

|    |   |                              |                          |  |                |                                       |
|----|---|------------------------------|--------------------------|--|----------------|---------------------------------------|
| 1  | <a href="#">Nature</a>                          | ChEMBL, BindingDB            | Graph CNN                | Graph-based molecular learning         | 85%            | ROC-AUC, PR-AUC                       |
| 2  | <a href="#">MolTrans</a>                        | BindingDB, Davis             | Transformer              | Attention-based sequence model         | 82.6 (CI)      | Concordance Index, MSE                |
| 3  | <a href="#">DeepDTA</a>                         | Davis, KIBA                  | CNN for SMILES & protein | End-to-end DL without features         | 0.863 (CI)     | MSE, RMSE, CI                         |
| 4  | <a href="#">GraphDTA</a>                        | KIBA, Davis                  | GCN + CNN                | Graphs for molecules, CNN for proteins | 0.891 (CI)     | CI, MSE                               |
| 5  | <a href="#">STGCN Model</a>                     | GDSC, CCLE                   | Spatio-Temporal GCN      | Time-based drug response prediction    | 76.4 %         | RMSE, R <sup>2</sup>                  |
| 6  | <a href="#">AlphaFold</a>                       | Protein structure DB         | Deep CNN                 | Near-atomic accuracy protein folding   | >90 % accuracy | RMSD, TM-score                        |
| 7  | <a href="#">Insilico Medicine (Fibrosis AI)</a> | Proprietary + ChEMBL         | GAN + RNN                | AI-designed fibrosis drugs             | N/A            | Chemical similarity, In vitro success |
| 8  | <a href="#">AI-CRISPR Screening</a>             | Genomics, Cancer cell lines  | ML over CRISPR data      | Identifies oncogenes using AI          | ~85 %          | Recall, Precision                     |
| 9  | <a href="#">Benevolent AI for COVID-19</a>      | COVID-related proteins       | Graph-based target ID    | JAK inhibitors found via AI            | N/A            | Literature validation                 |
| 10 | <a href="#">Personalized Medicine AI</a>        | Omics (genomics, proteomics) | ML + Feature Engineering | Predicts patient-specific response     | 70–88%         | Accuracy, AUC, F1-score               |

| Link   | Datas<br>et                  | Model /<br>Methodolog<br>y                    | Novelty   | Accur<br>acy<br>(%)                 | Evalua<br>tion<br>Metric<br>s    |
|--|------------------------------|---|---|-------------------------------------|----------------------------------|
| <a href="#">Nature:<br/>Deep<br/>learning for<br/>drug<br/>discovery</a> | ChEM<br>BL,<br>Bindin<br>gDB | Graph CNN,<br>SMILES-to-<br>vector DL         | Used message-passing<br>neural networks for<br>compound property<br>prediction  | 85%<br>(classif<br>ication<br>task) | ROC-<br>AUC,<br>PR-<br>AUC       |
| <a href="#">MolTrans:<br/>Transforme<br/>r for DTI</a>                   | Bindin<br>gDB,<br>Davis      | Transformer<br>+ Attention                    | Novel sequence-based<br>model using attention<br>for drug-target<br>interaction | 82.6<br>(CI<br>score)               | Concor<br>dance<br>Index,<br>MSE |
| DeepDTA:<br>Deep<br>learning for<br>DTI<br>prediction                    | Davis,<br>KIBA               | CNN for<br>SMILES and<br>protein<br>sequences | End-to-end DL from raw<br>sequences without<br>feature engineering              | 0.863<br>(CI)                       | MSE,<br>CI,<br>RMSE              |
| GraphDTA:<br>GCN for<br>DTI  | KIBA,<br>Davis               | Graph Conv.<br>Network<br>(GCN) +<br>CNN      | Uses molecular graph<br>structure + protein CNN                                 | 0.891<br>(CI)                       | CI, MSE                          |
| <a href="#">STGCN for<br/>Drug<br/>Response<br/>Prediction</a>           | GDSC<br>,<br>CCLE            | Spatial-<br>temporal<br>GCN                   | Captures gene-drug<br>interaction over time                                     | 76.4%                               | RMSE,<br>R <sup>2</sup>          |