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Supporting Information

Excited-State Proton Transfer Can Tune the Color of Protein Fluorescent Markers

Daiana T. Mancini,[a] Kakali Sen,*[b] Mario Barbatti,*[c] Walter Thiel,[c] and Teodorico C. Ramalho*[a]

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SECTION S1. MD CLASSIFICATION

The conformational evolution of the HABT and its surroundings was monitored during the molecular dynamics (MD) simulation. Three amino acids K721, E738 and T766 remain in close vicinity to HABT. The distances between HABT and these three residues are given in Figure S1. The amino group of HABT engages itself in forming H-bonds with either K721 or E738 or both, the other amino acid T766 is closer to the enol group of HABT. Since this enol group of HABT is directly involved in the ESPT process, depending on the nature of the surroundings of the enol group, we classify the conformations in three statistically relevant conformational sets (**Sets 1, 2, and 3**). This classification was based on the following criteria:

1. **Set 1**: No water around the enol and T766 OH groups.
2. **Set 2**: The enol and T766 OH groups are exposed to water, but there is no cross-link between them via water bridges. No distinction is made for the presence or absence of direct interactions between the enol and T766 OH groups in this selection. Also no distinction is made between water interacting with T766 or the enol group or both.
3. **Set 3**: The enol and T766 OH groups are exposed to water and are cross-linked with each other through one or two water bridges.
4. Species with more than two water bridges are considered as having individual interactions and are classified as belonging to **Set 2**.

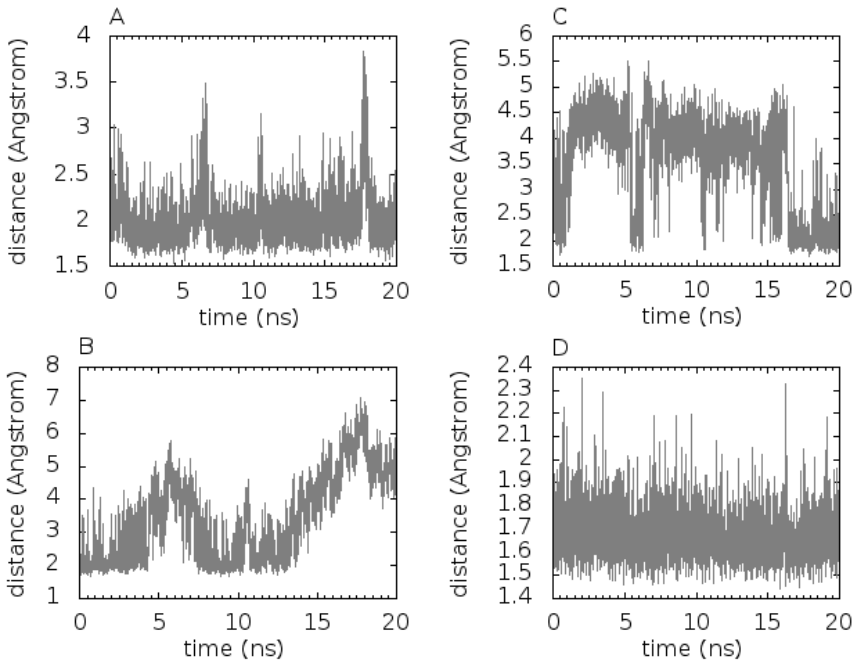


Figure S1 Relevant distances in the vicinity of HABT bound to TK: A) shortest distance between the H atom of the amino group of HABT and carboxylic side chain of E738; B) distance between enol O and T766 H; C) shortest distance between the N atom of the amino group of HABT and amino H of K721; and D) shortest distance between the amino H of K721 and carboxylic O of E738.

SECTION S2. ADDITIONAL RESULTS OF THE QM/MM CALCULATIONS

For each ensemble of conformations, a full path for the process starting with ESIPT and *cis-trans* isomerization of keto in S_1 state was studied for one of the selected snapshots. The other snapshots were used to study only the crucial first step, ESIPT, which is responsible for the dual fluorescence. The results for the three sets of conformers are provided in this section.

Conformational set 1: Four snapshots were selected at 0.2 (Conf-1-a1), 0.6 (Conf-1-a2), 0.8 (Conf-1-a3), and 0.9 ns (Conf-1-a4). The entire process, from absorption to internal conversion, was studied only for Conf-1-a2 (randomly chosen). In the main text and in the remaining sections of this SI, Conf-1-a2 is referred simply as Conf-1. The VE energies and ESIPT results for all four snapshots are given in Table S1 and Table S2. The QM region for these conformers consisted of HABT, the side chain of K721 modeled as methylamine, the side chain of E738 modeled as acetic acid, and the side chain of T766 modeled as ethanol.

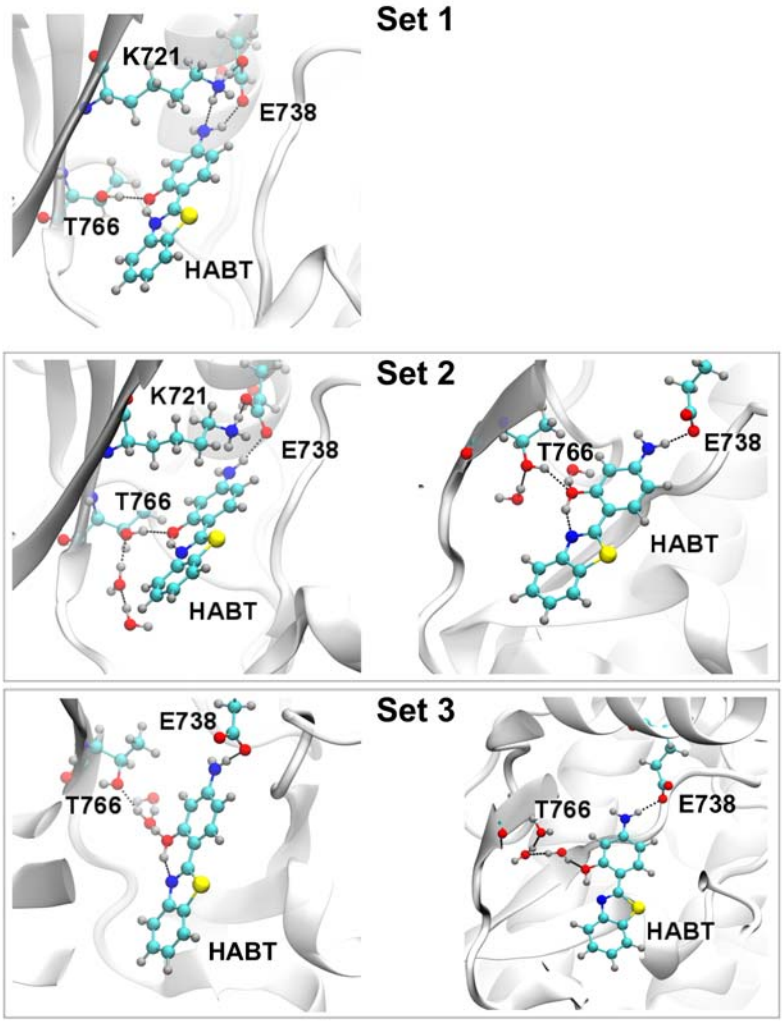


Figure S2 Representative structures (Conf-1, Conf-2, and Conf-3) of the statistically relevant conformational sets.

Table S1. Set 1: Relative energies of the singlet ground state (S_0) and the lowest singlet (S_1) excited states, evaluated at the optimized geometry of the enol (S_0) and enol (S_1) species. Also given are the relative energies of the transition state (TS) in the S_1 state. Energies refer to the minimum of the enol ground state (S_0) for each snapshot.

		Δ*E* (eV)			
	State	**Conf-1-a1**	**Conf-1-a2**	**Conf-1-a3**	**Conf-1-a4**
enol (S_0)	S_0	0.000	0.000	0.000	0.000
	S_1	3.797	3.747	3.687	3.741
enol (S_1)	S_0	0.220	0.139	0.152	0.174
	S_1	3.588	3.475	3.511	3.559
TS (S_1)	S_1	3.649	3.545	3.604	3.622

Table S2. Set 1: Energy barrier $\Delta E^{\neq}$ (eV) for ESIPT from enol (S_1).

$\Delta E^{\neq}$ (eV)			
Conf-1-a1	**Conf-1-a2**	**Conf-1-a3**	**Conf-1-a4**
0.06	0.07	0.09	0.06

Conformational set 2: Four snapshots at 7.6, 8.2, 11.1, and 11.4 ns were selected. They are named Conf-2-a1 to Conf-2-a4. Since the ESIPT barrier was very similar for all of them, the snapshot at 11.4 ns (Conf-2-a4) was randomly selected and used to study the entire process. For the other snapshots, we investigated only the ESIPT process. In the main text and in the remaining sections of this SI, Conf-2-a4 is referred as Conf-2. Results for all snapshots are reported in Table S3 and Table S4. The QM region for these conformers consisted of HABT, the side chain of E738 modeled as acetic acid, the side chain of T766 modeled as ethanol, the side chain of K721 modeled as methylamine (only if in hydrogen bond interaction with HABT), and two water molecules, either hydrogen bonded to T766 or forming individual hydrogen bonds with T766 and HABT.

Table S3. Set 2: Relative energies of the singlet ground state (S_0) and the lowest singlet (S_1) excited states, evaluated at the optimized geometries of the enol (S_0) and enol (S_1) species. Also given are the relative energies of the transition state (TS) in the S_1 state. Energies refer to the minimum of the enol ground state (S_0) for each snapshot.

		Δ*E* (eV)			
Geometry	**State**	**Conf-2-a1**	**Conf-2-a2**	**Conf-2-a3**	**Conf-2-a4**
enol (S_0)	S_0	0.000	0.000	0.000	0.000
	S_1	3.698	3.691	3.643	3.741
enol (S_1)	S_0	0.158	0.146	0.122	0.196
	S_1	3.540	3.542	3.516	3.539
TS (S_1)	S_1	3.597	3.638	3.605	3.629

Table S4. Set 2: Energy barriers $\Delta E^{\neq}$ (eV) for ESIPT from enol (S_1).

$\Delta E^{\neq}$ (eV)			
Conf-2-a1	**Conf-2-a2**	**Conf-2-a3**	**Conf-2-a4**
0.06	0.10	0.09	0.09

Conformational set 3: Four snapshots at 4.0, 6.0, 14.6, and 16.1 ns were selected. Those at 14.6 and 16.1 ns have one water bridge connecting the enol and T766 OH groups. Those at 4.0 and 6.0 ns have

two water molecules bridging enol with T766 OH. One snapshot (16.1 ns) with one water bridge was selected and used to study the entire process, Conf-3-a4. In the main text and in the remaining sections of this SI, Conf-3-a4 is referred as Conf-3. For the other snapshots, referred to as Conf-3-a1 (4.0 ns), Conf-3-a2 (6.0 ns), and Conf-3-a3 (14.6 ns), we investigated only the ESIPT process. Results for all snapshots are reported in Table S5 and Table S6. The QM region for these conformers consisted of HABT, the side chain of E738 modeled as acetic acid, the side chain of T766 modeled as ethanol, and the two water molecules; in two conformers (Conf-3-a3 and Conf-3-a4) one water molecule formed a hydrogen bridge between HABT and T766, and the other one was the immediately neighboring water molecule hydrogen bonded to the bridging water molecule. In the other two conformers (Conf-3-a1 and Conf-3-a2) the two water molecules formed the bridge between HABT and T766. Representative structures are illustrated in Figure S2.

Table S5. Set 3: Relative energies of the singlet ground state (S_0) and the lowest singlet (S_1) excited states, evaluated at the optimized geometries of the enol (S_0) and enol (S_1) species. Also given are the relative energies of the transition state (TS) in the S_1 state. Energies refer to the minimum of the enol ground state (S_0) for each snapshot.

		Δ*E* (eV)			
Geometry	**State**	**Conf-3-a1**	**Conf-3-a2**	**Conf-3-a3**	**Conf-3-a4**
enol (S_0)	S_0	0.000	0.000	0.000	0.000
	S_1	3.668	3.668	3.706	3.577
enol (S_1)	S_0	0.133	0.147	0.177	0.099
	S_1	3.535	3.532	3.542	3.476
TS (S_1)	S_1	3.646	3.682	3.665	3.726

Table S6. Set 3: Energy barriers $\Delta E^{\neq}$ (eV) for ESIPT from enol (S_1).

$\Delta E^{\neq}$ (eV)			
Conf-3-a1	**Conf-3-a2**	**Conf-3-a3**	**Conf-3-a4**
0.11	0.15	0.12	0.25

Table S7. Mean value and standard deviation of the data in Table S1, Table S3, and Table S5.

		Δ*E* (eV)		
	State	**Set 1**	**Set 2**	**Set 3**
enol (S_0)	S_0	0	0	0
	S_1	3.74 ± 0.04	3.69 ± 0.04	3.65 ± 0.05
enol (S_1)	S_0	0.17 ± 0.04	0.16 ± 0.03	0.14 ± 0.03
	S_1	3.53 ± 0.05	3.53 ± 0.01	3.52 ± 0.03
TS (S_1)	S_1	3.61 ± 0.04	3.62 ± 0.02	3.68 ± 0.03

Table S8. Mean values and standard deviations of the data in Table S2, Table S4, and Table S6.

$\langle\Delta E^{\neq}\rangle$ (eV)		
Set 1	**Set 2**	**Set 3**
0.07 ± 0.01	0.09 ± 0.02	0.16 ± 0.06

SECTION S3. POTENTIAL ENERGY SCANS

a) ESIPT step. The relaxed potential energy scans for the ESIPT process in Conf-1, Conf-2, and Conf-3 reported in the main text are given in Figure S3, Figure S4, and Figure S5.

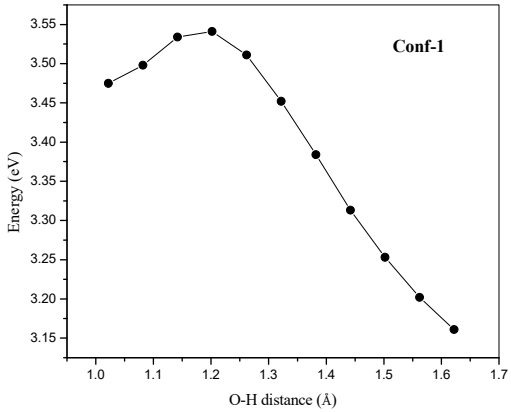


Figure S3 Potential energy curves obtained by a relaxed scan of the O-H distance for HABT (**Conf-1**).

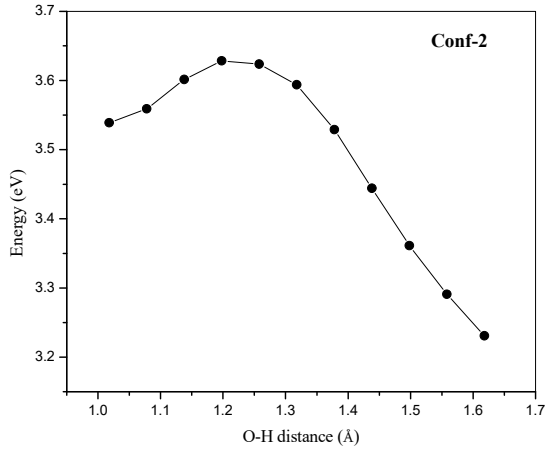


Figure S4 Potential energy curves obtained by a relaxed scan of the O-H distance for HABT (**Conf-2**).

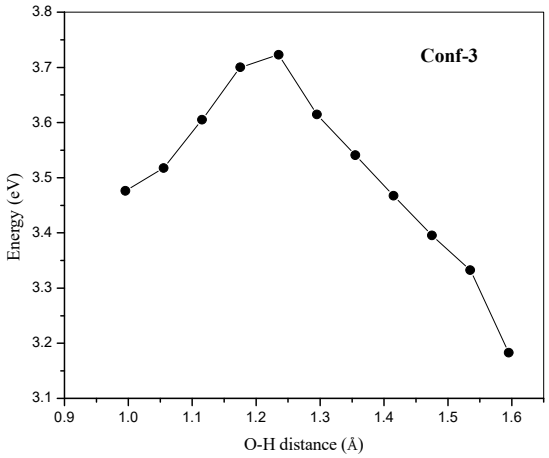


Figure S5 Potential energy curves obtained by a relaxed scan of the O-H distance for HABT (**Conf-3**).

b) cis-trans isomerization of the keto form in the S_1 state. The relaxed potential energy scans for the isomerization process in Conf-1, Conf-2, and Conf-3 reported in the main text are given in Figure S6, Figure S7, and Figure S8.

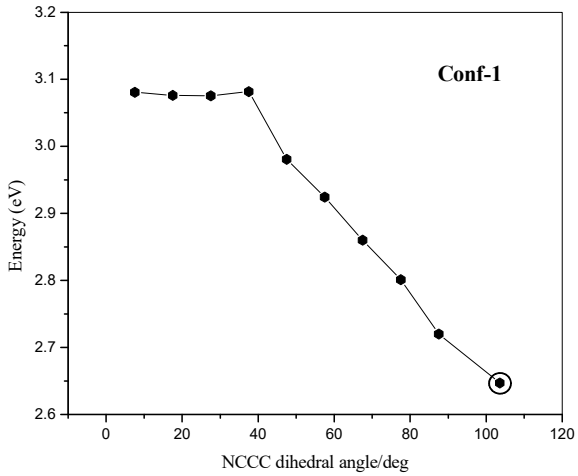


Figure S6 Potential energy curves obtained by a relaxed scan of the NCCC dihedral angle for HABT (**Conf-1**). The final point obtained from unconstrained optimization is surrounded by a black circle.

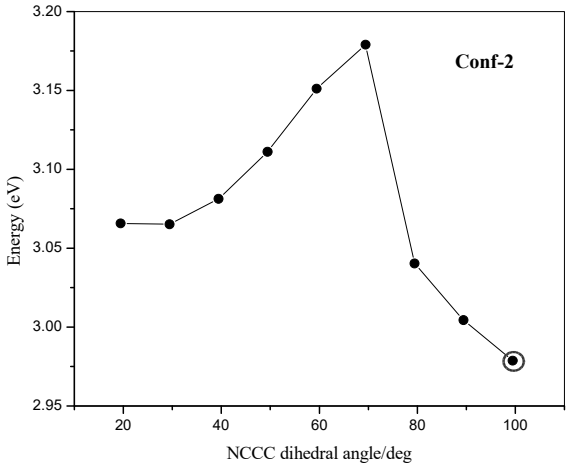


Figure S7 Potential energy curves obtained by a relaxed scan of the NCCC dihedral angle for HABT (**Conf-2**). The final point obtained from unconstrained optimization is surrounded by a black circle.

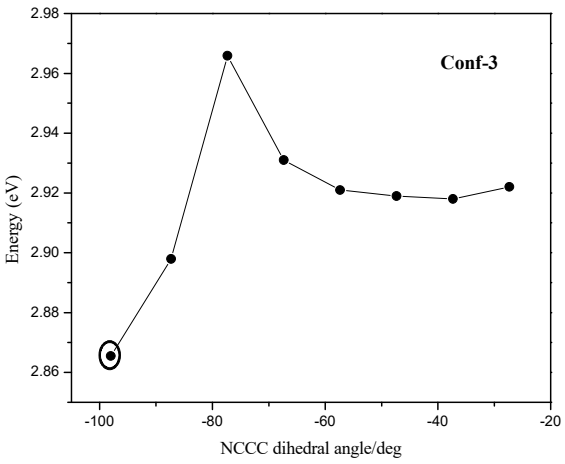
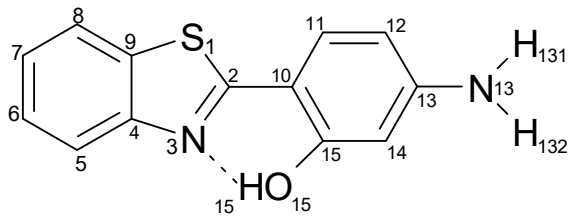


Figure S8 Potential energy curves obtained by a relaxed scan of the NCCC dihedral angle for HABT (**Conf-3**). The final point obtained from unconstrained optimization is surrounded by a black circle.

SECTION S4. PARTIAL CHARGES

Scheme S1 Partial Charges of HABT Atoms.

S1	-0.250
C2	0.340
N3	-0.690
C4	0.640
C5	-0.460
H5	0.260
C6	-0.290
H6	0.260
C7	-0.380
H7	0.260
C8	-0.240
H8	0.220
C9	0.330
C10	0.000
C11	-0.115
H11	0.115
C12	-0.115
H12	0.115
C13	0.072
N13	-0.834
H131	0.381
H132	0.381
C14	-0.115
H14	0.115
C15	0.110
O15	-0.530
H15	0.420



SECTION S5. SINGLE POINT CALCULATIONS WITH OTHER FUNCTIONALS

To assess the effects arising from long-range corrections or dispersion, the energies of all stationary points on the ESIPT and cis-trans isomerization pathways were recalculated with ωB97X-D functional and CAM-B3LYP for Conf-1, Conf-2 and Conf-3 (as discussed in the main text). The results are given in Tables S9 to S12. All energies were evaluated at QM(B3LYP)/CHARMM optimized geometries.

Table S9. ωB97X-D functional. Relative energies of the singlet ground state (S_0) and the lowest singlet (S_1) excited states for the three chosen conformers, evaluated at the optimized geometries of the enol (S_0), enol (S_1), and keto (S_1) species. Energies refer to the minimum of the enol ground state (S_0) for each conformer. TS denotes the transition state in the S_1 state.

Δ*E* (eV) ωB97X-D				
Geometry	***States***	**Conf-1**	**Conf-2**	**Conf-3**
enol (S_0)	S_0	0.000	0.000	0.000
	S_1	4.065	4.065	3.886
enol (S_1)	S_0	0.223	0.275	0.150
	S_1	3.774	3.850	3.766
enol (S_1)	TS	3.831	3.916	4.052
keto (S_1)	S_0	0.359	0.683	0.653
	S_1	3.559	3.622	3.439
keto (S_1)	TS	3.562	3.739	3.603
triplet-keto	T_1	2.645	2.827	2.669
twisted-keto	S_0	2.381	2.528	2.920
	S_1	3.271	3.692	3.559

Table S10. Energy barriers $\Delta E^{\neq}$ (eV) for ESIPT from enol (S_1) and for twisting from keto (S_1).

Relative energy barriers $\Delta E^{\neq}$ (eV) in S_1 (ωB97X-D)			
Process	**Conf-1**	**Conf-2**	**Conf-3**
ESIPT	0.057	0.066	0.286
cis-trans	0.003	0.117	0.164

Table S11. CAM-B3LYP functional. Relative energies of the singlet ground state (S_0) and the lowest singlet (S_1) excited states for the three chosen conformers, evaluated at the optimized geometries of the enol (S_0), enol (S_1), and keto (S_1) species. Energies refer to the minimum of the enol ground state (S_0) for each conformation. TS denotes the transition state in the S_1 state.

Δ*E* (eV) CAM-B3LYP				
Geometry	***States***	**Conf-1**	**Conf-2**	**Conf-3**
enol (S_0)	S_0	0.000	0.000	0.000
	S_1	4.035	4.033	3.856
enol (S_1)	S_0	0.231	0.280	0.158
	S_1	3.755	3.826	3.747
enol (S_1)	TS	3.820	3.891	4.027
keto (S_1)	S_0	0.620	0.699	0.669
	S_1	3.564	3.622	3.434
keto (S_1)	TS	3.575	3.763	3.613
triplet-keto	T1	2.623	2.814	2.596
twisted-keto	S_0	2.520	2.577	2.982
	S_1	3.358	3.690	3.562

Table S12. Energy barriers $\Delta E^{\neq}$ (eV) for ESIPT from enol (S_1) and for twisting from keto (S_1).

Relative energy barriers $\Delta E^{\neq}$ (eV) in S_1 (CAM-B3LYP)			
Process	**Conf-1**	**Conf-2**	**Conf-3**
ESIPT	0.065	0.065	0.280
cis-trans	0.011	0.141	0.179

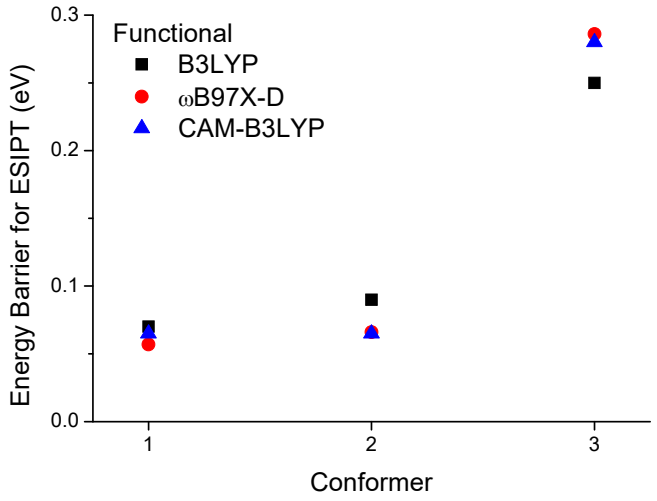


Figure S9 Energy barriers $\Delta E^{\neq}$ (eV) for ESIPT from enol (S_1) computed with three different functionals.

SECTION S6. ABSOLUTE ENERGIES OF ALL STATIONARY POINTS

Table S13. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-1**.

		Energy (a.u.) B3LYP		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1564.173546	-99.626453	-1663.800000
	S_1	-1564.035853	-99.626453	-1663.662306
enol (S_1)	S_0	-1564.165124	-99.629787	-1663.794911
	S_1	-1564.042510	-99.629787	-1663.672297
enol(S_1)	TS	-1564.039307	-99.630559	-1663.669866
keto (S_1)	S_0	-1564.150783	-99.629858	-1663.780641
	S_1	-1564.056922	-99.629858	-1663.686780
keto (S_1)	TS	-1564.057670	-99.629070	-1663.686740
triplet-keto	T_1	-1564.083191	-99.629858	-1663.713049
twisted-keto	S_0	-1564.083390	-99.627247	-1663.710637
	S_1	-1564.075474	-99.627247	-1663.702721

Table S14. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-2**.

		Energy (a.u.) B3LYP		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1717.095012	-99.394573	-1816.489585
	S_1	-1716.957524	-99.394573	-1816.352097
enol (S_1)	S_0	-1717.087172	-99.395196	-1816.482368
	S_1	-1716.964332	-99.395196	-1816.359528
enol (S_1)	TS	-1716.960827	-99.395414	-1816.356241
keto (S_1)	S_0	-1717.070746	-99.396383	-1816.467129
	S_1	-1716.980534	-99.396383	-1816.376917
keto (S_1)	TS	-1716.980113	-99.392645	-1816.372758
triplet-keto	T_1	-1717.000744	-99.396383	-1816.397127
twisted-keto	S_0	-1717.009401	-99.388905	-1816.398306
	S_1	-1716.991210	-99.388905	-1816.380114

Table S15. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-3**.

		Energy (a.u.) B3LYP		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1620.922156	-99.352549	-1720.274705
	S_1	-1620.790685	-99.352549	-1720.143234
enol (S_1)	S_0	-1620.916362	-99.354699	-1720.271061
	S_1	-1620.792255	-99.354699	-1720.146954
enol (S_1)	TS	-1620.785335	-99.352554	-1720.137890
keto (S_1)	S_0	-1620.895087	-99.358766	-1720.253853
	S_1	-1620.811714	-99.358766	-1720.170480
keto (S_1)	TS	-1620.816492	-99.349220	-1720.165712
triplet-keto	T_1	-1620.830791	-99.358766	-1720.189557
twisted-keto	S_0	-1620.821441	-99.347737	-1720.169178
	S_1	-1620.821658	-99.347737	-1720.169396

Table S16. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-1**.

		Energy (a.u.) ωB97X-D		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1564.5054	-99.6265	-1664.1319
	S_1	-1564.3560	-99.6265	-1663.9825
enol (S_1)	S_0	-1564.4939	-99.6298	-1664.1237
	S_1	-1564.3634	-99.6298	-1663.9932
enol(S_1)	TS	-1564.3605	-99.6306	-1663.9911
keto (S_1)	S_0	-1564.4799	-99.6299	-1664.1098
	S_1	-1564.3712	-99.6299	-1664.0011
keto (S_1)	TS	-1564.3719	-99.6291	-1664.0010
triplet-keto	T_1	-1564.4048	-99.6299	-1664.0347
twisted-keto	S_0	-1564.4172	-99.6272	-1664.0444
	S_1	-1564.3845	-99.6272	-1664.0117

Table S17. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-2**.

		Energy (a.u.) ωB97X-D		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1717.4552	-99.3946	-1816.8498
	S_1	-1717.3058	-99.3946	-1816.7004
enol (S_1)	S_0	-1717.4445	-99.3952	-1816.8397
	S_1	-1717.3131	-99.3952	-1816.7083
enol(S_1)	TS	-1717.3105	-99.3954	-1816.7059
keto (S_1)	S_0	-1717.4283	-99.3964	-1816.8247
	S_1	-1717.3203	-99.3964	-1816.7167
keto (S_1)	TS	-1717.3198	-99.3926	-1816.7124
triplet-keto	T_1	-1717.3495	-99.3964	-1816.7459
twisted-keto	S_0	-1717.3680	-99.3889	-1816.7569
	S_1	-1717.3252	-99.3889	-1816.7141

Table S18. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-3**.

		Energy (a.u.) ωB97X-D		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1621.2394	-99.3525	-1720.5919
	S_1	-1621.0966	-99.3525	-1720.4491
enol (S_1)	S_0	-1621.2317	-99.3547	-1720.5864
	S_1	-1621.0988	-99.3547	-1720.4535
enol(S_1)	TS	-1621.0904	-99.3526	-1720.4430
keto (S_1)	S_0	-1621.2091	-99.3588	-1720.5679
	S_1	-1621.1067	-99.3588	-1720.4655
keto (S_1)	TS	-1621.1103	-99.3492	-1720.4595
triplet-keto	T_1	-1621.1398	-99.3588	-1720.4938
twisted-keto	S_0	-1621.1369	-99.3477	-1720.4846
	S_1	-1621.1134	-99.3477	-1720.4611

Table S19. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-1**.

		Energy (a.u.) CAM-B3LYP		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1564.3329	-99.6265	-1663.9594
	S_1	-1564.1846	-99.6265	-1663.8111
enol (S_1)	S_0	-1564.3211	-99.6298	-1663.9509
	S_1	-1564.1916	-99.6298	-1663.8214
enol(S_1)	TS	-1564.1884	-99.6306	-1663.8190
keto (S_1)	S_0	-1564.3067	-99.6299	-1663.9366
	S_1	-1564.1985	-99.6299	-1663.8284
keto (S_1)	TS	-1564.1989	-99.6291	-1663.8280
triplet-keto	T_1	-1564.2330	-99.6299	-1663.8630
twisted-keto	S_0	-1564.2396	-99.6272	-1663.8668
	S_1	-1564.2089	-99.6272	-1663.8360

Table S20. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-2**.

		Energy (a.u.) CAM-B3LYP		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1717.2761	-99.3946	-1816.6707
	S_1	-1717.1279	-99.3946	-1816.5225
enol (S_1)	S_0	-1717.2653	-99.3952	-1816.6604
	S_1	-1717.1349	-99.3952	-1816.5301
enol(S_1)	TS	-1717.1323	-99.3954	-1816.5277
keto (S_1)	S_0	-1717.2486	-99.3964	-1816.6450
	S_1	-1717.1412	-99.3964	-1816.5376
keto (S_1)	TS	-1717.1398	-99.3926	-1816.5324
triplet-keto	T_1	-1717.1709	-99.3964	-1816.5673
twisted-keto	S_0	-1717.1871	-99.3889	-1816.5760
	S_1	-1717.1462	-99.3889	-1816.5351

Table S21. QM energies (a.u.), MM energies (a.u.), total QM/MM energies (a.u.) for **Conf-3**.

		Energy (a.u.) CAM-B3LYP		
Geometry	***States***	E_{QM}	E_{MM}	$E_{QM/MM}$
enol (S_0)	S_0	-1621.0931	-99.3525	-1720.4456
	S_1	-1621.9514	-99.3525	-1720.3039
enol (S_1)	S_0	-1621.0851	-99.3547	-1720.4398
	S_1	-1620.9532	-99.3547	-1720.3079
enol(S_1)	TS	-1620.9450	-99.3526	-1720.2976
keto (S_1)	S_0	-1621.0622	-99.3588	-1720.4210
	S_1	-1620.9606	-99.3588	-1720.3194
keto (S_1)	TS	-1620.9636	-99.3492	-1720.3128
triplet-keto	T_1	-1620.9914	-99.3588	-1720.3502
twisted-keto	S_0	-1620.9883	-99.3477	-1720.3360
	S_1	-1620.9670	-99.3477	-1720.3147

SECTION S7. CARTESIAN COORDINATES

Cartesian coordinates of the QM region of all species reported in the paper, from QM/MM geometries for Conf-1, Conf-2, and Conf-3.

Conf-1:

Enol(S_0)

C	30.1056806	1.3103506	49.1027594
H	29.9586223	1.7486493	48.1197128
H	31.0070621	0.7003878	49.0833001
N	30.3030350	2.4119968	50.0931476
H	30.1496861	2.0556929	51.0458094
H	29.6118442	3.1774584	49.9242076
H	31.2659597	2.8140995	50.1077630
C	34.1070037	2.4850694	52.8601363
H	34.2742846	3.1655740	53.6960164
H	33.8177150	1.5333123	53.3159339
C	32.8818255	3.0012385	52.0933885
O	32.9097037	3.1576812	50.8262212
O	31.8567892	3.2273466	52.7849434
C	27.0368355	-3.9234521	56.2655202
H	26.5656379	-3.5777490	57.1979705
O	26.2443404	-3.5833866	55.1391807
H	26.2317742	-2.6197430	55.0313067
C	28.4284092	-3.2966861	56.1930904
H	28.9517822	-3.5919463	55.2816824
H	29.0382531	-3.5557064	57.0629126
H	28.3347600	-2.2080819	56.1908865
S	22.8422428	2.0476011	52.3761911
C	23.9857719	0.9552835	53.1928779
N	23.4170211	-0.0332111	53.8346065
C	22.0399407	-0.0045902	53.7543409
C	21.1711729	-0.9098138	54.3721346
H	21.5875473	-1.7171914	54.9634401
C	19.8061890	-0.7338685	54.2129346
H	19.1068459	-1.4216928	54.6732463
C	19.3008425	0.3283491	53.4504020
H	18.2332503	0.4309816	53.3229454
C	20.1486449	1.2398602	52.8351416
H	19.7495720	2.0607280	52.2529267
C	21.5193072	1.0627801	52.9962969
C	25.4242514	1.1413707	53.1714629
C	26.0429555	2.2460828	52.5613825
H	25.4280534	3.0027600	52.0880272
C	27.4126698	2.4058205	52.5410083
H	27.8450846	3.2748413	52.0624009
C	28.2392017	1.4292104	53.1293740
N	29.6238719	1.5010154	53.0012555
H	30.1386771	0.8307674	53.5561657
H	30.0947451	2.4044506	53.0370935
C	27.6488042	0.3397157	53.7732668
H	28.2602561	-0.4100369	54.2610796
C	26.2651180	0.1963270	53.8185895
O	25.7584821	-0.8488759	54.5053036
H	24.7566229	-0.8058914	54.4345578
H	29.2529985	0.7049849	49.4102202
H	35.0593105	2.3551165	52.3460445
H	27.1147593	-5.0105117	56.2827143

Enol(S_1)

C	30.1018736	1.3001236	49.1054163
H	29.9405224	1.7298973	48.1208601
H	31.0093841	0.6997210	49.0812254
N	30.2990166	2.4131467	50.0828126
H	30.1815694	2.0646494	51.0412228
H	29.5895176	3.1650438	49.9248491
H	31.2522865	2.8346010	50.0693764
C	34.0926104	2.4986422	52.8440697
H	34.2569772	3.1826762	53.6778819
H	33.8054456	1.5479473	53.3030553
C	32.8680000	3.0104506	52.0736178
O	32.9048336	3.1893329	50.8120550
O	31.8321205	3.2130137	52.7608851
C	27.0043461	-3.9139835	56.2458318
H	26.5290682	-3.5690370	57.1763701
O	26.2155633	-3.5752778	55.1163406
H	26.1722063	-2.6100246	55.0313387
C	28.3943836	-3.2822808	56.1798808
H	28.9297065	-3.5826498	55.2770743
H	28.9940910	-3.5301590	57.0597306
H	28.2949684	-2.1943322	56.1670109
S	22.9197100	2.1659704	52.3360394
C	24.0503943	0.9820539	53.0986714
N	23.4178107	-0.0548923	53.7186398
C	22.0829600	0.0555045	53.6688255
C	21.1511310	-0.8357614	54.2604939
H	21.5283589	-1.6923141	54.8064015
C	19.8044066	-0.5803938	54.1259235
H	19.0752282	-1.2531366	54.5624910
C	19.3366041	0.5481645	53.4146598
H	18.2737264	0.7048064	53.3051176
C	20.2245324	1.4467646	52.8303461
H	19.8562429	2.3097657	52.2906497
C	21.5833065	1.2052735	52.9563313
C	25.4422463	1.1722318	53.1550799
C	26.1093530	2.2948456	52.5736210
H	25.5212699	3.0777298	52.1104734
C	27.4842237	2.3990516	52.5833360
H	27.9555623	3.2600447	52.1252503
C	28.2825174	1.3914199	53.1768710
N	29.6646430	1.4254154	53.0584798
H	30.1624972	0.7283272	53.5960075
H	30.1768204	2.3102240	53.0639936
C	27.6549121	0.3044459	53.8159962
H	28.2454867	-0.4488390	54.3242852
C	26.2789735	0.1987562	53.8497824
O	25.7123768	-0.8039377	54.5397659
H	24.7018266	-0.7519236	54.3945987
H	29.2575501	0.6887977	49.4239517
H	35.0461972	2.3704128	52.3319213
H	27.0862032	-5.0007463	56.2635143

Keto(S_1)

C	30.1108993	1.3014153	49.0733209
H	29.9356267	1.7322006	48.0917173
H	31.0194221	0.7033970	49.0367134
N	30.3180081	2.4135614	50.0498009
H	30.2198524	2.0621627	51.0081856
H	29.6006943	3.1609777	49.9063668
H	31.2668907	2.8414524	50.0202052
C	34.1113183	2.5217274	52.8226146
H	34.2776334	3.2121675	53.6506084
H	33.8153896	1.5772871	53.2889758
C	32.8948663	3.0354622	52.0418698
O	32.9327591	3.1956192	50.7787075
O	31.8598959	3.2582258	52.7248519
C	26.9869746	-3.9106163	56.2244242
H	26.5156034	-3.5637373	57.1572371
O	26.1937958	-3.5801585	55.0993255
H	26.1947237	-2.6142263	54.9702544
C	28.3758915	-3.2750241	56.1553204
H	28.9107186	-3.5761276	55.2521932
H	28.9777216	-3.5197574	57.0348533
H	28.2716471	-2.1878525	56.1395806
S	22.9311363	2.0158346	52.3814166
C	24.0731262	0.9311091	53.1731375
N	23.4032323	-0.0582784	53.8385557
C	22.0382731	-0.0193169	53.7815860
C	21.1322686	-0.9029807	54.3835122
H	21.5018368	-1.7321307	54.9755889
C	19.7740088	-0.6723558	54.2021819
H	19.0489526	-1.3442170	54.6463063

C	19.3139590	0.4082752	53.4456437
H	18.2537163	0.5526695	53.3026813
C	20.2120047	1.2936009	52.8451278
H	19.8552190	2.1323164	52.2609608
C	21.5668245	1.0684481	53.0185289
C	25.5163483	1.1010494	53.1974166
C	26.1474440	2.2051026	52.6695647
H	25.5469938	3.0055402	52.2496507
C	27.5709371	2.3826459	52.6192311
H	27.9650114	3.2840869	52.1692043
C	28.3884945	1.4056499	53.1268496
N	29.7717389	1.4119310	53.0287176
H	30.2440013	0.7310247	53.6070483
H	30.2944352	2.2913746	53.0195332
C	27.7648909	0.2616631	53.7329764
H	28.3758302	-0.5171683	54.1744661
C	26.3554354	0.0986239	53.8243874
O	25.8618717	-0.8977303	54.4561839
H	23.9736320	-0.7419432	54.3376837
H	29.2724863	0.6877257	49.4027371
H	35.0657709	2.3812059	52.3153273
H	27.0752888	-4.9967601	56.2480629

Twist-keto

C	30.0903373	1.3587593	48.9914945
H	30.0238051	1.8466881	48.0231921
H	30.9635359	0.7091224	48.9993151
N	30.2799424	2.4085580	50.0422933
H	30.2263373	1.9888171	50.9795037
H	29.5365090	3.1392884	49.9584118
H	31.2091326	2.8716716	50.0211179
C	34.0976801	2.4630344	52.8427474
H	34.2673668	3.1561615	53.6685054
H	33.8280728	1.5149540	53.3170757
C	32.8547644	2.9616531	52.0905200
O	32.8999865	3.2375820	50.8482412
O	31.8048100	3.0590552	52.7808347
C	26.8920980	-3.7982452	56.1908286
H	26.5056491	-3.4809420	57.1625054
O	25.9218050	-3.3584867	55.2439345
H	26.2478574	-3.4714647	54.3351405
C	28.2505972	-3.1309295	55.9848480
H	28.7073936	-3.4079842	55.0321244
H	28.9448237	-3.3852698	56.7909089
H	28.1249928	-2.0472296	55.9925978
S	23.7875192	0.5478587	52.3416556
C	24.7343458	-0.5833441	53.3078230
N	24.0165786	-0.9344478	54.4572078
C	22.6502239	-0.7454152	54.3160601
C	21.6274955	-1.2709112	55.1076983
H	21.8756128	-1.9098061	55.9468663
C	20.3088754	-0.9556197	54.7846092
H	19.4877225	-1.3520262	55.3697666
C	19.9927827	-0.1321395	53.7054503
H	18.9591039	0.0934361	53.4774881
C	21.0084456	0.3721480	52.8962755
H	20.7750563	0.9961248	52.0427305
C	22.3203254	0.0472572	53.2025257
C	26.2169368	-0.3764557	53.3396699
C	26.7675896	0.7837762	53.8076722
H	26.1145660	1.5424776	54.2176655
C	28.1214533	1.1196597	53.6041318
H	28.4596204	2.1226351	53.8287181
C	29.0105602	0.2074950	53.0150190
N	30.3054882	0.5985397	52.6878390
H	30.9804093	-0.1468634	52.5960967
H	30.7065757	1.4263765	53.1263570
C	28.5191026	-1.0421337	52.6695005
H	29.1662193	-1.8007006	52.2477711
C	27.1331556	-1.3921294	52.8119681
O	26.7495616	-2.5651194	52.5798619
H	24.3882815	-1.6876458	55.0286595
H	29.1928584	0.7854926	49.2237948
H	35.0482015	2.3439446	52.3227539
H	27.0107572	-4.8817384	56.1962226

Conf-2:

Enol(S_0)

C	28.4668184	0.3144039	48.8525910
H	28.6864508	0.4071594	47.7908164
H	29.0297614	-0.5218919	49.2614963
N	28.9224739	1.5668378	49.5388244
H	29.9501046	1.7776573	49.4181354
H	28.7646412	1.4831057	50.5453051
H	28.3403924	2.3896020	49.2664922
C	33.5061911	2.5464920	51.0549868
H	33.6981452	3.4212988	51.6735188
H	33.5785066	1.6756634	51.7159727
C	32.0525206	2.5990237	50.5771851
O	31.6852823	1.9635674	49.5471023
O	31.2411165	3.2558446	51.3056279
C	27.8074757	-3.6067910	56.6361366
H	27.6122735	-3.3874359	57.6932312
O	26.6194628	-3.3654571	55.8716235
H	26.6348359	-2.4763687	55.4754688
C	28.9784303	-2.7346005	56.1954280
H	29.8619364	-2.9172142	56.8125218
H	28.7130610	-1.6842241	56.3364013
H	29.2408585	-2.8941902	55.1479584
S	23.0621167	1.7599312	52.1449099
C	24.1633130	0.8326577	53.1880927
N	23.5764894	-0.0779814	53.9229500
C	22.2085304	-0.1255082	53.7201504
C	21.3130340	-0.9815092	54.3677107
H	21.6685266	-1.6730110	55.1219032
C	19.9680941	-0.9164808	54.0321922
H	19.2603087	-1.5654693	54.5318508
C	19.5084460	-0.0169244	53.0584308
H	18.4558108	0.0029751	52.8028541
C	20.3806669	0.8607223	52.4246199
H	20.0204676	1.5660682	51.6879858
C	21.7272704	0.7947365	52.7655362
C	25.5977342	1.0426271	53.1992500
C	26.2138363	2.0776334	52.4799597
H	25.6029065	2.7770427	51.9207732
C	27.5819624	2.2562562	52.4710830
H	27.9971881	3.0986192	51.9339505
C	28.4209954	1.3960671	53.2154093
N	29.7725908	1.5824086	53.2370191
H	30.3546095	0.9827654	53.7968657
H	30.2388074	2.2480702	52.6261350
C	27.8227238	0.3484222	53.9350537
H	28.4360998	-0.3397832	54.5020810
C	26.4438330	0.1806670	53.9509542
O	25.9359014	-0.8272626	54.6995662
H	24.9342097	-0.7957590	54.6098472
O	22.0068336	-2.3355100	58.1674205
H	22.1089246	-1.3792324	58.2081776
H	22.8581790	-2.6727851	57.8044545
O	24.4267938	-3.2913685	57.5807350
H	25.1390382	-3.3676297	56.9134075
H	24.7467715	-3.7305989	58.3894536
H	27.3970650	0.1744228	49.0078310
H	34.2938310	2.4692160	50.3055081
H	28.0712292	-4.6586595	56.5262591

Enol(S_1)

C	28.4456954	0.3290230	48.8374891
H	28.6684325	0.4260938	47.7766961
H	29.0061465	-0.5100941	49.2440632
N	28.9006538	1.5771192	49.5315237
H	29.9280861	1.7842632	49.4201938
H	28.7319491	1.4906546	50.5380707
H	28.3240742	2.4036392	49.2584292
C	33.5094873	2.5372773	51.0650077
H	33.7042135	3.4095028	51.6863855
H	33.5825780	1.6630350	51.7215643
C	32.0549874	2.5924213	50.5912047
O	31.6816528	1.9617560	49.5618458
O	31.2471064	3.2470057	51.3279439
C	27.8376085	-3.6204229	56.6513742

H	27.6443844	-3.4033096	57.7092417
O	26.6517456	-3.3652563	55.8881772
H	26.6756330	-2.4735926	55.4977996
C	29.0153973	-2.7565553	56.2129554
H	29.8984636	-2.9502923	56.8270724
H	28.7594112	-1.7048017	56.3606817
H	29.2727021	-2.9115389	55.1635798
S	23.1612877	1.8066657	52.1840118
C	24.2831924	0.8297187	53.2160454
N	23.6591005	-0.1176531	53.9660288
C	22.3322846	-0.1437990	53.7480086
C	21.4002057	-1.0051326	54.3746253
H	21.7404311	-1.7065862	55.1262823
C	20.0694535	-0.9180149	54.0249057
H	19.3455548	-1.5609858	54.5094153
C	19.6174194	0.0027695	53.0476005
H	18.5661480	0.0329856	52.7896647
C	20.5026259	0.8800420	52.4302780
H	20.1488709	1.5945922	51.6986862
C	21.8444875	0.8128168	52.7793583
C	25.6699596	1.0317752	53.2038504
C	26.2933957	2.0768935	52.4468891
H	25.6796740	2.7603013	51.8741066
C	27.6638975	2.2498830	52.4613385
H	28.0874179	3.0878347	51.9222207
C	28.5011700	1.4097932	53.2337729
N	29.8462036	1.6378403	53.3150011
H	30.4212926	1.0236142	53.8687920
H	30.3244316	2.2619492	52.6653584
C	27.9090887	0.3548842	53.9754724
H	28.5321927	-0.3115512	54.5577218
C	26.5443071	0.1720638	53.9860201
O	26.0179275	-0.8229024	54.7284760
H	25.0058418	-0.7917316	54.6235378
O	22.0591494	-2.3029264	58.1904202
H	22.1770247	-1.3484146	58.2291797
H	22.9001048	-2.6551471	57.8167874
O	24.4419636	-3.3227035	57.5719663
H	25.1635763	-3.3801129	56.9126476
H	24.7648410	-3.7511250	58.3852701
H	27.3753339	0.1902785	48.9896161
H	34.2952470	2.4624118	50.3133140
H	28.0917278	-4.6741106	56.5363433

Keto(S_1)

C	28.4532837	0.3294077	48.8560063
H	28.6947927	0.4046268	47.7975645
H	29.0063569	-0.5015095	49.2889533
N	28.8948593	1.5912240	49.5327116
H	29.9206718	1.7996698	49.4258129
H	28.7092476	1.5305124	50.5413207
H	28.3191504	2.4100880	49.2392933
C	33.5199535	2.5413332	51.0634298
H	33.7163905	3.4082311	51.6915067
H	33.5911471	1.6617035	51.7131918
C	32.0657835	2.6010135	50.5897952
O	31.6894141	1.9726527	49.5612276
O	31.2600657	3.2563552	51.3290036
C	27.8292861	-3.6085811	56.6465534
H	27.6471988	-3.3967803	57.7074939
O	26.6340164	-3.3530718	55.9053162
H	26.6886754	-2.5126244	55.4052975
C	28.9999578	-2.7355535	56.2049550
H	29.8879397	-2.9261042	56.8130107
H	28.7355713	-1.6867283	56.3567529
H	29.2540037	-2.8866671	55.1538905
S	23.1856441	1.5212647	52.0144588
C	24.2926184	0.6350115	53.0617235
N	23.5888148	-0.1677672	53.9256486
C	22.2302721	-0.2189406	53.7352065
C	21.3015747	-1.0087133	54.4206413
H	21.6113940	-1.6724366	55.2190861
C	19.9618285	-0.9086803	54.0598153
H	19.2292370	-1.5107188	54.5820688
C	19.5433322	-0.0485769	53.0395114
H	18.4951469	0.0005557	52.7724485
C	20.4656875	0.7521096	52.3604782
H	20.1387562	1.4264994	51.5799322
C	21.8009650	0.6530550	52.7144354
C	25.7221297	0.8866272	53.1320269
C	26.3139224	1.9581983	52.5038436
H	25.6922059	2.6829706	51.9881089
C	27.7261171	2.2071437	52.4664204
H	28.0704892	3.0937314	51.9538848
C	28.5818076	1.3945091	53.1739351
N	29.9250478	1.5856361	53.2816702
H	30.4841988	0.9161172	53.7835600
H	30.4129366	2.2485082	52.6787260
C	27.9948976	0.2661524	53.8604791
H	28.6348246	-0.4243140	54.3950606
C	26.5948931	-0.0084319	53.8645898
O	26.1521078	-1.0199132	54.5079832
H	24.1146776	-0.8004441	54.5188957
O	22.0392151	-2.2972077	58.1918812
H	22.1375831	-1.3442241	58.2853400
H	22.9049588	-2.6160845	57.8434183
O	24.4847849	-3.1760268	57.6223757
H	25.1899461	-3.2647104	56.9454390
H	24.7871421	-3.6624403	58.4105878
H	27.3807329	0.1904265	48.9915996
H	34.3053959	2.4684493	50.3112100
H	28.0920339	-4.6599185	56.5294218

Twist-keto

C	28.5151678	0.3511727	48.7999712
H	28.6652044	0.5008684	47.7320946
H	29.1068097	-0.5026559	49.1238936
N	29.0039764	1.5686620	49.5233455
H	29.9851957	1.8486310	49.2820090
H	29.0639812	1.3941224	50.5408570
H	28.3506041	2.3733139	49.4042323
C	33.5326873	2.5805196	51.0679677
H	33.7352223	3.4473340	51.6946063
H	33.5840918	1.7033628	51.7224254
C	32.0866613	2.6679161	50.5624055
O	31.7433733	2.0548425	49.5090170
O	31.2709005	3.3279122	51.2779689
C	27.7921969	-3.5741935	56.5940538
H	27.6626057	-3.3556777	57.6574339
O	26.5309302	-3.2980639	55.9854792
H	26.6062501	-3.0580728	55.0446001
C	28.9093914	-2.6777736	56.0674302
H	29.8357200	-2.8280343	56.6285693
H	28.6165626	-1.6334108	56.1929764
H	29.1169630	-2.8507062	55.0090496
S	22.9844359	0.5557526	51.9629722
C	23.9175285	0.0116270	53.3437406
N	23.1029689	-0.0740844	54.4767296
C	21.7640843	-0.2577082	54.1367656
C	20.7582216	-0.7812197	54.9438536
H	20.9625507	-1.1071452	55.9568318
C	19.4909310	-0.9426942	54.3912835
H	18.7189817	-1.4196238	54.9793812
C	19.2034719	-0.5307633	53.0877749
H	18.1997791	-0.6378447	52.6959472
C	20.2110125	-0.0176187	52.2749744
H	19.9946537	0.2886676	51.2594558
C	21.4914299	0.0702898	52.7993140
C	25.3642174	0.3652086	53.3893418
C	25.8132037	1.6572532	53.4272262
H	25.1040634	2.4715290	53.5190383
C	27.1581129	1.9849025	53.1364446
H	27.4096126	3.0233284	52.9647215
C	28.1187015	0.9817384	52.9372374
N	29.4058155	1.2875489	52.4851461
H	30.1259907	0.6223953	52.7292507
H	29.7493938	2.2386578	52.5497122
C	27.7228208	-0.3402950	53.0698391
H	28.4165918	-1.1608714	52.9537597
C	26.3619981	-0.7013479	53.3198247
O	26.0447688	-1.8964868	53.5599585
H	23.4692371	-0.5736416	55.2742103

O	21.9331537	-2.1928380	58.2432059
H	22.0284558	-1.2744595	58.5169338
H	22.8289501	-2.4581597	57.9248991
O	24.4818423	-2.8444600	57.7757382
H	25.1244722	-2.9863829	57.0504193
H	24.7553134	-3.4422681	58.4961184
H	27.4573086	0.1891952	49.0067648
H	34.3227233	2.4937753	50.3220555
H	28.0696513	-4.6223866	56.4828033

Conf-3:

Enol(S_0)

C	32.5387378	3.3400645	50.2215343
H	32.7622250	4.1845526	50.8744425
H	32.7960795	2.4327977	50.7780845
C	31.0206297	3.3261579	49.9527294
O	30.5534628	2.6821369	48.9804585
O	30.2988801	3.9647246	50.7902808
C	30.8134432	-3.0807865	56.7422679
H	30.8074711	-2.6386296	57.7402204
O	29.4240170	-3.1985269	56.3780205
H	29.2715613	-3.9111797	55.7356676
C	31.5540640	-2.1456358	55.7892329
H	31.0458968	-1.1797536	55.7789780
H	31.5764235	-2.5225635	54.7644851
H	32.5829996	-1.9761610	56.1202761
S	23.1206997	1.7932723	52.1524949
C	24.2225916	0.9622673	53.2829843
N	23.6311441	0.0802090	54.0613902
C	22.2667328	-0.0052167	53.8188572
C	21.3626009	-0.8438487	54.4774608
H	21.7119514	-1.5185339	55.2496908
C	20.0192648	-0.7891153	54.1216694
H	19.3002013	-1.4353738	54.6123447
C	19.5626296	0.0895145	53.1323998
H	18.5124816	0.1178141	52.8801160
C	20.4475473	0.9322539	52.4763095
H	20.0957295	1.6184094	51.7182615
C	21.7916318	0.8658793	52.8178712
C	25.6287487	1.2570358	53.2900093
C	26.1622247	2.2000320	52.3922814
H	25.4884785	2.7134108	51.7227257
C	27.4958317	2.5006918	52.3424558
H	27.8723848	3.2394071	51.6468981
C	28.3924783	1.8910901	53.2516789
N	29.7102082	2.2207896	53.2072212
H	30.3172104	2.0022239	53.9795036
H	30.0362283	2.8743409	52.5002481
C	27.8847322	0.9458081	54.1634200
H	28.5498566	0.4519590	54.8605413
C	26.5359063	0.6283412	54.1801416
O	26.0989484	-0.3157781	55.0684226
H	25.1336588	-0.4586999	54.9077346
O	27.4989056	-1.4293636	57.3214125
H	26.9519148	-1.0651989	56.5987388
H	28.0950262	-2.0914332	56.9092122
O	29.3555296	-1.4457830	59.5309029
H	29.2409701	-2.3368847	59.9264588
H	28.5563092	-1.3219618	58.9951411
H	33.1802655	3.3912810	49.3418266
H	31.3014935	-4.0545341	56.7833644

Enol(S_1)

C	32.5414068	3.3352162	50.2302875
H	32.7670761	4.1762802	50.8867721
H	32.8059007	2.4261360	50.7810622
C	31.0217451	3.3132696	49.9749514
O	30.5471243	2.6872089	48.9968720
O	30.3028004	3.9278149	50.8369507
C	30.8135730	-3.0795054	56.7417165
H	30.8060452	-2.6372041	57.7396030
O	29.4249769	-3.1954728	56.3741987
H	29.2719414	-3.9117336	55.7358781
C	31.5567415	-2.1445554	55.7902426
H	31.0489247	-1.1783610	55.7797401
H	31.5807375	-2.5213880	54.7654751
H	32.5850626	-1.9753331	56.1233064
S	23.1180828	1.7910052	52.1354871
C	24.2263553	0.9574843	53.2761532
N	23.6153342	0.0592599	54.0846658
C	22.2884128	-0.0254349	53.8362009
C	21.3536015	-0.8694352	54.4907699
H	21.6904463	-1.5517787	55.2615885
C	20.0217042	-0.7996885	54.1263139
H	19.2938716	-1.4412361	54.6117386
C	19.5629930	0.0871887	53.1322626
H	18.5132039	0.1202060	52.8805281
C	20.4581962	0.9282153	52.4781404
H	20.1133591	1.6168050	51.7185521
C	21.8001230	0.8585825	52.8143152
C	25.6235205	1.2597564	53.2824028
C	26.1494543	2.2119117	52.3769131
H	25.4692269	2.7242366	51.7139819
C	27.4905361	2.5136112	52.3322763
H	27.8686494	3.2544427	51.6398122
C	28.3907795	1.9008699	53.2388067
N	29.7081566	2.2432760	53.1963492
H	30.3151781	2.0332471	53.9735498
H	30.0391667	2.8761862	52.4651289
C	27.8924546	0.9457867	54.1564324
H	28.5668934	0.4562348	54.8480811
C	26.5501605	0.6247590	54.1810826
O	26.1004730	-0.3162484	55.0615707
H	25.1253098	-0.4410820	54.9069354
O	27.4956029	-1.4255583	57.3188171
H	26.9406423	-1.0684160	56.5988488
H	28.0883524	-2.0905459	56.9070510
O	29.3563966	-1.4453244	59.5270628
H	29.2425277	-2.3355716	59.9249814
H	28.5522278	-1.3196724	58.9994783
H	33.1781113	3.3903558	49.3473189
H	31.3016238	-4.0532260	56.7834437

Keto(S_1)

C	32.5555378	3.3331295	50.2335832
H	32.7796275	4.1784483	50.8854636
H	32.8194210	2.4281433	50.7907110
C	31.0356015	3.3149573	49.9755360
O	30.5652636	2.6930444	48.9897419
O	30.3172086	3.9289324	50.8335962
C	30.7960137	-3.0249012	56.7286375
H	30.7826482	-2.5835574	57.7269396
O	29.4098212	-3.1390812	56.3520757
H	29.2643188	-3.8617772	55.7201215
C	31.5480077	-2.0905125	55.7827904
H	31.0399390	-1.1248412	55.7623111
H	31.5837364	-2.4696586	54.7590999
H	32.5728227	-1.9188666	56.1260157
S	23.0112617	1.9067384	52.2449323
C	24.1283207	1.0415582	53.2982825
N	23.4793905	0.0069662	53.9288841
C	22.1185187	-0.0485712	53.7523544
C	21.2037469	-0.8926446	54.3898412
H	21.5349619	-1.5960895	55.1434052
C	19.8591870	-0.7810368	54.0506246
H	19.1291986	-1.3944260	54.5633943
C	19.4234418	0.1333160	53.0942291
H	18.3756236	0.1925782	52.8394156
C	20.3297531	0.9986360	52.4786644
H	19.9886276	1.7326546	51.7612626
C	21.6664730	0.9031300	52.8191105
C	25.5617921	1.2800134	53.3236791
C	26.1691937	1.9788515	52.3041022
H	25.5544800	2.2795355	51.4655915
C	27.5337149	2.3730369	52.2698434
H	27.9048882	3.0044467	51.4746064
C	28.3625927	2.0023631	53.2990740
N	29.6959385	2.2981107	53.3467100
H	30.1427385	2.3422322	54.2525757
H	30.0728048	2.8849454	52.6045352

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C    27.7853837    1.1985323   54.3498215
H    28.4129405    0.8661035   55.1651764
C    26.3937141    0.8525362   54.4105913
O    25.9539224    0.1835549   55.4198495
H    23.9606734   -0.4699935   54.6816597
O    27.4712412   -1.2684879   57.2783753
H    26.9169956   -0.8032263   56.6067668
H    28.0173687   -1.9317318   56.8117033
O    29.3304185   -1.4211149   59.5086663
H    29.2159026   -2.3065425   59.9167259
H    28.5434408   -1.3133966   58.9503075
H    33.1921222    3.3866346   49.3504275
H    31.2871210   -3.9969917   56.7724580

Twist-keto

C    32.5552555    3.3209351   50.2069194
H    32.7588207    4.1712258   50.8589070
H    32.8242683    2.4218767   50.7710790
C    31.0392133    3.2769718   49.9304732
O    30.5955836    2.6530552   48.9308555
O    30.2972989    3.8632411   50.7848365
C    30.7583032   -2.9795731   56.7262481
H    30.7622503   -2.5344580   57.7227879
O    29.3644829   -3.0957348   56.3783101
H    29.2200833   -3.7959510   55.7218806
C    31.4925380   -2.0495628   55.7620505
H    30.9867863   -1.0827020   55.7468864
H    31.5072501   -2.4333469   54.7393322
H    32.5251077   -1.8796062   56.0827480
S    23.1036872    2.4295197   52.9533737
C    24.1185349    1.1424304   53.5956442
N    23.5236823   -0.0899850   53.3164992
C    22.1557211   -0.0030635   53.1249485
C    21.2248201   -1.0317563   53.2165181
H    21.5433809   -2.0252169   53.5025845
C    19.8874021   -0.7401859   52.9791501
H    19.1460861   -1.5214876   53.0695117
C    19.4823385    0.5488761   52.6462579
H    18.4446158    0.7441568   52.4212741
C    20.4039271    1.5944335   52.6118569
H    20.0775721    2.5997456   52.3810777
C    21.7335569    1.3141231   52.8766434
C    25.6132674    1.2440250   53.5079934
C    26.2662598    1.3585026   52.3128543
H    25.6916535    1.3638611   51.3945435
C    27.6154064    1.7762879   52.2527650
H    28.0166436    2.1736250   51.3299914
C    28.4240709    1.8569275   53.4155371
N    29.7365408    2.2441630   53.3224953
H    30.2005875    2.4881171   54.1866115
H    30.0350701    2.7474578   52.4907529
C    27.8371362    1.4770238   54.6060005
H    28.4122074    1.4076265   55.5126497
C    26.4540799    1.1705728   54.7084725
O    25.9724270    0.6891161   55.7802100
H    23.8876049   -0.8873195   53.8153619
O    27.4937684   -1.1296265   57.3946817
H    26.9382471   -0.5516504   56.8262646
H    27.9652231   -1.7758010   56.8352278
O    29.3801161   -1.3908717   59.5459986
H    29.2430097   -2.2825549   59.9320031
H    28.6018669   -1.2497839   58.9812483
H    33.2009379    3.3795110   49.3307176
H    31.2541058   -3.9494324   56.7664855
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