Supporting Information

Correlation of TrpGly and GlyTrp Rotamer Structure with W7 and W10 UV Resonance Raman Modes and Fluorescence Emission Shifts

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Table S1. Calculated dihedral angles (χ^1, χ^2, ψ^1, φ^2, ψ^2) in degrees for the most stable tryptophan dipeptide conformers

TrpGly species	**(χ^1, χ^2, ψ^1, φ^2, ψ^2)/degrees**
Zwitterion (stretched)	(-171, 108, -80, -180, 0)
Zwitterion (folded)	(64, 80, 155, -175, -178)
Anion	(158, 96, -76, -126, 1)
GlyTrp species	
Zwitterion	(61, 92, 177, 140, 13)
Anion	(-66, 102, 160, -131, 168)

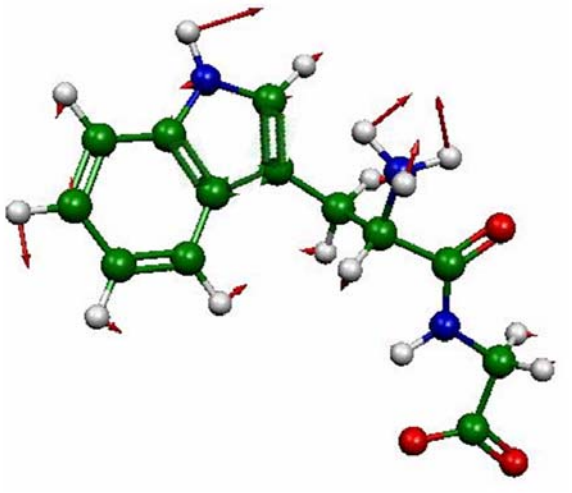
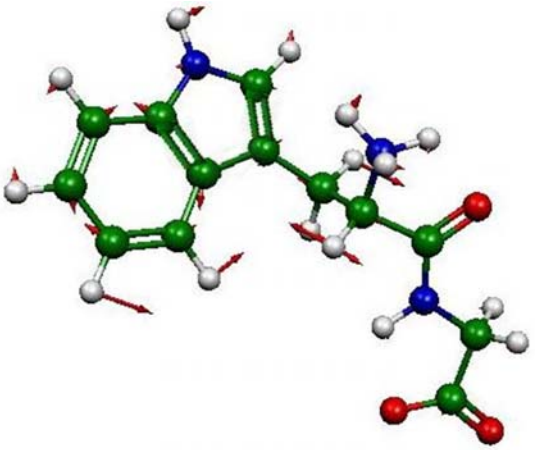
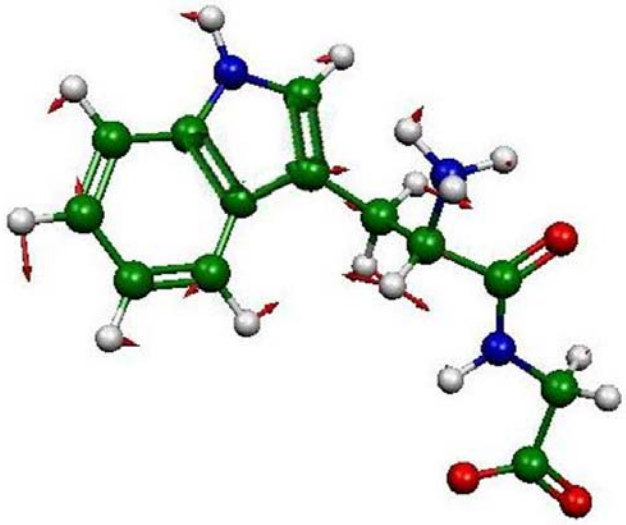


Figure S1. TrpGly zwitterion, calculated vibration at 1395 cm^{-1}. These motions are common to all dipeptides: C8---N1---C2, C5---C6---C7, and C9---C1---$C_{methylene}$ asymmetric stretches and N1---H and C6---H in-plane bending.



1310

Figure S2. Calculated vibration at 1310 cm^{-1} for the TrpGly zwitterion. Atom motions are similar to those for the 1320 cm^{-1} vibration.



1320

Figure S3. TrpGly zwitterion, calculated vibration at 1320 cm^{-1}. This vibration contains asymmetric stretches at C8---C9---C4, C9---C3---$C_{methylene}$, and C5---C6---C7, with an N1---C2---C3 bend. Prominent off-ring vibrations are the C3---$C_{methylene}$---C_{α} asymmetric stretch, the $C_{methylene}$---H bend, and the C_{α}---H bend for all Trp dipeptides**.**

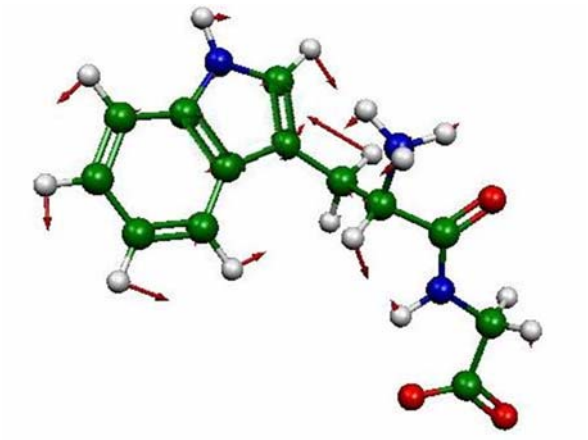


Figure S4. TrpGly zwitterion, calculated vibration at 1329 cm^{-1}. Vibrations for all Trp dipeptide species consists of synchronous, C---H in-plane bending for C4 to C7, with a C2---C3---C4 asymmetric stretch as well as off-ring H-bends at $C_{methylene}$ and C_{α}. All but the TrpGly zwitterion have an additional C4---C9 stretch.