Supporting Information

A Robust Heterogeneous Anisotropic Elastic Network Model Precisely Reproduces the Experimental B-factors of Biomolecules

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Figures and Captions

Table S1 The overlap values for each pair of the modes 7~11 between HANM and ANM are calculated according to Eq.(10). The values are listed from up to down in turn for crambin, trypsin inhibitor, HIV-1 protease and lysozyme.

Table S2 The overlap values for each pair of the modes 7~11 between the all-atom model of HIV-1 protease and HANM as well as ANM are calculated according to Eq.(10). The values are listed for HANM and ANM from up to down. The normal mode analysis of the all-atom model of HIV-1 protease is performed using the Gromos96 vacuum parameter set.[1] The normalized eigenvectors of the Cα atoms of the all-atom model were extracted to calculate the overlaps with the modes of HANM and ANM. The results show that the all-atom modes have higher overlaps with the modes of HANM than those of ANM.

Table S3 Overlaps between the first three NMR principle components and the first five low-frequency normal modes from ANM for the beta-neurotoxin.

Table S4 Overlaps between the first three NMR principle components and the first five low-frequency normal modes from HANM for the beta-neurotoxin.

Table S5 Time needed for the relatively large protein methionyl-tRNA synthetase (PDB ID: 1A8H)[2] to converge using correlation coefficient as a loose criterion.

Figure S1 A comprehensive comparison of the experimental and calculated B-factors for proteins with the PDB IDs: (a) 1HG7 (b) 1CC8 (c) 1IQZ (d) 1GNU (e) 1TU9 and (f) 1A6M. The experimental values are denoted by hollow red cycles. The blue curves of HANM are derived using the PFM method with the cut-off distances 15 Å. The calculated RMSDs between the experimental

B-factors and the HANM values are 0.073, 0.038, 0.029, 0.106, 0.038 and 0.079 $Å^2$ for (a)-(f), respectively. All calculated CCs for (a)-(f) are 0.99.

Table S1

Modes		HANM				
		7	**8**	**9**	**10**	**11**
ANM	**7**	0.095 0.363 0.120 0.979	0.812 0.601 0.736 0.057	0.412 0.578 0.285 0.151	0.150 0.193 0.367 0.052	0.046 0.009 0.050 0.017
	8	0.951 0.231 0.725 0.038	0.071 0.608 0.314 0.988	0.014 0.591 0.176 0.103	0.052 0.279 0.045 0.014	0.077 0.172 0.002 0.037
	9	0.139 0.751 0.407 0.164	0.322 0.252 0.152 0.096	0.221 0.053 0.457 0.962	0.136 0.227 0.121 0.092	0.215 0.210 0.141 0.029
	10	0.068 0.126 0.356 0.046	0.314 0.120 0.084 0.014	0.447 0.228 0.257 0.091	0.482 0.068 0.039 0.883	0.120 0.008 0.160 0.220
	11	0.100 0.132 0.034 0.034	0.103 0.019 0.405 0.045	0.231 0.185 0.256 0.063	0.019 0.107 0.439 0.114	0.492 0.011 0.074 0.604

Table S2

Modes		HANM ANM				
		7	**8**	**9**	**10**	**11**
All-atom	**7**	0.739 0.026	0.146 0.606	0.074 0.306	0.128 0.232	0.058 0.076
	8	0.065 0.664	0.709 0.300	0.297 0.002	0.162 0.164	0.132 0.185
	9	0.278 0.172	0.064 0.288	0.421 0.040	0.187 0.168	0.023 0.071
	10	0.524 0.452	0.516 0.193	0.151 0.210	0.167 0.222	0.243 0.248
	11	0.268 0.401	0.105 0.075	0.480 0.256	0.435 0.023	0.165 0.289

Table S3

ANM / PCA	Mode1	Mode2	Mode3	Mode4	Mode5
PC1	0.443064	0.308858	0.288996	0.044185	0.157861
PC2	0.018141	0.365115	0.20804	0.626305	0.036364
PC3	0.238578	0.045231	0.051463	0.068605	0.352327
PC4	0.314694	0.127458	0.061713	0.08507	0.027498
PC5	0.337046	0.124121	0.335573	0.058525	0.257465

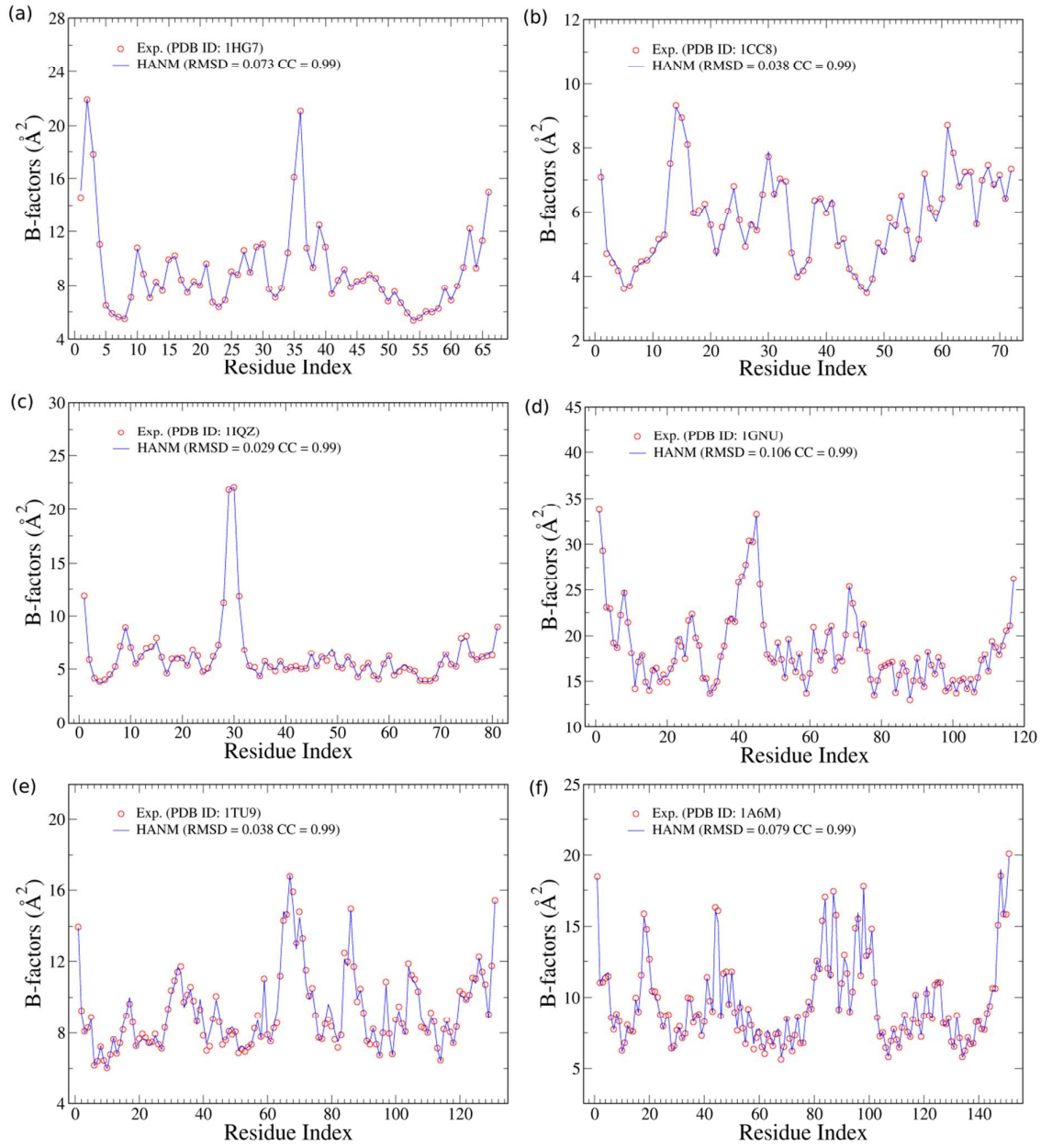
Table S4

HANM / PCA	Mode1	Mode2	Mode3	Mode4	Mode5
PC1	0.540367	0.122021	0.613042	0.002033	0.172391
PC2	0.307148	0.333615	0.077871	0.538221	0.070496
PC3	0.265255	0.341967	0.120507	0.047287	0.285156
PC4	0.134136	0.236982	0.226276	0.218619	0.292795
PC5	0.118402	0.011202	0.262686	0.038202	0.00925

Table S5

Correlation Coefficient	Iteration Number	Total Time
0.90	5	6h 34' 38"
0.95	8	10h 24' 41"
0.99	14	18h 04' 19"

Figure S1



The force constants of the ten X-ray crystal protein structures in this article can be found in the supporting information file "force_constants.zip". The source code of our method can be found in the file "HANM_code.zip". The files contained in the zip file can be viewed by Microsoft Word.

Reference:

[1] Scott, W. R. P.; Hünenberger, P. H.; Tironi, I. G.; Mark, A. E.; Billeter, S. R.; Fennen, J.; Torda, A. E.; Humber, T.; Krüger, P.; van Gunsteren, W. F. *J. Phys. Chem. A* **1999**, *103*, 3596-3607.

[2] Sugiura, I.; Nureki, O.; Ugaji-Yoshikawa, Y.; Kuwabara, S.; Shimada, A.; Tateno, M.; Lorber, B.; Giege, R.; Moras, D.; Yokoyama, S.; Konno, M. *Structure* **2000**, *8*, 197-208.