Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for

Combined Fragment-Based Machine Learning Force Field with Classical Force Field and its Application in the NMR Calculations of Macromolecules in Solutions

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1. The fragmentation of the oligopyridine-dicarboxamide molecule

For the oligopyridine-dicarboxamide molecule (123 atoms), we cut the bond between carbonyl carbon and α-carbon in the peptide bond (see Fig. S1), which is employed in the treatment of proteins. For the initial structure as shown in Fig. S1, the largest GEBF subsystem consists of three fragments with 58 atoms, as shown in Fig. S2.

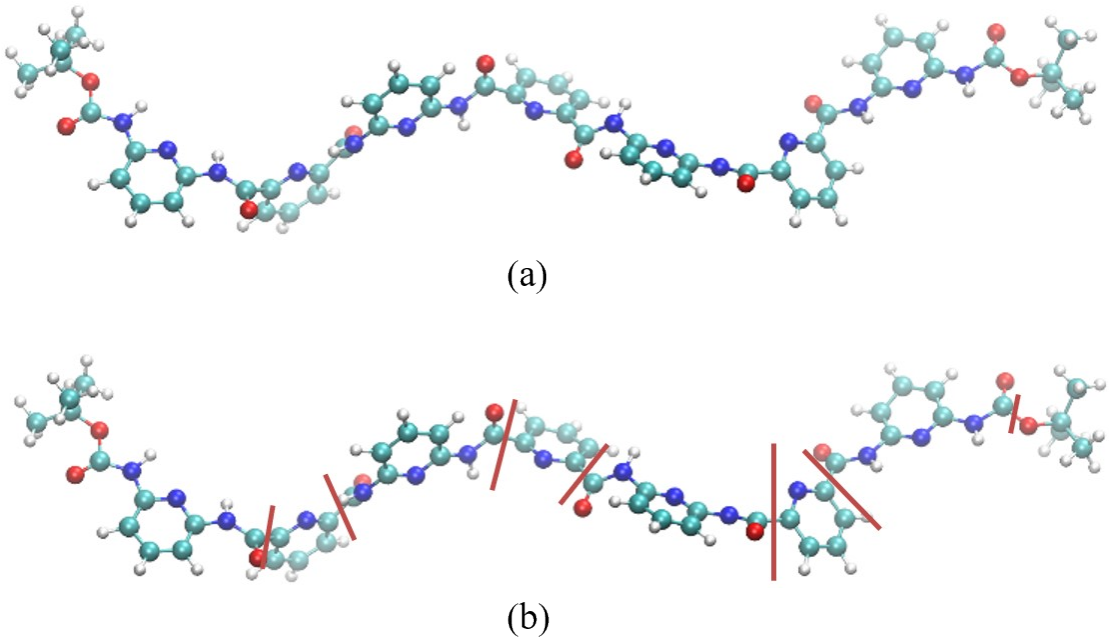

Fig. S1. The fragmentation of the oligopyridine-dicarboxamide molecule (123 atoms): (a) The initial structure of the heptamer; (b) The fragmentation scheme of the heptamer, where the red solid line represents the cut bonds.

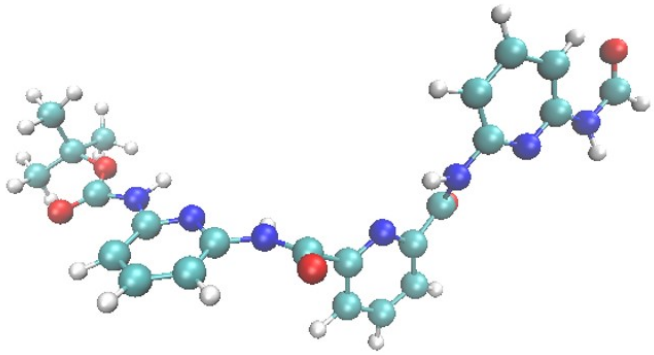

Fig. S2. The largest GEBF subsystem, which contains only 58 atoms.

2. The GEBF-NMR chemical shift without solvent molecules

Table S1. Comparisons of the average GEBF-B97-2 NMR chemical shifts (in ppm) for 15 snapshots from GEBF-NN/MM MD simulations (with and without explicit solvent molecules), and the experimental values for 7 types of hydrogen atoms in the heptamer.

Type	Without solvent molecules	With solvent molecules	Exp
1	10.08 (-0.19)	10.18 (-0.09)	10.27
2	10.35 (-0.08)	10.23 (-0.20)	10.43
3	9.78 (-1.08)	10.10 (-0.76)	10.86
4	8.05 (0.53)	8.23 (0.71)	7.52
5	8.45 (0.56)	8.59 (0.70)	7.89
6	8.22 (0.48)	8.43 (0.69)	7.74
7	8.44 (0.26)	8.64 (0.46)	8.18
MAE	0.45	0.52	
σ	0.55	0.33	