

Supplementary Material: One-Pot, One-Step Production of Dietary Nucleotides by Magnetic Biocatalysts

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1. Tables.

Table S1. Computed theoretical pKa values of the lysine residues in *Tt*HGXPRT using the server H++ (<http://biophysics.cs.vt.edu/H++>).

N-Terminal	Lys (#)	pK, int*	pKa**
N-Term His-tagged <i>Tt</i> HGXPRT		3.356	0.381
	18	9.405	9.295
	36	9.915	11.221
	37	9.554	9.847
	53	10.759	11.019
	94	10.182	10.408
	103	10.252	10.915
	138	10.481	10.451

pK, int*: computed pKa of a group assuming that there is not interaction with any other titratable group in the protein. pKa**It corresponds to the mid-point of a titration curve ($\text{pK } \frac{1}{2}$).

2. Figures

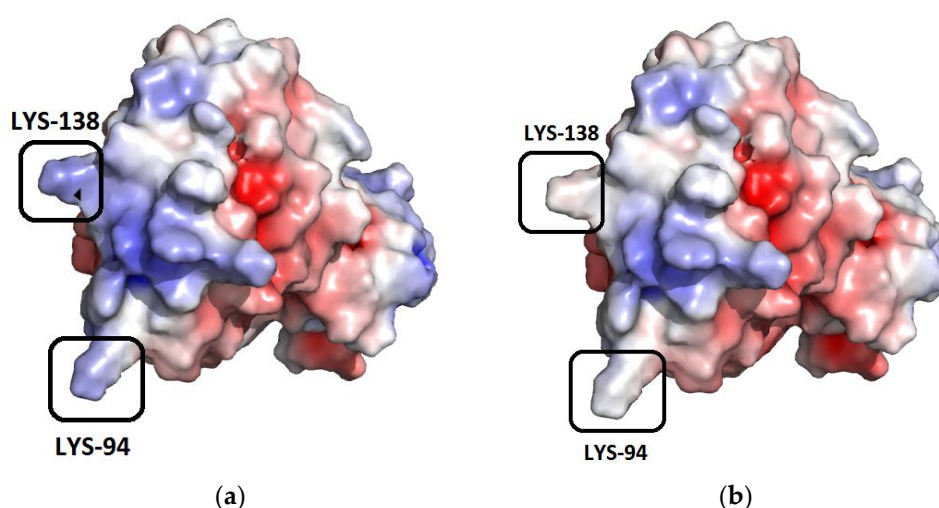


Figure S1. APBS-generated electrostatic surface of *Tt*HGXPRT. (a) Titratable state of the protein at pH 8.5; (b) Titratable state of the protein at pH 10.5.

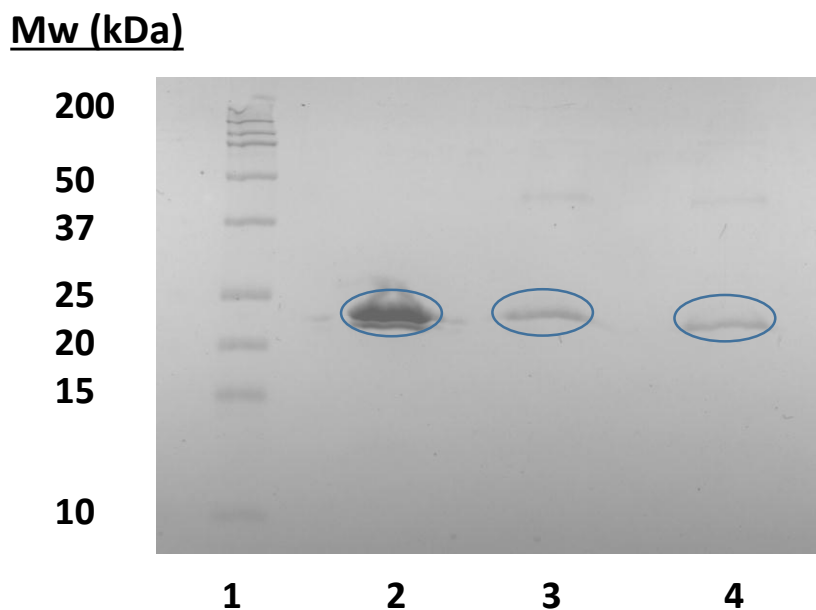


Figure S2. SDS-PAGE analysis of soluble and immobilized *Tt*HGXPRT. **Lane 1.** Prestained standard proteins from BioRad used as molecular weight markers. **Lane 2.** Supernatant obtained after boiling the soluble *Tt*HGXPRT in the presence of SDS and mercaptoethanol. **Lane 3.** Supernatant obtained after boiling the *MTt*HGXPRT3 in the presence of SDS and mercaptoethanol. **Lane 4.** Supernatant obtained after boiling the *MTt*HGXPRT5 in the presence of SDS and mercaptoethanol.