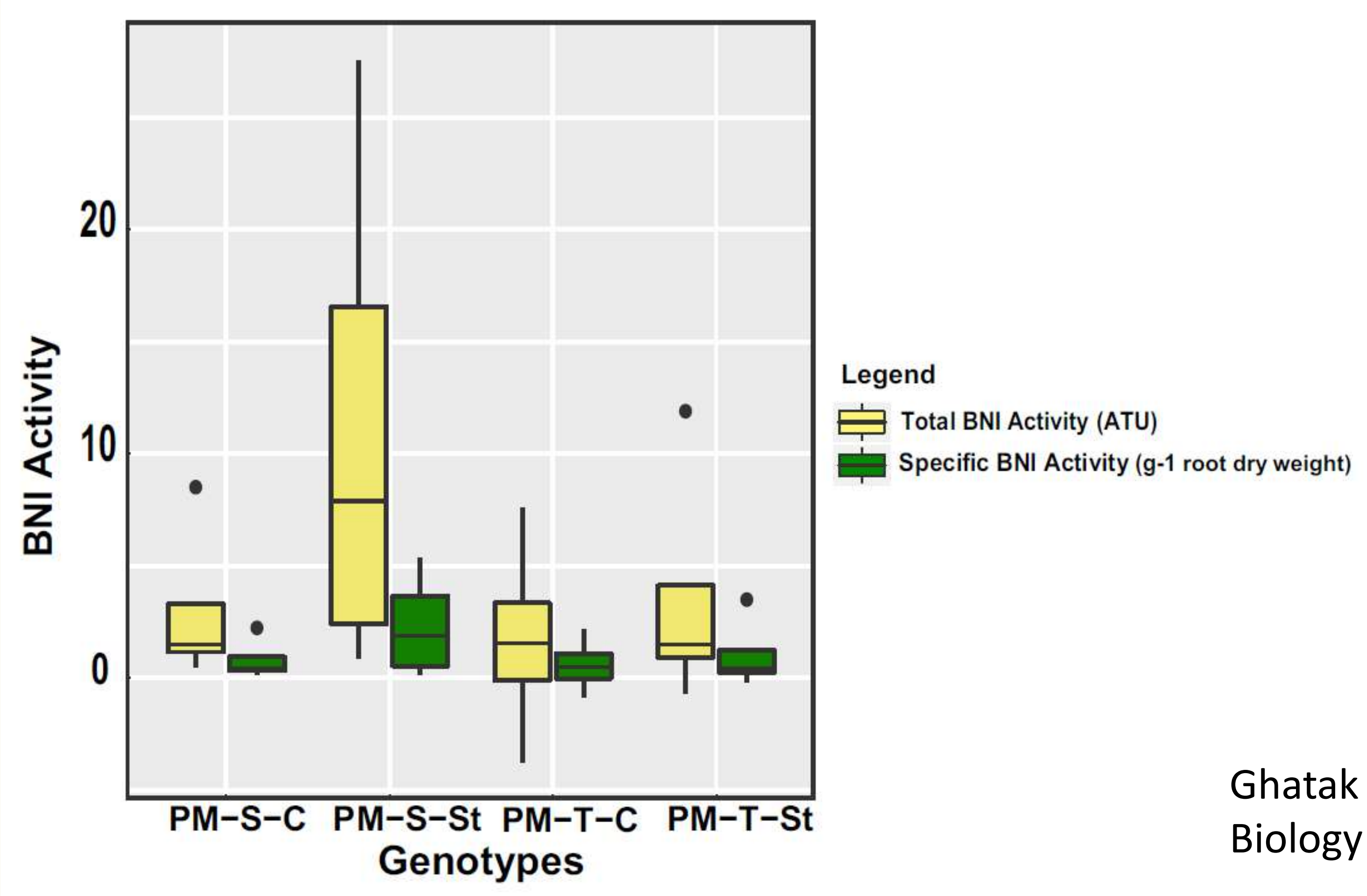

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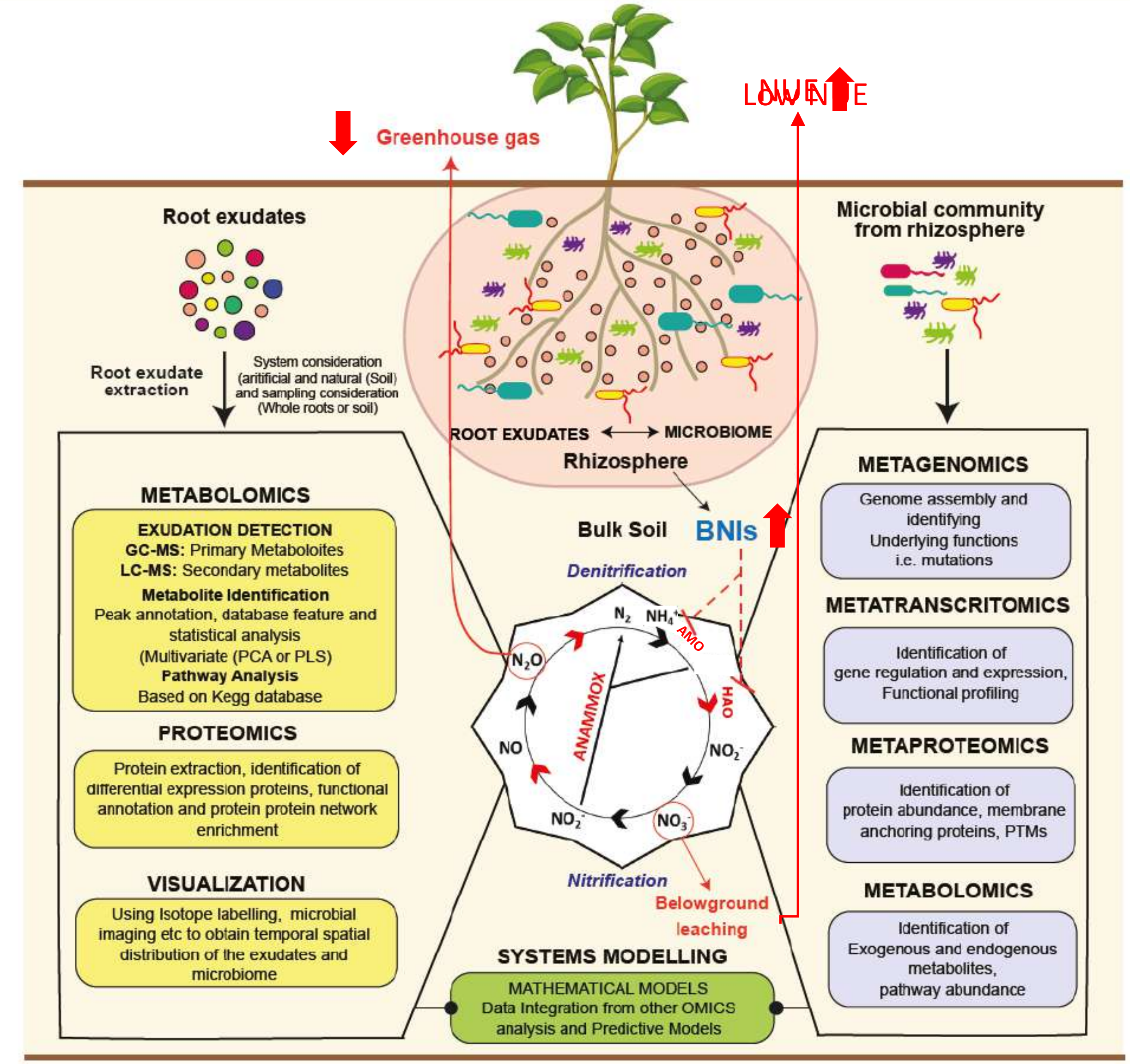
Germplasm collections offer climate smart crops – Biological nitrification inhibition (BNI)



Plant Soil (2016) 404:61–74
DOI 10.1007/s11104-016-2822-4

REGULAR ARTICLE

Identification of several wheat landraces with biological nitrification inhibition capacity

Cathryn A. O'Sullivan · Ian R. P. Fillery ·
Margaret M. Roper · Richard A. Richards

Received: 21 October 2015 / Accepted: 29 January 2016 / Published online: 13 February 2016

Abstract

Background and aims Nitrification is the first step in several pathways that lead to losses of nitrogen from agricultural systems. Biological nitrification inhibition (BNI) refers to the ability of some plant species to release chemicals from their roots that inhibit microbial ammonia oxidation thereby decreasing nitrification rates. BNI has been found in the wheat relative *Leymus racemosus* but not in *Triticum aestivum*. The aim of this work was to assess a number of landraces of *Triticum aestivum* for BNI ability.

Methods Samples of root exudates and root tissue extracts, collected from hydroponically grown plants, were tested for their impact on nitrification rates when inoculated with pure cultures of two ammonia oxidising bacteria, *Nitrosomonas europaea* and *Nitrosospira multiformis*. Pot experiments were then conducted to confirm the results.

Results The vast majority of the landraces tested caused some level of inhibition. However, of the 96 wheat landraces tested, 26 produced root exudates which caused a statistically significant reduction in nitrification rates of the two ammonia oxidising bacteria. Root exudates from four of the BNI positive landraces were shown to significantly inhibit nitrification rates in a sandy loam soil.

Conclusions This is the first evidence of significant levels of BNI in *Triticum aestivum*. The discovery of landraces with BNI ability raises the potential for breeding this trait into modern, elite wheat cultivars.

Keywords Biological nitrification inhibition · Wheat

Ghatak et al. PANOMICS meets root soil microbiome under review

PANOMICS resolution at subtissue and cellular level

In the framework of Green Systems Biology we propose three fundamental pillars for future breeding strategies:

(i) combining genome selection with environment-dependent PANOMICS analysis and deep learning to improve prediction accuracy for marker-dependent trait performance

(ii) PANOMICS resolution at subtissue, cellular and subcellular level provides information about fundamental functions of selected markers

(iii) combining PANOMICS with genome editing and speed breeding tools

Weckwerth et al. 2020 Panomics meets germplasm

PANOMICS resolution at subtissue and cellular level

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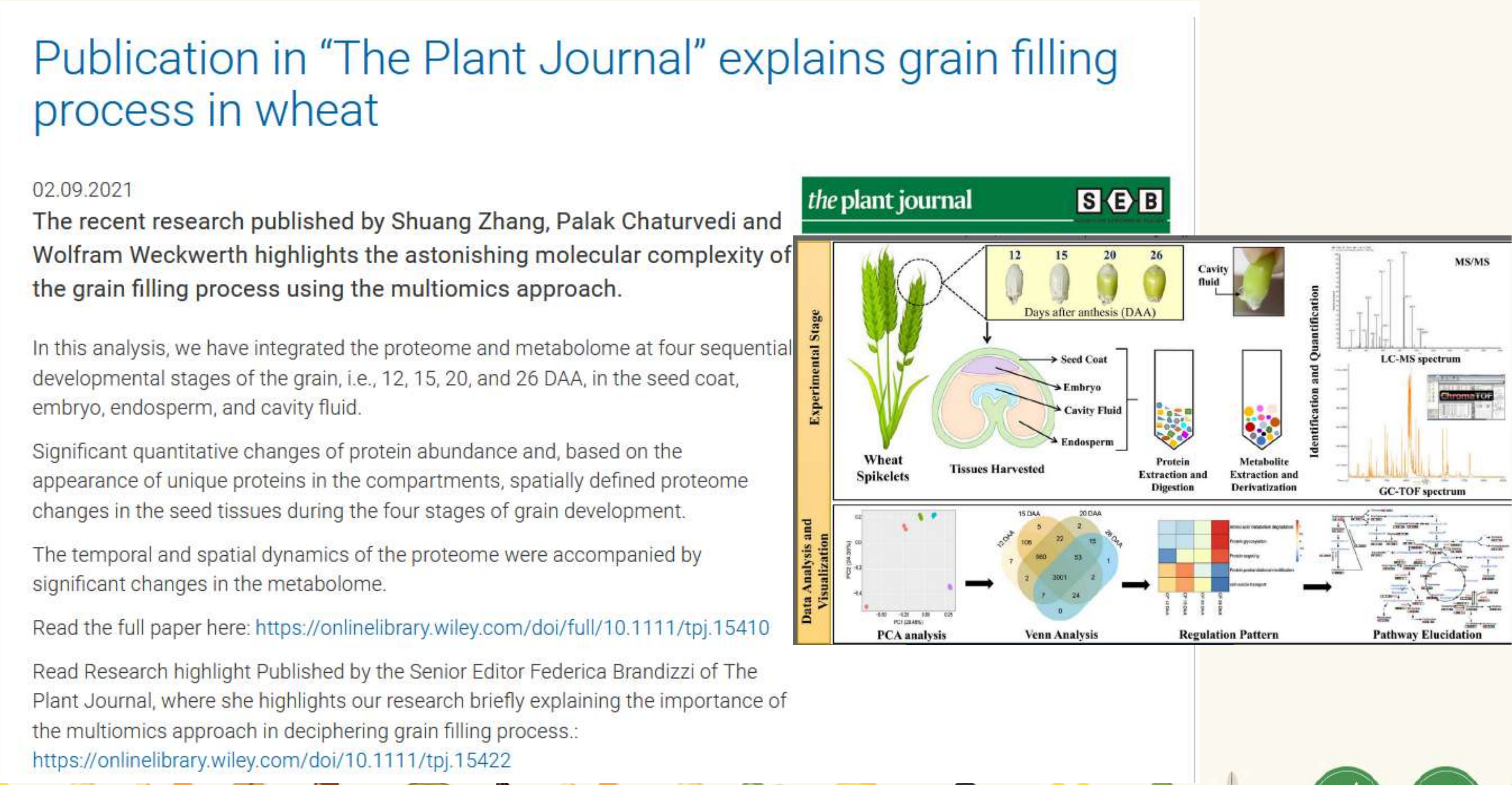
Weckwerth et al. 2020 Panomics meets germplasm

Wheat grain filling process

Shuang et al 2021 Plant Journal



Publication in “The Plant Journal” explains grain filling process in wheat

02.09.2021

The recent research published by Shuang Zhang, Palak Chaturvedi and Wolfram Weckwerth highlights the astonishing molecular complexity of the grain filling process using the multiomics approach.

In this analysis, we have integrated the proteome and metabolome at four sequential developmental stages of the grain, i.e., 12, 15, 20, and 26 DAA, in the seed coat, embryo, endosperm, and cavity fluid.

Significant quantitative changes of protein abundance and, based on the appearance of unique proteins in the compartments, spatially defined proteome changes in the seed tissues during the four stages of grain development.

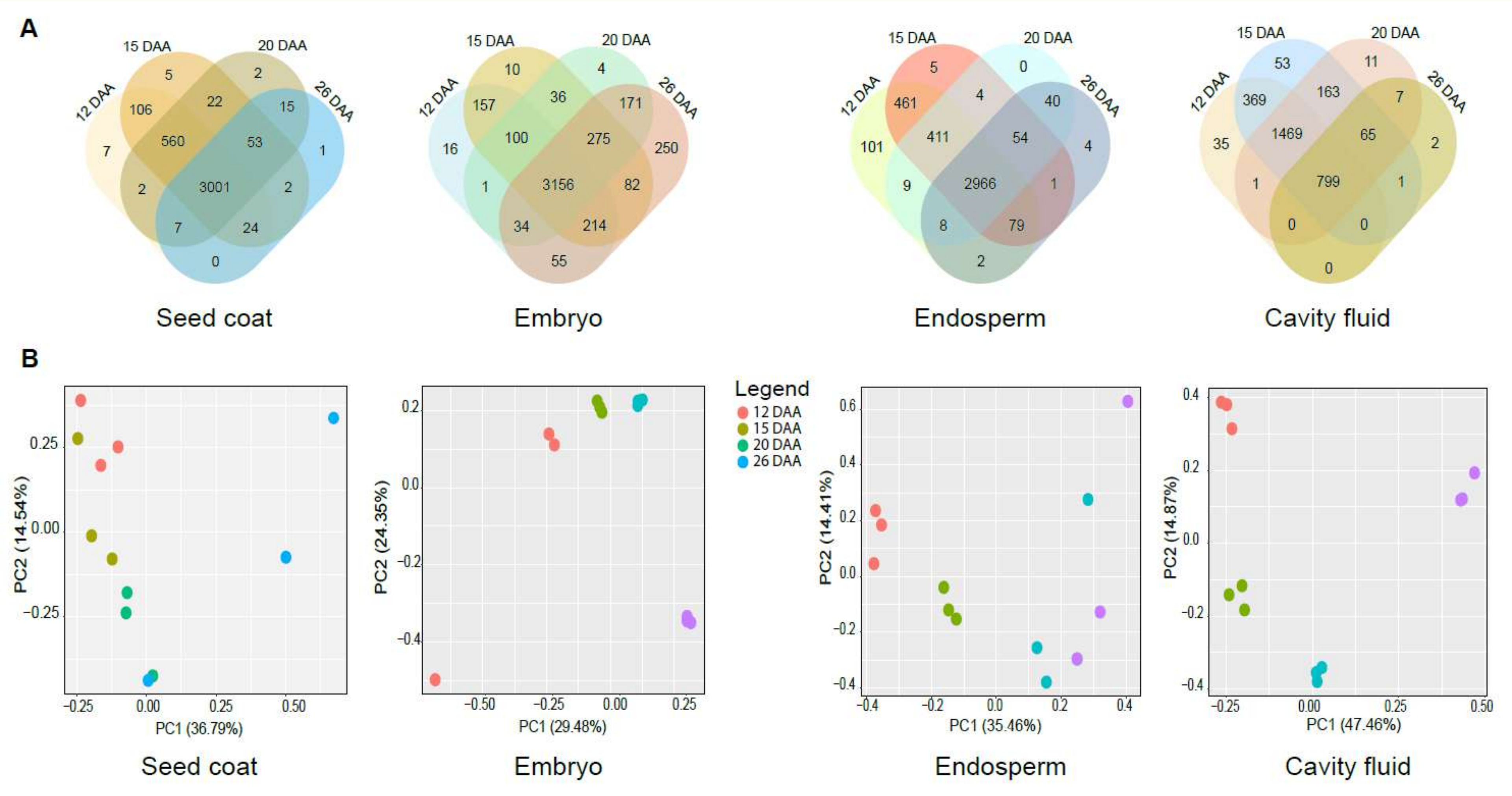
The temporal and spatial dynamics of the proteome were accompanied by significant changes in the metabolome.

Read the full paper here: https://onlinelibrary.wiley.com/doi/full/10.1111/tpj.15410

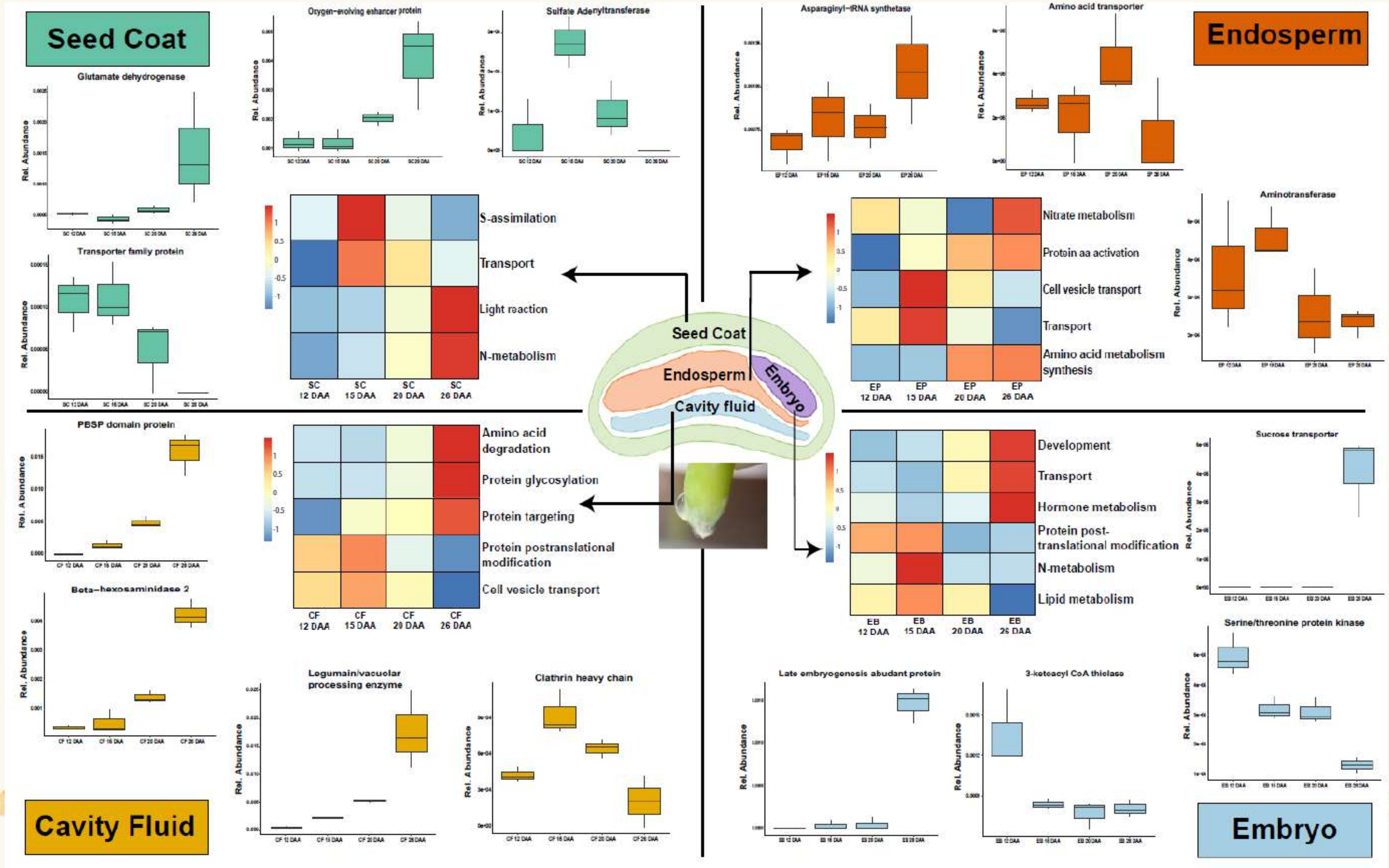
Read Research highlight Published by the Senior Editor Federica Brandizzi of The Plant Journal, where she highlights our research briefly explaining the importance of the multiomics approach in deciphering grain filling process.: https://onlinelibrary.wiley.com/doi/10.1111/tpj.15422

Wheat grain filling process at the tissue level

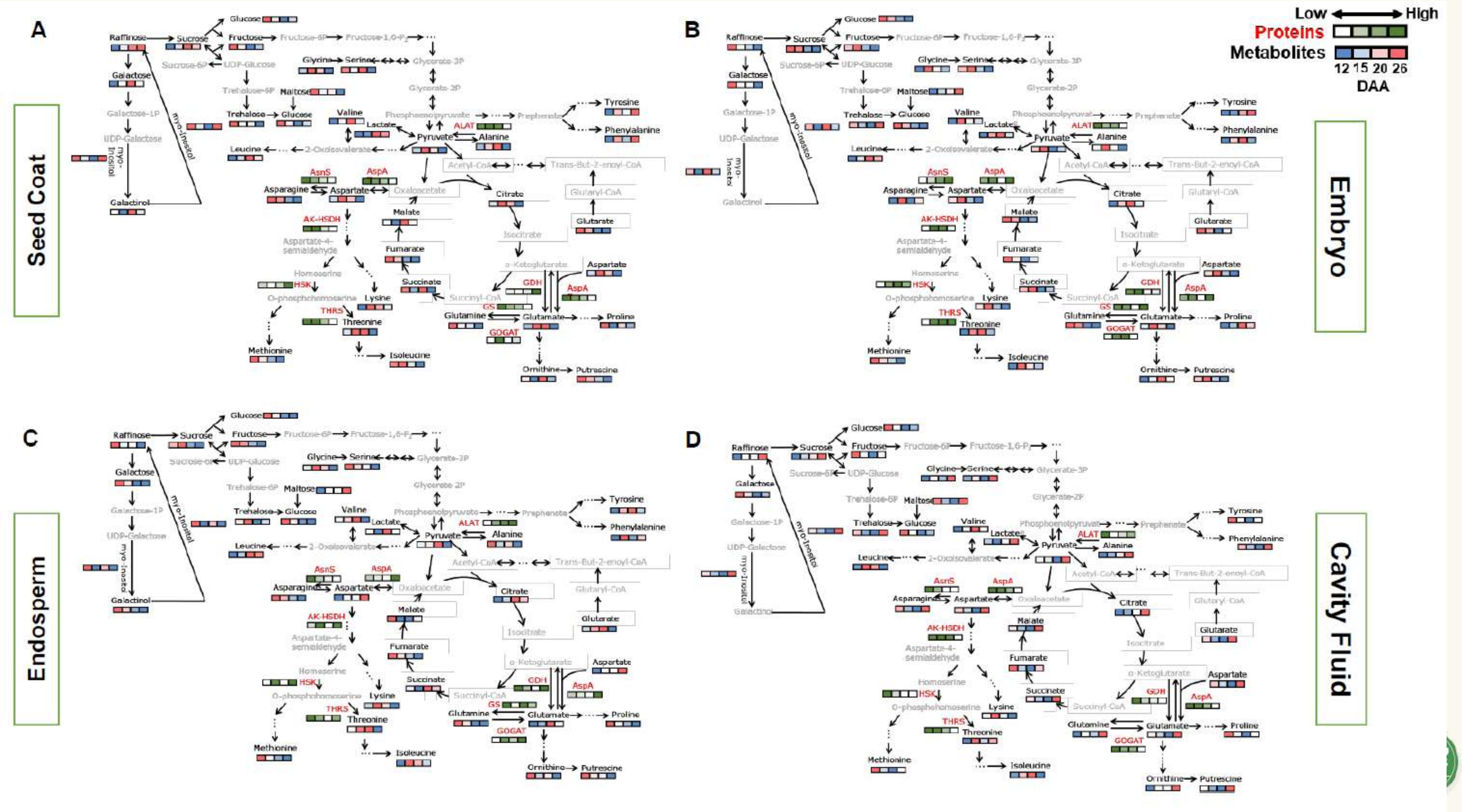
Shuang et al 2021 Plant Journal



Wheat grain filling process at the tissue level Shuang et al 2021 Plant Journal

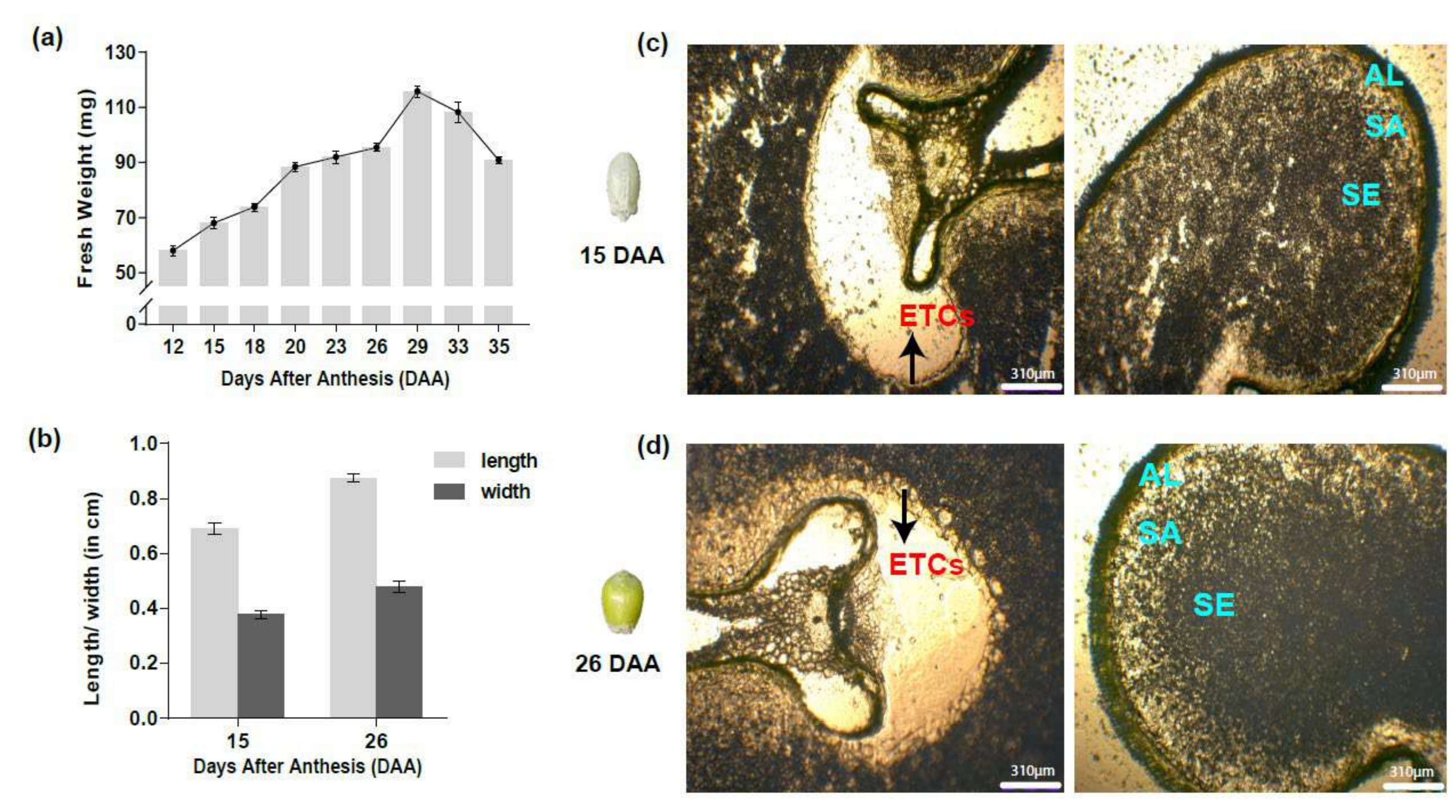


Wheat grain filling process at the tissue level Shuang et al 2021 Plant Journal



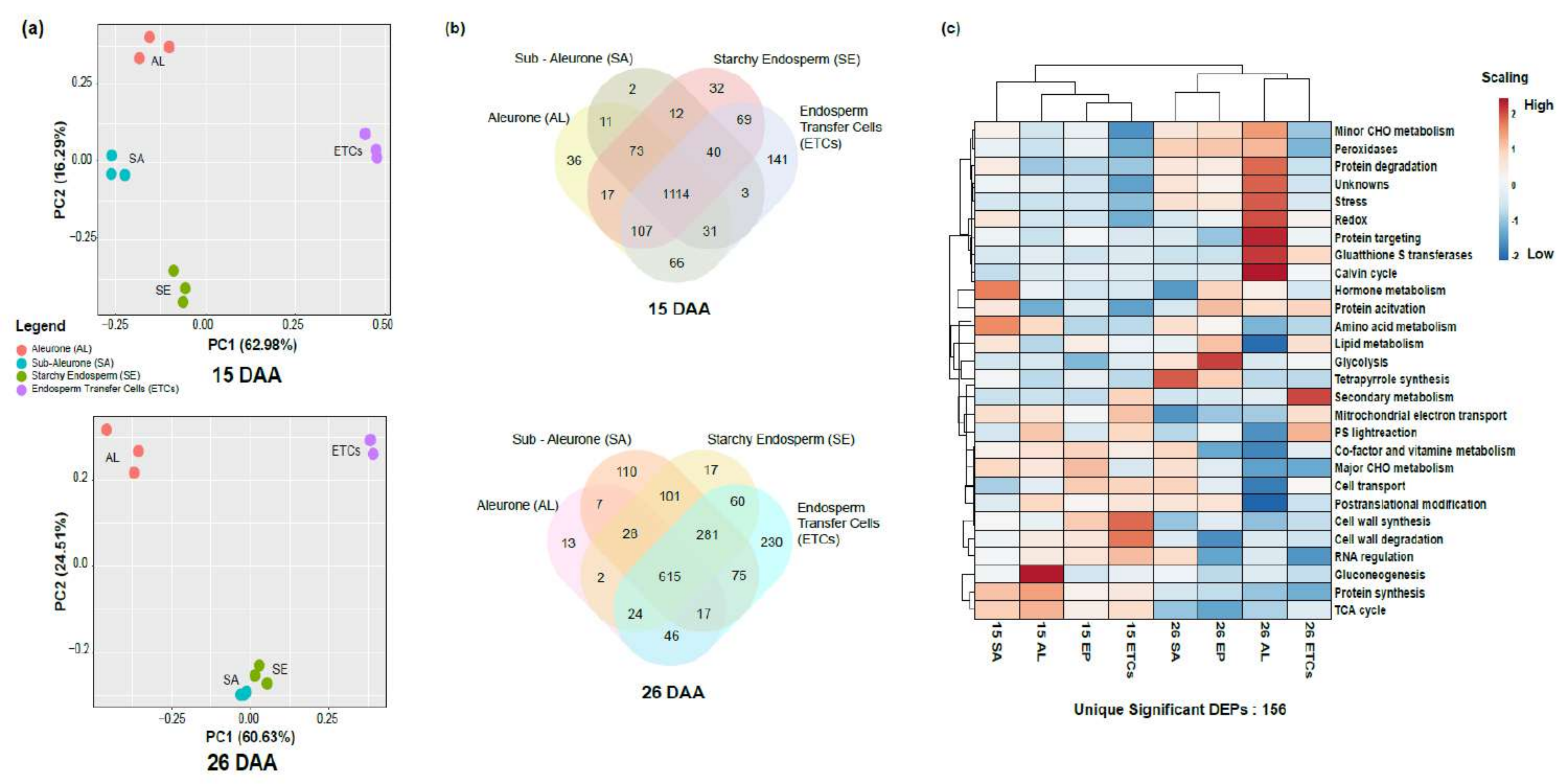
Wheat grain filling process at the cellular level

Shuang et al 2021 in preparation



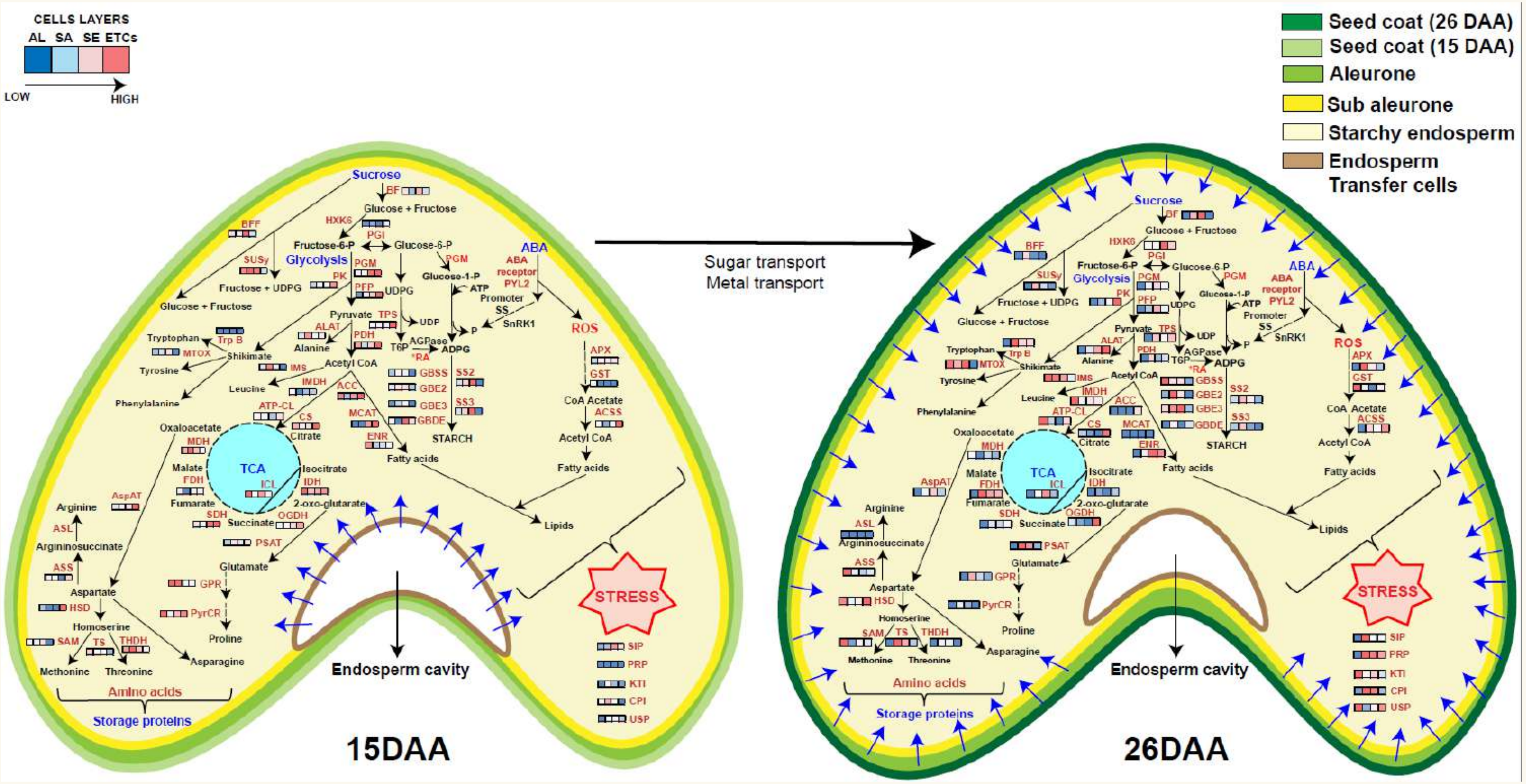
Wheat grain filling process at the cellular level

Shuang et al 2021 in preparation



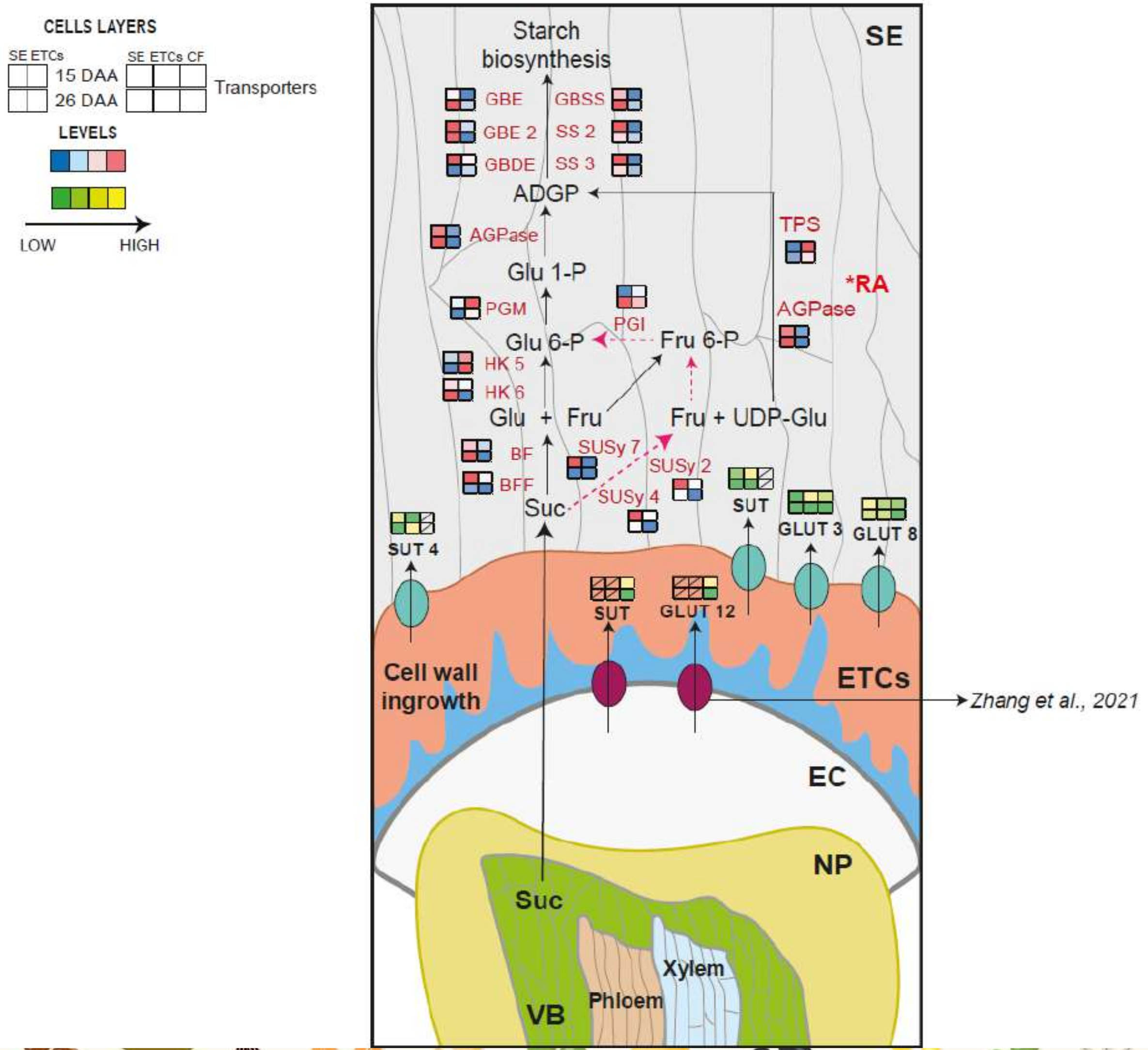
Wheat grain filling process at the cellular level

Shuang et al 2021 in preparation



Wheat grain filling process at the cellular level

Shuang et al 2021 in preparation



SUMMARY

- **More than 60% of phenotypic plasticity, pleiotropy, polygenic traits, physiology etc. is not explained by genomics** – application of metabolomics, proteomics, phosphoproteomics and biochemical modelling for genomic prediction
- **In situ molecular phenotype plasticity is enormeous**: Application of multiomics technology and Systems Biology from lab to field conditions reveals a new picture of the **genotype-environment-phenotype, phenotypic plasticity in a natural/agricultural environment and stress adaptation mechanisms**
- Application **to crop plants and natural ecosystems** reveal different adaptation strategies of the plant and can be used for correlation with traits, yield, stress tolerance, morphology, physiology etc.

International Cooperations

Rajeev Varshney

Dong Jiang

ICRISAT
INTERNATIONAL CROPS RESEARCH INSTITUTE FOR THE SEMI-ARID TROPICS

UNIVERSITY OF DELHI

BARC
ATOMS IN THE SERVICE OF THE NATION

NANJING AGRICULTURAL UNIVERSITY
1902

JIRCAS

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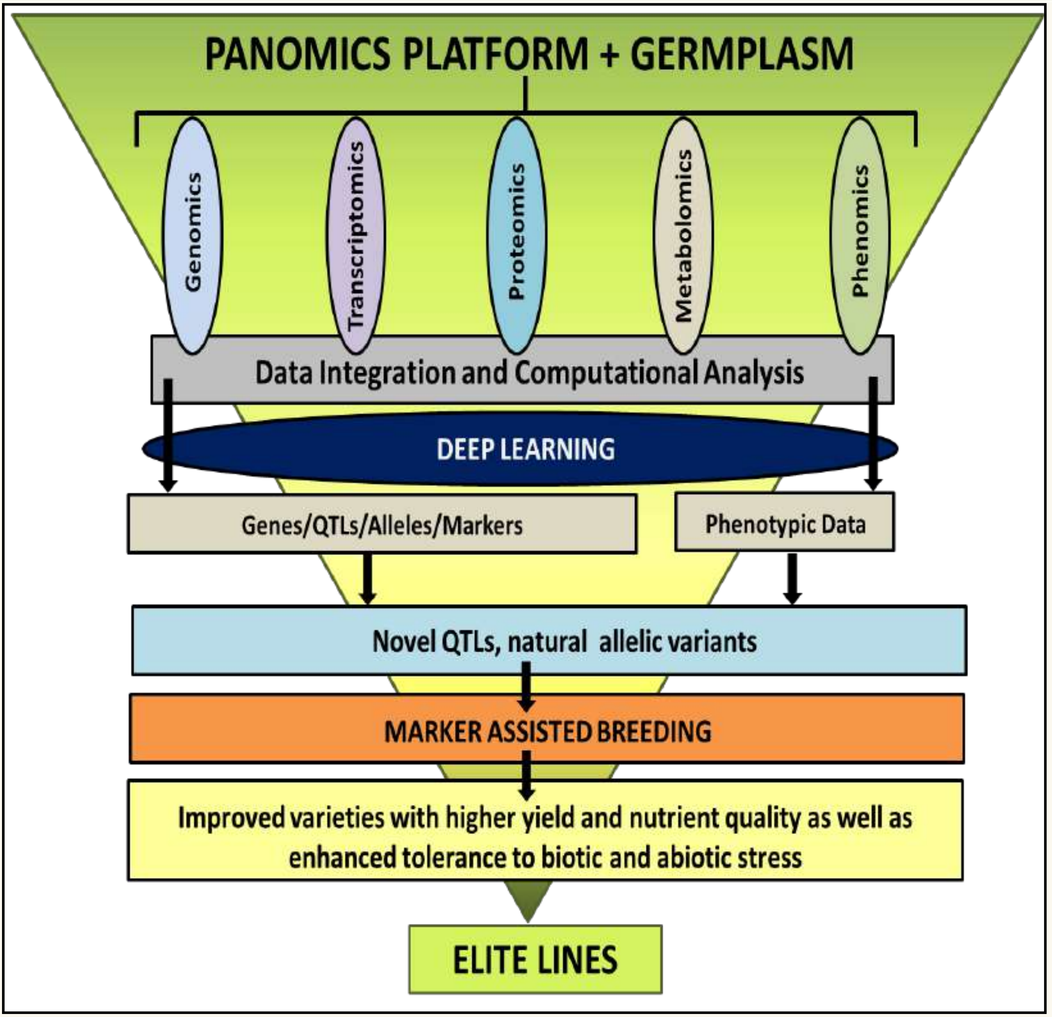

PANOMICS PLATFORM + GERMPLASM

Genomics
Transcriptomics
Proteomics
Metabolomics
Phenomics

Data Integration and Computational Analysis

DEEP LEARNING

Genes/QTLs/Alleles/Markers
Phenotypic Data

Novel QTLs, natural allelic variants

MARKER ASSISTED BREEDING

Improved varieties with higher yield and nutrient quality as well as enhanced tolerance to biotic and abiotic stress

ELITE LINES

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GEN-AU
GENOMFORSCHUNG IN ÖSTERREICH

ERA-NET PLANT GENOMICS

MARIE CURIE ACTIONS

WWTF
Wiener Wissenschafts-, Forschungs- und Technologiefonds

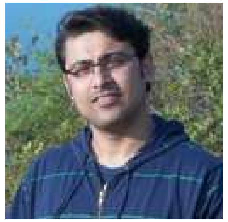
FWF

BIOCRATES
LIFE SCIENCES

BDI

Big hugs to the group

Palak Chaturvedi



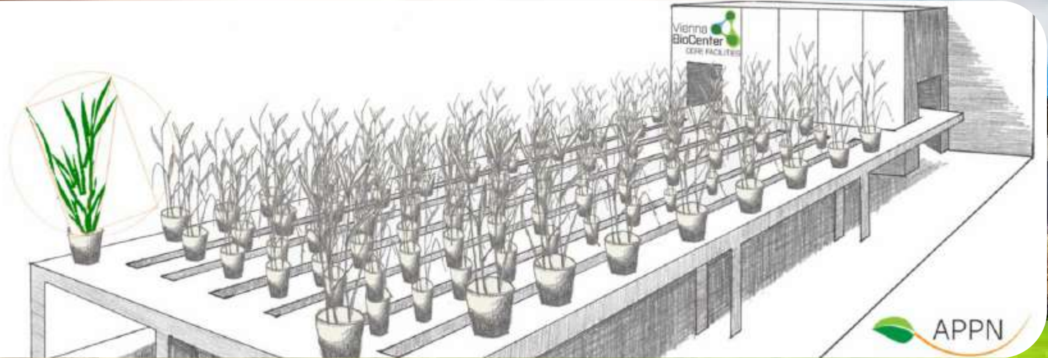
Arindam Ghatak

http://www.univie.ac.at/mosys/team.html

DOC.FUNDS PhD school:
MENTOR – Plant resilience in the climate crisis

FFG
Promoting Innovation.

PHENOPlant
launching
2021



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BOKU
Universität für Bodenkultur Wien
University of Natural Resources and Life Sciences, Vienna

GMI
GREGOR MENDEL INSTITUTE OF MOLECULAR PLANT BIOLOGY

AIT AUSTRIAN INSTITUTE OF TECHNOLOGY

MENTOR (First Plant PHD School in Austria)
Molecular Mechanisms to Improve Plant Resilience
Funding by FWF doc.funds (2.3 Million Euro)
Coordinated by
Wolfram Weckwerth

FWF
Der Wissenschaftsfonds.

universität wien

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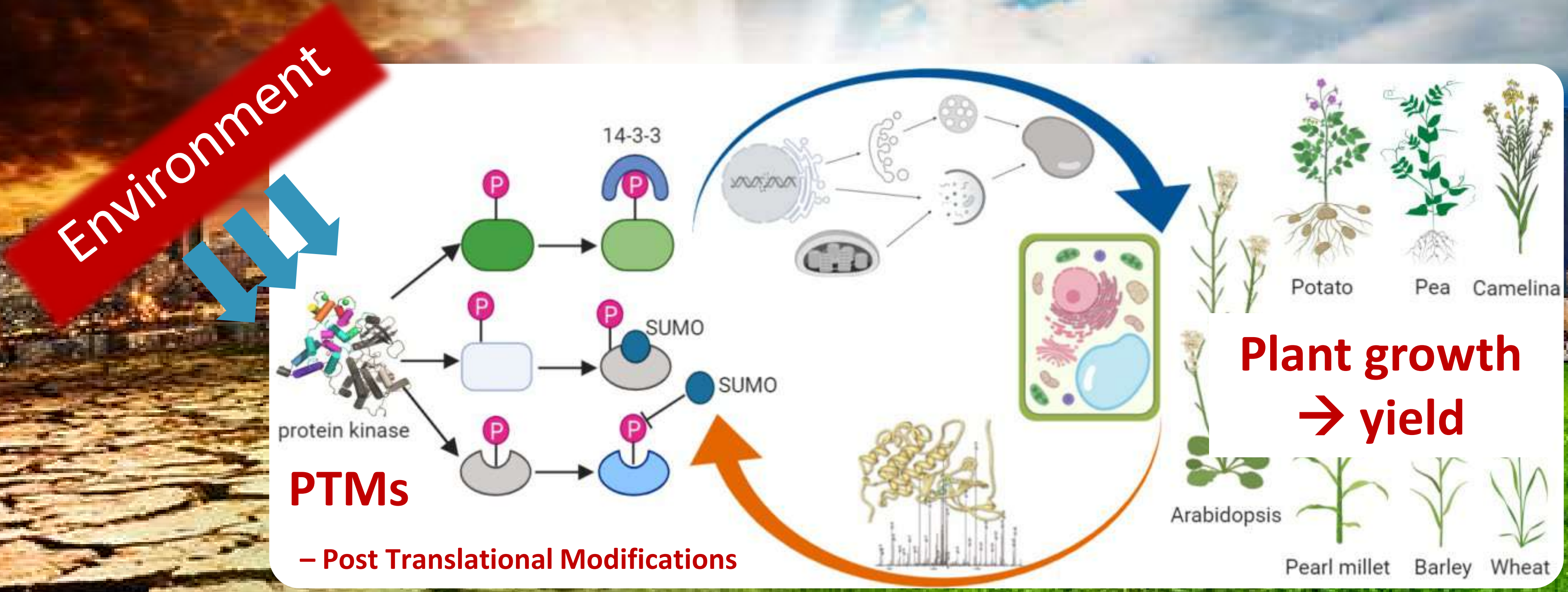
MENTOR – Plant resilience in the climate crisis



PTMs

– Post Translational Modifications

Plant growth
→ yield

Please, send applications to
wolfram.weckwerth@univie.ac.at

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MoSys

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