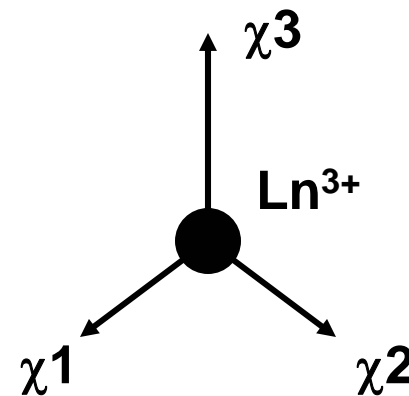


^1H - ^{15}N Structural Data and Assignment from Lanthanide Tagged Proteins: RDCs, PCSs, R_2

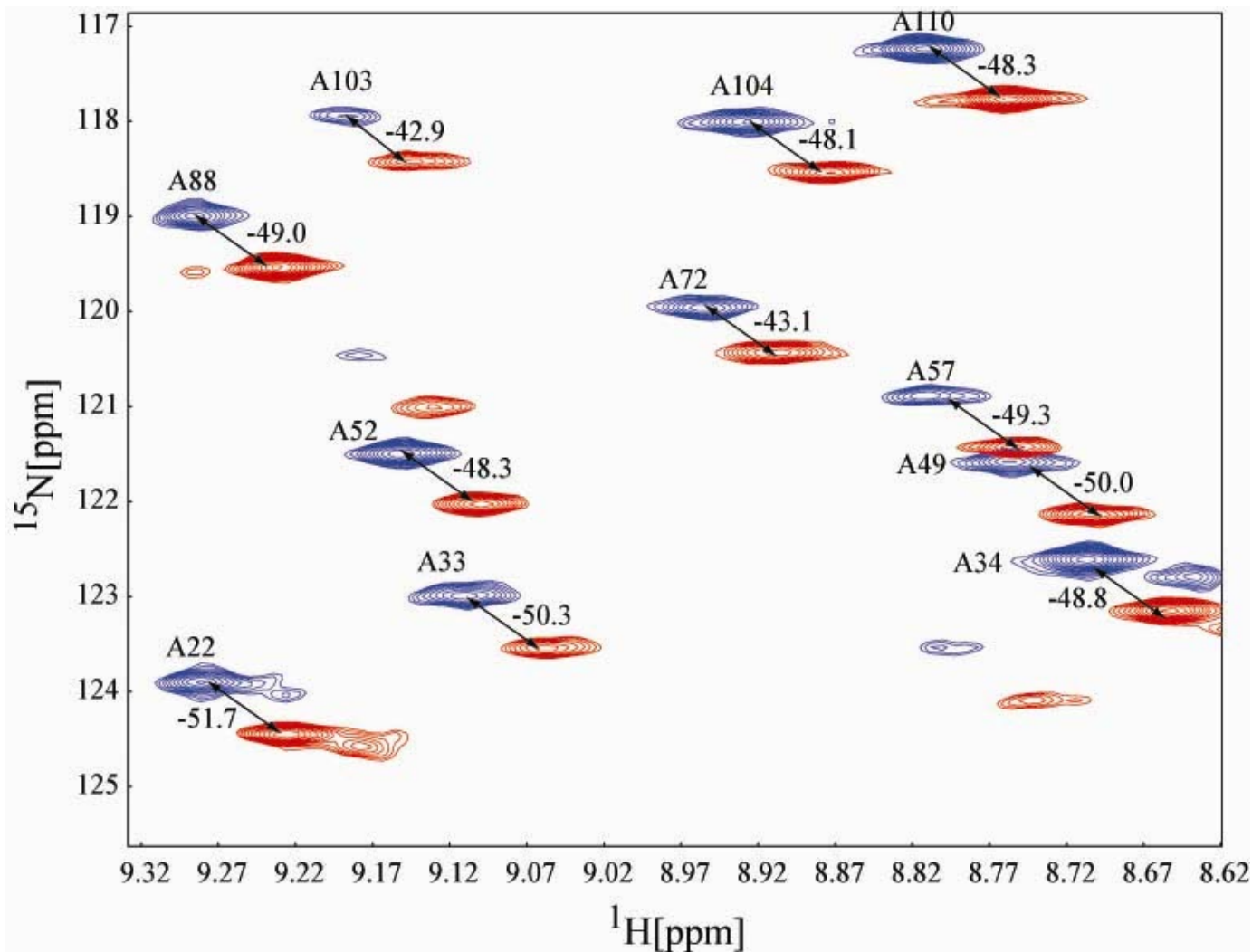


$$\text{RDC} = -(\gamma\gamma\hbar B^2)/(120\pi^3 r^3 kT) \\ \left[\frac{1}{2}\Delta\chi(3\cos^2\theta - 1) + \frac{3}{4}\delta\chi\sin^2\theta\cos\phi \right]$$

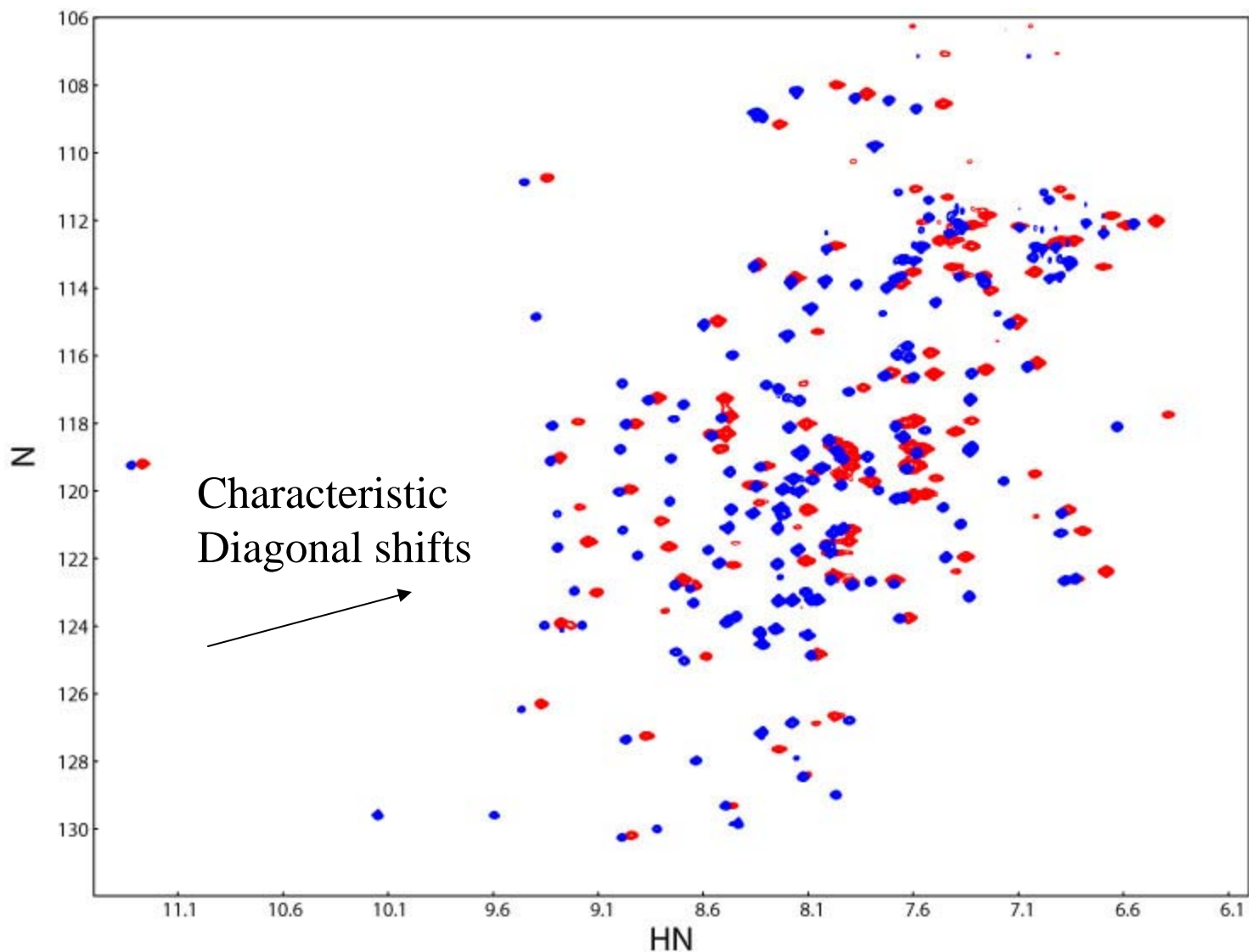
Note: B^2 dependence



TROSY-HSQC correlations give RDC data. 900 MHz Field-Induced Alignment



Comparison of Lu^{3+} and Dy^{3+} Complexes of Tagged Q15691 gives Pseudo-Contact Shifts



Pseudo-Contact Shifts Behave Like RDCs

These Provide Additional Orientation Data
and Distance Constraints

The pseudo-contact shift is due to the field from an induced dipole at the paramagnetic center. This field is given by:

$$\mathbf{B}' = \mathbf{u}/r^3 - 3\mathbf{r}(\mathbf{u}\cdot\mathbf{r})/r^5$$

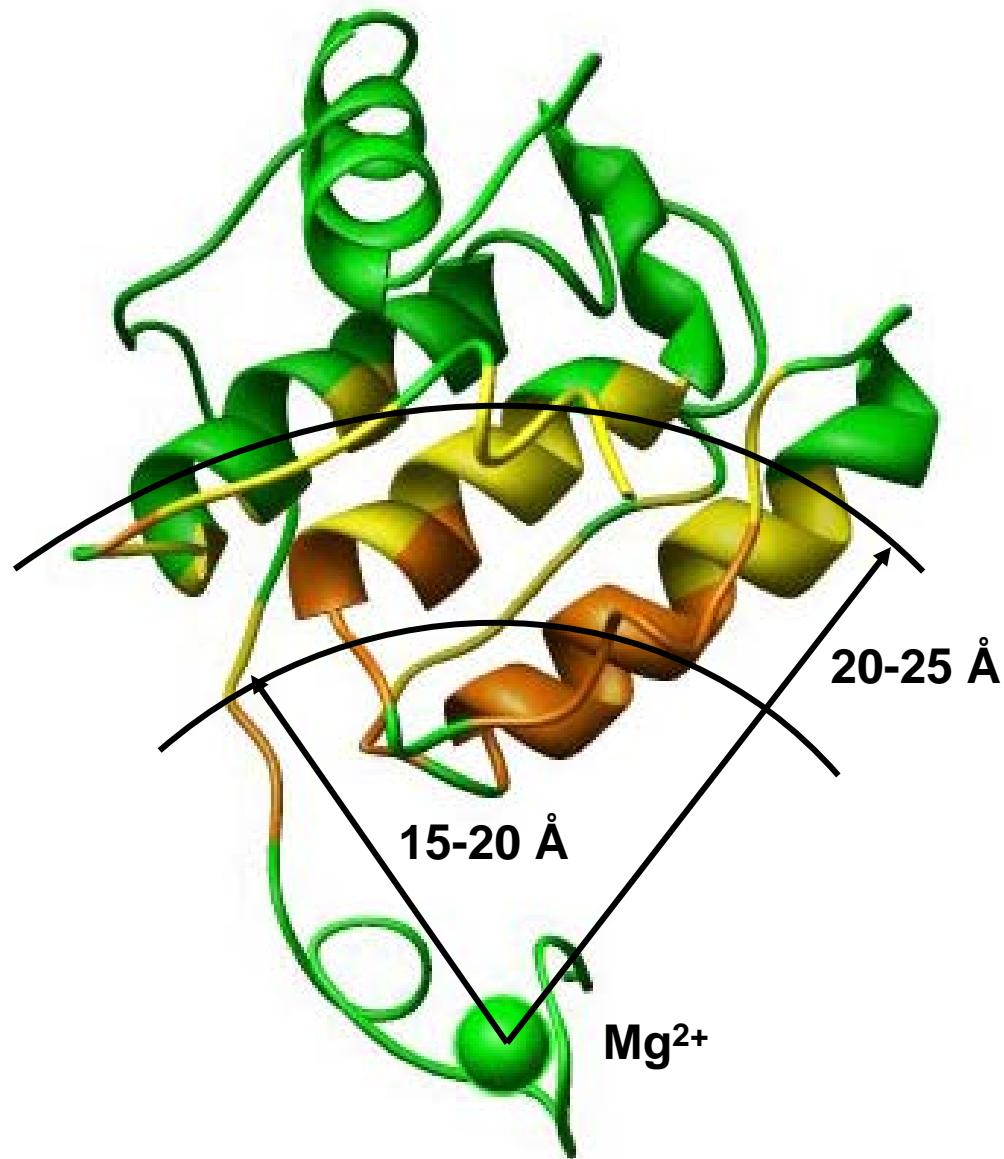
We want just the field contribution in the direction of the applied field B_0

$$\mathbf{v}\cdot\mathbf{B}' = \mathbf{v}\cdot\mathbf{u}/r^3 - 3\mathbf{v}\cdot\mathbf{r}(\mathbf{u}\cdot\mathbf{r})/r^5$$

$$= B_0/(3r^3)(X_{11} + X_{22} + X_{33}) + B_0/r^3 \sum_{ij} X_{ij} \cos\phi_i \cos\phi_j$$

The first term is the isotropic shift, the second is the anisotropic shift.
The second term is the same form as the RDC term.

$$S_{ij} = X_{ij} (2B_0^2/(15 \mu_0 kT)), \quad D_{\max} = \gamma \mu_0 kT / (4\pi B_0)$$



Other Approaches
to Limiting Sets:

1H - ^{15}N Groups
Selected by
Spin-Relaxation
Distance Mapping

Amide Exchange
Rate Groupings

Lanthanide -Tagged Hum-Q-15691