From Farm to FAIR

A Data Sharing Infrastructure for Designing Future Wheat

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Computational and Analytical Sciences - Rothamsted Research

DFW WP4 Lead: Rob Davey (EI) Co-Lead: Chris Rawlings (RRes)



Wide range of of data to be managed

In DFW combination of "traditional" breeding trials, bespoke research trials and fundamental research datasets creates a challenge

- Field trial datasets agronomic and developmental traits
- Diversity set genotyping
- Physical phenotyping
- Chemical phenotyping
- High Throughput phenotyping platform data and UAV imaging
- Pangenomic datasets i.e. Wheat 10+
- Epigenetic datasets
- Single cell genomics



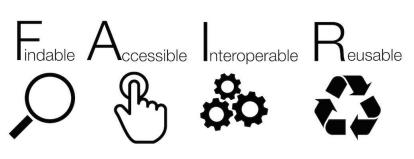
Data Sharing in DFW

- DFW has obligations because of it's significance and size as a UK publicly-funded (UKRI-BBSRC) R&D project
- Sharing data within the project is essential to the collaboration
- Important that data management and sharing is not solely the responsibility of the informatics teams, but shared across the project.
- Data Coordination Task Force brings different work streams together to coordinate efforts and share best practice.
 - Including breeder representative (Ruth Bryant RAGT)
 - Ensures development of the data sharing tools and ensures interoperability between the specialist bioinformatic and genomic data resources of individual partners



Sharing data with other stakeholders

- Breeders Toolkit data. Bringing data back into project after 2 year embargo https://designingfuturewheat.org.uk/breeders-toolkit/
- Funders (UKRI-BBSRC)
 - On demand access to catalogue of outputs from the project
 - Publications
 - Conference participation and presentations
 - Knowledge exchange outside research community
 - Digital outputs (datasets and software)
 - Public engagement
 - Collaborations
- Research Community commitment to data sharing <u>following FAIR</u> <u>principles</u>





- F The first step in (re)using data is to **find** them. Metadata and data should be easy to find for both humans and computers.
 - metadata are essential for automatic discovery of datasets and services, so this is an essential component of the FAIRification process
- A Once the user finds the required data, they need to know how they can be accessed
 - possibly including authentication and authorisation
- The data usually need to be **interoperable** with other data.
 - E.g. to interoperate with applications or workflows for analysis, storage, and processing
- R The ultimate goal of FAIR is to optimise the **reuse** of data.

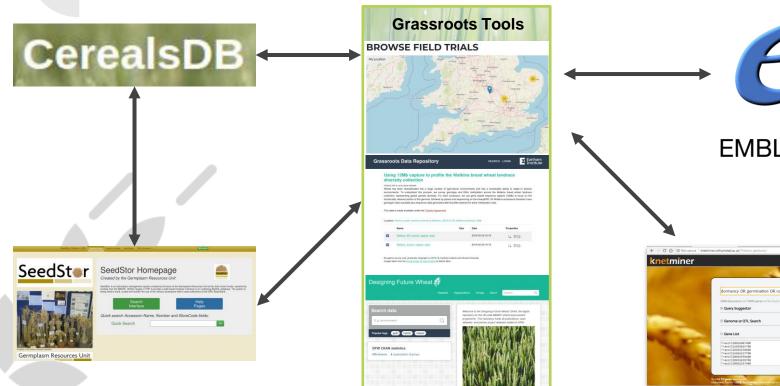
To achieve this, metadata and data should be well-described so that they can be replicated and/or combined in different settings.

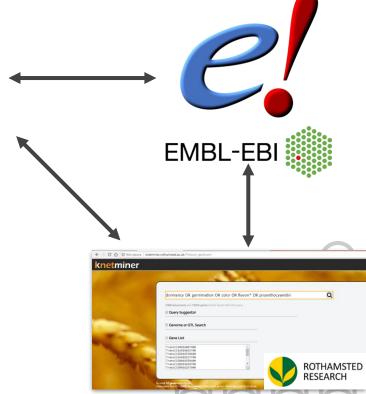


Main DFW-funded Data Resources

Wheat Germplasm Resource	www.seedstor.ac.uk
CerealsDB	www.cerealsdb.uk.net
DFW Field Trials	http://grassroots.tools/dfw
Ensembl Plants - Wheat	http://plants.ensembl.org/Triticum_aestivum
KnetMiner	https://knetminer.com/Triticum_aestivum
Wheat Expression Browser	www.wheat-expression.com
DFW Data Portal	http://opendata.earlham.ac.uk/wheat
DFW Digital Repository	http://ckan.grassroots.tools

Interoperability - Software and Data

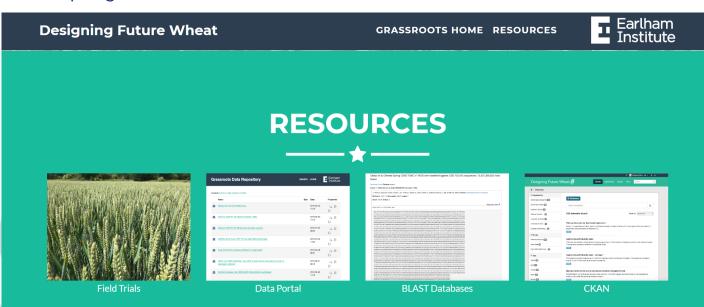






Grassroots Infrastructure

https://grassroots.tools/dfw





Field Trials Grassroots Service

- Provide a template for submitting metadata about DFW Field Experiments
 - To allow investigators to review ongoing and planned experiments and identify opportunities for adding value to experiments
 - Submitted using web-based forms and uploading spreadsheets
- Standardised template for submitting the genotype and phenotype data from DFW field trials
 - Working with field managers and biologists to standardize these spreadsheets and collection mechanisms
 - To facilitate publishing of data compliant with FAIR sharing principles
- Working with individual PIs to facilitate publication of datasets and integration with resources such as Ensembl Plants



Field Trials - Findable

- 55 Trials currently submitted
- The experimental data can be accessed using a map-based view and a searchable table of the data...

BROWSE FIELD TRIALS



Programme	Field Trial	Study	Team	Description	Sowing Date	Harvest Date	Plots	Address	Shape Data	Popup Info	Links
Designing Future Wheat	DFW - Designing Future Wheat - Work package 2 (WP2) - Added value and resilience	1st vs 3rd wheat take-all resistance trial	Rothamsted Research					Stackyard RES St Albans UK AL5 2BQ		• Study Info • Treatment Factors	• <u>Study</u>
Designing Future Wheat	6th Year Paragon Watkins Mapping populations 2017	2017 DFW Paragon x Watkins Mapping Populations 6th Year	Andrew Riche	7 PxW Mapping populations grown at 2 N levels plus 2 Robigus x Watkins mapping populations	2016-10- 19	2017-08- 15		Meadow, Rothamsted Experimental Farm Redbourn GB		• Study Info • Treatment Factors	• <u>Study</u>
Designing Future Wheat	DFW - Designing Future Wheat - Work package 2 (WP2) - Added value and resilience	AxC NILs (2)	Rothamsted Research					Black Horse St Albans United Kingdom AL3 7PX		• Study Info • Treatment Factors	• <u>Study</u>
Designing Future Wheat	DFW Academic Toolkit RRes	DFW Academic Tookit RRes, Harvest 2016	Andrew Riche					Blackhorse, Rothamsted Experimental Farm Rerlhourn		• Study Info • Treatment Factors	• <u>Study</u>



Field Trials - Findable

 ... or via a textbased search web page



SEARCH FIELD TRIALS

A service	to search fie	ld trial data				
or more	information	and help, go to the user documentation				
Simple o	ptions OA	lvanced options				
Search						
toolkit						
Гуре						
Any						-
age						
0						•
age size						
10						^ v
Submit						
how 10	✓ entries			Search:		
Rank	Type	Title	• Info		Link	
1	Study	DFW Toolkit lines	Broad Mead UK MK43 0XF		<u>View Study</u>	
2	Field Trial	DFW WP3 - DFW Academic Toolkit Trials	DFW WP3		View Field Trial	
3	Field Trial	DFW WP3 - DFW Breeders Toolkit Trials	DFW WP3		View Field Trial	
4	Field Trial	Andrew Riche - DFW Academic Toolkit RRes	Andrew Riche		View Field Trial	
5	Study	DFW Academic Toolkit Trial H2019	Black Horse St Albans United Kingdom AL3 7PX		View Study	
6	Study	DFW Toolkit lines 2nd year	Black Horse St Albans United Kingdom AL3 7PX		View Study	
			Meadow, Rothamsted Experimenta	al Farm		





Field Trials

Each Study has a plot-based tabular view

FIELD TRIAL DETAILS

Study: DFW Academic Toolkit RRes, Harvest 2020

20	Row:20	Row:20	Row:20	Row:20	Row:20	Row:20	Row:20	Row:20	Row:20									
	Column:1	Column:2	Column:3	Column:4	Column:5	Column:6	Column:7	Column:8	Column:9	Column:10	Column:11	Column:12	Column:13	Column:14	Column:15	Column:16	Column:17	Column:18
19	Row:19	Row:19	Row:19	Row:19	Row:19	Row:19	Row:19	Row:19	Row:19									
	Column:1	Column:2	Column:3	Column:4	Column:5	Column:6	Column:7	Column:8	Column:9	Column:10	Column:11	Column:12	Column:13	Column:14	Column:15	Column:16	Column:17	Column:18
18	Row:18	Row:18	Row:18	Row:18	Row:18	Row:18	Row:18	Row:18	Row:18									
	Column:1	Column:2	Column:3	Column:4	Column:5	Column:6	Column:7	Column:8	Column:9	Column:10	Column:11	Column:12	Column:13	Column:14	Column:15	Column:16	Column:17	Column:18
17	Row:17	Row:17	Row:17	Row:17	Row:17	Row:17	Row:17	Row:17	Row:17									
	Column:1	Column:2	Column:3	Column:4	Column:5	Column:6	Column:7	Column:8	Column:9	Column:10	Column:11	Column:12	Column:13	Column:14	Column:15	Column:16	Column:17	Column:18
16	Row:16	Row:16	Row:16	Row:16	Row:16	Row:16	Row:16	Row:16	Row:16									
	Column:1	Column:2	Column:3	Column:4	Column:5	Column:6	Column:7	Column:8	Column:9	Column:10	Column:11	Column:12	Column:13	Column:14	Column:15	Column:16	Column:17	Column:18
15	Row:15	Row:15	Row:15	Row:15	Row:15	Row:15	Row:15	Row:15	Row:15									
	Column:1	Column:2	Column:3	Column:4	Column:5	Column:6	Column:7	Column:8	Column:9	Column:10	Column:11	Column:12	Column:13	Column:14	Column:15	Column:16	Column:17	Column:18



Field Trial - Findable

PLOT DETAILS

Row: 20

Column: 1

Length: 3.594m Width: 1.8m

Study Design:

Sowing Date: 2019-10-30 Harvest Date: 2020-08-10

Treatment:

Comment: Slight height segregation



Replicate	Rack	Accession	Pedigree	Gene Bank	Links
1 (Current Plot)	1	DFW SEL 0208		Germplasm Resources Unit	
3 <u>(Plot Row:3 - Col:23)</u>	1	DFW SEL 0208		Germplasm Resources Unit	
2 (<u>Plot Row:14 - Col:15)</u>	1	DFW SEL 0208		Germplasm Resources Unit	

PHENOTYPES





Field Trial - Reusable Plot Phenotypes

Phenotypic traits, measurements & units are all ontological terms

PHENOTYPES

Replicate	Rack	Date	Raw Value	Corrected Value	Trait	Measurement		Unit
1 (Current Plot)	1		2020-07-31		Maturity time	Mat DS87 DT Computa	ion	day
1 (Current Plot)	1		57		Grain filling period	GFP pct Computation		day
1 (Current Plot)	1		1743.2		Anthesis thermal time	TTA Computation		°C day
1 (Current Plot)	1		2672.05		Physiological maturity thermal time	TTM Computation		°C day
1 (Current Plot)	1	2020-07-22	78.25		Plant height	PH Measurement		<u>cm</u>
1 (Current Plot)	1		6.858225978		Grain yield	GY Computation		t/ha
1 (Current Plot)	1	2020-08-05	0		Lodging incidence	Lodg Estimation		<u>%</u>
1 (Current Plot)	1	2020-07-06	0		Spike awnedness	Awns Estimation		0-9 AWNS scale
3 (<u>Plot Row:3 - Col:23)</u>	1		2020-08-04		Maturity time	Mat DS87 DT Computa	<u>ion</u>	day
3 (<u>Plot Row:3 - Col:23)</u>	1		59		Grain filling period	GFP pct Computation		day
3 (<u>Plot Row:3 - Col:23)</u>	1		1765.65		Anthesis thermal time	TTA Computation		°C day



Field Trials Grassroots Service

The service also integrates with other services and data repositories

- Any materials with publicly-available accessions automatically generates links to any data on the DFW data portal relevant to that accession
- The materials also automatically generate links to the Grassroots
 GRU service to view the seed details



DFW Data Portal

Grassroots Data Repository

SEARCH LOGIN



Using 12Mb capture to profile the Watkins bread wheat landrace diversity collection

Anthony Hall & Laura-Jayne Gardiner

Wheat has been domesticated into a large number of agricultural environments and has a remarkable ability to adapt to diverse environments. To understand this process, we survey genotype and DNA methylation across the Watkins bread wheat landrace collection, representing global genetic diversity. For each accession, we use gene based sequence capture (12Mb) to focus on the functionally relevant portion of the genome, followed by paired end sequencing on the Hiseq4000. All Watkins accessions therefore have genotypic data available plus sequence data generated after bisulfite treatment to allow methylation calls.

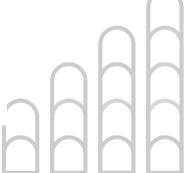
This data is made available under the Toronto Agreement

Location: Home > under license > toronto > Gardiner 2018-01-29 Watkins-diversity-12Mb

Name	Size	Date	Properties
Watkins BS exome capture data/		2018-02-20 18:18	Q ■{}
Watkins exome capture data/		2018-02-20 18:18	Q III{}

Brought to you by mod_eirods-dav Copyright (c) 2016-18, Earlham Institute and Utrecht University. Images taken from the <u>Amiga Image Storage System</u> by Martin Merz.

https://opendata.earlham.ac.uk/wheat/under_license/toronto/





DFW Data Portal datasets

24 TB data hosted

- 116M ./Ball_2018-06-13_Breeder_toolkit
- 1.6G ./Gardiner_2018-07-04_Wheat-gene-promoter-capture
- 4.7M ./Griffiths_2018-10-22_DFW-TK-NIL-Set2-2018-phenotypes
- 13T ./King_2018-05-09_Cadenza_RefSeqV1.0_Alignments
- 22G ./Clavijo_2017-04-25_Wheat-LoLa
- 279G ./Zhou_2019_RobxCla_UAV_Image_Data
- 14G ./Martin_etal_2018_Alabdullah_etal_2019_wheat_meiosis_transcriptome_and_co-expression_network
- 5.7G ./White_2020-02-06_consensus_evolved_fielder_wheat
- 4.0G ./Riche_2020-07-13_DFW_Academic_Toolkit_Harvest_2020
- 6.4T ./Wulff 2018-01-31 OWWC
- 1.5T ./Gardiner_2018-01-29_Watkins-diversity-12Mb
- 262G ./Brinton_etal_2020-05-20-Haplotypes-for-wheat-breeding
- 3.4T ./Wulff_2019-03-13_OWWC_lineage1
- 44G ./Gardiner_et_al_2017_Watkins_exome_capture_SNP_calls_VCF
- 13G ./Ramirez-Gonzalez_etal_2018-06025-Transcriptome-Landscape

Since July 2020 (new server) 418 unique visitors and over 23 TB of transferred data 4673 users in total from Apr 2018



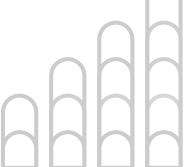
DFW Research Outputs - CKAN

Designing Future Wheat	Datasets Organizations Groups About Search Q
Search data E.g. environment	Welcome to the Designing Future Wheat CKAN, the digital repository for the UK-wide BBSRC wheat improvement programme. This repository holds all publications, open datasets, and partner project datasets related to DFW.
Popular tags gold hybrid closed	ANNAMOR
DFW CKAN statistics 370 datasets 8 organizations 3 groups	ALMANU.
Designing Future Wheat CKAN, the digital repository for the UKRI-BBSRC wheat improvement programme. This repository holds all publications, open datasets, and partner project datasets	



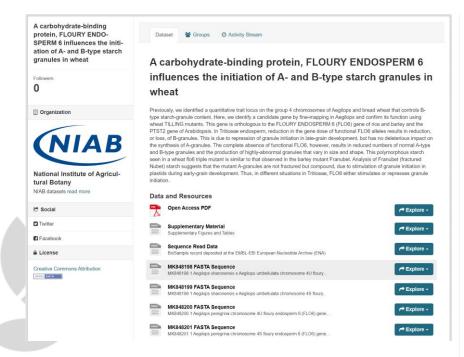
DFW Research Outputs in CKAN

▼ Organizations			
Rothamsted Research 215	Search datasets		Q
John Innes Centre 87	270 datasets found		
Earlham Institute 23	370 datasets found Order by:	Relevance	~
National Institute 18			
University of Bristol 13	Hidden variation in polyploid wheat drives local adaptation Wheat has been domesticated into a large number of agricultural environments and has the ability	to adapt to diverse	
University of Notti 11	environments. To understand this process, we survey		
European Bioinforma 2	POF		
Quadram Institute B	Uncovering hidden variation in polyploid wheat		
▼ Groups	Comprehensive reverse genetic resources, which have been key to understanding gene function in are missing in many polypiold crops. Young polypiold	diploid model org	anisms,
DFW Publications 360	COP CHARLE PARTY		
Open Data 6	LYS3 encodes a prolamin-box-binding transcription factor that controls embryo.		
Open Wild Wheat Con 2	Mutations at the LYS3 locus in barley have multiple effects on grain development, including an incredecrease in endosperm starch content. The gene	ease in embryo siz	te and a
▼ Tags	POF XML API		
gold 121	Transfer of a starch phenotype from wild wheat to bread wheat by deletion of		
hybrid 111	Our previous genetic analysis of a tetraploid wild wheat species, Aegilops peregrina, predicted that genome, Bgc-1, controls B-type starch granule	a single gene per	haploid
closed 54	POF		
green 44	A carbohydrate-binding protein, FLOURY ENDOSPERM 6 influences the initiation	1	
bronze 30	Previously, we identified a quantitative trait locus on the group 4 chromosomes of Aegilops and bre type starch-granule content. Here, we identify a	ad wheat that cont	trols B-
book chapter 14	rype starch-granule content. Here, we identify a		
grassroots 6			
toronto 🚯	Acrylamide in food: Progress in and prospects for genetic and agronomic solut. Acrylamide is a processing contaminant and Group 2a carcinogen that was discovered in foodstuff		ence in a
Toronto 🖪	range of popular foods has become one of the most		77.00
diversity 2	PDF XML		





CKAN Example entry



Additional Info

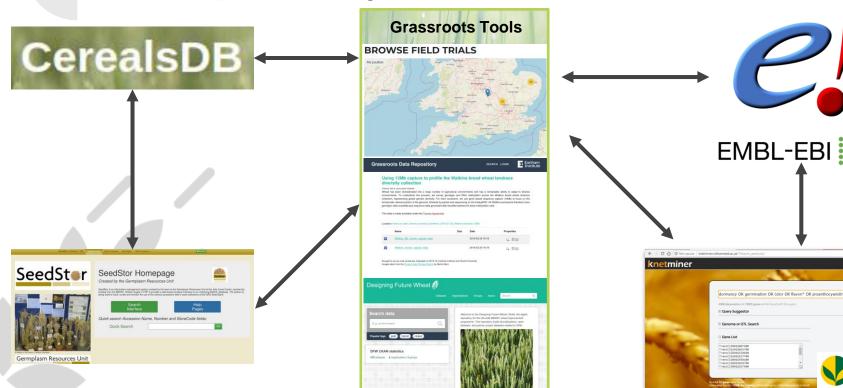
Field

Field	Value
Source	
Version	
Authors	 Name: Chia, Tansy, Type: Corresponding Author, Name: Chiroco, Marcoella, Type: Author, Name: King, Rob. Type: Author, Name: Ramiraz-Gonzalez, Ricardo, Type: Author, Name: Saccomanno, Bonedetta, Type: Author, Name: Seung, David, Type: Author, Name: Simmonds, James, Type: Author, Name: Trick, Martin, Type: Author, Name: Uauy, Cristobal, Type: Author, Name: Verhoeven, Tamara, Type: Author, Name: Trafford, Kay, Type: Author,
Maintainer	
Maintainer Email	
Article Host Type	publisher
Article Is Open Access	true
Article License Type	cc-by-nc-nd
Article Version Type	publishedVersion
Citation Report	https://scite.ai/reports/10.1101/643759
DFW Organisation	NIAB
DFW Work Package	2
DOI	10.1101/643759
Date Last Updated	2019-07-09T05:10:07.396155
Evidence	open (via page says license)
Journal Is Open Access	false
Open Access Status	hybrid
PDF URL	https://www.biorxiv.org/content/biorxiv/early/2019/05/23/6437 59.full.pdf
Publisher URL	https://doi.org/10.1101/643759

Value

Interoperability – Software and Data

ROTHAMSTED RESEARCH



Germplasm Resources Unit

DFW

www.seedstor.ac.uk

A display of the history of wheat cultivation.

Germplasm Resources Unit



KnetMiner 4.0 released with user workspaces for gene networks

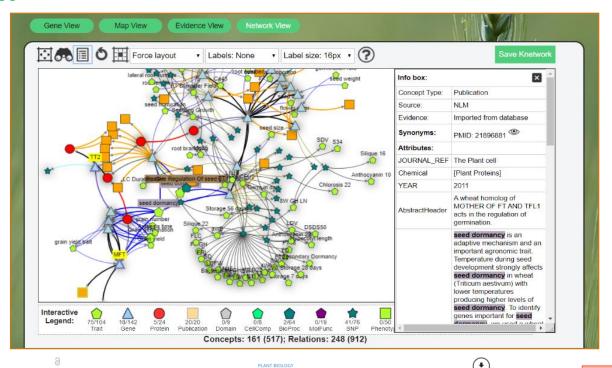
by Keywan Hassani-Pak

NEWS

https://knetminer.com



https://knetminer.com/Triticum_aestivum/



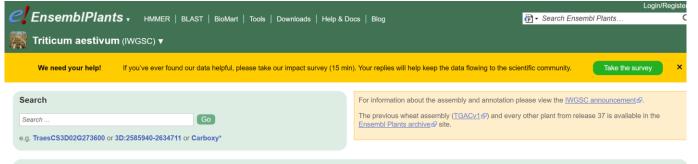
A roadmap for gene functional characterisation in crops with large genomes: Lessons from polyploid wheat

f 🛂 🖾 🕏

Featured in eLife

https://elifesciences.org/articles/55646





About Triticum aestivum

Triticum aestivum (bread wheat) is a major global cereal grain essential to human nutrition. Wheat was one of the first cereals to be domesticated, originating in the fertile crescent around 7000 years ago. Bread wheat is hexaploid, with a genome size estimated at ~17 Gb, composed of three closely-related and independently maintained genomes that are the result of a series of naturally occurring hybridisation events. The ancestral progenitor genomes are considered to be Triticum urartu (the A-genome donor) and an unknown grass thought to be related to Aegilops spelloides (the B-genome donor). This first hybridisation event produced tetraploid emmer wheat (AABB, T. dicoccoides) which hybridized again with Aegilops tauschii (the D-genome donor) to produce modern bread wheat.

Guidelines for gene nomenclature in wheat can be found in the 2013 edition of the Wheat Gene Catalogue available in GrainGenes 2. The Wheat Gene Catalogue is the internationally agreed rules of nomenclature for wheat genes.

Taxonomy ID 4565 ₽

Data source International Wheat Genome Sequencing Consortium ☑



More information and statistics

Genome assembly: IWGSC ₽

More information and statistics

Download DNA sequence (FASTA)

Convert your data to IWGSC coordinates

Display your data in Ensembl Plants

Other cultivars



View karyotype

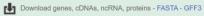


Example region

Gene annotation

What can I find? Protein-coding and non-coding genes, splice variants, cDNA and protein sequences, non-coding RNAs.

More about this genebuild



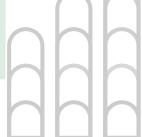
Update your old Ensembl IDs



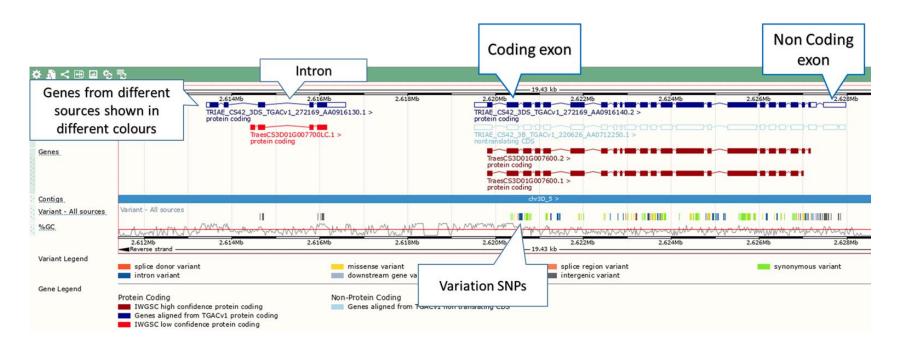
Example gene



Example transcript



The IWGSC RefSeq v1.0 in Ensembl Plants



The TILLING population in Ensembl Plants

Cadenza0225.chr3D.379537010 SNP

Most severe consequence missense variant | See all predicted consequences

Alleles G/A | Highest population MAF: < 0.01

Location Chromosome 3D:379537010 (forward strand) | VCF: 3D 379537010 Cadenza0225.chr3D.379537010 G A

HGVS names This variant has 5 HGVS names - Show

⊞

Original source EMS-induced mutations & from sequenced TILLING populations. Seeds can be ordered from UK SeedStor & or US Dubcovsky lab &.

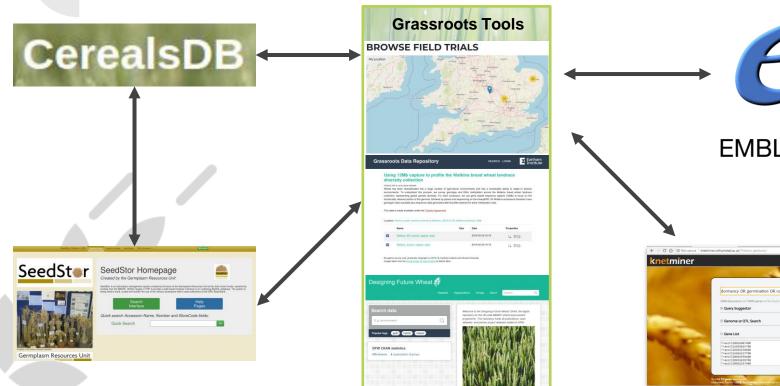
About this variant This variant overlaps 2 transcripts.

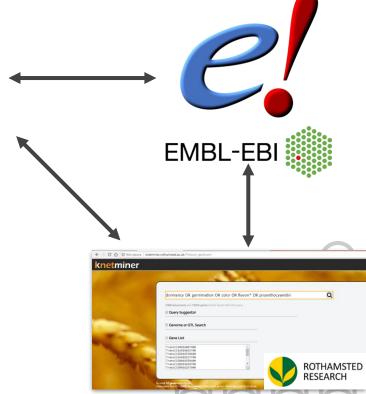
Gene and Transcript consequences

Show/hide columns								Filter	X
Gene	Transcript (strand)	Allele ▲ (transcript allele)	Consequence Type ▲	Position in transcript	Position in CDS	Position in protein	Amino acid	Codons	SIFT Detail
TraesCS3D01G273600	<u>TraesCS3D01G273600.1</u> (-) biotype: protein_coding	A (T)	missense variant	2171 (out of 2742)	2171 (out of 2742)	724 (out of 913)	A/V	GCG/GTG	0.01 Show
TraesCS3D01G273600	<u>TraesCS3D01G273600.2</u> (-) biotype: protein_coding	A (T)	missense variant	2261 (out of 2888)	2261 (out of 2688)	754 (out of 895)	A/V	GCG/GTG	deleterious

No overlap with Ensembl Regulatory features

Interoperability - Software and Data







What we have learned

- That the technical challenges of developing a data sharing infrastructure are significant but not overwhelming
 - Would not have been practical if we had started from scratch
- Ensuring that the tools we develop are useable by the project members takes longer and more resource than predicted
 - Major contributions needed by the trial managers who are already overcommitted
- Reaching other data submitters can almost require 1:1 support from DCTF or others
- Developing a common culture of data sharing takes time and effort
- Being open with our progress and research outputs benefits relationships:
 - With funders transparency
 - With community new collaborations

Acknowledgements



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 - Marco Brandizi

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 - > Xingdong Bian
 - Alice Minotto
 - Toni Etuk
 - Felix Shaw
 - Jon Wright
 - Paul Bailey
 - o Bernardo Clavijo
 - Luis Yanes
 - Catherine Hunter
- EMBL-EBI
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 - Dan Bolser
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