Supporting Information for:

Bond Specific Dissociation following Excitation Energy Transfer for Distance Constraint Determination in the Gas Phase

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Table S1. Ion mobility results for the polyalanine peptides.

Sequence	Predicted CCS (TM) (Å^2)	Experimental CCS (TWIMS) (Å^2)
$AcWA_8CK$-PM	383.1	372.8
$AcAWA_7CK$-PM	382.1[a]	366.5
AcA_2WA_6CK-PM	380.5	365.2
AcA_3WA_5CK-PM	383.9	363.3
AcA_4WA_4CK-PM	385.7	351.8
AcA_5WA_3CK-PM	377.0	349.7
AcA_6WA_2CK-PM	383.5	356.8
AcA_7WACK-PM	390.5	360.3
AcA_8WCK-PM	392.0	354.6

a) calculated in He and normalized to N_2

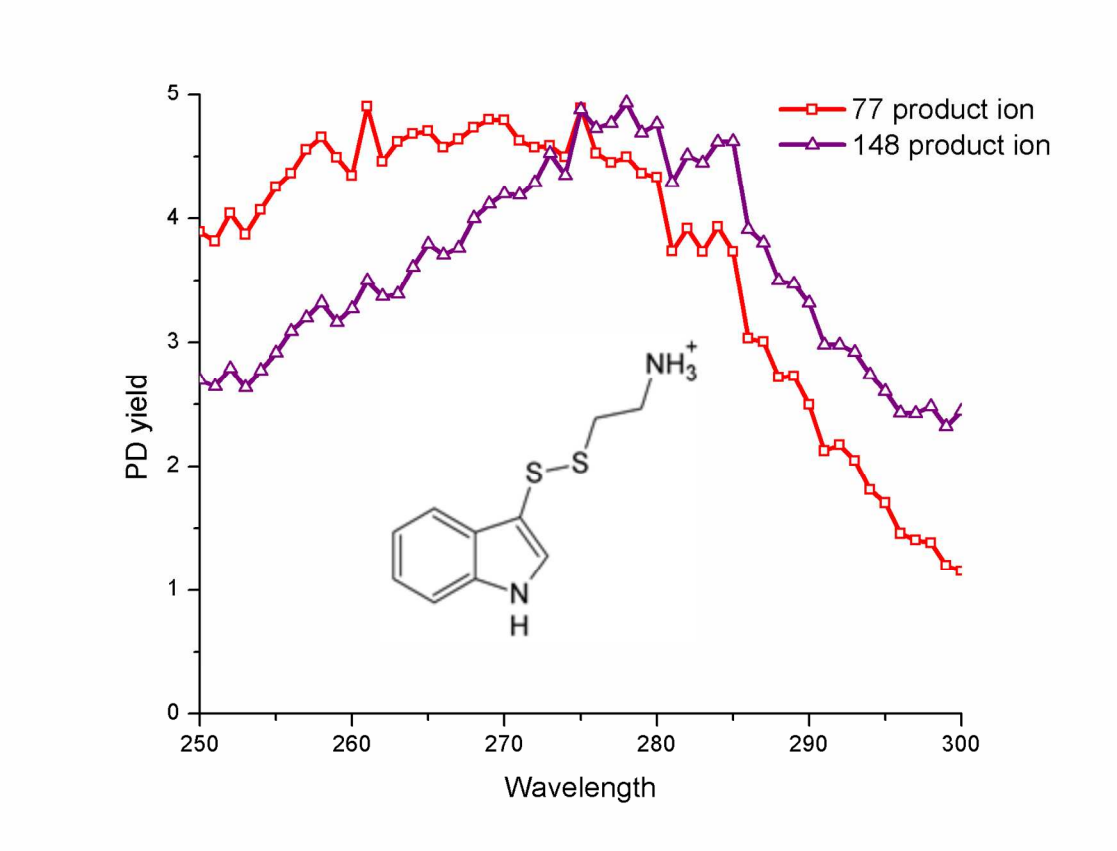

Figure S1: Action spectra of both the EET product (77Da) and electron transfer product (148Da) from the dissociation of the pictured structure.

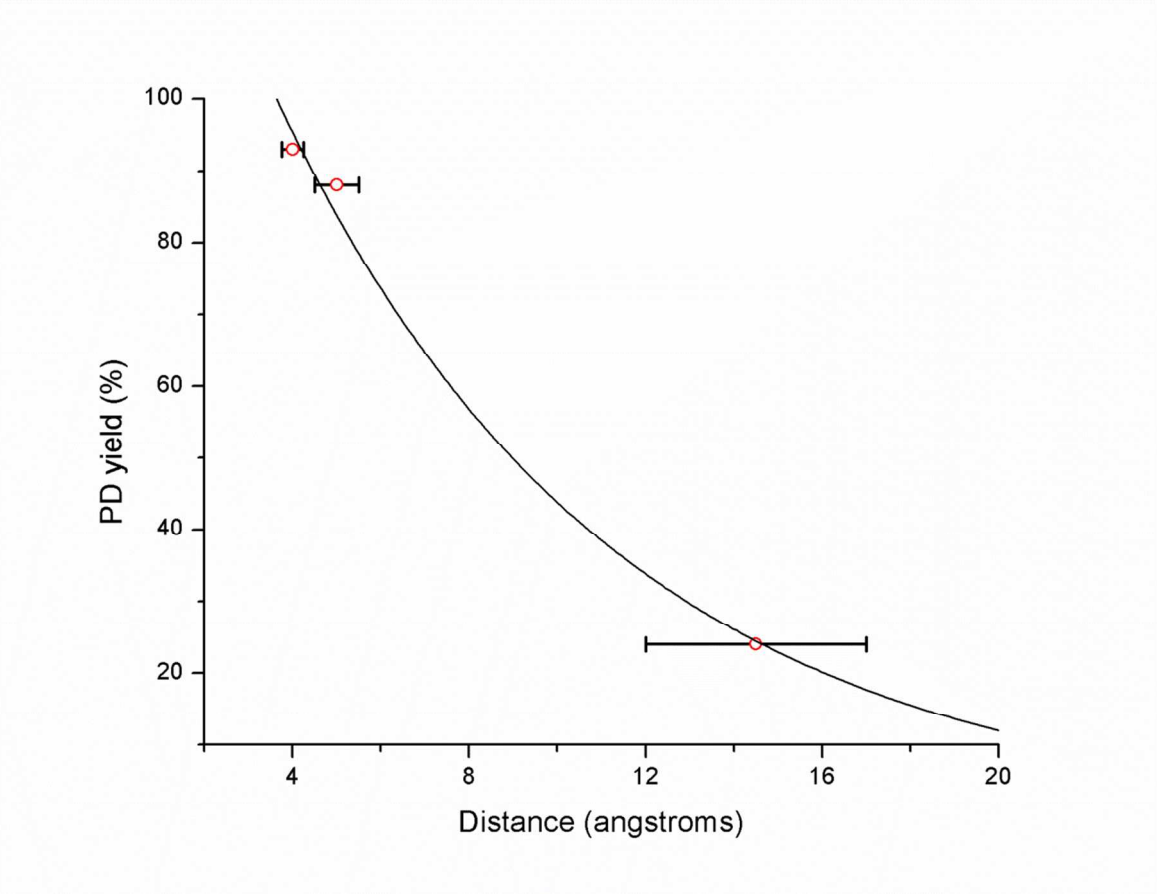

Figure S2. Fit of the Dexter equation to the experimental data.

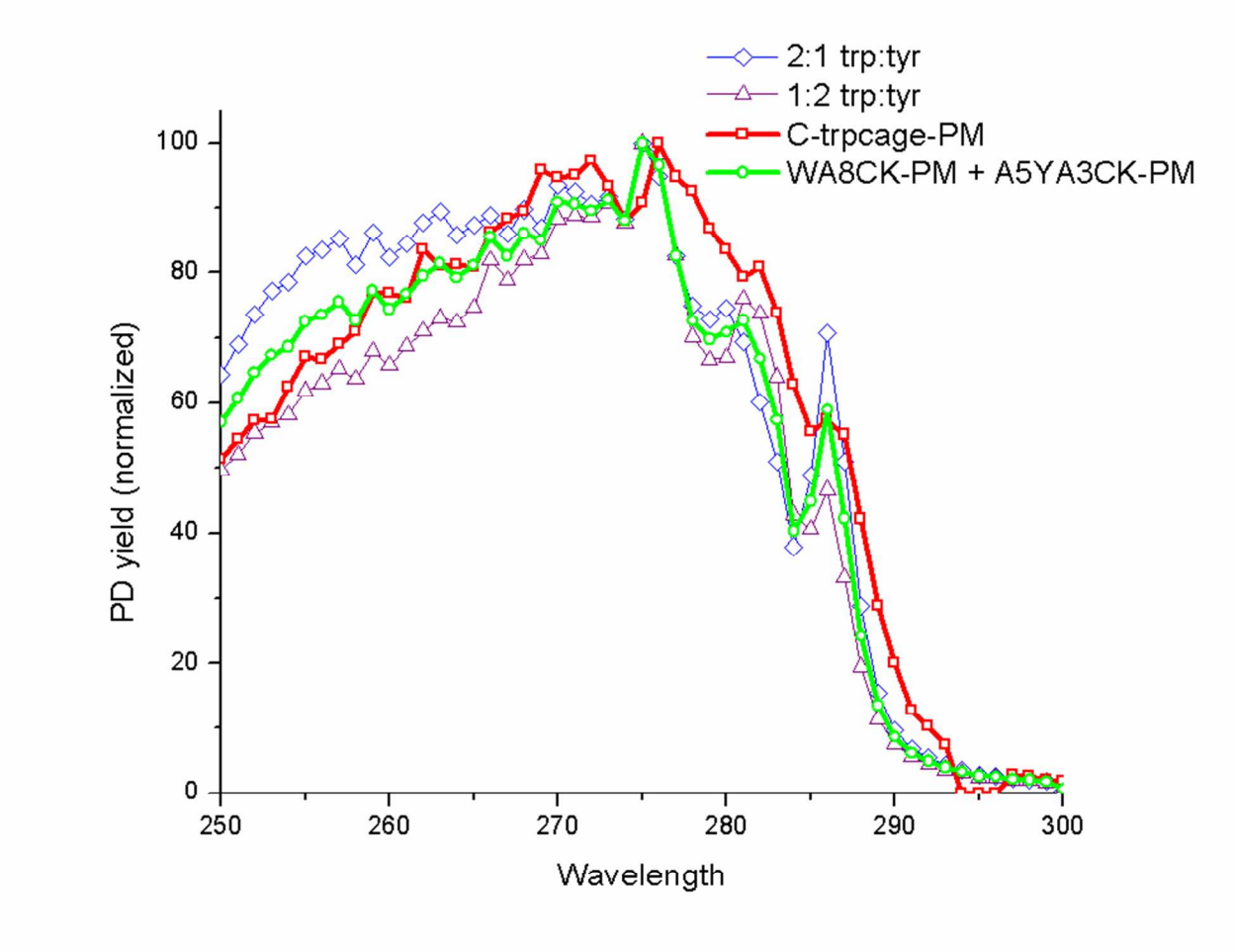

Figure S3: Various fits of combination spectra of tryptophan and tyrosine-induced EET compared to the C-trpcage-PM 2+ spectra (red). A one-to-one combination of the spectra from $AcWA_8CK$-PM and AcA_5YA_3CK-PM is shown (green) compared to the two-to-one (blue) and one-to-two combinations (purple).

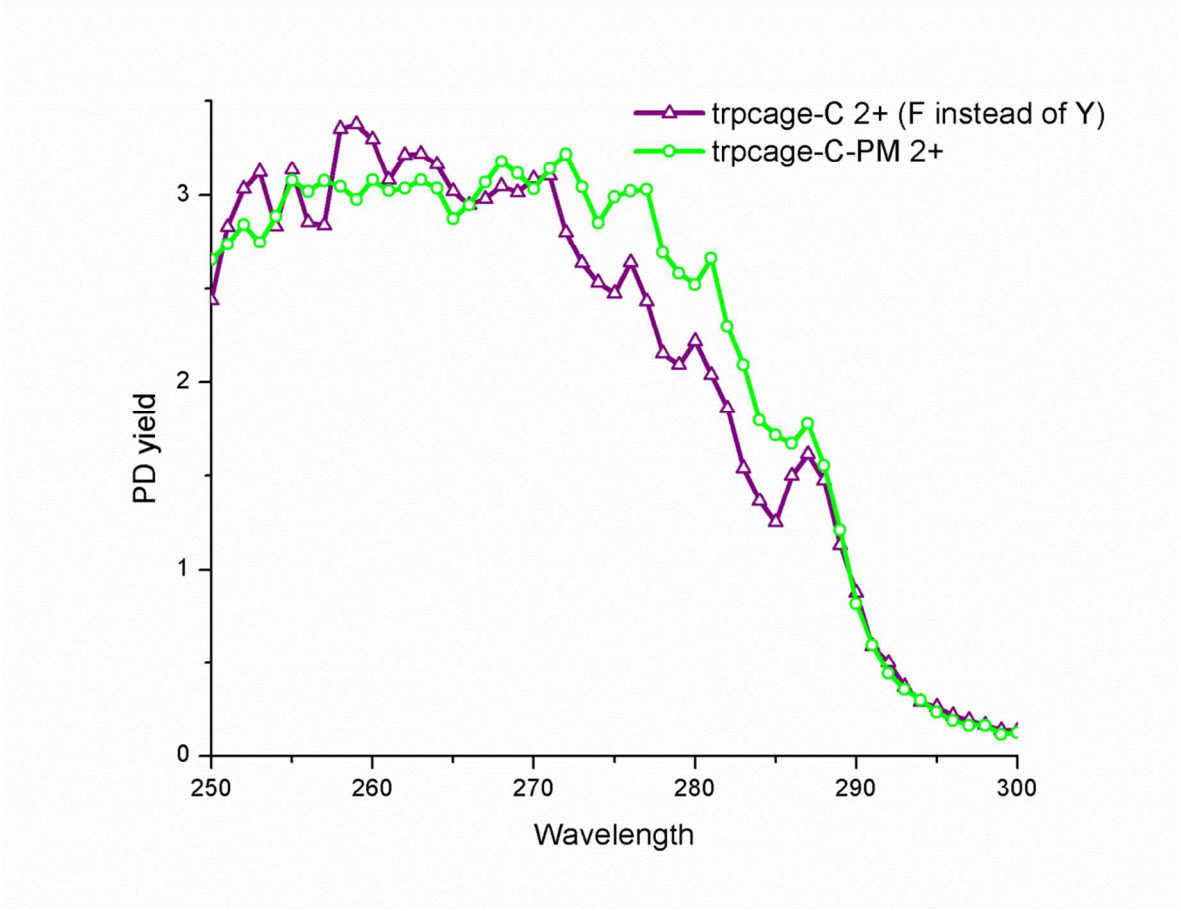

Figure S4. Action spectra of trpcage-C-PM and trpcage-C-PM with phenylalanine substituted for tyrosine.

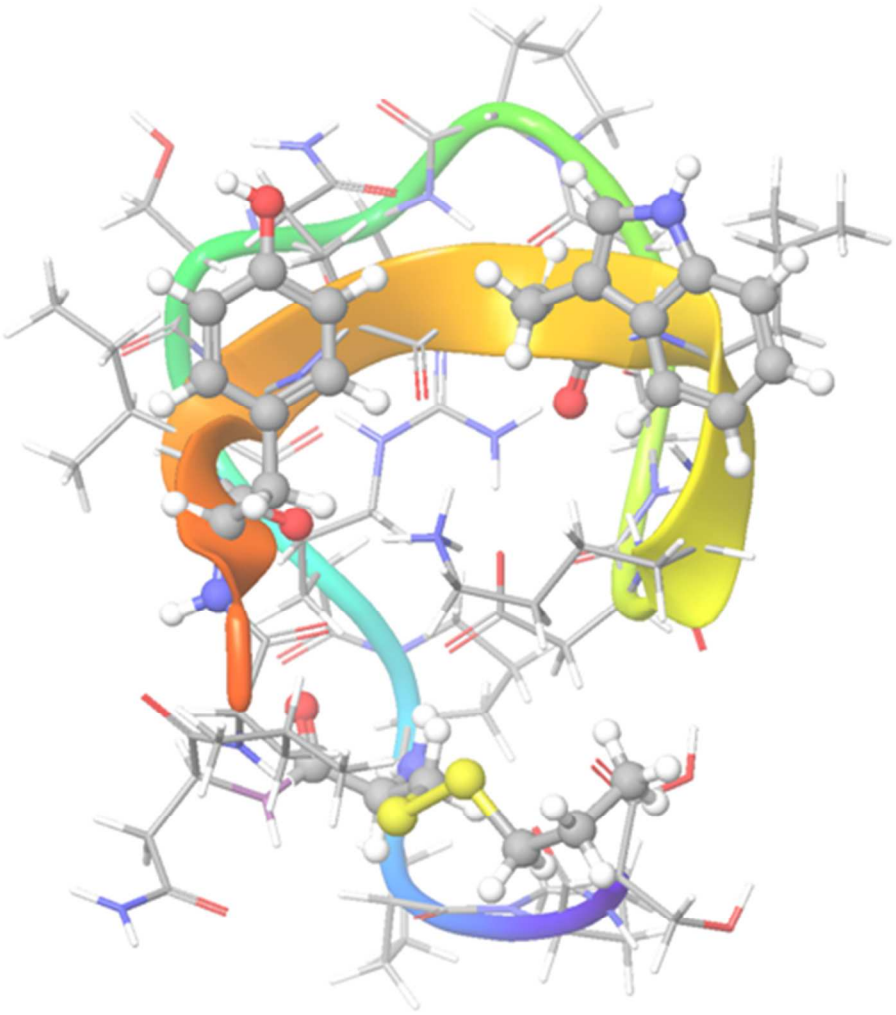

Figure S5. Lowest-energy structure generated from simulated annealing at 1000K. Tyrosine, tryptophan and cysteine are represented with ball-and-stick models.

Table S2. Effects of various perturbations of the Ctrpacage structure on PD yield.

Conditions	PD yield
Normal solvent and source conditions	35.0%

Native MS solvent (1mM NH_4oAc) and normal source conditions	33.8%
Normal solvent, CID enegery 18	31.3%
Normal solvent, spray voltage raised to 8	22.7%
Normal solvent, capillary temperature raised to 370	24.8%