

Relative Affinity — Validation Summary

Evidence disclosure of how LatticeZero ranks the effect of molecular changes within a series.

Version 1.0

June 2026

Executive summary

LatticeZero's relative-affinity validation measures how well the engine **ranks** the effect of molecular changes within a series — the question that matters for lead optimization. The promoted product mode ranks lead-optimization changes with strong agreement to experiment (Spearman $\rho = 0.8144$). A separate **beta** mode is under evaluation on broader holdout panels and is reported separately. All panels and their scope are defined so beta numbers are never mistaken for the shipped product number.

Panels (public level)

Promoted product mode — the shipped production default for relative ranking, evaluated on blind lead-optimization targets. **Beta broad-holdout mode** — a separate beta mode under evaluation on broader holdout panels.

holdout_27 (exp_schrodinger_holdout) — a lead-optimization holdout panel; **it is not a PDBbind-relative panel.**

global_69 — a broader holdout panel used for the beta mode.

Results — promoted product mode [Production]

Metric	Value
Rank agreement (Spearman ρ)	0.8144

Results — beta broad-holdout mode [Beta]

Separate evaluation track. Not the promoted product mode.

Panel	Spearman ρ
holdout_27 (exp_schrodinger_holdout)	0.8091
global_69	0.7334

CAVEATS

holdout_27 is not a PDBbind-relative panel — it is a separate lead-optimization holdout. **Beta modes are evaluated separately** from the promoted product mode and should not be quoted as the shipped product number.

Status

Production: the promoted relative product mode is the shipped default ($\rho = 0.8144$). **Beta:** the broad-holdout mode is under evaluation and clearly labeled beta.