

Online Resource 2

Additional comparisons and Pareto uncertainty

Breeding forage sorghum for biomass productivity and reduced early-stage cyanogenic potential: Pareto analysis and HCN-constrained ranking across two rainy seasons

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S1. Interpretation and confidence construction

The six-member nominal GFY–HCN-P frontier is a point-estimate description. A separate conservative candidate set uses approximate model-based simultaneous 95% confidence intervals over all 990 hybrid pairs and three traits (2,970 comparisons). A hybrid is excluded only when another has supported greater GFY and lower HCN-P in both simultaneous contrasts. Fourteen hybrids were excluded and 31 retained. Retention means that domination was not demonstrated; it does not establish Pareto optimality or predict a new environment.

For a difference of means, $SE = \sqrt{(2M/6)}$. The GFY and DFY comparisons use hybrid $\times$ season mean squares (44 df); HCN-P uses the residual mean square (176 df) after constraining its negative interaction component to zero. The nominal critical value is $t(.975, df)$, and the simultaneous value is $t[1 - .05/(2 \times 2970), df]$. The respective simultaneous half-widths are 15.641 kg plot⁻¹, 4.829 kg plot⁻¹ and 19.498 ppm. Common season and block intercepts cancel in pairwise differences. The family spans all hybrids to protect comparisons selected after viewing ranks. Raw-scale variance assumptions and the limited two-season archive remain limitations.

The exact hierarchical enumeration has 400 weighted configurations, with all hybrids and paired traits preserved within sampled blocks. Its frequencies have no Monte Carlo sampling error, but they are not calibrated population probabilities. Pareto-layer ranks are obtained by successively removing each non-dominated layer; layer 1 is the frontier. Yield-rank intervals at each HCN-P ceiling are conditional on eligibility and must be read with the eligibility frequency.

Table S1. Nominal frontier members and empirical Pareto-layer intervals

Code	Hybrid	Front frequency (%)	Layer interval ¹	Model set ²
L6×T1	MR750A ₂ × SSG59-3	76.2	1–2	Retained
L6×T3	MR750A ₂ × Pusa Chari 23	99.9	1–1	Retained
L6×T5	MR750A ₂ × UPMC503	32.7	1–3	Retained
L7×T5	A3N191 × UPMC503	100.0	1–1	Retained
L8×T5	A3N193 × UPMC503	98.9	1–1	Retained
L9×T1	A3N213 × SSG59-3	53.4	1–2	Retained

¹ Weighted 2.5th–97.5th empirical percentiles, not population confidence intervals. ² All six belong to the 31-hybrid conservative candidate set; this is distinct from proven optimality. Full 45-hybrid records are in pareto_confidence_and_rank.csv in Online Resource 1.

S2. Pairwise evidence for selected screening comparisons

Table S2 gives selected examples from the complete protected family. Differences are first code minus second code. GFY and DFY are kg plot⁻¹, HCN-P is ppm. Negative and positive bounds are not clipped. Full results, standard errors, degrees of freedom and adjusted P values are supplied in all_pairwise_contrasts.csv.

Contrast	Trait	Difference	Nominal 95% CI	Simultaneous 95% CI	Adjusted P
L8×T5 – L9×T5	GFY	2.800	-3.73, 9.33	-12.84, 18.44	1.000
L8×T5 – L9×T3	DFY	-0.038	-2.05, 1.98	-4.87, 4.79	1.000
L6×T3 – L8×T5	GFY	5.487	-1.04, 12.01	-10.15, 21.13	1.000
L6×T3 – L8×T5	HCN-P	38.934	30.24, 47.63	19.44, 58.43	<.001
L1×T2 – L8×T5	GFY	-16.133	-22.66, -9.61	-31.77, -0.49	0.030
L1×T2 – L8×T5	HCN-P	59.137	50.44, 67.83	39.64, 78.64	<.001

The first two comparisons do not support superiority of close point leaders. For L6×T3 versus L8×T5, HCN-P is demonstrably greater but GFY superiority is not established. The final pair illustrates a supported exclusion: L1×T2 has lower GFY and greater HCN-P than L8×T5, with both simultaneous intervals excluding zero. L1×T2 is therefore excluded from the candidate set.

At the first-quartile ceiling, the GFY point leader L8×T5 had a conditional empirical rank interval of 1–2, while the DFY point leader L9×T3 had an interval of 1–10 (median rank 2); both were eligible in all configurations. At the median ceiling, L6×T3 had a conditional GFY rank interval of 1–1 but was eligible in only 74.5% of configurations. Its DFY interval at the third-quartile ceiling was 1–5. These intervals show why eligibility, point rank and rank stability must be interpreted separately.

S3. Complete confidence-set membership and data boundary

Retained (31): L1×T1, L1×T3, L1×T5, L2×T1, L2×T2, L2×T3, L2×T5, L3×T2, L3×T3, L3×T4, L4×T1, L4×T3, L4×T4, L4×T5, L5×T1, L5×T5, L6×T1, L6×T3, L6×T4, L6×T5, L7×T3, L7×T4, L7×T5, L8×T1, L8×T3, L8×T4, L8×T5, L9×T1, L9×T3, L9×T4, L9×T5.

Excluded (14): L1×T2, L1×T4, L2×T4, L3×T1, L3×T5, L4×T2, L5×T2, L5×T3, L5×T4, L6×T2, L7×T1, L7×T2, L8×T2, L9×T2.

Names corresponding to every code and the demonstrated dominators for each excluded hybrid are given in pareto_confidence_and_rank.csv. Conditional yield-rank medians and intervals for all hybrids, ceilings and endpoints are given in conditional_screen_rank_intervals.csv. The main result files provide all hybrid means and conditional 95% intervals, season-specific means, diagnostics and fixed-season sensitivity frequencies.

The workbook audit compared 810 focal-trait cells in 270 records and found zero discrepancies. The identical DFY triplet for L7×T5 across seasons was retained unchanged: 6.669800204918032, 5.1095102505694765 and 7.80665 kg plot⁻¹. Original field/calculation sheets are needed to determine its provenance; this audit does not independently validate derived measurements.

Method reference: NIST/SEMATECH e-Handbook of Statistical Methods, “Bonferroni’s method”: <https://www.itl.nist.gov/div898/handbook/prc/section4/prc473.htm>. The simultaneous coverage interpretation depends on the validity of the component model intervals; the bootstrap percentile ranks are a separate empirical summary.