a

Peptide representation module

FIGKLISAASGLLSHL

Prototype

Encoder

Embedding space

Decoder

FIGKLSAASGLLSHC

Generated

Property evaluation module

AMP predictor

MIC predictor

Affinity predictor

Toxicity predictor

AMP landscape

MIC landscape

Affinity landscape

Toxicity landscape

Directed searching module

Low — High

Predicted value

$\nabla grad(z)$

Merged landscape

update the embedding using $\quad z_{t+1} = z_t - \alpha \cdot \nabla grad(z)$
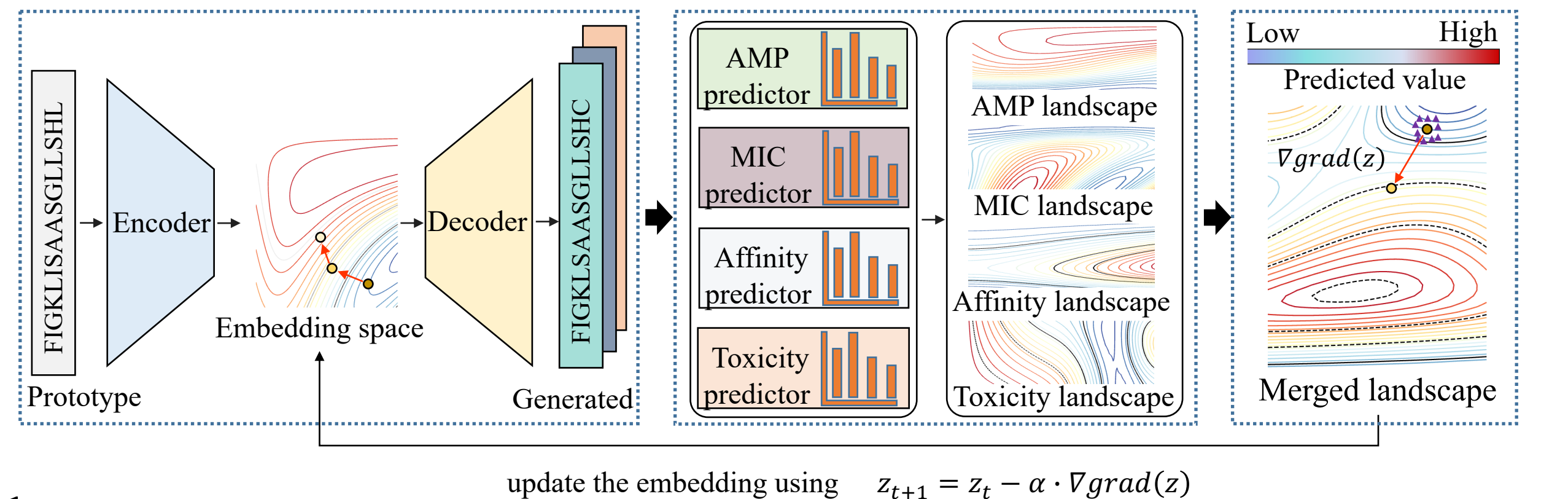
b

Task 1: Optimization of antimicrobial function and activity

Q R F S Q P T
M G L F D I V
G V F N A L T

prototype

case 1($P_{AMP} > 0.8$ and $P_{MIC} > 0.5$)

case 2($P_{AMP} > 0.8$ and $P_{MIC} \leq 0.5$)

case 3($P_{AMP} \leq 0.8$ or $P_{MIC} \leq 0.5$)

embedding

AMP direction

MIC direction

AMP and MIC optimized direction

Q R F S K P T
M G L G D E V
G K F R A L W
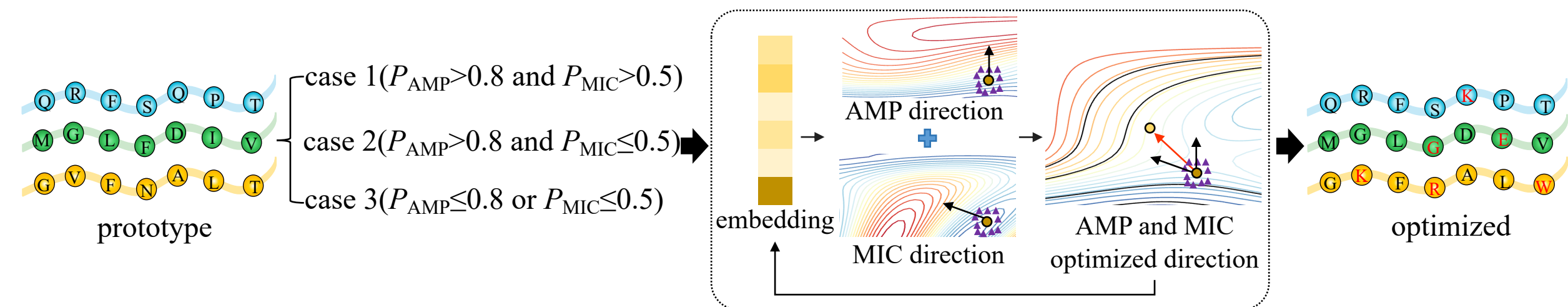
optimized

Task 2: Optimization of affinity and toxicity

SARS-CoV-2 binding target

Ligand

S protein

prototype

antiviral(low affinity and high toxicity)

embedding

Affinity direction

Toxicity direction

Affinity and Toxicity optimized direction

optimized