ryzue (Adiabatic scheme with single point correction for type III subm... 15.0 12.5 10.0 7.5 pKa (calc) 5.0 2.5 0.0 **-**2.5 -2.5 0.0 2.5 5.0 7.5 10.0 12.5 15.0 pKa (exp)