Supporting Information:

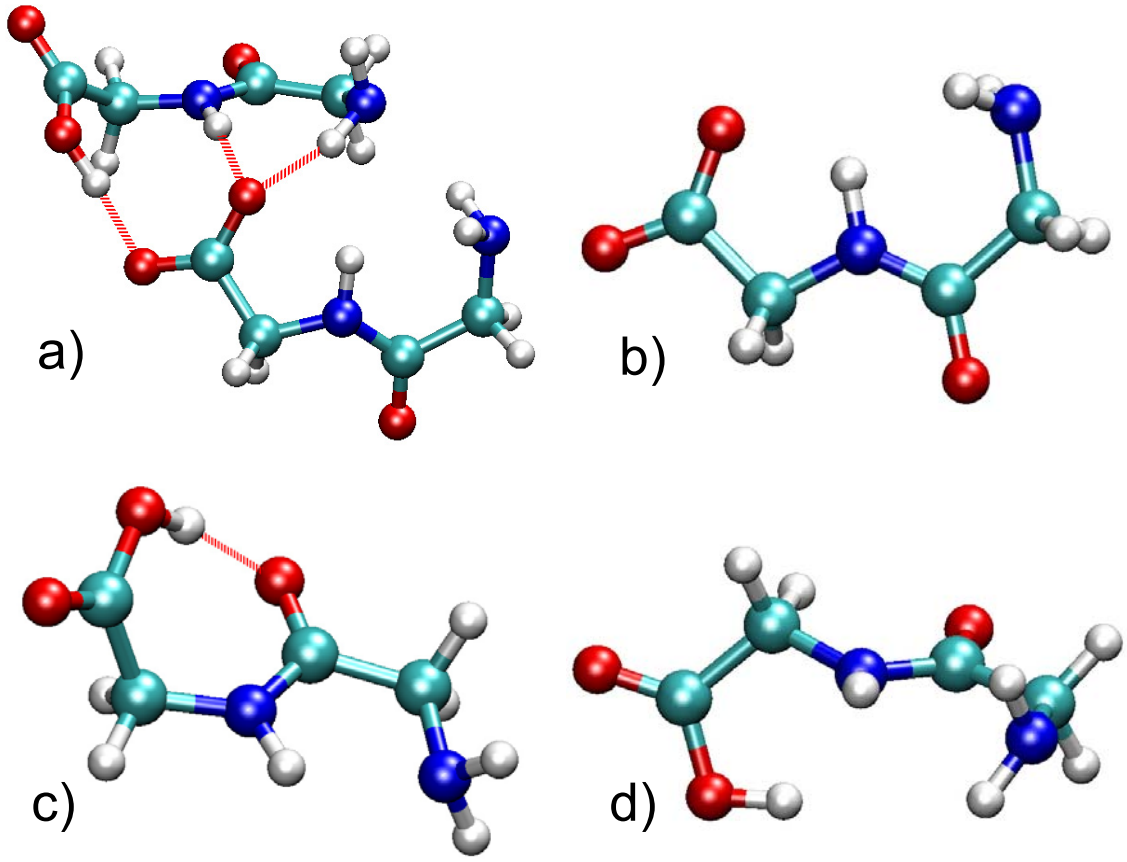

Figure S1. Optimized DFT structures for (a)deprotonated diglycine dimer $[GG\text{-}H]^{-}\cdot(GG)$ (lowest-energy structure), (b) deprotonated diglycine monomer $[GG\text{-}H]^{-}$ (lowest-energy structure), (c) neutral diglycine monomer (lowest-energy, H-bonded structure), and (d) neutral diglycine monomer (open structure). Typical hydrogen bonds (<3.0 Å, 180º ± 25º) are indicated as red dashed lines, loose "hydrogen-bond-like" interactions[48] (<3.5 Å, 180º ± 50º) as blue dotted lines. The white balls are H, the green C, the red O and the blue N. Graphics generated using VMD.[49]

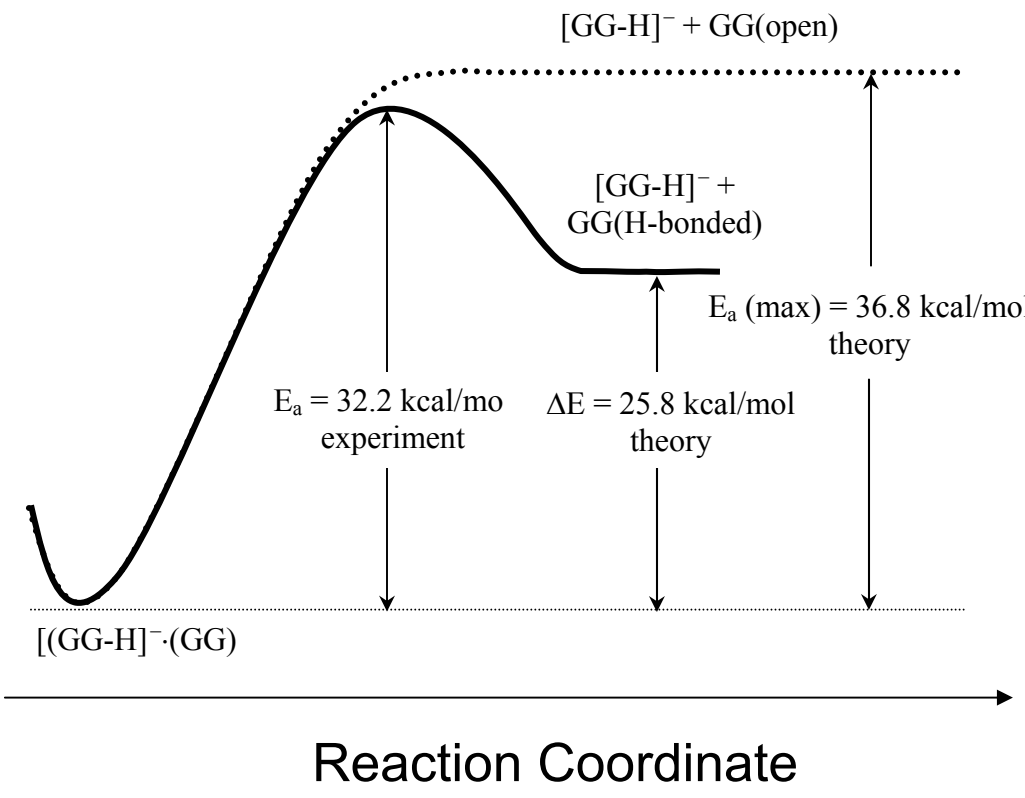

Figure S2. Schematic reaction coordinate diagram for deprotonated diglycine dimer dissociation, $[GG\text{-}H]^{-} \bullet (GG) \rightarrow [GG\text{-}H]^{-} + GG$, illustrating the experimental activation energy and the DFT dissociation energy (solid line). The dashed line represents dissociation to $[GG\text{-}H]^{-}$ and the open form of GG.