Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information of

Computational study on donor-acceptor optical markers for Alzheimer's disease: a game of charge transfer and electron delocalization.

by

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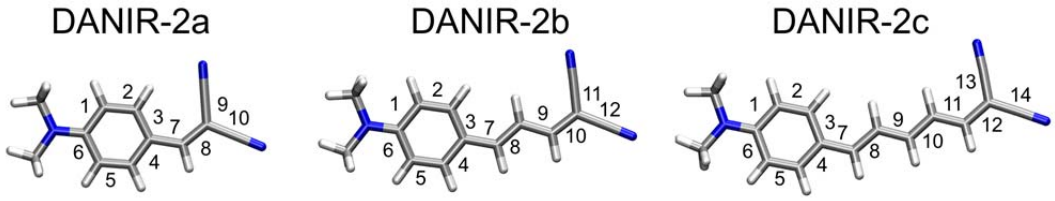
Table S1. Bond lengths (Å) of DANIR-2a, -2b and -2c at the S_0 and S_1 optimized geometries.



Bond lengths (Å) S_0	**2a**	**2b**	**2c**	**Bond lengths (Å) S_0**	**2a**	**2b**	**2c**
1	1.42	1.42	1.41	**8**	1.36	1.35	1.35
2	1.38	1.38	1.38	**9**	1.43	1.43	1.43
3	1.41	1.41	1.40	**10**	1.43	1.36	1.36
4	1.41	1.41	1.40	**11**	-	1.43	1.42
5	1.38	1.38	1.38	**12**	-	1.43	1.36
6	1.41	1.41	1.41	**13**	-	-	1.43
7	1.46	1.45	1.45	**14**	-	-	1.43
Bond lengths (Å) S_1	**2a**	**2b**	**2c**	**Bond lengths (Å) S_1**	**2a**	**2b**	**2c**
1	1.42	1.42	1.42	**8**	1.42	1.39	1.39
2	1.37	1.37	1.37	**9**	1.41	1.40	1.40
3	1.43	1.43	1.42	**10**	1.42	1.40	1.39
4	1.43	1.42	1.42	**11**	-	1.42	1.40
5	1.37	1.37	1.37	**12**	-	1.42	1.40
6	1.43	1.43	1.42	**13**	-	-	1.42
7	1.42	1.42	1.42	**14**	-	-	1.42

Table S2. PBE-D2 interaction energies and Grimme dispersion contribution (kJ/mol) of NIAD-4, DANIR-2a and DANIR-2c for selected marker-amyloid fibril complex models.

	I PELE (OPLS)	II PELE (OPLS)	I PBE-D	II PBE-D	I D	II D
NIAD-4	-337	-253	-339	-242	-255	-175
DANIR-2a	-179	-121	-195	-132	-195	-111
DANIR-2c	-251	-222	-265	-283	-232	-220

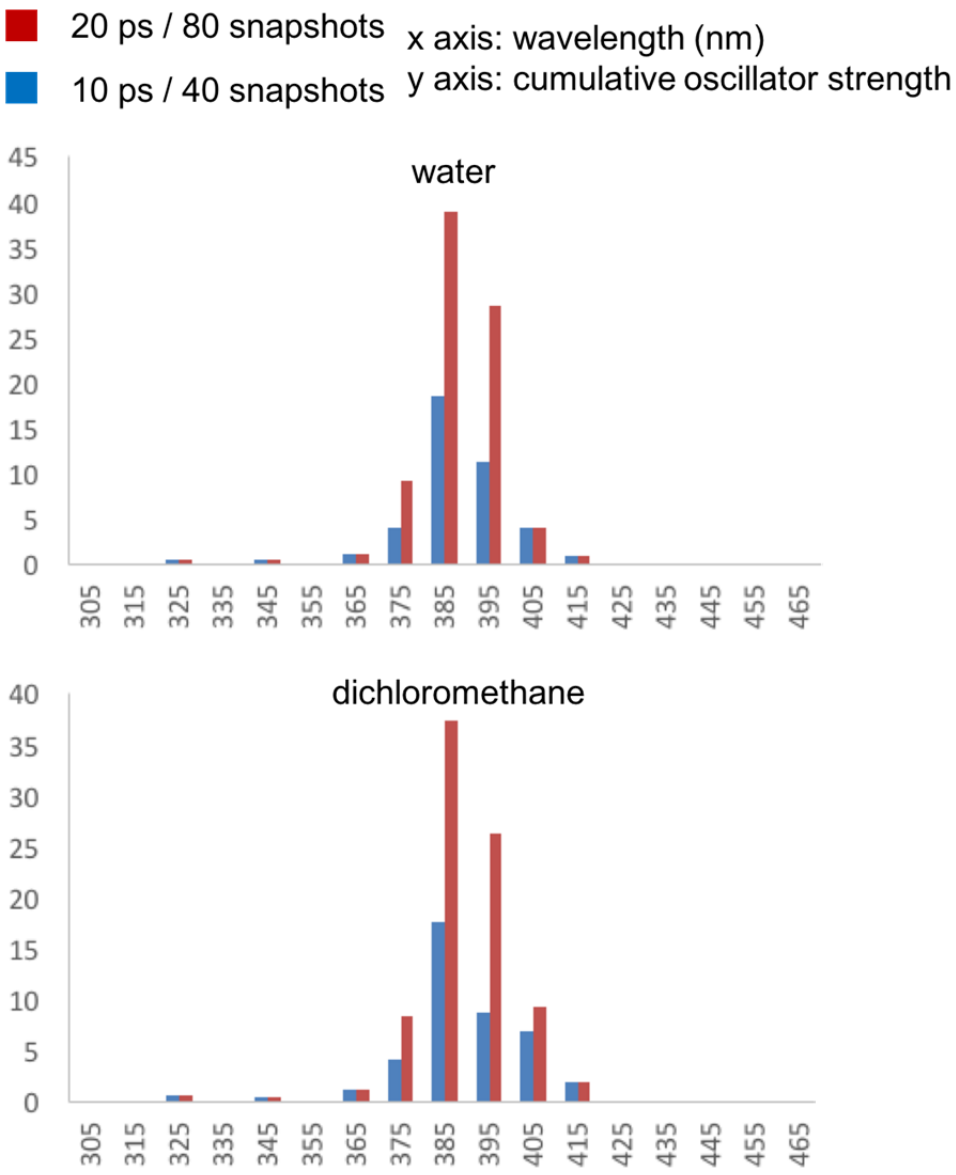


Figure S1. Computed TD-DFT(CAM-B3LYP) spectra from *ab initio* molecular dynamics simulations (PBE-D) of DANIR-2a in water and dichloromethane. Simulation time: 20 ps (80 evenly distributed snapshots) – red bars; 10 ps (40 evenly distributed snapshots) – blue bars.

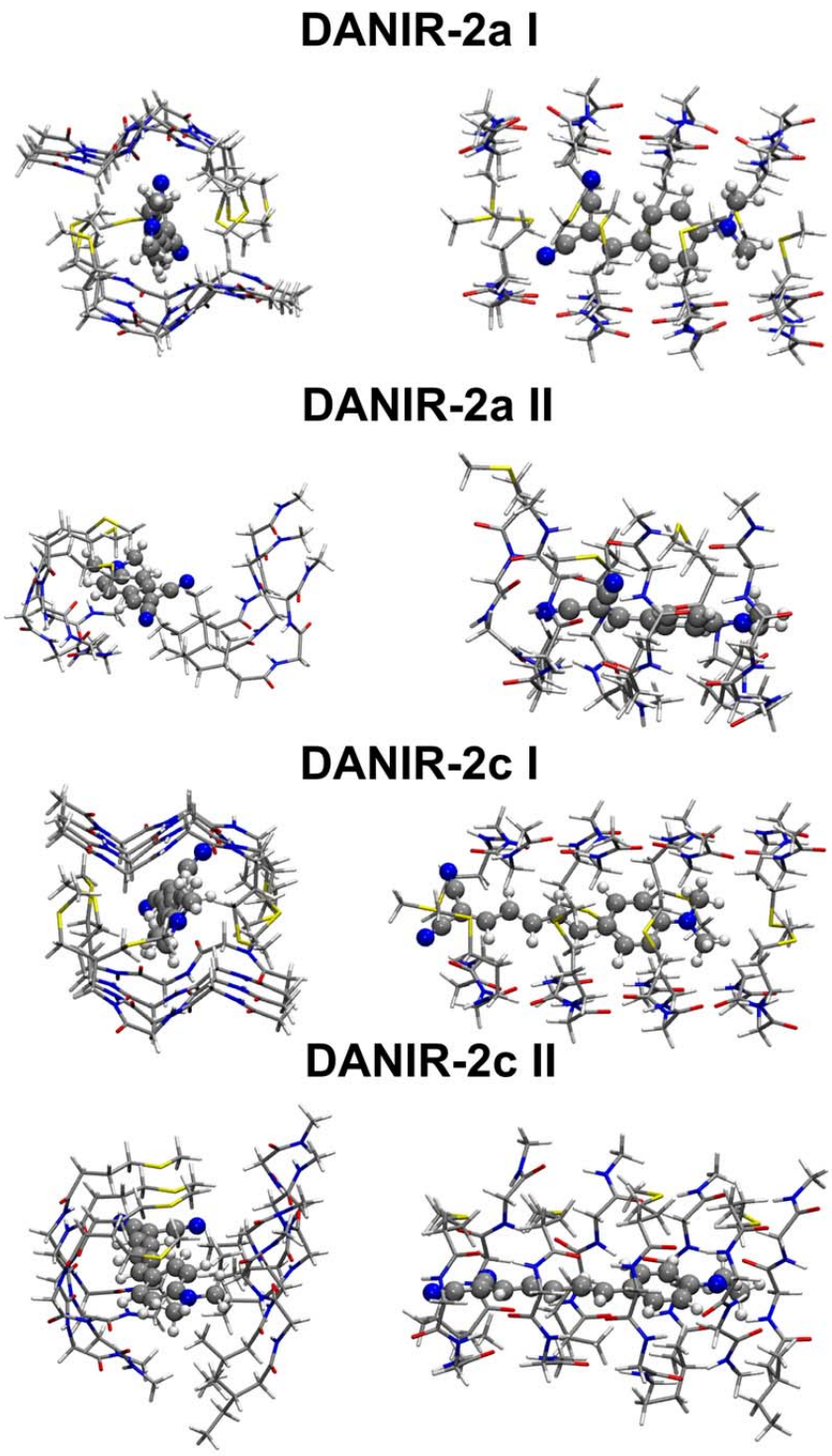


Figure S2. Selected models of fibril-marker interactions.

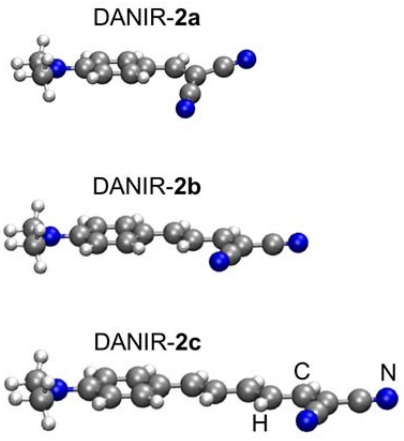


Figure S3. Optimized S_1 geometries of DANIR-2a, -2b and -2c.

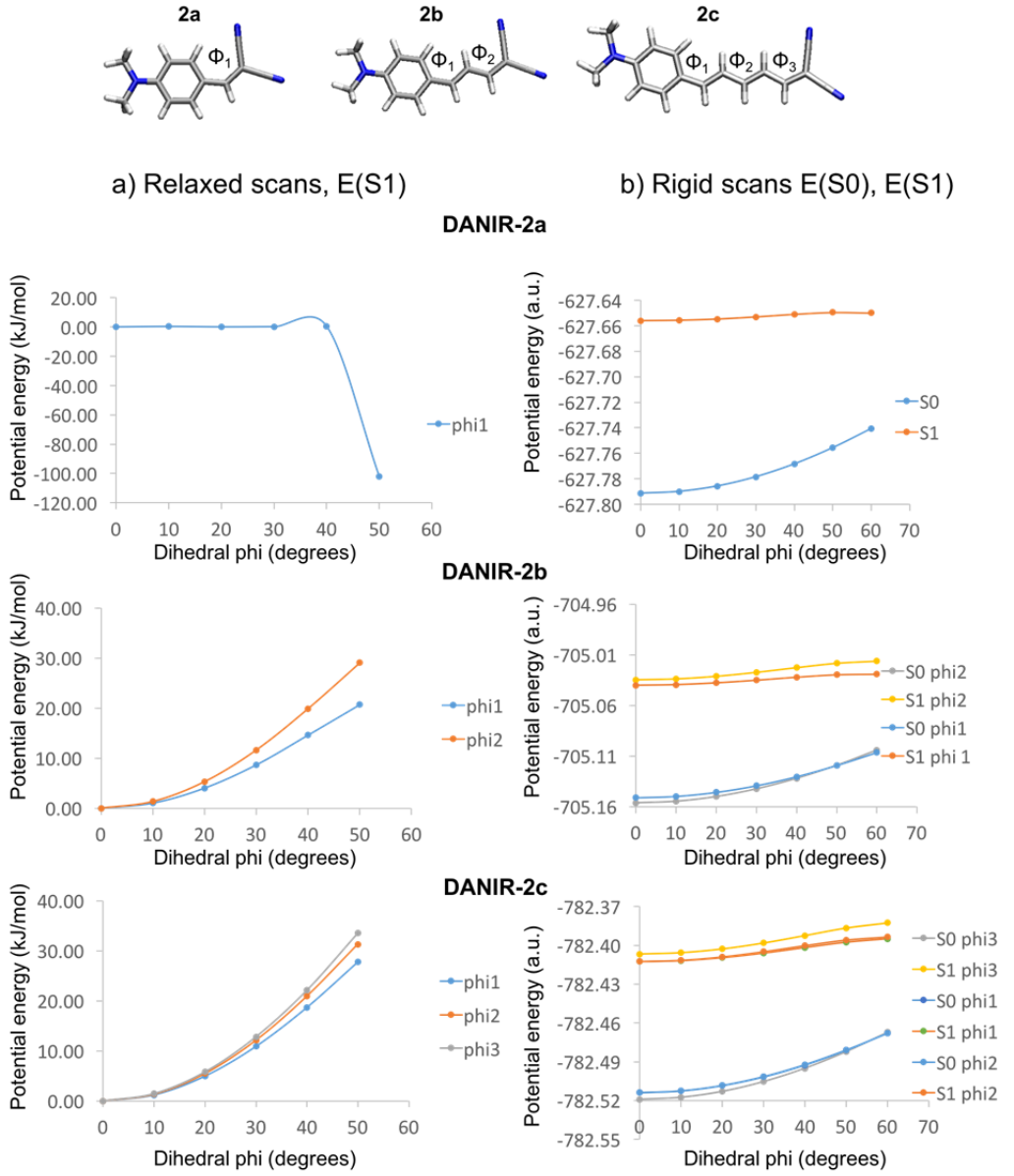


Figure S4 a) Relaxed and b) rigid potential energy scans around the double bonds of DANIR-2a, 2b and 2c.