**Novel** **1,2,3-****Triazole** **Erlotinib Derivatives as Potent IDO1 Inhibitors: Design, Drug-Target Interactions Prediction, Synthesis, Biological Evaluation, Molecular Docking and ADME Properties Studies**

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# Figure S1. The docking binding mode of compound a (wheat) with IDO1.



# Figure S2. The docking binding mode of compound c (purple) with IDO1.



# Figure S3. The docking binding mode of compound erlotinib (pale-yellow) with IDO1.



# Figure S4-1. 1H NMR spectrum (600MHz, DMSO-d6) of compound a

# Figure S4-2. 13C NMR spectrum (150MHz, DMSO-d6) of compound a



# Figure S5-1. 1H NMR spectrum (600MHz, DMSO-d6) of compound b





# Figure S5-2. 13C NMR spectrum (150MHz, DMSO-d6) of compound b



# Figure S6-1. 1H NMR spectrum (600MHz, DMSO-d6) of compound c





# Figure S6-2. 13C NMR spectrum (150MHz, DMSO-d6) of compound c



# Figure S7-1. 1H NMR spectrum (600MHz, DMSO-d6) of compound d





# Figure S7-2. 13C NMR spectrum (150MHz, DMSO-d6) of compound d



# Figure S8-1. 1H NMR spectrum (600MHz, DMSO-d6) of compound e





# Figure S8-2. 13C NMR spectrum (150MHz, DMSO-d6) of compound e

