Electronic Supporting Information for:

Chirality Effects on Proline-Substituted L-Serine Octamers Revealed by IRPD Spectroscopy

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Figures

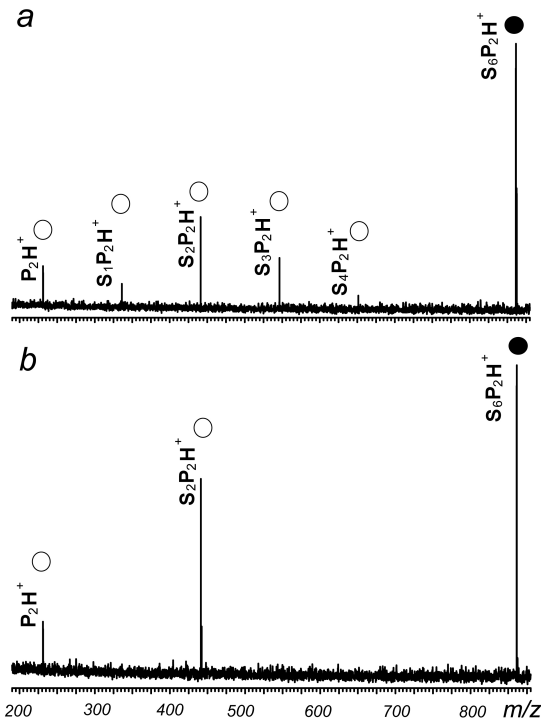

Figure S1. Sustained off-resonance irradiation (SORI) - CAD mass spectra of (a) $[L\text{-}Ser_7+L\text{-}Pro_1]H^+$, (b) $[L\text{-}Ser_7+D\text{-}Pro_1]H^+$, (c) $[L\text{-}Ser_6+L\text{-}Pro_2]H^+$ and (d) $[L\text{-}Ser_6+D\text{-}Pro_2]H^+$.

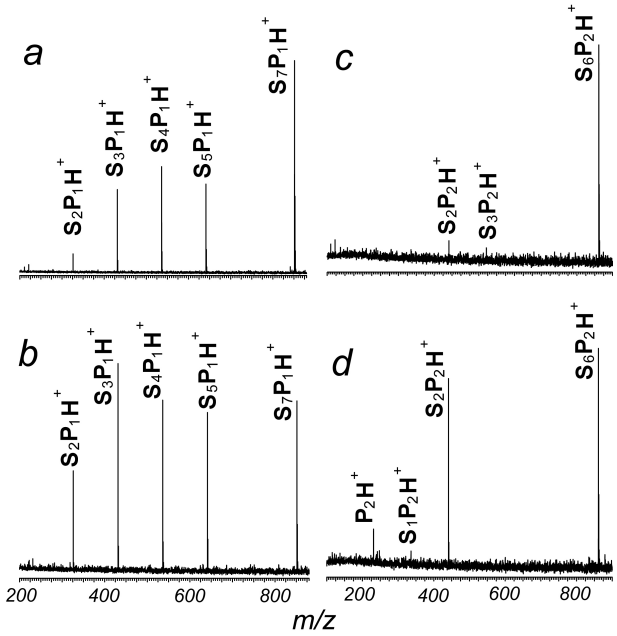

Figure S2. Based the results shown in Fig. 4, chiral differentiation of proline-substituted serine octamers can be fulfilled by choosing IR wavenumber in the range from 3460-3550 cm^{-1} (In fact, the chiral differentiation of $[L\text{-}Ser_6+L\text{-}Pro_2]H^+$ and $[L\text{-}Ser_6+D\text{-}Pro_2]H^+$ can be fulfilled at any wavenumbers where has an absorption, since their dissociation pathways are different). And the chiral differentiation effects can be optimized by selecting IR wavenumbers and irradiation time. Here are two examples: IRPD mass spectra of (a) $[L\text{-}Ser_7+L\text{-}Pro_1]H^+$ and (b) $[L\text{-}Ser_7+D\text{-}Pro_1]H^+$, which were obtained by 2s IR laser irradiations at 3470 cm^{-1}, (c) $[L\text{-}Ser_6+L\text{-}Pro_2]H^+$ and (d) $[L\text{-}Ser_6+D\text{-}Pro_2]H^+$, which were obtained by 2s IR laser irradiations at 3530 cm^{-1}. Chiral differentiation can be performed readily by comparing these spectra.

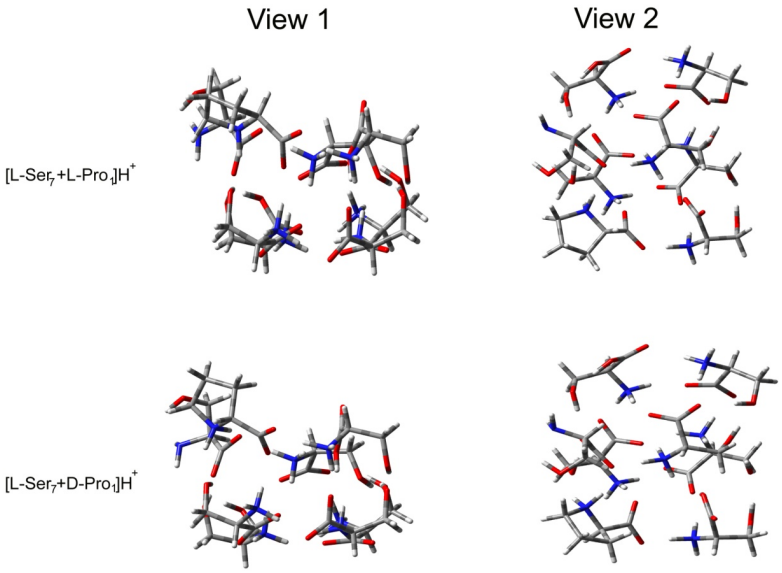

Figure S3. Isomers of (a) $[L\text{-}Ser_7+L\text{-}Pro_1]H^+$, and (b) $[L\text{-}Ser_7+D\text{-}Pro_1]H^+$. Both structures are optimized on the level of B3LYP/6-31G(d).

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics