

Incorporating RDC's into Traditional Structure Calculations

1. A rough initial structure is generated using NOE's and dihedral angles, or from homologous X-ray
2. Fitting of a subset of RDC's leads to alignment parameters and axes
3. RDC's are predicted and a pseudo-energy term is added to the total energy:

$$E_{\text{rdc}} = k_{\text{rdc}} (D_{\text{calc}} - D_{\text{obs}})^2$$

4. Continue energy minimization and return to step 2