

## Supporting Information

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### Molecular docking and antioxidant activity studies of imidodithiocarbonate derivatives containing pyrimidine

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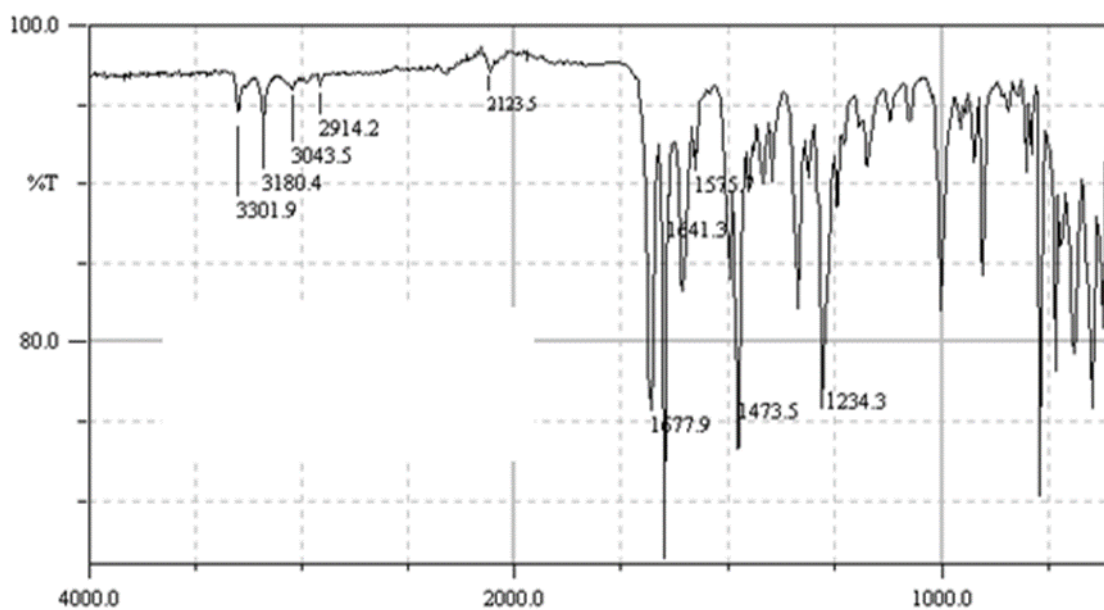
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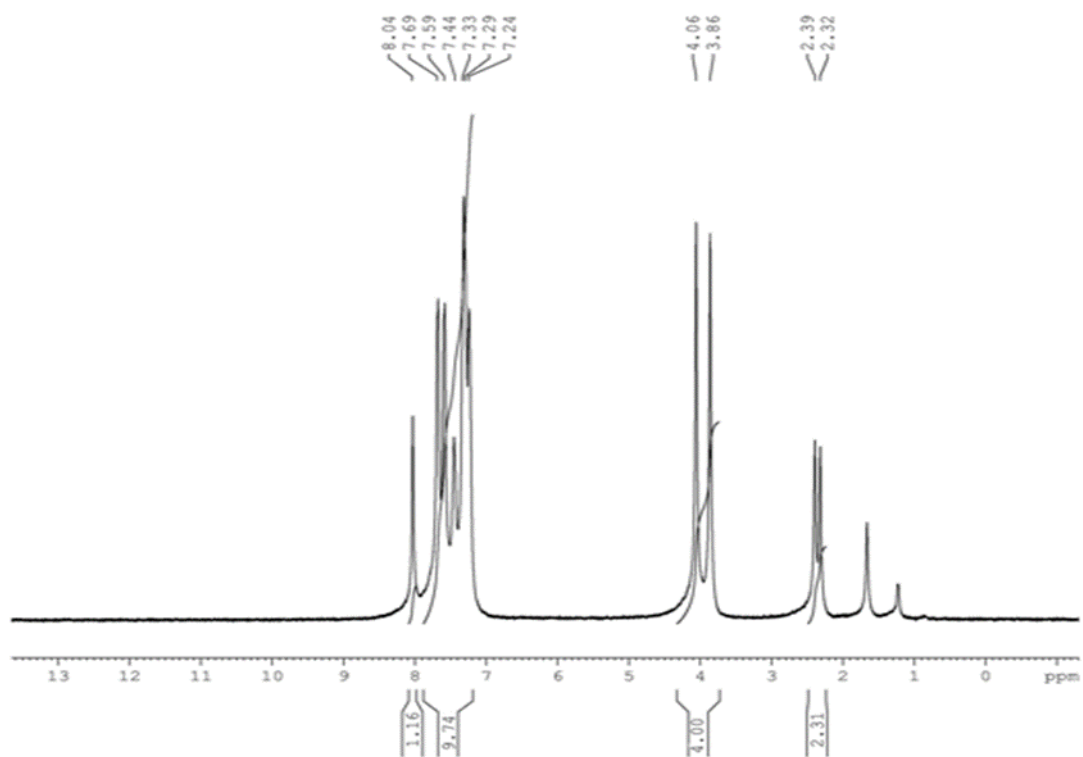
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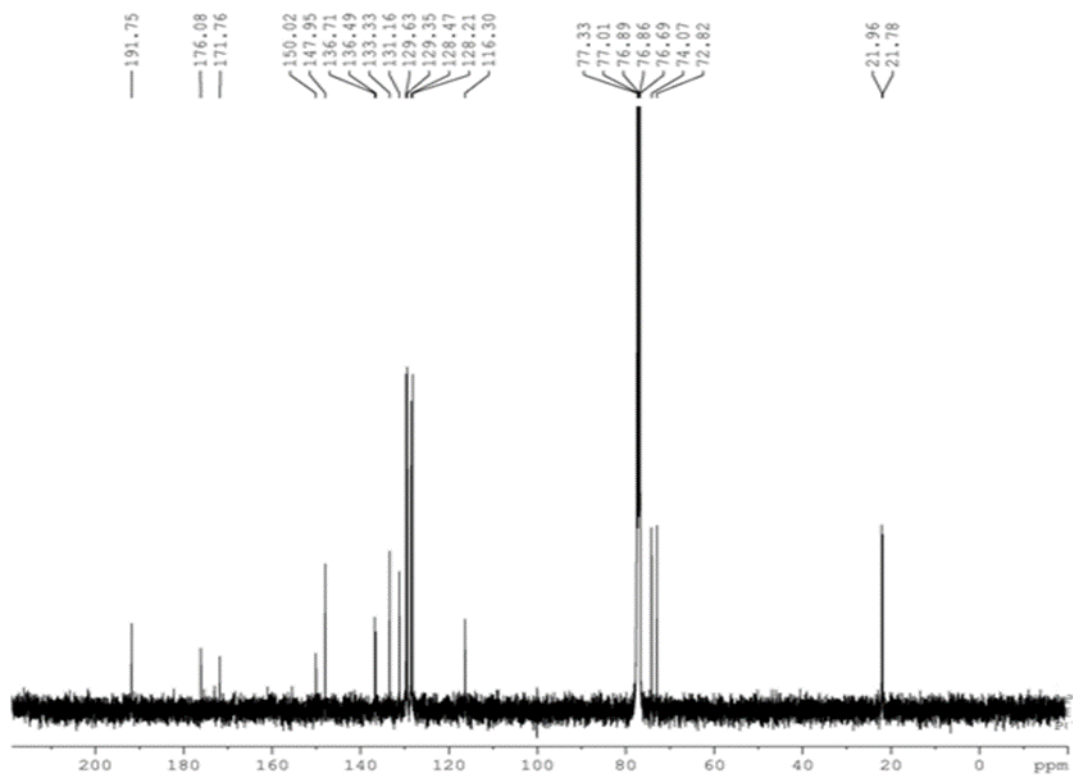
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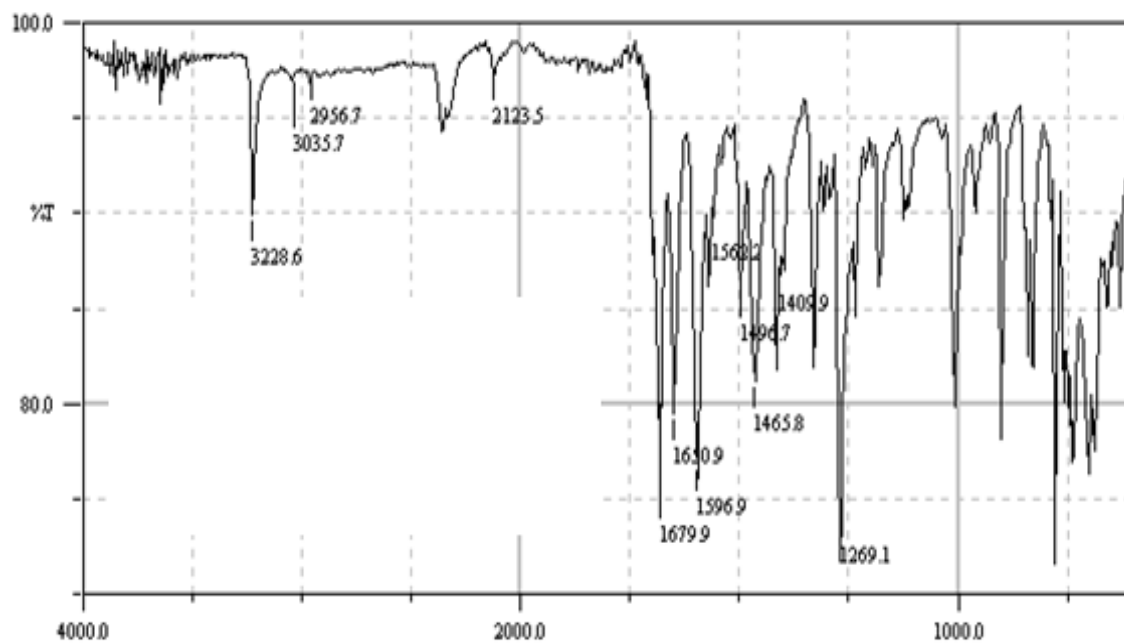
**Figure S1:** FT-IR Spectrum of **3a**



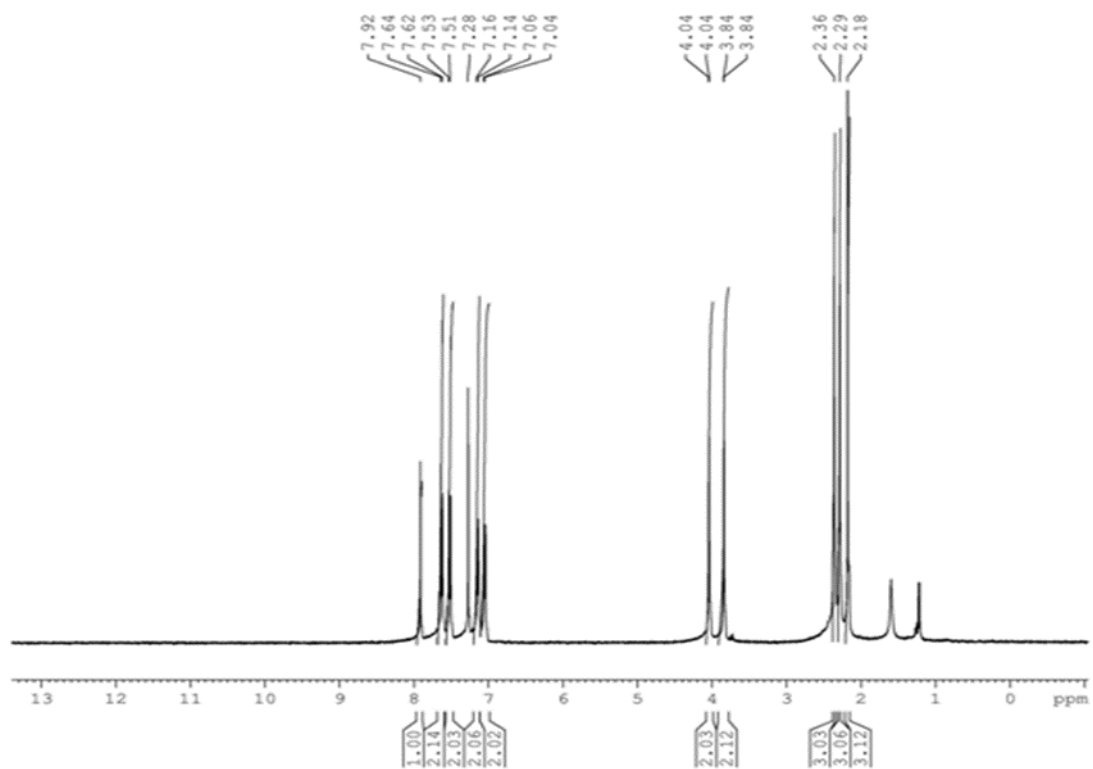
**Figure S2:**  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ ) Spectrum of **3a**



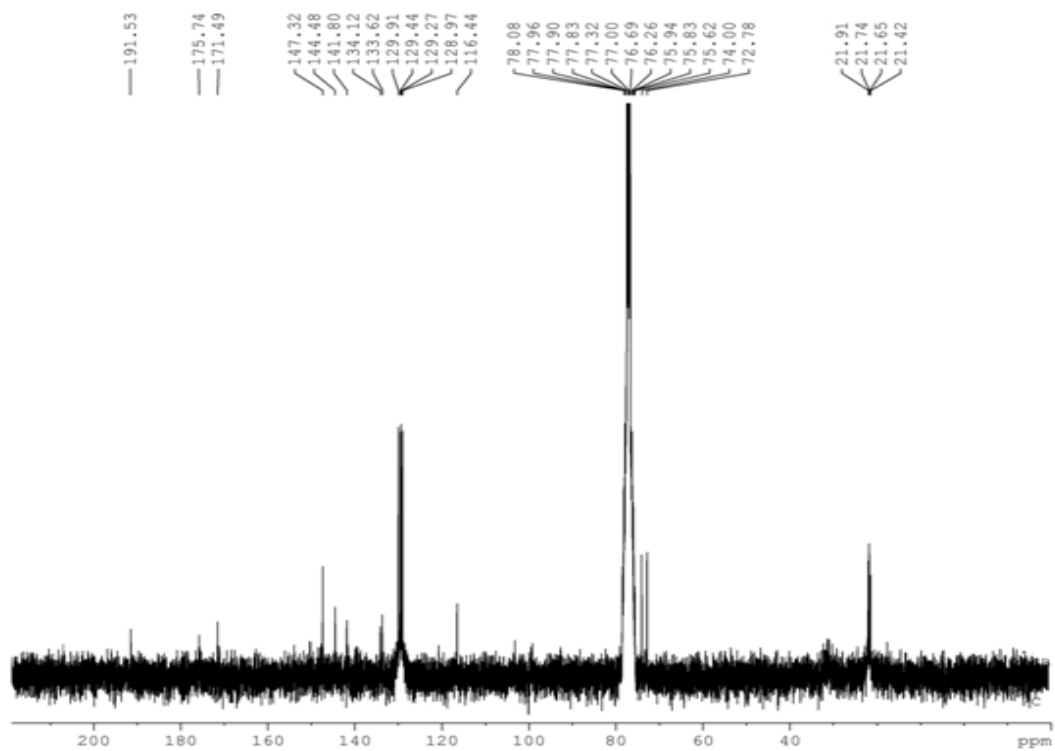
**Figure S3:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ ) Spectrum of **3a**



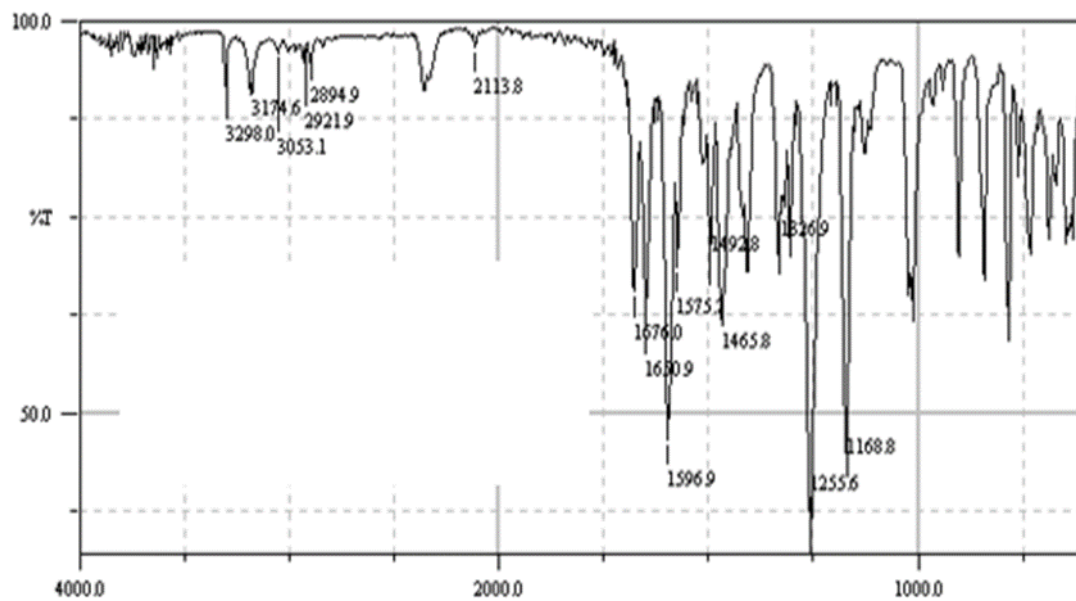
**Figure S4:** FT-IR Spectrum of **3b**



**Figure S5:** <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) Spectrum of **3b**

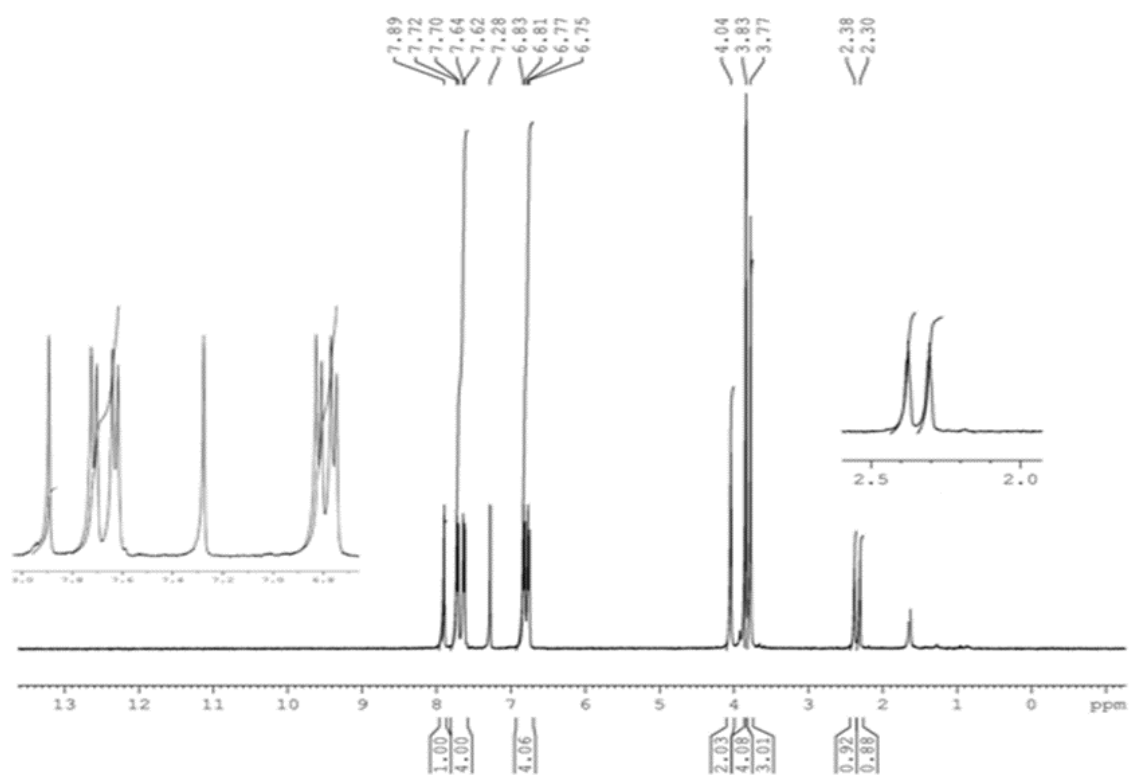


**Figure S6:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ ) Spectrum of **3b**

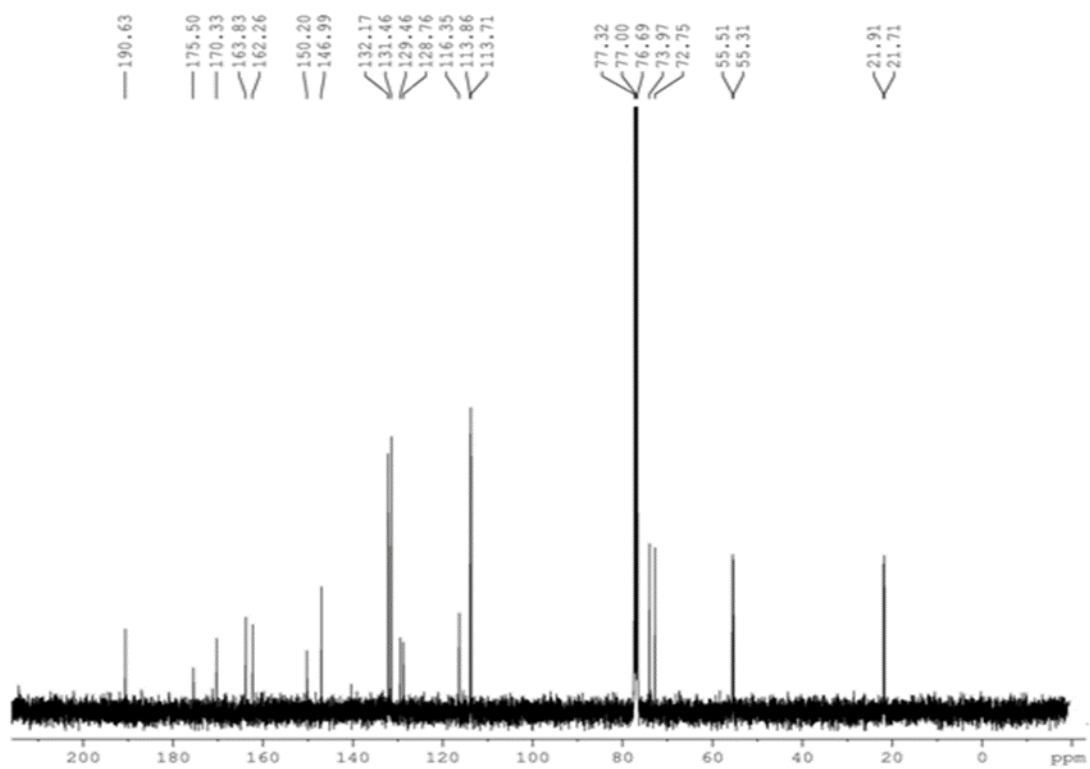


**Figure S7:** FT-IR Spectrum of **3c**





**Figure S8:**  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ ) Spectrum of **3c**



**Figure S9:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ ) Spectrum of **3c**