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SUPPLEMENTARY MATERIAL TO

3D-QSAR study of adenosine 5'-phosphosulfate (APS) analouges as ligands for APS reductase

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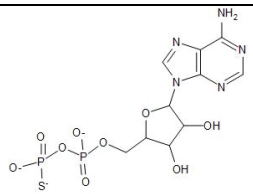
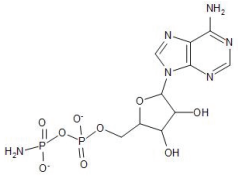
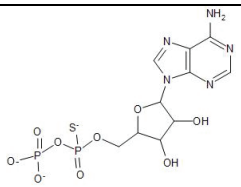
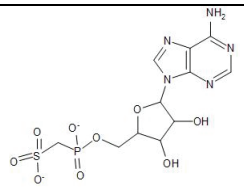
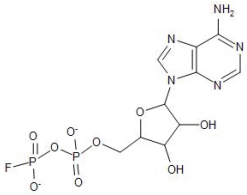
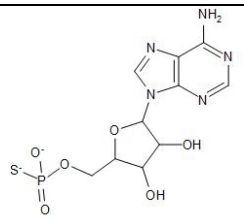
TABLE S-I. The structures of nucleoside analogues of APS and inhibition constants toward APSR

Compound	Structure	K_d / μM	Compound	Structure	K_d / μM
ADPβS		0.15	AMPPN		410
ADPαS		0.80	APSβM		700
ADPβF		2.5	5'–AMPS		3.3

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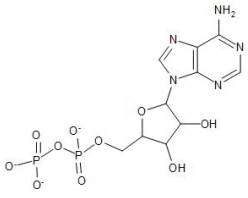
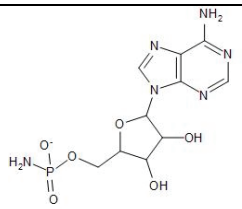
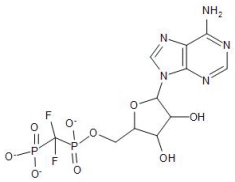
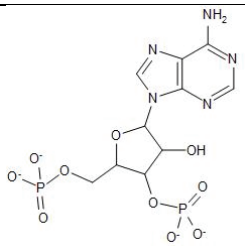
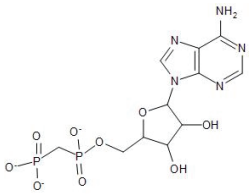
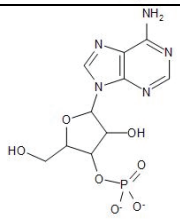
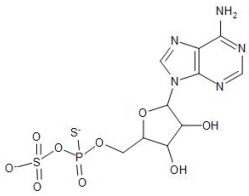
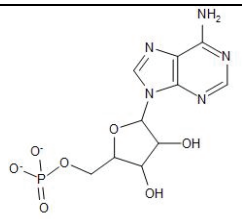
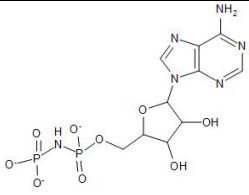
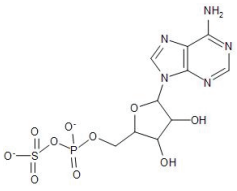
Compound	Structure	K_d / μM	Compound	Structure	K_d / μM
ADP		4.3	5'–AMPN		100
AMPCF$_2$P		13	3'5'–ADP		700
AMPCP		27	3'–AMP		3200
APSαS		43	AMP		5.4
AMPNP		260	APS		0.2

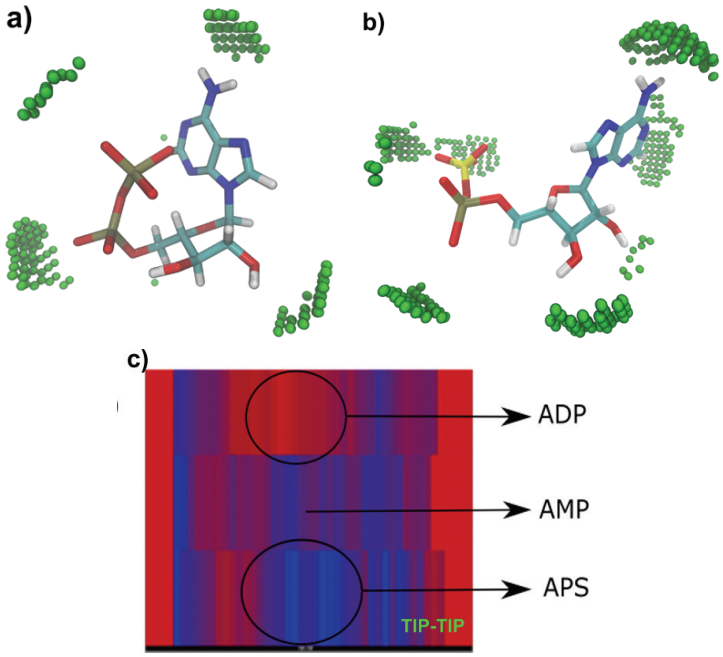


Fig. S-1. a) TIP – TIP interactions for ADP and b) APS, and c) TIP – TIP probe heatmap for ADP, AMP, and APS.

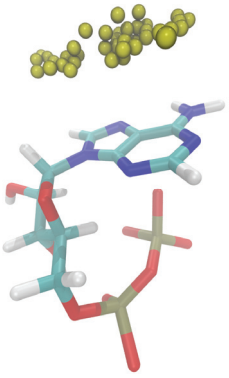


Fig. S-2. The location of favorable hydrophobic interactions of ADP mapped using DRY probe.

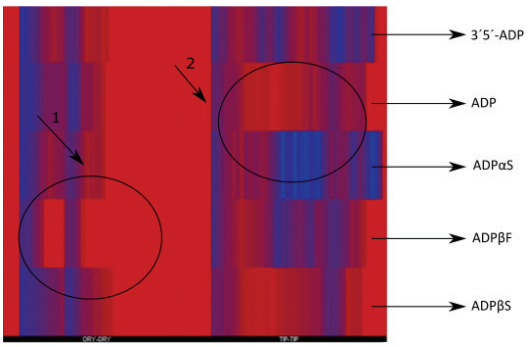


Fig. S-3. Differences in DRY – DRY interactions that ADPβF and ADPβS form with target (1) and differences in TIP – TIP interactions ADPαS and ADP (2).

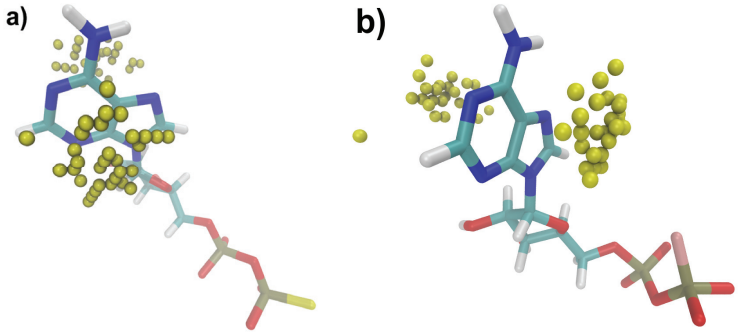


Fig. S-4. a) DRY – DRY interactions that ADPβS and b) ADPβF forms with enzyme.

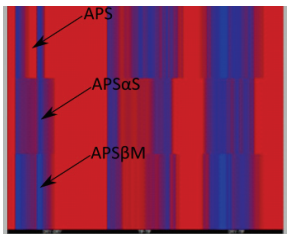


Fig. S-5. Differences in DRY – DRY interactions between APS, APSαS, and APSβM.

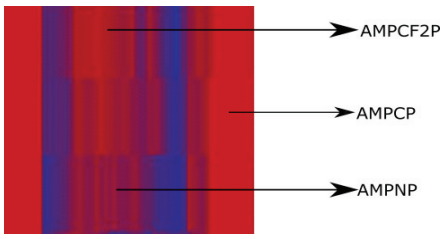


Fig. S-6. TIP – TIP interactions for AMPCF2P, AMPCP and AMPNP.

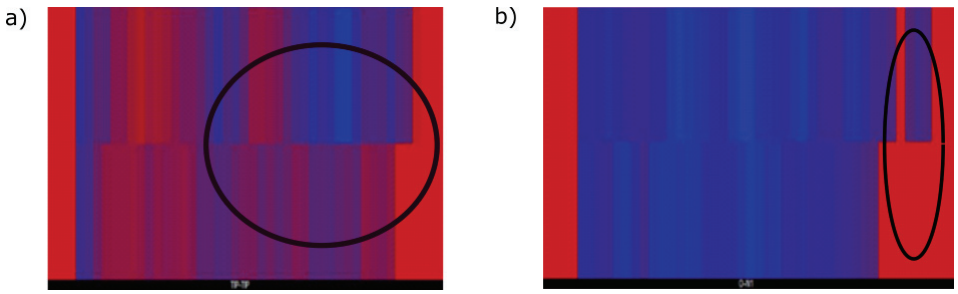


Fig. S-7. a) TIP – TIP interaction 5'AMPS and AMP and b) O – N1 interaction 5' AMPN and AMP.

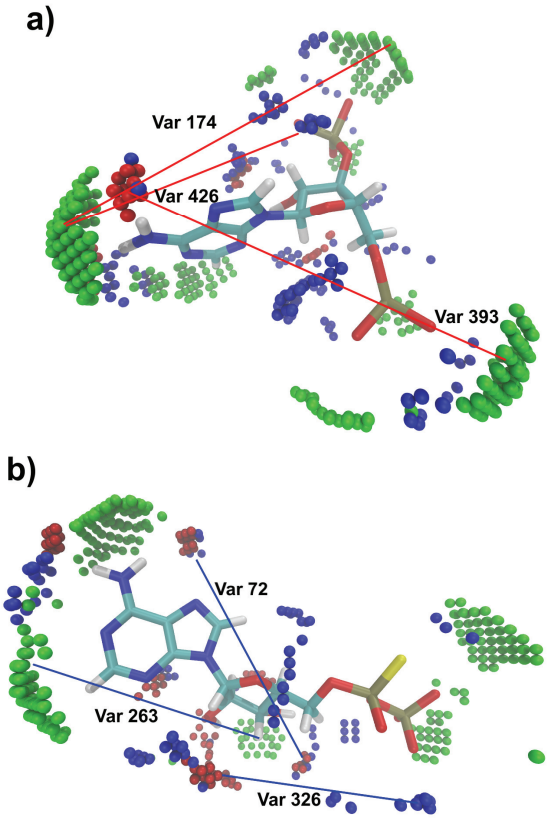


Fig. S-8. The structural features associated with the additional variables a) positively (red lines) and b) negatively (blue lines) correlated with the APS reductase inhibitory activity.