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In vitro Binding Effect Of Potential Inhibitors Identified By Docking To The Nickel Response Regulator (NikR) From *Helicobacter Pylori*

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Abstract: NikR protein is a regulator responsible for controlling the expression of certain genes such as ureA and ureB in Helicobacter pylori. The proteins ureA and ureB are the structural subunits of urease, an enzyme important for the H. pylori adaptation in low pH niche as an essential factor for living in human stomach. Thus, NikR is a good candidate for medicine targeting. Previously, we reported a molecular docking between X-ray structure of H. pylori NikR and a chemical database, and some potential inhibitors have been identified. The NikR from H. pylori strain 26695 was cloned into the plasmid pProExHTb for expression in Escherichia coli BL21 (DE3). Native H. pylori NikR with hexa-histidine tag was purified. In native conditions, HpNiKR was a tetrameric molecule as seen by N–PAGE and by size-exclusion chromatography, and confirmed by MALDI mass spectrometry. The ureA promoter fragment for HpNikR binding experiments was constructed via incubation by two synthesized complementary single oligonucleotide chains. The EMSAs competition assays showed the disassociation from DNA promoter–Holo-HpNikR complex as the addition of two compounds in range of 250-300 µM. The in vitro experiments showed that two compounds can bind to HpNikR, affecting the protein recognition with promoter of ureA.

Key words: Helicobacter pylori, NiKR, Inhibitors, binding, in vitro.

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