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Interaction of Synthetic Glycoconjugates with Glycosidases and Lectins

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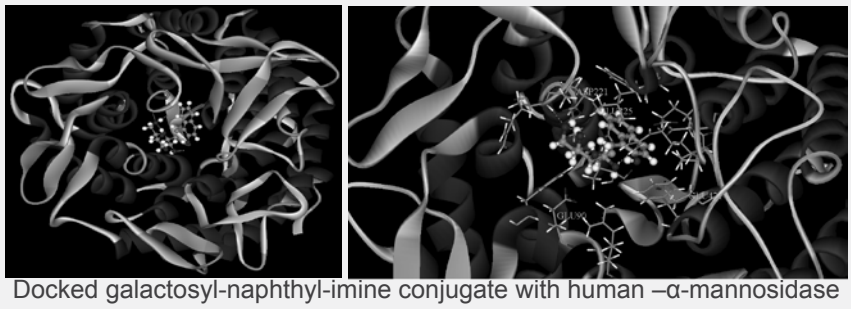
Inhibition of the glycosidases as well as alteration of lectin properties by chemically modified glycoconjugates can have profound effect in biology. Several C_1-imino conjugates of D-galactose, D-lactose and D-ribose and C_2-imino conjugates of D-glucose, where the nitrogen center was substituted by the salicylidene or naphthylidene, were synthesized and characterized. Those glyco-imino-aromatic conjugates, which are transition state analogues, exhibited 100% inhibition of glycosidases extracted from soybean and jack bean meal. Some of these conjugates exhibited IC_{50} values in the range of 20 to 50 μM and hence are potent inhibitors of glycosidases. The kinetic studies suggested non-competitive inhibition. Similar studies have been carried out by treating the lectins of both glucose/mannose specific (DLL-I, pea lectin, lentil lectin), galactose specific (DLL-II, PNA, SBA, moringa lectin) as well as lactose specific (unio lectin) with these glycoconjugates. Those conjugates which exhibit highest glycosidase inhibition also inhibit the agglutination of lectins and thereby modify the property of lectin accordingly. Both the experimental and computational docking studies revealed differences in the binding strengths of naphthylidene *vs.* salicylidene as well as galactosyl *vs.* lactosyl moieties present in these conjugates. The differential interactions of these glyco-conjugates have been addressed by computational docking studies to quantify the same exists between the enzyme (Figure) or lectin and the corresponding glycoconjugate. The present studies clearly supported the binding mainly through polar interactions in addition to exhibiting some nonpolar/hydrophobic ones.



Docked galactosyl-naphthyl-imine conjugate with human –α-mannosidase