Synthesis, Characterization, Spectroscopy, X-ray structure and Gaussian hybrid computational investigation of (−)-(S)-1-[2-(benzenesulfonamido)-3-phenylpropanoyl]-4-[(4-methyl)phenyl]thiosemicarbazide

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**Supplemental Materials**

# **Figure S 1** The calculated [DFT/B3LYP/6-31G(d, p) and DFT/B3LYP/6-31G+(d, p) levels] and experimental FT-IR spectra of the title compound (cm-1).

# **Figure S2** Correlation graphic of calculated and experimental vibrational frequencies of title compound (cm-1).

**Figure S 3** a) 1H-NMR and b) 13C-NMR spectra of the title compound.

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| **a)** |
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| **b)****C:\Users\Sibel\Desktop\Adsız.png** |

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**Figure S 4** Experimental UV-Vis spectra of the title compound.