

Supporting Information

Differentiation of Peptide Isomers by Excited-State Photodissociation and Ion-Molecule Interactions

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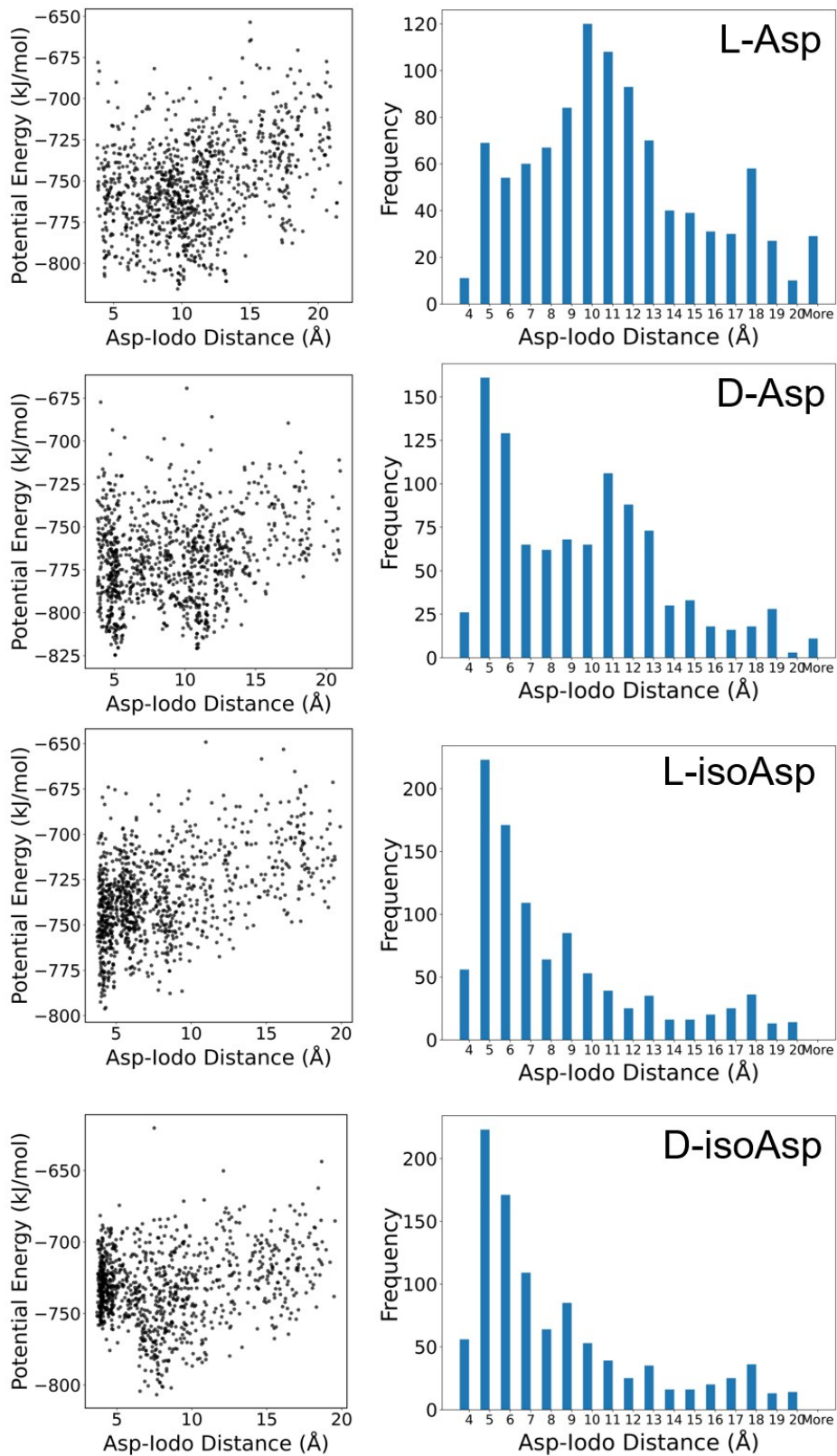


Figure S1: Full range of structures generated by simulated annealing of 4IB-VKLDHG, where Fig. 6 shows structures with potential energy within the lowest 50 kJ.

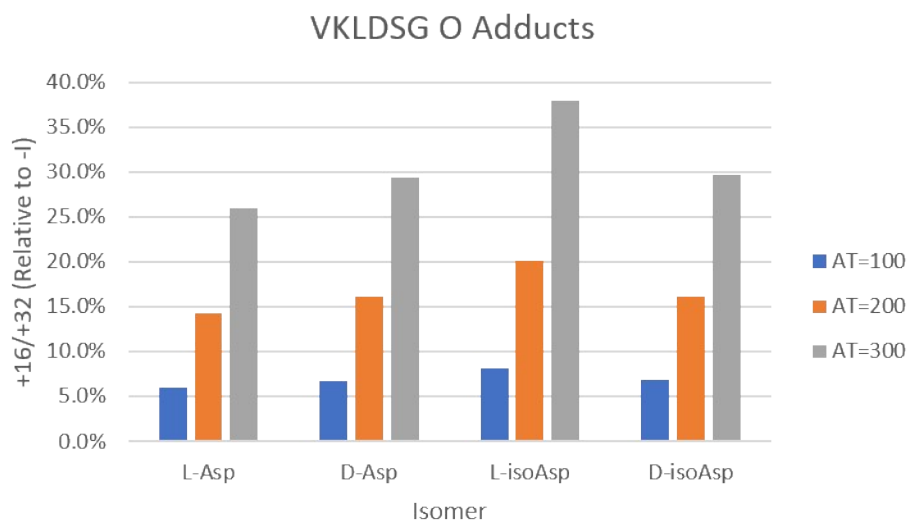


Figure S2: Ratio of +16/+32 Da oxygen adducts as a function of laser excitation time. Increased time corresponds to increased production of +16 Da. This is consistent with two-step process where O₂ initially adds to the radical site, followed by loss of O after a subsequent laser pulse.