ELECTRONIC SUPPLEMENTARY INFORMATION FOR:

The Role of Acid-Base Equilibria in Formal Hydrogen Transfer Reactions: Tryptophan Radicals Repair by Uric Acid as a Paradigmatic Case

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Contents:

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Table S1. Deprotonation free energies (ΔG, kcal/mol) for neutral (H_3Ur) and monoanionic (H_2Ur^-) fractions of uric acid at pH = 7.4.

H_nUr^q	NH	$\Delta G^{(pH=7.4)}$
H_3Ur	site 1	-0.23
	site 2	1.16
	site 3	8.26
	site 4	7.65
H_2Ur^-	site 2	11.31
	site 3	14.67
	site 4	19.90

Table S2. Proton transfer free energies (ΔG_{PT}, kcal/mol) between uric acid fractions (H_3Ur and H_2Ur^-) and tryptophanyl radical ($Trp_{(-H)}^{\bullet}$).

H_nUr^q	NH	ΔG_{PT}	Reactions step
H_3Ur	site 1	0.46	$Trp_{(-H)}^{\bullet} + H_3Ur \leftrightarrows [Trp^{+\bullet}\cdots H_2Ur^{-}]$
	site 2	3.13	
	site 3	6.98	
H_2Ur^-	site 2	15.23	$Trp_{(-H)}^{\bullet} + H_2Ur^{-} \leftrightarrows [Trp^{+\bullet}\cdots HUr^{2-}]$

Table S3. Activation free energies ($\Delta G^{\ddagger}$, kcal/mol) between uric acid fractions (H_3Ur, H_2Ur^- and HUr^{2-}) and tryptophanyl radicals ($Trp^{\bullet+}$ and $Trp_{(-H)}^{\bullet}$)

Trp radical	H_nUr^q	Mechanism[a]	$\Delta G^{\ddagger}$
$Trp^{\bullet}_{(-H)}$	H_3Ur (site 1)	PEST	4.93
	H_3Ur (site 2)	PEST	7.11
	H_3Ur (site 3)	PEST	10.33
	H_2Ur^- (site 2)	PEST	16.01
	H_2Ur^- (site 3)	PCET	15.56
	HUr^{2-} (site 3)	PCET	10.87
	HUr^{2-} (site 4)	EPST	16.60
$Trp^{\bullet+}$	H_2Ur^-	SPGET	4.41
	HUr^{2-}	SET	0.67

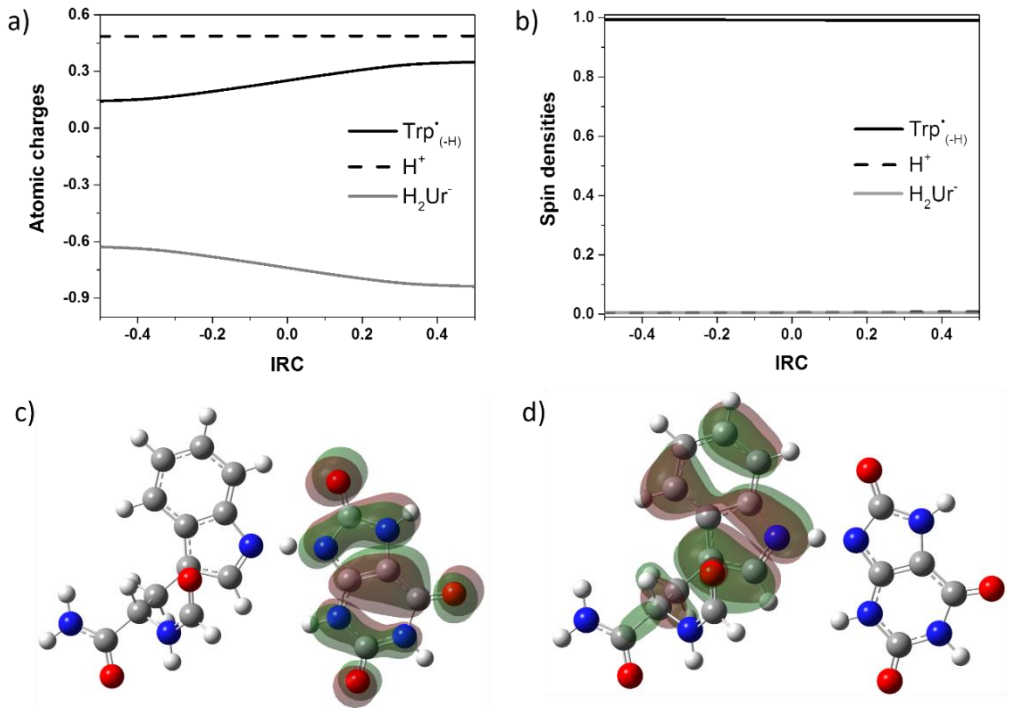

Figure S1. Information on the reaction involved in the repair of $Trp_{(-H)}^{\bullet}$ by H_3Ur (site 2). NPA atomic charge (a) and Hirshfeld spin density (b) along the reaction coordinate, HOMO (c) and (d) SOMO density surfaces (computed with isodensity value of 0.02 au) at the transition state geometry.

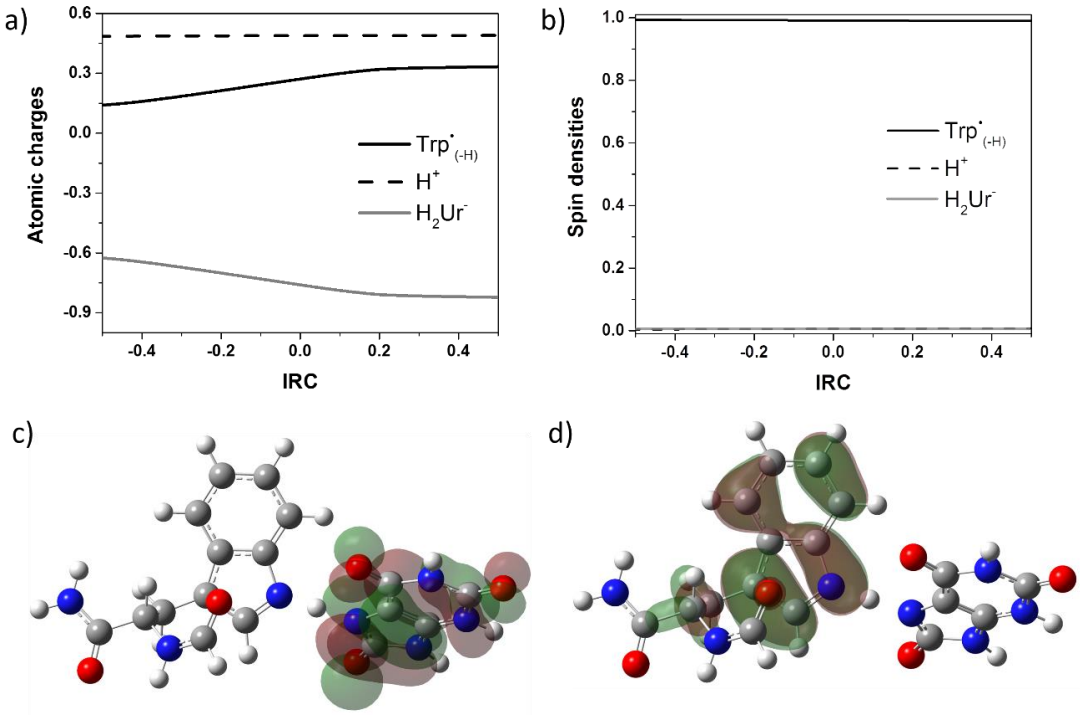

Figure S2. Information on the reaction involved in the repair of $Trp_{(-H)}^{\bullet}$ by H_3Ur (site 3). NPA atomic charge (a) and Hirshfeld spin density (b) along the reaction coordinate, HOMO (c) and (d) SOMO density surfaces (computed with isodensity value of 0.02 au) at the transition state geometry.

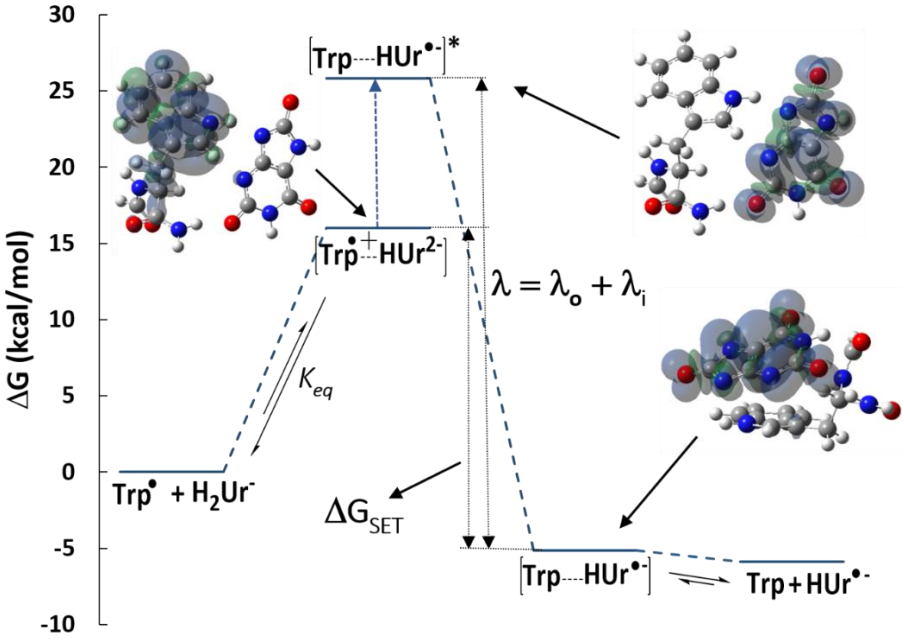

Figure S3. Pre-equilibrium reaction and parameters used to kinetic analysis of PEST mechanism between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and monoanionic fraction of uric acid (H_2Ur^{-}). Structures and spin densities to complexes are shown.

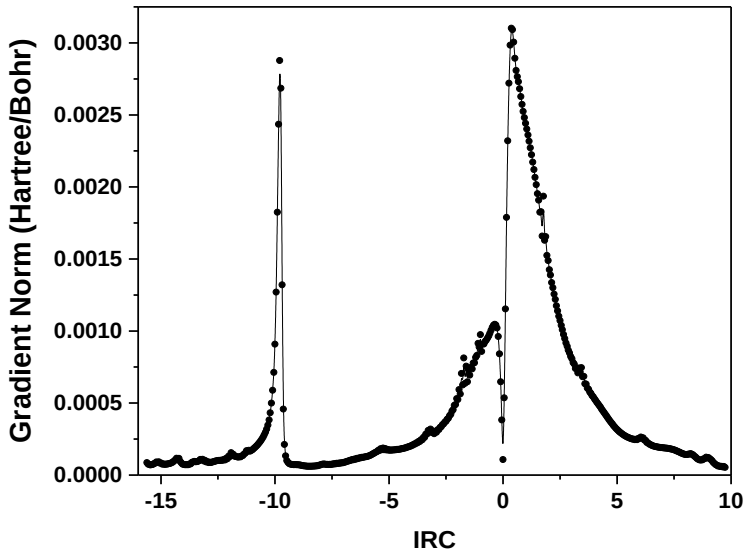

Figure S4. RMS gradient norm along the reaction pathway for repair reaction of $Trp_{(-H)}^{\bullet}$ by HUr^{2-} (site 3).

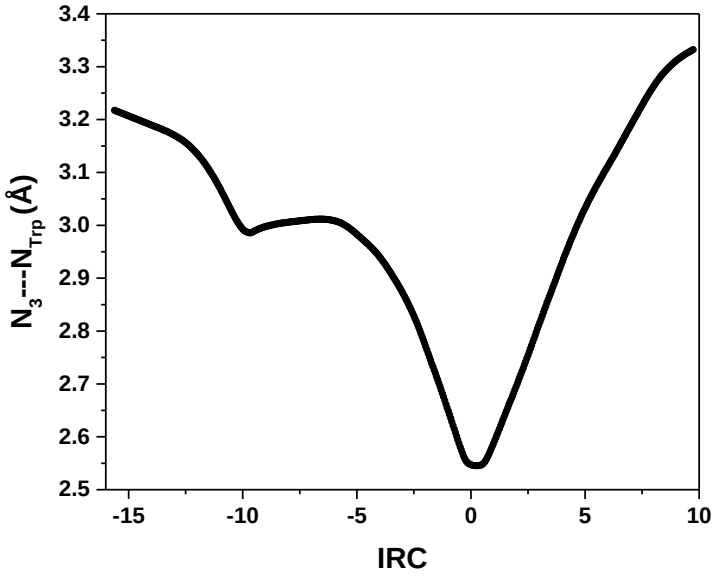

Figure S5. Distance between the H donor (N3 in HUr^{2-}) and the H acceptor (N atom in the side chain of tryptophan) along the reaction pathway for repair reaction of $Trp_{(-H)}^{\bullet}$ by HUr^{2-} (site 3).

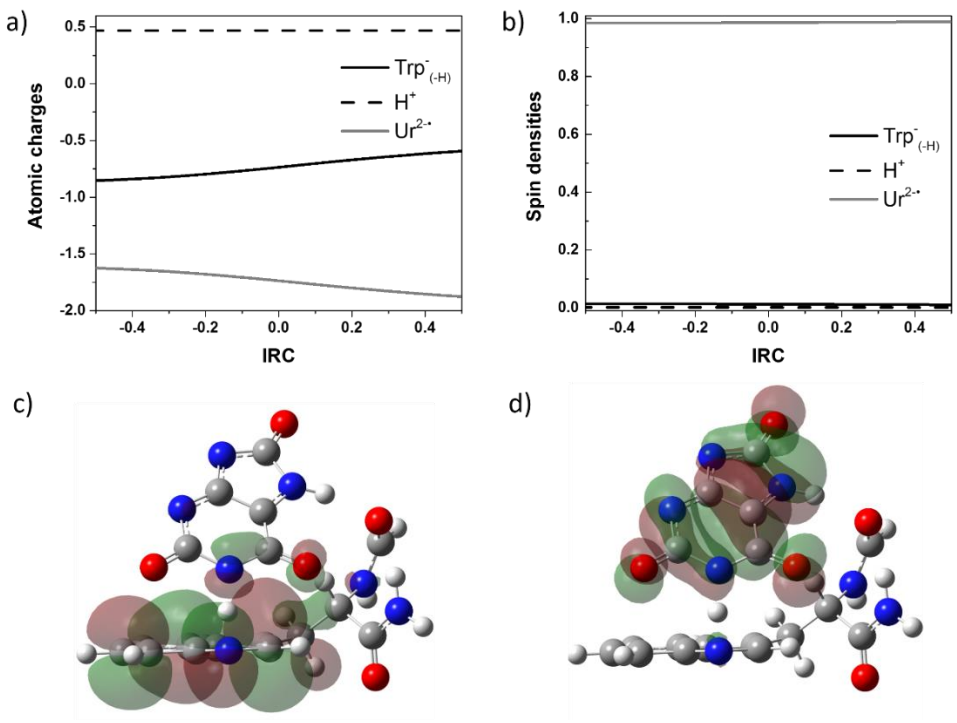

Figure S6. Information on the reaction involved in the repair of $Trp_{(-H)}^{\bullet}$ by HUr^{2-} (site 4). NPA atomic charge (a) and Hirshfeld spin density (b) along the reaction coordinate, HOMO (c) and (d) SOMO density surfaces (computed with isodensity value of 0.02 au) at the transition state geometry.

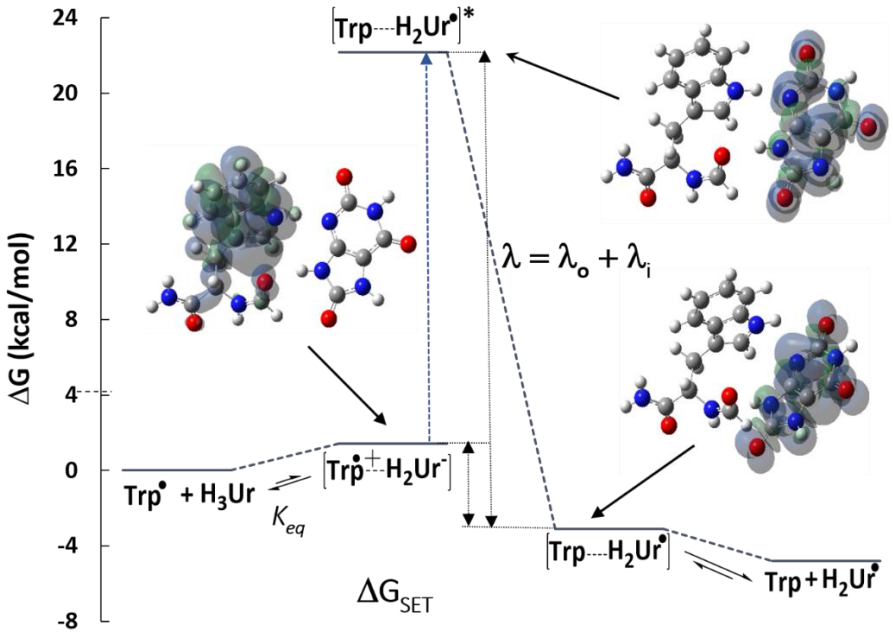

Figure S7. Pre-equilibrium reaction and parameters used to kinetic analysis of PEST mechanism between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 1). Structures and spin densities to complexes are shown.

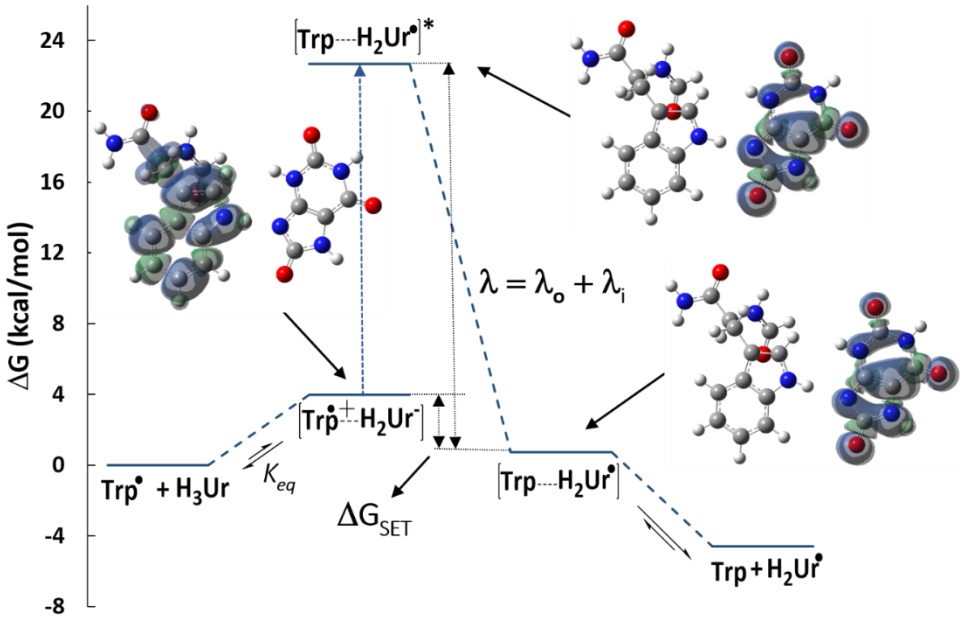

Figure S8. Pre-equilibrium reaction and parameters used to kinetic analysis of PEST mechanism between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 2). Structures and spin densities to complexes are shown.

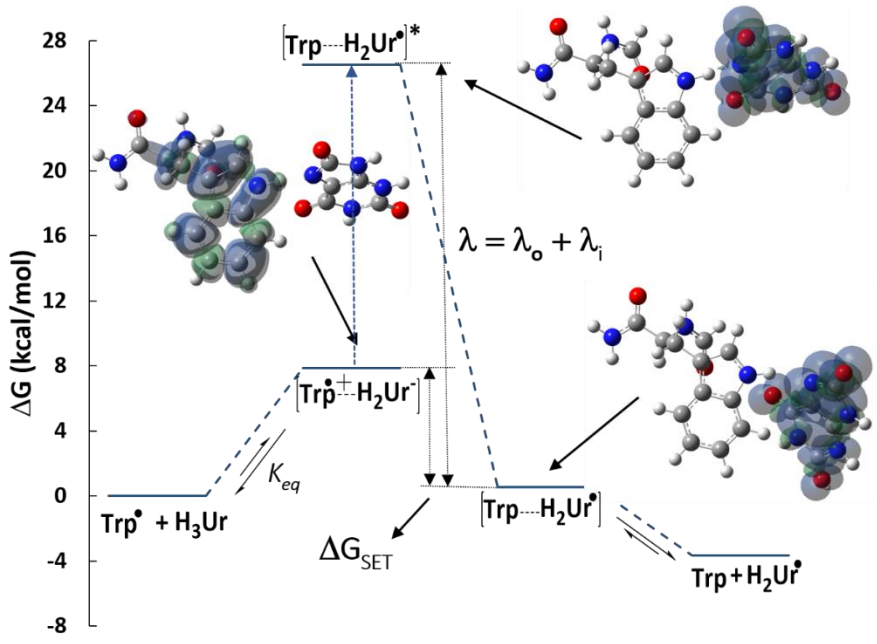

Figure S9. Pre-equilibrium reaction and parameters used to kinetic analysis of PEST mechanism between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 3). Structures and spin densities to complexes are shown.

Reactant and product structures (Å).

1. Tryptophanyl cation radical ($Trp^{\bullet+}$).

G= -779.447710

H= -779.387926

1 2

C	0.00795600	0.00924100	0.00455300
H	0.00446300	0.01001500	1.09581000
H	1.03790000	0.01202200	-0.35548600
C	-0.69572600	1.20433300	-0.51453500
C	-1.78348900	1.88468500	0.12974100
C	-0.50361300	1.86413300	-1.75587100
H	-2.22350500	1.67748100	1.09385800
N	-2.21273400	2.86228600	-0.64368600
C	-1.46526200	2.89709300	-1.83578800
C	0.38272100	1.65321800	-2.82369700
H	-2.97601000	3.48952700	-0.41476200
C	-1.58801200	3.72479900	-2.92497100
C	0.27257100	2.48232900	-3.93690100
H	1.12609200	0.86732200	-2.77828300
H	-2.33293400	4.50805700	-2.97197500
C	-0.69195300	3.49497800	-3.98521300
H	0.94021800	2.34564100	-4.77700800
H	-0.75414100	4.12488400	-4.86303200
C	-0.67640600	-1.29726700	-0.49280400
N	-2.02620000	-1.44020700	0.00434200
C	0.14399500	-2.47354400	0.02467400
H	-0.69546000	-1.29918000	-1.58255600
C	-3.09589300	-0.95182500	-0.63108600
H	-2.15538100	-1.93272800	0.87910200
N	1.16881500	-2.84626800	-0.73943400
O	-0.13321100	-3.00097700	1.11047800
O	-3.04695500	-0.32666600	-1.69953000
H	-4.04232900	-1.15658000	-0.12260900
H	1.35295600	-2.39384800	-1.62192400
H	1.79245200	-3.57044600	-0.41368100
H	1.80683100	-3.58231900	-0.40575700

2. Tryptophanyl neutral radical ($Trp_{(-H)}^{\bullet}$).

G= -779.009407

H= -778.950116

0 2

C	-0.01620800	0.01008800	-0.00334600
H	-0.01962800	0.01606200	1.08851300
H	1.01724900	0.01526900	-0.35698500
C	-0.73542600	1.19296300	-0.53416900
C	-1.78743300	1.94204400	0.11041300
C	-0.60318400	1.79143500	-1.82610100
H	-2.14816500	1.75914800	1.11431500
N	-2.28557600	2.89631300	-0.63887800
C	-1.56965600	2.82745400	-1.86035600
C	0.21645200	1.53858800	-2.92746800
C	-1.73019500	3.61716300	-2.98069000
C	0.05517400	2.33927800	-4.06241300
H	0.95582400	0.74642500	-2.90533600
H	-2.46871800	4.40889100	-3.01201700
C	-0.90056400	3.35852400	-4.08669100
H	0.67608500	2.16901400	-4.93275500
H	-1.00650800	3.96490400	-4.97765400
C	-0.68206700	-1.30828000	-0.48642800
N	-2.02861700	-1.45409800	0.02156100
C	0.15147600	-2.47144100	0.03420300
H	-0.71430500	-1.32237300	-1.57546000
C	-3.11767300	-1.06239700	-0.64657400
H	-2.13892500	-1.84207000	0.94930100
N	1.15432500	-2.86593400	-0.74930800
O	-0.08926800	-2.97068900	1.14284100
O	-3.10793200	-0.55905300	-1.77880500
H	-4.05015500	-1.23382100	-0.10075000
H	1.31195900	-2.43809100	-1.64884900
H	1.78891500	-3.57944300	-0.42144000

3. Tryptophan (Trp).

G= -779.648585

H= -779.589502

0 1

C	-0.00959600	0.00974200	0.01190100
H	-0.02246700	0.00806300	1.10450000
H	1.03284100	0.01654500	-0.31618400
C	-0.73394700	1.20376200	-0.51815600
C	-1.68818900	1.94858900	0.12583300
C	-0.64572700	1.73115800	-1.85539000
H	-2.05342300	1.86639600	1.13821800
N	-2.19322800	2.90657500	-0.72230700
C	-1.57331200	2.79815600	-1.94351700
C	0.12610700	1.39732600	-2.98181400
H	-2.89280100	3.58961800	-0.47774200
C	-1.74203800	3.54558300	-3.11496000
C	-0.03895900	2.13276200	-4.14558900
H	0.83878400	0.58104900	-2.93866000
H	-2.45295600	4.36156700	-3.16225700
C	-0.96502500	3.19708500	-4.20929100
H	0.54850300	1.89029200	-5.02285700
H	-1.07000800	3.75291700	-5.13317900
C	-0.66007600	-1.30907700	-0.47769800
N	-2.01264600	-1.44167100	0.01904400
C	0.16443900	-2.47536500	0.04231300
H	-0.68971300	-1.32340600	-1.56670300
C	-3.09831400	-1.08453900	-0.67188700
H	-2.12797600	-1.70032100	0.98994100
N	1.17182600	-2.87098100	-0.73708700
O	-0.07491100	-2.97745200	1.15151000
O	-3.10040600	-0.70510200	-1.85241800
H	-4.02650500	-1.17758500	-0.09980300
H	1.33354300	-2.44208000	-1.63522200

4. Tryptophanyl anion ($Trp_{(-H)}^{-}$).

G= -779.173317
H= -779.114732
-1 1

C	0.00450600	0.00575000	0.00661000
H	-0.00242600	0.00021700	1.10071100
H	1.04874000	0.01061500	-0.32018600
C	-0.73334400	1.19356600	-0.52044200
C	-1.71389800	1.94831100	0.12077800
C	-0.68734600	1.71693700	-1.84662700
H	-2.03158600	1.82434700	1.15050500
N	-2.28545900	2.90719600	-0.66202800
C	-1.66273900	2.77048000	-1.87453200
C	0.05462100	1.41066400	-3.00524900
C	-1.86385700	3.50929200	-3.05659300
C	-0.16292600	2.14859200	-4.16007200
H	0.78877300	0.61022800	-2.99658600
H	-2.59494800	4.31117700	-3.08491000
C	-1.11764600	3.19386300	-4.18306700
H	0.40203600	1.92515200	-5.05804800
H	-1.26623700	3.75519400	-5.09873900
C	-0.62976300	-1.32848500	-0.47206900
N	-1.98125200	-1.47053500	0.02521100
C	0.20505200	-2.48264200	0.05259200
H	-0.65940700	-1.34906400	-1.56087600
C	-3.07033100	-1.12562500	-0.66534600
H	-2.09295100	-1.69553400	1.00476600
N	1.22553700	-2.86236900	-0.71902700
O	-0.03129700	-2.99063400	1.16079400
O	-3.08425100	-0.78216100	-1.85746200
H	-3.99412100	-1.19939500	-0.08312900
H	1.38928900	-2.42757800	-1.61386400
H	1.87159100	-3.56054400	-0.38152600

5. Protonated fraction of uric acid (H_3Ur).

G= -637.613968
H= -637.569285
0 1

C	0.26163100	-0.75833900	-0.00000300
C	0.35118300	0.60384300	-0.00001100
C	-0.81597300	1.40955700	0.00000000
C	-2.10081400	-0.73163800	-0.00000100
C	2.44335500	-0.22801900	0.00000200
O	-0.87721100	2.64290300	0.00000900
O	-3.19451900	-1.29513000	-0.00000200
N	-1.98140800	0.63804700	-0.00000300
N	-0.91882900	-1.43029000	0.00000300
N	1.51918700	-1.27131600	0.00000700
H	1.78188500	-2.24841800	0.00001000
N	1.70883300	0.91640600	0.00000600
H	2.11206600	1.84210300	-0.00005200
H	-2.85819000	1.14772900	-0.00000100
O	3.67160900	-0.35291800	-0.00000300
H	-0.96557100	-2.44260900	0.00000400

6. Cation radical of H_3Ur

G= -637.396171
H= -637.351313
1 2

C	0.27812000	-0.81396600	-0.00000100
C	0.36626700	0.60213700	-0.00000600
C	-0.82842400	1.42911500	-0.00000700
C	-2.09445200	-0.71118000	0.00000300
C	2.44037100	-0.24222600	-0.00000500
O	-0.83184900	2.64571300	-0.00001200
O	-3.16063000	-1.28591400	0.00000700
N	-1.97986400	0.66217300	-0.00000300
N	-0.89174200	-1.43622100	0.00000400
N	1.51847800	-1.30231700	0.00000000
H	1.79364900	-2.28111000	0.00000300
N	1.66138400	0.92177300	-0.00000900
H	2.05406300	1.86033100	-0.00000900
H	-2.86392600	1.16505200	-0.00000300
O	3.64159600	-0.31941000	-0.00000600
H	-0.96580500	-2.45203700	0.00000900

7. Radical of H_3Ur in NH site 1.

G= -636.983379
H= -636.938949
0 2

C	-0.23004400	-0.83330700	0.00000000
C	-0.32787100	0.59095100	0.00000000
C	0.87066200	1.39238900	0.00000000
C	2.03338900	-0.80268000	0.00000000
C	-2.40979400	-0.23798700	0.00000000
O	0.90895400	2.61949000	0.00000000
O	3.13313400	-1.35030000	0.00000000
N	1.98991100	0.59417100	0.00000000
N	0.86233300	-1.53680700	0.00000000
N	-1.51626500	-1.29275700	0.00000000
H	-1.80587500	-2.26313100	0.00000000
N	-1.62713300	0.92336100	0.00000000
H	-2.01608000	1.86034300	0.00000600
H	2.89026400	1.06207600	0.00000000
O	-3.62312400	-0.28559700	0.00000000

8. Radical of H_3Ur in NH site 2.

G= -636.982941

H= -636.938286
0 2
C -0.33171000 -0.83526800 0.00000000
C -0.38931700 0.59609400 0.00000000
C 0.79608300 1.41629700 0.00000000
C 2.05676400 -0.72929800 0.00000000
C -2.40979200 -0.32600500 0.00000000
O 0.81863300 2.64080200 0.00000000
O 3.14387300 -1.28637800 0.00000000
N 1.94882300 0.64871200 0.00000000
N 0.87552800 -1.44437800 0.00000000
N -1.51809300 -1.39008700 0.00000000
N -1.68875100 0.89537200 0.00000000
H -2.10838200 1.81832600 0.00000000
H 2.83290600 1.14796700 0.00000000
O -3.62888500 -0.38045000 0.00000000
H 0.95178300 -2.45635000 0.00000000

9. Radical of H_3Ur in NH site 3.

G= -636.981865
H= -636.937443
0 2
C 0.00021100 0.00000000 0.00256500
C -0.00087300 0.00000000 1.42191200
C 1.26971900 0.00000000 2.12307100
C 2.36322600 0.00000000 -0.11805900
C -2.06526300 0.00000000 0.79852100
O 1.42290300 0.00000000 3.33677200
O 3.39200900 0.00000000 -0.77335300
N 2.35835000 0.00000000 1.25816300
N 1.11732100 0.00000000 -0.73239700
N -1.27364400 0.00000000 -0.38042700
H -1.63662900 0.00000000 -1.32661700
N -1.23683300 0.00000000 1.90651000
H 3.27817400 0.00000000 1.68843000
O -3.28929400 0.00000000 0.78398000
H 1.09700800 0.00000000 -1.74788000

10. Radical of H_3Ur in NH site 4.

G= -636.963990
H= -636.919480
0 2
C -0.00044900 0.00000000 -0.00016000
C 0.00011300 0.00000000 1.41342300
C 1.26152800 0.00000000 2.15478600
C 2.38007300 0.00000000 0.07040300
C -2.12584900 0.00000000 0.69414300
O 1.23926200 0.00000000 3.39665900
O 3.39150000 0.00000000 -0.63518600
N 2.38876600 0.00000000 1.41425800
N 1.13947900 0.00000000 -0.65703900
N -1.27609000 0.00000000 -0.41849800
H -1.60883100 0.00000000 -1.37698900
N -1.28134600 0.00000000 1.80657700
H -1.61609200 0.00000000 2.76512700
O -3.33530500 0.00000000 0.68984800
H 1.18488800 0.00000000 -1.67188900

11. Mono-anionic fraction of uric acid (H_2Ur^-, NH site 1).

G= -637.174729
H= -637.130618
-1 1
C -0.21719500 -0.78206600 0.00000000
C -0.32280800 0.59626400 0.00000100
C 0.84373400 1.37762000 0.00000000
C 2.03529900 -0.81341400 0.00000000
C -2.41600600 -0.22825400 0.00000000
O 0.93849500 2.62694500 -0.00000100
O 3.17622900 -1.34341700 0.00000000
N 1.97887600 0.57908600 0.00000000
N 0.89228900 -1.52653200 0.00000000
N -1.50551400 -1.26879200 0.00000000
H -1.77865700 -2.24111900 -0.00000100
N -1.68416000 0.91572700 0.00000000
H -2.09070000 1.83899300 0.00000200
H 2.86932100 1.06065800 0.00000000
O -3.65329300 -0.34051000 0.00000000

12. Anion radical of H_2Ur^- NH in site 2.

G= -636.545594
H= -636.501558
-1 2
C 0.00035100 -0.00002800 -0.00025700
C -0.00001800 -0.00003200 1.44466600
C 1.22323900 -0.00003700 2.19314800
C 2.28274100 -0.00003100 -0.05224500
C -2.06866500 -0.00002700 0.63339900
O 1.32261400 -0.00004100 3.42542000
O 3.38397000 -0.00003100 -0.62592600
N 2.30718200 -0.00003600 1.35226400
N 1.10621100 -0.00002800 -0.73164400
N -1.26058400 -0.00002500 -0.46236500
N -1.28007600 -0.00003100 1.82041800
H -1.64711900 -0.00003200 2.76377900

H 3.22644300 -0.00003900 1.77867300
O -3.30111200 -0.00002400 0.67833900

13. Anion radical of H_2Ur^- NH in site 3.

G= -636.553483
H= -636.509563
-1 2
C -0.00034800 0.00000700 0.00058000
C -0.00047000 -0.00000600 1.43397000
C 1.27657700 0.00000000 2.10087200
C 2.24681900 0.00003200 -0.19188900
C -2.07201200 -0.00002600 0.84477600
O 1.46851400 -0.00001000 3.32229500
O 3.31135000 0.00004800 -0.82742500
N 2.32351200 0.00001800 1.20265500
N 1.02933500 0.00002700 -0.81304500
N -1.31516100 -0.00000500 -0.33309200
H -1.70385200 -0.00000200 -1.26584800
N -1.23208400 -0.00002500 1.94272100
H 3.26001000 0.00002400 1.59037000
O -3.30639200 -0.00004300 0.86387300

14. Anion radical of H_2Ur^- NH in site 4.

G= -636.533115
H= -636.488895
-1 2
C 0.00004500 -0.00000100 0.00039300
C 0.00013500 0.00000400 1.41923600
C 1.26908400 -0.00001200 2.12218000
C 2.26838100 -0.00002700 -0.02260800
C -2.13786100 0.00002500 0.73194800
O 1.29716600 -0.00001200 3.37805200
O 3.31310800 -0.00003700 -0.71043600
N 2.36145800 -0.00002700 1.34129700
N 1.05606000 -0.00001600 -0.74861300
N -1.32333800 0.00001300 -0.37926200
H -1.67851800 0.00001300 -1.32590500
N -1.28310900 0.00001900 1.83463400
H -1.61012800 0.00002600 2.79321900
O -3.35878500 0.00003900 0.76420600

15. Bi-anionic fraction of uric acid (HUr^{2-}, NH site 1 and 2).

G= -636.715546
H= -636.671301
-2 1
C 0.00002200 -0.00040900 -0.00140000
C 0.00027800 0.00190000 1.39842200
C 1.19139100 -0.00505600 2.11906600
C 2.27654100 0.00221800 -0.11875200
C -2.08543400 -0.00500400 0.61143400
O 1.35753200 -0.01370500 3.37366400
O 3.40614300 0.00514200 -0.69891800
N 2.29478900 0.00098200 1.27344900
N 1.11265500 0.00033000 -0.77632500
N -1.27345500 -0.00517700 -0.48116200
N -1.34232700 -0.01347100 1.76850600
H -1.72409300 0.03143100 2.69929200
H 3.20612300 -0.00093200 1.71176300
O -3.35383200 0.00077400 0.60650700

16. Bi-anion radical of H_2Ur^- NH in site 3.

G= -636.096478
H= -636.053178
-2 2
C 0.00017300 -0.00000200 0.00084700
C -0.00013900 -0.00000100 1.44964700
C 1.24958000 0.00000000 2.14940000
C 2.27533200 -0.00000200 -0.11675400
C -2.01415900 -0.00000200 0.73448500
O 1.41981600 0.00000100 3.38404100
O 3.38186400 -0.00000200 -0.70710600
N 2.32197900 -0.00000100 1.28411300
N 1.09689100 -0.00000300 -0.76873200
N -1.26574300 -0.00000300 -0.42706500
N -1.24551700 -0.00000100 1.91282900
H 3.24721400 0.00000000 1.69482400
O -3.26770900 -0.00000200 0.76139500

17. Bi-anion radical of H_2Ur^- NH in site 4.

G= -636.084777
H= -636.041038
-2 2
C 0.00020600 -0.00000600 -0.00106300
C 0.00020200 0.00002700 1.43252200
C 1.24264300 -0.00003900 2.16623100
C 2.28618200 -0.00014200 0.04597300
C -2.07315800 0.00013400 0.61959900
O 1.24436500 -0.00001400 3.43142400
O 3.37199500 -0.00021200 -0.59958700
N 2.35685300 -0.00012300 1.41943500
N 1.11456800 -0.00008700 -0.70255300
N -1.27405600 0.00006300 -0.47292400

N	-1.28723500	0.00011200	1.80477200
H	-1.65570800	0.00016700	2.74607800
O	-3.31531700	0.00021900	0.67005500

Transition states and complexes structures (Å).

1. Transition state for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 1).

G= -1416.614584
H= -1416.529131
0 2

C	-3.51736600	0.05225000	-1.15386100
H	-3.44865500	-0.42551200	-2.13291200
H	-4.34003300	0.76948500	-1.16118000
C	-2.25345600	0.75137600	-0.82358700
C	-0.91952300	0.34264300	-1.19032000
C	-2.07907600	1.90735600	-0.00985600
H	-0.64929000	-0.50619800	-1.80394000
N	-0.01283900	1.14003000	-0.67781700
C	-0.68373700	2.12948800	0.07143700
C	-2.96813500	2.76103500	0.65457700
C	-0.14464400	3.17527200	0.78790600
C	-2.43257400	3.82160400	1.38560400
H	-4.03820500	2.60197700	0.60074300
H	0.92451600	3.33997000	0.83838800
C	-1.04967400	4.02405900	1.44978800
H	-3.09356000	4.49953300	1.90970600
H	-0.66327100	4.85739000	2.02266400
C	-3.83935200	-1.04175700	-0.09592500
N	-2.87646000	-2.12161800	-0.10469700
C	-5.20503500	-1.62463300	-0.43854500
H	-3.85760500	-0.59119800	0.89595400
C	-1.79272200	-2.15564500	0.67631100
H	-3.05779900	-2.90315400	-0.72171900
N	-6.25356700	-0.98942500	0.08210500
O	-5.29859300	-2.60517000	-1.19009900
O	-1.47204500	-1.26270600	1.47346400
H	-1.19424900	-3.06350700	0.55344000
H	-6.13095600	-0.19853500	0.69593900
H	-7.18711900	-1.27962700	-0.17097900
H	1.24931100	0.89980000	-0.66147400
N	2.48056400	0.57690400	-0.57152000
C	2.89094000	-0.60901100	-0.07987700
C	3.44543500	1.47579500	-0.89778300
C	4.19459200	-0.99950500	0.09526300
N	2.09444100	-1.64253900	0.33158000
O	3.18096000	2.60818800	-1.33933000
N	4.76517800	1.09286500	-0.72824600
C	5.24680000	-0.11589400	-0.23114000
N	4.17009600	-2.29029500	0.62691900
C	2.88172900	-2.69594100	0.77744700
H	1.08331400	-1.65993300	0.34847400
H	5.46075300	1.78482500	-0.98220200
O	6.46877600	-0.31603900	-0.11942300
H	4.96793400	-2.85991400	0.86713500
O	2.46563000	-3.77649900	1.21652300

2. Metastable complex for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 1).

G= -1416.615571
H= -1416.530200
0 2

C	-3.39505500	-0.06091100	-1.27663000
H	-3.25995600	-0.53029400	-2.25173000
H	-4.29058900	0.56238900	-1.29704200
C	-2.22976800	0.78345700	-0.92766500
C	-0.86391200	0.56152000	-1.31545900
C	-2.20338000	1.89827900	-0.04797700
H	-0.47421200	-0.21662300	-1.95608200
N	-0.08127700	1.45198100	-0.74437500
C	-0.85346000	2.30077500	0.07106200
C	-3.20050800	2.57306900	0.67228300
C	-0.45303600	3.34348600	0.87382800
C	-2.81176400	3.63115600	1.48928400
H	-4.23863400	2.27421500	0.59410000
H	0.58479900	3.63850200	0.95610600
C	-1.46639200	4.00705600	1.58731800
H	-3.55646200	4.17187200	2.05819100
H	-1.19477300	4.83369300	2.23100900
C	-3.60273200	-1.17748800	-0.21030000
N	-2.58464300	-2.20427600	-0.27165600
C	-4.94991500	-1.84095200	-0.47783900
H	-3.60085500	-0.72933400	0.78369100
C	-1.40460500	-2.11563800	0.34006400
H	-2.78860100	-3.02665100	-0.82645400
N	-6.00934100	-1.21119300	0.02691000
O	-5.02035600	-2.87884500	-1.14927100
O	-1.04482800	-1.14435800	1.02669600
H	-0.75678200	-2.98337800	0.18550900
H	-5.90354100	-0.36731000	0.56999300
H	-6.93620300	-1.55611700	-0.17667000
H	0.96480300	1.38840300	-0.73744000
N	2.62969800	0.82702600	-0.45921900
C	2.84484100	-0.36923700	0.10804100
C	3.72681500	1.42670900	-0.96690600
C	4.04754200	-1.03494500	0.22625700

N	1.88815900	-1.16945000	0.68569900
O	3.69001800	2.54636400	-1.53075400
N	4.95747600	0.78635900	-0.86234800
C	5.21930400	-0.45151500	-0.28791900
N	3.79238100	-2.24666100	0.87448900
C	2.46620200	-2.33416700	1.15826700
H	0.88838400	-0.98805000	0.77421800
H	5.74913000	1.27659800	-1.26053800
O	6.37918100	-0.91814600	-0.27290600
H	4.46427600	-2.96084100	1.11244200
O	1.86860900	-3.26345300	1.72622500

3. Product complex for repair reaction between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 1).

G= -1416.623718
H= -1416.537193
0 2

C	3.99075700	0.41751900	0.72643400
H	4.41223400	0.28898400	1.72614800
H	4.75443600	0.87384200	0.09182300
C	2.77112000	1.27855800	0.77900400
C	1.97946500	1.53191700	1.86969300
C	2.13584100	1.92606200	-0.33952800
H	2.10484000	1.21781100	2.89470700
N	0.89964900	2.30040800	1.50214500
C	0.96730000	2.55602700	0.15404700
C	2.44029000	2.01990200	-1.70871100
C	0.10417500	3.28294500	-0.67447900
C	1.58690300	2.73558200	-2.53444400
H	3.32643500	1.54052400	-2.11001500
H	-0.78563300	3.75730400	-0.27775400
C	0.43002800	3.36149800	-2.02016600
H	1.80600600	2.81762900	-3.59216300
H	-0.21650600	3.91345700	-2.69164800
C	3.66861200	-0.98615800	0.15431800
N	2.73814300	-1.69584700	1.00714000
C	4.95785700	-1.78832500	0.07369100
H	3.22427700	-0.88784300	-0.83537400
C	1.42799300	-1.74366900	0.79925700
H	3.10756400	-2.12305400	1.84694700
N	5.67956200	-1.61383900	-1.03425800
O	5.31692400	-2.51164100	1.01523800
O	0.85047500	-1.25453500	-0.19203600
H	0.87119600	-2.27573900	1.57487400
H	5.35133800	-1.01796900	-1.77890400
H	6.58588400	-2.05139900	-1.11330200
H	0.18033300	2.63172600	2.12546600
N	-2.52139200	0.51189100	0.66440100
C	-2.76724600	-0.63934400	0.10820800
C	-3.62970100	1.28211200	0.94461600
C	-4.05569900	-1.16190900	-0.22369000
N	-1.86061000	-1.58316100	-0.27092000
O	-3.52770100	2.39139400	1.46677200
N	-4.91085800	0.81272100	0.63856900
C	-5.23870800	-0.38753000	0.05351100
N	-3.88137900	-2.36969500	-0.77738400
C	-2.50972000	-2.66365400	-0.83040200
H	-0.82249500	-1.49118800	-0.22161200
H	-5.67689700	1.43336500	0.87791900
O	-6.39262600	-0.73302700	-0.18997200
H	-4.60223300	-2.99271200	-1.12462900
O	-2.01934600	-3.67985100	-1.28606200

4. Transition state for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 2).

G= -1416.611472
H= -1416.526311
0 2

C	-3.38874000	-0.47518500	-1.18848300
H	-3.09498600	-1.19882400	-1.95066200
H	-4.23278000	0.11246900	-1.55452700
C	-2.26013200	0.42849500	-0.86704600
C	-0.85637400	0.13056000	-0.99585400
C	-2.31548000	1.73167200	-0.29116500
H	-0.42342400	-0.77514500	-1.40000600
N	-0.11258100	1.11878800	-0.55813800
C	-0.97406900	2.13770200	-0.09851400
C	-3.36769800	2.56932000	0.09381500
C	-0.64561000	3.35101400	0.46461500
C	-3.04613500	3.80182400	0.66502600
H	-4.39920900	2.27013300	-0.04679200
H	0.38449000	3.65166200	0.60840700
C	-1.71312400	4.18361200	0.84582600
H	-3.83729100	4.47287700	0.97306900
H	-1.49390400	5.14550900	1.29157500
C	-3.85182400	-1.25288300	0.07638800
N	-2.82179900	-2.13138700	0.58415200
C	-5.05632600	-2.10383200	-0.30882000
H	-4.12842600	-0.54244700	0.85505700
C	-1.92468400	-1.76116300	1.50329800
H	-2.78282100	-3.07127300	0.21158600
N	-6.23308500	-1.47977300	-0.28731200
O	-4.91118400	-3.28589700	-0.65006000
O	-1.87777500	-0.63918100	2.02649500
H	-1.21751600	-2.55216800	1.76911800
H	-6.30536500	-0.51616000	0.00254800

H	-7.06001500	-1.96603300	-0.60199200
H	1.15950600	1.08763600	-0.51010900
N	2.43691000	0.95485500	-0.44107300
C	3.10994300	-0.19317000	-0.22365700
C	3.37299100	1.97304200	-0.44073700
C	4.45712200	0.04123600	-0.09296900
N	2.57896000	-1.44827600	-0.13847900
N	4.60581500	1.41857700	-0.23391500
O	3.13170400	3.18617000	-0.60222800
C	5.36595600	-1.00796300	0.15309700
C	3.38667300	-2.52897600	0.09256600
H	1.58435600	-1.61191800	-0.24389400
H	5.46592900	1.94374400	-0.18604900
O	6.59638300	-0.93416800	0.29964900
N	4.72518700	-2.25260100	0.22686000
O	2.94242100	-3.67781800	0.17518200
H	5.31826600	-3.05602100	0.40138200

5. Metastable complex for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 2).

G= -1416.611312
H= -1416.524678
0 2

C	-3.40619500	-0.67879900	-1.09075300
H	-3.04558200	-1.48738000	-1.72939300
H	-4.22282000	-0.15825200	-1.59278600
C	-2.31160700	0.27797400	-0.80615400
C	-0.91446300	-0.04610100	-0.70173500
C	-2.40669800	1.66605300	-0.51668400
H	-0.44749800	-1.00780100	-0.85857700
N	-0.22254800	1.02476900	-0.37992300
C	-1.09577600	2.12128000	-0.24518100
C	-3.48397100	2.56164700	-0.45075900
C	-0.81091300	3.42447500	0.08742000
C	-3.21227400	3.88658500	-0.11510400
H	-4.49429100	2.23042200	-0.65564300
H	0.19910000	3.75502900	0.29199000
C	-1.90427600	4.30779800	0.14777700
H	-4.02197000	4.60184800	-0.05680400
H	-1.72357700	5.34360500	0.40444400
C	-3.95653500	-1.30167800	0.22463200
N	-2.95397500	-2.06254400	0.93404500
C	-5.09981100	-2.24227000	-0.14068700
H	-4.32143600	-0.50510300	0.87340200
C	-2.16059500	-1.53057700	1.86897000
H	-2.87418800	-3.04895800	0.72219000
N	-6.27768700	-1.65937800	-0.35817700
O	-4.90514100	-3.46001100	-0.25597500
O	-2.18665000	-0.34033900	2.21146100
H	-1.46907400	-2.24707200	2.32115500
H	-6.39894800	-0.66502600	-0.23735800
H	-7.05959900	-2.22010000	-0.66395700
H	0.82885000	1.04888100	-0.24702100
N	2.52609700	0.95585700	-0.06243900
C	3.26467900	-0.16230900	-0.12263300
C	3.42507100	1.97754600	0.15087700
C	4.61329000	0.08495200	0.03969000
N	2.79445400	-1.43402200	-0.31669700
N	4.69621000	1.46364900	0.21005800
O	3.14168900	3.19361700	0.27384300
C	5.56600800	-0.94613600	0.01599900
C	3.64765300	-2.50092700	-0.35165200
H	1.80631400	-1.61763000	-0.43920800
H	5.52836700	2.00774200	0.37711000
O	6.80125000	-0.85953800	0.15053600
N	4.97753000	-2.20522200	-0.18832200
O	3.24971000	-3.66003600	-0.52120600
H	5.60740200	-2.99859400	-0.21275600

6. Product complex for repair reaction between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 2).

G= -1416.616489
H= -1416.528990
0 2

C	-3.43151600	-0.76239800	-1.15822000
H	-3.07079300	-1.66129900	-1.66375500
H	-4.19199000	-0.29854200	-1.79156200
C	-2.30696400	0.18798400	-0.90785900
C	-0.96816100	-0.10535800	-0.83907600
C	-2.43138800	1.58111800	-0.56651500
H	-0.46643700	-1.04539400	-1.01564800
N	-0.25363000	1.01461800	-0.48602200
C	-1.12381100	2.06200100	-0.31011900
C	-3.52261200	2.45863800	-0.43973400
C	-0.87434600	3.39067600	0.05400400
C	-3.28150800	3.77417300	-0.07393800
H	-4.53349100	2.11159300	-0.62351600
H	0.13415200	3.73999900	0.24112100
C	-1.96835800	4.23474800	0.16904900
H	-4.11042900	4.46398800	0.02925500
H	-1.81378800	5.26898800	0.45198800
C	-4.10813300	-1.19432600	0.16829700
N	-3.18418400	-1.91553600	1.01713200
C	-5.27790500	-2.10641900	-0.16237400
H	-4.45607100	-0.31348400	0.70688300
C	-2.46760800	-1.34691200	1.99045700
H	-2.99421800	-2.88118100	0.78347000
N	-6.44340200	-1.50000900	-0.39245000

O	-5.11909400	-3.33324400	-0.26034600
O	-2.57588400	-0.16889100	2.36235500
H	-1.76385000	-2.03486800	2.46897700
H	-6.53813200	-0.50044900	-0.29645500
H	-7.23605800	-2.04558000	-0.69760400
H	0.75211700	1.06577900	-0.37588100
N	2.84877000	1.09879900	-0.05017900
C	3.41984000	-0.07960000	-0.09579100
C	3.89001500	1.99902800	0.13913900
C	4.84119200	-0.00880500	0.05818200
N	2.83159600	-1.28379500	-0.26417400
N	5.11568400	1.28827200	0.20321200
O	3.81097800	3.21162500	0.24117300
C	5.67662200	-1.18411300	0.03272500
C	3.56284500	-2.45602200	-0.29953700
H	1.82571400	-1.36302500	-0.38162700
H	6.02689300	1.71463300	0.32909200
O	6.89485900	-1.19665600	0.15459600
N	4.93232200	-2.33761200	-0.15122300
O	3.02571000	-3.54120800	-0.45611900
H	5.44451700	-3.21382800	-0.18423400

7. Transition state for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 3).

G= -1416.606606
H= -1416.521517
0 2

C	-3.82422200	-0.49604600	-0.91365600
H	-3.87504600	-1.47363700	-1.39609100
H	-4.48054600	0.20010200	-1.43887200
C	-2.43654300	0.02201800	-0.93426200
C	-1.22752200	-0.76174800	-0.95043400
C	-2.00540400	1.37810400	-0.85848400
H	-1.15392300	-1.83904900	-1.00762400
N	-0.16279100	0.00235900	-0.89255400
C	-0.59164200	1.34562400	-0.82457800
C	-2.68467100	2.60013000	-0.79251000
C	0.16874300	2.49032900	-0.72826800
C	-1.92454900	3.76596000	-0.69407400
H	-3.76693100	2.63777000	-0.81676400
H	1.25033000	2.45846800	-0.69771400
C	-0.52749800	3.71065100	-0.66323000
H	-2.42011600	4.72642600	-0.64023300
H	0.03684400	4.63123300	-0.58656900
C	-4.33995300	-0.63840500	0.54654000
N	-3.58095700	-1.60590300	1.30665900
C	-5.78954700	-1.10753500	0.49036800
H	-4.27929800	0.32894600	1.04504900
C	-2.51229100	-1.28907400	2.04429800
H	-3.89606300	-2.56719900	1.28906100
N	-6.69671000	-0.15156100	0.29647500
O	-6.06896600	-2.31082900	0.58365100
O	-2.04487900	-0.14653800	2.14806600
H	-2.07185300	-2.14294300	2.56704000
H	-6.42734200	0.81926700	0.24398800
H	-7.66809900	-0.40291000	0.18468100
H	1.00492400	-0.38458000	-0.88629900
N	2.27309300	-0.79956700	-0.89177200
C	3.29351800	-0.39602000	-0.03489600
C	2.84140200	-1.53199500	-1.86485900
C	4.48362700	-0.90132800	-0.48871300
C	3.26854800	0.39003600	1.14459600
N	4.22372800	-1.60719700	-1.61389400
O	2.29536700	-2.08076400	-2.85051800
N	5.68286100	-0.69585200	0.12468300
O	2.28207000	0.90763400	1.68813300
N	4.54177000	0.56227700	1.70359400
H	4.88603600	-2.10306900	-2.19436000
C	5.74317800	0.06540900	1.26103800
H	6.54718500	-1.08114300	-0.23711000
H	4.58953200	1.11551100	2.55184400
O	6.80470500	0.28902900	1.84996500

8. Metastable complex for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 3).

G= -1416.605172
H= -1416.518830
0 2

C	-3.85886500	-0.48784900	-0.90841600
H	-3.91410000	-1.46435600	-1.39233600
H	-4.50876400	0.21387000	-1.43368500
C	-2.46805600	0.02108900	-0.92745400
C	-1.27100200	-0.77723900	-0.93178200
C	-2.02647400	1.37240300	-0.86832600
H	-1.19732000	-1.85440300	-0.97560500
N	-0.20621200	-0.00971800	-0.88155400
C	-0.61356500	1.33839300	-0.83056200
C	-2.69938600	2.60054500	-0.81987800
C	0.15572000	2.47622400	-0.74674000
C	-1.93335500	3.76216200	-0.73425300
H	-3.78114800	2.64270600	-0.84809200
H	1.23674400	2.43700000	-0.71362500
C	-0.53634300	3.69998700	-0.69911400
H	-2.42335500	4.72596100	-0.69441900
H	0.03241000	4.61850100	-0.63310100
C	-4.37769800	-0.62878100	0.55111400
N	-3.62528800	-1.59895600	1.31389000
C	-5.82877900	-1.09401000	0.49033900

H -4.31537800 0.33888200 1.04885200
C -2.55135300 -1.28656100 2.04580600
H -3.95200600 -2.55657300 1.30655900
N -6.73263600 -0.13611300 0.29191200
O -6.11109700 -2.29633100 0.58531900
O -2.07069800 -0.14817600 2.13350600
H -2.11921000 -2.13923300 2.57720300
H -6.46086700 0.83403000 0.23903900
H -7.70437800 -0.38534700 0.17823200
H 0.83530200 -0.36162000 -0.87556300
N 2.32025700 -0.85212100 -0.88078600
C 3.33530800 -0.41845300 -0.03421400
C 2.91253500 -1.57498500 -1.83934500
C 4.54380100 -0.89256300 -0.47924600
C 3.29020700 0.37846100 1.13680500
N 4.30285900 -1.61461800 -1.59641700
O 2.38775700 -2.15537800 -2.82662400
N 5.73635900 -0.64936200 0.13608200
O 2.28964000 0.87887200 1.67445000
N 4.55685600 0.58960300 1.69979700
H 4.97743800 -2.09705100 -2.17344300
C 5.77175100 0.11777700 1.26802600
H 6.61171900 -1.01768800 -0.21608800
H 4.58619100 1.14768800 2.54554700
O 6.82498500 0.36814300 1.86378600

9. Product complex for repair reaction between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and protonated fraction of uric acid (H_3Ur, site 3).

G= -1416.616817
H= -1416.529843
0 2
C -3.86656500 -0.73097100 -0.88411000
H -4.17220000 -1.77983900 -0.89192900
H -4.38875500 -0.21862200 -1.69600600
C -2.38695700 -0.61835200 -1.05217100
C -1.44964900 -1.57889100 -0.77028100
C -1.65190700 0.56458100 -1.41850400
H -1.59227100 -2.59781400 -0.44318900
N -0.18326300 -1.07868900 -0.95805400
C -0.27497300 0.23753900 -1.34037300
C -2.02948400 1.86765100 -1.78685200
C 0.72943200 1.16980900 -1.63045000
C -1.03826900 2.79569400 -2.06772200
H -3.07731500 2.14073500 -1.84774600
H 1.77891600 0.90369600 -1.57480500
C 0.32823600 2.44779400 -1.99009500
H -1.31107000 3.80521900 -2.35061000
H 1.07871800 3.19531400 -2.21721700
C -4.33277000 -0.10533100 0.45615100
N -3.74983700 -0.79178600 1.58960000
C -5.84491600 -0.22810700 0.53830100
H -4.03655700 0.94206000 0.49661400
C -2.62795900 -0.39978000 2.20065200
H -4.14312300 -1.68897500 1.84102100
N -6.53952200 0.77625100 0.00231800
O -6.37459500 -1.23660200 1.03065800
O -2.01679300 0.65305700 1.96602100
H -2.28819100 -1.09656800 2.97304100
H -6.07233000 1.58289900 -0.38280400
H -7.54565700 0.71387200 -0.05085300
H 0.67595900 -1.56228300 -0.73154200
N 2.70052600 -1.87718700 0.05285800
C 3.18006200 -0.71807700 0.48808900
C 3.71622400 -2.43983700 -0.69964300
C 4.50655900 -0.50276400 0.02952500
C 2.53919300 0.30277200 1.29859600
N 4.83648500 -1.56807800 -0.69635300
O 3.69798600 -3.51199700 -1.28879900
N 5.21181500 0.59609800 0.31858600
O 1.40990300 0.24659000 1.76304900
N 3.35734400 1.40680700 1.51095900
H 5.71094300 -1.74351400 -1.17747000
C 4.64891900 1.61314900 1.08169700
H 6.16131400 0.73662700 -0.01428700
H 2.96993800 2.15793000 2.07399400
O 5.27672100 2.62445900 1.34626200

10. Transition state for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and monoanionic fraction of uric acid (H_2Ur^{-}, site 2).

G= -1416.152648
H= -1416.070146
-1 2
C -2.76843400 0.22799300 -1.42154800
H -3.82063500 -0.04303700 -1.51820000
H -2.44379600 0.70393400 -2.34797900
C -1.90381400 -0.94976200 -1.15604000
C -0.49860800 -0.95259500 -1.45912800
C -2.12526800 -2.12493400 -0.38871100
H 0.03906900 -0.19528100 -2.00755000
N 0.11187500 -1.97955100 -0.91818900
C -0.85713200 -2.74607500 -0.23378500
C -3.26329000 -2.69593600 0.20094000
C -0.68967900 -3.90262800 0.49247800

C	-3.10325600	-3.87004200	0.93342800
H	-4.23682900	-2.23480400	0.08615200
H	0.28137700	-4.36538500	0.61212900
C	-1.84160000	-4.45838300	1.07808600
H	-3.96275500	-4.33480500	1.39831100
H	-1.74623200	-5.36905800	1.65540200
C	-2.60033800	1.24229500	-0.25795600
N	-3.49804100	0.89542200	0.82481900
C	-2.89307100	2.64703900	-0.78451200
H	-1.57188500	1.21927400	0.10944700
C	-3.54037300	1.61995100	1.94602000
H	-4.14392000	0.12534300	0.71853400
N	-1.81785100	3.39491300	-1.03228800
O	-4.05696200	3.00773000	-1.01503400
O	-2.81919600	2.60696600	2.14472300
H	-4.26873200	1.27024500	2.68291500
H	-0.88638800	3.11899900	-0.72876600
H	-1.95056000	4.31663900	-1.42280900
H	1.27774300	-1.86846800	-0.73812400
N	2.53543300	-1.30644600	-0.45823500
C	2.62059200	0.02970700	-0.16619000
C	3.77850600	-1.84504100	-0.26548800
C	3.92420900	0.33965100	0.20584800
N	1.58967800	0.89585300	-0.24030400
N	4.63872800	-0.85702800	0.13618300
O	4.09813800	-3.05157800	-0.42545100
C	4.26737600	1.65193800	0.54614000
C	1.87888700	2.16417600	0.06883000
H	5.61327200	-1.00277200	0.34758700
O	5.38856000	2.09915600	0.90603200
N	3.17310200	2.50624300	0.44897100
O	1.01996800	3.09648500	0.03006100
H	3.33749800	3.47913500	0.67312600
C	3.10000900	3.91722900	0.95001000
H	4.24210900	2.24954900	0.18131300
H	-0.27179000	4.43458700	0.51534500
C	1.83956100	4.52068000	1.04042600
H	3.94850200	4.38710100	1.42925600
H	1.73587800	5.44728700	1.58997300
C	2.61310600	-1.24503400	-0.20863600
N	3.44978500	-0.90294900	0.92303800
C	2.94656100	-2.63671500	-0.74754100
H	1.56715200	-1.24181400	0.10692200
C	3.43152700	-1.63388000	2.04145900
H	4.11075800	-0.14152100	0.84892300
N	1.89224800	-3.37326800	-1.09546800
O	4.12377500	-2.99626800	-0.89813500
O	2.69530300	-2.61736500	2.19758900
H	4.12285600	-1.29188200	2.81658300
H	0.93908000	-3.09576600	-0.86684700
H	2.05291200	-4.28356800	-1.50185300
H	-1.10847500	2.03245300	-0.90354800
N	-2.71892800	1.29042200	-0.67650700
C	-2.71521600	-0.03596700	-0.34742100
C	-3.92217600	1.78356600	-0.26356800
C	-3.91897000	-0.38710000	0.26482000
N	-1.68716600	-0.88247800	-0.58609700
N	-4.67747100	0.78200000	0.29601900
O	-4.31457600	2.98060700	-0.36906600
C	-4.14855000	-1.69647900	0.68961500
C	-1.85955000	-2.14103300	-0.17421400
H	-5.58853100	0.91306700	0.70535300
O	-5.17703300	-2.17391900	1.24441400
N	-3.05301700	-2.51663600	0.43333900
O	-0.97491300	-3.04296400	-0.31154600
H	-3.13075400	-3.48402500	0.71872500

11. Metastable complex for proton transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and monoanionic fraction of uric acid (H_2Ur^-, site 2).

G= -1416.152785
H= -1416.066891
-1 2

C	2.82634300	-0.20994900	-1.34496000
H	3.87867800	0.07250900	-1.39059800
H	2.54666200	-0.67080200	-2.29344400
C	1.94349000	0.95789600	-1.09951200
C	0.54989300	0.94397600	-1.44219300
C	2.14492400	2.14739000	-0.35609600
H	0.01351900	0.18187900	-1.98209700
N	-0.05809900	1.99625100	-0.94336500
C	0.88100200	2.78584200	-0.25011800
C	3.27151300	2.72417200	0.25490900
C	0.69811800	3.96154500	0.43689200

12. Product complex for repair reaction between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and monoanionic fraction of uric acid (H_2Ur^-, site 2).

G= -1416.186504
H= -1416.101838
-1 2

C	-0.90566400	-1.89067000	-1.44843100
H	-1.01474700	-2.97507300	-1.36675000
H	-1.24037900	-1.59703800	-2.44492200
C	0.52609900	-1.48583400	-1.25072500
C	1.12357300	-0.35574900	-1.75220500
C	1.54072600	-2.17285900	-0.49108700
H	0.70887700	0.41317300	-2.38638800
N	2.43921100	-0.30155700	-1.36084500
C	2.72227300	-1.39401900	-0.57900800
C	1.56965100	-3.37335700	0.24311600
C	3.91611500	-1.76937400	0.04826000

C	2.74933500	-3.74908000	0.86607100
H	0.68556400	-3.99787000	0.31696400
H	4.80595300	-1.15671700	-0.03194500
C	3.91134100	-2.95210800	0.77078800
H	2.78537000	-4.66995600	1.43529700
H	4.81708500	-3.27359600	1.27040300
C	-1.84683900	-1.22201200	-0.43323100
N	-1.55272100	-1.68788500	0.91044800
C	-3.29227600	-1.53694400	-0.80747700
H	-1.69521500	-0.14465200	-0.48308600
C	-2.24799400	-1.26605300	1.96719500
H	-0.79149600	-2.33480100	1.06352500
N	-3.96080600	-0.54116100	-1.39286200
O	-3.76465700	-2.67175100	-0.63845100
O	-3.20077600	-0.47426400	1.88644200
H	-1.91746600	-1.68104200	2.92306700
H	-3.60271500	0.40663900	-1.36811900
H	-4.91721100	-0.69809000	-1.67568000
H	3.08357600	0.44078900	-1.58655300
N	1.54321100	3.21514600	-1.05636100
C	0.38315300	2.82248100	-0.50745900
C	2.51532800	2.90493500	-0.15406300
C	0.61776900	2.26283500	0.80440900
N	-0.81982100	2.91199700	-1.05962200
N	1.93404000	2.32724900	1.01080600
O	3.73395100	3.06674900	-0.25601300
C	-0.46354200	1.77842800	1.61275200
C	-1.85601900	2.42458700	-0.33145300
H	2.45081900	2.00666100	1.82019600
O	-0.36070100	1.26430300	2.73235200
N	-1.66933400	1.96357600	0.98083100
O	-3.01466800	2.36238600	-0.78273400
H	-2.47784700	1.51938500	1.40975200
C	2.99123900	-1.88816200	2.28596400
H	0.96462600	-1.50269900	2.92004900
H	4.09696300	-2.08921800	-0.95034400
C	3.86820000	-2.05684900	1.19875400
H	3.37548800	-1.97077100	3.29549000
H	4.91367600	-2.26801500	1.38905100
C	-2.61432600	-0.82267900	0.10474500
N	-3.73565900	-0.37407500	0.91998900
C	-3.02178500	-2.16007400	-0.51398800
H	-2.47089800	-0.08004200	-0.67815300
C	-4.27969300	0.84264700	0.83218100
H	-4.07561500	-0.99330800	1.64438100
N	-3.33805800	-2.14380600	-1.80874800
O	-3.09355800	-3.17747400	0.19142900
O	-3.93869200	1.71918800	0.02245400
H	-5.08746800	1.01219400	1.54956200
H	-3.23730500	-1.30371600	-2.35754600
H	-3.63557400	-2.99718600	-2.25932200
H	1.80155500	-0.24904800	-1.93918600
N	1.99301900	0.94559600	-1.70428500
C	0.99682400	1.47654800	-0.93795100
C	3.17485800	1.13762700	-0.97734800
C	1.51607400	1.98189100	0.28289700
C	-0.38352200	1.71840800	-1.23459200
N	2.86586300	1.78188800	0.21106400
O	4.29804500	0.80044300	-1.33280700
N	0.85913900	2.54053000	1.27078500
O	-0.97089500	1.48553100	-2.30045100
N	-1.04134700	2.28817900	-0.16088700
H	3.54743800	2.01814200	0.91983500
C	-0.49442400	2.62821300	1.07287400
H	-2.05946800	2.32713100	-0.21960900
O	-1.26319000	3.03096500	1.95946600

13. Transition state for formal hydrogen transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and monoanionic fraction of uric acid (H_2Ur^-, site 3).

G= -1416.152263
H= -1416.071475
-1 2

C	-1.35890100	-0.96726200	0.96282700
H	-1.23011100	-0.03223400	1.51956100
H	-1.52745600	-1.75141500	1.70711900
C	-0.11455900	-1.25122500	0.18234400
C	0.08910600	-1.27717500	-1.19023300
C	1.17741800	-1.52441600	0.76227300
H	-0.64045900	-1.08722800	-1.96382100
N	1.39473100	-1.50796300	-1.54448400
C	2.06643800	-1.68668600	-0.32602300
C	1.64039700	-1.62533200	2.08097200
C	3.41784400	-1.96118300	-0.11600100

14. Transition state for formal hydrogen transfer between tryptophanyl radical ($Trp_{(-H)}^{\bullet}$) and dianionic fraction of uric acid (HUr^{2-}, site 3).

G= -1415.700562
H= -1415.620905
-2 2

C	1.55252600	0.88525500	0.93000800
H	1.39023700	-0.05795900	1.46477300
H	1.81257400	1.63515300	1.68336300
C	0.29802200	1.27441000	0.20483100
C	0.03371800	1.31731700	-1.14739900
C	-0.95082800	1.60971900	0.84180400
H	0.70739900	1.08179100	-1.95758400
N	-1.28029100	1.62865100	-1.44770000
C	-1.88140100	1.82576600	-0.20775800
C	-1.35371700	1.72488600	2.18176900
C	-3.21022100	2.16572300	0.07319500

C	-2.67696600	2.05155000	2.45123400
H	-0.64898700	1.56003500	2.98976100
H	-3.92020600	2.33529000	-0.72789600
C	-3.59527500	2.27323800	1.40427500
H	-3.01066600	2.14356800	3.47808700
H	-4.61972500	2.53316100	1.64373800
C	2.76401600	0.67700200	0.01921600
N	3.90244700	0.18860600	0.78844900
C	3.21344400	1.98903000	-0.61940000
H	2.54578800	-0.06292800	-0.74928500
C	4.22695900	-1.10278700	0.88583600
H	4.38942500	0.84565800	1.38435900
N	3.38355800	1.98636900	-1.94111800
O	3.44914900	2.97658300	0.09387300
O	3.65835100	-2.02538800	0.28174900
H	5.07102800	-1.29323600	1.55450200
H	3.15261500	1.17478200	-2.49363800
H	3.68610600	2.83088700	-2.40507200
H	-1.76840500	0.42445800	-1.89184100
N	-2.07950500	-0.76958400	-1.76018700
C	-1.20165700	-1.45134900	-0.99840700
C	-3.31700500	-0.92666100	-1.06259800
C	-1.88594700	-1.96475600	0.16367900
C	0.18412600	-1.75214000	-1.20285900
N	-3.19263300	-1.66320500	0.08373300
O	-4.36738000	-0.43272400	-1.50492300
N	-1.28936700	-2.61226400	1.16308800
O	0.86044700	-1.51250900	-2.21813000
N	0.72540300	-2.40376100	-0.11767100
C	0.05250800	-2.76964200	1.05152300
H	1.73969500	-2.49295700	-0.09398900
O	0.74593600	-3.26855400	1.96328900

15. Transition state for proton transfer between tryptophanyl anion ($Trp_{(-H)}^{-}$) and radical anion fraction of uric acid ($HUr^{-\bullet}$, site 3) for repair reaction between ($Trp_{(-H)}^{\bullet}$) and dianionic fraction of uric acid (HUr^{2-}, site 4).

G= -1415.691423
H= -1415.611373
-2 2

C	-1.00368000	-2.22404700	1.03692000
H	-0.85873700	-1.80047400	2.03367500
H	-1.29175500	-3.27042100	1.16893000
C	0.27892300	-2.05774300	0.26787000
C	0.44333800	-1.81912600	-1.07631900
C	1.59730700	-1.93631000	0.83329500
H	-0.32177800	-1.78887600	-1.83809700
N	1.74642300	-1.51178200	-1.43283100
C	2.46040200	-1.60132800	-0.24727600
C	2.11350100	-2.06592100	2.13451100
C	3.83178900	-1.40512400	-0.03041000
C	3.47169800	-1.86382200	2.33796400
H	1.46405300	-2.32088600	2.96524900
H	4.49098700	-1.15554600	-0.85378400
C	4.32436500	-1.53860400	1.26142200
H	3.88691200	-1.96125600	3.33433900
H	5.38194200	-1.39178200	1.44744200
C	-2.14633800	-1.45726200	0.37501300
N	-3.21807000	-1.16883000	1.32387600
C	-2.74885000	-2.20624800	-0.82235500
H	-1.77751800	-0.49444500	0.01971800
C	-3.92853600	-0.04050600	1.27962600
H	-3.40520000	-1.82594300	2.06984500
N	-3.48310700	-1.44901800	-1.64180300
O	-2.58584500	-3.42325300	-0.98894500
O	-3.79659200	0.83452800	0.40573500
H	-4.65776700	0.06094700	2.08750100
H	-3.59323300	-0.46056300	-1.46138600
H	-3.95862400	-1.87480400	-2.42391500
H	1.67004700	-0.23620700	-1.85675700
N	-1.32384300	2.53889400	0.09283800
C	-0.19589600	2.13515600	-0.50549800
C	-0.94868700	3.47716300	1.09388900
C	0.87939200	2.86052400	0.11622000
C	0.06119100	1.22016800	-1.58218400
N	0.39455000	3.68131800	1.07277400
O	-1.79020200	3.99211700	1.84362600
N	2.14424500	2.70362700	-0.23342800
O	-0.84524900	0.66894800	-2.23830500
N	1.38961000	0.99879800	-1.81540800
C	2.38778600	1.74034800	-1.18452600
O	3.56761600	1.49769400	-1.52267500
H	-2.24204900	2.10506100	0.02067400

Table 4. The $k_{overall}$ ($M^{-1}s^{-1}$) and k_{hyp} ($M^{-1}s^{-1}$) for different pHs.

pH	$k_{overall}$ ($M^{-1}s^{-1}$)	k_{hyp} ($M^{-1}s^{-1}$)
2	$9.37X10^{5}$	$6.00X10^{0}$
2.2	$1.48X10^{6}$	$1.50X10^{1}$
2.4	$2.35X10^{6}$	$3.77X10^{1}$
2.6	$3.71X10^{6}$	$9.44X10^{1}$
2.8	$5.85X10^{6}$	$2.36X10^{2}$
3	$9.19X10^{6}$	$5.88X10^{2}$
3.2	$1.44X10^{7}$	$1.46X10^{3}$
3.4	$2.24X10^{7}$	$3.60X10^{3}$
3.6	$3.44X10^{7}$	$8.77X10^{3}$
3.8	$5.21X10^{7}$	$2.10X10^{4}$
4	$7.71X10^{7}$	$4.93X10^{4}$
4.2	$1.10X10^{8}$	$1.12X10^{5}$
4.4	$1.51X10^{8}$	$2.43X10^{5}$
4.6	$1.96X10^{8}$	$4.99X10^{5}$
4.8	$2.38X10^{8}$	$9.63X10^{5}$
5	$2.71X10^{8}$	$1.73X10^{6}$
5.2	$2.86X10^{8}$	$2.90X10^{6}$
5.4	$2.81X10^{8}$	$4.51X10^{6}$
5.6	$2.56X10^{8}$	$6.53X10^{6}$
5.8	$2.18X10^{8}$	$8.80X10^{6}$
6	$1.73X10^{8}$	$1.11X10^{7}$
6.2	$1.30X10^{8}$	$1.32X10^{7}$
6.4	$9.26X10^{7}$	$1.49X10^{7}$
6.6	$6.36X10^{7}$	$1.62X10^{7}$
6.8	$4.24X10^{7}$	$1.71X10^{7}$
7	$2.78X10^{7}$	$1.78X10^{7}$
7.2	$1.80X10^{7}$	$1.82X10^{7}$
7.4	$1.15X10^{7}$	$1.85X10^{7}$
7.6	$7.33X10^{6}$	$1.87X10^{7}$
7.8	$4.65X10^{6}$	$1.88X10^{7}$
8	$2.95X10^{6}$	$1.88X10^{7}$
8.2	$1.86X10^{6}$	$1.89X10^{7}$
8.4	$1.17X10^{6}$	$1.89X10^{7}$
8.6	$7.40X10^{5}$	$1.89X10^{7}$
8.8	$4.66X10^{5}$	$1.88X10^{7}$
9	$2.93X10^{5}$	$1.87X10^{7}$
9.2	$1.83X10^{5}$	$1.86X10^{7}$
9.4	$1.14X10^{5}$	$1.83X10^{7}$
9.6	$7.06X10^{4}$	$1.80X10^{7}$
9.8	$4.32X10^{4}$	$1.74X10^{7}$
10	$2.60X10^{4}$	$1.66X10^{7}$
10.2	$1.53X10^{4}$	$1.55X10^{7}$
10.4	$8.73X10^{3}$	$1.40X10^{7}$
10.6	$4.77X10^{3}$	$1.22X10^{7}$
10.8	$2.49X10^{3}$	$1.00X10^{7}$
11	$1.23X10^{3}$	$7.88X10^{6}$
11.2	$5.78X10^{2}$	$5.87X10^{6}$
11.4	$2.60X10^{2}$	$4.18X10^{6}$
11.6	$1.13X10^{2}$	$2.87X10^{6}$
11.8	$4.75X10^{1}$	$1.92X10^{6}$
12	$1.96X10^{1}$	$1.26X10^{6}$