*Supplementary Material*

**Optical and electrical properties of thiarubrine A simulated via the Hückel method and the nonequilibrium Green's function**

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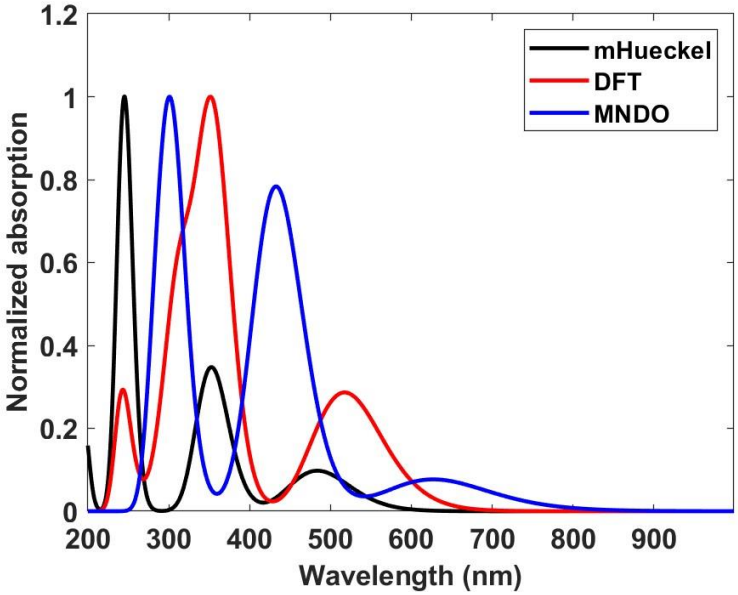


**Figure A1**. Calculated absorption spectrum, with modified Hückel method, modified neglect of diatomic overlap method (MNDO), and density functional theory (DFT), of thiarubrine A (isosurface value = 0.02) calculated with the density functional theory.

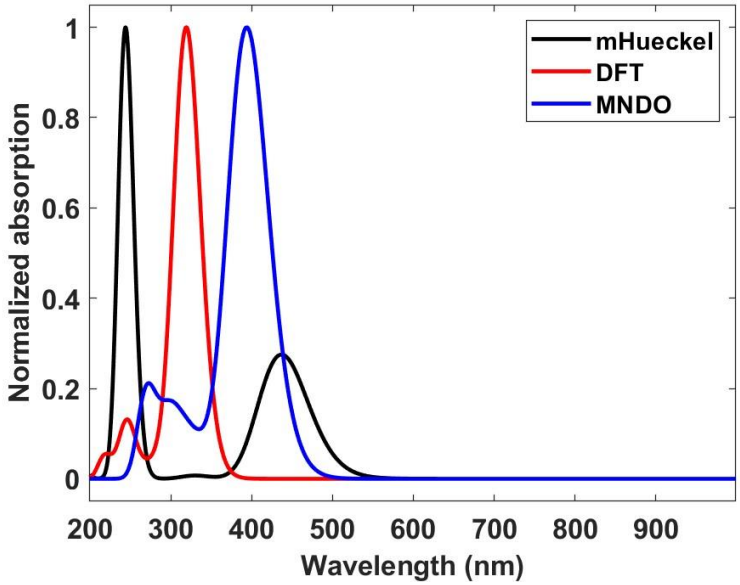


**Figure A2**. Calculated absorption spectrum, with modified Hückel method, modified neglect of diatomic overlap method (MNDO), and density functional theory (DFT), of thiophene A (isosurface value = 0.02) calculated with the density functional theory.

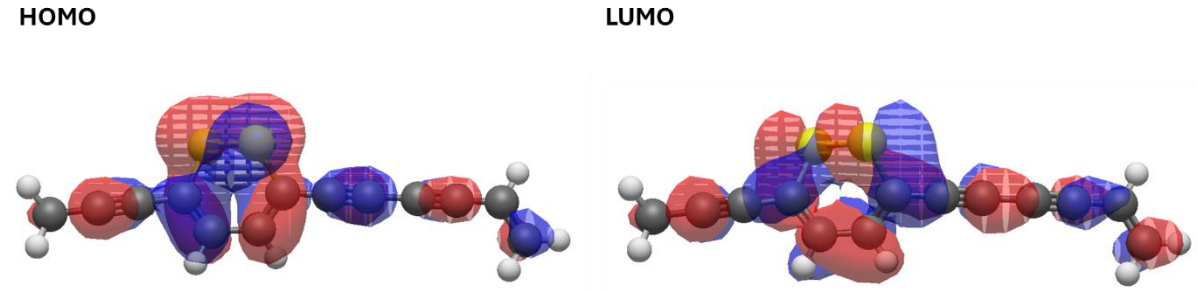


**Figure A3**. HOMO and LUMO orbitals for thiarubrine A (isosurface value = 0.02) calculated with the density functional theory.

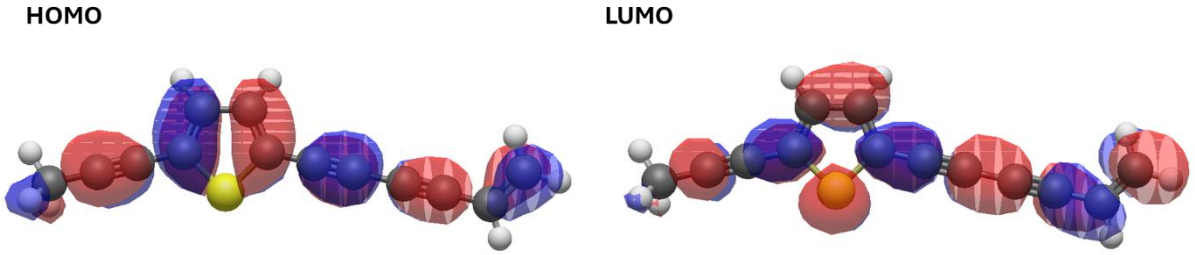


**Figure A4**. HOMO and LUMO orbitals for thiophene A (isosurface value = 0.02) calculated with the density functional theory.

**Table A1**. Electronic transitions (#, wavelength in nm, and oscillator strength) of thiarubrine A (first twelve transitions) calculated with density functional theory.

| | | |
|---|---|---|
| 1 | 517.4 | 0.142398051 |

| | | |
|---|---|---|
| 2 | 355.2 | 0.454431813 |
| 3 | 328.9 | 0.015401400 |
| 4 | 317.8 | 0.199099720 |
| 5 | 304.0 | 0.043034603 |
| 6 | 302.0 | 0.045413391 |
| 7 | 290.4 | 0.008473551 |
| 8 | 286.9 | 0.025172441 |
| 9 | 260.9 | 0.005657426 |
| 10 | 258.6 | 0.009540445 |
| 11 | 248.4 | 0.005199597 |
| 12 | 242.2 | 0.127650371 |

**Table A2**. Electronic transitions (#, wavelength in nm, and oscillator strength) of thiophene A (first twelve transitions) calculated with density functional theory.

| | | |
|---|---|---|
| 1 | 319.3 | 1.211177137 |
| 2 | 286.8 | 0.036479509 |
| 3 | 283.0 | 0.001541003 |
| 4 | 268.8 | 0.022100216 |
| 5 | 255.3 | 0.000651788 |
| 6 | 248.6 | 0.078045378 |
| 7 | 243.4 | 0.077535108 |
| 8 | 228.5 | 0.003177762 |
| 9 | 225.9 | 0.022600486 |
| 10 | 222.2 | 0.008799227 |
| 11 | 216.8 | 0.003942661 |
| 12 | 215.8 | 0.035973649 |

**Table A3**. Electronic transitions (#, wavelength in nm, and oscillator strength) of thiarubrine A (first twelve transitions) calculated with modified neglect of diatomic overlap method.

| | | |
|---|---|---|
| 1 | 627.1 | 0.016473231 |
| 2 | 433.5 | 0.197129486 |
| 3 | 396.3 | 0.012208586 |
| 4 | 334.5 | 0.003237810 |
| 5 | 325.8 | 0.002427542 |
| 6 | 320.2 | 0.015653732 |
| 7 | 305.2 | 0.084314754 |
| 8 | 304.8 | 0.115963247 |
| 9 | 302.8 | 0.005067813 |
| 10 | 294.7 | 0.004058414 |
| 11 | 286.2 | 0.102999996 |
| 12 | 282.7 | 0.003845221 |

**Table A4**. Electronic transitions (#, wavelength in nm, and oscillator strength) of thiophene A (first twelve transitions) calculated with modified neglect of diatomic overlap method.

| | | |
|---|---|---|
| 1 | 394.0 | 0.513356058 |
| 2 | 332.8 | 0.000088741 |
| 3 | 328.5 | 0.039900484 |
| 4 | 314.3 | 0.000392276 |
| 5 | 305.3 | 0.009553895 |
| 6 | 299.4 | 0.061106816 |
| 7 | 291.5 | 0.003236926 |
| 8 | 285.4 | 0.000810199 |
| 9 | 279.5 | 0.000185687 |
| 10 | 271.2 | 0.012052830 |
| 11 | 270.3 | 0.037653285 |
| 12 | 270.2 | 0.052659876 |

**Table A5**. Optimized geometry of thiarubrine A.

| | | | |
|---|---|---|---|
| C | -5.29990 | -0.01121 | 0.24805 |
| C | -3.85242 | 0.17377 | 0.15299 |
| H | -5.75820 | -0.01196 | -0.74547 |
| C | -2.66398 | 0.33140 | 0.07498 |
| H | -5.75741 | 0.79273 | 0.83243 |
| H | -5.53952 | -0.96222 | 0.73316 |
| S | 1.00023 | 2.11756 | 0.84401 |
| C | -1.25410 | 0.51941 | -0.01594 |
| C | 1.75213 | 0.63577 | 0.30754 |
| H | 9.04531 | 1.28642 | -0.33547 |
| S | -0.63617 | 2.10338 | -0.41309 |
| C | 1.02082 | -0.46424 | 0.04370 |
| H | 1.51263 | -1.38912 | -0.25013 |
| C | 9.17437 | -0.79154 | -0.02443 |
| C | 5.89581 | 0.46806 | 0.02279 |
| C | 8.50799 | 0.36035 | -0.15329 |
| C | -0.42877 | -0.53211 | 0.14937 |
| C | 4.36914 | 0.53289 | 0.12650 |
| H | -0.83921 | -1.51806 | 0.35648 |
| C | 3.17218 | 0.58069 | 0.20886 |
| C | 7.09250 | 0.41543 | -0.05764 |
| H | 10.25658 | -0.81547 | -0.10002 |
| H | 8.66308 | -1.73187 | 0.15844 |

**Table A5**. Optimized geometry of thiophene A.

| | | | |
|---|---|---|---|
| C | -0.12356 | -0.10944 | -0.00572 |
| C | 1.30031 | 0.22136 | -0.03091 |
| H | -0.37320 | -0.81574 | -0.80322 |
| C | 2.47106 | 0.48841 | -0.05135 |
| H | -0.73417 | 0.78793 | -0.14368 |
| H | -0.40050 | -0.56483 | 0.94984 |
| S | 5.09361 | -0.37391 | 0.02209 |
| C | 3.86103 | 0.80484 | -0.07582 |
| C | 4.37785 | 2.07813 | -0.17978 |
| C | 5.80568 | 2.07964 | -0.17872 |
| H | 3.76571 | 2.96906 | -0.25347 |
| C | 6.32441 | 0.80709 | -0.07397 |
| H | 6.41488 | 2.97271 | -0.25159 |
| C | 8.88475 | 0.22539 | -0.02549 |
| C | 7.71437 | 0.49181 | -0.04743 |
| C | 10.37753 | -0.11641 | 0.00208 |
| C | 11.54726 | -0.38587 | 0.02342 |
| C | 12.92849 | -0.71360 | 0.04771 |
| H | 13.20812 | -1.75930 | -0.04059 |
| C | 13.86966 | 0.22737 | 0.17518 |
| H | 13.61882 | 1.28000 | 0.26545 |
| H | 14.92091 | -0.04105 | 0.19195 |