Rapid Characterization of Cross-links, Mono-adducts, and Non-covalent Binding of Psoralens to Deoxyoligonucleotides by LC-UV/ESI-MS and IRMPD Mass Spectrometry

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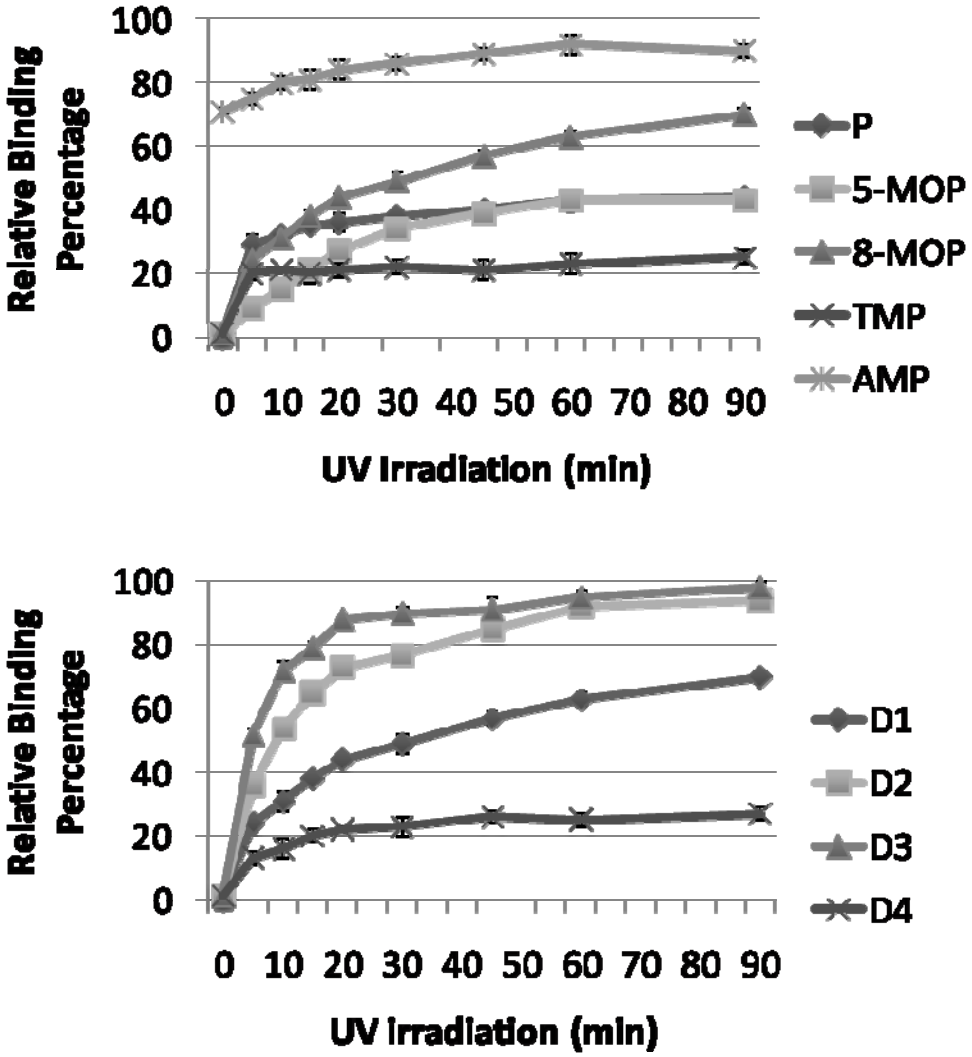
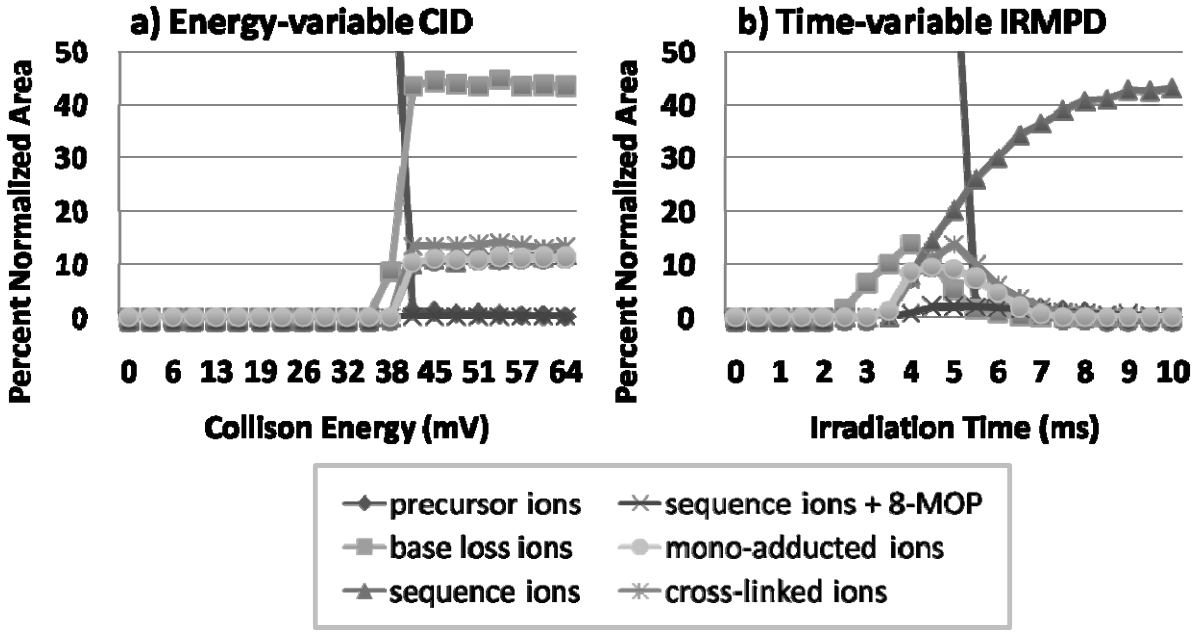


Supplementary Figure 1. Relative binding percentage of (a) each psoralen analog with D1 and (b) 8-MOP with each duplex. The relative binding percentages include all possible DNA/psoralen products: mono-adducts, cross-links, and non-covalent complexes. ESI-MS measurements were performed in triplicate on separate samples on different days.



Supplementary Figure 2. Variable energy dissociation comparison for $[D1 + 8\text{-MOP}]^{6-}$ obtained by a) CID and b) IRMPD at 10 W. Product ion types are grouped by ion type including precursor ions, base loss ions, backbone sequence ions, sequence ions retaining the 8-MOP adduct, mono-adducted ions, and cross-linked product ions.