Supplementary Material

Substitution by *tert*-butyl groups facilitates excited state proton transfer in hydroxylated triphenylimidazole frameworks more than it does for oxazole and thiazole analogs

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Table of Contents

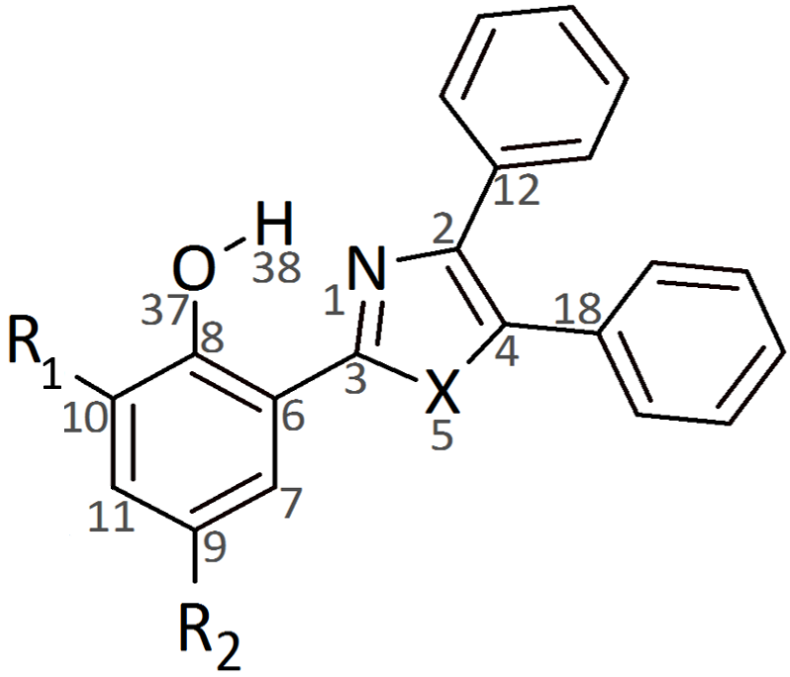


Figure SM1. Atomic numbering scheme adopted along the text.

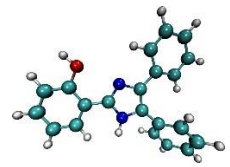
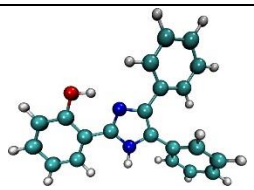
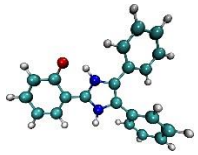
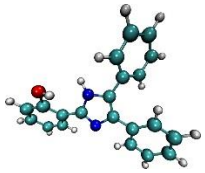
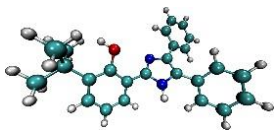
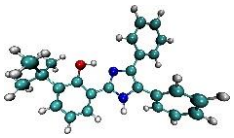
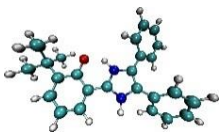
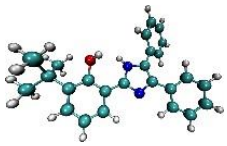
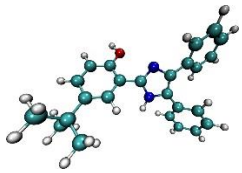
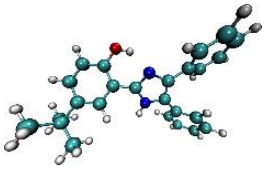
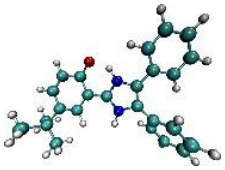
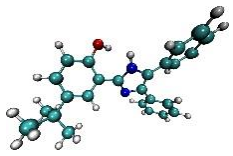
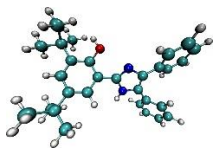
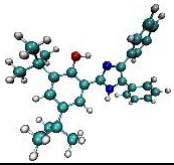
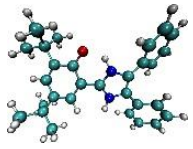
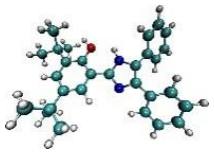
	Open	Closed (enol)	Keto	Rotamer
1a				
1b				
1c				
1d				

Figure SM2. Optimized structures obtained for the imidazole derivatives in open, closed (enol), keto and rotamer forms.

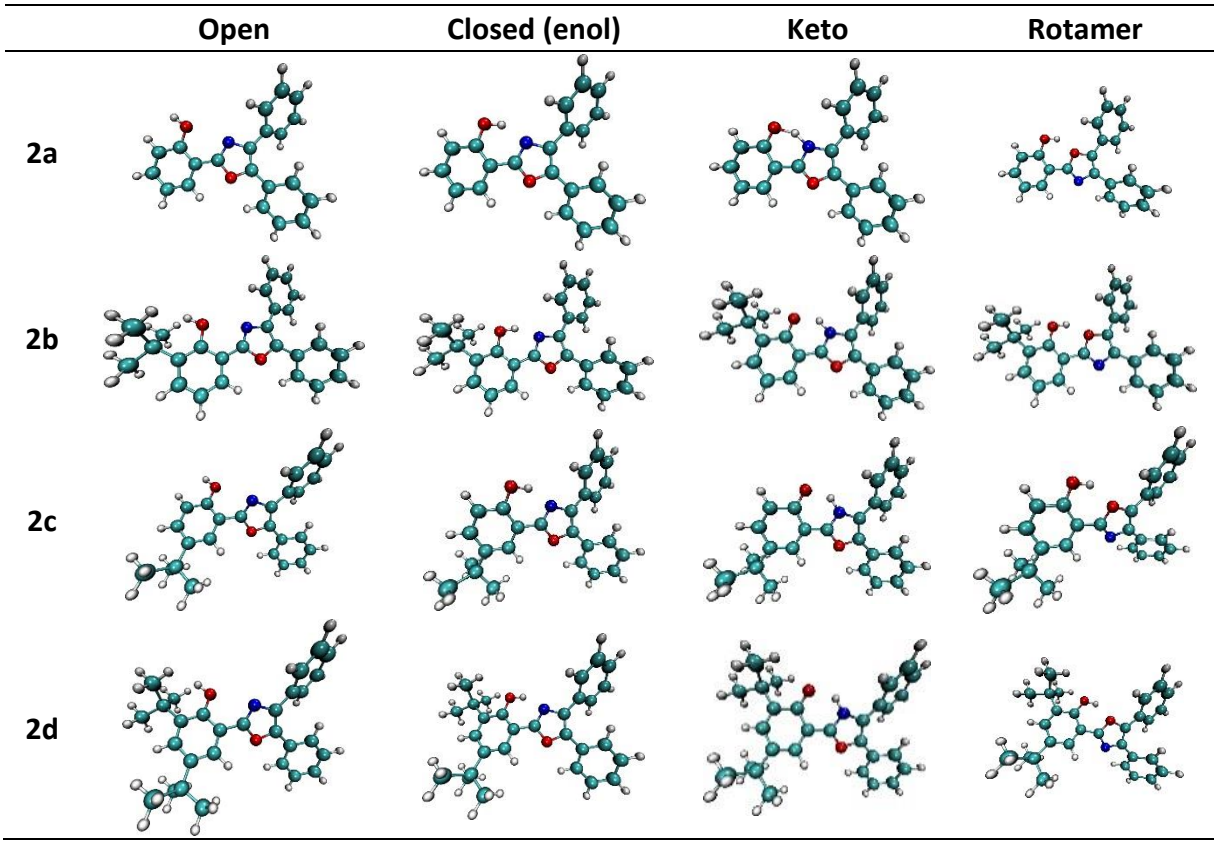


Figure SM3. Optimized structures obtained for the oxazole derivatives in open, closed (enol), keto and rotamer forms.

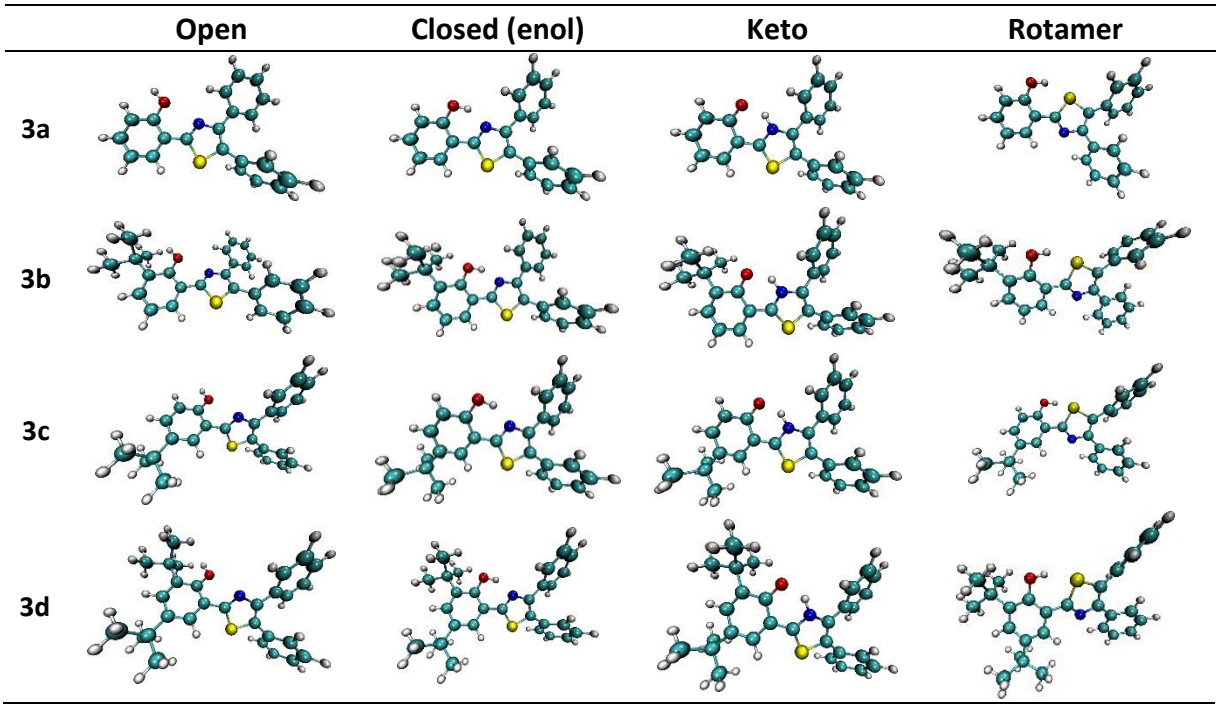


Figure SM4. Optimized structures obtained for the thiazole derivatives in open, closed (enol), keto and rotamer forms.

Table SM1. Bond distances and angles obtained for different forms of imidazole compounds in ground state

	Closed (enol)				Open				Rotamer			
	1a	**1b**	**1c**	**1d**	**1a**	**1b**	**1c**	**1d**	**1a**	**1b**	**1c**	**1d**
O – H	0.992	0.995	0.984	0.988	0.964	0.960	0.964	0.959	0.966	0.965	0.965	0.967
C_8 – O	1.341	1.346	1.346	1.351	1.355	1.363	1.359	1.362	1.376	1.392	1.382	1.369
N_1 – C_2	1.380	1.380	1.381	1.382	1.376	1.379	1.378	1.378	1.381	1.376	1.377	1.383
N_1 – C_3	1.328	1.328	1.328	1.329	1.319	1.318	1.320	1.322	1.317	1.321	1.322	1.320
N_5 – C_3	1.364	1.366	1.363	1.363	1.374	1.372	1.370	1.372	1.375	1.375	1.371	1.368
N_5 – C_4	1.388	1.387	1.385	1.384	1.382	1.382	1.381	1.380	1.388	1.387	1.383	1.383
C_2 – C_4	1.392	1.389	1.389	1.389	1.395	1.393	1.393	1.394	1.394	1.394	1.394	1.393
C_3 – C_6	1.456	1.458	1.458	1.459	1.464	1.471	1.469	1.473	1.466	1.468	1.466	1.485
C_6 – C_7	1.404	1.402	1.406	1.405	1.406	1.400	1.406	1.404	1.404	1.404	1.406	1.400
C_6 – C_8	1.420	1.421	1.411	1.412	1.416	1.412	1.406	1.409	1.408	1.409	1.404	1.401
C_7 – C_9	1.386	1.381	1.393	1.386	1.388	1.386	1.396	1.390	1.388	1.382	1.393	1.389
C_9 – C_{11}	1.399	1.398	1.407	1.405	1.393	1.391	1.402	1.400	1.396	1.394	1.406	1.405
C_8 – C_{10}	1.401	1.419	1.399	1.417	1.398	1.416	1.397	1.417	1.394	1.411	1.392	1.415
C_{10} – C_{11}	1.386	1.394	1.385	1.392	1.388	1.401	1.388	1.396	1.391	1.399	1.387	1.396
$\theta_{(C8\text{-}C10\text{-}C11)}$	120.7	116.9	120.6	117.0	121.3	116.9	121.1	117.1	120.1	116.3	120.2	116.3
$\theta_{(C7\text{-}C9\text{-}C11)}$	119.3	119.5	116.6	116.8	119.3	119.4	116.5	116.7	119.6	120.1	117.1	116.9
$\theta_{(C9\text{-}C11\text{-}C10)}$	120.5	122.9	122.2	124.6	119.5	122.6	121.5	124.2	120.3	122.4	121.7	124.6
D°$_{(C8\text{-}C6\text{-}C3\text{-}N1)}$	-0.4	-7.3	2.6	2.2	0.3	– 44.8	42.9	37.8	– 32.2	– 14.9	29.9	– 94.3
D°$_{(C12\text{-}C2\text{-}C4\text{-}C18)}$	3.4	7.8	-3.6	-0.8	2.9	7.0	3.5	5.3	6.8	1.3	3.6	2.4

Table SM2. Bond distances and angles obtained for different forms of oxazole compounds in ground state

	Closed (enol)				Open				Rotamer			
	2a	**2b**	**2c**	**2d**	**2a**	**2b**	**2c**	**2d**	**2a**	**2b**	**2c**	**2d**
O – H	0.986	0.987	0.986	0.985	0.964	0.960	0.964	0.960	0.967	0.967	0.967	0.967
C_8 – O	1.342	1.349	1.342	1.351	1.355	1.358	1.359	1.360	1.355	1.360	1.356	1.362
N_1 – C_2	1.389	1.392	1.390	1.393	1.387	1.389	1.390	1.390	1.391	1.391	1.390	1.391
N_1 – C_3	1.309	1.308	1.309	1.309	1.302	1.301	1.300	1.301	1.301	1.299	1.299	1.301
O_5 – C_3	1.351	1.351	1.351	1.351	1.365	1.366	1.361	1.364	1.367	1.370	1.369	1.371
O_5 – C_4	1.385	1.384	1.387	1.383	1.377	1.376	1.377	1.376	1.383	1.388	1.386	1.386
C_2 – C_4	1.377	1.379	1.378	1.377	1.379	1.380	1.381	1.381	1.375	1.376	1.374	1.373
C_3 – C_6	1.447	1.450	1.447	1.450	1.458	1.463	1.463	1.465	1.455	1.460	1.455	1.460
C_6 – C_7	1.406	1.404	1.408	1.406	1.406	1.403	1.407	1.405	1.408	1.406	1.409	1.408
C_6 – C_8	1.419	1.419	1.415	1.413	1.413	1.415	1.406	1.408	1.416	1.416	1.409	1.412
C_7 – C_9	1.385	1.380	1.389	1.384	1.387	1.382	1.394	1.388	1.384	1.379	1.389	1.385
C_9 – C_{11}	1.400	1.398	1.410	1.407	1.394	1.393	1.404	1.402	1.399	1.398	1.409	1.407
C_8 – C_{10}	1.401	1.419	1.399	1.417	1.398	1.419	1.397	1.417	1.399	1.418	1.399	1.416
C_{10} – C_{11}	1.386	1.395	1.382	1.392	1.389	1.397	1.387	1.394	1.395	1.394	1.384	1.392
$\theta_{(C8\text{-}C10\text{-}C11)}$	120.4	116.7	120.5	116.8	121.1	117.0	121.0	117.0	120.7	116.8	120.7	116.8
$\theta_{(C7\text{-}C9\text{-}C11)}$	119.4	119.7	117.0	116.9	119.4	119.7	116.6	116.9	119.5	119.7	116.8	117.0
$\theta_{(C9\text{-}C11\text{-}C10)}$	120.8	123.2	122.3	124.8	119.8	122.5	121.7	124.3	120.3	122.9	122.0	124.6
$D°_{(C8\text{-}C6\text{-}C3\text{-}N1)}$	0.3	– 2.2	– 3.8	15.6	– 2.0	– 8.3	35.5	29.3	0.9	– 3.5	15.9	20.2
$D°_{(C12\text{-}C2\text{-}C4\text{-}C18)}$	4.3	3.6	7.8	– 2.6	4.9	3.2	1.8	3.2	5.8	3.9	3.9	1.9

Table SM3. Bond distances and angles obtained for different forms of thiazole compounds in ground state

	Closed (enol)				Open				Rotamer			
	3a	**3b**	**3c**	**3d**	**3a**	**3b**	**3c**	**3d**	**3a**	**3b**	**3c**	**3d**
O – H	0.989	0.993	0.989	0.987	0.964	0.960	0.964	0.960	0.963	0.963	0.967	0.968
C_8 – O	1.342	1.347	1.343	1.350	1.358	1.361	1.359	1.361	1.361	1.366	1.361	1.371
N_1 – C_2	1.379	1.380	1.379	1.382	1.377	1.377	1.379	1.379	1.373	1.377	1.378	1.376
N_1 – C_3	1.315	1.314	1.314	1.314	1.299	1.300	1.300	1.302	1.307	1.306	1.303	1.304
S_5 – C_3	1.751	1.751	1.750	1.750	1.765	1.769	1.755	1.764	1.759	1.759	1.767	1.765
S_5 – C_4	1.747	1.747	1.750	1.746	1.744	1.738	1.744	1.741	1.745	1.744	1.744	1.748
C_2 – C_4	1.380	1.380	1.381	1.380	1.386	1.383	1.385	1.384	1.382	1.382	1.381	1.384
C_3 – C_6	1.455	1.457	1.454	1.458	1.466	1.471	1.474	1.475	1.469	1.474	1.468	1.472
C_6 – C_7	1.406	1.404	1.408	1.405	1.406	1.403	1.403	1.403	1.412	1.408	1.410	1.408
C_6 – C_8	1.421	1.422	1.416	1.415	1.416	1.417	1.405	1.410	1.413	1.415	1.417	1.409
C_7 – C_9	1.383	1.379	1.387	1.384	1.387	1.382	1.395	1.389	1.383	1.377	1.391	1.384
C_9 – C_{11}	1.400	1.399	1.410	1.407	1.394	1.392	1.403	1.401	1.398	1.396	1.407	1.406
C_8 – C_{10}	1.402	1.419	1.401	1.418	1.400	1.418	1.397	1.418	1.400	1.425	1.397	1.417
C_{10} – C_{11}	1.386	1.394	1.383	1.392	1.388	1.398	1.387	1.396	1.384	1.394	1.384	1.395
$\theta_{(C8\text{-}C10\text{-}C11)}$	120.6	116.9	120.7	117.0	121.3	117.2	120.8	117.0	120.9	116.9	120.6	116.8
$\theta_{(C7\text{-}C9\text{-}C11)}$	119.2	119.5	116.6	116.7	119.2	119.4	116.7	116.8	119.5	119.7	116.9	117.0
$\theta_{(C9\text{-}C11\text{-}C10)}$	120.6	122.9	122.2	124.6	119.2	119.4	116.7	116.8	119.9	122.5	121.9	124.4
$D°_{(C8\text{-}C6\text{-}C3\text{-}N1)}$	– 0.2	– 9.0	– 3.5	20.5	0.2	– 23.4	50.7	38.1	0.5	0.5	33.3	26.0
$D°_{(C12\text{-}C2\text{-}C4\text{-}C18)}$	6.7	9.9	7.4	0.3	4.4	6.5	3.0	5.6	8.9	– 0.3	10.2	8.7

Table SM4. Bond distances and angles obtained for tautomers of imidazole compounds in ground (S_0) and excited (S_1) states

	S_0 enol (≡closed form)				S_1 enol				S_0 keto				S_1 keto			
	1a	**1b**	**1c**	**1d**	**1a**	**1b**	**1c**	**1d**	**1a**	**1b**	**1c**	**1d**	**1a**	**1b**	**1c**	**1d**
O – H	0.992	0.995	0.984	0.988	1.009	0.995	1.032	1.011	1.606	1.595	1.585	1.671	1.964	1.971	1.926	1.941
H···N	1.711	1.684	1.841	1.783	1.653	1.639	1.572	1.578	1.030	1.039	1.040	1.029	1.030	1.039	1.040	1.029
C_8 – O	1.341	1.346	1.346	1.351	1.324	1.328	1.315	1.318	1.274	1.281	1.275	1.277	1.257	1.257	1.257	1.258
N_1 – C_2	1.380	1.380	1.381	1.382	1.367	1.367	1.372	1.373	1.387	1.387	1.388	1.389	1.417	1.417	1.417	1.417
N_1 – C_3	1.328	1.328	1.328	1.329	1.331	1.331	1.329	1.327	1.344	1.345	1.344	1.347	1.317	1.319	1.318	1.319
N_5 – C_3	1.364	1.366	1.363	1.363	1.382	1.383	1.374	1.375	1.359	1.360	1.359	1.358	1.328	1.329	1.329	1.330
N_5 – C_4	1.388	1.387	1.385	1.384	1.379	1.379	1.386	1.387	1.399	1.399	1.400	1.399	1.419	1.419	1.420	1.420
C_2 – C_4	1.392	1.389	1.389	1.389	1.447	1.446	1.442	1.441	1.382	1.381	1.382	1.382	1.422	1.422	1.423	1.422
C_3 – C_6	1.456	1.458	1.458	1.459	1.431	1.433	1.437	1.440	1.421	1.423	1.421	1.419	1.484	1.485	1.483	1.484
C_6 – C_7	1.404	1.402	1.406	1.405	1.411	1.408	1.403	1.399	1.413	1.412	1.415	1.414	1.370	1.368	1.373	1.371
C_6 – C_8	1.420	1.421	1.411	1.412	1.440	1.443	1.444	1.446	1.457	1.455	1.452	1.450	1.461	1.462	1.458	1.458
C_7 – C_9	1.386	1.381	1.393	1.386	1.382	1.378	1.393	1.390	1.375	1.371	1.380	1.373	1.419	1.416	1.424	1.420
C_9 – C_{11}	1.399	1.398	1.407	1.405	1.409	1.408	1.423	1.421	1.416	1.414	1.426	1.425	1.392	1.389	1.406	1.403
C_8 – C_{10}	1.401	1.419	1.399	1.417	1.406	1.423	1.410	1.428	1.436	1.454	1.434	1.456	1.443	1.468	1.441	1.466
C_{10} – C_{11}	1.386	1.394	1.385	1.392	1.382	1.390	1.376	1.384	1.373	1.381	1.371	1.378	1.384	1.394	1.377	1.387
$\theta_{(O-H\cdots N)}$	148.8	150.6	146.6	149.0	149.7	151.1	150.9	152.0	139.9	139.2	141.0	136.3	125.7	123.7	127.0	125.3
$\theta_{(C8\text{-}C10\text{-}C11)}$	120.7	116.9	120.6	117.0	120.2	116.5	120.2	116.5	121.9	118.4	121.9	118.5	121.8	118.0	122.0	118.2
$\theta_{(C7\text{-}C9\text{-}C11)}$	119.3	119.5	116.6	116.8	120.1	120.4	117.7	117.9	119.0	119.2	116.4	116.5	120.2	120.6	117.3	117.6
$\theta_{(C9\text{-}C11\text{-}C10)}$	120.5	122.9	122.2	124.6	120.7	123.0	122.1	124.4	121.7	123.9	123.2	125.4	119.7	122.2	121.6	124.0
D°$_{(C8\text{-}C6\text{-}C3\text{-}N1)}$	-0.4	-7.3	2.6	2.2	– 3.1	– 3.3	– 3.0	– 3.4	0	3.0	5.8	6.0	1.0	13.8	4.8	7.9
D°$_{(C12\text{-}C2\text{-}C4\text{-}C18)}$	3.4	7.8	-3.6	-0.8	14.7	14.3	14.3	14.2	3.8	4.3	0	3.6	16.1	17.0	16.6	16.6

Table SM5. Bond distances and angles obtained for tautomers of oxazole compounds in ground (S_0) and excited (S_1) states

	S_0 enol (≡closed form)				S_1 enol				S_0 keto				S_1 keto			
	2a	**2b**	**2c**	**2d**	**2a**	**2b**	**2c**	**2d**	**2a**	**2b**	**2c**	**2d**	**2a**	**2b**	**2c**	**2d**
O – H	0.986	0.987	0.986	0.985	1.005	1.006	1.039	1.001	1.280	1.629	1.611	1.712	1.646	1.946	1.928	1.940
H···N	1.765	1.755	1.764	1.806	1.692	1.658	1.545	1.629	1.162	1.041	1.041	1.029	1.162	1.041	1.041	1.029
C_8 – O	1.342	1.349	1.342	1.351	1.324	1.322	1.305	1.314	1.298	1.276	1.272	1.272	1.265	1.258	1.258	1.259
N_1 – C_2	1.389	1.392	1.390	1.393	1.373	1.378	1.395	1.391	1.391	1.394	1.393	1.396	1.427	1.433	1.434	1.434
N_1 – C_3	1.309	1.308	1.309	1.309	1.316	1.310	1.299	1.300	1.323	1.335	1.335	1.338	1.294	1.300	1.299	1.301
O_5 – C_3	1.351	1.351	1.351	1.351	1.360	1.355	1.338	1.344	1.340	1.343	1.342	1.344	1.304	1.302	1.301	1.302
O_5 – C_4	1.385	1.384	1.387	1.383	1.393	1.399	1.416	1.411	1.397	1.398	1.400	1.398	1.436	1.434	1.435	1.435
C_2 – C_4	1.377	1.379	1.378	1.377	1.429	1.427	1.423	1.423	1.374	1.369	1.371	1.368	1.416	1.412	1.412	1.411
C_3 – C_6	1.447	1.450	1.447	1.450	1.430	1.439	1.456	1.454	1.421	1.407	1.404	1.402	1.473	1.474	1.473	1.473
C_6 – C_7	1.406	1.404	1.408	1.406	1.405	1.393	1.379	1.379	1.409	1.416	1.420	1.419	1.368	1.369	1.373	1.373
C_6 – C_8	1.419	1.419	1.415	1.413	1.441	1.447	1.444	1.443	1.444	1.459	1.456	1.455	1.457	1.457	1.453	1.453
C_7 – C_9	1.385	1.380	1.389	1.384	1.387	1.389	1.417	1.411	1.378	1.367	1.375	1.369	1.422	1.416	1.425	1.421
C_9 – C_{11}	1.400	1.398	1.410	1.407	1.410	1.407	1.419	1.417	1.411	1.418	1.430	1.429	1.393	1.390	1.407	1.404
C_8 – C_{10}	1.401	1.419	1.399	1.417	1.406	1.430	1.418	1.437	1.421	1.457	1.436	1.459	1.441	1.468	1.442	1.466
C_{10} – C_{11}	1.386	1.395	1.382	1.392	1.383	1.389	1.374	1.385	1.379	1.379	1.369	1.376	1.385	1.396	1.378	1.388
$\theta_{(O-H\cdots N)}$	147.0	149.1	146.9	148.1	148.9	151.0	151.4	151.7	150.8	136.6	138.4	133.5	135.3	124.1	126.3	124.7
$\theta_{(C8\text{-}C10\text{-}C11)}$	120.4	116.7	120.5	116.8	119.9	116.1	120.0	116.3	120.9	118.0	121.7	118.1	121.3	117.8	121.8	118.0
$\theta_{(C7\text{-}C9\text{-}C11)}$	119.4	119.7	117.0	116.9	120.4	121.0	118.1	118.3	119.3	119.5	116.7	116.8	120.4	120.6	117.3	117.6
$\theta_{(C9\text{-}C11\text{-}C10)}$	120.8	123.2	122.3	124.8	120.7	122.7	121.6	123.9	121.8	124.2	123.5	125.8	120.1	122.5	122.0	124.3
D°$_{(C8\text{-}C6\text{-}C3\text{-}N1)}$	0.3	– 2.2	– 3.8	15.6	– 0.4	– 0.4	-0.4	– 0.1	0	1.8	0.7	8.2	2.0	4.0	2.8	2.8
D°$_{(C12\text{-}C2\text{-}C4\text{-}C18)}$	4.3	3.6	7.8	– 2.6	15.9	15.9	17.4	16.8	5.8	4.0	4.9	– 1.4	19.4	18.7	18.4	19.1

Table SM6. Bond distances and angles obtained for tautomers of thiazole compounds in ground (S_0) and excited (S_1) states

	S_0 enol (≡closed form)				S_1 enol				S_0 keto				S_1 keto			
	3a	**3b**	**3c**	**3d**	**3a**	**3b**	**3c**	**3d**	**3a**	**3b**	**3c**	**3d**	**3a**	**3b**	**3c**	**3d**
O – H	0.989	0.993	0.989	0.987	1.003	1.046	1.042	1.007	1.610	1.608	1.582	1.629	1.807	1.772	1.789	1.789
H···N	1.742	1.686	1.736	1.778	1.678	1.492	1.541	1.610	1.030	1.036	1.039	1.029	1.030	1.036	1.039	1.029
C_8 – O	1.342	1.347	1.343	1.350	1.330	1.310	1.311	1.319	1.270	1.274	1.271	1.273	1.262	1.264	1.261	1.263
N_1 – C_2	1.379	1.380	1.379	1.382	1.354	1.365	1.365	1.362	1.384	1.385	1.383	1.386	1.418	1.414	1.418	1.417
N_1 – C_3	1.315	1.314	1.314	1.314	1.328	1.317	1.317	1.318	1.343	1.343	1.343	1.344	1.306	1.306	1.307	1.307
S_5 – C_3	1.751	1.751	1.750	1.750	1.776	1.746	1.748	1.754	1.742	1.743	1.742	1.744	1.706	1.709	1.707	1.709
S_5 – C_4	1.747	1.747	1.750	1.746	1.767	1.780	1.776	1.776	1.769	1.770	1.771	1.770	1.775	1.777	1.775	1.776
C_2 – C_4	1.380	1.380	1.381	1.380	1.435	1.426	1.428	1.428	1.370	1.370	1.371	1.370	1.417	1.417	1.416	1.416
C_3 – C_6	1.455	1.457	1.454	1.458	1.435	1.467	1.462	1.463	1.411	1.412	1.410	1.410	1.482	1.483	1.480	1.480
C_6 – C_7	1.406	1.404	1.408	1.405	1.410	1.376	1.385	1.383	1.419	1.418	1.420	1.418	1.374	1.372	1.377	1.375
C_6 – C_8	1.421	1.422	1.416	1.415	1.442	1.450	1.444	1.445	1.463	1.461	1.457	1.456	1.459	1.458	1.456	1.455
C_7 – C_9	1.383	1.379	1.387	1.384	1.386	1.413	1.416	1.411	1.370	1.366	1.373	1.368	1.417	1.414	1.421	1.417
C_9 – C_{11}	1.400	1.399	1.410	1.407	1.405	1.392	1.414	1.411	1.420	1.419	1.431	1.430	1.392	1.388	1.406	1.403
C_8 – C_{10}	1.402	1.419	1.401	1.418	1.403	1.441	1.415	1.433	1.440	1.458	1.438	1.458	1.441	1.464	1.440	1.463
C_{10} – C_{11}	1.386	1.394	1.383	1.392	1.386	1.396	1.379	1.389	1.370	1.378	1.368	1.376	1.386	1.397	1.378	1.389
$\theta_{(O-H\cdots N)}$	147.9	150.2	147.9	148.4	149.7	153.9	152.1	152.4	141.5	106.3	142.3	140.0	134.2	134.0	124.8	133.7
$\theta_{(C8\text{-}C10\text{-}C11)}$	120.6	116.9	120.7	117.0	120.3	116.6	120.3	116.6	121.8	118.2	121.9	118.4	121.8	118.1	122.0	118.3
$\theta_{(C7\text{-}C9\text{-}C11)}$	119.2	119.5	116.6	116.7	120.1	121.2	117.8	118.1	119.1	119.4	116.5	116.8	120.0	120.3	117.1	117.4
$\theta_{(C9\text{-}C11\text{-}C10)}$	120.6	122.9	122.2	124.6	120.5	121.7	121.3	123.6	121.8	123.9	123.3	125.4	120.0	122.3	121.7	124.1
D°$_{(C8\text{-}C6\text{-}C3\text{-}N1)}$	– 0.2	– 9.0	– 3.5	20.5	1.8	1.5	0.5	1.2	– 0.6	4.5	0.6	6.2	1.1	3.7	5.2	3.7
D°$_{(C12\text{-}C2\text{-}C4\text{-}C18)}$	6.7	9.9	7.4	0.3	20.0	17.9	18.2	17.7	4.8	6.2	3.9	5.7	20.7	19.6	19.4	20.2

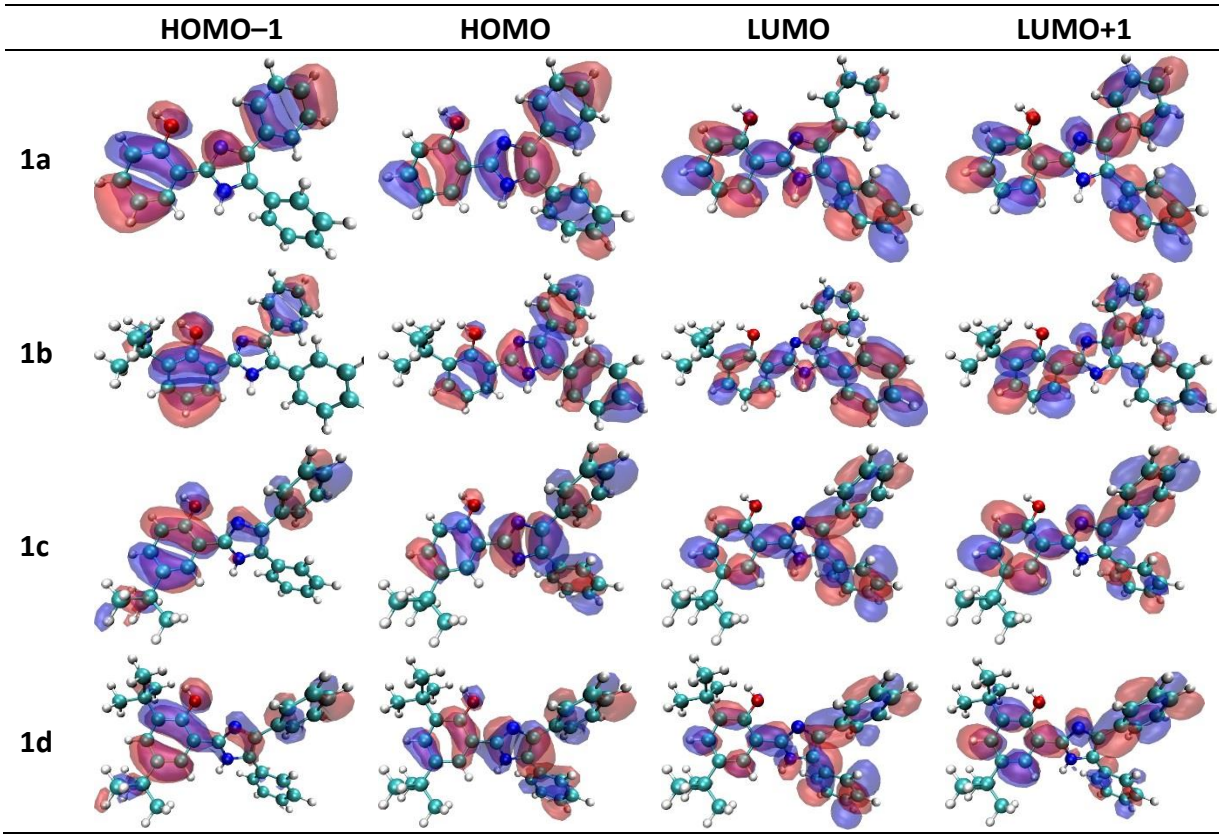


Figure SM5. Molecular orbitals obtained for the open form of the imidazole derivatives.

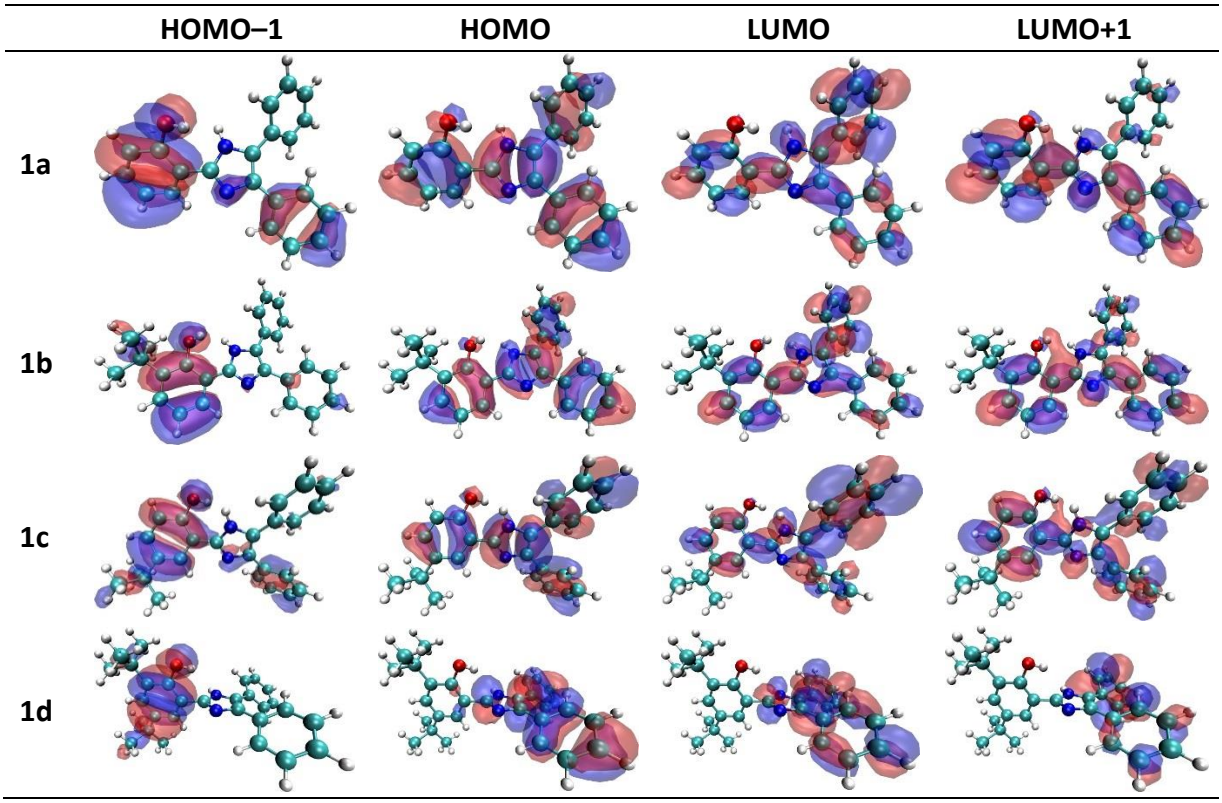


Figure SM6. Molecular orbitals obtained for the rotamer form of the imidazole derivatives.

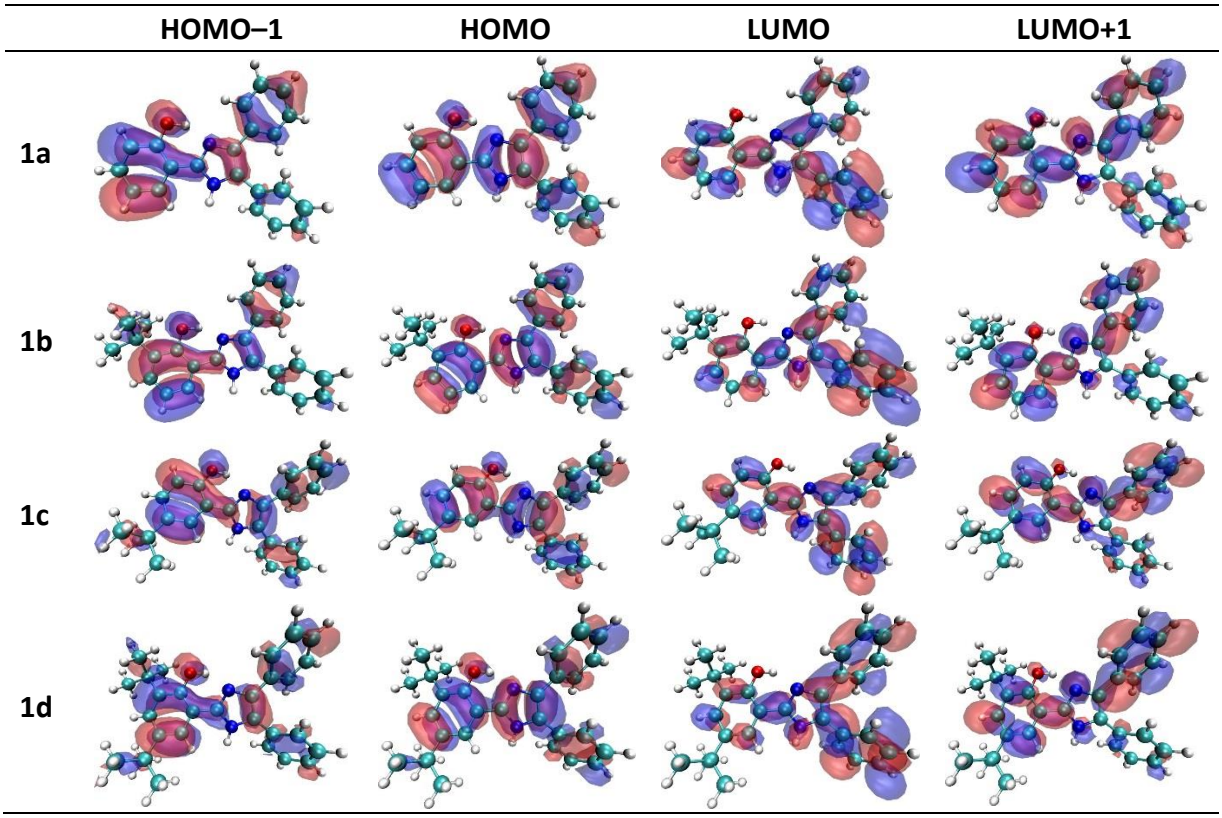


Figure SM7. Molecular orbitals obtained for the closed (enol) form of the imidazole derivatives.

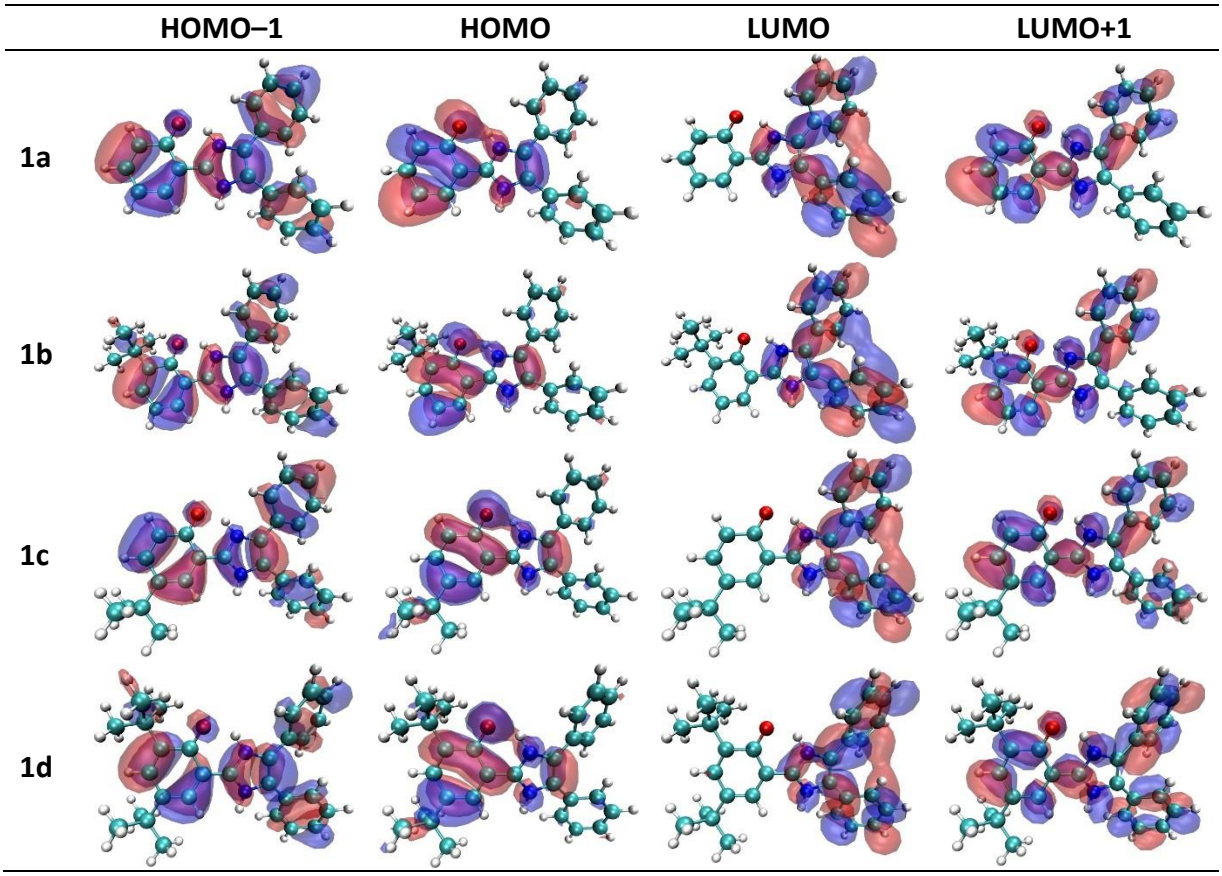


Figure SM8. Molecular orbitals obtained for the keto form of the imidazole derivatives.

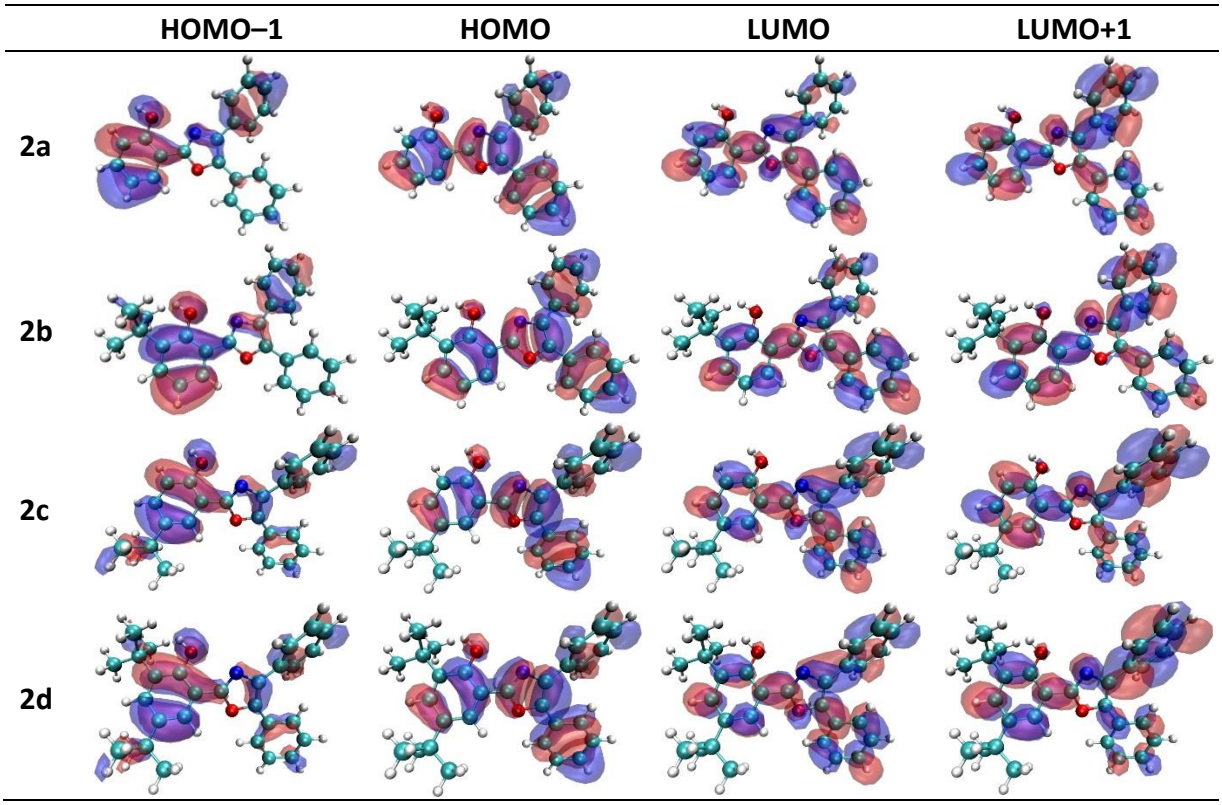


Figure SM9. Molecular orbitals obtained for the open form of the oxazole derivatives.

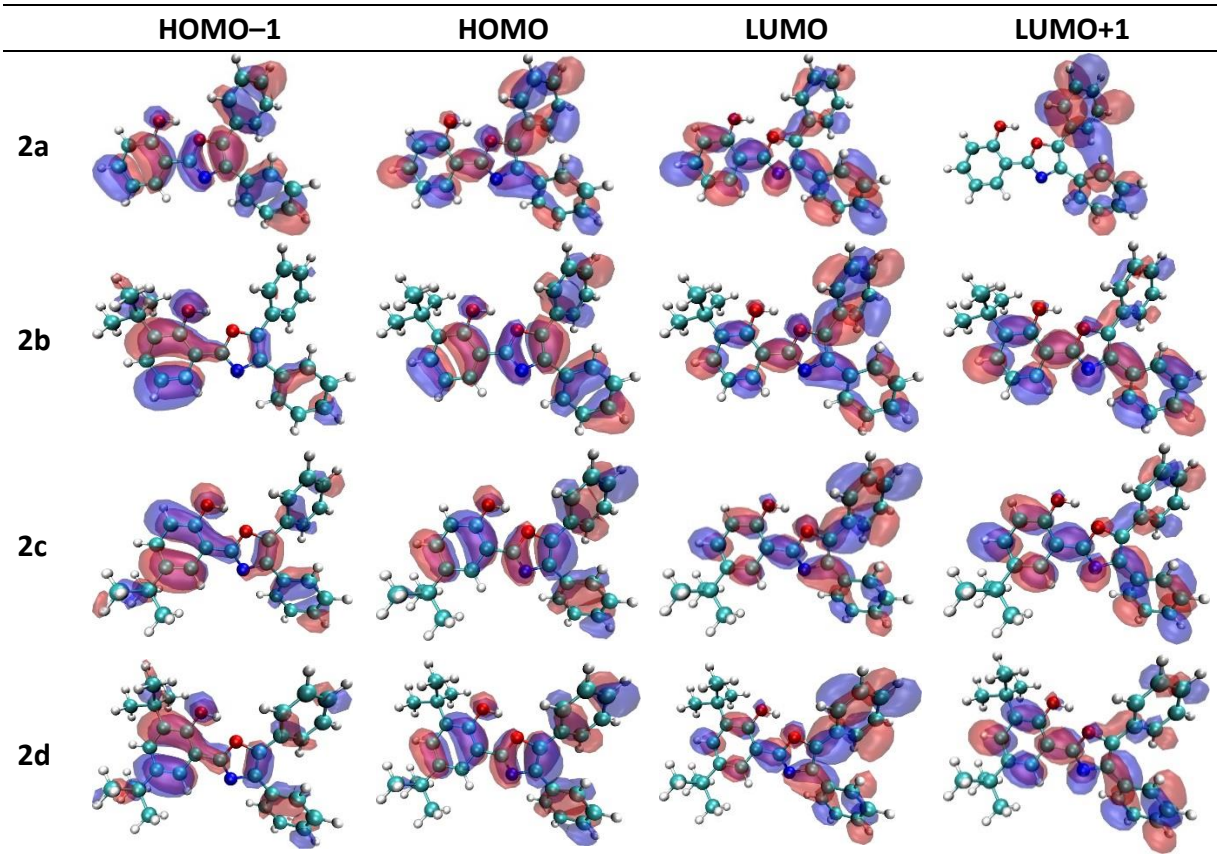


Figure SM10. Molecular orbitals obtained for the rotamer form of the oxazole derivatives.

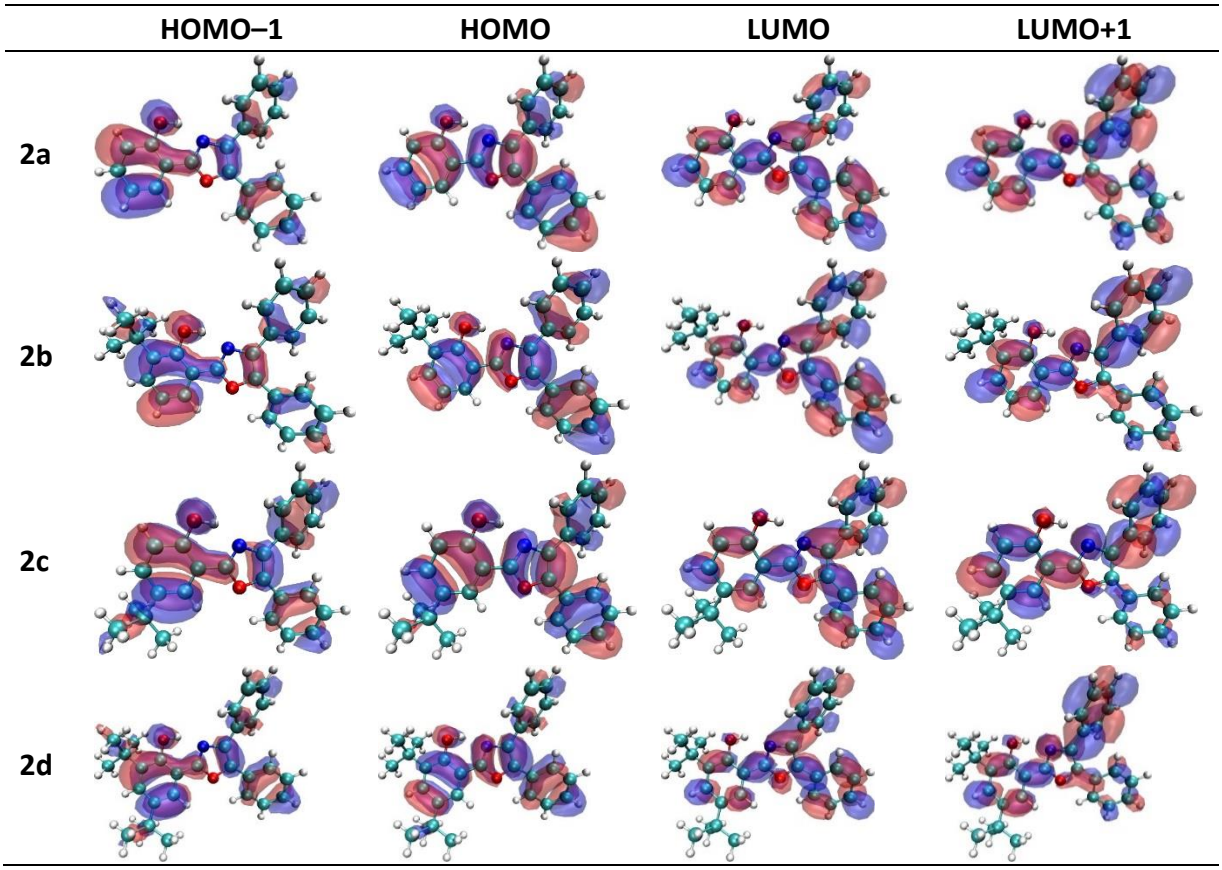


Figure SM11. Molecular orbitals obtained for the closed (enol) form of the oxazole derivatives.

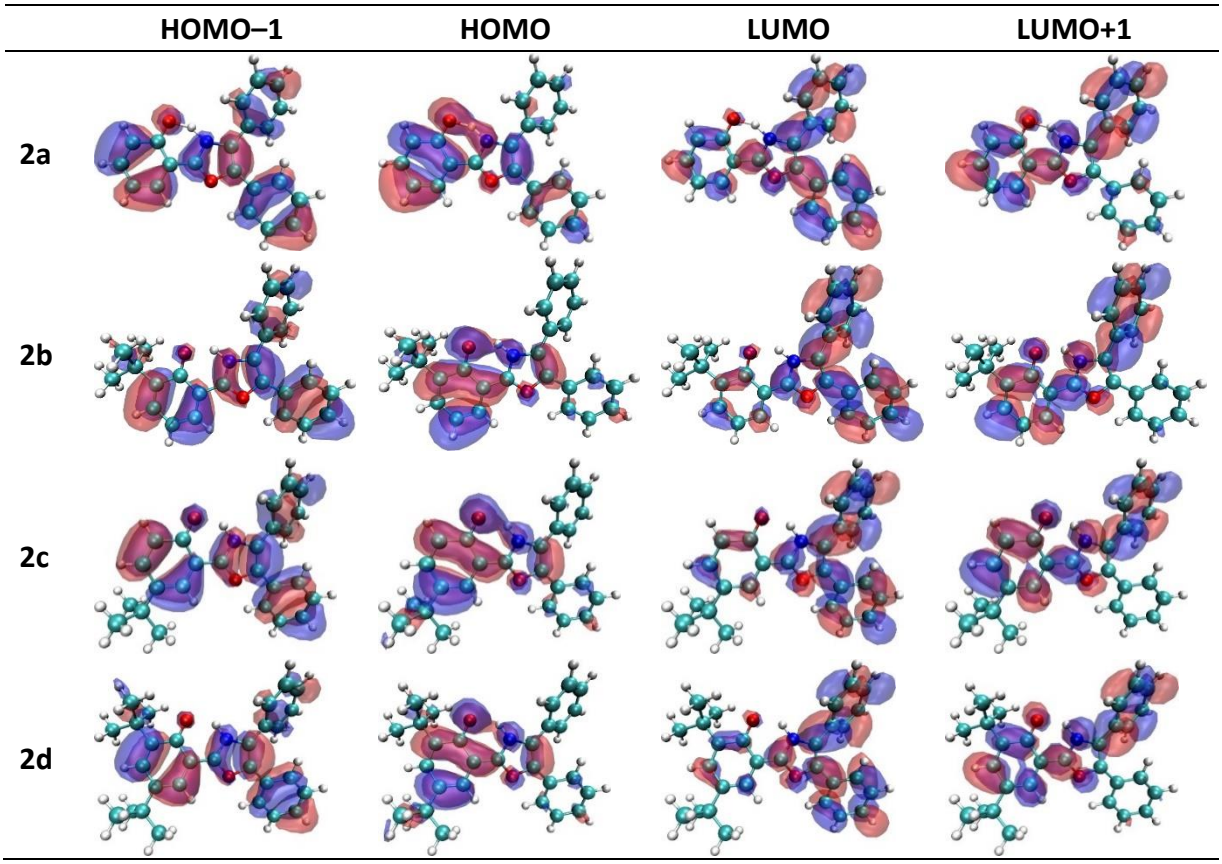


Figure SM12. Molecular orbitals obtained for the keto form of the oxazole derivatives.

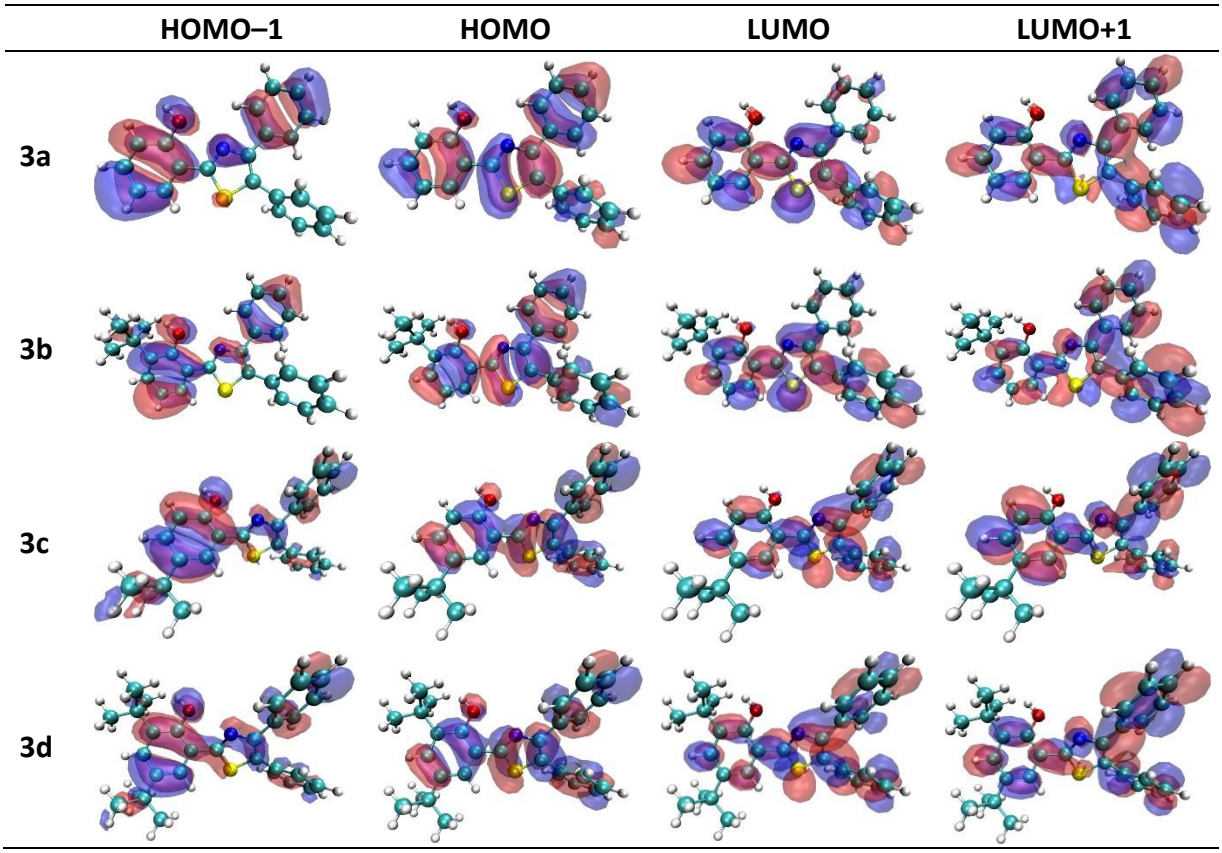


Figure SM13. Molecular orbitals obtained for the open form of the thiazole derivatives.

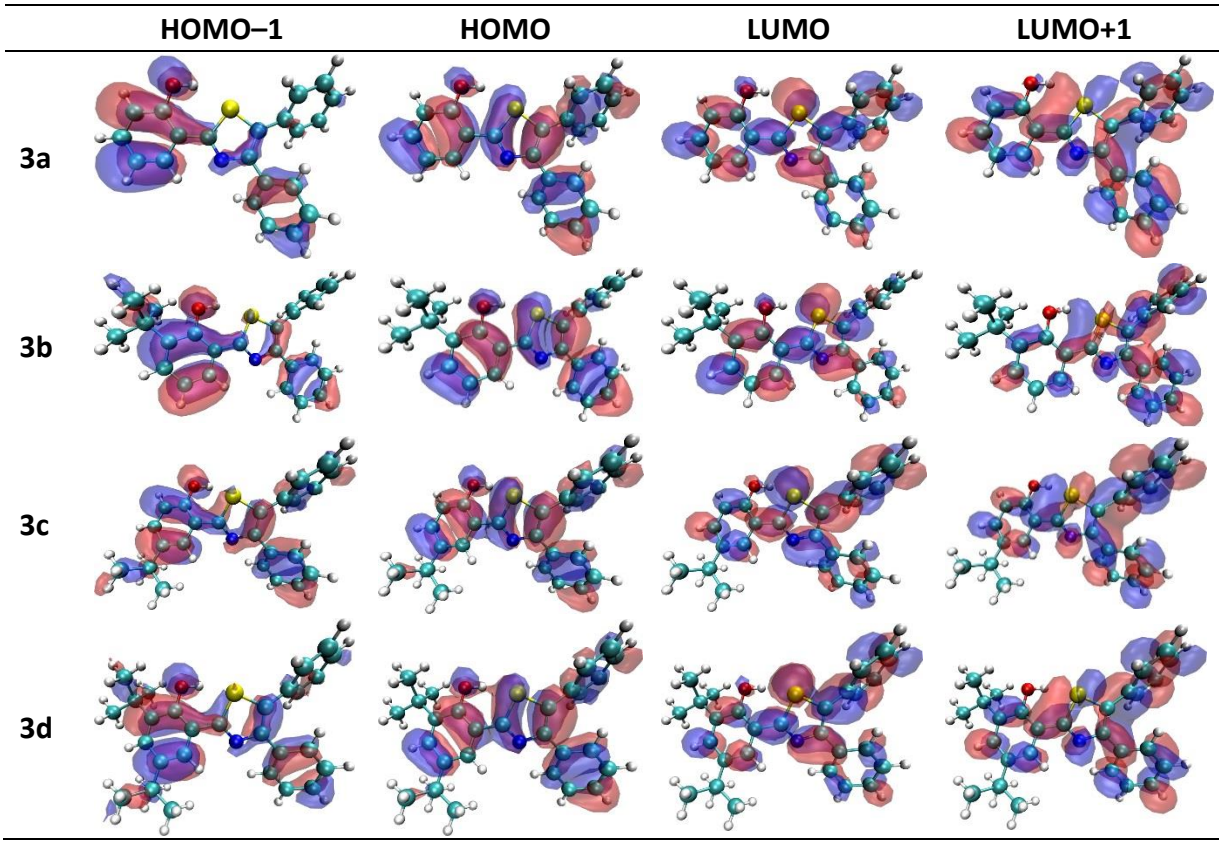


Figure SM14. Molecular orbitals obtained for the rotamer form of the thiazole derivatives.

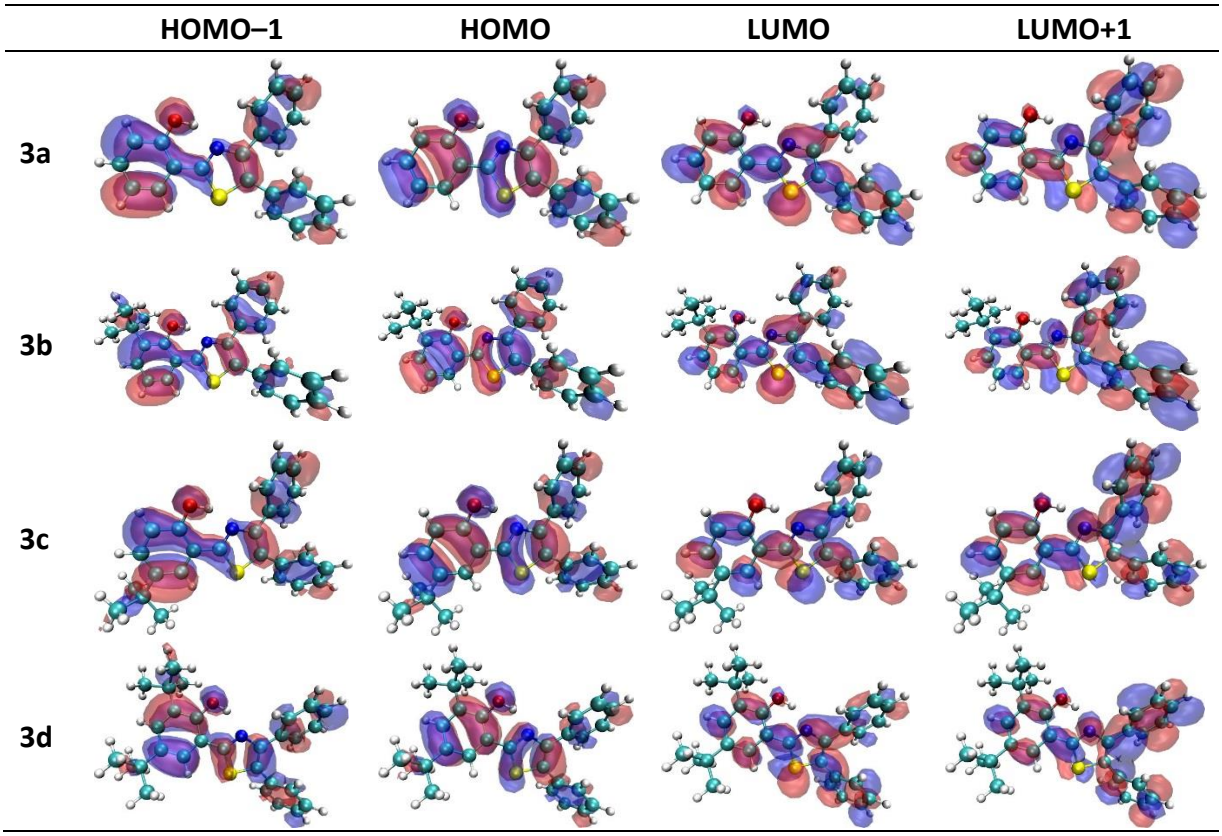


Figure SM15. Molecular orbitals obtained for the enol (closed) form of the thiazole derivatives.

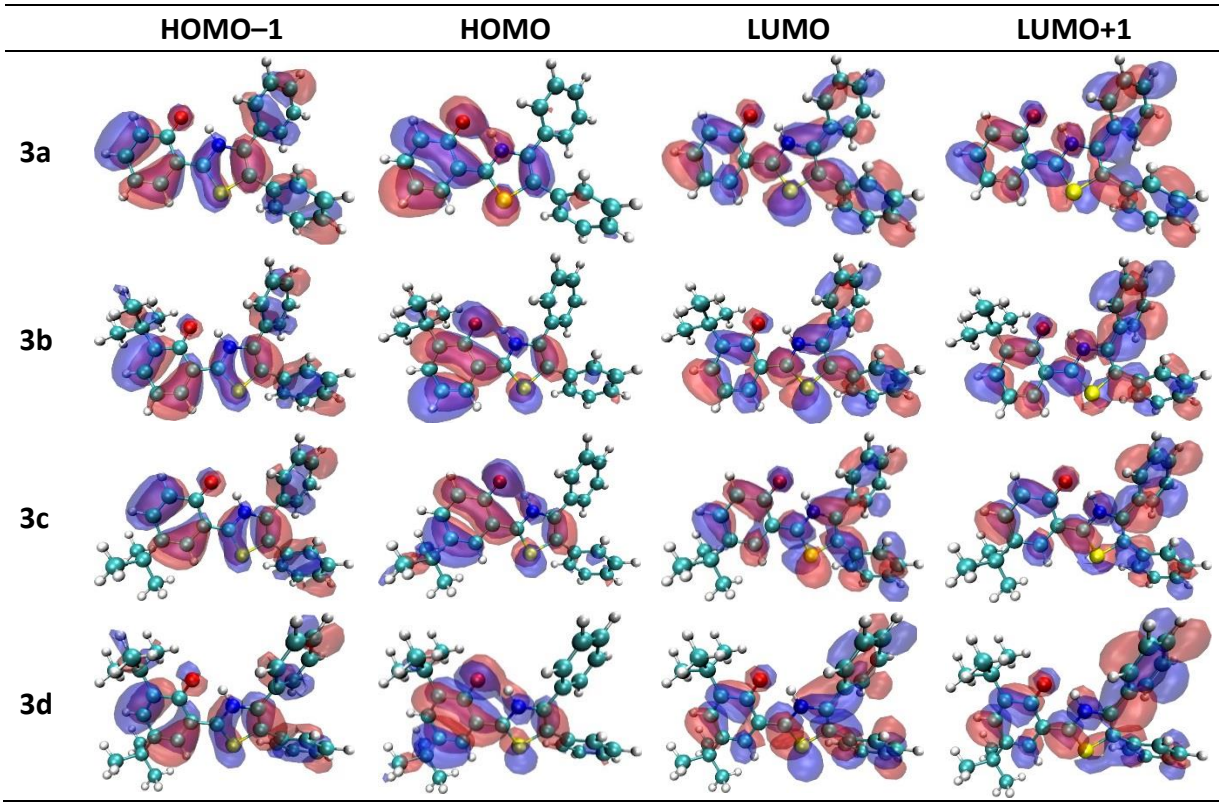


Figure SM16. Molecular orbitals obtained for the keto form of the thiazole derivatives.