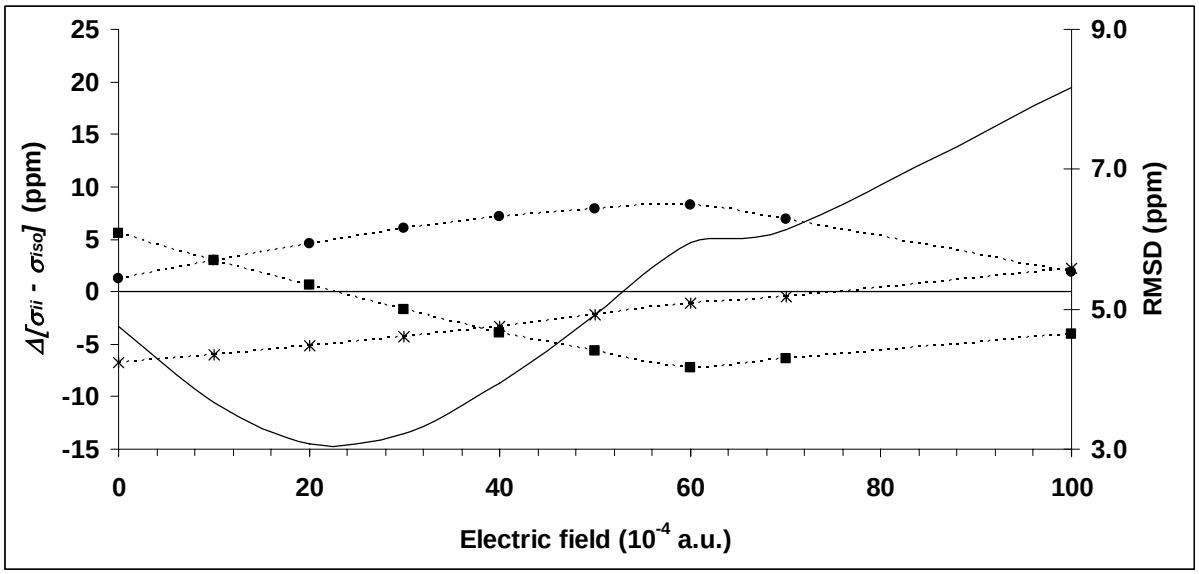
Electronic Supplementary Information

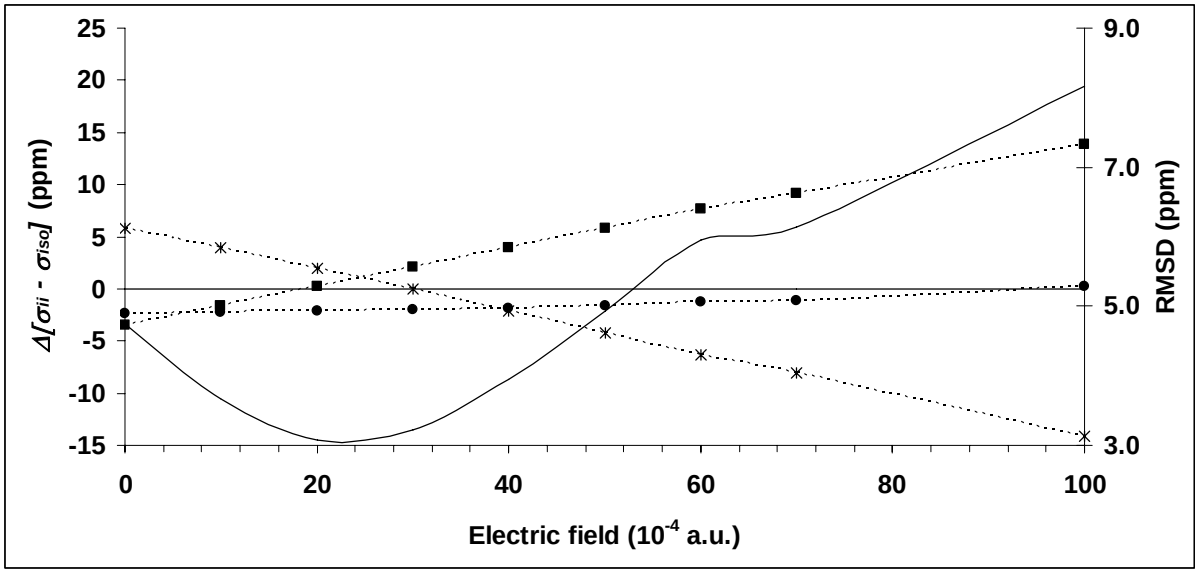
# Modelling the influence of hydrogen bond network on chemical shielding tensors description. GIAO - DFT study of WALP23 transmembrane α-helix as a test case.

**Léa Rougier,[a,b,c] Alain Milon,[b,c] Valérie Réat[b,c] and Franck Jolibois[a,c]**

[a] *Laboratoire de Physique et Chimie des Nano-Objets, Université de Toulouse, INSA-UPS, 135 av. de Rangueil 31077 Toulouse France, Fax: (+33) 561559697, E-mail: franck.jolibois@univ-tlse3.fr*
[b] *Institut de Pharmacologie et Biologie Structurale, Université de Toulouse, UPS, 205 rte de Narbonne, 31077 Toulouse, France*
[c] *CNRS, UMR 5089 and UMR 5215, Toulouse, France*

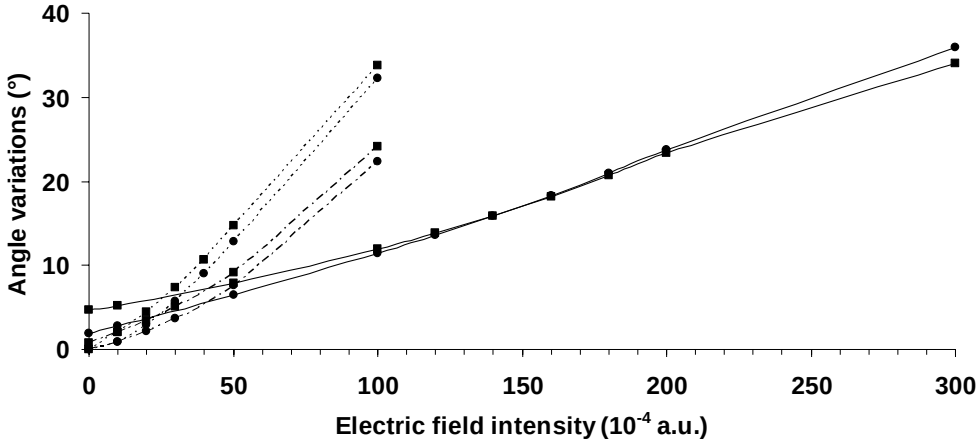



a)

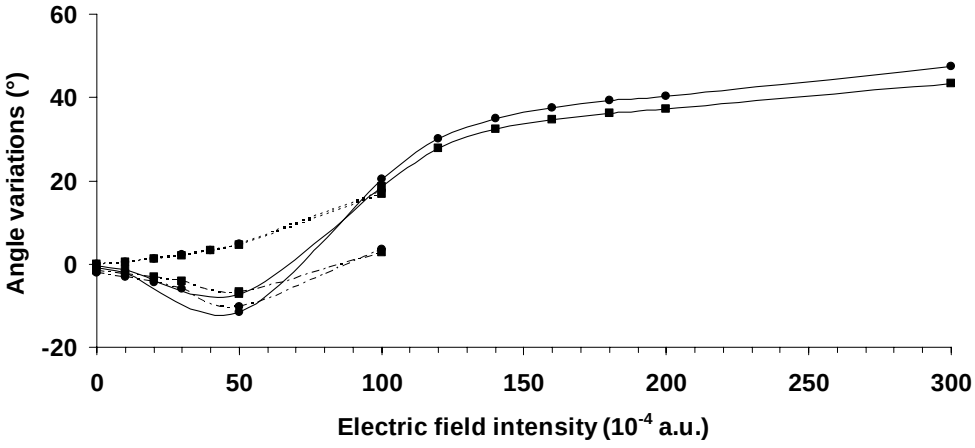



b)

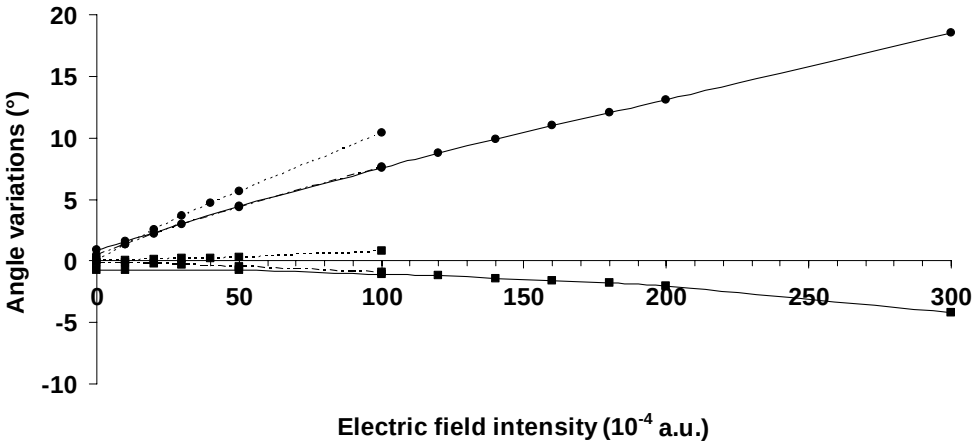
**Fig.S1** $Ala_{13}$ $^{13}C_1$ (a) and $Leu_{14}$ $^{15}N$ (b) $\sigma_{ii}$-$\sigma_{iso}$ (*i=1-3*) difference between theory and experiment as a function of electric field applied to **WALP23 (**$\Delta[\sigma_{ii}\text{-}\sigma_{iso}] = (\sigma_{ii}\text{-}\sigma_{iso})_{theo} - (\sigma_{ii}\text{-}\sigma_{iso})_{exp}$) Circle *i=1*, square, *i=2*, star *i=3*. In solid line is represented the total RMSD between theory and experience calculated using the 6 $\sigma_{ii}$-$\sigma_{iso}$ values as a function of electric fied.




(a)




(b)




(c)

**Fig.S2** Variation of eigenvector orientation relative to molecular frame as a function of applied electric field. Reference as been set to calculation performed without electric field. a) $Ala_{13}$ $^{13}C_1$ alpha (square) and beta (circle) variations. b) $Leu_{14}$ $^{15}N$ alpha (square) and beta (circle) variations. c) $Leu_{14}$ $^{15}N$ (square) and $Ala_{13}$ $^{13}C_1$ (circle) gamma variation. Plain line = WALP_7, Dashed line = WALP23 and Dashed – Point line = polyGLY-AL.