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Supporting Information for

Chirality recognition of the protonated serine dimer and octamer by infrared multiphoton dissociation spectroscopy

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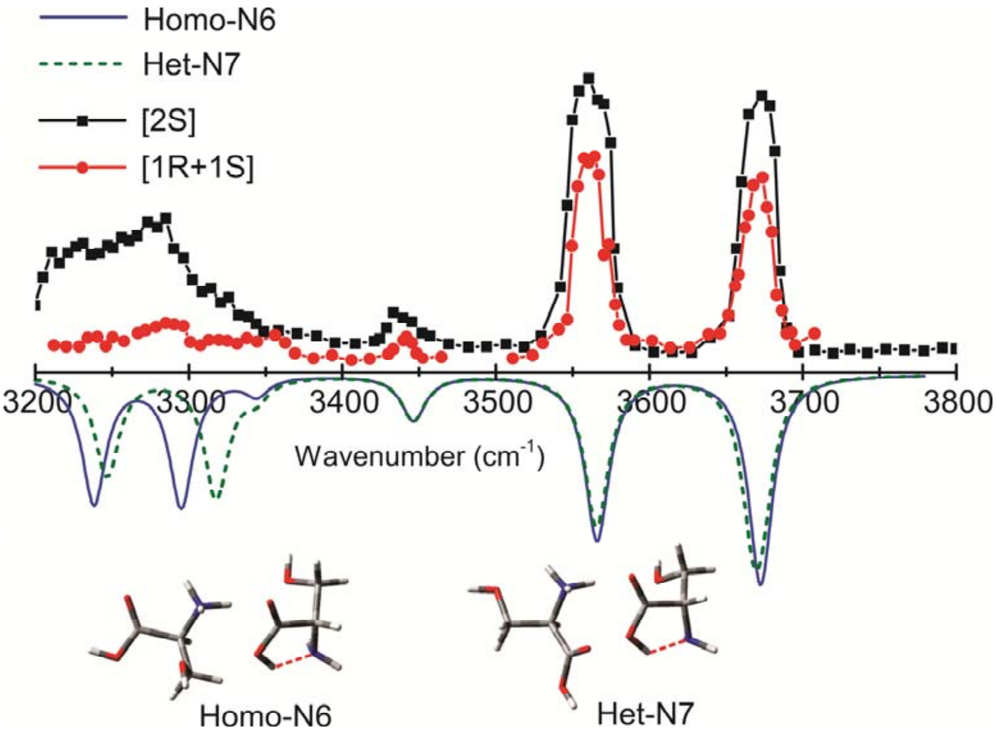

Fig. S1 Comparison of the experimental homochiral and heterochiral dimer spectra with the calculated spectra of homo-N6 and het-N7. The structures of these two conformers are also included at the bottom.

Table S1. Calculated Gibbs free energies (in kcal/mol) of the three Zwitterionic conformers of the homochiral protonated serine dimers at room temperature.

Species	Approach I[a]		Approach II[b]		
	Without dispersion correction		With dispersion correction		MP2/ 6-311++G(d,p)
	B3LYP/ 6-31G(d)	B3LYP/ 6-311++G(d,p)	B3LYP/ 6-31G(d)	B3LYP/ 6-311++G(d,p)	
	ΔG_{298}[c]	ΔG_{298}[d]	ΔG_{298}[c]	ΔG_{298}[d]	ΔG_{298}[e]
Z1	0.00	0.00	0.00	0.00	0.00
Z2	0.59	0.30	0.69	0.38	0.70
Z3	2.18	1.87	1.99	1.84	1.94

[a] Exactly the same approach used for the calculations of the Zwitterionic conformers of the protonated serine octamers is used here. The geometry optimizations and harmonic frequency calculations were carried out at the B3LYP/6-31G(d) level. Further single point energy calculations were obtained at the B3LYP/6-311++G(d,p).

[b] The same calculations as in approach I were repeated with the dispersion correction using B3LYP/6-31G(d) S=1.05 and B3LYP/6-311++G(d,p) S=1.05. These calculations were carried out using Gaussian 09, Revision C.01 (M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.) where the scaling factor S=1.05 for B3LYP for dispersion corrections (S. Grimme, *J. Comput. Chem.* 2006, **27**, 1787) was implemented.

[c] ΔG_{298} for Z1 is set to 0 kcal/mol. ΔG_{298} (Z1) = -798.117104 and -798.149160 Hartree without and with dispersion, respectively.

[c] ΔG_{298} values are calculated using the ΔG_{corr} values obtained at the B3LYP/6-31G(d) level. ΔG_{298} (Z1) = -798.3998796 and -798.431569 Hartree without and with dispersion, respectively.

[e] See Table 1 in the main text.