One-pot Synthesis, theoretical study and antimicrobial activity of

5,5`-(1,4-phenylenebis-(methanylylidene))bis(3-aryl(alkyl)-2-thioxoimidazolidin-4-one) derivatives

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**Table S 1.** Relativeenergies for *Z*- and *E*-isomer of **4a**, calculated at B3LYP/6-31+G\* level of theory.

|  |  |  |
| --- | --- | --- |
| ***Conformer*** | **Electronic energy (au)** | ***Δ*E (kcal/mol)** |
| **4a-1** | -2167.534460 | 0.00 |
| **4a-2** | -2167.534328 | 0.08 |
| **4a-3** | -2167.531661 | 1.76 |
| **4a-4** | -2167.531494 | 1.86 |
| **4a-5** | -2167.528627 | 3.66 |
| **4a-6** | -2167.527312 | 4.49 |

**Table S 2.** Relative energies for thioamide-**4α** and iminothiol-**4β** forms of **4a**, calculated at B3LYP/6-31+G\* level of theory.

|  |  |  |  |
| --- | --- | --- | --- |
| ***Conformer*** | **Electronic energy (au)** | | ***Δ*E (kcal/mol)** |
| ***E*thioamide-4α form** | ***E*iminothiol-4β form** |
| **4a-1 (*Z*,*Z*)** | -2167.53446 | -2167.49805 | -22.85 |
| **4a-3 (*E*,*Z*)** | -2167.53166 | -2167.49288 | -24.34 |
| **4a-5 (*E*,*E*)** | -2167.52863 | -2167.48838 | -25.26 |

**Table S 3.** Relativeenergies for *Z*- and *E*-isomer of **6a**, calculated at B3LYP/6-31+G\* level of theory.

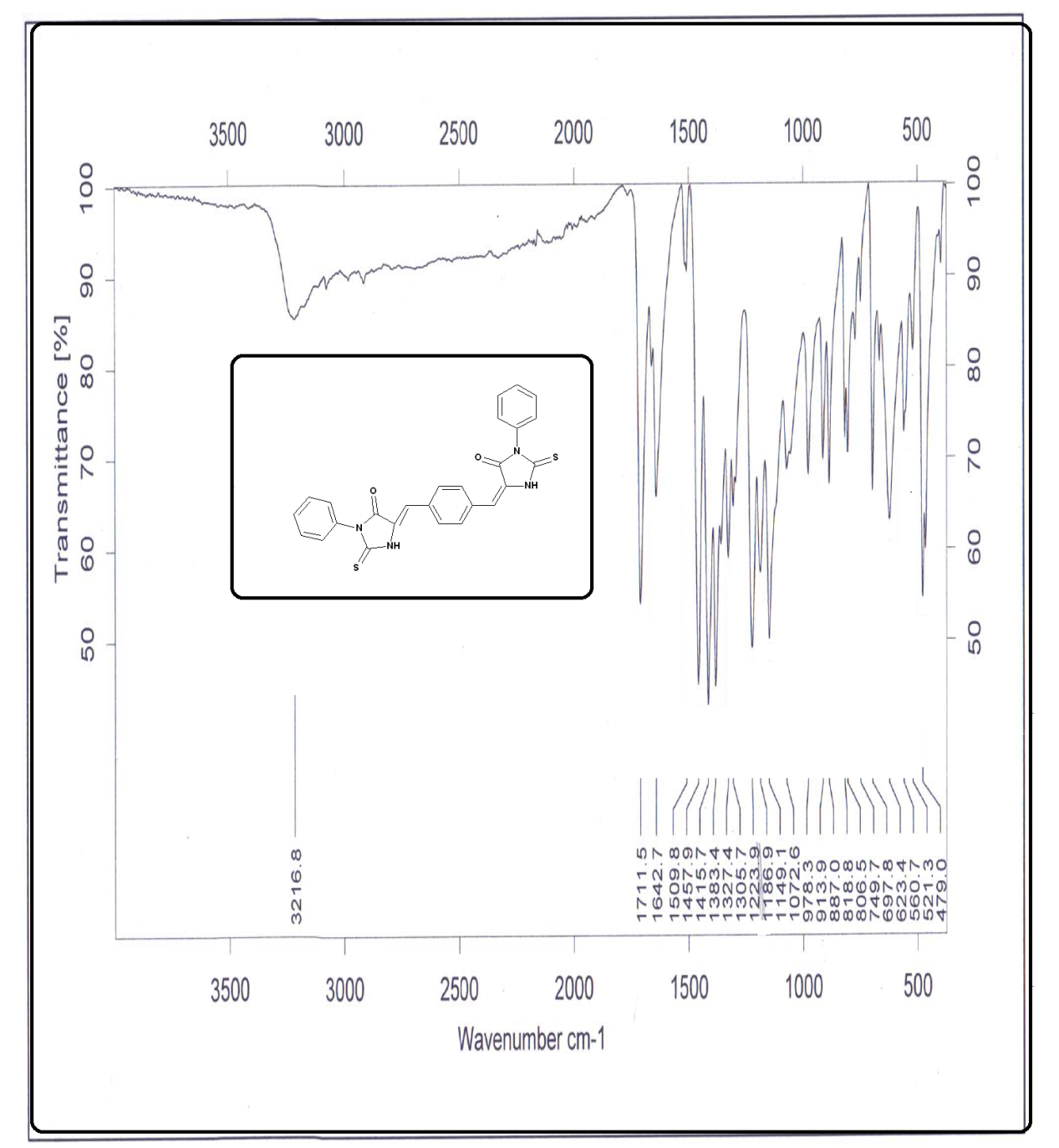
|  |  |  |
| --- | --- | --- |
| ***Conformer*** | **Electronic energy (au)** | ***Δ*E (kcal/mol)** |
| **6a-1** | -2246.135813 | 0.00 |
| **6a-2** | -2246.135402 | 0.26 |
| **6a-3** | -2246.130759 | 3.17 |
| **6a-4** | -2246.130718 | 3.20 |
| **6a-5** | -2246.126039 | 6.13 |
| **6a-6** | -2246.124809 | 6.91 |

**Table S 4.** Relativeenergies for *Z*- and *E*-isomer of **8a**, calculated at B3LYP/6-31+G\* level of theory.

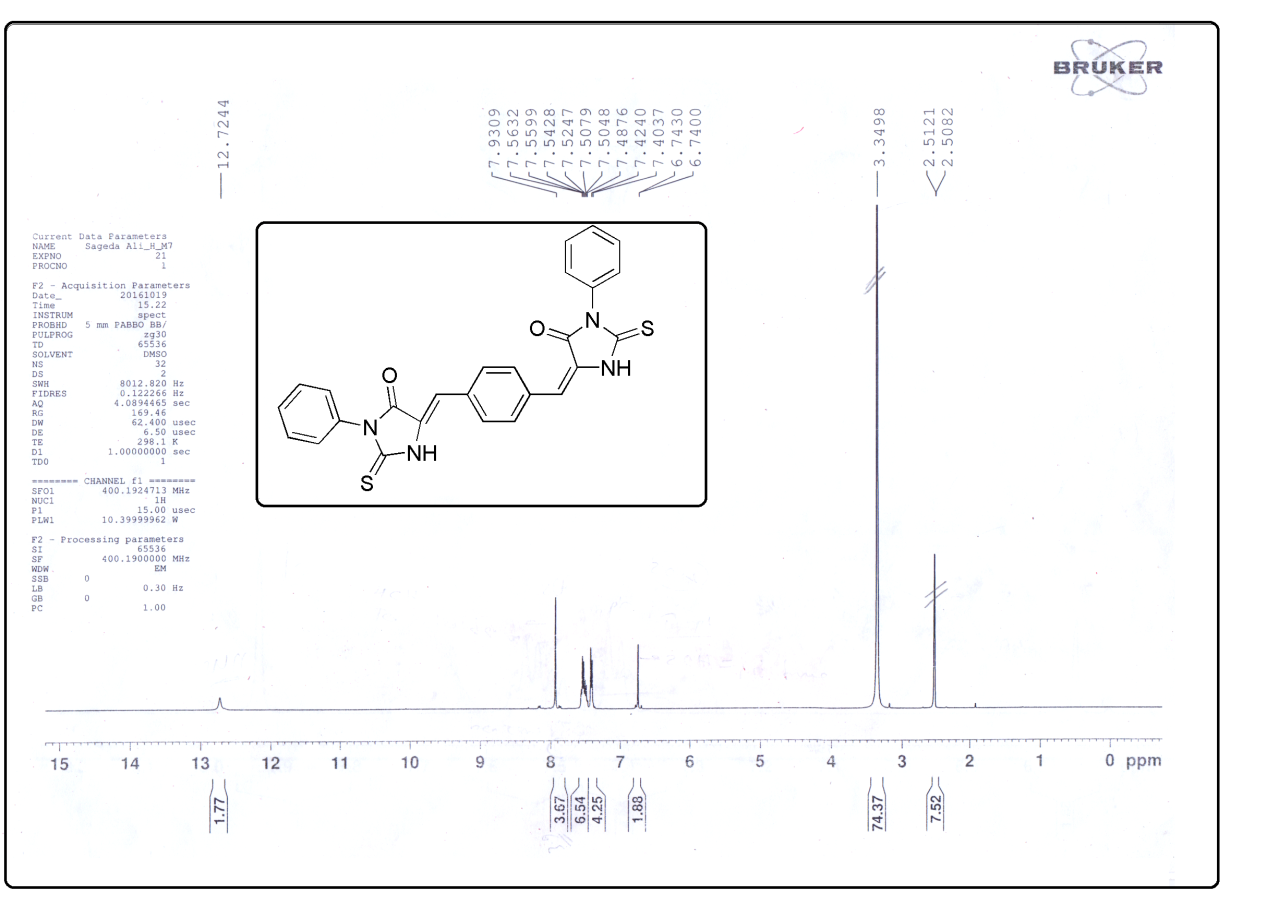
|  |  |  |
| --- | --- | --- |
| ***Conformer*** | **Electronic energy (au)** | ***Δ*E (kcal/mol)** |
| **8a-1** | -2246.153108 | 0.00 |
| **8a-2** | -2246.151548 | 0.98 |
| **8a-3** | -2246.148737 | 2.74 |
| **8a-4** | -2246.148544 | 2.86 |
| **8a-5** | -2246.144289 | 5.53 |
| **8a-6** | -2246.144075 | 5.67 |

**Table S 5.** *In-vitro* antimicrobial activity of the synthesized compounds.

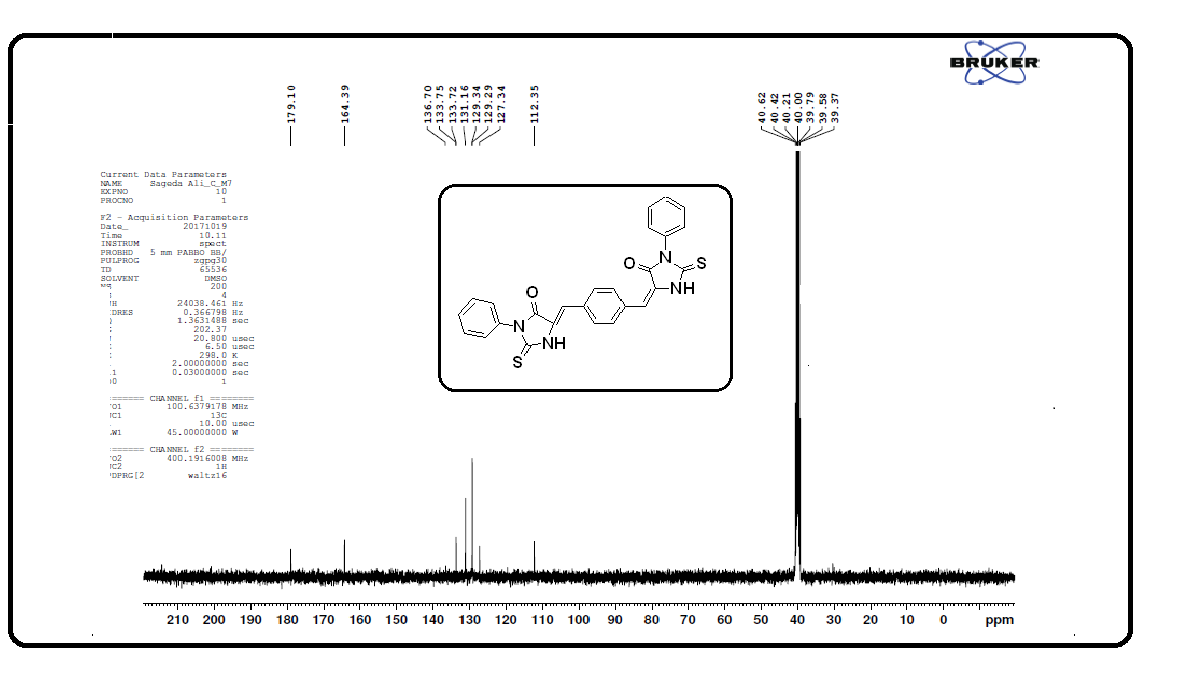
|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compounds** | **MIC in 1mg/mL (zone of inhibition in mm)** | | | | |
| **Gram-positive bacteria**  ***B. cereus*** |  | **Gram-negative bacteria**  ***E. coli*** |  | **Fungi**  ***F. oxysporum*** |
| **4a** | 2 |  | - |  | 2 |
| **4b** | - |  | - |  | 8 |
| **6a** | - |  | - |  | 2 |
| **6b** | 2 |  | - |  | 2 |
| **8a** | - |  | - |  | 4 |
| **8b** | 3 |  | - |  | 2 |
| **8c** | 2 |  | - |  | 4 |



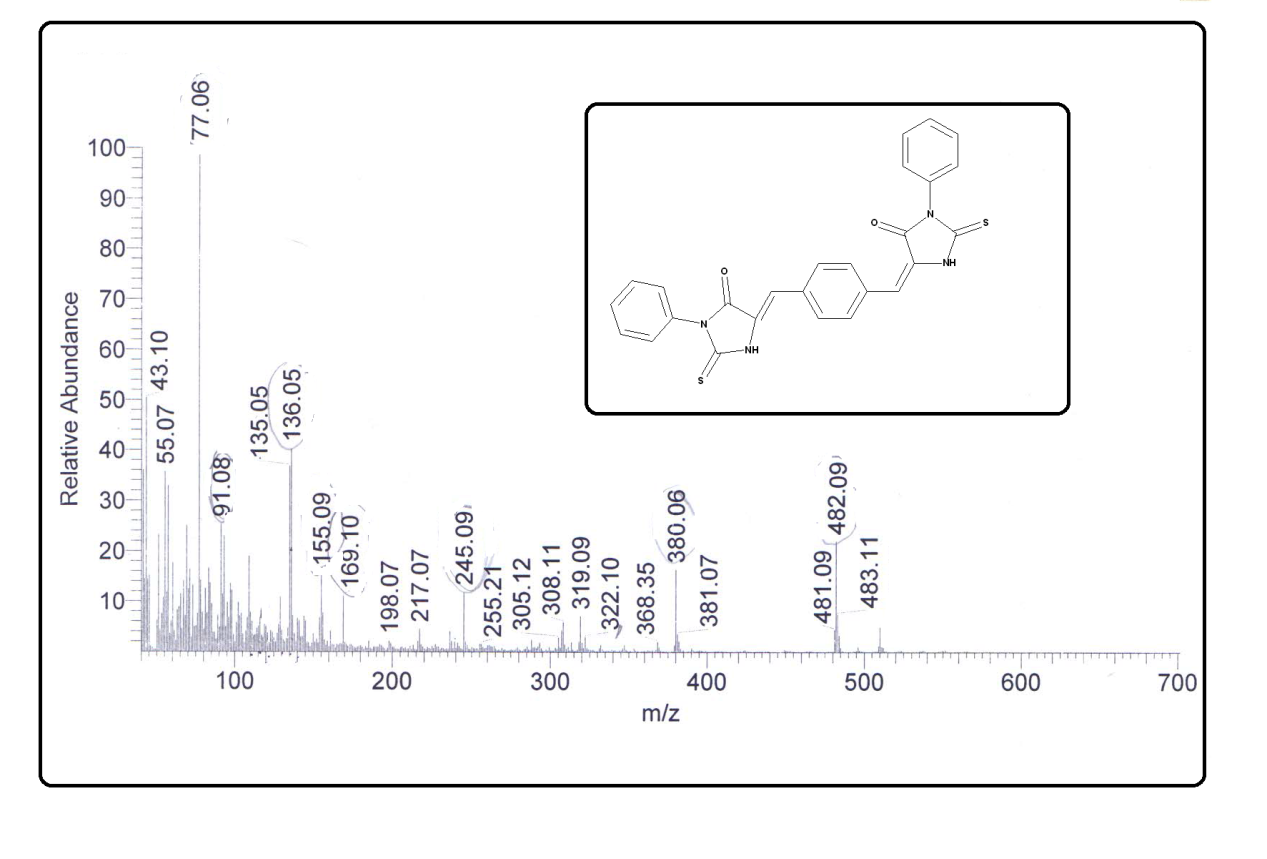
**Figure S 1**.IR spectrum of compound **4a**.



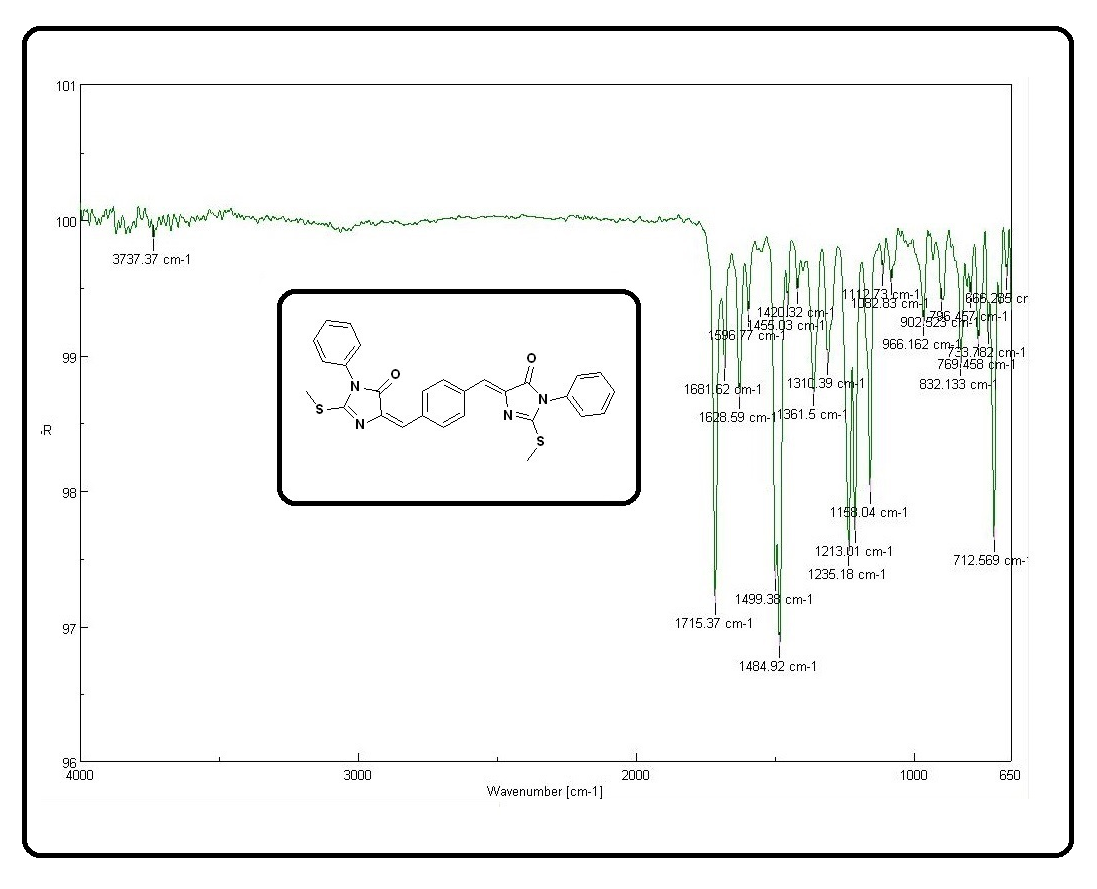
**Figure S 2**.1H NMR of compound **4a**.



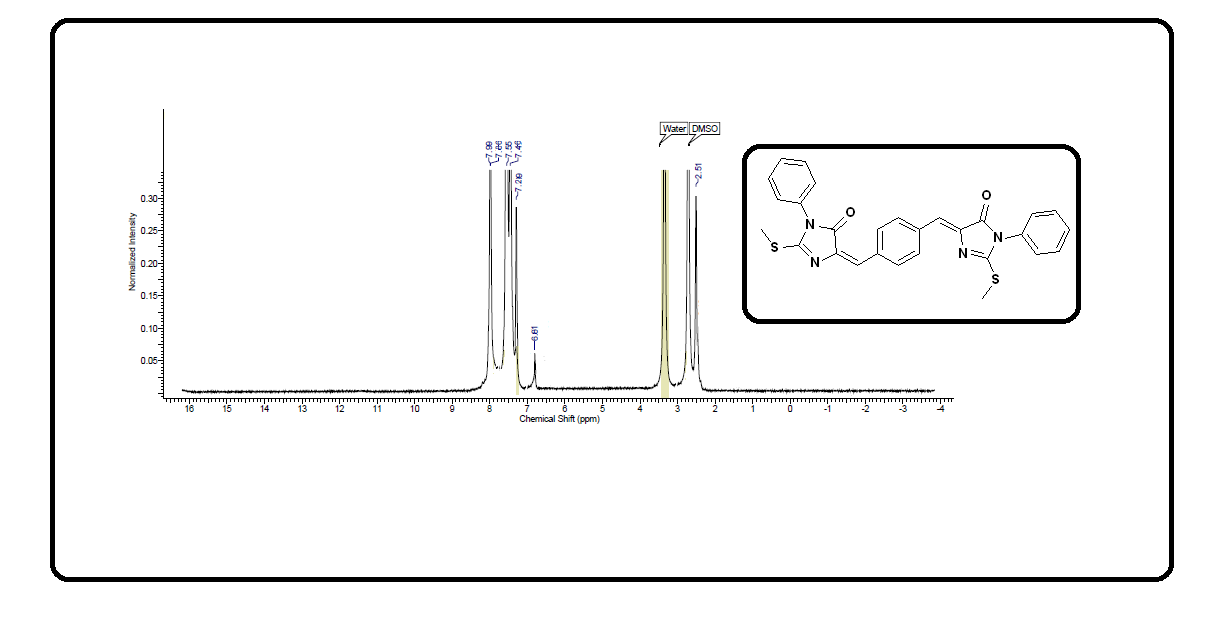
**Figure S 3**.13C NMR of compound **4a**.



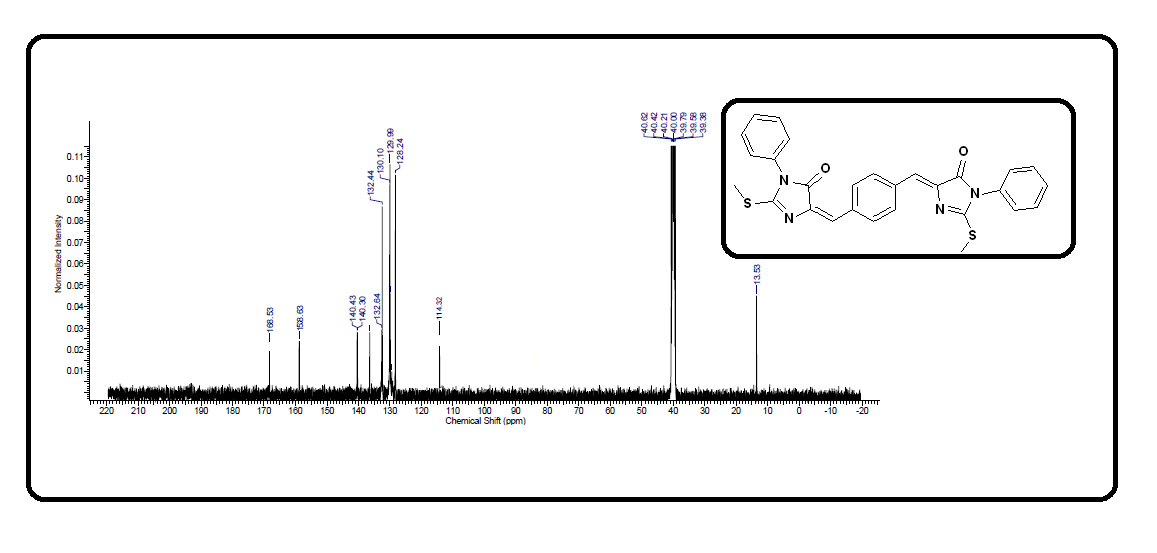
**Figure S 4**.Mass spectrum of compound **4a**.



**Figure S 5**.IR spectrum of compound **6a**.



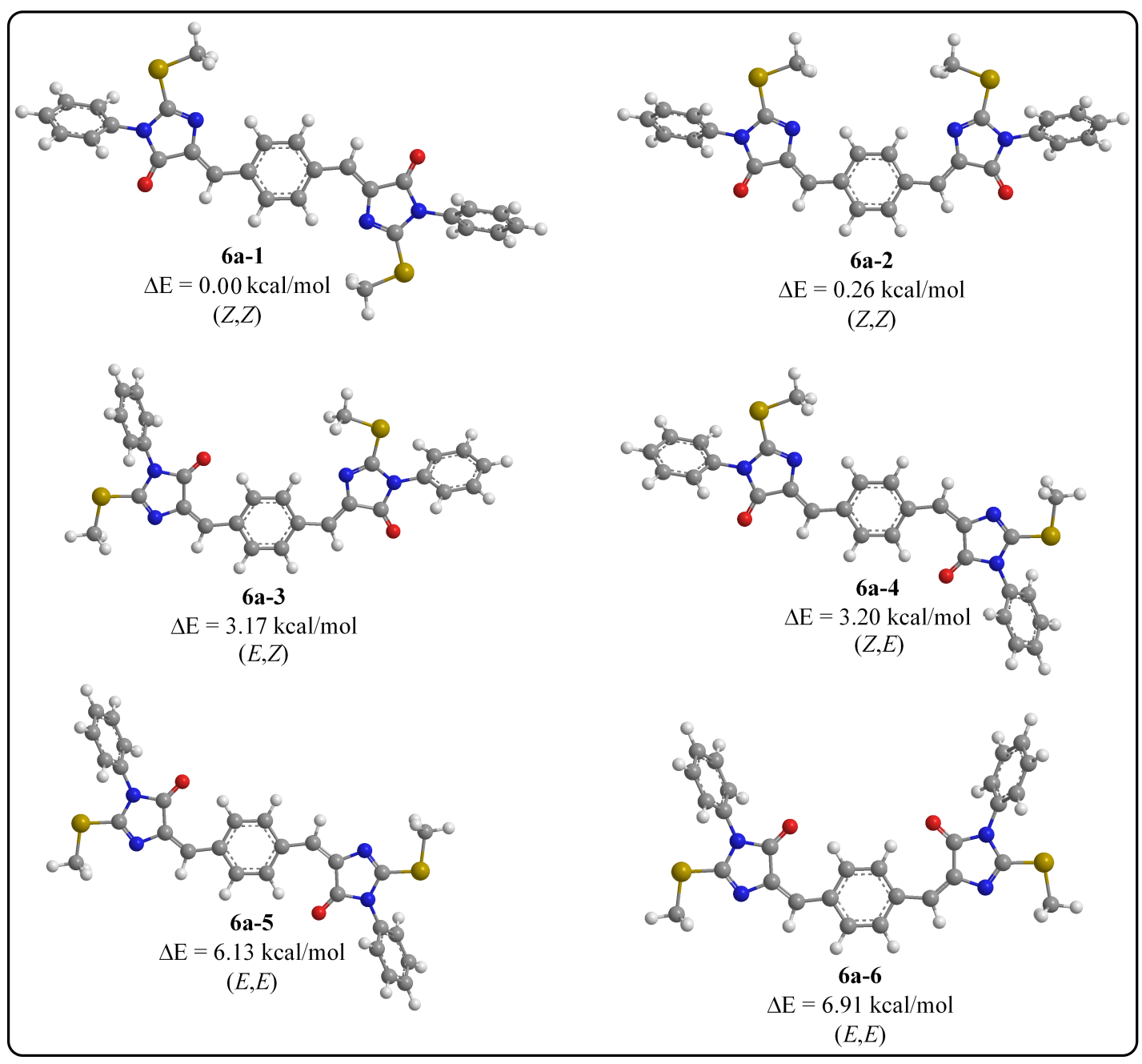
**Figure S 6**.1H NMR of compound **6a**.



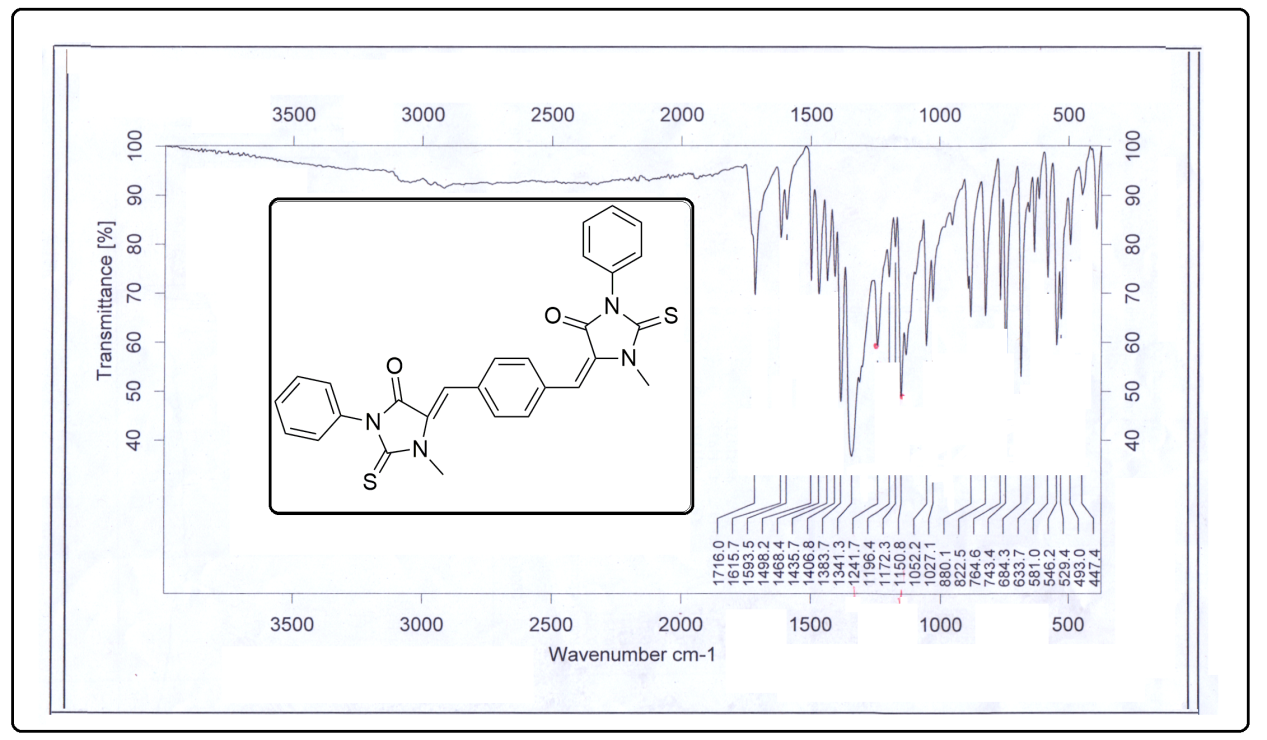
**Figure S 7**.13C NMR of compound **6a**.



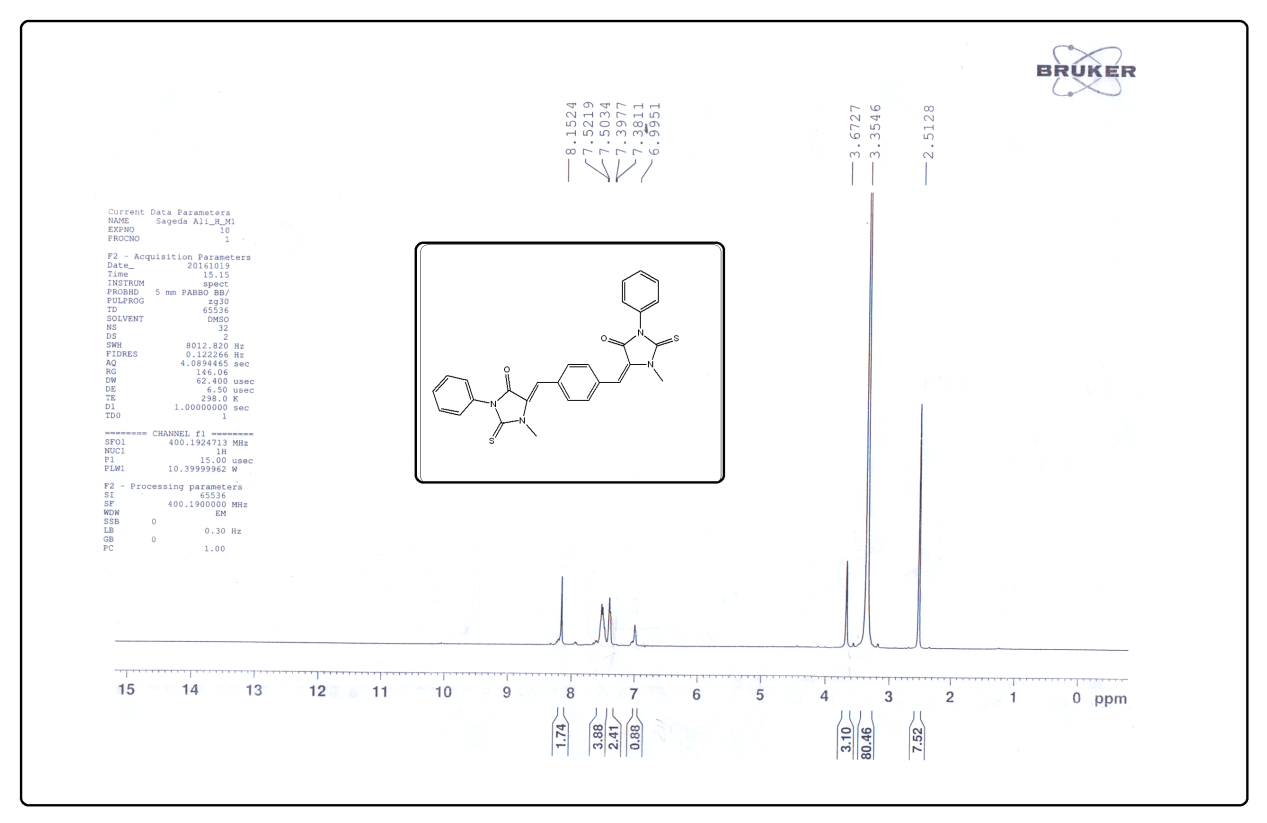
**Figure S 8**.Mass spectrum of compound **6a**.



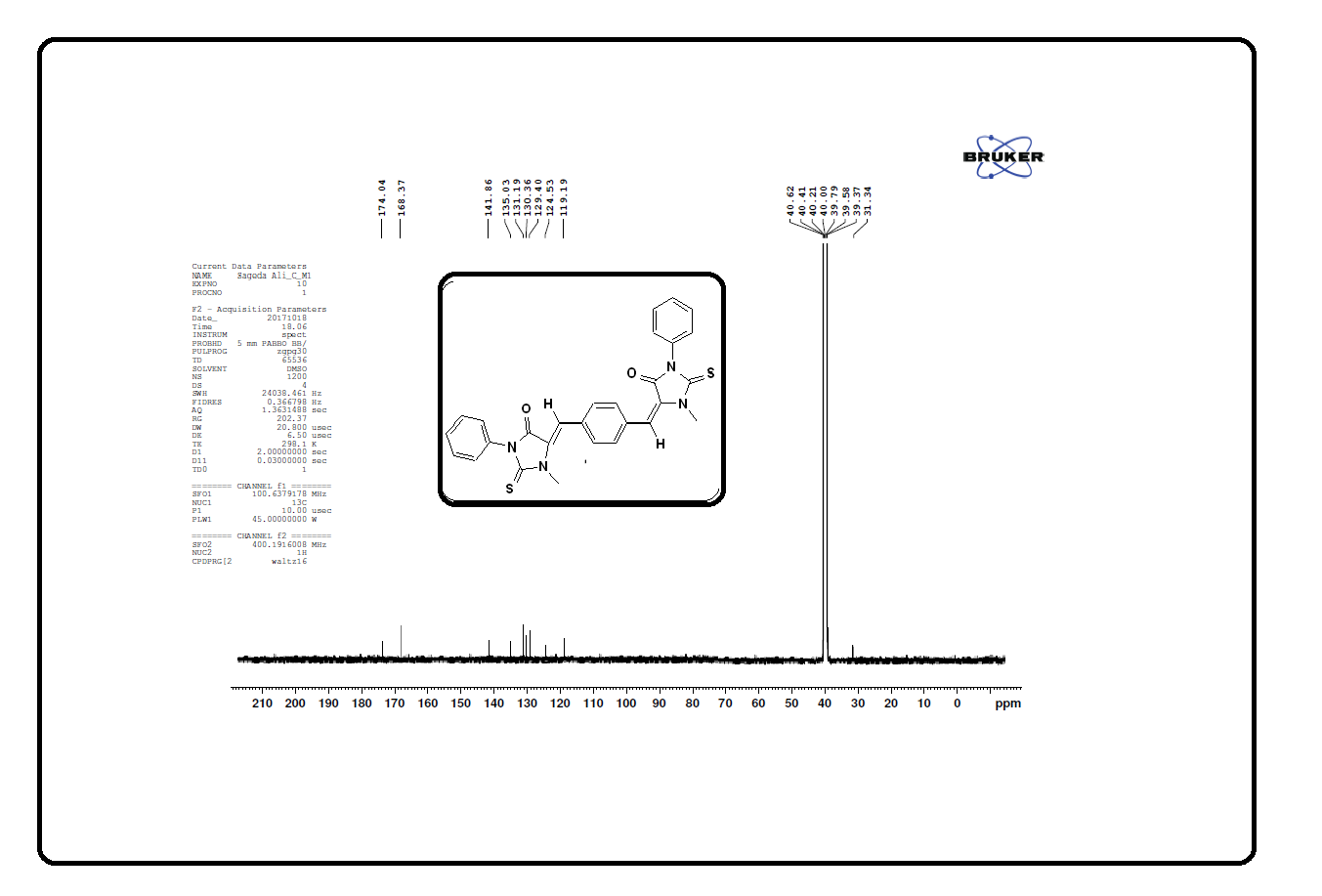
**Figure S 9.** 3D optimized structures and relative energies calculated at B3LYP/6-31+G\* of *Z*- and *E*-isomers for **6a**.



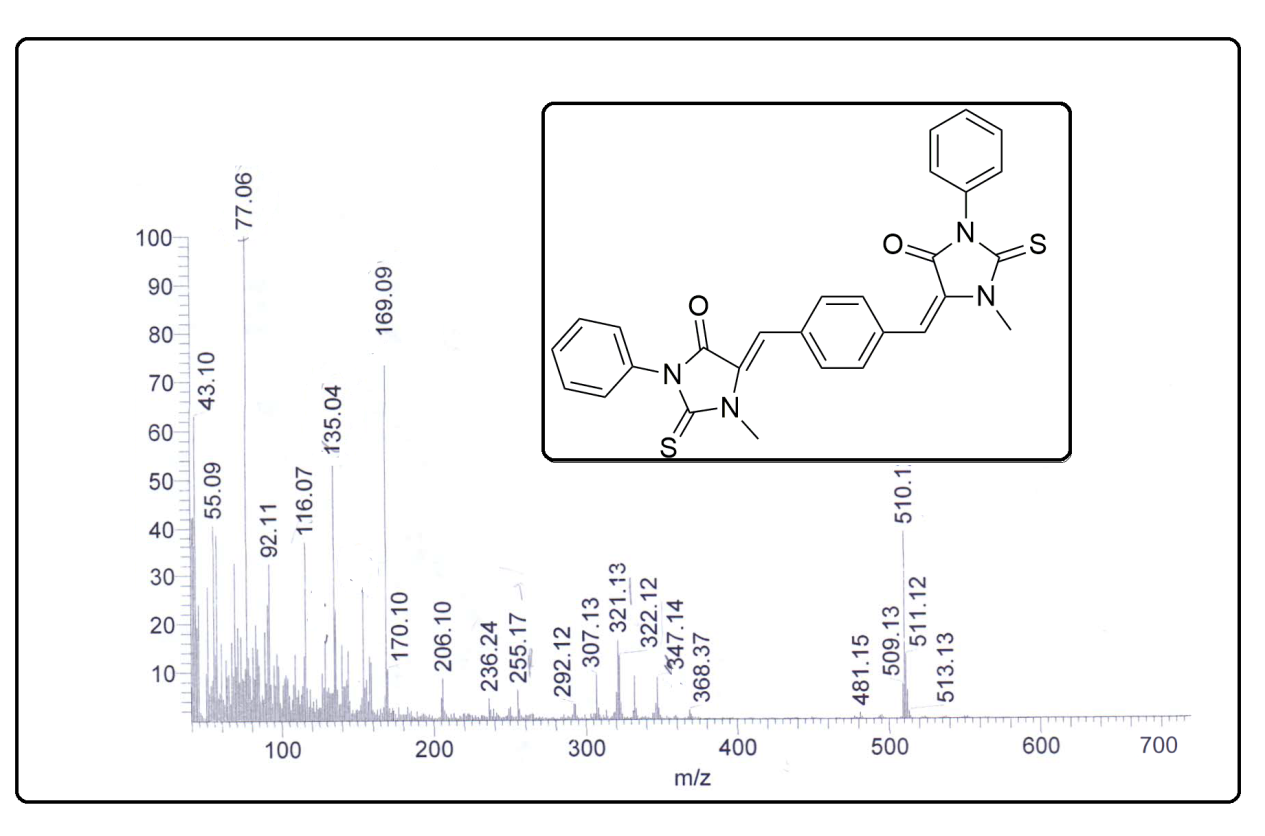
**Figure S 10**.IR spectrum of compound **8a**.



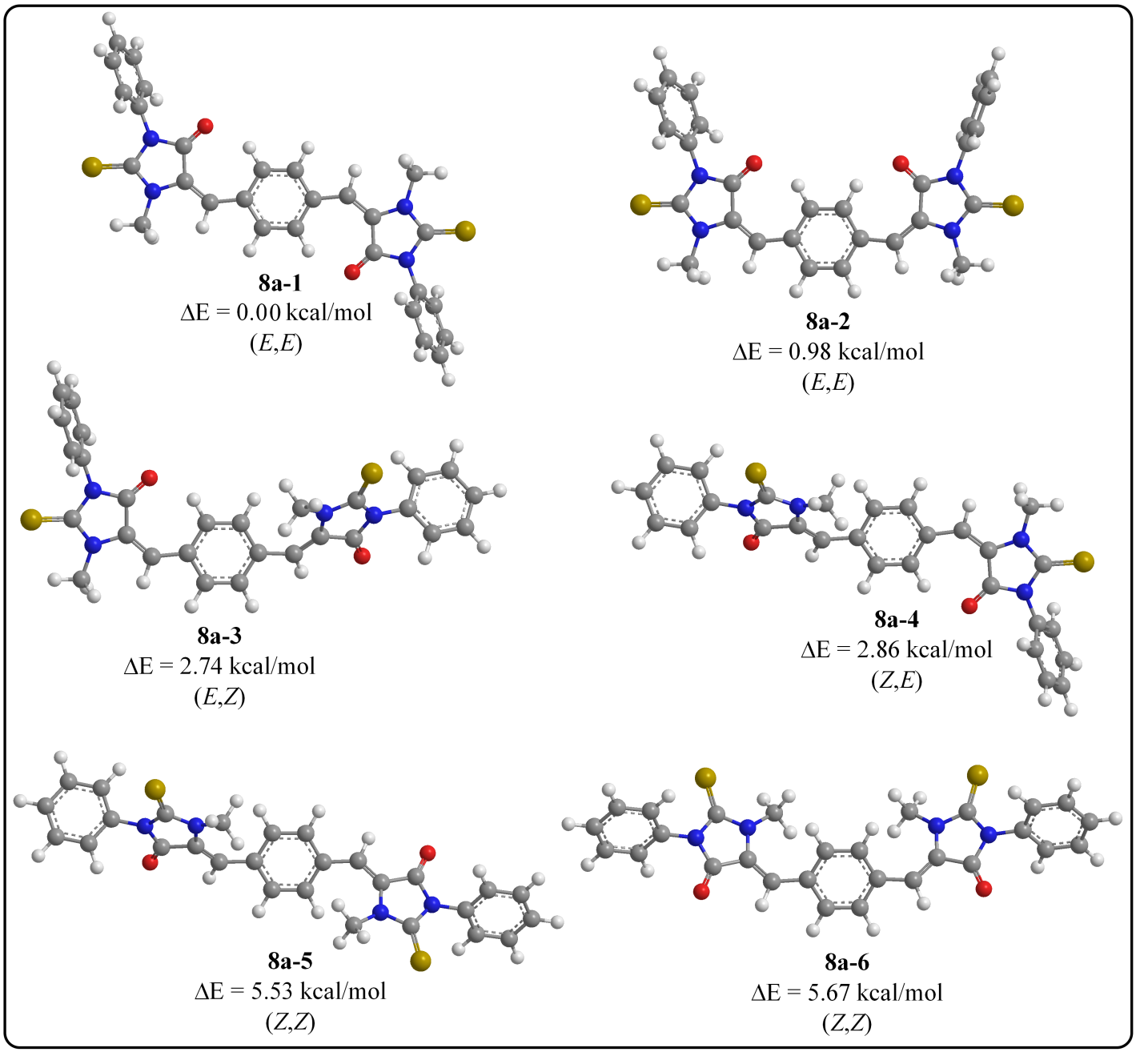
**Figure S 11**.1H-NMR of compound **8a**.



**Figure S 12**.13C-NMR of compound **8a**.



**Figure S 13**.Mass spectrum of compound **8a**.



**Figure S 14.** 3D optimized structures and relative energies calculated at B3LYP/6-31+G\* of *Z*- and *E*-isomers for **8a**.