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

SUPPLEMENTARY INFORMATION

A molecular dynamics study on the glucose molecular recognition by a non-enzymatic selective sensor based on a conducting polymer

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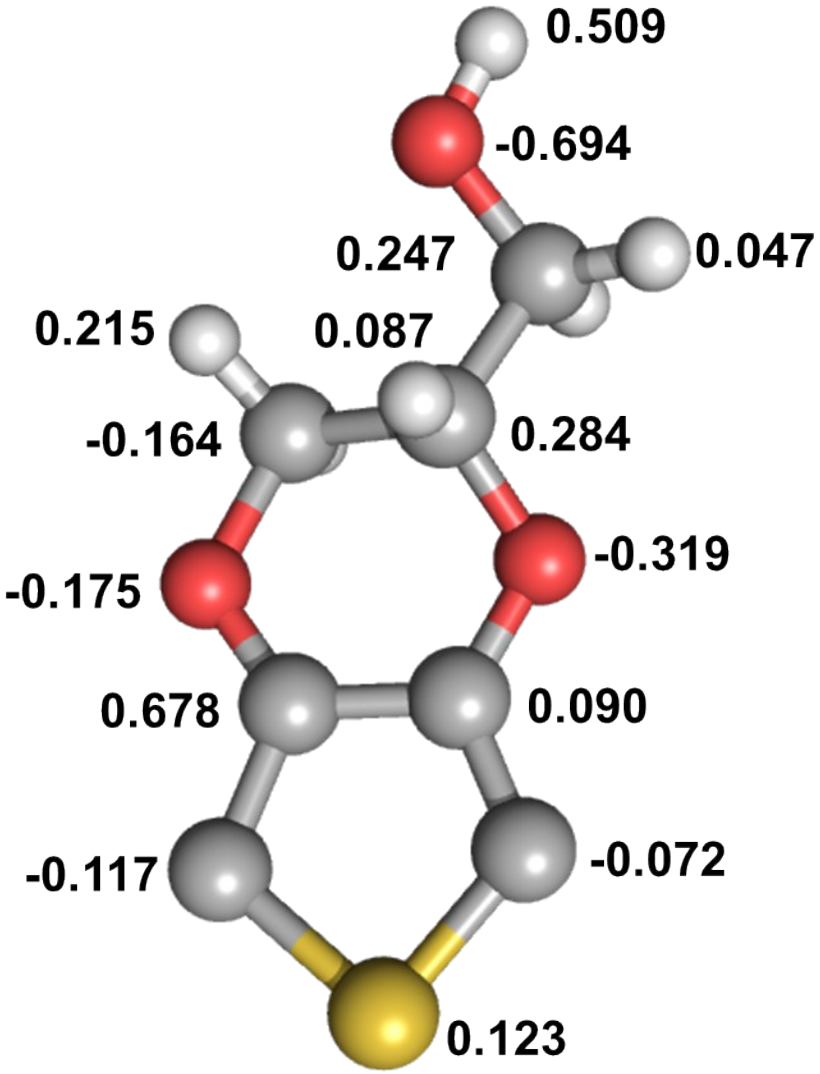

Figure S1. Electrostatic parameters for the repeat unit of PHMeDOT.

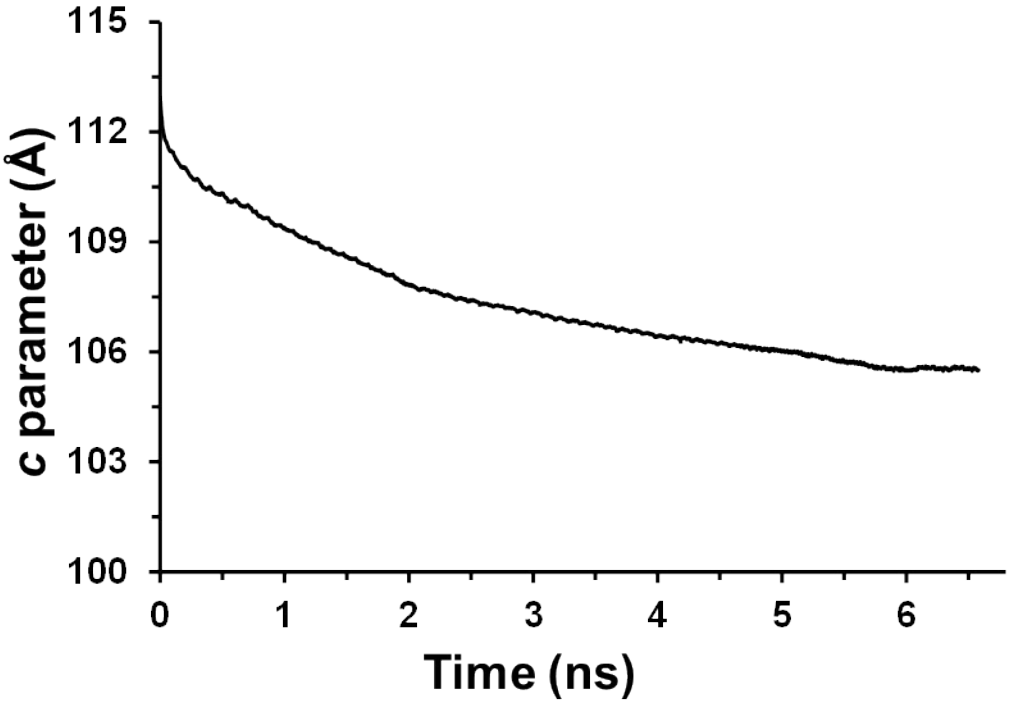

Figure S2. Temporal evolution of *c*-parameter (*z*-direction) with simulated time during the equilibration of the model that was built to study the sugar···PHMeDOT interactions.

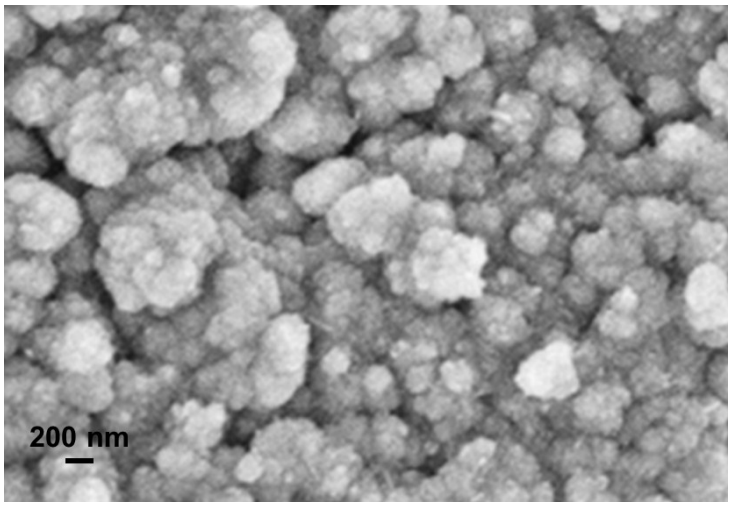

Figure S3. SEM micrograph of PHMeDOT.

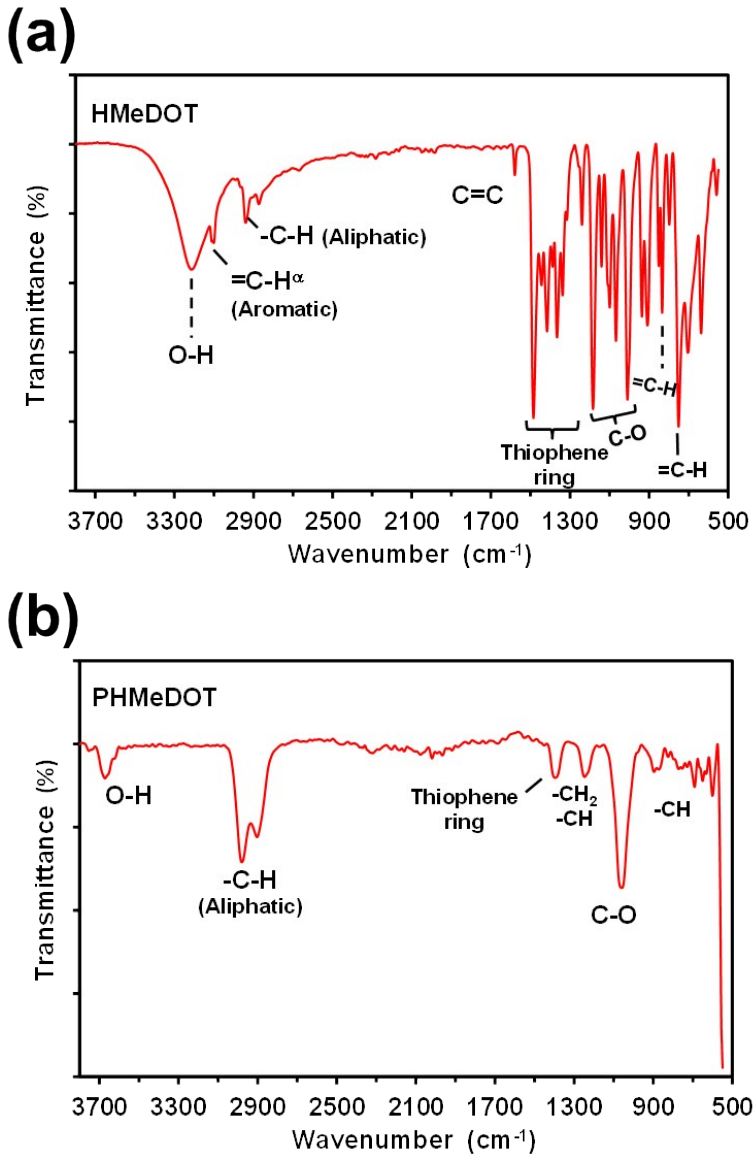

Figure S4. FTIR spectra of (a) the HMeDOT monomer and (b) PHMeDOT monomer obtained by anodic polymerization. The most relevant bands in the PHMeDOT spectrum are observed at 3669 cm^{1} (O–H stretching) and 2980-2900 cm^{-1} (–C–H aliphatic stretching) and 1238 cm^{-1} (-CH deformation), from CH_2 lateral groups and methylenedioxy groups. The strong and broad band vibrations at 1388 and 1059 cm^{-1} are attributed to the stretching modes of thiophene ring and ether group, respectively, while the main bands in the monomer spectrum are centered at 3208 cm^{-1} (O–H stretching), 3099 cm^{-1} (=C–H stretching), 2937-2869 cm^{-1} (–C–H stretching), 1578 cm^{-1} (C=C stretching) and 1484 to 1339 cm^{-1} (C-C thiophene ring vibrations).