

## 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

Fabricio de Carvalho, Mauricio D. Coutinho-Neto, Fernando H. Bartoloni,\* and Paula Homem-de-Mello\*

*Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André/SP, Brazil*

Email: [fernando.bartoloni@ufabc.edu.br](mailto:fernando.bartoloni@ufabc.edu.br); [paula.mello@ufabc.edu.br](mailto:paula.mello@ufabc.edu.br)

### Table of Contents

Atomic numbering scheme adopted along the text .....	S2
Optimized structures obtained for the imidazole derivatives in open, closed (enol), keto and rotamer forms .....	S2
Optimized structures obtained for the oxazole derivatives in open, closed (enol), keto and rotamer forms .....	S3
Optimized structures obtained for the thiazole derivatives in open, closed (enol), keto and rotamer forms .....	S3
Bond distances and angles obtained for different forms of imidazole compounds in ground state .....	S4
Bond distances and angles obtained for different forms of oxazole compounds in ground state .....	S5
Bond distances and angles obtained for different forms of thiazole compounds in ground state .....	S6
Bond distances and angles obtained for tautomers of imidazole compounds in ground ( $S_0$ ) and excited ( $S_1$ ) states ..	S7
Bond distances and angles obtained for tautomers of oxazole compounds in ground ( $S_0$ ) and excited ( $S_1$ ) states .....	S8
Bond distances and angles obtained for tautomers of thiazole compounds in ground ( $S_0$ ) and excited ( $S_1$ ) states ....	S9
Molecular orbitals obtained for the open form of the imidazole derivatives .....	S10
Molecular orbitals obtained for the rotamer form of the imidazole derivatives .....	S10
Molecular orbitals obtained for the closed (enol) form of the imidazole derivatives .....	S11
Molecular orbitals obtained for the keto form of the imidazole derivatives .....	S11
Molecular orbitals obtained for the open form of the oxazole derivatives .....	S12
Molecular orbitals obtained for the rotamer form of the oxazole derivatives .....	S12
Molecular orbitals obtained for the closed (enol) form of the oxazole derivatives .....	S13
Molecular orbitals obtained for the keto form of the oxazole derivatives .....	S13
Molecular orbitals obtained for the open form of the thiazole derivatives .....	S14
Molecular orbitals obtained for the rotamer form of the thiazole derivatives .....	S14
Molecular orbitals obtained for the enol (closed) form of the thiazole derivatives .....	S15
Molecular orbitals obtained for the keto form of the thiazole derivatives .....	S15

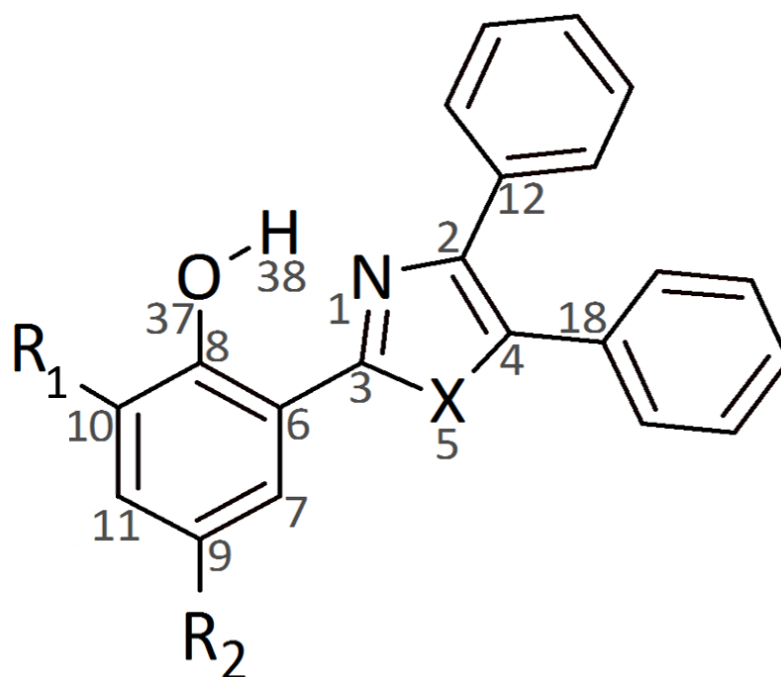


Figure SM1. Atomic numbering scheme adopted along the text.

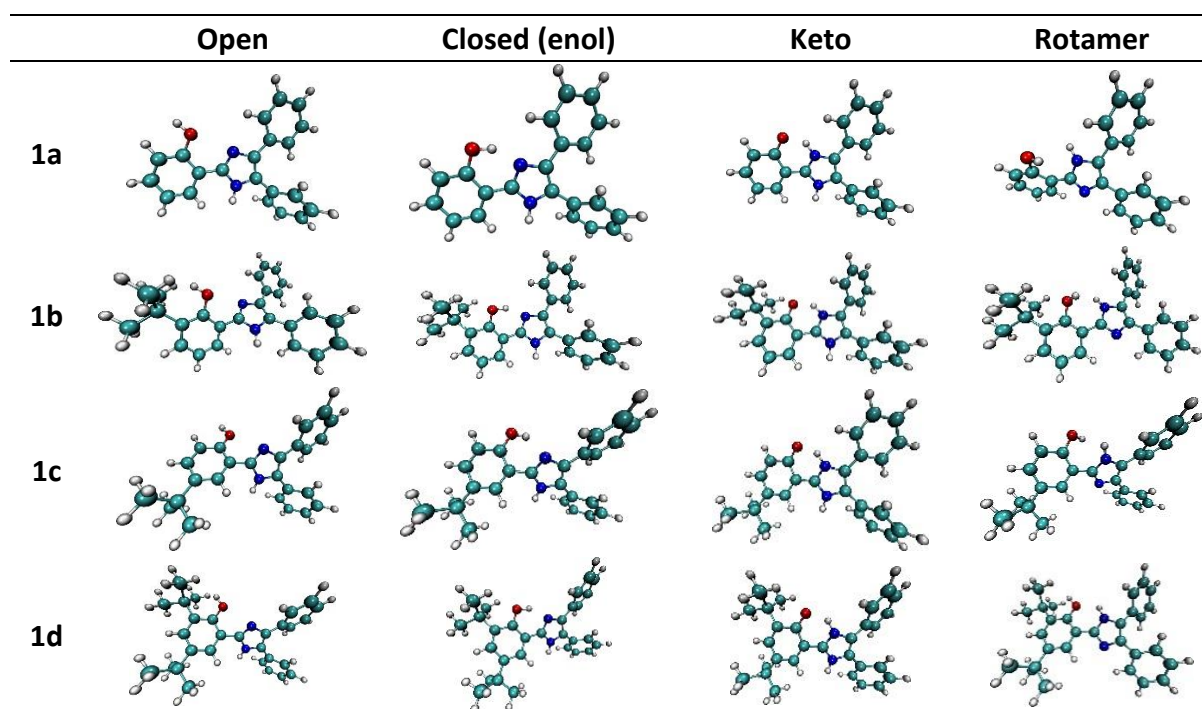
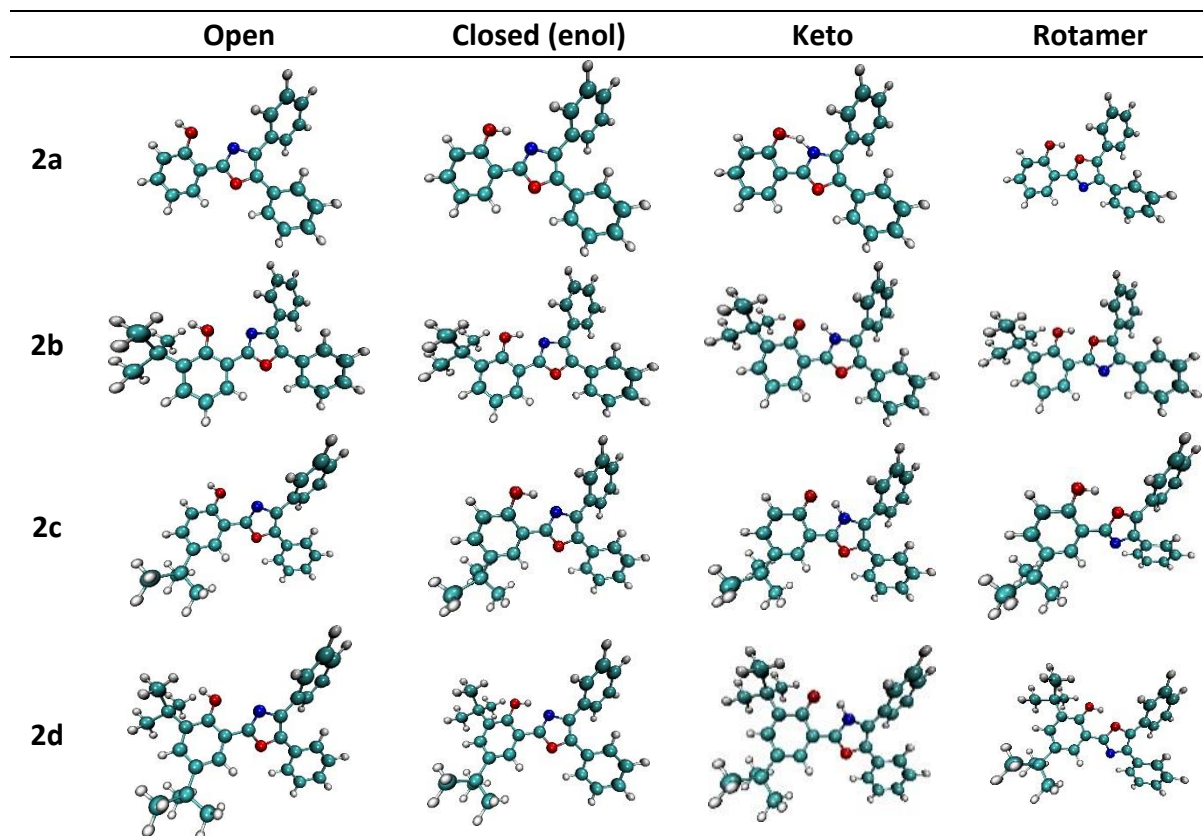
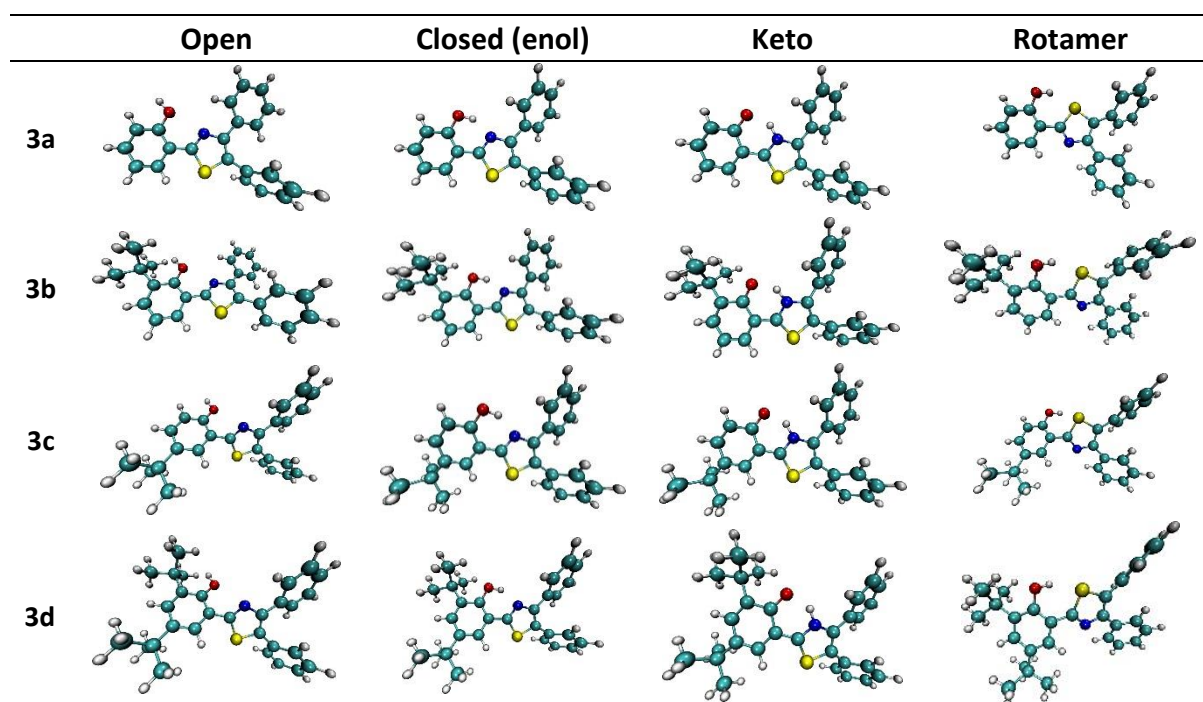


Figure SM2. Optimized structures obtained for the imidazole derivatives in open, closed (enol), keto and rotamer forms.



**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
<b>O – H</b>	0.992	0.995	0.984	0.988	0.964	0.960	0.964	0.959	0.966	0.965	0.965	0.967
<b>C<sub>8</sub> – O</b>	1.341	1.346	1.346	1.351	1.355	1.363	1.359	1.362	1.376	1.392	1.382	1.369
<b>N<sub>1</sub> – C<sub>2</sub></b>	1.380	1.380	1.381	1.382	1.376	1.379	1.378	1.378	1.381	1.376	1.377	1.383
<b>N<sub>1</sub> – C<sub>3</sub></b>	1.328	1.328	1.328	1.329	1.319	1.318	1.320	1.322	1.317	1.321	1.322	1.320
<b>N<sub>5</sub> – C<sub>3</sub></b>	1.364	1.366	1.363	1.363	1.374	1.372	1.370	1.372	1.375	1.375	1.371	1.368
<b>N<sub>5</sub> – C<sub>4</sub></b>	1.388	1.387	1.385	1.384	1.382	1.382	1.381	1.380	1.388	1.387	1.383	1.383
<b>C<sub>2</sub> – C<sub>4</sub></b>	1.392	1.389	1.389	1.389	1.395	1.393	1.393	1.394	1.394	1.394	1.394	1.393
<b>C<sub>3</sub> – C<sub>6</sub></b>	1.456	1.458	1.458	1.459	1.464	1.471	1.469	1.473	1.466	1.468	1.466	1.485
<b>C<sub>6</sub> – C<sub>7</sub></b>	1.404	1.402	1.406	1.405	1.406	1.400	1.406	1.404	1.404	1.404	1.406	1.400
<b>C<sub>6</sub> – C<sub>8</sub></b>	1.420	1.421	1.411	1.412	1.416	1.412	1.406	1.409	1.408	1.409	1.404	1.401
<b>C<sub>7</sub> – C<sub>9</sub></b>	1.386	1.381	1.393	1.386	1.388	1.386	1.396	1.390	1.388	1.382	1.393	1.389
<b>C<sub>9</sub> – C<sub>11</sub></b>	1.399	1.398	1.407	1.405	1.393	1.391	1.402	1.400	1.396	1.394	1.406	1.405
<b>C<sub>8</sub> – C<sub>10</sub></b>	1.401	1.419	1.399	1.417	1.398	1.416	1.397	1.417	1.394	1.411	1.392	1.415
<b>C<sub>10</sub> – C<sub>11</sub></b>	1.386	1.394	1.385	1.392	1.388	1.401	1.388	1.396	1.391	1.399	1.387	1.396
<b><math>\theta</math> (C8-C10-C11)</b>	120.7	116.9	120.6	117.0	121.3	116.9	121.1	117.1	120.1	116.3	120.2	116.3
<b><math>\theta</math> (C7-C9-C11)</b>	119.3	119.5	116.6	116.8	119.3	119.4	116.5	116.7	119.6	120.1	117.1	116.9
<b><math>\theta</math> (C9-C11-C10)</b>	120.5	122.9	122.2	124.6	119.5	122.6	121.5	124.2	120.3	122.4	121.7	124.6
<b>D° (C8-C6-C3-N1)</b>	-0.4	-7.3	2.6	2.2	0.3	-44.8	42.9	37.8	-32.2	-14.9	29.9	-94.3
<b>D° (C12-C2-C4-C18)</b>	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
<b>O – H</b>	0.986	0.987	0.986	0.985	0.964	0.960	0.964	0.960	0.967	0.967	0.967	0.967
<b>C<sub>8</sub> – O</b>	1.342	1.349	1.342	1.351	1.355	1.358	1.359	1.360	1.355	1.360	1.356	1.362
<b>N<sub>1</sub> – C<sub>2</sub></b>	1.389	1.392	1.390	1.393	1.387	1.389	1.390	1.390	1.391	1.391	1.390	1.391
<b>N<sub>1</sub> – C<sub>3</sub></b>	1.309	1.308	1.309	1.309	1.302	1.301	1.300	1.301	1.301	1.299	1.299	1.301
<b>O<sub>5</sub> – C<sub>3</sub></b>	1.351	1.351	1.351	1.351	1.365	1.366	1.361	1.364	1.367	1.370	1.369	1.371
<b>O<sub>5</sub> – C<sub>4</sub></b>	1.385	1.384	1.387	1.383	1.377	1.376	1.377	1.376	1.383	1.388	1.386	1.386
<b>C<sub>2</sub> – C<sub>4</sub></b>	1.377	1.379	1.378	1.377	1.379	1.380	1.381	1.381	1.375	1.376	1.374	1.373
<b>C<sub>3</sub> – C<sub>6</sub></b>	1.447	1.450	1.447	1.450	1.458	1.463	1.463	1.465	1.455	1.460	1.455	1.460
<b>C<sub>6</sub> – C<sub>7</sub></b>	1.406	1.404	1.408	1.406	1.406	1.403	1.407	1.405	1.408	1.406	1.409	1.408
<b>C<sub>6</sub> – C<sub>8</sub></b>	1.419	1.419	1.415	1.413	1.413	1.415	1.406	1.408	1.416	1.416	1.409	1.412
<b>C<sub>7</sub> – C<sub>9</sub></b>	1.385	1.380	1.389	1.384	1.387	1.382	1.394	1.388	1.384	1.379	1.389	1.385
<b>C<sub>9</sub> – C<sub>11</sub></b>	1.400	1.398	1.410	1.407	1.394	1.393	1.404	1.402	1.399	1.398	1.409	1.407
<b>C<sub>8</sub> – C<sub>10</sub></b>	1.401	1.419	1.399	1.417	1.398	1.419	1.397	1.417	1.399	1.418	1.399	1.416
<b>C<sub>10</sub> – C<sub>11</sub></b>	1.386	1.395	1.382	1.392	1.389	1.397	1.387	1.394	1.395	1.394	1.384	1.392
<b><math>\theta</math> (C8-C10-C11)</b>	120.4	116.7	120.5	116.8	121.1	117.0	121.0	117.0	120.7	116.8	120.7	116.8
<b><math>\theta</math> (C7-C9-C11)</b>	119.4	119.7	117.0	116.9	119.4	119.7	116.6	116.9	119.5	119.7	116.8	117.0
<b><math>\theta</math> (C9-C11-C10)</b>	120.8	123.2	122.3	124.8	119.8	122.5	121.7	124.3	120.3	122.9	122.0	124.6
<b>D° (C8-C6-C3-N1)</b>	0.3	-2.2	-3.8	15.6	-2.0	-8.3	35.5	29.3	0.9	-3.5	15.9	20.2
<b>D° (C12-C2-C4-C18)</b>	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
<b>O – H</b>	0.989	0.993	0.989	0.987	0.964	0.960	0.964	0.960	0.963	0.963	0.967	0.968
<b>C<sub>8</sub> – O</b>	1.342	1.347	1.343	1.350	1.358	1.361	1.359	1.361	1.361	1.366	1.361	1.371
<b>N<sub>1</sub> – C<sub>2</sub></b>	1.379	1.380	1.379	1.382	1.377	1.377	1.379	1.379	1.373	1.377	1.378	1.376
<b>N<sub>1</sub> – C<sub>3</sub></b>	1.315	1.314	1.314	1.314	1.299	1.300	1.300	1.302	1.307	1.306	1.303	1.304
<b>S<sub>5</sub> – C<sub>3</sub></b>	1.751	1.751	1.750	1.750	1.765	1.769	1.755	1.764	1.759	1.759	1.767	1.765
<b>S<sub>5</sub> – C<sub>4</sub></b>	1.747	1.747	1.750	1.746	1.744	1.738	1.744	1.741	1.745	1.744	1.744	1.748
<b>C<sub>2</sub> – C<sub>4</sub></b>	1.380	1.380	1.381	1.380	1.386	1.383	1.385	1.384	1.382	1.382	1.381	1.384
<b>C<sub>3</sub> – C<sub>6</sub></b>	1.455	1.457	1.454	1.458	1.466	1.471	1.474	1.475	1.469	1.474	1.468	1.472
<b>C<sub>6</sub> – C<sub>7</sub></b>	1.406	1.404	1.408	1.405	1.406	1.403	1.403	1.403	1.412	1.408	1.410	1.408
<b>C<sub>6</sub> – C<sub>8</sub></b>	1.421	1.422	1.416	1.415	1.416	1.417	1.405	1.410	1.413	1.415	1.417	1.409
<b>C<sub>7</sub> – C<sub>9</sub></b>	1.383	1.379	1.387	1.384	1.387	1.382	1.395	1.389	1.383	1.377	1.391	1.384
<b>C<sub>9</sub> – C<sub>11</sub></b>	1.400	1.399	1.410	1.407	1.394	1.392	1.403	1.401	1.398	1.396	1.407	1.406
<b>C<sub>8</sub> – C<sub>10</sub></b>	1.402	1.419	1.401	1.418	1.400	1.418	1.397	1.418	1.400	1.425	1.397	1.417
<b>C<sub>10</sub> – C<sub>11</sub></b>	1.386	1.394	1.383	1.392	1.388	1.398	1.387	1.396	1.384	1.394	1.384	1.395
<b><math>\theta</math> (C8-C10-C11)</b>	120.6	116.9	120.7	117.0	121.3	117.2	120.8	117.0	120.9	116.9	120.6	116.8
<b><math>\theta</math> (C7-C9-C11)</b>	119.2	119.5	116.6	116.7	119.2	119.4	116.7	116.8	119.5	119.7	116.9	117.0
<b><math>\theta</math> (C9-C11-C10)</b>	120.6	122.9	122.2	124.6	119.2	119.4	116.7	116.8	119.9	122.5	121.9	124.4
<b>D° (C8-C6-C3-N1)</b>	-0.2	-9.0	-3.5	20.5	0.2	-23.4	50.7	38.1	0.5	0.5	33.3	26.0
<b>D° (C12-C2-C4-C18)</b>	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 ( $\equiv$ 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
<b>O – H</b>	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
<b>H<math>\cdots</math>N</b>	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
<b>C<sub>8</sub> – O</b>	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
<b>N<sub>1</sub> – C<sub>2</sub></b>	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
<b>N<sub>1</sub> – C<sub>3</sub></b>	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
<b>N<sub>5</sub> – C<sub>3</sub></b>	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
<b>N<sub>5</sub> – C<sub>4</sub></b>	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
<b>C<sub>2</sub> – C<sub>4</sub></b>	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
<b>C<sub>3</sub> – C<sub>6</sub></b>	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
<b>C<sub>6</sub> – C<sub>7</sub></b>	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
<b>C<sub>6</sub> – C<sub>8</sub></b>	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
<b>C<sub>7</sub> – C<sub>9</sub></b>	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
<b>C<sub>9</sub> – C<sub>11</sub></b>	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
<b>C<sub>8</sub> – C<sub>10</sub></b>	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
<b>C<sub>10</sub> – C<sub>11</sub></b>	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
<b><math>\theta</math> (O – H <math>\cdots</math> N)</b>	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
<b><math>\theta</math> (C<sub>8</sub>-C<sub>10</sub>-C<sub>11</sub>)</b>	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
<b><math>\theta</math> (C<sub>7</sub>-C<sub>9</sub>-C<sub>11</sub>)</b>	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
<b><math>\theta</math> (C<sub>9</sub>-C<sub>11</sub>-C<sub>10</sub>)</b>	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
<b>D<sup>o</sup> (C<sub>8</sub>-C<sub>6</sub>-C<sub>3</sub>-N<sub>1</sub>)</b>	-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
<b>D<sup>o</sup> (C<sub>12</sub>-C<sub>2</sub>-C<sub>4</sub>-C<sub>18</sub>)</b>	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 ( $\equiv$ 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 $\cdots$ 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 <sub>8</sub> – 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 <sub>1</sub> – C <sub>2</sub>	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 <sub>1</sub> – C <sub>3</sub>	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 <sub>5</sub> – C <sub>3</sub>	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 <sub>5</sub> – C <sub>4</sub>	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 <sub>2</sub> – C <sub>4</sub>	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 <sub>3</sub> – C <sub>6</sub>	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 <sub>6</sub> – C <sub>7</sub>	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 <sub>6</sub> – C <sub>8</sub>	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 <sub>7</sub> – C <sub>9</sub>	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 <sub>9</sub> – C <sub>11</sub>	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 <sub>8</sub> – C <sub>10</sub>	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 <sub>10</sub> – C <sub>11</sub>	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
$\theta$ (C <sub>8</sub> -C <sub>10</sub> -C <sub>11</sub> )	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
$\theta$ (C <sub>7</sub> -C <sub>9</sub> -C <sub>11</sub> )	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
$\theta$ (C <sub>9</sub> -C <sub>11</sub> -C <sub>10</sub> )	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 $^\circ$ (C <sub>8</sub> -C <sub>6</sub> -C <sub>3</sub> -N <sub>1</sub> )	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 $^\circ$ (C <sub>12</sub> -C <sub>2</sub> -C <sub>4</sub> -C <sub>18</sub> )	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 ( $\equiv$ 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 $\cdots$ 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 <sub>8</sub> – 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 <sub>1</sub> – C <sub>2</sub>	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 <sub>1</sub> – C <sub>3</sub>	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 <sub>5</sub> – C <sub>3</sub>	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 <sub>5</sub> – C <sub>4</sub>	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 <sub>2</sub> – C <sub>4</sub>	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 <sub>3</sub> – C <sub>6</sub>	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 <sub>6</sub> – C <sub>7</sub>	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 <sub>6</sub> – C <sub>8</sub>	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 <sub>7</sub> – C <sub>9</sub>	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 <sub>9</sub> – C <sub>11</sub>	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 <sub>8</sub> – C <sub>10</sub>	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 <sub>10</sub> – C <sub>11</sub>	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
$\theta$ (C <sub>8</sub> -C <sub>10</sub> -C <sub>11</sub> )	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
$\theta$ (C <sub>7</sub> -C <sub>9</sub> -C <sub>11</sub> )	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
$\theta$ (C <sub>9</sub> -C <sub>11</sub> -C <sub>10</sub> )	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 $^\circ$ (C <sub>8</sub> -C <sub>6</sub> -C <sub>3</sub> -N <sub>1</sub> )	-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 $^\circ$ (C <sub>12</sub> -C <sub>2</sub> -C <sub>4</sub> -C <sub>18</sub> )	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

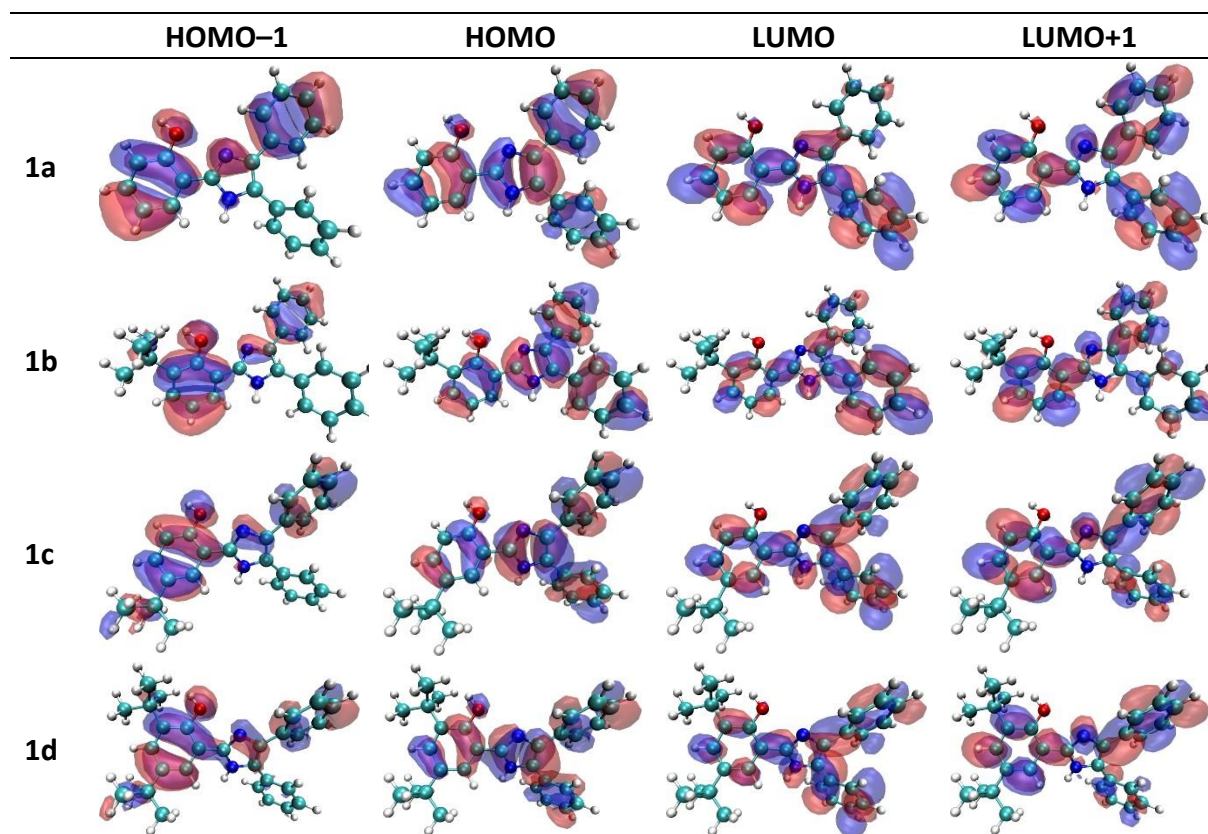


Figure SM5. Molecular orbitals obtained for the open form of the imidazole derivatives.

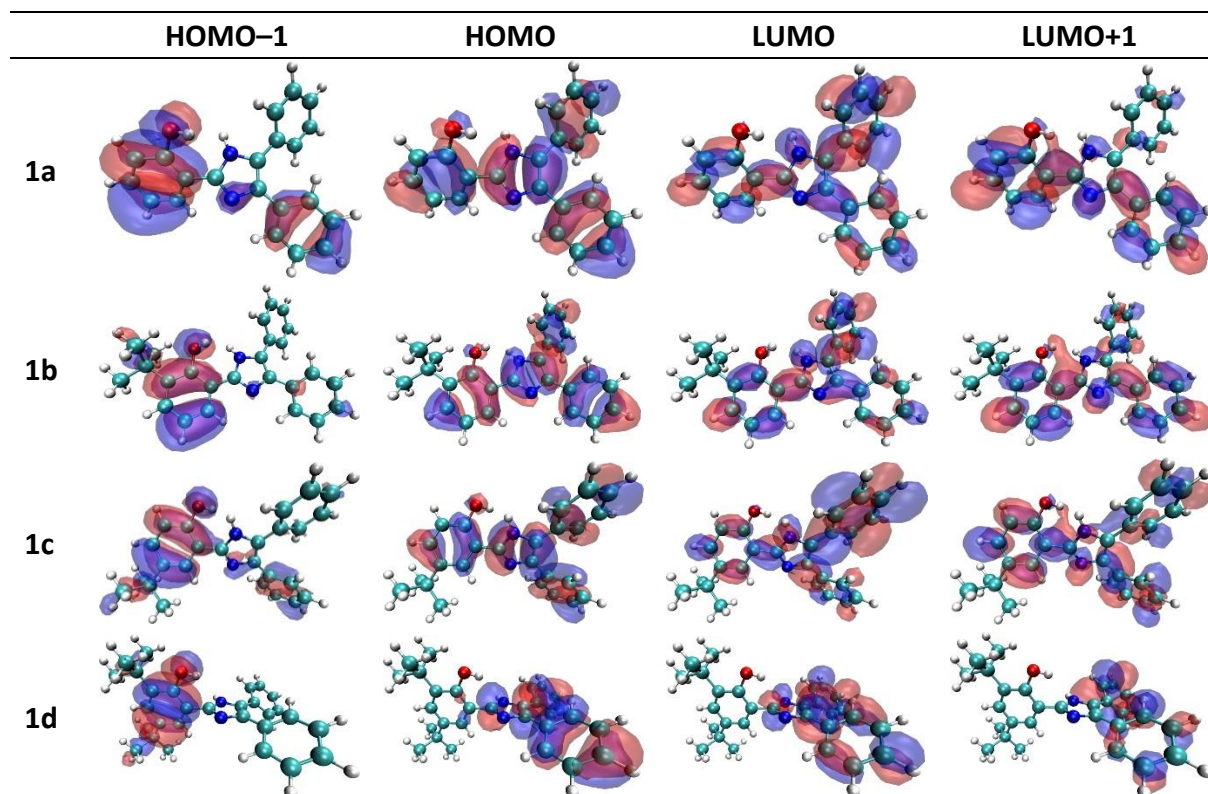


Figure SM6. Molecular orbitals obtained for the rotamer form of the imidazole derivatives.

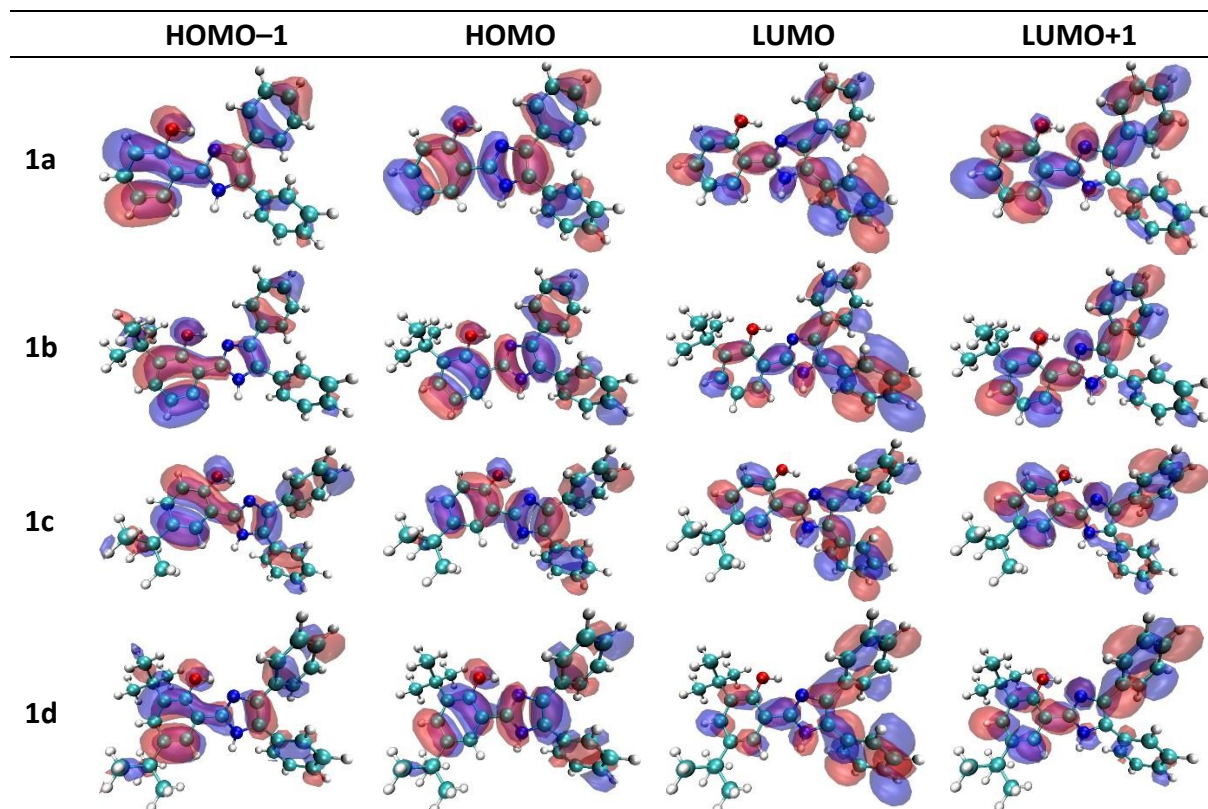


Figure SM7. Molecular orbitals obtained for the closed (enol) form of the imidazole derivatives.

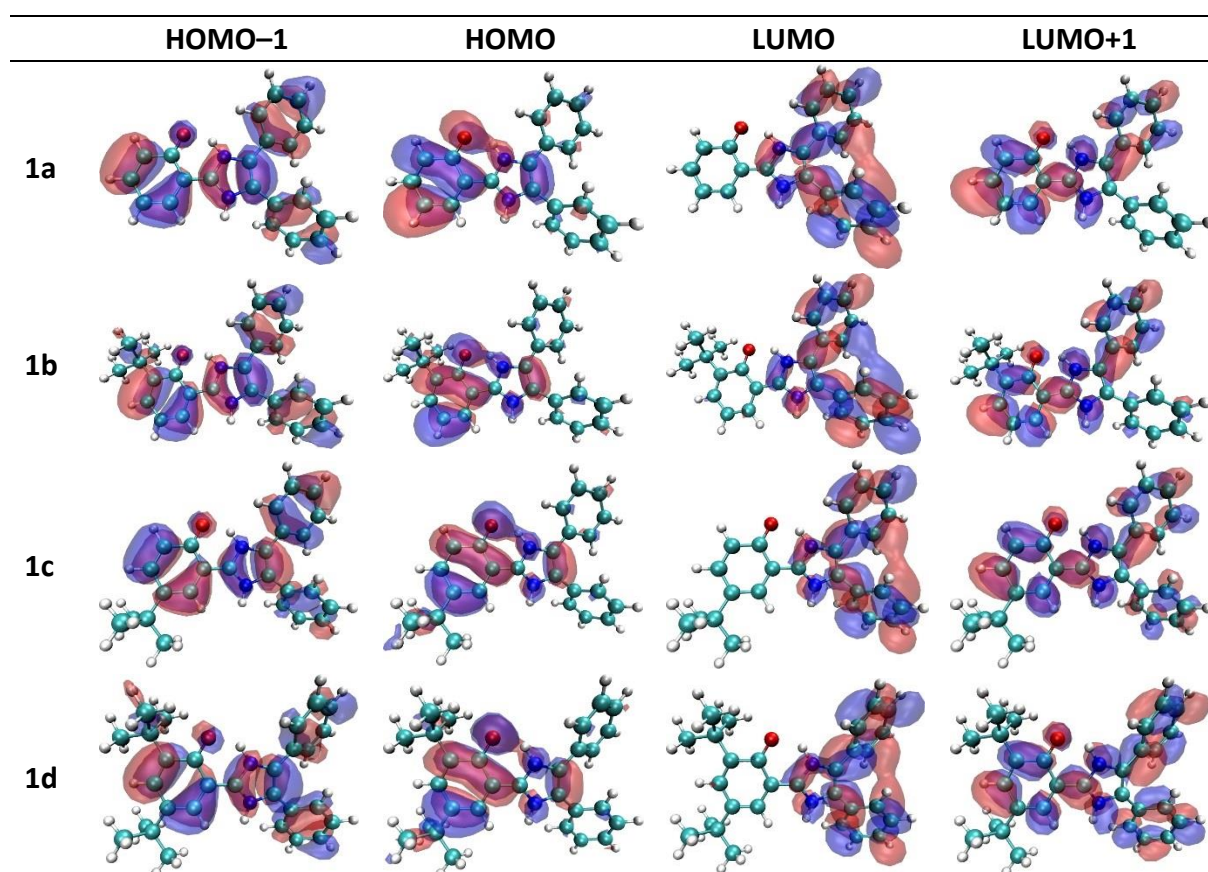


Figure SM8. Molecular orbitals obtained for the keto form of the imidazole derivatives.

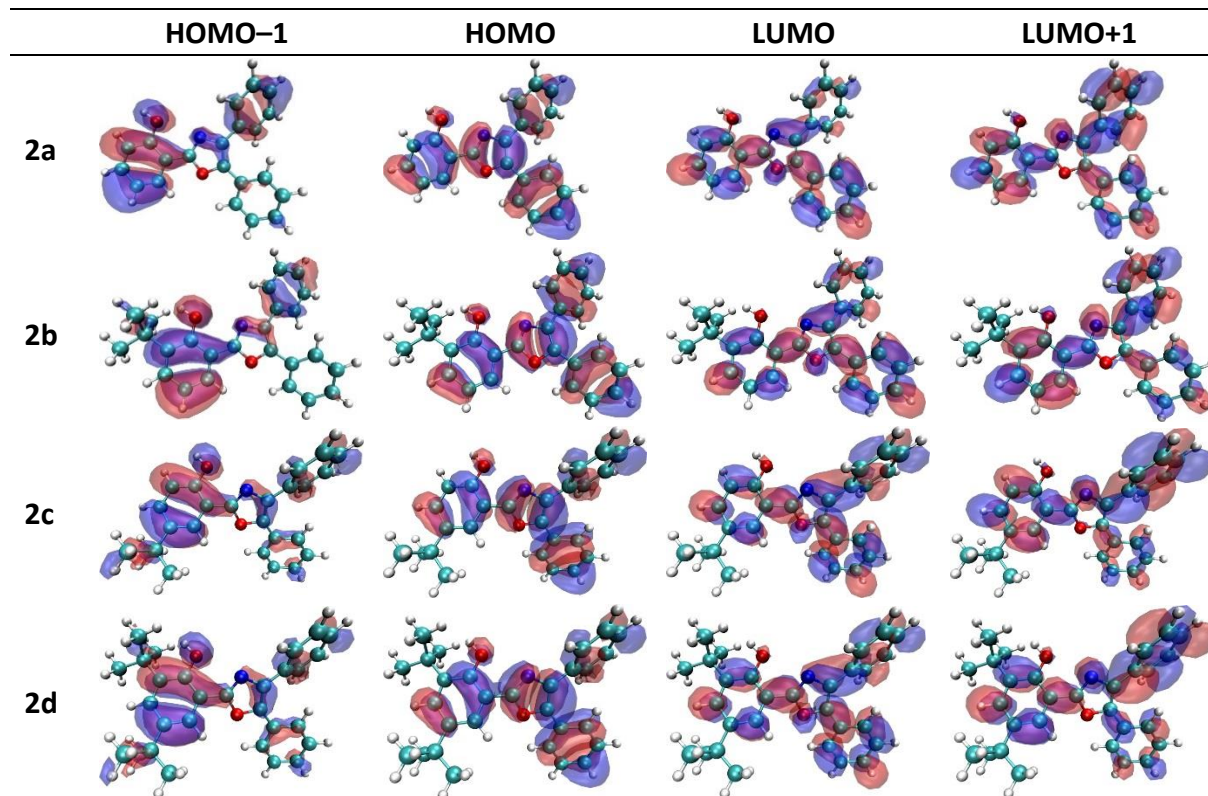


Figure SM9. Molecular orbitals obtained for the open form of the oxazole derivatives.

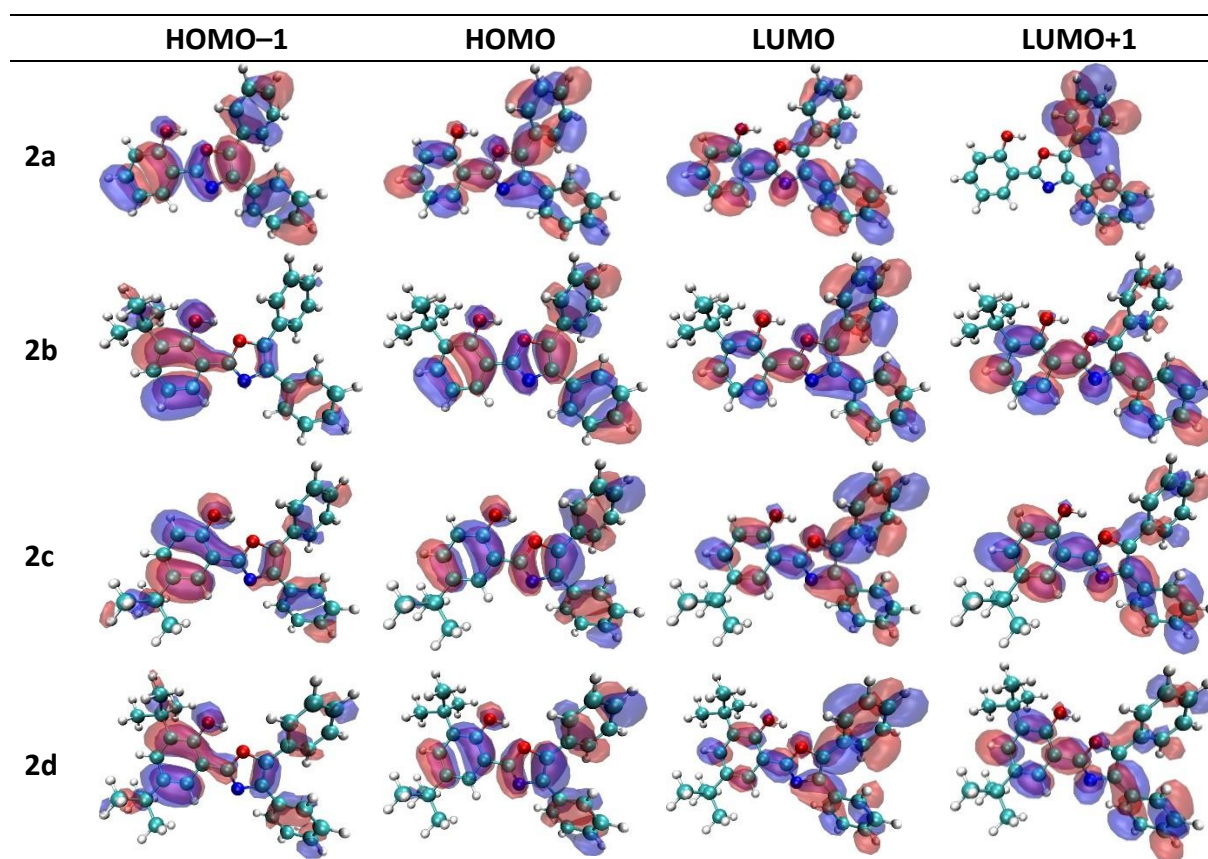


Figure SM10. Molecular orbitals obtained for the rotamer form of the oxazole derivatives.

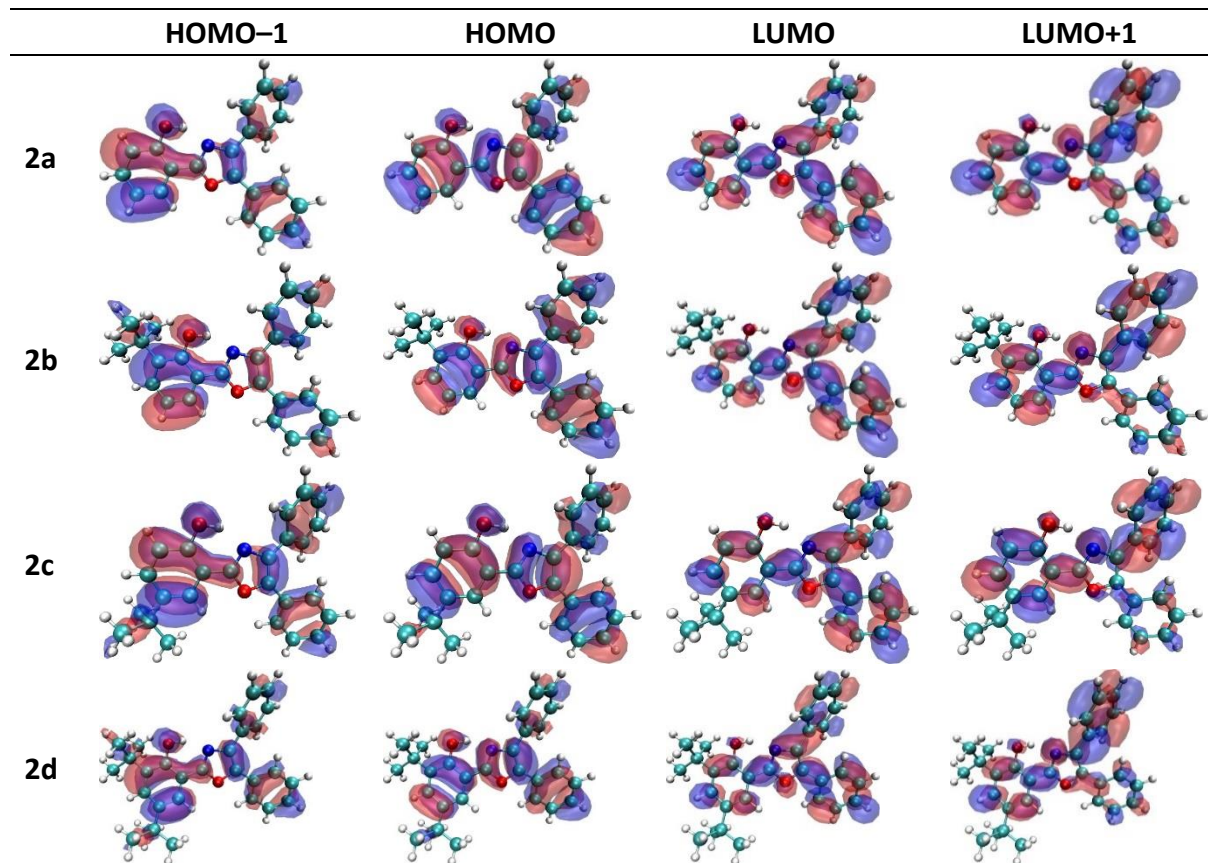


Figure SM11. Molecular orbitals obtained for the closed (enol) form of the oxazole derivatives.

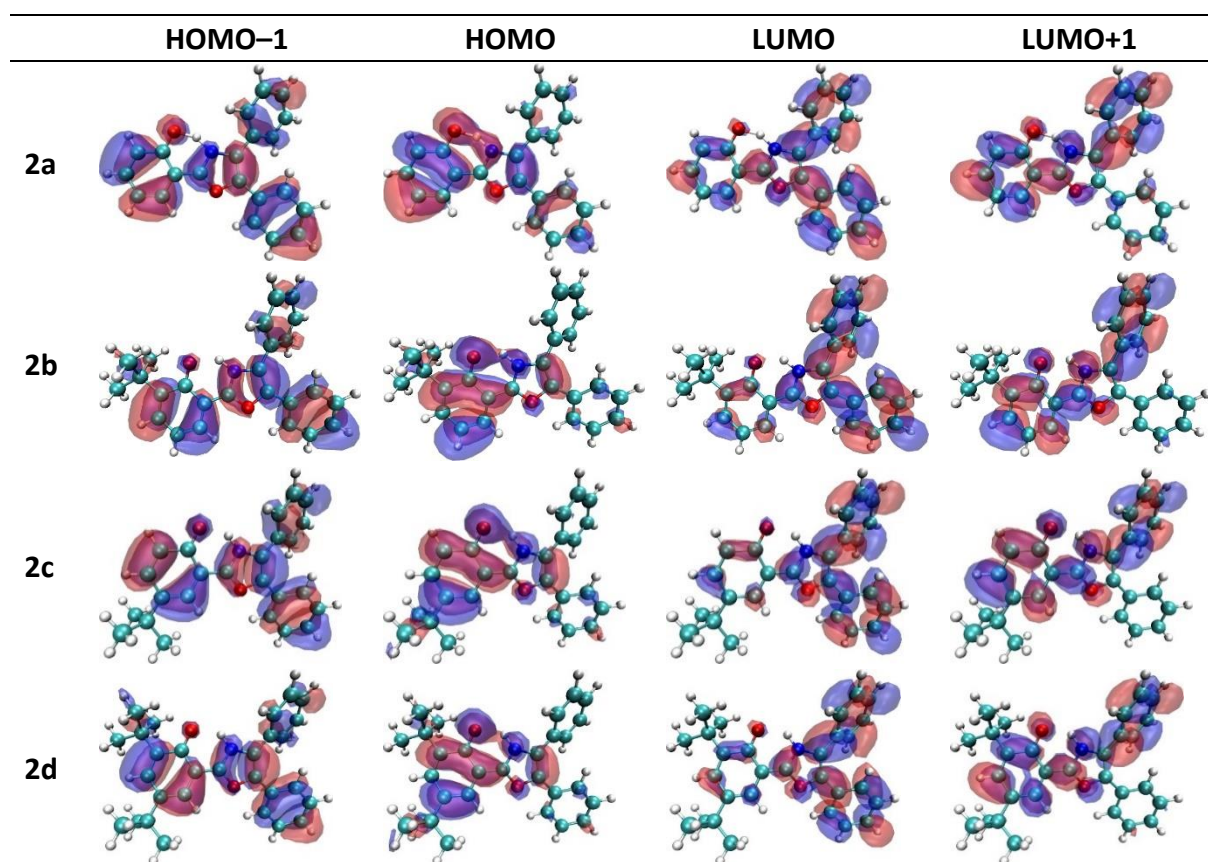


Figure SM12. Molecular orbitals obtained for the keto form of the oxazole derivatives.

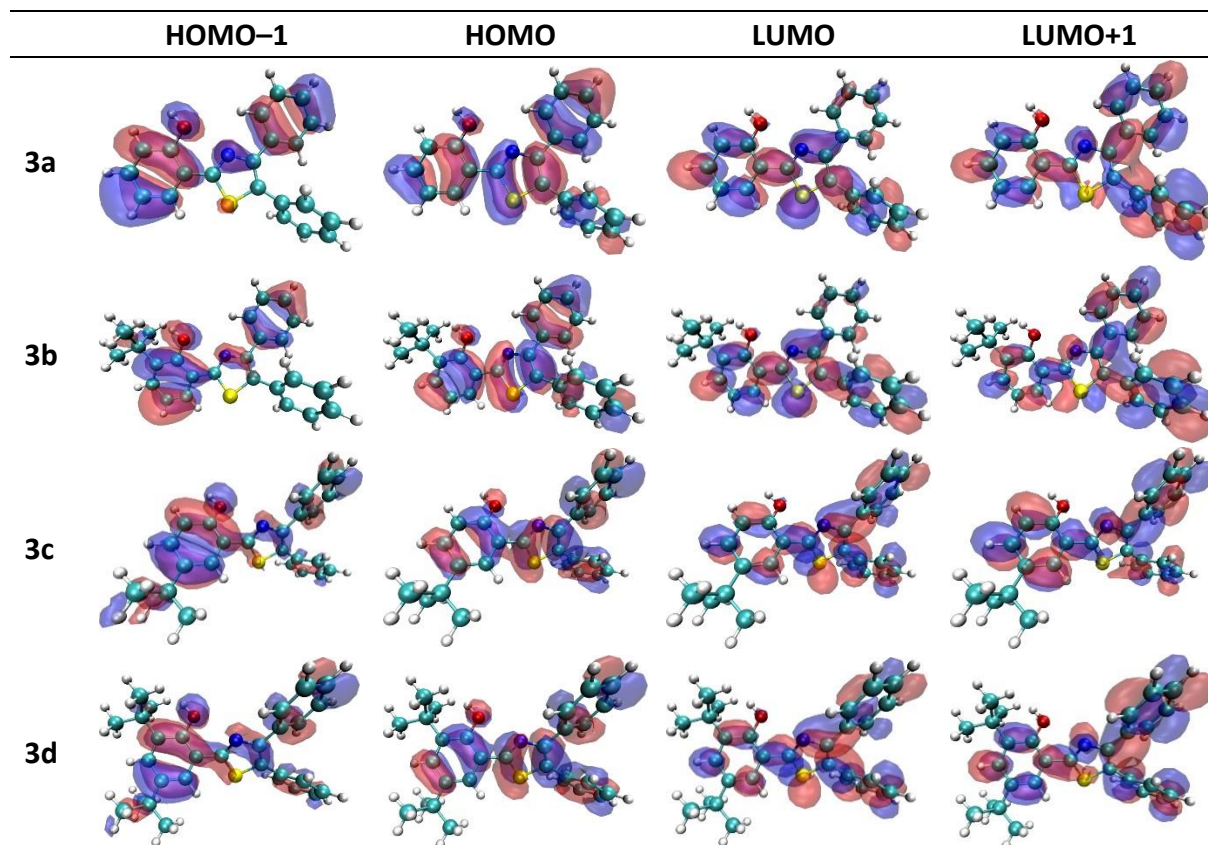


Figure SM13. Molecular orbitals obtained for the open form of the thiazole derivatives.

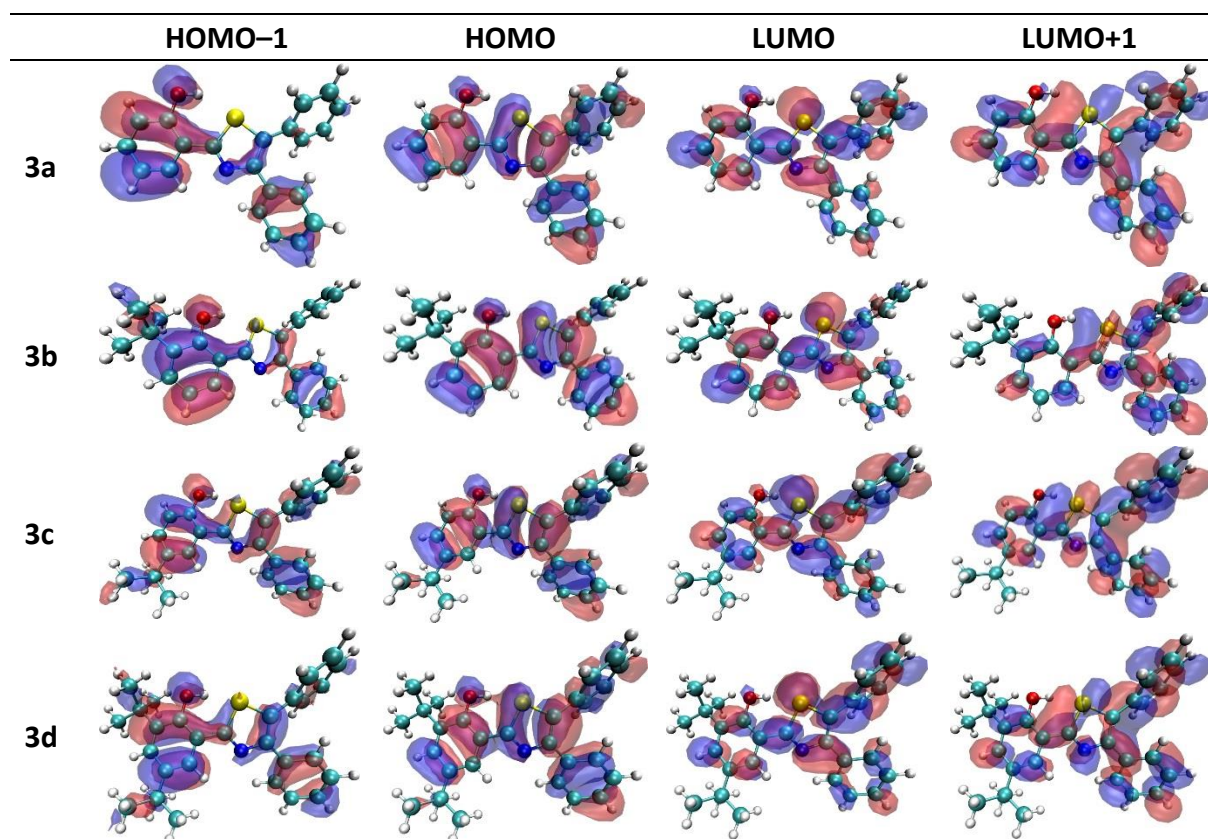


Figure SM14. Molecular orbitals obtained for the rotamer form of the thiazole derivatives.

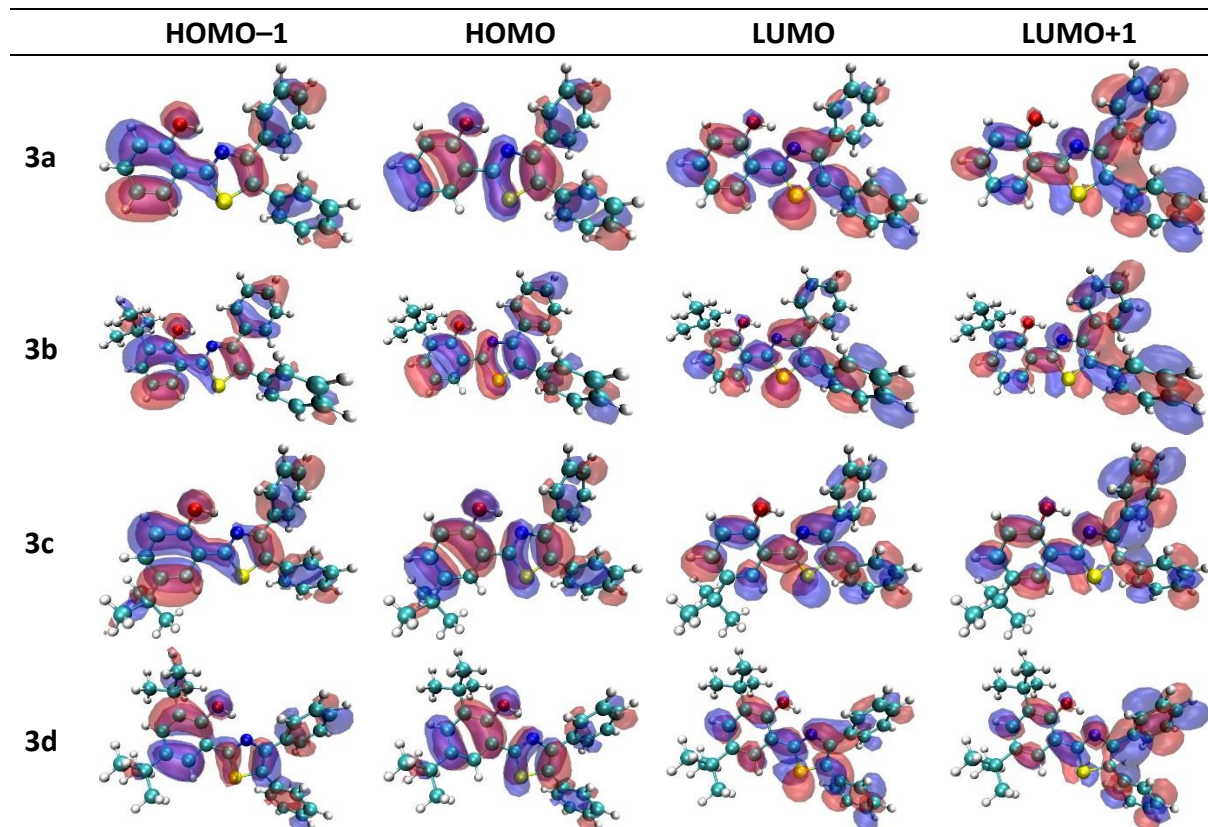


Figure SM15. Molecular orbitals obtained for the enol (closed) form of the thiazole derivatives.

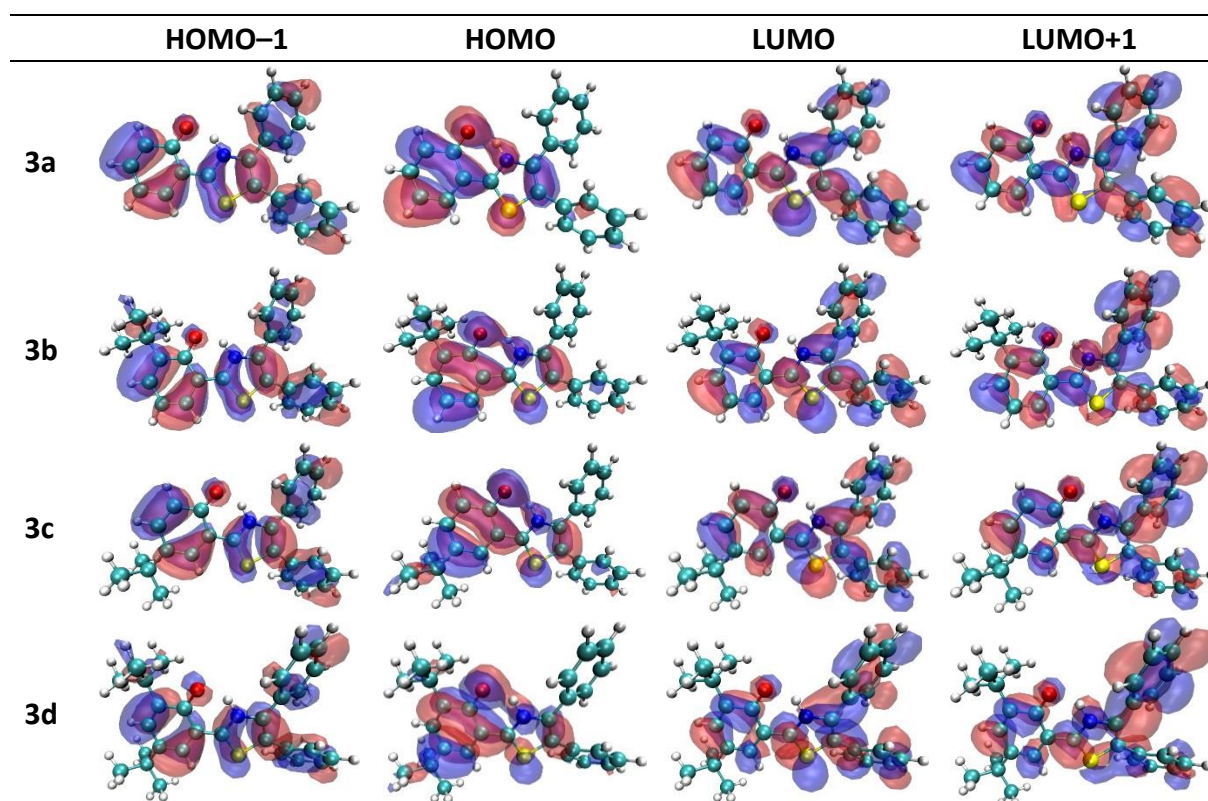


Figure SM16. Molecular orbitals obtained for the keto form of the thiazole derivatives.