# Supplementary Materials: Synthesis, Molecular Structure Optimization, and Cytotoxicity Assay of a Novel 2-Acetyl-3-amino-5-[(2-oxopropyl)sulfanyl]-4-cyanothiophene

**Yahia N. Mabkhot, Fahad D. Aldawsari, Salim S. Al-Showiman, Assem Barakat, Saied M. Soliman, Muhammad I. Choudhary, Sammer Yousuf, Taibi Ben Hadda, and Mohammad S. Mubarak**

**Table S1.** Calculated electronic transition bands of compound **4** using TD-DFT method.

| $\lambda_{max}$ (nm) | f | Major contributions |
|---|---|---|
| **336.9** | **0.1493** | **H→L (78%)** |
| 309.7 | 0.0002 | H-2→L (84%), H-2→L + 3 (11%) |
| 301.9 | 0.0002 | H→L + 1 (94%) |
| 288.0 | 0.0000 | H→L + 2 (94%) |
| **285.8** | **0.2552** | **H-1→L (70%), H→L + 3 (11%)** |
| 274.0 | 0.0001 | H-3→L + 1 (92%) |
| 261.2 | 0.0077 | H-1→L + 1 (94%) |
| **257.9** | **0.1364** | **H→L + 3 (71%)** |
| 254.6 | 0.0000 | H-1→L + 2 (84%), H→L + 4 (12%) |
| 243.6 | 0.0003 | H-1→L + 2 (12%), H→L + 4 (79%) |
| 236.2 | 0.0000 | H-3→L (55%), H-2→L + 3 (36%) |
| 233.9 | 0.0000 | H-3→L (44%), H-2→L + 3 (47%) |
| 230.5 | 0.0000 | H-2→L + 1 (98%) |
| **230.3** | **0.0781** | **H-4→L (14%), H-1→L + 3 (75%)** |
| **219.5** | **0.0077** | **H-4→L (20%), H-2→L + 2 (72%)** |
| 216.7 | 0.0660 | H-4→L (56%), H-2→L + 2 (23%), H-1→L + 3 (10%) |
| 216.1 | 0.0000 | H-1→L + 4 (88%) |
| 209.1 | 0.0004 | H→L + 5 (94%) |
| 201.4 | 0.0009 | H-4→L + 1 (98%) |
| 201.2 | 0.0017 | H→L + 6 (79%) |
| 198.7 | 0.0147 | H-3→L + 2 (93%) |
| 197.4 | 0.0000 | H-1→L + 5 (67%) |
| 196.2 | 0.0000 | H→L + 7 (75%) |
| 194.2 | 0.0014 | H-5→L (12%), H-4→L + 2 (62%) |
| 193.8 | 0.0001 | H-5→L (69%), H-1→L + 5 (15%) |
| 193.1 | 0.0155 | H-2→L + 4 (87%) |
| 188.8 | 0.0009 | H→L + 8 (89%) |
| 188.2 | 0.0000 | H-3→L + 3 (99%) |
| 185.7 | 0.0971 | H-4→L + 3 (80%) |
| 181.9 | 0.0020 | H-1→L + 6 (73%), H→L + 10 (17%) |
| 181.5 | 0.0383 | H-6→L (47%), H→L + 9 (30%) |
| 181.5 | 0.0007 | H-8→L (32%), H-1→L + 7 (30%), H→L + 10 (25%) |
| 180.0 | 0.0005 | H-8→L (59%), H→L + 10 (18%) |
| 178.2 | 0.0784 | H-3→L + 4 (87%) |
| 177.2 | 0.0000 | H-1→L + 6 (11%), H-1→L + 7 (51%), H→L + 10 (29%) |
| 176.2 | 0.0971 | H-6→L (22%), H→L + 9 (46%) |
| 175.0 | 0.0006 | H-4→L + 4 (43%), H→L + 12 (20%), H→L + 13 (21%) |
| 174.7 | 0.0091 | H-7→L (78%) |
| 172.4 | 0.0000 | H-4→L + 4 (42%), H→L + 12 (17%), H→L + 13 (30%) |
| 171.5 | 0.0102 | H-2→L + 5 (89%) |

**Table S2.** Calculated chemical shifts δ (ppm) of the compound **4** using GIAO method.

| Atom | $\delta_{calc}$ (ppm) | $\delta_{exp.}$(ppm) | Atom | $\delta_{calc}$ (ppm) | $\delta_{exp.}$(ppm) |
|---|---|---|---|---|---|
| H6 | 8.34 | 7.51 | C9 | 36.88 | 28.7 |
| H7 | 4.54 | 7.51 | C12 | 37.89 | 28.4 |
| H10 | 1.70 | 2.26 | C15 | 122.19 | 108.7 |
| H11 | 1.98 | 2.26 | C16 | 168.84 | 153.9 |
| H13 | 1.97 | 2.24 | C17 | 109.32 | 99.6 |
| H14 | 2.07 | 2.24 | C18 | 180.06 | 156 |
| H22 | 3.70 | 4.42 | C19 | 198.40 | 188.4 |
| H24 | 1.98 | 2.26 | C20 | 122.83 | 112.6 |
| H25 | 2.07 | 2.24 | C21 | 62.23 | 45.8 |
| H26 | 3.70 | 4.42 | C23 | 211.45 | 201.2 |