

Supporting_MT

Robin Lindner

2025-01-08

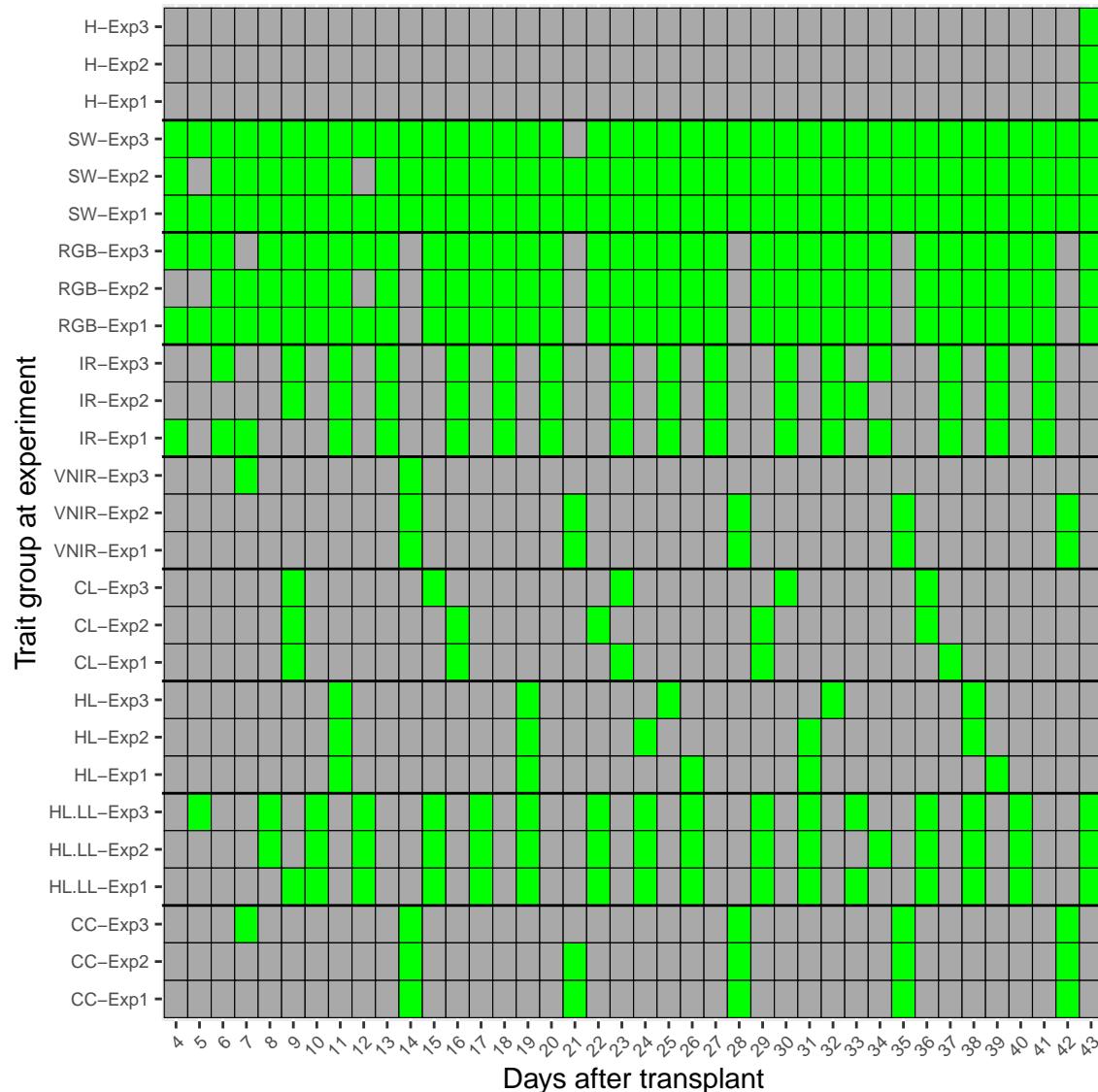


Figure 1: Experiment-wise measurement log for each group. The y-axis labels consist of a group prefix and an experiment suffix, denoting the group-experiment pair. A green rectangle indicates that a measurement protocol was conducted.

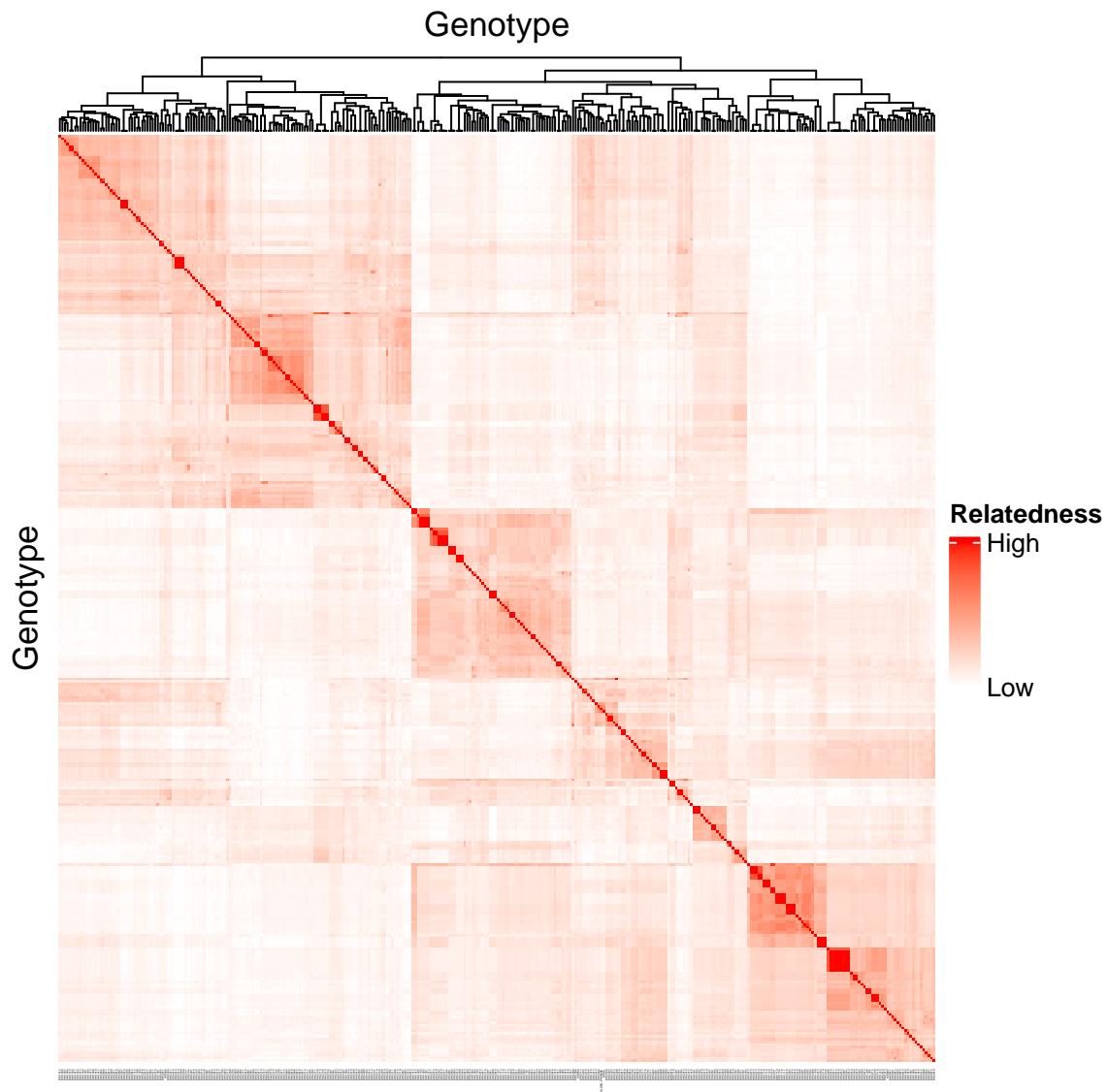


Figure 2: Kinship between 340 B1K accessions Relatedness is indicated in red. Above the heatmap columns, a dendrogram of a hierarchical clustering is plotted. The clustering is calculated using `hclust` in r.

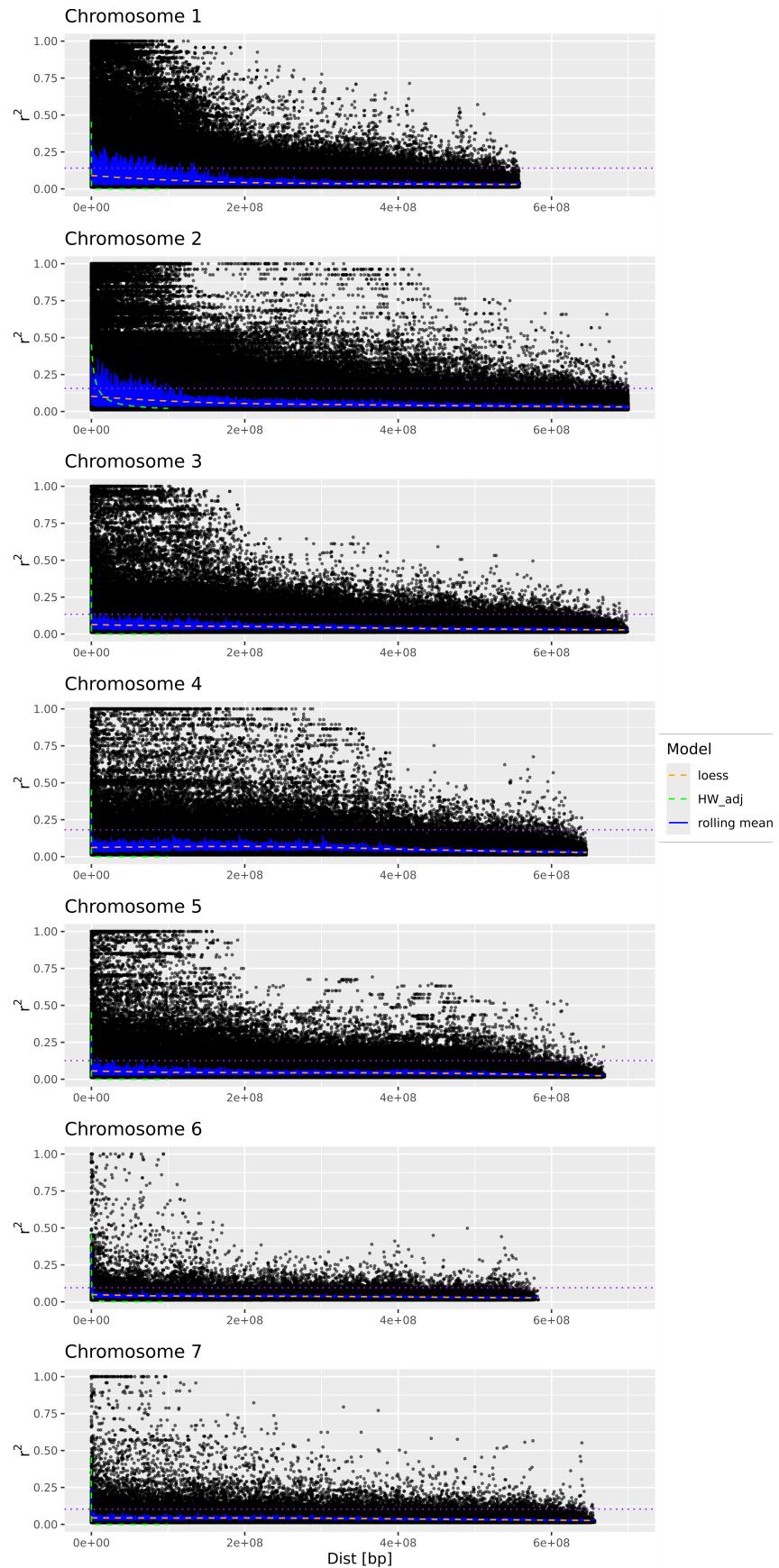


Figure 3: LD for marker pairs on all seven chromosomes. The rolling mean of a 100 marker window is shown in blue. The dotted line indicates the background LD as defined in Materials and Methods. Best fits for a standard loess and the utilized Hill and Weir model are shown as dashed lines and plotted for 100000 distance values equally spaced on the x-axis.

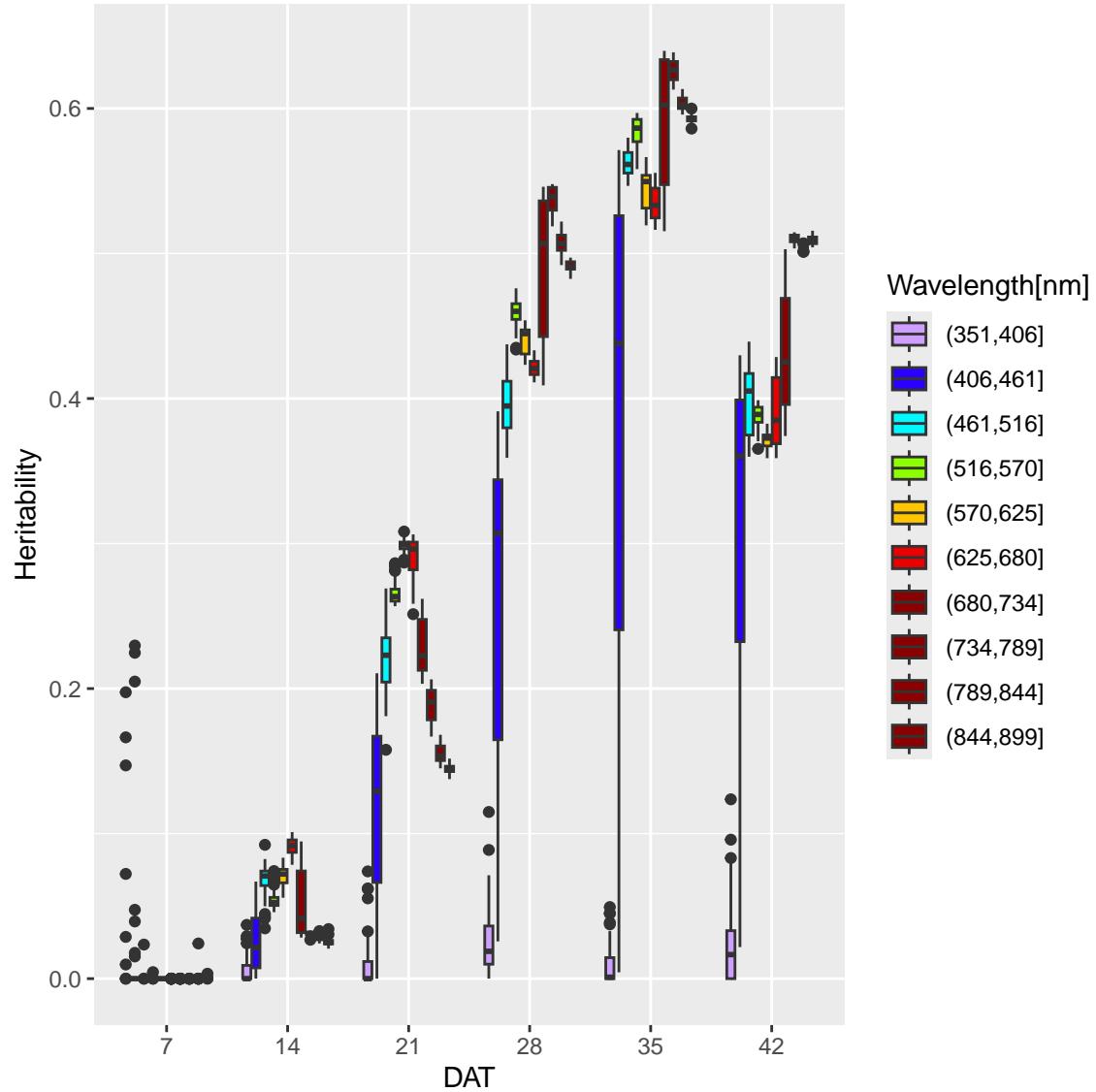


Figure 4: Heritability estimates for HSR-data for six measured time points. The measured wavelengths are binned and color coded based on their length.

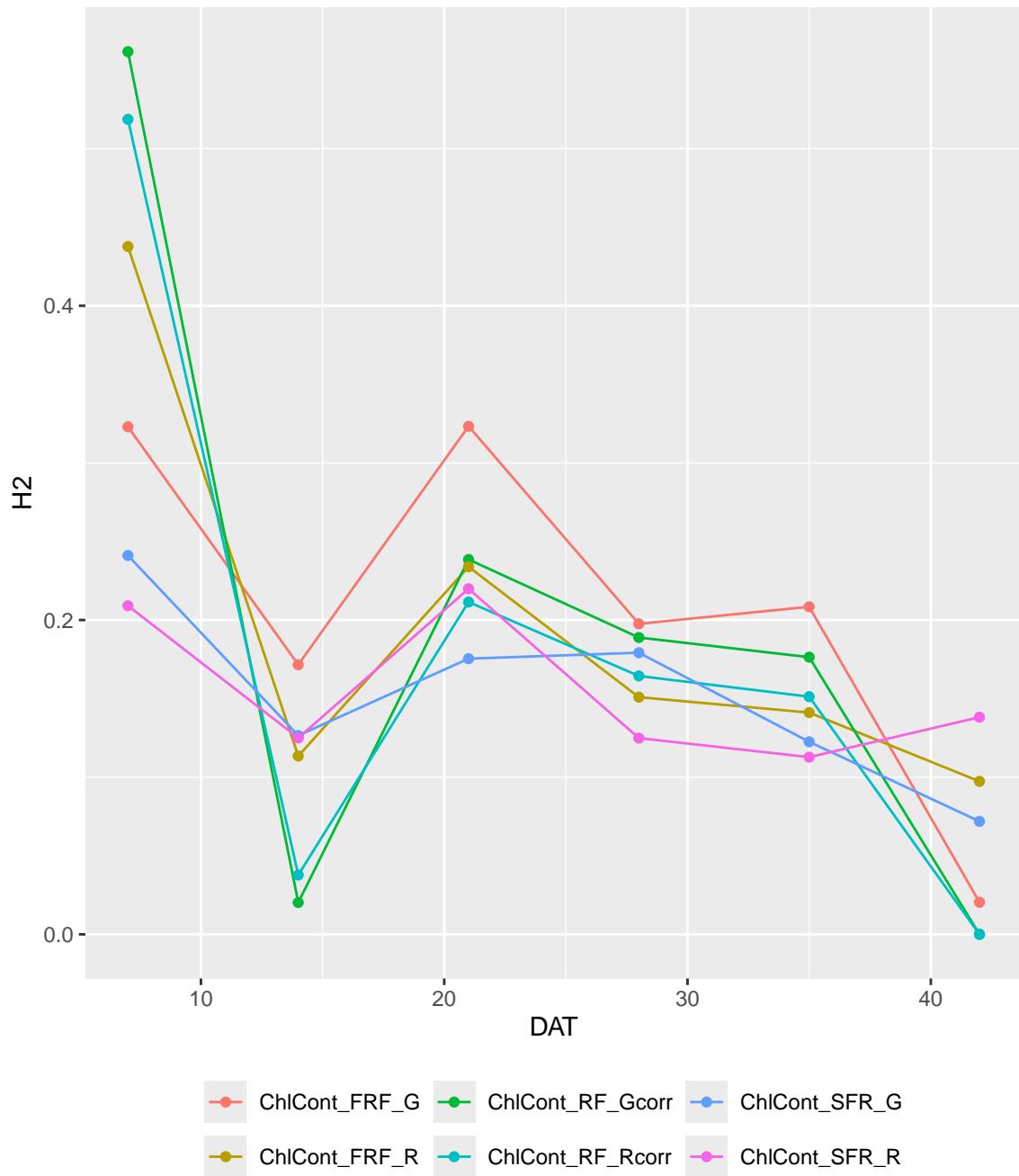


Figure 5: Heritability estimates for CC traits through time.

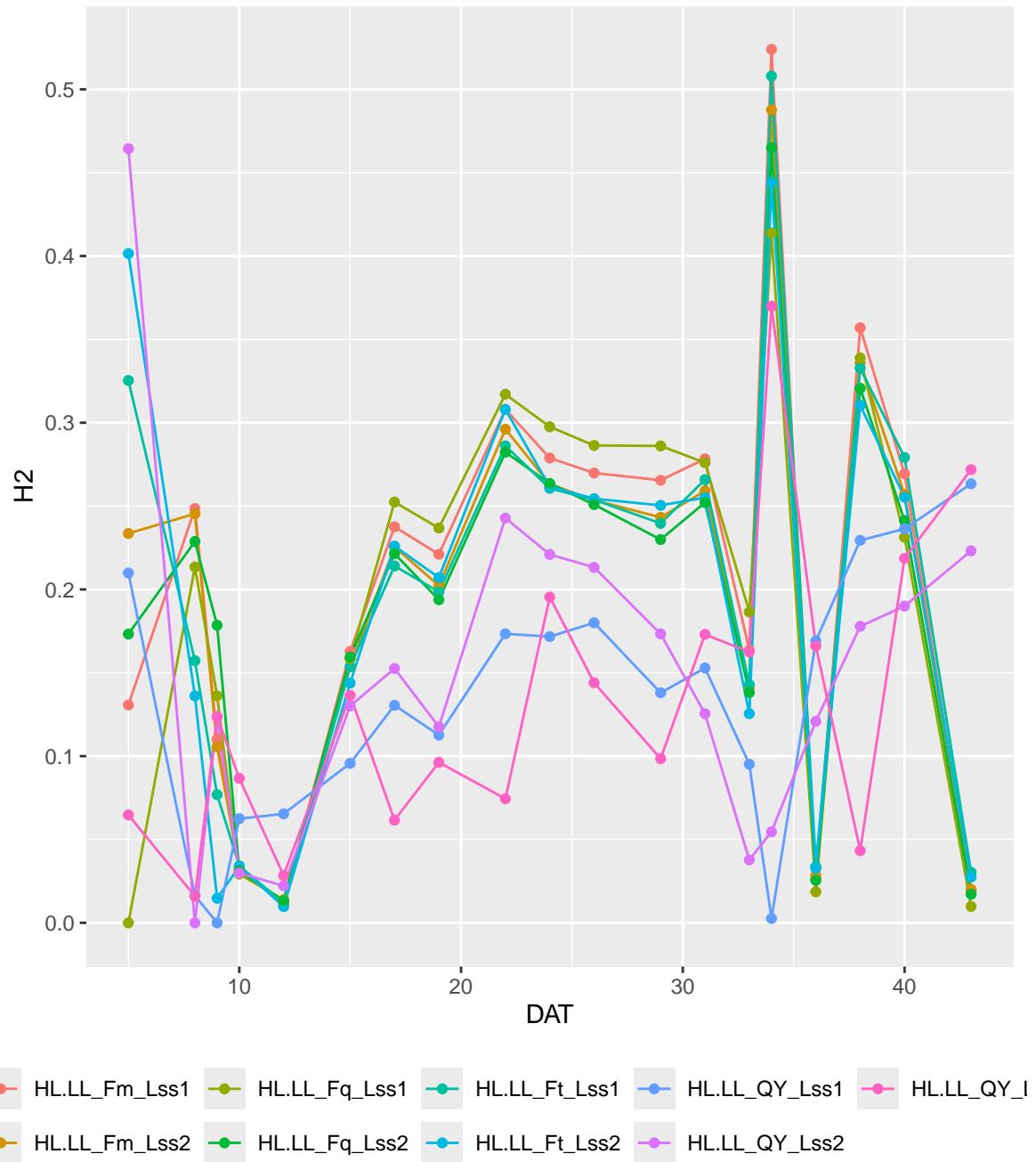


Figure 6: Heritability estimates for HL.LL traits through time.

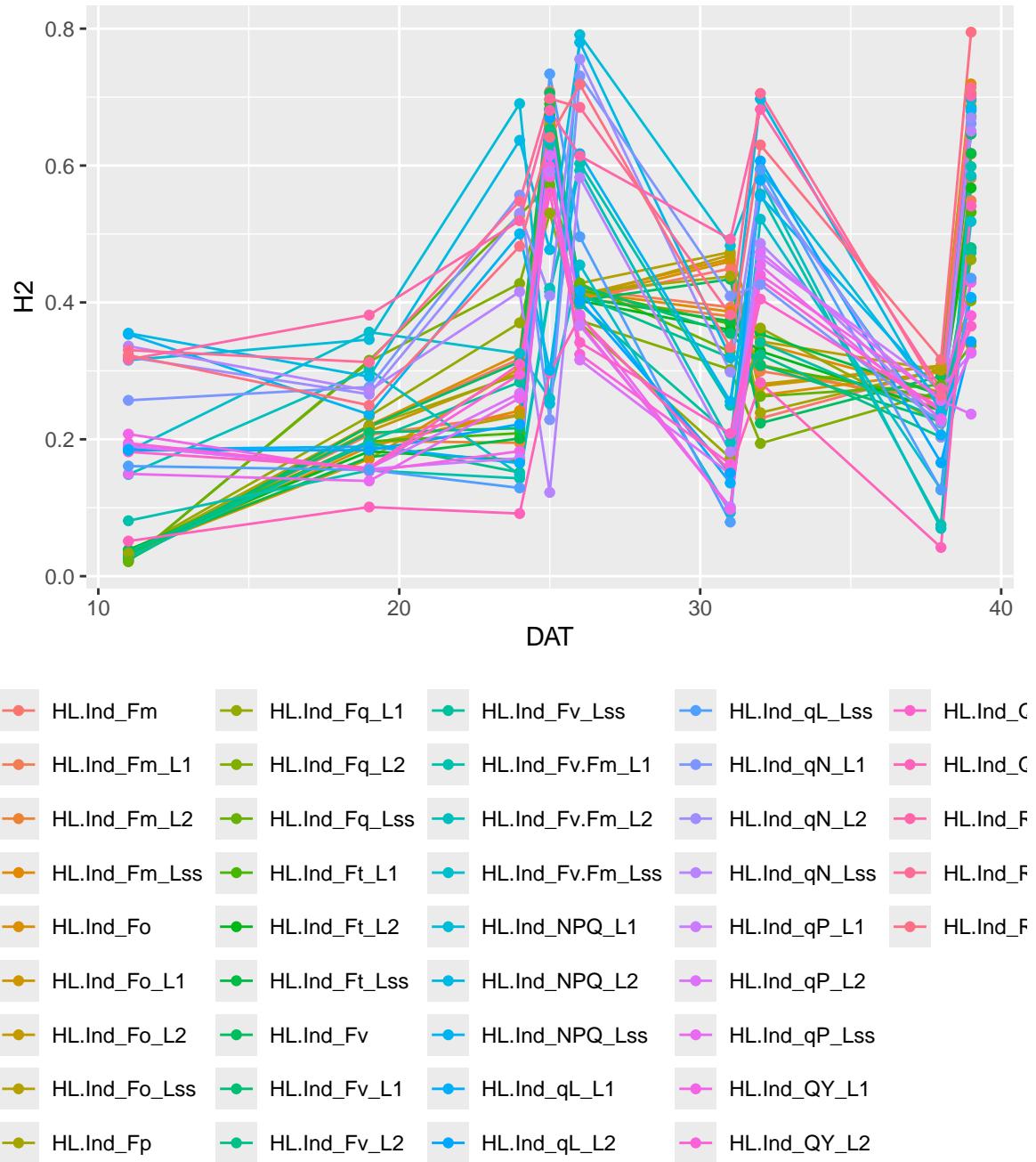


Figure 7: Heritability estimates for HL traits through time.

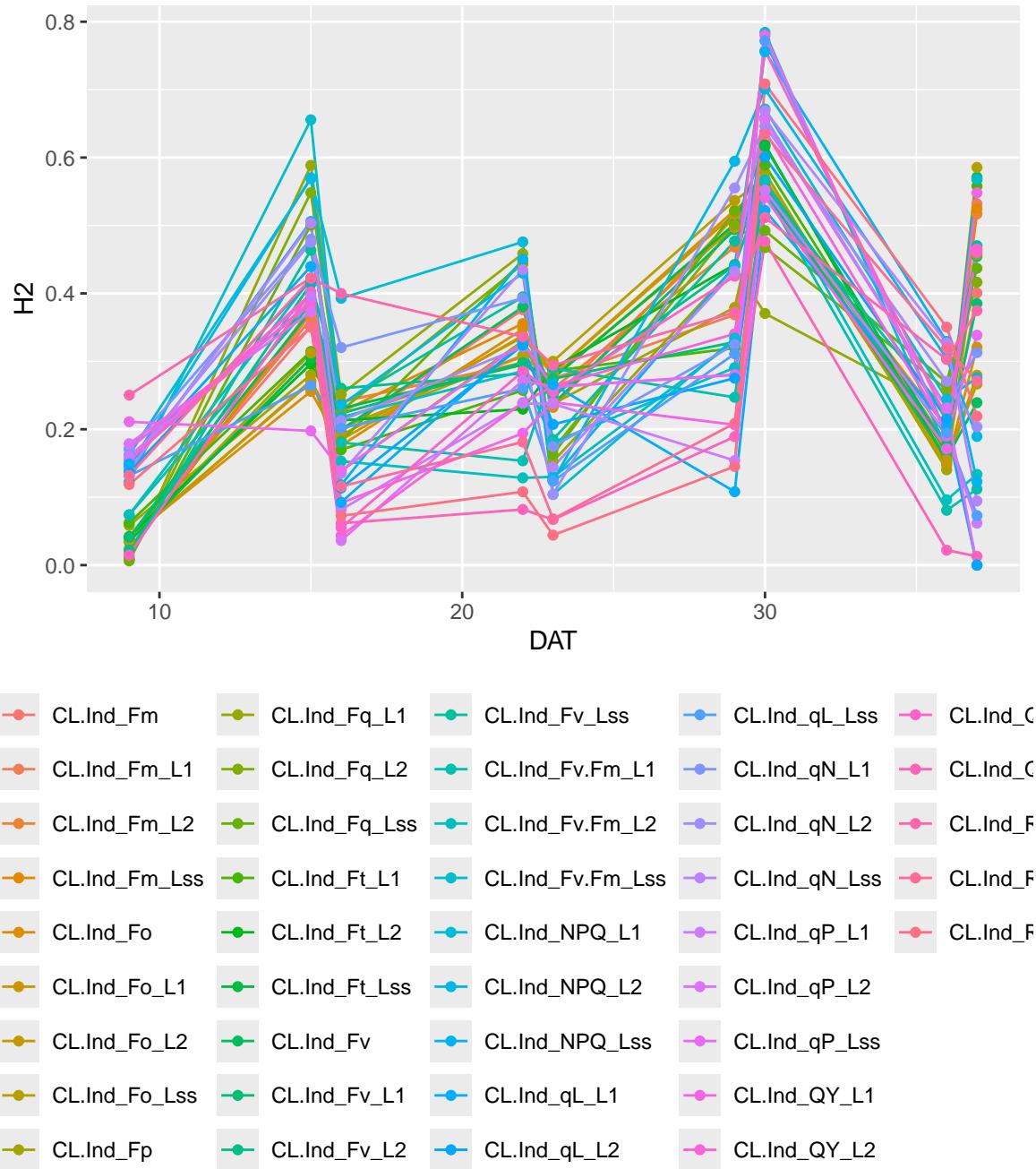


Figure 8: Heritability estimates for CL traits through time.

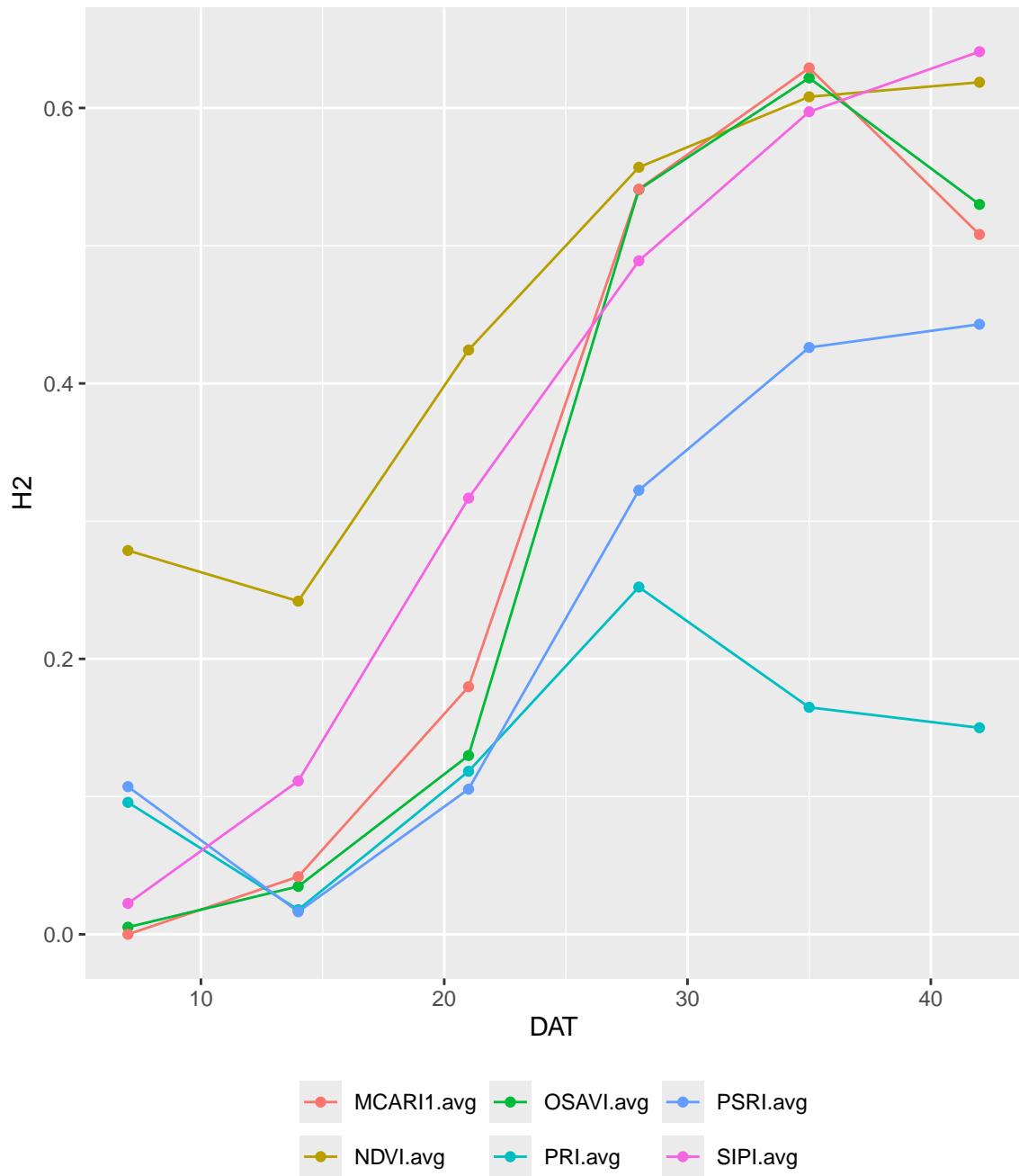


Figure 9: Heritability estimates for VNIR traits through time.

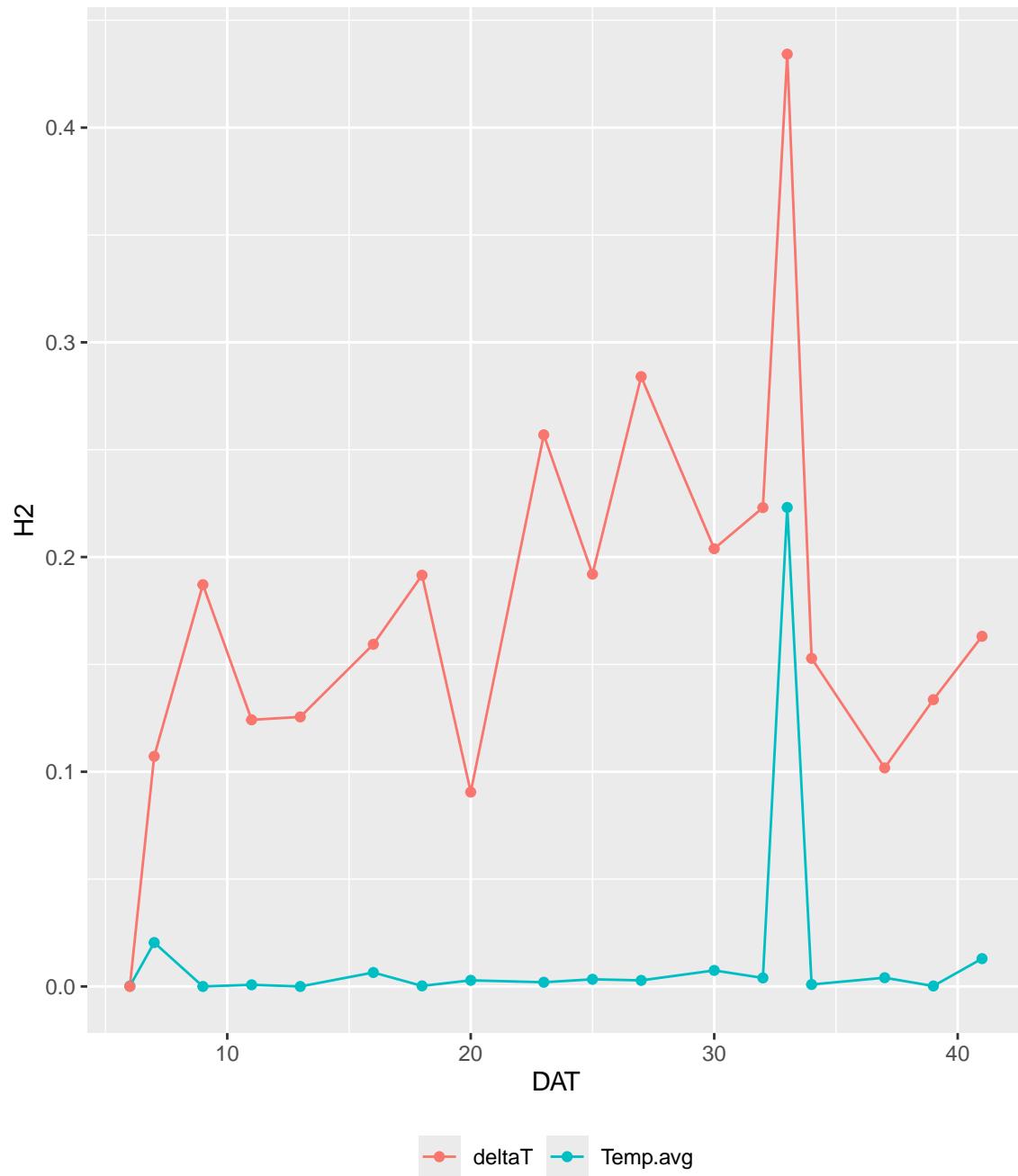


Figure 10: Heritability estimates for IR traits through time.

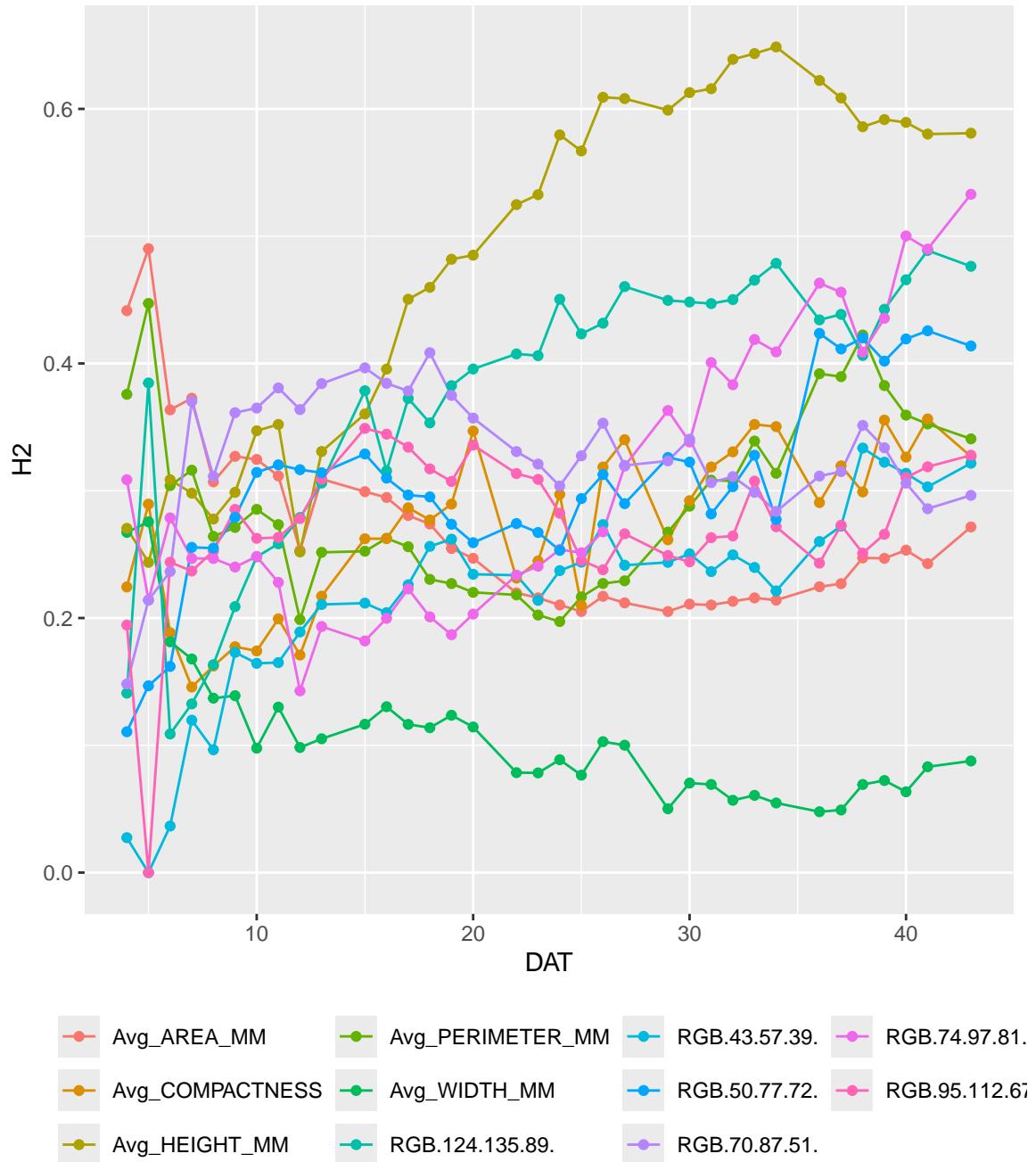


Figure 11: Heritability estimates for RGB traits through time.

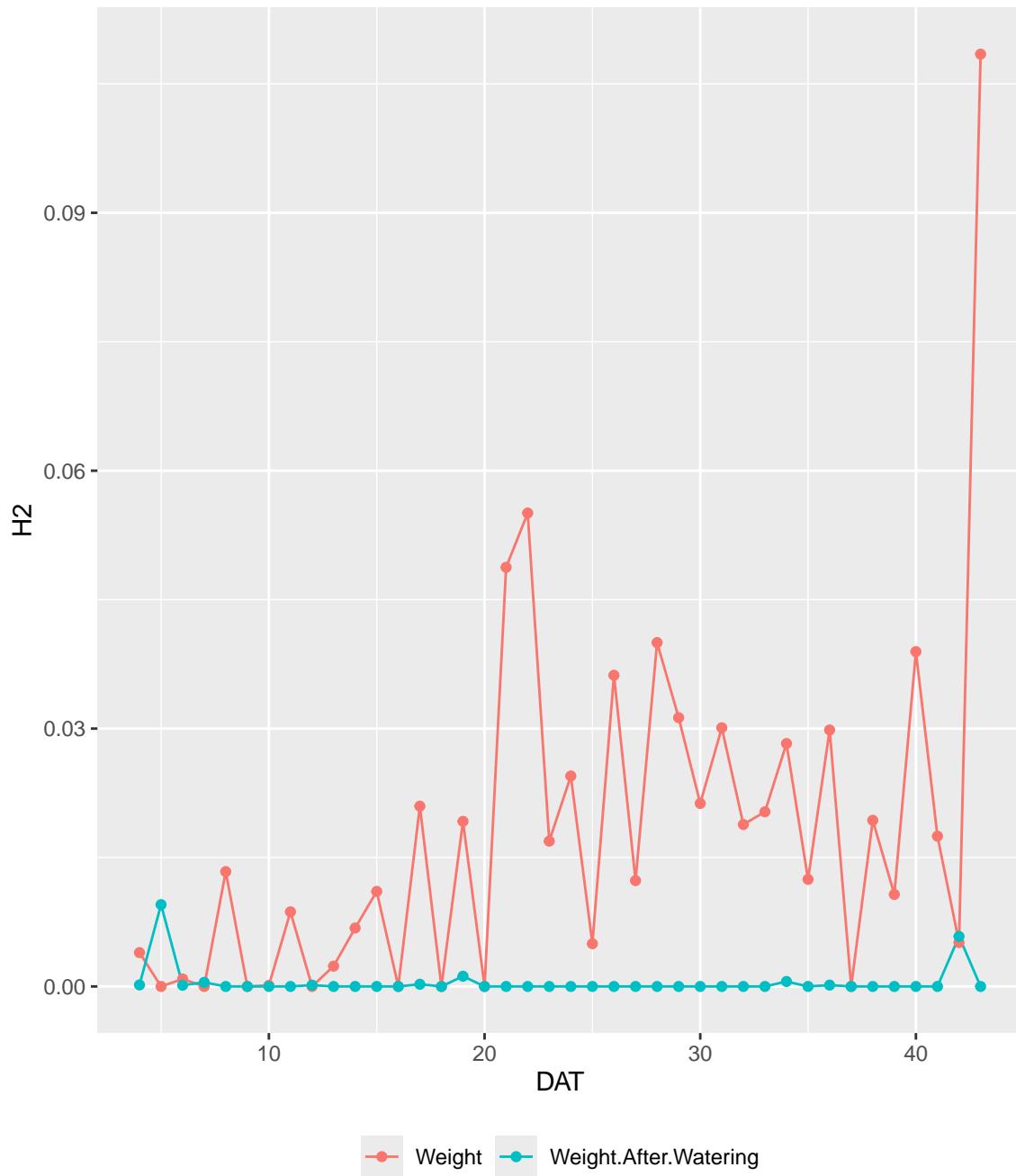


Figure 12: Heritability estimates for SW traits through time.

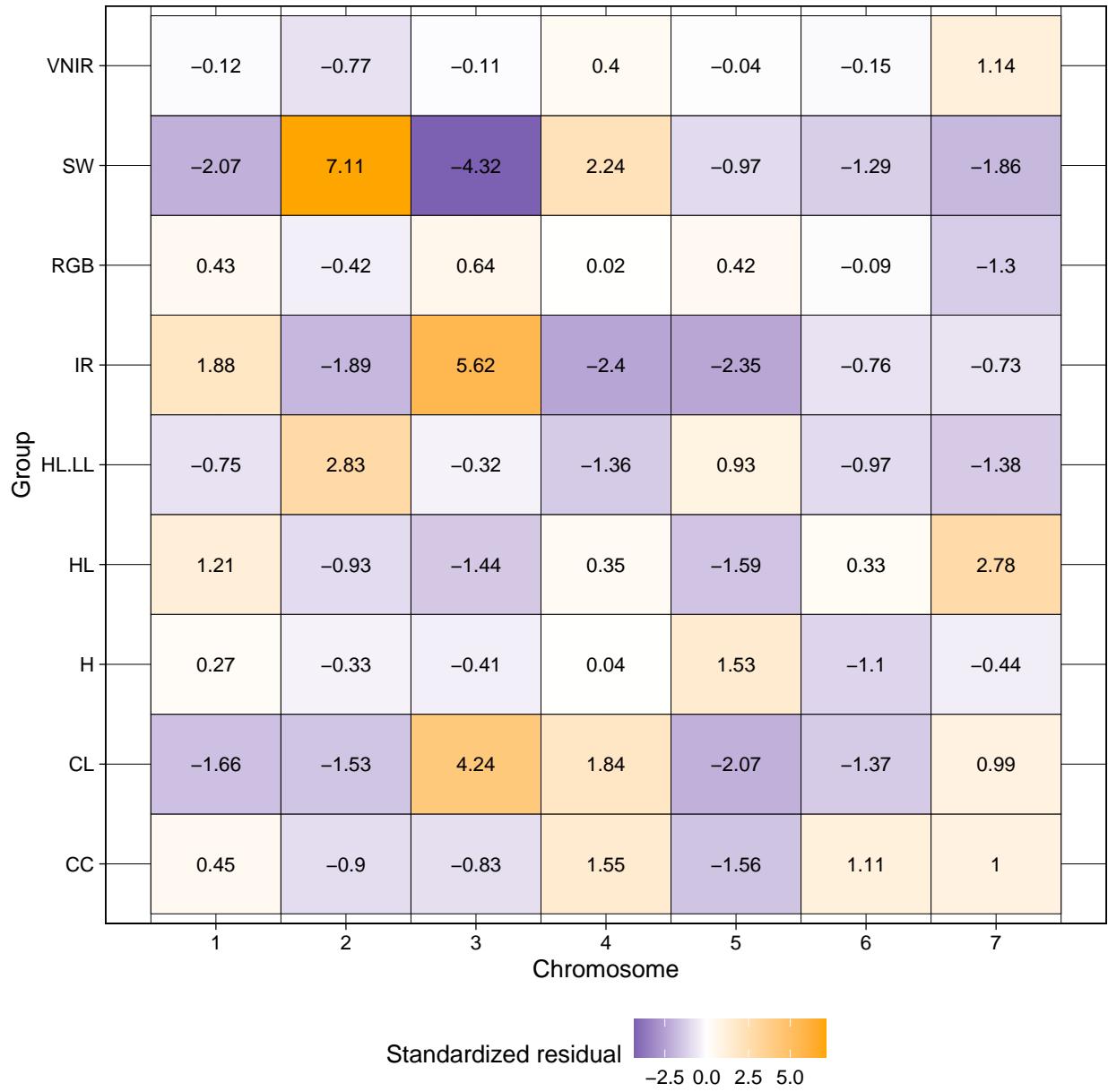


Figure 13: Enrichment of associations per chromosome-group pair Standardized residuals of a chi²-test for homogeneity of the distribution of associated SNP. P-values for chi²-test can be found in STab.3

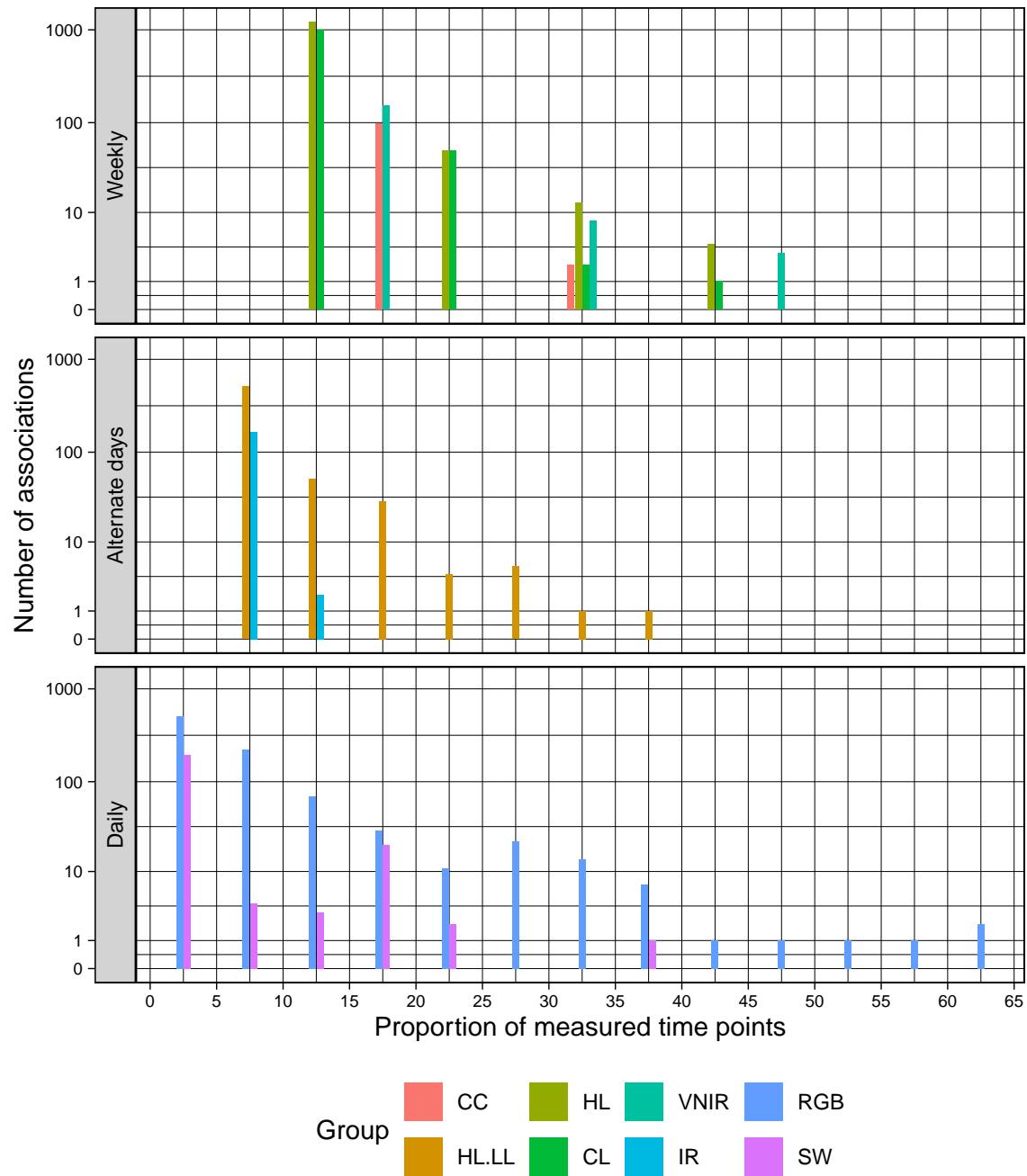


Figure 14: Marker stability for groups with different measurement frequencies.

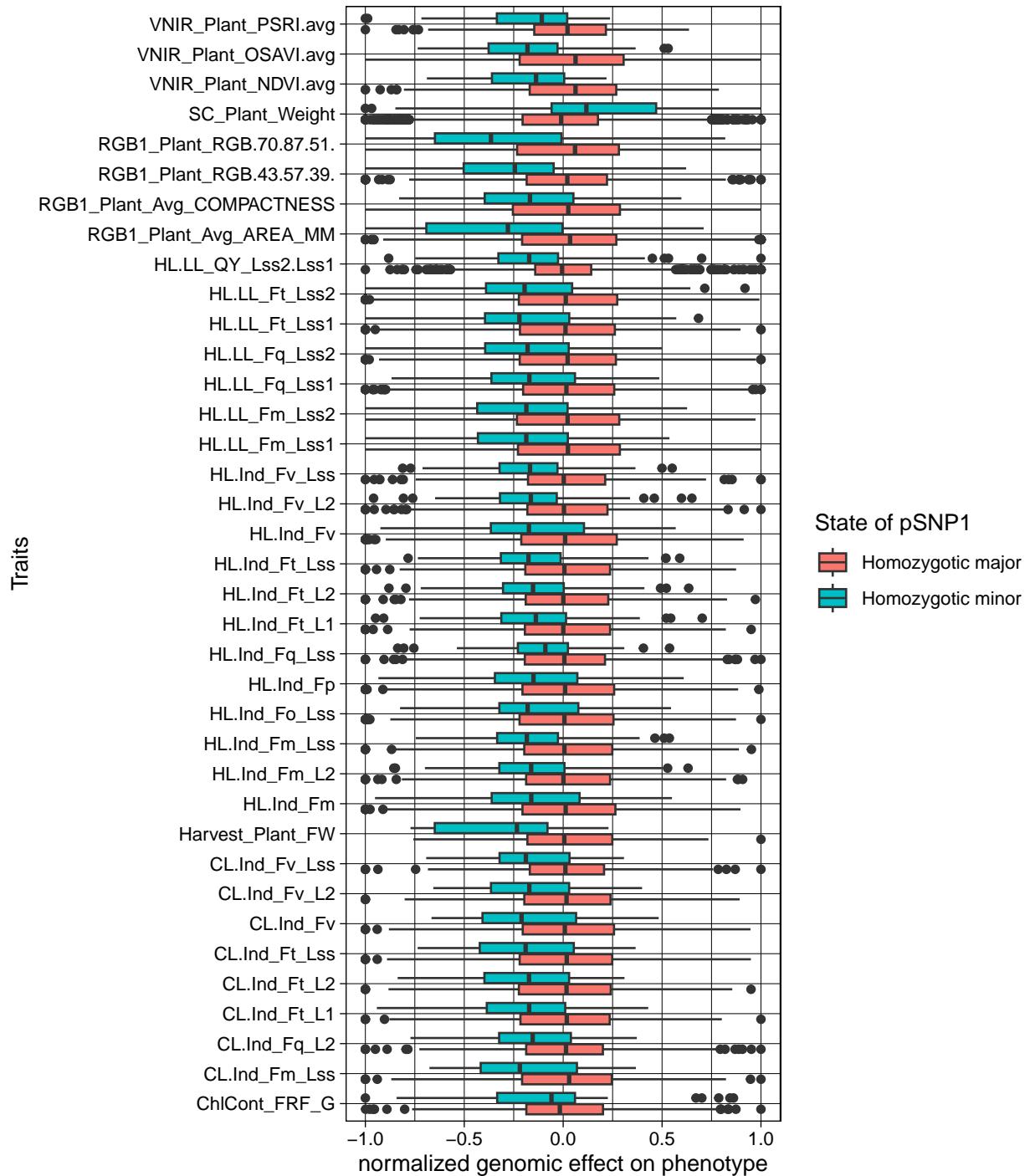


Figure 15: Effect of allele state in pSNP1 Normalized genomic BLUP predictions in associated traits between lines with differing allele states in pSNP1

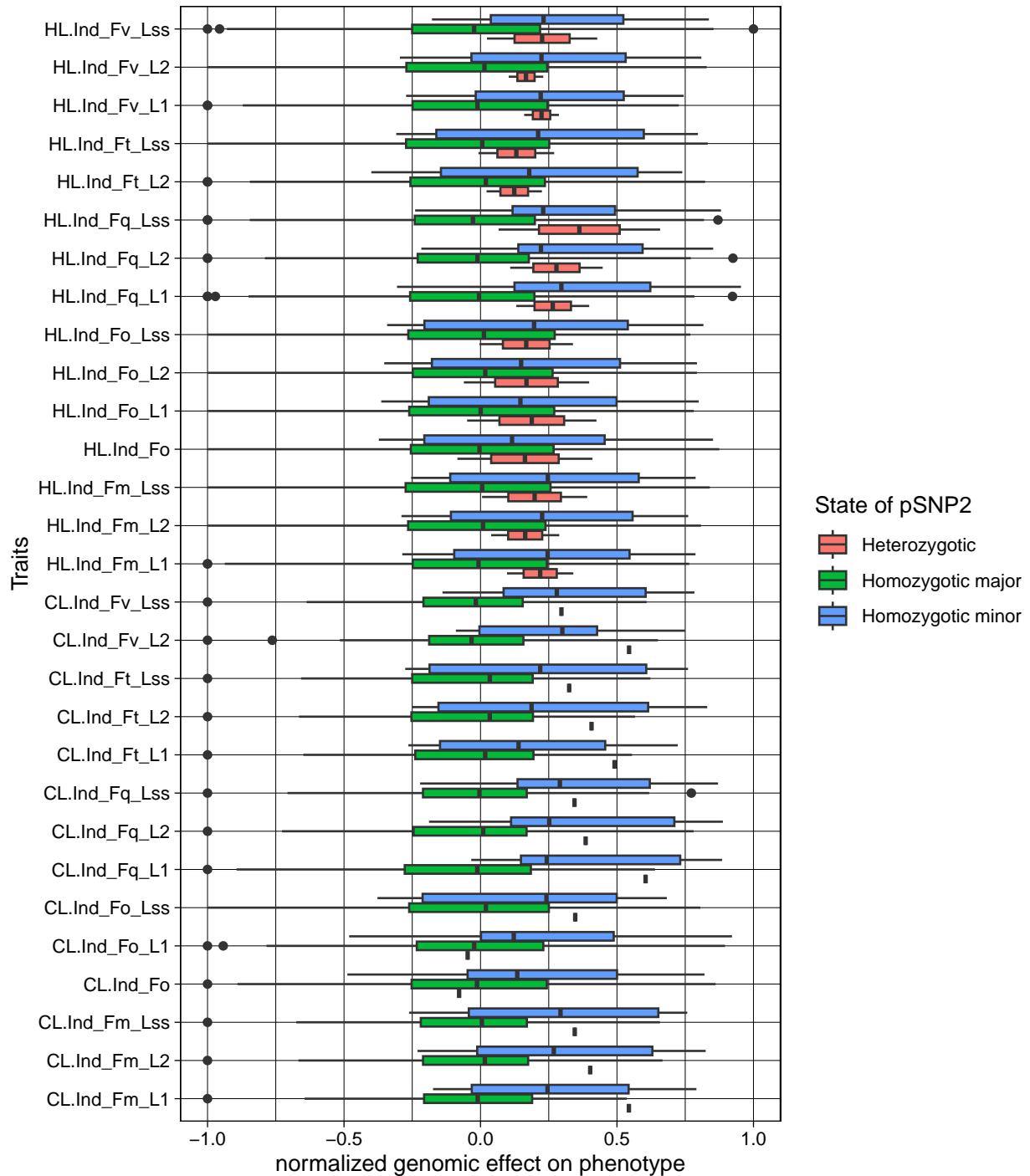


Figure 16: Effect of allele state in pSNP2 Normalized genomic BLUP predictions in associated traits between lines with differing allele states in pSNP2

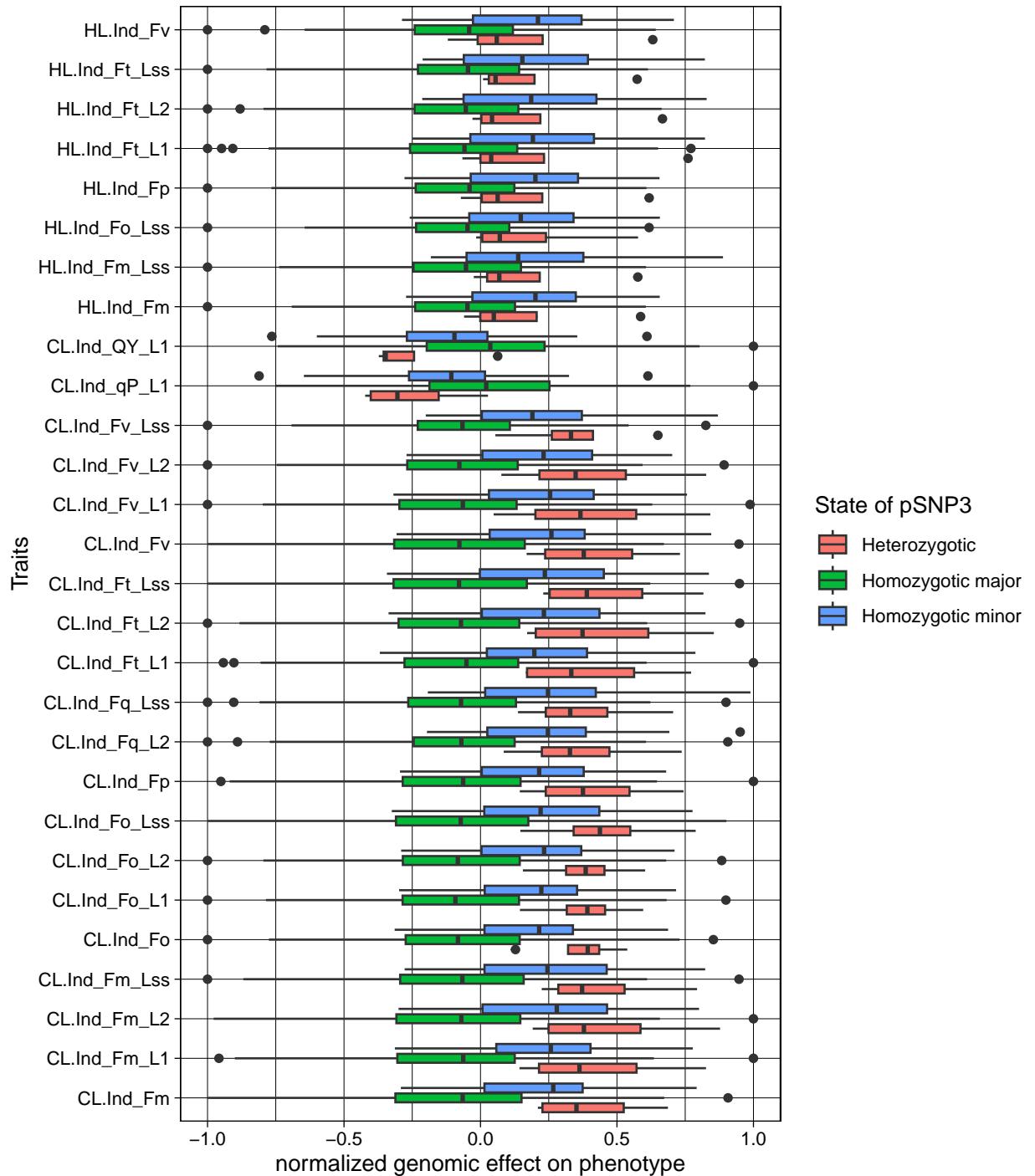


Figure 17: Effect of allele state in pSNP3 Normalized genomic BLUP predictions in associated traits between lines with differing allele states in pSNP3

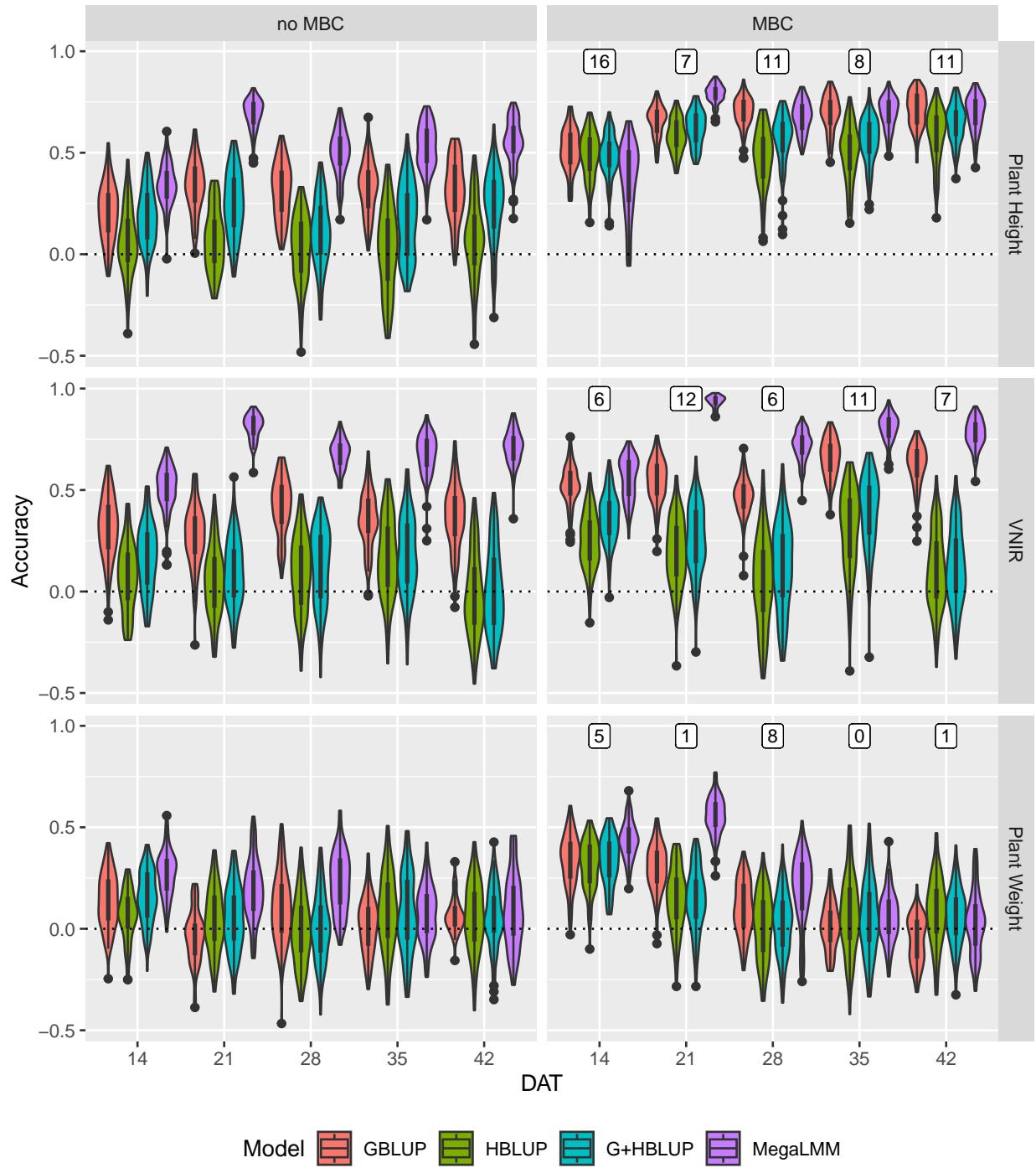


Figure 18: Time specific genomic prediction performance GP accuracy for three yield-related traits at 5 time points. The number of fixed effect covariates added in the MBC models is indicated above the violin plots.

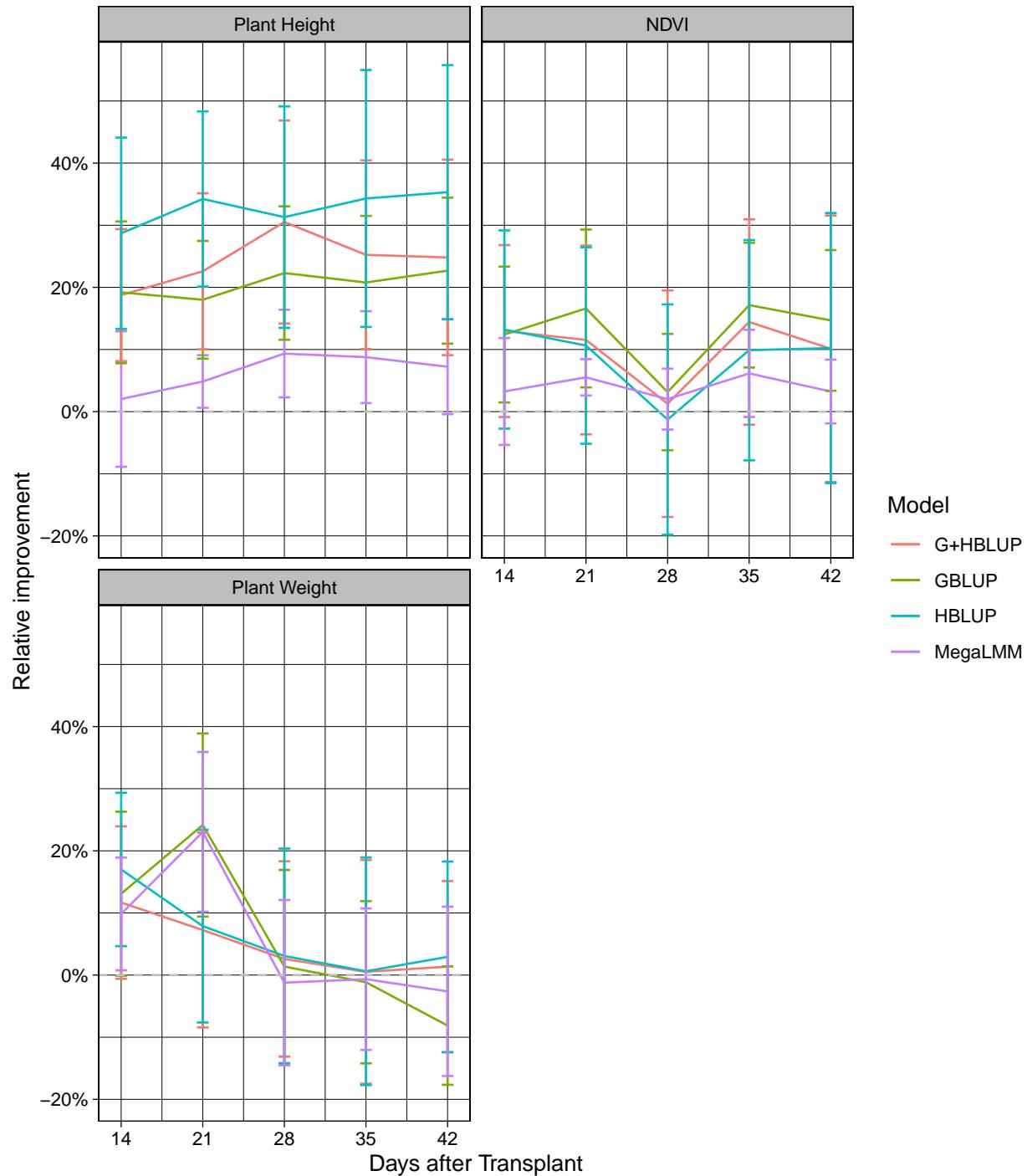


Figure 19: Genomic prediction performance improvement Improvement of prediction accuracy observed after inclusion of marker based covariates.

Table 1: Group assignment (1/2) of all recorded traits. Column names indicate the resspective group, while entries are the assigned traits.

HL.LL	HL	CL	RGB
HL.LL_Fm_Lss1	HL.Ind_Fo	CL.Ind_Fo	Avg_AREA_MM
HL.LL_Fm_Lss2	HL.Ind_Fm	CL.Ind_Fm	Avg_PERIMETER_MM
HL.LL_Ft_Lss1	HL.Ind_Fv	CL.Ind_Fv	Avg_COMPACTNESS
HL.LL_Ft_Lss2	HL.Ind_Fp	CL.Ind_Fp	Avg_WIDTH_MM
HL.LL_Fq_Lss1	HL.Ind_Fm_L1	CL.Ind_Fm_L1	Avg_HEIGHT_MM
HL.LL_Fq_Lss2	HL.Ind_Fm_L2	CL.Ind_Fm_L2	RGB.43.57.39.
HL.LL_QY_Lss1	HL.Ind_Fm_Lss	CL.Ind_Fm_Lss	RGB.124.135.89.
HL.LL_QY_Lss2	HL.Ind_Ft_L1	CL.Ind_Ft_L1	RGB.95.112.67.
HL.LL_QY_Lss2.Lss1	HL.Ind_Ft_L2	CL.Ind_Ft_L2	RGB.74.97.81.
	HL.Ind_Ft_Lss	CL.Ind_Ft_Lss	RGB.50.77.72.
	HL.Ind_Fo_L1	CL.Ind_Fo_L1	RGB.70.87.51.
	HL.Ind_Fo_L2	CL.Ind_Fo_L2	
	HL.Ind_Fo_Lss	CL.Ind_Fo_Lss	
	HL.Ind_Fv_L1	CL.Ind_Fv_L1	
	HL.Ind_Fv_L2	CL.Ind_Fv_L2	
	HL.Ind_Fv_Lss	CL.Ind_Fv_Lss	
	HL.Ind_Fq_L1	CL.Ind_Fq_L1	
	HL.Ind_Fq_L2	CL.Ind_Fq_L2	
	HL.Ind_Fq_Lss	CL.Ind_Fq_Lss	
	HL.Ind_QY_max	CL.Ind_QY_max	
	HL.Ind_Fv.Fm_L1	CL.Ind_Fv.Fm_L1	
	HL.Ind_Fv.Fm_L2	CL.Ind_Fv.Fm_L2	
	HL.Ind_Fv.Fm_Lss	CL.Ind_Fv.Fm_Lss	
	HL.Ind_QY_L1	CL.Ind_QY_L1	
	HL.Ind_QY_L2	CL.Ind_QY_L2	
	HL.Ind_QY_Lss	CL.Ind_QY_Lss	
	HL.Ind_NPQ_L1	CL.Ind_NPQ_L1	
	HL.Ind_NPQ_L2	CL.Ind_NPQ_L2	
	HL.Ind_NPQ_Lss	CL.Ind_NPQ_Lss	
	HL.Ind_qN_L1	CL.Ind_qN_L1	
	HL.Ind_qN_L2	CL.Ind_qN_L2	
	HL.Ind_qN_Lss	CL.Ind_qN_Lss	
	HL.Ind_qP_L1	CL.Ind_qP_L1	
	HL.Ind_qP_L2	CL.Ind_qP_L2	
	HL.Ind_qP_Lss	CL.Ind_qP_Lss	
	HL.Ind_qL_L1	CL.Ind_qL_L1	
	HL.Ind_qL_L2	CL.Ind_qL_L2	
	HL.Ind_qL_Lss	CL.Ind_qL_Lss	
	HL.Ind_Rfd_L1	CL.Ind_Rfd_L1	
	HL.Ind_Rfd_L2	CL.Ind_Rfd_L2	
	HL.Ind_Rfd_Lss	CL.Ind_Rfd_Lss	

Table 2: Group assignment(1/2) of all recorded traits. Column names indicate the respective group, while entries are the assigned traits.

CC	VNIR	IR	SW	H
ChlCont_FRF_G	PRI.avg	Temp.avg	Weight	FW
ChlCont_RF_Gcorr	NDVI.avg	deltaT	Weight.After.Watering	DW
ChlCont_SFR_G	PSRI.avg			FWDWratio
ChlCont_FRF_R	OSAVI.avg			
ChlCont_RF_Rcorr	SIP1.avg			
ChlCont_SFR_R	MCARI1.avg			

Table 3: Chi^2-test for homogeneous distribution. Tests the distribution of the set of associated SNP across all chromosomes. The alternative hypothesis is that there is no difference in number of associated SNP between chromosomes.

Trait Group	p-value	Number of associated SNP
HL.LL	0.0667	387
CL	7.87e-05	522
RGB	0.892	687
SW	7.47e-13	222
TCI	1.04e-07	139
HL	0.0424	604
CC	0.272	83
VNIR	0.933	127
H	0.737	17

Table 4: Improvement by implementing MFE Paired t-test results of changes in prediction accuracy between models with and without marker fixed effects.

Trait	Dat	Model	Statistic	p_value
RGB1_Plant_Avg_HEIGHT_MM	14	GBLUP	-18.347	1.28e-33
RGB1_Plant_Avg_HEIGHT_MM	14	HBLUP	-22.142	3.95e-40
RGB1_Plant_Avg_HEIGHT_MM	14	G_HBLUP	-20.028	1.35e-36
RGB1_Plant_Avg_HEIGHT_MM	14	MegaLMM	-1.665	0.099
VNIR_Plant_NDVI.avg	14	GBLUP	-11.979	5.69e-21
VNIR_Plant_NDVI.avg	14	HBLUP	-8.096	1.49e-12
VNIR_Plant_NDVI.avg	14	G_HBLUP	-9.357	2.76e-15
VNIR_Plant_NDVI.avg	14	MegaLMM	-3.485	0.000736
SC_Plant_Weight	14	GBLUP	-10.214	3.74e-17
SC_Plant_Weight	14	HBLUP	-12.448	4.33e-19
SC_Plant_Weight	14	G_HBLUP	-9.771	3.46e-16
SC_Plant_Weight	14	MegaLMM	-11.078	4.94e-19
RGB1_Plant_Avg_HEIGHT_MM	21	GBLUP	-21.457	5.19e-39
RGB1_Plant_Avg_HEIGHT_MM	21	HBLUP	-29.466	8.42e-51
RGB1_Plant_Avg_HEIGHT_MM	21	G_HBLUP	-20.872	4.91e-38
RGB1_Plant_Avg_HEIGHT_MM	21	MegaLMM	-12.019	4.67e-21
VNIR_Plant_NDVI.avg	21	GBLUP	-14.629	1.73e-26
VNIR_Plant_NDVI.avg	21	HBLUP	-6.415	4.86e-09
VNIR_Plant_NDVI.avg	21	G_HBLUP	-7.324	6.54e-11
VNIR_Plant_NDVI.avg	21	MegaLMM	-19.803	3.31e-36
SC_Plant_Weight	21	GBLUP	-12.999	1.71e-16
SC_Plant_Weight	21	HBLUP	-4.573	1.39e-05
SC_Plant_Weight	21	G_HBLUP	-4.091	8.75e-05
SC_Plant_Weight	21	MegaLMM	-20.112	9.65e-37
RGB1_Plant_Avg_HEIGHT_MM	28	GBLUP	-24.012	4.49e-43
RGB1_Plant_Avg_HEIGHT_MM	28	HBLUP	-20.946	3.69e-38
RGB1_Plant_Avg_HEIGHT_MM	28	G_HBLUP	-21.946	8.19e-40
RGB1_Plant_Avg_HEIGHT_MM	28	MegaLMM	-13.872	6.04e-25
VNIR_Plant_NDVI.avg	28	GBLUP	-2.838	0.0055
VNIR_Plant_NDVI.avg	28	HBLUP	1.490	0.139
VNIR_Plant_NDVI.avg	28	G_HBLUP	0.053	0.958
VNIR_Plant_NDVI.avg	28	MegaLMM	-3.945	0.000149
SC_Plant_Weight	28	GBLUP	-0.006	0.995
SC_Plant_Weight	28	HBLUP	-0.969	0.335
SC_Plant_Weight	28	G_HBLUP	-0.889	0.376
SC_Plant_Weight	28	MegaLMM	1.468	0.145
RGB1_Plant_Avg_HEIGHT_MM	35	GBLUP	-21.578	3.28e-39
RGB1_Plant_Avg_HEIGHT_MM	35	HBLUP	-19.977	1.65e-36
RGB1_Plant_Avg_HEIGHT_MM	35	G_HBLUP	-18.650	3.61e-34
RGB1_Plant_Avg_HEIGHT_MM	35	MegaLMM	-12.573	3.1e-22
VNIR_Plant_NDVI.avg	35	GBLUP	-18.714	2.78e-34
VNIR_Plant_NDVI.avg	35	HBLUP	-5.008	2.4e-06
VNIR_Plant_NDVI.avg	35	G_HBLUP	-8.594	1.26e-13
VNIR_Plant_NDVI.avg	35	MegaLMM	-9.101	1e-14
SC_Plant_Weight	35	GBLUP	1.149	0.256
SC_Plant_Weight	35	HBLUP	0.546	0.586
SC_Plant_Weight	35	G_HBLUP	0.629	0.531
SC_Plant_Weight	35	MegaLMM	1.205	0.231
RGB1_Plant_Avg_HEIGHT_MM	42	GBLUP	-22.622	6.66e-41

Trait	Dat	Model	Statistic	p_value
RGB1_Plant_Avg_HEIGHT_MM	42	HBLUP	-21.907	9.5e-40
RGB1_Plant_Avg_HEIGHT_MM	42	G_HBLUP	-19.493	1.15e-35
RGB1_Plant_Avg_HEIGHT_MM	42	MegaLMM	-9.705	4.82e-16
VNIR_Plant_NDVI.avg	42	GBLUP	-13.813	7.99e-25
VNIR_Plant_NDVI.avg	42	HBLUP	-3.972	0.000135
VNIR_Plant_NDVI.avg	42	G_HBLUP	-3.924	0.000161
VNIR_Plant_NDVI.avg	42	MegaLMM	-6.207	1.27e-08
SC_Plant_Weight	42	GBLUP	5.059	1.34e-05
SC_Plant_Weight	42	HBLUP	-1.132	0.26
SC_Plant_Weight	42	G_HBLUP	-0.243	0.809
SC_Plant_Weight	42	MegaLMM	2.678	0.00868

Table 5: Trait- and time point-specific influential markers. Relative effect size of most influential markers for each time point and trait.

Trait	DAT	Chromosome	Position	Relative effect size	p-value
Plant height	14	4	603676865	-0.76 ± 0.029	7.80e-15
Plant height	21	2	462299201	0.67 ± 0.109	3.41e-13
Plant height	28	3	539544166	-0.33 ± 0.058	2.85e-03
Plant height	35	7	370020277	0.26 ± 0.049	2.50e-01
Plant height	42	2	462299201	0.55 ± 0.147	8.74e-11
NDVI-score	14	3	617851427	1.42 ± 1.155	4.64e-18
NDVI-score	21	3	563926632 - 563926908	0.29 ± 0.105	5.86e-02
NDVI-score	28	5	581820381	-0.45 ± 0.083	4.69e-07
NDVI-score	35	1	347256694	-0.45 ± 0.057	3.77e-07
NDVI-score	42	2	657275399	-0.96 ± 0.567	5.41e-17
Plant weight	14	6	483571436	0.86 ± 0.063	5.33e-16
Plant weight	21	1	348245457	0.52 ± 0.003	1.46e-09
Plant weight	28	4	64884408	1.76 ± 0.623	4.23e-18
Plant weight	42	2	210159676	0.11 ± 0.799	1.00e+00

Table 6: Fixed effect coefficient averages across models. In the case of linear dependence between SNP the position of the MFE is written as nr(POS):min(POS)-max(POS)

Chromosome	Position	Trait	DAT	Avg. effect size	SD effect size
1	9:128611549 - 140895082	Plant height	14	0.0370	0.082
1	8:128611549 - 140895082	Plant height	14	-0.8600	11.000
1	134409984	Plant height	14	0.8600	11.000
1	134410435	Plant height	14	0.1200	0.098
1	363153663	Plant height	14	0.0850	0.046
2	56835696	Plant height	14	0.1100	0.070
2	56835854	Plant height	14	0.2100	0.072
4	424886468	Plant height	14	0.1500	0.034
4	603676865	Plant height	14	-0.7600	0.057
7	175300725	Plant height	14	-0.4100	0.063
1	128611549	Plant height	21	0.3100	0.093
2	462299201	Plant height	21	0.7000	0.210
2	56835854	Plant height	21	0.2700	0.074
2	605605659	Plant height	21	0.1900	0.037
3	3468738	Plant height	21	-0.4800	0.150
3	559836151	Plant height	21	-0.4700	0.060
4	406737028	Plant height	21	0.3900	0.150
1	476745338	Plant height	28	0.2400	0.043
2	278063816	Plant height	28	0.2600	0.043
2	462299201	Plant height	28	0.5100	0.150
2	53653197	Plant height	28	0.3400	0.065
2	589285600	Plant height	28	0.2200	0.043
2	56835854	Plant height	28	0.2400	0.061
3	539544166	Plant height	28	-0.3600	0.075
3	585751509	Plant height	28	0.1300	0.043
3	62069228	Plant height	28	0.2200	0.044
7	15066593	Plant height	28	0.2700	0.061
7	370020277	Plant height	28	0.3300	0.039
1	476745338	Plant height	35	0.2000	0.044
2	278063816	Plant height	35	0.2900	0.070
2	429379061	Plant height	35	0.1400	0.061
2	462299201	Plant height	35	0.4300	0.250
2	56835854	Plant height	35	0.2000	0.073
2	631074842	Plant height	35	0.2200	0.069
7	15066593	Plant height	35	0.2200	0.067
7	370020277	Plant height	35	0.2800	0.058
1	395860012	Plant height	42	-0.2600	0.043
1	476745338	Plant height	42	0.2500	0.030
2	151507496	Plant height	42	0.1300	0.029
2	309338682	Plant height	42	0.2300	0.043
2	462299201	Plant height	42	0.5700	0.150
2	550482269	Plant height	42	0.1700	0.040
2	56835854	Plant height	42	0.2100	0.036
2	620540722	Plant height	42	0.1600	0.036
2	631074842	Plant height	42	0.3000	0.043
7	15066593	Plant height	42	0.2400	0.059
7	370020277	Plant height	42	0.3800	0.053
1	3:361593490 - 363154334	Plant weight	14	-0.4000	0.059
4	430727396	Plant weight	14	0.2800	0.075

Chromosome	Position	Trait	DAT	Avg. effect size	SD effect size
6	483571436	Plant weight	14	0.4000	0.057
1	348245457	Plant weight	21	0.7000	0.110
4	3:112440916 - 127406250	Plant weight	28	0.2100	0.860
4	4:66875798 - 127406250	Plant weight	28	-0.1700	0.091
4	3:132679529 - 135659099	Plant weight	28	-0.2700	0.650
4	64884408	Plant weight	28	0.5200	2.900
4	2:64884408 - 66875798	Plant weight	28	0.2700	0.100
4	66875798	Plant weight	28	-0.2300	3.300
2	210159676	Plant weight	42	0.0021	0.054
1	496710773	NDVI	14	-0.1900	0.130
2	650852302	NDVI	14	0.1700	0.085
3	503169955	NDVI	14	-0.1600	0.130
3	617851427	NDVI	14	0.2100	0.160
5	377686445	NDVI	14	-0.2800	0.110
7	455108620	NDVI	14	0.1100	0.072
1	48317122	NDVI	21	0.1100	0.094
1	51221636	NDVI	21	0.0850	0.200
2	80232245	NDVI	21	0.0990	0.130
3	51800478	NDVI	21	-0.0790	0.095
3	2:563926632 - 563926908	NDVI	21	0.2900	0.100
4	92086066	NDVI	21	0.1500	0.190
5	258309983	NDVI	21	0.1100	0.190
5	548720813	NDVI	21	0.2300	0.130
5	552997447	NDVI	21	-0.0630	0.067
6	539994614	NDVI	21	-0.1100	0.150
7	156649522	NDVI	21	-0.1800	0.099
1	331407118	NDVI	28	-0.1900	0.180
2	631512943	NDVI	28	0.1200	0.160
2	656785598	NDVI	28	0.0590	0.084
5	581820381	NDVI	28	-0.1800	0.120
5	60186708	NDVI	28	-0.0960	0.110
7	609303563	NDVI	28	-0.1100	0.120
1	329646879	NDVI	35	0.1300	0.087
1	347256694	NDVI	35	-0.3200	0.230
2	110518829	NDVI	35	0.1200	0.110
2	25384315	NDVI	35	-0.0960	0.065
2	511828192	NDVI	35	-0.2300	0.150
4	9957163	NDVI	35	-0.1500	0.120
4	532153356	NDVI	35	0.1700	0.099
5	499522580	NDVI	35	-0.0660	0.100
5	60186708	NDVI	35	-0.1200	0.100
6	154022486	NDVI	35	-0.1200	0.069
7	491194205	NDVI	35	-0.1200	0.088
1	347256694	NDVI	42	-0.3000	0.240
2	657275399	NDVI	42	-0.2500	0.260
4	532153356	NDVI	42	0.1700	0.100
4	596783225	NDVI	42	0.0010	0.130
5	258309983	NDVI	42	0.1700	0.150
5	501842475	NDVI	42	0.1600	0.130
5	60186708	NDVI	42	-0.0510	0.079

Supplementary Section 1: MegaLMM parameterization

```

library(MegaLMM)
run_parameters = MegaLMM_control(
  h2_divisions = 20,
  # Each variance component is allowed to explain between 0% and 100% of the
  # total variation. How many segments should the range [0,100) be divided
  # into for each random effect?
  burn = 1000,
  # number of burn in samples before saving posterior samples.
  thin = 2, #,
  # during sampling, we'll save every 2nd sample to the posterior database.
  K = 100 # number of factors.
)
Lambda_prior = list(
  sampler = sample_Lambda_prec_horseshoe,
  # function that implements the horseshoe-based Lambda prior
  # described in Runcie et al 2020.
  #See code to see requirements for this function.
  # other options are:
  # ?sample_Lambda_prec_ARD,
  # ?sample_Lambda_prec_BayesC
  prop_0 = 0.1,
  # prior guess at the number of non-zero loadings in the first and most important factor
  delta = list(shape = 3, scale = 1),
  # parameters of the gamma distribution giving the expected change
  # in proportion of non-zero loadings in each consecutive factor
  delta_iterations_factor = 100
  # parameter that affects mixing of the MCMC sampler. This value is generally fine.
)
priors = MegaLMM_priors(
  tot_Y_var = list(V = 0.5, nu = 5),
  # Prior variance of trait residuals after accounting for fixed effects and factors
  # See MCMCglmm for meaning of V and nu
  tot_F_var = list(V = 18/20, nu = 20),
  # Prior variance of factor traits. This is included to improve MCMC mixing,
  # but can be turned off by setting nu very large
  h2_priors_resids_fun = function(h2s,n) 1,
  # Function that returns the prior density for any value of the h2s vector
  # (ie the vector of random effect proportional variances across all random effects.
  # 1 means constant prior.
  # n is the number of h2 divisions above (here=20)
  # 1-n*sum(h2s)/n linearly interpolates between 1 and 0,
  # giving more weight to lower values
  h2_priors_factors_fun = function(h2s,n) 1,
  # See above.
  # sum(h2s) linearly interpolates between 0 and 1,
  # giving more weight to higher values
  # Another choice is one that gives 50% weight to h2==0: ifelse(h2s == 0,n,n/(n-1))
  Lambda_prior = Lambda_prior
  # from above
)

```