

Kinetic Method

Name _____

	height tyr	height gln or asp	branching ratio	$\Delta\Delta H/RT$	$\Delta\Delta H(@900K)$ (kJ/mol)
tyr + gln					
tyr + gln					
tyr + gln					
Average					
tyr + asp					
tyr + asp					
tyr + asp					
Average					

Molecular Mechanics (CHARMM2.2 forcefield—gas phase)

Charges	Tyr-Na ⁺	Gln [±]	Tyr [±]	Gln-Na ⁺	$\Delta\Delta H$
Forcefield					
Gasteiger (PEOE)					

units? _____

Charges	Tyr-Na ⁺	Asp [±]	Tyr [±]	Asp-Na ⁺	$\Delta\Delta H$
Forcefield					
Gasteiger (PEOE)					