

In `test2media.m`, backcalculation is tested for N-H RDCs in two media. Two alignment tensors are calculated, one for each medium, using `updateTen()` with the correct assignments.

Results are included for 1D3Z N-H RDCs in two media, with normalized N-H vectors from the 1D3Z NMR structure (Fig. 1) and the 1UBI crystal structure (Fig. 2).

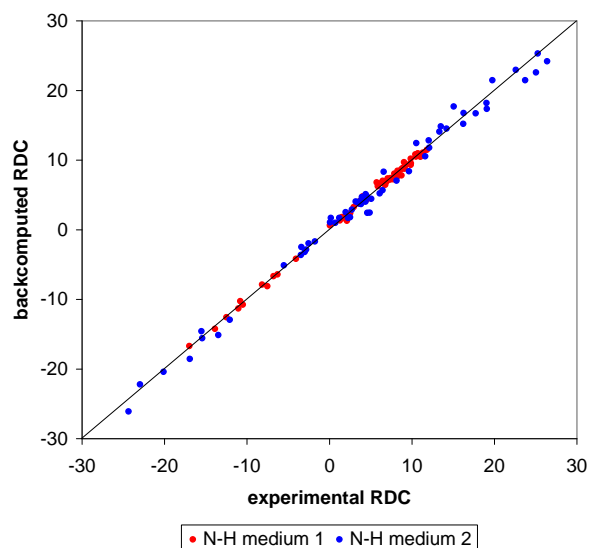


Fig 1. 1D3Z N-H RDCs in two media, 1D3Z vectors  
RDC RMSD N-H medium 1: 0.3818  
RDC RMSD N-H medium 2: 1.1364

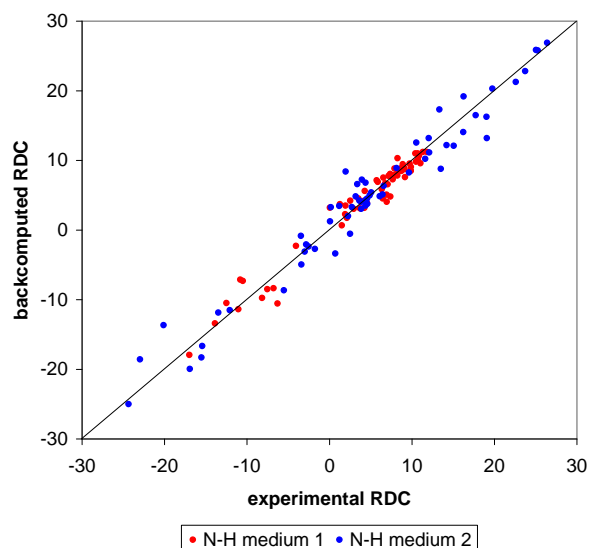


Fig 2. 1D3Z N-H RDCs in two media, 1UBI vectors  
RDC RMSD N-H medium 1: 1.4223  
RDC RMSD N-H medium 2: 2.4019

In `test1medium.m`, backcalculation is tested for N-H and  $C_\alpha-H_\alpha$  RDCs in one medium. One alignment tensor is calculated using `updateTen.CH()` with the correct assignments.

Results are included for 1D3Z N-H and  $C_\alpha-H_\alpha$  RDCs in two media, with normalized N-H and  $C_\alpha-H_\alpha$  vectors from both the 1D3Z NMR structure (Figs. 3, 4) and the 1UBI crystal structure (Figs. 5, 6).  $C_\alpha-H_\alpha$  RDCs are scaled as described in the documentation.

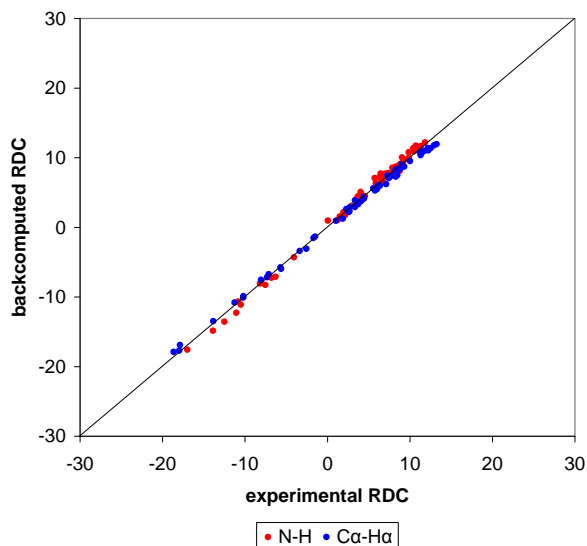


Fig 3. 1D3Z N-H and  $C_\alpha-H_\alpha$  RDCs in medium 1, 1D3Z vectors  
RDC RMSD N-H: 0.5926  
RDC RMSD  $C_\alpha-H_\alpha$ : 0.5624

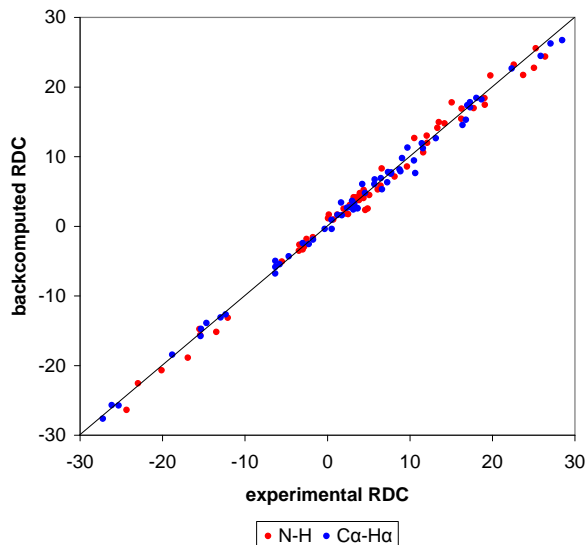


Fig 4. 1D3Z N-H and  $C_\alpha-H_\alpha$  RDCs in medium 2, 1D3Z vectors  
RDC RMSD N-H: 1.1469  
RDC RMSD  $C_\alpha-H_\alpha$ : 0.9532

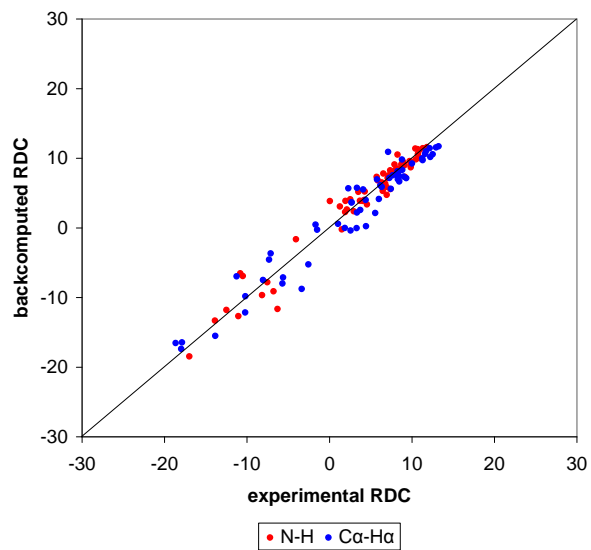


Fig 5. 1D3Z N-H and C $\alpha$ -H $\alpha$  RDCs in medium 1, 1UBI vectors  
RDC RMSD N-H: 1.5181  
RDC RMSD C $\alpha$ -H $\alpha$ : 1.9526

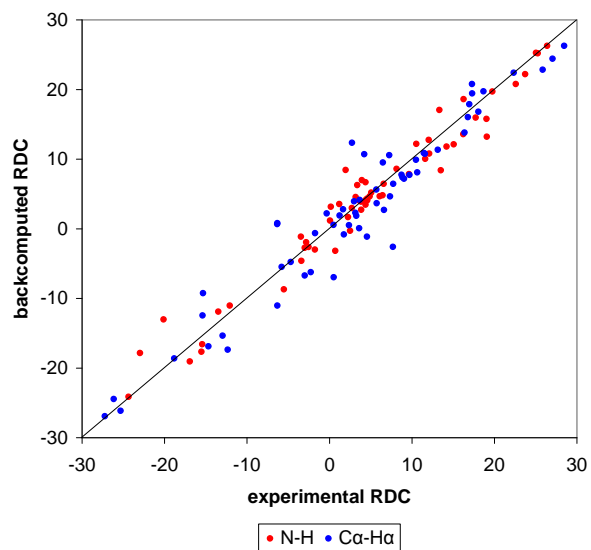


Fig 6. 1D3Z N-H and C $\alpha$ -H $\alpha$  RDCs in medium 2, 1UBI vectors  
RDC RMSD N-H: 2.4329  
RDC RMSD C $\alpha$ -H $\alpha$ : 3.4070