

Supporting Information

Mol-Zero-GAN: Zero-Shot Adaptation of Molecular Generative Adversarial Network for Specific Protein Targets

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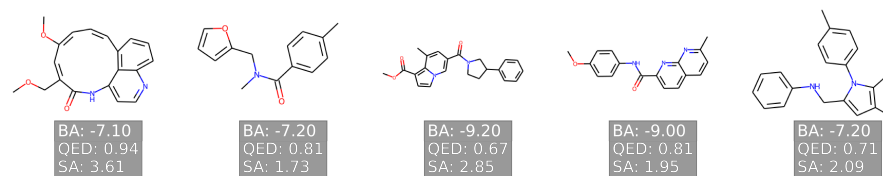


Figure S1: Example of generated molecules from the BA optimization model of *DRD3* protein.

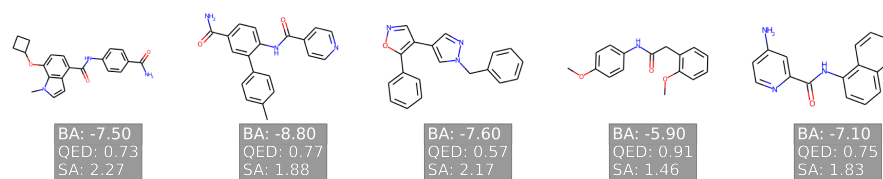


Figure S2: Example of generated molecules from the BA optimization model of *SARS – CoV – 2 M_{pro}* protein.

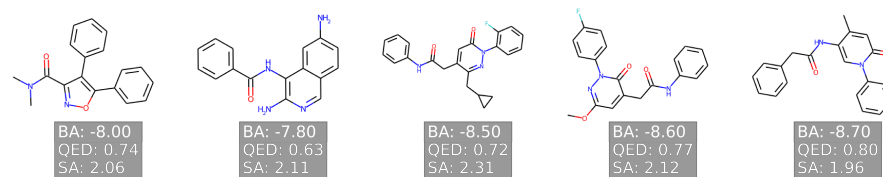


Figure S3: Example of generated molecules from the BA optimization model of *TTBK1* protein.

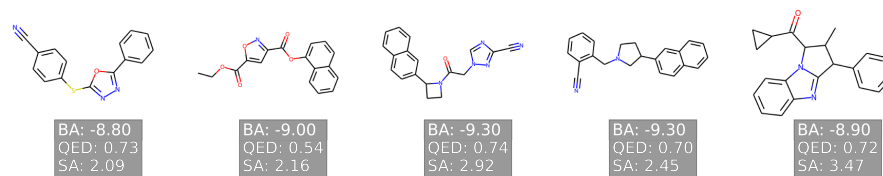


Figure S4: Example of generated molecules from the BA optimization model of *EGFR* protein.

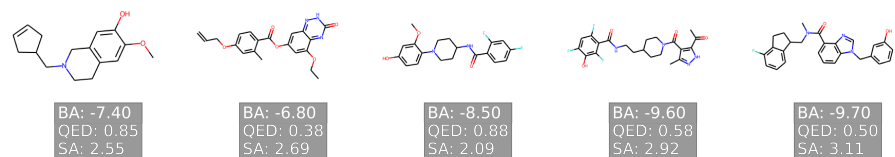


Figure S5: Example of generated molecules from the BA optimization model of *HTR1A* protein.

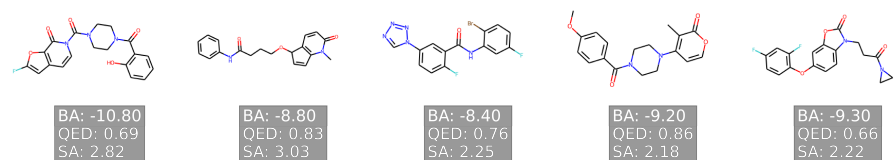


Figure S6: Example of generated molecules from the BA optimization model of *S1PR1* protein.

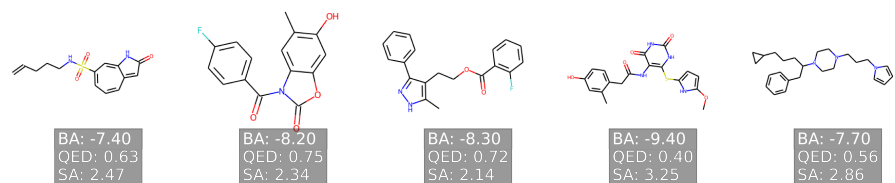


Figure S7: Example of generated molecules from the BA optimization model of *AKT1* protein.

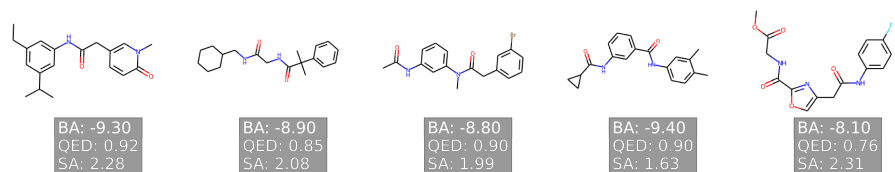


Figure S8: Example of generated molecules from the weighted sum optimization model of *DRD3* protein.

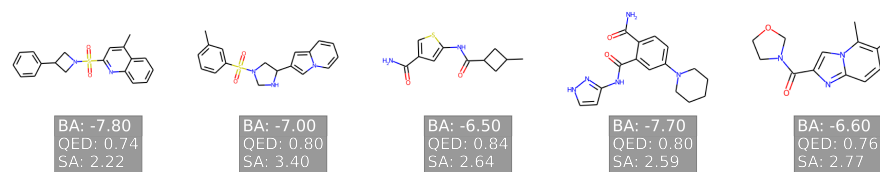


Figure S9: Example of generated molecules from the weighted sum optimization model of *SARS – CoV – 2 M_{pro}* protein.

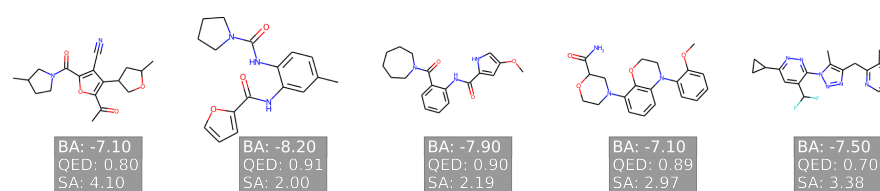


Figure S10: Example of generated molecules from the weighted sum optimization model of *TTBK1* protein.

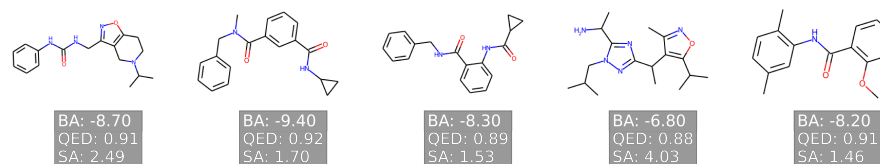


Figure S11: Example of generated molecules from the weighted sum optimization model of *EGFR* protein.

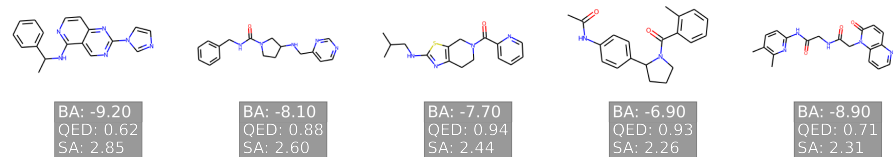


Figure S12: Example of generated molecules from the weighted sum optimization model of *HTR1A* protein.

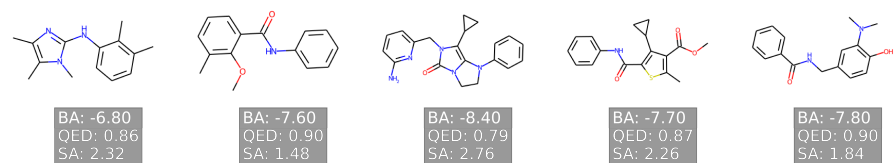


Figure S13: Example of generated molecules from the weighted sum optimization model of *S1PR1* protein.

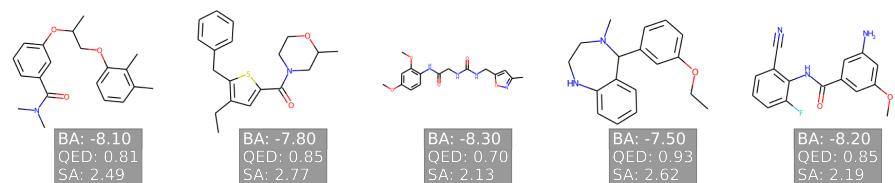


Figure S14: Example of generated molecules from the weighted sum optimization model of *AKT1* protein.