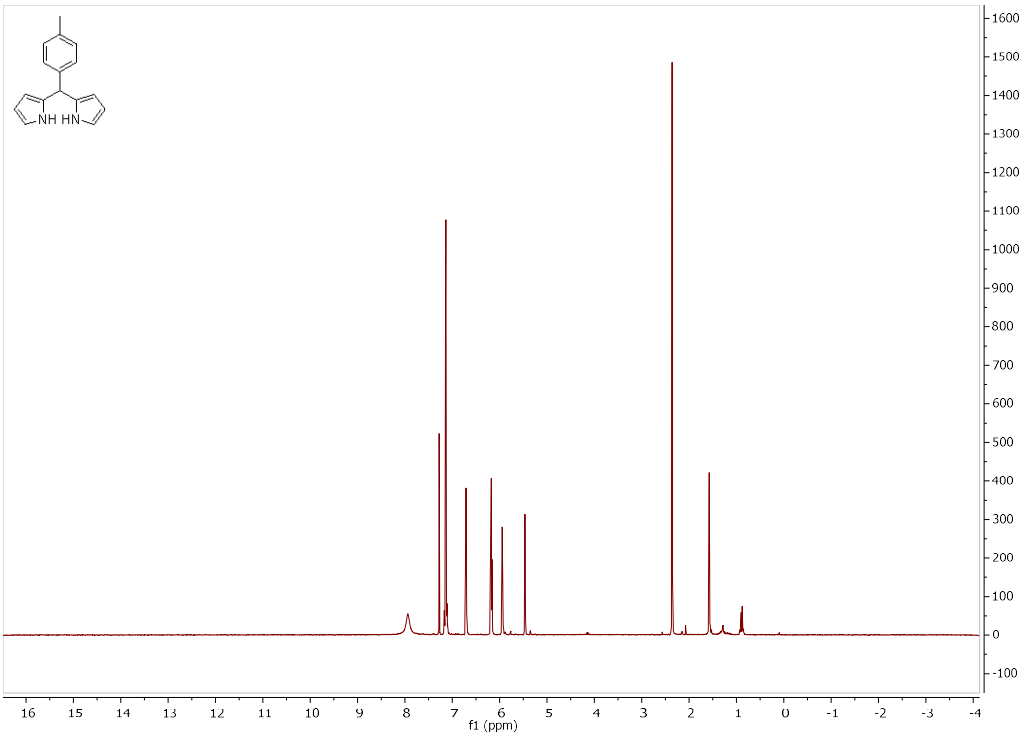
Supplementary Information

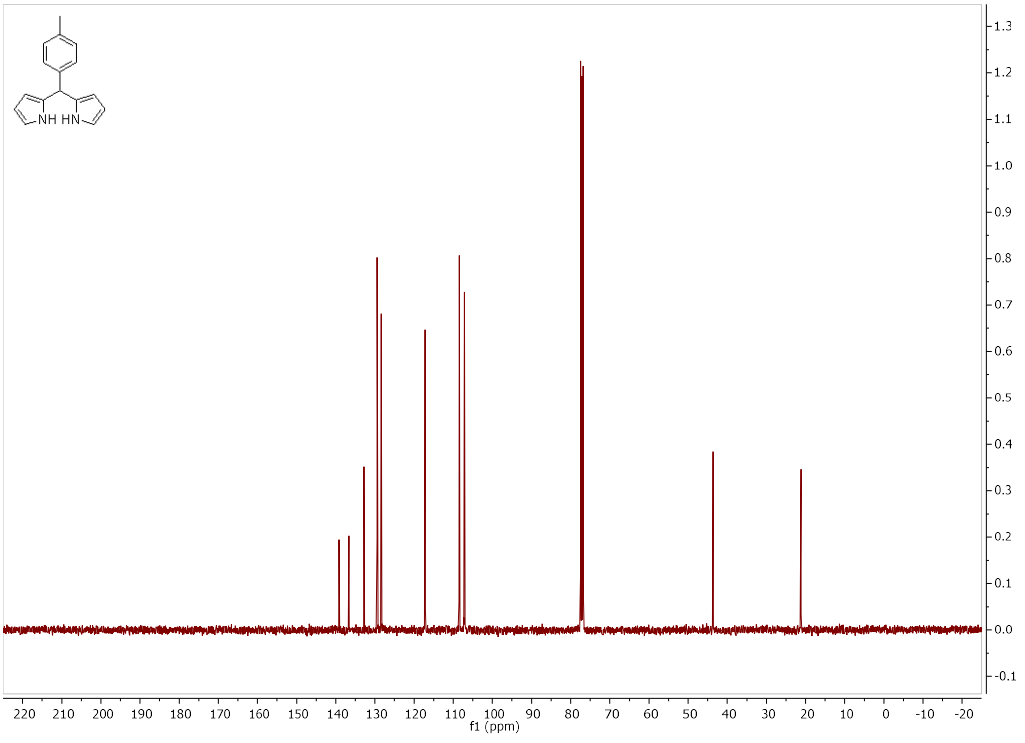
A New Chiral Boron–dipyrromethene (BODIPY)–based Fluorescent Probe: Molecular docking, DFT, Antibacterial and Antioxidant approaches.

Rua B. Alnoman,[a]* Shazia Parveen,[a]* Mohamad Hagar,[a,b] Hoda A. Ahmed,[a,c] & Julian G. Knight[d]

[a]Faculty of Science, Chemistry Department, Taibah University, Yanbu Branch, 46423, Yanbu, Saudi Arabia.
[b]Faculty of Science, Chemistry Department, Alexandria University, Alexandria, Egypt.
[c]Faculty of Science, Department of Chemistry, Cairo University, Cairo, Egypt.
[d]School of Chemistry, Bedson Building, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK.
**Corresponding authors: email: rua–b–n@live.co.uk (R.B. Alnoman), shazia021@gmail.com (S. Parveen).*



(a)



(b)

Figure S1. (a) ^{1}H NMR (300 MHz, $CDCl_3$) and (b) ^{13}C NMR (101 MHz, $CDCl_3$) spectra of compound **1.**

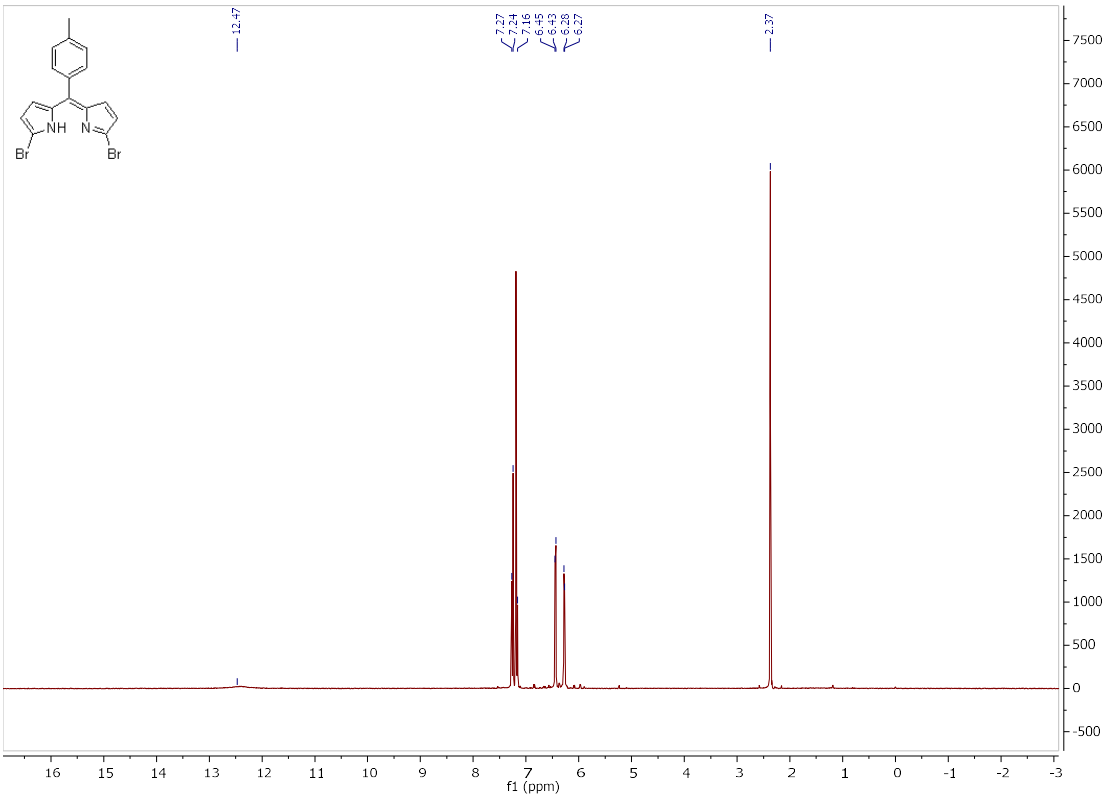
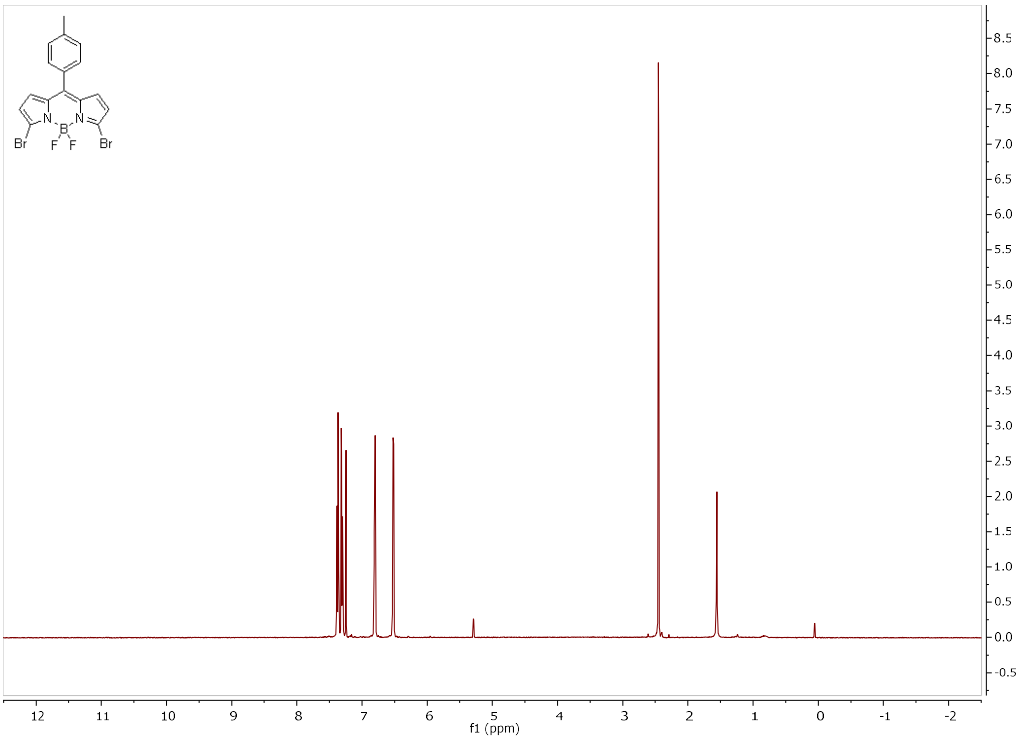
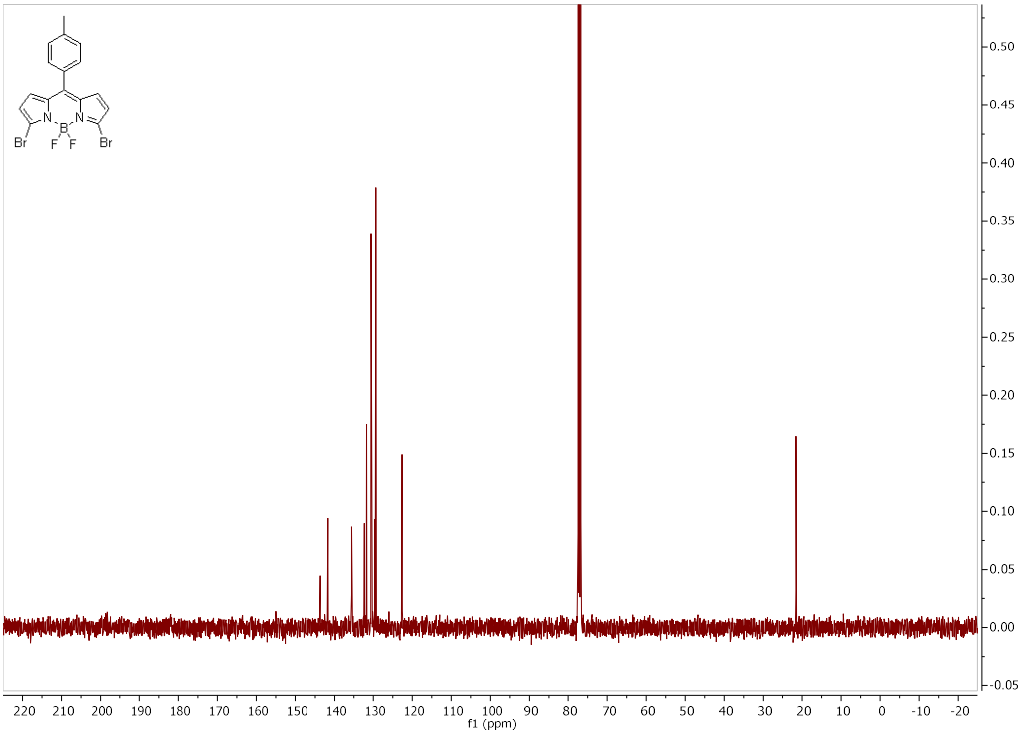


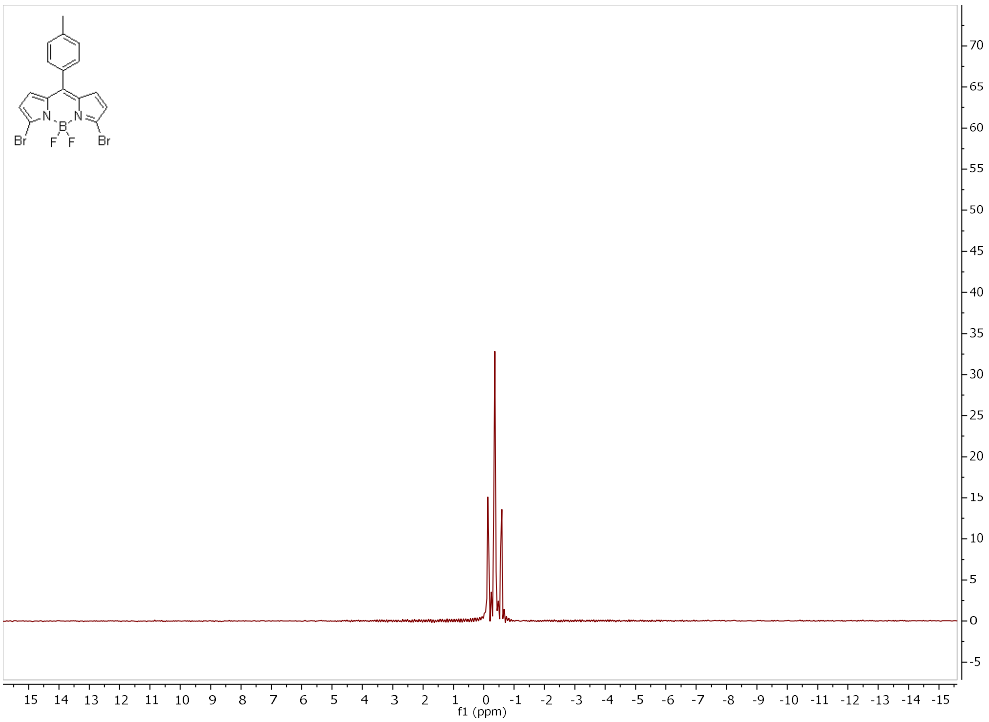
Figure S2. (a) ^{1}H NMR (300 MHz, $CDCl_3$) spectra of compound **2.**



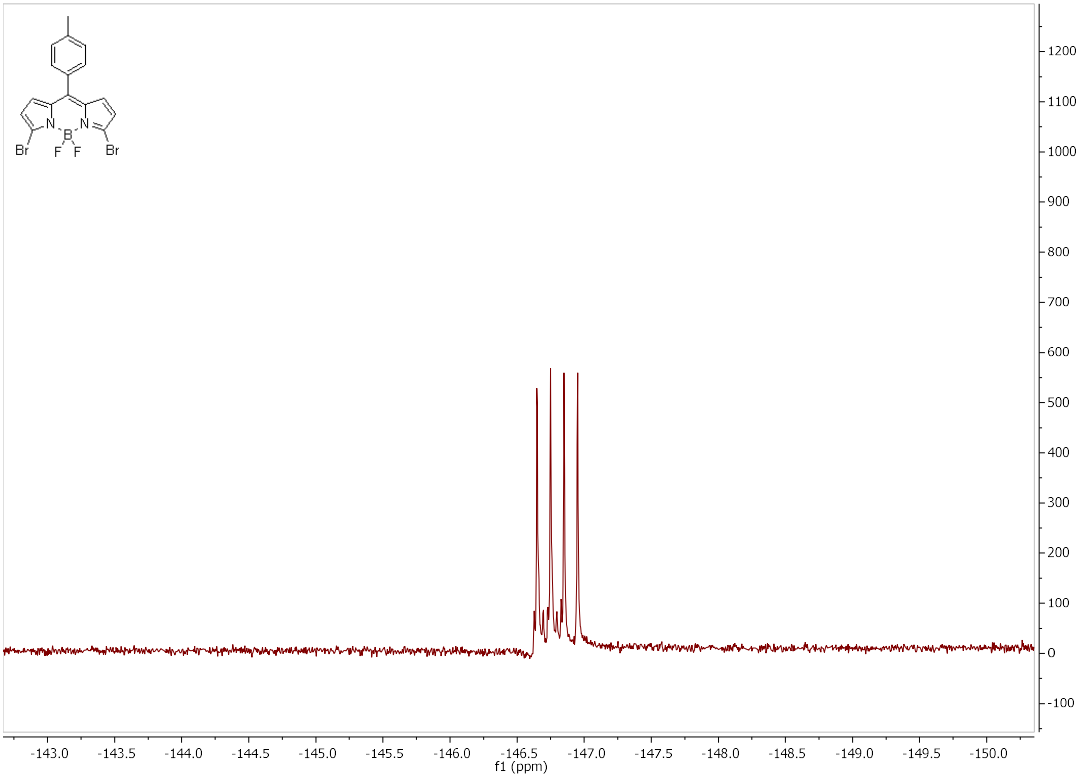
(a)



(b)

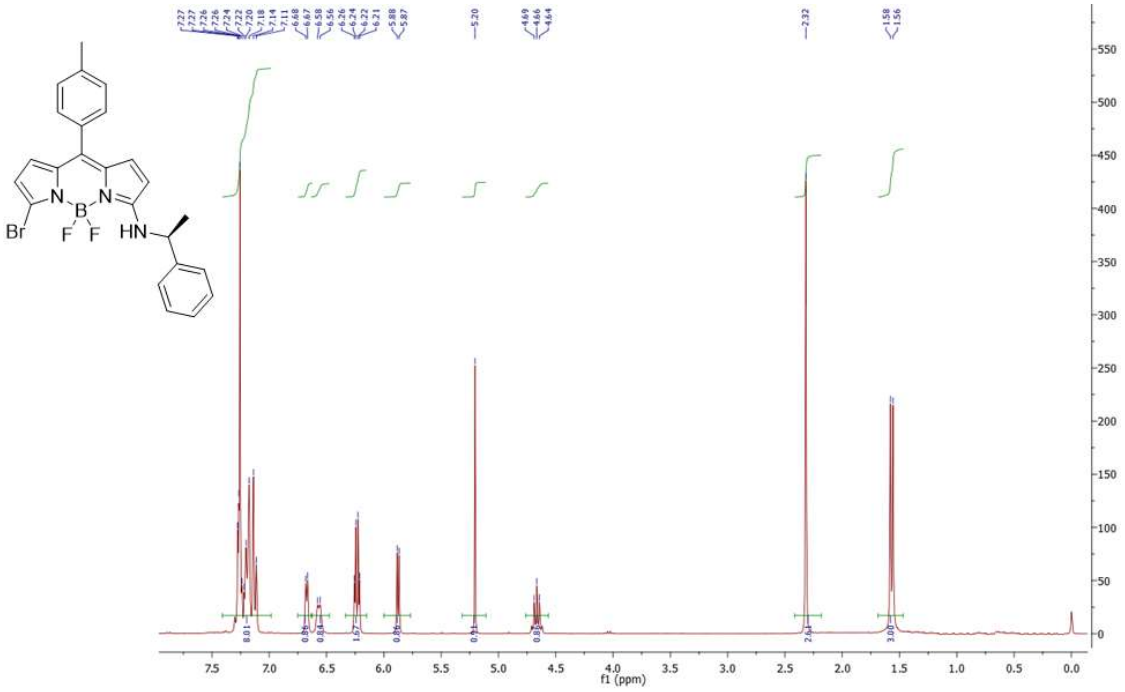


(c)

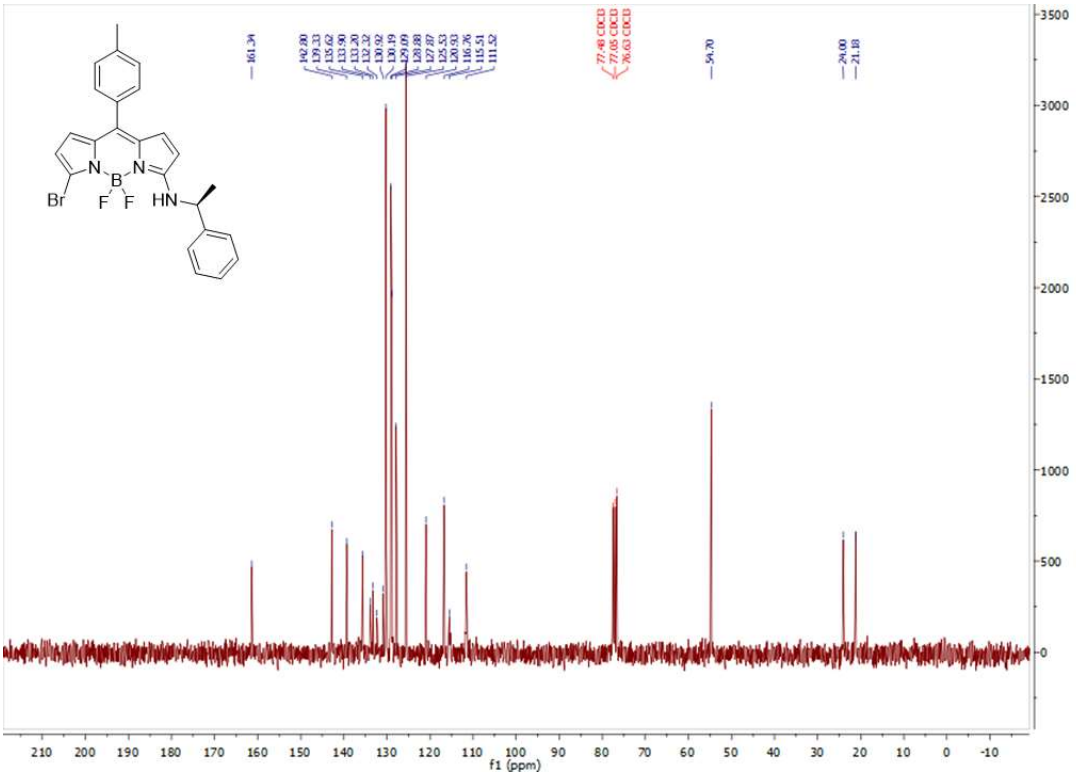


(d)

Figure S3. (a) ^{1}H NMR (300 MHz, $CDCl_3$), (b) ^{13}C NMR (101 MHz, $CDCl_3$), (c) ^{11}B NMR (128 MHz, $CDCl_3$) and (d) ^{19}F NMR (282 MHz, $CDCl_3$) spectra of compound **3.**



(a)



(b)

Figure S4. (a) ^{1}H NMR (300 MHz, $CDCl_3$) and (b) ^{13}C NMR (101 MHz, $CDCl_3$ spectra of compound **4.**