Supporting information: Enzyme-Specific Sensors via Aggregation of Charged *p*-Phenylene Ethynylenes

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Table S1. Detailed Simulation Information

Simulation	**# OPEs**	**# DOPG**	**# Na^+**	**# Cl^-**	**# Waters**	**# atoms**	**Periodic box size (Å)**	**Simulation length (ns)**
0_1	**0**	42	44	2	30500	97052	100	150
2_1	2	6	17	15	15804	48426	80	100
2_2	2	21	15	5	30500	94472	100	150
3_1	3	6	15	15	15804	48522	80	100
4_1	4	42	44	10	30500	97444	100	250
5_1	5	20	25	15	15804	50562	80	100

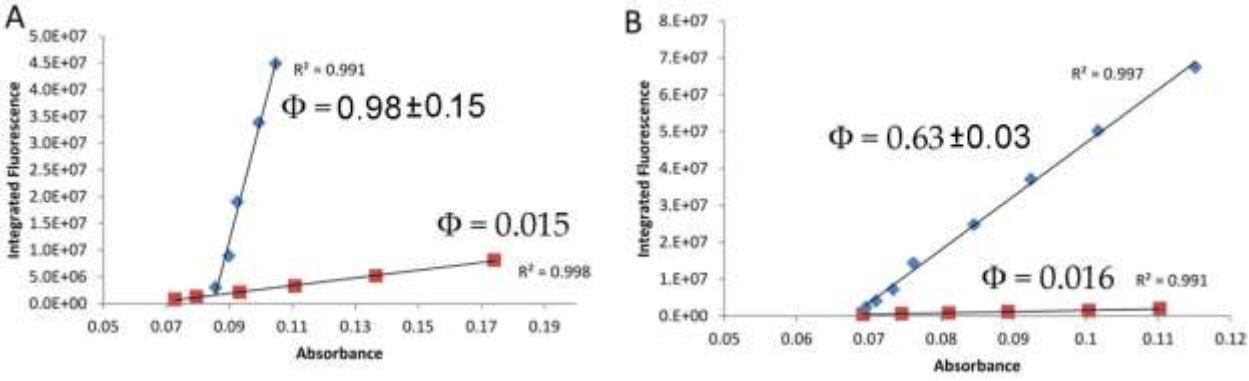

Figure S1. Integrated Fluorescence versus Absorbance for (A) 5 µM -1C (squares) and 5 µM -1C with 32 µM LaCh (diamonds), and (B) 1.4 µM +2C (squares) and 1.4 µM +2C with 16 µM DLPG (diamonds). This data was used to calculate the fluorescence quantum yields by the comparative method, and the new values for the quantum yields that were corrected from a previous study are given next to the line. Excitation was 370 nm for A and 375 nm for B, with fluorescence excitation wavelengths from 390 to 600 nm.

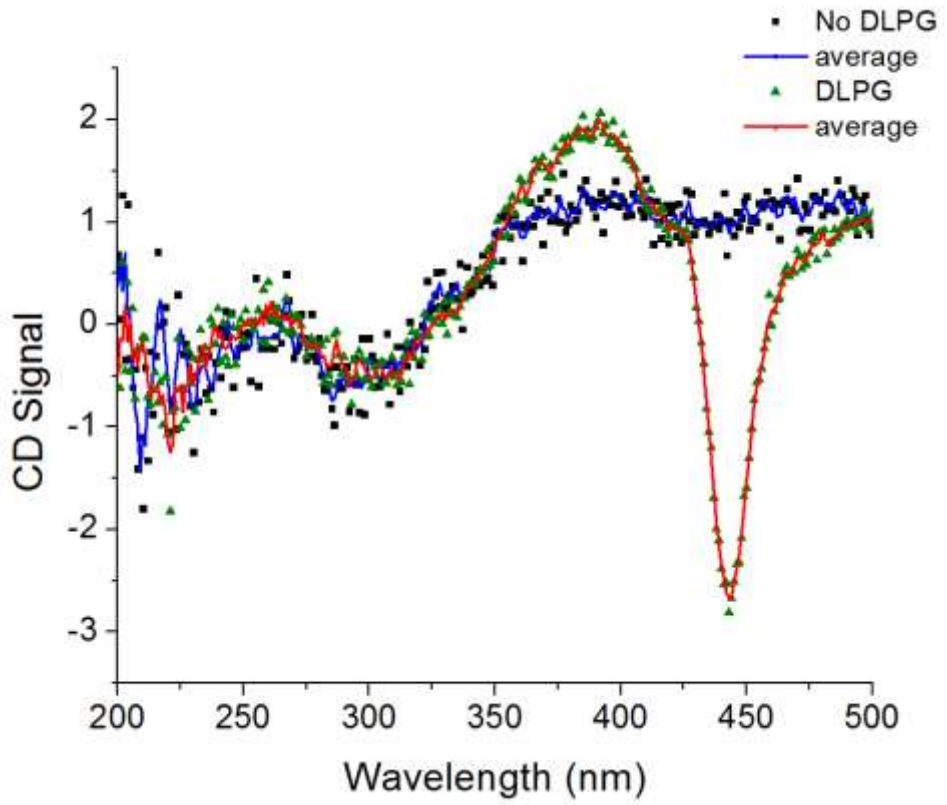

Figure S2. Circular Dichroism spectrum of 1.4 µM +2C with and without 16 µM DLPG added.

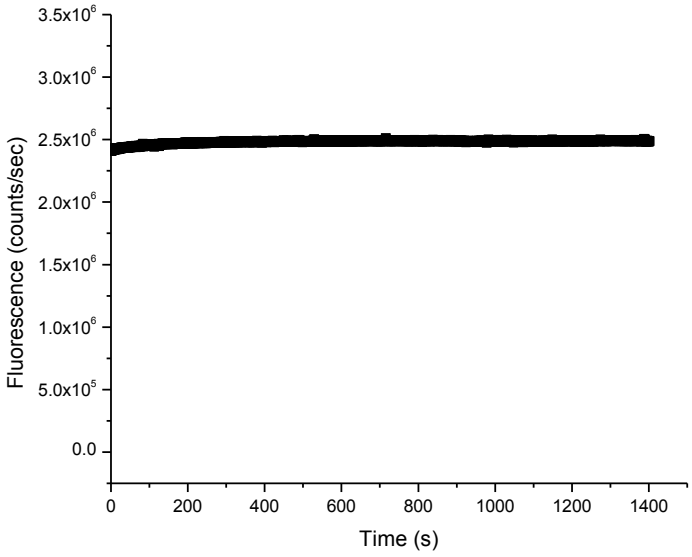

Figure S3. Fluorescence of PLA sensor (Ex. 375 nm; Em. 440 nm) composed of 1.4 µM +2C and 16 µM DLPG following addition of 0.4U of PLC.

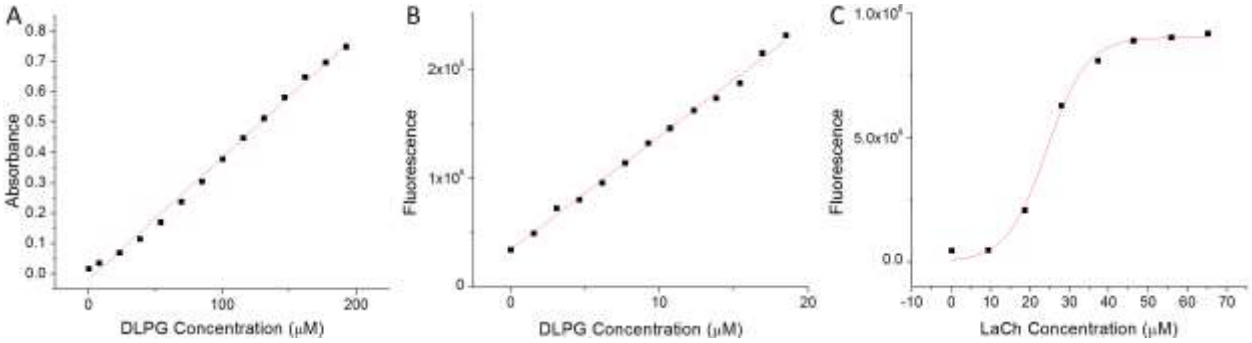

Figure S4. Linear regression of (A) Absorbance of 10 µM OPE-2+; (B) Fluorescence of 1.4 µM OPE-2+ (Ex: 375 nm, Em: 440 nm), with increasing DLPG concentration; (C) Fluorescence of OPE-1- with increasing LaCh concentration (Ex:370 nm, Em: 440 nm).

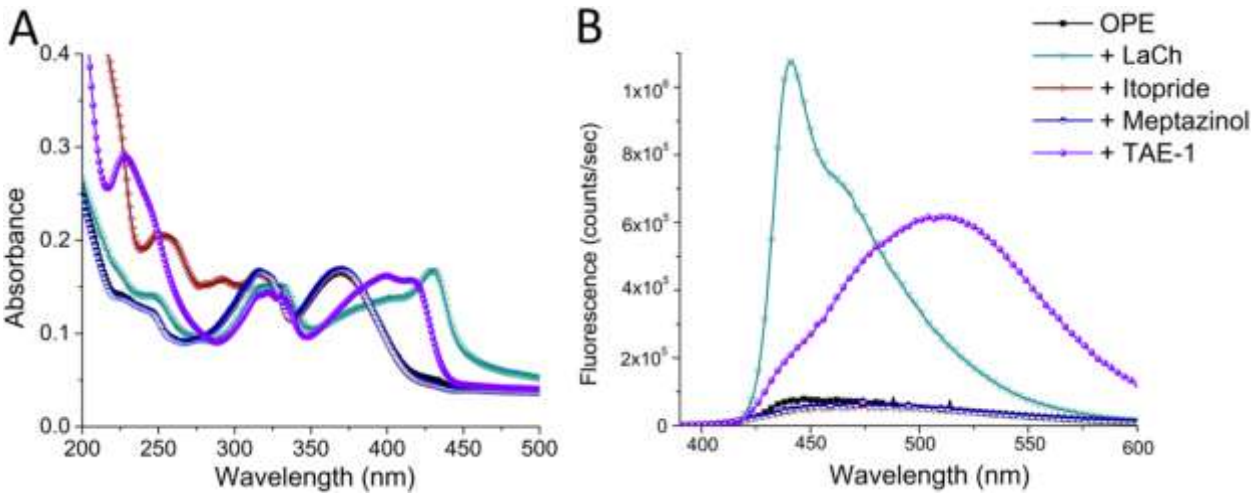

Figure S5. (A) Absorbance and (B) Fluorescence (Ex: 370 nm) of 5 µM -1C with 5 µg/mL of either LaCh or one of the three AChE Inhibitors used in this study.

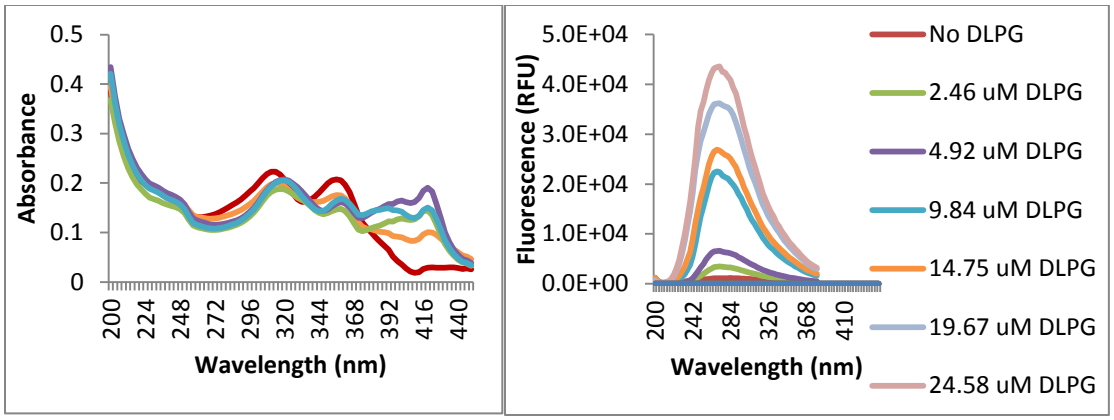

Figure S6. (A) Absorbance and (B) Fluorescence (Ex: 370) of 4.3 µM +1C with various concentrations of DLPG.

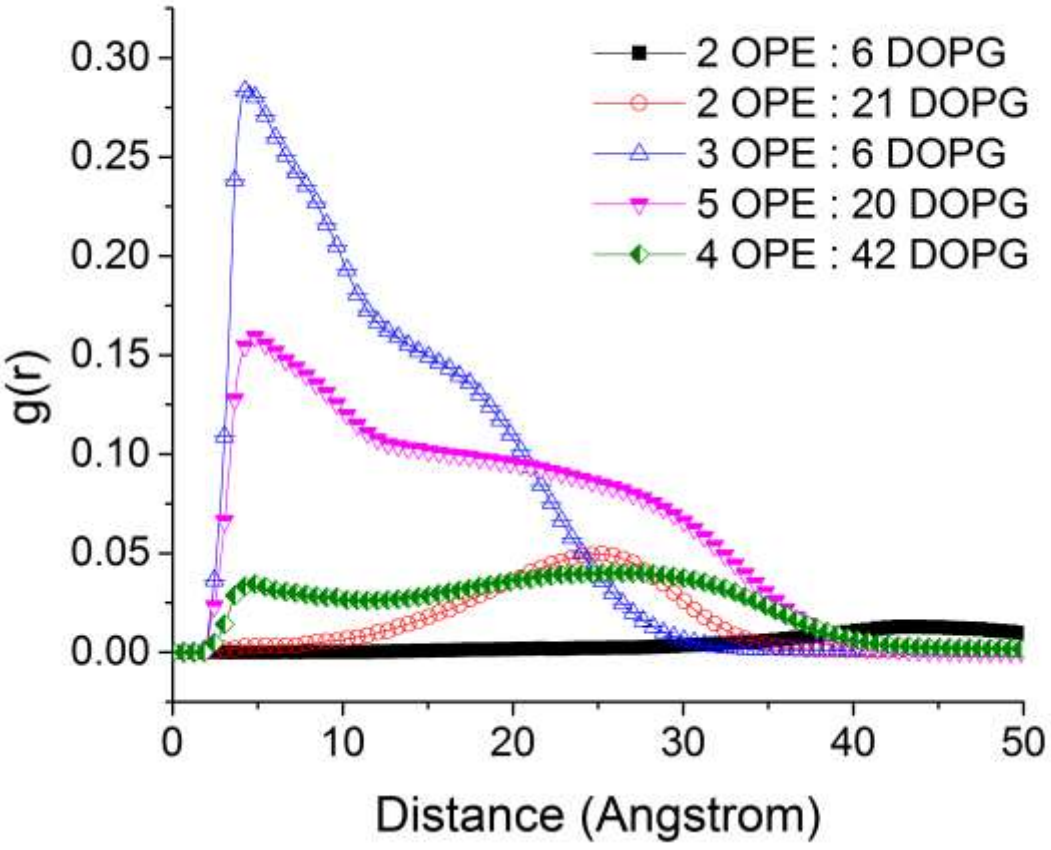

Figure S7. Radial pair distributions between OPEs in the different systems simulated with classical MD. The different simulations are annotated in the legend.

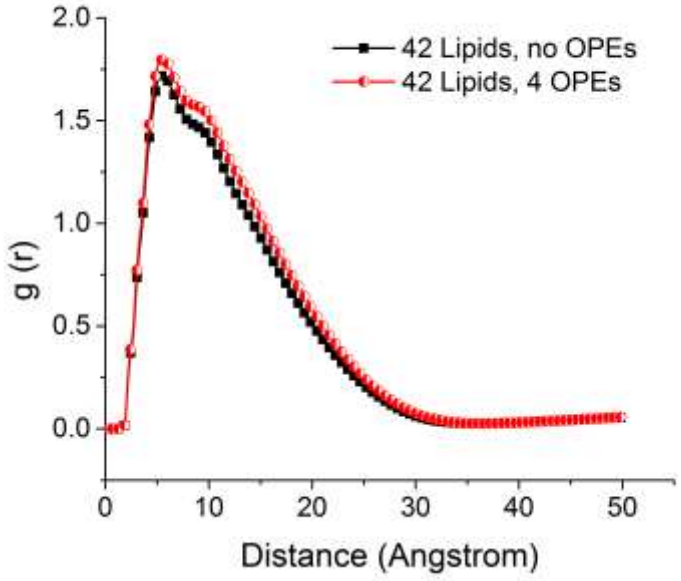

Figure S8. Radial pair distributions of oleyl chains of DOPG in a simulation with 42 lipids and either 0 or 4 OPEs.

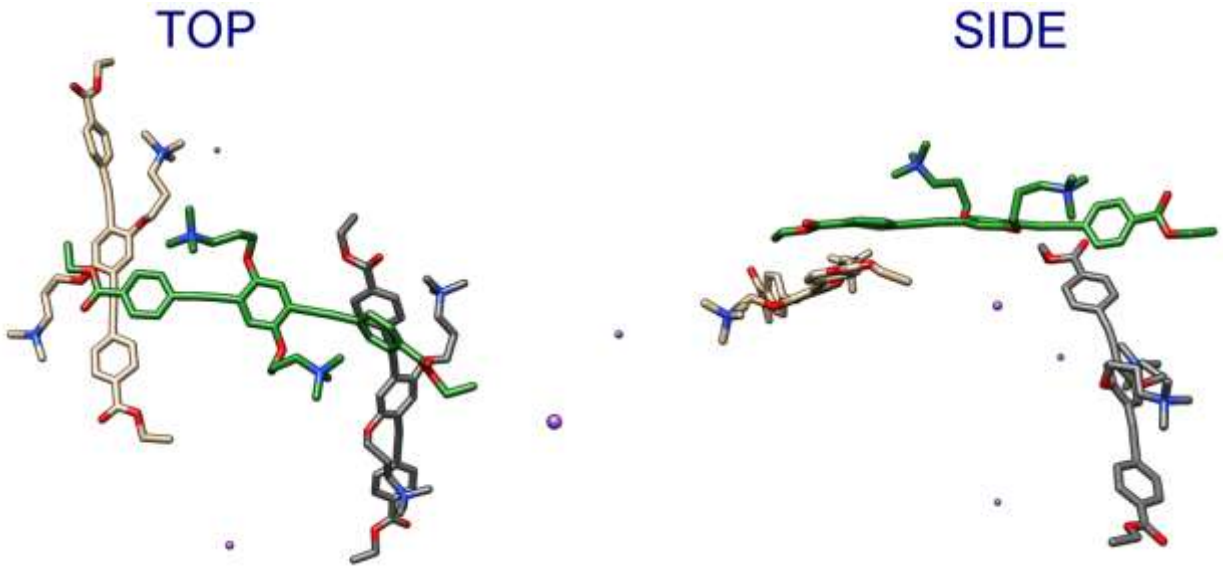

Figure S9. Trimeric aggregate which lasts for final 40 ns of 3 OPE/ 6 DOPG Molecular Dynamics Simulation