## Supplement information

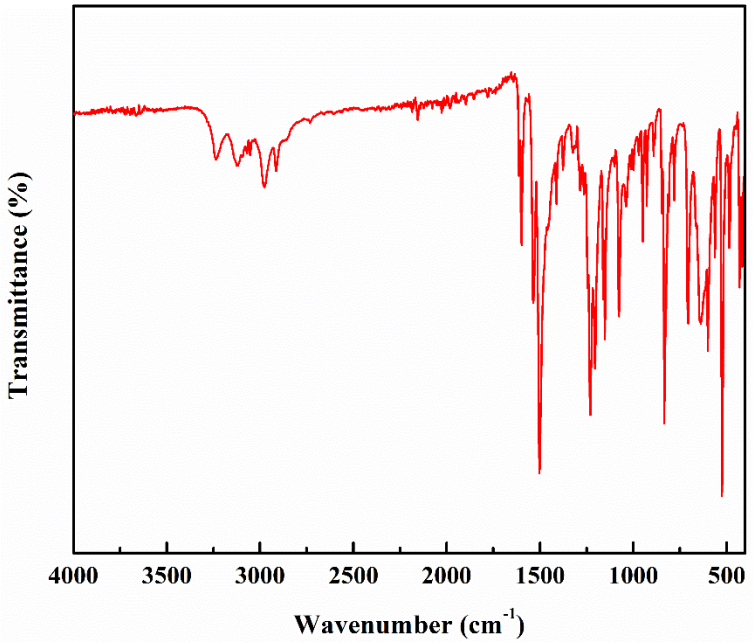



Figure S1. FT-IR spectrum of the synthetized compound.

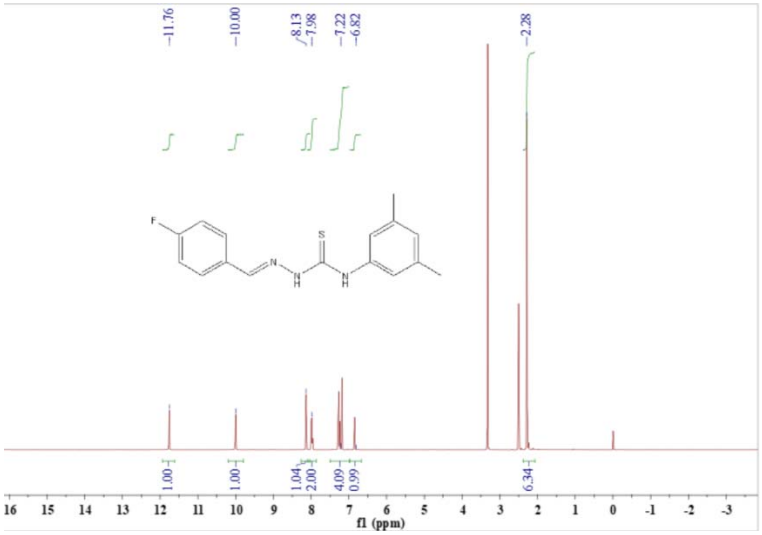



Figure S2. $^{1}$H NMR spectrum of the synthetized compound.

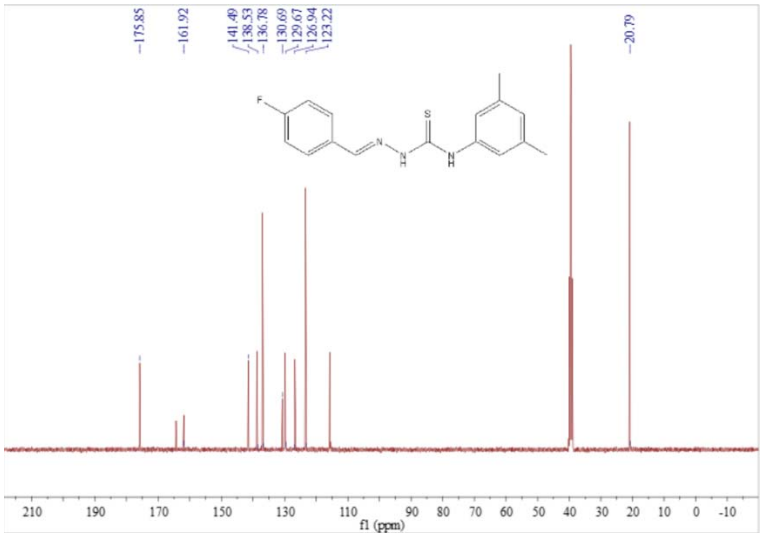



Figure S3. $^{13}C$ NMR spectrum of the synthetized compound.

Table S1. Selected experimental and theoretical geometrical parameters of the synthetized compound at B3LYP/6-31+G(d,p) level.

| Parameters | Experimental | Calculated |
|---|---|---|
| Bond length (Å) | | |
| S(1)—C(9) | 1.691 | 1.678 |
| N(1)—C(3) | 1.427 | 1.414 |
| N(2)—C(9) | 1.351 | 1.387 |
| N(3)—C(10) | 1.284 | 1.290 |
| C(2)—C(3) | 1.387 | 1.353 |
| C(14)—F(1) | 1.365 | 1.357 |
| Bond angle (°) | | |
| C(4)—C(3)—N(1) | 119.4 | 115.3 |
| C(3)—N(1)—C(9) | 124.2 | 133.1 |
| N(1)—C(9)—S(1) | 124.9 | 130.0 |
| C(9)—N(2)—N(3) | 120.0 | 123.0 |
| C(13)—C(14)—F(1) | 118.8 | 118.9 |
| Dihedral angle (°) | | |
| C(3)—N(1)—C(9)—S(1) | -5.5 | -0.01 |
| N(1)—C(9)—N(2)—N(3) | 0.2 | -0.002 |
| S(1)—C(9)—N(2)—N(3) | -178.8 | 180.0 |
| C(9)—N(2)—N(3)—C(10) | -178.9 | 180.0 |

Table S2. Conformers of the minimum and maximum energy of the synthetized compound.

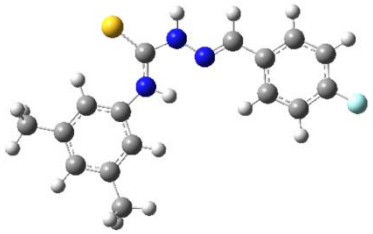
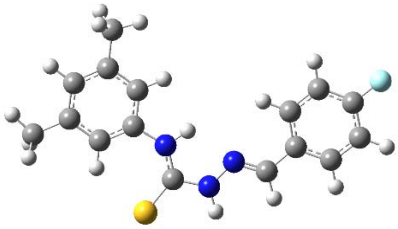
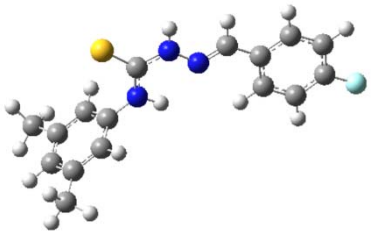
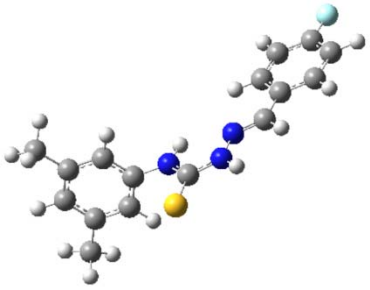
| | |
|---|---|
|  |  |
| Scan co-ordinate angle = 182.1°<br>Total energy = -804266 Kcal/mol | Scan co-ordinate angle = 362.1°<br>Total energy = -804266 Kcal/mol |
|  |  |
| Scan co-ordinate angle = 267.1°<br>Total energy = -804264 Kcal/mol | Scan co-ordinate angle = 452.1°<br>Total energy = -804264 Kcal/mol |

Table S3. The $\lambda_{max}$ of experimental and theoretical maximum absorbance, excitation energy (*E*), oscillator strength (*f*) and assignments of the synthetized compound at TD-DFT/ B3LYP/6-31+G(d,p) basis set.

| Excited state | Wavelength (nm) | | Excitation energies (eV) | Oscillator strengths | Assignment |
|---|---|---|---|---|---|
| | Theoretical | Experimental ($\varepsilon_{max}$) | | | |
| S1 | 329 | 320 (70000) | 3.77 | 0.75 | HOMO LUMO (51%) |
| S2 | 298 | - | 4.17 | 0.23 | HOMO-2 LUMO (68%) |
| S3 | 230 | 209 (35000) | 5.08 | 0.08 | HOMO-5 LUMO (39%) |

Table S4. Docking energy, hydrogen bond, the residue of active site and inhibition constant Ki for the synthetized compound and co-crystal ligand.

| 1NMT | Docking energy(Kcal/mol) | Hydrogen bond | The residues of active site | Ki(μmol/L) |
|---|---|---|---|---|
| Compound | -4.99 | ASN421 | LYS167;ASP64;ASN166;LYS161;ILE63;ASN421;ARG423;THR218;LEU220;TYR422;LEU419; TYR418;PHE420;PRO217;VAL168 | 220.81 |
| Co-crystal ligand | -3.06 | LEU419; ASN421 | PRO219;LEU220;THR218;LEU419;TYR418;PRO217;PHE420;ASN421;ILE63;TYR422 | 5.7 |