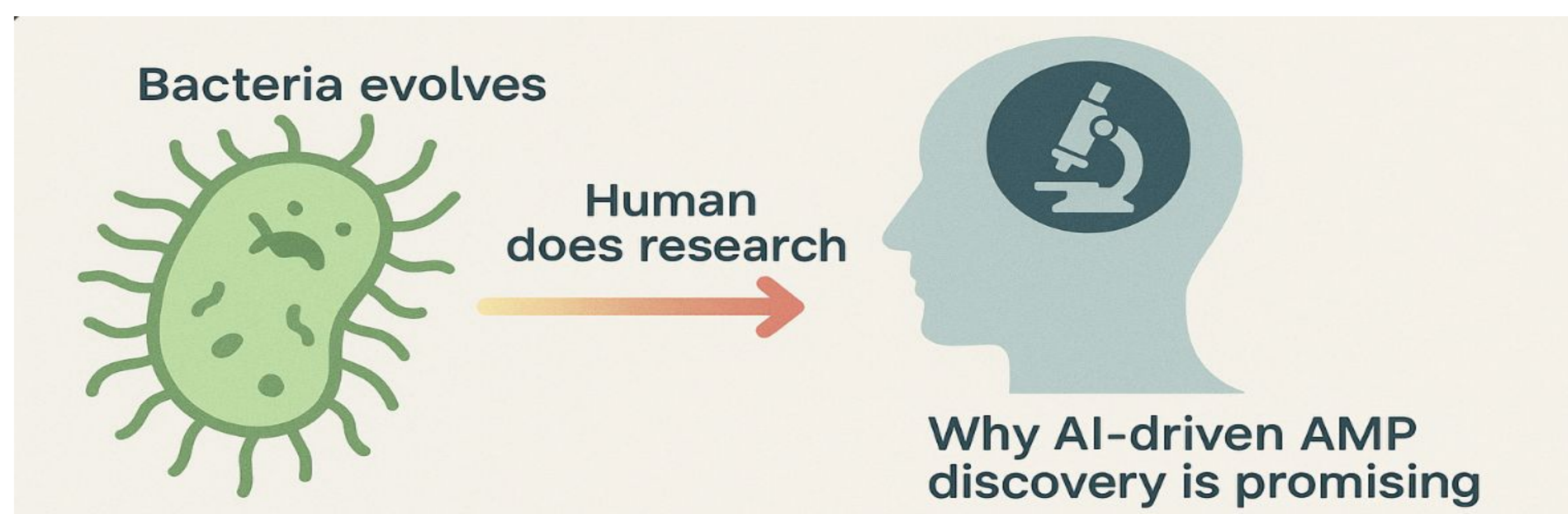


Design novel AMPs using Optimized Binder Design methods

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Motivation

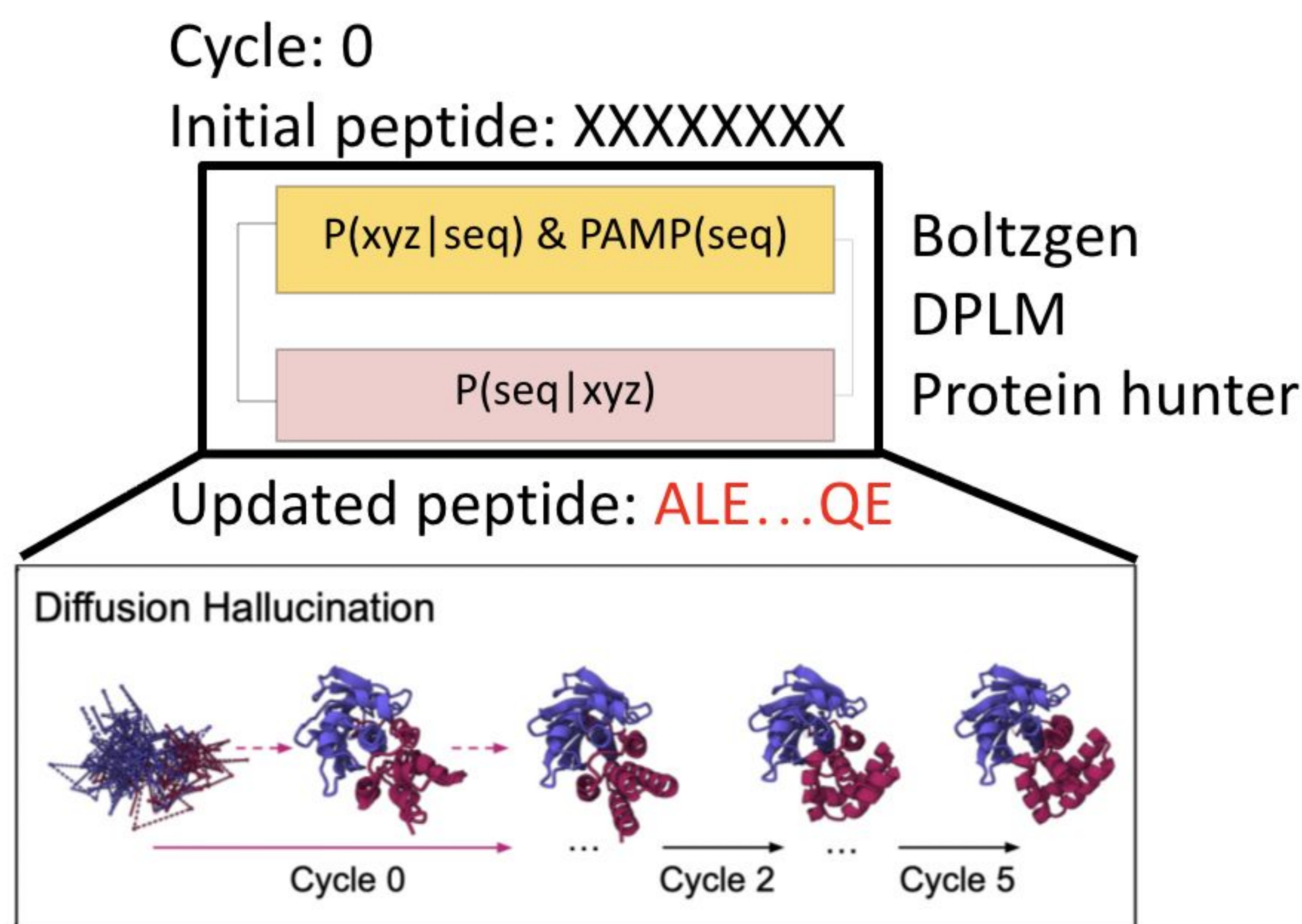
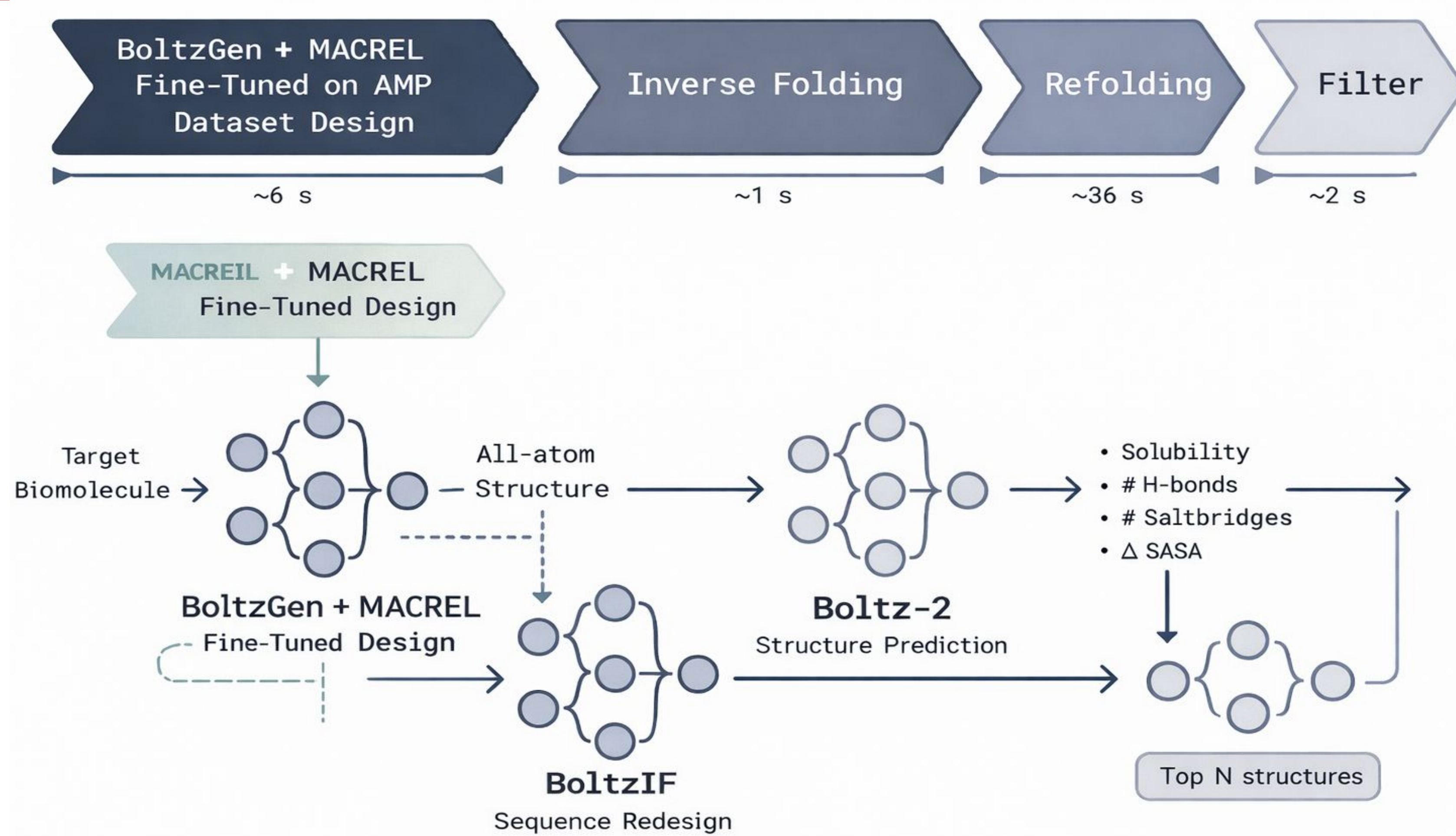
Antimicrobial resistance (AMR) poses a critical global health threat, demanding rapid discovery of novel antimicrobial peptides (AMPs).



Key Mission

Antimicrobial peptides (AMPs) are a promising alternative to conventional antibiotics due to their broad-spectrum activity, rapid mechanism of action, and lower propensity for inducing resistance. As antimicrobial resistance (AMR) continues to threaten global health, the discovery and design of novel AMPs has become increasingly important. In this work, we focus on two biologically relevant targets derived from **antimicrobial resistance genes**, aiming to design effective AMP candidates using AI-driven generative models. The designed peptides are currently in the **activity testing stage**, where their antimicrobial efficacy is being experimentally evaluated.

Method



Evaluation

Method	Instability	Charge	Isoelectric Point	Hydrophobic Ratio	Aromaticity	Boman Index	TM_tend
bg_hall	22.94	-1.46	5.39	0.48	0.01	0.47	-0.33
bg_binder	45.11	-1.40	5.38	0.35	0.02	1.32	-0.58
hf_hall	40.60	-1.07	5.86	0.35	0.03	1.19	-0.51
random	43.66	0.15	7.20	0.35	0.15	1.60	-0.42

Table 1: Evaluation metrics across different design methods.

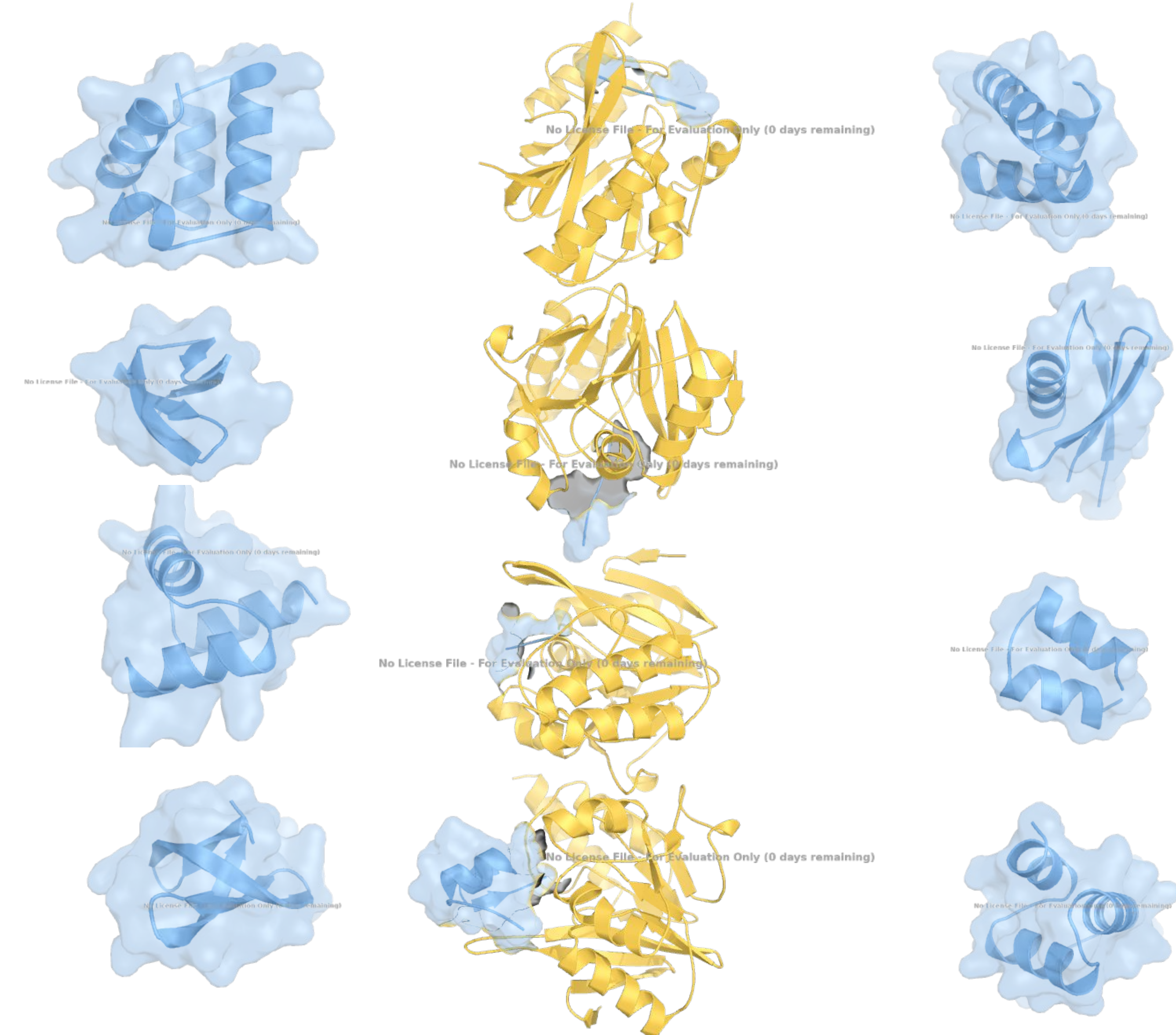
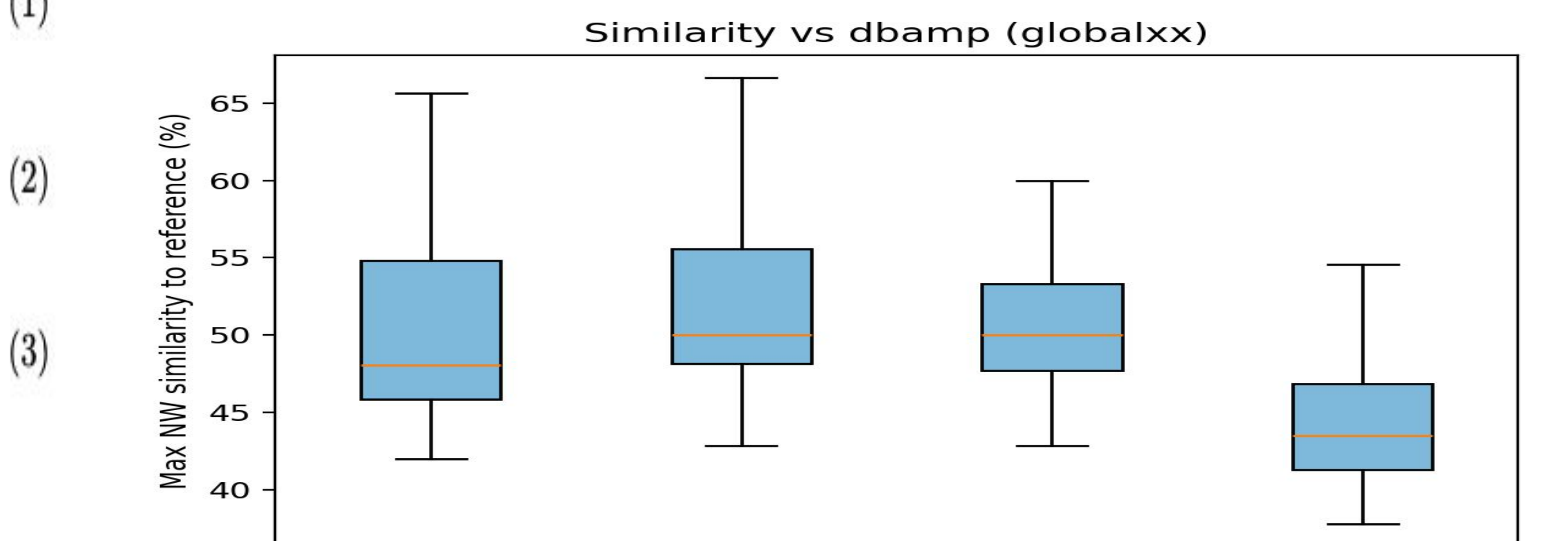
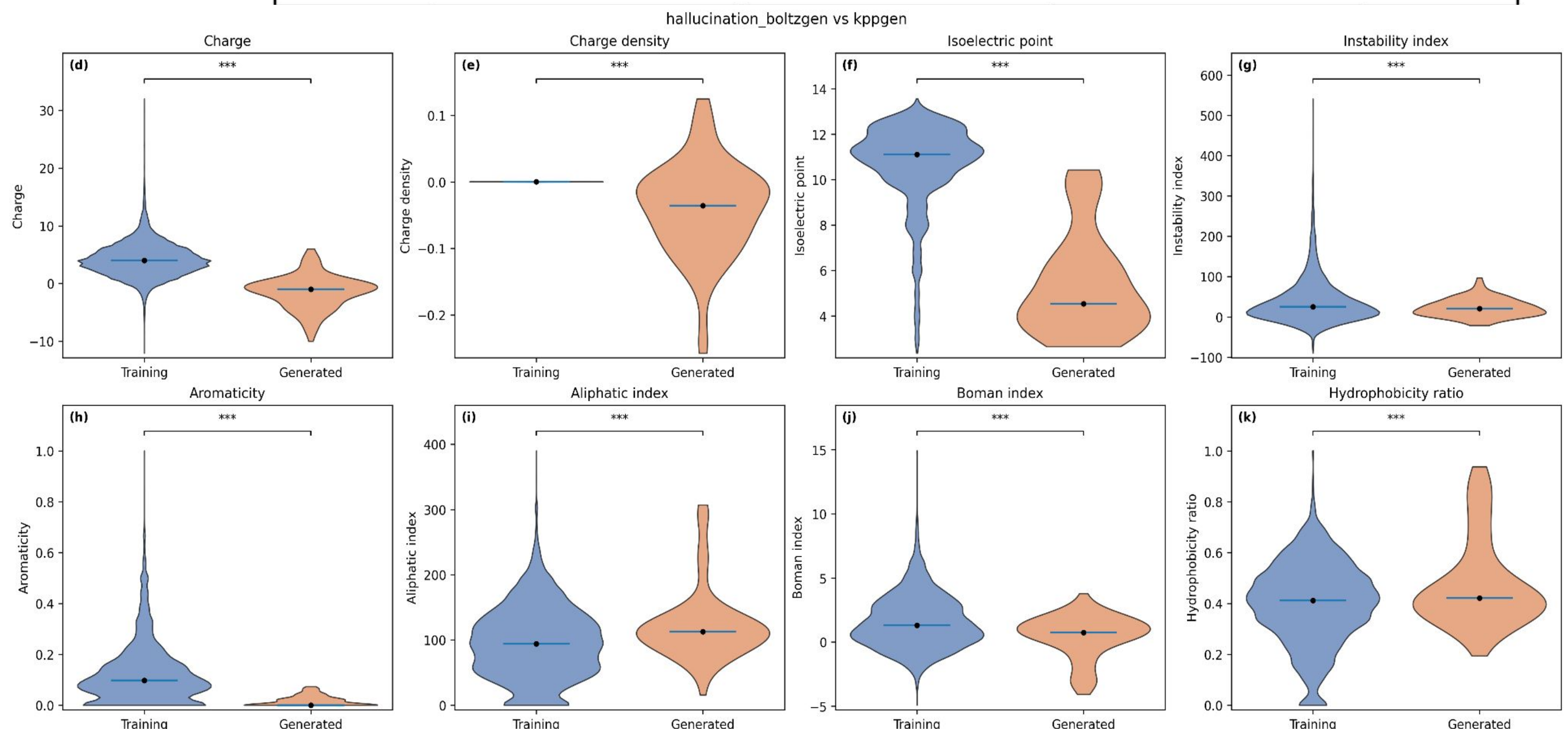
$$\mathcal{L}(\theta) = \mathbb{E}_{X \sim p_{\text{data}}, t \sim p_{\text{noise}}, \epsilon \sim \mathcal{N}} [\mathcal{L}_{\text{MSE}}(\theta; X, t, \epsilon) + \mathcal{L}_{\text{bond}}(\theta; X, t, \epsilon) + \mathcal{L}_{\text{smooth_IDDT}}(\theta; X, t, \epsilon) + \mathcal{L}_{\text{Macrel}}(\theta; X, t, \epsilon)] \quad (1)$$

$$\hat{X} = D_{\theta}(X + t\epsilon; t; z)$$

$$\mathcal{L}_{\text{MSE}}(\theta; X, t, \epsilon) = \frac{1}{3} \sum_l w_l \left\| \hat{X}_l - X_l^{\text{aligned}} \right\|_w^2$$

Results

Protein hunter hallucination Protein hunter hallucination Protein hunter hallucination



References

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