Supporting information

Quantitative analysis of pheromone-binding protein specificity

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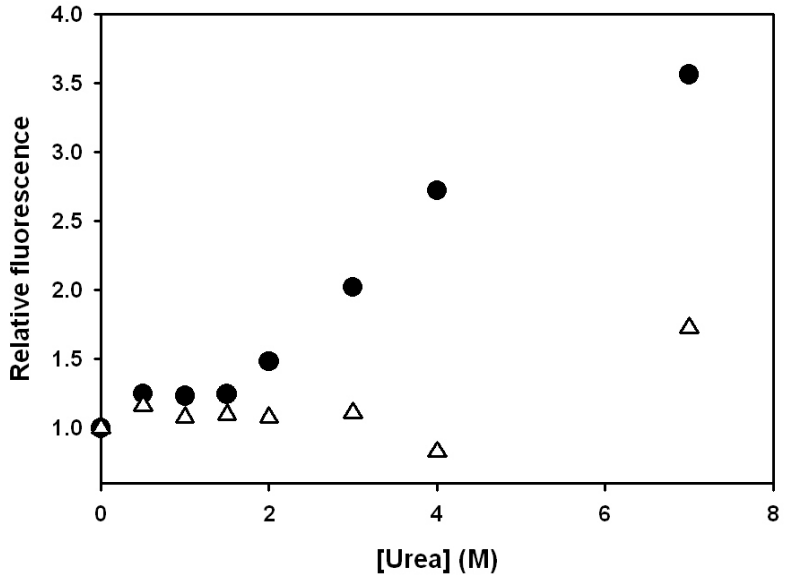

Figure S1. LUSH Tryptophan fluorescence in urea. Fluorescence emission at 355 nm in urea (20 mM phosphate, pH 6.5) relative to emission in the absence of urea. Circles: LUSH (1 μM) refolded by the cystine/cysteine method; triangles: LUSH (1 μM) not refolded.

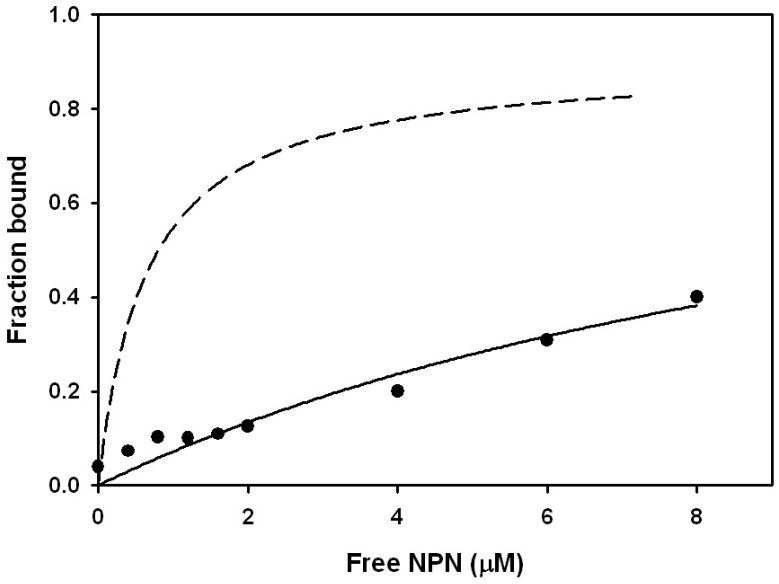

Figure S2. NPN binding to unfolded LUSH. Similar to figure 1A, except that LUSH is not fully refolded. Solid line: binding curve fit with dissociation constant of 12.9 μM; correlation coefficient = 0.97. Dashed line: binding curve fit to data in figure 1A.

Table S1

Atomic coordinates for NPN Model 1. To display the LUSH-NPN complex in a molecular viewer (e.g. figure 2), take atoms 1-1080 from Protein Data Bank file 2GTE (LUSH, molecule A) and append the atoms below, which were positioned by AutoDock (Table 1).

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REMARK                  MODEL   FOR   NPN   BINDING   TO   LUSH   (2GTE,   MOLECULE   A)
REMARK            NPN  COORDINATES  FROM  LOWEST  ENERGY  STRUCTURE  AFTER  AUTODOCK  RUN
ATOM    2001   C2   NPN B    1       -2.515    1.586   -4.909                           C
ATOM    2002   C3   NPN B    1       -2.046    0.257   -5.076                           C
ATOM    2003   C4   NPN B    1       -0.759   -0.121   -4.578                           C
ATOM    2004   C5   NPN B    1        0.062    0.851   -3.921                           C
ATOM    2005   C6   NPN B    1       -0.422    2.199   -3.753                           C
ATOM    2006   C7   NPN B    1        0.381    3.186   -3.092                           C
ATOM    2007   C8   NPN B    1       -0.118    4.569   -2.929                           C
ATOM    2008   C9   NPN B    1       -1.400    4.944   -3.418                           C
ATOM    2009   C10  NPN B    1       -2.196    3.969   -4.066                           C
ATOM    2010   C11  NPN B    1       -1.686    2.571   -4.234                           C
ATOM    2011   N1   NPN B    1       -3.826    1.980   -5.402                           N
ATOM    2012   C12  NPN B    1       -4.947    1.845   -4.541                           C
ATOM    2013   C13  NPN B    1       -6.258    2.043   -5.047                           C
ATOM    2014   C14  NPN B    1       -7.379    1.908   -4.187                           C
ATOM    2015   C15  NPN B    1       -7.190    1.576   -2.819                           C
ATOM    2016   C16  NPN B    1       -5.878    1.378   -2.312                           C
ATOM    2017   C17  NPN B    1       -4.756    1.513   -3.173                           C
TER
END
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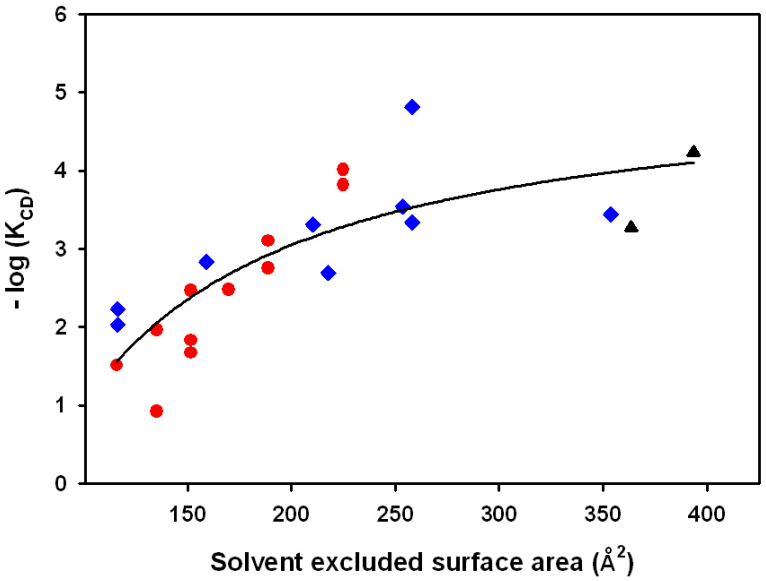

Figure S3. Relationship between β-cyclodextrin-guest affinities and molecular surface area. Solvent-excluded surface areas were calculated from the molecular structures (obtained from Cambridge Structural Database) using Python Molecular Viewer. β-cyclodextrin-guest 1:1 association constants ($1/K_{CD}$) were obtained from reference (*33*). Circles: fatty acids; diamonds: aromatics; triangles: cholesterol and prostaglandin E2. Line fit to equation $f = y_0+ax/(b+x)$, with $y_0 = -61.6$, $a = 66.8$, $b = 6.75$; correlation coefficient = 0.81.

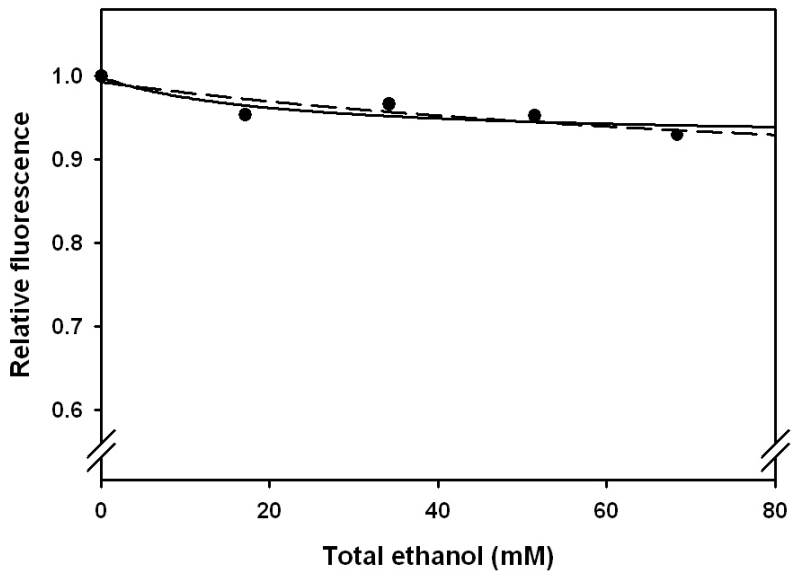

Figure S4. Ethanol binding only weakly affects LUSH tryptophan emission. Same conditions as figure 3. Lines fit with hyperbolic decay function $f = y_o + ab/(b+x)$. Dissociation constants: solid line, 21 mM (correlation coefficient = 0.92); dashed line, 107 mM (correlation coefficient = 0.84).