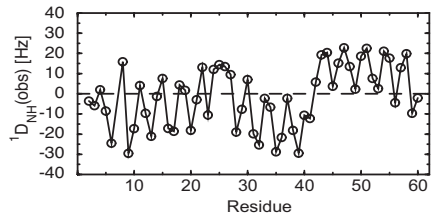
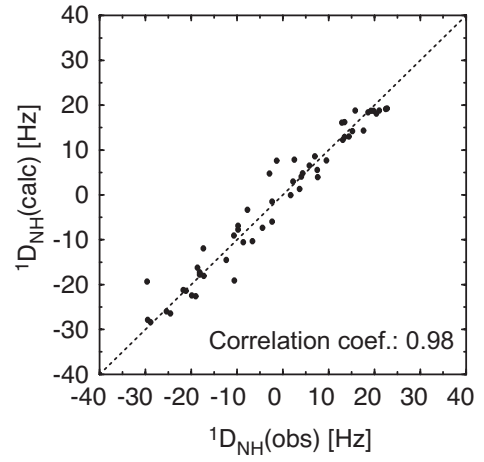


A

Fitting against structure

Experimental $^1D_{NH}$ (specific complex)Optimization of
 D_a , R , α , β , γ +
Structure (specific complex)**B**

PALES prediction

Structure (specific complex)

Based on
shape and charge distribution