Supporting Information for "Modest influence of FRET chromophores on the properties of unfolded proteins"

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Parameterization of chromophores

Our priority in determining parameters was to obtain reasonable non-bonded interactions, as the most critical feature of the model is how the chromophores interact with each other and with the protein. We use standard Amber atom types for all of the atoms in the two chromophores, thus fixing the Lennard-Jones parameters; angle and torsion terms were added by analogy with similar terms in the AMBER force field. Charges were determined using the restrained electrostatic potential (RESP) fitting[1] as implemented in the Antechamber program. For consistency with AMBER charges, electrostatic potentials were determined with unrestricted Hartree-Fock, assuming all carboxylate groups to be deprotonated, i.e. net charge of -2 for each dye; the geometry of each molecule was first optimized with the same

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method. We used the 6-31+G* basis set in place of the standard 6-31G*, the diffuse basis functions being included due to the presence of the sulfur atoms in these molecules. We also found that using this basis set gave more reasonable results in the geometry optimizations. Gromacs parameters for the dyes are available upon request from the authors.

Table S1: Sequences of molecules simulated in this study. *Dyes are attached to cysteine residues given in red.

	Sequences
CSP	MRGKVKWFDS KKGYGFITKD EGGDVFVHWS AIEMEGFKTL KEGQVVEFEI QEGKKGPQAA HVKVVE
CSP Dyes*	MCRGKVKWFD SKKGYGFITK DEGGDVFVHW SAIEMEGFKT LKEGQVVEFE IQEGKKGPQA AHVKVVEC
LR	GPCLTQEQLE DARRLKAIYE KKKNELGLSQ ESVADKMGMG QSGVGALFNG INALNAYNAA LLAKILKVSV EEFSPSIARE CR
LR Dyes*	GPCLTQEQLE DARRLKAIYE KKKNELGLSQ ESVADKMGMG QSGVGALFNG INALNAYNAA LLAKILKVSV EEFSPSIARE CR
IN	CFLDGIDKAQ EEHEKYHSNW RAMASDFNLP PVVAKGIVAS CDKCQLKGEA MHGQVDC
IN Dyes*	CFLDGIDKAQ EEHEKYHSNW RAMASDFNLP PVVAKGIVAS CDKCQLKGEA MHGQVDC

Table S2: Number of non-protein molecules in simulated systems.

	CSP	**CSP Dyes**	**LR**	**LR Dyes**	**IN**	**IN Dyes**
Water	8339	8329	8294	8234	8422	8353
Sodium ions	10	10	9	11	12	16
Chloride ions	10	6	10	8	8	8

References

(1) Cieplak, P.; Cornell, W. D.; Bayly, C.; Kollman, P. A. *J. Comput. Chem.* **1995**, *16*, 1357–1377.

(2) Cross, S.; Kuttel, M. M.; Stone, J. E.; Gain, J. E. *J. Mol. Graph. Model.* **2009**, *28*, 131–139.

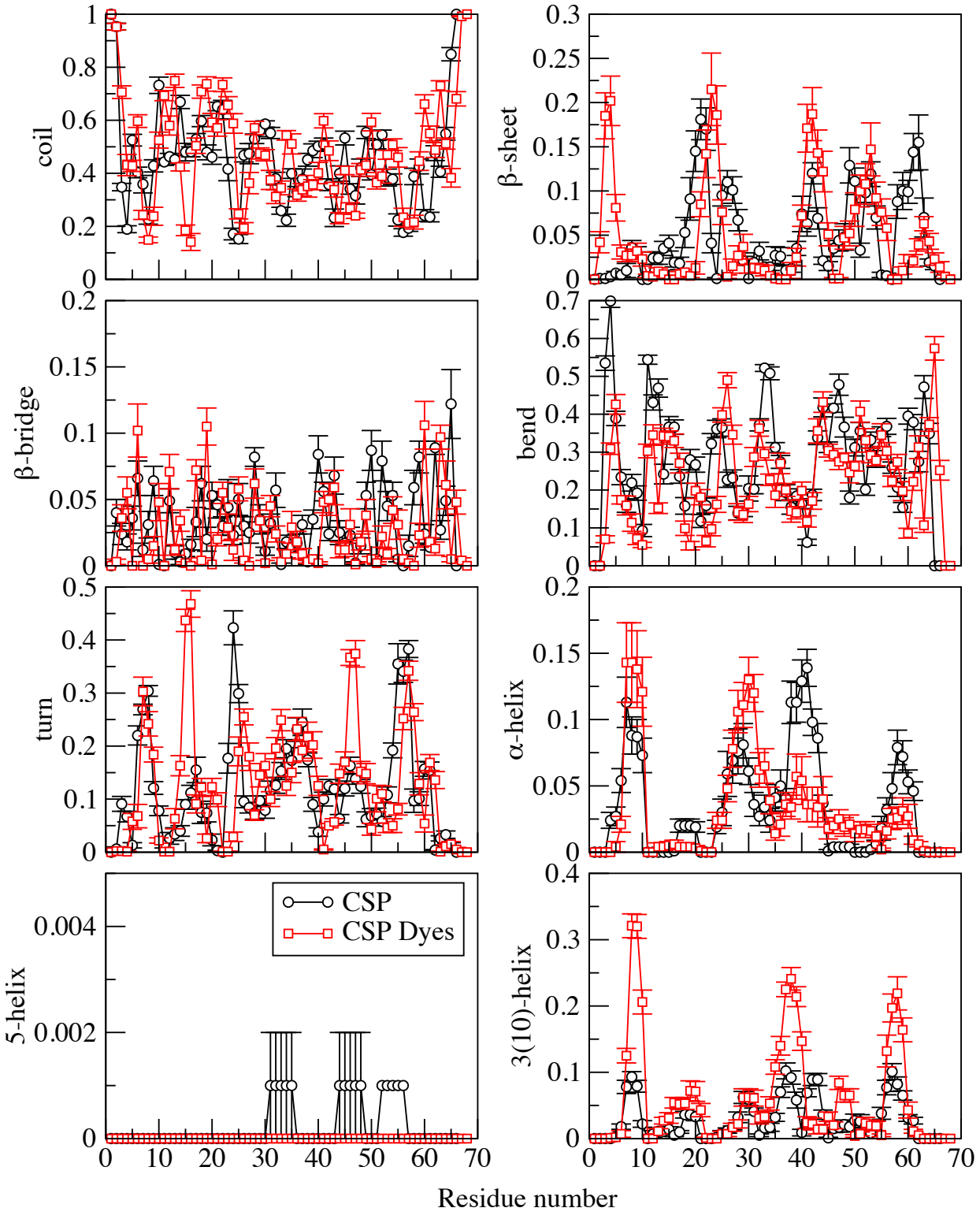

Figure S1: Per-residue secondary structure propensities calculated based on DSSP definition of CSP and CSP Dyes. Standard errors are calculated using block averaging.

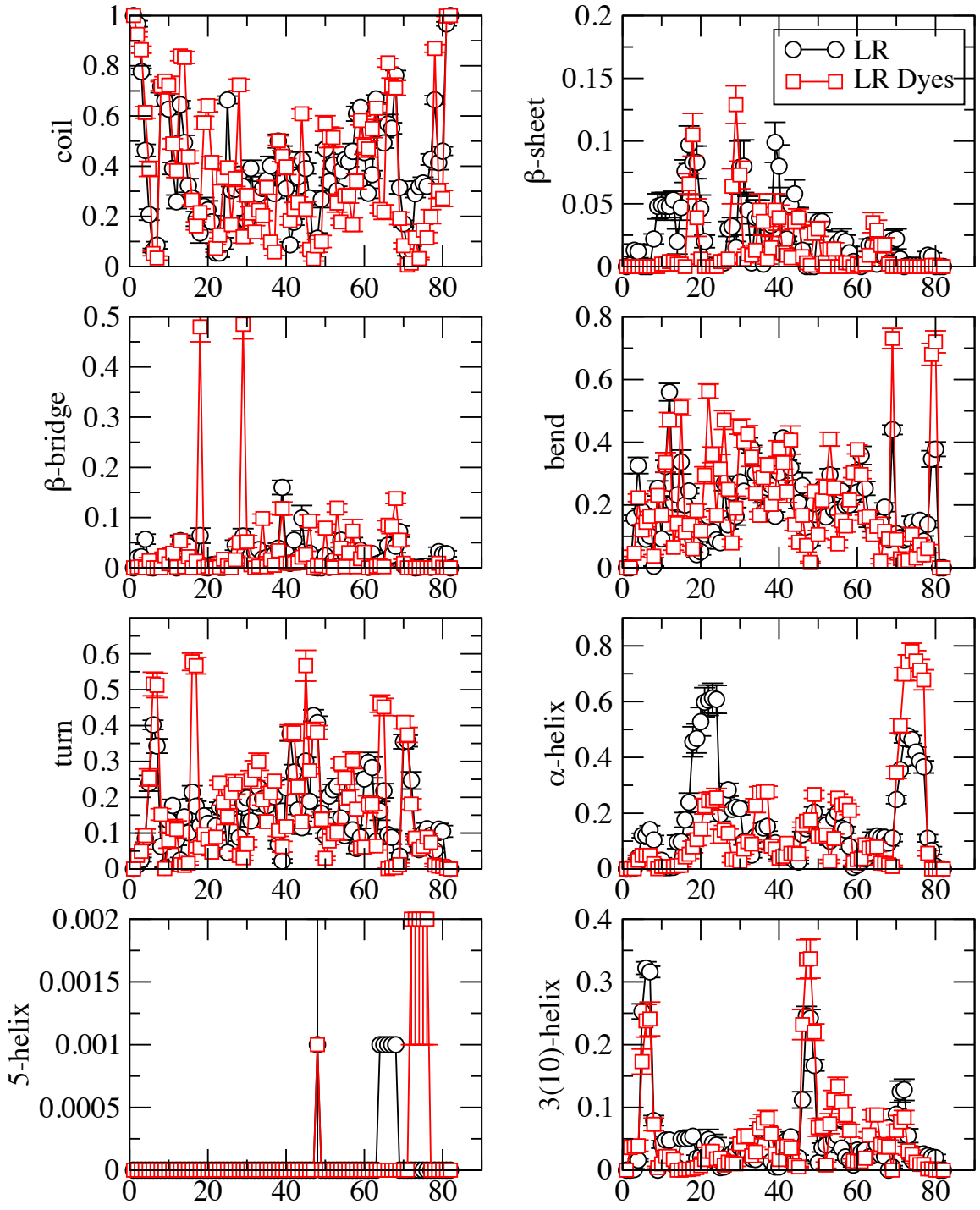

Figure S2: Per-residue secondary structure propensities calculated based on DSSP definition of LR and LR Dyes. Standard errors are calculated using block averaging.

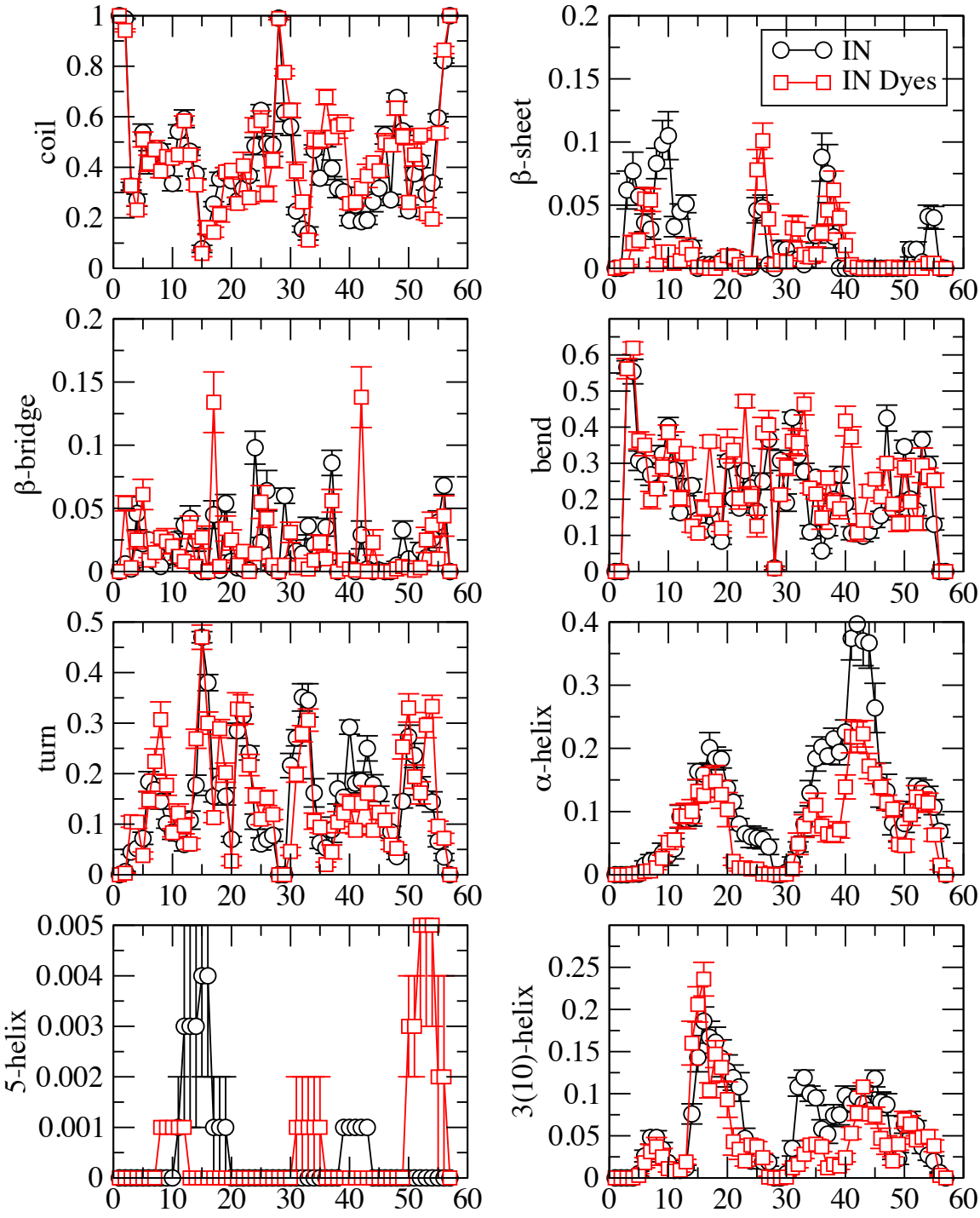

Figure S3: Per-residue secondary structure propensities calculated based on DSSP definition of IN and IN Dyes. Standard errors are calculated using block averaging.

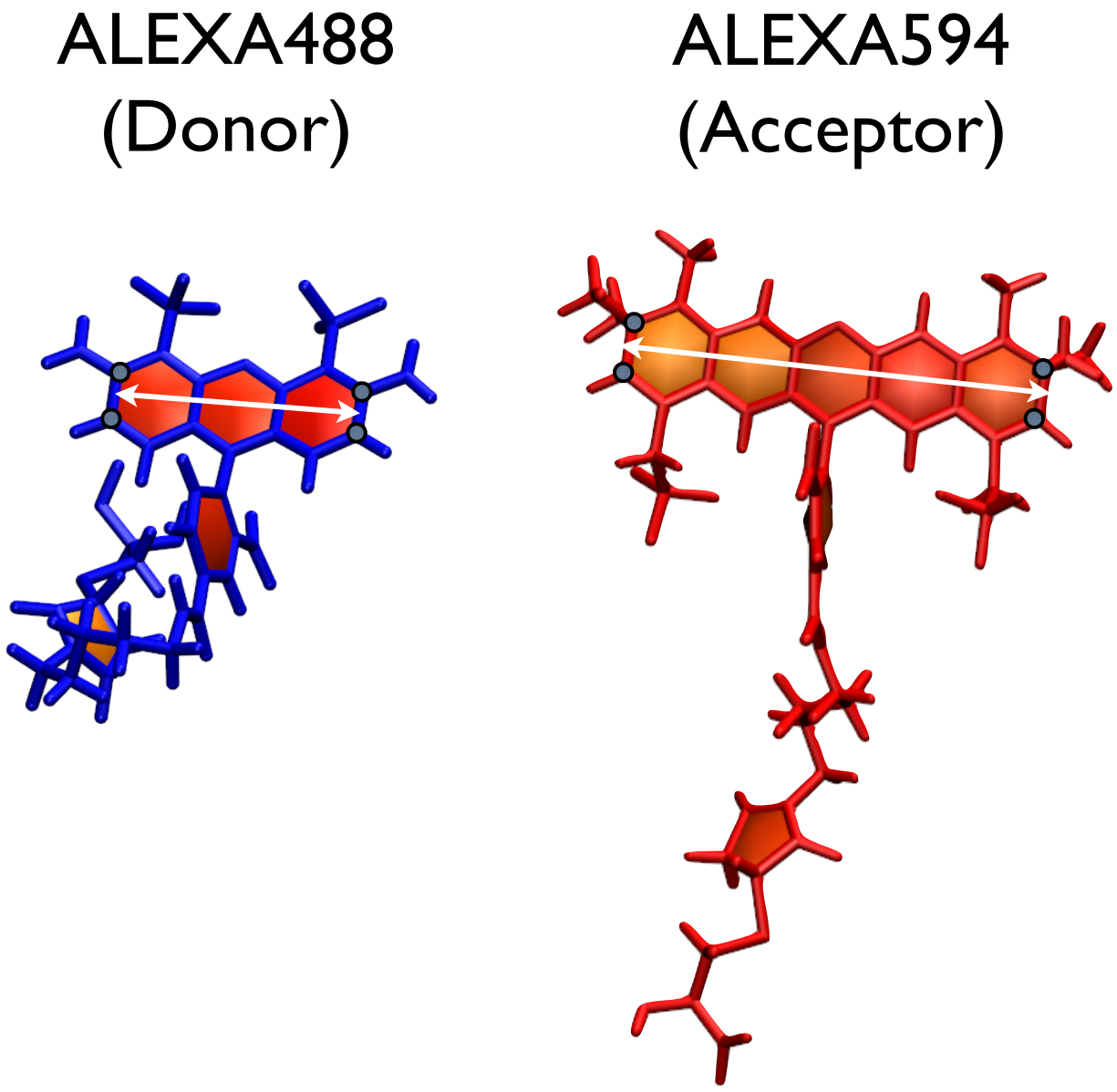

Figure S4: Blue molecule is the Alexa 488 attached at the N-terminus and red molecule is the Alexa 594 attached at the C-terminus. Both are shown with the paperchain representation in VMD.[2] Transition dipole vectors used for orientational factor κ^2 calculation are shown with white arrows.