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Electronic Supplementary Information

Fragmentation and rearrangement of Breslow intermediates: branches to both of radical and ionic pathways

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1. Computational details

All structures are first optimized in the gas phase at the level of open-shell density functional theory (DFT) using the M06-2X functional[1] with D3 dispersion correction[2] incorporating the 6-31+G(d,p) basis set,[3] denoted as UM06-2X-D3/6-31+G(d,p). Frequencies are calculated to confirm the stationary points. All of the computed wavefunctions are confirmed stable. For model systems, single-point energies are calculated by coupled-cluster theory with single, double, and perturbative triple excitations (CCSD(T))[4, 5] combined with Dunning's aug-cc-pVDZ basis set[6] to assess the accuracy in energies. The open-shell UCCSD(T) calculations are carried out based on unrestricted Hartree-Fock determinant as the reference wavefunction. For the systems of thiamin and *N*-allyl benzothiazole, Truhlar's universal solvent model (SMD)[7] is additionally employed to optimize the geometries and to calculate the Gibbs free energies of each species at 298.15K. In the DFT calculations, the radical character could be verified by the plots of spin densities, while the ionic character and charge could be assigned by the Mulliken charges. The DFT and CCSD(T) calculations are performed with Gaussian 16 program.[8] Comparison between the DFT and CCSD(T) energies show that the deviations between the two methods are less than 5 kcal/mol, suggesting the accuracy in the combination of the functional and the basis set (Table S1 and S2) for the NHC systems. For detailed mechanisms of model systems, see Section 2. The notations of total energy and Gibbs free energy are E and G, respectively.

Table S1. Comparison between energies (kcal/mol) calculated at DFT and CCSD(T) levels in the enol system.

	UM06-2X-D3/ 6-31+G(d,p)	UCCSD(T)/aug-cc-pVDZ// UM06-2X-D3/6-31+G(d,p)
neutral singlet		
2a	0.0	0.0
TSa$_{2\text{-}67}$	37.2	34.7
[6a 7a]	32.8	30.6
TSa$_{2\text{-}5}$	27.9	25.8
5a	–27.1	–31.7
doublet cation		
2a^{+}	137.7	136.9
TSa$_{2\text{-}67}^{+}$	178.1	174.7
[6a 7a]$^{+}$	177.6	173.2

Table S2. Comparison between energies (kcal/mol) calculated at DFT and CCSD(T) levels in the enolate system.

	UM06-2X-D3/ 6-31+G(d,p)	UCCSD(T)/aug-cc-pVDZ// UM06-2X-D3/6-31+G(d,p)
singlet anion		
2'a	0.0	0.0
TSa'$_{2\text{-}67}$	20.4	21.4
[6a 7'a]	13.9	14.5
[8a 4a]	8.5	8.0
TS'a$_{2\text{-}5}$	16.4	16.0
5'a	–18.2	–22.5
neutral doublet[a]		
2'a^{+}	19.3	20.7
TS'a$_{2\text{-}84}^{+}$	47.9	45.3
[8a 4a]$^{+}$	32.8	28.8

[a] The neutral doublet compounds have one less electron compared to the singlet anion species. To keep consistency with the compound names in the enol system in Table S1, we denote the corresponding neutral doublet compounds with the superscript "+" next to the neutral doublet compounds.

Multireference theories are exclusively carried out to examine the electronic configurations of each geometry in each system, and to quantify the radical and the ionic characters. State-average complete active space self-consistent field (SA-CASSCF)[9] with the multi-state dynamical correlation in the second-order perturbation theory (MS-CASPT2)[10] is performed along the intrinsic reaction coordinate (IRC), which are determined at DFT level with local quadratic approximation (LQA).[11, 12] The active spaces consist of the π and π* orbitals of NHC, π and π* orbitals of allyl group as well as σ and σ* orbitals of the C–N bond, resulting in the combination of 8 active electrons in 8 active orbitals (denoted as SA-CAS(8,8)) for the enol system (Figure S1) and SA-CAS(10,10) for the enolate system (Figure S2), respectively. Rydberg states found in the enolate system are depicted with additional 7 s and 7 p functions, whose exponents are set from 0.025 to 0.000025 in an even-tempered manner at the center of mass.[13] Two-electron integrals are accelerated by the resolution of identity combined with Cholesky decomposition, abbreviated as RICD.[14] In the MS-CASPT2 calculation, the IPEA value is set as 0.25 by default while the imaginary shift is set at 0.1 to eliminate intruder states.[15, 16] The MS-CASPT2 calculations performed in this work aim to provide a quantitative description rather than qualitative picture. The multireference calculations are performed with the OpenMolcas suite of programs.[17]

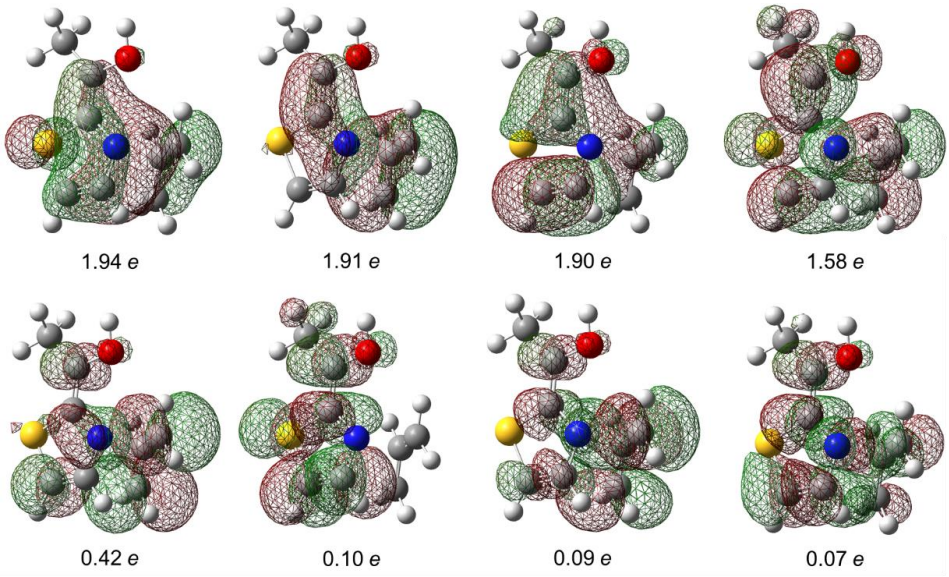


Figure S1. Active space of SA-CAS(8,8) wavefunction of the enol system (**TSa**$_{2\text{-}67}$). Ground-state electron occupation numbers are listed below each natural orbital. The isovalue is 0.02, and natural orbitals are calculated at the level of SA-CASSCF/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p).

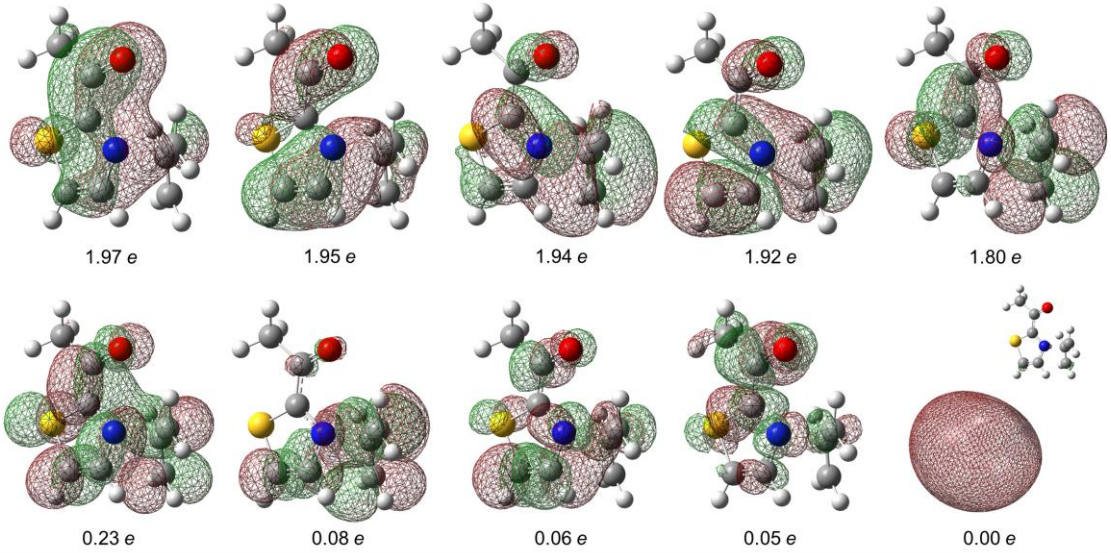


Figure S2. Active space of SA-CAS(10,10) wavefunction of the enolate system (**TS'a**$_{2\text{-}67}$). Ground-state electron occupation numbers are listed below each natural orbital. The isovalue is 0.02 except for the Rydberg state, whose isovalue is 0.00053. Natural orbitals are calculated at the level of SA-CASSCF/aug-cc-pVDZ+7s7p//UM06-2X-D3/6-31+G(d,p).

2. Breslow intermediate of the model system

Structures in Scheme 2 are utilized as our model system to investigate the C–N bond scission regarding the protonation state of the hydroxyl group. Similar to the system of *N*-allyl benzothiazole (**2c**), the model systems could proceed with a Claisen rearrangement (**2a** → **5a** and **2'a** → **5'a**) with lower energy barriers (*c.a.* 25.8 and 16.0 kcal/mol in the enol and the enolate systems, respectively, at UCCSD(T)/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p) level) compared to the fragmentation (Figure S3). As a result, the rearrangement product (**5a**/**5'a**) is excepted to be the major product. One may propose that the Breslow intermediate could be oxidized first before the fragmentation; however, according to our calculation shown in Figure S4, the required activation energies for C–N bond cleavage are 3~4 kcal/mol higher than the singlet state (37.8 and 24.6 kcal/mol, respectively, for enol and enolate systems at the same level). In addition, the doublet states are energetically higher than the singlet state throughout the reaction coordinate. It should be noted that the energies in Figure S4 are total energies (E) in the gas phase and should not be compared directly to other energy profiles.

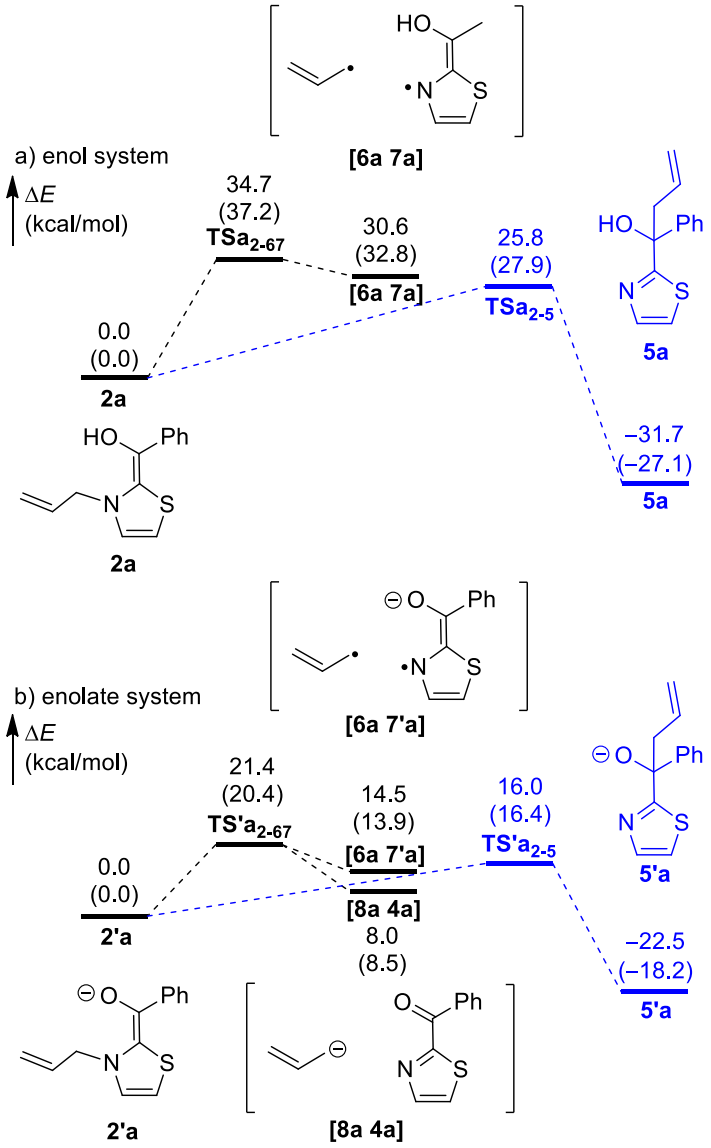


Figure S3. Energy profiles of the fragmentation and rearrangement of a) the enol and b) the enolate forms of model Breslow intermediates. The energies are calculated at the levels of UCCSD(T)/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p), and UM06-2X-D3/6-31+G(d,p) in parentheses.

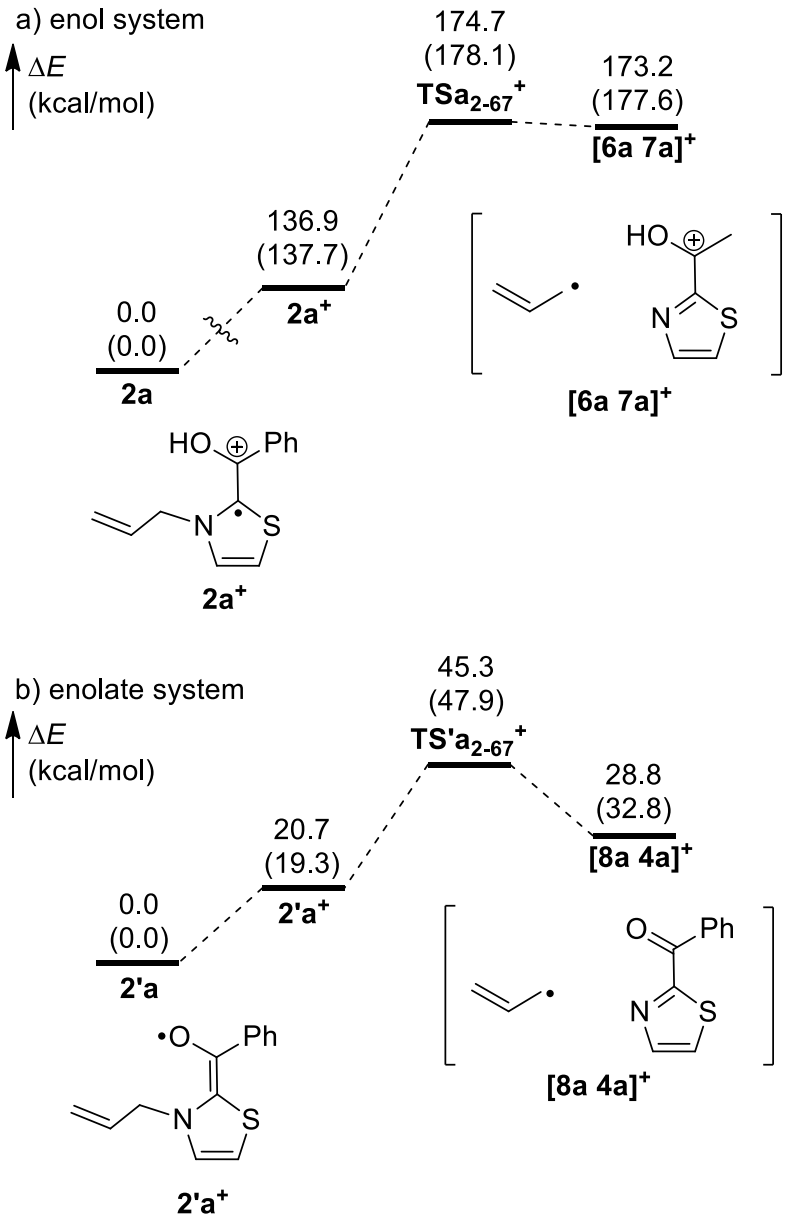


Figure S4. Energy profile of the doublet systems of a) the enol and b) the enolate forms of model Breslow intermediates. The energies are calculated at the levels of UCCSD(T)/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p), and UM06-2X-D3/6-31+G(d,p) in parentheses.

To investigate the C–N bond cleavage, we perform three-state and five-state MS-CASPT2 calculations for the enol and the enolate systems, respectively. Rydberg states are observed in Breslow intermediates of both systems. For the enol system, a Rydberg-

like orbital, which is not as diffused as the Rydberg orbital, is found at the geometry of Breslow intermediate **2a** and is included in the active space (Figure S5). This Rydberg-like state is 87.9 kcal/mol higher than the ground state at the level of MS-CASPT2/aug-cc-pVDZ//UM06-2X-D3//6-31+G(d,p). In addition, when the C–N distance increases, the Rydberg-like state vanishes (Figure S6). The observation indicates that the fragmentation reaction does not relate to the high-energy Rydberg-like state for the enol system. The third state (for clarity, we denote the third state as the first excited state hereafter) results from a $\pi \rightarrow \pi^*$ transition and has a relative energy of 96.2 kcal/mol at the geometry of **2a** (Figure S5). The potential energy surfaces (PESs) of the three states in the enol system are shown in Figure S6, where the three states do not cross each other. The comparison between the PESs obtained from MS-CASPT2 and DFT shows that at the geometry of the transition state located by DFT, the energy is overestimated by around 4 kcal/mol (Figure S7). The PES calculated with MS-CASPT2 reveals a barrierless process. It should be noted again that the calculated barrier at UCCSD(T)/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p) level is 34.7 kcal/mol (Table S1), which is closer to the DFT energy.

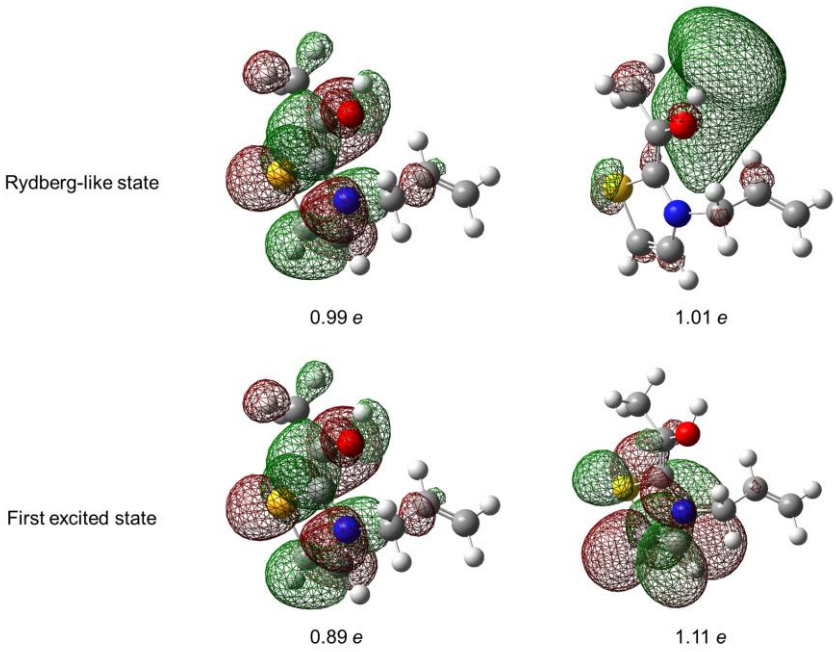


Figure S5. Two representative orbitals of Rydberg-like state (top) and the first excited state (bottom) of the enol Breslow intermediate (**2a**) plotted with an isovalue of 0.02. The natural orbitals are calculated at the level of SA-CASSCF/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p).

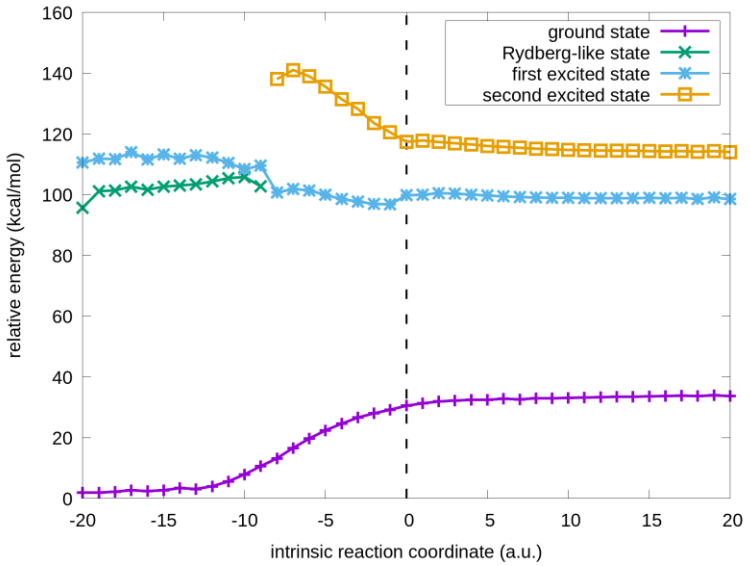


Figure S6. Potential energy surfaces of the enol system calculated at the level of three-state MS-CASPT2/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p). The vertical dashed line indicates the transition-state geometry in the ground state located by DFT.

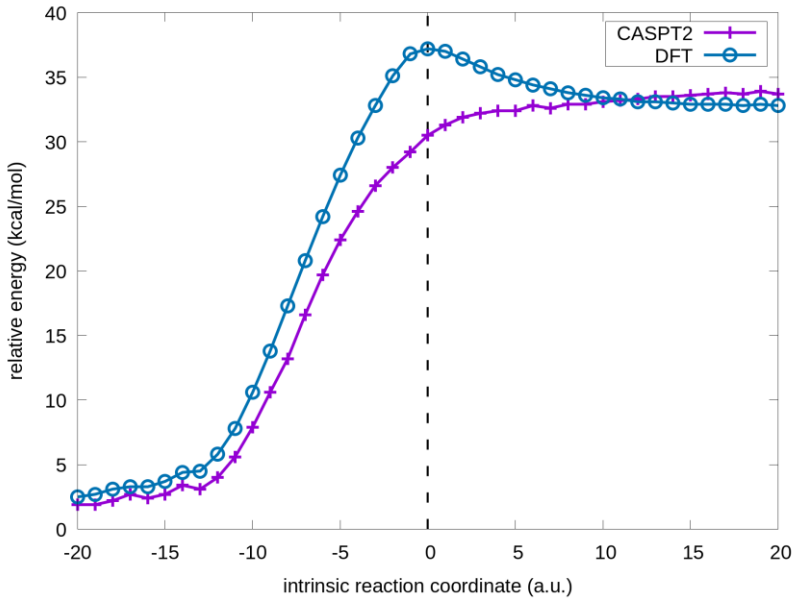


Figure S7. Comparison between the potential energy surfaces of the enol obtained by MS-CASPT2 and UM06-2X-D3 methods. The vertical dashed line indicates the transition-state geometry in the ground state located by DFT.

The enolate system, on the other hand, has a very diffused Rydberg orbital (Figure S8). To describe the Rydberg state and separate it from the other excited states, we augment additional 7 s and 7 p diffuse functions with exponents from 0.025 to 0.000025 in an even-tempered manner at the center of mass.[13] This Rydberg state is approximately 30 kcal/mol above the ground state through the IRC (green curve in Figure S9). The first excited state involves the transition from π on the NHC to π* on the allyl group and is 77.6 kcal/mol higher than the ground state at the geometry of **2'a**. The second and third Rydberg states are transitions from different π orbitals to the Rydberg states and are 118.1 and 129.9 kcal/mol higher, respectively, than the ground state at the geometry of **2'a** (Figure S8). Figure S9 shows the PESs of the five states in the enolate system. The energy difference between the ground and the first excited states decreases as the fragmentation occurs, while the potential energy curves of the

first excited state and Rydberg state cross each other. Given the small coupling between the Rydberg state, the ground, and the first excited state, the Rydberg state is unlikely to participate in this reaction. The comparison between the PESs obtained from MS-CASPT2 and DFT shows that the energy barrier of the transition state is overestimated by around 8 kcal/mol using DFT (Figure S10). The energy calculated with UCCSD(T) method is 21.4 kcal/mol (Table S1), which is closer to the result of DFT. On the other hand, closed-shell CCSD(T) calculation gives an energy of 16.6 kcal/mol, resembling the MS-CASPT2 calculation with a deviation around 4 kcal/mol. This may be due to nature of the complicated ionic-radical mixing state, which is more suitably characterized as ionic at the transition-state geometry. That is, the closed-shell CCSD(T) and MS-CASPT2 may depict the transition state better than the open-shelled UCCSD(T). Electron occupation numbers of **[8a 4a]** show that the active orbitals are either doubly occupied or empty (Figure S11), while those of **[6a 7'a]** show that the π orbital on the NHC and nonbonding orbital the allyl group are singly-occupied (Figure S12). This confirms the ionic and radical characters of **[8a 4a]** and **[6a 7'a]**, respectively.

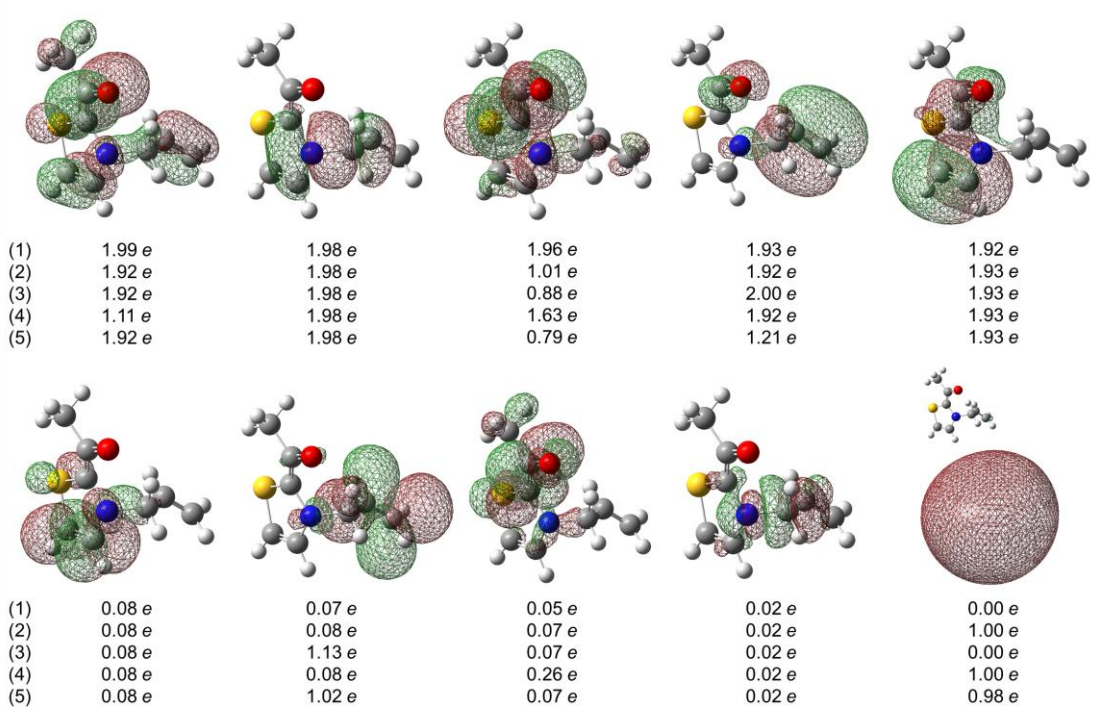


Figure S8. Electron occupation numbers of (1) the ground state, (2) the Rydberg state, (3) the first excited state, (4) the second, and (5) the third Rydberg states (from top to bottom) of the enolate Breslow intermediate (**2'a**) with an isovalue of 0.02 except for the Rydberg orbital (isovalue = 0.00042). The natural orbitals are calculated at the level of SA-CASSCF/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p).

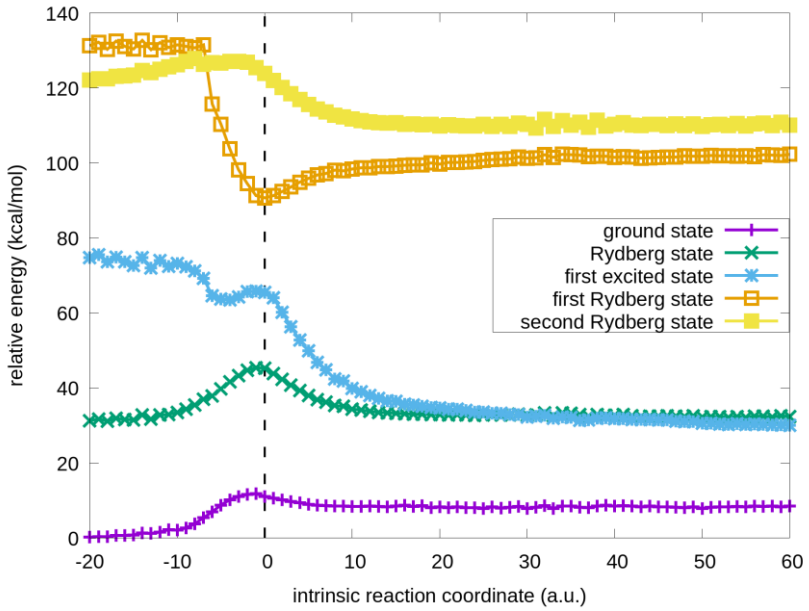


Figure S9. Potential energy surfaces of the enolate system calculated at the level of five-state MS-CASPT2/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p). The vertical dashed line indicates the transition-state geometry in the ground state located by DFT.

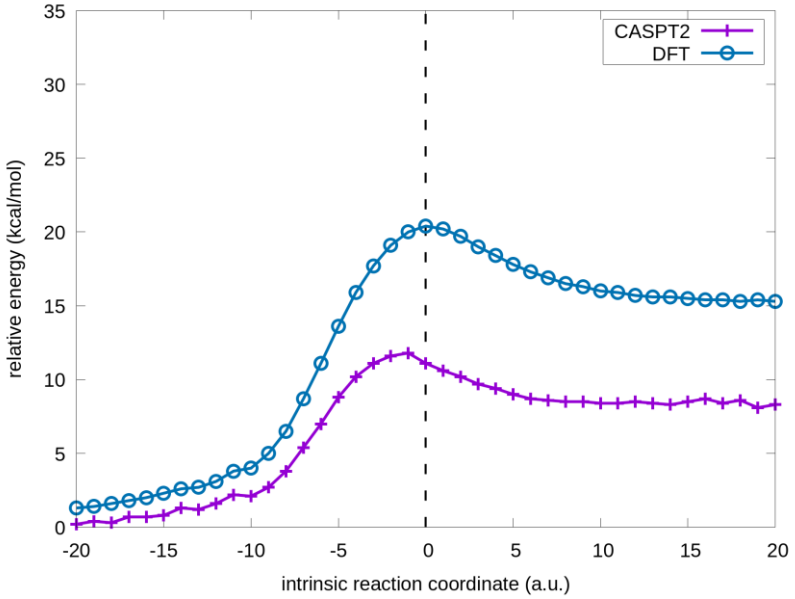


Figure S10. Comparison between the potential energy surfaces of the enolate obtained from MS-CASPT2 and UM06-2X-D3 methods. The vertical dashed line indicates the transition-state geometry in the ground state located by DFT.

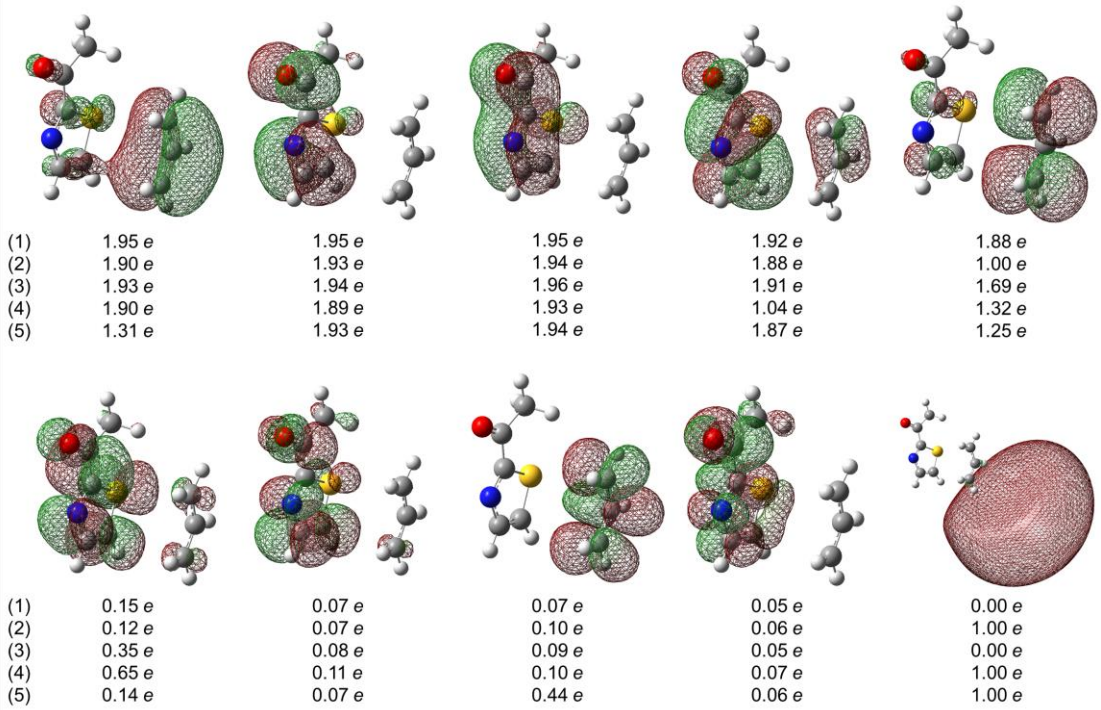


Figure S11. Electron occupation numbers of (1) the ground state, (2) the Rydberg state, (3) the first excited state, (4) the second, and (5) the third Rydberg states (from top to bottom) of the ionic intermediates (**[8a 4a]**) with an isovalue of 0.02 except for the Rydberg state (isovalue = 0.0015). The natural orbitals are calculated at the level of SA-CASSCF/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p).

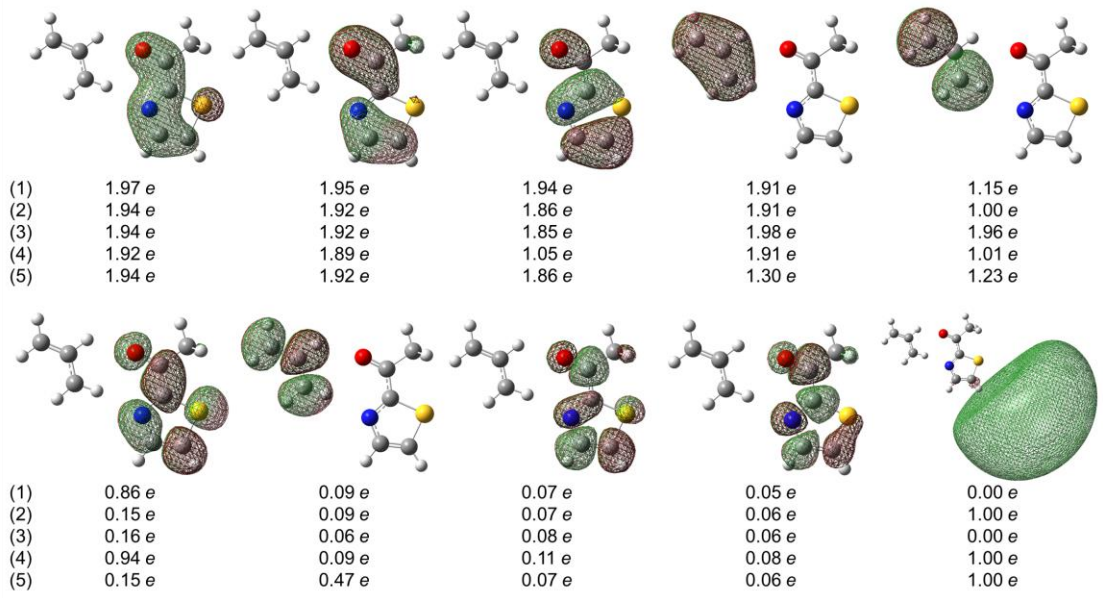


Figure S12. Electron occupation numbers of (1) the ground state, (2) the Rydberg state, (3) the first excited state, (4) the second, and (5) the third Rydberg states (from top to bottom) of the radical pair (**[6a 7'a]**) with an isovalue of 0.02 except for the Rydberg state (isovalue = 0.0018). The natural orbitals are calculated at the level of SA-CASSCF/aug-cc-pVDZ//UM06-2X-D3/6-31+G(d,p).

3. Calculation of pKa values

The pKa values are calculated with an efficient and reliable methodology proposed by Thapa and Schlegel.[18] They introduce the combination of the explicit solvent (up to three water molecules) and the implicit solvent model (SMD) to calculate the Gibbs free energies of the deprotonated and the protonated species ($G^*_{aq,RO-} - G^*_{aq,ROH}$). The pKa value is then given by

$$\text{pKa} = \frac{\Delta G^*_{aq}}{2.303RT} = \frac{G^*_{aq,RO-} + G^*_{aq,H+} - G^*_{aq,ROH}}{2.303RT}$$

$$G^*_{aq,H+} = G^\circ_{g,H+} + \Delta G^*_{aq,H+} + \Delta G^{1atm \to 1M}$$

$$G^\circ_{g,H+} = H^\circ_{g,H+} - TS^\circ_{g,H+}$$

$$H^\circ_{g,H+} = \frac{5RT}{2} = 1.48\ kcal/mol$$

$$S^\circ_{g,H+} = 26.05\ cal/mol$$

$$\Delta G^*_{aq,H+} = -265.9\ kcal/mol$$

$$\Delta G^{1atm \to 1M} = RT \ln(24.4) = 1.89\ kcal/mol$$

where the symbols * and ° denote the standard state of 1 mol/L and 1 atm, respectively. The value $\Delta G^*_{aq,H+}$ is taken directly from the literature,[18] and therefore, at 298.15 K, the pKa is estimated as

$$\mathrm{pKa} = \frac{G^*_{aq,RO-} - G^*_{aq,ROH} - 270.30}{2.303 \times 0.001987 \times 298.15}$$

Thapa and Schlegel reported that the mean signed error (MSE) and the standard deviation (STDEV) for alcohols, phenols, and hydroperoxides are -0.02 ± 0.55 when three explicit water molecules are employed at the level of B3LYP/6-311++G(d,p). The MSE and STDEV are 0.95 ± 0.72 at the level of ωB97XD/6-311++G(d,p).

Following this methodology, we calculate the pKa values of the hydroxyl group of Breslow intermediates (**2a**, **2c**, and **2d**) with three explicit waters at the levels of B3LYP/6-311++G(d,p) and ωB97XD/6-311++G(d,p). The calculated pKa values are above 9 for all NHC systems in our study, showing that Breslow intermediate prefers the enol form in neutral solution (Figure S13). The pKa values of the nitrogen atoms (N1 and N3) on the pyrimidine of thiamin Breslow intermediates (**2c**) are calculated with one explicit water at the level of B3LYP/6-311++G(d,p) and ωB97XD/6-311++G(d,p). The calculated pKa values show that N3 is deprotonated in neutral solution, while the proton on N1 is likely to shuttle between solvent molecules and thiamin in the enol form but could be protonated in the enolate form (Figure S14).

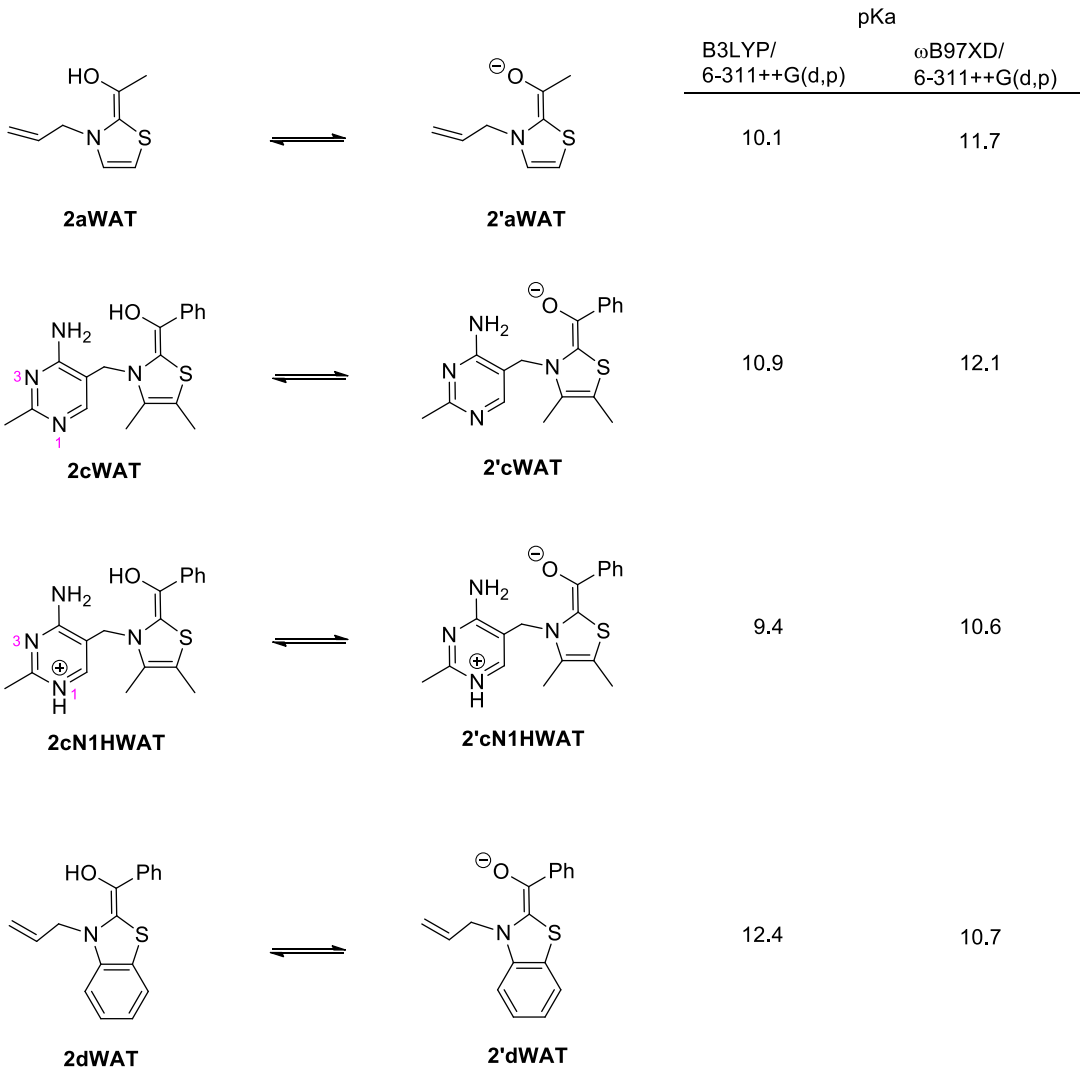


Figure S13. Calculated pKa values of the hydroxyl groups. The three explicit water molecules added in each structure are not shown.

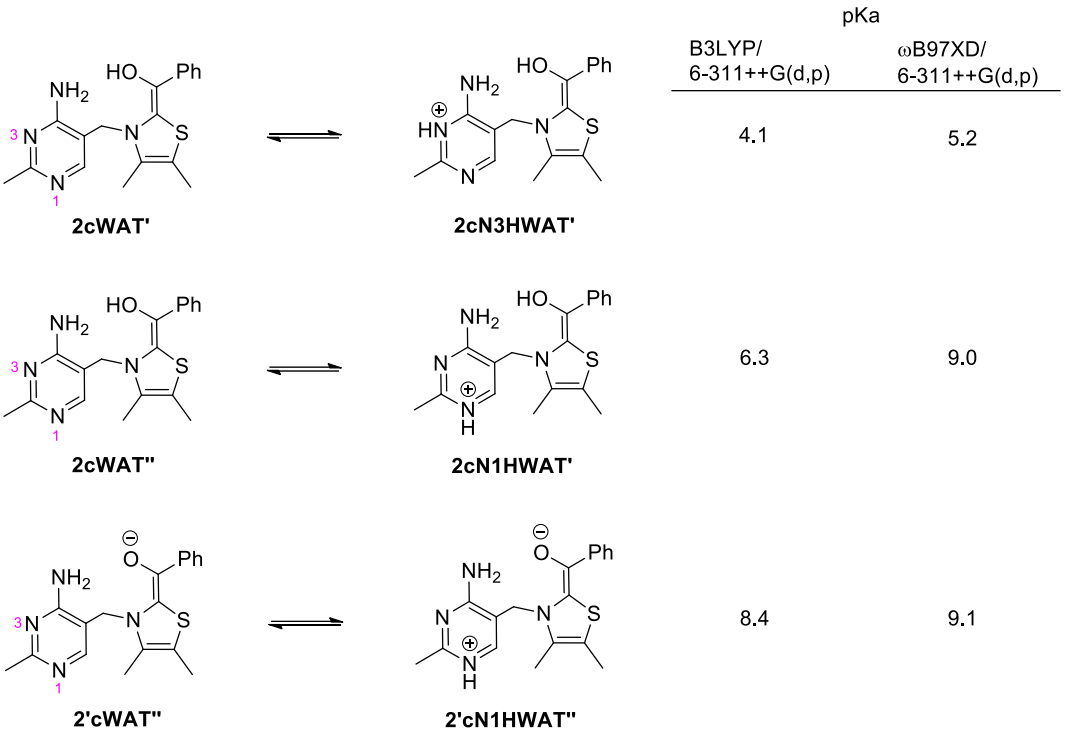


Figure S14. Calculated pKa values of the nitrogen atoms. The single explicit water molecule added in each structure is not shown.

4. Breslow intermediate of N1-protonated thiamin

Given that the pKa value of N1 atom is close to 7 (see Session 3 of ESI), we calculate different protonation states regarding that on N1 and the hydroxyl group with DFT and SMD solvent model. The N1-deprotonated systems are shown in the main text (Figure 3). Figure S15 displays the N1-protonated (denoted as **N1H**) enol and enolate systems with an amine group on the pyrimidine ring, while Figure S16 shows the N1-protonated imine system (denoted as **i**).

N1-protonated amine systems (Figure S15) have slightly smaller activation free energies (25.8 and 19.5 kcal/mol for the enol and the enolate systems, respectively, at the level of UM06-2X-D3/6-31+G(d,p)) compared to N1-deprotonated systems (Figure 3). The enol system proceeds through the radical mechanisms, while the enolate system undergoes only the ionic dissociation. This may result from the zwitterionic character of **2'cN1H**.

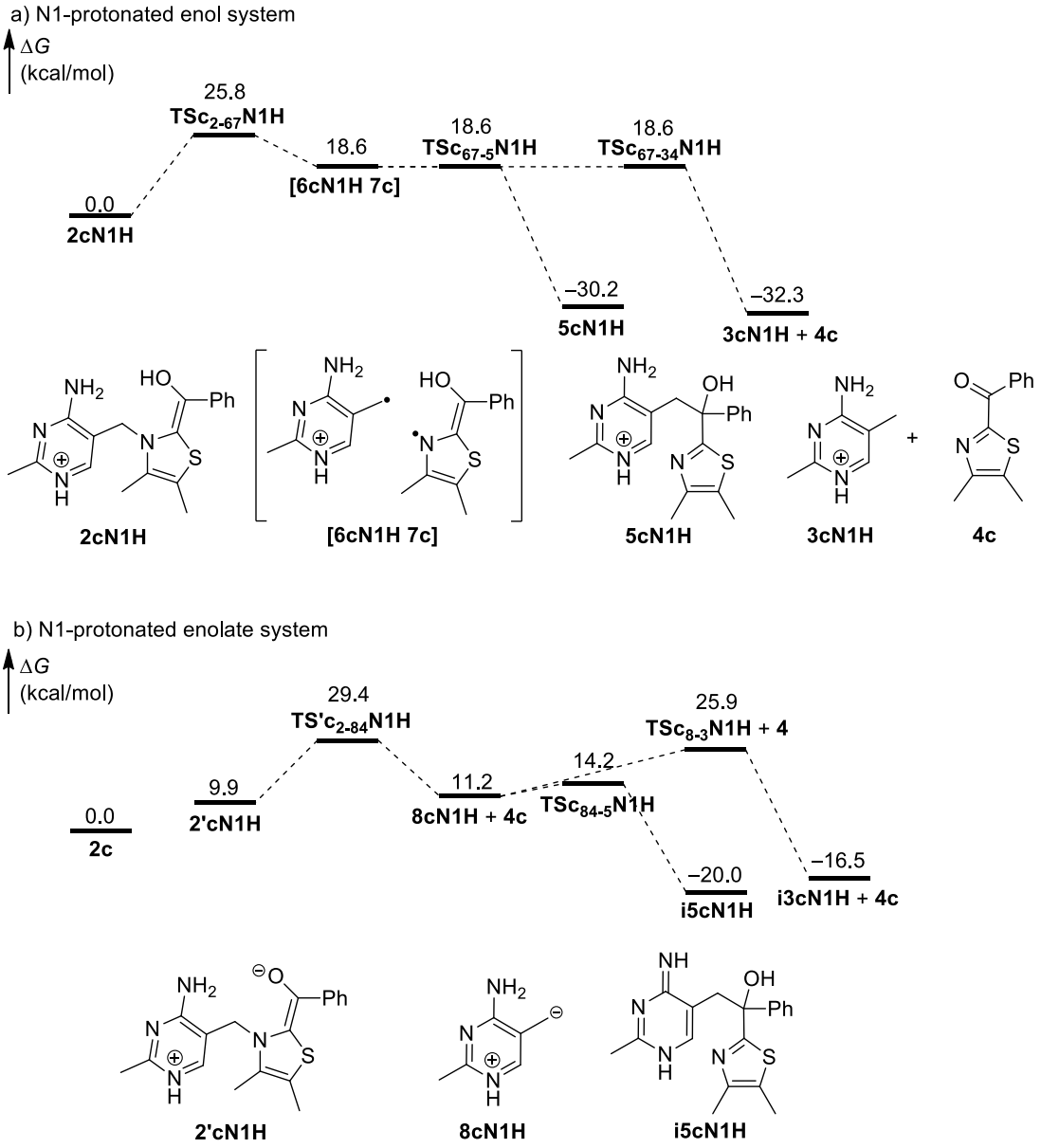


Figure S15. Free energy profiles of a) the enol, and b) the enolate of N1-protonated thiamin. The energies are calculated at the level of UM06-2X-D3/6-31+G(d,p) with solvent effect.

The Breslow intermediate in the imine system (**i2cN1H** in Figure S16) has a similar energy to that in the N1-protonated enolate system (**2'cN1H** in Figure S15). These two compounds correlate each other as a result of proton transfer between the amine group and the hydroxyl group. The imine system undergoes only the radical route

with a free energy barrier of 29.1 kcal/mol (Figure S16a). In addition, the radical pathway of imine (Figure S16a) and the ionic pathway of amine (Figure S15b) could be connected through a hydrogen transfer between the imine of **i6cN1H** and the hydroxyl group of **7c** (Figure S16b). Figure S17 summarizes reactions of these two systems.

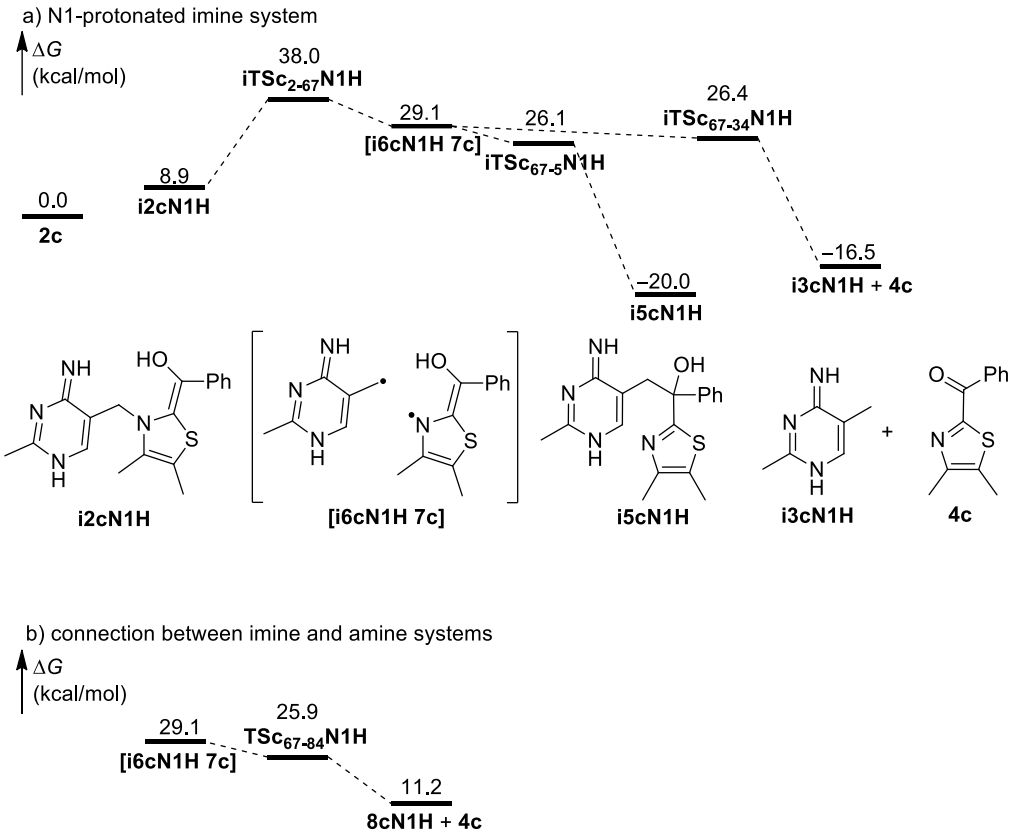


Figure S16. Free energy profile of a) N1-protonated imine thiamin, and b) connection between the amine and imine systems. The energies are calculated at the level of UM06-2X-D3/6-31+G(d,p) with solvent effect.

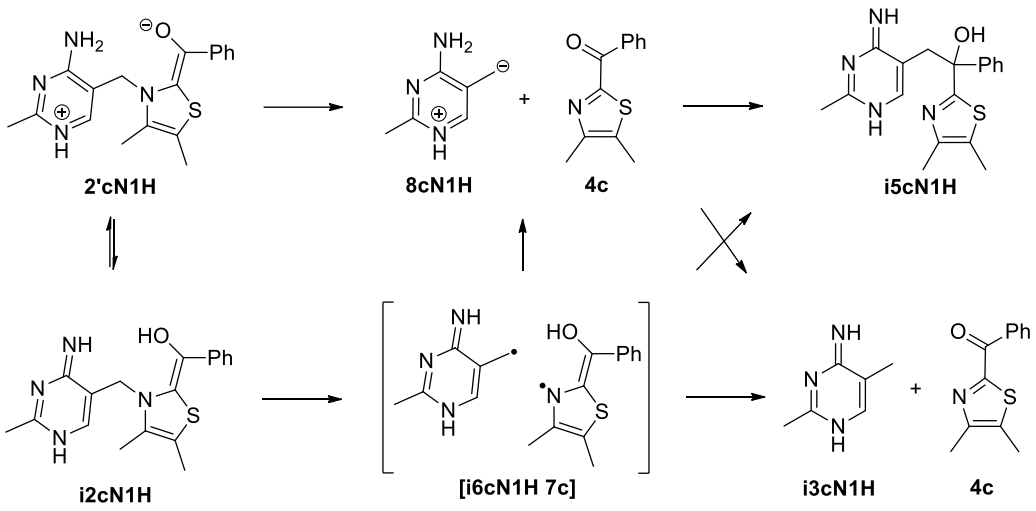


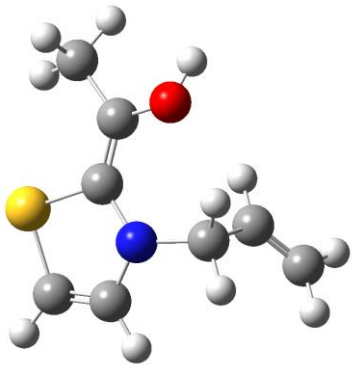
Figure S17. Summary of reactions in the enolate amine (**2'cN1H**) and enol imine systems (**i2cN1H**).

5. List of absolute energies and optimized structures

The geometries, total energy (E), zero-point energy (ZPE), enthalpy (H), Gibbs free energy (G), and the expectation value of the square of spin quantum number (<S^2>) reported here are calculated with DFT. Single-point energies calculated at the levels of CCSD(T) and MS-CASPT2 are denoted by the subscripts. The units of the Cartesian coordinates and the energies are angstroms and hartree, respectively.

2a neutral singlet, optimized in gas phase

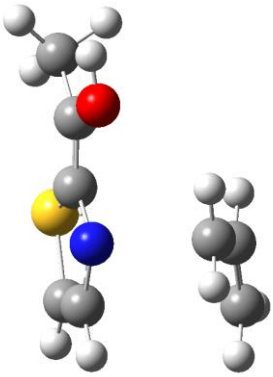
E	-839.360173
E+ZPE	-839.182143
H	-839.169048
G	-839.221301
<S^2>	0.0000
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.9482401
$E_{MS\text{-}CASPT2}$	
state 1	-837.7992007
state 2	-837.6591241
state 3	-837.6459076



C	-0.541187	-1.897051	-0.476306
C	0.551938	-2.453145	0.054619
C	0.694131	0.052245	-0.175013
N	-0.477094	-0.524515	-0.709006
S	1.805016	-1.247548	0.346095
H	-1.448123	-2.416153	-0.760231
H	0.726116	-3.497009	0.262361
C	1.025444	1.353661	-0.088716
O	0.211394	2.308708	-0.684385
H	0.236795	3.115143	-0.155378
C	2.307677	1.858879	0.491094
H	2.791122	1.107411	1.119355
H	3.013313	2.160331	-0.292826
H	2.121746	2.737754	1.123041
C	-1.732511	0.226318	-0.809726
H	-1.549124	1.122266	-1.402276
H	-2.440368	-0.406882	-1.353791
C	-2.292177	0.588216	0.539082
H	-1.626839	1.154669	1.189855
C	-3.511627	0.249733	0.952007
H	-3.881452	0.533211	1.932038
H	-4.185058	-0.321164	0.316206

TSa2-67 neutral singlet, optimized in gas phase

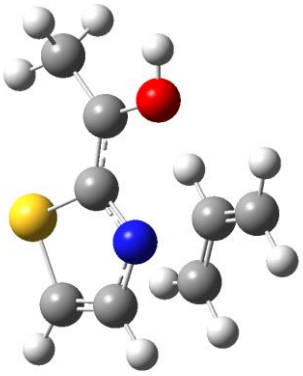
E	-839.300812
E+ZPE	-839.128152
H	-839.114989
G	-839.166674
$\langle S^2 \rangle$	0.5915
imaginary freq.	526.4*i*
$E_{UCCSD(T)}$	-837.892884
$E_{MS\text{-}CASPT2}$	
state 1	-837.7506269
state 2	-837.6426196
state 3	-837.6096679



C	-1.247950	-0.618613	-1.372747
C	-1.263642	-1.713910	-0.557299
C	0.702169	-0.259367	-0.352005
N	-0.203327	0.242247	-1.243457
S	0.156103	-1.765727	0.436187
H	-2.037567	-0.380716	-2.077331
H	-2.001138	-2.502761	-0.520418
C	1.888791	0.346611	-0.047370
O	2.132648	1.552947	-0.630581
H	3.034374	1.833696	-0.437815
C	2.901389	-0.168902	0.919297
H	2.672342	-1.188393	1.233508
H	3.899015	-0.180026	0.462160
H	2.948988	0.461359	1.816493
C	-1.189875	1.978207	-0.114258
H	-0.242916	2.503223	-0.100057
H	-1.845031	2.176558	-0.956282
C	-1.685222	1.311987	1.021575
H	-1.025999	1.222356	1.883859
C	-2.894665	0.677845	1.056352
H	-3.219853	0.117411	1.925412
H	-3.583737	0.746472	0.219054

[6a 7a] neutral singlet, optimized in gas phase

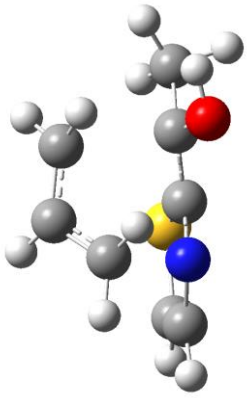
E	-839.307895
E+ZPE	-839.137048
H	-839.122185
G	-839.180584
$\langle S^2 \rangle$	1.0352
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.8994725
$E_{MS\text{-}CASPT2}$	
state 1	-837.7450073
state 2	-837.6412943
state 3	-837.6171288



C	-0.989350	1.056397	1.492085
C	-1.176684	1.850358	0.388349
C	0.778045	0.381010	0.353359
N	0.087925	0.237826	1.485906
S	0.081704	1.575364	-0.756910
H	-1.651576	1.050989	2.350503
H	-1.965044	2.563751	0.199565
C	1.920161	-0.349474	0.026645
O	2.314845	-1.286976	0.919201
H	3.143143	-1.688499	0.632092
C	2.703334	-0.210023	-1.233675
H	2.340001	0.616752	-1.845582
H	3.762014	-0.019636	-1.014960
H	2.643898	-1.126031	-1.836130
C	-1.395816	-2.176454	0.316783
H	-0.442483	-2.689523	0.345423
H	-1.978489	-2.157646	1.232154
C	-1.838294	-1.517047	-0.817333
H	-1.207400	-1.549700	-1.705117
C	-3.017062	-0.795798	-0.889111
H	-3.314028	-0.281066	-1.794781
H	-3.677532	-0.728005	-0.030181

TSa2-5 neutral singlet, optimized in gas phase

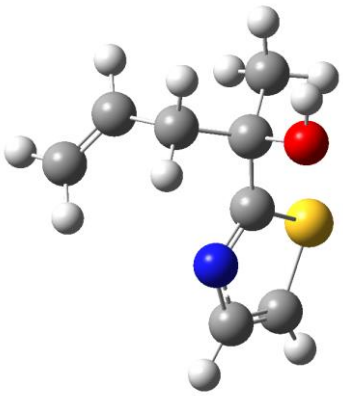
E	-839.315779
E+ZPE	-839.139267
H	-839.127442
G	-839.175036
$\langle S^2 \rangle$	0.0000
imaginary freq.	567.1*i*
$E_{UCCSD(T)}$	-837.9071827



C	-2.074379	-0.698712	-0.670152
C	-2.543229	0.347057	0.035297
C	-0.129944	0.413956	-0.435562
N	-0.695766	-0.722090	-0.902586
S	-1.253249	1.440287	0.465727
H	-2.675775	-1.514492	-1.052976
H	-3.567390	0.561011	0.304104
C	1.247288	0.584338	-0.371575
O	1.943727	-0.089839	-1.359112
H	2.890141	0.017914	-1.207216
C	1.888113	1.837447	0.147472
H	1.332491	2.245249	0.995234
H	2.906366	1.627997	0.496397
H	1.946982	2.602136	-0.636769
C	0.060938	-2.239134	-0.041765
H	-0.796927	-2.900470	-0.120468
H	0.843115	-2.417166	-0.774769
C	0.437879	-1.729840	1.214289
H	-0.323433	-1.650303	1.987890
C	1.553501	-0.907798	1.273107
H	1.754548	-0.330019	2.173013
H	2.421415	-1.156997	0.668265

5a neutral singlet, optimized in gas phase

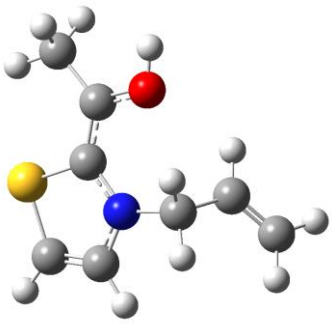
E	-839.403342
E+ZPE	-839.224361
H	-839.212119
G	-839.262429
$<S^2>$	0.0000
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.9986923



C	-1.979712	1.419117	0.682960
C	-2.746096	0.661713	-0.151043
C	-0.466722	-0.109119	0.199215
N	-0.694751	0.975299	0.874470
S	-1.829378	-0.672083	-0.729453
H	-2.309536	2.320433	1.183798
H	-3.771880	0.818609	-0.450693
C	0.834073	-0.887740	0.262455
O	0.649962	-1.796959	1.346848
H	1.463262	-2.305109	1.460662
C	1.086978	-1.668960	-1.027598
H	1.107436	-1.010121	-1.899428
H	2.051837	-2.184435	-0.962188
H	0.309144	-2.424731	-1.169717
C	2.043438	2.299906	-0.554227
H	2.323403	2.938004	-1.386561
H	1.483303	2.748774	0.261797
C	2.359945	1.006075	-0.533300
H	2.911143	0.580466	-1.371844
C	1.997492	0.070411	0.587305
H	2.864298	-0.560216	0.830711
H	1.724809	0.631817	1.484042

2a^{+} cation doublet, optimized in gas phase

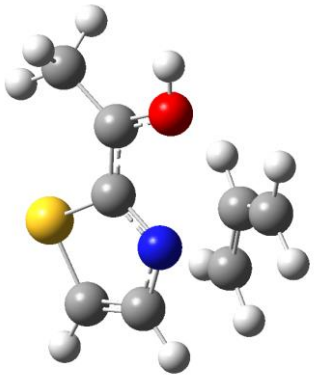
E	-839.140660
E+ZPE	-838.961039
H	-838.948377
G	-839.000489
$<S^2>$	0.7657
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.7300819



C	-0.448343	-1.920005	-0.330741
C	0.750514	-2.422840	0.049072
C	0.715753	0.039640	-0.116970
N	-0.475169	-0.552212	-0.442778
S	1.900377	-1.167642	0.298729
H	-1.346735	-2.481952	-0.548520
H	1.015528	-3.460604	0.189414
C	1.015513	1.400580	-0.077289
O	0.027829	2.260575	-0.344394
H	0.331894	3.179219	-0.308722
C	2.356717	1.951175	0.269195
H	3.110864	1.176549	0.405698
H	2.703092	2.615494	-0.530554
H	2.295091	2.532284	1.196624
C	-1.739185	0.143321	-0.808777
H	-1.483599	0.974726	-1.463962
H	-2.322579	-0.579770	-1.382143
C	-2.489118	0.586237	0.415526
H	-2.006169	1.338893	1.034565
C	-3.692129	0.111355	0.727953
H	-4.224434	0.459825	1.606215
H	-4.193776	-0.628297	0.108504

TSa2-67^{+} cation doublet, optimized in gas phase

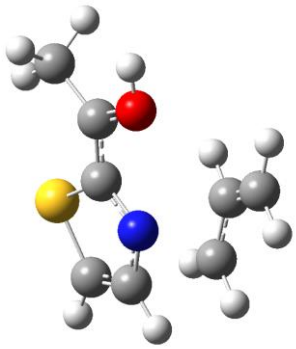
E	-839.076275
E+ZPE	-838.901288
H	-838.888470
G	-838.940465
$\langle S^2 \rangle$	0.7869
imaginary freq.	133.4*i*
$E_{UCCSD(T)}$	-837.6698215



C	1.206977	-0.674550	1.385659
C	1.212150	-1.744782	0.507229
C	-0.694491	-0.271956	0.340750
N	0.173462	0.174250	1.268691
S	-0.185954	-1.745194	-0.462628
H	1.982980	-0.484227	2.117944
H	1.939476	-2.543922	0.442086
C	-1.889258	0.387170	0.041404
O	-2.076237	1.535887	0.654198
H	-2.938723	1.929180	0.449346
C	-2.922941	-0.105252	-0.908532
H	-2.656666	-1.063776	-1.352779
H	-3.876542	-0.226984	-0.381722
H	-3.069917	0.623968	-1.713315
C	1.309822	2.053875	0.106694
H	0.413332	2.662840	0.111547
H	1.947142	2.118594	0.982432
C	1.722477	1.347200	-1.024480
H	1.099165	1.365628	-1.915267
C	2.861494	0.582652	-1.017339
H	3.171349	0.012544	-1.886270
H	3.521948	0.576267	-0.154680

[6a 7a]$^{+}$ cation doublet, optimized in gas phase

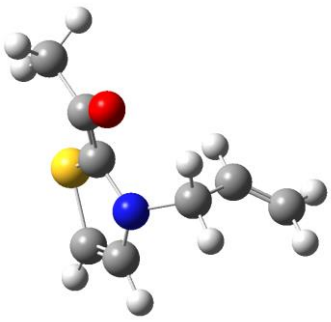
E	-839.077129
E+ZPE	-838.902542
H	-838.888746
G	-838.943617
$<S^2>$	0.7943
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.672236



C	-1.073959	0.616279	1.493393
C	-1.228730	1.600500	0.509372
C	0.770991	0.263352	0.354726
N	0.012216	-0.139226	1.384422
S	0.102307	1.619629	-0.533634
H	-1.786449	0.440195	2.290902
H	-2.017635	2.337854	0.430550
C	1.992896	-0.338276	0.028393
O	2.323859	-1.382381	0.742715
H	3.190755	-1.744634	0.500456
C	2.903858	0.120794	-1.054445
H	2.513861	0.984580	-1.591545
H	3.874148	0.393674	-0.623465
H	3.066772	-0.692160	-1.771015
C	-1.463266	-2.185141	-0.173693
H	-0.659861	-2.856621	-0.454246
H	-1.898962	-2.320952	0.811361
C	-1.954579	-1.235943	-1.044348
H	-1.509924	-1.146139	-2.033152
C	-2.982198	-0.367830	-0.697288
H	-3.373561	0.358670	-1.400504
H	-3.502523	-0.477308	0.249456

2'a singlet anion, optimized in gas phase

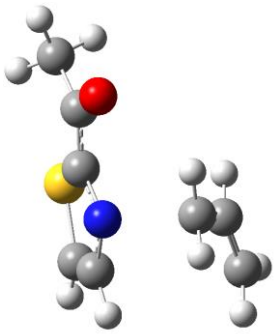
E	-838.795234
E+ZPE	-838.631182
H	-838.618600
G	-838.669432
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.3850201
$E_{MS\text{-}CASPT2}$	
state 1	-837.2309448
state 2	-837.1857585
state 3	-837.1073580
state 4	-837.0427500
state 5	-837.0239410



C	1.002232	1.271063	-1.107952
C	0.395479	2.270718	-0.448143
C	-0.748694	0.057553	-0.175617
N	0.476715	-0.005337	-0.925759
S	-0.884951	1.672236	0.627266
H	1.864274	1.385524	-1.759850
H	0.641494	3.322473	-0.505158
C	-1.642785	-0.987514	-0.147114
O	-1.450254	-2.109690	-0.732603
C	-2.916251	-0.832211	0.677031
H	-3.137601	0.206871	0.946191
H	-3.746994	-1.238638	0.090197
H	-2.844584	-1.423923	1.598178
C	1.405447	-1.082252	-0.566183
H	0.793875	-1.993577	-0.567804
H	2.172594	-1.166873	-1.348848
C	2.052533	-0.853329	0.770384
H	1.359357	-0.586908	1.569713
C	3.364373	-0.918984	1.009235
H	3.779089	-0.724752	1.994453
H	4.068728	-1.171356	0.217976

TS'a$_{2\text{-}67}$ singlet anion, optimized in gas phase

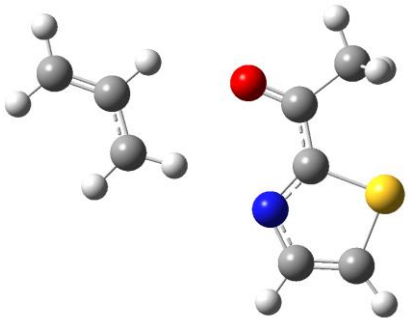
E	-838.762719
E+ZPE	-838.602766
H	-838.589995
G	-838.641462
$\langle S^2 \rangle$	0.2320
imaginary freq.	478.3*i*
$E_{UCCSD(T)}$	-837.3509907
$E_{ROCCSD(T)}$	-837.3586414
$E_{MS\text{-}CASPT2}$	
state 1	-837.2132451
state 2	-837.1587813
state 3	-837.1265172
state 4	-837.0864080
state 5	-837.0334419



C	1.153315	0.765522	-1.287603
C	0.956795	1.870699	-0.526744
C	-0.796239	0.138993	-0.381013
N	0.245953	-0.263324	-1.159248
S	-0.477334	1.707224	0.445770
H	2.017187	0.617301	-1.928352
H	1.582322	2.751071	-0.474668
C	-1.923702	-0.664814	-0.087867
O	-2.072330	-1.830562	-0.517062
C	-2.983482	-0.082663	0.844484
H	-3.116434	0.996530	0.712143
H	-3.927430	-0.596488	0.648448
H	-2.706888	-0.260593	1.891692
C	1.369495	-1.730215	-0.222634
H	0.483859	-2.350057	-0.134733
H	2.014741	-1.947398	-1.072521
C	1.950845	-1.139036	0.929719
H	1.303561	-1.056758	1.805248
C	3.182472	-0.551770	1.001341
H	3.512450	-0.026376	1.891499
H	3.873950	-0.595340	0.162060

[6a 7'a] singlet anion, optimized in gas phase

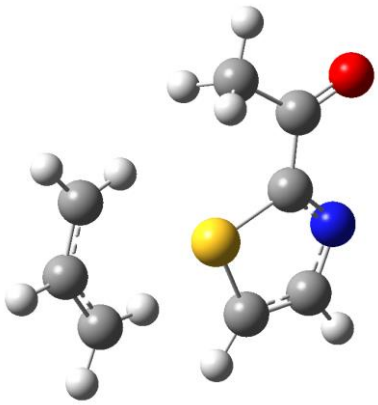
E	-838.773130
E+ZPE	-838.614982
H	-838.600705
G	-838.657796
$\langle S^2 \rangle$	1.0343
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.3618775
$E_{MS\text{-}CASPT2}$	
state 1	-837.2098957
state 2	-837.1746500
state 3	-837.1631147
state 4	-837.0643345
state 5	-837.0500486



C	1.564527	2.044406	0.000326
C	2.858023	1.578382	-0.000376
C	1.041809	-0.114821	0.000296
N	0.560934	1.143890	0.000689
S	2.840362	-0.167740	-0.000599
H	1.316843	3.103254	0.000603
H	3.778512	2.143013	-0.000702
C	0.269445	-1.308849	0.000453
O	-0.989906	-1.316889	0.000884
C	1.030902	-2.629048	-0.000049
H	1.678884	-2.726357	0.881783
H	0.301623	-3.441547	0.000904
H	1.676924	-2.726738	-0.883282
C	-2.912284	1.189510	0.000336
H	-1.833305	1.057047	0.000734
H	-3.326466	2.196853	0.000341
C	-3.766107	0.089942	-0.000230
H	-3.276161	-0.882428	-0.000180
C	-5.144997	0.165108	-0.000821
H	-5.764068	-0.725504	-0.001253
H	-5.653786	1.126345	-0.000883

[8a 4a] singlet anion, optimized in gas phase

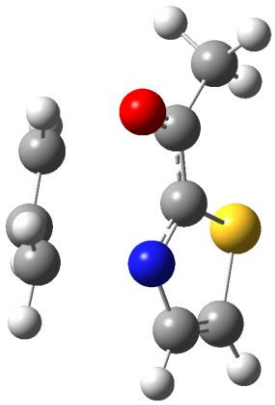
E	-838.781623
E+ZPE	-838.622182
H	-838.608343
G	-838.663261
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.3722612
$E_{MS\text{-}CASPT2}$	
state 1	-837.2303540
state 2	-837.1772954
state 3	-837.1664286
state 4	-837.0659634
state 5	-837.0568384



C	0.085021	-2.236544	0.181577
C	0.899263	-1.489535	-0.662095
C	-1.217144	-0.482223	-0.028019
N	-1.085276	-1.676980	0.532566
S	0.160888	0.010702	-0.980692
H	0.349378	-3.214713	0.567245
H	1.880894	-1.720815	-1.043674
C	-2.339539	0.432517	0.202063
O	-3.350372	0.106709	0.809933
C	-2.176233	1.843439	-0.340195
H	-2.083942	1.832522	-1.431705
H	-3.049286	2.430783	-0.054095
H	-1.262048	2.303219	0.056178
C	1.929181	1.813721	0.608764
H	1.767860	2.823012	0.242965
H	1.292977	1.469732	1.421410
C	3.044521	1.077465	0.211563
H	3.662188	1.545356	-0.563197
C	3.441441	-0.190770	0.605957
H	4.346629	-0.642137	0.211092
H	2.921979	-0.721414	1.399733

TS'a$_{2\text{-}5}$ singlet anion, optimized in gas phase

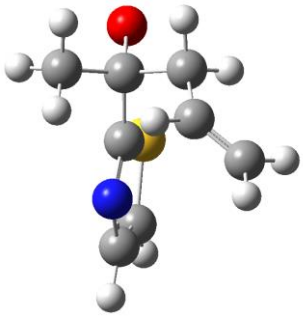
E	-838.769056
E+ZPE	-838.607756
H	-838.595493
G	-838.645084
$\langle S^2 \rangle$	0.0000
imaginary freq.	338.8*i*
$E_{UCCSD(T)}$	-837.3594471



C	-2.044335	-0.046014	-0.868553
C	-2.292577	0.964167	-0.007872
C	0.095466	0.450841	-0.410791
N	-0.717436	-0.405650	-1.075320
S	-0.806481	1.586778	0.669197
H	-2.814552	-0.609533	-1.387208
H	-3.256093	1.370041	0.269367
C	1.511757	0.441501	-0.556473
O	2.112267	-0.330921	-1.332568
C	2.345261	1.432545	0.249790
H	1.759744	2.097362	0.890630
H	3.047464	0.870026	0.873653
H	2.934255	2.035301	-0.450285
C	-0.553505	-2.278683	-0.291399
H	-1.525488	-2.683197	-0.564219
H	0.265217	-2.517289	-0.963590
C	-0.251011	-2.024561	1.064744
H	-1.080486	-1.967391	1.771770
C	0.975541	-1.552766	1.452319
H	1.148732	-1.198760	2.465401
H	1.829239	-1.620279	0.784526

5'a singlet anion, optimized in gas phase

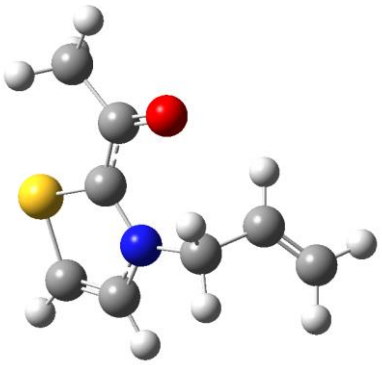
E	-838.824313
E+ZPE	-838.660290
H	-838.648229
G	-838.698086
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.4209169



C	-1.880462	-1.462278	0.816802
C	-2.671314	-0.826803	-0.095651
C	-0.467781	0.136783	0.256940
N	-0.634417	-0.909761	1.013579
S	-1.842395	0.546133	-0.743706
H	-2.161330	-2.345019	1.382622
H	-3.678454	-1.091286	-0.388062
C	0.734713	1.078664	0.092478
O	0.376088	2.160514	-0.604982
C	1.256902	1.405076	1.515850
H	1.446999	0.514262	2.127377
H	2.176166	1.994285	1.415789
H	0.505532	2.025817	2.013884
C	2.330802	-2.195133	-0.693486
H	2.703781	-3.089086	-0.200741
H	1.893219	-2.317655	-1.682182
C	2.368813	-0.996941	-0.103819
H	2.798068	-0.930014	0.897748
C	1.848618	0.274081	-0.694270
H	2.659591	1.008331	-0.793092
H	1.445224	0.095762	-1.698326

2'a^{+} neutral doublet, optimized in gas phase

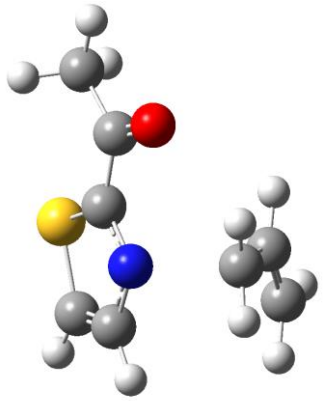
E	-838.764402
E+ZPE	-838.597790
H	-838.585344
G	-838.636869
$<S^2>$	0.7627
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.3520923



C	0.371239	1.930629	-0.320806
C	-0.838903	2.374334	0.075025
C	-0.699061	-0.103474	-0.134541
N	0.463169	0.567257	-0.469891
S	-1.949104	1.046360	0.303990
H	1.243216	2.535797	-0.532238
H	-1.143122	3.396686	0.234555
C	-0.885394	-1.516659	-0.111838
O	0.033764	-2.313910	-0.386895
C	-2.263725	-2.016751	0.276154
H	-2.533125	-1.695562	1.288948
H	-3.034036	-1.642559	-0.407531
H	-2.250435	-3.105935	0.238639
C	1.733124	-0.085803	-0.823125
H	1.504931	-0.924118	-1.481203
H	2.325879	0.656055	-1.366370
C	2.471119	-0.560984	0.397488
H	1.977627	-1.349743	0.961068
C	3.654621	-0.075883	0.766128
H	4.170497	-0.446296	1.645784
H	4.153812	0.701939	0.191989

TS'a$_{2\text{-}84}^{+}$ cation doublet, optimized in gas phase

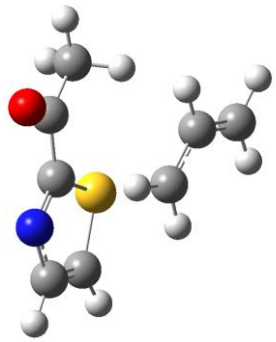
E	-838.718938
E+ZPE	-838.556545
H	-838.543980
G	-838.596081
$\langle S^2 \rangle$	0.7785
imaginary freq.	631.7*i*
$E_{UCCSD(T)}$	-837.312865



C	1.187980	-1.101150	1.117278
C	0.791356	-2.123819	0.316012
C	-0.698767	-0.197710	0.358401
N	0.369452	0.006202	1.129154
S	-0.687492	-1.734576	-0.479421
H	2.091557	-1.094251	1.714903
H	1.276568	-3.078266	0.169571
C	-1.724429	0.826404	0.135415
O	-1.601599	1.937130	0.630374
C	-2.900048	0.466694	-0.747092
H	-2.566405	0.286920	-1.775067
H	-3.393581	-0.443794	-0.392961
H	-3.607420	1.295388	-0.739844
C	1.514908	1.608956	0.571722
H	0.768946	2.338295	0.861703
H	2.304373	1.411540	1.291666
C	1.782592	1.372588	-0.812952
H	1.046945	1.739872	-1.527351
C	2.836108	0.653201	-1.267389
H	2.977244	0.454724	-2.323826
H	3.590073	0.271358	-0.583492

[8a 4a]$^{+}$ neutral doublet, optimized in gas phase

E	-838.742901
E+ZPE	-838.742901
H	-838.567941
G	-838.624499
$<S^2>$	0.7834
imaginary freq.	N/A
$E_{UCCSD(T)}$	-837.3390849



C	-2.422249	0.453772	-0.930354
C	-2.367497	1.101286	0.274063
C	-0.725245	-0.646807	-0.073664
N	-1.492537	-0.528978	-1.117123
S	-1.100099	0.452178	1.227335
H	-3.135779	0.667716	-1.715996
H	-2.997640	1.901131	0.635493
C	0.430121	-1.605731	0.008438
O	0.744692	-2.257219	-0.959733
C	1.156037	-1.696987	1.329447
H	1.567962	-0.717973	1.599064
H	0.469785	-2.007320	2.124033
H	1.964126	-2.421954	1.236970
C	1.350931	1.163790	-1.491351
H	1.271884	0.504511	-2.346920
H	0.565550	1.901605	-1.348779
C	2.397405	1.062060	-0.587701
H	3.157386	0.305266	-0.778414
C	2.525882	1.844062	0.546725
H	3.365267	1.731269	1.222283
H	1.790954	2.608831	0.779018

Table S3. Absolute energies of IRC points of enol system.

	UM06-2X-D3/	MS-CASPT2/aug-cc-pVDZ//M06-2X-D3/6-31+G(d,p)			
	6-31+G(d,p)	state 1	state 2	state 3	state 4
-20	-839.3561398	-837.7962154	-837.6467762	-837.6229582	N/A
-19	-839.3558932	-837.7961601	-837.6381522	-837.6209866	N/A
-18	-839.3552057	-837.7956629	-837.6376224	-837.6211639	N/A
-17	-839.3549536	-837.7948969	-837.6356363	-837.6176121	N/A
-16	-839.3548935	-837.7954448	-837.6372189	-837.6214211	N/A
-15	-839.3542467	-837.7949182	-837.6356995	-837.6188383	N/A
-14	-839.3531392	-837.7938459	-837.6350433	-837.6209626	N/A
-13	-839.3529401	-837.7942525	-837.6344087	-837.6190803	N/A
-12	-839.3509736	-837.7928409	-837.6329394	-837.6203974	N/A
-11	-839.3477478	-837.7903270	-837.6312553	-837.6232787	N/A
-10	-839.3433600	-837.7866617	-837.6305980	-837.6263736	N/A
-9	-839.3381770	-837.7822803	-837.6354619	-837.6247528	N/A
-8	-839.3326000	-837.7781473	N/A	-837.6387895	-837.5793264
-7	-839.3269730	-837.7726833	N/A	-837.6369340	-837.5745515
-6	-839.3215578	-837.7678227	N/A	-837.6376824	-837.5777895
-5	-839.3165239	-837.7635666	N/A	-837.6399647	-837.5833208
-4	-839.3119521	-837.7600314	N/A	-837.6422983	-837.5898300
-3	-839.3078451	-837.7567952	N/A	-837.6434286	-837.5949371
-2	-839.3042009	-837.7546314	N/A	-837.6448430	-837.6023903
-1	-839.3015457	-837.7526292	N/A	-837.6449398	-837.6071534
0 ($TSa_{2\text{-}67}$)	-839.3008120	-837.7506073	N/A	-837.6401447	-837.6121623
1	-839.3012628	-837.7493858	N/A	-837.6399497	-837.6115341
2	-839.3021297	-837.7483781	N/A	-837.6391148	-837.6122300
3	-839.3030985	-837.7479207	N/A	-837.6393431	-837.6129218
4	-839.3039980	-837.7475210	N/A	-837.6398346	-837.6135886
5	-839.3047479	-837.7475212	N/A	-837.6402995	-837.6142844
6	-839.3053781	-837.7469503	N/A	-837.6407882	-837.6148239
7	-839.3058328	-837.7472398	N/A	-837.6410517	-837.6152938
8	-839.3063276	-837.7468026	N/A	-837.6414207	-837.6157883
9	-839.3066833	-837.7466974	N/A	-837.6416286	-837.6161009
10	-839.3069647	-837.7464307	N/A	-837.6416415	-837.6163732
11	-839.3071783	-837.7462467	N/A	-837.6417378	-837.6166271
12	-839.3073553	-837.7460837	N/A	-837.6417033	-837.6167307
13	-839.3074939	-837.7458840	N/A	-837.6416807	-837.6169120
14	-839.3076047	-837.7457763	N/A	-837.6417030	-837.6169629
15	-839.3076883	-837.7456001	N/A	-837.6416267	-837.6170364
16	-839.3077498	-837.7455659	N/A	-837.6417646	-837.6171317
17	-839.3077933	-837.7454137	N/A	-837.6416284	-837.6170952
18	-839.3078246	-837.7454653	N/A	-837.6420011	-837.6173592
19	-839.3078133	-837.7452409	N/A	-837.6414669	-837.6169754
20	-839.3078571	-837.7454376	N/A	-837.6422123	-837.6175938

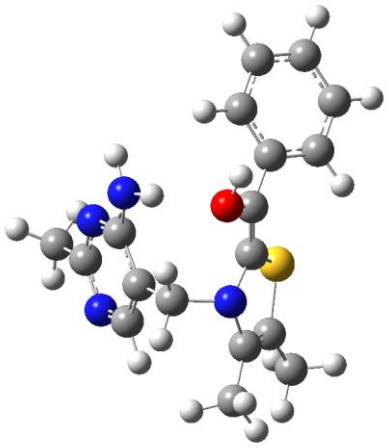
Table S4. Absolute energies of IRC points of enolate system.

	UM06-2X-D3/	MS-CASPT2/aug-cc-pVDZ//M06-2X-D3/6-31+G(d,p)				
	6-31+G(d,p)	state 1	state 2	state 3	state 4	state 5
-20	-838.7931922	-837.2306288	-837.1810676	-837.1117937	-837.0216768	-837.0364374
-19	-838.7929702	-837.2302838	-837.1804615	-837.1107029	-837.0201957	-837.0357489
-18	-838.7926509	-837.2303900	-837.1811544	-837.1137003	-837.0232249	-837.0357921
-17	-838.7923274	-837.2297575	-837.1800820	-837.1116074	-837.0197263	-837.0347729
-16	-838.7921250	-837.2298804	-837.1805314	-837.1134201	-837.0220492	-837.0345486
-15	-838.7916359	-837.2296636	-837.1807303	-837.1151137	-837.0231301	-837.0343360
-14	-838.7911445	-837.2288155	-837.1786179	-837.1118670	-837.0194738	-837.0324261
-13	-838.7908746	-837.2289894	-837.1804603	-837.1162049	-837.0234757	-837.0332127
-12	-838.7903597	-837.2284017	-837.1786340	-837.1130823	-837.0204776	-837.0316648
-11	-838.7892247	-837.2274431	-837.1785873	-837.1155694	-837.0225050	-837.0305798
-10	-838.7889104	-837.2275862	-837.1775662	-837.1142412	-837.0213364	-837.0298600
-9	-838.7873270	-837.2266725	-837.1761922	-837.1157622	-837.0220641	-837.0283578
-8	-838.7848193	-837.2249348	-837.1743633	-837.1174480	-837.0227178	-837.0271146
-7	-838.7813984	-837.2223081	-837.1720355	-837.1206432	-837.0213220	-837.0296555
-6	-838.7774660	-837.2198081	-837.1704706	-837.1280448	-837.0465764	-837.0288026
-5	-838.7735053	-837.2169311	-837.1674850	-837.1294323	-837.0550963	-837.0290739
-4	-838.7699212	-837.2146800	-837.1646567	-837.1297131	-837.0655155	-837.0283584
-3	-838.7669825	-837.2132785	-837.1620009	-837.1284852	-837.0744945	-837.0284067
-2	-838.7647801	-837.2123953	-837.1596357	-837.1262337	-837.0803059	-837.0287869
-1	-838.7632902	-837.2121930	-837.1585684	-837.1261374	-837.0853806	-837.0311097
0 ($TS'a_{2\text{-}67}$)	-838.7627186	-837.2132451	-837.1587813	-837.1265172	-837.0864080	-837.0334419
1	-838.7630809	-837.2141029	-837.1609258	-837.1288807	-837.0854997	-837.0364510
2	-838.7639028	-837.2147141	-837.1635917	-837.1350619	-837.0837214	-837.0394808
3	-838.7649031	-837.2154385	-837.1660554	-837.1412347	-837.0817470	-837.0421791
4	-838.7659098	-837.2159981	-837.1683597	-837.1468014	-837.0797424	-837.0446167
5	-838.7668499	-837.2165746	-837.1703215	-837.1513491	-837.0781296	-837.0467409
6	-838.7676786	-837.2170140	-837.1720906	-837.1563384	-837.0766469	-837.0485976
7	-838.7683505	-837.2172457	-837.1732281	-837.1595617	-837.0759844	-837.0499468
8	-838.7689023	-837.2173652	-837.1746817	-837.1632957	-837.0746312	-837.0513784
9	-838.7692406	-837.2174554	-837.1750332	-837.1641528	-837.0749365	-837.0519281
10	-838.7696749	-837.2175687	-837.1761534	-837.1673011	-837.0740700	-837.0529996
11	-838.7699370	-837.2175832	-837.1766790	-837.1688237	-837.0736028	-837.0535585
12	-838.7701592	-837.2173639	-837.1770765	-837.1703285	-837.0735893	-837.0539790
13	-838.7703206	-837.2176030	-837.1775849	-837.1716901	-837.0730086	-837.0543779
14	-838.7704272	-837.2176681	-837.1777224	-837.1725786	-837.0729767	-837.0546984
15	-838.7704866	-837.2173207	-837.1779221	-837.1730094	-837.0728223	-837.0545759
16	-838.7706675	-837.2171236	-837.1782246	-837.1740894	-837.0726181	-837.0551773
17	-838.7707661	-837.2175233	-837.1783197	-837.1744502	-837.0724172	-837.0550729
18	-838.7708483	-837.2172806	-837.1784143	-837.1749456	-837.0723639	-837.0553599
19	-838.7706781	-837.2180496	-837.1784856	-837.1755298	-837.0715838	-837.0551388
20	-838.7708967	-837.2176632	-837.1785754	-837.1756600	-837.0721055	-837.0558706
21	-838.7709581	-837.2181014	-837.1786597	-837.1761947	-837.0713067	-837.0552820
22	-838.7706316	-837.2176679	-837.1784783	-837.1763400	-837.0712006	-837.0556961
23	-838.7709072	-837.2180097	-837.1786445	-837.1767238	-837.0710494	-837.0558577
24	-838.7711930	-837.2180108	-837.1788471	-837.1774263	-837.0708778	-837.0558828
25	-838.7710363	-837.2184197	-837.1786414	-837.1773841	-837.0704475	-837.0551839
26	-838.7706872	-837.2177108	-837.1785660	-837.1777996	-837.0701542	-837.0561558
27	-838.7711426	-837.2181986	-837.1786711	-837.1779146	-837.0699732	-837.0552147
28	-838.7710287	-837.2178918	-837.1786460	-837.1785152	-837.0697819	-837.0561572
29	-838.7709153	-837.2175444	-837.1783280	-837.1784391	-837.0690899	-837.0546725
30	-838.7711709	-837.2183733	-837.1788098	-837.1794867	-837.0695510	-837.0551717

31	-838.7707406	-837.2178766	-837.1785959	-837.1791951	-837.0694109	-837.0567127
32	-838.7703374	-837.2171724	-837.1777246	-837.1788371	-837.0680216	-837.0530573
33	-838.7711517	-837.2183431	-837.1790177	-837.1801423	-837.0691711	-837.0561213
34	-838.7705356	-837.2174573	-837.1776609	-837.1794930	-837.0678654	-837.0535747
35	-838.7705525	-837.2173527	-837.1781058	-837.1798105	-837.0680002	-837.0555388
36	-838.7713384	-837.2178907	-837.1784477	-837.1808378	-837.0682824	-837.0542211
37	-838.7713504	-837.2179740	-837.1791524	-837.1807983	-837.0688523	-837.0564950
38	-838.7712609	-837.2174111	-837.1784724	-837.1801825	-837.0687822	-837.0533422
39	-838.7710829	-837.2170836	-837.1788048	-837.1799054	-837.0687723	-837.0558341
40	-838.7711790	-837.2173714	-837.1788617	-837.1802990	-837.0691497	-837.0551147
41	-838.7710227	-837.2172410	-837.1785413	-837.1803459	-837.0688432	-837.0543839
42	-838.7711056	-837.2173351	-837.1790519	-837.1805135	-837.0689800	-837.0555594
43	-838.7714874	-837.2177042	-837.1792952	-837.1806527	-837.0695228	-837.0556185
44	-838.7715565	-837.2174428	-837.1792246	-837.1806341	-837.0693705	-837.0552133
45	-838.7713552	-837.2177047	-837.1791278	-837.1808064	-837.0691652	-837.0552314
46	-838.7713739	-837.2176692	-837.1790145	-837.1807537	-837.0689921	-837.0555760
47	-838.7714539	-837.2177997	-837.1791066	-837.1811598	-837.0690628	-837.0550424
48	-838.7716401	-837.2180327	-837.1793524	-837.1815351	-837.0686341	-837.0557130
49	-838.7716245	-837.2177761	-837.1789207	-837.1815524	-837.0687825	-837.0549727
50	-838.7715328	-837.2182834	-837.1795118	-837.1821881	-837.0687446	-837.0559438
51	-838.7717282	-837.2178110	-837.1792582	-837.1821848	-837.0683848	-837.0553436
52	-838.7718059	-837.2177721	-837.1793632	-837.1824855	-837.0684994	-837.0552320
53	-838.7718677	-837.2177068	-837.1795894	-837.1826750	-837.0685791	-837.0556331
54	-838.7719122	-837.2175143	-837.1792525	-837.1823800	-837.0686707	-837.0549140
55	-838.7719366	-837.2176803	-837.1796493	-837.1826743	-837.0685015	-837.0557325
56	-838.7719035	-837.2173864	-837.1791669	-837.1825292	-837.0688443	-837.0549592
57	-838.7718947	-837.2175602	-837.1792273	-837.1826121	-837.0680118	-837.0547548
58	-838.7718993	-837.2173841	-837.1793952	-837.1828100	-837.0682746	-837.0556826
59	-838.7719575	-837.2176726	-837.1789225	-837.1827938	-837.0683837	-837.0542843
60	-838.7720743	-837.2174723	-837.1793449	-837.1831890	-837.0678459	-837.0554145

2c neutral singlet, optimized with SMD mimicking the water solution

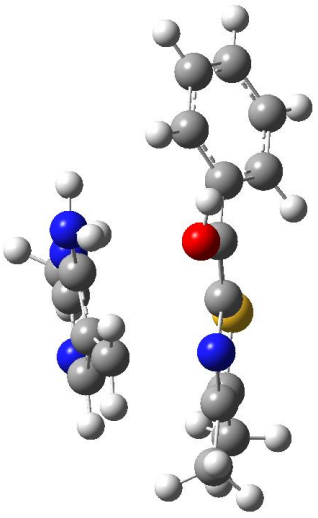
E	-1390.009029
E+ZPE	-1389.650551
H	-1389.626874
G	-1389.702971
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.713603	2.222301	0.397604
C	1.401203	2.321592	-0.902981
C	-0.370929	1.154981	0.440173
N	0.789794	1.476091	1.196782
S	-0.118902	1.485553	-1.288966
C	2.897515	2.833652	1.081041
H	2.588634	3.306572	2.018161
H	3.667459	2.092231	1.320041
H	3.354999	3.593526	0.446439
C	1.422552	0.319920	1.898855
H	2.324999	0.699429	2.381520
H	0.755630	-0.008774	2.694333
C	1.776091	-0.804623	0.958186
N	1.298832	-2.883297	-0.151039
C	2.403359	-2.688994	-0.879784
C	2.714524	-3.734683	-1.907237
H	1.881867	-3.827413	-2.610528
H	3.621616	-3.480926	-2.455518
H	2.846722	-4.707023	-1.423575
C	2.904134	-0.739271	0.166253
H	3.592553	0.095219	0.279781
C	0.973311	-1.959531	0.768345
N	-0.115482	-2.224606	1.535541
H	-0.724733	-2.961858	1.205270
H	-2.384029	0.360129	2.678300
C	2.100442	3.040694	-2.010212
H	3.044972	3.464108	-1.664821
H	2.319482	2.352360	-2.833742
H	1.481728	3.849988	-2.411659
C	-1.500203	0.649572	0.976652
O	-1.476990	0.373733	2.337927
C	-2.708552	0.223011	0.242200
C	-3.371045	-0.953706	0.630115
C	-3.247690	0.983298	-0.807181
C	-4.522370	-1.371956	-0.033947
H	-2.980259	-1.548413	1.451515
C	-4.397116	0.560282	-1.469785
H	-2.783465	1.922157	-1.090943
C	-5.036390	-0.621218	-1.091047
H	-5.015814	-2.288233	0.275282
H	-4.802236	1.164787	-2.275474
H	-5.932722	-0.947811	-1.608817
N	3.243005	-1.657714	-0.759181
H	-0.566729	-1.474018	2.046248

TSc2-67 neutral singlet, optimized with SMD mimicking the water solution

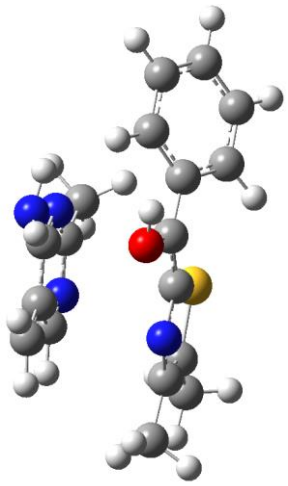
E	-1389.958651
E+ZPE	-1389.606414
H	-1389.582307
G	-1389.658640
$\langle S^2 \rangle$	0.4116
imaginary freq.	540.4*i*



C	2.418823	1.611411	-0.251486
C	2.234560	0.848243	-1.373153
C	0.181564	1.391190	-0.117558
N	1.298302	1.893070	0.489519
S	0.540564	0.510104	-1.618729
C	3.756156	2.092054	0.230104
H	3.623464	2.817210	1.035336
H	4.361973	1.261841	0.611617
H	4.318710	2.569091	-0.576831
C	1.728698	0.436814	2.256026
H	2.759251	0.770272	2.301887
H	1.042886	0.889290	2.961891
C	1.422146	-0.747678	1.569689
N	-0.187670	-2.331986	0.716745
C	0.766487	-2.761942	-0.125990
C	0.359074	-3.820971	-1.103542
H	-0.517421	-3.492506	-1.669677
H	1.172249	-4.043957	-1.794357
H	0.081388	-4.737315	-0.572023
C	2.348267	-1.355116	0.699896
H	3.382828	-1.017582	0.710605
C	0.118437	-1.354253	1.570347
N	-0.813471	-1.020502	2.503095
H	-1.751234	-1.353022	2.311619
H	-1.980209	2.242339	1.977392
C	3.253463	0.396284	-2.365395
H	4.259645	0.573573	-1.978877
H	3.150574	-0.673914	-2.573377
H	3.150135	0.928630	-3.317528
C	-1.067976	1.465946	0.463587
O	-1.079863	1.985325	1.727657
C	-2.325278	0.941331	-0.074554
C	-3.327106	0.491998	0.807962
C	-2.584572	0.892375	-1.457036
C	-4.525679	-0.022198	0.321336
H	-3.169332	0.526261	1.882238
C	-3.784246	0.376518	-1.936333
H	-1.868535	1.298472	-2.163307
C	-4.757587	-0.092123	-1.052191
H	-5.277992	-0.373286	1.020677
H	-3.964588	0.355543	-3.006560
H	-5.691847	-0.494716	-1.430126
N	2.044315	-2.360659	-0.126930
H	-0.773778	-0.089237	2.900568

[6c 7c] neutral singlet, optimized with SMD mimicking the water solution

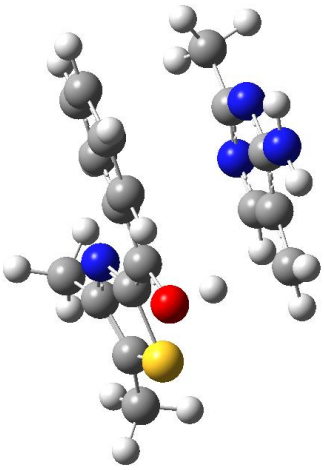
E	-1389.966893
E+ZPE	-1389.616306
H	-1389.590578
G	-1389.673640
$<S^2>$	0.9995
imaginary freq.	N/A



C	-2.446947	-1.661145	-0.381575
C	-2.258554	-0.766087	-1.411203
C	-0.227242	-1.490198	-0.229871
N	-1.319980	-2.077287	0.261712
S	-0.570753	-0.421617	-1.587419
C	-3.787797	-2.167049	0.063440
H	-3.681973	-2.721717	0.997582
H	-4.484349	-1.339421	0.229182
H	-4.233195	-2.831471	-0.683952
C	-2.072607	0.016578	2.549436
H	-3.129775	-0.218482	2.487213
H	-1.491555	-0.485635	3.313083
C	-1.523134	0.949933	1.660037
N	0.340688	2.201966	0.756513
C	-0.514426	2.737496	-0.130956
C	0.075136	3.674879	-1.138536
H	0.742249	3.121777	-1.809377
H	-0.706778	4.148552	-1.732261
H	0.673813	4.444361	-0.643163
C	-2.305396	1.603842	0.689367
H	-3.372353	1.390156	0.645832
C	-0.131878	1.322579	1.639478
N	0.733677	0.838088	2.565797
H	1.716628	0.980692	2.366035
H	1.918997	-2.534504	1.828870
C	-3.281690	-0.141810	-2.301195
H	-4.279719	-0.476807	-2.009923
H	-3.252433	0.950905	-2.232959
H	-3.122953	-0.415363	-3.349505
C	1.041824	-1.625772	0.372110
O	1.021945	-2.280371	1.564456
C	2.292318	-1.041738	-0.089717
C	3.288179	-0.691194	0.846722
C	2.556014	-0.820691	-1.456555
C	4.480746	-0.108987	0.431324
H	3.124119	-0.850749	1.909142
C	3.750048	-0.234886	-1.862639
H	1.850281	-1.150144	-2.211273
C	4.715195	0.132746	-0.923287
H	5.226398	0.164317	1.171265
H	3.933235	-0.080156	-2.921326
H	5.644937	0.590903	-1.244654
N	-1.830125	2.495425	-0.185190
H	0.512362	-0.036700	3.023146

TSc$_{67\text{-}34}$ neutral singlet, optimized with SMD mimicking the water solution

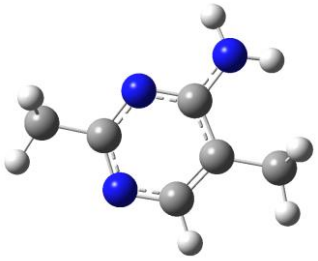
E	-1389.968095
E+ZPE	-1389.619399
H	-1389.595008
G	-1389.672305
$\langle S^2 \rangle$	0.5944
imaginary freq.	381.9*i*



C	-3.395802	1.095878	-0.114271
C	-4.000520	-0.137424	-0.057960
C	-1.655553	-0.058055	0.661354
N	-2.084247	1.131679	0.296366
S	-2.875069	-1.311741	0.542497
C	-4.026719	2.374652	-0.571560
H	-4.018406	3.111986	0.237043
H	-3.462127	2.794208	-1.409728
H	-5.058071	2.227152	-0.892940
C	1.023808	-3.058280	-0.371396
H	0.057337	-3.503636	-0.593405
H	1.772506	-3.706541	0.071827
C	1.352729	-1.833950	-0.967681
N	2.905202	-0.020266	-1.405990
C	1.878979	0.655931	-1.946594
C	2.184344	2.014301	-2.495149
H	2.523586	1.920172	-3.533681
H	1.293069	2.644113	-2.484028
H	2.982407	2.490768	-1.922596
C	0.384133	-1.018806	-1.591981
H	-0.624797	-1.409250	-1.711976
C	2.668539	-1.234146	-0.904542
N	3.693122	-1.887090	-0.340824
H	4.600670	-1.442907	-0.304199
H	0.374683	-2.247947	1.034230
C	-5.394717	-0.537905	-0.422758
H	-5.991790	0.341155	-0.670134
H	-5.399737	-1.208419	-1.288084
H	-5.885076	-1.058720	0.405101
C	-0.353909	-0.419076	1.147893
O	-0.268394	-1.679592	1.602074
C	0.785848	0.461467	1.324074
C	1.894065	-0.014409	2.062725
C	0.853701	1.758207	0.769867
C	3.020441	0.777068	2.237735
H	1.858848	-1.007687	2.498477
C	1.986024	2.545726	0.961979
H	0.020775	2.141762	0.195897
C	3.074022	2.063360	1.689395
H	3.860821	0.393356	2.808336
H	2.019661	3.540763	0.528221
H	3.954984	2.681373	1.831789
N	0.628898	0.194523	-2.092751
H	3.591603	-2.816281	0.038919

3c neutral singlet, optimized with SMD mimicking the water solution

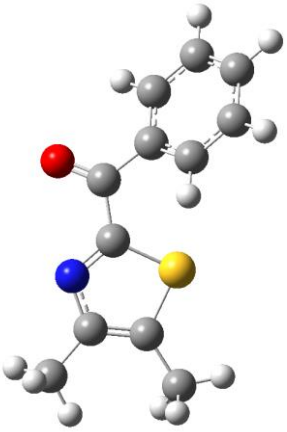
E	-398.202925
E+ZPE	-398.053043
H	-398.043178
G	-398.086607
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A



C	2.607592	-0.802620	0.004237
H	2.800543	-1.877723	0.004520
H	3.085285	-0.367127	0.889264
C	1.132676	-0.537522	-0.000482
N	-0.707291	1.017713	0.001213
C	-1.529248	-0.041168	-0.000089
C	-2.998003	0.260382	0.000817
H	-3.259896	0.850496	0.883989
H	-3.260497	0.853033	-0.880485
H	-3.582341	-0.659747	-0.000384
C	0.184978	-1.533855	-0.004647
H	0.503025	-2.574345	-0.008080
C	0.612174	0.782429	0.001553
N	1.440867	1.853900	0.038734
H	1.042282	2.769652	-0.116774
H	3.092984	-0.368241	-0.877433
N	-1.148957	-1.318447	-0.004051
H	2.425261	1.735960	-0.154224

4c neutral singlet, optimized with SMD mimicking the water solution

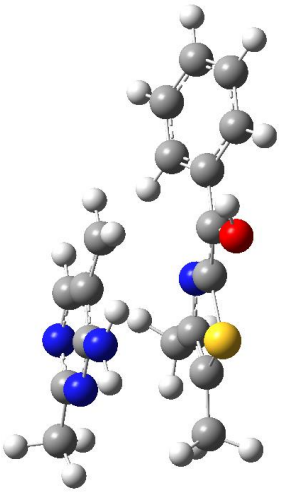
E	-991.823544
E+ZPE	-991.620972
H	-991.605994
G	-991.663916
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.893214	0.462755	0.187924
C	-2.632580	-0.825030	-0.230221
C	-0.687748	0.614262	0.049354
N	-1.790837	1.261133	0.326613
S	-0.938321	-1.032044	-0.427049
C	-4.252022	1.007829	0.493087
H	-5.032554	0.302363	0.202752
H	-4.352018	1.209183	1.564287
H	-4.414638	1.947560	-0.041738
C	-3.611729	-1.929089	-0.482025
H	-4.127190	-2.198734	0.444611
H	-4.364352	-1.608820	-1.208005
H	-3.119611	-2.821867	-0.871413
C	0.643057	1.276815	0.024182
O	0.707511	2.497143	-0.066560
C	1.876715	0.445026	0.068896
C	2.977310	0.857174	-0.693817
C	1.974479	-0.689283	0.884471
C	4.157868	0.123081	-0.662097
H	2.891667	1.741608	-1.317804
C	3.167438	-1.408653	0.928556
H	1.142620	-0.988673	1.514298
C	4.253125	-1.010081	0.149593
H	5.003911	0.432715	-1.267022
H	3.247759	-2.277411	1.573656
H	5.177114	-1.579122	0.177941

TSc67-5 neutral singlet, optimized with SMD mimicking the water solution

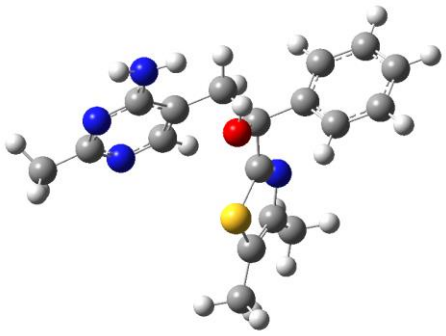
E	-1389.969802
E+ZPE	-1389.619342
H	-1389.594494
G	-1389.673609
$<S^2>$	0.7812
imaginary freq.	133.5*i*



C	-1.062183	2.008551	-0.237507
C	-1.805474	1.400515	-1.220154
C	0.486710	0.561235	-0.928289
N	0.220571	1.544094	-0.083435
S	-0.846975	0.180255	-2.001547
C	-1.523227	3.112782	0.662727
H	-0.990648	4.041730	0.433378
H	-1.311084	2.856599	1.704965
H	-2.593637	3.299450	0.564467
C	0.649208	-2.046472	0.832882
H	0.911806	-2.839816	0.142540
H	1.425919	-1.690774	1.499938
C	-0.666417	-1.594716	1.015771
N	-2.998869	-1.482350	0.377460
C	-3.138231	-0.479197	1.254249
C	-4.479226	0.182009	1.348487
H	-5.128299	-0.130976	0.530197
H	-4.363891	1.270065	1.326535
H	-4.959208	-0.078269	2.298283
C	-0.976409	-0.581330	1.944283
H	-0.187073	-0.214887	2.598696
C	-1.794006	-2.048013	0.247600
N	-1.688422	-3.096500	-0.600888
H	-2.454838	-3.247797	-1.243401
H	2.403676	-1.709068	-1.971905
C	-3.211295	1.655472	-1.661959
H	-3.674955	2.421773	-1.037847
H	-3.818831	0.746685	-1.591771
H	-3.245405	1.998847	-2.701222
C	1.683177	-0.195813	-1.004713
O	1.740069	-1.013655	-2.098558
C	2.899636	0.053405	-0.239630
C	4.152018	-0.269256	-0.797536
C	2.863764	0.593846	1.062474
C	5.326221	-0.048762	-0.081844
H	4.217575	-0.668615	-1.804930
C	4.040985	0.810972	1.767586
H	1.907910	0.823053	1.518202
C	5.279389	0.493774	1.201734
H	6.280882	-0.296231	-0.535683
H	3.991835	1.222022	2.771288
H	6.195505	0.665261	1.757888
N	-2.182935	-0.035500	2.087042
H	-0.776459	-3.406124	-0.904632

5c neutral singlet, optimized with SMD mimicking the water solution

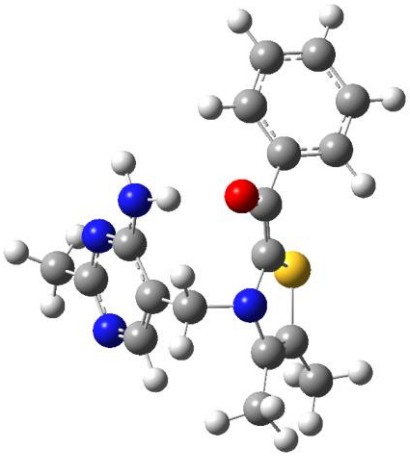
E	-1390.050781
E+ZPE	-1389.692817
H	-1389.668838
G	-1389.747039
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.399938	2.800594	0.673349
C	-0.256446	3.009572	-0.508599
C	0.594716	0.747665	-0.151867
N	0.878385	1.511220	0.856919
S	-0.273606	1.534554	-1.427177
C	0.647914	3.805447	1.754597
H	1.722814	3.934440	1.914946
H	0.210230	3.463642	2.697669
H	0.218485	4.777259	1.509008
C	0.074256	-1.461881	0.876834
H	0.358784	-2.520497	0.879081
H	0.338057	-1.051205	1.855384
C	-1.406918	-1.291580	0.667766
N	-3.518541	-1.945690	-0.278475
C	-4.055077	-0.862066	0.292740
C	-5.515588	-0.632691	0.046156
H	-5.873450	0.226768	0.612885
H	-6.090610	-1.518654	0.328963
H	-5.688653	-0.454061	-1.019651
C	-2.085678	-0.225083	1.220046
H	-1.544529	0.484746	1.843522
C	-2.206985	-2.174427	-0.100906
N	-1.713964	-3.317742	-0.641778
H	-2.304167	-3.798237	-1.307707
H	0.913170	-2.032958	-1.671740
C	-0.888069	4.253690	-1.051637
H	-0.808296	5.065250	-0.326316
H	-1.948409	4.096689	-1.269955
H	-0.398890	4.574760	-1.976192
C	0.913563	-0.735386	-0.202474
O	0.515141	-1.166607	-1.500089
C	2.420162	-0.932035	-0.025969
C	3.262007	-0.521177	-1.068256
C	2.985475	-1.482930	1.125270
C	4.642195	-0.665380	-0.964278
H	2.829895	-0.085787	-1.965540
C	4.371665	-1.626432	1.229842
H	2.361533	-1.805568	1.951727
C	5.202407	-1.220580	0.188656
H	5.280744	-0.342942	-1.780964
H	4.797295	-2.058482	2.130275
H	6.278786	-1.334027	0.272637
N	-3.399530	0.019122	1.051551
H	-0.717912	-3.421431	-0.767640

2'c singlet anion, optimized with SMD mimicking the water solution

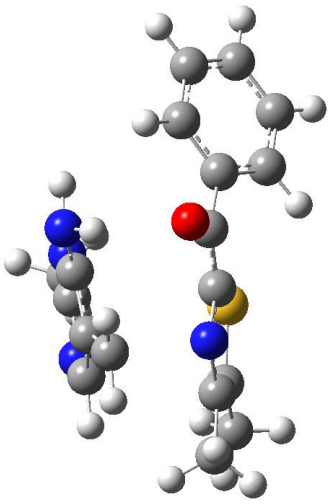
E	-1389.535283
E+ZPE	-1389.190165
H	-1389.166857
G	-1389.242693
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.583890	2.301028	0.384221
C	1.204283	2.392425	-0.900930
C	-0.432426	1.099473	0.513728
N	0.755712	1.492714	1.222166
S	-0.252789	1.433633	-1.239777
C	2.768824	2.974283	1.008628
H	2.492816	3.412483	1.972869
H	3.592813	2.274452	1.187332
H	3.146421	3.770384	0.365434
C	1.494110	0.377859	1.874928
H	2.397341	0.801752	2.319391
H	0.876255	0.003314	2.690840
C	1.862706	-0.729374	0.922774
N	1.421517	-2.840779	-0.139861
C	2.496048	-2.618171	-0.906432
C	2.812073	-3.669639	-1.927527
H	1.974843	-3.778145	-2.623495
H	3.710327	-3.408762	-2.487118
H	2.960425	-4.636763	-1.438441
C	2.957862	-0.632902	0.092100
H	3.617245	0.229403	0.169884
C	1.091099	-1.911839	0.773508
N	0.035134	-2.186178	1.583568
H	-0.544908	-2.960289	1.284907
C	1.805774	3.174931	-2.023572
H	2.728872	3.667722	-1.713064
H	2.042649	2.514084	-2.865195
H	1.112191	3.938053	-2.392880
C	-1.501421	0.509473	1.117728
O	-1.507555	0.175554	2.402022
C	-2.705351	0.105921	0.319585
C	-3.266441	-1.162974	0.528182
C	-3.347109	0.975469	-0.574318
C	-4.408386	-1.565824	-0.162449
H	-2.802038	-1.838022	1.241841
C	-4.495066	0.578449	-1.259425
H	-2.954567	1.977167	-0.721996
C	-5.026687	-0.697072	-1.063134
H	-4.818485	-2.557334	0.006322
H	-4.981555	1.272033	-1.939167
H	-5.919757	-1.006232	-1.597619
N	3.298540	-1.554181	-0.833015
H	-0.464857	-1.407988	2.024826

TS'c$_{2\text{-}84}$ singlet anion, optimized with SMD mimicking the water solution

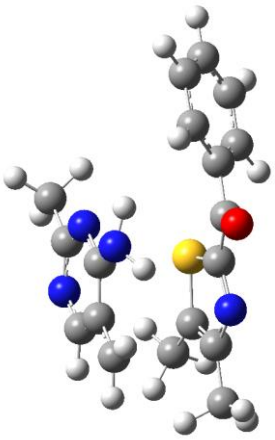
E	-1389.496932
E+ZPE	-1389.156149
H	-1389.132808
G	-1389.207512
$\langle S^2 \rangle$	0.0000
imaginary freq.	315.1*i*



C	-2.327349	-1.669054	-0.149617
C	-2.087929	-1.024737	-1.329142
C	-0.108333	-1.353962	0.110392
N	-1.253498	-1.797877	0.710280
S	-0.400632	-0.619743	-1.493422
C	-3.676697	-2.166871	0.281913
H	-3.576166	-2.792423	1.171291
H	-4.353016	-1.338092	0.522391
H	-4.149428	-2.761203	-0.504930
C	-1.884566	-0.303092	2.200430
H	-2.913334	-0.644821	2.244306
H	-1.249677	-0.616204	3.021698
C	-1.583888	0.842933	1.446149
N	0.058624	2.358249	0.525784
C	-0.841061	2.678160	-0.421932
C	-0.390583	3.649827	-1.472833
H	0.577887	3.349784	-1.882281
H	-1.119152	3.707551	-2.282626
H	-0.269419	4.650348	-1.041689
C	-2.463020	1.355517	0.470586
H	-3.500631	1.025457	0.466103
C	-0.290369	1.467793	1.451375
N	0.583016	1.249730	2.495029
H	1.509212	1.616492	2.301581
C	-3.052938	-0.734095	-2.431766
H	-4.077244	-0.919409	-2.099703
H	-2.979730	0.312619	-2.746107
H	-2.857643	-1.355677	-3.312717
C	1.122388	-1.338198	0.792863
O	1.195963	-1.652795	2.031557
C	2.379751	-0.882582	0.118064
C	3.331007	-0.185584	0.878632
C	2.680162	-1.178578	-1.219841
C	4.523897	0.249101	0.305413
H	3.129802	0.011489	1.927181
C	3.879910	-0.755690	-1.789770
H	1.990825	-1.770008	-1.813987
C	4.800804	-0.029223	-1.034030
H	5.240879	0.800492	0.906275
H	4.098750	-1.003896	-2.823960
H	5.732305	0.304294	-1.480899
N	-2.115329	2.268621	-0.442382
H	0.631385	0.280404	2.808076

[8c 4c] singlet anion, optimized with SMD mimicking the water solution

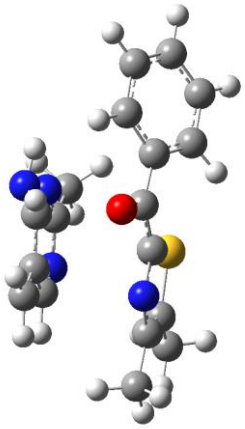
E	-1389.508991
E+ZPE	-1389.169364
H	-1389.144484
G	-1389.223649
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A



C	-2.254074	-1.780975	0.278585
C	-1.943079	-1.478708	-1.034763
C	-0.105918	-1.321472	0.550378
N	-1.218605	-1.692243	1.154332
S	-0.279887	-1.092408	-1.163318
C	-3.633601	-2.136510	0.740213
H	-3.631416	-2.341343	1.812191
H	-4.328163	-1.310926	0.546655
H	-4.014240	-3.017935	0.214320
C	-2.827472	1.364567	1.996348
H	-3.885007	1.146056	1.876478
H	-2.448100	1.453413	3.007402
C	-2.040600	1.612131	0.872230
N	0.121298	2.173704	-0.114879
C	-0.453928	2.133496	-1.339701
C	0.435070	2.429370	-2.513637
H	1.315702	1.776527	-2.511025
H	-0.104785	2.277020	-3.450363
H	0.799215	3.463512	-2.489672
C	-2.502933	1.602666	-0.470843
H	-3.555833	1.395169	-0.661830
C	-0.622870	1.907041	0.943868
N	-0.036072	2.006409	2.196823
H	0.976420	1.957383	2.156957
C	-2.865523	-1.514631	-2.210071
H	-3.843798	-1.114803	-1.926890
H	-2.480772	-0.923952	-3.043984
H	-3.009863	-2.543069	-2.559131
C	1.127472	-1.025469	1.297700
O	1.100748	-0.952620	2.527855
C	2.400580	-0.761445	0.562986
C	3.239264	0.250954	1.047512
C	2.797409	-1.518097	-0.546648
C	4.439537	0.533236	0.403298
H	2.939767	0.819578	1.923058
C	4.010942	-1.246111	-1.176433
H	2.185325	-2.342832	-0.897952
C	4.825249	-0.213628	-0.711941
H	5.075337	1.332126	0.771277
H	4.320315	-1.844795	-2.027083
H	5.764198	0.003047	-1.211865
N	-1.744266	1.876055	-1.543102
H	-0.411734	1.349338	2.874998

[6c 7'c] singlet anion, optimized with SMD mimicking the water solution

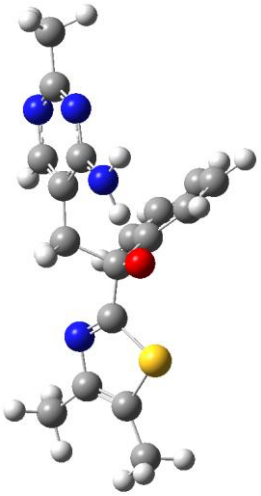
E	-1389.505381
E+ZPE	-1389.166745
H	-1389.141820
G	-1389.221459
$<S^2>$	0.8486
imaginary freq.	N/A



C	-2.520867	-1.606717	-0.264376
C	-2.306526	-0.832498	-1.376770
C	-0.288580	-1.472781	-0.086607
N	-1.405501	-1.975830	0.439852
S	-0.599692	-0.559557	-1.571328
C	-3.857404	-2.050945	0.249466
H	-3.877329	-3.138694	0.368850
H	-4.048858	-1.608980	1.233859
H	-4.671805	-1.763947	-0.417194
C	-1.903346	0.218851	2.677936
H	-2.962258	-0.015170	2.696002
H	-1.283598	-0.187405	3.468098
C	-1.396484	1.042848	1.670599
N	0.432114	2.189956	0.572105
C	-0.456874	2.643511	-0.328454
C	0.090210	3.490438	-1.436665
H	0.834907	2.926107	-2.007737
H	-0.706330	3.808625	-2.109762
H	0.591328	4.375130	-1.030900
C	-2.218598	1.611249	0.673662
H	-3.289580	1.415750	0.703144
C	-0.005916	1.402943	1.552295
N	0.889379	1.020326	2.511678
H	1.856475	1.155078	2.236628
C	-3.275037	-0.264719	-2.364368
H	-4.296626	-0.555126	-2.111613
H	-3.229197	0.829896	-2.380027
H	-3.065342	-0.617484	-3.380035
C	0.977515	-1.559904	0.592878
O	1.006115	-2.025577	1.790442
C	2.238270	-1.058728	-0.001323
C	3.279798	-0.682500	0.871718
C	2.484767	-0.969774	-1.385305
C	4.486191	-0.188519	0.385859
H	3.129352	-0.781613	1.942133
C	3.696150	-0.480314	-1.869423
H	1.752263	-1.328020	-2.100014
C	4.699990	-0.072505	-0.989893
H	5.264449	0.106543	1.083700
H	3.859195	-0.431474	-2.942090
H	5.640938	0.312437	-1.370278
N	-1.776097	2.413062	-0.296928
H	0.729338	0.103662	2.920642

5'c singlet anion, optimized with SMD mimicking the water solution

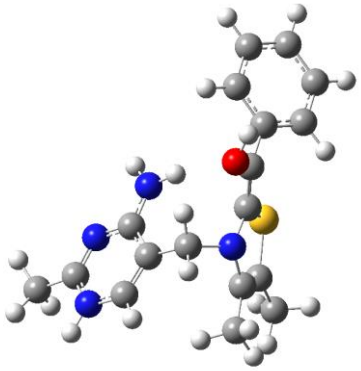
E	-1389.567319
E+ZPE	-1389.224238
H	-1389.200686
G	-1389.279095
$<S^2>$	0.0000
imaginary freq.	N/A



C	-3.774303	-0.573715	1.119691
C	-4.366727	-0.385729	-0.096603
C	-1.911462	-0.461705	-0.103272
N	-2.383844	-0.612768	1.096721
S	-3.139823	-0.275566	-1.324833
C	-4.460002	-0.750016	2.439245
H	-4.137486	0.022884	3.144086
H	-4.204786	-1.721342	2.875087
H	-5.544989	-0.693942	2.342265
C	0.384641	-1.265542	0.462852
H	0.026638	-1.089416	1.480982
H	0.158352	-2.309802	0.207707
C	1.873225	-1.039733	0.456806
N	4.041791	-1.168297	-0.590372
C	4.562144	-0.717052	0.558369
C	6.053642	-0.560270	0.594158
H	6.384943	-0.224248	1.576840
H	6.372609	0.167553	-0.158139
H	6.538591	-1.511560	0.356622
C	2.533495	-0.571417	1.568599
H	1.963178	-0.328978	2.463952
C	2.705945	-1.310685	-0.667369
N	2.161353	-1.745392	-1.823738
H	2.787728	-1.782300	-2.618075
C	-5.819079	-0.309557	-0.453472
H	-6.436635	-0.373407	0.444317
H	-6.106793	-1.127561	-1.121360
H	-6.054704	0.631525	-0.959529
C	-0.443301	-0.384776	-0.533547
O	-0.331067	-0.823448	-1.837230
C	0.021176	1.079690	-0.349935
C	0.682319	1.739705	-1.386796
C	-0.134749	1.744206	0.874398
C	1.173840	3.036787	-1.210874
H	0.814398	1.230550	-2.335909
C	0.353387	3.037010	1.053633
H	-0.638917	1.243713	1.697069
C	1.011396	3.690841	0.008686
H	1.685885	3.533083	-2.030350
H	0.221957	3.534670	2.010169
H	1.392903	4.697957	0.146940
N	3.871588	-0.391544	1.651152
H	1.153091	-1.464978	-1.971270

2cN1H singlet cation, optimized with SMD mimicking the water solution

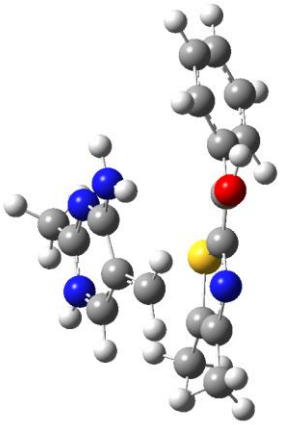
E	-1390.460585
E+ZPE	-1390.088728
H	-1390.064610
G	-1390.142224
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.984714	2.217084	0.386320
C	0.491035	2.440747	-0.840423
C	-0.904120	0.828948	0.495416
N	0.287162	1.232066	1.147259
S	-0.935514	1.433102	-1.179966
C	2.129241	2.926377	1.038643
H	1.861649	3.211484	2.060711
H	3.028728	2.305472	1.088759
H	2.382466	3.830729	0.484076
C	1.131405	0.207808	1.800569
H	1.702120	0.701010	2.591365
H	0.473157	-0.515728	2.281691
C	2.117201	-0.501600	0.895878
N	2.693247	-2.050158	-0.901895
C	3.961623	-1.781627	-0.705532
C	5.008579	-2.382535	-1.576338
H	5.122527	-1.757832	-2.468113
H	5.968466	-2.432631	-1.060104
H	4.698196	-3.379299	-1.888715
C	3.454150	-0.304219	1.062612
H	3.865079	0.343038	1.829214
C	1.758005	-1.457615	-0.114231
N	0.505397	-1.838136	-0.321644
H	0.315005	-2.521556	-1.044595
H	-2.568297	-0.556395	2.751249
C	0.922852	3.415501	-1.886432
H	1.845253	3.917887	-1.590050
H	1.107154	2.901883	-2.836044
H	0.153748	4.174277	-2.064162
C	-1.891181	0.106067	1.065054
O	-1.707187	-0.327851	2.371086
C	-3.096495	-0.390903	0.365526
C	-3.447671	-1.743950	0.490996
C	-3.919386	0.458944	-0.386550
C	-4.586726	-2.239489	-0.139680
H	-2.818942	-2.407895	1.078801
C	-5.055889	-0.041123	-1.018717
H	-3.680073	1.515360	-0.461431
C	-5.391425	-1.390675	-0.900655
H	-4.842744	-3.289780	-0.040157
H	-5.687488	0.628682	-1.594066
H	-6.278449	-1.776724	-1.393009
N	4.357746	-0.940902	0.273355
H	-0.273951	-1.448461	0.194695
H	5.351757	-0.776885	0.416382

TSc2-67N1H singlet cation, optimized with SMD mimicking the water solution

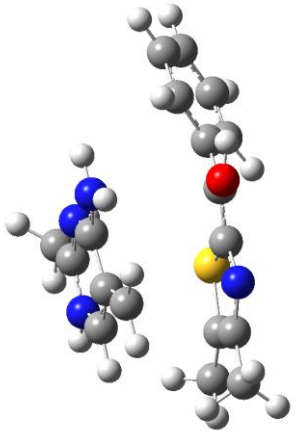
E	-1390.416621
E+ZPE	-1390.049950
H	-1390.026057
G	-1390.101108
$\langle S^2 \rangle$	0.3304
imaginary freq.	456.5*i*



C	2.375278	1.569151	-0.421353
C	2.171138	0.656741	-1.431434
C	0.145794	1.362235	-0.227093
N	1.274452	1.935751	0.297097
S	0.476100	0.309274	-1.622676
C	3.723165	2.101501	-0.038201
H	3.612331	2.897906	0.699812
H	4.350779	1.313400	0.394108
H	4.247691	2.503066	-0.909304
C	1.780654	0.714651	2.208932
H	2.803120	1.073455	2.198814
H	1.098394	1.212142	2.886031
C	1.487027	-0.527639	1.636562
N	-0.186107	-2.164501	0.915704
C	0.694350	-2.649047	0.056663
C	0.298017	-3.737051	-0.879829
H	-0.572840	-3.413650	-1.455304
H	1.110170	-3.990093	-1.561842
H	0.015712	-4.624754	-0.306964
C	2.386805	-1.161137	0.777460
H	3.432201	-0.888051	0.703403
C	0.177900	-1.154826	1.725896
N	-0.693810	-0.783506	2.659559
H	-1.618051	-1.197317	2.655847
H	-2.002869	2.367487	1.818236
C	3.178551	0.083765	-2.370414
H	4.188417	0.285098	-2.006432
H	3.054111	-1.001069	-2.463030
H	3.078222	0.513370	-3.373075
C	-1.091246	1.495582	0.362649
O	-1.097212	2.142447	1.554883
C	-2.349854	0.915436	-0.124426
C	-3.302057	0.442615	0.795866
C	-2.639505	0.840012	-1.497375
C	-4.493499	-0.122796	0.349744
H	-3.110221	0.497128	1.863909
C	-3.832346	0.274198	-1.936118
H	-1.952052	1.260005	-2.224516
C	-4.759931	-0.217084	-1.016133
H	-5.212412	-0.494304	1.072989
H	-4.043440	0.230895	-2.999867
H	-5.689080	-0.658823	-1.361700
N	1.973846	-2.224881	0.045414
H	-0.537099	0.026243	3.243733
H	2.626896	-2.657970	-0.603892

[6cN1H 7c] singlet cation, optimized with SMD mimicking the water solution

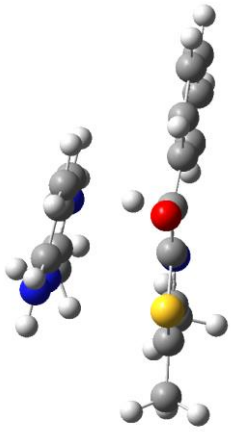
E	-1390.423761
E+ZPE	-1390.058333
H	-1390.032992
G	-1390.112648
$\langle S^2 \rangle$	0.9647
imaginary freq.	N/A



C	-2.451950	-1.602856	-0.376511
C	-2.241786	-0.745664	-1.436463
C	-0.230886	-1.458331	-0.212058
N	-1.339222	-2.010090	0.292352
S	-0.545141	-0.444241	-1.621705
C	-3.806217	-2.064611	0.074262
H	-3.705671	-2.710242	0.948279
H	-4.439516	-1.212847	0.344137
H	-4.320158	-2.622594	-0.714134
C	-2.068070	-0.050798	2.568060
H	-3.119506	-0.302190	2.491098
H	-1.487198	-0.542239	3.337126
C	-1.522828	0.888402	1.683729
N	0.384683	2.132699	0.772748
C	-0.409691	2.634303	-0.154316
C	0.148126	3.530981	-1.203163
H	0.884915	2.973772	-1.789269
H	-0.631750	3.905434	-1.866538
H	0.659540	4.371278	-0.727689
C	-2.295751	1.489094	0.695358
H	-3.359357	1.311352	0.589308
C	-0.124089	1.291072	1.692688
N	0.702427	0.862385	2.636709
H	1.678789	1.128296	2.590790
H	1.892867	-2.438989	1.898433
C	-3.250361	-0.143511	-2.358084
H	-4.257519	-0.392035	-2.016037
H	-3.161327	0.948104	-2.394385
H	-3.133797	-0.518886	-3.380254
C	1.028320	-1.585772	0.403722
O	0.997290	-2.203333	1.611836
C	2.288228	-1.028440	-0.073771
C	3.270393	-0.627339	0.854925
C	2.568950	-0.888729	-1.446952
C	4.470480	-0.073275	0.422561
H	3.090416	-0.724987	1.922161
C	3.770617	-0.331253	-1.870590
H	1.871882	-1.260404	-2.190184
C	4.723523	0.087593	-0.940563
H	5.207329	0.240920	1.154959
H	3.969327	-0.239885	-2.933766
H	5.659538	0.522775	-1.275426
N	-1.729892	2.361061	-0.172646
H	0.423253	0.180706	3.328524
H	-2.306132	2.769607	-0.905689

TSc67-34N1H singlet cation, optimized with SMD mimicking the water solution

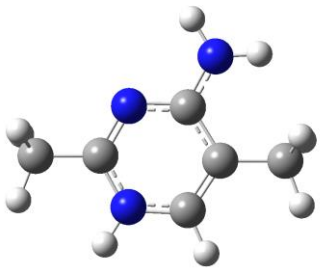
E	-1390.421575
E+ZPE	-1390.059160
H	-1390.034788
G	-1390.112571
$\langle S^2 \rangle$	0.5993
imaginary freq.	583.6*i*



C	2.063528	-1.869619	-0.141733
C	2.772006	-1.085897	-1.027569
C	0.361215	-0.665990	-0.926105
N	0.716908	-1.626765	-0.090731
S	1.699596	-0.009970	-1.849515
C	2.645601	-2.953054	0.716977
H	2.723105	-3.891269	0.157368
H	2.002323	-3.127188	1.581914
H	3.643824	-2.690784	1.074504
C	-1.334246	3.088309	-0.267412
H	-0.954269	3.906144	-0.868543
H	-2.410555	3.020276	-0.139102
C	-0.512447	2.316272	0.563606
N	1.700019	1.543892	1.307195
C	1.117656	0.608957	2.031237
C	1.936891	-0.311651	2.863415
H	2.855082	-0.563548	2.329455
H	1.386115	-1.220014	3.112509
H	2.209992	0.203044	3.791031
C	-1.038599	1.298404	1.359121
H	-2.104697	1.131688	1.458475
C	0.944142	2.384452	0.571994
N	1.585662	3.284688	-0.152216
H	2.598321	3.305026	-0.128043
H	-1.260420	1.758630	-1.561549
C	4.236198	-1.104128	-1.325808
H	4.738847	-1.835690	-0.690701
H	4.688578	-0.123628	-1.147600
H	4.423336	-1.373728	-2.369893
C	-0.948666	-0.133967	-1.143012
O	-0.987842	0.891115	-2.013993
C	-2.210455	-0.647911	-0.632955
C	-3.400982	-0.003481	-1.031664
C	-2.296208	-1.727641	0.272753
C	-4.630734	-0.415130	-0.528645
H	-3.359169	0.816121	-1.740683
C	-3.531833	-2.132738	0.761777
H	-1.394986	-2.234207	0.591991
C	-4.704107	-1.478353	0.371908
H	-5.535234	0.094617	-0.845516
H	-3.581113	-2.965007	1.457149
H	-5.664615	-1.799691	0.761958
N	-0.227407	0.499324	2.084810
H	1.103532	3.965908	-0.722790
H	-0.638822	-0.255099	2.631533

3cN1H singlet cation, optimized with SMD mimicking the water solution

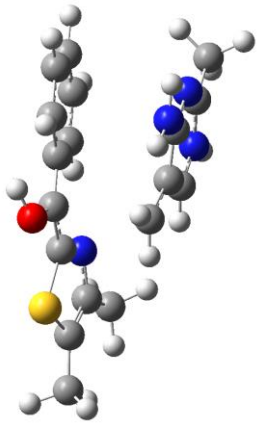
E	-398.660414
E+ZPE	-398.496416
H	-398.486629
G	-398.529815
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.634372	-0.805711	0.000002
H	-2.825668	-1.879894	0.000001
H	-3.107429	-0.367163	-0.885204
C	-1.162009	-0.539987	0.000001
N	0.681226	1.063314	-0.000002
C	1.526153	0.055246	-0.000002
C	2.993350	0.310240	0.000003
H	3.254067	0.895960	0.884809
H	3.561264	-0.620409	-0.000044
H	3.254060	0.896048	-0.884746
C	-0.230274	-1.528649	-0.000001
H	-0.479036	-2.583140	-0.000001
C	-0.645795	0.798327	-0.000001
N	-1.471554	1.838388	-0.000001
H	-1.093415	2.777342	0.000000
H	-3.107427	-0.367166	0.885211
N	1.097965	-1.220653	-0.000002
H	1.783064	-1.972079	-0.000004
H	-2.475262	1.716363	0.000004

TSc67-5N1H singlet cation, optimized with SMD mimicking the water solution

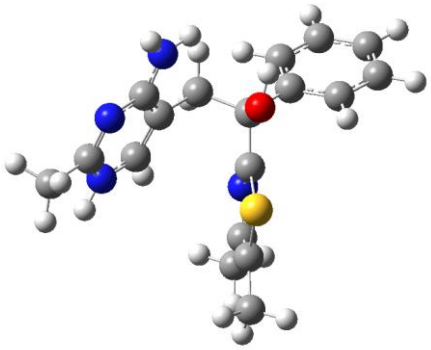
E	-1390.423122
E+ZPE	-1390.058139
H	-1390.033288
G	-1390.112579
$<S^2>$	0.7214
imaginary freq.	283.0*i*



C	-3.065647	1.219230	0.574918
C	-4.051653	0.440563	0.022668
C	-1.864656	-0.639862	0.312037
N	-1.844956	0.605228	0.740669
S	-3.426473	-1.147635	-0.304448
C	-3.195887	2.645926	1.011973
H	-3.019867	2.730206	2.088903
H	-2.449116	3.264644	0.504325
H	-4.184719	3.049932	0.793091
C	-0.185642	-0.252628	-2.062161
H	-1.168904	0.202766	-2.073402
H	-0.063007	-1.192080	-2.585929
C	0.901640	0.492216	-1.574305
N	3.277174	0.682452	-1.005165
C	3.012523	1.795732	-0.346901
C	4.100052	2.505932	0.381416
H	4.587667	1.805404	1.064308
H	4.847357	2.856312	-0.335938
H	3.715370	3.356152	0.946085
C	0.719610	1.700305	-0.918184
H	-0.242775	2.189737	-0.840831
C	2.277901	0.027180	-1.623352
N	2.607322	-1.056626	-2.315970
H	3.568418	-1.374370	-2.302153
H	1.917688	-1.630850	-2.779603
C	-5.479373	0.769391	-0.277963
H	-5.681275	1.819475	-0.060909
H	-5.714476	0.588564	-1.331293
H	-6.160700	0.160333	0.324744
C	-0.757649	-1.546361	0.230759
O	-1.112871	-2.750460	-0.293689
C	0.545137	-1.378478	0.855940
C	1.566267	-2.323353	0.617965
C	0.845988	-0.272954	1.680415
C	2.822700	-2.178954	1.194256
H	1.406853	-3.164453	-0.051437
C	2.111077	-0.130871	2.242693
H	0.084733	0.469093	1.877456
C	3.105482	-1.081198	2.010074
H	3.589548	-2.919553	0.989866
H	2.318151	0.731916	2.869551
H	4.091221	-0.964668	2.449532
N	1.773852	2.323465	-0.334752
H	1.617165	3.198483	0.160167
H	-0.473774	-3.443731	-0.072825

5cN1H singlet cation, optimized with SMD mimicking the water solution

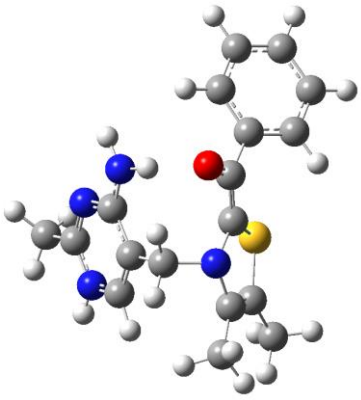
E	-1390.506833
E+ZPE	-1390.135089
H	-1390.111000
G	-1390.190313
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.450606	2.805991	0.673472
C	-0.172916	3.027252	-0.524211
C	0.625485	0.750182	-0.148347
N	0.898060	1.507306	0.868427
S	-0.197569	1.552888	-1.443356
C	0.692746	3.806850	1.759548
H	1.765739	3.911046	1.947614
H	0.222575	3.477516	2.691312
H	0.293052	4.787782	1.500524
C	0.079278	-1.446580	0.892954
H	0.352033	-2.507188	0.915367
H	0.332533	-1.025009	1.868670
C	-1.397956	-1.267675	0.666464
N	-3.526136	-1.944366	-0.316006
C	-4.089564	-0.885007	0.215539
C	-5.545932	-0.634750	0.034516
H	-5.800908	0.403137	0.250997
H	-6.100575	-1.285932	0.717225
H	-5.833739	-0.883875	-0.987313
C	-2.055142	-0.198055	1.194662
H	-1.571805	0.547261	1.816924
C	-2.201979	-2.163162	-0.114619
N	-1.703385	-3.264640	-0.661837
H	-2.312956	-3.867926	-1.199687
H	0.872559	-2.049604	-1.651278
C	-0.764789	4.283847	-1.082799
H	-0.714515	5.085558	-0.344044
H	-1.813919	4.139804	-1.356574
H	-0.226239	4.610919	-1.977323
C	0.922815	-0.738034	-0.195014
O	0.506256	-1.167949	-1.484946
C	2.425754	-0.958436	-0.019708
C	3.269031	-0.600834	-1.079797
C	2.985547	-1.474202	1.150391
C	4.647159	-0.763978	-0.974175
H	2.840727	-0.192784	-1.991432
C	4.369306	-1.636327	1.255952
H	2.360044	-1.754617	1.991069
C	5.202399	-1.284018	0.197159
H	5.287791	-0.483742	-1.804608
H	4.791144	-2.040848	2.170769
H	6.277050	-1.412034	0.281946
N	-3.381444	-0.013858	0.962470
H	-0.718302	-3.484657	-0.615807
H	-3.851989	0.793094	1.365617

2'cN1H neutral singlet, optimized with SMD mimicking the water solution

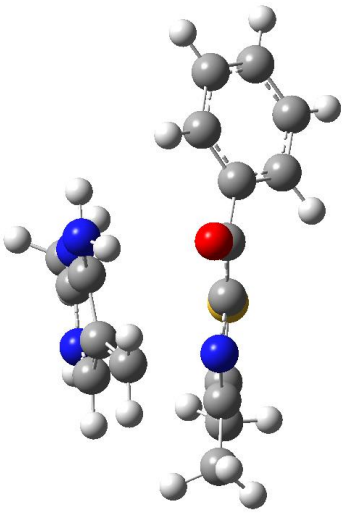
E	-1389.993950
E+ZPE	-1389.635135
H	-1389.611843
G	-1389.687159
$<S^2>$	0.0000
imaginary freq.	N/A



C	-1.527733	-2.342191	0.386918
C	-1.148502	-2.433651	-0.898249
C	0.475372	-1.110021	0.506562
N	-0.704694	-1.522533	1.219535
S	0.301139	-1.466404	-1.241606
C	-2.702134	-3.026933	1.018322
H	-2.417017	-3.456889	1.983501
H	-3.534991	-2.337327	1.196491
H	-3.070771	-3.830657	0.379685
C	-1.453413	-0.429431	1.884204
H	-2.348713	-0.862529	2.333561
H	-0.838438	-0.038034	2.693255
C	-1.849205	0.672712	0.934391
N	-1.441505	2.838410	-0.114361
C	-2.505260	2.651376	-0.860368
C	-2.897370	3.667115	-1.876756
H	-2.204111	3.604737	-2.720945
H	-3.912451	3.498257	-2.237970
H	-2.818445	4.664889	-1.442873
C	-2.949333	0.558058	0.142117
H	-3.633834	-0.281779	0.182593
C	-1.079170	1.874968	0.774023
N	-0.006991	2.118125	1.517565
H	0.516194	2.961238	1.313164
H	0.476647	1.364618	2.033826
C	-1.739436	-3.231546	-2.015539
H	-2.661535	-3.725678	-1.704516
H	-1.974125	-2.581748	-2.866067
H	-1.038959	-3.994865	-2.370852
C	1.525568	-0.483823	1.106418
O	1.499295	-0.118213	2.383758
C	2.727829	-0.066615	0.315709
C	3.277935	1.205907	0.532017
C	3.377439	-0.925486	-0.583168
C	4.415529	1.622815	-0.157451
H	2.810394	1.872981	1.250864
C	4.520752	-0.513961	-1.267005
H	2.996545	-1.931083	-0.734446
C	5.040524	0.765423	-1.064177
H	4.817084	2.616748	0.017289
H	5.013185	-1.199481	-1.950564
H	5.930077	1.085956	-1.597767
N	-3.260078	1.539094	-0.750048
H	-4.082799	1.438856	-1.339234

TS'c$_{2\text{-}84}$N1H neutral singlet, optimized with SMD mimicking the water solution

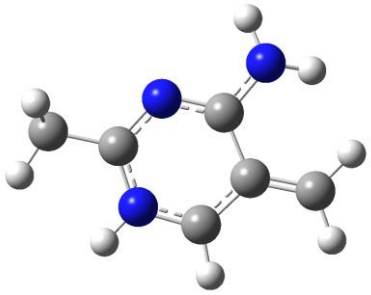
E	-1389.961275
E+ZPE	-1389.605973
H	-1389.582847
G	-1389.656181
$\langle S^2 \rangle$	0.0000
imaginary freq.	502.0*i*



C	2.252963	1.685803	-0.290843
C	2.015967	0.921487	-1.398066
C	0.041299	1.336899	0.024480
N	1.187196	1.850330	0.579096
S	0.341695	0.449105	-1.497503
C	3.590538	2.262332	0.070074
H	3.474269	3.007027	0.860166
H	4.279361	1.488209	0.429017
H	4.055290	2.745354	-0.793284
C	1.837420	0.630247	2.136180
H	2.850568	1.014038	2.184620
H	1.179618	0.970982	2.927082
C	1.627795	-0.617389	1.518917
N	0.024934	-2.279614	0.709747
C	0.896682	-2.634705	-0.224116
C	0.537145	-3.678225	-1.227000
H	1.301660	-3.764789	-2.000764
H	0.424379	-4.645501	-0.727596
H	-0.417869	-3.422890	-1.691195
C	2.533702	-1.135971	0.595264
H	3.561752	-0.804652	0.514184
C	0.354021	-1.309654	1.572928
N	-0.509429	-1.058107	2.579205
H	-1.426202	-1.479106	2.481300
H	-0.517151	-0.124051	2.976871
C	2.976602	0.535363	-2.474768
H	3.996955	0.800818	-2.189556
H	2.940557	-0.546053	-2.651691
H	2.739446	1.030928	-3.422097
C	-1.188234	1.371339	0.706491
O	-1.270930	1.798398	1.905226
C	-2.435121	0.840204	0.064289
C	-3.352551	0.139928	0.860108
C	-2.750009	1.072586	-1.281728
C	-4.532572	-0.359158	0.313106
H	-3.136505	-0.010036	1.913673
C	-3.937824	0.585884	-1.825533
H	-2.080775	1.660814	-1.902049
C	-4.826846	-0.141923	-1.033904
H	-5.225377	-0.912848	0.939507
H	-4.172143	0.784139	-2.866993
H	-5.748675	-0.525464	-1.460177
N	2.150315	-2.140271	-0.226452
H	2.804190	-2.476445	-0.929223

8cN1H neutral singlet, optimized with SMD mimicking the water solution

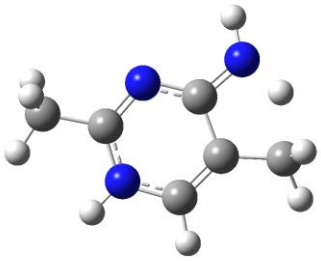
E	-398.136358
E+ZPE	-397.987704
H	-397.977729
G	-398.021178
$<S^2>$	0.0000
imaginary freq.	N/A



C	2.607613	-0.862808	0.024665
H	2.951683	-1.891711	0.020504
H	3.360853	-0.088172	0.082715
C	1.249145	-0.595895	0.004688
N	-0.591283	1.058238	0.004098
C	-1.496446	0.068750	0.003726
C	-2.955521	0.377429	0.013948
H	-3.222469	0.976870	-0.861568
H	-3.550416	-0.538091	0.004964
H	-3.214921	0.954199	0.906799
C	0.226552	-1.566080	-0.021634
H	0.419170	-2.630125	-0.030843
C	0.702647	0.767246	-0.001032
N	1.574984	1.802030	0.031623
H	1.203393	2.728583	-0.131458
H	2.533151	1.642853	-0.245244
N	-1.083535	-1.196655	-0.016582
H	-1.785546	-1.931557	-0.026008

TSc8-3N1H neutral singlet, optimized with SMD mimicking the water solution

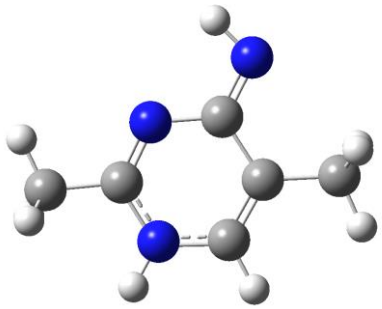
E	-398.108987
E+ZPE	-397.963973
H	-397.954933
G	-397.997823
$<S^2>$	0.0000
imaginary freq.	1448.7*i*



C	2.649816	-0.659775	-0.012198
H	3.104017	-0.494390	0.974353
H	3.025616	-1.592937	-0.439679
C	1.183383	-0.595123	0.050214
N	-0.633978	1.100662	0.012396
C	-1.497302	0.100446	-0.002233
C	-2.962488	0.384079	0.028336
H	-3.205467	1.131426	-0.729682
H	-3.549344	-0.518097	-0.150330
H	-3.230075	0.793607	1.006579
C	0.224475	-1.554226	-0.018022
H	0.415234	-2.619873	-0.050846
C	0.683602	0.781645	0.026737
N	1.671141	1.647999	-0.034198
H	1.469096	2.624469	-0.219768
H	2.571875	0.880406	-0.293420
N	-1.104870	-1.182967	-0.043999
H	-1.815917	-1.906743	-0.073605

i3cN1H neutral singlet, optimized with SMD mimicking the water solution

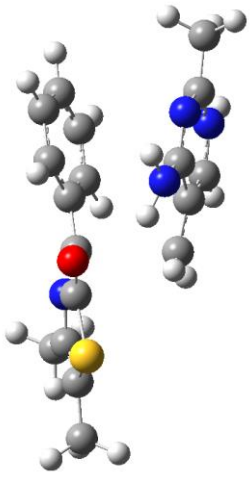
E	-398.182582
E+ZPE	-398.031888
H	-398.022345
G	-398.065410
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.683672	-0.722661	0.000000
H	-2.897479	-1.794177	0.000000
H	-3.152267	-0.270094	-0.880069
C	-1.207459	-0.478297	0.000000
N	0.693937	1.085264	-0.000000
C	1.492612	0.057269	-0.000000
C	2.977422	0.232927	0.000000
H	3.411447	-0.241806	0.884843
H	3.411447	-0.241807	-0.884843
H	3.224611	1.293207	-0.000000
C	-0.310722	-1.486505	0.000000
H	-0.588526	-2.534239	0.000000
C	-0.694328	0.892439	-0.000000
N	-1.511761	1.896793	0.000000
H	-0.961763	2.757580	0.000000
H	-3.152267	-0.270094	0.880069
N	1.040140	-1.222438	-0.000000
H	1.705461	-1.986930	-0.000000

TSc84-5N1H neutral singlet, optimized with SMD mimicking the water solution

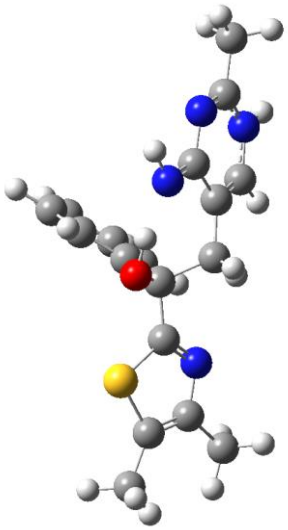
E	-1389.980490
E+ZPE	-1389.626979
H	-1389.602796
G	-1389.680295
$<S^2>$	0.0000
imaginary freq.	166.7*i*



C	3.654809	1.165255	0.376836
C	4.331743	-0.027088	0.404018
C	2.058587	-0.114477	-0.489632
N	2.374103	1.099750	-0.138957
S	3.329988	-1.279092	-0.256762
C	4.166368	2.496661	0.832660
H	4.130618	3.216696	0.009455
H	3.544294	2.887840	1.643655
H	5.195610	2.434851	1.187470
C	0.087855	-1.373797	1.299463
H	0.801420	-0.928242	1.986744
H	0.373510	-2.313491	0.843462
C	-1.242654	-0.955803	1.357369
N	-3.516211	-1.032266	0.409173
C	-3.872005	-0.000441	1.179244
C	-5.258330	0.544605	1.107383
H	-5.490645	0.828359	0.077246
H	-5.977369	-0.219471	1.417436
H	-5.371711	1.418982	1.750395
C	-1.709058	0.100558	2.144369
H	-1.091688	0.621251	2.864490
C	-2.266086	-1.487209	0.461389
N	-1.942960	-2.520245	-0.345254
H	-2.605644	-2.749978	-1.075520
H	-0.966961	-2.654853	-0.579605
C	5.718872	-0.330726	0.876129
H	6.157918	0.543235	1.359772
H	5.718725	-1.152820	1.597676
H	6.364857	-0.619369	0.041048
C	0.799290	-0.579162	-1.135690
O	0.833377	-1.674333	-1.729548
C	-0.355671	0.345411	-1.312110
C	-1.246867	0.072515	-2.361360
C	-0.628565	1.421627	-0.453894
C	-2.378618	0.859155	-2.555392
H	-1.045321	-0.764455	-3.022434
C	-1.764588	2.204368	-0.646550
H	0.031131	1.625397	0.380548
C	-2.645457	1.925160	-1.692581
H	-3.056115	0.636801	-3.373974
H	-1.970960	3.024583	0.034824
H	-3.533840	2.533403	-1.834456
N	-2.994798	0.534498	2.029868
H	-3.293326	1.319591	2.602611

i5cN1H neutral singlet, optimized with SMD mimicking the water solution

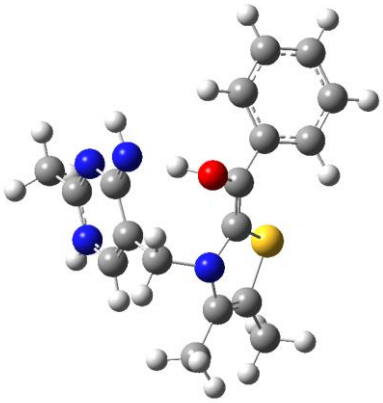
E	-1390.038420
E+ZPE	-1389.680604
H	-1389.657097
G	-1389.734899
$<S^2>$	0.0000
imaginary freq.	N/A



C	-3.766602	-0.640176	-1.110155
C	-4.375246	-0.406417	0.090886
C	-1.927670	-0.463859	0.129576
N	-2.377889	-0.667477	-1.069070
S	-3.165039	-0.227249	1.325779
C	-4.436740	-0.876196	-2.427669
H	-4.105424	-0.135172	-3.161708
H	-4.176669	-1.866236	-2.815316
H	-5.522462	-0.815779	-2.344205
C	0.373448	-1.342404	-0.317077
H	0.011348	-1.307432	-1.347289
H	0.158118	-2.343542	0.077241
C	1.858566	-1.097966	-0.336028
N	4.056099	-1.037128	0.762560
C	4.592607	-0.779938	-0.396929
C	6.067893	-0.596815	-0.539679
H	6.449385	-1.202290	-1.365981
H	6.286119	0.452915	-0.759276
H	6.566893	-0.879953	0.385573
C	2.494220	-0.824031	-1.497677
H	1.983339	-0.739033	-2.450188
C	2.674079	-1.163509	0.871948
N	2.115057	-1.339611	2.032280
H	2.818544	-1.359605	2.769230
H	0.548269	-0.940860	2.094777
C	-5.831224	-0.329958	0.430659
H	-6.435848	-0.403858	-0.474888
H	-6.124149	-1.142874	1.102237
H	-6.073945	0.615570	0.924222
C	-0.465737	-0.343740	0.526274
O	-0.408945	-0.660454	1.899998
C	0.003097	1.095359	0.259488
C	0.504492	1.886436	1.293359
C	-0.025201	1.614307	-1.041576
C	0.968922	3.179252	1.033918
H	0.534590	1.493011	2.303862
C	0.436691	2.902142	-1.300236
H	-0.407630	1.006563	-1.857435
C	0.936344	3.691245	-0.260827
H	1.356197	3.782805	1.849397
H	0.408718	3.290062	-2.314045
H	1.297044	4.695266	-0.462007
N	3.853734	-0.648671	-1.527142
H	4.319110	-0.452115	-2.406572

i2cN1H neutral singlet, optimized with SMD mimicking the water solution

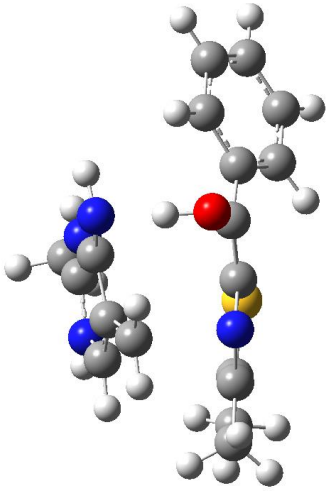
E	-1389.995282
E+ZPE	-1389.636609
H	-1389.613586
G	-1389.688820
$<S^2>$	0.0000
imaginary freq.	N/A



C	-1.697996	2.310255	-0.428206
C	-1.222151	2.659783	0.775794
C	0.366098	1.180793	-0.522732
N	-0.860634	1.441488	-1.189062
S	0.358846	1.925901	1.094040
C	-2.975555	2.792519	-1.044875
H	-2.816302	3.049116	-2.096585
H	-3.769654	2.039539	-1.000477
H	-3.332294	3.682872	-0.525779
C	-1.573832	0.284339	-1.793021
H	-2.526143	0.662720	-2.164386
H	-1.015944	-0.072994	-2.653348
C	-1.815934	-0.840499	-0.816931
N	-1.243103	-3.029555	0.135557
C	-2.202114	-2.866411	1.001740
C	-2.487475	-3.897048	2.043615
H	-2.345002	-3.467203	3.039485
H	-3.525911	-4.231183	1.964925
H	-1.819698	-4.747121	1.916261
C	-2.802802	-0.757012	0.105535
H	-3.490482	0.078542	0.177045
C	-0.996207	-2.046982	-0.820754
N	-0.063332	-2.220703	-1.712093
H	0.406458	-3.111764	-1.556263
H	0.765812	-0.959325	-2.208162
C	-1.783593	3.589806	1.801308
H	-2.776496	3.935805	1.509419
H	-1.872492	3.085804	2.769655
H	-1.138330	4.463545	1.941601
C	1.396762	0.464271	-1.033746
O	1.285369	-0.076387	-2.304614
C	2.643680	0.122022	-0.313765
C	3.215087	-1.145301	-0.527800
C	3.312099	1.010493	0.544312
C	4.387865	-1.522360	0.120868
H	2.728375	-1.841340	-1.204728
C	4.489046	0.632626	1.189479
H	2.936748	2.018361	0.687162
C	5.029566	-0.637161	0.989122
H	4.801717	-2.511328	-0.052515
H	4.990596	1.341878	1.841186
H	5.944768	-0.929810	1.494250
N	-2.994296	-1.763482	1.013117
H	-3.735920	-1.688468	1.701251

iTSc2-67N1H neutral singlet, optimized with SMD mimicking the water solution

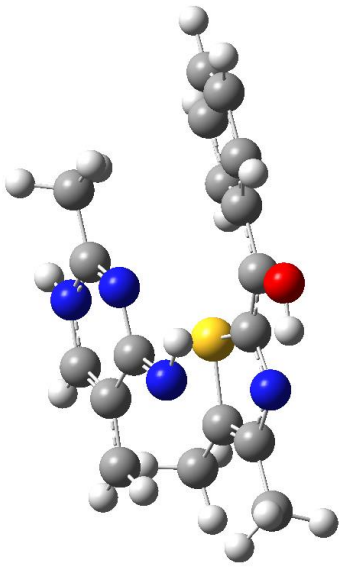
E	-1389.943070
E+ZPE	-1389.590945
H	-1389.567675
G	-1389.642448
$\langle S^2 \rangle$	0.3262
imaginary freq.	514.9*i*



C	2.433298	1.595669	-0.047597
C	2.191285	1.042438	-1.278669
C	0.200259	1.369117	0.147958
N	1.353389	1.746606	0.780849
S	0.479322	0.823586	-1.525560
C	3.799704	1.978408	0.440327
H	3.722147	2.499101	1.396611
H	4.434974	1.095811	0.578187
H	4.300803	2.637593	-0.273912
C	1.958820	0.015984	2.257413
H	2.995908	0.329085	2.242432
H	1.352128	0.333986	3.094841
C	1.527291	-1.006142	1.413615
N	-0.319798	-2.325023	0.461276
C	0.472017	-2.653230	-0.524272
C	-0.006832	-3.521830	-1.640878
H	0.373466	-3.162333	-2.600405
H	0.354658	-4.544693	-1.491874
H	-1.095787	-3.531203	-1.657384
C	2.315046	-1.443077	0.354851
H	3.363642	-1.191581	0.247192
C	0.150159	-1.519873	1.484441
N	-0.598227	-1.217423	2.510849
H	-1.514070	-1.653264	2.390800
H	-0.807542	0.403177	2.496438
C	3.165201	0.740092	-2.367867
H	4.187076	0.880359	-2.008404
H	3.059841	-0.297876	-2.704834
H	3.012140	1.387188	-3.238508
C	-1.023412	1.267298	0.786463
O	-1.029141	1.349573	2.150717
C	-2.306025	0.948133	0.149704
C	-3.301677	0.302245	0.908335
C	-2.601423	1.280521	-1.185931
C	-4.523169	-0.041567	0.336931
H	-3.111529	0.066998	1.950190
C	-3.827016	0.939752	-1.750844
H	-1.891880	1.847853	-1.779015
C	-4.790485	0.266572	-0.998013
H	-5.270388	-0.550715	0.938082
H	-4.034079	1.214475	-2.780611
H	-5.744348	0.000037	-1.442150
N	1.783106	-2.279400	-0.568884
H	2.349280	-2.574327	-1.358889

[i6cN1H 7c] neutral singlet, optimized with SMD mimicking the water solution

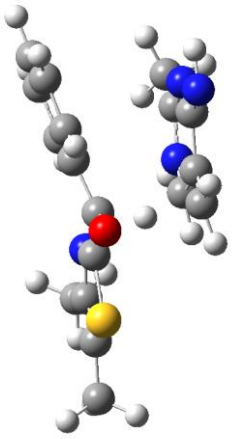
E	-1389.954363
E+ZPE	-1389.602503
H	-1389.577497
G	-1389.656648
$<S^2>$	1.0480
imaginary freq.	N/A



C	-2.800834	-1.056303	0.751691
C	-2.597256	-1.679921	-0.456642
C	-0.562158	-1.032125	0.763879
N	-1.668371	-0.712066	1.433783
S	-0.893501	-1.845143	-0.748183
C	-4.135446	-0.741916	1.356411
H	-4.075325	0.194999	1.915574
H	-4.907777	-0.638972	0.591754
H	-4.444124	-1.530946	2.050478
C	-2.983120	2.035019	-0.390697
H	-3.686985	1.634649	-1.112880
H	-3.362696	2.505959	0.505775
C	-1.610059	1.946104	-0.628334
N	0.740013	2.418390	0.002983
C	1.120022	1.845873	-1.104095
C	2.562406	1.784448	-1.492076
H	2.876506	0.743104	-1.624153
H	2.714741	2.307047	-2.441606
H	3.173161	2.249455	-0.719811
C	-1.106577	1.349351	-1.772895
H	-1.737711	0.914296	-2.538728
C	-0.614980	2.461217	0.344631
N	-1.003346	2.953219	1.472362
H	-0.174613	3.246593	1.993293
H	-0.283858	0.262572	2.628909
C	-3.592185	-2.174281	-1.455971
H	-4.604117	-2.072385	-1.059872
H	-3.530087	-1.605673	-2.390331
H	-3.427251	-3.229315	-1.695330
C	0.700229	-0.639371	1.279461
O	0.654617	0.092652	2.420461
C	2.026355	-0.871969	0.748921
C	3.108494	-0.141488	1.288559
C	2.297589	-1.796920	-0.281494
C	4.396884	-0.312113	0.798104
H	2.926903	0.571986	2.084353
C	3.590553	-1.956322	-0.768645
H	1.518588	-2.429296	-0.689668
C	4.647377	-1.213068	-0.239295
H	5.209994	0.268277	1.223345
H	3.772806	-2.676151	-1.560433
H	5.653986	-1.341571	-0.624029
N	0.240852	1.299852	-1.988111
H	0.599124	0.853393	-2.825599

iTSc$_{67\text{-}34}$N1H neutral singlet, optimized with SMD mimicking the water solution

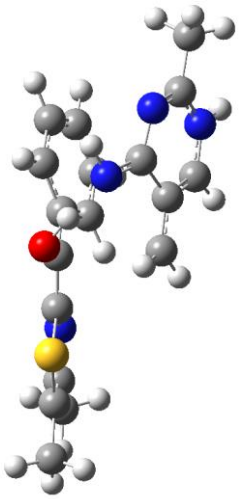
E	-1389.959984
E+ZPE	-1389.609453
H	-1389.586179
G	-1389.660859
$\langle S^2 \rangle$	0.0000
imaginary freq.	1135.3*i*



C	-3.311122	1.080323	-0.219668
C	-3.997740	-0.076811	0.037912
C	-1.595746	-0.135661	0.505925
N	-1.953884	1.029605	0.046027
S	-2.904972	-1.278342	0.649420
C	-3.878110	2.362497	-0.744687
H	-3.719110	3.170599	-0.024030
H	-3.378330	2.644715	-1.676391
H	-4.948029	2.281771	-0.938857
C	0.941509	-3.073538	-0.569880
H	-0.007014	-3.501400	-0.888512
H	1.727244	-3.766060	-0.288741
C	1.293179	-1.810482	-1.048554
N	2.940042	0.008905	-1.401938
C	1.955350	0.779573	-1.773727
C	2.227361	2.172435	-2.244497
H	2.421919	2.154074	-3.321939
H	1.372593	2.826760	-2.057967
H	3.109612	2.565657	-1.738795
C	0.298619	-0.878455	-1.364673
H	-0.710885	-1.194541	-1.600055
C	2.688857	-1.298400	-0.987593
N	3.631846	-2.075517	-0.584260
H	4.511639	-1.556065	-0.619295
H	0.400733	-2.497141	0.659717
C	-5.453739	-0.383002	-0.120773
H	-5.977504	0.474922	-0.545127
H	-5.607497	-1.238454	-0.785070
H	-5.914171	-0.620816	0.843062
C	-0.238974	-0.588776	0.872020
O	-0.202399	-1.809445	1.348933
C	0.854832	0.330181	1.256817
C	1.942765	-0.208859	1.969226
C	0.883455	1.689576	0.903036
C	3.035137	0.584226	2.297726
H	1.927135	-1.255410	2.255334
C	1.982411	2.479754	1.240728
H	0.052521	2.125352	0.363831
C	3.063283	1.932409	1.928428
H	3.868226	0.150947	2.842643
H	1.992320	3.526946	0.953435
H	3.919037	2.550019	2.183080
N	0.663507	0.366622	-1.826173
H	-0.060227	1.037910	-2.060700

iTSc$_{67\text{-}5}$N1H neutral singlet, optimized with SMD mimicking the water solution

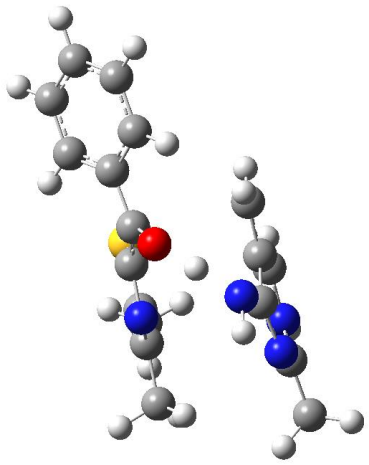
E	-1389.958831
E+ZPE	-1389.608069
H	-1389.584156
G	-1389.661406
$\langle S^2 \rangle$	0.8552
imaginary freq.	82.1*i*



C	-3.976841	0.897845	-0.459935
C	-4.479648	-0.361570	-0.242689
C	-2.137546	-0.009322	0.416643
N	-2.668442	1.092108	-0.082223
S	-3.251644	-1.363661	0.469660
C	-4.715833	2.057028	-1.055749
H	-4.740926	2.893809	-0.350872
H	-4.209522	2.402812	-1.962300
H	-5.742257	1.796230	-1.315609
C	0.205767	-1.351210	-1.404541
H	-0.339297	-0.840774	-2.191645
H	-0.266574	-2.185495	-0.902616
C	1.552998	-1.040904	-1.172859
N	3.662018	-1.426817	0.046742
C	4.226847	-0.517096	-0.705014
C	5.669930	-0.176582	-0.527475
H	6.092001	0.258387	-1.435297
H	5.767068	0.551216	0.285114
H	6.227664	-1.072448	-0.253074
C	2.224889	-0.077223	-1.901284
H	1.766810	0.488113	-2.703429
C	2.300165	-1.642874	-0.053547
N	1.666908	-2.342634	0.840984
H	2.318920	-2.666986	1.555141
H	0.284478	-1.792034	1.320704
C	-5.843148	-0.913099	-0.516262
H	-6.494633	-0.138409	-0.923909
H	-5.801238	-1.735802	-1.237324
H	-6.305598	-1.297173	0.398456
C	-0.811040	-0.199294	0.911786
O	-0.627774	-1.363021	1.577761
C	0.232014	0.815998	0.932351
C	1.292483	0.695329	1.853562
C	0.276881	1.876116	0.001669
C	2.353672	1.595867	1.843015
H	1.282056	-0.112094	2.578643
C	1.337069	2.775791	0.003048
H	-0.508402	1.969629	-0.738468
C	2.385003	2.641676	0.918309
H	3.159146	1.479969	2.562408
H	1.354835	3.577717	-0.729201
H	3.215837	3.340399	0.908064
N	3.539525	0.180041	-1.643183
H	4.026077	0.887938	-2.183842

TSc$_{67\text{-}84}$N1H neutral singlet, optimized with SMD mimicking the water solution

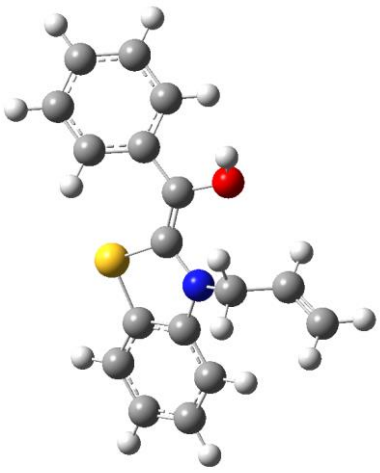
E	-1389.956071
E+ZPE	-1389.608784
H	-1389.584610
G	-1389.661737
$\langle S^2 \rangle$	0.9810
imaginary freq.	1063.7*i*



C	-1.539145	-1.409538	-1.087440
C	-1.160352	-2.218283	-0.047324
C	0.534285	-0.597852	-0.832889
N	-0.590705	-0.519801	-1.531230
S	0.476845	-1.850414	0.406993
C	-2.874749	-1.441614	-1.771108
H	-2.844976	-2.080359	-2.660767
H	-3.657664	-1.820085	-1.109415
H	-3.153296	-0.434653	-2.092823
C	0.400080	1.672794	1.455306
H	0.854737	1.203271	2.320488
H	0.965076	2.414823	0.906528
C	-0.928044	1.378231	1.116413
N	-2.911253	1.798967	-0.272136
C	-3.588309	0.975275	0.493073
C	-5.047806	0.765538	0.262143
H	-5.434778	-0.053893	0.869711
H	-5.585744	1.682946	0.519304
H	-5.224477	0.552792	-0.794314
C	-1.708322	0.506294	1.857185
H	-1.344206	-0.025562	2.727625
C	-1.559930	1.928500	-0.089475
N	-0.827047	2.532164	-0.990697
H	-1.391143	2.835492	-1.782413
H	0.325624	2.007159	-1.295615
C	-1.943940	-3.253725	0.693261
H	-2.901683	-3.429358	0.199324
H	-1.407780	-4.206748	0.739034
H	-2.143287	-2.935663	1.723657
C	1.590763	0.363080	-0.943210
O	1.357917	1.504377	-1.583746
C	2.933643	0.170255	-0.394360
C	3.701076	1.307225	-0.067484
C	3.514378	-1.099095	-0.205601
C	4.981278	1.176899	0.458238
H	3.272215	2.292815	-0.217982
C	4.797032	-1.223297	0.321954
H	2.982001	-1.994459	-0.509178
C	5.536106	-0.089537	0.663210
H	5.548962	2.066776	0.713510
H	5.226479	-2.212196	0.451287
H	6.536015	-0.190336	1.073241
N	-3.010500	0.302082	1.514178
H	-3.566670	-0.361937	2.044722

2d neutral singlet, optimized with SMD mimicking the water solution

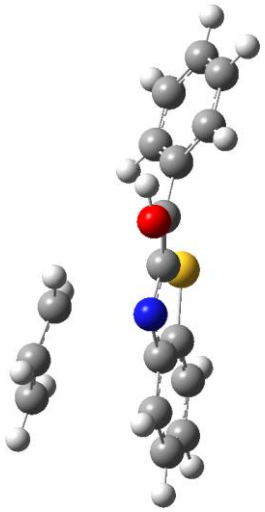
E	-1184.654198
E+ZPE	-1184.374904
H	-1184.356533
G	-1184.421013
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A



C	-2.176883	-0.334776	0.004867
C	-1.696449	-1.646643	0.129312
C	0.121366	0.084820	-0.146250
N	-1.175210	0.610056	-0.197894
S	0.059048	-1.701595	-0.046581
C	1.258128	0.811565	-0.030981
O	1.126393	2.166145	0.244393
H	1.790063	2.663349	-0.256906
C	-1.490343	1.879470	-0.862975
H	-0.609150	2.174499	-1.435917
H	-2.303383	1.692868	-1.574079
C	-1.889031	2.969165	0.094351
H	-1.184439	3.186693	0.894966
C	-3.024417	3.657781	-0.016606
H	-3.272561	4.457495	0.674918
H	-3.738892	3.443188	-0.809365
C	-3.549058	-0.088635	0.057953
C	-2.556895	-2.719605	0.307336
C	-3.932691	-2.471126	0.368486
H	-4.620470	-3.297653	0.512139
C	-4.416616	-1.169372	0.240732
H	-5.484996	-0.983805	0.287028
H	-2.171428	-3.730815	0.392748
H	-3.934246	0.921614	-0.030201
C	2.621261	0.262711	-0.019570
C	2.994321	-0.829232	-0.819844
C	3.597176	0.857358	0.800150
C	4.290960	-1.337156	-0.769832
H	2.280908	-1.262708	-1.514627
C	4.893653	0.352196	0.840194
H	3.331065	1.711390	1.415444
C	5.245797	-0.752505	0.062128
H	4.558713	-2.180824	-1.398644
H	5.630678	0.820106	1.485839
H	6.257010	-1.145526	0.095384

TSd2-67 neutral singlet, optimized with SMD mimicking the water solution

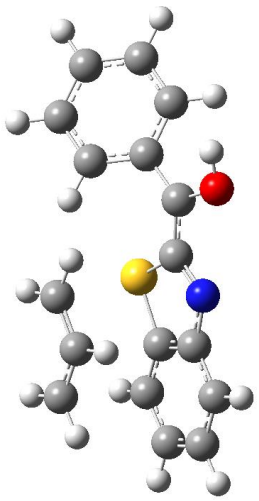
E	-1184.591385
E+ZPE	-1184.317915
H	-1184.299210
G	-1184.364801
$<S^2>$	0.5697
imaginary freq.	617.3*i*



C	2.013513	-0.113319	-0.662955
C	1.702754	-1.351896	-0.053810
C	-0.198145	0.200057	-0.409360
N	0.969798	0.773688	-0.800850
S	-0.002723	-1.418086	0.337067
C	-1.419945	0.807097	-0.596479
O	-1.401590	1.983178	-1.292881
H	-2.254978	2.434876	-1.208370
C	1.289165	2.129022	1.087967
H	0.500170	2.789837	0.749471
H	0.999802	1.263245	1.677487
C	2.636572	2.524839	1.062782
H	2.889303	3.464185	0.574601
C	3.642251	1.726302	1.529596
H	4.684701	2.016472	1.449685
H	3.419248	0.775520	2.009172
C	3.334917	0.138747	-1.065435
C	2.671729	-2.326630	0.155581
C	3.977544	-2.061908	-0.266533
H	4.745214	-2.815301	-0.121619
C	4.302561	-0.845597	-0.876908
H	5.322610	-0.661383	-1.198577
H	2.422089	-3.273800	0.623184
H	3.578113	1.084665	-1.538709
C	-2.722486	0.266813	-0.187187
C	-2.905574	-0.348735	1.061255
C	-3.821719	0.385052	-1.055669
C	-4.151439	-0.858220	1.418472
H	-2.085031	-0.395147	1.770981
C	-5.064678	-0.123402	-0.691839
H	-3.694288	0.856531	-2.026371
C	-5.232816	-0.751861	0.543429
H	-4.280009	-1.325435	2.389735
H	-5.901570	-0.035509	-1.377466
H	-6.202895	-1.148786	0.825275

[6d 7d] neutral singlet, optimized with SMD mimicking the water solution

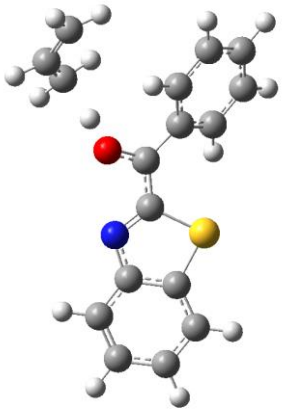
E	-1184.604985
E+ZPE	-1184.332299
H	-1184.312411
G	-1184.381558
$\langle S^2 \rangle$	1.0510
imaginary freq.	N/A



C	2.072553	1.024212	0.141237
C	1.894466	0.280569	-1.047098
C	-0.134534	0.801217	0.242680
N	0.926001	1.317133	0.840058
S	0.203534	-0.056781	-1.274627
C	-1.453348	0.978202	0.722821
O	-1.572401	1.870880	1.733375
H	-2.450959	1.811023	2.140487
C	0.634927	-2.226846	1.514393
H	-0.174503	-1.842474	2.125732
H	0.379275	-2.882635	0.686649
C	1.956318	-1.910645	1.784056
H	2.162056	-1.253581	2.628690
C	3.034153	-2.365757	1.039365
H	4.052128	-2.093119	1.293582
H	2.880714	-3.015988	0.182345
C	3.372057	1.386325	0.535939
C	2.974378	-0.112839	-1.838822
C	4.251868	0.251380	-1.426855
H	5.109017	-0.044072	-2.023251
C	4.446377	0.995230	-0.248361
H	5.454348	1.264653	0.050765
H	2.823511	-0.690544	-2.745212
H	3.515763	1.955922	1.448938
C	-2.654428	0.348902	0.182094
C	-2.652715	-0.990732	-0.248031
C	-3.855723	1.081001	0.124674
C	-3.815843	-1.569387	-0.745997
H	-1.754285	-1.593045	-0.153466
C	-5.013887	0.493813	-0.373636
H	-3.873570	2.119346	0.444653
C	-4.998059	-0.830581	-0.815134
H	-3.801661	-2.606612	-1.065185
H	-5.929423	1.074492	-0.424211
H	-5.903112	-1.286248	-1.203846

TSd67-34 neutral singlet, optimized with SMD mimicking the water solution

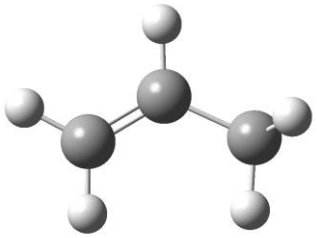
E	-1184.586706
E+ZPE	-1184.318093
H	-1184.299268
G	-1184.366434
$<S^2>$	0.6363
imaginary freq.	3071.8*i*



C	2.871095	0.850150	0.079017
C	3.132061	-0.514425	-0.169714
C	0.770027	0.158872	-0.081008
N	1.539539	1.202203	0.111781
S	1.627127	-1.365338	-0.352314
C	-0.665534	0.260839	-0.209067
O	-1.134703	1.454822	-0.468146
H	-1.964461	1.777088	0.192386
C	-4.847077	2.474698	-0.537471
H	-5.391864	3.048985	-1.279320
H	-5.167627	1.451200	-0.354794
C	-3.807577	3.015811	0.152499
H	-3.511995	4.039358	-0.073974
C	-3.026410	2.307922	1.116870
H	-2.382956	2.872799	1.787588
H	-3.411882	1.364266	1.502898
C	3.944950	1.735459	0.270072
C	4.434438	-1.015611	-0.232060
C	5.481740	-0.122969	-0.042107
H	6.503744	-0.484951	-0.086592
C	5.237551	1.240900	0.207625
H	6.076413	1.913790	0.352996
H	4.622818	-2.066920	-0.423173
H	3.747782	2.785361	0.462274
C	-1.609576	-0.841789	-0.080980
C	-1.341450	-1.999039	0.676700
C	-2.882206	-0.694251	-0.667464
C	-2.309631	-2.987557	0.811496
H	-0.398902	-2.109470	1.201564
C	-3.844044	-1.687598	-0.528809
H	-3.102648	0.200256	-1.242393
C	-3.559965	-2.840389	0.206213
H	-2.093355	-3.868962	1.406554
H	-4.816617	-1.562395	-0.994545
H	-4.311984	-3.615128	0.317389

3d neutral singlet, optimized with SMD mimicking the water solution

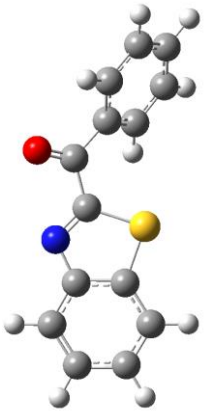
E	-117.845271
E+ZPE	-117.765256
H	-117.760232
G	-117.790256
$<S^2>$	0.0000
imaginary freq.	N/A



H	1.802777	0.150853	-0.879501
C	-1.279136	-0.222140	0.000016
H	-2.240261	0.284141	0.000009
H	-1.289276	-1.310539	-0.000126
C	-0.131832	0.458996	-0.000002
H	-0.164642	1.548695	-0.000023
C	1.231131	-0.164850	-0.000023
H	1.802871	0.151399	0.879239
H	1.167552	-1.256585	0.000454

4d neutral singlet, optimized with SMD mimicking the water solution

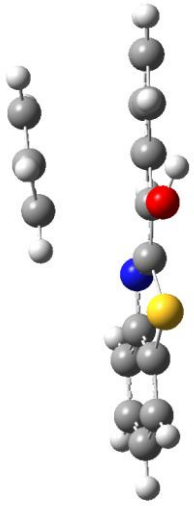
E	-1066.817026
E+ZPE	-1066.622105
H	-1066.608292
G	-1066.662966
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A



C	2.406447	0.625648	0.243305
C	2.222849	-0.664584	-0.295400
C	0.217180	0.686240	0.005575
N	1.249135	1.368648	0.387366
S	0.533159	-0.930852	-0.591577
C	-1.158009	1.288266	-0.042513
O	-1.261128	2.494773	-0.201034
C	3.695964	1.066734	0.581046
C	3.301995	-1.529013	-0.512596
C	4.567110	-1.073740	-0.174816
H	5.423024	-1.722265	-0.331214
C	4.763205	0.212652	0.368059
H	5.768017	0.534545	0.620792
H	3.154462	-2.520199	-0.927987
H	3.834038	2.059685	0.996607
C	-2.346572	0.405606	0.061501
C	-2.348395	-0.731558	0.879602
C	-3.501586	0.766706	-0.645415
C	-3.503420	-1.503838	0.984215
H	-1.471050	-0.994201	1.462588
C	-4.643430	-0.020592	-0.553789
H	-3.486790	1.652728	-1.272765
C	-4.644172	-1.155420	0.261621
H	-3.511235	-2.375368	1.630421
H	-5.532621	0.247842	-1.114769
H	-5.538305	-1.766491	0.335900

TSd67-5 neutral singlet, optimized with SMD mimicking the water solution

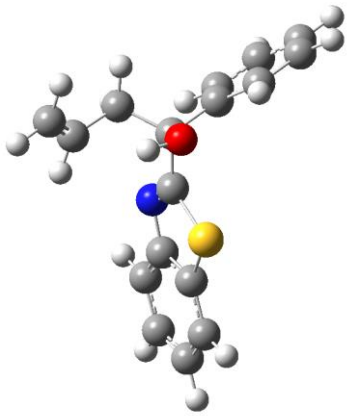
E	-1184.607028
E+ZPE	-1184.333940
H	-1184.315037
G	-1184.381710
$<S^2>$	0.8477
imaginary freq.	70.5*i*



C	-2.402381	0.752328	0.229648
C	-2.997086	-0.383851	-0.361408
C	-0.545941	-0.228054	-0.487136
N	-1.026423	0.814668	0.147589
S	-1.760185	-1.398827	-1.048801
C	0.827292	-0.528100	-0.760420
O	0.972645	-1.736871	-1.364516
C	3.394308	-1.435372	1.961462
H	4.330979	-1.974674	1.873064
H	3.441576	-0.373033	2.188067
C	2.178538	-2.067844	1.810831
H	2.172863	-3.134436	1.590986
C	0.956657	-1.404692	1.873035
H	0.017578	-1.938299	1.773039
H	0.914889	-0.347480	2.119369
C	-3.215840	1.716463	0.846152
C	-4.379807	-0.575866	-0.348494
C	-5.168952	0.389871	0.266951
H	-6.246367	0.262192	0.289382
C	-4.589649	1.526387	0.858789
H	-5.228316	2.265063	1.332486
H	-4.827753	-1.452334	-0.805565
H	-2.761336	2.590886	1.301353
C	1.969733	0.348695	-0.604069
C	1.839230	1.695817	-0.194625
C	3.270385	-0.144805	-0.849911
C	2.959426	2.503567	-0.055635
H	0.856977	2.101195	0.005221
C	4.385050	0.680648	-0.722962
H	3.439045	-1.179785	-1.131779
C	4.239541	2.006354	-0.322456
H	2.832382	3.535634	0.256390
H	5.371297	0.273792	-0.923619
H	5.109486	2.646598	-0.216989
H	1.820432	-1.811073	-1.826093

5d neutral singlet, optimized with SMD mimicking the water solution

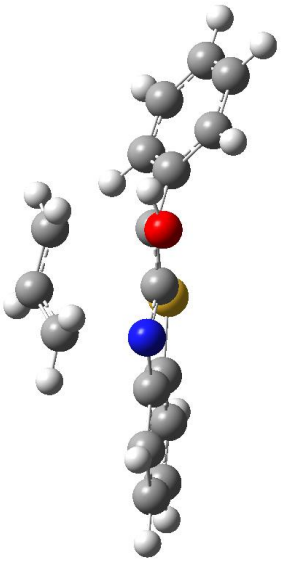
E	-1184.691751
E+ZPE	-1184.411770
H	-1184.393886
G	-1184.458076
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A



C	2.216902	-0.254567	0.646571
C	2.484574	-0.323018	-0.734468
C	0.242181	0.404217	-0.090542
N	0.930882	0.164508	0.973327
S	1.068759	0.165810	-1.623965
C	-1.224650	0.814156	-0.114008
O	-1.505840	1.411153	-1.366346
H	-1.189460	2.329228	-1.344984
C	-1.291013	4.224102	0.442784
H	-0.692262	5.122660	0.325817
H	-2.349871	4.292622	0.200550
C	-0.755461	3.083324	0.883015
H	0.307551	3.045239	1.118974
C	-1.532675	1.806142	1.031738
H	-1.301261	1.323097	1.984862
H	-2.608288	2.008140	0.994901
C	3.214473	-0.592883	1.569889
C	3.735306	-0.719503	-1.216381
C	4.712967	-1.054015	-0.287979
H	5.691559	-1.368533	-0.636131
C	4.454667	-0.991503	1.093249
H	5.238369	-1.258922	1.794557
H	3.936704	-0.766764	-2.281578
H	3.005545	-0.540273	2.633767
C	-2.085019	-0.444558	0.009590
C	-2.022871	-1.219178	1.174291
C	-2.937931	-0.836675	-1.024490
C	-2.806681	-2.363057	1.303836
H	-1.357033	-0.934184	1.983566
C	-3.721288	-1.985628	-0.892774
H	-2.994953	-0.247927	-1.932449
C	-3.659755	-2.751343	0.269086
H	-2.749216	-2.951991	2.213993
H	-4.379854	-2.278359	-1.704832
H	-4.269480	-3.643850	0.369463

TSd2-5 neutral singlet, optimized with SMD mimicking the water solution

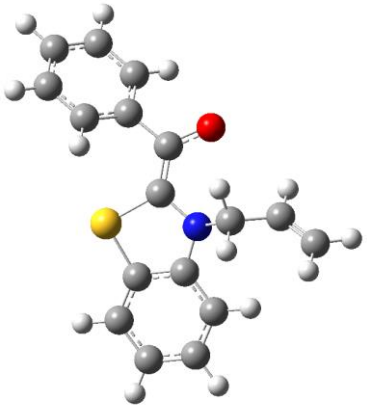
E	-1184.608455
E+ZPE	-1184.330878
H	-1184.313512
G	-1184.374526
$\langle S^2 \rangle$	0.0000
imaginary freq.	511.6*i*



C	2.401765	0.161908	-0.472872
C	2.164638	-1.135357	0.006691
C	0.148297	0.244646	-0.396166
N	1.260026	0.963660	-0.632992
S	0.448210	-1.384756	0.256763
C	-1.118522	0.832579	-0.414823
O	-1.186698	1.944326	-1.243633
H	-2.006898	2.429774	-1.066710
C	1.355183	2.436290	0.719955
H	2.435319	2.432737	0.828543
H	0.952967	3.197253	0.057214
C	0.538836	1.946566	1.743179
H	0.975471	1.278621	2.483866
C	-0.834887	1.938407	1.543894
H	-1.484921	1.415665	2.240785
H	-1.293541	2.744206	0.977837
C	3.708369	0.572838	-0.745157
C	3.207003	-2.035077	0.222401
C	4.506939	-1.612852	-0.049514
H	5.333829	-2.297153	0.110665
C	4.754532	-0.319921	-0.529437
H	5.773506	-0.010846	-0.738890
H	3.013999	-3.036810	0.592869
H	3.892444	1.576033	-1.118266
C	-2.379619	0.068591	-0.237134
C	-2.596355	-0.759268	0.875210
C	-3.391537	0.174146	-1.203654
C	-3.779310	-1.483180	1.000767
H	-1.851560	-0.817921	1.663409
C	-4.578657	-0.543775	-1.069252
H	-3.245483	0.807834	-2.072824
C	-4.776098	-1.379315	0.029339
H	-3.928177	-2.116553	1.869789
H	-5.347603	-0.452134	-1.830210
H	-5.700769	-1.938188	0.133176

2'd singlet anion, optimized with SMD mimicking the water solution

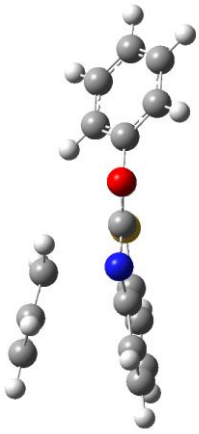
E	-1184.176826
E+ZPE	-1183.910574
H	-1183.892661
G	-1183.956183
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A



C	-2.121778	-0.353378	0.109809
C	-1.588647	-1.655715	0.084399
C	0.156715	0.161520	-0.137734
N	-1.181588	0.654890	-0.077864
S	0.139763	-1.635666	-0.288870
C	1.245414	0.950793	0.106373
O	1.146218	2.231451	0.415168
C	-1.566225	1.827422	-0.873225
H	-0.676135	2.146845	-1.421811
H	-2.328352	1.532877	-1.607838
C	-2.082817	2.967268	-0.038673
H	-1.429962	3.301108	0.767174
C	-3.252239	3.569506	-0.253532
H	-3.579378	4.408898	0.353147
H	-3.918304	3.238832	-1.048629
C	-3.497227	-0.175007	0.269643
C	-2.401379	-2.769284	0.239508
C	-3.779278	-2.585289	0.416502
H	-4.424844	-3.448788	0.539028
C	-4.316277	-1.299340	0.422588
H	-5.385170	-1.159919	0.551844
H	-1.978256	-3.768923	0.207562
H	-3.921005	0.823990	0.285456
C	2.619738	0.365791	0.045662
C	3.015948	-0.561162	-0.929056
C	3.571080	0.779464	0.992687
C	4.310729	-1.082911	-0.938885
H	2.320371	-0.855034	-1.710774
C	4.861954	0.257513	0.986811
H	3.284951	1.511853	1.741919
C	5.237723	-0.680766	0.021716
H	4.597317	-1.793237	-1.708929
H	5.577738	0.582112	1.736506
H	6.245595	-1.084349	0.013414

TS'd$_{2\text{-}67}$ singlet anion, optimized with SMD mimicking the water solution

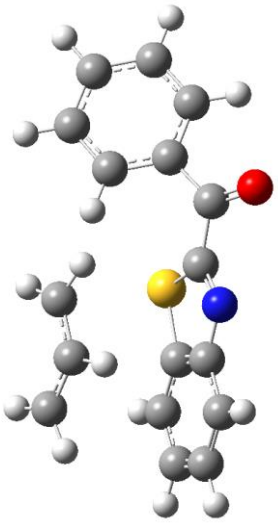
E	-1184.128442
E+ZPE	-1183.867146
H	-1183.848890
G	-1183.914035
$\langle S^2 \rangle$	0.4377
imaginary freq.	637.4*i*



C	1.989712	-0.168700	-0.633572
C	1.614539	-1.369800	0.011073
C	-0.215228	0.263198	-0.421982
N	0.990480	0.779551	-0.782050
S	-0.087290	-1.324984	0.422218
C	-1.426059	0.932167	-0.661354
O	-1.475407	2.052471	-1.291871
C	1.393625	2.103044	0.911398
H	0.579470	2.750986	0.606929
H	1.144483	1.292411	1.593109
C	2.728086	2.574850	0.881040
H	2.925004	3.492424	0.326792
C	3.784536	1.899760	1.416727
H	4.802727	2.262743	1.318446
H	3.632693	0.973793	1.968136
C	3.314701	-0.010436	-1.063012
C	2.531106	-2.392043	0.239655
C	3.846153	-2.218136	-0.201238
H	4.571315	-3.009750	-0.040711
C	4.229937	-1.042140	-0.853528
H	5.253828	-0.926077	-1.195178
H	2.231459	-3.308716	0.738458
H	3.607073	0.903126	-1.570774
C	-2.723132	0.330894	-0.216094
C	-2.932012	-0.134811	1.088380
C	-3.788198	0.286725	-1.127651
C	-4.171519	-0.652868	1.466542
H	-2.134608	-0.065598	1.823420
C	-5.021922	-0.239203	-0.753719
H	-3.637248	0.661649	-2.136169
C	-5.216956	-0.713399	0.545951
H	-4.320930	-0.999769	2.484605
H	-5.832830	-0.279612	-1.474824
H	-6.180120	-1.119103	0.839898

[8d 4d] singlet anion, optimized with SMD mimicking the water solution

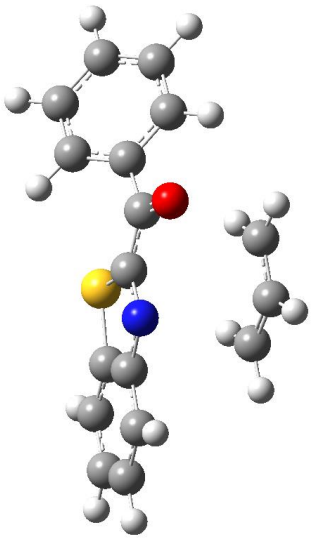
E	-1184.134912
E+ZPE	-1183.874924
H	-1183.855080
G	-1183.923921
$\langle S^2 \rangle$	0.0000
imaginary freq.	N/A



C	2.020763	-0.973622	-0.400265
C	1.845168	-0.620419	0.953557
C	-0.180070	-0.951197	-0.356546
N	0.850522	-1.171302	-1.109256
S	0.149609	-0.516412	1.307098
C	-1.580760	-1.161509	-0.853642
O	-1.772018	-1.995021	-1.726364
C	0.640372	2.600471	-1.096555
H	-0.061004	2.185461	-1.814564
H	0.225639	3.099621	-0.221287
C	2.014076	2.416712	-1.250719
H	2.299178	1.865221	-2.155475
C	3.087485	2.811331	-0.453055
H	4.107563	2.560797	-0.727393
H	2.937425	3.353038	0.479998
C	3.315655	-1.108272	-0.926223
C	2.936595	-0.401307	1.801745
C	4.206655	-0.542433	1.264135
H	5.072148	-0.374217	1.896912
C	4.395440	-0.891755	-0.088664
H	5.404291	-0.989462	-0.475942
H	2.794308	-0.127067	2.841687
H	3.447590	-1.375764	-1.969848
C	-2.692775	-0.380010	-0.256807
C	-2.512187	0.943372	0.167177
C	-3.957126	-0.979578	-0.177951
C	-3.596900	1.658719	0.670792
H	-1.543274	1.426436	0.067772
C	-5.029240	-0.266966	0.346284
H	-4.082881	-2.004620	-0.513115
C	-4.849135	1.052982	0.768819
H	-3.462825	2.689026	0.983690
H	-6.004508	-0.736029	0.425193
H	-5.688987	1.610318	1.172020

[6d 7'd] singlet anion, optimized with SMD mimicking the water solution

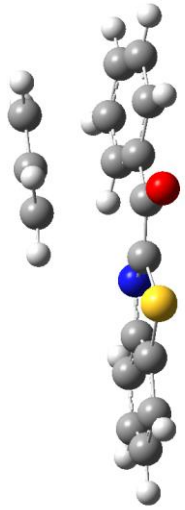
E	-1184.147516
E+ZPE	-1183.887612
H	-1183.868042
G	-1183.936819
$\langle S^2 \rangle$	1.0227
imaginary freq.	N/A



C	2.322347	-0.138618	0.864688
C	2.106732	-0.941426	-0.281173
C	0.086941	-0.084154	0.883427
N	1.195489	0.316258	1.503454
S	0.391503	-1.120594	-0.544695
C	-1.222270	0.366138	1.249049
O	-1.369888	1.255521	2.165380
C	-0.628880	2.452165	-1.146963
H	-1.330721	2.999328	-0.527700
H	-1.029541	1.726175	-1.849370
C	0.738614	2.676767	-1.060333
H	1.087917	3.407511	-0.331436
C	1.686769	2.017316	-1.821472
H	2.746449	2.214741	-1.700015
H	1.390007	1.281554	-2.563626
C	3.644139	0.143316	1.250873
C	3.160856	-1.451282	-1.034527
C	4.465058	-1.151462	-0.638510
H	5.301675	-1.533545	-1.214559
C	4.698458	-0.360551	0.497022
H	5.719474	-0.137095	0.791383
H	2.974228	-2.060681	-1.913746
H	3.825992	0.759417	2.126574
C	-2.433921	-0.139590	0.547592
C	-2.620569	-1.489384	0.209370
C	-3.468904	0.767607	0.260989
C	-3.789702	-1.910954	-0.424032
H	-1.866855	-2.225556	0.472273
C	-4.633270	0.347211	-0.374525
H	-3.344340	1.811810	0.533466
C	-4.797453	-0.995385	-0.726026
H	-3.916879	-2.961376	-0.668586
H	-5.414452	1.067528	-0.598742
H	-5.706005	-1.324562	-1.220696

TS'd$_{67\text{-}5}$ singlet anion, optimized with SMD mimicking the water solution

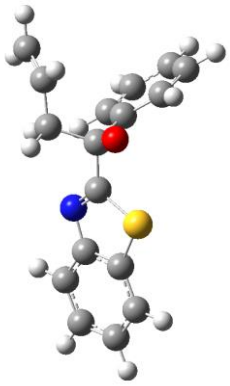
E	-1184.150331
E+ZPE	-1183.890088
H	-1183.871651
G	-1183.936886
$\langle S^2 \rangle$	0.6603
imaginary freq.	267.7*i*



C	2.391696	-0.803988	0.107288
C	2.964232	0.417565	-0.316137
C	0.508677	0.225881	-0.476762
N	1.018361	-0.890250	-0.002698
S	1.704071	1.485607	-0.879264
C	-0.869712	0.573835	-0.781125
O	-1.071924	1.682970	-1.386254
C	-3.305349	1.753870	1.730689
H	-4.094484	2.483080	1.580276
H	-3.599456	0.723204	1.918508
C	-1.978730	2.115031	1.711738
H	-1.740809	3.163389	1.529141
C	-0.905309	1.228217	1.844511
H	0.115794	1.591987	1.885606
H	-1.076644	0.180519	2.074701
C	3.227937	-1.821106	0.594413
C	4.340755	0.635658	-0.261345
C	5.154783	-0.384467	0.226442
H	6.228318	-0.233772	0.278015
C	4.598796	-1.602477	0.650123
H	5.250115	-2.384945	1.027163
H	4.769524	1.577277	-0.590502
H	2.794740	-2.761654	0.921313
C	-1.999044	-0.360668	-0.580795
C	-1.922461	-1.577650	0.127306
C	-3.254906	0.029222	-1.083285
C	-3.053527	-2.366932	0.308770
H	-0.976045	-1.896951	0.543360
C	-4.384265	-0.769209	-0.904841
H	-3.336762	0.964786	-1.625524
C	-4.292566	-1.971685	-0.206492
H	-2.968553	-3.298285	0.861277
H	-5.339043	-0.443960	-1.308046
H	-5.171009	-2.592978	-0.061134

5'd singlet anion, optimized with SMD mimicking the water solution

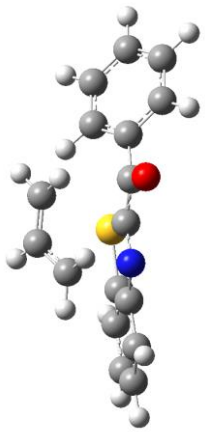
E	-1184.204573
E+ZPE	-1183.938230
H	-1183.920668
G	-1183.983580
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.380371	0.230540	-0.706286
C	-2.767900	-0.114806	0.603740
C	-0.434616	0.576576	0.296424
N	-1.050382	0.619621	-0.839903
S	-1.412090	0.085570	1.679225
C	1.045533	0.865766	0.576314
O	1.216695	1.195267	1.894978
C	3.823858	2.245036	-1.231695
H	4.874682	2.477172	-1.081655
H	3.521398	1.929594	-2.228963
C	2.936347	2.344326	-0.239160
H	3.275052	2.659623	0.747613
C	1.478943	2.026188	-0.375191
H	0.875795	2.895763	-0.083097
H	1.244816	1.789450	-1.417468
C	-3.311934	0.164407	-1.750403
C	-4.074041	-0.522176	0.891159
C	-4.985921	-0.586644	-0.155818
H	-6.004512	-0.904511	0.043006
C	-4.607438	-0.245638	-1.466363
H	-5.339088	-0.304980	-2.265869
H	-4.368086	-0.784089	1.902677
H	-3.011739	0.429906	-2.759484
C	1.807181	-0.426420	0.174732
C	1.832799	-0.890237	-1.148456
C	2.506411	-1.148138	1.143628
C	2.544078	-2.038515	-1.491325
H	1.292010	-0.352195	-1.922159
C	3.219353	-2.301999	0.804909
H	2.492471	-0.795654	2.169501
C	3.242800	-2.751348	-0.513606
H	2.553822	-2.377337	-2.523266
H	3.757360	-2.847151	1.575330
H	3.798079	-3.645682	-0.779879

TS'd$_{2\text{-}5}$ singlet anion, optimized with SMD mimicking the water solution

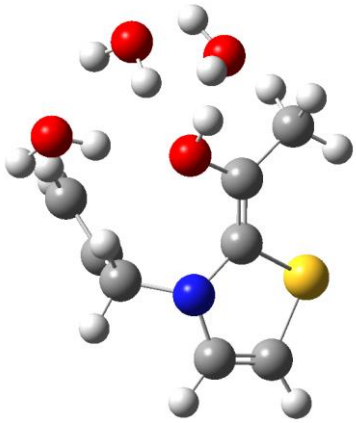
E	-1184.137992
E+ZPE	-1183.875004
H	-1183.857457
G	-1183.919595
$\langle S^2 \rangle$	0.0000
imaginary freq.	318.2*i*



C	2.354155	0.104804	-0.552683
C	2.093779	-1.131127	0.068999
C	0.111667	0.294811	-0.415535
N	1.245560	0.927197	-0.767236
S	0.380765	-1.289779	0.399277
C	-1.166328	0.859240	-0.666622
O	-1.288821	1.928067	-1.362765
C	1.533367	2.528032	0.686679
H	2.617910	2.494111	0.718868
H	1.094634	3.259180	0.013441
C	0.766340	2.022713	1.737913
H	1.265489	1.416724	2.494475
C	-0.611258	2.000813	1.675869
H	-1.196682	1.504580	2.444835
H	-1.143573	2.662238	0.999309
C	3.667765	0.428438	-0.907672
C	3.115416	-2.037258	0.347188
C	4.421321	-1.698540	-0.009424
H	5.229724	-2.392480	0.197883
C	4.692710	-0.474578	-0.633838
H	5.712993	-0.225652	-0.908763
H	2.902274	-2.985739	0.830893
H	3.874314	1.380729	-1.387973
C	-2.418046	0.098581	-0.330666
C	-2.629708	-0.581180	0.877223
C	-3.438383	0.079863	-1.293573
C	-3.816943	-1.276292	1.104936
H	-1.880652	-0.541671	1.661736
C	-4.623198	-0.617679	-1.068577
H	-3.290556	0.612033	-2.228328
C	-4.816773	-1.301727	0.132375
H	-3.964617	-1.787361	2.051602
H	-5.395696	-0.627257	-1.831783
H	-5.741452	-1.841368	0.312597

2aWAT neutral singlet, optimized with SMD mimicking the water solution at the level of ωB97XD/6-311++G(d,p).

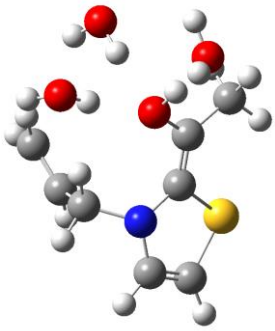
E	-1068.914969
E+ZPE	-1068.664539
H	-1068.641476
G	-1068.717351
$<S^2>$	0.0000
imaginary freq.	N/A



C	2.791176	0.693270	-1.044961
C	3.538764	-0.197544	-0.398028
C	1.069293	-0.590914	-0.152981
N	1.398889	0.552867	-0.931243
S	2.554569	-1.337864	0.522283
H	3.166312	1.507613	-1.650297
H	4.615437	-0.272556	-0.395100
C	-0.149434	-1.109474	0.045877
O	-1.257092	-0.476943	-0.493886
H	-1.942932	-1.142414	-0.729098
C	-0.437795	-2.310511	0.886110
H	0.468166	-2.870077	1.124085
H	-0.920319	-2.026337	1.827224
H	-1.116652	-2.986693	0.357003
C	0.661480	1.808713	-0.698579
H	1.154757	2.568659	-1.309780
H	-0.358043	1.710309	-1.063813
C	0.668315	2.225559	0.743162
H	1.645145	2.267826	1.223278
C	-0.428540	2.531530	1.426489
H	-0.384239	2.843698	2.464893
H	-1.409926	2.489959	0.960010
O	-3.337991	-2.079186	-1.162949
H	-4.077319	-1.715887	-0.665260
H	-3.555504	-1.911574	-2.085086
O	-3.038379	1.717880	-1.259244
H	-2.631465	2.557911	-1.029776
H	-2.395922	1.057164	-0.965777
O	-2.888877	0.105543	1.901436
H	-2.708202	0.982352	2.250121
H	-2.315459	0.033683	1.124165

2aWAT neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

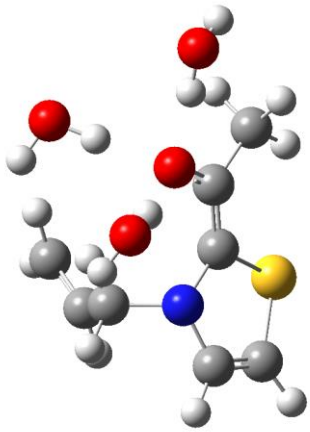
E	-1069.151458
E+ZPE	-1068.905116
H	-1068.881638
G	-1068.958926
$<S^2>$	0.0000
imaginary freq.	N/A



C	2.689010	0.551026	-1.212393
C	3.478606	-0.311723	-0.567549
C	1.020010	-0.612206	-0.064922
N	1.309938	0.467744	-0.948829
S	2.557994	-1.343553	0.544482
H	3.020536	1.303290	-1.915203
H	4.547859	-0.424424	-0.658695
C	-0.186041	-1.115079	0.254374
O	-1.342983	-0.513454	-0.249325
H	-1.982191	-1.214691	-0.523421
C	-0.412795	-2.256648	1.194970
H	0.499302	-2.831106	1.367551
H	-0.781793	-1.910663	2.167500
H	-1.163381	-2.940071	0.784795
C	0.611938	1.769017	-0.790675
H	1.009776	2.415063	-1.578376
H	-0.449379	1.637014	-0.983005
C	0.831688	2.407156	0.553342
H	1.867152	2.490227	0.879050
C	-0.149073	2.873161	1.324617
H	0.054566	3.350462	2.277645
H	-1.190030	2.806266	1.018989
O	-3.201866	-2.317284	-1.170270
H	-4.051509	-2.180614	-0.730459
H	-3.371883	-2.112579	-2.099324
O	-3.190818	1.499727	-1.537863
H	-3.033304	2.369991	-1.151571
H	-2.554930	0.921769	-1.088688
O	-2.892103	0.486828	2.011816
H	-2.435446	1.275532	2.328853
H	-2.360717	0.192403	1.249003

2'aWAT singlet anion, optimized with SMD mimicking the water solution at the level of ωB97XD/6-311++G(d,p).

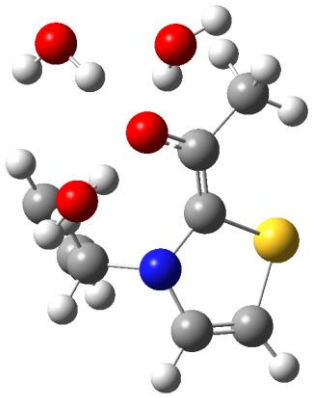
E	-1068.447951
E+ZPE	-1068.210370
H	-1068.188859
G	-1068.261175
$<S^2>$	0.0000
imaginary freq.	N/A



C	2.431539	0.168984	-1.312048
C	3.083335	-0.850305	-0.753340
C	0.677906	-0.712922	-0.065330
N	1.100361	0.370878	-0.902839
S	2.103822	-1.686944	0.460711
H	2.849372	0.855111	-2.038670
H	4.094305	-1.168239	-0.962557
C	-0.611643	-1.011645	0.202355
O	-1.629350	-0.301030	-0.282019
C	-0.990154	-2.158928	1.100091
H	-0.135591	-2.759647	1.418183
H	-1.494146	-1.784818	1.997952
H	-1.695450	-2.815724	0.579893
C	0.814802	1.734348	-0.409379
H	1.117571	2.427804	-1.199994
H	-0.262804	1.829725	-0.273607
C	1.533985	2.059424	0.868369
H	2.621927	2.067177	0.818707
C	0.924450	2.297546	2.025071
H	1.485538	2.515202	2.928751
H	-0.159430	2.286029	2.105691
O	-4.059379	-1.420739	-0.226829
H	-4.041787	-2.047171	0.500916
H	-3.147135	-1.033526	-0.236997
O	-1.911543	1.185511	-2.478107
H	-1.296205	1.921703	-2.436981
H	-1.708698	0.642374	-1.675703
O	-2.694162	1.653019	1.207964
H	-2.156403	2.430679	1.039053
H	-2.264597	0.935181	0.681052

2'aWAT singlet anion, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

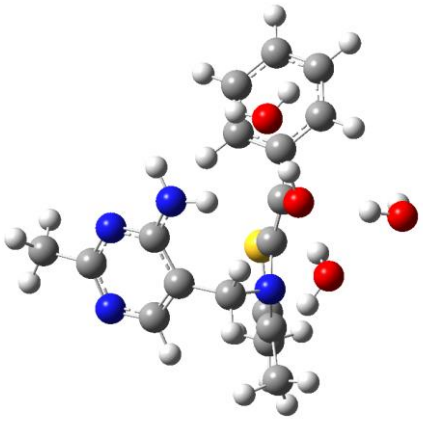
E	-1068.687463
E+ZPE	-1068.453981
H	-1068.431891
G	-1068.506164
$<S^2>$	0.0000
imaginary freq.	N/A



C	2.473651	-0.070375	-1.325685
C	3.080302	-1.066645	-0.671242
C	0.686052	-0.700362	0.043665
N	1.163420	0.251117	-0.923607
S	2.072921	-1.716522	0.642643
H	2.913822	0.509452	-2.127301
H	4.065450	-1.467799	-0.857353
C	-0.613347	-0.895002	0.381574
O	-1.619954	-0.174371	-0.138814
C	-1.013414	-1.921428	1.412648
H	-0.192137	-2.577506	1.708857
H	-1.395240	-1.434441	2.317687
H	-1.822202	-2.546372	1.017766
C	0.921402	1.695062	-0.665553
H	1.286074	2.227741	-1.549785
H	-0.153412	1.857712	-0.597439
C	1.611137	2.217310	0.565231
H	2.688251	2.064436	0.610034
C	0.990907	2.836019	1.569151
H	1.533920	3.203716	2.434099
H	-0.082642	3.005918	1.555911
O	-3.962818	-1.455237	-0.577496
H	-3.972618	-2.239556	-0.016519
H	-3.088745	-1.021040	-0.384325
O	-2.038540	0.906473	-2.567759
H	-1.427286	1.643760	-2.679740
H	-1.798869	0.514136	-1.686704
O	-2.878806	1.504188	1.536376
H	-2.295788	2.266393	1.630104
H	-2.388459	0.884065	0.930480

2cWAT neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

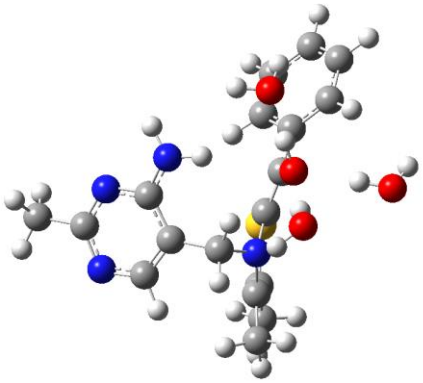
E	-1619.701093
E+ZPE	-1619.269941
H	-1619.236176
G	-1619.336122
$<S^2>$	0.0000
imaginary freq.	N/A



C	-1.620911	-2.255803	-0.689528
C	-1.582514	-1.761272	-1.932038
C	0.204093	-0.817273	-0.447700
N	-0.692062	-1.680512	0.226894
S	-0.364739	-0.472929	-2.099932
C	-2.503149	-3.354651	-0.191144
H	-1.914429	-4.090736	0.363028
H	-3.283278	-2.982155	0.479666
H	-2.995141	-3.863179	-1.019546
C	-1.295328	-1.095795	1.451314
H	-1.986089	-1.831505	1.861984
H	-0.507664	-0.966564	2.190733
C	-2.014950	0.201746	1.175878
N	-2.097953	2.593360	1.024400
C	-3.283339	2.465015	0.425446
C	-3.942941	3.730892	-0.024527
H	-3.324082	4.223919	-0.779457
H	-4.925545	3.529607	-0.449210
H	-4.048665	4.422260	0.815094
C	-3.258035	0.206966	0.585903
H	-3.771263	-0.733018	0.407391
C	-1.459384	1.481470	1.414623
N	-0.299673	1.664275	2.096367
H	0.130608	2.573563	2.018092
H	2.337300	-0.245823	1.752580
C	-2.368696	-2.142643	-3.141292
H	-3.139946	-2.872748	-2.893894
H	-2.863444	-1.265275	-3.570035
H	-1.726534	-2.569652	-3.917753
C	1.367105	-0.386178	0.064491
O	1.790702	-0.909390	1.271794
C	2.256259	0.597898	-0.580538
C	1.754484	1.811608	-1.056051
C	3.628776	0.342305	-0.684264
C	2.602774	2.741817	-1.647666
H	0.699486	2.038142	-0.942764
C	4.474395	1.275541	-1.267708
H	4.029285	-0.591771	-0.305262
C	3.963307	2.476604	-1.755031
H	2.200537	3.680927	-2.010978
H	5.535110	1.064722	-1.346711
H	4.625700	3.204431	-2.210167
N	-3.916438	1.314293	0.202465
H	0.336932	0.892073	2.210795
O	3.189789	1.022536	2.569627
H	4.030370	1.075789	2.102364
H	2.720137	1.820529	2.304204
O	1.117793	-3.020763	3.104682
H	0.159725	-3.075934	3.154643
H	1.284586	-2.328595	2.447068
O	3.131362	-3.172153	0.064358
H	2.745325	-2.474035	0.614276
H	3.160837	-2.779339	-0.812784

2cWAT neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

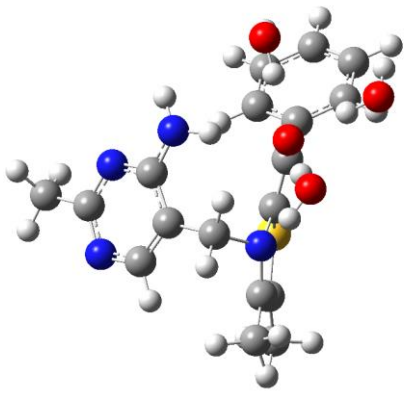
E	-1620.111654
E+ZPE	-1619.687093
H	-1619.652506
G	-1619.755850
$<S^2>$	0.0000
imaginary freq.	N/A



C	-1.340628	-2.404267	-0.630564
C	-1.199098	-2.149658	-1.942684
C	0.337937	-0.762198	-0.490096
N	-0.571593	-1.568667	0.235293
S	-0.077800	-0.785030	-2.233837
C	-2.136459	-3.519275	-0.023347
H	-1.493697	-4.150734	0.598469
H	-2.950231	-3.158597	0.611631
H	-2.577430	-4.143805	-0.799312
C	-1.289696	-0.933790	1.381111
H	-1.861774	-1.721316	1.869809
H	-0.544268	-0.604035	2.098902
C	-2.219485	0.199688	0.993993
N	-2.776965	2.528832	0.741191
C	-3.939886	2.147176	0.203423
C	-4.854490	3.239296	-0.267277
H	-4.389431	3.788740	-1.091613
H	-5.804986	2.832383	-0.609943
H	-5.039768	3.956850	0.536307
C	-3.467986	-0.060361	0.461894
H	-3.802989	-1.086942	0.358369
C	-1.913071	1.578911	1.148943
N	-0.784640	2.028398	1.759327
H	-0.583719	3.014916	1.679784
H	2.146161	0.263872	1.824478
C	-1.781294	-2.837975	-3.134459
H	-2.523140	-3.579849	-2.837202
H	-2.274735	-2.117803	-3.796165
H	-1.010175	-3.343979	-3.725219
C	1.452889	-0.194347	0.035480
O	1.781242	-0.522950	1.349680
C	2.398255	0.670769	-0.684412
C	1.972620	1.590187	-1.659693
C	3.777054	0.601289	-0.399137
C	2.890008	2.383834	-2.345794
H	0.915796	1.716394	-1.860987
C	4.688615	1.400109	-1.082042
H	4.135020	-0.092620	0.351680
C	4.252360	2.292990	-2.063587
H	2.534012	3.088018	-3.089728
H	5.745289	1.321629	-0.850750
H	4.964748	2.914713	-2.593821
N	-4.343943	0.880105	0.055319
H	0.007050	1.419380	1.895548
O	2.762971	1.579753	2.786680
H	3.392854	2.052890	2.226203
H	2.067814	2.224569	2.973838
O	1.118921	-2.156750	3.757275
H	0.157268	-2.148110	3.837633
H	1.290641	-1.677677	2.930304
O	3.693873	-2.695010	1.413670
H	3.063640	-1.951643	1.386341
H	4.398929	-2.432046	0.809966

2'cWAT neutral singlet, optimized with SMD mimicking the water solution at the level of ωB97XD/6-311++G(d,p).

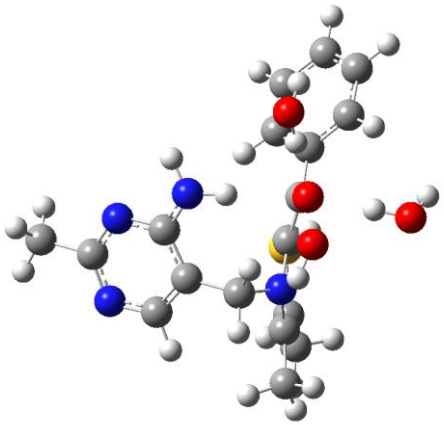
E	-1619.234412
E+ZPE	-1618.815744
H	-1618.783378
G	-1618.879131
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.809022	2.297996	-0.642792
C	1.738062	1.855680	-1.904731
C	-0.108597	0.966758	-0.447367
N	0.846476	1.758798	0.258438
S	0.454363	0.640857	-2.117413
C	2.774783	3.309910	-0.111784
H	2.253788	4.048625	0.503617
H	3.548244	2.848320	0.510057
H	3.276201	3.834967	-0.924324
C	1.413463	1.119518	1.467954
H	2.166879	1.792402	1.877491
H	0.626004	1.045942	2.215964
C	2.022511	-0.231952	1.198061
N	1.903578	-2.624396	1.099030
C	3.118134	-2.609719	0.544265
C	3.690870	-3.939243	0.162062
H	3.061553	-4.411218	-0.597665
H	4.700301	-3.830492	-0.232670
H	3.713546	-4.605083	1.028368
C	3.275087	-0.352554	0.645971
H	3.869010	0.538543	0.463899
C	1.343538	-1.452008	1.429599
N	0.134459	-1.501274	2.048694
H	-0.354876	-2.380828	1.966274
C	2.544187	2.244415	-3.099406
H	3.353307	2.923857	-2.828634
H	2.992642	1.360718	-3.565361
H	1.924854	2.733830	-3.857908
C	-1.286057	0.541650	0.053091
O	-1.708656	0.800404	1.295742
C	-2.153145	-0.373317	-0.752631
C	-1.742132	-1.678488	-1.031486
C	-3.424548	0.034896	-1.164186
C	-2.582957	-2.558578	-1.706665
H	-0.761065	-2.008508	-0.705315
C	-4.264257	-0.841226	-1.841828
H	-3.754989	1.045985	-0.951368
C	-3.846607	-2.142098	-2.112026
H	-2.252298	-3.571296	-1.910650
H	-5.246553	-0.509206	-2.160263
H	-4.503996	-2.827006	-2.636345
N	3.848263	-1.521613	0.306170
H	-0.467640	-0.683514	1.999175
O	-4.145022	2.038731	1.546120
H	-3.277578	1.594967	1.415939
H	-4.779817	1.419085	1.177574
O	-1.201285	2.984818	2.807476
H	-0.254902	3.136546	2.865762
H	-1.296749	2.203890	2.212067
O	-3.285583	-1.270691	2.181108
H	-2.729603	-0.515468	1.881662
H	-3.409269	-1.795308	1.384745

2'cWAT neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

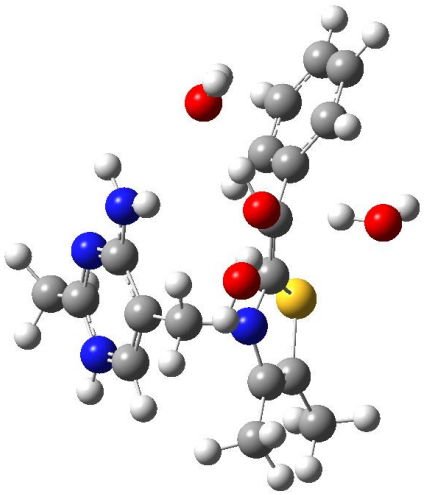
E	-1619.645909
E+ZPE	-1619.234228
H	-1619.200780
G	-1619.301496
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.431931	2.549946	-0.136673
C	1.239786	2.587576	-1.467003
C	-0.278994	0.927471	-0.288328
N	0.665404	1.575742	0.568237
S	0.097570	1.321271	-2.009227
C	2.318946	3.466743	0.651697
H	1.774198	3.904325	1.494178
H	3.191738	2.947985	1.060594
H	2.685974	4.280096	0.026532
C	1.408297	0.715576	1.531076
H	2.085045	1.364325	2.085080
H	0.693178	0.326943	2.249501
C	2.192264	-0.418220	0.910311
N	2.452774	-2.728070	0.285512
C	3.643375	-2.402779	-0.232131
C	4.420748	-3.513397	-0.876030
H	3.857783	-3.932096	-1.715461
H	5.383371	-3.156466	-1.240039
H	4.588049	-4.324741	-0.162050
C	3.442362	-0.217449	0.363215
H	3.886747	0.772896	0.394140
C	1.717594	-1.756167	0.859310
N	0.543561	-2.134792	1.432306
H	0.217627	-3.064855	1.209525
C	1.805659	3.508905	-2.499288
H	2.556862	4.173361	-2.070507
H	2.283527	2.942763	-3.306892
H	1.027387	4.128113	-2.959133
C	-1.373203	0.242828	0.156139
O	-1.657870	0.129119	1.467484
C	-2.323824	-0.410327	-0.785943
C	-1.904732	-1.114559	-1.926958
C	-3.706470	-0.352765	-0.524825
C	-2.826971	-1.711151	-2.787539
H	-0.846957	-1.229336	-2.131860
C	-4.627104	-0.944920	-1.384696
H	-4.059318	0.171279	0.355030
C	-4.193360	-1.626535	-2.524788
H	-2.472853	-2.255600	-3.656471
H	-5.687315	-0.873714	-1.166018
H	-4.910682	-2.091143	-3.192051
N	4.188214	-1.180582	-0.217778
H	-0.178488	-1.443080	1.610695
O	-3.268767	2.311219	2.012771
H	-2.706352	1.520814	1.821990
H	-3.899924	2.339059	1.284086
O	-1.179132	0.650308	4.153513
H	-0.293489	1.007069	4.289038
H	-1.250614	0.522552	3.182483
O	-2.972427	-2.034497	2.397017
H	-2.507202	-1.245541	2.006621
H	-3.621328	-2.285282	1.729124

2cN1HWAT neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

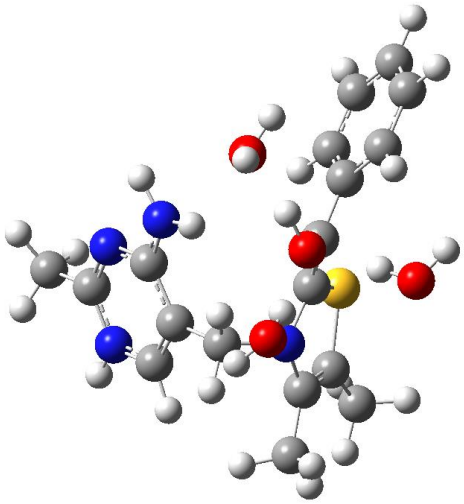
E	-1620.164337
E+ZPE	-1619.718868
H	-1619.685219
G	-1619.784171
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.590855	2.259373	-0.750315
C	1.615783	1.699701	-1.965459
C	-0.214275	0.789404	-0.510895
N	0.635848	1.707526	0.153636
S	0.435883	0.374931	-2.115510
C	2.423567	3.404822	-0.271472
H	1.792589	4.152101	0.217063
H	3.181192	3.087633	0.451747
H	2.940428	3.882940	-1.102669
C	1.196209	1.200109	1.426107
H	1.858685	1.962519	1.833039
H	0.384802	1.083696	2.140188
C	1.955962	-0.090903	1.227912
N	2.074792	-2.519719	1.138097
C	3.256792	-2.425303	0.585056
C	3.981656	-3.641392	0.133276
H	3.670913	-3.869835	-0.890701
H	5.060739	-3.485055	0.138752
H	3.723239	-4.485877	0.769601
C	3.203077	-0.072602	0.689638
H	3.751743	0.836009	0.484264
C	1.413487	-1.389948	1.489889
N	0.255281	-1.572229	2.109717
H	-0.087909	-2.512747	2.234449
H	-2.345579	0.304097	1.690215
C	2.438827	2.041152	-3.161893
H	3.179444	2.805183	-2.923887
H	2.972563	1.157578	-3.525902
H	1.815292	2.409604	-3.982077
C	-1.386691	0.364493	-0.011678
O	-1.857597	0.961112	1.140265
C	-2.236361	-0.677920	-0.613124
C	-1.683492	-1.861424	-1.110353
C	-3.626234	-0.509823	-0.658496
C	-2.496694	-2.840273	-1.671075
H	-0.615102	-2.032418	-1.033508
C	-4.436149	-1.492329	-1.210791
H	-4.070578	0.395222	-0.259433
C	-3.873947	-2.658589	-1.724775
H	-2.052440	-3.753433	-2.051131
H	-5.510036	-1.346060	-1.244202
H	-4.508536	-3.424349	-2.156578
N	3.841804	-1.228761	0.383105
H	-0.339454	-0.808039	2.387717
O	-3.110048	-0.891883	2.657768
H	-3.868312	-0.508187	3.109484
H	-3.489176	-1.508096	2.021765
O	-1.253157	3.192262	2.861282
H	-0.314633	3.382062	2.780588
H	-1.406000	2.468750	2.235004
O	-3.431498	3.072616	-0.022865
H	-2.944613	2.383765	0.455383
H	-3.693764	2.644861	-0.842649
H	4.770492	-1.192669	-0.021157

2cN1HWAT neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

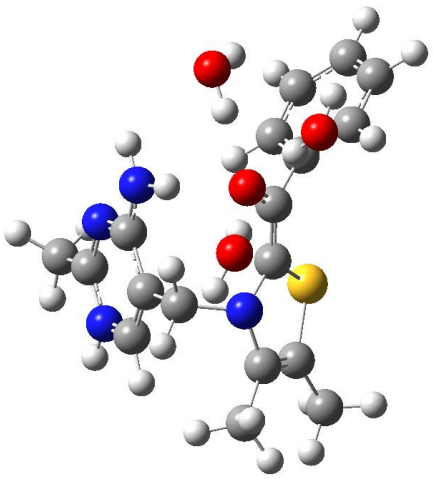
E	-1620.572346
E+ZPE	-1620.133672
H	-1620.099129
G	-1620.200714
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.324049	2.387518	-0.719375
C	1.206475	2.064907	-2.018900
C	-0.362558	0.753511	-0.529746
N	0.536352	1.595836	0.173319
S	0.088273	0.688886	-2.262698
C	2.106142	3.533290	-0.152871
H	1.448394	4.197131	0.417277
H	2.903522	3.208192	0.521485
H	2.567702	4.114461	-0.950159
C	1.235273	1.018244	1.353342
H	1.799870	1.821674	1.822874
H	0.485798	0.705932	2.074221
C	2.180895	-0.122486	1.021940
N	2.738646	-2.491620	0.822049
C	3.913958	-2.165466	0.341433
C	4.877939	-3.211605	-0.098843
H	4.697273	-3.441189	-1.154196
H	5.908362	-2.868618	0.003485
H	4.729926	-4.121972	0.479753
C	3.432576	0.140692	0.546614
H	3.823932	1.140465	0.424439
C	1.860878	-1.513843	1.177931
N	0.712025	-1.941642	1.696809
H	0.554423	-2.936722	1.778796
H	-2.173533	-0.190589	1.808170
C	1.810397	2.692275	-3.233190
H	2.545467	3.450188	-2.960977
H	2.315934	1.939451	-3.847658
H	1.049046	3.165174	-3.862530
C	-1.481670	0.205729	0.005497
O	-1.826064	0.584364	1.300706
C	-2.409389	-0.702922	-0.684797
C	-1.959348	-1.674264	-1.596091
C	-3.793201	-0.623977	-0.430539
C	-2.859113	-2.512020	-2.252455
H	-0.897984	-1.804519	-1.769129
C	-4.687349	-1.466243	-1.083729
H	-4.168416	0.111318	0.270768
C	-4.227056	-2.412380	-2.002291
H	-2.485521	-3.256420	-2.946912
H	-5.748814	-1.380650	-0.878557
H	-4.925858	-3.068273	-2.508896
N	4.279437	-0.868761	0.210569
H	-0.031011	-1.317332	1.972780
O	-2.684792	-1.522688	2.807099
H	-3.059978	-1.204282	3.638977
H	-3.422594	-1.949128	2.350397
O	-1.212018	2.277679	3.675904
H	-0.251192	2.278160	3.765966
H	-1.371388	1.787395	2.853167
O	-3.795842	2.713324	1.322221
H	-3.151117	1.982678	1.300801
H	-4.489153	2.438408	0.710264
H	5.205661	-0.647000	-0.141692

2'cN1HWAT neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

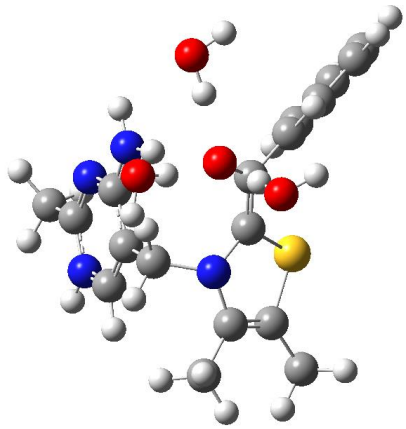
E	-1619.699626
E+ZPE	-1619.266611
H	-1619.234172
G	-1619.330282
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.774273	-2.335972	0.617129
C	1.700902	-1.915266	1.886247
C	-0.136978	-0.986447	0.440385
N	0.814054	-1.776705	-0.275735
S	0.418765	-0.703599	2.119278
C	2.735573	-3.342911	0.069112
H	2.211319	-4.068046	-0.559355
H	3.512746	-2.875066	-0.543732
H	3.233061	-3.884270	0.873133
C	1.382387	-1.134072	-1.476047
H	2.131534	-1.802305	-1.898703
H	0.598977	-1.033651	-2.224440
C	2.007957	0.206741	-1.184227
N	1.898264	2.633383	-1.059097
C	3.097268	2.639529	-0.531278
C	3.733633	3.922983	-0.133824
H	3.124129	4.397448	0.638275
H	4.742750	3.770677	0.248095
H	3.767091	4.591314	-0.995991
C	3.253195	0.291266	-0.654238
H	3.883576	-0.568397	-0.471706
C	1.326258	1.449940	-1.386852
N	0.121615	1.505440	-1.943147
H	-0.341729	2.402414	-1.970689
C	2.500018	-2.330510	3.076596
H	3.309684	-3.005180	2.796110
H	2.946132	-1.457496	3.564115
H	1.874832	-2.835136	3.819988
C	-1.301004	-0.529982	-0.063364
O	-1.701530	-0.740305	-1.322515
C	-2.170686	0.367875	0.758459
C	-1.755266	1.661182	1.082023
C	-3.449645	-0.044752	1.140982
C	-2.600134	2.526090	1.771514
H	-0.767589	1.995064	0.780911
C	-4.293581	0.816425	1.832286
H	-3.782552	-1.047283	0.894636
C	-3.871951	2.106065	2.146372
H	-2.266195	3.529980	2.010622
H	-5.282116	0.481418	2.127307
H	-4.532524	2.779431	2.681483
N	3.781656	1.499184	-0.327986
H	-0.471586	0.677626	-2.002525
O	-4.172313	-1.930296	-1.639267
H	-3.298410	-1.510113	-1.486904
H	-4.796904	-1.312141	-1.251115
O	-1.254288	-2.936437	-2.850543
H	-0.312764	-3.118779	-2.899171
H	-1.331687	-2.158223	-2.250624
O	-3.281984	1.367336	-2.156677
H	-2.736139	0.599947	-1.874795
H	-3.449261	1.843909	-1.338358
H	4.711859	1.543849	0.071111

2'cN1HWAT neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

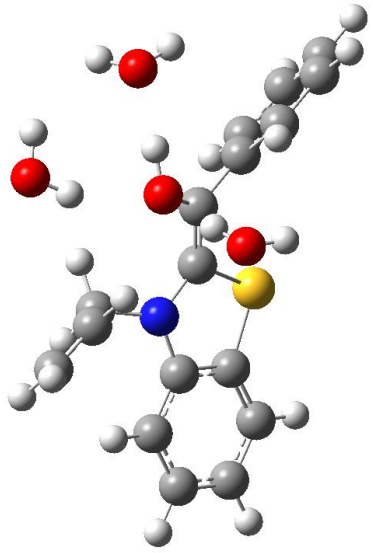
E	-1620.108516
E+ZPE	-1619.683191
H	-1619.649611
G	-1619.749585
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.401639	-2.573824	-0.255558
C	1.159692	-2.862359	1.035180
C	-0.319985	-0.997494	0.140803
N	0.650507	-1.486595	-0.791252
S	-0.016006	-1.726781	1.761209
C	2.318480	-3.327382	-1.172442
H	1.804621	-3.590864	-2.102168
H	3.206604	-2.747112	-1.442443
H	2.659994	-4.248890	-0.702392
C	1.397991	-0.493664	-1.597938
H	2.080069	-1.042347	-2.244337
H	0.693912	0.015260	-2.248474
C	2.189066	0.517776	-0.795679
N	2.443416	2.721602	0.223720
C	3.633090	2.370023	0.651631
C	4.453897	3.306064	1.470634
H	4.077463	3.304523	2.498290
H	5.503182	3.010129	1.485245
H	4.361207	4.319186	1.079425
C	3.438390	0.228553	-0.337798
H	3.938515	-0.711410	-0.525780
C	1.698890	1.832418	-0.489214
N	0.513331	2.260694	-0.915257
H	0.211898	3.184281	-0.634690
C	1.693100	-3.961798	1.896023
H	2.474203	-4.525082	1.384127
H	2.123983	-3.558778	2.819480
H	0.904315	-4.663231	2.189628
C	-1.382612	-0.210753	-0.194796
O	-1.589970	0.200946	-1.461903
C	-2.380489	0.235294	0.816747
C	-2.022124	0.699204	2.092740
C	-3.748594	0.222142	0.484281
C	-2.990850	1.110412	3.009353
H	-0.976199	0.772288	2.366697
C	-4.715348	0.628392	1.399405
H	-4.052368	-0.120468	-0.497768
C	-4.342328	1.074171	2.670190
H	-2.684360	1.472995	3.984744
H	-5.763573	0.596255	1.121909
H	-5.095372	1.395454	3.381031
N	4.141577	1.144901	0.384093
H	-0.185140	1.626681	-1.307758
O	-3.079476	-1.807494	-2.618036
H	-2.558458	-1.073730	-2.207646
H	-3.856847	-1.897449	-2.054638
O	-1.022577	0.540318	-4.190486
H	-0.432435	-0.162317	-4.487755
H	-1.151651	0.362970	-3.236244
O	-2.940958	2.507818	-1.943102
H	-2.479224	1.657474	-1.719109
H	-3.689810	2.541880	-1.336154
H	5.072166	0.910818	0.715135

2dWAT neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

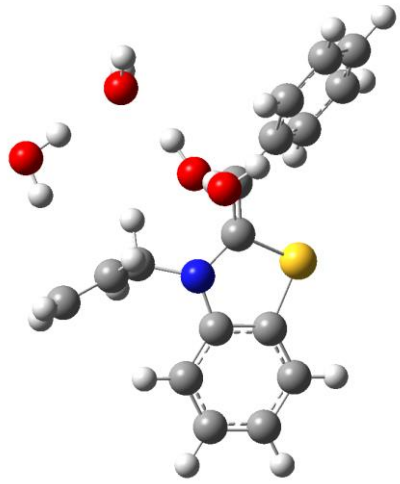
E	-1414.270885
E+ZPE	-1413.918738
H	-1413.890339
G	-1413.978436
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.570620	-0.420330	-0.136542
C	-2.319341	-1.793848	-0.050245
C	-0.233134	-0.381918	-0.260745
N	-1.426783	0.347960	-0.317136
S	-0.596706	-2.136334	-0.218162
C	1.018684	0.095010	-0.125718
O	1.223170	1.442638	0.119845
H	2.135394	1.687214	-0.157464
C	-1.522110	1.700036	-0.864214
H	-0.616309	1.887127	-1.440869
H	-2.360370	1.723961	-1.566792
C	-1.703950	2.755292	0.190714
H	-0.945383	2.785548	0.969189
C	-2.709048	3.622702	0.197498
H	-2.793756	4.385028	0.965057
H	-3.479685	3.601300	-0.569227
C	-3.880125	0.046095	-0.068003
C	-3.344437	-2.710115	0.098723
C	-4.656856	-2.240169	0.170921
H	-5.472039	-2.943782	0.291837
C	-4.914592	-0.876695	0.085005
H	-5.935553	-0.516440	0.141884
H	-3.134012	-3.772054	0.154765
H	-4.095759	1.105607	-0.122871
C	2.216050	-0.767943	-0.067249
C	2.487451	-1.713318	-1.059402
C	3.119733	-0.625018	0.994184
C	3.620993	-2.515911	-0.981206
H	1.819906	-1.808000	-1.908946
C	4.256256	-1.418793	1.063922
H	2.926678	0.112593	1.766004
C	4.508393	-2.371233	0.078962
H	3.817033	-3.244145	-1.760323
H	4.944969	-1.299049	1.892910
H	5.395810	-2.991598	0.135652
O	3.721197	2.184200	-0.662566
H	4.256099	1.383184	-0.650898
H	3.688498	2.448553	-1.587378
O	1.109995	4.261942	-1.042509
H	0.908987	3.404430	-0.649211
H	2.029624	4.183001	-1.311046
O	0.734860	1.501339	2.896436
H	0.981994	0.591664	3.084332
H	0.908797	1.597464	1.944659

2dWAT neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

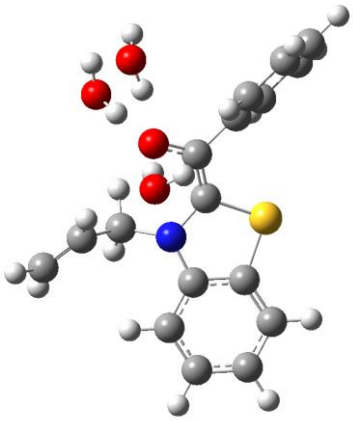
E	-1414.633198
E+ZPE	-1414.286343
H	-1414.257794
G	-1414.347125
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.559904	-0.495763	-0.032164
C	-2.375689	-1.886726	-0.030532
C	-0.212710	-0.558797	-0.152422
N	-1.372996	0.229861	-0.154778
S	-0.663262	-2.301057	-0.208930
C	1.061826	-0.109854	0.011834
O	1.219808	1.207359	0.440428
H	1.833652	1.700791	-0.148186
C	-1.399411	1.598266	-0.706153
H	-0.463658	1.745988	-1.244361
H	-2.206806	1.647288	-1.441964
C	-1.577580	2.683192	0.322946
H	-0.941651	2.620402	1.201097
C	-2.424426	3.701880	0.179956
H	-2.493216	4.488328	0.924037
H	-3.075141	3.784636	-0.686328
C	-3.851950	0.027681	0.053613
C	-3.447913	-2.763873	0.051796
C	-4.740120	-2.235503	0.142881
H	-5.588839	-2.905459	0.212771
C	-4.933192	-0.853972	0.140408
H	-5.936572	-0.449881	0.210985
H	-3.288314	-3.835761	0.042265
H	-4.016780	1.096995	0.063240
C	2.281064	-0.923431	-0.071612
C	2.408586	-2.009717	-0.958208
C	3.388587	-0.607199	0.742346
C	3.574432	-2.771107	-0.998576
H	1.608030	-2.243441	-1.649310
C	4.553793	-1.365840	0.692694
H	3.326597	0.232370	1.423692
C	4.653502	-2.457797	-0.172112
H	3.644818	-3.600249	-1.694145
H	5.387390	-1.105650	1.336015
H	5.562120	-3.047870	-0.208417
O	2.725199	2.857097	-1.182196
H	3.552276	3.162063	-0.785300
H	2.974098	2.509747	-2.049334
O	0.675579	4.866925	-1.232742
H	-0.092548	4.469559	-0.798632
H	1.358982	4.171259	-1.213524
O	1.509052	1.623636	3.210613
H	2.216376	1.032092	3.494162
H	1.431872	1.465906	2.248559

2'dWAT neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

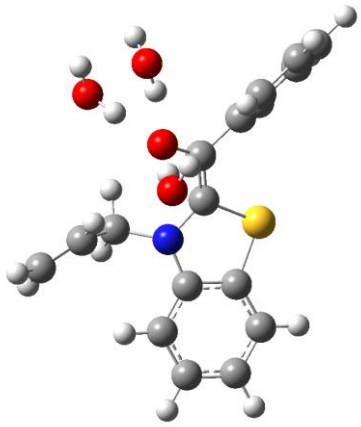
E	-1413.803033
E+ZPE	-1413.464434
H	-1413.436962
G	-1413.524413
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.565865	-0.350023	0.001850
C	-2.319388	-1.730394	0.038310
C	-0.235674	-0.329460	-0.236649
N	-1.436881	0.425129	-0.229585
S	-0.621409	-2.087578	-0.300503
C	1.003756	0.180634	-0.053114
O	1.223903	1.477246	0.181502
C	-1.560709	1.661640	-1.003345
H	-0.656647	1.760656	-1.605420
H	-2.404372	1.563248	-1.695900
C	-1.740268	2.887335	-0.153098
H	-0.987074	3.044616	0.615202
C	-2.731876	3.757016	-0.310356
H	-2.809964	4.645226	0.308322
H	-3.498764	3.610372	-1.067218
C	-3.867124	0.119417	0.159283
C	-3.342785	-2.639109	0.240562
C	-4.645615	-2.163308	0.409076
H	-5.455870	-2.864789	0.570569
C	-4.899378	-0.797695	0.361217
H	-5.912269	-0.431951	0.488164
H	-3.140276	-3.704209	0.256991
H	-4.073337	1.182744	0.135186
C	2.196493	-0.712505	-0.069904
C	2.474731	-1.565862	-1.139664
C	3.082337	-0.685185	1.013696
C	3.600396	-2.385703	-1.121761
H	1.815272	-1.577876	-2.001369
C	4.204102	-1.503038	1.033666
H	2.879786	-0.021839	1.848238
C	4.466734	-2.358334	-0.035105
H	3.803579	-3.038959	-1.963462
H	4.875070	-1.477125	1.885556
H	5.344381	-2.995193	-0.020445
O	3.621398	2.631718	0.665542
H	4.117280	2.526765	-0.150278
H	2.783039	2.136825	0.506864
O	1.768067	2.721241	-2.149214
H	1.542947	2.278537	-1.296019
H	2.666725	3.035047	-2.019667
O	0.670415	1.852427	2.777464
H	1.270009	1.231300	3.198587
H	0.851730	1.748349	1.810904

2'dWAT neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

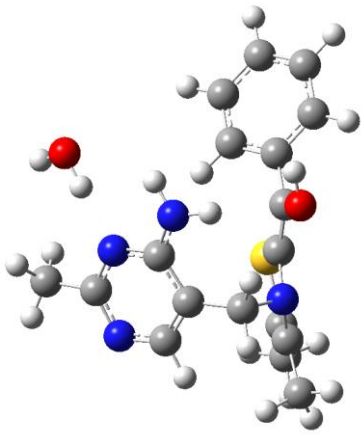
E	-1414.163587
E+ZPE	-1413.829490
H	-1413.801787
G	-1413.889325
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.572760	-0.354135	0.031140
C	-2.346827	-1.742270	0.093299
C	-0.231011	-0.367466	-0.228667
N	-1.428951	0.403468	-0.225456
S	-0.650269	-2.133256	-0.248900
C	1.027844	0.126643	-0.056668
O	1.263198	1.430195	0.172475
C	-1.544136	1.623592	-1.048766
H	-0.623081	1.703315	-1.626378
H	-2.365827	1.491026	-1.760851
C	-1.752346	2.888497	-0.259381
H	-1.040186	3.070489	0.540993
C	-2.712742	3.775557	-0.513501
H	-2.800636	4.694518	0.056733
H	-3.441188	3.616351	-1.304160
C	-3.872820	0.133766	0.189255
C	-3.384640	-2.636060	0.318112
C	-4.684010	-2.139404	0.485307
H	-5.502351	-2.827183	0.663755
C	-4.919611	-0.767541	0.414441
H	-5.926173	-0.384817	0.540913
H	-3.195743	-3.703046	0.352804
H	-4.068390	1.197500	0.149549
C	2.209122	-0.783233	-0.082791
C	2.413022	-1.725358	-1.102888
C	3.173615	-0.694458	0.936788
C	3.528644	-2.564237	-1.095228
H	1.707745	-1.788196	-1.923878
C	4.285143	-1.532425	0.946767
H	3.040413	0.029633	1.731917
C	4.468359	-2.473829	-0.069647
H	3.667469	-3.279332	-1.899008
H	5.009620	-1.454215	1.750378
H	5.336573	-3.123403	-0.063339
O	3.588153	2.762249	0.770994
H	4.056893	2.866077	-0.065350
H	2.805599	2.199760	0.549805
O	1.794369	2.801809	-2.123985
H	1.591711	2.304254	-1.290104
H	2.584926	3.312002	-1.911694
O	0.685980	2.118288	2.725511
H	1.529325	2.008574	3.180371
H	0.877588	1.868331	1.782736

2cWAT' neutral singlet, optimized with SMD mimicking the water solution at the level of ωB97XD/6-311++G(d,p).

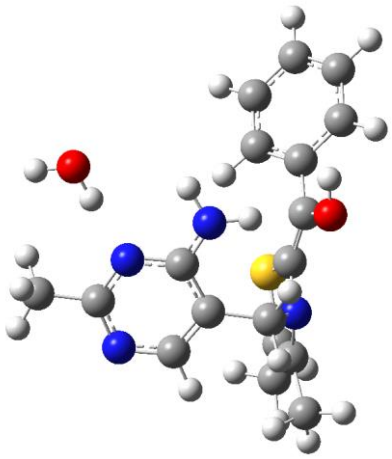
E	-1466.793660
E+ZPE	-1466.412411
H	-1466.384961
G	-1466.470905
$<S^2>$	0.0000
imaginary freq.	N/A



C	-2.009364	-2.317836	0.010392
C	-1.682651	-2.218377	-1.283051
C	0.156232	-1.471725	0.248735
N	-1.038145	-1.819785	0.928875
S	-0.094428	-1.449181	-1.514227
C	-3.257802	-2.919617	0.570652
H	-3.014768	-3.613157	1.380136
H	-3.932101	-2.159884	0.977080
H	-3.802829	-3.467424	-0.197473
C	-1.535581	-0.773480	1.859353
H	-2.480656	-1.122930	2.272648
H	-0.840744	-0.702385	2.693708
C	-1.730038	0.552626	1.168636
N	-0.950599	2.682496	0.407565
C	-2.049087	2.768667	-0.347626
C	-2.155322	3.973948	-1.227942
H	-1.408874	3.911133	-2.025726
H	-3.144617	4.039724	-1.678534
H	-1.952640	4.883460	-0.658537
C	-2.837794	0.778764	0.385258
H	-3.634294	0.041358	0.361111
C	-0.776663	1.598938	1.179040
N	0.309783	1.606889	1.987274
H	1.033133	2.276277	1.769359
H	2.198500	-1.065066	2.570418
C	-2.426359	-2.664468	-2.496922
H	-3.416113	-3.038975	-2.234189
H	-2.557145	-1.831426	-3.194987
H	-1.888340	-3.456166	-3.027265
C	1.333418	-1.258899	0.856596
O	1.406751	-1.486539	2.221415
C	2.555651	-0.776784	0.188388
C	2.513761	0.329258	-0.665481
C	3.785213	-1.400507	0.431905
C	3.671139	0.784208	-1.286589
H	1.575228	0.848820	-0.826261
C	4.940915	-0.939079	-0.184452
H	3.831706	-2.255217	1.098674
C	4.886455	0.150867	-1.049252
H	3.624612	1.644520	-1.944875
H	5.886005	-1.435347	0.005827
H	5.789734	0.508730	-1.530478
N	-3.029203	1.871181	-0.376651
H	0.618788	0.749080	2.417551
O	1.149620	4.490416	-0.201906
H	0.819339	4.955098	-0.975265
H	0.420371	3.881158	0.043343

2cWAT' neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

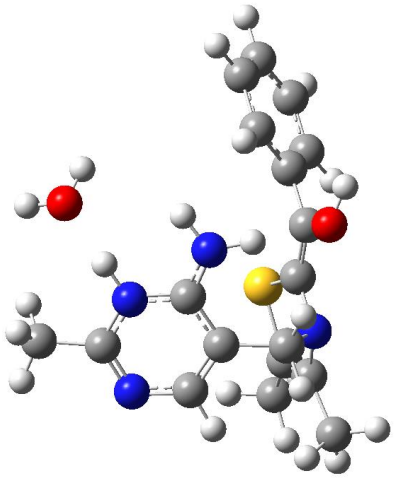
E	-1467.160907
E+ZPE	-1466.783505
H	-1466.756091
G	-1466.841893
$<S^2>$	0.0000
imaginary freq.	N/A



C	-0.339646	-2.998127	0.351824
C	0.200472	-3.123508	-0.872375
C	0.974845	-1.042252	0.348492
N	0.007162	-1.802927	1.046927
S	1.192135	-1.699134	-1.302536
C	-1.183817	-4.017271	1.054854
H	-0.778625	-4.232653	2.048391
H	-2.217566	-3.684812	1.186707
H	-1.207029	-4.947976	0.489419
C	-1.080143	-1.087735	1.772075
H	-1.686420	-1.850530	2.256789
H	-0.627505	-0.503404	2.567911
C	-1.964749	-0.226773	0.892564
N	-2.689280	1.886228	0.003291
C	-3.572458	1.220966	-0.752917
C	-4.431635	2.044358	-1.666143
H	-3.810114	2.649258	-2.331946
H	-5.079709	1.406930	-2.265811
H	-5.051982	2.732643	-1.084627
C	-2.934853	-0.791438	0.089097
H	-3.086736	-1.865618	0.108221
C	-1.885466	1.190343	0.832922
N	-1.061919	1.919657	1.627543
H	-0.954238	2.899480	1.405427
H	1.959153	1.002538	2.509946
C	0.120057	-4.242212	-1.859611
H	-0.586095	-5.005511	-1.531339
H	-0.214262	-3.876501	-2.836659
H	1.093971	-4.720669	-2.009338
C	1.740725	-0.064969	0.898966
O	1.596532	0.137741	2.275474
C	2.758333	0.738098	0.213007
C	2.616669	1.146039	-1.126221
C	3.921028	1.137277	0.904566
C	3.609648	1.892255	-1.756297
H	1.710354	0.913873	-1.671619
C	4.905856	1.890332	0.272764
H	4.066036	0.838777	1.936608
C	4.760388	2.267925	-1.063268
H	3.472531	2.196888	-2.787996
H	5.794484	2.175951	0.824824
H	5.529677	2.852832	-1.554242
N	-3.744257	-0.103475	-0.742572
H	-0.280588	1.473140	2.085910
O	-2.615675	4.745784	-0.073585
H	-3.185287	5.007049	-0.807021
H	-2.654539	3.760023	-0.066212

2cN3HWAT' neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

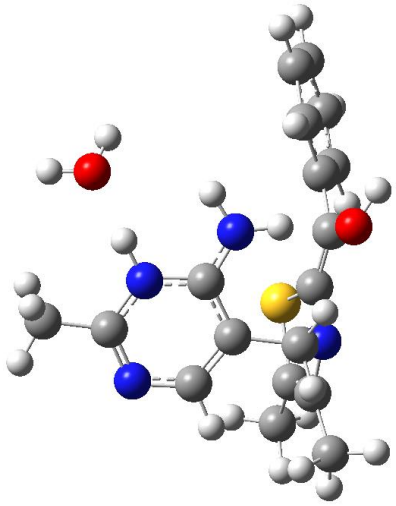
E	-1467.249868
E+ZPE	-1466.855060
H	-1466.827471
G	-1466.912919
$<S^2>$	0.0000
imaginary freq.	N/A



C	-1.476461	-2.651844	0.289429
C	-1.109623	-2.689732	-0.995886
C	0.482927	-1.378172	0.436590
N	-0.667514	-1.831659	1.135619
S	0.322270	-1.683232	-1.308427
C	-2.602967	-3.407642	0.917990
H	-2.264456	-3.898071	1.834544
H	-3.443260	-2.758044	1.180747
H	-2.979867	-4.172385	0.239827
C	-1.424684	-0.798071	1.880154
H	-2.293827	-1.281609	2.322297
H	-0.817740	-0.444714	2.709437
C	-1.877186	0.336837	0.996106
N	-1.628651	2.461871	0.000935
C	-2.705643	2.239393	-0.791071
C	-3.050564	3.319822	-1.752857
H	-2.227775	3.462257	-2.458569
H	-3.953793	3.055939	-2.297991
H	-3.204275	4.262144	-1.221556
C	-2.973465	0.211628	0.183072
H	-3.577908	-0.686464	0.240913
C	-1.172028	1.561839	0.902810
N	-0.133962	1.908196	1.655000
H	0.360004	2.768118	1.460824
H	2.369426	-0.361027	2.697679
C	-1.681373	-3.463291	-2.136218
H	-2.588810	-3.989075	-1.838549
H	-1.937123	-2.794790	-2.964310
H	-0.966054	-4.198990	-2.516209
C	1.545664	-0.786575	1.004236
O	1.479185	-0.507793	2.361277
C	2.740304	-0.290886	0.286689
C	3.192042	1.016511	0.499391
C	3.465288	-1.123958	-0.570987
C	4.327415	1.485456	-0.150236
H	2.653057	1.671047	1.175354
C	4.597308	-0.651078	-1.222769
H	3.150237	-2.150660	-0.716768
C	5.029644	0.655774	-1.018341
H	4.661445	2.502808	0.020390
H	5.150565	-1.310367	-1.882253
H	5.914748	1.022442	-1.525970
N	-3.400439	1.135381	-0.713900
H	0.355981	1.210426	2.204458
O	-0.194035	4.829240	-0.267235
H	0.737743	4.611167	-0.370770
H	-0.445859	5.246905	-1.097185
H	-1.115613	3.360487	-0.106032

2cN3HWAT' neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

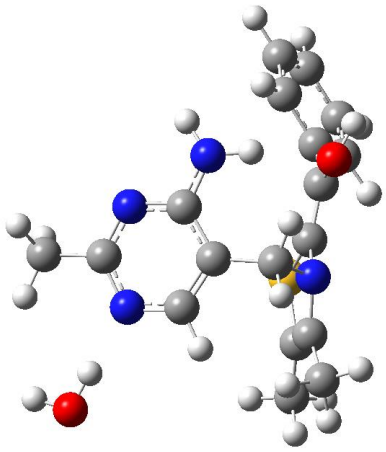
E	-1467.614031
E+ZPE	-1467.223654
H	-1467.196001
G	-1467.281479
$<S^2>$	0.0000
imaginary freq.	N/A



C	-0.558095	-2.984391	0.393248
C	-0.038741	-3.128201	-0.836495
C	0.949289	-1.169285	0.434499
N	-0.100850	-1.838011	1.117704
S	1.104715	-1.812627	-1.226252
C	-1.475078	-3.947292	1.084574
H	-1.080444	-4.207642	2.071554
H	-2.481732	-3.544874	1.229478
H	-1.569141	-4.864740	0.504899
C	-1.157395	-1.029938	1.791937
H	-1.835357	-1.735831	2.266074
H	-0.700319	-0.460037	2.593803
C	-1.963326	-0.134716	0.870469
N	-2.536617	1.945906	-0.115459
C	-3.527910	1.357508	-0.836831
C	-4.313564	2.239652	-1.745550
H	-3.656154	2.696874	-2.490481
H	-5.081181	1.657929	-2.250661
H	-4.784365	3.046927	-1.177702
C	-3.003970	-0.637313	0.123318
H	-3.259850	-1.686561	0.210090
C	-1.728571	1.262363	0.742289
N	-0.816169	1.956404	1.418530
H	-0.686903	2.940551	1.220893
H	2.209029	0.630603	2.650591
C	-0.220570	-4.214616	-1.845893
H	-0.990600	-4.918435	-1.529106
H	-0.524220	-3.799869	-2.813022
H	0.707662	-4.772426	-2.009206
C	1.737618	-0.197796	0.955002
O	1.421522	0.237725	2.249559
C	2.806940	0.552205	0.270211
C	2.946936	1.933202	0.510177
C	3.742694	-0.068847	-0.576690
C	3.968293	2.664555	-0.091124
H	2.246494	2.438962	1.164746
C	4.760387	0.667045	-1.177283
H	3.692518	-1.136162	-0.749075
C	4.877854	2.037867	-0.942665
H	4.049508	3.728109	0.104448
H	5.473678	0.162793	-1.819863
H	5.672397	2.607381	-1.411052
N	-3.782076	0.074148	-0.734756
H	-0.073684	1.478773	1.924948
O	-2.065364	4.713356	-0.346239
H	-1.128716	4.906781	-0.485839
H	-2.511152	5.075138	-1.123820
H	-2.378937	2.967975	-0.229527

2cWAT'' neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

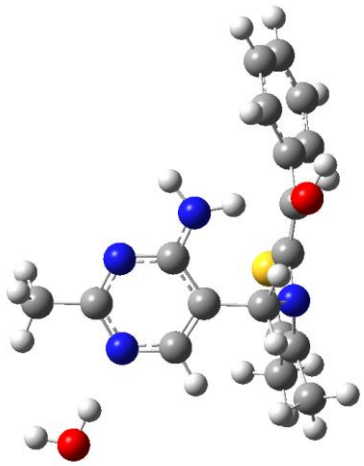
E	-1466.792000
E+ZPE	-1466.409689
H	-1466.382762
G	-1466.467360
$<S^2>$	0.0000
imaginary freq.	N/A



C	1.024628	2.491746	0.548241
C	0.798269	2.537234	-0.768727
C	-0.867391	1.118352	0.463673
N	0.172703	1.617291	1.289805
S	-0.536546	1.465717	-1.249778
C	2.041919	3.284935	1.304239
H	1.587706	3.736986	2.190068
H	2.881063	2.668815	1.640908
H	2.448061	4.082916	0.683663
C	0.897085	0.604231	2.100020
H	1.688130	1.127242	2.635310
H	0.219774	0.218517	2.857179
C	1.490667	-0.503241	1.265459
N	1.443430	-2.703336	0.301729
C	2.541771	-2.378191	-0.377050
C	3.091335	-3.404914	-1.316427
H	2.401798	-3.541868	-2.154447
H	4.060972	-3.097097	-1.706858
H	3.192203	-4.367669	-0.811211
C	2.637061	-0.298110	0.536136
H	3.169991	0.644513	0.610274
C	0.907862	-1.786875	1.123566
N	-0.171409	-2.179730	1.842074
H	-0.620309	-3.030037	1.535493
H	-2.947812	0.002142	2.494350
C	1.454263	3.356221	-1.829339
H	2.304019	3.909761	-1.428870
H	1.823066	2.715183	-2.636292
H	0.754279	4.071832	-2.271478
C	-1.953242	0.462794	0.903417
O	-2.031432	0.181061	2.259933
C	-3.020705	-0.099872	0.047300
C	-3.402639	-1.437996	0.196463
C	-3.693936	0.693679	-0.886601
C	-4.418533	-1.973471	-0.585971
H	-2.899849	-2.063208	0.926213
C	-4.705628	0.154313	-1.671432
H	-3.432873	1.740502	-0.990460
C	-5.068949	-1.181160	-1.526602
H	-4.698924	-3.013664	-0.462981
H	-5.219655	0.783240	-2.389779
H	-5.860121	-1.599973	-2.138349
N	3.178674	-1.210675	-0.289324
H	-0.789066	-1.480315	2.234743
O	5.455008	-0.592092	-1.801788
H	5.590183	-1.346695	-2.380613
H	4.656669	-0.827232	-1.273747

2cWAT'' neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

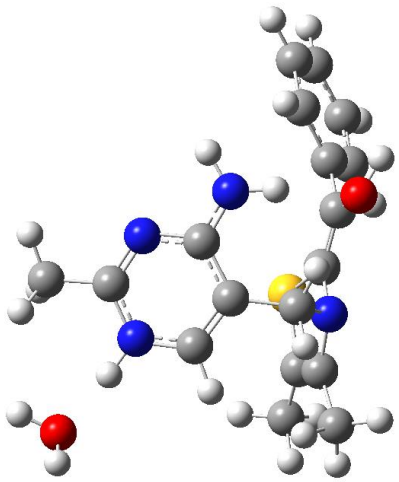
E	-1467.159385
E+ZPE	-1466.782838
H	-1466.755265
G	-1466.842495
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.793049	2.510031	0.662699
C	0.420748	2.795290	-0.595702
C	-1.007398	0.999613	0.480978
N	0.079963	1.435922	1.282898
S	-0.891910	1.718548	-1.152802
C	1.796986	3.266548	1.479412
H	1.354244	3.584383	2.428720
H	2.685157	2.674204	1.715600
H	2.130128	4.156156	0.946174
C	0.918486	0.413874	1.983612
H	1.651629	0.968138	2.566225
H	0.290741	-0.107420	2.698570
C	1.640350	-0.560337	1.074330
N	1.897267	-2.706669	0.003557
C	3.000340	-2.236027	-0.581284
C	3.729410	-3.160751	-1.510267
H	3.075765	-3.456836	-2.335651
H	4.620217	-2.683940	-1.917661
H	4.021481	-4.073266	-0.983329
C	2.808468	-0.201009	0.434514
H	3.234232	0.784169	0.592318
C	1.210367	-1.895774	0.833958
N	0.138175	-2.444762	1.457508
H	-0.176530	-3.338532	1.106402
H	-2.776541	-0.616104	2.483095
C	0.876104	3.873907	-1.524253
H	1.715431	4.426622	-1.101524
H	1.201493	3.452641	-2.481556
H	0.072178	4.585824	-1.739721
C	-2.007479	0.179449	0.884334
O	-1.898826	-0.352318	2.175835
C	-3.136852	-0.319190	0.076213
C	-3.549142	-1.659285	0.209333
C	-3.868675	0.513610	-0.789534
C	-4.634609	-2.149765	-0.512652
H	-3.009832	-2.323961	0.874415
C	-4.951187	0.018324	-1.511093
H	-3.605895	1.559308	-0.883817
C	-5.338713	-1.316359	-1.381403
H	-4.926330	-3.187959	-0.398392
H	-5.503088	0.683106	-2.166475
H	-6.182729	-1.698645	-1.944098
N	3.501169	-1.007874	-0.395697
H	-0.571241	-1.848363	1.868886
O	5.915866	-0.053209	-1.477646
H	6.248855	-0.741224	-2.065834
H	5.067336	-0.420083	-1.120058

2cN1HWAT' neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

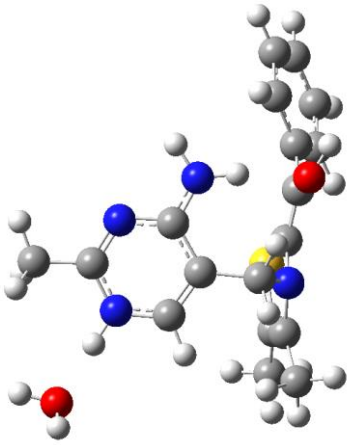
E	-1467.254910
E+ZPE	-1466.859551
H	-1466.832128
G	-1466.917655
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.921161	2.539256	0.497235
C	0.706720	2.536248	-0.822615
C	-0.934231	1.112547	0.436883
N	0.087836	1.660941	1.256969
S	-0.592898	1.413620	-1.282736
C	1.901927	3.389227	1.239664
H	1.419694	3.857103	2.102055
H	2.754757	2.812584	1.610600
H	2.292812	4.177507	0.597447
C	0.834964	0.691668	2.091982
H	1.606116	1.244183	2.625723
H	0.167073	0.291556	2.849613
C	1.475155	-0.407015	1.278579
N	1.484639	-2.638033	0.311655
C	2.582992	-2.330643	-0.332563
C	3.225621	-3.304147	-1.255429
H	3.115942	-2.952735	-2.285126
H	4.293333	-3.383185	-1.039814
H	2.755349	-4.279681	-1.157021
C	2.629520	-0.176326	0.596944
H	3.177662	0.753955	0.657374
C	0.911499	-1.709970	1.116932
N	-0.179340	-2.099891	1.769120
H	-0.565522	-3.007389	1.555086
H	-2.983995	-0.006214	2.495808
C	1.345735	3.345434	-1.900857
H	2.178991	3.930710	-1.510990
H	1.733798	2.694628	-2.690598
H	0.628362	4.031009	-2.362047
C	-2.005981	0.444071	0.891026
O	-2.073292	0.189738	2.252383
C	-3.062465	-0.159370	0.049823
C	-3.436545	-1.493283	0.248112
C	-3.735236	0.593580	-0.917547
C	-4.443554	-2.065253	-0.519825
H	-2.936346	-2.086795	1.005464
C	-4.738272	0.017709	-1.687078
H	-3.481456	1.637830	-1.058793
C	-5.093161	-1.313957	-1.493862
H	-4.718074	-3.101752	-0.358587
H	-5.252537	0.615399	-2.431386
H	-5.877769	-1.761271	-2.093733
N	3.169580	-1.126692	-0.199208
H	-0.772309	-1.441728	2.260059
O	5.507595	-0.742383	-1.683731
H	6.264391	-0.497654	-1.142431
H	5.712306	-1.624171	-2.011302
H	4.045258	-0.933590	-0.717024

2cN1HWAT' neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

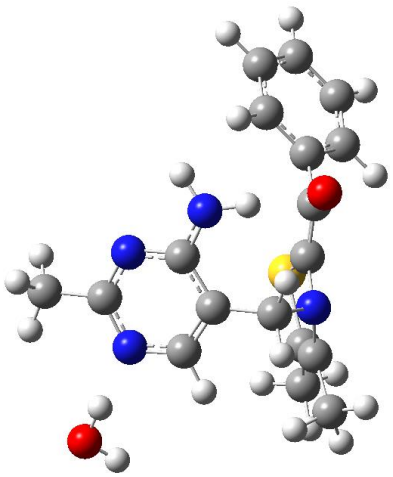
E	-1467.619607
E+ZPE	-1467.229251
H	-1467.201604
G	-1467.286953
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.714280	2.524528	0.670287
C	0.333594	2.811506	-0.585196
C	-1.060381	0.980878	0.478831
N	0.020443	1.432704	1.282896
S	-0.960788	1.716118	-1.147994
C	1.700599	3.296033	1.493952
H	1.245952	3.605994	2.440240
H	2.597209	2.719207	1.736896
H	2.022733	4.191018	0.963160
C	0.868062	0.431714	1.989357
H	1.585061	0.992996	2.584508
H	0.246788	-0.112713	2.692172
C	1.626003	-0.523642	1.085695
N	1.950089	-2.696775	0.023324
C	3.043572	-2.242122	-0.542624
C	3.856241	-3.106734	-1.445389
H	3.872620	-2.682141	-2.453239
H	4.888670	-3.159892	-1.090497
H	3.433332	-4.107872	-1.484149
C	2.785733	-0.134291	0.478379
H	3.223904	0.844612	0.613651
C	1.222561	-1.875804	0.830917
N	0.142325	-2.421762	1.389776
H	-0.103935	-3.366574	1.127522
H	-2.782353	-0.702162	2.466608
C	0.765818	3.906936	-1.504874
H	1.596005	4.471186	-1.079449
H	1.095314	3.500751	-2.467197
H	-0.052255	4.605392	-1.710461
C	-2.041436	0.135712	0.875371
O	-1.912106	-0.418513	2.155378
C	-3.169981	-0.364758	0.066974
C	-3.553195	-1.715890	0.166860
C	-3.929081	0.478611	-0.763904
C	-4.638916	-2.206703	-0.554560
H	-2.992139	-2.387563	0.806414
C	-5.011668	-0.016910	-1.485144
H	-3.687309	1.531566	-0.830575
C	-5.370975	-1.362266	-1.388884
H	-4.909372	-3.253146	-0.466594
H	-5.585789	0.655289	-2.113246
H	-6.215537	-1.744629	-1.950697
N	3.474817	-0.976996	-0.331420
H	-0.553017	-1.862417	1.875282
O	5.836577	-0.016640	-1.558121
H	6.536628	0.183490	-0.922770
H	6.205507	-0.712185	-2.118747
H	4.350113	-0.647869	-0.777308

2'cWAT" neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

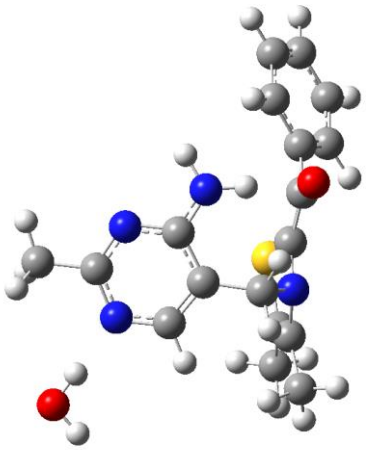
E	-1466.314628
E+ZPE	-1465.946097
H	-1465.919430
G	-1466.004447
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.980674	2.496001	0.542795
C	0.698335	2.532693	-0.765814
C	-0.876699	1.062183	0.538477
N	0.194088	1.602492	1.326730
S	-0.595295	1.393281	-1.202197
C	2.018984	3.314709	1.244647
H	1.616117	3.729034	2.172948
H	2.901613	2.721441	1.504125
H	2.352867	4.142236	0.619092
C	0.985021	0.613249	2.096081
H	1.799540	1.148199	2.584219
H	0.351119	0.216997	2.886554
C	1.542700	-0.498459	1.247825
N	1.432109	-2.708472	0.312451
C	2.516636	-2.406807	-0.400795
C	3.041797	-3.464929	-1.319742
H	2.261757	-3.775879	-2.018992
H	3.902024	-3.101511	-1.880906
H	3.338240	-4.345895	-0.744192
C	2.663618	-0.314092	0.478800
H	3.206816	0.625598	0.522178
C	0.930221	-1.771787	1.134022
N	-0.142548	-2.121438	1.884904
H	-0.594946	-2.979572	1.604248
C	1.285479	3.379656	-1.846135
H	2.123130	3.973069	-1.477377
H	1.655110	2.754887	-2.666124
H	0.541129	4.062736	-2.267981
C	-1.927690	0.370564	1.044178
O	-2.048598	0.044772	2.320769
C	-2.996271	-0.139578	0.121426
C	-3.263091	-1.510276	0.048924
C	-3.790999	0.733211	-0.626368
C	-4.280450	-1.996953	-0.764341
H	-2.665807	-2.202099	0.633516
C	-4.814184	0.249881	-1.436057
H	-3.608797	1.801090	-0.568408
C	-5.059767	-1.117690	-1.511514
H	-4.466284	-3.064583	-0.814676
H	-5.424639	0.943820	-2.004153
H	-5.856127	-1.495632	-2.143336
N	3.166808	-1.244911	-0.354134
H	-0.778748	-1.384454	2.205400
O	5.364323	-0.497418	-1.909321
H	5.276658	0.456171	-1.981998
H	4.589066	-0.780132	-1.368672

2'cWAT" neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

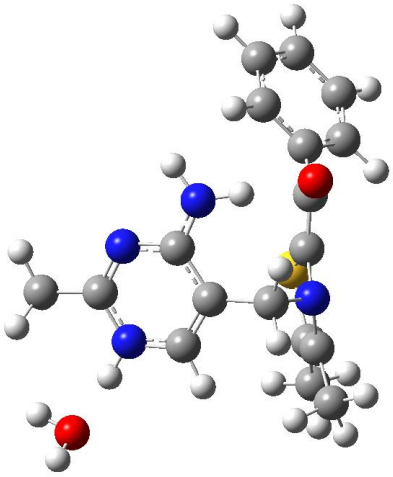
E	-1466.684672
E+ZPE	-1466.321250
H	-1466.294256
G	-1466.380182
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.725870	2.546952	0.628465
C	0.319230	2.776109	-0.633142
C	-1.012883	0.946190	0.526411
N	0.076923	1.471293	1.305192
S	-0.922181	1.598961	-1.154266
C	1.731642	3.362520	1.386491
H	1.328740	3.669294	2.357141
H	2.657102	2.810844	1.578161
H	1.998015	4.261602	0.831508
C	0.972745	0.500541	2.000049
H	1.717659	1.085894	2.537406
H	0.374178	-0.014828	2.746102
C	1.672968	-0.496710	1.105106
N	1.870457	-2.677072	0.087752
C	2.966223	-2.238629	-0.531745
C	3.683783	-3.183925	-1.450449
H	3.731958	-2.766665	-2.460240
H	4.712898	-3.333079	-1.111513
H	3.180436	-4.148818	-1.489645
C	2.828133	-0.169616	0.425914
H	3.266120	0.816760	0.545581
C	1.212087	-1.827307	0.910831
N	0.140033	-2.324307	1.574583
H	-0.189979	-3.224439	1.253030
C	0.711223	3.852625	-1.593794
H	1.523406	4.463778	-1.198271
H	1.049775	3.423465	-2.543772
H	-0.131011	4.514847	-1.824100
C	-1.963273	0.085347	0.997581
O	-1.910538	-0.446250	2.219991
C	-3.091089	-0.383830	0.125632
C	-3.398957	-1.754254	0.066713
C	-3.929718	0.505087	-0.566671
C	-4.480224	-2.220037	-0.679105
H	-2.782196	-2.460108	0.611614
C	-5.018198	0.042318	-1.305460
H	-3.737984	1.570099	-0.514295
C	-5.296191	-1.323852	-1.371992
H	-4.688076	-3.284245	-0.717191
H	-5.656904	0.752141	-1.820619
H	-6.141914	-1.684046	-1.947228
N	3.488027	-1.009898	-0.395972
H	-0.583903	-1.679159	1.925965
O	5.830753	-0.176804	-1.698982
H	5.938756	0.752384	-1.464531
H	4.997795	-0.461963	-1.240824

2'cN1HWAT'' neutral singlet, optimized with SMD mimicking the water solution at the level of *ω*B97XD/6-311++G(d,p).

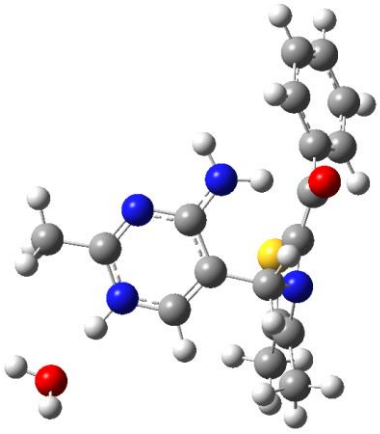
E	-1466.780119
E+ZPE	-1466.397855
H	-1466.370976
G	-1466.455075
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.794106	2.601472	0.486333
C	0.509644	2.603272	-0.822027
C	-0.979848	1.059663	0.503726
N	0.055052	1.678824	1.283032
S	-0.725182	1.394755	-1.239272
C	1.781734	3.488730	1.177365
H	1.352094	3.895344	2.096960
H	2.695782	2.951577	1.449675
H	2.069997	4.323008	0.538493
C	0.892118	0.763593	2.085761
H	1.668823	1.354258	2.569953
H	0.275846	0.342023	2.876273
C	1.530252	-0.331484	1.270749
N	1.570070	-2.602636	0.401315
C	2.641184	-2.293705	-0.287123
C	3.293545	-3.294554	-1.174974
H	3.169764	-2.991276	-2.218227
H	4.363953	-3.346939	-0.965284
H	2.841559	-4.273069	-1.030244
C	2.650546	-0.095697	0.539863
H	3.170344	0.853211	0.542678
C	0.985782	-1.650046	1.173152
N	-0.087639	-2.018189	1.865619
H	-0.450925	-2.942354	1.681160
C	1.045608	3.468198	-1.914549
H	1.861398	4.099367	-1.559962
H	1.431061	2.855022	-2.735747
H	0.266549	4.115639	-2.329692
C	-1.976511	0.298775	1.020173
O	-2.049373	-0.040206	2.298935
C	-3.020646	-0.282077	0.113269
C	-3.233868	-1.663901	0.086216
C	-3.846460	0.533363	-0.665390
C	-4.226777	-2.216829	-0.714754
H	-2.615344	-2.312594	0.697476
C	-4.845413	-0.016454	-1.462456
H	-3.708909	1.609072	-0.640568
C	-5.035928	-1.394466	-1.494147
H	-4.370803	-3.291933	-0.729585
H	-5.480726	0.633901	-2.054272
H	-5.813513	-1.824353	-2.116026
N	3.190732	-1.066158	-0.235357
H	-0.755207	-1.316545	2.223985
O	5.429480	-0.645316	-1.874548
H	6.254250	-0.664119	-1.379698
H	5.449025	-1.441769	-2.414668
H	4.035121	-0.869384	-0.798798

2'cN1HWAT'' neutral singlet, optimized with SMD mimicking the water solution at the level of B3LYP/6-311++G(d,p).

E	-1467.147695
E+ZPE	-1466.770962
H	-1466.743713
G	-1466.829098
$<S^2>$	0.0000
imaginary freq.	N/A



C	0.635027	2.573355	0.621709
C	0.211612	2.811285	-0.632389
C	-1.077990	0.939340	0.514146
N	0.005930	1.480654	1.290580
S	-1.023365	1.628476	-1.151839
C	1.631529	3.397067	1.382664
H	1.227352	3.688971	2.357312
H	2.567541	2.860546	1.566368
H	1.880000	4.305009	0.834081
C	0.914220	0.536139	1.993872
H	1.640299	1.134253	2.541465
H	0.324811	-0.004395	2.728105
C	1.654736	-0.438462	1.103622
N	1.922970	-2.643989	0.091167
C	3.018068	-2.221155	-0.496538
C	3.811542	-3.124265	-1.380266
H	3.843521	-2.721392	-2.396505
H	4.840937	-3.198399	-1.019818
H	3.363230	-4.114933	-1.400843
C	2.807513	-0.079949	0.469764
H	3.259201	0.897315	0.572426
C	1.216982	-1.788164	0.886642
N	0.131698	-2.279397	1.480870
H	-0.140901	-3.220142	1.227065
C	0.577542	3.905315	-1.583293
H	1.388905	4.519249	-1.190682
H	0.906325	3.493309	-2.544073
H	-0.275322	4.561194	-1.791012
C	-1.993746	0.037844	0.977737
O	-1.889935	-0.527595	2.184864
C	-3.125472	-0.444048	0.121330
C	-3.423500	-1.817522	0.076959
C	-3.976789	0.431802	-0.572905
C	-4.505514	-2.298348	-0.657985
H	-2.798763	-2.513628	0.624860
C	-5.065632	-0.046379	-1.300764
H	-3.796516	1.499047	-0.529457
C	-5.332809	-1.415293	-1.354109
H	-4.705277	-3.364425	-0.684615
H	-5.713648	0.653987	-1.817171
H	-6.179094	-1.787306	-1.920873
N	3.472142	-0.957171	-0.328210
H	-0.599767	-1.655455	1.883507
O	5.846254	-0.065013	-1.614105
H	6.553402	0.140096	-0.988331
H	6.199276	-0.783394	-2.155781
H	4.344689	-0.656328	-0.794686

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