



THE UNIVERSITY OF
TOLEDO
1872

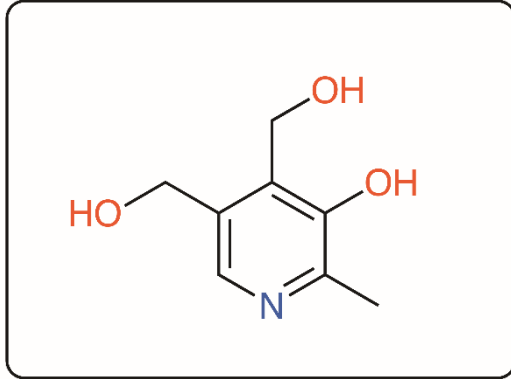


Using Neutron Scattering, Diffraction, and
Computational Methods to Identify the Molecular
Determinants that Govern Pyridoxal 5'-Phosphate-
Dependent Catalysis

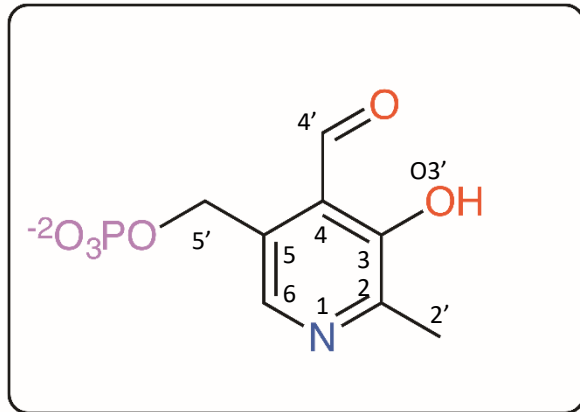
Steven Dajnowicz

Catalytic versatility

Pyridoxine (vitamin B6)

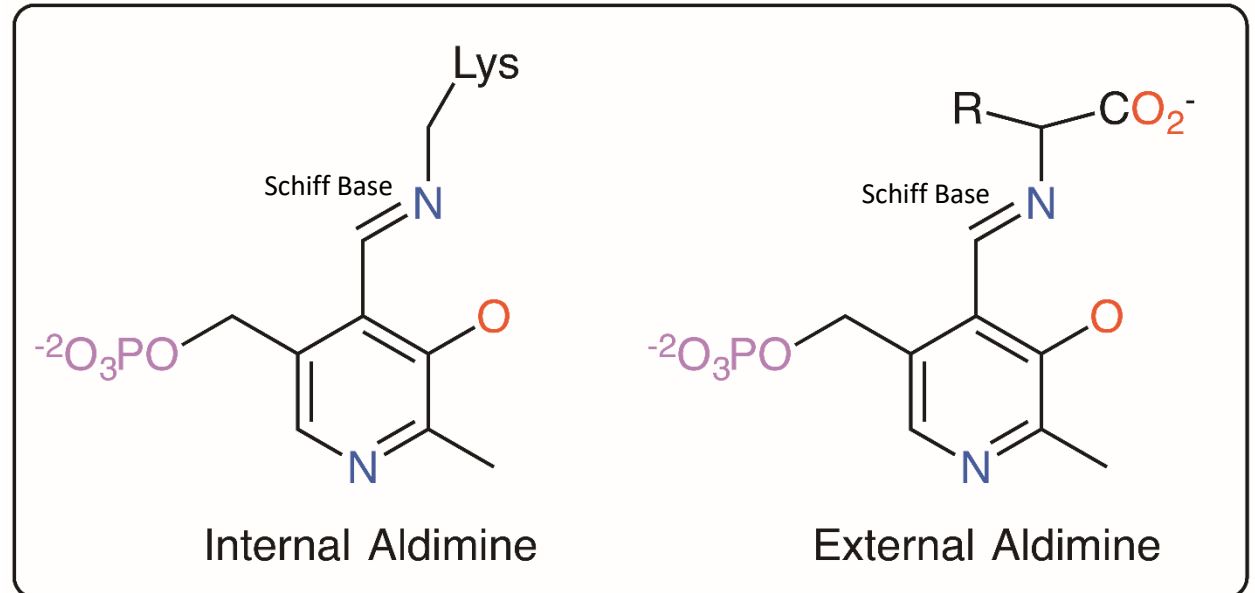


Pyridoxal 5'-phosphate (PLP)



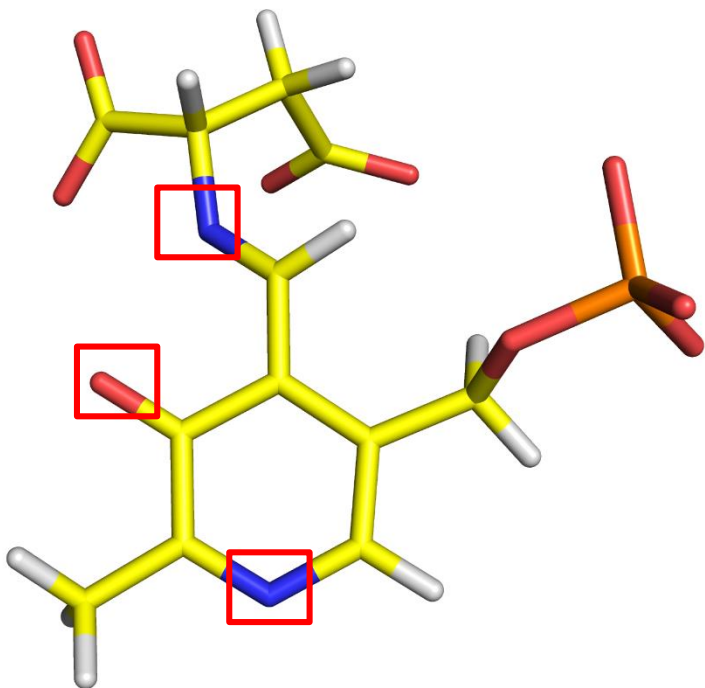
PLP-dependent reactions

- Decarboxylation
- Racemization
- **Transamination** **Aspartate Aminotransferase (AAT)**
- β/γ -elimination
- Retro Aldol Cleavage
- Phosphorylation
- Replacement

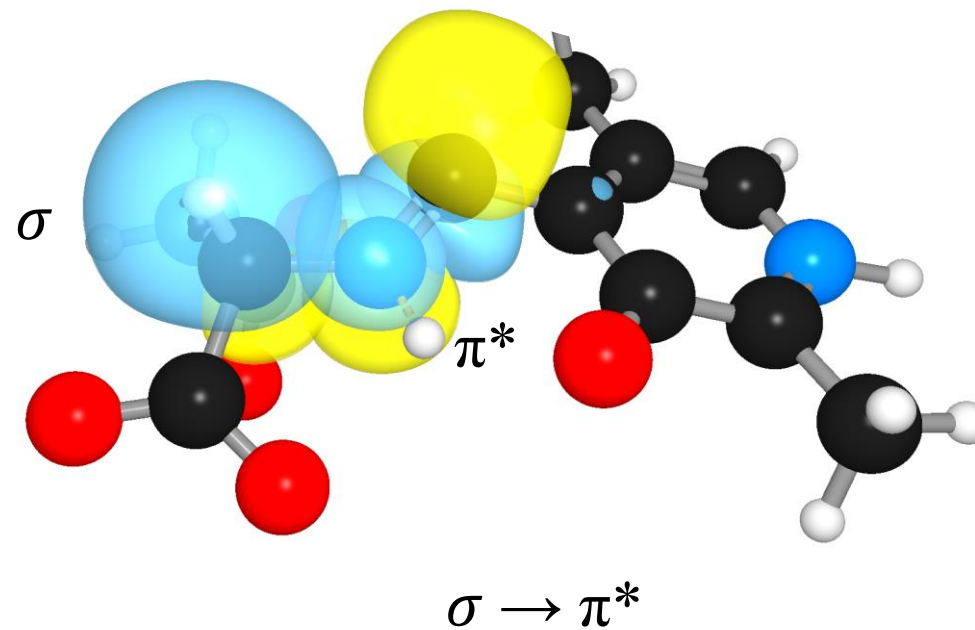


Electronic modulation of PLP

Selective protonation



Stereoelectronic control



Dunathan, H. (1966). *PNAS* **55**, 712-716

Dutta, S. (2014). *J. Phys. Chem. B.* **118**, 11077-11089

Weinhold, F. (2013). *J. Comp. Chem.* **34**, 1429-1437