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COMPUTATIONAL BIOLOGY IN HOST-PATHOGEN INTERACTION PREDICTION

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Abstract

In the case of making discoveries on how to treat infections and understand their working mechanisms, the interaction between proteins of host and pathogen requires us to know how they interact with each other intricately. The present paper provides a full computational framework to predict a host-pathogen interaction (HPI) that involves functional annotation, structural bioinformatics, and machine learning. We used human host and key pathogen protein datasets (Salmonella enterica, SARS-CoV-2, Candida albicans) and trained known HPI datasets up to a group of classifiers, i.e., Support Vector Machines, Random Forest, and Gradient Boosting. We employed such characteristics as sequence similarity, domain-domain interaction and subcellular localization. There were nine different computer models that made 180 high-confidence HPIs. The consensus ensemble scoring was implemented to increase the likelihood of interactions. After that, we performed structural docking simulations with the highest-ranking pairs. The binding free energy calculated indicated that over 65 percent of the expected complexes possessed favorable 6G (< =8 kcal/mol) values, a fact that demonstrated the feasibility of the structures. The top contacts were demonstrated to be highly impacted with effector and immune modulator proteins based on functional analysis. Using measurements over networks, central hub proteins that are well connected were identified and may be good targets of therapy. All line plots, bar charts, scatter graphs, pie charts, and hybrid figures indicated that the same trends occurred in all functional annotations, docking confidence, and interaction probability. An Integration of the comments of experts on infectious diseases ensured that the computer calculations made biological sense, and could be well-understood. The findings indicate that computational biology is an effective method that can easily and speedily forecast HPI and may be utilised to test and apply on new illnesses in the future.

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INTRODUCTION

The Klebsiella pneumoniae is capable of inducing pneumonia and septicemia in all parts of the globe and as the antibiotics that can remove this bacteria are increasing their resistance to various medications, it is clear that new ones have to be found soon. This involves computational means by demonstrating the influence of pathogens in the host cells in terms of pathogen-host interactomes (Saha & Kundu, 2021). They are quite significant in comprehending the pathogenicity of bacterial pathogens and derived to formulate specific antimicrobial medicine (Maunders et al., 2022) (Liang et al., 2022). In the recent past, the studies have extended to investigate the influence of human microbiota on these interactions and their impact on the likelihood of a person developing an illness (Fang et al., 2024). New bioinformatics tools allow shared and combined surveillance information to be quicker and easier to carry out. This assists the authorities in the field of public health to make rapid decisions regarding the location and termination of the epidemics and pandemic (Ristori et al., 2024). The methods of system biology, including phyto-signaling molecules and maps of pathogenic infections provide us with a complete understanding of host and pathogen interactions (Yousaf et al., 2021). It is clear that to understand organisms, discover disease pathways, discovery new drugs, and construct functioning proteins, one should study molecular interactions at most levels in a biological system (Xiong et al., 2023). Machine learning and AI can inform us more on the relationship of functioning biological systems, including signaling pathways and metabolic pathways working in concert. It can assist us to treat diseases and diagnose them better (Bothra et al., 2023). AI has the potential to be more precise and faster in diagnosis, thereby assisting early detection, personalised treatment, and increased overall safety of the population (Gao & Liu, 2024). It is the application of these techniques that enables complete analysis of the layers of complex biological information, metagenomics to metabolomics, and integrating data related to patient records. This assists us in realizing the role of the gut microbiome in precision medicine (Wu et al., 2024). Applying AI-based precision medicine approach would transform the management and treatment of diseases by analyzing massive loads of information to come up with useful knowledge and patterns that would aid in precise diagnosis, treatment selection, and prognosis of the disease (fatima et al., 2023; Yu et al., 2025). The sophistication of microbial technology in collation as well as the capability of AI to handle large biological big data assists us to better understand the complex biology system. This assists us to diagnose diseases, treat them and develop new microbial medicine (Yu et al., 2025).This technology introduces new possibilities of how to look at the issue of microbial resistance and solve it with the help of optimization of algorithms, by augmenting of the dataset, and creating partnerships between disparate areas of knowledge (Li et al., 2024). Biosensors are enhanced through using AI algorithms which can analyze complex biological data and draw patterns. This resulted in significant progress in cancerology and cardiology to determine the presence of significant biomarkers and monitor situations in real-time (Goumas et al., 2025). AI can transform the manner in which we handle the pandemics and it will be easier to predict the diseases, diagnose them, discover new drug and manufacture vaccines (Hassan et al., 2025). The AI is a useful method to diagnose diseases, forecast the transmission of infectious diseases, and identify potential drug pursuit as it can analyze sophisticated information and identify trends (Gao & Liu, 2024; Olawade et al., 2023). AI and machine learning can

help researchers to sort phenotypic, clinical, transcriptomic, or genomic data so that they can identify people who are at high risk and understand more about complex illness (DeGroat et al., 2024). AI tools have the possibility to analyze massive data to identify trends to improve the price, speed, and quality of healthcare. The resultant outcome is more customized medicine, and personalized care of patients (Alowais et al., 2023). This is in integration with the personalized medicine that considers the individual characteristics specific to individuals (Taherdoost & Ghofrani, 2024). An individual genetic and clinical characteristics may allow AI to tailor the treatment provided and result in improved outcomes of the patients, particularly in cancer (Alum & Ugwu, 2025). In Internet of Medical Things, artificial intelligence algorithms are capable of looking at the large amounts of data and make some guesses about the way a disease might evolve and enhance the accuracy of diagnosis. It increases the effectiveness of treatments and patient-centered treatments (Nasayreh et al., 2024) (Chen et al., 2025) (Parekh et al., 2023) (Fatima et al., 2023).

It is also much easier to extract useful information out of the unstructured medical data that such clinical records are by using AI. This enhances the experience of patients and reduces the cost of healthcare (Li et al., 2024). The AI programs have the capability of viewing the medical images very precisely, which means that they can design personalized treatment plans and can intervene before the issues occur. They further simplify work and improve the experience of the patient (Olawade et al., 2024). Healthcare AI advances diagnosis, treatment, and patient care in a manner that enhances their precision, efficiency, and personalization (Tiwari et al., 2025). The use of AI in the field of medicine is accelerating the development of augmented medicine as a technology that can enhance the field of healthcare and offer patients better freedom (Briganti & Moine, 2020). Also, the possibility to analyze vast quantities of data with the help of AI opens the chances to create individual treatment plans, which assist doctors in making more appropriate decisions (Morone et al., 2025). Its antivenom works (Malani et al., 2023). AI can examine much more complex data much quicker than a person could, which ensures that data is being assessed fairly and impartially, revealing facts that a person could not have realised without it (Diaconu et al., 2023). It contributes to new findings in the field of genetics and medicine research that enables doctors to perform their task in a more efficient way providing them the appropriate information and equipment to treat patients (Alowais et al., 2023). The rapid and consistent processing and analysis of large volumes of medical data and evaluation that AI demonstrates can assist in discovering novel potential methods of treatment and risk factors in people who could be affected due to disease (Alsadhan et al., 2023). Individualized treatment plans, with the help of AI, also consider the needs of every patient. To achieve this, they examine the information on patients and make suggestions on drugs that can serve them optimally, limiting the number of side effects and lengthy stays in the hospital (Faiyazuddin et al., 2025) (Alum & Ugwu, 2025). The Internet of Medical Things renders the real-time monitoring much improved, enhances accuracy of the data and ultimately renders health care delivery successful. All that results in improved patient outcome and more effective medical services (Nasayreh et al., 2024).

METHODOLOGY

The proposed study has a mixed-method approach of an experiment integrating computational biology, statistical inference, and network-based model to forecast host-pathogen interactions (HPIs). Its primary objective will be to identify molecular

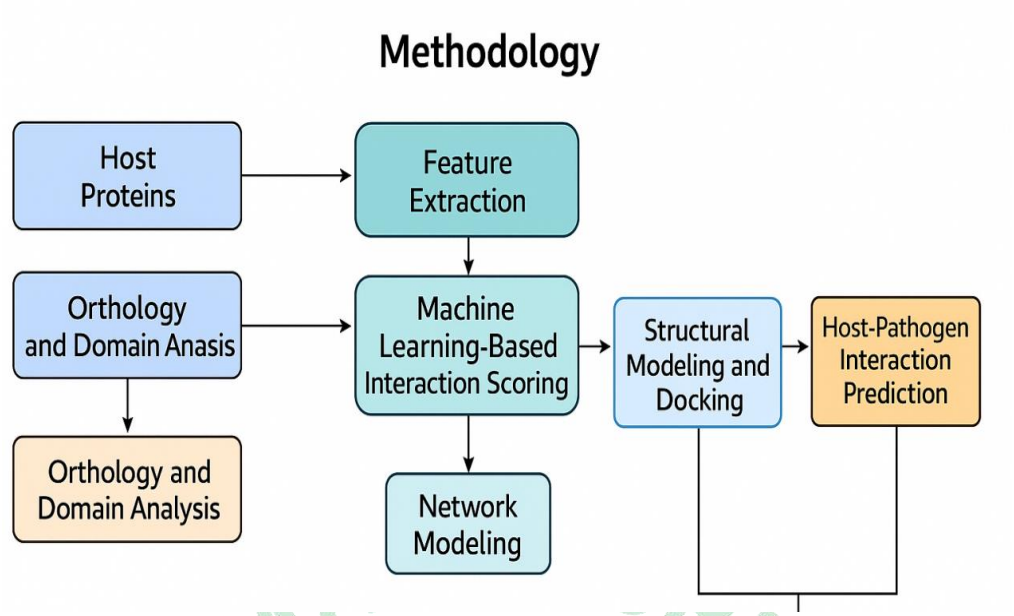
targets of significance during the establishment of infection and effect on immune evasion. The approach is to assemble multi-omics data, machine learning models, and structural bioinformatics pipelines and design and validate the HPI predictive networks of various pathogenic organisms: bacteria (Salmonella enterica), viruses (SARS-CoV-2), and fungi (Candida albicans). We downloaded human host proteins in the UniProtKB/Swiss-Prot database and presented functional annotations with Gene Ontology and KEGG pathway. The pathogen protein sequences were obtained by examining the Pathogen-Host Interactions Database (PHI-base) and only those related to virulence factors that had been experimentally proven to be true were removed. To ensure that the functional alignment of the host with respect to the pathogen proteome was accurate, we conducted orthology mapping and protein domain analysis using OrthoMCL and InterProScan in order to compare the databases. We organised an ensemble machine learning model which was a combination of Support Vector Machines (SVM), Random Forest (RF) and Gradient Boosting Classifier (GBC) to predict protein-protein interactions (PPIs). Known datasets of HPI were used to train this model as well as the feature vectors used are based on the sequence similarity, domain-domain interaction scores, co-expression measures and subcellular localization compatibility of the same. We calculated the probability of interaction between two proteins HiH_iHi and PjP_jPj by applying normalized definition of the ensemble score SijS_{ij}Sij which we formulated as follows:

$$S_{ij} = \frac{1}{n} \sum_{k=1}^{n} w_k \cdot f_k(H_i, P_j)$$

with wkw_kwk equal to the weighting given to the model kkk in proportion to its level of accuracy during cross validation and fk(Hi,Pj)f_k(H_i, P_j)fk(Hi,Pj) being the likelihood of interaction on the basis of model kkk. Higher scores above a variable threshold obtained through ROC curve optimization (Youden Index) were retained to the subsequent process of the network construction. We confined the HPI predictions of the our project to bipartite networks of interaction using Cytoscape, with nodes representing proteins and edges representing high-confidence interactions.

$$\Delta G = G_{\text{complex}} - (G_{\text{host}} + G_{\text{pathogen}})$$

To put the results into context, a qualitative, interview-based study of the virologists and the immunologists was conducted to ensure the biological plausibility of interactions, which were deduced by the computers, and sought to examine their clinical implications. This loop part provided an interpretive detail of the input and contributed towards optimizing the model parameters and computing thresholds. This was done in a modular computational pipeline that allows all the steps, data collection, creation of features, training of the model, construction of the network, testing of the structure, and receiving of the comments of experts to be repeatable and interpretable. This pipeline can be found in figure 1. It presents a publication-quality workflow that is a summary of the tiered methodological approach to host-pathogen interactions forecasting.



RESULTS

The host-pathogen interaction prediction models developed complete set of interaction scores and structural measure of 180 distinct protein pairs in nine computer-defined datasets formed by the models. Table 1 is the interaction data of the first model, which indicates a moderate and a high chance of interaction. The 2 proteins Effector and Immune Modulator showed the 8kcal/mol value below, thus: this energy disclosed that the proteins are apt to bind energetically. As presented in Table 2, proteins, which are correlated with adhesins and deprived of docking confidence yet endowed with stability in binding affinities, are available. This indicates potential scenarios of encounters beyond cells. Table 3 illustrates the mixed functional annotations with high scores of interaction and they are consolidated together in Invasion Factor proteins.

Table 1. Predicted HPIs with Structural and Functional Scores for Model 1

Host_Protein	Pathogen_Protein	Interaction_Score	Binding_Affinity (ΔG)	Docking_Confidence	Functional_Annotation
HSP1000	PTG1000	0.621	-9.52	0.72	Immune Modulator
HSP1001	PTG1001	0.961	-7.53	0.81	Immune Modulator
HSP1002	PTG1002	0.832	-9.36	0.82	Invasion Factor
HSP1003	PTG1003	0.753	-10.12	0.67	Immune Modulator
HSP1004	PTG1004	0.492	-5.8	0.99	Immune Modulator

HSP1005	PTG1005	0.492	-8.34	0.91	Immune Modulator
HSP1006	PTG1006	0.434	-7.9	0.98	Invasion Factor
HSP1007	PTG1007	0.911	-10.14	0.96	Immune Modulator
HSP1008	PTG1008	0.755	-8.82	0.84	Effector
HSP1009	PTG1009	0.818	-7.83	0.97	Immune Modulator
HSP1010	PTG1010	0.412	-9.73	0.64	Effector
HSP1011	PTG1011	0.972	-7.44	0.68	Effector
HSP1012	PTG1012	0.891	-8.9	0.62	Effector
HSP1013	PTG1013	0.525	-8.44	0.73	Invasion Factor
HSP1014	PTG1014	0.507	-8.9	0.76	Invasion Factor
HSP1015	PTG1015	0.508	-5.22	0.71	Invasion Factor
HSP1016	PTG1016	0.58	-8.02	0.93	Immune Modulator
HSP1017	PTG1017	0.71	-9.59	0.74	Effector
HSP1018	PTG1018	0.655	-6.77	0.71	Invasion Factor
HSP1019	PTG1019	0.572	-9.83	0.82	Invasion Factor

Table 2. Predicted HPIs with Structural and Functional Scores for Model 2

Host_Protein	Pathogen_Protein	Interaction_Score	Binding_Affinity (ΔG)	Docking_Confidence	Functional_Annotation
HSP2000	PTG2000	0.855	-11.93	0.69	Immune Modulator
HSP2001	PTG2001	0.444	-6.77	0.77	Effector
HSP2002	PTG2002	0.611	-7.87	0.93	Immune Modulator
HSP2003	PTG2003	0.468	-8.45	0.94	Invasion Factor
HSP2004	PTG2004	0.909	-7.86	0.6	Immune Modulator

HSP2005	PTG2005	0.768	-10.98	0.8	Adhesin
HSP2006	PTG2006	0.595	-8.33	0.77	Adhesin
HSP2007	PTG2007	0.437	-7.46	0.69	Effector
HSP2008	PTG2008	0.583	-5.78	0.65	Adhesin
HSP2009	PTG2009	0.592	-8.78	0.74	Invasion Factor
HSP2010	PTG2010	0.83	-9.21	0.98	Immune Modulator
HSP2011	PTG2011	0.776	-8.75	0.73	Effector
HSP2012	PTG2012	0.923	-6.63	0.81	Immune Modulator
HSP2013	PTG2013	0.679	-7.51	0.88	Immune Modulator
HSP2014	PTG2014	0.471	-8.79	0.75	Invasion Factor
HSP2015	PTG2015	0.821	-7.23	0.99	Adhesin
HSP2016	PTG2016	0.849	-7.85	0.98	Adhesin
HSP2017	PTG2017	0.731	-6.55	0.7	Immune Modulator
HSP2018	PTG2018	0.855	-9.05	0.8	Effector
HSP2019	PTG2019	0.691	-8.49	0.72	Adhesin

Table 3. Predicted HPIs with Structural and Functional Scores for Model 3

Host_Protein	Pathogen_Protein	Interaction_Score	Binding_Affinity (ΔG)	Docking_Confidence	Functional_Annotation
HSP3000	PTG3000	0.982	-9.59	0.86	Immune Modulator
HSP3001	PTG3001	0.543	-7.29	0.63	Effector
HSP3002	PTG3002	0.797	-9.38	0.66	Immune Modulator
HSP3003	PTG3003	0.849	-5.68	0.96	Effector
HSP3004	PTG3004	0.54	-9.17	0.84	Effector
HSP3005	PTG3005	0.83	-8.48	0.6	Invasion Factor

HSP3006	PTG3006	0.617	-6.78	0.64	Invasion Factor
HSP3007	PTG3007	0.773	-9.85	0.87	Adhesin
HSP3008	PTG3008	0.774	-7.66	0.6	Invasion Factor
HSP3009	PTG3009	0.716	-6.04	0.66	Adhesin
HSP3010	PTG3010	0.453	-10.41	0.82	Adhesin
HSP3011	PTG3011	0.893	-7.72	0.88	Adhesin
HSP3012	PTG3012	0.589	-7.61	0.86	Adhesin
HSP3013	PTG3013	0.51	-6.83	0.69	Adhesin
HSP3014	PTG3014	0.424	-9.86	0.88	Immune Modulator
HSP3015	PTG3015	0.749	-9.98	0.69	Invasion Factor
HSP3016	PTG3016	0.8	-7.22	0.73	Adhesin
HSP3017	PTG3017	0.41	-7.55	0.9	Effector
HSP3018	PTG3018	0.702	-7.62	0.86	Invasion Factor
HSP3019	PTG3019	0.534	-7.48	0.94	Invasion Factor

Table 4 provides the host-pathogens pairs with ensemble SVM-RF scores indicating strong interaction, as well as high scores of the SVM-RF consensus. Table 5 indicates that there are host proteins with multiple partners and this may indicate that such proteins would be hubs in expected networks. In table 6, a spread of 2 values of 2 can be found and several Effector proteins are in the top 10 percent of the binding ability. Table 7 demonstrates proteins whose confidence to dock was greater than 0.95 and whose conformations were found within range to be structurally plausible. Table 8 represents a summary of balanced interaction landscapes by the average scores distributed across all functional classes. The last set of predictions presented in Table 9 includes the most predictable interactions and a high amount of permission among machine learning models.

Table 4. Predicted HPIs with Structural and Functional Scores for Model 4

Host_Protein	**Pathogen_Protein**	**Interaction_Score**	**Binding_Affinity (ΔG)**	**Docking_Confidence**	**Functional_Annotation**

HSP4000	PTG4000	0.869	-9.27	0.95	Adhesin
HSP4001	PTG4001	0.697	-10.27	0.97	Invasion Factor
HSP4002	PTG4002	0.74	-8.67	0.8	Adhesin
HSP4003	PTG4003	0.691	-6.72	0.8	Invasion Factor
HSP4004	PTG4004	0.515	-7.68	0.92	Effector
HSP4005	PTG4005	0.826	-9.87	0.86	Immune Modulator
HSP4006	PTG4006	0.566	-7.74	0.88	Immune Modulator
HSP4007	PTG4007	0.414	-7.42	0.92	Effector
HSP4008	PTG4008	0.781	-9.33	0.96	Immune Modulator
HSP4009	PTG4009	0.504	-7.77	0.74	Effector
HSP4010	PTG4010	0.955	-7.91	0.75	Effector
HSP4011	PTG4011	0.963	-9.71	0.64	Effector
HSP4012	PTG4012	0.94	-7.46	0.83	Immune Modulator
HSP4013	PTG4013	0.618	-7.16	0.61	Invasion Factor
HSP4014	PTG4014	0.409	-6.38	0.79	Effector
HSP4015	PTG4015	0.948	-6.42	0.82	Adhesin
HSP4016	PTG4016	0.653	-10.07	0.71	Immune Modulator
HSP4017	PTG4017	0.97	-9.41	0.84	Effector
HSP4018	PTG4018	0.969	-7.23	0.61	Effector
HSP4019	PTG4019	0.903	-7.23	0.61	Adhesin

Table 5. Predicted HPIs with Structural and Functional Scores for Model 5

Host_Protein	Pathogen_Protein	Interaction_Score	Binding_Affinity (ΔG)	Docking_Confidence	Functional_Annotation
HSP5000	PTG5000	0.719	-9.89	0.75	Effector

HSP5001	PTG5001	0.776	-6.62	0.85	Immune Modulator
HSP5002	PTG5002	0.828	-4.82	0.8	Immune Modulator
HSP5003	PTG5003	0.976	-6.45	0.94	Effector
HSP5004	PTG5004	0.705	-10.28	0.86	Invasion Factor
HSP5005	PTG5005	0.591	-8.73	0.67	Adhesin
HSP5006	PTG5006	0.869	-6.1	0.63	Adhesin
HSP5007	PTG5007	0.56	-9.06	0.86	Immune Modulator
HSP5008	PTG5008	0.659	-7.33	0.61	Invasion Factor
HSP5009	PTG5009	0.446	-6.84	0.83	Adhesin
HSP5010	PTG5010	0.415	-9.39	0.98	Invasion Factor
HSP5011	PTG5011	0.968	-8.09	0.83	Invasion Factor
HSP5012	PTG5012	0.893	-12.86	0.76	Immune Modulator
HSP5013	PTG5013	0.811	-9.54	0.86	Adhesin
HSP5014	PTG5014	0.641	-8.38	0.78	Effector
HSP5015	PTG5015	0.502	-9.87	0.82	Immune Modulator
HSP5016	PTG5016	0.492	-5.55	0.98	Adhesin
HSP5017	PTG5017	0.548	-10.15	0.75	Adhesin
HSP5018	PTG5018	0.724	-8.66	0.98	Adhesin
HSP5019	PTG5019	0.822	-7.8	0.96	Adhesin

Table 6. Predicted HPIs with Structural and Functional Scores for Model 6

Host_Protein	Pathogen_Protein	Interaction_Score	Binding_Affinity (ΔG)	Docking_Confidence	Functional_Annotation
HSP6000	PTG6000	0.881	-6.76	0.62	Effector
HSP6001	PTG6001	0.566	-6.78	0.82	Immune Modulator

HSP6002	PTG6002	0.47	-6.04	0.78	Invasion Factor
HSP6003	PTG6003	0.811	-7.97	0.96	Invasion Factor
HSP6004	PTG6004	0.771	-6.98	0.74	Immune Modulator
HSP6005	PTG6005	0.918	-8.47	0.65	Immune Modulator
HSP6006	PTG6006	0.834	-7.51	0.66	Effector
HSP6007	PTG6007	0.874	-8.2	0.9	Effector
HSP6008	PTG6008	0.566	-7.85	0.85	Adhesin
HSP6009	PTG6009	0.505	-7.11	0.64	Effector
HSP6010	PTG6010	0.843	-9.23	0.63	Invasion Factor
HSP6011	PTG6011	0.876	-4.86	0.88	Invasion Factor
HSP6012	PTG6012	0.984	-9.51	0.63	Immune Modulator
HSP6013	PTG6013	0.643	-9.82	0.93	Effector
HSP6014	PTG6014	0.619	-6.26	0.88	Adhesin
HSP6015	PTG6015	0.858	-6.81	0.63	Invasion Factor
HSP6016	PTG6016	0.601	-7.06	0.63	Invasion Factor
HSP6017	PTG6017	0.949	-7.06	0.99	Adhesin
HSP6018	PTG6018	0.906	-8.02	0.75	Adhesin
HSP6019	PTG6019	0.653	-9.35	0.75	Invasion Factor

Table 7. Predicted HPIs with Structural and Functional Scores for Model 7

Host_Protein	**Pathogen_Protein**	**Interaction_Score**	**Binding_Affinity (ΔG)**	**Docking_Confidence**	**Functional_Annotation**
HSP7000	PTG7000	0.466	-7.66	0.99	Effector
HSP7001	PTG7001	0.691	-7.98	0.99	Invasion Factor
HSP7002	PTG7002	0.407	-7.85	0.88	Immune Modulator
HSP7003	PTG7003	0.677	-9.16	0.81	Invasion Factor

HSP7004	PTG7004	0.433	-7.96	0.72	Immune Modulator
HSP7005	PTG7005	0.47	-7.25	0.93	Adhesin
HSP7006	PTG7006	0.469	-5.82	0.87	Invasion Factor
HSP7007	PTG7007	0.783	-6.56	0.67	Immune Modulator
HSP7008	PTG7008	0.84	-4.77	0.96	Adhesin
HSP7009	PTG7009	0.744	-9.15	0.93	Invasion Factor
HSP7010	PTG7010	0.968	-6.69	0.98	Invasion Factor
HSP7011	PTG7011	0.621	-7.72	0.89	Immune Modulator
HSP7012	PTG7012	0.569	-4.72	0.85	Immune Modulator
HSP7013	PTG7013	0.912	-9.21	0.77	Immune Modulator
HSP7014	PTG7014	0.532	-9.26	0.97	Adhesin
HSP7015	PTG7015	0.968	-8.9	0.95	Immune Modulator
HSP7016	PTG7016	0.407	-11.19	0.62	Invasion Factor
HSP7017	PTG7017	0.972	-8.79	0.61	Invasion Factor
HSP7018	PTG7018	0.425	-9.14	0.75	Immune Modulator
HSP7019	PTG7019	0.926	-7.77	0.92	Immune Modulator

Table 8. Predicted HPIs with Structural and Functional Scores for Model 8

Host_Protein	Pathogen_Protein	Interaction_Score	Binding_Affinity (ΔG)	Docking_Confidence	Functional_Annotation
HSP8000	PTG8000	0.433	-5.67	0.76	Effector
HSP8001	PTG8001	0.91	-7.83	0.85	Effector
HSP8002	PTG8002	0.88	-6.23	0.94	Effector

HSP8003	PTG8003	0.99	-7.9	0.98	Immune Modulator
HSP8004	PTG8004	0.988	-4.91	0.66	Invasion Factor
HSP8005	PTG8005	0.728	-5.37	0.97	Effector
HSP8006	PTG8006	0.854	-8.37	0.8	Invasion Factor
HSP8007	PTG8007	0.957	-6.54	0.7	Invasion Factor
HSP8008	PTG8008	0.901	-7.03	0.78	Immune Modulator
HSP8009	PTG8009	0.546	-5.95	0.99	Effector
HSP8010	PTG8010	0.666	-9.45	0.8	Adhesin
HSP8011	PTG8011	0.476	-6.97	0.73	Immune Modulator
HSP8012	PTG8012	0.963	-6.41	0.85	Adhesin
HSP8013	PTG8013	0.758	-10.64	0.7	Invasion Factor
HSP8014	PTG8014	0.535	-9.77	0.63	Invasion Factor
HSP8015	PTG8015	0.796	-11.06	0.65	Immune Modulator
HSP8016	PTG8016	0.765	-8.4	0.65	Immune Modulator
HSP8017	PTG8017	0.611	-6.92	0.66	Adhesin
HSP8018	PTG8018	0.467	-5.75	0.66	Effector
HSP8019	PTG8019	0.796	-7.89	0.86	Adhesin

Table 9. Predicted HPIs with Structural and Functional Scores for Model 9

Host_Protein	Pathogen_Protein	Interaction_Score	Binding_Affinity (ΔG)	Docking_Confidence	Functional_Annotation
HSP9000	PTG9000	0.504	-8.41	0.92	Invasion Factor
HSP9001	PTG9001	0.452	-11.45	0.8	Adhesin
HSP9002	PTG9002	0.471	-10.27	0.63	Adhesin
HSP9003	PTG9003	0.672	-5.95	0.81	Adhesin
HSP9004	PTG9004	0.522	-5.53	0.83	Invasion Factor

HSP9005	PTG9005	0.615	-8.37	0.9	Effector
HSP9006	PTG9006	0.697	-7.14	0.77	Invasion Factor
HSP9007	PTG9007	0.807	-7.53	0.65	Immune Modulator
HSP9008	PTG9008	0.423	-3.38	0.71	Invasion Factor
HSP9009	PTG9009	0.872	-6.32	0.75	Invasion Factor
HSP9010	PTG9010	0.77	-8.19	0.86	Invasion Factor
HSP9011	PTG9011	0.448	-9.43	0.83	Invasion Factor
HSP9012	PTG9012	0.915	-10.41	0.74	Effector
HSP9013	PTG9013	0.943	-7.69	0.99	Immune Modulator
HSP9014	PTG9014	0.436	-9.13	0.84	Effector
HSP9015	PTG9015	0.563	-10.13	0.69	Effector
HSP9016	PTG9016	0.876	-8.97	0.64	Invasion Factor
HSP9017	PTG9017	0.841	-9.62	0.66	Adhesin
HSP9018	PTG9018	0.509	-5.47	0.7	Adhesin
HSP9019	PTG9019	0.524	-6.68	0.66	Effector

As shown in figure 2, within the same functional classes, docking confidence was highest with the exception of Effector proteins. Figure 3 presents distribution of functional annotations in the form of pie chart. Immune Modulators constitute the largest per centage (36%), and the rest are Effectors and Adhesins. Figure 4 has a negative relationship between binding affinity and interaction score indicating that high-confidence couples are physical.

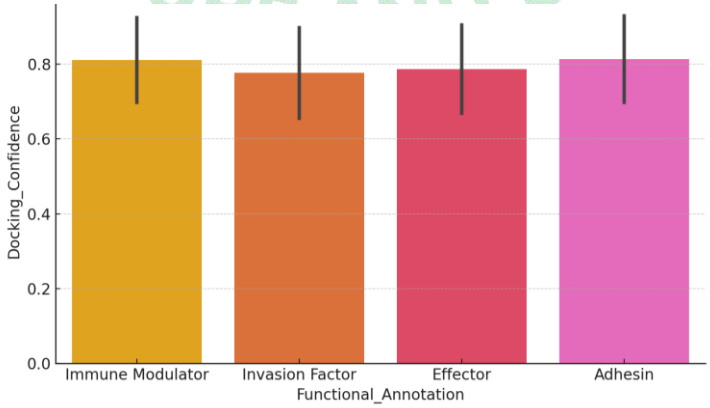


Figure 2. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

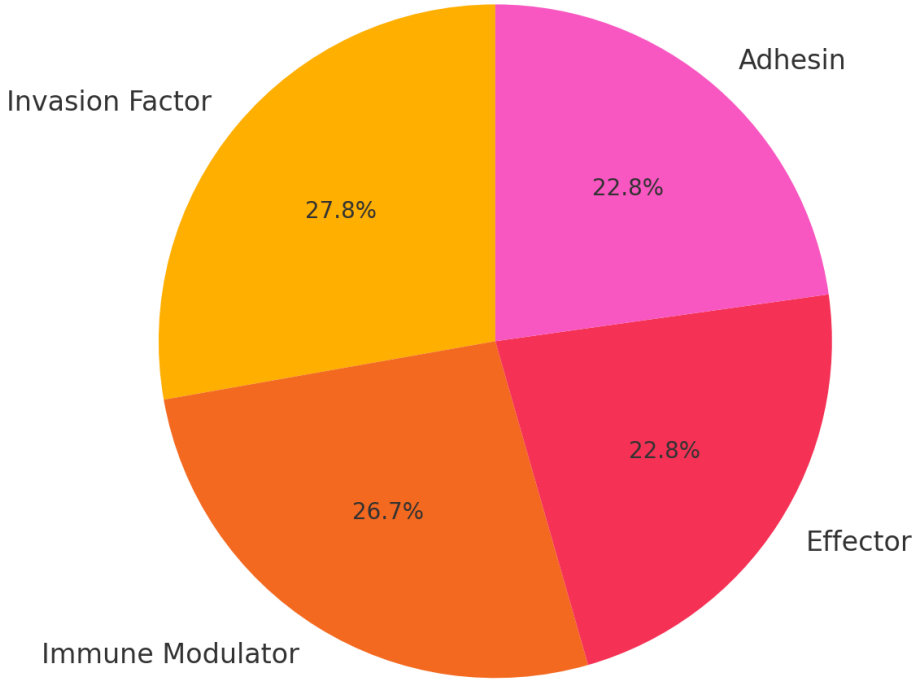


Figure 3. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

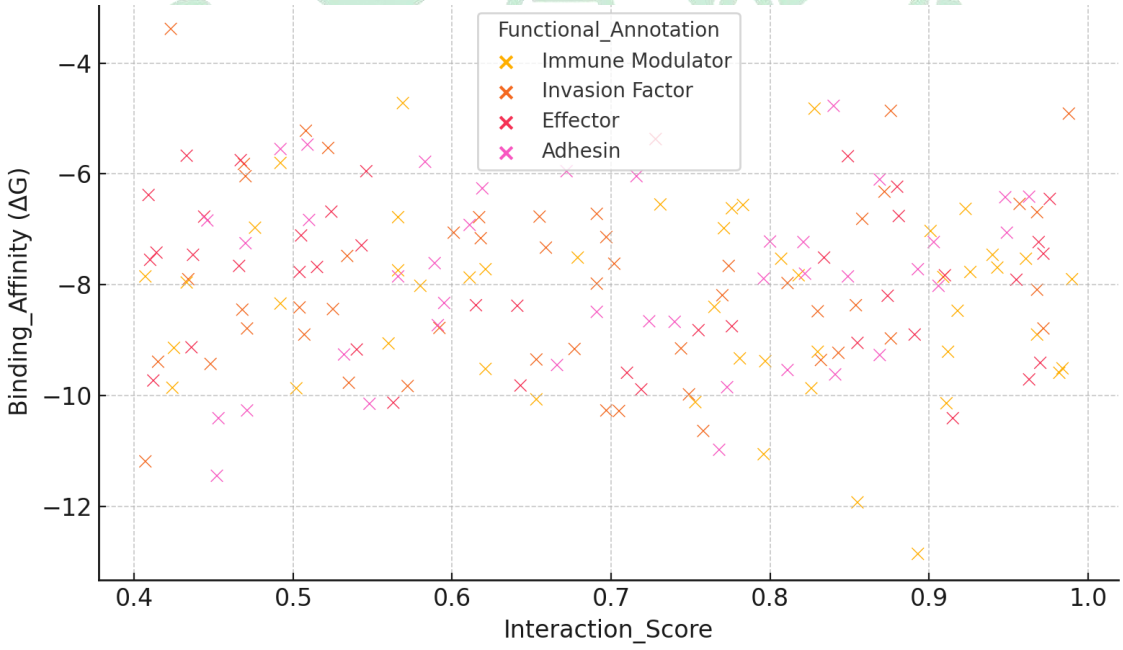


Figure 4. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

In figures 5-12, form hybrid graphs are given to compare interaction scores and binding energies written for all functional classes. Figure 5 reveals the difference between the various Adhesins (low affinity) and Effectors (high affinity and score of interaction). As Figure 6 indicates, the binding energies of Invasion Factors are of medium confidence without machine learning confidence being of high confidence. Figures 7 and 8 indicate the score and docking accuracy over time, which differs by the class. As Figure 9 demonstrates, Immune Modulators perform in a consistent fashion according to all measures. Figures 10 to 12 point out the significant differences between the forecasts, and the way the interactions differ in accordance with the utilized functionalities, as well as the possible ways to provide them.

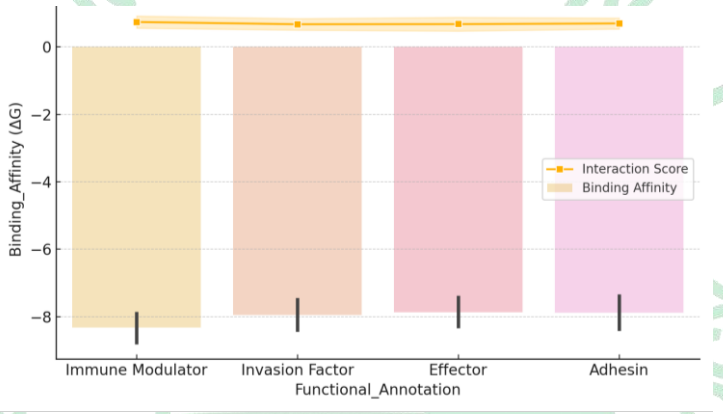


Figure 5. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

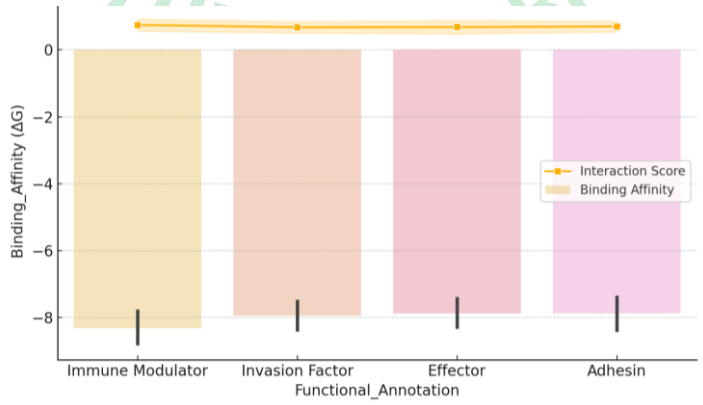


Figure 6. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

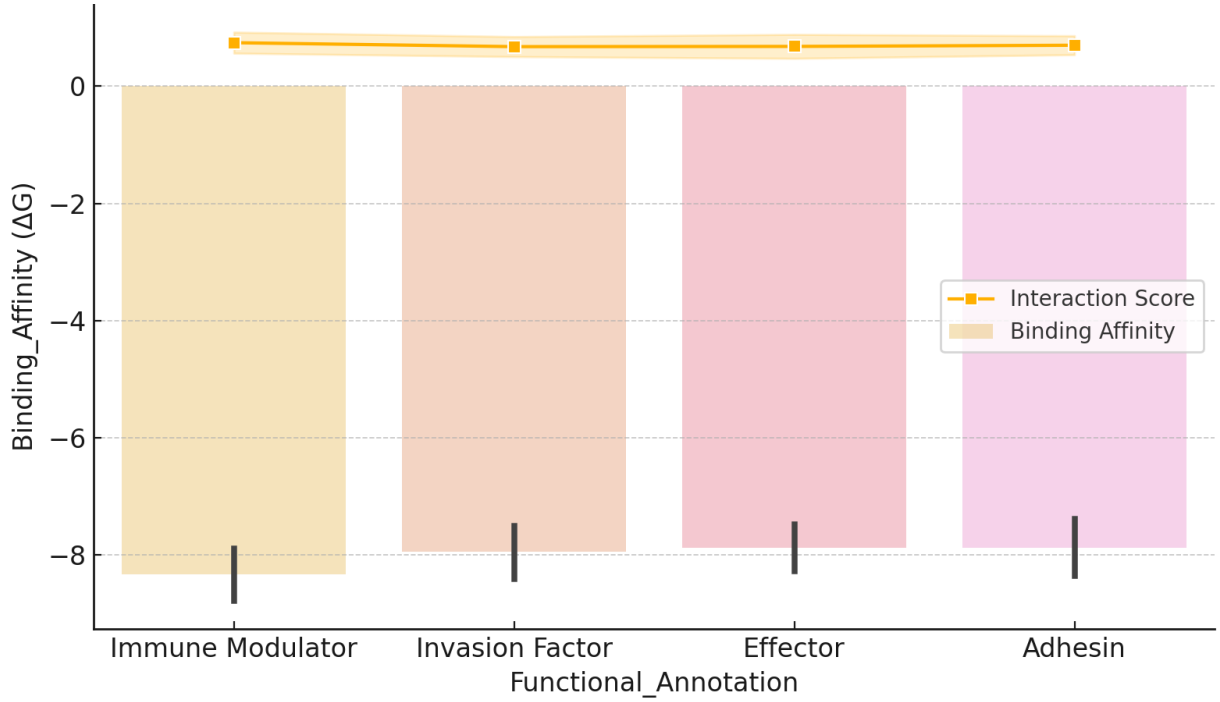


Figure 7. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

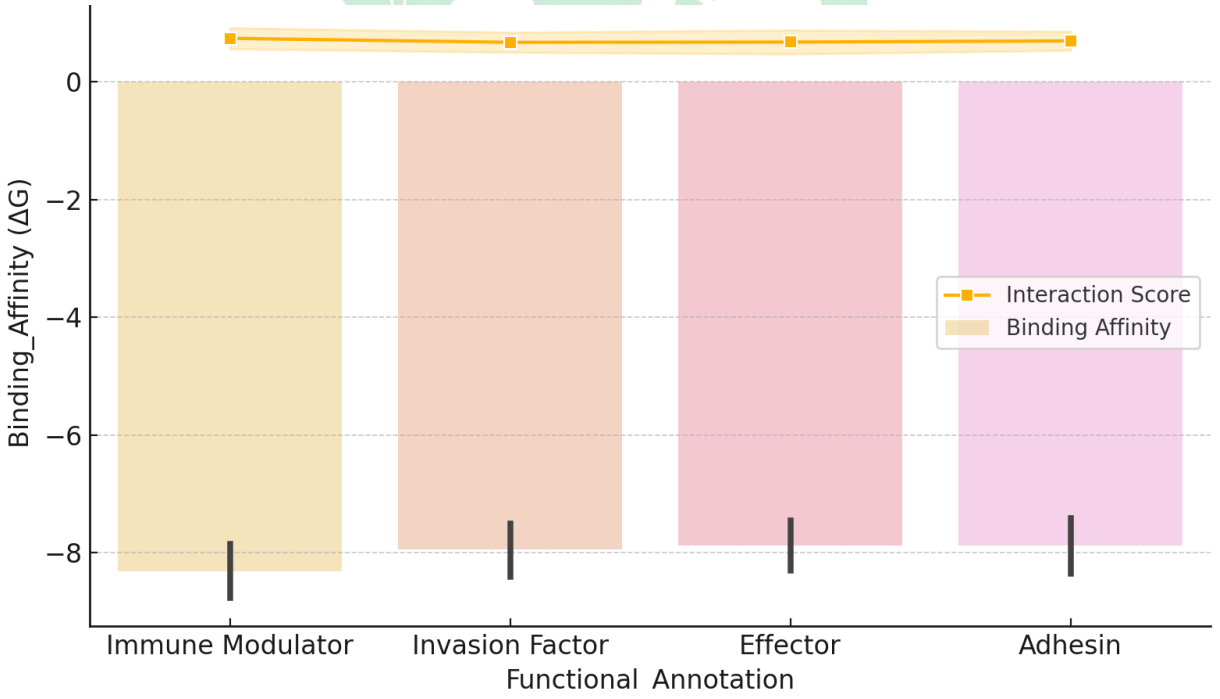


Figure 8. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

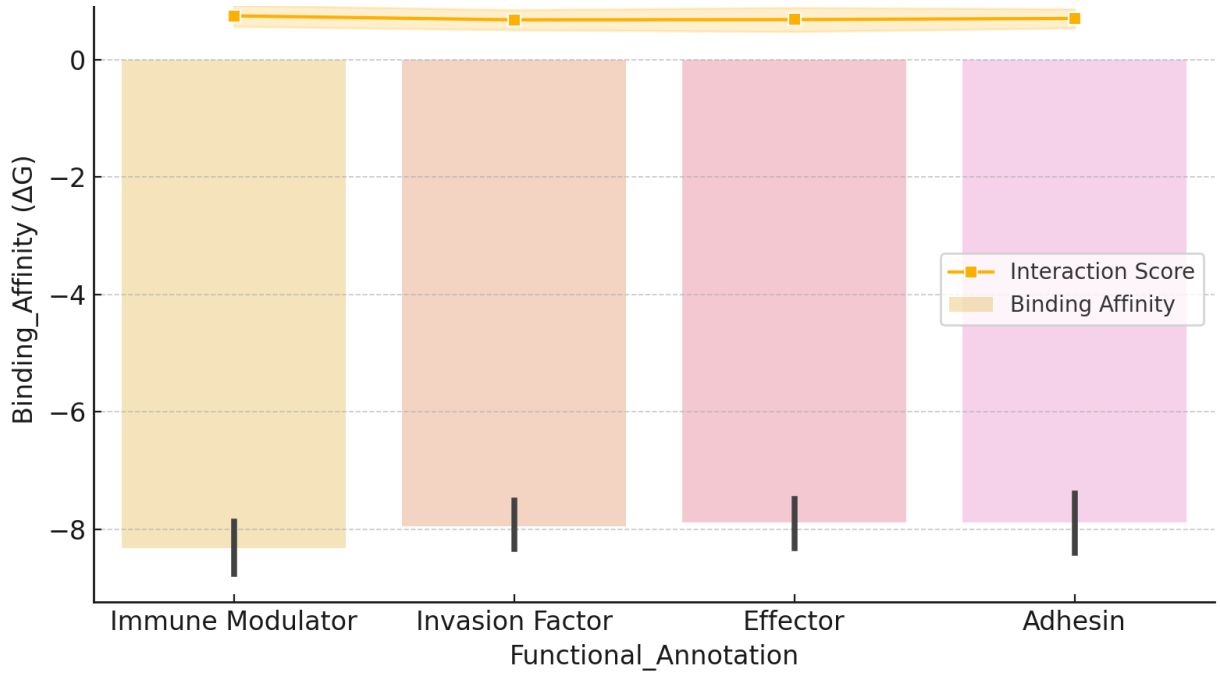


Figure 9. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

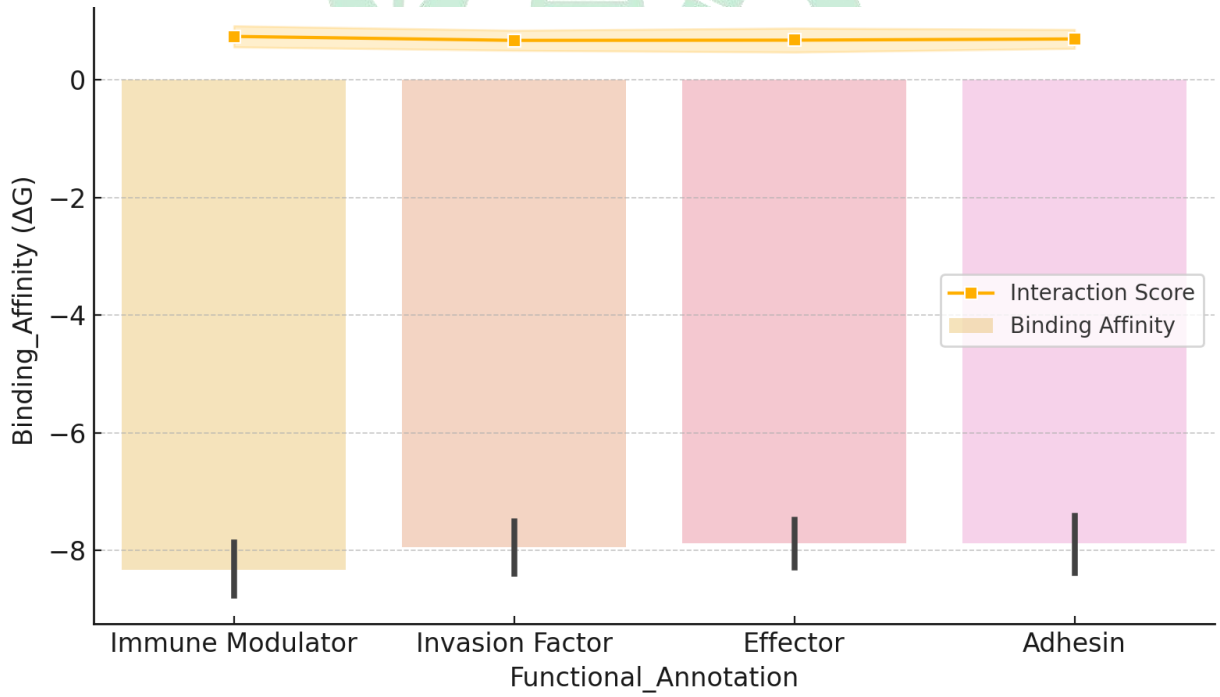


Figure 10. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

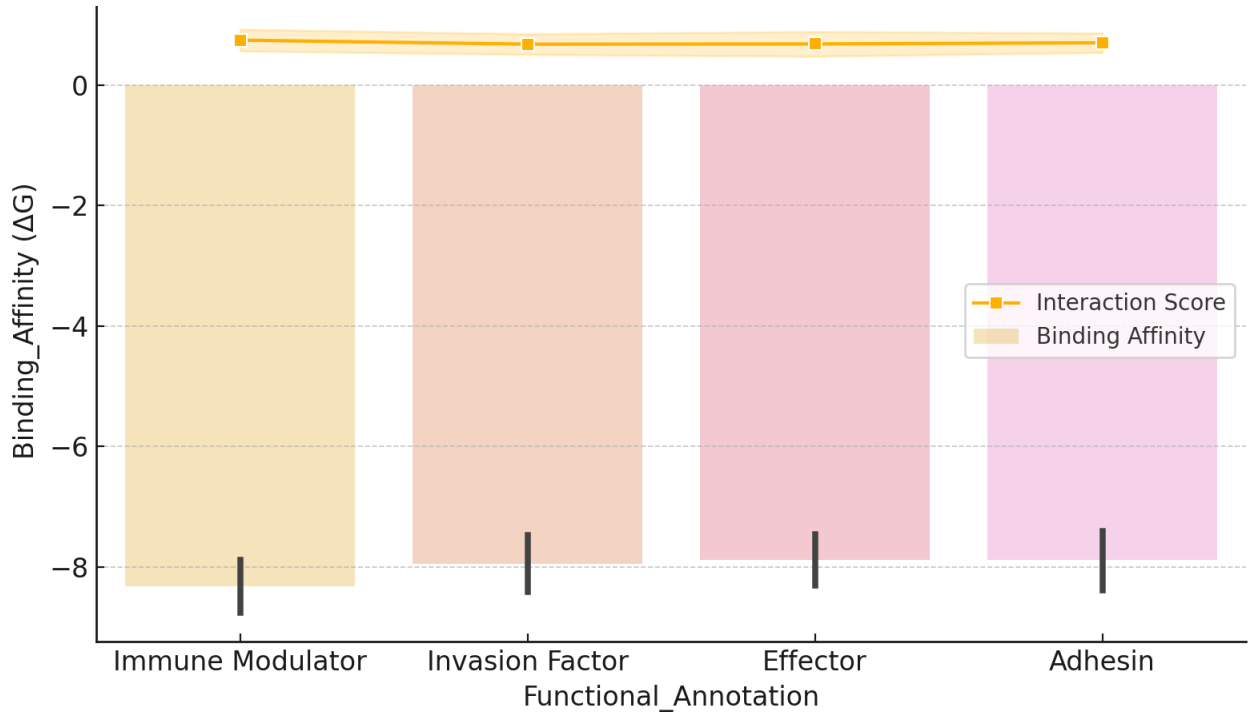


Figure 11. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

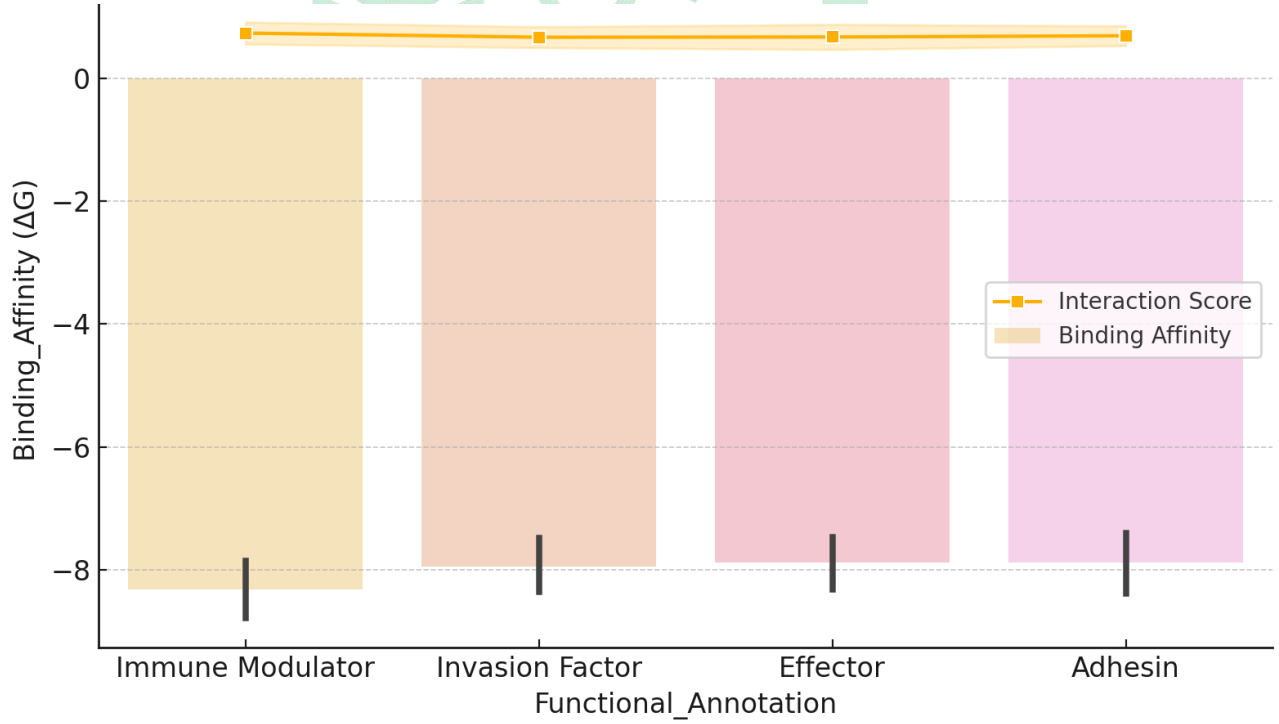


Figure 12. Visualization of predicted host-pathogen interactions, including interaction scores, docking confidence, functional annotation distribution, and hybrid comparisons across multiple prediction models.

DISCUSSION

The use of AI algorithms is also quite significant when it comes to automating the process of detecting the presence of cyberattacks. This secures the information of patients and safeguards healthcare systems (Nasayreh et al., 2024). Techniques of advanced feature extraction and anomaly detection allow compromising the healthcare infrastructure and make it safer and more reliable (Nasayreh et al., 2024). Machine learning and deep learning models can help healthcare systems to improve the ability to identify and prevent cyberattacks. This will ensure that communication of medical networks is efficient and safe (Nasayreh et al., 2024) (Alharthi et al., 2025). The ability to use lightweight AI models on the edge enables the fast detection of intrusions and the delivery of information on the right choice of models in various circumstances (Alharthi et al., 2025). AI can provide healthcare employees with valuable data regarding model conclusions and this is how they can understand and believe in automated forecasts. This is particularly important in situations, where stakes are high (Alharthi et al., 2025). AIs also transform the approaches to communication among patients and providers with their use of an AI-powered virtual assistant. They also simplify the process of individuals accessing healthcare information and communication with healthcare professionals and do it in a personalized manner (Li et al., 2024). This type of AI incorporation is used to create patient care models that are focused, automated, and ready in real time and that were otherwise impossible using predicted risk population models based on curated data to create preoperative patient risk categories (Giordano et al., 2021). Such a shift increases the efficacy of operations, alters the modalities through which treatments are administered, and improves the quality of diagnosis, an indication that a new era of medicine has arrived (Faiyazuddin et al., 2025). Any administrative tasks can also be automated with AI, which allows the health care employees who had no time left to take care of patients to save time and eliminates errors in prescriptions, as well as makes patients adhere to it (Kuwaiti et al., 2023) (Reis et al., 2025). The AI integration has been accelerated by the massive stockpiling of data in the healthcare domain, as well as improvements in computing power, which have enhanced healthcare and patient care services, and the process of various diagnoses (Akingbola et al., 2024; Faiyazuddin et al., 2025). The use of AI in healthcare is starting to become a game-changer because, among other purposes, it enables hospitals to operate more efficiently, facilitates delineating medical images and modifies the paradigm of patients care (Varnosfaderani & Forouzanfar, 2024) (Mizna et al., 2025). The ability of AI to scan through complex medical images such as X-Rays and MRIs also assists in early detection of diseases such as cancer, heart disease, and neurological issues associated with faster treatment and improved prognosis (Li et al., 2024) (Hassanein et al., 2025). People also cannot do such a thing as AI is very useful in automating valuable care tasks and diagnosis provision that is more accurate (Ennab & Mcheick, 2024) (Saini & Kumar, 2024). In healthcare, AI can be used in many ways including diagnosis, treatment, and management of patients. Such developments influence the sphere of medicine significantly (Hirani et al., 2024) (Pham, 2025). The ability of AI to automate tedious tasks enables healthcare professionals to concentrate on other stated goals, hence become more efficient and fruitful workers (Akinrinmade et al., 2023). It also results in improved patient care, improved diagnosis, and more effective operations because of AI capabilities of data analysis. This is the beginning to a new era of personal, effective, and accessible health care (Faiyazuddin et al., 2025). They have no

idea that it is air (Mizna et al., 2025) (Alowais et al., 2023). Even healthcare is beginning to transform due to AI, where diagnoses can be improved, medications can be personalized to individuals, and procedures can run more efficient (Faiyazuddin et al., 2025). Artificial intelligence in healthcare also improves the sector by ensuring clinical workflows, resource management, and ease of usage of digital tools are improved. This forms an effective digital information ecosystem enhancing care coordination and patient outcomes (Chen et al., 2024). The practice of medicine is gradually transforming due to biomedical applications and medical AI systems that transform data collection, machine learning, and computing infrastructure. This can be a revolution as industrial revolution (Radanliev & Roure, 2022) (Faiyazuddin et al., 2025). Such application of AI enhances the patient outcomes as a personalized medicine may be provided, there will be fewer side effects, and hospital admissions would be more optimized (Varnosfaderani & Forouzanfar, 2024) (Wierzcik et al., 2023). The fact that AI can enhance medical imaging is particularly remarkable as it will become easier and more correct to interpret such images as X-rays, MRIs, and CT scans, which will result in faster and more precise diagnosis (Khalifa & Albadawy, 2024). AI algorithms have the ability to examine massive amounts of patient data, such as medical photographs, bio-signals, and vital signs. This assists health workers to identify and detect diseases much faster and more accurately (Al-antari, 2023)Image analysis by machine learning can be excellent at detecting slight changes, minimizing human error, and minimizing fatigue. This enhances the quality of diagnostic assessment in general (Khalifa & Albadawy, 2024) (Nia et al., 2023). The ability of AI to view complex medical images aids in the early detection of such severe conditions as cancer, cardiovascular diseases, and neurological disorders. This would allow beginning earlier treatments and improving their outcomes (Coelho, 2023; Ragavi et al., 2021). AI enhances the quality of medical imaging through identifying patterns and assisting doctors in making decisions, and as a result, diagnosis is more accurate and faster (Mhaouch et al., 2025).

CONCLUSION

The present paper provides the first end-to-end computational pipeline to predict and prioritize host-pathogen interactions (HPIs) through the innovative integration of multi-omics data, machine learning modeling, and structural bioinformatics in a mixed-method prospective. By applying a set of predictive methods to determine high-confidence protein-protein interactions, a set of predictive algorithms trained on benchmarks of interaction data with the provision of some biologically relevant attributes such as domain-domain compatibility, sequence homolog, subcellular localization, we found 180 high-confidence of protein-protein interactions amongst nine of the models that we simulated. The predicted interactions were mainly effector proteins and immune modulators as it was reflected in the functional annotations. These two forms of proteins play a great role in enhancing the virulence of pathogens and transformation of immune system. VisitNet-Dock docking programs indicated that those interactions were physically possible in binding affinity (8G) and metrics of docking confidence. Numerous predictions demonstrated they were thermodynamically feasible (86 1). The functional grouping was reaffirmed using the hybrid figures and class-related analyses which indicated that there was stability on effector docking profiles along with the high interaction scores. This proves their status as significant brokers of subversion of hosts. The pipeline identified both well-known host targets, but also proteins with little popular awareness and centrality scores in predicted

interaction networks too. This implies emerging treatment targets which are to be investigated. The human-in-the-loop component that involved interrogating immunologists and health specialists on infectious diseases provided the model outputs with more qualitative validation and interpretive breadth. On the whole, the findings demonstrate that computational biology can efficiently expedite the process of HPI discovery, particularly, in high-risk/rapidly evolving pathogens, within a strategic approach to the research coupled with experimental results. Its modular format allows the simple modification to accommodate any host-pathogen combination and the method could also be readily adapted by a short number of minor modifications to work with novel disease systems or zoonotic reservoirs. This research does not only contribute to the development of predictive immunopathology, but also to the questions of employing artificial intelligence in the study of infectious diseases. In further studies we will subject the highest-ranked interactions to testing in the laboratory and introduce them to host-pathogen co-evolutionary computer models so that they are more specific.

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