Supporting information for

Nonadiabatic Photodynamics of Retinal Models in Polar and Nonpolar Environment

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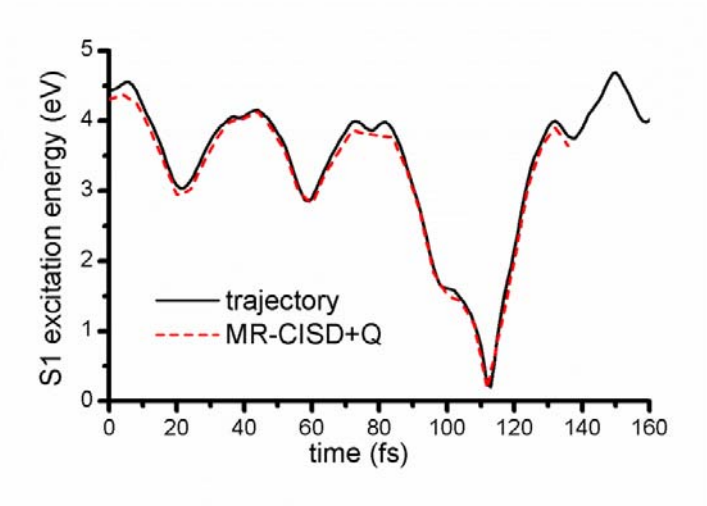

Figure S1: S_1 excitation energy along a trajectory using the MR-CIS(4,5) method in comparison to the MR-CISD(4,5)-FC6+Q/6-31G(d) reference level.

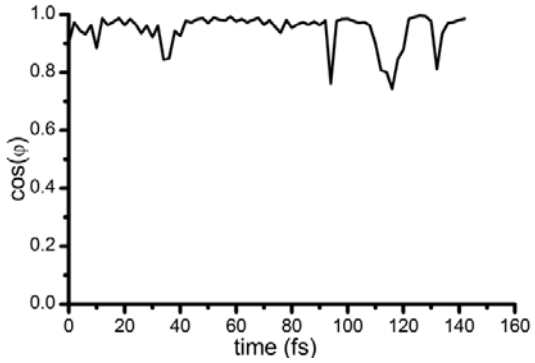

Figure S2: Cosine of angle φ between the energy gradient computed at the dynamics level [MR-CIS(4,5)] and the MR-CISD(4,5)-FC6/6-31G(d) reference along one trajectory.

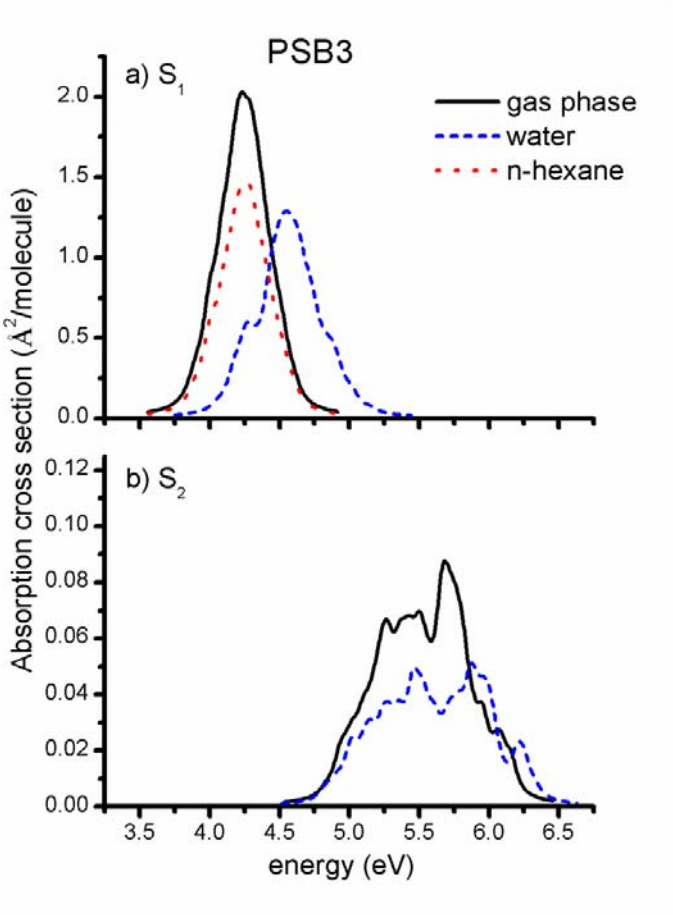

Figure S3: a) S_1 absorption spectra of PSB3 in the gas phase water and n-hexane and b) S_2 absorption spectra in gas phase and water.

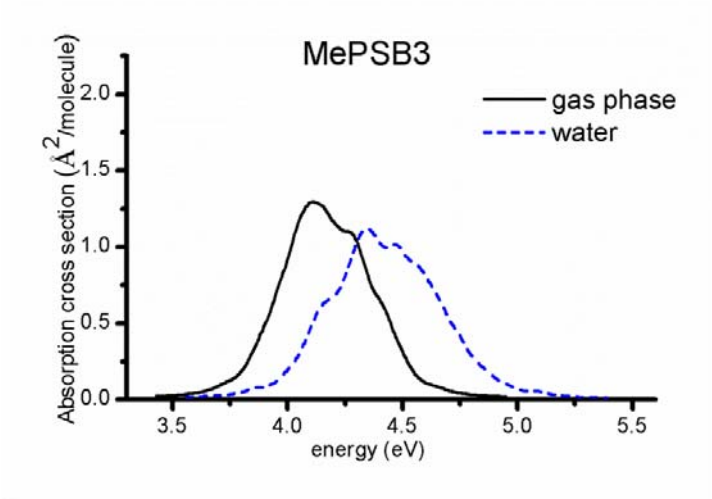

Figure S4: S_1 absorption spectrum of MePSB3 in the gas phase and water.

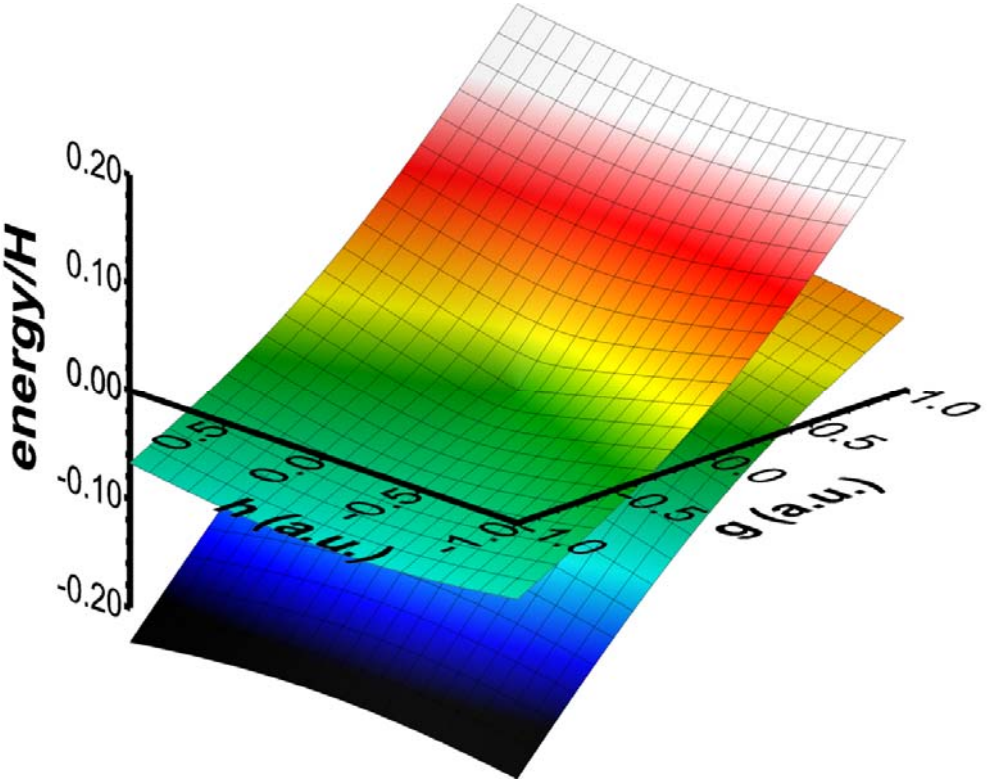

Figure S5: Double cone of the energy surfaces in the *g*-*h* subspace at the MXS of PSB3 in the gas phase.

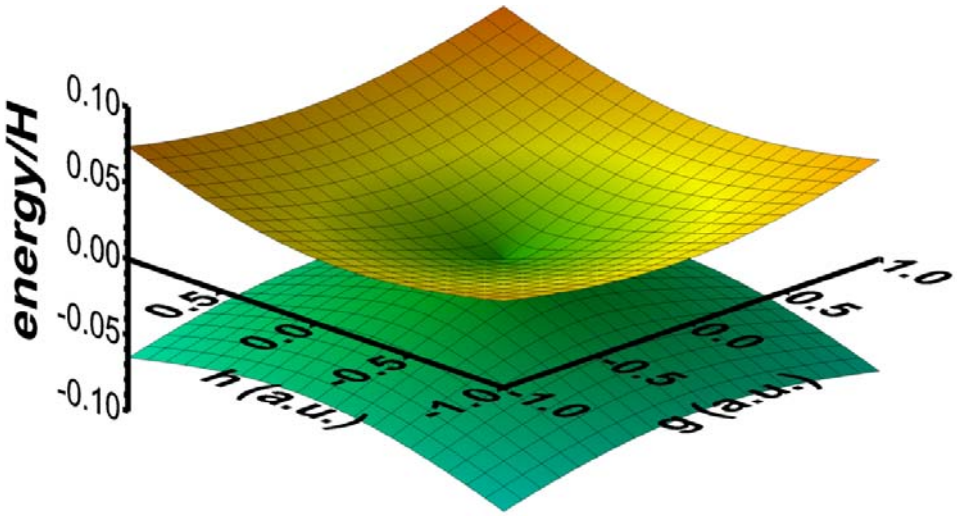

Figure S6: Double cone in the *g*-*h* subspace at the MXS of PSB3 in water for one selected solvent distribution.

Table S1: Lennard-Jones parameters used for PSB3 and MePSB3

Atom		σ-diameter (Å)	ε-well depth (kcal/mol)
(Me)PSB3	N	3.250	0.170
(Me)PSB3	C (-CH, -CH_2)	3.550	0.076
MePSB3	C (-CH_3)	3.500	0.066
(Me)PSB3	H (-CH, -$CH_{2,3}$)	2.420	0.030
(Me)PSB3	H (-NH_2)	0.000	0.000