

Supporting Information

S1 Text

Abbreviations in alphabetical order	1
AdK, <u>A</u> denylate <u>K</u> inase;	2
ANM, <u>A</u> nisotropic <u>N</u> etwork <u>M</u> odel;	3
CADD, <u>C</u> omputer- <u>A</u> sisted <u>D</u> rug <u>D</u> iscovery;	4
CASP, <u>C</u> ritical <u>Assessment of protein <u>S</u>tructure <u>P</u>rediction;</u>	5
cryo-EM, cryo- <u>E</u> lectron <u>M</u> icroscopy;	6
DIMS, <u>D</u> ynamic <u>I</u> mportance <u>S</u> ampling;	7
EA, <u>E</u> volutionary <u>A</u> lgorithm;	8
ENM, <u>E</u> lastic <u>N</u> etwork <u>M</u> odel;	9
EST, <u>E</u> xpansive <u>S</u> paces <u>T</u> ree;	10
GA, <u>G</u> enetic <u>A</u> lgorithm;	11
IDP, <u>I</u> ntrinsically- <u>D</u> isordered <u>P</u> rotein;	12
IMP, <u>I</u> ntegrative <u>M</u> odeling <u>P</u> latform;	13
MA, <u>M</u> emetic <u>E</u> volutionary <u>A</u> lgorithm;	14
MC, <u>M</u> onte <u>C</u> arlo MC-SA, <u>M</u> onte <u>C</u> arlo- <u>S</u> imulated <u>A</u> nnealing;	15
MD, <u>M</u> olecular <u>D</u> ynamics;	16
MEP, <u>M</u> inimum <u>E</u> nergy <u>P</u> ath	17
MFEP, <u>M</u> inimum <u>F</u> ree <u>E</u> nergy <u>P</u> ath	18
MGA, <u>M</u> emetic <u>G</u> enetic <u>A</u> lgorithm;	19
MM, <u>M</u> olecular <u>M</u> echanics;	20
MO-EA, <u>M</u> ulti <u>O</u> bjective EA;	21
MO-GA, <u>M</u> ulti <u>O</u> bjective GA	22
MSM, <u>M</u> arkov <u>S</u> tate <u>M</u> odel;	23
MWC, <u>M</u> onod- <u>W</u> yman- <u>C</u> hangeaux;	24
NEB, <u>N</u> udged <u>E</u> lastic <u>B</u> and;	25
NMA, <u>N</u> ormal <u>M</u> ode <u>A</u> nalysis	26
NMR, <u>N</u> uclear <u>M</u> agnetic <u>R</u> esonance;	27
NOE, <u>N</u> uclear <u>O</u> verhauser <u>E</u> ffect;	28
PDB, <u>P</u> rotein <u>D</u> ata <u>B</u> ank;	29
PDST, <u>P</u> ath-directed <u>S</u> ubdivision <u>T</u> ree;	30
PNM, <u>P</u> lastic <u>N</u> etwork <u>M</u> odel;	31
PRM, <u>P</u> robabilistic <u>R</u> oad <u>M</u> ap;	32
QM, <u>Q</u> uantum <u>M</u> echanics;	33
RDC, <u>R</u> esidual <u>D</u> ipolar <u>C</u> oupling;	34
RMSD, <u>R</u> oot- <u>M</u> ean- <u>S</u> quared <u>D</u> evelopment;	35
RRT, <u>R</u> apidly-exploring <u>R</u> andom <u>T</u> ree;	36
TPS, <u>T</u> ransition <u>P</u> ath <u>S</u> ampling;	37
TST, <u>T</u> ransition <u>S</u> <u>T</u> heory;	38
VMD, <u>V</u> isual <u>M</u> olecular <u>D</u> ynamics;	39
WEM, <u>W</u> eighted <u>E</u> nsemble <u>M</u> ethod;	40
	41