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**Molecular basis for the affinity and specificity in the binding of five-membered iminocyclitols with glycosidases: An experimental and theoretical synergy**

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**Highlights**

- Design and synthesis of novel five membered iminocyclitols.
- Inhibition of glycosidases.
- Atomistic level explanation for specificity via molecular dynamics simulation.
- Direct correlation between theoretically calculated binding energies and observed IC<sub>50</sub> values.

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