

Fig. S1 DEER profiles before background subtraction: (a) N53C-T110C cyan, (b) N53C-A103C green, (c) T34C-T117C magenta, and background subtractions used (black) superimposed.

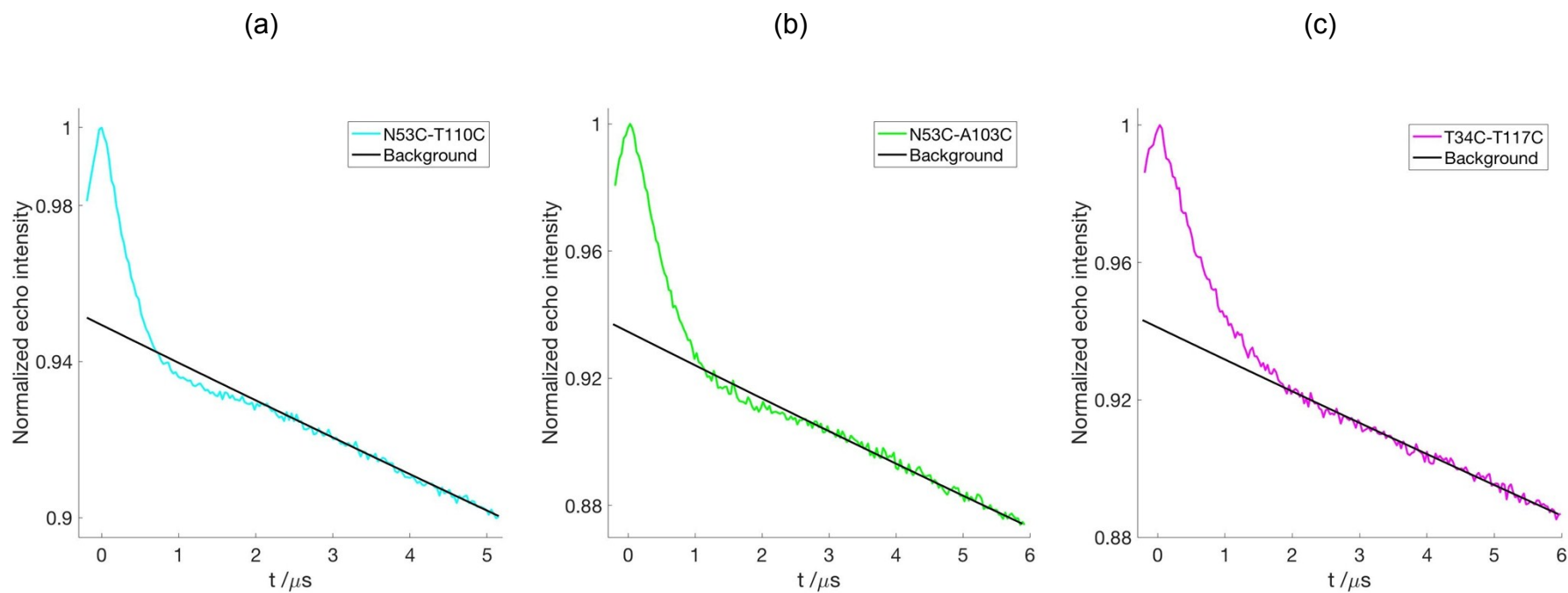


Fig. S2 Correlation between calculated and observed PCS (a) and RDC (b) values obtained with NMR and SAXS data (green) and with NMR, SAXS and DEER data (magenta).

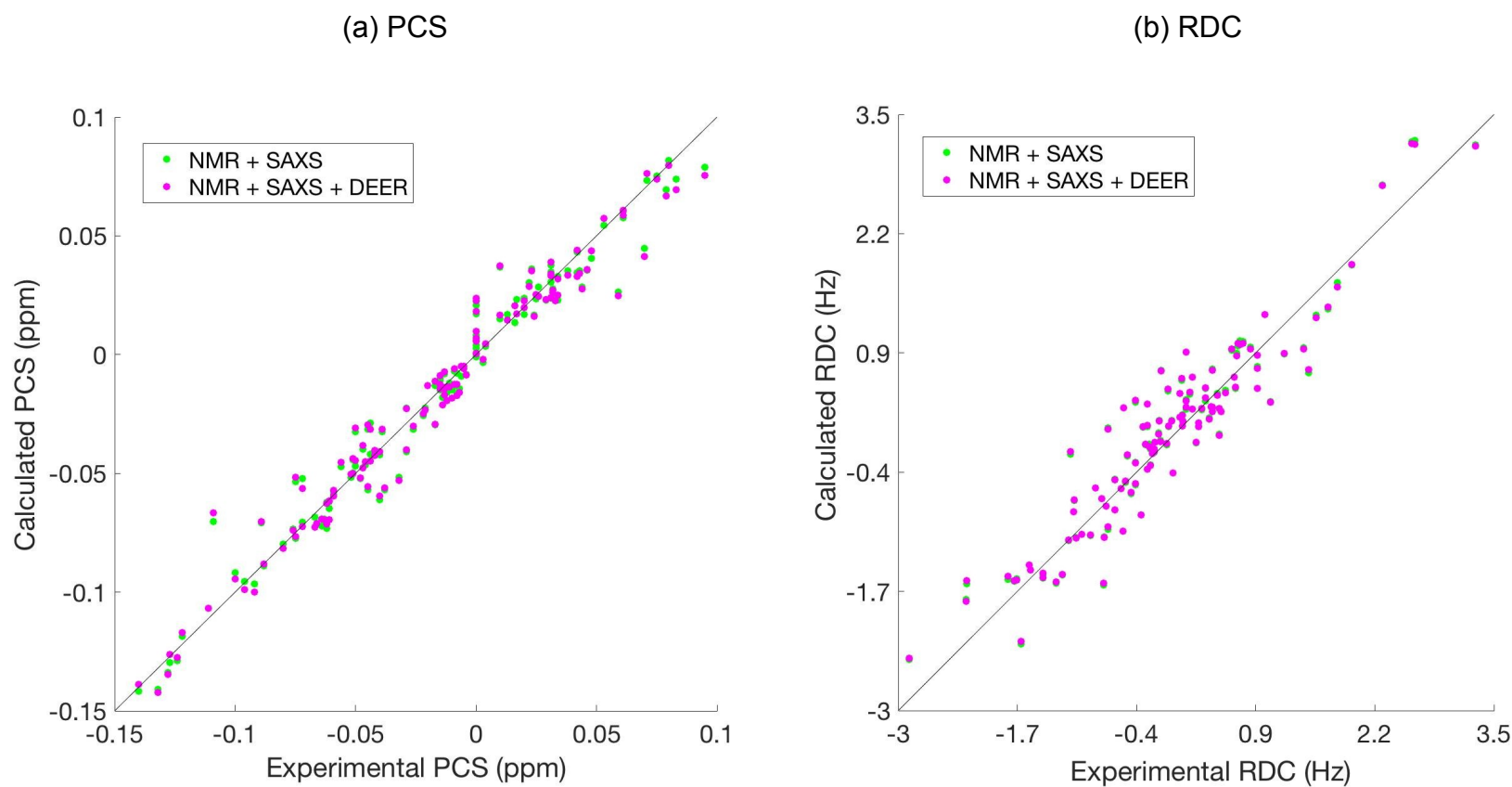


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calculated with NMR and SAXS data (green) and with NMR, SAXS and DEER data (magenta).

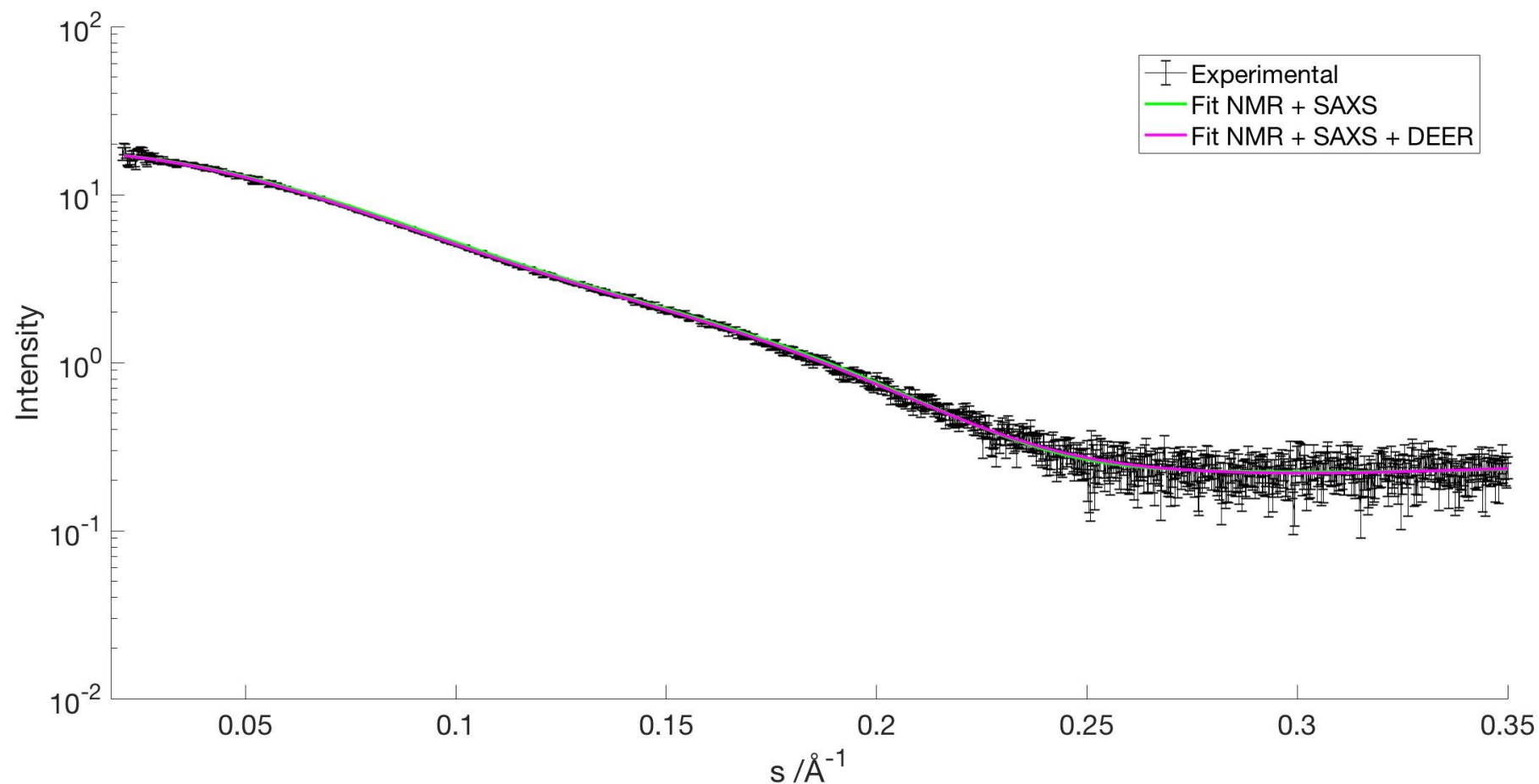


Fig. S4 (a) MaxOcc_D values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_D values of the selected conformations. Each conformation is color coded according to MaxOcc_D from low ($< 5\%$, blue) to high ($> 60\%$, red).

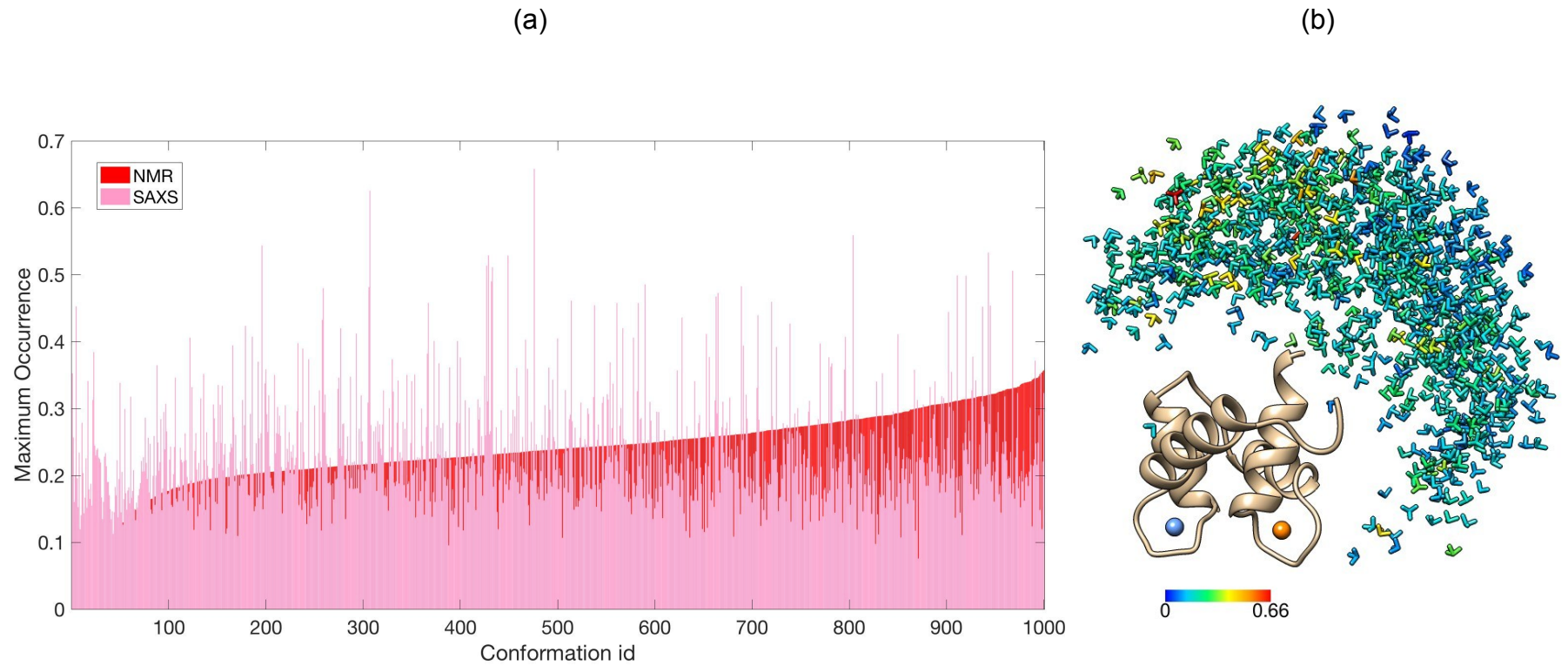


Fig. S5 (a) MaxOcc_E values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_E values of the selected conformations. Each conformation is color coded according to MaxOcc_E from low (< 5%, blue) to high (> 60%, red).

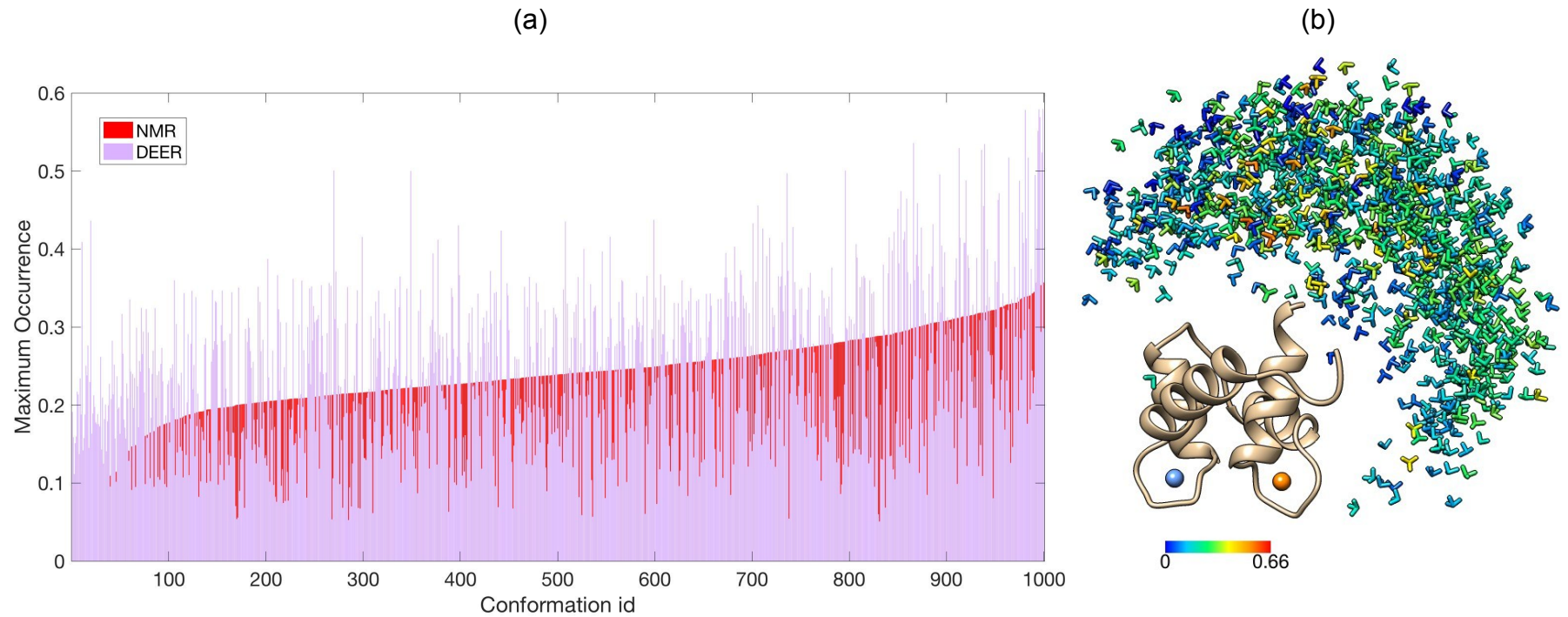


Fig. S6 (a) MaxOcc_F values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_F values of the selected conformations. Each conformation is color coded according to MaxOcc_F from low (< 5%, blue) to high (> 60%, red).

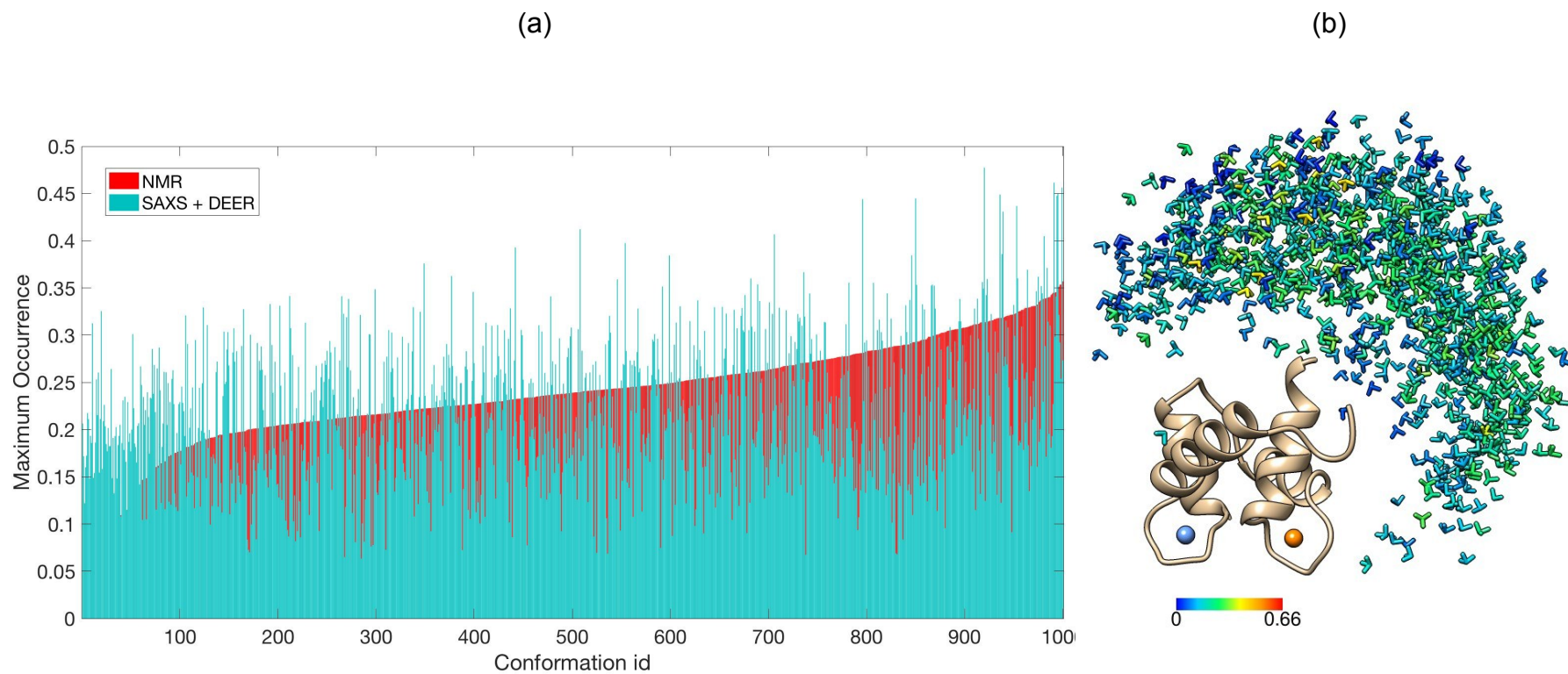


Fig. S7 (a) MaxOcc_G values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_G values of the selected conformations. Each conformation is color coded according to MaxOcc_G from low ($< 5\%$, blue) to high ($> 34\%$, red).

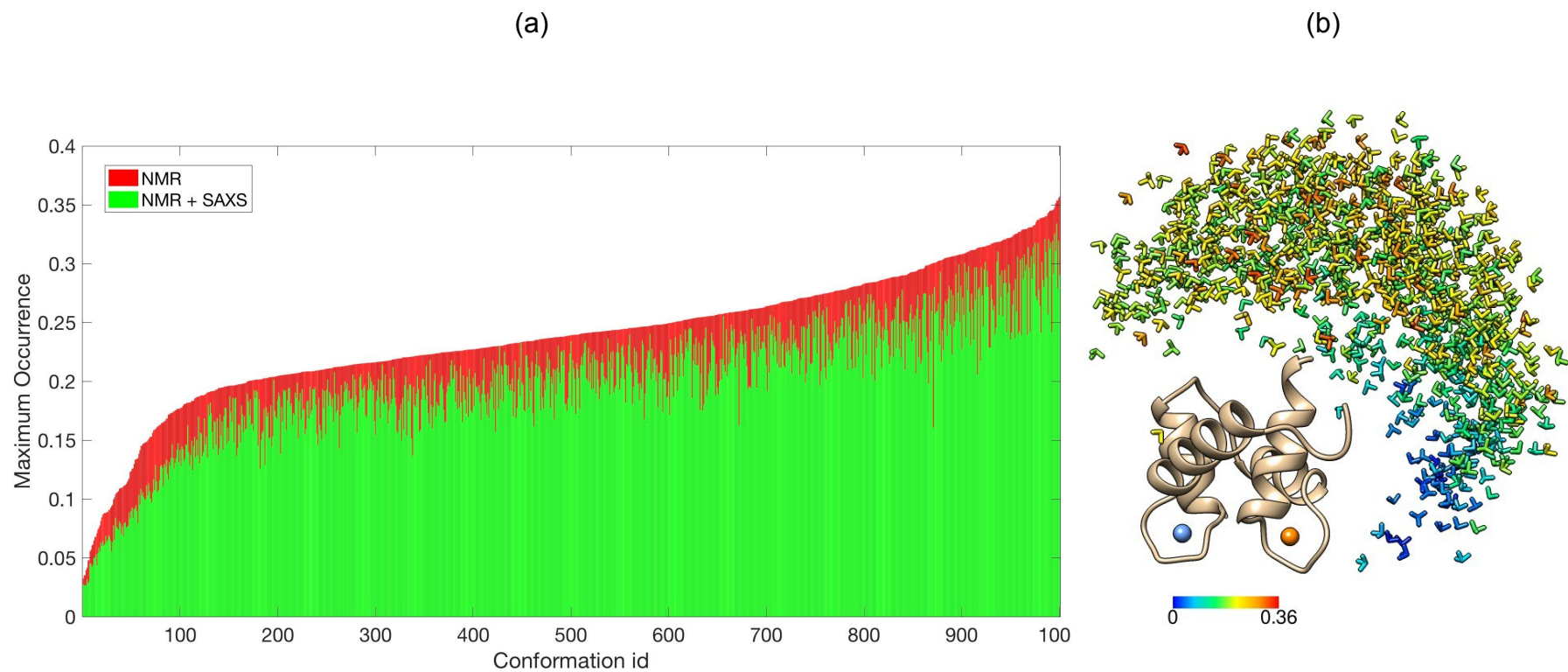


Fig. S8 (a) MaxOcc_H values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_H values of the selected conformations. Each conformation is color coded according to MaxOcc_H from low (< 5%, blue) to high (> 34%, red).

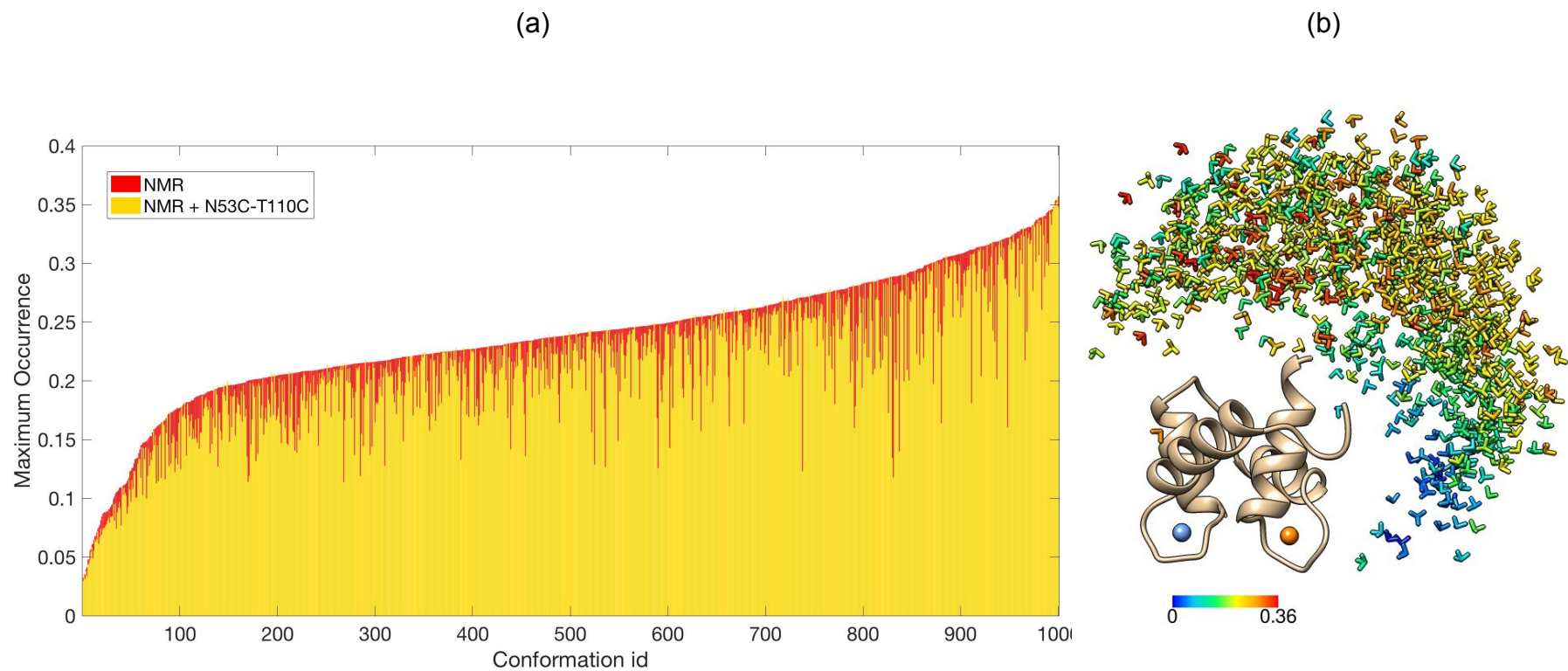


Fig. S9 (a) MaxOcc_i values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_i values of the selected conformations. Each conformation is color coded according to MaxOcc_i from low ($< 5\%$, blue) to high ($> 34\%$, red).

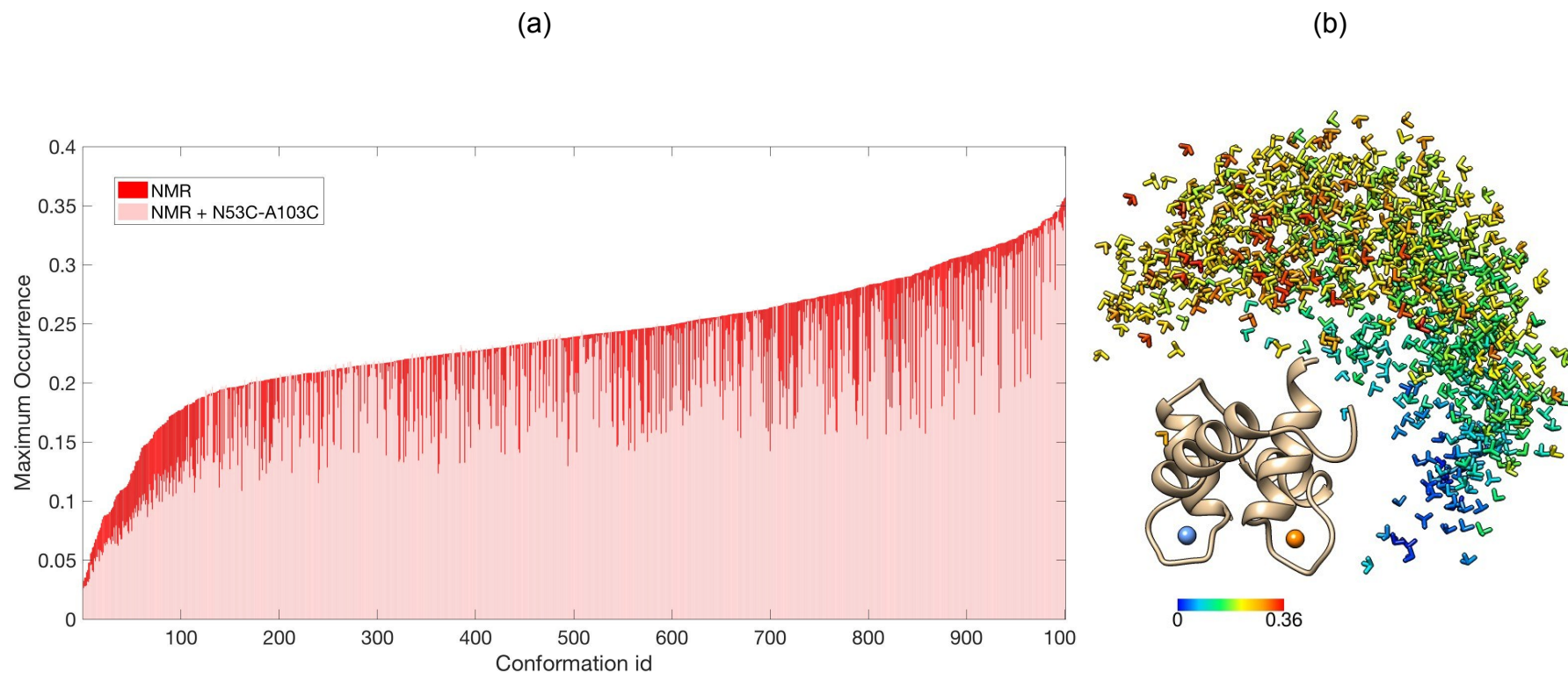


Fig. S10 (a) MaxOcc_L values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_L values of the selected conformations. Each conformation is color coded according to MaxOcc_L from low (< 5%, blue) to high (> 34%, red).

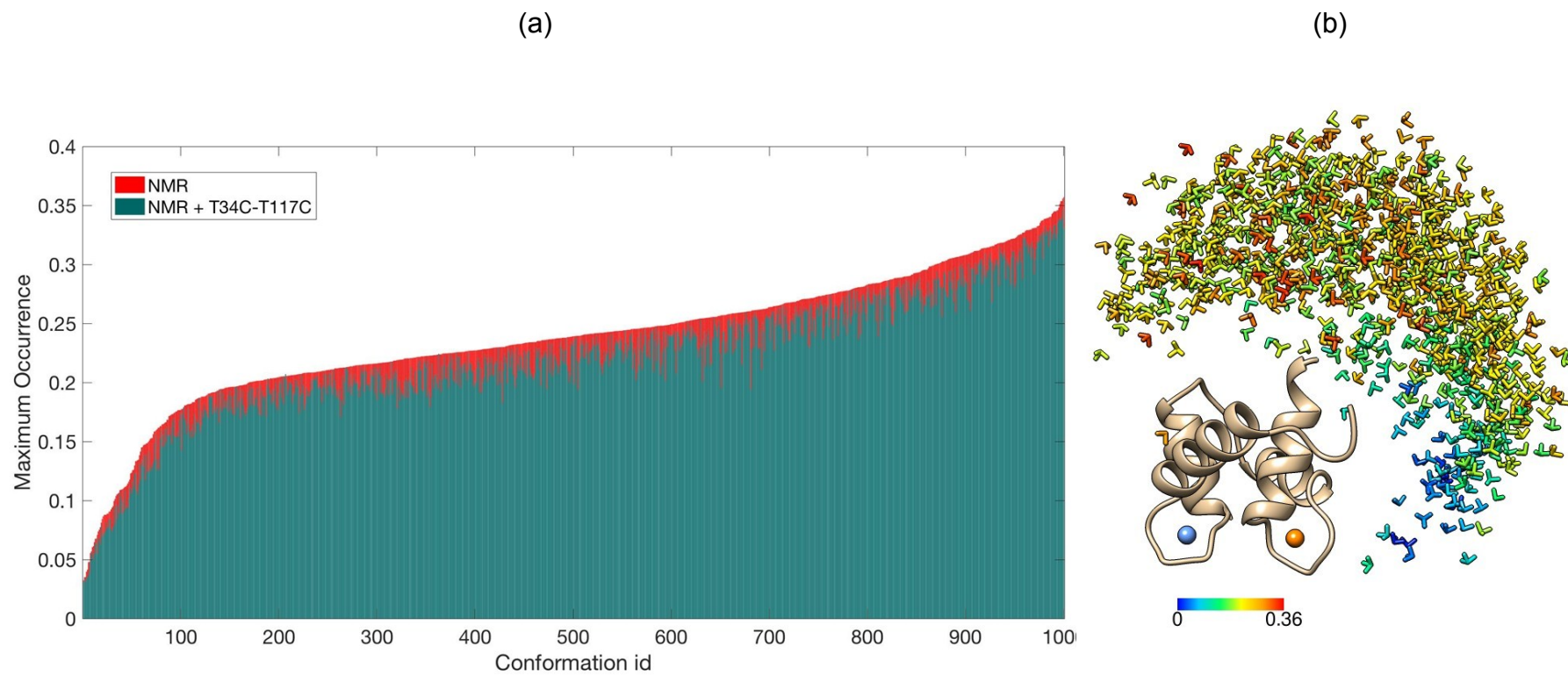


Fig. S11 MaxOcc_M values for 1000 conformations, sorted by ascending MaxOcc_A values.

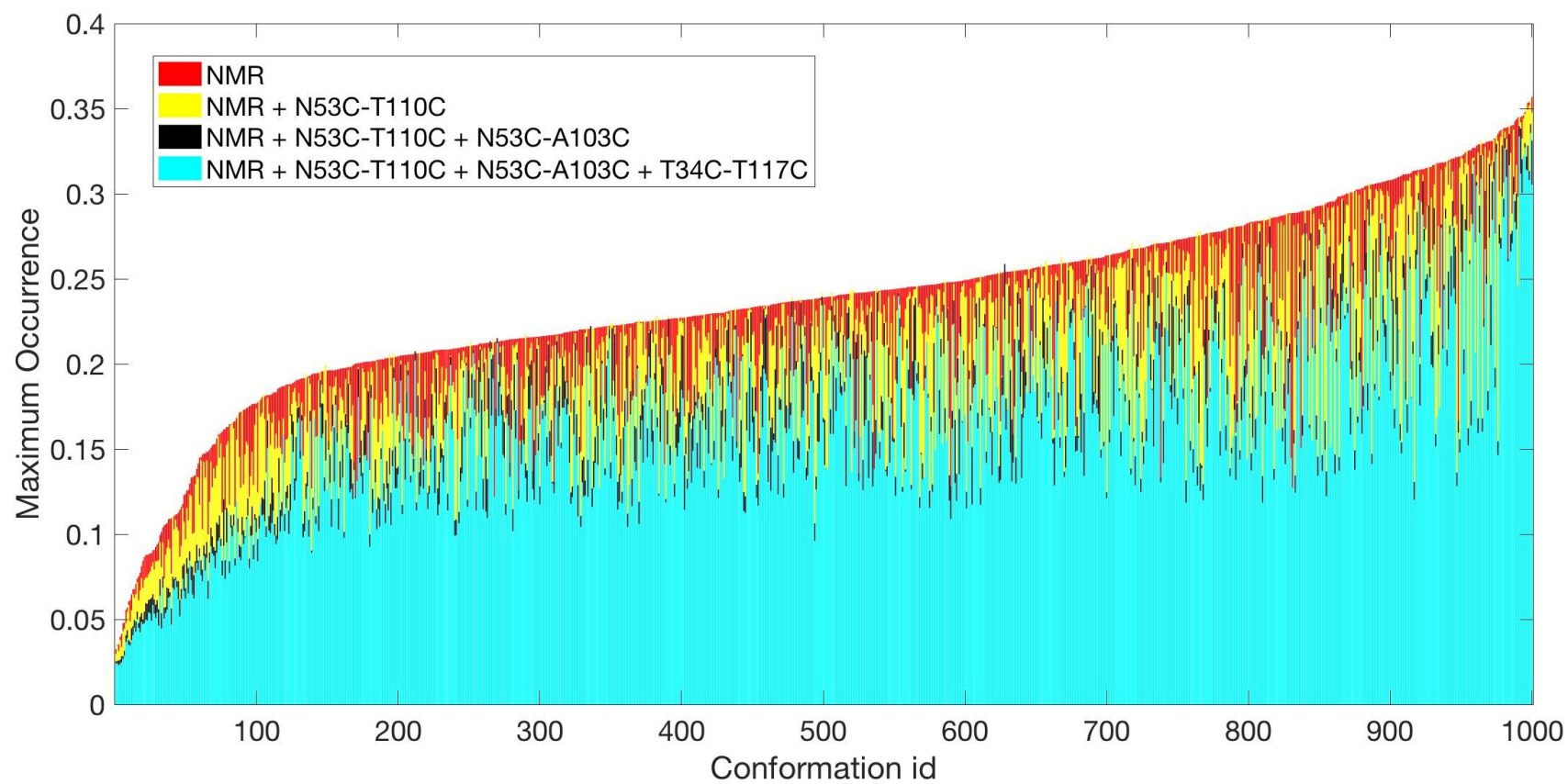
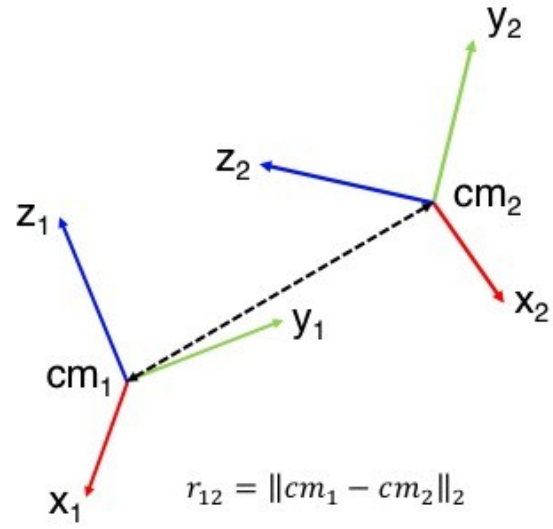


Fig. S12 Graphical representation of r and ρ distances.



$$r_{12} = \|cm_1 - cm_2\|_2$$

$$\rho_{12} = 1 - \frac{\sqrt{x_1 \cdot x_2 + y_1 \cdot y_2 + z_1 \cdot z_2 + 1}}{2}$$