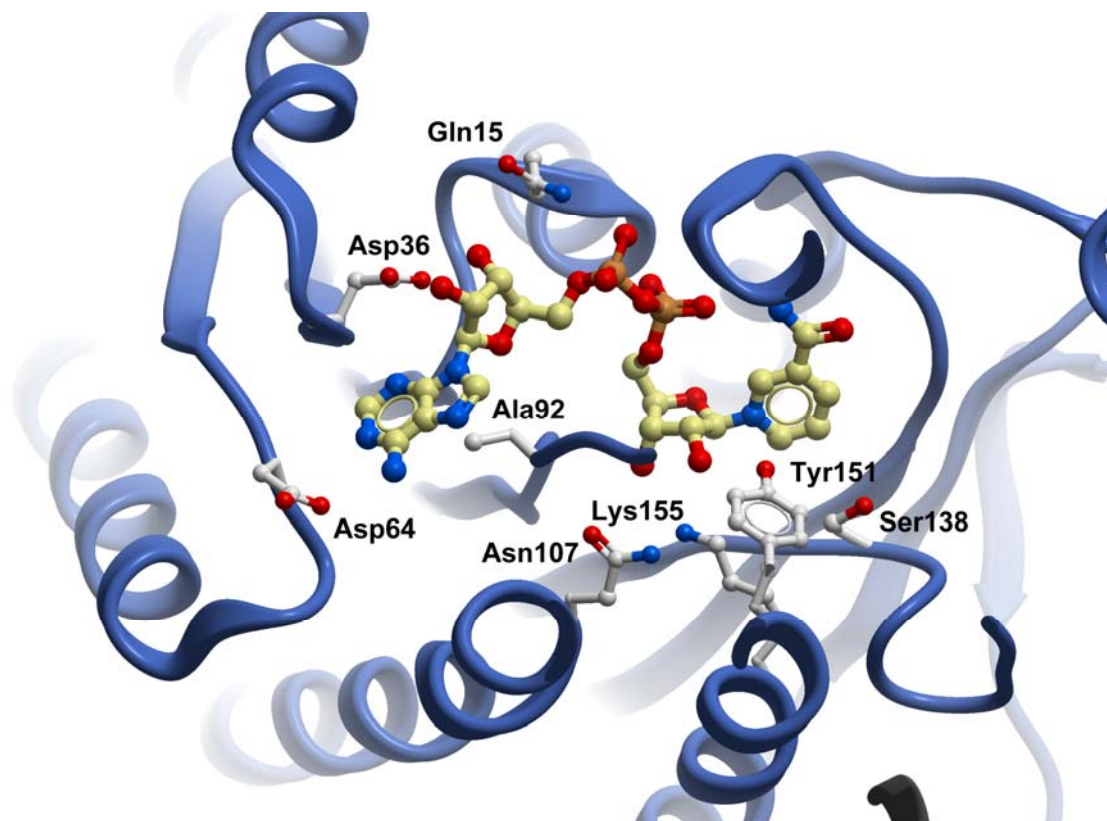


High-affinity Inhibitors of Human NAD⁺-dependent 15-Hydroxyprostaglandin Dehydrogenase: Mechanisms of Inhibition and Structure-activity Relationships

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SUPPLEMENTARY INFORMATION FIGURE S2



Binding of the cofactor NAD⁺ in the active site of human 15-PGDH. The acidic residue Asp36 forms hydrogen bonds to the 2'- and 3'-hydroxyl groups of the adenine ribose moiety, while Asp64 forms a hydrogen bond to the amino group of the adenine moiety. The nicotinamide moiety of NAD⁺ is positioned close to the catalytic tetrad (Asn107, Ser138, Tyr151 and Lys155).