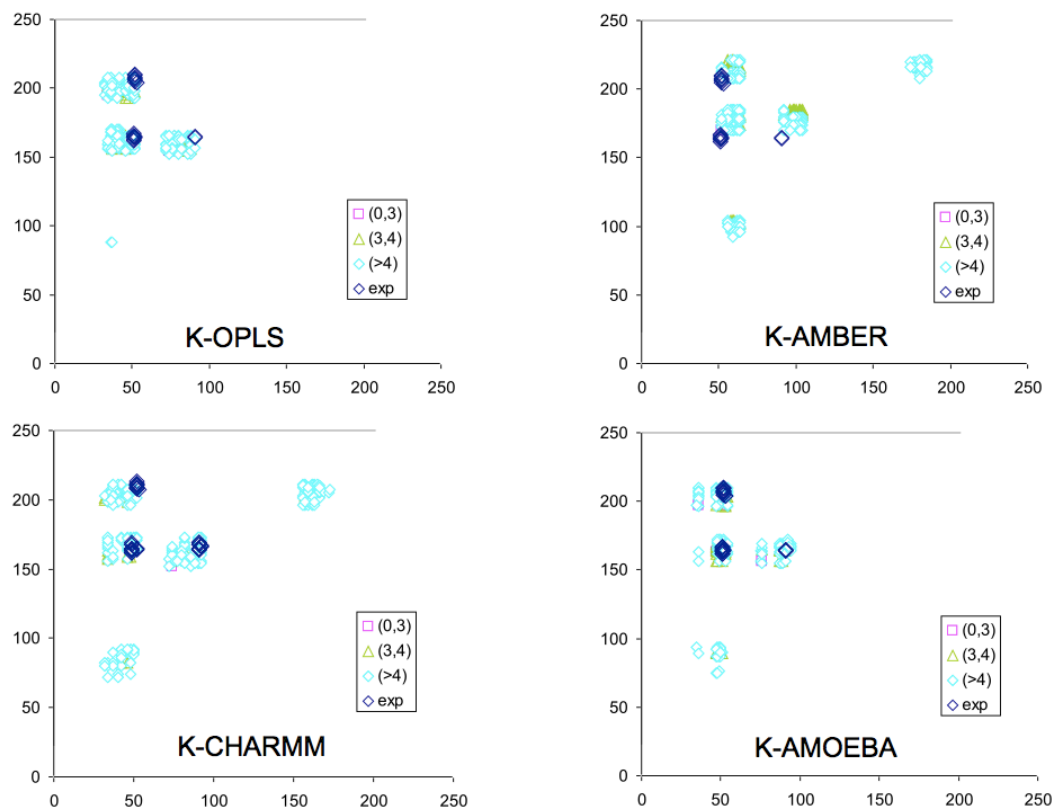
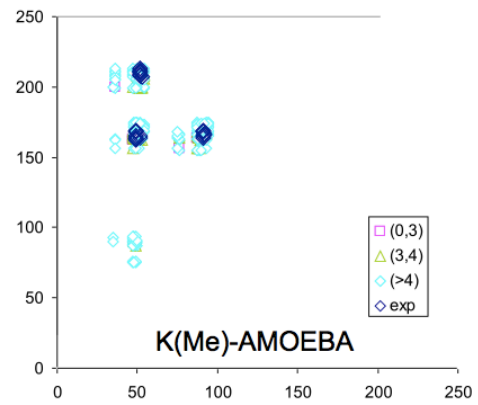
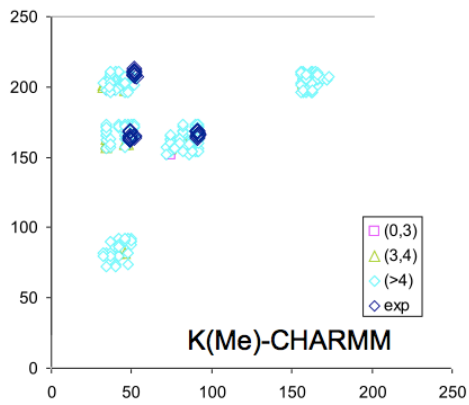
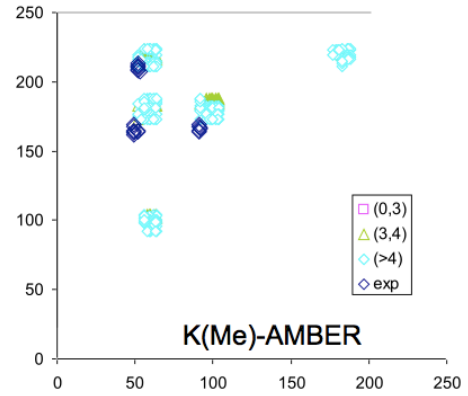
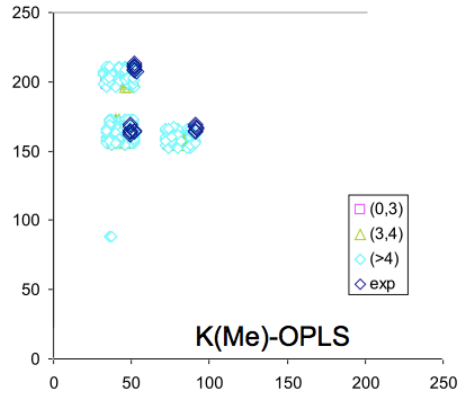


Supplemental Figure 1. Comparison of Experimental (dark blue) NOEs with predicted NOEs from 100 nsec MD simulations in explicit solvent.

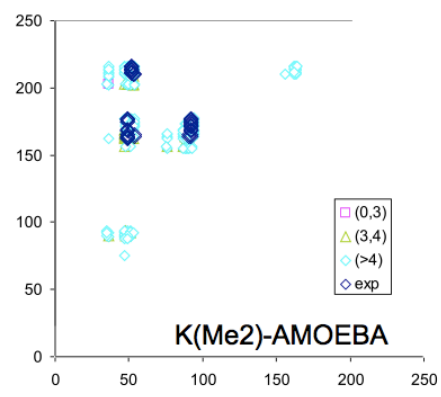
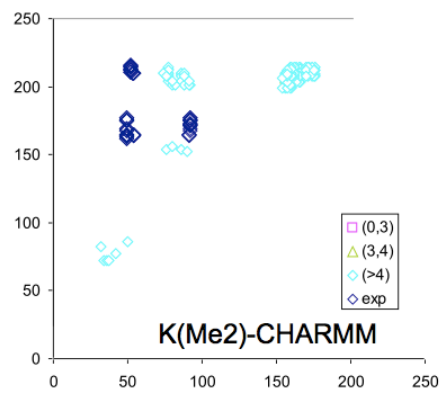
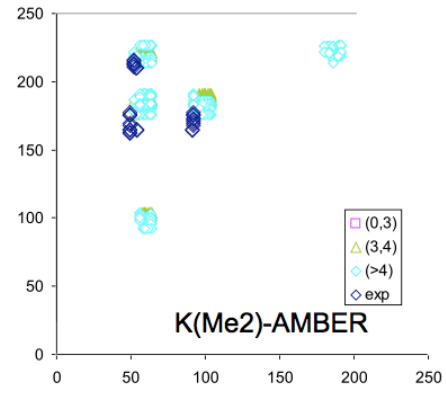
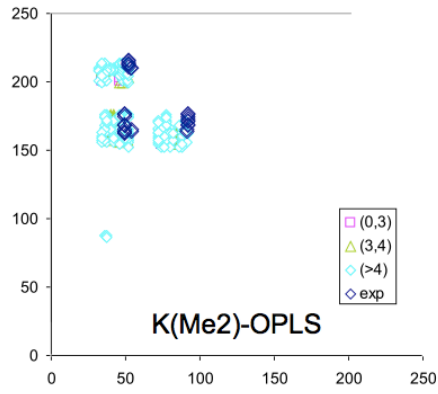
Suppl. Fig. 1a = data for Lys-9 hairpin model.



Supplemental Figure 1b. Data for Lys(Me)-9 hairpin model.



Supplemental Figure 1c. Data for Lys(Me2)-9 hairpin model.



Supplemental Figure 1d. Data for Lys(Me3)-9 hairpin model.

