Supporting Information for -

Selective Stabilization of Aspartic Acid Protonation State within a Given Protein Conformation Occurs via Specific 'Molecular Association'

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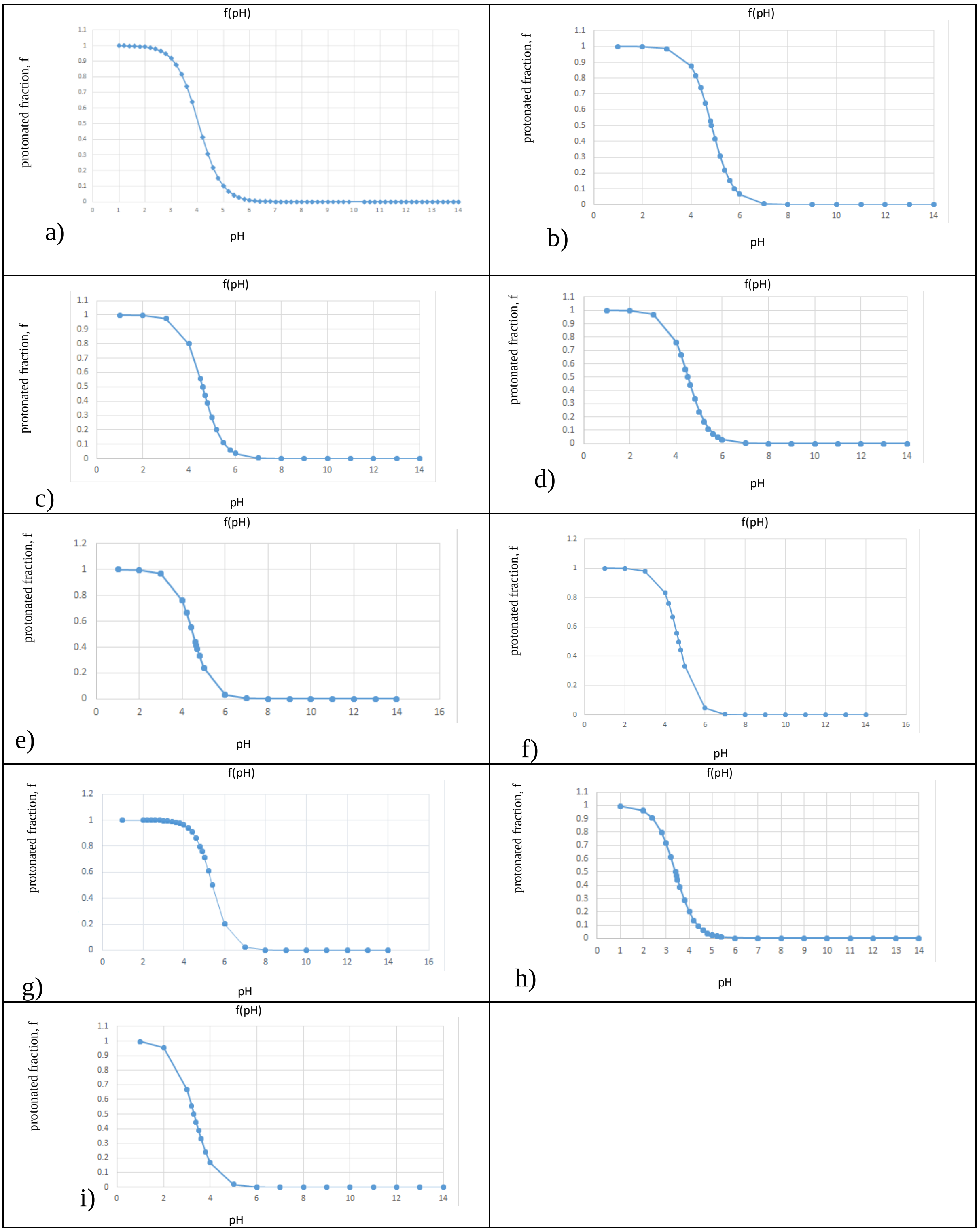
Table S1: The best fitted equation, fairly reproduce the dielectric values within the range of 2 to 47.

Solvent name	Bond order (x) of Carboxylic acid O-H in Asp side chain	Dielectric constants (y) derived based on the equation; $y = 0.0563x^{-15.89}$	Dielectric value for the respective solvents[1]	Error between computed and experimental dielectric values
Water	0.693	19.1	80.1	Too high
DMSO	0.658	43.5	46.7	3.2
Methanol	0.659	42.5	32.7	9.8
Ethanol	0.669	33.4	24.5	8.9
Acetone	0.688	21.4	20.7	0.7
Tetrahydrofuran	0.7	16.3	7.6	8.7
Chlorobenzene	0.779	3.0	5.62	2.62
Benzene	0.779	3.0	2.27	0.73
Cyclohexane	0.773	3.4	2.02	1.38

Table S2: Mulliken charges on OD2 and HD2 atoms of capped aspartic acid in different liquid media. Cases are highlighted where magnitude of negative and positive charge differences is less than 0.02, in order to identify the existence of a dipole. Electric dipole is defined as the product of either charge separated by a certain distance. In case, where the magnitude of charge difference is larger than 0.02 (choice of this threshold is empirical, based on the observation from this table), those are not considered as true dipoles

Liquid media	Mulliken charge on OD2 atom	Mulliken charge on HD2 atom
Water	-0.49	0.51
DMSO	-0.44	0.50
Methanol	-0.55	0.53
Ethanol	-0.45	0.47
Acetone	-0.51	0.39
Tetrahydrofuran	-0.41	0.39
Chlorobenzene	-0.44	0.38
Benzene	-0.44	0.45
Cyclohexane	-0.40	0.41

Figure S1: Titration curves obtained from constant pH MD simulations for aspartic acid in solvent systems a) water b) methanol c) ethanol d) tetrahydrofuran e) dimethyl sulphoxide f) acetone g) cyclohexane h) benzene and i) chlorobenzene



(1) Arthur A Maryott; Edgar Reynolds Smith. *Table of Dielectric Constants of Pure Liquids*, National g.; Washington, U.S. Govt. Print. Off., National Bureau of Standards circular, 514, 1951.