

SUPPORTING INFORMATION

Adenylate Kinase-Catalyzed Reactions of AMP in Pieces: Specificity for Catalysis at the Nucleoside Activator and Dianion Catalytic Sites

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Figure S1 shows the Michaelis–Menten plot of $v_{\text{obs}}/[E]$ against $[\text{AMP}]$ for rabbit muscle adenylate kinase (RAdK)-catalyzed phosphoryl transfer from 1.0 mM ATP to AMP. Figure S2 shows the Michaelis–Menten plot of $v_{\text{obs}}/[E]$ against $[2'\text{-dAMP}]$ for HAdK1-catalyzed phosphoryl transfer from 1 mM ATP (saturating) to 2'-dAMP. These plots give the Michaelis–Menten parameters reported in Table 1.

Figures S3A and S3B show kinetic data for EA-activated RAdK-catalyzed phosphoryl transfer from ATP to FPO_3^{2-} . Figures S4A and S4B show kinetic data for adenosine-activated HAdK-catalyzed phosphoryl transfer from ATP to HPO_3^{2-} . The kinetic parameter $(k_{\text{cat}})_{\text{XPi}\cdot\text{EA}}/K_{\text{XPi}}K_{\text{EA}}$ for the EA- and Ado-activated reactions, respectively, reported in Table 2 were determined from the fits of these plots to eq 1 and 2 from the main text. Figure S5 and S6 show, respectively, the effect of increasing $[2'\text{-dAdo}]$ and $[3'\text{-dAdo}]$ on $v_{\text{obs}}/[E]$ for *HsAdK1*-catalyzed reactions of saturating (1 mM) ATP with 23 mM $[\text{HPO}_3^{2-}]$ at pH 7.5, $I = 0.150$ (NaCl), and 25 °C.

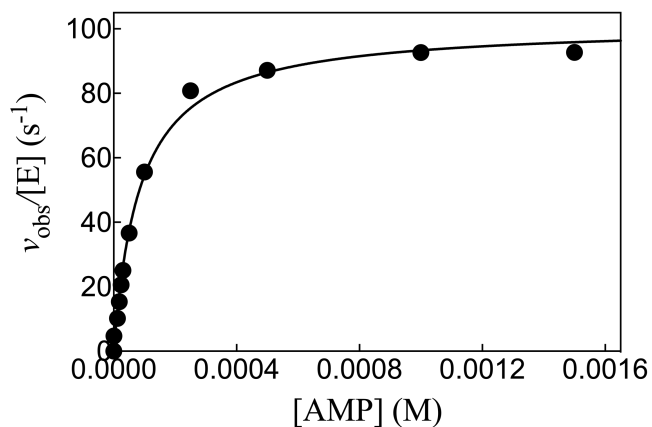


Figure S1. The increase in $v_{\text{obs}}/[E]$ with increasing $[\text{AMP}]$ for RAdK1-catalyzed phosphoryl transfer from ATP (1 mM) to AMP at pH 7.5, $I = 0.150$ (NaCl) and 25 °C.

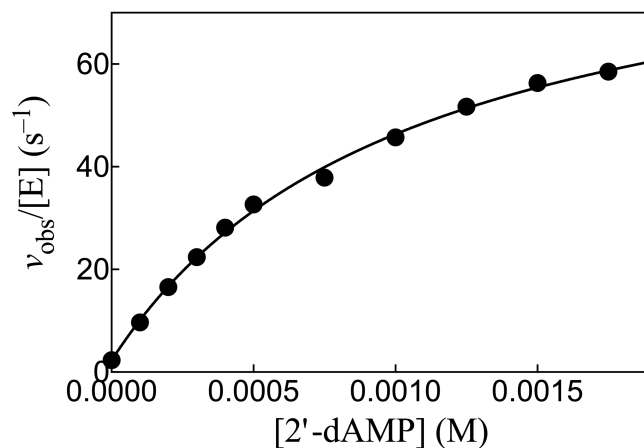


Figure S2. The increase in $v_{\text{obs}}/[E]$ with increasing $[\text{2'-dAMP}]$ for HAdK1-catalyzed phosphoryl transfer from ATP (1 mM) to 2'-dAMP at pH 7.5, $I = 0.150$ (NaCl), and 25 °C.

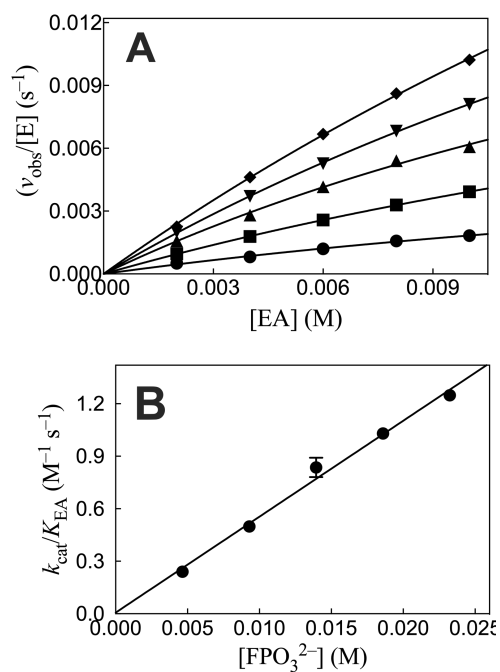


Figure S3. (A) The increase in $v_{\text{obs}}/[E]$ with increasing $[EA]$ for RAdK1-catalyzed reactions of ATP (1 mM) with FPO_3^{2-} at pH 7.5, $I = 0.150$ (NaCl), and 25 °C. Key: \blacklozenge , 25 mM $[FPO_3^{2-}]$; \blacktriangledown , 20 mM $[FPO_3^{2-}]$; \blacktriangle , 15 mM $[FPO_3^{2-}]$; \blacksquare , 10 mM $[FPO_3^{2-}]$; \bullet , 5 mM $[FPO_3^{2-}]$. (B) The effect of increasing $[FPO_3^{2-}]$ on the values of $(k_{\text{cat}}/K_{EA})_{\text{obs}}$ determined for Figure 3A.

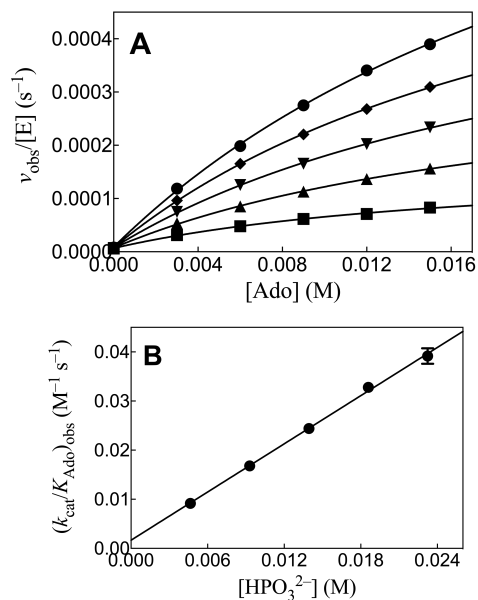


Figure S4. (A) The increase in $v_{\text{obs}}/[E]$ with increasing [Ado] for HAdK1-catalyzed reactions of ATP (1 mM) with phosphite dianion at pH 7.5, $I = 0.150$ (NaCl), and 25 °C. Key: ●, 23 mM [HPO₃²⁻] (93% dianion); ◆, 19 mM [HPO₃²⁻]; ▼, 14 mM [HPO₃²⁻]; ▲, 9.2 mM [HPO₃²⁻]; ■, 4.6 mM [HPO₃²⁻]. (B) The effect of increasing [HPO₃²⁻] on the values of $(k_{\text{cat}}/K_{\text{Ado}})_{\text{obs}}$ determined for Figure S4A.

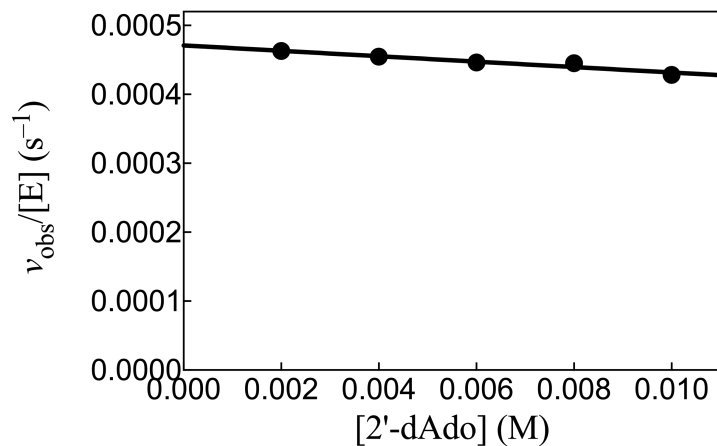


Figure S5. The effect of increasing [2'-dAdo] on $v_{\text{obs}}/[E]$ for HAdK1-catalyzed reactions of ATP (1 mM) with 23 mM HPO_3^{2-} at pH 7.5, $I = 0.150$ (NaCl), and 25 °C.

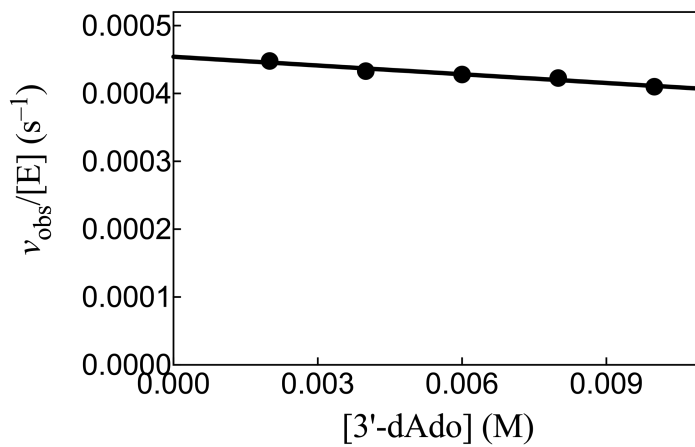


Figure S6. The effect of increasing [3'-dAdo] on $v_{\text{obs}}/[E]$ for HAdK1-catalyzed reactions of ATP (1 mM) with 23 mM $[\text{HPO}_3^{2-}]$ at pH 7.5, $I = 0.150$ (NaCl), and 25 °C.