Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information: Ultrafast Excited-State Dynamics of Promising Nucleobase Ancestor 2,4,6-Triaminopyrimidine

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Table S1: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the S_0 minimum-energy geometry of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.532899825$			
N	-0.676279	-0.004583	-1.182556
N	-0.676279	-0.004585	1.182556
N	1.264601	0.046540	-2.422370
N	1.264602	0.046541	2.422371
N	-2.651212	0.048845	-0.000000
C	-1.278311	0.005441	0.000000
C	1.385743	0.017123	-0.000000
C	0.648870	0.007873	-1.188596
C	0.648871	0.007874	1.188596
H	2.192724	-0.318867	-2.480882
H	2.192725	-0.318867	2.480882
H	0.672652	-0.199691	-3.190563
H	0.672653	-0.199690	3.190563
H	-3.100591	-0.225345	-0.848702
H	-3.100592	-0.225347	0.848701
H	2.466048	0.048286	-0.000000

Table S2: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the S_0 minimum-energy geometry of TAP at the SA5-CASSCF(16,11)/*def*2-SV(P) level

$E = -427.538788521$			
N	-0.679565	-0.006038	-1.183331
N	-0.679565	-0.006049	1.183331
N	1.259169	0.044489	-2.418211
N	1.259170	0.044491	2.418211
N	-2.650097	0.045504	0.000000
C	-1.281000	0.002455	-0.000000
C	1.383592	0.011414	0.000000
C	0.645859	0.003944	-1.188733
C	0.645859	0.003946	1.188733
H	2.199099	-0.287264	-2.481271
H	2.199100	-0.287257	2.481271
H	0.672376	-0.189467	-3.193764
H	0.672377	-0.189467	3.193764
H	-3.105503	-0.210227	-0.850973
H	-3.105503	-0.210235	0.850971
H	2.464094	0.040899	0.000000

Table S3: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the S_0 minimum-energy geometry of TAP at the MR-CISD/*def*2-SV(P) level

$E = -428.509673984$			
N	-0.678640	-0.007701	-1.184013
N	-0.678639	-0.007697	1.184013
N	1.256588	0.043545	-2.410576
N	1.256588	0.043544	2.410576
N	-2.635350	0.038106	0.000000
C	-1.275072	0.000687	0.000000
C	1.385301	0.012926	-0.000000
C	0.649391	0.003531	-1.184067
C	0.649391	0.003529	1.184067
H	2.205859	-0.276314	-2.477868
H	2.205858	-0.276317	2.477869
H	0.660761	-0.185110	-3.187742
H	0.660761	-0.185110	3.187742
H	-3.100727	-0.178110	-0.862084
H	-3.100726	-0.178106	0.862085
H	2.469544	0.044051	-0.000000

Table S4: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $\pi\pi^*$ S_1 minimum-energy geometry of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.340374627$			
N	-0.700844	-0.009324	-1.216046
N	-0.700844	-0.009324	1.216046
N	1.287626	0.073730	-2.466133
N	1.287626	0.073730	2.466133
N	-2.669212	0.060588	0.000000
C	-1.300747	0.002462	-0.000000
C	1.406580	0.031470	-0.000000
C	0.663916	-0.011544	-1.227787
C	0.663916	-0.011544	1.227787
H	2.149924	-0.430842	-2.548580
H	2.149924	-0.430842	2.548580
H	0.664957	-0.120588	-3.227223
H	0.664957	-0.120587	3.227223
H	-3.125043	-0.202729	-0.849339
H	-3.125043	-0.202729	0.849339
H	2.482801	0.122295	-0.000000

Table S5: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $\pi\pi^*$ S_1 minimum-energy geometry of TAP at the SA5-CASSCF(16,11)/*def*2-SV(P) level

$E = -427.347859694$			
N	-0.702391	-0.008364	-1.216057
N	-0.702391	-0.008363	1.216057
N	1.281753	0.091385	-2.463256
N	1.281753	0.091385	2.463256
N	-2.660670	0.057286	-0.000000
C	-1.297385	0.000660	-0.000000
C	1.402999	0.025670	0.000000
C	0.662299	-0.024326	-1.226779
C	0.662299	-0.024326	1.226779
H	2.168971	-0.366539	-2.548872
H	2.168971	-0.366539	2.548872
H	0.669361	-0.118162	-3.228586
H	0.669361	-0.118162	3.228586
H	-3.129787	-0.160050	-0.854409
H	-3.129787	-0.160050	0.854409
H	2.479611	0.116956	0.000000

Table S6: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $\pi\pi^*$ S_1 minimum-energy geometry of TAP at the MR-CISD/*def*2-SV(P) level

$E = -428.265287580$			
N	-0.708666	-0.036852	-1.198177
N	-0.708666	-0.036852	1.198177
N	1.255556	0.140293	-2.461995
N	1.255556	0.140293	2.461995
N	-2.608111	0.033946	-0.000000
C	-1.274067	-0.011200	0.000000
C	1.409604	0.035218	0.000000
C	0.645303	-0.035074	-1.238186
C	0.645303	-0.035074	1.238186
H	2.164304	-0.284230	-2.562920
H	2.164304	-0.284231	2.562920
H	0.640724	-0.069927	-3.232916
H	0.640724	-0.069927	3.232916
H	-3.096219	0.088645	-0.874140
H	-3.096219	0.088645	0.874139
H	2.489079	0.136264	0.000000

Table S7: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $^1\mathbf{S}_4$ S_1/S_0 minimum-energy crossing point of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.355192344$			
N	-0.710462	-0.109370	-1.068698
N	-0.777975	0.115718	1.253632
N	1.215193	-0.040547	-2.452555
N	1.216000	-0.157346	2.414550
N	-1.086453	2.046168	-0.118285
C	-1.166688	0.643541	-0.000543
C	1.298668	0.235791	-0.003656
C	0.607911	0.109977	-1.217015
C	0.510962	0.082387	1.252448
H	2.133383	-0.440567	-2.441951
H	2.058936	-0.689462	2.321914
H	0.618612	-0.470903	-3.133773
H	0.639978	-0.455558	3.178982
H	-1.745418	2.416289	-0.778189
H	-1.169519	2.518672	0.762653
H	2.373662	0.124483	0.034393

Table S8: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $^1\mathbf{H}_6$ S_1/S_0 minimum-energy crossing point of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.356320661$			
N	-1.156126	0.198825	0.697977
N	1.105858	0.501847	0.493772
N	-1.554490	2.301370	-0.280232
N	2.113612	0.290439	-1.595946
N	0.161313	0.563557	2.633763
C	0.071054	0.493581	1.261703
C	-0.317579	0.541214	-1.473426
C	-1.375934	0.917460	-0.502493
C	0.916188	0.433410	-0.907159
H	-1.374745	2.867652	-1.087612
H	2.030111	-0.054761	-2.531556
H	-2.443440	2.536226	0.123320
H	2.824818	-0.181460	-1.071767
H	-0.567239	0.081141	3.123735
H	1.078672	0.385890	2.994565
H	-0.464396	0.583241	-2.544519

Table S9: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $\mathbf{E}_5$ S_1/S_0 minimum-energy crossing point of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.302429857$			
N	-0.964454	0.470353	0.935323
N	1.309283	0.304956	0.798673
N	-1.756382	-0.138646	-1.211428
N	1.727682	-0.460657	-1.407007
N	0.307901	0.527518	2.922012
C	0.209054	0.415600	1.551521
C	0.157954	1.461529	-1.052859
C	-0.731978	0.470017	-0.463463
C	0.918457	0.324475	-0.567317
H	-1.572131	-0.194967	-2.194007
H	1.407410	-0.509530	-2.354695
H	-2.038212	-1.030034	-0.845628
H	1.906311	-1.378113	-1.040326
H	-0.531926	0.308386	3.419571
H	1.137968	0.134644	3.318793
H	0.112469	1.643452	-2.122402

Table S10: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $\mathbf{B}_{4,5}$ S_1/S_0 minimum-energy crossing point of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.357276630$			
N	-0.742370	0.073277	-1.229004
N	-0.743757	0.085033	1.206547
N	1.344343	-0.181477	-2.291726
N	1.342240	-0.157224	2.275379
N	-2.351183	1.367364	-0.016427
C	-1.130580	0.739372	-0.014527
C	1.086076	0.842342	-0.013569
C	0.529147	0.213658	-1.250782
C	0.527892	0.226087	1.229493
H	2.244826	-0.538198	-2.037490
H	2.246127	-0.509333	2.027440
H	0.880893	-0.739041	-2.984258
H	0.880546	-0.709802	2.972978
H	-2.878528	1.305425	-0.864166
H	-2.886535	1.294505	0.825521
H	1.966222	1.472537	-0.016327

Table S11: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $\mathbf{B}_{1,6'}$ S_1/S_0 minimum-energy crossing point of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.337093549$			
N	-0.724337	0.159893	-1.267609
N	-0.490191	0.948704	0.862830
N	1.186682	1.228712	-2.250773
N	0.971462	-0.164722	2.448077
N	-2.511109	-0.182849	0.248567
C	-1.266168	0.261296	-0.131727
C	1.416518	0.126911	-0.015051
C	0.589551	0.719649	-1.107610
C	0.715171	0.214200	1.133426
H	2.139561	0.964701	-2.414599
H	1.774698	-0.756685	2.541012
H	0.616328	1.165084	-3.072043
H	0.182822	-0.560348	2.926266
H	-2.894725	-0.915183	-0.314777
H	-2.688466	-0.267445	1.228315
H	2.392656	-0.324958	-0.143309

Table S12: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $n\pi^*$ S_1 minimum-energy geometry of TAP at the SA5-CASSCF(10,8)/*def*2-SV(P) level

$E = -427.340993452$			
N	2.336584	0.025394	1.227754
N	1.083963	0.039388	-0.624183
N	1.485144	-0.099753	3.371157
N	-1.221687	-0.073765	-0.649944
N	3.391450	0.497582	-0.903304
C	2.264640	0.546303	-0.076073
C	-0.028198	0.006268	1.469498
C	1.271179	-0.019242	2.015430
C	-0.051027	-0.007565	0.063660
H	0.786188	-0.571046	3.908713
H	-1.989751	-0.543725	-0.215913
H	2.423950	-0.310281	3.645355
H	-1.124169	-0.255140	-1.628827
H	4.170629	0.971466	-0.484779
H	3.662663	-0.446065	-1.136024
H	-0.922389	0.044022	2.072886

Table S13: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $n\pi^*$ S_1 minimum-energy geometry of TAP at the SA5-CASSCF(16,11)/*def*2-SV(P) level

$E = -427.347822717$			
N	2.340786	0.001544	1.224420
N	1.088860	0.021226	-0.631127
N	1.488838	-0.115958	3.359876
N	-1.207956	-0.095370	-0.648222
N	3.384481	0.528359	-0.898020
C	2.255067	0.550731	-0.071619
C	-0.025269	0.030751	1.468039
C	1.271460	-0.023941	2.013214
C	-0.045720	-0.011372	0.061808
H	0.762757	-0.504845	3.925194
H	-2.010001	-0.483059	-0.196638
H	2.420969	-0.337340	3.646077
H	-1.125998	-0.281952	-1.627024
H	4.165401	0.978017	-0.456506
H	3.649077	-0.407633	-1.166335
H	-0.920135	0.072220	2.070506

Table S14: Optimised Cartesian coordinates in Å and energy, E, in atomic units (a.u.) for the $n\pi^*$ S_1 minimum-energy geometry of TAP at the MR-CISD/*def*2-SV(P) level

$E = -428.300524771$			
N	2.329631	-0.068752	1.206273
N	1.106328	-0.043989	-0.610585
N	1.489895	-0.132483	3.333614
N	-1.175550	-0.123167	-0.640023
N	3.360631	0.607609	-0.889341
C	2.240935	0.552278	-0.060846
C	-0.021660	0.077890	1.466880
C	1.265566	-0.031657	2.002996
C	-0.032953	-0.021463	0.069345
H	0.740183	-0.411164	3.939386
H	-2.032482	-0.368036	-0.180656
H	2.426725	-0.341141	3.630279
H	-1.107466	-0.270395	-1.631091
H	4.145503	1.018853	-0.406735
H	3.622684	-0.310422	-1.236659
H	-0.919935	0.144732	2.069042