



STRUCTURAL  
CHEMISTRY

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2 **Volume 79 (2023)**

3 **Supporting information for article:**

4 **Crystallographic, spectroscopic, and thermal studies of 1-(4-bromophenyl)-5-**  
5 **(2,5-dimethyl-1*H*-pyrrol-1-yl)-3-methyl-1*H*-pyrazole**

6 **Erika Moreno-Suárez, Rafael Avila-Acosta, Karen Sánchez-Ramírez, Juan-Carlos Castillo and Mario**

7 **A. Macías**

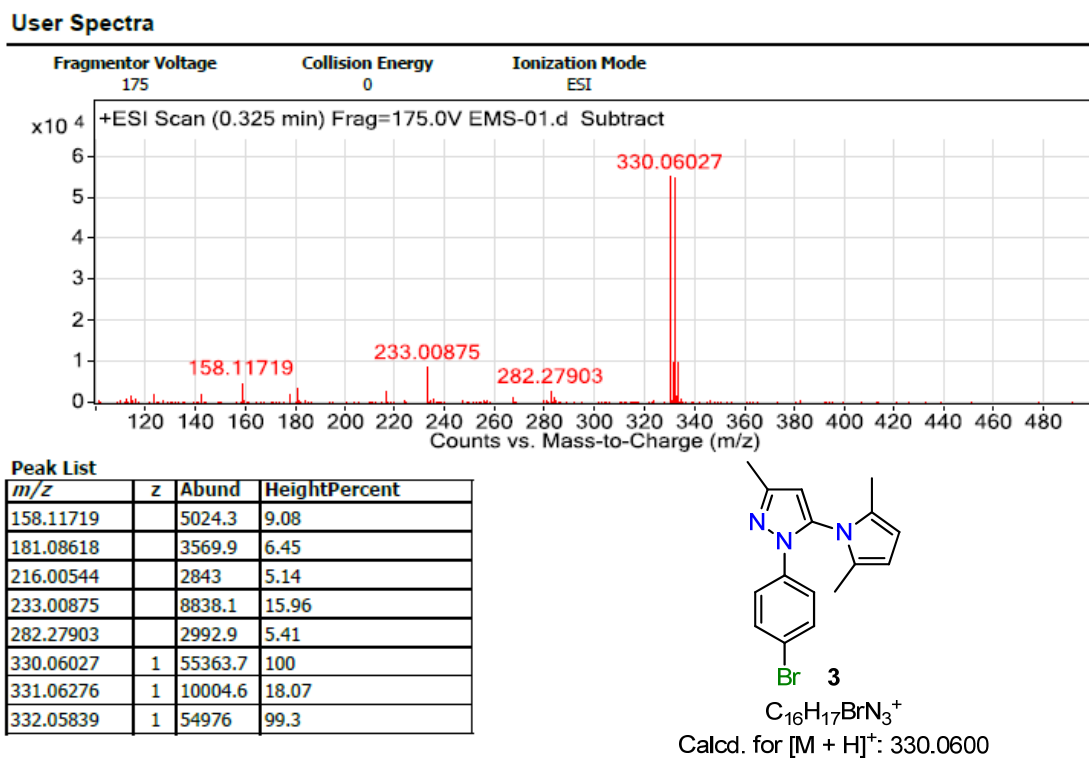
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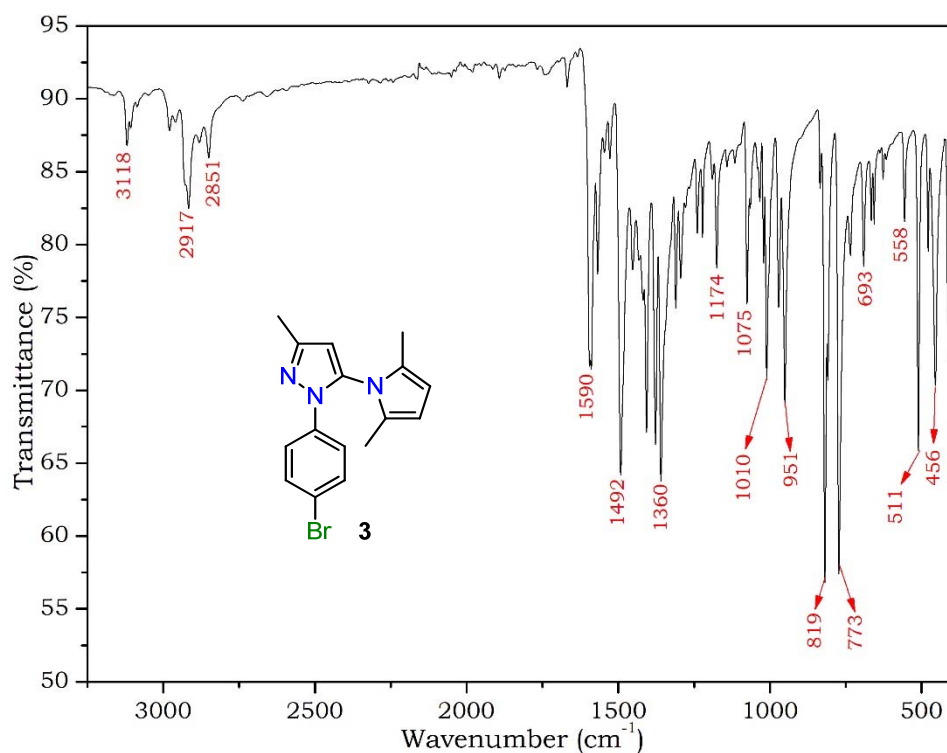
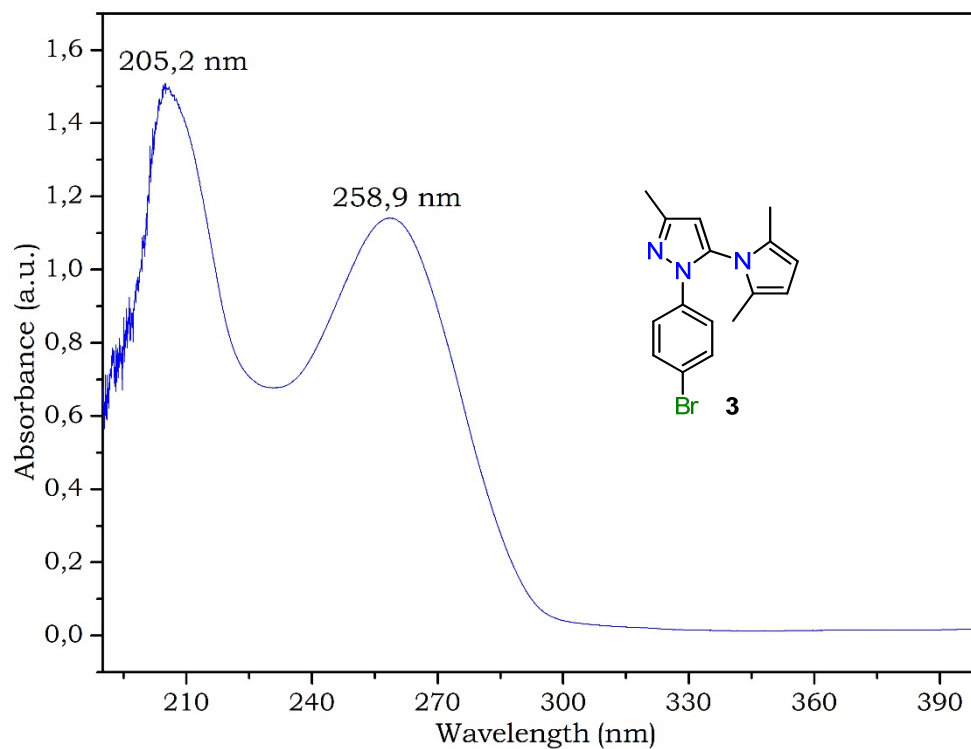
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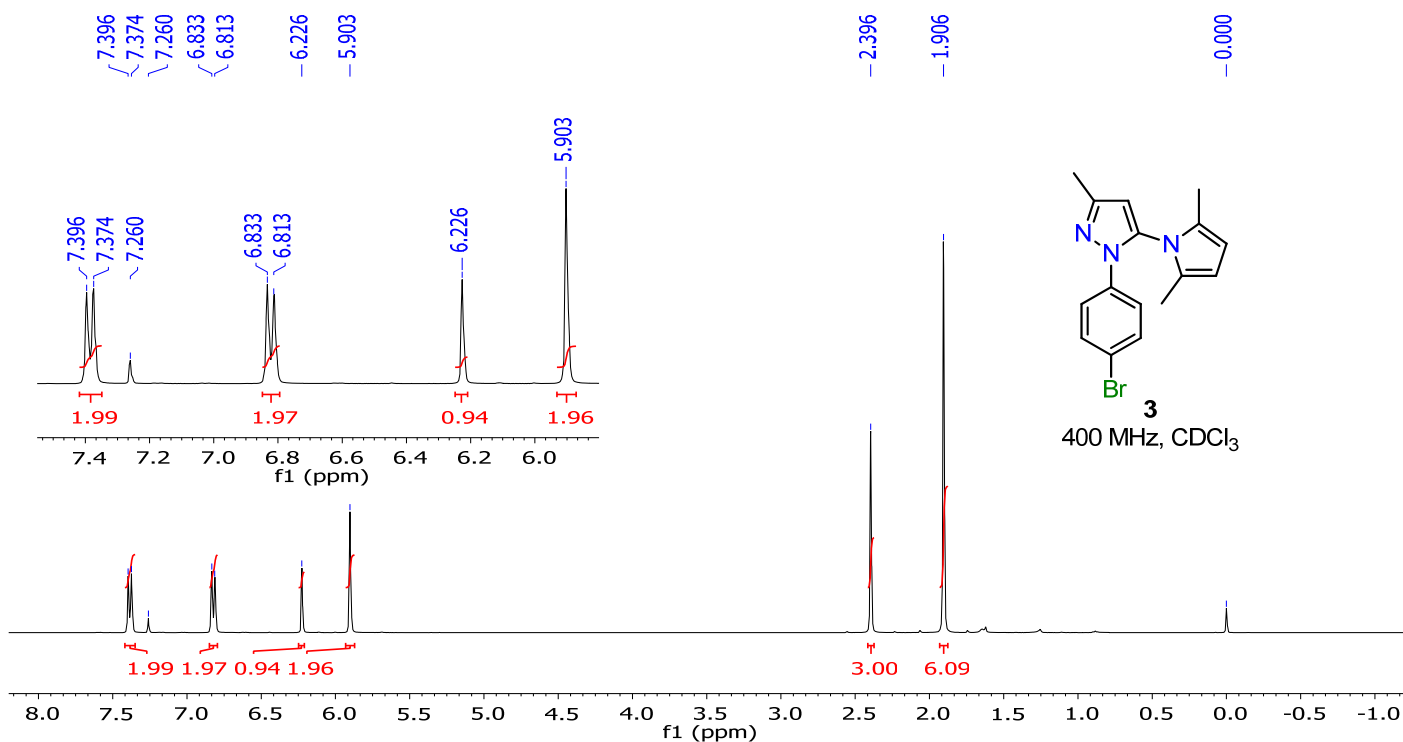
## SUPPORTING INFORMATION

## Content

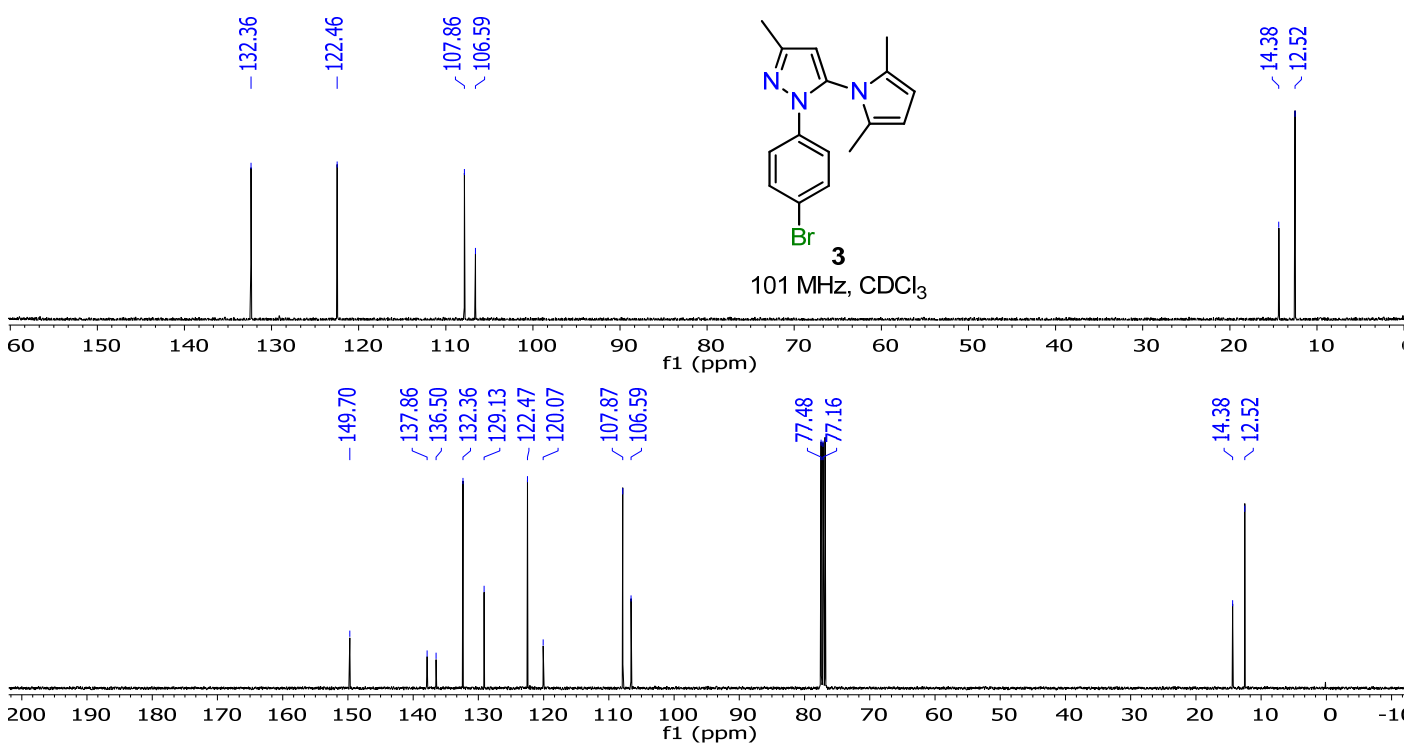
1. Copy of the HRMS spectrum for compound **3**.....p. S2
2. Copy of the IR spectrum for compound **3**.....p. S2
3. Copy of the UV–Vis spectrum for compound **3**.....p. S3
4. Copies of NMR spectra for compound **3**.....p. S3

1. Copy of the HRMS spectrum for compound **3**Figure S1: HRMS spectrum for the compound **3**.

39 **2. Copy of the IR spectrum for compound 3**40  
41 **Figure S2:** IR spectrum for the compound 3 (ATR technique).  
4243 **3. Copy of the UV–Vis spectrum for compound 3**  
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46 **Figure S3:** UV–Vis spectrum for the compound 3 (50 μM in MeOH).  
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48 **4. Copies of NMR spectra for compound 3**

49 **Figure S4:**  $^1\text{H}$ -NMR spectrum for the compound **3**.



52 **Figure S5:**  $^{13}\text{C}\{^1\text{H}\}$ -NMR and DEPT-135 spectra for the compound **3**.

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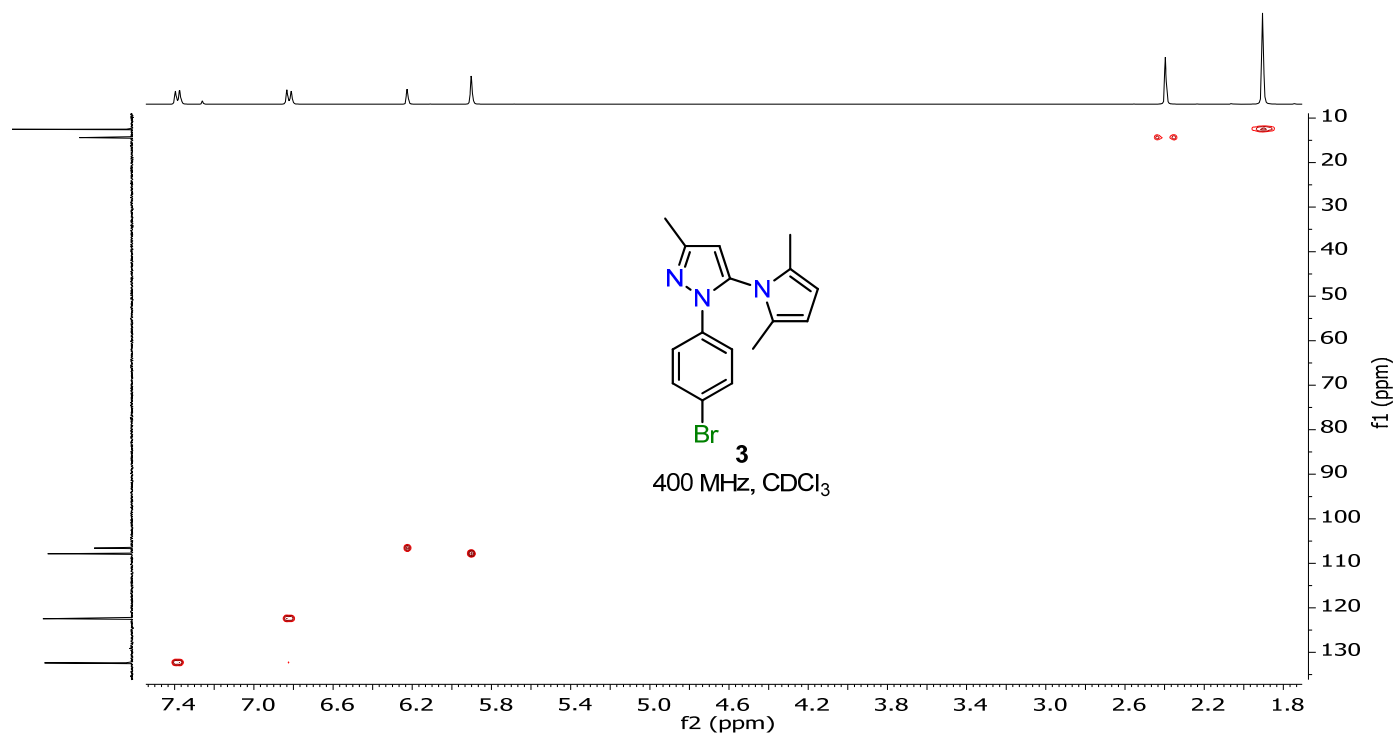


Figure S6: HSQC spectrum for the compound **3**.

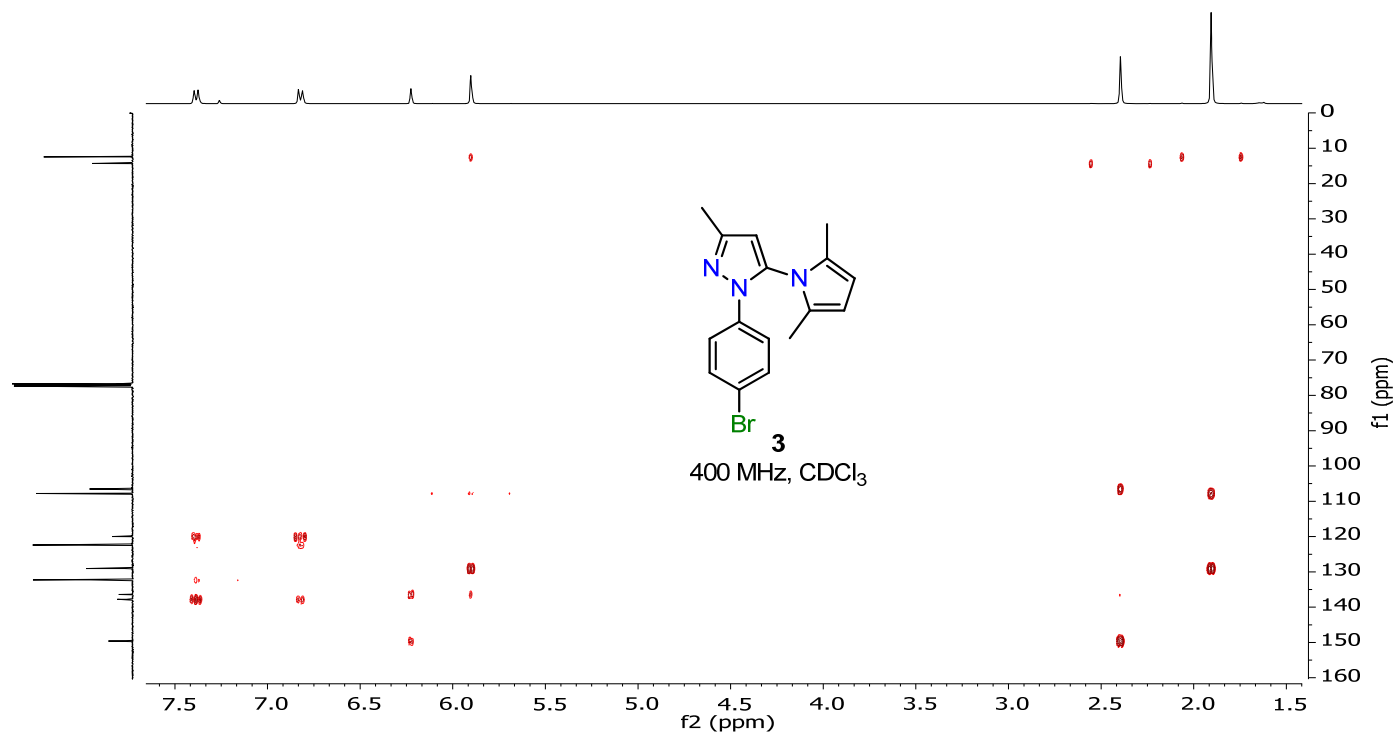
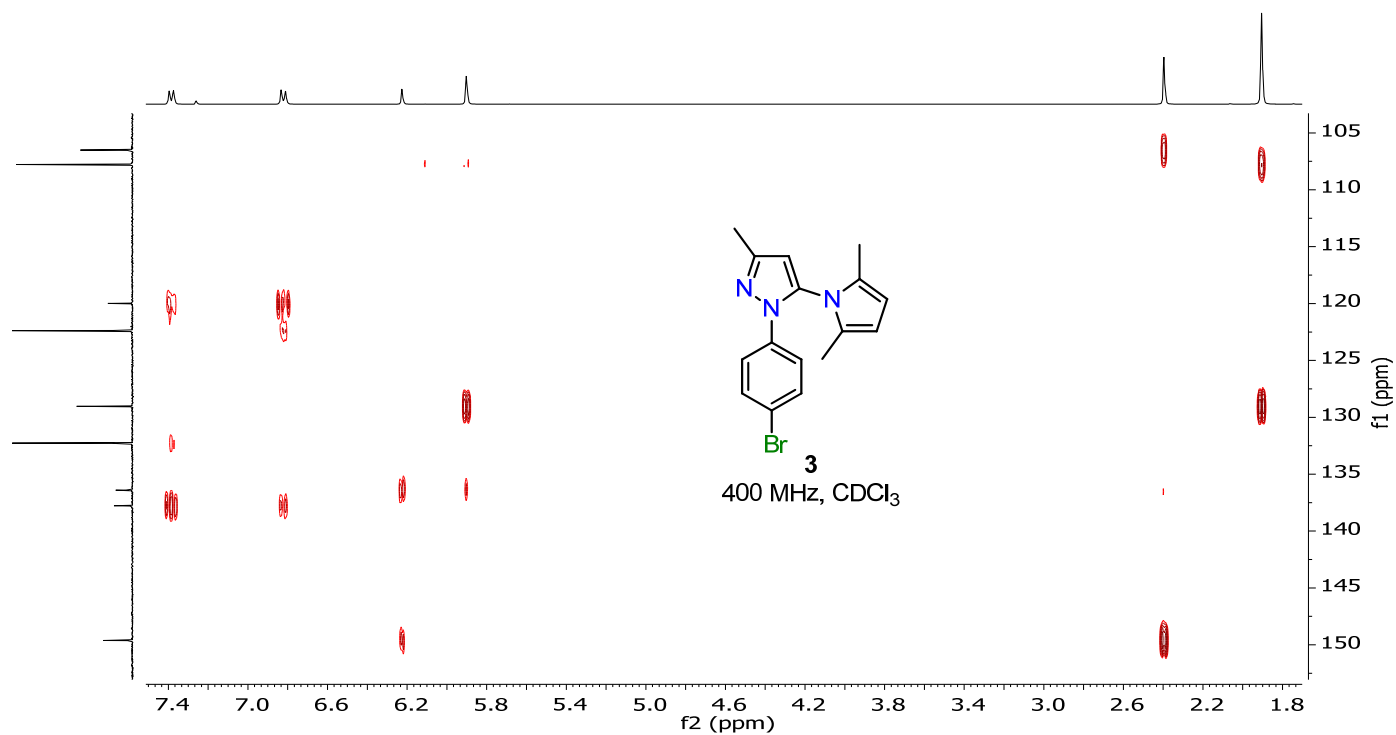
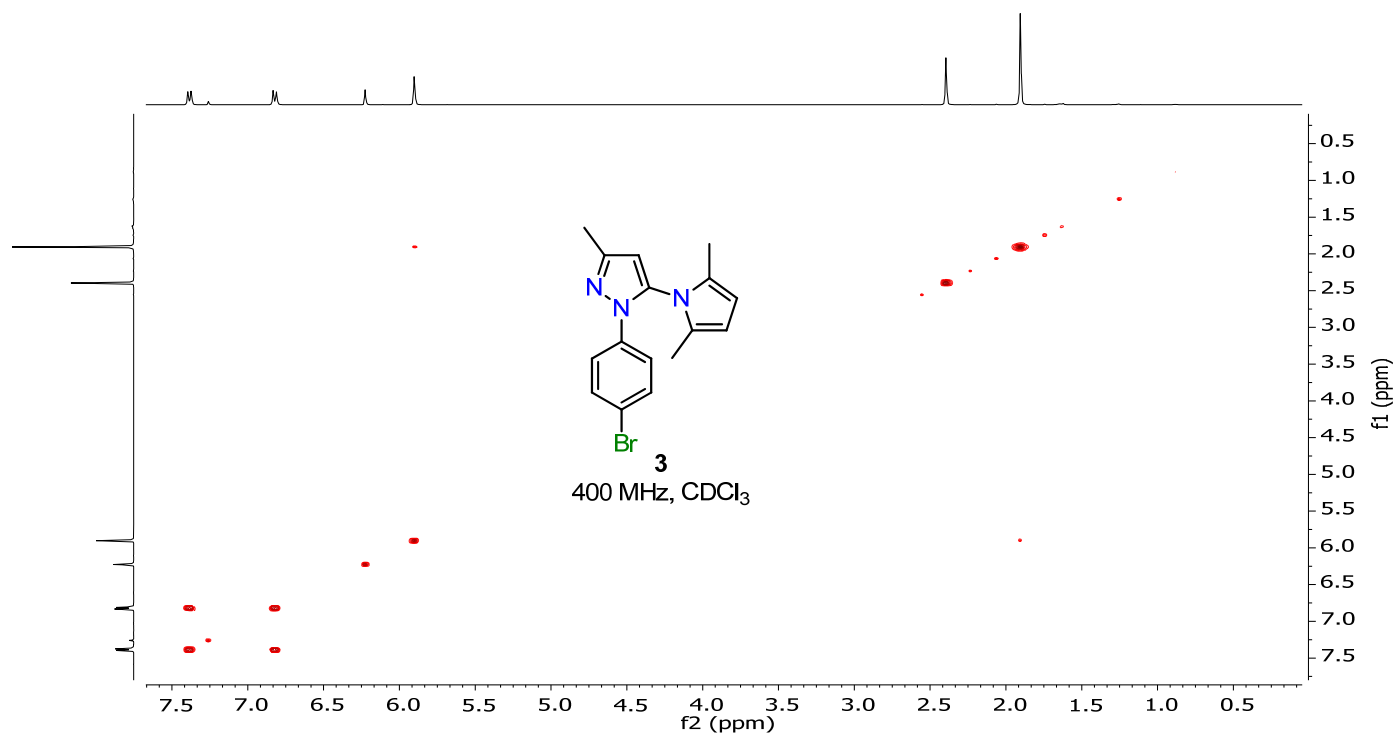


Figure S7: HMBC spectrum for the compound **3**.



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**Figure S8:** Expansion of the HMBC spectrum for the compound 3.



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**Figure S9:** COSY spectrum for the compound 3.