Supporting Information

Evolution of Oxidation Dynamics of Histidine: Non-Reactivity in the Gas Phase, Peroxides in Hydrated Clusters, and pH Dependence in Solution

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Summary of literature proposed His photooxidation pathways

We have summarized literature proposed oxidation pathways of single His in Fig. S1.[1-4] The photooxidation of His was initiated by the formation of endoperoxide via [4+2] Diels-Alder cycloaddition of $^1O_2$ to the conjugated double bonds of the imidazole ring. Note that $^1O_2$ does not really favor a Diels-Alder reaction, due to high activation barriers and relatively weak O-C bonding formed. Consequently, the endoperoxides were only detected at low temperature.[2, 5] The endoperoxides may in one pathway lose O_2 to regenerate starting materials. In another pathway, the endoperoxides decomposed by ring-opening to a number of poorly characterized intermediates, including hydroperoxides which may eliminate water and be hydrolyzed to hydrated imidazolone. Hydrated imidazolone intermediate (**2a** and/or **2a′**) was assumed to be a key intermediate. Hydrated imidazolone may either undergo intramolecular nucleophilic attack to form 6α-hydoxy-2-oxo-octahydro-pyrrolo[2,3-d]imidazole-5-carboxylic acid (**2d**), or cross-link with another His molecule to produce a dimeric product (see Fig. 8 of the paper). Hydrated imidazolone may also evolve to hydroxyimidazolidinedione (**4**) via hydration and dehydrogenation. Ring rupture of **4** and subsequent degradation produce various stable end-products, of which asparagine (**6**), aspartic acid (**8**) and urea (**9**) were mostly identified.

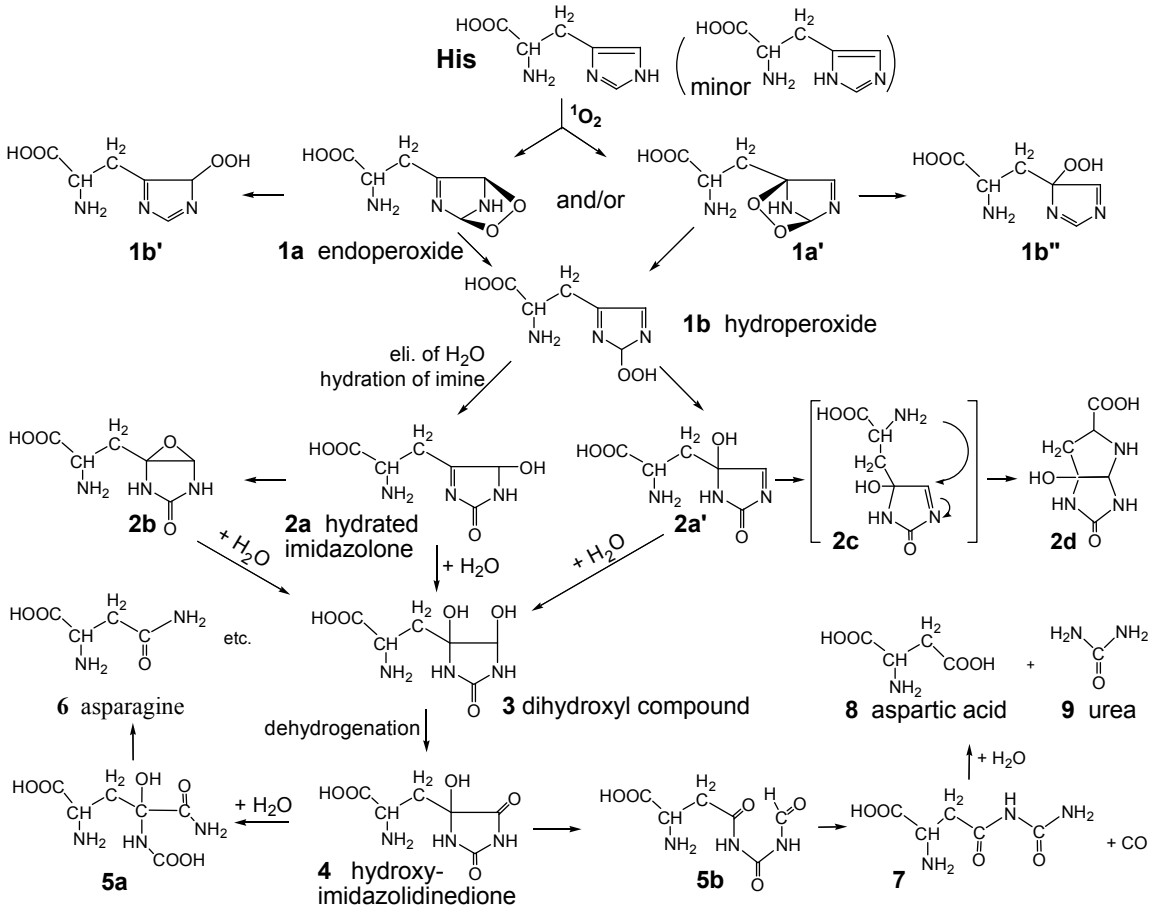

Fig. S1 Literature proposed photooxidation pathways of histidine. [1-4]

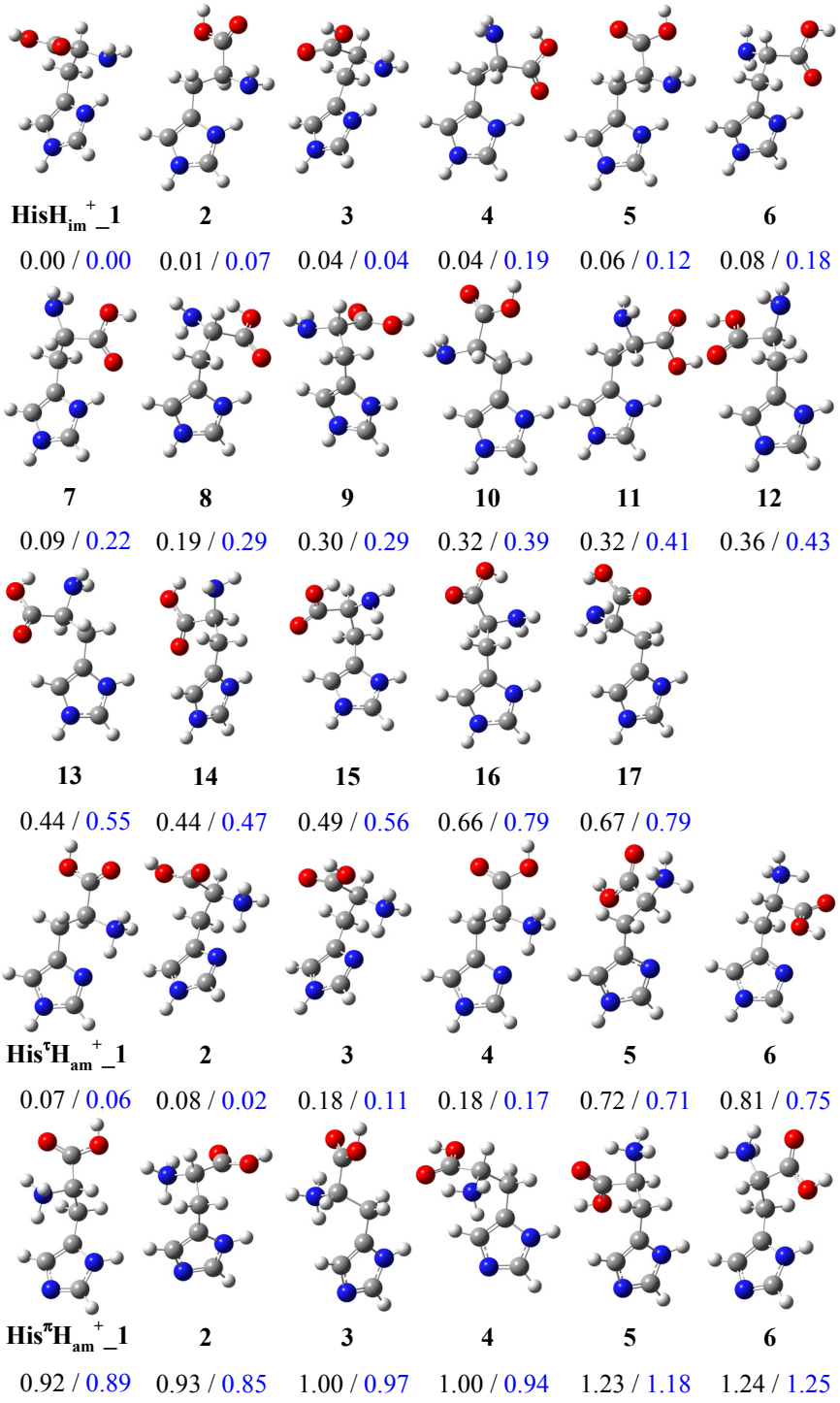

Fig. S2 Stable conformers and tautomers of $HisH^{+}$. Relative energies (eV) shown before slashes are derived from B3LYP/6-311++G(d,p), followed by the values (in blue) from MP2/6-311++G(d,p).

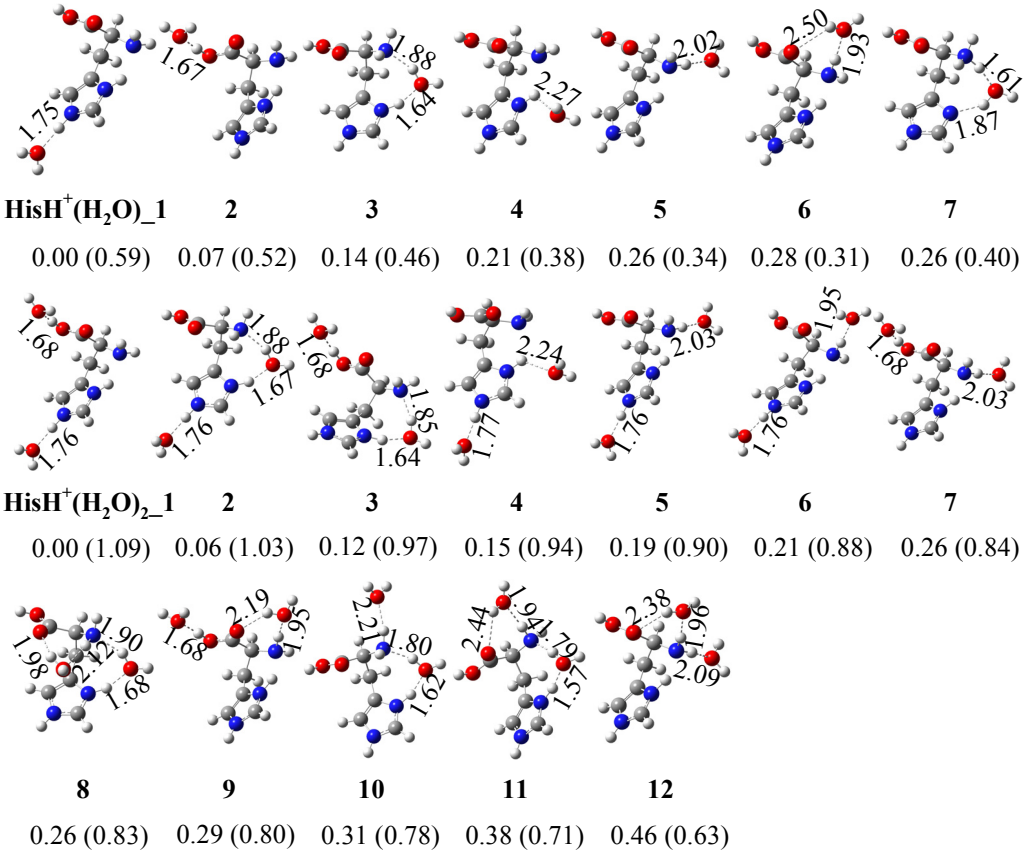

Fig. S3 Stable conformers and tautomers of $HisH^+(H_2O)_{1,2}$. Hydrogen bonds (---) between His and water(s) are shown in Å. B3LYP/6-311++G(d,p) calculated relative energies (eV) are indicated below each structure, along with hydration energies presented in parentheses.

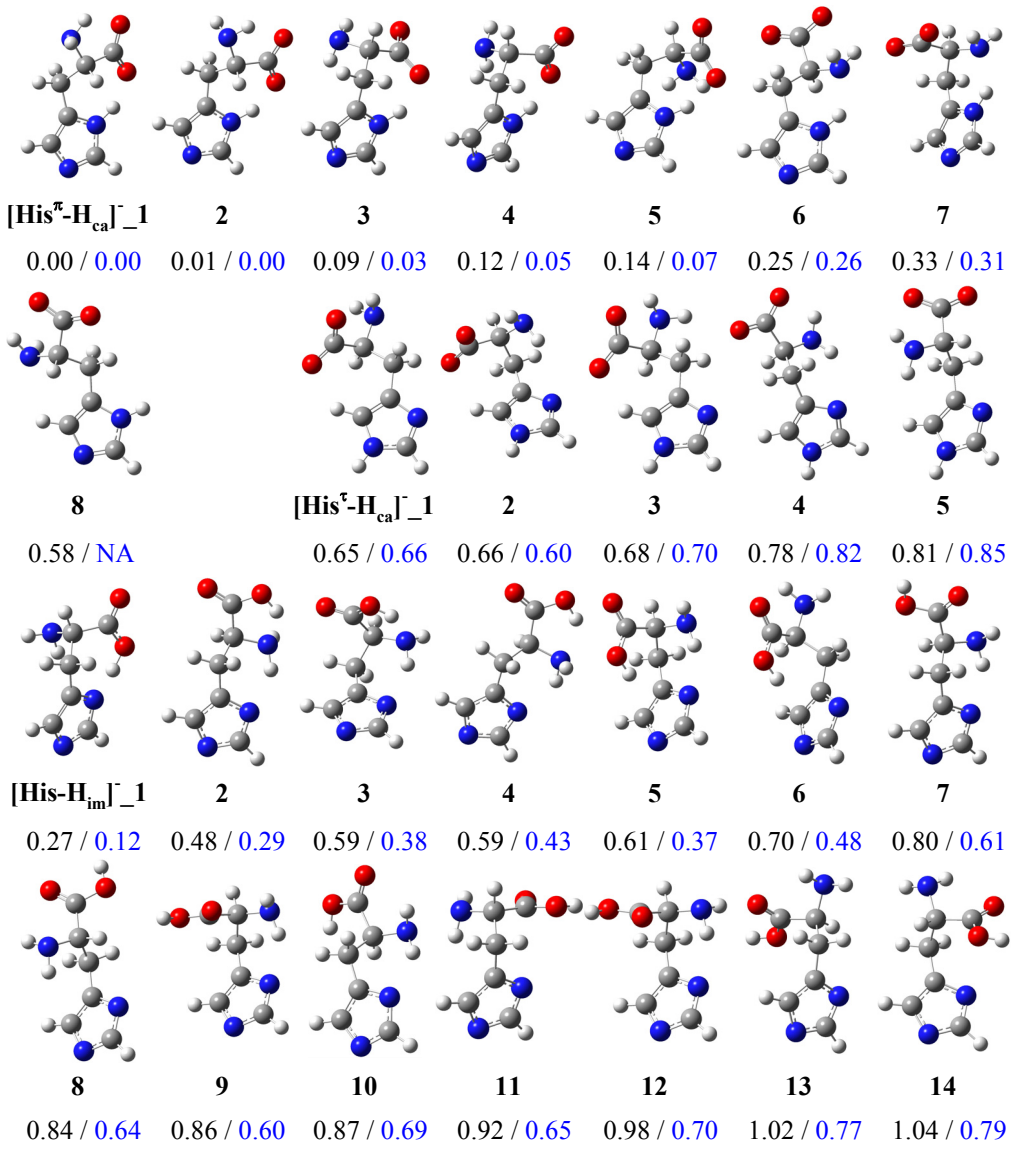

Fig. S4 Stable conformers and tautomers of [His-H]$^-$. Relative energies (eV) shown before slashes are derived from B3LYP/6-311++G(d,p), followed by the values (in blue) from MP2/6-311++G(d,p). Note that MP2 calculation for [His$^{\pi}$-H$_{ca}$]$^-$_8 ran into convergence failure.

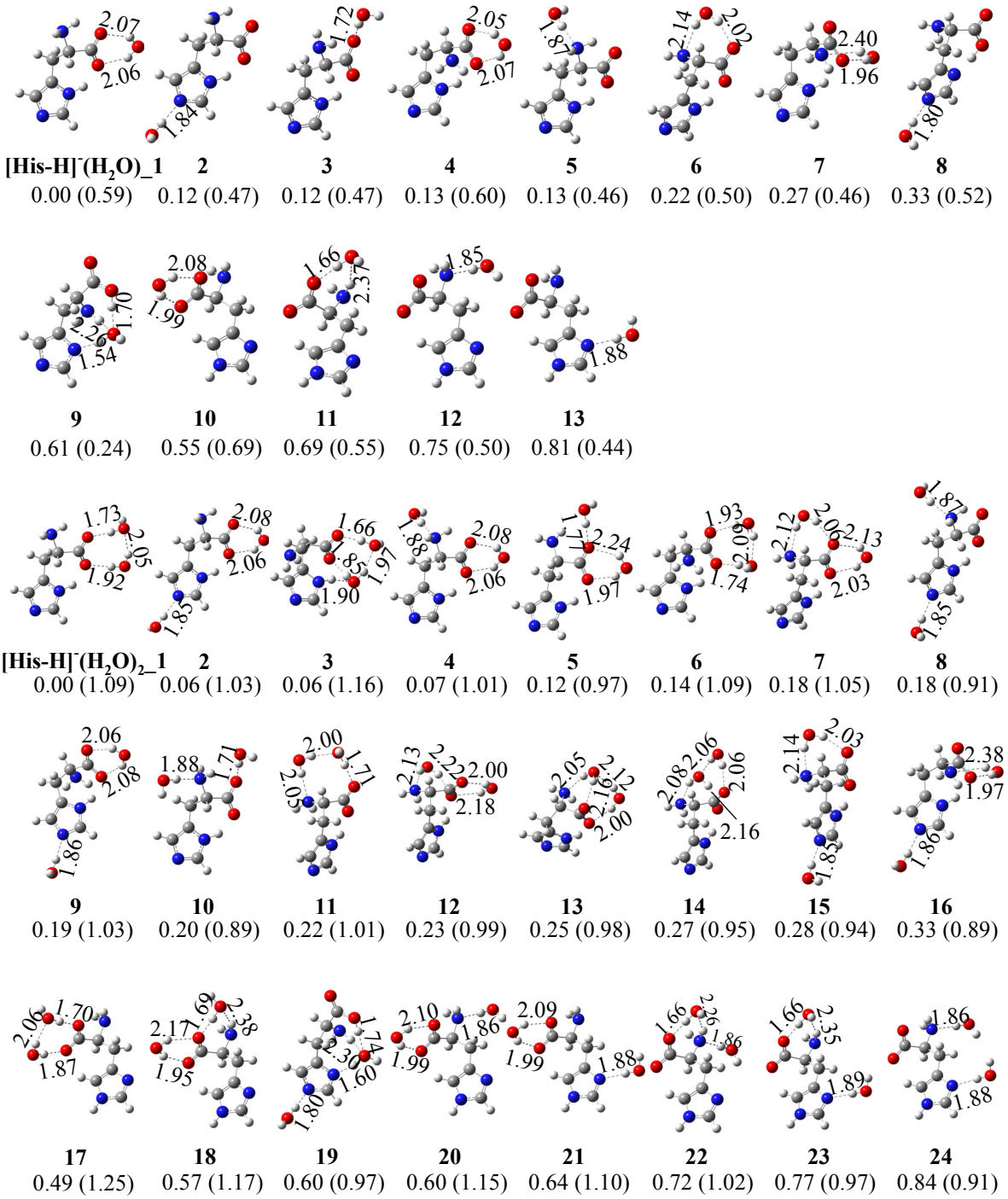

Fig. S5 Stable conformers and tautomers of [His-H]$^-(H_2O)_{1,2}$. Hydrogen bonds (---) between His and water(s) are shown in Å. B3LYP/6-311++G(d,p) calculated relative energies (eV) are indicated below each structure, along with hydration energies presented in parentheses.

The reactions of $^1O_2$ with dihydrated $[HisH]^+(H_2O)_2$ and $[His\text{-}H]^-(H_2O)_2$

The potential energy surfaces (PESs) associated with the reaction coordinates for $^1O_2$ with $HisH^+(H_2O)_2$ and $[His\text{-}H]^-(H_2O)_2$ are presented in Fig. S6. Dihydrates follow the similar routes as the corresponding monohydrates. For $HisH^+(H_2O)_2$, the energetically most favorable pathway is $HisH^+(H_2O)_2 + {}^1O_2 \rightarrow PC(2W) \rightarrow TS1(2W) \rightarrow HisH\text{-}2,5\text{-}OO^+(H_2O)_2\_a \rightarrow HisH\text{-}2,5\text{-}OO^+(H_2O)_2\_b \rightarrow TS2(2W) \rightarrow His\text{-}5\text{-}OOH^+(H_2O)_2$ (*m/z* 224) $\rightarrow His\text{-}5\text{-}OOH^+(H_2O)$ (*m/z* 206) + H_2O. A large fraction of $His\text{-}5\text{-}OOH^+(H_2O)$ may undergo secondary reaction, eliminating the remaining water ligand. Consequently, $His\text{-}5\text{-}OOH^+$(*m/z* 188) accounts for ~30% of the total product ions at $E_{col} \leq 0.1$ eV. Note that the density of states in dihydrates is much higher than that in monohydrates, because dihydrates have more low frequency modes, *e.g.*, $HisH\text{-}2,5\text{-}OO^+(H_2O)_2$_a/b have six vibrational modes below 100 cm^{-1} and $His\text{-}5\text{-}OOH^+(H_2O)_2$ has seven. This improves intramolecular vibrational relaxation (IVR) and thus the stability of dihydrates. Consequently, a small fraction (~5%) of $HisH\text{-}2,5\text{-}OO^+(H_2O)_2$ and/or $His\text{-}5\text{-}OOH^+(H_2O)_2$ survived intact and were detected (at *m/z* 224) at our lowest E_{col}.

Just as that for $[His\text{-}H]^-(H_2O)$, the favorable pathway for $[His\text{-}H]^-(H_2O)_2$ corresponds to reactants $\rightarrow PC^-(2W) \rightarrow TS1^-(2W) \rightarrow [His\text{-}H]\text{-}2,4\text{-}OO^-(H_2O)_2 \rightarrow [His\text{-}H]\text{-}2,4\text{-}OO^-(H_2O)$ (*m/z* 204) + $H_2O \rightarrow [His\text{-}H]\text{-}2,4\text{-}OO^-$ (*m/z* 186) + $2H_2O$, and the product ions have 2,4-endoperoxide structures.

The formation and subsequent ring-opening of endoperoxides are site-specific in all hydrated systems: protonated hydrates produce 2,5-endoperoxides and 5-hydroperoxides preferentially, while deprotonated hydrates produce 2,4-endoperoxides and 2-hydroperoxides.

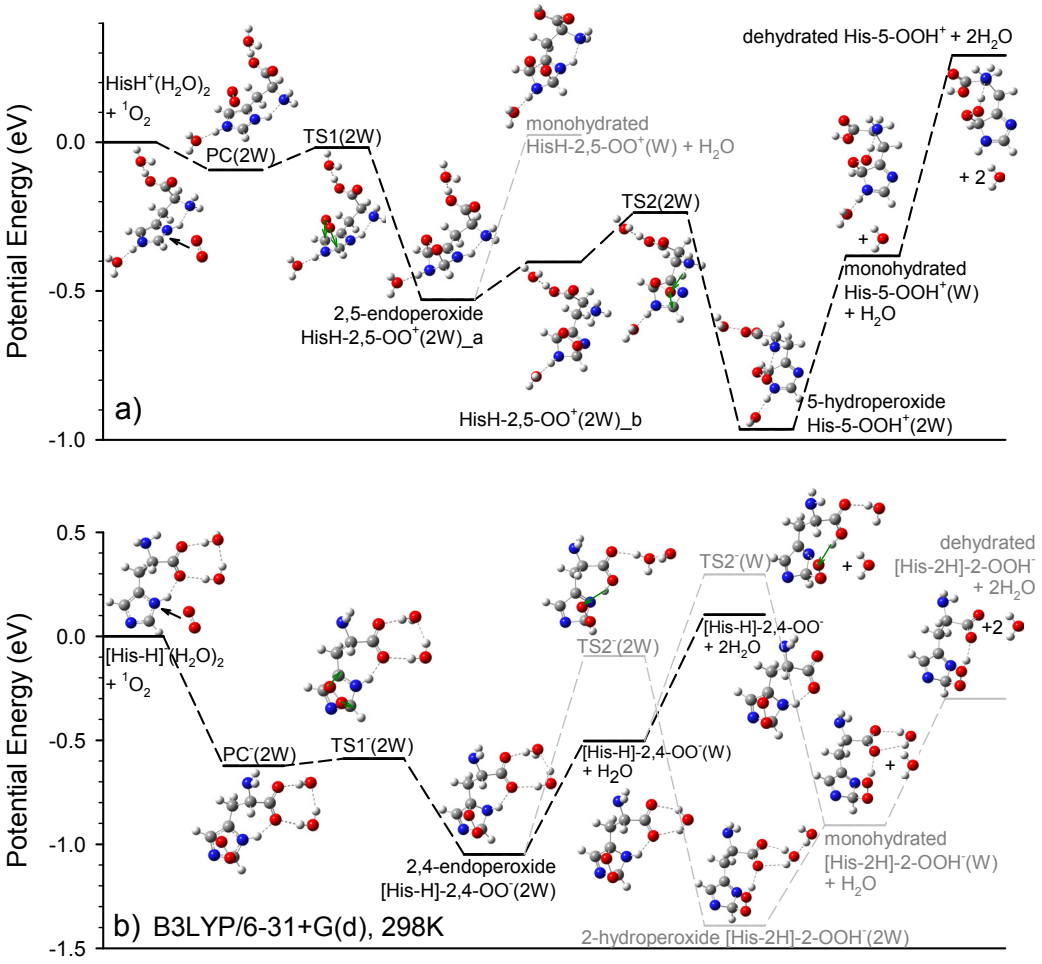

Fig. S6 Schematic reaction coordinates for a) $HisH^+(H_2O)_2 + {}^1O_2$ and b) $[His\text{-}H]^-(H_2O)_2 + {}^1O_2$. Favorable pathways are indicated by heavy dashed lines. Transition vectors in each TS are indicated by green arrows.

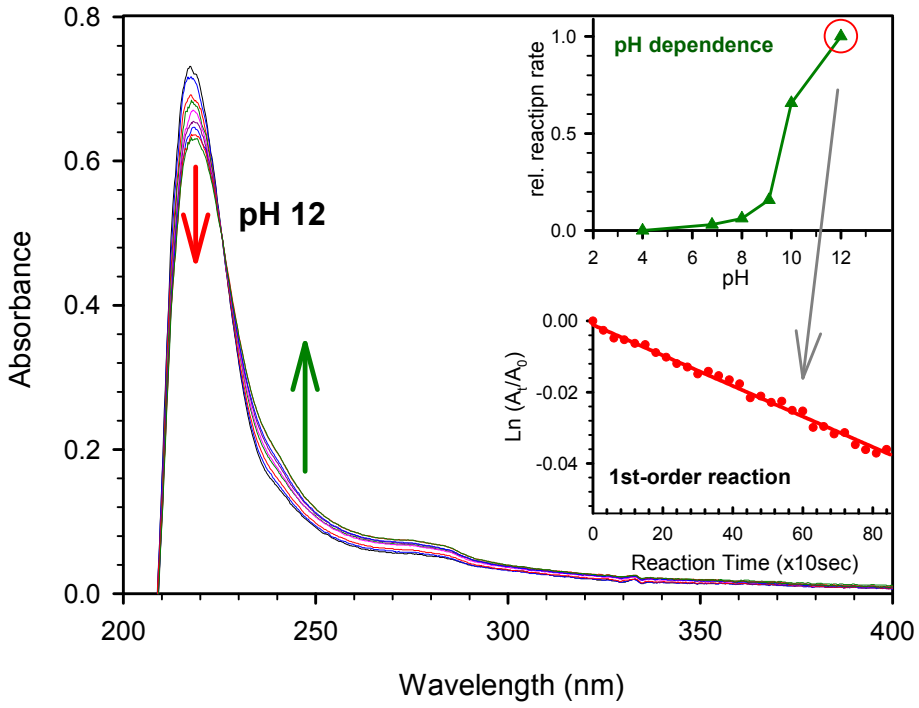

Fig. S7 UV-Vis absorption spectra of His over the course of the reaction with $^1O_2$, recorded at pH 12. Spectral changes reveal that the band belonging to His decreased, where the product absorption at wavelength longer than 230 nm increased as a function of reaction time.

Bottom insert: the plot of $\ln(A_t/A_0)$ as a function of reaction time t at pH 12, where A_t and A_0 are the absorbance of His at 218 nm at any time and time zero, respectively. Note the occasional signal drifts from linearity arose mostly from transient cavitation within the flow cell.

Top insert: dependence of relative reaction rate (based on UV-Vis kinetics analysis) on solution pH. Spectra were measured in 0.1mM aqueous solution of His prepared in potassium acetate buffer (pH 4.0), phosphate buffer (pH 6.8 and 8.0), $Na_2B_4O_7$/HCl buffer (pH 9.13), borax/NaOH buffer (pH 10.0), or 0.01 M NaOH (pH 12). All chemicals were of the highest purity available and were used without further purification. Control experiments were performed using $^3O_2$ under the same conditions, and no obvious spectral changes were observed.

Cartesian coordinates for all the structures in Figures S2, S3, S4 and S5, optimized at B3LYP/6-311++G(d,p)

$HisH^+$

$HisH_{im}^+$_1
O1 2.049739 -1.687553 -0.161426
C2 1.890342 -0.389221 -0.466146
O3 2.067543 0.080469 -1.559321
C4 1.474885 0.426031 0.759142
N5 1.206384 1.811593 0.333114
C6 0.240697 -0.178709 1.477954
H7 2.369752 -2.154480 -0.950236
H8 2.316318 0.359932 1.459928
H9 1.804888 2.046836 -0.456229
H10 1.408869 2.465614 1.083266
C11 -0.993360 -0.182408 0.629044
H12 0.053517 0.411743 2.381206
H13 0.462339 -1.195725 1.801561
C14 -1.999260 -1.089045 0.451522
N15 -2.886292 -0.525230 -0.450325
C16 -2.445651 0.680557 -0.824178
N17 -1.308627 0.902546 -0.174415
H18 -2.159611 -2.063831 0.878858
H19 -3.740705 -0.953752 -0.781509
H20 -2.925034 1.341742 -1.526783
H21 -0.614759 1.673002 -0.246725

$HisH_{im}^+$_2
O1 -2.917022 -1.340886 -0.525469
C2 -2.592479 -0.125100 -0.056103
O3 -3.333990 0.599242 0.550952
C4 -1.130521 0.222644 -0.369299
N5 -0.842170 1.646567 -0.133450
C6 -0.200862 -0.672582 0.492017
H7 -3.842224 -1.529940 -0.297900
H8 -0.951646 -0.001615 -1.424291
H9 -1.331853 1.949390 0.708865
H10 -1.235548 2.207719 -0.884977
C11 1.252078 -0.435063 0.220461
H12 -0.433322 -1.723043 0.313786
H13 -0.403698 -0.474573 1.551418
C14 2.330009 -1.270123 0.138502
N15 3.434734 -0.468867 -0.096915
C16 3.057794 0.812198 -0.164461
N17 1.744022 0.846322 0.031257
H18 2.407924 -2.339927 0.228477
H19 4.386418 -0.795323 -0.203149
H20 3.703484 1.654803 -0.348225
H21 1.056353 1.625666 -0.020809

$HisH_{im}^+$_3
O1 2.792693 -0.276515 -1.063821
C2 1.831797 -0.677887 -0.211193
O3 1.359775 -1.783021 -0.193879
C4 1.449886 0.444164 0.758120
N5 1.319800 1.735662 0.043250
C6 0.150974 0.102454 1.513745
H7 3.048418 -1.025118 -1.626733
H8 2.263002 0.470869 1.496737
H9 2.085698 1.845120 -0.616739
H10 1.395160 2.505715 0.703631
C11 -1.051311 -0.004370 0.627994
H12 -0.021508 0.878878 2.267223
H13 0.278832 -0.838712 2.048605
C14 -2.123523 -0.848964 0.625062
N15 -2.932296 -0.461283 -0.429239
C16 -2.383688 0.579455 -1.062582
N17 -1.250689 0.870271 -0.428990
H18 -2.369122 -1.683178 1.259013
H19 -3.805955 -0.898617 -0.691458
H20 -2.786670 1.083608 -1.924934
H21 -0.510117 1.556076 -0.655756

$HisH_{im}^+$_4
O1 -3.117562 -0.995311 -0.073139
C2 -1.821138 -0.804927 -0.020116
O3 -1.044109 -1.712917 0.216709
C4 -1.366338 0.649395 -0.318744
N5 -2.533866 1.522812 -0.218884
C6 -0.161655 1.097242 0.559326
H7 -3.521673 -0.111357 -0.245156
H8 -1.054899 0.638065 -1.369011
H9 -2.537676 2.269597 -0.903047
H10 -2.659516 1.925058 0.705109
C11 1.180725 0.524200 0.213067
H12 -0.383059 0.880387 1.610689
H13 -0.079522 2.182399 0.473460
C14 2.385146 1.134946 0.001643
N15 3.306718 0.129228 -0.230323
C16 2.696013 -1.059372 -0.170459
N17 1.416216 -0.835501 0.099663
H18 2.663413 2.174824 0.006650
H19 4.291729 0.262895 -0.418592
H20 3.160139 -2.020114 -0.321032
H21 0.614444 -1.500605 0.170883

$HisH_{im}^+$_5
O1 -3.452510 0.664990 -0.329551

C2 -2.560768 -0.320264 -0.118886
O3 -2.849375 -1.464060 0.106656
C4 -1.120878 0.203914 -0.240799
N5 -0.900820 1.562332 0.296903
C6 -0.144589 -0.799747 0.402893
H7 -4.347138 0.290231 -0.284166
H8 -0.919560 0.252405 -1.317672
H9 -1.242816 1.625175 1.254281
H10 -1.439903 2.240299 -0.235383
C11 1.289392 -0.460699 0.140434
H12 -0.358348 -1.803178 0.035951
H13 -0.320434 -0.827698 1.484874
C14 2.393373 -1.229967 -0.095367
N15 3.462166 -0.360364 -0.233134
C16 3.040224 0.900330 -0.095014
N17 1.731802 0.853142 0.135309
H18 2.509967 -2.297274 -0.172598
H19 4.420508 -0.629909 -0.413421
H20 3.650538 1.785458 -0.163123
H21 1.029714 1.609880 0.241291

$HisH_{im}^{+}$_6
O1 -3.335422 -0.471715 0.046769
C2 -2.014396 -0.501465 -0.102898
O3 -1.379061 -1.542769 -0.123378
C4 -1.414803 0.908622 -0.173299
N5 -1.193219 1.475476 1.153866
C6 -0.129413 0.973827 -1.031759
H7 -3.671017 -1.378347 0.147690
H8 -2.153520 1.537777 -0.673104
H9 -0.721189 0.841346 1.789473
H10 -2.056572 1.780959 1.588370
C11 1.115692 0.390034 -0.438647
H12 0.068464 2.029309 -1.222475
H13 -0.317334 0.501839 -2.002100
C14 2.335256 0.952861 -0.190147
N15 3.150514 -0.051954 0.300569
C16 2.464427 -1.197178 0.361446
N17 1.237918 -0.946141 -0.085291
H18 2.685588 1.961951 -0.322539
H19 4.118836 0.054440 0.573645
H20 2.837858 -2.144689 0.712920
H21 0.417678 -1.570583 -0.111195

$HisH_{im}^{+}$_7
O1 -3.149855 -0.889362 -0.191492
C2 -1.839959 -0.740337 -0.033658
O3 -1.109689 -1.669155 0.268110
C4 -1.362645 0.700761 -0.305833
N5 -2.366360 1.740028 -0.188293
C6 -0.147840 1.078883 0.589429
H7 -3.384690 -1.820785 -0.042844
H8 -1.028675 0.689592 -1.351306
H9 -2.816258 1.742128 0.721763
H10 -3.092592 1.648009 -0.889205
C11 1.182795 0.500115 0.223530
H12 -0.370899 0.835080 1.634101
H13 -0.063390 2.164104 0.530434
C14 2.375503 1.114121 -0.038087
N15 3.301523 0.112243 -0.270355
C16 2.708292 -1.080299 -0.162426
N17 1.432773 -0.860816 0.138659
H18 2.640056 2.157083 -0.069476
H19 4.279140 0.251654 -0.490226
H20 3.178862 -2.039618 -0.300335
H21 0.662373 -1.538770 0.246339

$HisH_{im}^{+}$_8
O1 2.742676 -0.891171 -0.854944
C2 1.812009 -0.718205 0.064467
O3 1.242072 -1.648679 0.596848
C4 1.526577 0.758110 0.419823
N5 1.816579 1.586587 -0.744531
C6 0.156591 0.942142 1.130570
H7 2.977399 -0.003352 -1.200597
H8 2.283692 1.004530 1.173110
H9 2.102802 2.528373 -0.505283
H10 1.056626 1.633053 -1.415702
C11 -1.059606 0.439039 0.416474
H12 0.019949 2.006367 1.331014
H13 0.210172 0.443250 2.102392
C14 -2.148564 1.086455 -0.096241
N15 -3.011834 0.113008 -0.569841
C16 -2.481971 -1.095829 -0.361996
N17 -1.309019 -0.916075 0.234572
H18 -2.389726 2.134612 -0.142745
H19 -3.911669 0.280401 -1.001284
H20 -2.923692 -2.040258 -0.634733
H21 -0.603826 -1.623088 0.478617

$HisH_{im}^{+}$_9
O1 1.634170 -1.801533 0.092932
C2 1.850791 -0.555013 -0.385681
O3 2.245746 -0.327809 -1.496604
C4 1.559582 0.516125 0.663704
N5 1.495628 1.819817 0.016642
C6 0.254930 0.230769 1.452628
H7 1.928058 -2.435700 -0.580795
H8 2.381779 0.432799 1.389678
H9 2.048598 1.815162 -0.836181

H10 1.853366 2.551150 0.621102
C11 -0.958943 0.182565 0.578741
H12 0.133393 1.025106 2.194037
H13 0.352992 -0.707503 2.001728
C14 -1.449158 1.060442 -0.348123
N15 -2.600155 0.497249 -0.869812
C16 -2.830401 -0.684872 -0.299591
N17 -1.845498 -0.888747 0.578350
H18 -1.054735 2.007365 -0.670730
H19 -3.186197 0.914104 -1.582004
H20 -3.652583 -1.349154 -0.507159
H21 -1.754625 -1.716926 1.153376

$HisH_{im}^{+}$_10
O1 -2.789177 -1.440810 -0.517917
C2 -2.608878 -0.181250 -0.071129
O3 -3.448884 0.467635 0.489312
C4 -1.179791 0.313022 -0.352134
N5 -1.011851 1.741216 -0.134713
C6 -0.196973 -0.488049 0.540970
H7 -3.700219 -1.712972 -0.320347
H8 -0.956257 0.083587 -1.397800
H9 -1.528750 2.027248 0.694749
H10 -1.413479 2.266864 -0.905104
C11 1.239274 -0.191221 0.242826
H12 -0.380986 -1.557688 0.414419
H13 -0.402337 -0.251009 1.590874
C14 1.909892 0.979708 0.022131
N15 3.237723 0.652610 -0.189902
C16 3.404192 -0.666189 -0.104745
N17 2.204051 -1.190688 0.156293
H18 1.532686 1.986490 -0.004149
H19 3.980653 1.312865 -0.381307
H20 4.327890 -1.207153 -0.225776
H21 2.029525 -2.180928 0.274027

$HisH_{im}^{+}$_11
O1 -1.199484 -1.742591 -0.038526
C2 -2.049892 -0.655154 -0.005073
O3 -3.199690 -0.767942 0.293481
C4 -1.343896 0.658343 -0.383128
N5 -2.246086 1.785445 -0.468528
C6 -0.197416 0.991362 0.628758
H7 -1.721334 -2.530039 0.190222
H8 -0.899721 0.508491 -1.372737
H9 -2.849318 1.843981 0.347211
H10 -2.853464 1.713509 -1.277766
C11 1.158822 0.468618 0.280431
H12 -0.469610 0.663264 1.638034
H13 -0.133418 2.079383 0.658018
C14 2.359019 1.114368 0.182345
N15 3.306278 0.161721 -0.149601
C16 2.722815 -1.032803 -0.262038
N17 1.427744 -0.864015 -0.002327
H18 2.612928 2.151130 0.321822
H19 4.293144 0.335661 -0.290962
H20 3.210171 -1.958577 -0.519403
H21 0.691759 -1.572997 -0.038652

$HisH_{im}^{+}$_12
O1 -2.767484 -1.052934 -0.947312
C2 -1.794589 -0.740662 -0.079005
O3 -1.329332 -1.522166 0.717909
C4 -1.384570 0.732722 -0.211890
N5 -2.457121 1.663408 0.120594
C6 -0.169088 1.048936 0.688192
H7 -3.038100 -1.973672 -0.801183
H8 -1.123228 0.902690 -1.261479
H9 -2.852883 1.480692 1.038149
H10 -3.208883 1.625827 -0.558894
C11 1.110953 0.374661 0.307941
H12 -0.410958 0.777923 1.718462
H13 -0.032531 2.132248 0.664719
C14 1.569365 -0.900449 0.490335
N15 2.839381 -0.959053 -0.053500
C16 3.175175 0.226768 -0.560340
N17 2.139556 1.042848 -0.351481
H18 1.086840 -1.747064 0.946652
H19 3.434563 -1.777735 -0.066544
H20 4.104638 0.479333 -1.042906
H21 2.118889 2.018280 -0.622437

$HisH_{im}^{+}$_13
O1 -3.202130 -0.944282 -0.288521
C2 -1.913330 -0.786818 -0.024418
O3 -1.204098 -1.686386 0.354996
C4 -1.376345 0.643278 -0.276398
N5 -2.481651 1.589144 -0.175976
C6 -0.156012 0.956276 0.637835
H7 -3.565883 -0.058946 -0.499724
H8 -1.046659 0.647319 -1.321437
H9 -2.357554 2.423213 -0.736688
H10 -2.700094 1.860164 0.777971
C11 1.147193 0.314799 0.256128
H12 -0.398548 0.676566 1.667369
H13 -0.013540 2.040563 0.630965
C14 1.545972 -0.986840 0.119268
N15 2.885617 -0.968058 -0.219924
C16 3.324178 0.287301 -0.296570
N17 2.284153 1.075306 -0.013549

H18 0.974915 -1.891271 0.235213
H19 3.455830 -1.787536 -0.388353
H20 4.323525 0.606684 -0.541324
H21 2.331072 2.085871 0.015274

$HisH_{im}^{+}$_14
O1 2.687246 1.437173 0.267007
C2 1.510525 0.937240 -0.074847
O3 0.506548 1.599338 -0.182272
C4 1.512008 -0.584699 -0.373687
N5 2.806596 -1.169970 -0.037835
C6 0.321042 -1.307908 0.321437
H7 3.325635 0.689912 0.253163
H8 1.388632 -0.651917 -1.459766
H9 3.167994 -1.800710 -0.742227
H10 2.825231 -1.638348 0.861805
C11 -1.019260 -0.655436 0.203816
H12 0.539802 -1.392606 1.389552
H13 0.271465 -2.330552 -0.066339
C14 -1.860013 -0.194089 1.173637
N15 -2.956373 0.356745 0.536097
C16 -2.815976 0.240091 -0.782182
N17 -1.659942 -0.388665 -0.999253
H18 -1.757274 -0.185696 2.244729
H19 -3.745813 0.795327 0.992723
H20 -3.507736 0.584067 -1.532951
H21 -1.280215 -0.559525 -1.920672

$HisH_{im}^{+}$_15
O1 2.768514 -0.752928 -0.958685
C2 1.916447 -0.658137 0.056719
O3 1.506711 -1.615991 0.663383
C4 1.500880 0.787435 0.415252
N5 1.615794 1.637956 -0.761818
C6 0.160337 0.791820 1.199966
H7 2.895579 0.145698 -1.323476
H8 2.262602 1.129611 1.124542
H9 1.792737 2.611945 -0.549380
H10 0.840753 1.565821 -1.411909
C11 -1.020641 0.214884 0.480029
H12 -0.063146 1.819497 1.498813
H13 0.309390 0.217202 2.116181
C14 -1.339776 -1.073138 0.143972
N15 -2.575128 -1.037904 -0.474518
C16 -3.026318 0.214396 -0.529042
N17 -2.095176 0.985017 0.040153
H18 -0.784822 -1.982616 0.300217
H19 -3.073140 -1.844025 -0.831848
H20 -3.961865 0.543103 -0.950289
H21 -2.183889 1.986070 0.161473

$HisH_{im}^{+}$_16
O1 -3.603212 0.361482 -0.310910
C2 -2.560533 -0.421848 -0.046098
O3 -2.657810 -1.567505 0.299210
C4 -1.174766 0.252258 -0.275461
N5 -1.304914 1.702690 -0.276516
C6 -0.157631 -0.373147 0.716584
H7 -3.259080 1.245966 -0.542921
H8 -0.898257 -0.046583 -1.292208
H9 -0.696409 2.197017 -0.914448
H10 -1.303204 2.136492 0.639511
C11 1.268671 -0.273322 0.294810
H12 -0.413636 -1.429230 0.821107
H13 -0.289914 0.075401 1.706865
C14 2.058309 -1.156449 -0.388016
N15 3.304356 -0.572738 -0.527429
C16 3.309553 0.628844 0.046636
N17 2.085145 0.827438 0.543521
H18 1.838925 -2.139381 -0.769224
H19 4.104336 -0.993938 -0.983678
H20 4.144147 1.307983 0.104679
H21 1.807537 1.654711 1.056164

$HisH_{im}^{+}$_17
O1 -3.640242 0.379078 0.043172
C2 -2.579995 -0.373463 -0.234657
O3 -2.645674 -1.519256 -0.588622
C4 -1.217821 0.371273 -0.112305
N5 -1.364116 1.559911 0.719891
C6 -0.144651 -0.655393 0.304743
H7 -3.311389 1.251041 0.340993
H8 -1.016461 0.710693 -1.134700
H9 -0.767367 2.334346 0.460482
H10 -1.267031 1.379269 1.713542
C11 1.267143 -0.237735 0.052626
H12 -0.349746 -1.584244 -0.238751
H13 -0.268439 -0.890131 1.368099
C14 1.839091 0.628550 -0.836682
N15 3.211206 0.554158 -0.660071
C16 3.497142 -0.319605 0.301592
N17 2.334514 -0.804009 0.744531
H18 1.401343 1.271989 -1.579555
H19 3.901527 1.081573 -1.180145
H20 4.479513 -0.582784 0.658132
H21 2.248703 -1.502507 1.473150

$His^{\tau}H_{am}^{+}$_1
O1 -2.992699 -1.319904 -0.445021
C2 -2.578358 -0.121549 -0.043479
O3 -3.232272 0.694377 0.553702

C4 -1.111929 0.110476 -0.406556
N5 -0.825578 1.574603 -0.182934
C6 -0.160184 -0.747206 0.457565
H7 -3.918189 -1.451997 -0.178106
H8 -0.948267 -0.100323 -1.464572
H9 -1.325319 1.892472 0.655454
H10 0.245564 1.667320 -0.072754
H11 -1.158580 2.147891 -0.959804
C12 1.285790 -0.436979 0.195765
H13 -0.398544 -0.581097 1.515629
H14 -0.373192 -1.796064 0.247540
C15 2.371977 -1.262856 0.091282
N16 3.451407 -0.425429 -0.094458
C17 3.005140 0.851955 -0.104914
N18 1.697783 0.880166 0.071139
H19 2.474855 -2.333898 0.136856
H20 4.413110 -0.715164 -0.202906
H21 3.648427 1.706654 -0.240987

$His^{\tau}H_{am}^{+}$_2
O1 2.086117 -1.673348 -0.217072
C2 1.952646 -0.369047 -0.435382
O3 2.246503 0.211872 -1.448922
C4 1.413876 0.358862 0.802085
N5 1.119269 1.769068 0.347826
C6 0.168722 -0.278255 1.451867
H7 2.474741 -2.094064 -1.002378
H8 2.229536 0.394662 1.529020
H9 1.719025 1.987692 -0.458333
H10 0.083650 1.775144 0.026780
H11 1.261631 2.455654 1.088350
C12 -1.046095 -0.219866 0.571841
H13 0.414370 -1.308906 1.708747
H14 -0.023834 0.242776 2.396825
C15 -2.024171 -1.144659 0.325180
N16 -2.914672 -0.518174 -0.520778
C17 -2.464097 0.734066 -0.766174
N18 -1.336223 0.948411 -0.116389
H19 -2.167685 -2.155735 0.667003
H20 -3.762705 -0.922701 -0.891775
H21 -2.973597 1.435544 -1.407404

$His^{\tau}H_{am}^{+}$_3
O1 2.447407 0.192073 -1.291147
C2 1.890835 -0.582237 -0.335011
O3 1.821858 -1.773877 -0.363666
C4 1.404311 0.257477 0.853402
N5 1.182458 1.696637 0.430888
C6 0.121195 -0.309217 1.484726
H7 2.794816 -0.370395 -2.003173
H8 2.217549 0.246984 1.584395
H9 1.879966 1.987289 -0.258460
H10 1.218121 2.329779 1.231182
C11 -1.068686 -0.194071 0.575172
H12 -0.062422 0.217760 2.428376
H13 0.312514 -1.352452 1.737453
C14 -2.110977 -1.050611 0.350024
N15 -2.927045 -0.405444 -0.554833
C16 -2.372728 0.790785 -0.856355
N17 -1.246779 0.951928 -0.186186
H18 -2.338253 -2.030046 0.735465
H19 -3.792998 -0.765157 -0.930647
H20 -2.808880 1.492990 -1.548709
H21 0.181327 1.723081 0.001786

$His^{\tau}H_{am}^{+}$_4
O1 -3.328395 0.710676 0.222553
C2 -2.553906 -0.332847 -0.142053
O3 -2.928562 -1.456068 -0.299709
C4 -1.097878 0.087481 -0.345252
N5 -0.860046 1.539562 0.007421
C6 -0.125922 -0.800851 0.454073
H7 -4.245881 0.407405 0.328797
H8 -0.877979 -0.004201 -1.412013
H9 -1.231542 1.760582 0.933943
H10 -1.310029 2.172560 -0.655430
C11 1.308380 -0.440480 0.189419
H12 -0.326779 -1.836659 0.179058
H13 -0.356442 -0.711757 1.523628
C14 2.420662 -1.228848 0.073380
N15 3.469257 -0.356286 -0.127226
C16 2.981655 0.905241 -0.135076
N17 1.675761 0.889840 0.056653
H18 2.558835 -2.296015 0.116195
H19 4.438222 -0.614623 -0.249765
H20 3.594255 1.780458 -0.281454
H21 0.220237 1.655399 0.009397

$His^{\tau}H_{am}^{+}$_5
O1 1.138266 1.813624 -0.103992
C2 1.953139 0.775436 -0.155740
O3 3.160338 0.820789 -0.226638
C4 1.207091 -0.559826 -0.140331
N5 2.309519 -1.602050 -0.022457
C6 0.124055 -0.737923 0.944042
H7 1.655586 2.636100 -0.148916
H8 0.729195 -0.708276 -1.113956
H9 3.191473 -1.136189 -0.308342
H10 2.429632 -1.921350 0.942660
H11 2.128349 -2.419849 -0.608277

C12 -1.211988 -0.311228 0.412024
H13 0.080575 -1.805225 1.199742
H14 0.383241 -0.195914 1.856692
C15 -2.234567 0.364375 1.024720
N16 -3.236074 0.421664 0.081288
C17 -2.786225 -0.201237 -1.042163
N18 -1.564005 -0.656184 -0.873073
H19 -2.343388 0.789669 2.008306
H20 -4.140304 0.854405 0.201167
H21 -3.378296 -0.290258 -1.939645

$His^{\tau}H_{am}^{+}$_6
O1 -0.904924 1.609181 0.997700
C2 -1.600710 0.851402 0.175069
O3 -2.363984 1.220699 -0.685978
C4 -1.390064 -0.646965 0.435085
N5 -2.699491 -1.272547 -0.033588
C6 -0.238122 -1.268671 -0.392507
H7 -0.987582 2.541905 0.735043
H8 -1.271634 -0.847471 1.499355
H9 -3.040416 -0.664540 -0.802708
H10 -2.573005 -2.229830 -0.370838
H11 -3.416135 -1.276929 0.697000
C12 1.090124 -0.609861 -0.198234
H13 -0.171139 -2.328554 -0.127342
H14 -0.505963 -1.199184 -1.453698
C15 2.200425 -1.068267 0.467324
N16 3.150680 -0.092005 0.285502
C17 2.589774 0.896853 -0.468211
N18 1.345411 0.613574 -0.775631
H19 2.401983 -1.972179 1.018076
H20 4.099713 -0.115234 0.629036
H21 3.130684 1.782879 -0.762837

$His^{\pi}H_{am}^{+}$_1
O1 3.051396 -1.303623 -0.019660
C2 2.562727 -0.073205 0.022559
O3 3.142112 0.944489 -0.264055
C4 1.094716 -0.070879 0.448526
N5 0.756205 1.367797 0.756920
C6 0.160285 -0.592800 -0.687006
H7 3.973659 -1.286943 -0.329296
H8 0.954427 -0.653709 1.358603
H9 1.385041 1.968764 0.198813
H10 -0.239090 1.539677 0.515469
H11 0.902714 1.604269 1.740922
C12 -1.276928 -0.303785 -0.413545
H13 0.444649 -0.113374 -1.628295
H14 0.360366 -1.660076 -0.804578
C15 -2.054206 0.781178 -0.769524
N16 -3.307714 0.685512 -0.219709
C17 -3.310097 -0.435046 0.458865
N18 -2.098837 -1.070843 0.393822
H19 -1.797899 1.588308 -1.443100
H20 -1.893153 -1.983982 0.774113
H21 -4.145350 -0.839902 1.010579

$His^{\pi}H_{am}^{+}$_2
O1 2.251406 -1.397912 0.586577
C2 1.993153 -0.388743 -0.235383
O3 2.237420 -0.350968 -1.414869
C4 1.355238 0.797557 0.499641
N5 0.944842 1.754149 -0.595192
C6 0.139844 0.459928 1.406836
H7 2.724298 -2.099849 0.106695
H8 2.140803 1.275411 1.089556
H9 -0.068574 1.611098 -0.784953
H10 1.106000 2.734371 -0.356869
H11 1.469296 1.503238 -1.450957
C12 -1.083993 0.100856 0.630573
H13 0.450769 -0.332721 2.089920
H14 -0.075079 1.335145 2.025363
C15 -2.095777 0.899320 0.133228
N16 -2.991373 0.157832 -0.594685
C17 -2.549254 -1.074364 -0.546404
N18 -1.385977 -1.168575 0.169384
H19 -2.262225 1.952543 0.318084
H20 -0.905188 -2.025520 0.403403
H21 -3.018425 -1.933839 -1.001401

$His^{\pi}H_{am}^{+}$_3
O1 3.067128 -1.042108 0.785102
C2 2.579731 -0.088756 0.006327
O3 3.138689 0.448366 -0.916646
C4 1.139398 0.259730 0.386225
N5 0.822534 1.549768 -0.337229
C6 0.148508 -0.847037 -0.041069
H7 3.971095 -1.271955 0.507975
H8 1.058531 0.452292 1.456331
H9 1.323404 1.553114 -1.238439
H10 -0.201631 1.611059 -0.467827
H11 1.137769 2.373076 0.182168
C12 -1.277534 -0.391509 0.054444
H13 0.378273 -1.161435 -1.065586
H14 0.349787 -1.709092 0.602121
C15 -1.923418 0.480760 0.908090
N16 -3.258589 0.561894 0.605106
C17 -3.440493 -0.249046 -0.407990
N18 -2.271584 -0.845354 -0.792967
H19 -1.516732 1.026360 1.748936

H20 -2.171723 -1.530949 -1.528201
H21 -4.378990 -0.441539 -0.905652

$His^{\pi}H_{am}^{+}$_4
O1 -2.340229 -0.384914 -1.509567
C2 -2.108874 -0.333644 -0.208920
O3 -2.473724 -1.129909 0.620104
C4 -1.330709 0.934266 0.180668
N5 -1.002582 0.753263 1.646495
C6 -0.063426 1.232234 -0.646348
H7 -2.865425 -1.175044 -1.725003
H8 -2.028418 1.770548 0.097098
H9 -0.043260 0.364751 1.713065
H10 -1.058644 1.619555 2.184478
H11 -1.654100 0.046490 2.029862
C12 1.090097 0.334035 -0.306171
H13 -0.350690 1.153936 -1.699116
H14 0.216687 2.277674 -0.481671
C15 1.172147 -0.976603 0.124393
N16 2.480759 -1.354591 0.291342
C17 3.195496 -0.306969 -0.036070
N18 2.405766 0.750391 -0.394183
H19 0.372989 -1.685530 0.292158
H20 2.733039 1.650393 -0.715716
H21 4.273457 -0.247549 -0.030347

$His^{\pi}H_{am}^{+}$_5
O1 0.793875 1.620787 -0.917012
C2 1.602979 0.882500 -0.185877
O3 2.436475 1.270254 0.598795
C4 1.385842 -0.618545 -0.413312
N5 2.711172 -1.246150 -0.002543
C6 0.258771 -1.208959 0.484272
H7 0.905951 2.563325 -0.701017
H8 1.215775 -0.833879 -1.467595
H9 2.591780 -2.183749 0.390245
H10 3.377225 -1.303771 -0.777832
H11 3.117615 -0.610190 0.710514
C12 -1.076507 -0.571712 0.317251
H13 0.212931 -2.287830 0.285288
H14 0.556768 -1.084919 1.530848
C15 -1.729990 0.345113 1.105991
N16 -2.940869 0.680492 0.561642
C17 -3.039526 -0.019847 -0.542588
N18 -1.933249 -0.796632 -0.749591
H19 -1.395096 0.771157 2.040806
H20 -1.818581 -1.459946 -1.501363
H21 -3.875952 -0.013806 -1.225140

$His^{\pi}H_{am}^{+}$_6
O1 1.200516 1.781608 -0.014269
C2 2.001491 0.731818 -0.133675
O3 3.207203 0.766218 -0.160838
C4 1.235321 -0.592864 -0.255785
N5 2.324644 -1.653440 -0.134762
C6 0.091902 -0.842347 0.766722
H7 1.736419 2.593899 0.017929
H8 0.841410 -0.666743 -1.272075
H9 2.413963 -1.988275 0.829666
H10 2.147283 -2.461378 -0.735871
H11 3.224112 -1.204990 -0.387571
C12 -1.257261 -0.396265 0.309313
H13 0.019288 -1.923959 0.921661
H14 0.366303 -0.404134 1.733082
C15 -2.310629 -1.135948 -0.178043
N16 -3.380476 -0.330691 -0.461092
C17 -2.999213 0.885842 -0.150344
N18 -1.718912 0.908562 0.324765
H19 -2.359107 -2.206041 -0.320365
H20 -1.201268 1.726470 0.607085
H21 -3.596621 1.780106 -0.244188

$HisH^+(H_2O)_{1,2}$

$HisH^+(H_2O)$_1
O1 -2.255263 1.980726 0.233099
C2 -2.318906 0.815727 -0.434308
O3 -2.443519 0.724016 -1.627462
C4 -2.240300 -0.379240 0.515421
N5 -2.189640 -1.614840 -0.284979
C6 -1.025616 -0.292056 1.475020
H7 -2.367666 2.705845 -0.402316
H8 -3.142586 -0.320508 1.137489
H9 -2.702756 -1.478960 -1.153467
H10 -2.621048 -2.386234 0.214772
C11 0.294414 -0.319293 0.768263
H12 -1.083879 -1.140287 2.165560
H13 -1.095136 0.614153 2.076925
C14 1.463293 0.364308 0.953907
N15 2.359728 -0.097494 0.008477
C16 1.768986 -1.027722 -0.741664
N17 0.524262 -1.180518 -0.292341
H18 1.728791 1.125216 1.667311
H19 3.336155 0.220027 -0.107551
H20 2.219000 -1.554972 -1.565985
H21 -0.264131 -1.739145 -0.658357
O22 4.998051 0.722880 -0.335241
H23 5.775002 0.361613 0.106633
H24 5.312425 1.451896 -0.882117

$HisH^+(H_2O)$_2
O1 1.918188 -0.328464 0.964372
C2 1.521372 0.489303 0.001350
O3 1.894616 0.445603 -1.150835
C4 0.534022 1.546863 0.508565
N5 -0.022266 2.270071 -0.651434
C6 -0.594538 0.934789 1.376300
H7 2.595289 -0.962718 0.596593
H8 1.118704 2.204334 1.164001
H9 0.675181 2.287000 -1.393763
H10 -0.245294 3.230604 -0.408922
C11 -1.472168 -0.008531 0.614048
H12 -1.205082 1.753892 1.771265
H13 -0.159730 0.415672 2.230076
C14 -2.047754 -1.207640 0.923686
N15 -2.767331 -1.601257 -0.192381
C16 -2.637457 -0.686610 -1.159582
N17 -1.865034 0.282880 -0.682813
H18 -2.007591 -1.803819 1.818782
H19 -3.311149 -2.450140 -0.272545
H20 -3.076216 -0.736012 -2.142099
H21 -1.446759 1.124168 -1.134382
O22 3.636124 -1.909093 -0.301820
H23 3.752549 -1.494876 -1.165961
H24 4.480233 -2.303373 -0.056600

$HisH^+(H_2O)$_3
O1 2.730032 -1.257166 0.502483
C2 2.123725 -0.385165 -0.321551
O3 2.067576 -0.510442 -1.517508
C4 1.474935 0.767718 0.449296
N5 1.065938 1.843846 -0.465962
C6 0.304250 0.236161 1.332435
H7 3.147632 -1.951922 -0.032295
H8 2.216595 1.154980 1.151431
H9 0.994009 1.460467 -1.408960
H10 1.800810 2.544016 -0.515121
C11 -0.793011 -0.479115 0.605790
H12 -0.115571 1.087451 1.872192
H13 0.721855 -0.445878 2.074746
C14 -1.016029 -1.815714 0.422208
N15 -2.179114 -1.932012 -0.315097
C16 -2.662626 -0.713055 -0.577024
N17 -1.840833 0.174034 -0.029133
H18 -0.461621 -2.675487 0.756708
H19 -2.608784 -2.798986 -0.609162
H20 -3.560866 -0.494814 -1.130373
H21 -1.938651 1.218785 -0.059464
O22 -1.511067 2.794984 0.064168
H23 -1.848995 3.672176 -0.139473
H24 -0.548142 2.744149 -0.148945

$HisH^+(H_2O)$_4
O1 2.714753 -0.896167 -0.842924
C2 2.082767 0.264948 -0.596352
O3 1.890690 1.118825 -1.422428
C4 1.660262 0.372511 0.867783
N5 0.879485 1.601800 1.049078
C6 0.845041 -0.859371 1.335643
H7 3.012723 -0.894008 -1.766688
H8 2.594783 0.371339 1.444324
H9 1.194475 2.310863 0.391749
H10 0.997625 1.970128 1.987341
C11 -0.427833 -1.060118 0.573925
H12 0.613522 -0.720511 2.396908
H13 1.452672 -1.761141 1.255928
C14 -1.013456 -2.186598 0.069926
N15 -2.197826 -1.788345 -0.528026
C16 -2.338916 -0.464403 -0.406712
N17 -1.282966 -0.014622 0.260622
H18 -0.697283 -3.215201 0.086809
H19 -2.858903 -2.397925 -0.989953

H20 -3.143309 0.145365 -0.781418
H21 -1.059197 0.969120 0.458525
O22 -2.532870 2.530897 -0.276972
H23 -3.077095 3.077408 0.301558
H24 -2.248647 3.122479 -0.983498

$HisH^+(H_2O)$_5
O1 0.509607 2.659316 -0.821306
C2 0.814065 1.851821 0.210797
O3 0.766401 2.184467 1.366111
C4 1.253294 0.469739 -0.270026
N5 1.464679 -0.402458 0.897477
C6 0.233185 -0.167765 -1.250220
H7 0.293920 3.538285 -0.470539
H8 2.176993 0.632922 -0.839553
H9 1.826150 0.146988 1.673485
H10 2.142239 -1.131259 0.666470
C11 -1.092647 -0.440963 -0.608873
H12 0.664108 -1.108450 -1.608019
H13 0.095915 0.477338 -2.117859
C14 -2.385335 -0.335795 -1.037405
N15 -3.184357 -0.745967 0.017330
C16 -2.416545 -1.083945 1.060286
N17 -1.153001 -0.912748 0.692477
H18 -2.799239 -0.012116 -1.976680
H19 -4.194795 -0.785382 0.009288
H20 -2.767613 -1.425527 2.019671
H21 -0.238911 -0.963243 1.212356
O22 3.339144 -2.467648 -0.269575
H23 3.298249 -3.421206 -0.136272
H24 4.254414 -2.287767 -0.512520

$HisH^+(H_2O)$_6
O1 -1.122701 2.310400 -0.683555
C2 -1.257908 0.986608 -0.490306
O3 -1.589976 0.212067 -1.350607
C4 -0.932540 0.614563 0.956355
N5 -1.139813 -0.829334 1.156028
C6 0.529025 1.002578 1.314319
H7 -1.367017 2.516540 -1.599937
H8 -1.592058 1.229170 1.580883
H9 -2.010529 -1.140632 0.713323
H10 -1.227826 -1.025659 2.149840
C11 1.540191 0.253763 0.498838
H12 0.685269 0.784280 2.376245
H13 0.673059 2.075246 1.184355
C14 2.747539 0.593855 -0.042129
N15 3.221329 -0.535930 -0.688294
C16 2.337704 -1.533189 -0.558783
N17 1.323608 -1.072397 0.161539
H18 3.299849 1.517527 -0.025860
H19 4.099492 -0.605049 -1.185010
H20 2.436835 -2.523534 -0.970808
H21 0.388044 -1.477149 0.430482
O22 -3.661254 -1.568258 -0.198547
H23 -4.455516 -2.109045 -0.142157
H24 -3.558078 -1.320802 -1.124355

$HisH^+(H_2O)$_7
O1 -2.723506 -1.300818 -0.550699
C2 -2.126199 -0.457653 0.289392
O3 -2.103287 -0.556403 1.489647
C4 -1.434552 0.680315 -0.461987
N5 -1.011592 1.677950 0.585208
C6 -0.243553 0.195048 -1.325216
H7 -3.153652 -2.009757 -0.043958
H8 -2.158524 1.173055 -1.113392
H9 -0.692778 1.163791 1.415099
H10 -0.222144 2.314874 0.263663
H11 -1.803872 2.247500 0.887804
C12 0.872316 -0.466828 -0.572508
H13 -0.658674 -0.494904 -2.061700
H14 0.142205 1.056137 -1.876928
C15 1.193212 -1.797971 -0.495490
N16 2.316636 -1.862181 0.296733
C17 2.639206 -0.599120 0.669390
N18 1.788073 0.270731 0.163107
H19 0.748090 -2.675047 -0.934761
H20 2.823014 -2.700506 0.543263
H21 3.489216 -0.367513 1.291963
O22 1.196766 2.920859 -0.209119
H23 1.761738 2.128321 -0.046780
H24 1.711194 3.726695 -0.099722

$HisH^+(H_2O)_2$_1
O1 -2.168864 0.881297 1.001596
C2 -2.140804 0.031645 -0.014872
O3 -2.439691 0.304084 -1.158251
C4 -1.712482 -1.375246 0.414040
N5 -1.489893 -2.193304 -0.792163
C6 -0.455380 -1.363108 1.318897
H7 -2.499420 1.763357 0.675758
H8 -2.540458 -1.756378 1.025763
H9 -2.104115 -1.862122 -1.533796
H10 -1.710369 -3.168322 -0.614922
C11 0.764277 -0.833671 0.631136
H12 -0.266323 -2.390108 1.649824
H13 -0.652910 -0.769102 2.210983
C14 1.779839 -0.012408 1.033465
N15 2.648559 0.113686 -0.034473

C16 2.187105 -0.596320 -1.064401
N17 1.054543 -1.181354 -0.677885
H18 1.953352 0.485638 1.971551
H19 3.519086 0.668325 -0.045439
H20 2.648119 -0.675393 -2.034426
H21 0.357876 -1.735689 -1.205733
O22 -3.008619 3.077988 -0.240392
H23 -3.228336 2.706511 -1.104642
H24 -3.653521 3.767679 -0.050071
O25 5.011785 1.594933 -0.117291
H26 5.102484 2.525351 -0.352453
H27 5.889855 1.295288 0.144375

$HisH^+(H_2O)_2$_2
O1 -1.895132 -2.596379 -0.578155
C2 -1.868891 -1.604730 0.330331
O3 -1.590189 -1.759834 1.491260
C4 -2.199702 -0.249376 -0.299679
N5 -2.447583 0.765779 0.734464
C6 -1.084211 0.165582 -1.307050
H7 -1.701545 -3.434279 -0.127530
H8 -3.104093 -0.376347 -0.898927
H9 -1.980974 0.477105 1.594636
H10 -3.438252 0.783259 0.960578
C11 0.294040 0.305849 -0.738044
H12 -1.386198 1.111725 -1.760980
H13 -1.051854 -0.581020 -2.102153
C14 1.349419 -0.565116 -0.722280
N15 2.395709 0.066390 -0.082422
C16 2.006217 1.288037 0.283516
N17 0.743012 1.454291 -0.102210
H18 1.441557 -1.562121 -1.117248
H19 3.334389 -0.328889 0.085484
H20 2.612252 2.014564 0.798307
H21 0.153969 2.303570 0.042712
O22 -1.238540 3.223674 0.141579
H23 -1.547062 4.089045 0.425574
H24 -1.886987 2.531245 0.413292
O25 4.948047 -0.955472 0.394156
H26 5.710631 -0.901236 -0.193044
H27 5.231488 -1.469230 1.158992

$HisH^+(H_2O)_2$_3
O1 -2.318868 -0.199320 0.937867
C2 -1.584191 -0.787530 0.002958
O3 -1.808495 -0.738849 -1.187743
C4 -0.374938 -1.525612 0.590199
N5 0.356702 -2.250907 -0.462120
C6 0.521515 -0.542123 1.401551
H7 -3.095563 0.250766 0.503892
H8 -0.760281 -2.238805 1.323387
H9 0.019259 -1.920728 -1.367336
H10 0.114274 -3.236731 -0.425898
C11 0.999748 0.666602 0.657677
H12 1.380824 -1.101069 1.777705
H13 -0.051275 -0.200721 2.264491
C14 0.496111 1.937237 0.612398
N15 1.321763 2.667140 -0.221836
C16 2.302665 1.879628 -0.676551
N17 2.124526 0.671612 -0.155658
H18 -0.360882 2.371409 1.097537
H19 1.213208 3.645586 -0.452258
H20 3.094990 2.177268 -1.342864
H21 2.711790 -0.180072 -0.333762
O22 3.100360 -1.769093 -0.397681
H23 3.764005 -2.350882 -0.779579
H24 2.200785 -2.174558 -0.486430
O25 -4.201845 0.953539 -0.547423
H26 -5.156661 1.049835 -0.461076
H27 -4.030095 0.554353 -1.410061

$HisH^+(H_2O)_2$_4
O1 -2.248992 -2.142961 0.845849
C2 -2.336937 -0.802143 0.774665
O3 -2.447448 -0.082709 1.733438
C4 -2.304375 -0.313922 -0.671575
N5 -2.282368 1.152721 -0.679014
C6 -1.092398 -0.876503 -1.455199
H7 -2.328541 -2.404888 1.776849
H8 -3.206420 -0.729913 -1.140540
H9 -2.774774 1.510798 0.135154
H10 -2.740324 1.516693 -1.508076
C11 0.233338 -0.493080 -0.875932
H12 -1.162712 -0.503546 -2.482558
H13 -1.154523 -1.963991 -1.505547
C14 1.371520 -1.220178 -0.664522
N15 2.311656 -0.362897 -0.123812
C16 1.775190 0.851042 0.002788
N17 0.525172 0.793174 -0.451392
H18 1.586683 -2.257670 -0.853216
H19 3.275710 -0.612684 0.142639
H20 2.245883 1.730818 0.406353
H21 -0.163863 1.551897 -0.424558
O22 4.937787 -1.012961 0.596334
H23 5.711016 -0.996856 0.021042
H24 5.243497 -1.338768 1.450398
O25 0.410690 3.537591 0.437234
H26 -0.003643 3.801135 1.266928
H27 0.496470 4.353012 -0.069536

$HisH^+(H_2O)_2$_5
O1 1.328913 2.626200 -0.809326
C2 1.570751 1.788702 0.216895
O3 1.561317 2.121991 1.373240
C4 1.886028 0.377340 -0.273227
N5 2.031022 -0.516839 0.885728
C6 0.808275 -0.162310 -1.249909
H7 1.190055 3.516616 -0.449419
H8 2.815881 0.466517 -0.850090
H9 2.430388 -0.001760 1.666406
H10 2.654657 -1.290308 0.651123
C11 -0.537500 -0.311878 -0.610264
H12 1.152250 -1.137411 -1.609878
H13 0.729182 0.493400 -2.116967
C14 -1.812696 -0.065603 -1.036861
N15 -2.660472 -0.410956 -0.000555
C16 -1.937879 -0.847521 1.032523
N17 -0.655419 -0.803129 0.678838
H18 -2.182589 0.318592 -1.971654
H19 -3.690020 -0.344415 -0.011675
H20 -2.327763 -1.171509 1.982672
H21 0.224966 -0.962589 1.213422
O22 3.784954 -2.717480 -0.255648
H23 3.672009 -3.665626 -0.126400
H24 4.715072 -2.603757 -0.480873
O25 -5.450055 -0.250533 0.024933
H26 -6.070818 -0.921003 -0.282140
H27 -5.982085 0.505913 0.296865

$HisH^+(H_2O)_2$_6
O1 1.697527 2.124837 1.072527
C2 1.807836 0.831386 0.718082
O3 1.960397 -0.066738 1.506294
C4 1.717704 0.675131 -0.799195
N5 1.868143 -0.741398 -1.164844
C6 0.370420 1.228564 -1.337667
H7 1.793420 2.188741 2.035973
H8 2.513715 1.308875 -1.210402
H9 2.635845 -1.174944 -0.643495
H10 2.106169 -0.812293 -2.150718
C11 -0.818675 0.487948 -0.804084
H12 0.389931 1.148993 -2.430082
H13 0.279698 2.287832 -1.096836
C14 -2.072282 0.879398 -0.424662
N15 -2.747857 -0.258303 -0.024079
C16 -1.940807 -1.314148 -0.143325
N17 -0.775370 -0.883793 -0.619794
H18 -2.533189 1.851828 -0.406297
H19 -3.722228 -0.297964 0.313744
H20 -2.191464 -2.331035 0.107495
H21 0.136897 -1.363993 -0.780952
O22 4.099712 -1.803943 0.483222
H23 4.841808 -2.414644 0.533168
H24 3.799391 -1.654754 1.387065
O25 -5.381433 -0.429342 0.888313
H26 -5.687773 -0.344379 1.798335
H27 -6.171431 -0.535989 0.346281

$HisH^+(H_2O)_2$_7
O1 -2.048689 -0.568404 1.019490
C2 -1.316411 -0.930634 -0.025225
O3 -1.730280 -1.035019 -1.160449
C4 0.132627 -1.242875 0.359309
N5 0.934664 -1.409909 -0.866021
C6 0.750565 -0.158981 1.279610
H7 -2.988260 -0.424971 0.720233
H8 0.086227 -2.167295 0.949300
H9 0.350768 -1.820248 -1.591437
H10 1.724848 -2.031349 -0.686424
C11 0.874099 1.169235 0.599409
H12 1.743979 -0.504484 1.583961
H13 0.149764 -0.054127 2.182439
C14 0.690712 2.460100 1.006439
N15 0.960460 3.260736 -0.091510
C16 1.289522 2.494198 -1.138773
N17 1.249765 1.231618 -0.732496
H18 0.394139 2.871306 1.955674
H19 0.915723 4.270612 -0.108251
H20 1.535305 2.846045 -2.126626
H21 1.333365 0.303173 -1.230715
O22 -4.403910 -0.210008 -0.164015
H23 -4.199605 -0.558277 -1.041626
H24 -5.318631 -0.438831 0.032487
O25 3.235491 -3.129122 0.109838
H26 3.145144 -4.047179 0.388829
H27 4.165422 -3.027332 -0.121175

$HisH^+(H_2O)_2$_8
O1 -3.203131 -0.576759 -0.869995
C2 -2.259249 -0.292239 0.037258
O3 -2.074114 -0.955859 1.031886
C4 -1.444241 0.940635 -0.371150
N5 -0.830889 1.636476 0.760095
C6 -0.391263 0.540412 -1.451649
H7 -3.694049 -1.363937 -0.581868
H8 -2.132649 1.626633 -0.868709
H9 -0.394024 0.975499 1.406868
H10 -1.541793 2.133987 1.288841
C11 0.739296 -0.309226 -0.960442
H12 0.014762 1.464158 -1.868612

H13 -0.903424 0.018306 -2.261979
C14 0.920327 -1.663696 -0.964225
N15 2.141344 -1.906623 -0.366545
C16 2.696099 -0.747062 -0.002717
N17 1.871806 0.226364 -0.364346
H18 0.299927 -2.458936 -1.339502
H19 2.550823 -2.816743 -0.207337
H20 3.644087 -0.628490 0.494020
H21 2.005181 1.248472 -0.195320
O22 1.566903 2.856909 -0.026229
H23 1.935128 3.700761 0.252128
H24 0.659235 2.751541 0.342874
O25 0.414364 -0.730945 2.375485
H26 0.563354 -0.840025 3.320539
H27 -0.480373 -1.064447 2.202006

$HisH^+(H_2O)_2$_9
O1 1.444452 -1.489447 0.824079
C2 1.308042 -0.237212 0.411551
O3 1.806626 0.212776 -0.597871
C4 0.455348 0.582904 1.387276
N5 0.176877 1.918451 0.831998
C6 -0.874569 -0.141231 1.730821
H7 2.036301 -1.994794 0.203602
H8 1.042119 0.628499 2.313823
H9 0.976808 2.303567 0.321095
H10 -0.042041 2.569434 1.580921
C11 -1.772626 -0.286552 0.539536
H12 -1.390346 0.442022 2.501423
H13 -0.664955 -1.122550 2.154953
C14 -2.611373 -1.274208 0.107317
N15 -3.179773 -0.819613 -1.071402
C16 -2.704554 0.398430 -1.360584
N17 -1.861449 0.733937 -0.393131
H18 -2.847431 -2.238977 0.521609
H19 -3.851853 -1.324203 -1.633427
H20 -2.961125 0.988970 -2.224105
H21 -1.200867 1.547055 -0.252925
O22 2.998350 -2.851246 -0.881674
H23 3.452446 -2.330415 -1.553632
H24 3.565693 -3.603244 -0.679219
O25 2.211231 3.032319 -1.003558
H26 2.522096 2.162443 -1.284084
H27 2.926686 3.654759 -1.165610

$HisH^+(H_2O)_2$_10
O1 -0.960100 -2.679676 -0.472421
C2 -1.037713 -1.614682 0.349022
O3 -0.986461 -1.690066 1.549575
C4 -1.165691 -0.304231 -0.429452
N5 -1.450591 0.817603 0.473197
C6 0.090003 -0.081903 -1.328917
H7 -0.914405 -3.482823 0.070970
H8 -2.004977 -0.421432 -1.119698
H9 -1.235634 0.532043 1.428178
H10 -2.455253 1.001313 0.447664
C11 1.406771 -0.045470 -0.616894
H12 -0.053727 0.855736 -1.870008
H13 0.126869 -0.882783 -2.068722
C14 2.360279 -1.013269 -0.460036
N15 3.386832 -0.451495 0.275720
C16 3.082492 0.819094 0.562572
N17 1.894387 1.080640 0.032149
H18 2.396968 -2.029662 -0.811953
H19 4.240692 -0.917247 0.551718
H20 3.697000 1.504862 1.121623
H21 1.367216 1.991185 0.089332
O22 -4.396456 0.940563 -0.087682
H23 -4.870087 1.572631 -0.639467
H24 -5.075105 0.500233 0.435959
O25 0.125476 3.027816 -0.000198
H26 -0.616502 2.395269 0.203460
H27 -0.093965 3.907111 0.321543

$HisH^+(H_2O)_2$_11
O1 0.582960 -2.510792 -0.155749
C2 1.094289 -1.267822 -0.274152
O3 1.553876 -0.831520 -1.296407
C4 1.011745 -0.524561 1.054720
N5 1.640136 0.798925 0.942683
C6 -0.454441 -0.447341 1.584221
H7 0.700658 -2.969179 -1.002973
H8 1.549185 -1.159253 1.771160
H9 2.508640 0.730998 0.400483
H10 1.915236 1.101207 1.874470
C11 -1.541367 -0.175100 0.587167
H12 -0.480305 0.310339 2.372876
H13 -0.695830 -1.399581 2.058113
C14 -2.551436 -1.002580 0.180913
N15 -3.314405 -0.293899 -0.726948
C16 -2.792865 0.928576 -0.879623
N17 -1.728696 1.021231 -0.092615
H18 -2.784836 -2.015247 0.460754
H19 -4.138884 -0.634950 -1.202363
H20 -3.168385 1.699437 -1.531930
H21 -1.088959 1.867278 -0.050699
O22 4.109761 0.460628 -0.663638
H23 4.995163 0.802443 -0.823581
H24 3.781149 0.133760 -1.509114
O25 0.129948 2.857319 -0.095419

H26 0.821172 2.231432 0.257792
H27 0.298840 3.745409 0.233398

$HisH^+(H_2O)_2$_12
O1 -0.797465 -1.870610 -1.960790
C2 -0.997401 -1.340072 -0.740419
O3 -1.220114 -1.998260 0.244419
C4 -0.905818 0.183831 -0.788278
N5 -1.163324 0.751509 0.544674
C6 0.486801 0.648689 -1.299556
H7 -0.894708 -2.834001 -1.897298
H8 -1.644062 0.504820 -1.533345
H9 -1.982514 0.317501 0.978550
H10 -1.349797 1.749873 0.439120
C11 1.591541 0.244914 -0.369868
H12 0.453555 1.740138 -1.378512
H13 0.675171 0.250334 -2.296298
C14 2.878540 -0.175035 -0.553276
N15 3.399863 -0.401877 0.710248
C16 2.466492 -0.139639 1.635318
N17 1.374932 0.259574 0.998070
H18 3.457288 -0.330936 -1.447142
H19 4.338925 -0.717607 0.911390
H20 2.589149 -0.242287 2.700505
H21 0.366653 0.478707 1.290137
O22 -3.481082 -0.765298 1.632918
H23 -4.256457 -0.779298 2.202651
H24 -3.130253 -1.663404 1.615968
O25 -1.265136 3.668972 -0.393659
H26 -1.990512 4.013777 -0.926875
H27 -0.923282 4.433378 0.083582

[His-H]$^-$

[His$^{\pi}$-H$_{ca}$]$^-$_1
O1 -1.066728 -1.743839 0.105011
C2 -1.906475 -0.799952 0.009199
O3 -3.141884 -0.880762 0.139818
C4 -1.326722 0.627894 -0.340614
N5 -2.402050 1.633248 -0.284727
C6 -0.154897 1.066215 0.585352
H7 -0.923033 0.543485 -1.359654
H8 -3.265957 1.102097 -0.161629
H9 -2.468468 2.136904 -1.162179
C10 1.196788 0.511710 0.249287
H11 -0.094598 2.156627 0.537884
H12 -0.424086 0.819731 1.620546
C13 2.443824 1.087047 0.111212
N14 3.389579 0.132669 -0.202238
C15 2.712254 -1.002078 -0.256352
N16 1.392908 -0.824886 0.012625
H17 2.709589 2.128670 0.222314
H18 0.550482 -1.453632 0.004680
H19 3.133279 -1.969302 -0.488719

[His$^{\pi}$-H$_{ca}$]$^-$_2
O1 -3.143435 -0.904202 0.062454
C2 -1.903895 -0.807511 0.003667
O3 -1.059633 -1.741260 0.165298
C4 -1.333876 0.620432 -0.365450
N5 -2.384643 1.658004 -0.355587
C6 -0.154842 1.098842 0.516879
H7 0.536078 -1.448425 0.066734
H8 -0.964106 0.534548 -1.395728
H9 -3.257168 1.148731 -0.505222
H10 -2.470888 2.009582 0.596793
C11 1.194157 0.523208 0.209074
H12 -0.410947 0.907998 1.569161
H13 -0.079731 2.185288 0.402454
C14 2.443024 1.088703 0.052050
N15 3.387648 0.116668 -0.202256
C16 2.706857 -1.017785 -0.201350
N17 1.386377 -0.824242 0.047450
H18 2.710066 2.134477 0.106444
H19 3.127016 -1.996843 -0.379129

[His$^{\pi}$-H$_{ca}$]$^-$_3
O1 2.860493 -0.724167 -0.790383
C2 1.926547 -0.646193 0.030780
O3 1.347897 -1.595691 0.641369
C4 1.459512 0.825906 0.353264
N5 1.453703 1.696232 -0.839658
C6 0.128018 0.955292 1.120763
H7 -0.374981 -1.547463 0.290942
H8 2.237923 1.217719 1.022869
H9 2.232739 1.374169 -1.413049
H10 0.615883 1.485965 -1.380152
C11 -1.084816 0.407125 0.430192
H12 -0.046874 2.016405 1.326671
H13 0.247331 0.447514 2.083111
C14 -2.271521 0.962605 0.000103
N15 -3.091232 0.000315 -0.554029
C16 -2.400477 -1.122152 -0.460955
N17 -1.193154 -0.930504 0.131339
H18 -2.577895 1.996778 0.062160
H19 -2.730041 -2.090024 -0.808890

[His$^{\pi}$-H$_{ca}$]$^-$_4
O1 3.117815 0.513957 -0.831975
C2 2.059348 0.510003 -0.180450
O3 1.434176 1.518274 0.284414
C4 1.430558 -0.901945 0.113477
N5 1.121147 -1.154650 1.534663
C6 0.183030 -1.192078 -0.757070
H7 2.192514 -1.626896 -0.183532
H8 0.477279 -0.436511 1.858036
H9 1.970871 -1.012459 2.074717
C10 -1.084148 -0.475884 -0.381509
H11 0.448941 -0.959744 -1.796510
H12 -0.024520 -2.266310 -0.714096
C13 -2.404301 -0.875175 -0.364641
N14 -3.225431 0.162421 0.023148
C15 -2.402492 1.172999 0.244314
N16 -1.105806 0.842562 0.007228
H17 -2.803681 -1.849753 -0.606296
H18 -0.201545 1.356982 0.169677
H19 -2.697132 2.156982 0.578503

[His$^{\pi}$-H$_{ca}$]$^-$_5
O1 -2.877669 -0.502016 -1.096014
C2 -2.031879 -0.485742 -0.189535
O3 -1.536928 -1.474909 0.441523
C4 -1.450905 0.923400 0.195666
N5 -1.184785 1.010688 1.640173
C6 -0.213370 1.246578 -0.690368
H7 -2.222571 1.648510 -0.078214
H8 -0.317269 1.506990 1.822429
H9 -1.058865 0.057887 1.976241
C10 1.045413 0.491546 -0.367920
H11 -0.507955 1.075223 -1.733338
H12 0.016413 2.316295 -0.607049
C13 2.373460 0.864903 -0.372976

N14 3.185154 -0.195797 -0.029549
C15 2.349912 -1.195576 0.188330
N16 1.054301 -0.836833 -0.010775
H17 2.785623 1.835625 -0.609451
H18 0.170252 -1.350281 0.192544
H19 2.632668 -2.191907 0.494639

[His^{π}-H_{ca}]$^{-}$_6
O1 -2.813657 -1.511368 -0.198902
C2 -2.634786 -0.275777 -0.144061
O3 -3.476713 0.653095 -0.065621
C4 -1.134070 0.205749 -0.242845
N5 -0.945195 1.607508 0.223219
C6 -0.150892 -0.732990 0.470655
H7 -0.891724 0.195558 -1.314194
H8 -1.085212 1.600937 1.234331
H9 -1.776491 2.096816 -0.112573
C10 1.293252 -0.436301 0.187670
H11 -0.339935 -0.672616 1.553533
H12 -0.393469 -1.755215 0.180024
C13 2.426177 -1.211184 0.065605
N14 3.535716 -0.429506 -0.191406
C15 3.079472 0.806309 -0.229014
N16 1.737256 0.854917 -0.000514
H17 2.501586 -2.285587 0.142969
H18 1.068200 1.631125 -0.015557
H19 3.670644 1.689891 -0.419504

[His^{π}-H_{ca}]$^{-}$_7
O1 2.152297 -1.675657 -0.402365
C2 2.049621 -0.435373 -0.473923
O3 2.418118 0.352092 -1.381791
C4 1.419682 0.259790 0.800955
N5 1.188928 1.702270 0.529878
C6 0.158254 -0.463689 1.323344
H7 2.184834 0.137013 1.580148
H8 1.732283 1.867702 -0.325862
H9 1.580491 2.277179 1.268869
C10 -1.082016 -0.300578 0.497042
H11 0.401325 -1.525940 1.388619
H12 -0.051660 -0.110062 2.344529
C13 -2.124565 -1.140895 0.174990
N14 -3.078047 -0.479559 -0.573559
C15 -2.613822 0.746772 -0.708507
N16 -1.422527 0.907504 -0.068365
H17 -2.231657 -2.185112 0.427593
H18 -0.748143 1.676362 -0.051260
H19 -3.092184 1.543717 -1.258481

[His^{π}-H_{ca}]$^{-}$_8
O1 -2.617191 -1.626073 -0.266071
C2 -2.626192 -0.377438 -0.155854
O3 -3.601652 0.401934 -0.035873
C4 -1.210429 0.328384 -0.235602
N5 -1.223029 1.733484 0.219228
C6 -0.143689 -0.492688 0.493995
H7 -0.952085 0.331770 -1.303540
H8 -1.185010 1.728883 1.237995
H9 -2.173782 2.049838 0.017703
C10 1.280662 -0.147300 0.179673
H11 -0.315354 -0.403117 1.578079
H12 -0.342118 -1.538621 0.243784
C13 1.943868 1.012656 -0.148053
N14 3.296032 0.782218 -0.330095
C15 3.462669 -0.502184 -0.116881
N16 2.277379 -1.109799 0.198006
H17 1.502329 1.988854 -0.264928
H18 2.127010 -2.091305 0.369693
H19 4.395751 -1.043089 -0.176870

[His^{τ}-H_{ca}]$^{-}$_1
O1 1.434618 1.874937 -0.416528
C2 1.845551 0.819545 0.132181
O3 2.573418 0.698349 1.146684
C4 1.400650 -0.538950 -0.529226
N5 2.508172 -1.525644 -0.538024
C6 0.209198 -1.185672 0.204671
H7 1.111081 -0.341579 -1.566175
H8 2.962811 -1.408950 0.369940
C9 -1.113438 -0.483574 0.087530
H10 0.088302 -2.203578 -0.179420
H11 0.477221 -1.286240 1.264924
C12 -1.375246 0.826074 -0.231427
N13 -2.751917 0.950477 -0.189171
C14 -3.261638 -0.271143 0.150521
N15 -2.306630 -1.155733 0.322460
H16 -0.689810 1.631197 -0.457567
H17 -3.273282 1.792175 -0.370203
H18 -4.322212 -0.452184 0.249990
H19 3.203755 -1.198511 -1.205103

[His^{τ}-H_{ca}]$^{-}$_2
O1 1.800083 -1.461017 0.894160
C2 1.931160 -0.615038 -0.026134
O3 2.394872 -0.781067 -1.179967
C4 1.484913 0.857075 0.328015
N5 1.394941 1.739612 -0.851710
C6 0.192000 0.898028 1.166914
H7 2.284287 1.244491 0.976400

H8 1.933686 1.255417 -1.572530
H9 0.434834 1.732724 -1.189437
C10 -1.005157 0.280524 0.500653
H11 0.398010 0.368800 2.099753
H12 -0.054912 1.937426 1.407330
C13 -1.181012 -1.036702 0.149025
N14 -2.426389 -1.102344 -0.443685
C15 -2.951100 0.159221 -0.429739
N16 -2.124801 1.013090 0.132784
H17 -0.514439 -1.877570 0.251568
H18 -2.847101 -1.924560 -0.844276
H19 -3.925086 0.388781 -0.836488

[His^{τ}-H_{ca}]$^{-}$_3
O1 3.012825 -1.407974 -0.111717
C2 2.653227 -0.214783 -0.013477
O3 3.282546 0.833245 -0.307008
C4 1.177010 -0.000396 0.503984
N5 0.996734 1.377463 0.973806
C6 0.226079 -0.406884 -0.657831
H7 1.008875 -0.702083 1.326898
H8 1.735843 1.916747 0.518699
H9 0.090741 1.754088 0.711183
C10 -1.230055 -0.235434 -0.362696
H11 0.484350 0.196202 -1.536213
H12 0.432974 -1.452771 -0.897003
C13 -2.052259 0.802969 -0.736000
N14 -3.293031 0.530736 -0.181554
C15 -3.169024 -0.648668 0.496947
N16 -1.954687 -1.133145 0.408450
H17 -1.872339 1.679804 -1.335715
H18 -4.120599 1.098850 -0.255558
H19 -3.995785 -1.099200 1.027041

[His^{τ}-H_{ca}]$^{-}$_4
O1 -2.854340 -1.507705 0.026283
C2 -2.641342 -0.274413 -0.030957
O3 -3.425282 0.678594 0.197521
C4 -1.165823 0.121767 -0.431050
N5 -1.050482 1.555696 -0.726563
C6 -0.210845 -0.364194 0.688108
H7 -0.928107 -0.461981 -1.330138
H8 -1.918817 1.967408 -0.379047
H9 -0.270150 1.974338 -0.230162
C10 1.243203 -0.238844 0.354058
H11 -0.415212 0.206467 1.600425
H12 -0.460144 -1.410349 0.881534
C13 2.041857 -1.145997 -0.301918
N14 3.283445 -0.545827 -0.425048
C15 3.189433 0.684602 0.158652
N16 1.985741 0.899040 0.636568
H17 1.836601 -2.128403 -0.693251
H18 4.098329 -0.942381 -0.863186
H19 4.024653 1.367901 0.207339

[His^{τ}-H_{ca}]$^{-}$_5
O1 3.012825 -1.407974 -0.111717
C2 2.653227 -0.214783 -0.013477
O3 3.282546 0.833245 -0.307008
C4 1.177010 -0.000396 0.503984
N5 0.996734 1.377463 0.973806
C6 0.226079 -0.406884 -0.657831
H7 1.008875 -0.702083 1.326898
H8 1.735843 1.916747 0.518699
H9 0.090741 1.754088 0.711183
C10 -1.230055 -0.235434 -0.362696
H11 0.484350 0.196202 -1.536213
H12 0.432974 -1.452771 -0.897003
C13 -2.052259 0.802969 -0.736000
N14 -3.293031 0.530736 -0.181554
C15 -3.169024 -0.648668 0.496947
N16 -1.954687 -1.133145 0.408450
H17 -1.872339 1.679804 -1.335715
H18 -4.120599 1.098850 -0.255558
H19 -3.995785 -1.099200 1.027041

[His-H_{im}]$^{-}$_1
O1 3.281678 0.438938 -0.439016
C2 2.096555 0.429795 -0.146284
O3 1.390905 1.531105 -0.006719
C4 1.371000 -0.920114 0.085694
N5 1.067271 -1.059812 1.521735
C6 0.149873 -1.141346 -0.859915
H7 2.126882 -1.669755 -0.156728
H8 0.326036 -0.406304 1.764446
C9 -1.101557 -0.427420 -0.437295
H10 0.452141 -0.853482 -1.877937
H11 -0.055684 -2.218293 -0.897300
C12 -2.422228 -0.838442 -0.369638
N13 -3.206135 0.187864 0.101429
C14 -2.334398 1.176780 0.311996
N15 -1.050472 0.870764 0.007912
H16 -2.844038 -1.800260 -0.633717
H17 -2.618602 2.147662 0.698170
H18 0.680182 -1.985821 1.685968
H19 0.322307 1.358691 0.058095

[His-H_{im}]$^{-}$_2
O1 3.073052 -1.366968 0.269632
C2 2.545587 -0.293625 0.090116

O3 3.181329 0.736457 -0.494422
C4 1.091262 0.035736 0.458517
N5 0.909872 1.501289 0.410206
C6 0.126859 -0.655641 -0.544972
H7 0.900981 -0.382581 1.452315
H8 -0.058219 1.697761 0.107908
C9 -1.316883 -0.364632 -0.266903
H10 0.315127 -1.731357 -0.505076
H11 0.401651 -0.315620 -1.553778
C12 -2.356334 -1.218374 0.081561
N13 -3.508271 -0.493676 0.243426
C14 -3.112700 0.765130 -0.007713
N15 -1.809045 0.918733 -0.325708
H16 -2.334478 -2.294109 0.212035
H17 -3.795552 1.606869 0.035671
H18 1.018254 1.901644 1.336921
H19 2.502550 1.465504 -0.446769

[His-H_{im}]$^-$_3
O1 2.435711 -1.567851 -0.024025
C2 2.057314 -0.449099 -0.282371
O3 2.263000 0.132658 -1.470171
C4 1.359692 0.477051 0.737618
N5 1.057333 1.768242 0.084812
C6 0.124286 -0.193367 1.395417
H7 2.118800 0.633149 1.514478
H8 0.033240 1.834755 -0.051575
H9 1.353284 2.547184 0.660868
C10 -1.108567 -0.199361 0.540691
H11 -0.068299 0.351667 2.330899
H12 0.399717 -1.215661 1.667992
C13 -1.881363 -1.258662 0.082476
N14 -2.937829 -0.775250 -0.643934
C15 -2.754534 0.553967 -0.599493
N16 -1.678918 0.975790 0.100027
H17 -1.728817 -2.320554 0.233684
H18 -3.427044 1.249167 -1.090691
H19 1.864356 1.037184 -1.344452

[His-H_{im}]$^-$_4
O1 2.880360 1.494414 -0.136397
C2 2.526594 0.340750 -0.150327
O3 3.413690 -0.677172 -0.171868
C4 1.071080 -0.144758 -0.204852
N5 1.033009 -1.564525 0.212616
C6 0.063485 0.750060 0.530961
H7 0.809739 -0.130350 -1.271143
H8 1.036531 -1.585527 1.232773
C9 -1.357905 0.373300 0.207354
H10 0.246804 1.794188 0.263560
H11 0.274219 0.666398 1.611182
C12 -2.459409 1.191867 -0.009120
N13 -3.562352 0.420097 -0.270488
C14 -3.077765 -0.829697 -0.204712
N15 -1.760982 -0.936907 0.079745
H16 -2.510692 2.274520 0.005060
H17 -3.699278 -1.702649 -0.373795
H18 0.085199 -1.888951 -0.023070
H19 2.840870 -1.485353 -0.147386

[His-H_{im}]$^-$_5
O1 3.115459 -0.901394 -0.293508
C2 1.939981 -0.634527 -0.146326
O3 0.997094 -1.476611 -0.594670
C4 1.493795 0.695534 0.495292
N5 1.360406 1.759225 -0.513015
C6 0.195717 0.613642 1.329095
H7 0.097405 -1.146563 -0.351782
H8 2.322246 0.959780 1.161368
H9 2.080643 1.677388 -1.223224
H10 0.436504 1.695266 -0.949024
C11 -1.039735 0.219735 0.563642
H12 0.065269 1.605409 1.780658
H13 0.348658 -0.094434 2.151782
C14 -1.923157 -0.839021 0.785366
N15 -2.930707 -0.796408 -0.137443
C16 -2.614202 0.280617 -0.878909
N17 -1.496200 0.939717 -0.518663
H18 -1.882765 -1.602976 1.553574
H19 -3.217280 0.596552 -1.723041

[His-H_{im}]$^-$_6
O1 -2.866869 1.219591 -0.327500
C2 -1.741837 0.853659 -0.057267
O3 -0.720040 1.712700 -0.073554
C4 -1.425885 -0.591313 0.385914
N5 -2.595033 -1.469190 0.279919
C6 -0.221463 -1.213660 -0.354998
H7 0.130593 1.229735 0.094828
H8 -1.159188 -0.514381 1.448492
H9 -3.431857 -0.910216 0.426750
H10 -2.662852 -1.807005 -0.676984
C11 1.104963 -0.545396 -0.111804
H12 -0.415363 -1.198454 -1.434591
H13 -0.196505 -2.269628 -0.055542
C14 1.673476 -0.065087 1.074322
N15 2.933160 0.403847 0.815159
C16 3.068418 0.181425 -0.505052
N17 2.012360 -0.378775 -1.125743
H18 1.261083 -0.050619 2.077032

H19 3.969922 0.453304 -1.043598

[His-H_{im}]$^-$_7
O1 -2.889023 -1.328787 -0.535869
C2 -2.501718 -0.110014 -0.055789
O3 -3.252259 0.555598 0.622012
C4 -1.073709 0.224083 -0.405597
N5 -0.914424 1.673655 -0.508388
C6 -0.132522 -0.453174 0.652470
H7 -3.780732 -1.479474 -0.189655
H8 -0.847851 -0.231750 -1.373503
H9 -1.358531 2.103623 0.299486
H10 0.090213 1.863069 -0.426589
C11 1.317537 -0.286562 0.317372
H12 -0.368102 -1.521984 0.711833
H13 -0.373343 -0.005361 1.627473
C14 2.276257 -1.259300 0.051176
N15 3.474420 -0.656617 -0.225951
C16 3.182432 0.652049 -0.123277
N17 1.906863 0.949857 0.202834
H18 2.164953 -2.337986 0.053459
H19 3.925979 1.424609 -0.289252

[His-H_{im}]$^-$_8
O1 2.959069 -1.352747 -0.003247
C2 2.500971 -0.068418 0.017076
O3 3.201165 0.847503 -0.356758
C4 1.067178 0.028489 0.461469
N5 0.843351 1.328633 1.091324
C6 0.139042 -0.264991 -0.775019
H7 3.849226 -1.312178 -0.382326
H8 0.869489 -0.759680 1.191004
H9 1.205138 2.057288 0.480656
H10 -0.165553 1.464090 1.146887
C11 -1.308543 -0.178796 -0.412789
H12 0.386582 -1.263729 -1.154835
H13 0.375710 0.464516 -1.559577
C14 -2.243901 0.805652 -0.731629
N15 -3.446853 0.492856 -0.159281
C16 -3.176552 -0.659245 0.485917
N17 -1.914190 -1.119377 0.379222
H18 -2.115226 1.688959 -1.348097
H19 -3.932571 -1.188239 1.057330

[His-H_{im}]$^-$_9
O1 2.065048 -1.604507 0.257852
C2 1.870659 -0.404130 -0.358432
O3 2.123112 -0.257189 -1.531185
C4 1.416028 0.682546 0.612709
N5 1.195709 1.969682 -0.033588
C6 0.162450 0.249890 1.420815
H7 2.324323 -2.223875 -0.439359
H8 2.253730 0.766075 1.325746
H9 1.746455 2.021541 -0.885346
H10 0.209519 2.011837 -0.313497
C11 -1.058615 0.009675 0.584595
H12 -0.014199 1.055797 2.145173
H13 0.406371 -0.651615 1.988495
C14 -1.780882 -1.162414 0.382282
N15 -2.829255 -0.913536 -0.463391
C16 -2.688665 0.395827 -0.737634
N17 -1.650032 1.016539 -0.140530
H18 -1.602768 -2.147589 0.798868
H19 -3.369523 0.924238 -1.396862

[His-H_{im}]$^-$_10
O1 -3.314052 0.548305 0.535997
C2 -2.521042 -0.133824 -0.057972
O3 -2.888196 -1.396313 -0.448011
C4 -1.083342 0.242220 -0.372141
N5 -0.951047 1.689621 -0.479782
C6 -0.139099 -0.412829 0.694979
H7 -2.148692 -1.806216 -0.914186
H8 -0.817010 -0.198867 -1.342631
H9 -1.456437 2.118850 0.291056
H10 0.043610 1.908157 -0.363233
C11 1.307791 -0.262860 0.341353
H12 -0.371355 -1.481206 0.795712
H13 -0.374525 0.060032 1.658675
C14 2.257159 -1.246145 0.079821
N15 3.450656 -0.654149 -0.237421
C16 3.164668 0.657361 -0.161036
N17 1.896606 0.967562 0.183537
H18 2.145388 -2.324384 0.117778
H19 3.906696 1.422924 -0.361417

[His-H_{im}]$^-$_11
O1 2.225750 -1.158666 0.940848
C2 1.915233 -0.401152 -0.143427
O3 2.182160 -0.761201 -1.266370
C4 1.340722 0.958495 0.244451
N5 1.029546 1.787307 -0.915103
C6 0.105554 0.838325 1.180607
H7 2.496010 -2.021676 0.597057
H8 2.145811 1.435132 0.825380
H9 1.584999 1.479500 -1.708180
H10 0.056778 1.606160 -1.165126
C11 -1.092372 0.223409 0.524638
H12 -0.135368 1.854849 1.510512
H13 0.408156 0.267470 2.064329

C14 -2.299366 0.811835 0.150673
N15 -3.100662 -0.128927 -0.439847
C16 -2.334978 -1.236164 -0.401295
N17 -1.118189 -1.098690 0.163180
H18 -2.626144 1.836912 0.289121
H19 -2.677152 -2.185724 -0.800410

[His-H_{im}]$^-$_12
O1 2.254978 -1.523872 0.301604
C2 1.853973 -0.413819 -0.398665
O3 1.861019 -0.402345 -1.601051
C4 1.444495 0.704380 0.545028
N5 1.274709 1.949099 -0.202121
C6 0.200038 0.277899 1.388941
H7 2.414254 -2.207613 -0.364373
H8 2.289390 0.827144 1.236335
H9 0.386854 1.874903 -0.707539
H10 1.114128 2.688271 0.477577
C11 -1.039865 0.022978 0.588365
H12 0.040703 1.095844 2.108347
H13 0.453124 -0.614119 1.971174
C14 -1.801162 -1.138272 0.491627
N15 -2.860827 -0.922606 -0.348201
C16 -2.688203 0.357446 -0.723850
N17 -1.618544 0.990870 -0.198898
H18 -1.641687 -2.094206 0.978492
H19 -3.367770 0.854303 -1.408580

[His-H_{im}]$^-$_13
O1 1.109692 1.600300 -1.049662
C2 1.682686 0.789663 -0.139029
O3 2.351592 1.218196 0.777549
C4 1.380764 -0.675587 -0.367725
N5 2.642158 -1.417637 -0.188500
C6 0.234055 -1.121380 0.595164
H7 1.239947 2.508544 -0.738202
H8 1.027629 -0.805885 -1.391382
H9 3.044860 -1.156598 0.708640
H10 2.429035 -2.409986 -0.139252
C11 -1.108446 -0.520749 0.326377
H12 0.555507 -0.907520 1.621984
H13 0.181572 -2.215079 0.490561
C14 -1.818573 0.430933 1.054507
N15 -3.002944 0.696741 0.421030
C16 -2.947825 -0.106808 -0.659306
N17 -1.840646 -0.866481 -0.779742
H18 -1.543765 0.918669 1.983684
H19 -3.751000 -0.144890 -1.388574

[His-H_{im}]$^-$_14
O1 1.056368 -1.571924 1.050477
C2 1.663056 -0.780749 0.146374
O3 2.329110 -1.217076 -0.766848
C4 1.414372 0.691735 0.394547
N5 2.677748 1.407409 0.144901
C6 0.229558 1.180374 -0.504562
H7 1.057027 -2.469114 0.686273
H8 1.127094 0.819978 1.440387
H9 3.074645 1.057206 -0.724005
H10 2.475676 2.392845 0.001487
C11 -1.108010 0.553492 -0.268330
H12 0.542739 1.037134 -1.547149
H13 0.160095 2.262948 -0.331120
C14 -2.198076 1.046311 0.445577
N15 -3.218157 0.135016 0.406864
C16 -2.693402 -0.865467 -0.327707
N17 -1.432698 -0.681404 -0.768233
H18 -2.298266 1.994124 0.964381
H19 -3.256070 -1.764444 -0.559404

[His-H]$^-$(H$_2$O)$_{1,2}$

[His-H]$^-$(H$_2$O)_1
O1 -1.157514 -1.013498 -0.003219
C2 -1.614560 0.165462 -0.103350
O3 -2.819256 0.493726 -0.073116
C4 -0.572657 1.318532 -0.320698
N5 -1.240036 2.623413 -0.194072
C6 0.640129 1.257102 0.652158
H7 -0.184236 1.168580 -1.339004
H8 -2.242437 2.437019 -0.207678
H9 -1.017266 3.221960 -0.981236
C10 1.742852 0.312664 0.281851
H11 1.063295 2.263553 0.701443
H12 0.264096 1.034290 1.658391
C13 3.109815 0.463122 0.174063
N14 3.706002 -0.725938 -0.191478
C15 2.705366 -1.580731 -0.307065
N16 1.507172 -1.003807 -0.027164
H17 3.692645 1.357126 0.343168
H18 0.525500 -1.340517 -0.072871
H19 2.798225 -2.618239 -0.592135
O20 -3.781698 -2.218736 0.182001
H21 -2.809601 -2.232294 0.157501
H22 -3.900120 -1.255996 0.114342

[His-H]$^-$(H$_2$O)_2
O1 1.793308 -1.717565 -0.035553
C2 2.589795 -0.737829 0.093064
O3 3.831214 -0.776179 0.049419
C4 1.935518 0.674114 0.366328
N5 2.973089 1.717824 0.354042
C6 0.813691 1.046883 -0.646615
H7 1.468010 0.597704 1.358525
H8 3.863744 1.220523 0.303768
H9 2.960309 2.249038 1.217387
C10 -0.530243 0.432142 -0.395620
H11 0.700723 2.133618 -0.621904
H12 1.164837 0.798564 -1.656125
C13 -1.808654 0.946221 -0.359095
N14 -2.717410 -0.057479 -0.090721
C15 -1.989014 -1.157587 0.037288
N16 -0.671852 -0.909216 -0.142863
H17 -2.125765 1.966725 -0.513828
H18 0.214760 -1.486703 -0.061245
H19 -2.379864 -2.138858 0.259435
O20 -5.498878 0.198215 0.348487
H21 -4.539850 0.096166 0.122895
H22 -5.485410 0.445881 1.276973

[His-H]$^-$(H$_2$O)_3
O1 -0.490436 -1.780853 0.066846
C2 -1.299692 -0.817424 0.153989
O3 -2.483059 -0.886154 0.564568
C4 -0.769675 0.595229 -0.294633
N5 -1.782740 1.660522 -0.298766
C6 0.429113 1.066292 0.575517
H7 -0.411631 0.485701 -1.324310
H8 -2.199551 1.705459 0.628989
H9 -2.556329 1.380799 -0.896520
C10 1.774692 0.513547 0.212421
H11 0.479141 2.154461 0.486264
H12 0.204644 0.845688 1.628638
C13 3.017812 1.097074 0.082285
N14 3.966780 0.154427 -0.254163
C15 3.296871 -0.982187 -0.329545
N16 1.976995 -0.817874 -0.051793
H17 3.277443 2.137983 0.210748
H18 1.155081 -1.462581 -0.071232
H19 3.721214 -1.942291 -0.583708
O20 -4.816378 0.133434 -0.334158
H21 -5.213509 -0.672495 -0.674571
H22 -3.959498 -0.178853 0.050506

[His-H]$^-$(H$_2$O)_4
O1 2.524906 -0.617968 -0.862512
C2 1.630886 -0.472776 -0.009200
O3 1.462001 0.524454 0.766205
C4 0.563870 -1.608746 0.089179
N5 0.155508 -1.824135 1.484055
C6 -0.617456 -1.312164 -0.881891
H7 1.054429 -2.509056 -0.290711
H8 0.299319 -0.949942 1.984106
C9 -1.575070 -0.236924 -0.455262
H10 -0.182871 -1.075201 -1.861034
H11 -1.199733 -2.231234 -1.018750
C12 -2.945324 -0.130591 -0.564781
N13 -3.389531 1.071517 -0.056185
C14 -2.296702 1.680298 0.363736
N15 -1.178454 0.939740 0.138316
H16 -3.630904 -0.851404 -0.986864
H17 -2.261215 2.650418 0.836671
H18 -0.833617 -2.046042 1.545485
H19 -0.205219 1.093025 0.452237
O20 3.827175 1.876736 -0.220225
H21 3.711751 1.045847 -0.714123
H22 3.061511 1.783389 0.371246

[His-H]$^-$(H$_2$O)_5
O1 -0.132599 2.125288 -0.541839

C2 -1.152820 1.586060 -0.027836
O3 -2.309786 2.046534 0.018984
C4 -0.937583 0.186186 0.672035
N5 -2.261829 -0.397596 0.976825
C6 -0.089994 -0.822000 -0.148629
H7 -0.389401 0.403993 1.599871
H8 -2.911742 0.393023 0.940176
H9 -2.279390 -0.785750 1.914750
C10 1.395417 -0.640797 -0.066572
H11 -0.323325 -1.828810 0.208941
H12 -0.421280 -0.785793 -1.193874
C13 2.435845 -1.505072 0.204837
N14 3.645517 -0.844797 0.147205
C15 3.331028 0.404131 -0.151082
N16 1.991070 0.573744 -0.295157
H17 2.379112 -2.559698 0.433061
H18 1.376253 1.403964 -0.459253
H19 4.035425 1.214310 -0.269247
O20 -3.580897 -2.253219 -0.748541
H21 -3.715284 -1.734606 -1.547032
H22 -3.078787 -1.639958 -0.154845

[His-H]$^-$(H_2O)_6
O1 -2.704477 1.193878 0.589419
C2 -1.514232 0.974757 0.293934
O3 -0.680239 1.802493 -0.180770
C4 -1.014449 -0.501228 0.503727
N5 -1.033806 -1.179477 -0.809527
C6 0.332906 -0.630161 1.274862
H7 -1.774521 -0.985330 1.120972
H8 -0.480805 -0.644321 -1.473794
C9 1.589197 -0.350503 0.506917
H10 0.275284 0.022194 2.156375
H11 0.408657 -1.654901 1.659000
C12 2.773535 -1.042667 0.361731
N13 3.646778 -0.349807 -0.449908
C14 2.987812 0.743535 -0.793109
N15 1.749625 0.792585 -0.235997
H16 3.044307 -1.993029 0.799332
H17 3.363993 1.521552 -1.440861
H18 -0.596330 -2.095498 -0.741703
H19 0.924066 1.429621 -0.352910
O20 -4.062461 -1.015175 -0.767447
H21 -3.156387 -1.241831 -1.037988
H22 -3.897653 -0.213528 -0.238391

[His-H]$^-$(H_2O)_7
O1 2.069617 -1.596880 -1.374048
C2 1.554473 -0.686228 -0.716989
O3 1.415350 0.541693 -1.048532
C4 0.934660 -1.082923 0.665580
N5 1.092160 0.006524 1.641092
C6 -0.533040 -1.565805 0.464546
H7 1.504622 -1.946565 1.016267
H8 0.789939 0.873886 1.204488
C9 -1.545960 -0.498289 0.162127
H10 -0.517975 -2.316982 -0.335249
H11 -0.866511 -2.085570 1.371296
C12 -2.859270 -0.340919 0.550932
N13 -3.409915 0.789667 -0.014471
C14 -2.433658 1.313359 -0.731345
N15 -1.294569 0.572694 -0.666315
H16 -3.435647 -0.982909 1.201648
H17 -2.497205 2.224461 -1.307455
H18 0.496556 -0.147386 2.450729
H19 2.728939 1.702081 -0.178553
O20 3.232436 2.060654 0.577222
H21 2.985415 1.435807 1.272149
H22 -0.344324 0.782074 -1.023701

[His-H]$^-$(H_2O)_8
O1 -3.936522 -0.483149 -0.401253
C2 -2.750448 -0.456549 -0.126212
O3 -2.030936 -1.558330 -0.008575
C4 -2.035528 0.896218 0.108495
N5 -1.709739 1.023930 1.539440
C6 -0.838317 1.143654 -0.860947
H7 -2.805841 1.637535 -0.112014
H8 -0.939168 0.398118 1.762017
C9 0.439030 0.462350 -0.462762
H10 -1.151728 0.845486 -1.872221
H11 -0.659618 2.224637 -0.904789
C12 1.745613 0.914209 -0.437078
N13 2.563876 -0.091382 0.021412
C14 1.726272 -1.106438 0.265197
N15 0.433747 -0.834110 -0.005638
H16 2.138733 1.882619 -0.716027
H17 2.053126 -2.062140 0.653176
H18 -1.364924 1.963544 1.717563
H19 -0.996642 -1.374166 0.056616
O20 5.352749 -0.065858 0.174498
H21 4.355810 -0.052604 0.190279
H22 5.552995 -0.414068 -0.698615

[His-H]$^-$(H_2O)_9
O1 3.457991 -1.075137 -0.260685
C2 2.502138 -0.356156 -0.063854
O3 2.586364 0.962413 -0.298183
C4 1.147463 -0.887272 0.409244
N5 0.744251 -0.204351 1.645407

C6 0.120125 -0.860829 -0.800937
H7 1.324580 -1.930621 0.673885
H8 0.592343 0.786458 1.477705
C9 -1.293120 -0.537034 -0.428632
H10 0.458572 -0.130866 -1.543082
H11 0.163588 -1.839473 -1.288601
C12 -2.399012 -1.347938 -0.221300
N13 -3.485064 -0.579859 0.118607
C14 -2.997505 0.664975 0.111942
N15 -1.687341 0.764148 -0.209891
H16 -2.470388 -2.424768 -0.312749
H17 -3.599922 1.535059 0.344802
H18 -0.168918 -0.564434 1.912540
H19 1.725140 1.454380 -0.192040
O20 0.308924 2.395592 -0.080003
H21 0.246073 3.109594 -0.719980
H22 -0.580743 1.827676 -0.159156

[His-H]$^-$(H_2O)_10
O1 1.520452 -0.864977 0.952129
C2 1.583175 0.126061 0.172682
O3 2.304368 0.250262 -0.849088
C4 0.670987 1.352238 0.506977
N5 1.397982 2.631495 0.341177
C6 -0.582720 1.406587 -0.386588
H7 0.359131 1.271915 1.552392
H8 1.917629 2.538063 -0.532486
C9 -1.610648 0.333855 -0.167978
H10 -1.063885 2.376762 -0.228978
H11 -0.255562 1.390526 -1.434448
C12 -1.477903 -0.892636 0.434918
N13 -2.725556 -1.482840 0.354595
C14 -3.551352 -0.603723 -0.286434
N15 -2.916067 0.498053 -0.611969
H16 -0.611284 -1.362134 0.875701
H17 -2.966888 -2.399153 0.694309
H18 -4.592446 -0.818121 -0.479449
H19 2.118416 2.675835 1.058380
O20 3.476192 -2.364666 -0.477434
H21 3.373463 -1.529594 -0.966303
H22 2.829583 -2.170292 0.227934

[His-H]$^-$(H_2O)_11
O1 -0.724481 2.313957 -0.019304
C2 -1.276280 1.192947 -0.081577
O3 -2.097525 0.799349 -0.960520
C4 -0.910057 0.165898 1.047844
N5 -2.082091 -0.496820 1.656737
C6 0.041328 -0.937648 0.550782
H7 -0.406043 0.730140 1.838478
H8 -2.594718 -0.992024 0.927560
C9 1.423639 -0.502866 0.157310
H10 0.131338 -1.685595 1.345474
H11 -0.431456 -1.448504 -0.297926
C12 1.896287 0.756620 -0.118056
N13 3.232511 0.591063 -0.433425
C14 3.510761 -0.743112 -0.339302
N15 2.448818 -1.428713 0.014875
H16 1.383222 1.706856 -0.129189
H17 3.871213 1.323462 -0.695740
H18 4.493501 -1.147672 -0.533565
H19 -2.721367 0.221167 1.987709
O20 -3.549130 -1.419942 -1.203904
H21 -3.036142 -0.566430 -1.118348
H22 -3.029203 -1.938061 -1.823955

[His-H]$^-$(H_2O)_12
O1 -0.186961 -2.544906 -0.646733
C2 -0.952206 -1.843889 0.059988
O3 -1.604926 -2.171550 1.079401
C4 -1.134274 -0.340417 -0.376221
N5 -2.546587 0.085721 -0.177296
C6 -0.236570 0.618101 0.429563
H7 -0.894758 -0.247812 -1.439235
H8 -2.819982 -0.360320 0.703056
C9 1.241570 0.531359 0.176184
H10 -0.545038 1.646195 0.212764
H11 -0.435797 0.454550 1.496925
C12 1.978102 -0.500556 -0.350162
N13 3.287637 -0.057532 -0.349381
C14 3.291602 1.205572 0.171598
N15 2.079413 1.591422 0.496242
H16 1.657242 -1.474970 -0.690625
H17 4.086091 -0.579705 -0.670363
H18 4.195215 1.787243 0.282178
H19 -3.111238 -0.392220 -0.877067
O20 -3.369567 2.798509 -0.337797
H21 -3.068094 1.853334 -0.276178
H22 -2.644601 3.298992 0.046919

[His-H]$^-$(H_2O)_13
O1 -2.455393 -1.545018 -0.126309
C2 -2.429836 -0.348245 0.261845
O3 -2.987947 0.163509 1.260701
C4 -1.587153 0.656597 -0.611089
N5 -2.257711 1.972896 -0.728015
C6 -0.185115 0.906380 -0.020331
H7 -1.475703 0.236943 -1.615707
H8 -2.667559 2.135796 0.194179
C9 0.775233 -0.247158 -0.054976

H10 0.261881 1.741551 -0.570059
H11 -0.309401 1.246746 1.016348
C12 0.523002 -1.590185 -0.177061
N13 1.760023 -2.207254 -0.140323
C14 2.703975 -1.236100 0.002342
N15 2.146163 -0.046097 0.055034
H16 -0.424066 -2.105232 -0.266026
H17 1.925172 -3.198334 -0.200396
H18 3.762038 -1.443395 0.055520
H19 -3.061829 1.856056 -1.340328
O20 3.638677 2.385265 0.298108
H21 2.961808 3.066822 0.340789
H22 3.125009 1.548443 0.214435

[His-H]$^-$(H_2O)$_2$_1
O1 -0.855437 -0.686694 0.031941
C2 -1.142647 0.529552 -0.136494
O3 -2.296425 1.017608 -0.213904
C4 0.044358 1.533373 -0.308354
N5 -0.444604 2.910966 -0.154665
C6 1.222554 1.288227 0.674711
H7 0.421201 1.350318 -1.326944
H8 -1.451614 2.888284 -0.303797
H9 -0.028875 3.523033 -0.847870
C10 2.199613 0.219415 0.291808
H11 1.775188 2.227917 0.755961
H12 0.805807 1.092093 1.669878
C13 3.572956 0.210861 0.168115
N14 4.024576 -1.038997 -0.201105
C15 2.932761 -1.774300 -0.303127
N16 1.811912 -1.062675 -0.011064
H17 4.256205 1.032301 0.328833
H18 0.807694 -1.295922 -0.044864
H19 2.901614 -2.815982 -0.585663
O20 -2.914709 -2.713230 0.077685
H21 -2.163230 -2.089896 0.078686
H22 -3.672119 -2.112349 0.000545
O23 -4.650776 -0.309644 0.058897
H24 -3.791493 0.160062 -0.097767
H25 -4.842363 -0.132006 0.983936

[His-H]$^-$(H_2O)$_2$_2
O1 -1.669449 -1.076450 -0.051307
C2 -2.256647 0.047044 -0.131645
O3 -3.488124 0.237950 -0.084825
C4 -1.349130 1.310719 -0.338220
N5 -2.159637 2.532636 -0.233833
C6 -0.160509 1.388384 0.663876
H7 -0.922940 1.203075 -1.346164
H8 -3.134296 2.232941 -0.228661
H9 -2.016828 3.132112 -1.038412
C10 1.044832 0.564841 0.327039
H11 0.149975 2.434689 0.714226
H12 -0.533333 1.131547 1.663004
C13 2.390525 0.855016 0.274704
N14 3.108409 -0.268809 -0.080692
C15 2.203585 -1.220930 -0.245876
N16 0.951980 -0.764174 -0.006439
H17 2.879707 1.797336 0.470468
H18 0.002101 -1.192504 -0.085690
H19 2.414350 -2.237610 -0.540087
O20 -4.137015 -2.574670 0.187687
H21 -3.171282 -2.474278 0.139292
H22 -4.372088 -1.634083 0.122202
O23 5.931402 -0.517846 -0.223964
H24 6.120919 -0.695164 0.701383
H25 4.947997 -0.417954 -0.244804

[His-H]$^-$(H_2O)$_2$_3
O1 -2.054473 0.744373 -0.885063
C2 -1.391396 1.034521 0.148437
O3 -1.625865 0.666165 1.327068
C4 -0.145564 1.934209 -0.101865
N5 0.536133 2.370923 1.122358
C6 0.825182 1.251426 -1.098347
H7 -0.537306 2.815209 -0.626091
H8 -0.089779 2.152131 1.895756
C9 1.646489 0.116316 -0.560961
H10 0.224988 0.924903 -1.952183
H11 1.533964 2.001920 -1.464169
C12 3.016018 -0.016220 -0.467575
N13 3.368023 -1.240300 0.057888
C14 2.217870 -1.842688 0.285725
N15 1.151217 -1.078036 -0.073380
H16 3.761785 0.709170 -0.759853
H17 2.093041 -2.826091 0.713570
H18 1.356067 1.788384 1.273833
H19 0.174458 -1.356894 0.088533
O20 -3.627559 -1.400669 -0.859587
H21 -3.092362 -0.555552 -0.904829
H22 -4.337713 -1.190589 -0.246341
O23 -1.412271 -2.058554 0.857937
H24 -1.582557 -1.180989 1.262882
H25 -2.142440 -2.125621 0.215508

[His-H]$^-$(H_2O)$_2$_4
O1 0.607729 -1.619851 -0.185269
C2 1.325624 -0.697964 0.300032
O3 2.562205 -0.732445 0.478491
C4 0.592422 0.608555 0.765819

N5 1.602856 1.659847 1.004326
C6 -0.486473 1.126190 -0.221413
H7 0.085448 0.336769 1.703115
H8 2.485420 1.167020 1.155346
H9 1.382359 2.190192 1.841321
C10 -1.825763 0.461202 -0.132937
H11 -0.632794 2.192179 -0.027293
H12 -0.089118 1.054497 -1.240988
C13 -3.107280 0.951417 0.003183
N14 -4.025047 -0.077824 0.021471
C15 -3.301355 -1.175917 -0.097904
N16 -1.973872 -0.902288 -0.199747
H17 -3.415592 1.983754 0.083138
H18 -1.130104 -1.500671 -0.244480
H19 -3.689520 -2.183508 -0.112874
O20 2.837919 -3.441914 -0.521843
H21 1.904881 -3.175622 -0.580846
H22 3.189692 -2.617332 -0.147219
O23 2.334692 3.570687 -1.006515
H24 2.039839 2.913740 -0.329751
H25 2.718501 3.028115 -1.701408

[His-H]$^-$$(H_2O)_2$_5
O1 0.456032 1.310986 0.296337
C2 1.135928 0.270172 0.079624
O3 2.379155 0.241195 -0.100371
C4 0.370850 -1.086927 -0.026748
N5 1.253636 -2.194470 0.363811
C6 -0.923724 -1.163682 0.823231
H7 0.076584 -1.151530 -1.088653
H8 2.208787 -1.973495 0.099392
H9 0.991364 -3.047056 -0.119858
C10 -2.139623 -0.497910 0.256821
H11 -1.164191 -2.222697 0.956169
H12 -0.699570 -0.771660 1.821501
C13 -3.408919 -0.954632 -0.028739
N14 -4.196732 0.062716 -0.525760
C15 -3.407999 1.121057 -0.542840
N16 -2.163811 0.834270 -0.075803
H17 -3.796305 -1.954832 0.101142
H18 -1.298774 1.388348 -0.001520
H19 -3.687925 2.106721 -0.883670
O20 2.612707 3.188424 0.283918
H21 1.709319 2.829938 0.361472
H22 3.073781 2.361227 0.083375
O23 4.523197 -1.328557 -0.778456
H24 5.063278 -1.163002 -0.000821
H25 3.744205 -0.744419 -0.643783

[His-H]$^-$$(H_2O)_2$_6
O1 2.042734 -1.172908 -0.672578
C2 1.142778 -0.787536 0.088545
O3 1.072816 0.339074 0.690427
C4 -0.063203 -1.749324 0.303309
N5 -0.506375 -1.721125 1.702654
C6 -1.186199 -1.446225 -0.735672
H7 0.313888 -2.746762 0.063569
H8 -0.320059 -0.793961 2.075337
C9 -2.030469 -0.233463 -0.470926
H10 -0.711794 -1.379548 -1.722871
H11 -1.861154 -2.308881 -0.779609
C12 -3.379870 -0.000417 -0.627652
N13 -3.701149 1.294648 -0.280121
C14 -2.557097 1.835437 0.091205
N15 -1.519958 0.960852 -0.014564
H16 -4.132408 -0.692942 -0.976260
H17 -2.425997 2.846632 0.446564
H18 -1.506503 -1.881680 1.773690
H19 -0.542459 1.052103 0.300508
O20 4.636643 0.096808 -0.825712
H21 3.804065 -0.412599 -0.852860
H22 4.390932 0.848051 -0.264663
O23 3.042113 2.220530 0.538696
H24 2.358597 1.509362 0.637143
H25 2.815185 2.640737 -0.295852

[His-H]$^-$$(H_2O)_2$_7
O1 -2.603406 0.172727 0.544727
C2 -1.382960 0.263330 0.295357
O3 -0.779114 1.293526 -0.135231
C4 -0.532893 -1.031410 0.511772
N5 -0.382379 -1.703234 -0.795569
C6 0.801469 -0.808698 1.283053
H7 -1.149216 -1.685474 1.132411
H8 0.040446 -1.063012 -1.462465
C9 1.955924 -0.251204 0.507764
H10 0.584623 -0.171821 2.150573
H11 1.121993 -1.775919 1.687833
C12 3.263353 -0.661843 0.356234
N13 3.958545 0.208844 -0.455838
C14 3.075279 1.130158 -0.794424
N15 1.858260 0.901233 -0.233403
H16 3.739665 -1.528644 0.791422
H17 3.267078 1.974259 -1.439985
H18 0.253550 -2.492682 -0.712392
H19 0.930517 1.352316 -0.346771
O20 -3.108017 2.998802 -0.038300
H21 -3.419447 2.119395 0.229803
H22 -2.177216 2.769574 -0.202402

O23 -3.323949 -2.377877 -0.760133
H24 -2.390732 -2.331896 -1.030014
H25 -3.407395 -1.553425 -0.251391

[His-H]$^-$(H_2O)$_2$_8
O1 1.087019 -2.203174 -0.456980
C2 1.999373 -1.492066 0.055520
O3 3.207795 -1.771676 0.152554
C4 1.555471 -0.109160 0.677859
N5 2.765756 0.672400 1.007749
C6 0.615215 0.730820 -0.227676
H7 0.999255 -0.362807 1.591477
H8 3.528737 -0.010791 1.006973
H9 2.695717 1.072630 1.937971
C10 -0.828556 0.330209 -0.209947
H11 0.678149 1.773766 0.093998
H12 1.003878 0.704400 -1.253097
C13 -1.998722 1.038009 -0.042591
N14 -3.083629 0.188946 -0.123525
C15 -2.568029 -1.013449 -0.332097
N16 -1.217423 -0.973093 -0.396337
H17 -2.123023 2.097755 0.122126
H18 -0.461817 -1.703602 -0.479902
H19 -3.137101 -1.924233 -0.439054
O20 -5.819032 0.793036 0.309403
H21 -4.875254 0.596689 0.087256
H22 -5.833203 0.773772 1.270140
O23 3.796867 2.748381 -0.668151
H24 3.399100 2.041890 -0.100797
H25 4.042921 2.284039 -1.473314

[His-H]$^-$(H_2O)$_2$_9
O1 3.223752 -0.228034 -0.858480
C2 2.302722 -0.251489 -0.024564
O3 1.930420 0.702013 0.737396
C4 1.471458 -1.569943 0.068788
N5 1.131193 -1.872310 1.464509
C6 0.244925 -1.496258 -0.889345
H7 2.119935 -2.356735 -0.325313
H8 1.066002 -0.993077 1.970718
C9 -0.893283 -0.623037 -0.444482
H10 0.614144 -1.174036 -1.870977
H11 -0.154446 -2.507737 -1.028835
C12 -2.258523 -0.768990 -0.550522
N13 -2.903582 0.325911 -0.013979
C14 -1.937623 1.118681 0.418564
N15 -0.713111 0.593877 0.174166
H16 -2.809730 -1.591347 -0.981407
H17 -2.080877 2.066664 0.913860
H18 0.229230 -2.333406 1.534253
H19 0.228395 0.913645 0.479224
O20 4.018419 2.479718 -0.218612
H21 4.080577 1.641443 -0.708344
H22 3.273841 2.241280 0.358393
O23 -5.699989 0.841486 0.032002
H24 -4.736134 0.630432 0.075621
H25 -5.791307 1.315270 -0.799150

[His-H]$^-$(H_2O)$_2$_10
O1 -0.247561 -2.220632 -0.167988
C2 -1.131821 -1.367430 0.104434
O3 -2.301252 -1.606554 0.490145
C4 -0.719121 0.142012 -0.055095
N5 -1.817432 1.101022 0.175551
C6 0.470275 0.516897 0.872579
H7 -0.393791 0.272891 -1.093079
H8 -2.159274 0.972133 1.126328
H9 -2.615489 0.842136 -0.402596
C10 1.835715 0.187232 0.349756
H11 0.433452 1.595594 1.046075
H12 0.315544 0.038205 1.849256
C13 3.009764 0.907816 0.288200
N14 4.016464 0.151829 -0.274640
C15 3.449896 -1.008802 -0.551673
N16 2.140443 -1.038040 -0.189409
H17 3.182173 1.922124 0.617841
H18 1.385464 -1.745758 -0.305438
H19 3.942821 -1.850871 -1.014538
O20 -4.591555 -0.520797 -0.418268
H21 -4.878495 -1.169780 -1.065989
H22 -3.788865 -0.930603 -0.009035
O23 -1.068075 3.810776 -0.371177
H24 -1.366122 2.888218 -0.170547
H25 -0.254455 3.693340 -0.869697

[His-H]$^-$(H_2O)$_2$_11
O1 1.961697 -1.751948 0.359455
C2 0.959467 -1.190174 -0.141361
O3 0.152867 -1.687745 -0.972187
C4 0.669047 0.275607 0.323617
N5 0.608808 1.154186 -0.857903
C6 -0.577062 0.356833 1.256761
H7 1.523105 0.586893 0.929023
H8 0.123970 0.662941 -1.604321
C9 -1.927230 0.279368 0.607387
H10 -0.472236 -0.431495 2.014159
H11 -0.535083 1.307069 1.801919
C12 -3.088408 0.996327 0.804980
N13 -4.095854 0.534202 -0.014580
C14 -3.542605 -0.446332 -0.704301

N15 -2.242465 -0.645140 -0.359956
H16 -3.252315 1.812477 1.493976
H17 -4.037434 -1.035877 -1.461781
H18 0.076555 1.997089 -0.658515
H19 -1.500961 -1.242267 -0.775832
O20 3.485268 2.023942 -0.877515
H21 2.558268 1.764637 -1.035968
H22 3.861950 1.259909 -0.408961
O23 4.272655 -0.385136 0.652589
H24 3.447513 -0.929089 0.550174
H25 4.374092 -0.277708 1.601959

[His-H]$^-$$(H_2O)_2$_12
O1 -2.036535 0.637765 1.496427
C2 -1.364268 0.078917 0.613335
O3 -1.311367 0.380094 -0.625097
C4 -0.426773 -1.073921 1.082250
N5 -0.296356 -2.103070 0.039634
C6 0.925244 -0.477751 1.576785
H7 -0.912415 -1.525813 1.949833
H8 0.001024 -1.657596 -0.824818
C9 1.860527 0.007443 0.506902
H10 0.684991 0.333307 2.275294
H11 1.459974 -1.239111 2.156819
C12 3.230163 -0.075119 0.381672
N13 3.660985 0.553632 -0.767028
C14 2.560333 1.004843 -1.335239
N15 1.449753 0.711136 -0.604970
H16 3.926036 -0.547826 1.059704
H17 2.509954 1.543196 -2.269784
H18 0.421280 -2.777132 0.293220
H19 0.456992 0.834757 -0.850524
O20 -3.054081 2.732150 -0.185254
H21 -2.917012 2.215622 0.629713
H22 -2.557499 2.164817 -0.793951
O23 -2.704687 -2.087784 -1.748376
H24 -2.072066 -2.426862 -1.093080
H25 -2.559936 -1.133511 -1.661717

[His-H]$^-$$(H_2O)_2$_13
O1 2.274222 -0.918476 -1.477877
C2 1.256916 -0.431185 -0.956645
O3 0.813447 0.752783 -1.101423
C4 0.481749 -1.343986 0.052068
N5 0.675600 -0.768575 1.398958
C6 -0.999579 -1.622602 -0.339404
H7 0.997258 -2.306682 0.034925
H8 0.339264 0.191441 1.407018
C9 -1.996122 -0.533023 -0.080437
H10 -1.010881 -1.904135 -1.401148
H11 -1.338605 -2.508151 0.211507
C12 -3.258127 -0.543119 0.475003
N13 -3.803988 0.722618 0.471822
C14 -2.874995 1.486896 -0.073162
N15 -1.772401 0.776784 -0.430636
H16 -3.801146 -1.390349 0.868879
H17 -2.950148 2.553506 -0.223431
H18 0.133615 -1.279586 2.091065
H19 3.566562 -0.599508 0.229101
O20 3.616686 -0.327370 1.159598
H21 2.711944 -0.518434 1.475962
H22 -0.835629 1.066039 -0.781153
O23 2.735784 2.462590 0.314841
H24 2.114771 2.048778 -0.310333
H25 3.198347 1.697191 0.690951

[His-H]$^-$$(H_2O)_2$_14
O1 1.878466 -1.083597 -1.311877
C2 1.117361 -0.321749 -0.694083
O3 0.773558 0.861579 -1.014173
C4 0.498935 -0.873879 0.630901
N5 0.500339 0.180929 1.661124
C6 -0.890411 -1.523962 0.365060
H7 1.166589 -1.669368 0.967284
H8 -0.040063 0.972800 1.321917
C9 -2.028633 -0.578310 0.108446
H10 -0.768138 -2.214472 -0.479350
H11 -1.166731 -2.140847 1.228543
C12 -3.349482 -0.602530 0.501930
N13 -4.036880 0.476825 -0.010667
C14 -3.136176 1.150333 -0.700252
N15 -1.914004 0.553342 -0.668510
H16 -3.839986 -1.340513 1.120258
H17 -3.314476 2.071919 -1.233986
H18 0.051292 -0.148953 2.511709
H19 -0.996235 0.891671 -1.010571
O20 4.594085 -0.434793 -0.234680
H21 4.219555 0.348714 0.200208
H22 3.833444 -0.786999 -0.725630
O23 2.888366 1.776105 0.872052
H24 2.277464 1.248338 1.420114
H25 2.385731 1.836268 0.043284

[His-H]$^-$$(H_2O)_2$_15
O1 -3.420407 1.102345 0.405183
C2 -2.208835 0.931429 0.182577
O3 -1.397607 1.774353 -0.310657
C4 -1.640162 -0.495644 0.516871
N5 -1.544621 -1.254879 -0.747058
C6 -0.338086 -0.495770 1.371673

H7 -2.407344 -0.983427 1.121926
H8 -0.986095 -0.734207 -1.417843
C9 0.942344 -0.167602 0.665350
H10 -0.491618 0.195477 2.210814
H11 -0.220827 -1.492061 1.814717
C12 2.184094 -0.764144 0.652778
N13 3.046593 -0.050013 -0.152951
C14 2.326358 0.957580 -0.623292
N15 1.058372 0.930163 -0.151842
H16 2.505863 -1.654198 1.172730
H17 2.685602 1.714548 -1.303562
H18 -1.069561 -2.141573 -0.596422
H19 0.181088 1.486359 -0.357969
O20 -4.579721 -1.276031 -0.867479
H21 -3.649268 -1.459987 -1.080388
H22 -4.494676 -0.432636 -0.388037
O23 5.825552 -0.507974 -0.504614
H24 6.161273 -0.024000 0.254767
H25 4.846329 -0.387838 -0.442974

[His-H]$^-$$(H_2O)_2$_16
O1 2.906217 -1.335885 -1.369039
C2 2.246220 -0.521530 -0.717643
O3 1.909348 0.667495 -1.054827
C4 1.693643 -1.007199 0.664659
N5 1.702312 0.088560 1.644862
C6 0.308763 -1.692747 0.465563
H7 2.380490 -1.783186 1.009878
H8 1.253135 0.901543 1.231555
C9 -0.844594 -0.780114 0.158150
H10 0.428133 -2.435926 -0.332960
H11 0.050673 -2.252526 1.372699
C12 -2.169933 -0.822317 0.529526
N13 -2.863386 0.226990 -0.036647
C14 -1.963639 0.899373 -0.734542
N15 -0.738208 0.327318 -0.654697
H16 -2.661451 -1.543542 1.165188
H17 -2.153906 1.799274 -1.298807
H18 1.171875 -0.163902 2.474694
H19 3.061043 2.013776 -0.184784
O20 3.507892 2.425929 0.578030
H21 3.352867 1.759777 1.261396
H22 0.185360 0.665513 -1.001415
O23 -5.669085 0.665549 0.094573
H24 -4.686926 0.560748 0.105978
H25 -5.944072 0.140874 -0.662219

[His-H]$^-$$(H_2O)_2$_17
O1 -1.241422 -0.321983 -1.183387
C2 -1.122059 0.627199 -0.370537
O3 -1.835927 0.864239 0.644306
C4 0.025993 1.650719 -0.626896
N5 -0.445182 3.047468 -0.498245
C6 1.202004 1.461191 0.348342
H7 0.382992 1.507045 -1.650425
H8 -0.996410 3.081871 0.359167
C9 1.993409 0.192102 0.212053
H10 1.884179 2.306422 0.215834
H11 0.811224 1.535999 1.371398
C12 1.656090 -0.991124 -0.397809
N13 2.738429 -1.828907 -0.207150
C14 3.673227 -1.131125 0.502222
N15 3.260925 0.086732 0.767796
H16 0.756067 -1.286098 -0.913823
H17 2.802164 -2.785507 -0.514466
H18 4.624439 -1.556312 0.787267
H19 -1.114280 3.226642 -1.243333
O20 -2.926590 -2.557917 -0.664992
H21 -3.337228 -2.191472 0.133973
H22 -2.336971 -1.823002 -0.933840
O23 -3.896774 -0.685046 1.430598
H24 -4.620822 -0.256654 0.965663
H25 -3.100836 -0.144090 1.169331

[His-H]$^-$$(H_2O)_2$_18
O1 -0.941686 1.528637 1.084664
C2 -1.183299 0.436999 0.512686
O3 -1.951579 0.273261 -0.481606
C4 -0.480025 -0.833072 1.084457
N5 -1.416933 -1.931328 1.393154
C6 0.599910 -1.380829 0.136042
H7 -0.005312 -0.534722 2.023494
H8 -1.912965 -2.201430 0.544471
C9 1.804959 -0.507710 -0.063884
H10 0.935521 -2.343905 0.533386
H11 0.139249 -1.591770 -0.837152
C12 1.972949 0.826240 0.216157
N13 3.265306 1.127815 -0.171784
C14 3.818862 -0.018853 -0.665267
N15 2.971829 -1.020080 -0.612807
H16 1.289086 1.551880 0.627729
H17 3.701366 2.033414 -0.116404
H18 4.831495 -0.061928 -1.038903
H19 -2.132332 -1.582145 2.025365
O20 -2.613150 3.134231 -0.552839
H21 -2.704656 2.252669 -0.946988
H22 -2.000612 2.889099 0.168058
O23 -3.056952 -1.934591 -1.526368
H24 -3.981161 -1.674350 -1.562464
H25 -2.594290 -1.120614 -1.192503

[His-H]$^-$(H$_2$O)$_2$_19
O1 3.905719 -1.464004 -0.185774
C2 3.056673 -0.616914 -0.018643
O3 3.347791 0.679851 -0.215247
C4 1.617618 -0.950386 0.384320
N5 1.276482 -0.241429 1.624755
C6 0.652700 -0.736107 -0.852850
H7 1.627866 -2.013890 0.625544
H8 1.162493 0.750833 1.434475
C9 -0.729776 -0.278527 -0.502759
H10 1.093698 -0.001642 -1.534207
H11 0.608563 -1.679917 -1.404563
C12 -1.912636 -0.979546 -0.341204
N13 -2.917264 -0.105811 -0.002916
C14 -2.307727 1.087072 0.032299
N15 -0.993052 1.052280 -0.258256
H16 -2.097901 -2.038876 -0.459454
H17 -2.830132 2.004755 0.271343
H18 0.356118 -0.557757 1.919244
H19 2.569298 1.287029 -0.138232
O20 -5.644096 -0.635060 0.280068
H21 -4.663382 -0.456075 0.250816
H22 -5.903259 -0.585804 -0.644053
O23 1.238939 2.412762 -0.152131
H24 0.284417 2.009693 -0.212828
H25 1.181116 3.244421 0.324529

[His-H]$^-$(H$_2$O)$_2$_20
O1 1.399535 -1.431690 0.954698
C2 1.549829 -0.470970 0.154053
O3 2.298471 -0.416688 -0.853182
C4 0.715755 0.823554 0.433994
N5 1.542377 2.034746 0.192841
C6 -0.535187 0.918055 -0.459445
H7 0.409795 0.822429 1.483369
H8 2.062876 1.834341 -0.664150
C9 -1.631504 -0.073322 -0.192835
H10 -0.963056 1.918966 -0.344505
H11 -0.214733 0.837099 -1.506281
C12 -1.581372 -1.288163 0.444588
N13 -2.869414 -1.786338 0.391885
C14 -3.635741 -0.867750 -0.266907
N15 -2.925057 0.174467 -0.630107
H16 -0.747846 -1.806005 0.894195
H17 -3.174236 -2.670877 0.763553
H18 -4.691737 -1.009983 -0.444065
H19 2.259092 2.070898 0.915090
O20 3.288395 -3.108011 -0.381947
H21 3.261261 -2.287575 -0.902535
H22 2.640507 -2.846107 0.298970
O23 0.421465 4.658757 0.183348
H24 0.795017 3.740584 0.181474
H25 -0.425887 4.568737 -0.261480

[His-H]$^-$(H$_2$O)$_2$_21
O1 -2.271172 -0.740951 -0.723198
C2 -1.988452 0.344211 -0.143564
O3 -2.500608 0.808774 0.904797
C4 -0.875475 1.227947 -0.797509
N5 -1.242153 2.661123 -0.791726
C6 0.476101 1.091350 -0.070240
H7 -0.752033 0.910781 -1.836968
H8 -1.652942 2.834066 0.126685
C9 1.161633 -0.240145 -0.173787
H10 1.146471 1.857778 -0.472185
H11 0.319262 1.337637 0.988194
C12 0.652016 -1.463488 -0.528570
N13 1.711058 -2.348322 -0.444572
C14 2.806743 -1.645642 -0.046664
N15 2.512231 -0.375081 0.122109
H16 -0.355639 -1.742804 -0.798714
H17 1.667856 -3.337057 -0.628733
H18 3.777178 -2.095448 0.098113
H19 -2.012971 2.790358 -1.442823
O20 -4.299391 -1.446740 1.155007
H21 -3.936115 -0.600450 1.467904
H22 -3.735608 -1.536561 0.363428
O23 4.503272 1.504998 0.976185
H24 4.003496 2.248136 1.325246
H25 3.810900 0.875479 0.668844

[His-H]$^-$(H$_2$O)$_2$_22
O1 -0.222304 -1.930731 -1.711289
C2 -0.903572 -1.433002 -0.790670
O3 -1.643786 -2.047906 0.030317
C4 -0.827546 0.127518 -0.632148
N5 -2.151329 0.765442 -0.428660
C6 0.082421 0.553517 0.534936
H7 -0.415673 0.524804 -1.564275
H8 -2.550057 0.433404 0.450962
C9 1.552306 0.301268 0.359436
H10 -0.052812 1.627035 0.705815
H11 -0.267044 0.057086 1.449058
C12 2.195510 -0.549941 -0.504603
N13 3.543451 -0.395964 -0.239646
C14 3.659984 0.527536 0.760082
N15 2.483983 0.967903 1.142666
H16 1.793499 -1.231481 -1.239425
H17 4.294030 -0.882845 -0.701084
H18 4.615196 0.837458 1.158024

H19 -2.785764 0.422985 -1.146570
O20 -3.200716 -1.113982 1.967841
H21 -2.639543 -1.506327 1.239336
H22 -2.710667 -1.302263 2.772487
O23 -2.130188 3.598263 -0.747513
H24 -2.163606 2.615944 -0.609534
H25 -1.228965 3.835996 -0.512357

[His-H]$^-$(H_2O)$_2$_23
O1 1.741011 -2.292618 0.089905
C2 1.935094 -1.062108 -0.025605
O3 2.611932 -0.480426 -0.921655
C4 1.260967 -0.143138 1.054527
N5 2.157954 0.882722 1.622180
C6 0.019052 0.584691 0.507877
H7 0.948245 -0.795664 1.875440
H8 2.494729 1.481876 0.869132
C9 -1.147829 -0.278902 0.127031
H10 -0.311545 1.294515 1.274005
H11 0.322470 1.184930 -0.359668
C12 -1.204880 -1.634009 -0.079508
N13 -2.518063 -1.905549 -0.417574
C14 -3.200180 -0.727405 -0.406913
N15 -2.406951 0.269676 -0.081607
H16 -0.421125 -2.376003 -0.032903
H17 -2.892572 -2.812300 -0.642879
H18 -4.252555 -0.651551 -0.634655
H19 2.987235 0.421347 1.986401
O20 3.306455 2.066593 -1.262104
H21 3.082161 1.100893 -1.138700
H22 2.757914 2.338664 -2.002508
O23 -3.372821 2.968480 0.058005
H24 -2.582153 3.508196 0.144985
H25 -3.029344 2.046143 0.022691

[His-H]$^-$(H_2O)$_2$_24
O1 -1.686251 -2.538984 -0.268489
C2 -1.978915 -1.481695 0.342695
O3 -2.577807 -1.339557 1.434037
C4 -1.536548 -0.131179 -0.339341
N5 -2.578427 0.912862 -0.153927
C6 -0.220107 0.410967 0.249506
H7 -1.407198 -0.300274 -1.412017
H8 -2.907627 0.774273 0.805536
C9 1.022237 -0.375021 -0.055831
H10 -0.068349 1.430432 -0.120991
H11 -0.343680 0.491909 1.337666
C12 1.157410 -1.681581 -0.451008
N13 2.517790 -1.892402 -0.578944
C14 3.150243 -0.729514 -0.260404
N15 2.279713 0.204014 0.057027
H16 0.396240 -2.431497 -0.617077
H17 2.956051 -2.756559 -0.851896
H18 4.223325 -0.614817 -0.279461
H19 -3.378947 0.650857 -0.726061
O20 -2.159855 3.636205 -0.880367
H21 -2.281842 2.690758 -0.605172
H22 -1.206377 3.754100 -0.913366
O23 3.128440 2.821289 0.857696
H24 2.817616 1.934370 0.562641
H25 2.465122 3.101646 1.494386

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