General Applicable Frequency Map for the Amide-I Mode in β-Peptides

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Table S1. A comparison of the amide-I vibrational frequency maps for peptides, based on NMA or NEPA.

	NMA-based								NEPA-based		
	Skinner[1]	Cho[2]	Cho[3]	Bour[4]	Tokmakoff[5]	Ge[6]	Wang[7]	Cai[8]	Wang[9, a]	GA[b]	GA_GD3[c]
Unit	cm^{-1}/a.u.	cm^{-1}/a.u.	cm^{-1}/a.u.	cm^{-1}/a.u.	$cm^{-1}a_o e/E_h$	1/e	cm^{-1}/V^{-1}	cm^{-1}/V^{-1}	cm^{-1}/V^{-1}	cm^{-1}/V^{-1}	cm^{-1}/V^{-1}
CH_3(C)	1203	263	--	590	--	--	--	--	--	--	--
C	-2715	-66	351	-1370	1123.5	0.01179	79.441	121.966	51.640	156.350	156.225
O	-203	-1185	-1216	-713	-1383.4	-0.00756	-19.880	-64.995	-48.859	-70.528	-70.460
N	2417	1405	1051	1492	-11.819	-0.00549	-121.026	-79.300	109.331	-92.102	-92.022
H	-273	-307	-189	--	271.66	0.00126	54.817	22.329	-5.933	6.281	6.257
CH_3(N)	-429	-241	--	--	--	--	--	--	--	--	--

a. Map is constructed based on NEPA solvated in D_2O.

b. This work. Partially based on DFT computations on the NEPA-*n*-$CHCl_3$ clusters.

c. This work. Partially based on DFT computations on the NEPA-*n*-$CHCl_3$ clusters, using the Grimme's DFT-D3 method for dispersion correction.

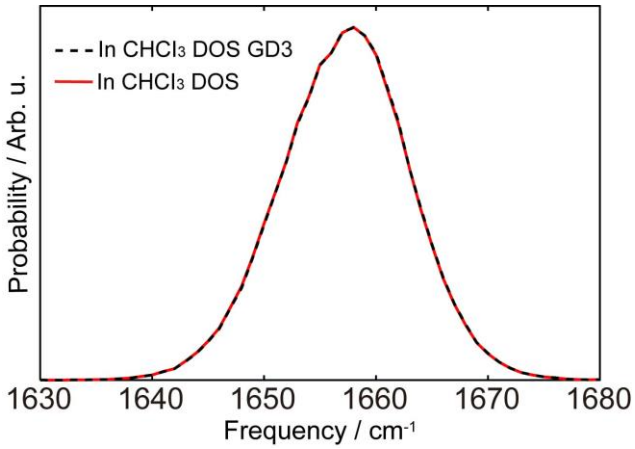

Figure S1. A comparison of the amide-I frequency distributions of NEPA in $CHCl_3$, obtained using the GA and GA_GD3 frequency maps respectively.

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