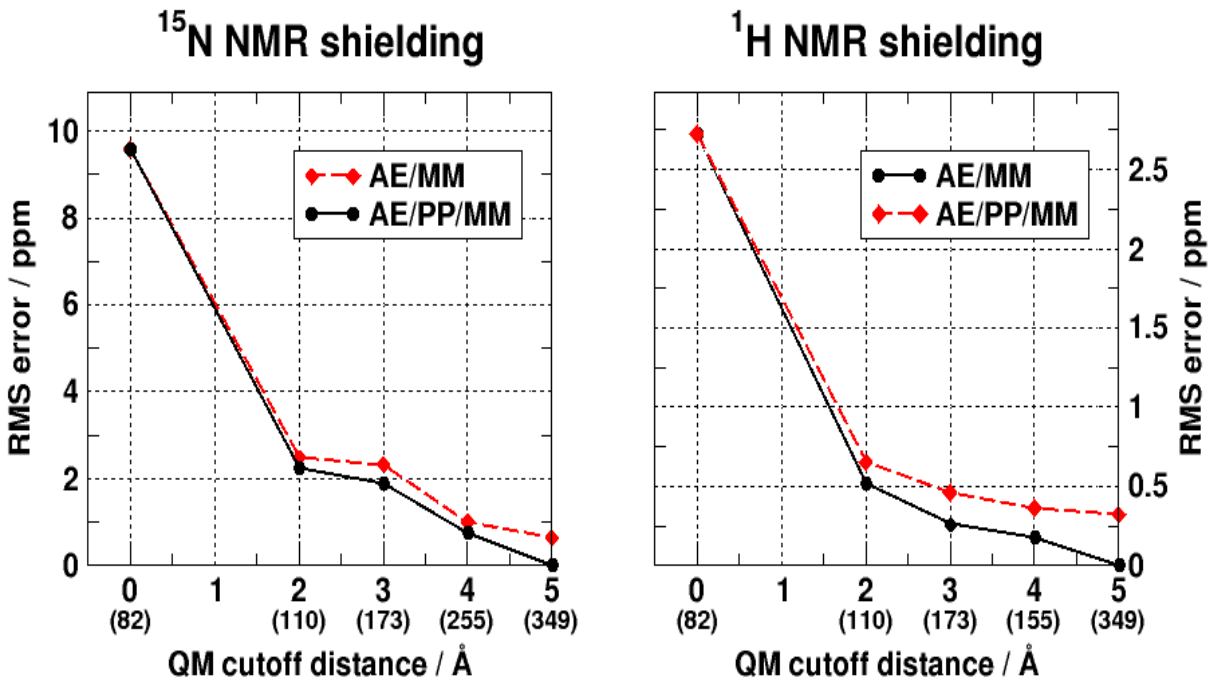

Figure S1: Convergence of computed NMR shieldings with respect to size of QM region. The x-axis shows the distance cutoff that defines the QM region (corresponding number of QM atoms between brackets). The QM region is defined such that it includes PCB and any solvent or protein residue within the cutoff from any PCB pyrrole hydrogen or nitrogen. In this work we chose a cutoff of 3 Å for our NMR calculations, and the entire QM region was treated at an all-electron level.

AE/MM: The entire QM region is treated at an all-electron level, the rest of the system MM. AE/PP/MM: QM region is split into two part, PCB is treated at an all-electron level, the rest of the QM region using pseudopotentials. All RMS values are relative to the largest AE/MM system.

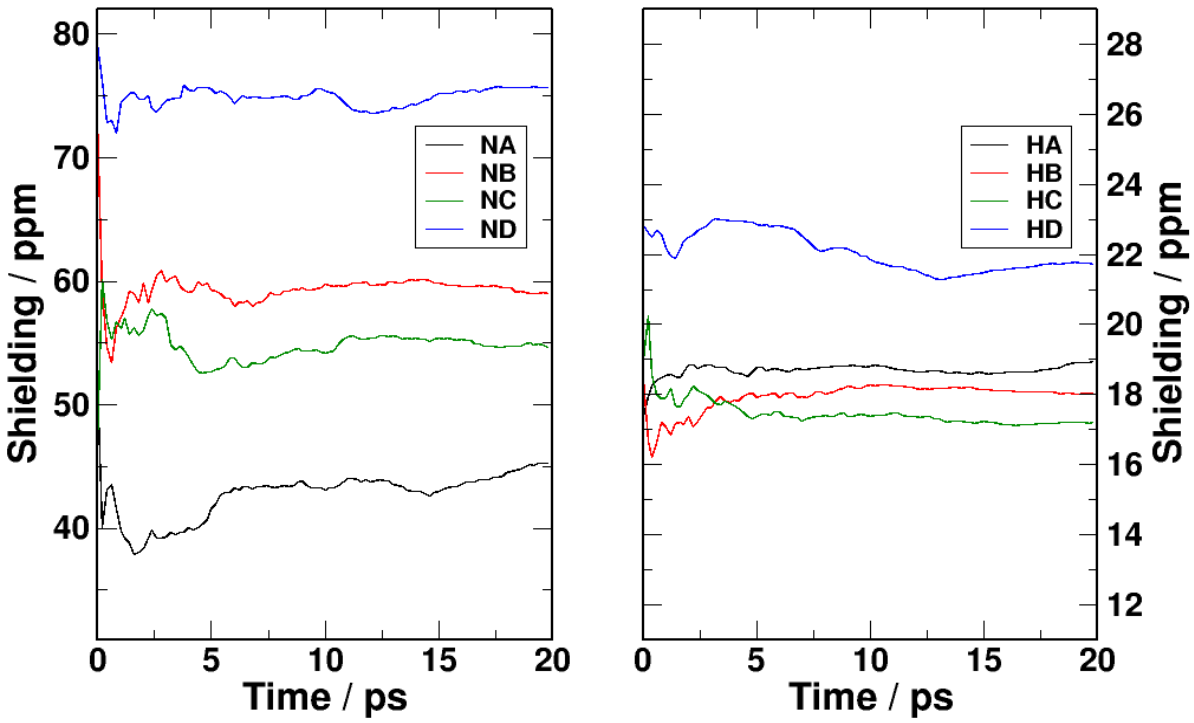

Figure S2: Cumulative average of the computed nuclear shieldings for the Nitrogens (left) and hydrogens (right) along the MD trajectory.