Electronic Supplementary Material (ESI) for Soft Matter.

Understanding Selective Molecular Recognition in Integrated Carbon Nanotube-Polymer Sensors by Simulating Physical Analyte Binding on Carbon Nanotube-Polymer Scaffolds

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Electronic Supplementary Information (ESI)

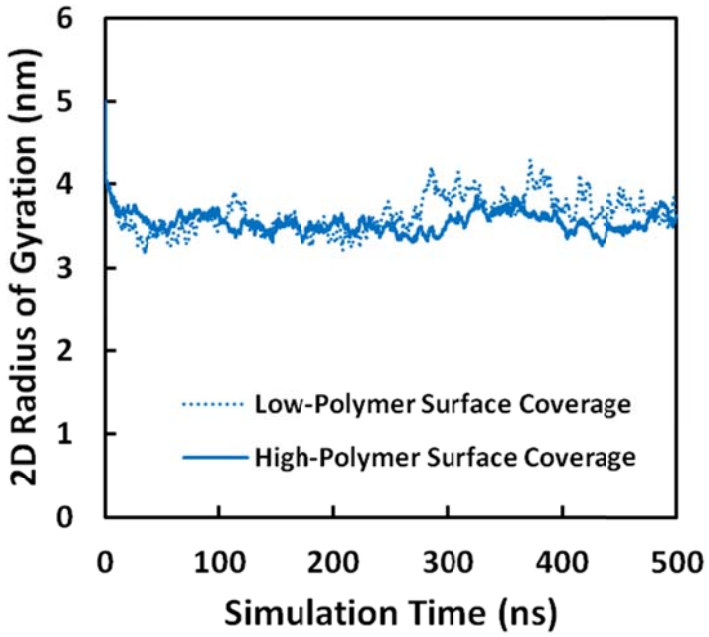
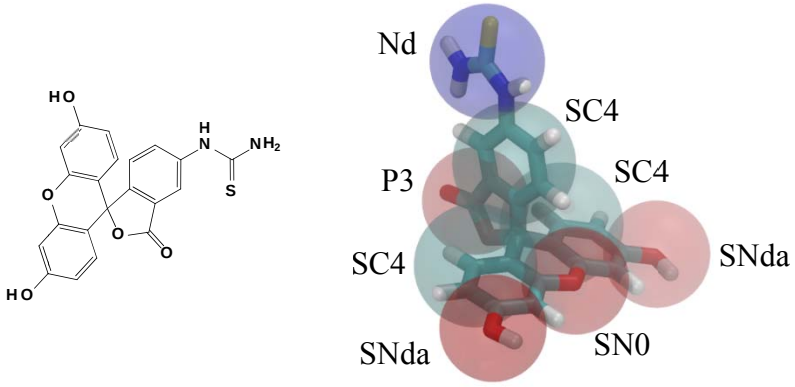
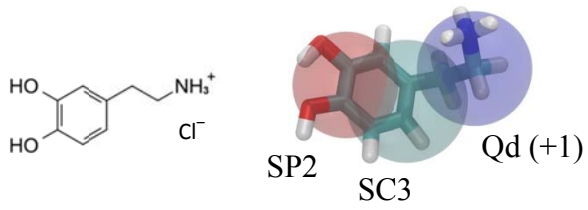


Figure S1. 2D radius of gyration of the PEG backbone under low-polymer and high-polymer surface coverages. The profiles are quite stable after 300 ns, with small fluctuations within about 0.5 nm.

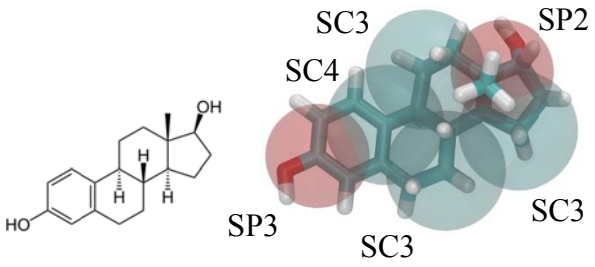
Table S1. Chemical structures (left in each panel), overlapped AA and CG molecular structures (right in each panel), and CG force-field parameters (labeled with the MARTINI particle types[1] and assigned charges for non-neutral particles) of FITC and the 5 analytes missing the original MARTINI parameters, as a result of the calibration method presented in Computational Methods. The AA structures are shown in an opaque bond fashion, while the CG structures are shown in a transparent volume fashion. Color code for the AA structures: white – hydrogen, red – oxygen, light blue – carbon, dark blue – nitrogen, and purple – iodine. The same color code applies for the CG structures to represent the primary atom type composing the CG particle.



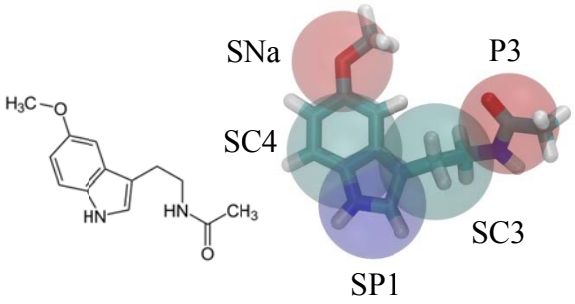
FITC



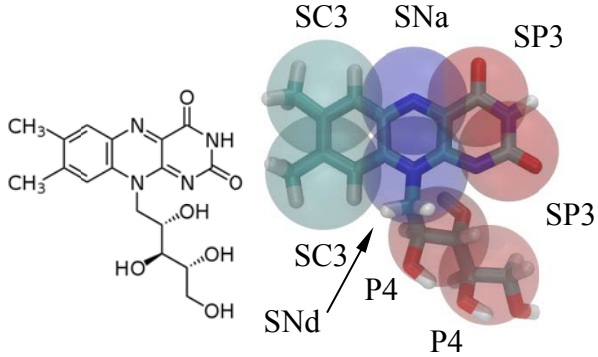
Dopamine



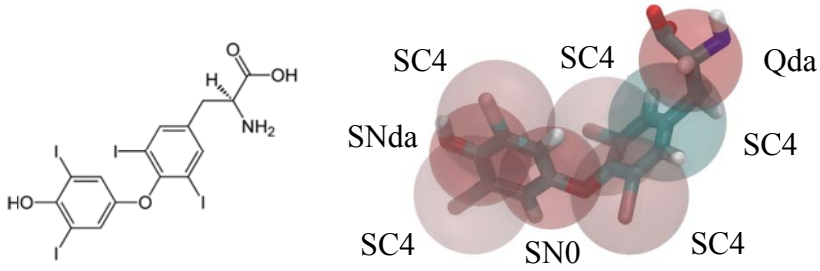
Estradiol



Melatonin



Riboflavin



Thyroxine

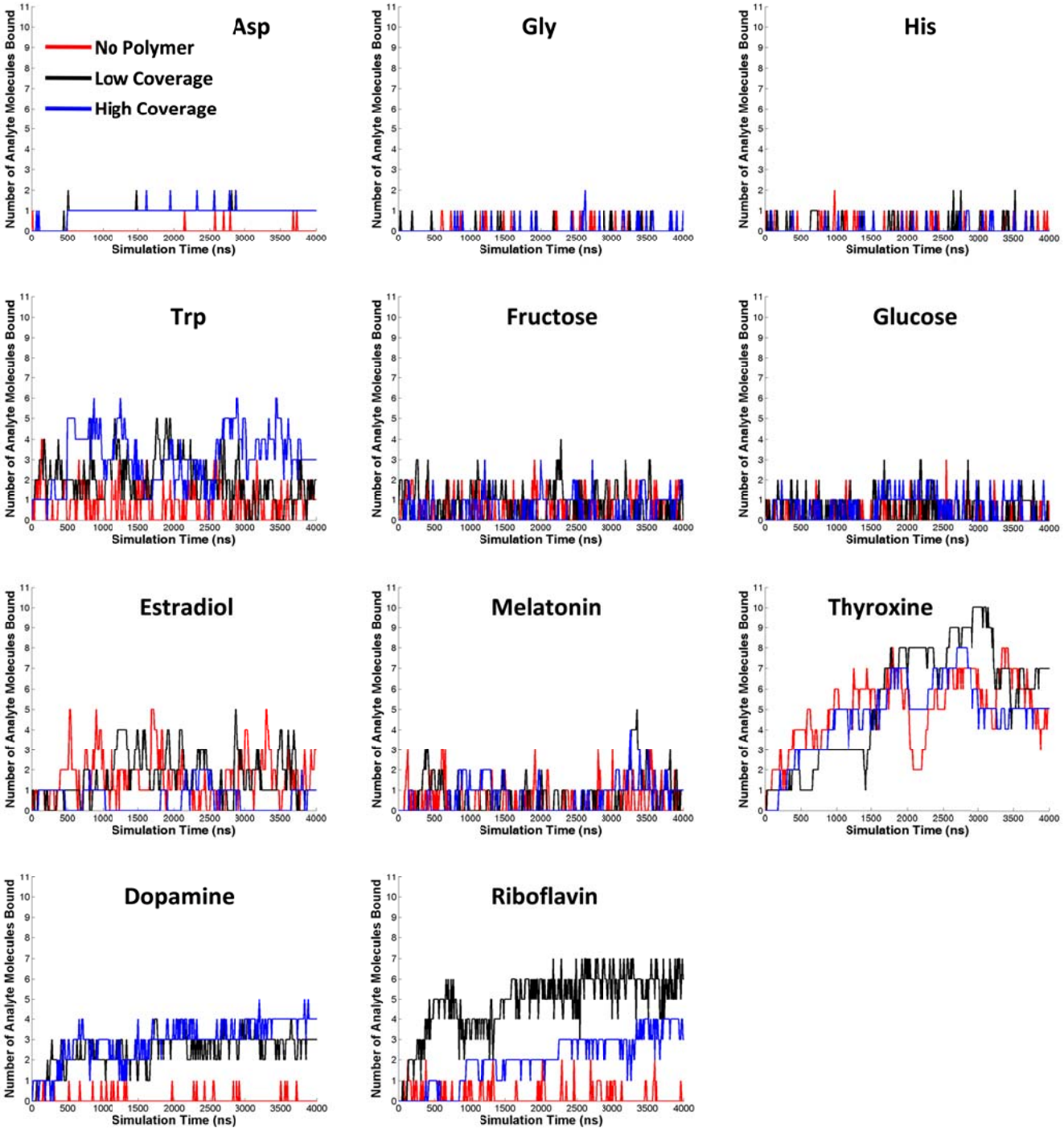


Figure S2. Binding/adsorption kinetics ("on" and "off" events) of the analyte molecules on the SWCNT-polymer scaffold during the 4 μs simulation period, as quantified by the number of bound analyte molecules $N(r \leq R_1, t)$ (within Phase I, where $R_1 = 1.3$ nm) around the cylindrical central axis of the SWCNT.

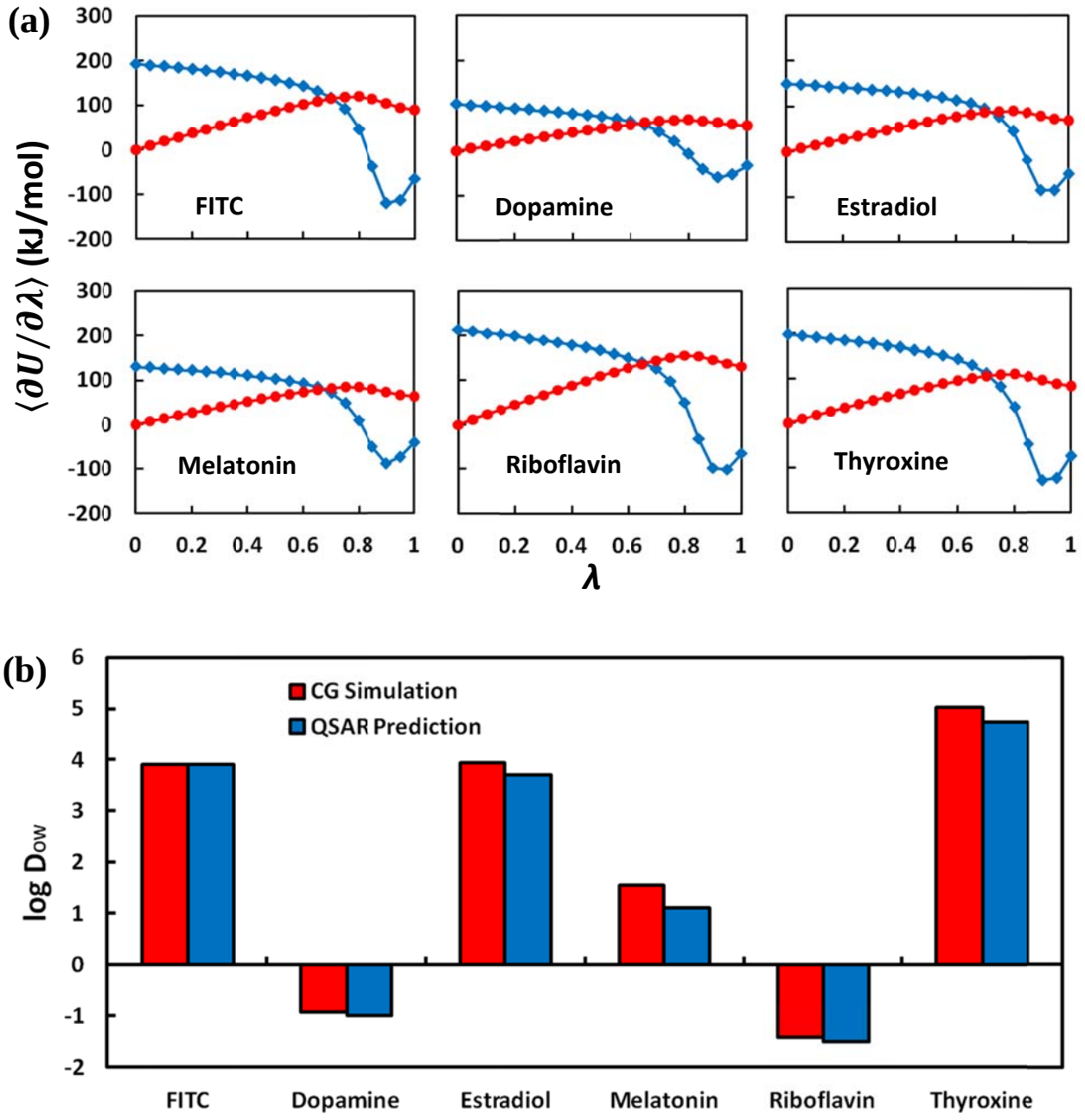
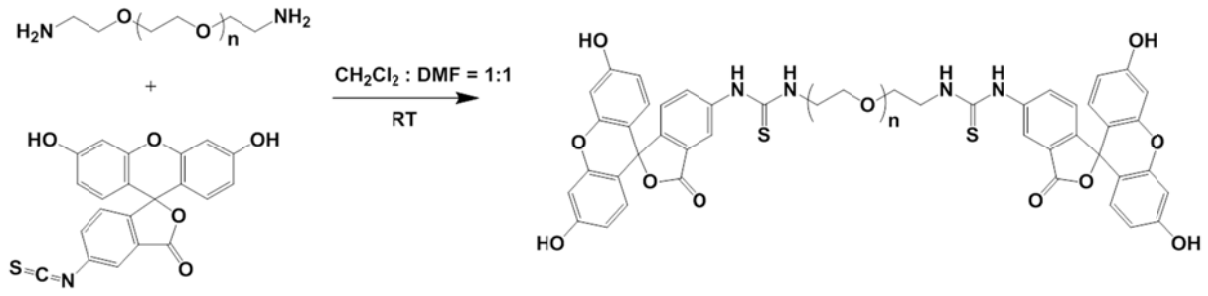


Figure S3. (a) Energy derivatives, $\langle \partial U/\partial \lambda \rangle$, as a function of the integration parameter, λ, for the FITC groups and 5 additional analytes in water (red circles connected by the red lines) and water-saturated octanol (blue diamonds connected by the blue lines). (b) Comparison between the CG-simulated and the QSAR-predicted log D_{OW} values for FITC and the 5 additional analytes.



Scheme S1: Schematic of the synthesis of FITC-PEG-FITC.

Table S2. Bulk concentrations of the 11 analytes in the high-throughput screening assay.

Analyte	Concentration (mM)	Analyte	Concentration (mM)
Asp	0.02	Estradiol	0.10
Gly	0.50	Melatonin	0.49
His	0.10	Thyroxine	0.10
Trp	0.25	Dopamine	0.49
Fructose	10.80	Riboflavin	0.10
Glucose	10.90		

References

1. S. J. Marrink, H. J. Risselada, S. Yefimov, D. P. Tieleman and A. H. de Vries, *The Journal of Physical Chemistry B*, 2007, **111**, 7812-7824.