

Supporting Information section for

Conformations of Antipyridines

Michael Roumanos and Miklos Kertesz*

Department of Chemistry, Georgetown University, Washington, DC 20057-1227, USA

Torsions were used to measure α and β values because they are simple to calculate and are platform-versatile. Moreover, they were chosen since a torsion-defined α/β angle closely describes the actual out-of-plane bending at each nitrogen, as seen in Fig. S1 and Fig. S2 below.

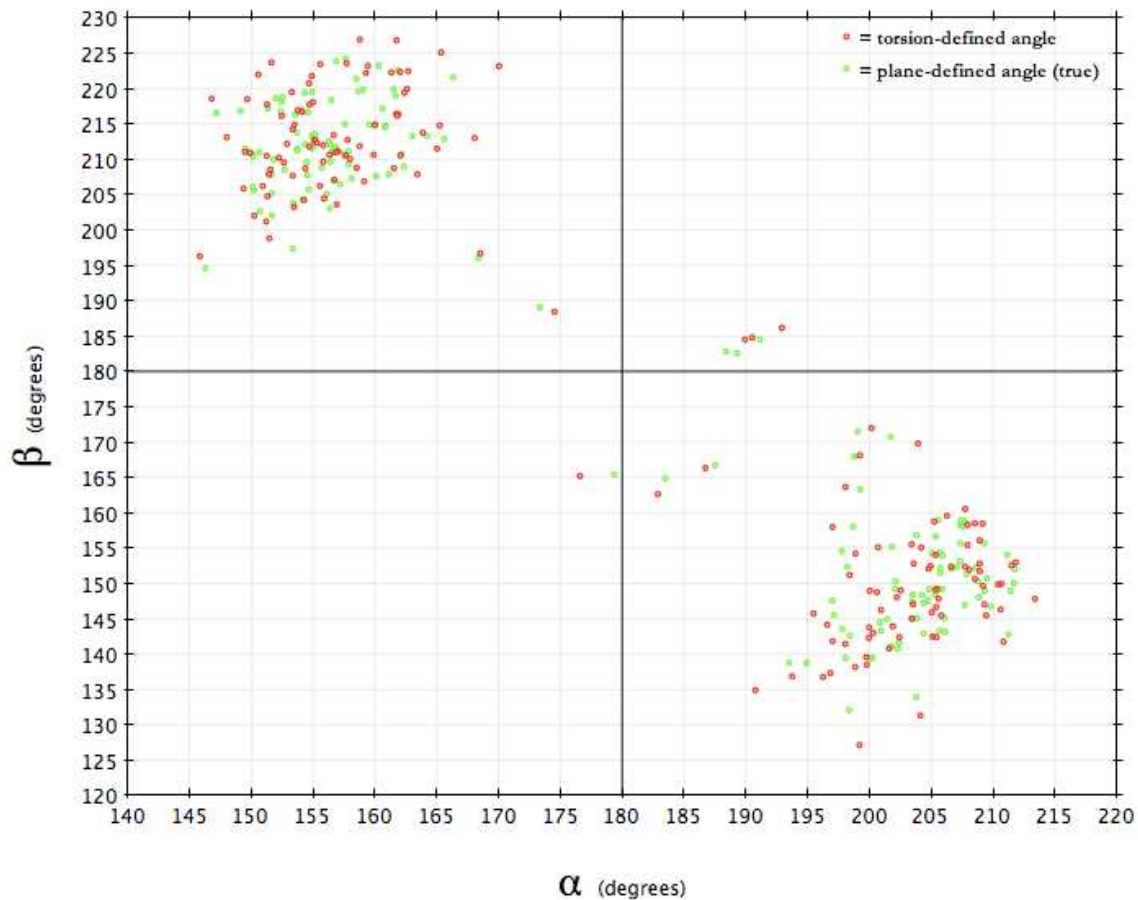


Figure S1: Torsion-defined angles are compared with true out-of-plane bending angles at the antipyrine substructure nitrogens. For graph clarity, calculated symmetry partners from space groups with an inversion center or glide plane were excluded.

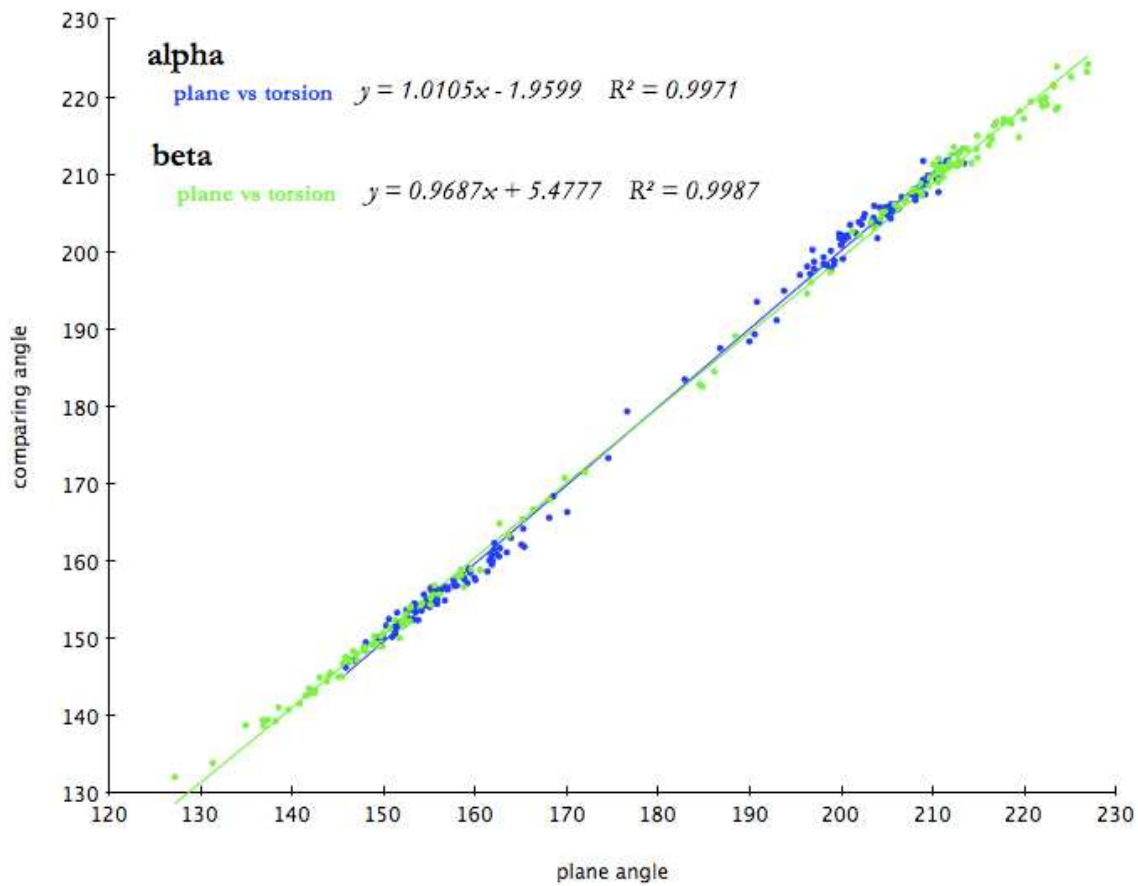


Figure S2: Torsion-defined α and β angles are directly compared with true out-of-plane bending angles at the antipyrine substructure nitrogens.