Synthesis, Evaluation of Antimicrobial, Antioxidant and Anticancer Properties of a New Series of Linked Tris-Heterocycles

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In search of versatile lead molecules with potential pharmacological properties, a new series of linked heterocyles, 4-(3,5-dimethyl-1-(2-phenylquinazolin-4-yl)-1*H*-pyrazol-4-yl)-6-aryl pyrimidin-2-amines **8a-j**, have been synthesized efficiently both quantitavely and qualitatively *via* one-pot three-component cyclo-condensation reaction of guanidine hydrochloride with the corresponding chalcones **7a-j**. Structures of all the newly synthesized compounds **8a-j** were confirmed by spectral data and elemental analysis, and further screened for their *in vitro* antimicrobial, antioxidant and anticancer activities. Antimicrobial studies revealed that, compounds **8d (**4-nitrophenyl), **8h (**2-pyridyl), **8i (**2-furyl**)**, and **8j** (5-thiazolyl) displayed appreciable activity against the tested microbes. Antioxidant assay revealed that, compounds **8e** (2-hydroxyphenyl), **8f** (4-aminophenyl), **8g** (4-hydroxyphenyl) and **8h** (2-pyridyl) showed prominent antioxidant activity with IC_{50} values lower than the positive control Trolox. Similarly, *In vitro* anticancer screening revealed that the compounds **8d (**4-nitrophenyl), **8e (**2-hydroxyphenyl), **8g (**4-hydroxyphenyl) and **8h** (2-pyridyl) evolved as potent anti-cancer agents, further supported by docking studies as well.

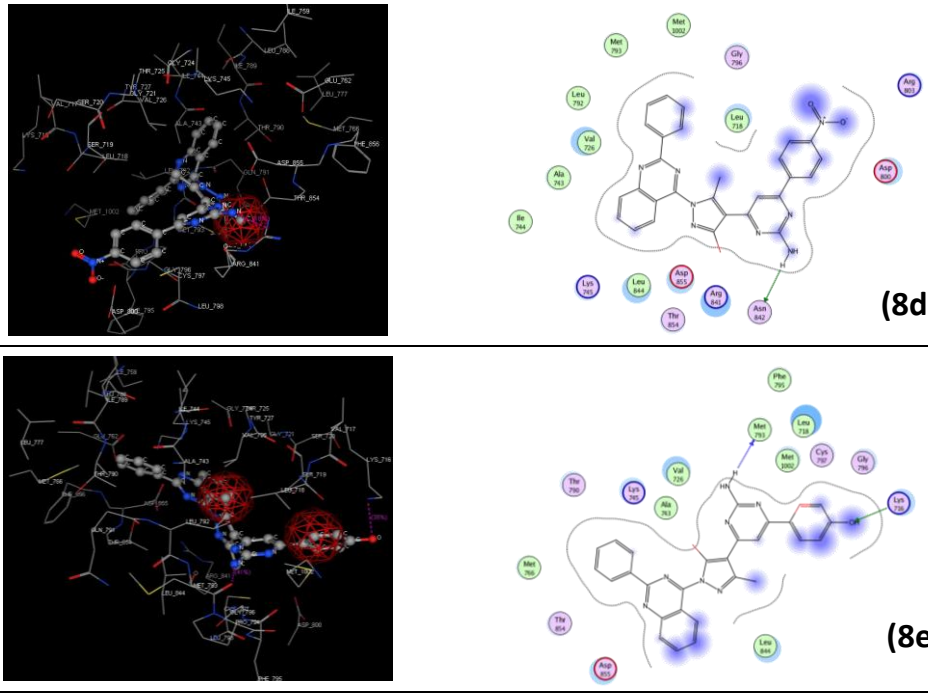

Fig. *In silico* orientation and interactions of ligand **8d** and **8e**, showing key hydrophobic and H-bonding interactions in active pocket of 2ITO