

Supporting Information:

A selective supramolecular photochemical sensor for dopamine

Setu Kasera, Zarah Walsh, Jesús del Barrio, and Oren A. Scherman*

Melville Laboratory for Polymer Synthesis, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK. Email: oas23@cam.ac.uk

Table S1: Association constants of PDI·CB[8] towards catecholamines and their mixtures in the presence and absence of ascorbic acid

Second guest	K_a (M^{-1}) without Asc	R^2	K_a (M^{-1}) with Asc	R^2
Dopamine	$(1.0 \pm 0.009) \cdot 10^6$	0.99	$(1.0 \pm 0.013) \cdot 10^6$	0.98
Epinephrine	$(1.0 \pm 0.007) \cdot 10^3$	0.99	$(1.3 \pm 0.008) \cdot 10^3$	0.99
Norepinephrine	$(2.9 \pm 0.099) \cdot 10^2$	0.51	$(5.3 \pm 0.087) \cdot 10^2$	-0.45
Mixture 1 (EPI + NE)	$(1.4 \pm 0.003) \cdot 10^3$	0.98	$(1.5 \pm 0.005) \cdot 10^3$	0.98
Mixture 2 (EPI + NE + DA)	$(0.9 \pm 0.006) \cdot 10^6$	0.99	$(1.0 \pm 0.014) \cdot 10^6$	0.99

\pm error values denote standard deviation;

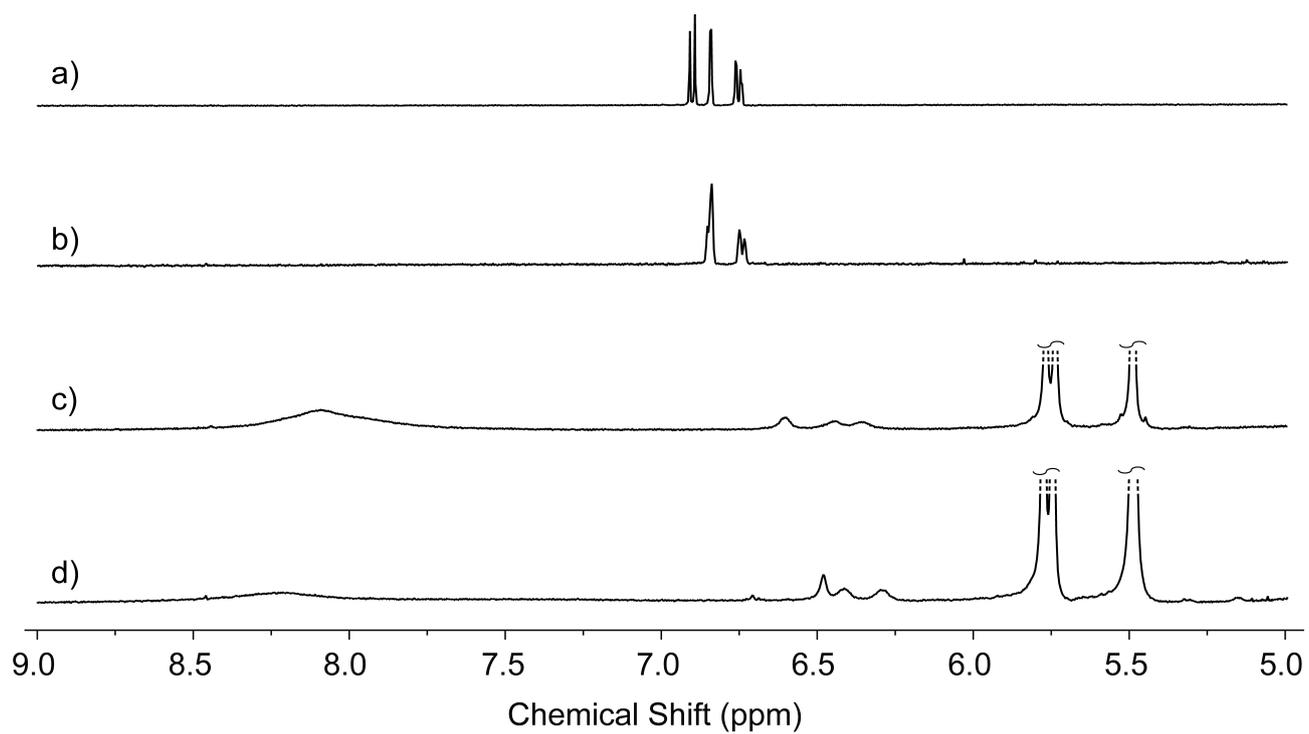


Figure S1: Partial ¹H NMR spectra (500 MHz, D₂O, 298 K) of a) DA, b) EPI, c) DA·PDI·CB[8] and d) EPI·PDI·CB[8].

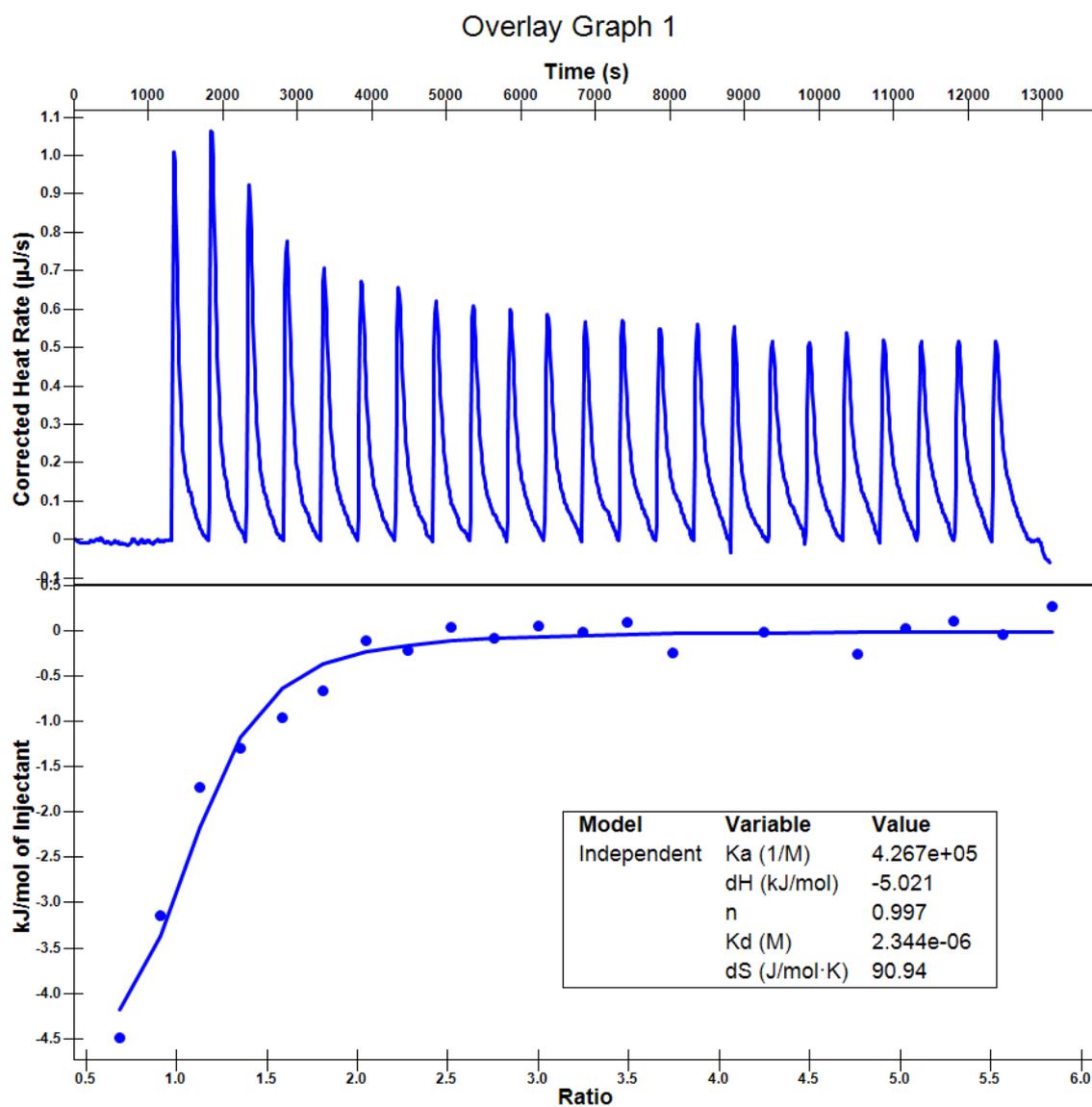


Figure S2: Isothermal Titration Calorimetry measurements of DA and PDI-CB[8].

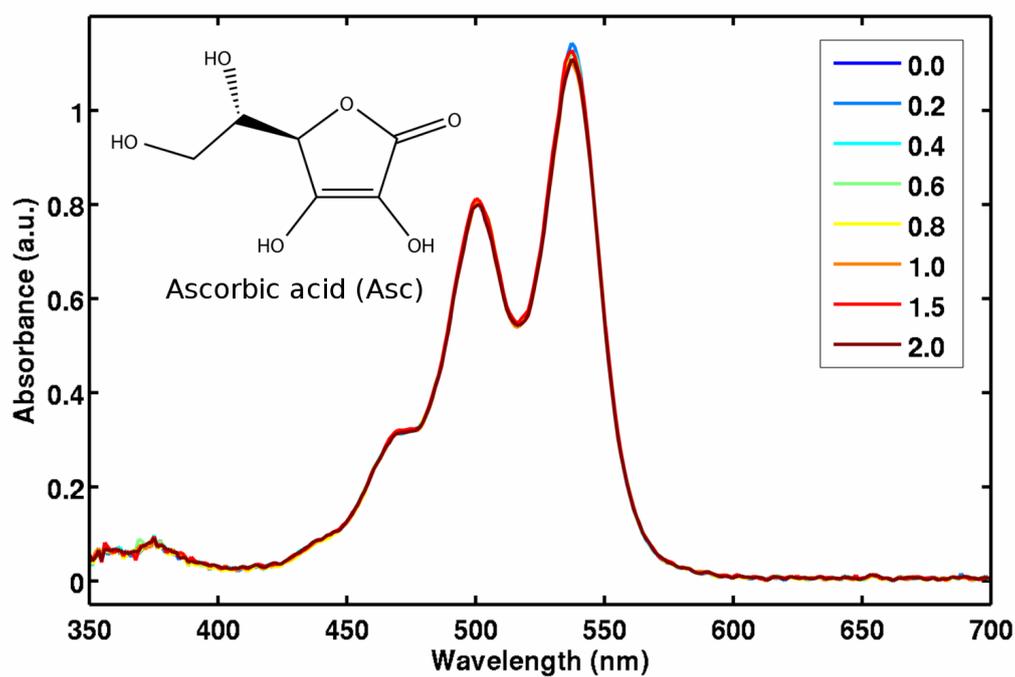


Figure S3: Titration of ascorbic acid into 1:1 PDI·CB[8] (3×10^{-5} M) solution does not show any marked change in the absorbance bands of PDI.

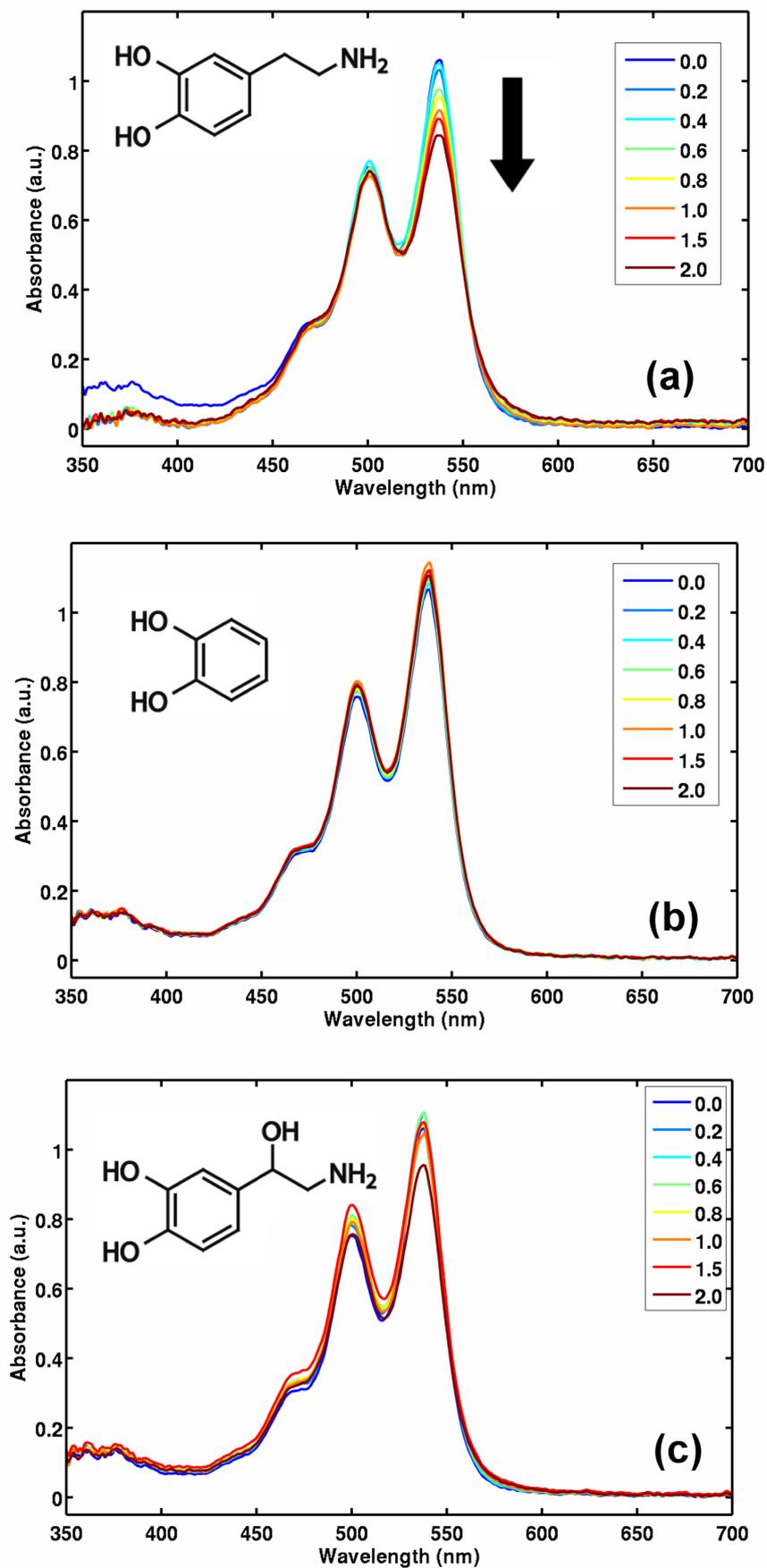


Figure S4: Titration of (a) DA, (b) Cat and (c) NE into 1:1 PDI-CB[8] (3×10^{-5} M) solution also containing ascorbic acid (3×10^{-5} M). The presence of ascorbic acid does not affect binding behaviour of the three compounds.

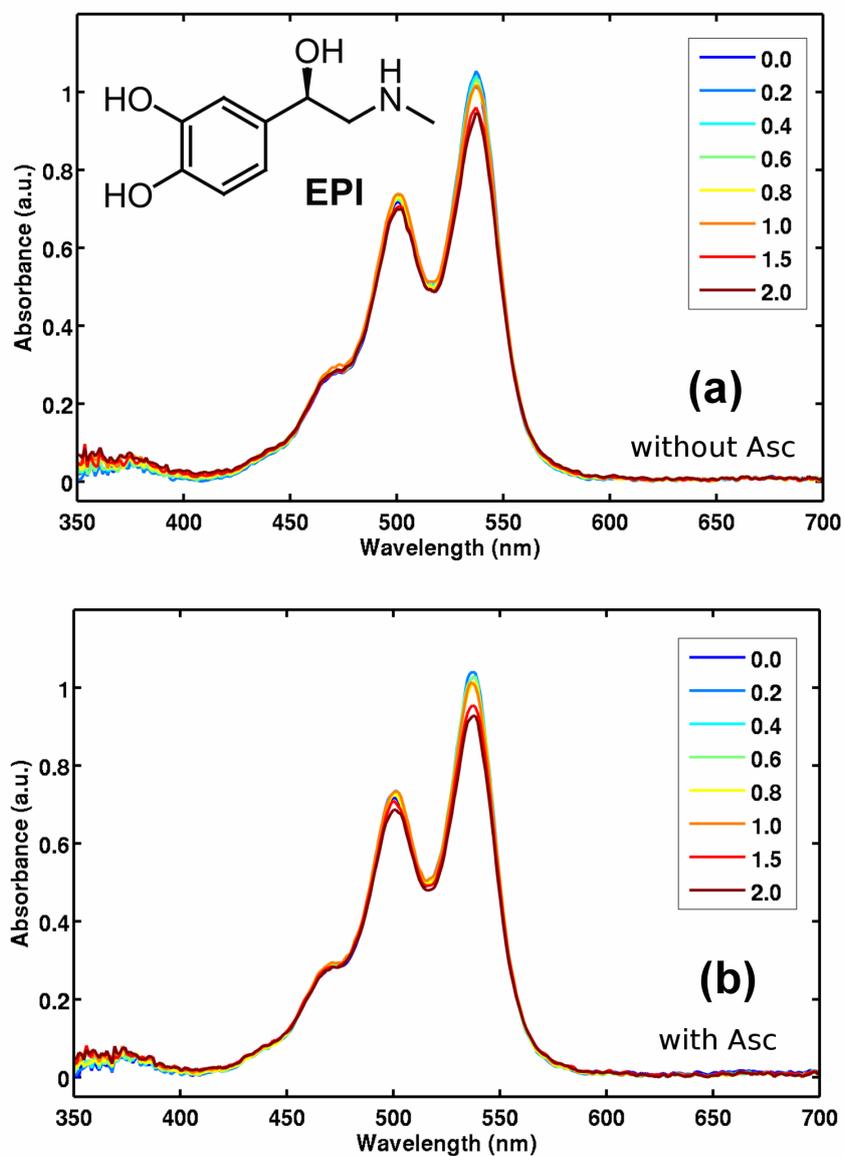


Figure S5: Titration of EPI into 1:1 PDI-CB[8] (3×10^{-5} M) (a) without ascorbic acid present and (b) with ascorbic acid (3×10^{-5} M) present in the solution. The presence of ascorbic acid does not affect binding behaviour of EPI.

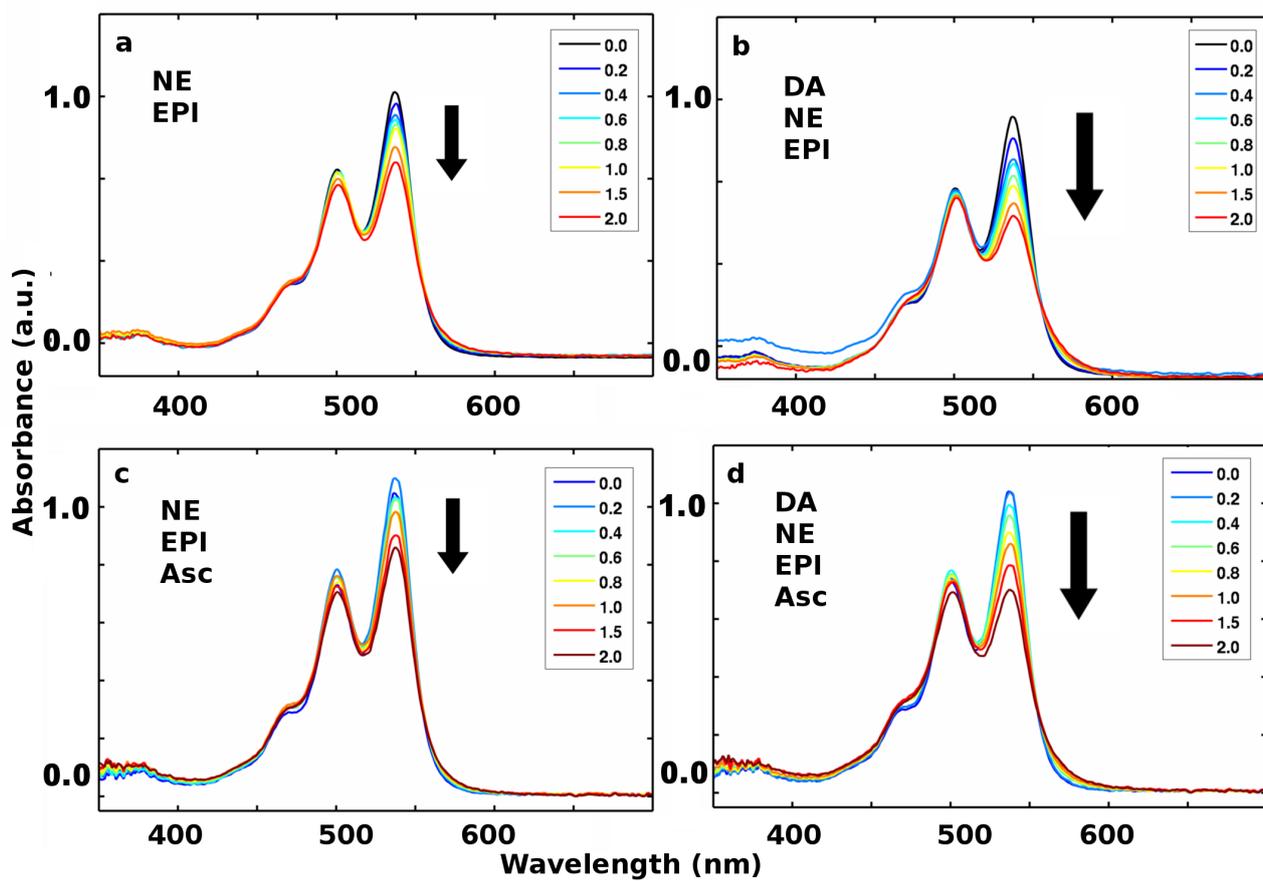


Figure S6: Titration of (a) Mixture 1 (EPI + NE), (b) Mixture 2 (EPI + NE + DA), (c) Mixture 1 (EPI + NE) with Asc and (d) Mixture 2 (EPI + NE + DA) into 1:1 PDI-CB[8] (3×10^{-5} M) solution. The presence of ascorbic acid does not show interference within the mixtures.