

Supplementary materials: 3-(3,4-Dimethoxyphenyl)-5-(2-fluorophenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

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==== Shimadzu LCsolution Analysis Report ====
Department of Chemistry, University of Riau

D:\HPLC Data\PA\PF-SW.lcd

Acquired by : Admin
Sample Name : PF-SW
Sample ID : PF-SW
Vial # :
Injection Volume : 20 uL
Data File Name : PF-SW.lcd
Method File Name : Gr-kalkon 50-90asn.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 03/10/2017 18:38:18
Data Processed : 03/10/2017 19:03:21

<Chromatogram>

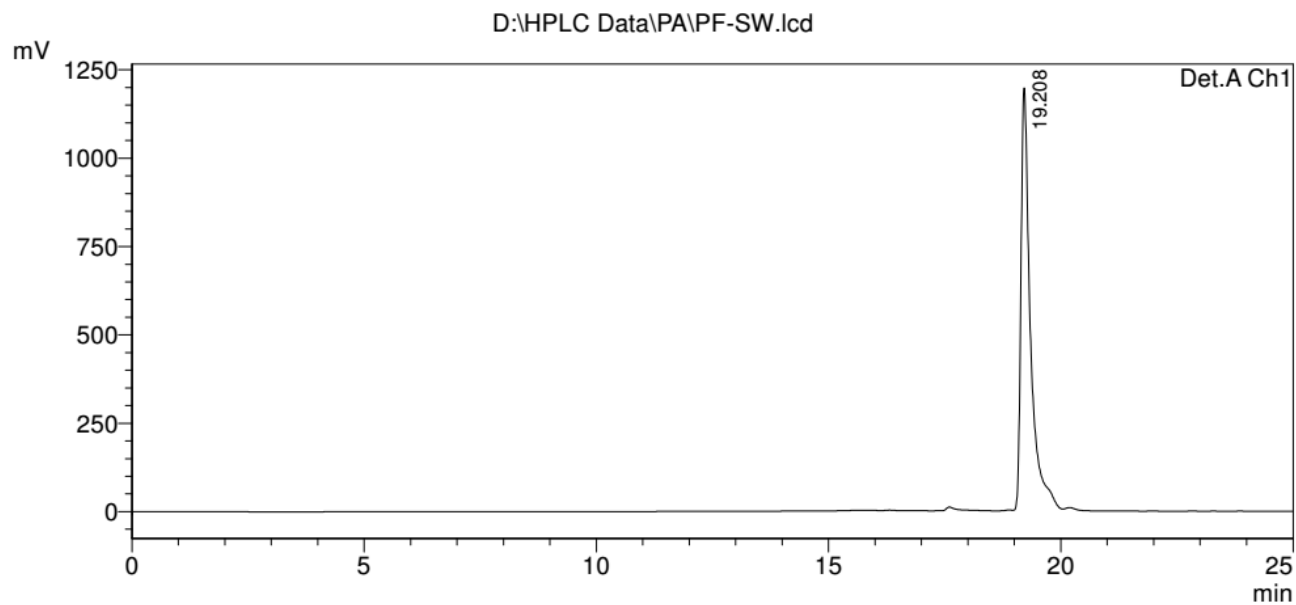


Figure S1. HPLC chromatogram of compound 1.

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

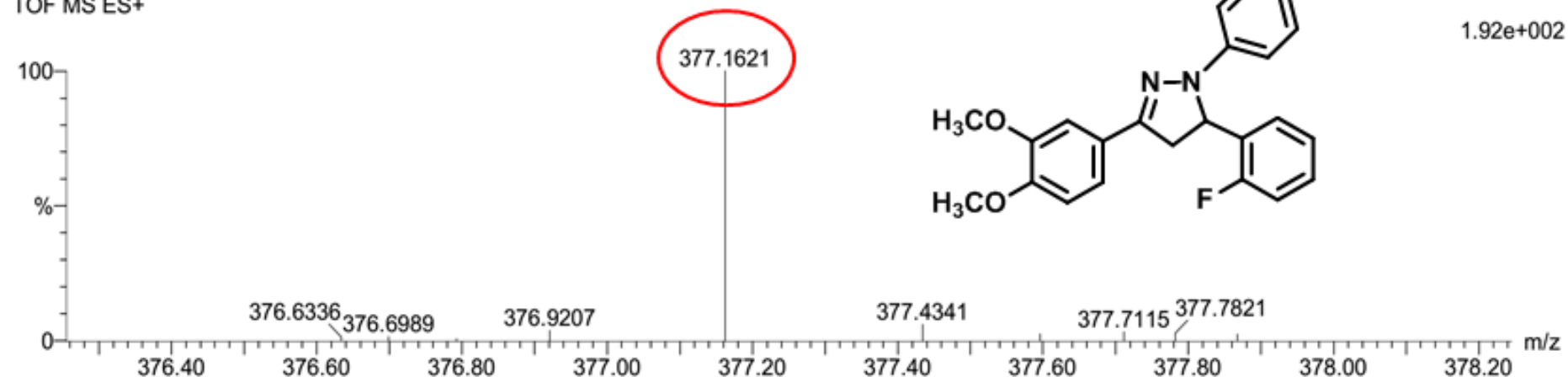
Monoisotopic Mass, Even Electron Ions

1980 formula(e) evaluated with 46 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-1

TOF MS ES+



Minimum: -1.5
Maximum: 10.0 3.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
377.1621	377.1665	-4.4	-11.7	13.5	39.6	4.6	C23 H22 N2 O2 F

Figure S2. TOF HRMS ES+ spectrum of compound 1.

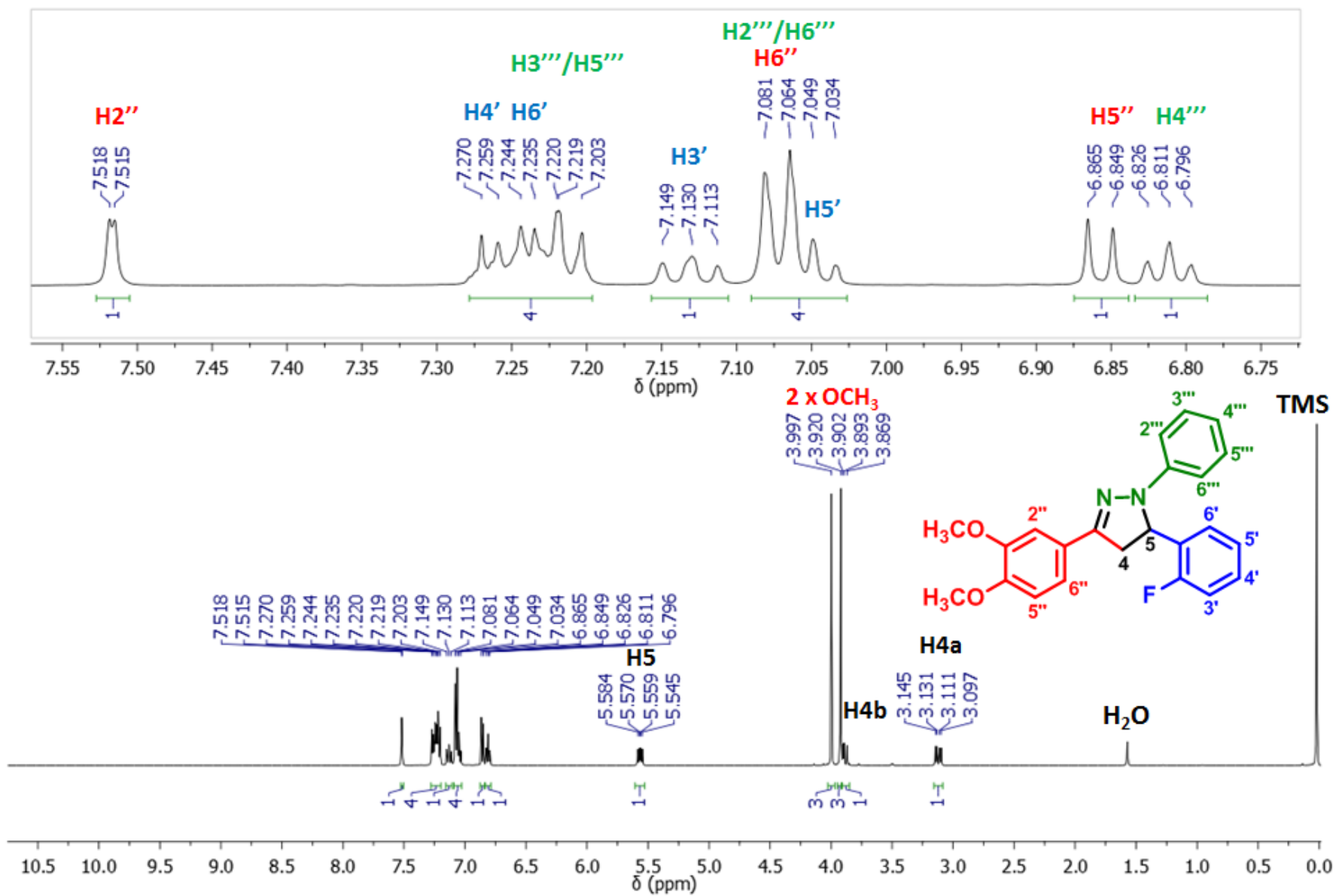


Figure S4. ¹H NMR spectra of compound 1, expanded aromatic region.

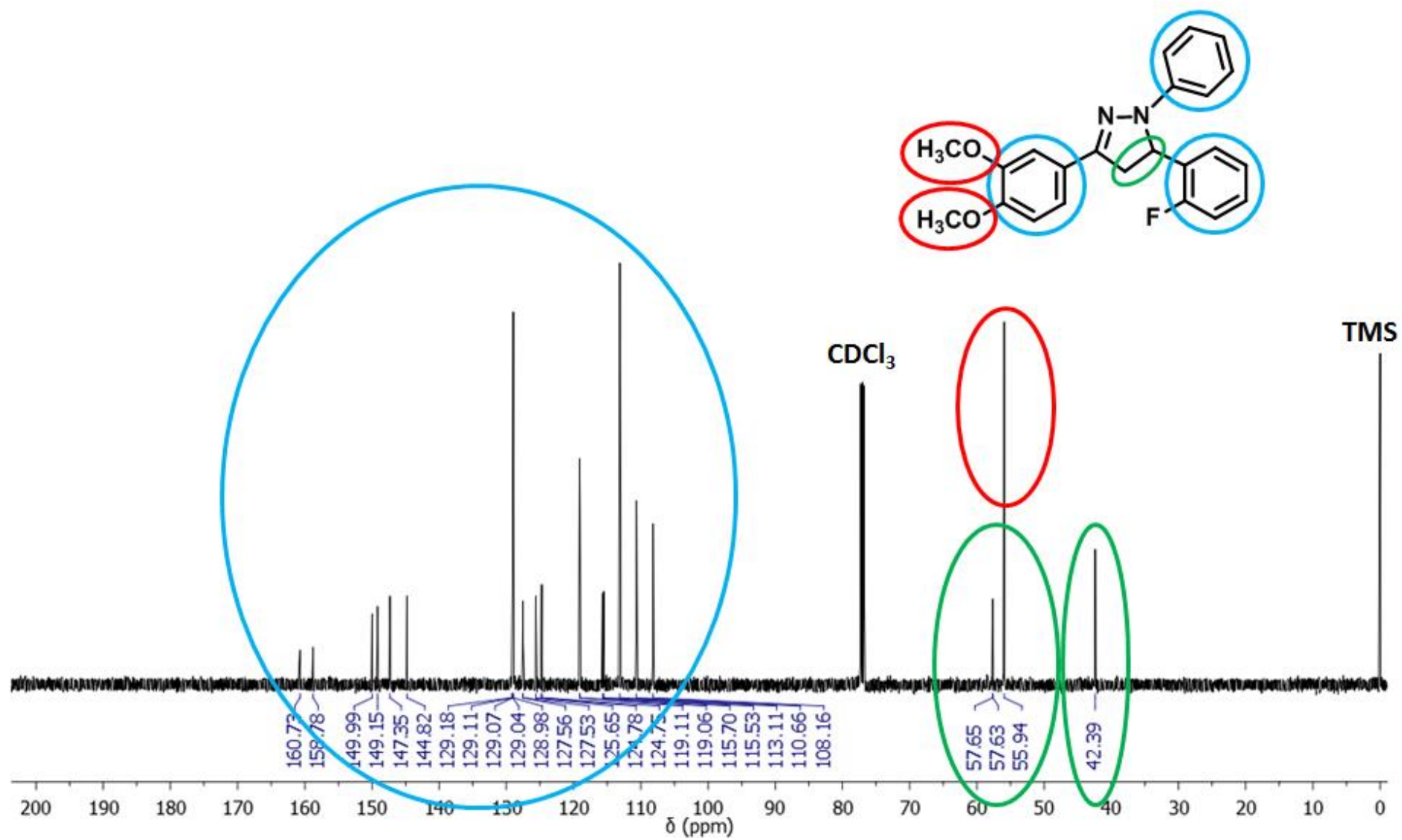


Figure S5. ¹³C NMR spectra of compound 1 (125 MHz, CDCl₃).

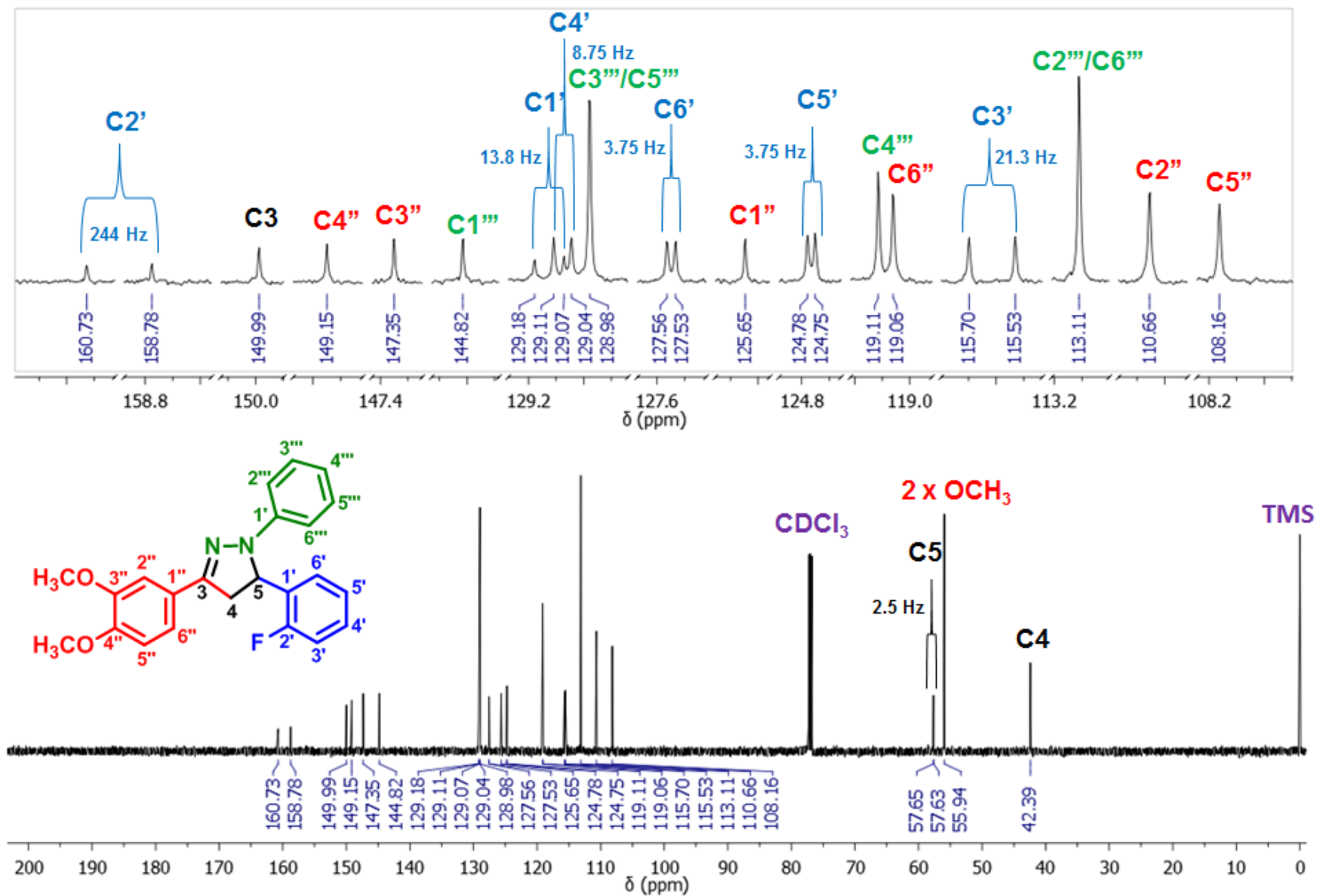


Figure S6. ^{13}C NMR spectra of compound 1, expanded aromatic region.