SUPPORTING INFORMATION

Kinetic Isotope Effects and Transition State Structure for Hypoxanthine-Guanine-Xanthine Phosphoribosyltransferase from *Plasmodium falciparum*

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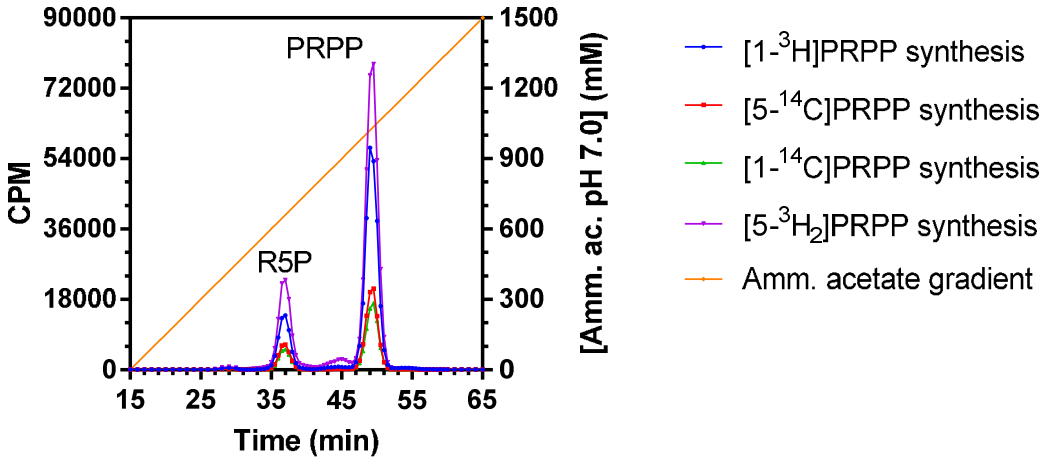
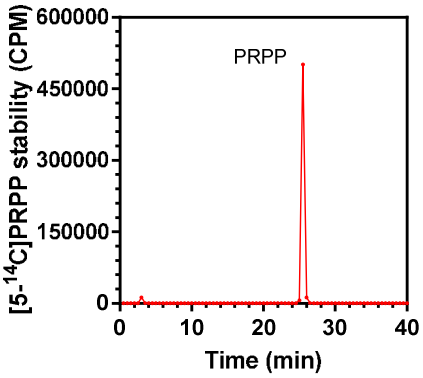
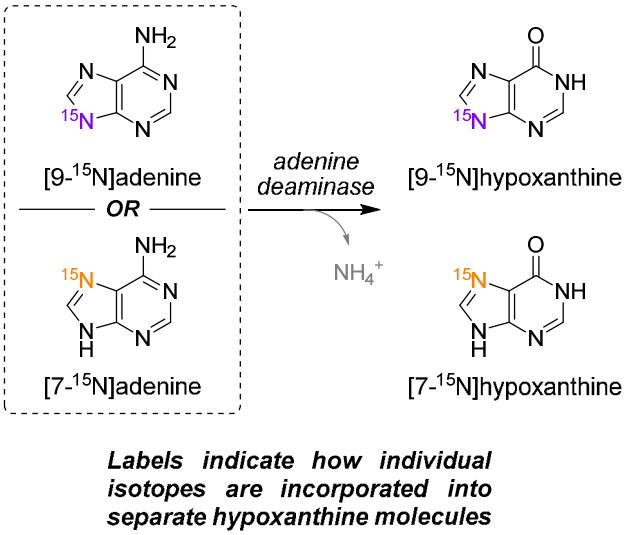


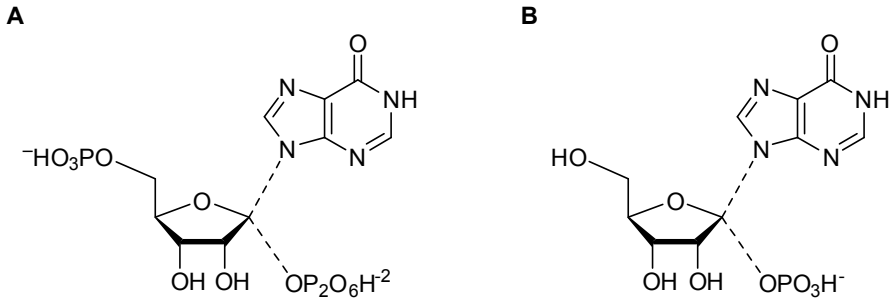
Supporting Information Figure S1. HPLC purification of radiolabeled PRPP synthesis. The R5P is the product of PRPP hydrolysis. This analysis demonstrates the labile properties of PRPP. PRPP, 5-phospho-α-D-ribosyl 1-pyrophosphate; R5P, ribose 5-phosphate.



Supporting Information Figure S2. HPLC trace of radiolabeled PRPP following the purification and lyophilization processes used here to prepare PRPP for KIE analysis.



Supporting Information Figure S3. Synthesis of isotopically labeled hypoxanthine from adenine.



Supporting Information Figure S4. The full transition state (A) was simplified by truncating the 5-phosphate and the 1-pyrophosphate on PRPP (B).

TS

C	-2.90565939	3.28337037	-0.42449917
O	-4.13939751	3.78479777	0.05060849
C	-2.92775289	1.75501965	-0.48445613
C	-2.73595755	0.99195591	0.84935738
O	-3.43482693	-0.19821362	0.93588156
C	-1.17316996	0.83215866	0.87068991
O	-0.59747813	-0.06834644	1.73581249
C	-0.89882476	0.69324443	-0.60971062
N	4.14205097	-1.02476813	0.07296452
C	2.90822147	-1.43949242	-0.34790278
N	1.91333732	-0.64319677	-0.61407019
C	2.18447845	0.68395411	-0.41037623
C	3.41564356	1.17276681	0.00538080
C	4.53844165	0.32216508	0.29119000
O	5.66000572	0.62568366	0.66340859
N	3.26426196	2.53768779	0.08496757
C	1.98017651	2.80995307	-0.27156958
H	-2.05472835	3.63836185	0.17968828
H	-2.78183982	3.68067982	-1.43591348
H	-3.81064093	1.41121448	-1.02518121
H	-3.04693642	1.61977400	1.69434830
H	-3.02302175	-0.86792696	0.30984762
H	-0.76598743	1.81994611	1.12981709
H	-0.95783193	-0.97985761	1.61137879
H	-0.17948093	0.07714554	-1.11625865
H	2.76672354	-2.51161256	-0.45335493
H	1.59080517	3.81853332	-0.29535930
O	-1.77218574	1.28848293	-1.32891681
N	1.29180956	1.72108322	-0.57700590
H	4.85840303	-1.71809796	0.26356160
O	-1.96675856	-1.67619119	-0.68246536
P	-1.32341126	-3.00630140	-0.25611155
O	-2.01384520	-4.31226594	-0.38495328
O	0.16575607	-3.04182607	-0.94195121
O	-0.93341490	-2.74986463	1.35869537
H	-1.31117482	-3.48170661	1.87176221
H	0.48834219	-2.13000713	-1.06179417
H	-4.23868929	3.53708996	0.98320416
H	3.98058686	3.19671620	0.36035478

Supporting Information Figure S5. Atomic coordinates for the *Pf*HGXPRT transition state structure

GS Ribose 1-phosphate

C	2.88298090	-1.15854098	0.47572696
O	3.83274378	-1.12237006	-0.57581431
C	1.56329132	-0.65829653	-0.10640680
C	1.57707784	0.81783957	-0.49304455
O	0.74649935	1.03462867	-1.63748788
C	0.94520097	1.51947428	0.73647401
O	0.31825538	2.73210862	0.38082338
C	-0.02929344	0.44280295	1.26270373
O	-3.56981000	0.05708275	-0.36169860
P	-2.20180049	-0.43639258	-0.16299432
O	-1.30975704	-0.76780849	-1.45535034
O	-2.09162959	-1.77090606	0.72245661
O	-1.29678462	0.68877642	0.64127677
H	3.18207025	-0.52209280	1.32487892
H	2.72624819	-2.17570998	0.86300920
H	1.27844085	-1.28237253	-0.95699219
H	2.59303727	1.16484492	-0.70679048
H	0.48086607	1.97374281	-1.57634629
H	1.71184797	1.72384427	1.49182732
H	-0.64045320	2.54645811	0.36030099
O	0.54676615	-0.79590116	0.93211302
H	-0.19514867	0.45919210	2.34233388
H	-0.66863729	-0.04757338	-1.68378905
H	4.66688132	-1.49081363	-0.24894682
H	-1.15395806	-2.02819242	0.81216019

Supporting Information Figure S6. Atomic coordinates for *Pf*HGXPRT reactant state structure for α-D-ribose 1-phosphate.

GS Hypoxanthine

N	1.92123497	0.32248594	-0.00001254
C	1.41758202	1.59085067	-0.00001990
N	0.14786265	1.88297650	0.00010865
C	-0.63266981	0.76665593	0.00017598
C	-0.24534889	-0.57422608	-0.00001708
C	1.16421394	-0.89877863	0.00004131
O	1.73803013	-1.97207406	-0.00013936
N	-1.34475913	-1.40529259	0.00020669
C	-2.37138192	-0.59023737	-0.00020685
H	2.15030897	2.39390201	-0.00019886
H	-3.41057490	-0.89149241	0.00015308
N	-2.00387008	0.73911481	0.00017524
H	2.92610492	0.18435016	-0.00006437
H	-2.60773095	1.54925297	-0.00196193

Supporting Information Figure S7. Atomic coordinates for the *Pf*HGXPRT reactant state structure for hypoxanthine.