

Table S10 Comparison of Genomic Prediction Methods for 24 Grain Carotenoid Traits using Three Marker Sets as Predictors

		Carotenoid QTL-Targeted Prediction			Pathway-Level Prediction			Genome-Wide Prediction			
	Trait	Heritability	RR-BLUP <sup>a</sup>	LASSO <sup>b</sup>	eNet <sup>c</sup>	RR-BLUP	LASSO	eNet	RR-BLUP	LASSO	eNet
15 priority traits	Lutein	0.94	0.582 (0.039)	0.534 (0.091)	0.516 (0.117)	0.461 (0.185)	0.514 (0.163)	0.521 (0.160)	0.509 (0.204)	0.476 (0.157)	0.471 (0.156)
	Zeinoxanthin	0.88	0.443 (0.166)	0.451 (0.099)	0.488 (0.051)	0.427 (0.136)	0.512 (0.070)	0.520 (0.075)	0.442 (0.172)	0.549 (0.085)	0.560 (0.082)
	$\alpha$ -Carotene	0.25	0.65 (0.338)	0.212 (0.206) <sup>d</sup>	0.187 (0.198)	0.676 (0.238)	0.111 (0.582) <sup>d</sup>	0.030 (0.025) <sup>d</sup>	0.769 (0.282)	0.500 (0.289)	0.374 (0.200)
	$\alpha$ -Carotene/Zeinoxanthin	0.9	0.443 (0.155)	0.576 (0.153)	0.561 (0.13)	0.462 (0.118)	0.470 (0.199)	0.451 (0.199)	0.411 (0.110)	0.589 (0.200)	0.590 (0.193)
	Zeinoxanthin/Lutein	0.89	0.467 (0.11)	0.483 (0.121)	0.487 (0.121)	0.393 (0.233)	0.457 (0.183)	0.502 (0.187)	0.387 (0.243)	0.363 (0.266)	0.350 (0.241)
	Zeaxanthin	0.94	0.566 (0.076)	0.619 (0.078)	0.611 (0.079)	0.433 (0.223)	0.516 (0.127)	0.544 (0.134)	0.346 (0.278)	0.519 (0.132)	0.512 (0.170)
	$\beta$ -Cryptoxanthin	0.95	0.49 (0.137)	0.3 (0.107)	0.316 (0.132)	0.501 (0.190)	0.441 (0.194)	0.434 (0.190)	0.464 (0.144)	0.530 (0.104)	0.478 (0.111)
	$\beta$ -Carotene	0.82	0.282 (0.205)	0.168 (0.191)	0.169 (0.167)	0.336 (0.127)	0.159 (0.180)	0.166 (0.167)	0.254 (0.123)	0.152 (0.101)	0.185 (0.062) <sup>d</sup>
	$\beta$ -Cryptoxanthin/Zeaxanthin	0.9	0.372 (0.188)	0.358 (0.134)	0.377 (0.119)	0.388 (0.184)	0.339 (0.074)	0.314 (0.155)	0.384 (0.185)	0.215 (0.193)	0.243 (0.127) <sup>d</sup>
	$\beta$ -Carotene/ $\beta$ -Cryptoxanthin	0.89	0.351 (0.098)	0.312 (0.101)	0.317 (0.126)	0.399 (0.110)	0.434 (0.095)	0.444 (0.100)	0.402 (0.065)	0.455 (0.116)	0.444 (0.064)
	Total Carotenoids	0.91	0.367 (0.151)	0.228 (0.015) <sup>d</sup>	0.19 (0.072) <sup>d</sup>	0.267 (0.208)	0.336 (0.186)	0.358 (0.152)	0.191 (0.228)	0.065 (0.170) <sup>d</sup>	0.084 (0.160) <sup>d</sup>
	Ayclic and Monocyclic Carotenes	0.57	0.342 (0.199)	0.242 (0.247)	0.224 (0.254)	0.456 (0.153)	0.328 (0.395)	0.331 (0.397)	0.407 (0.126)	0.384 (0.173)	0.389 (0.175)
	$\beta$ -Xanthophylls/ $\alpha$ -Xanthophylls	0.83	0.716 (0.073)	0.717 (0.056)	0.719 (0.042)	0.663 (0.166)	0.774 (0.101)	0.779 (0.108)	0.587 (0.237)	0.732 (0.187)	0.736 (0.195)
	Provitamin A	0.8	0.325 (0.158)	0.352 (0.182)	0.335 (0.062) <sup>d</sup>	0.434 (0.142)	0.293 (0.161)	0.292 (0.093)	0.390 (0.147)	0.328 (0.116) <sup>d</sup>	0.330 (0.115) <sup>d</sup>
	$\beta$ -Carotenoids/ $\alpha$ -Carotenoids	0.98	0.566 (0.076)	0.615 (0.056)	0.617 (0.058)	0.535 (0.161)	0.586 (0.176)	0.598 (0.152)	0.555 (0.192)	0.610 (0.101)	0.605 (0.107)
9 additional traits	$\zeta$ -Carotene	0.45	0.346 (0.073)	0.409 (0.2)	0.385 (0.241)	0.457 (0.247)	0.431 (0.111)	0.447 (0.123)	0.465 (0.205)	0.469 (0.124)	0.431 (0.111)
	Phytofluene	0.65	0.358 (0.273)	0.283 (0.16)	0.262 (0.161)	0.549 (0.150)	0.499 (0.185)	0.494 (0.182)	0.497 (0.149)	0.397 (0.086)	0.499 (0.185)
	Tetrahydrolycopene	0.6	0.369 (0.122)	0.197 (0.096)	0.208 (0.102)	0.522 (0.148)	0.451 (0.154)	0.463 (0.162)	0.541 (0.151)	0.682 (0.132)	0.451 (0.154)
	Total $\beta$ -Xanthophylls	0.96	0.41 (0.135)	0.446 (0.086)	0.449 (0.097)	0.396 (0.251)	0.554 (0.158)	0.559 (0.188)	0.313 (0.287)	0.428 (0.204)	0.554 (0.158)
	Total $\alpha$ -Xanthophylls	0.91	0.546 (0.09)	0.51 (0.102)	0.503 (0.107)	0.400 (0.210)	0.540 (0.119)	0.542 (0.120)	0.479 (0.226)	0.455 (0.159)	0.540 (0.119)
	Provitamin A/Total Carotenoids	0.86	0.335 (0.224)	0.281 (0.272)	0.275 (0.271)	0.286 (0.124)	-0.101 (0.17) <sup>d</sup>	-0.031 (0.15) <sup>d</sup>	0.321 (0.089)	-0.054 (0.119) <sup>d</sup>	0.065 (0.259) <sup>d</sup>
	$\beta$ -Carotene/( $\beta$ -Cryptoxanthin+Zeaxanthin)	0.93	0.308 (0.221)	0.428 (0.12)	0.411 (0.146)	0.251 (0.182)	0.361 (0.118)	0.355 (0.111)	0.290 (0.148)	0.396 (0.095)	0.361 (0.118)
	Ayclic Carotenes/Cyclic Carotenes	0.74	0.149 (0.106)	0.142 (0.09) <sup>d</sup>	0.221 (0.083) <sup>d</sup>	0.577 (0.155)	0.729 (0.150)	0.734 (0.156)	0.565 (0.219)	0.743 (0.198)	0.729 (0.150)
	Total Carotenes/Total Xanthophylls	0.62	0.286 (0.367)	0.378 (0.28)	0.376 (0.273)	0.351 (0.088)	0.327 (0.098) <sup>d</sup>	0.310 (0.093) <sup>d</sup>	0.294 (0.059)	0.291 (0.121)	0.327 (0.098) <sup>d</sup>

The three marker sets tested were carotenoid quantitative trait loci (QTL)-targeted prediction (the 944 SNP markers and 7 indels within  $\pm$  250 kb of 8 *a priori* candidate genes), pathway-level prediction (the 7,408 SNP markers and 7 indels within  $\pm$  250 kb of 58 *a priori* candidate genes,) and genome-wide prediction (all 284,180 SNP markers and 7 indels used in our genome-wide association studies). Standardized average correlations resulting from the 5-fold cross-validation are reported, with standardized standard deviations in parentheses. Standardization was conducted as follows: Raw correlations were divided by the square root of a trait's broad-sense heritability to obtain standardized average correlations, also called prediction accuracy. Raw standard deviations were squared to obtain variance, divided by heritability, and the square root was taken to obtain standardized standard deviation.

<sup>a</sup>RR-BLUP, Ridge Regression Best Linear Unbiased Prediction

<sup>b</sup>LASSO, Least Absolute Shrinkage and Selection Operator

<sup>c</sup>eNet, Elastic net

<sup>d</sup>indicates that no markers were selected in one or two of the five folds, or in three of the five folds in one case ( $\alpha$ -Carotene, Pathway-Level Prediction, eNet)