



STRUCTURAL  
CHEMISTRY

1

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**

8

9

10

11

12  
13  
14 Content

15

- 16 1. Copy of the HRMS spectrum for compound 3.....p. S2  
 17 2. Copy of the IR spectrum for compound 3.....p. S2  
 18 3. Copy of the UV–Vis spectrum for compound 3.....p. S3  
 19 4. Copies of NMR spectra for compound 3.....p. S3

20

21

22

23

24

25

26

27

28

29

30

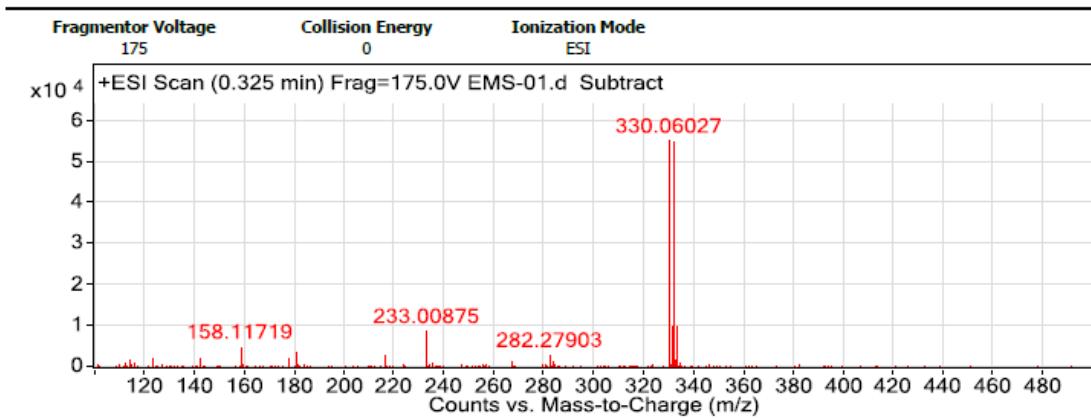
31

32

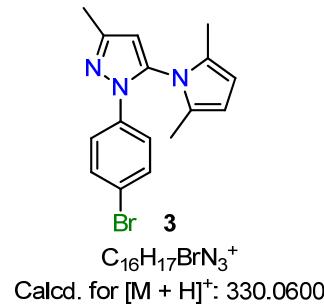
33

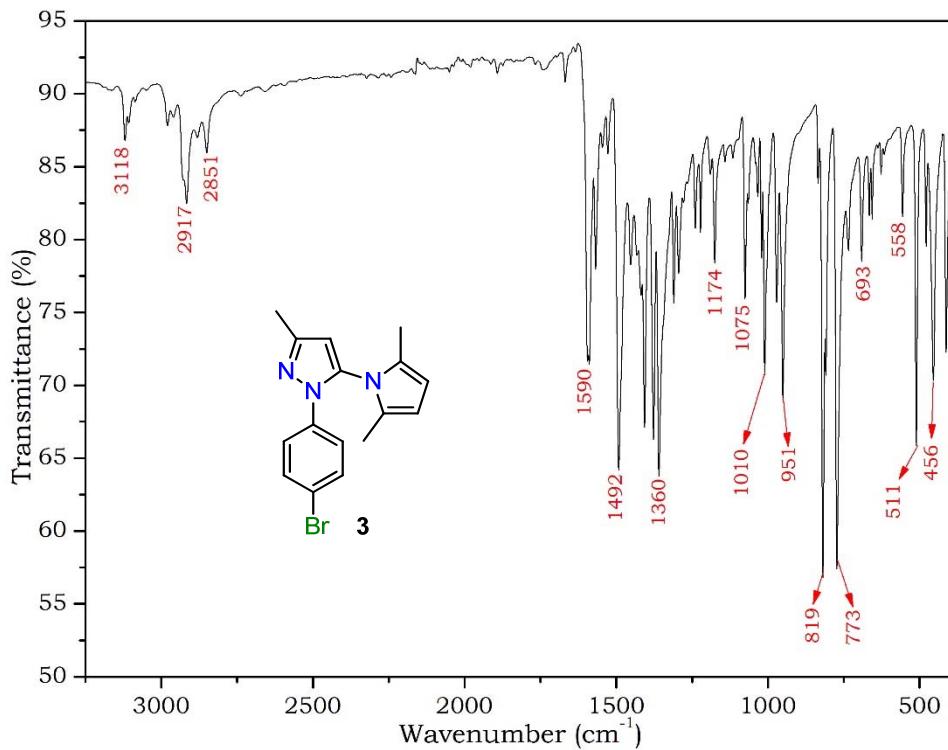
34

35

36 **1. Copy of the HRMS spectrum for compound 3****User Spectra****Peak List**

m/z	z	Abund	HeightPercent
158.11719		5024.3	9.08
181.08618		3569.9	6.45
216.00544		2843	5.14
233.00875		8838.1	15.96
282.27903		2992.9	5.41
330.06027	1	55363.7	100
331.06276	1	10004.6	18.07
332.05839	1	54976	99.3

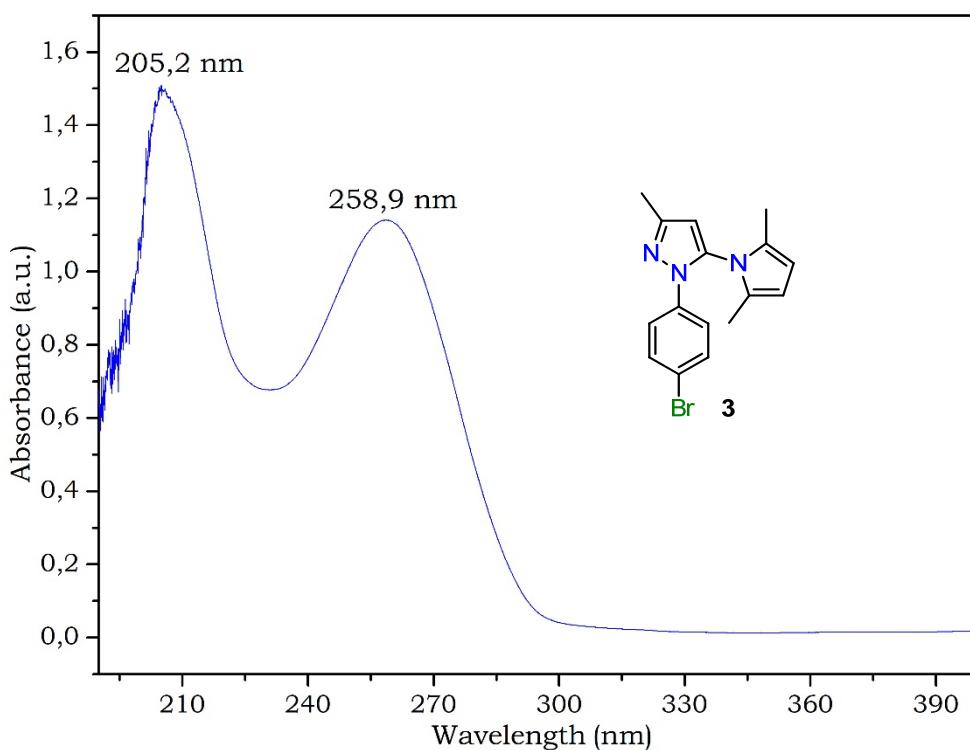
37  
38 **Figure S1:** HRMS spectrum for the compound 3.

39 **2. Copy of the IR spectrum for compound 3**40 **Figure S2:** IR spectrum for the compound 3 (ATR technique).41 **3. Copy of the UV–Vis spectrum for compound 3**

42

43 **3. Copy of the UV–Vis spectrum for compound 3**

44

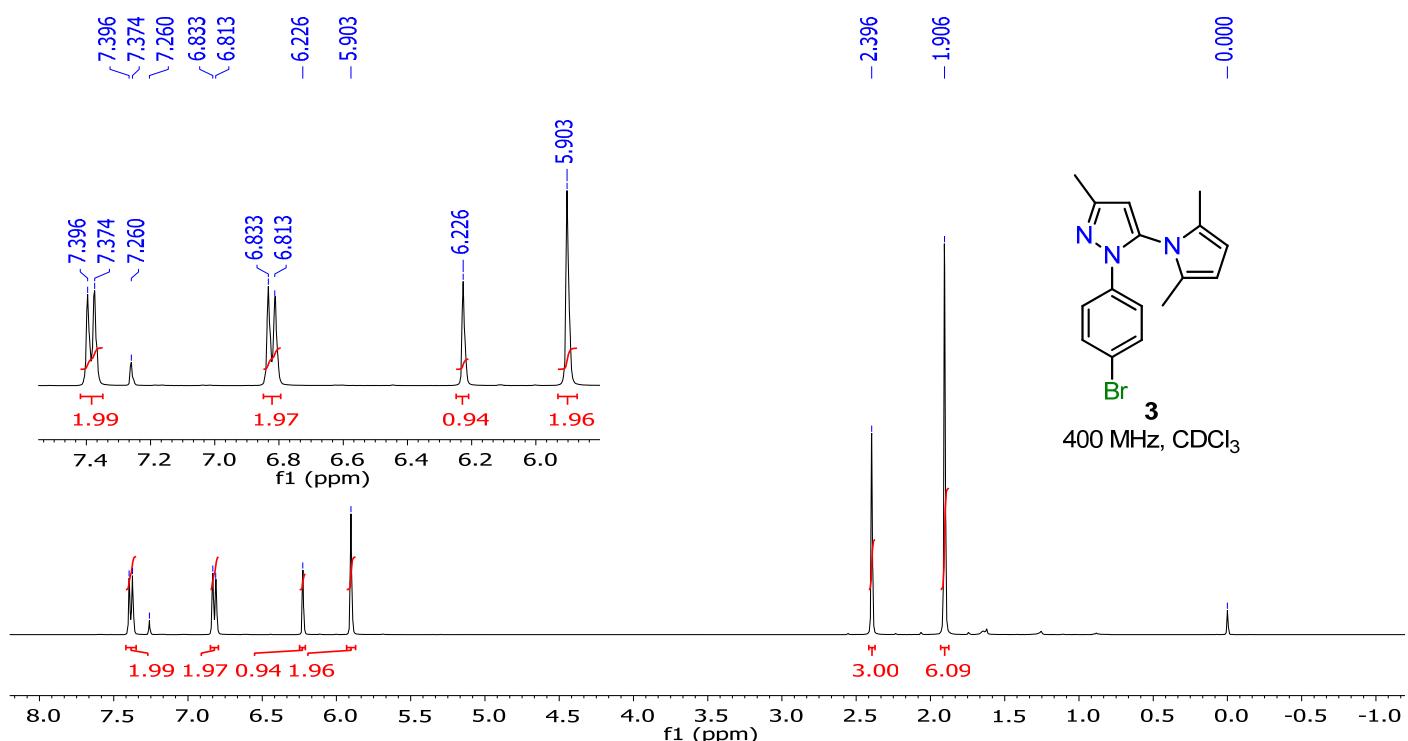
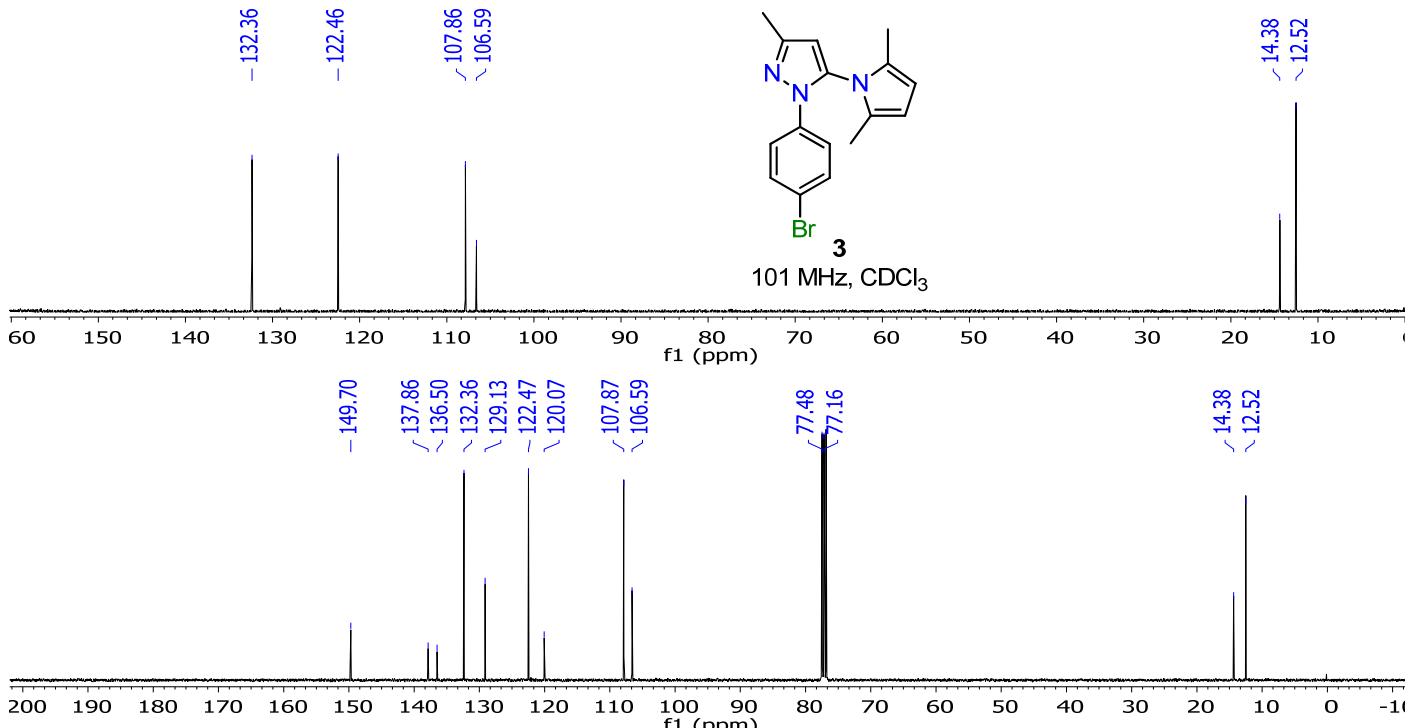


45

46 **Figure S3:** UV–Vis spectrum for the compound 3 (50  $\mu\text{M}$  in MeOH).

47

## 48 4. Copies of NMR spectra for compound 3

50 **Figure S4:**  $^1\text{H}$ -NMR spectrum for the compound 3.53 **Figure S5:**  $^{13}\text{C}\{^1\text{H}\}$ -NMR and DEPT-135 spectra for the compound 3.  
54  
55  
56

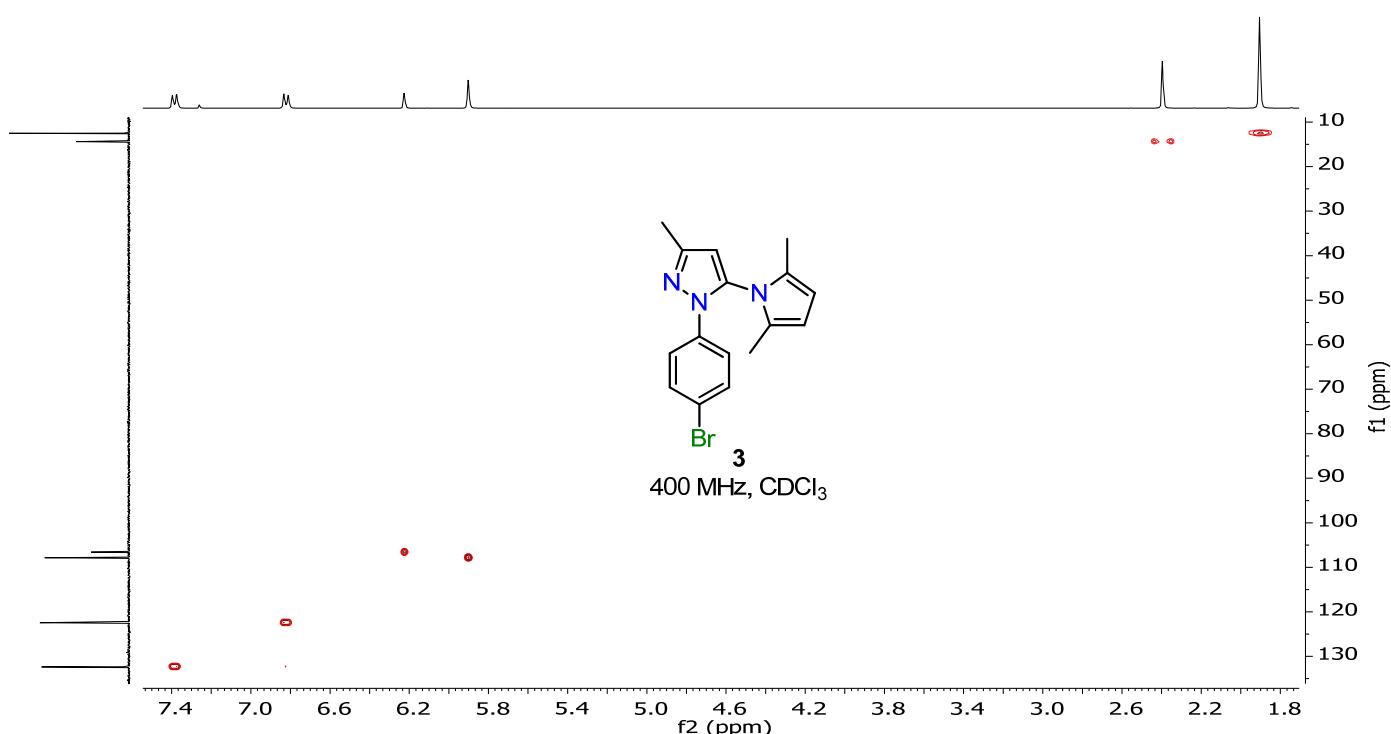


Figure S6: HSQC spectrum for the compound 3.

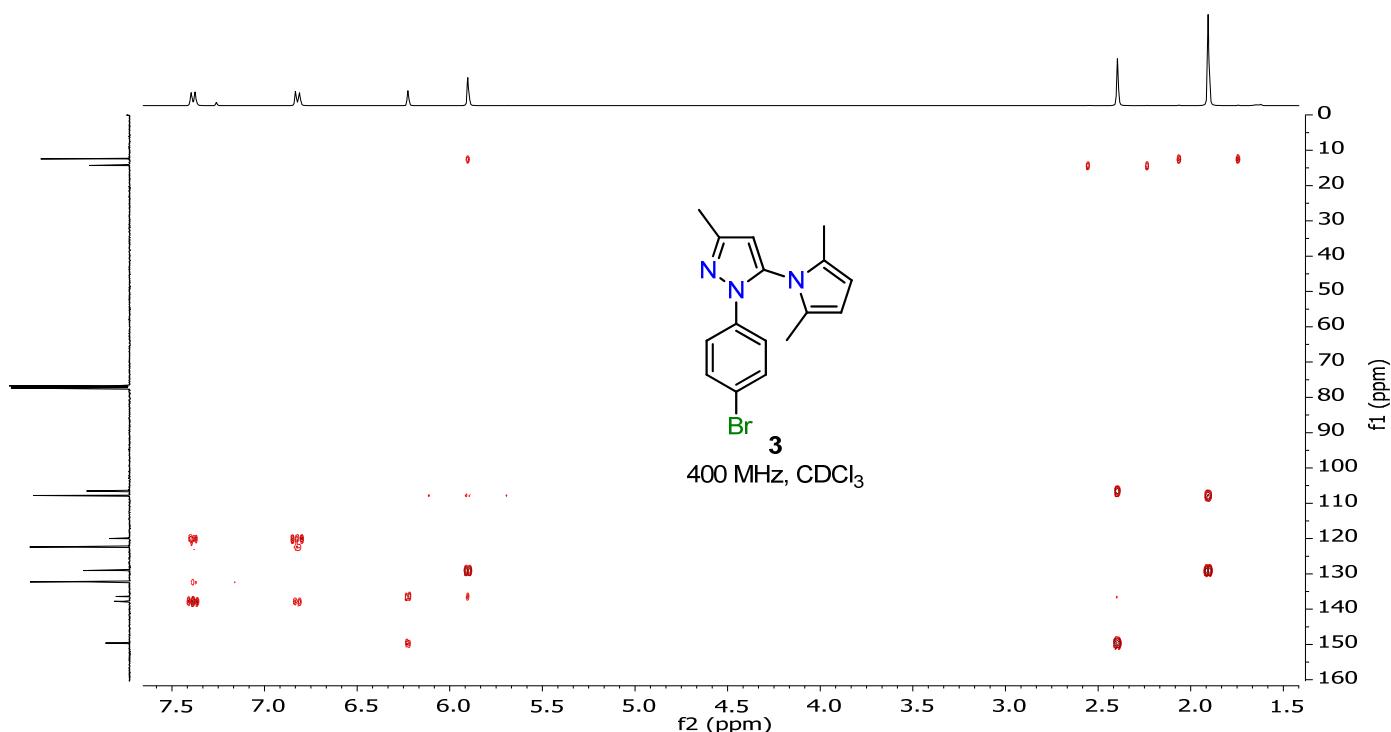
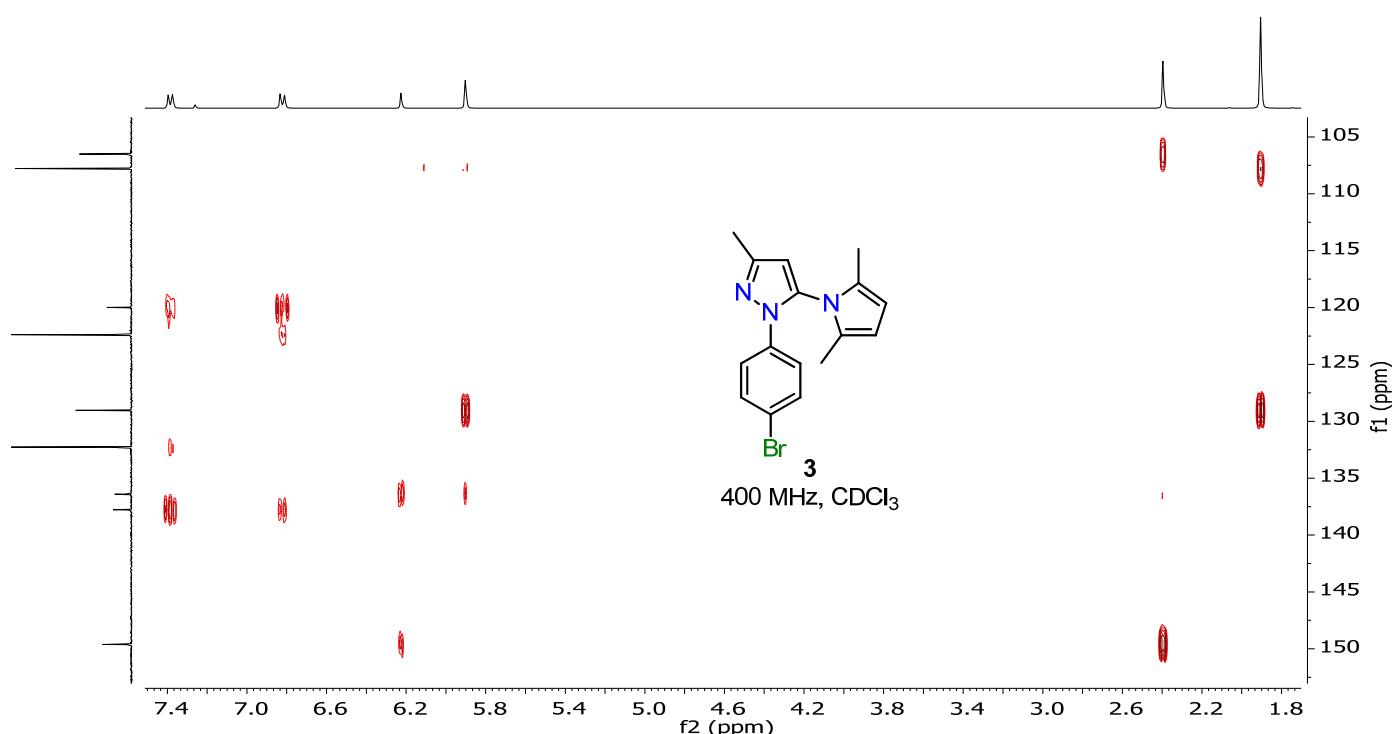
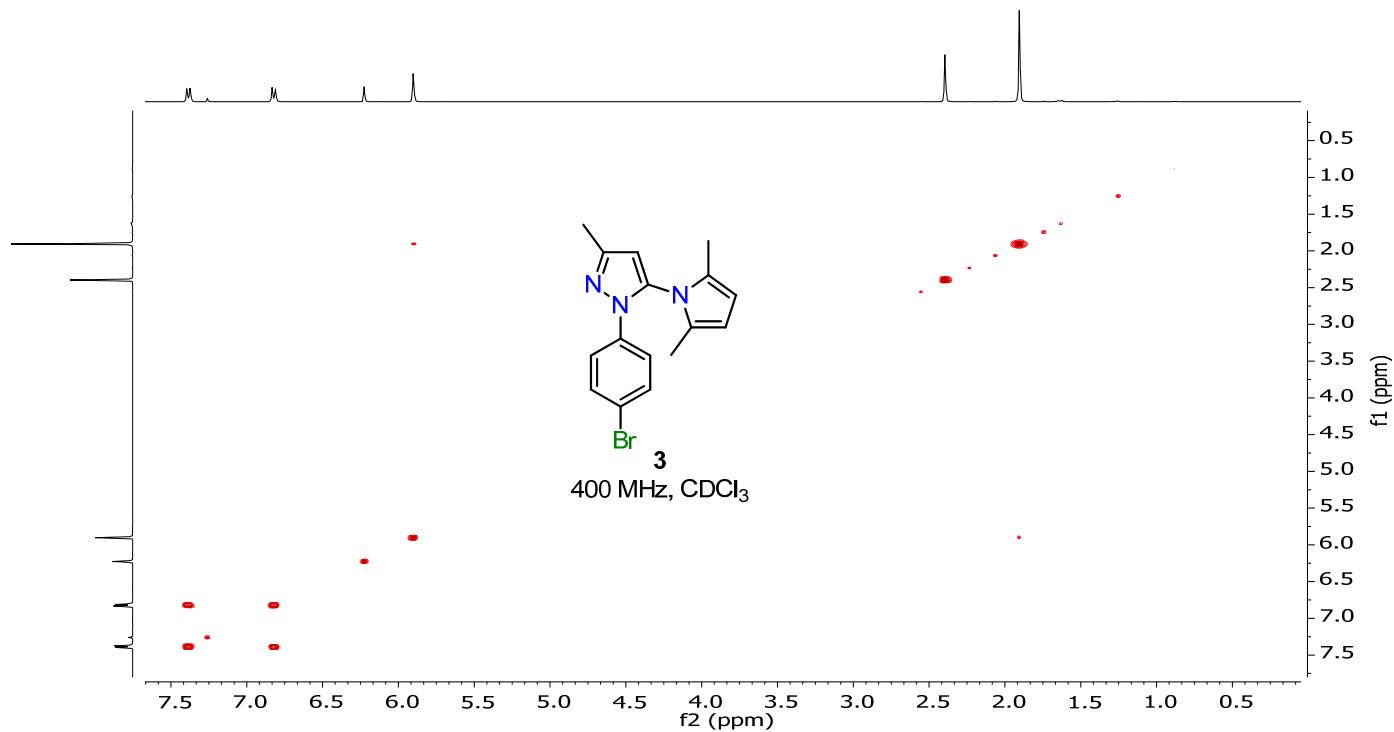


Figure S7: HMBC spectrum for the compound 3.



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



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