

# Synthesis, Biological Activity and Molecular Modelling Studies of Naphthoquinone

## Derivatives as Promising Anticancer Candidates Targeting COX-2

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Content:

Supplemental Figures S1–S16, representing <sup>1</sup>H and <sup>13</sup>C NMR spectra of all the newly synthesized compounds **9–16**.

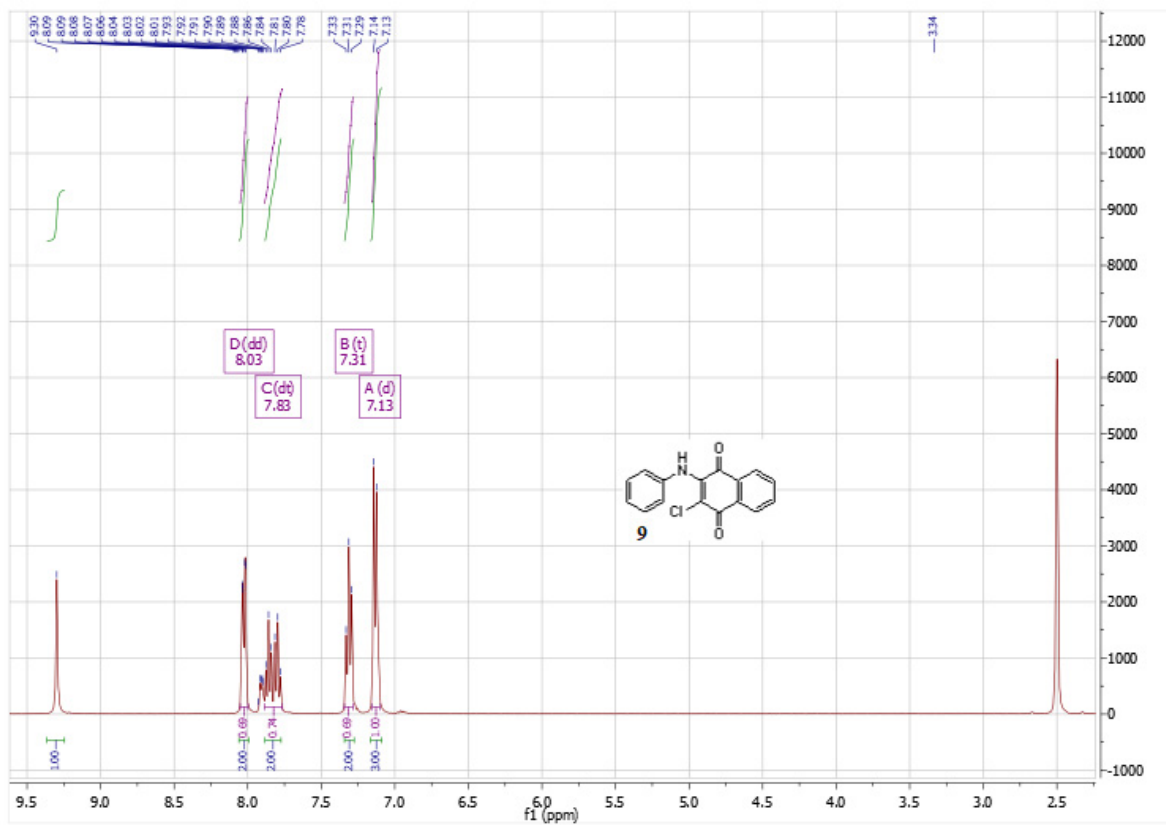


Figure S1:  $^1\text{H-NMR}$  spectrum of compound 9.

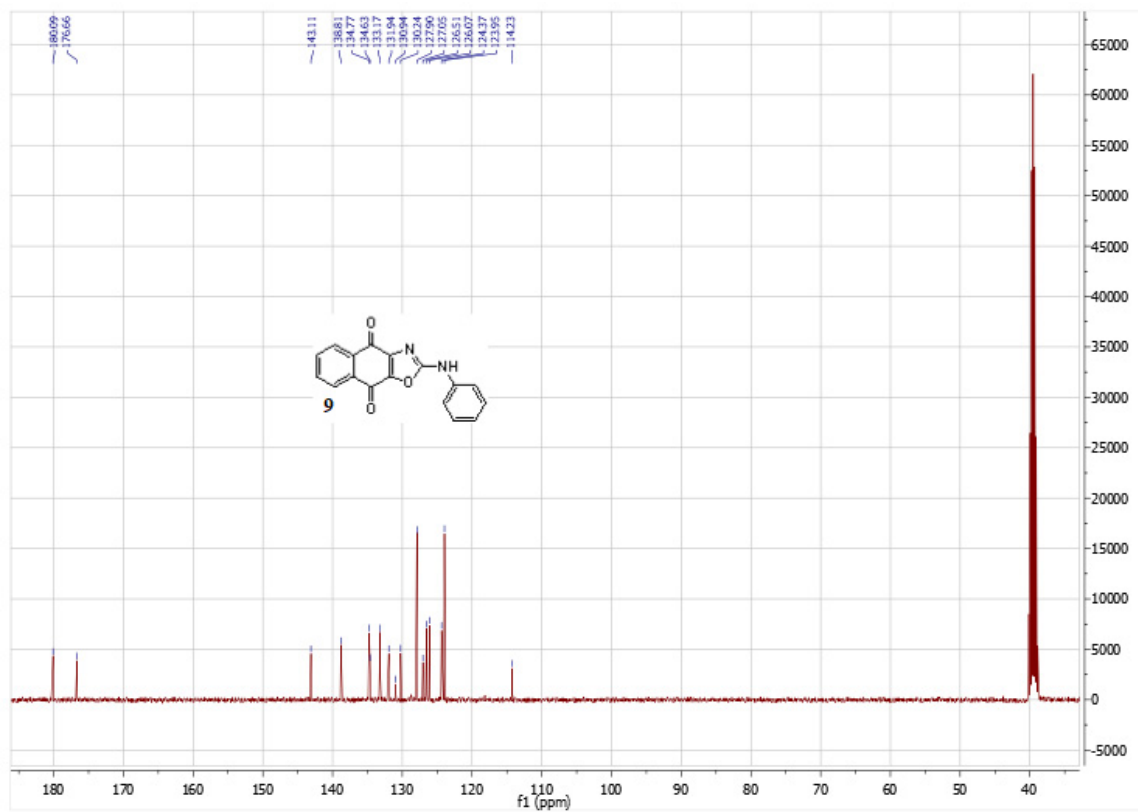


Figure S2:  $^{13}\text{C-NMR}$  spectrum of compound 9.

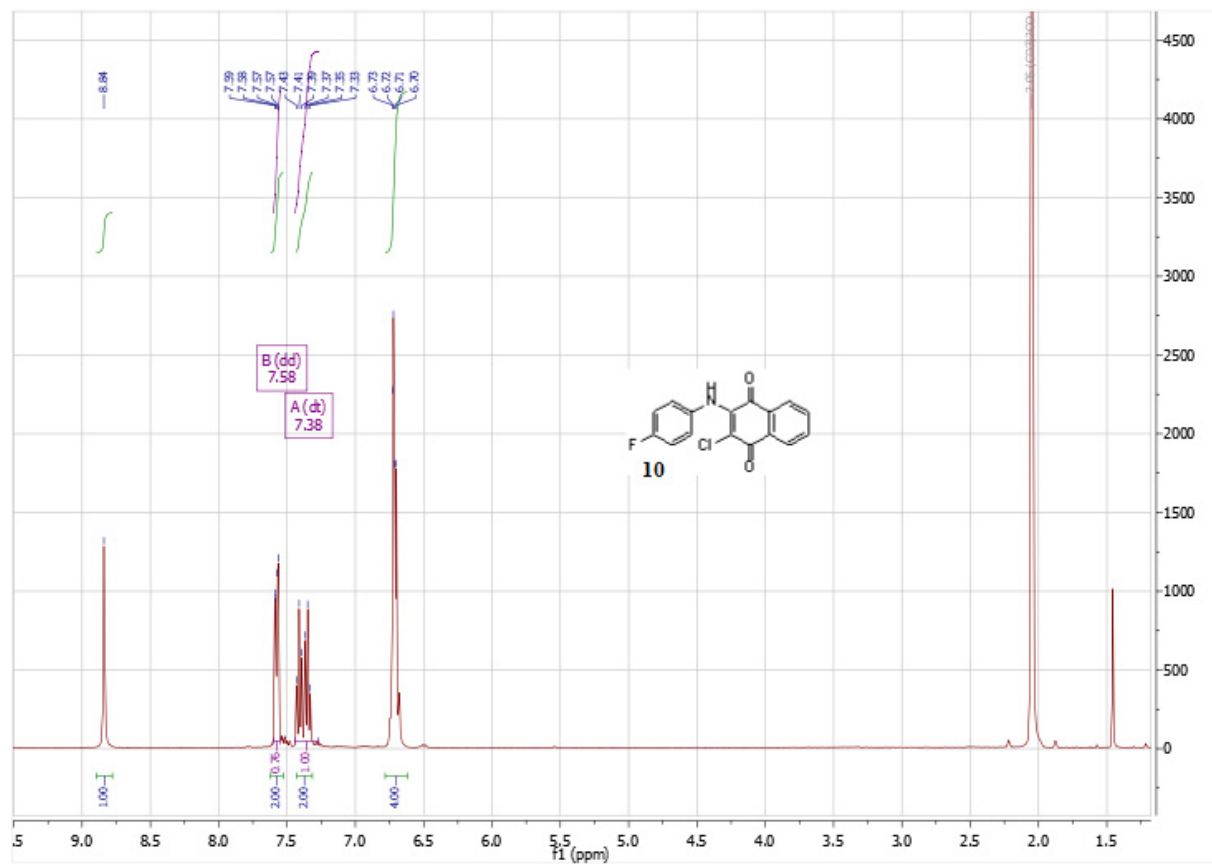


Figure S3: <sup>1</sup>H-NMR spectrum of compound 10.

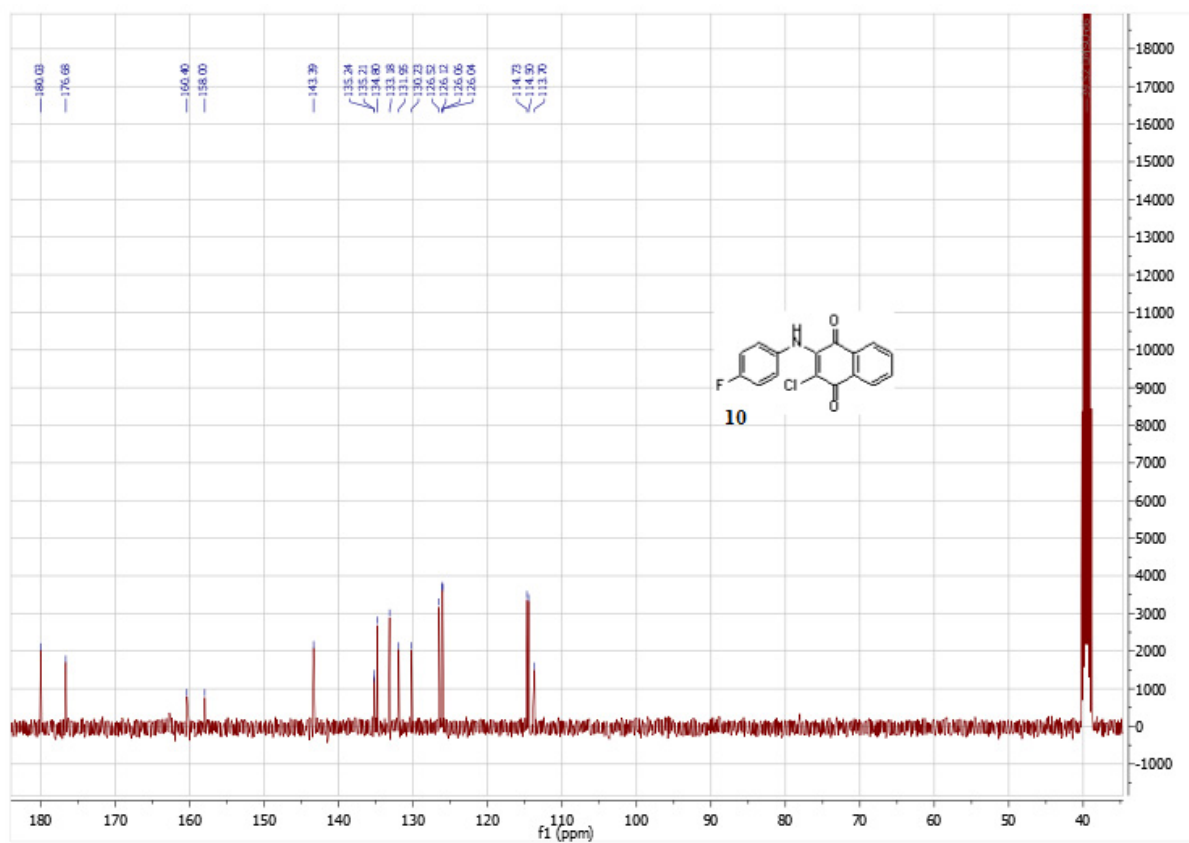
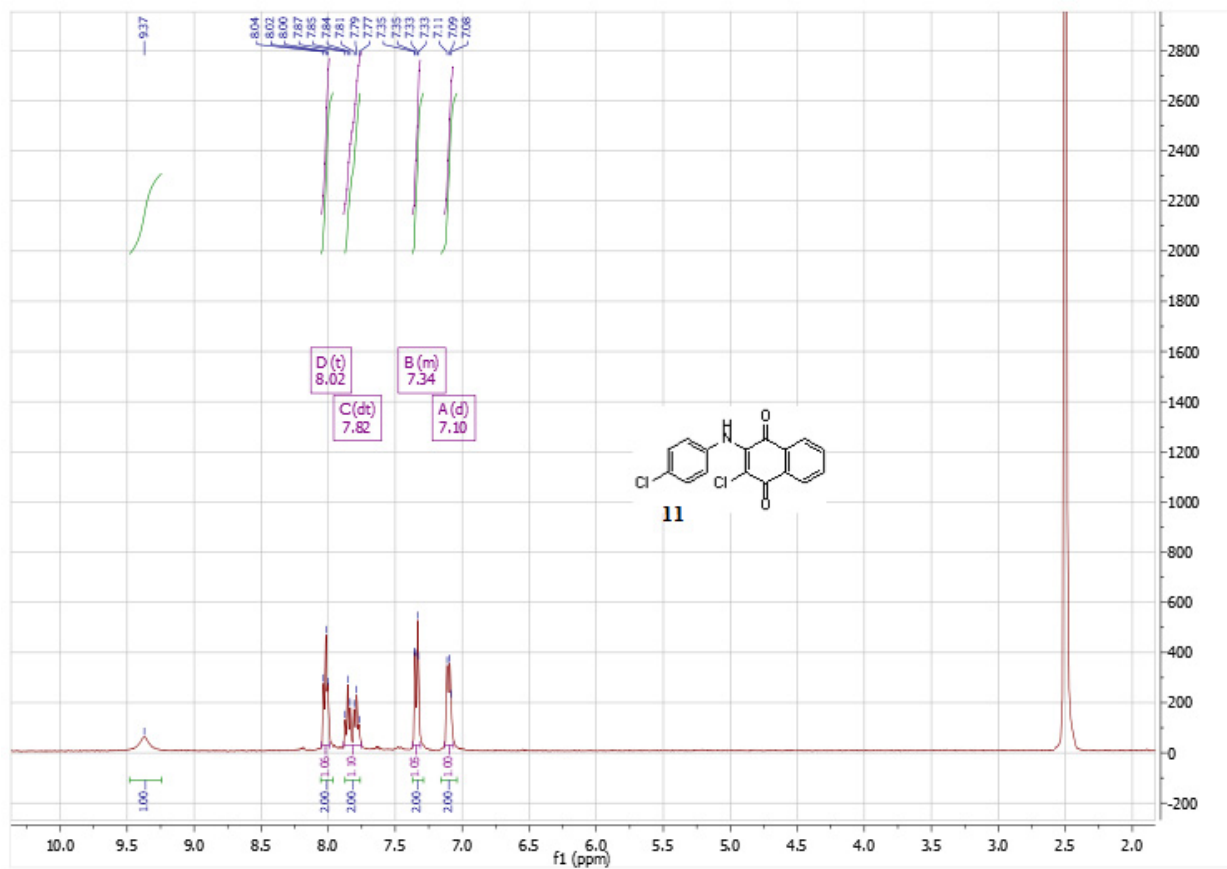
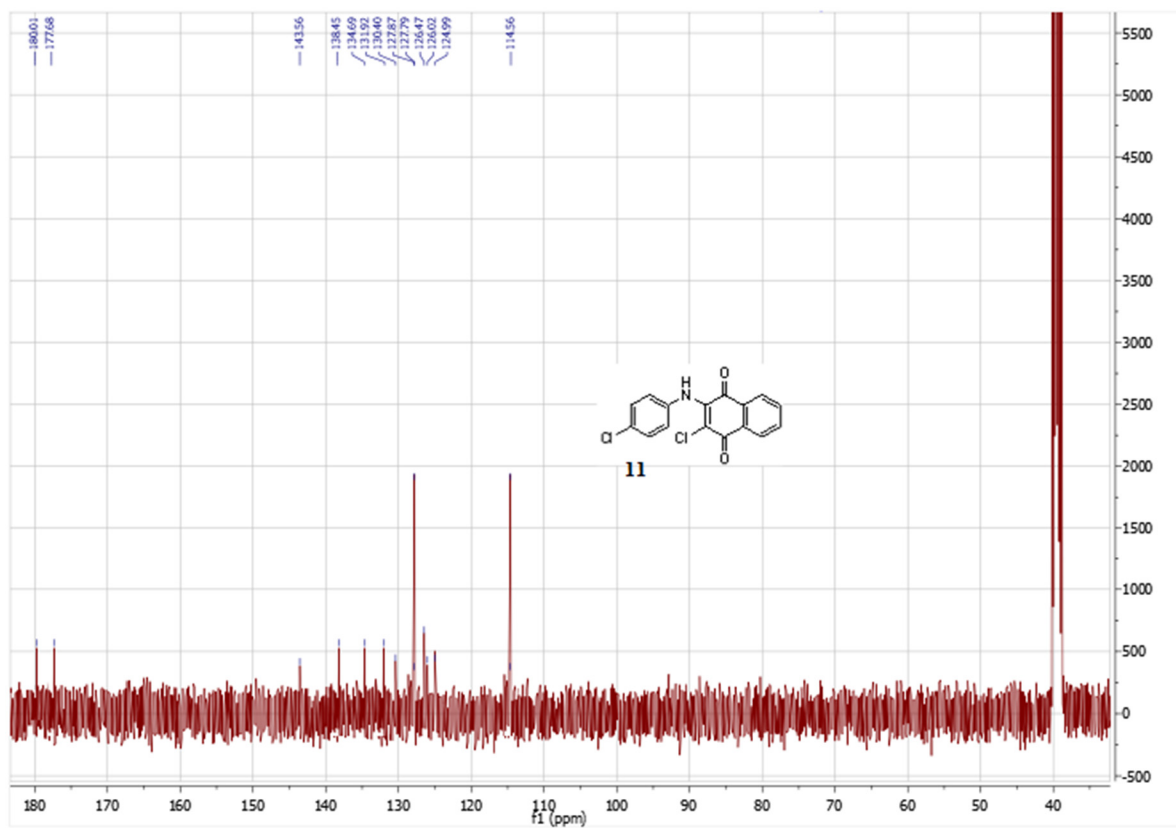


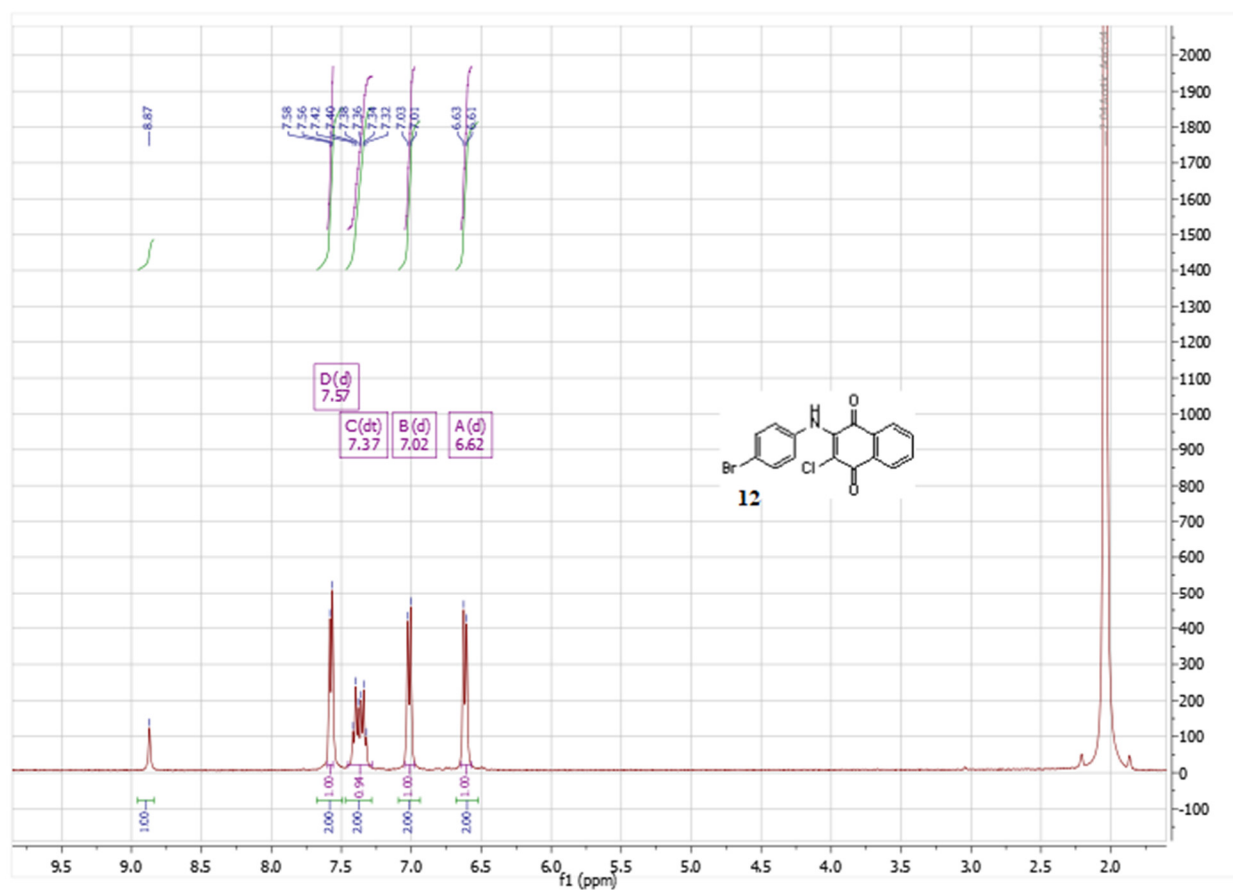
Figure S4: <sup>13</sup>C-NMR spectrum of compound 10.



**Figure S5:  $^1\text{H}$ -NMR spectrum of compound 11.**



**Figure S6:  $^{13}\text{C}$ -NMR spectrum of compound 11.**



**Figure S7:**  $^1\text{H}$ -NMR spectrum of compound **12**.

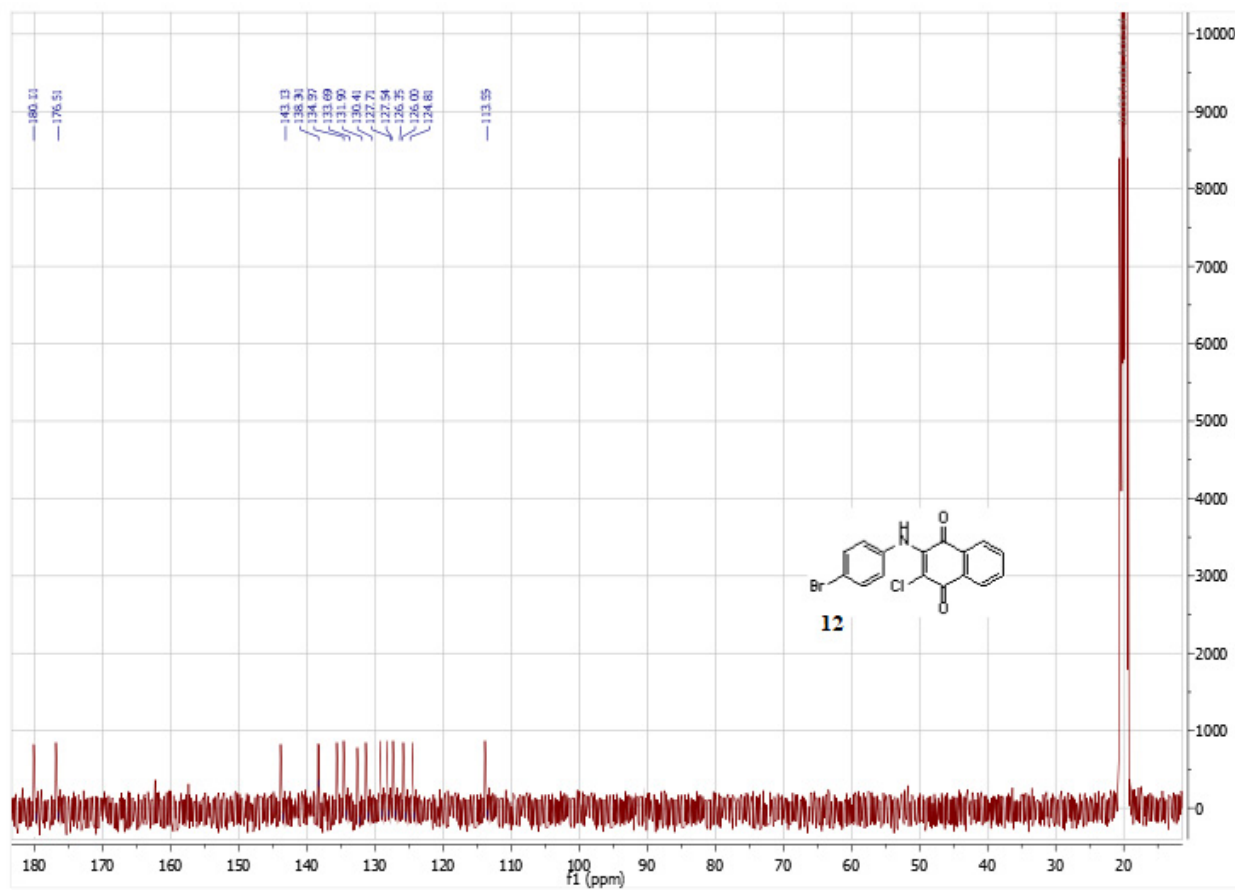


Figure S8:  $^{13}\text{C}$ -NMR spectrum of compound 12.

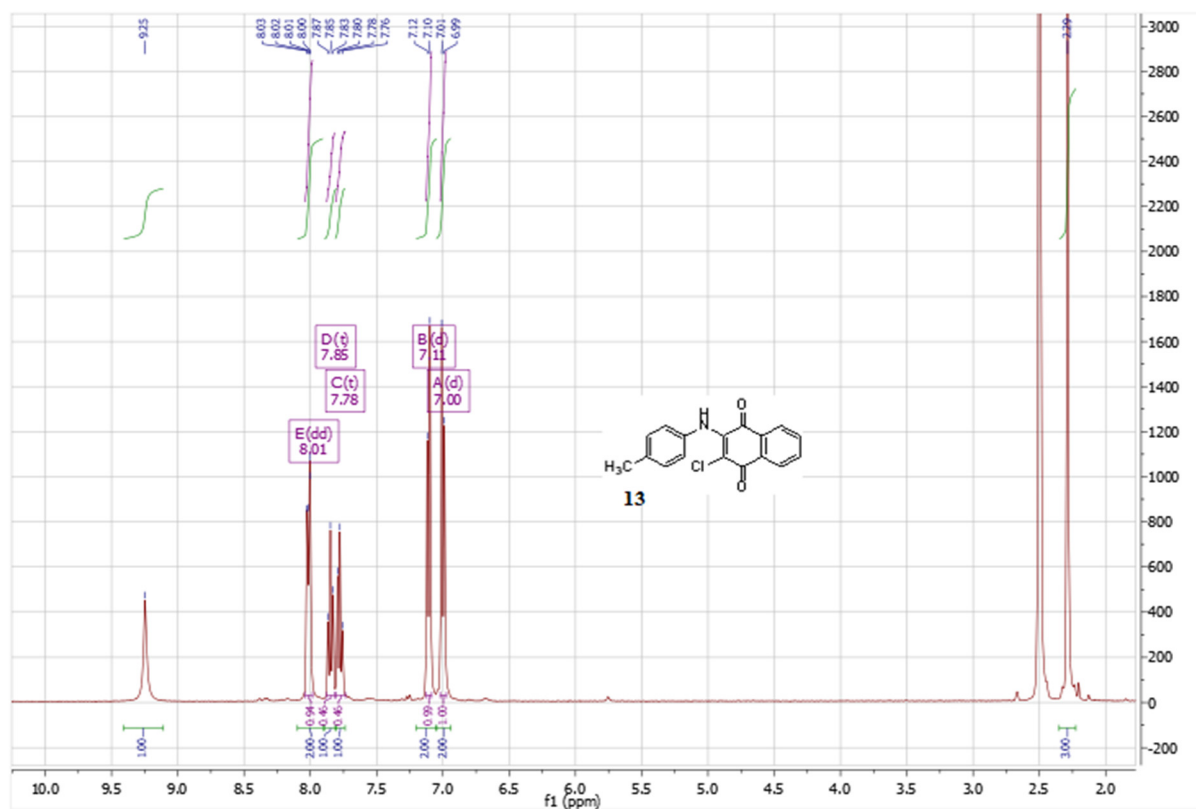


Figure S9:  $^1\text{H}$ -NMR spectrum of compound 13.

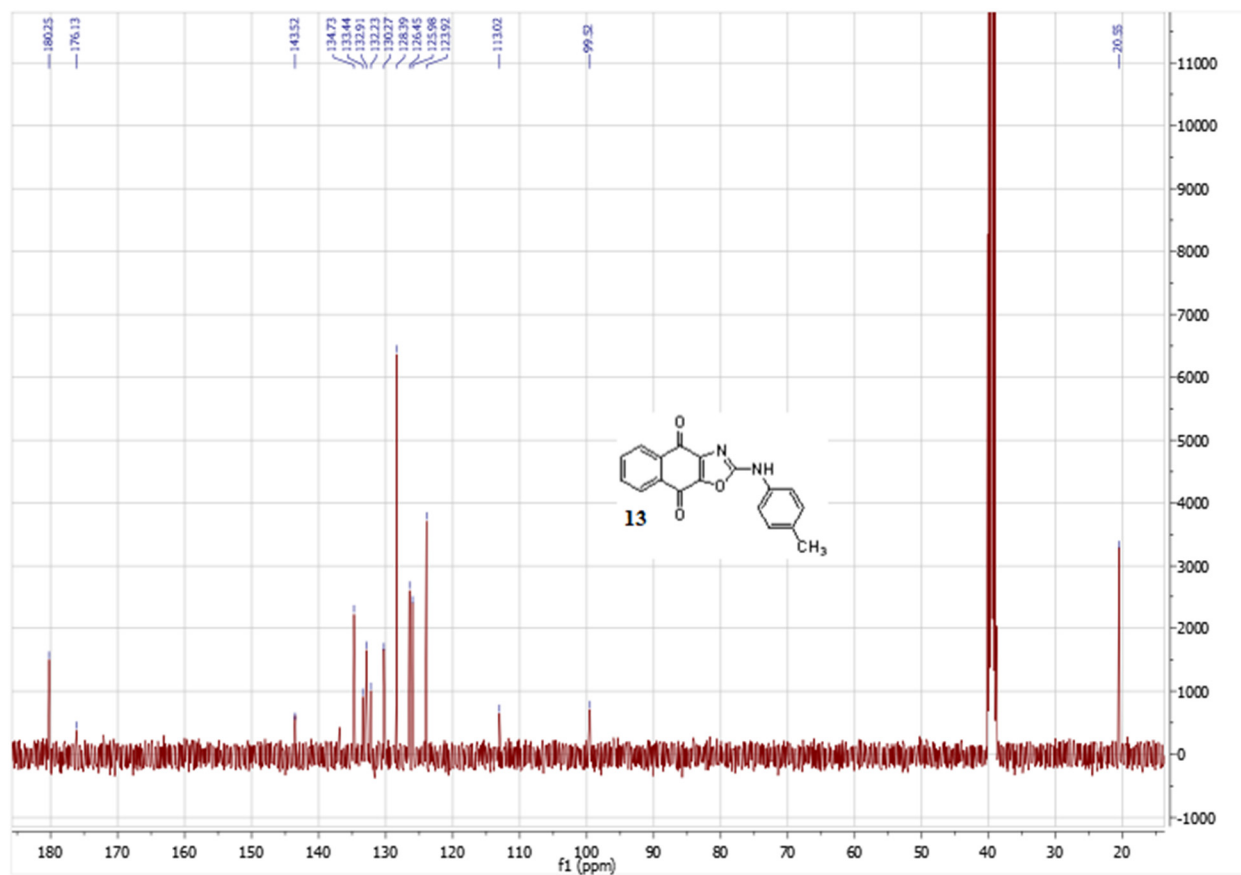


Figure S10: <sup>13</sup>C-NMR spectrum of compound 13.

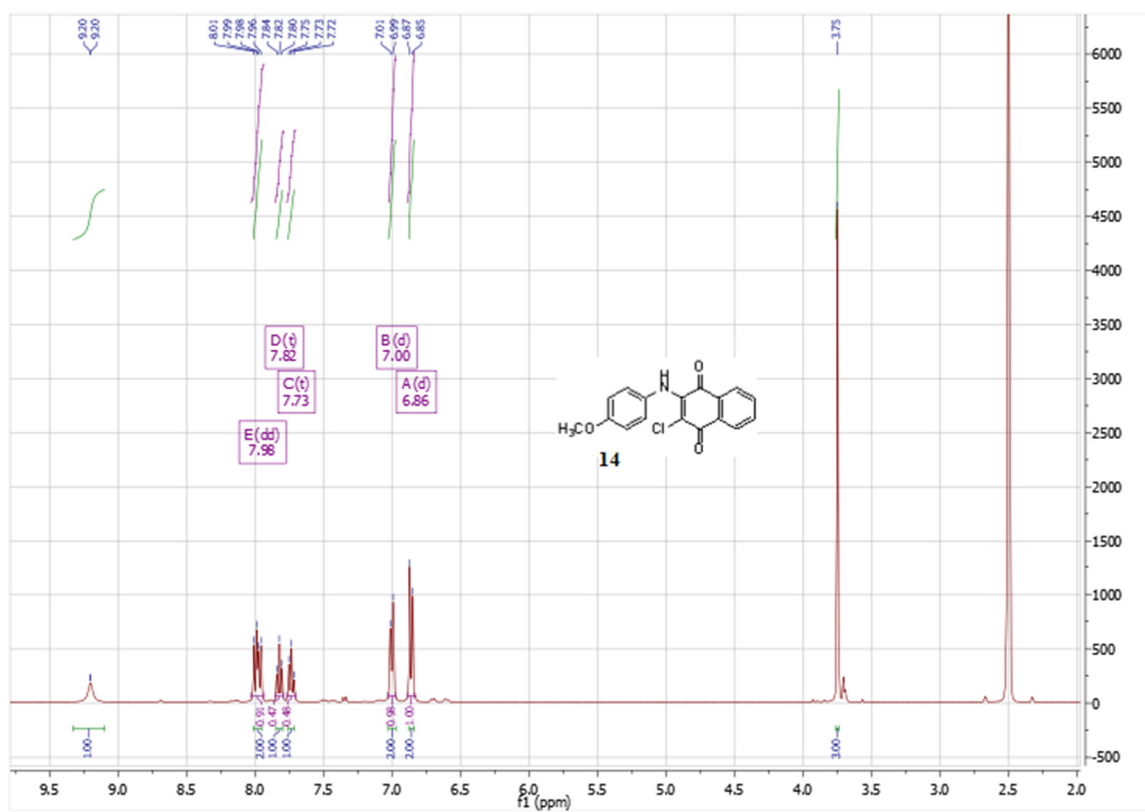


Figure S11: <sup>1</sup>H-NMR spectrum of compound 14.

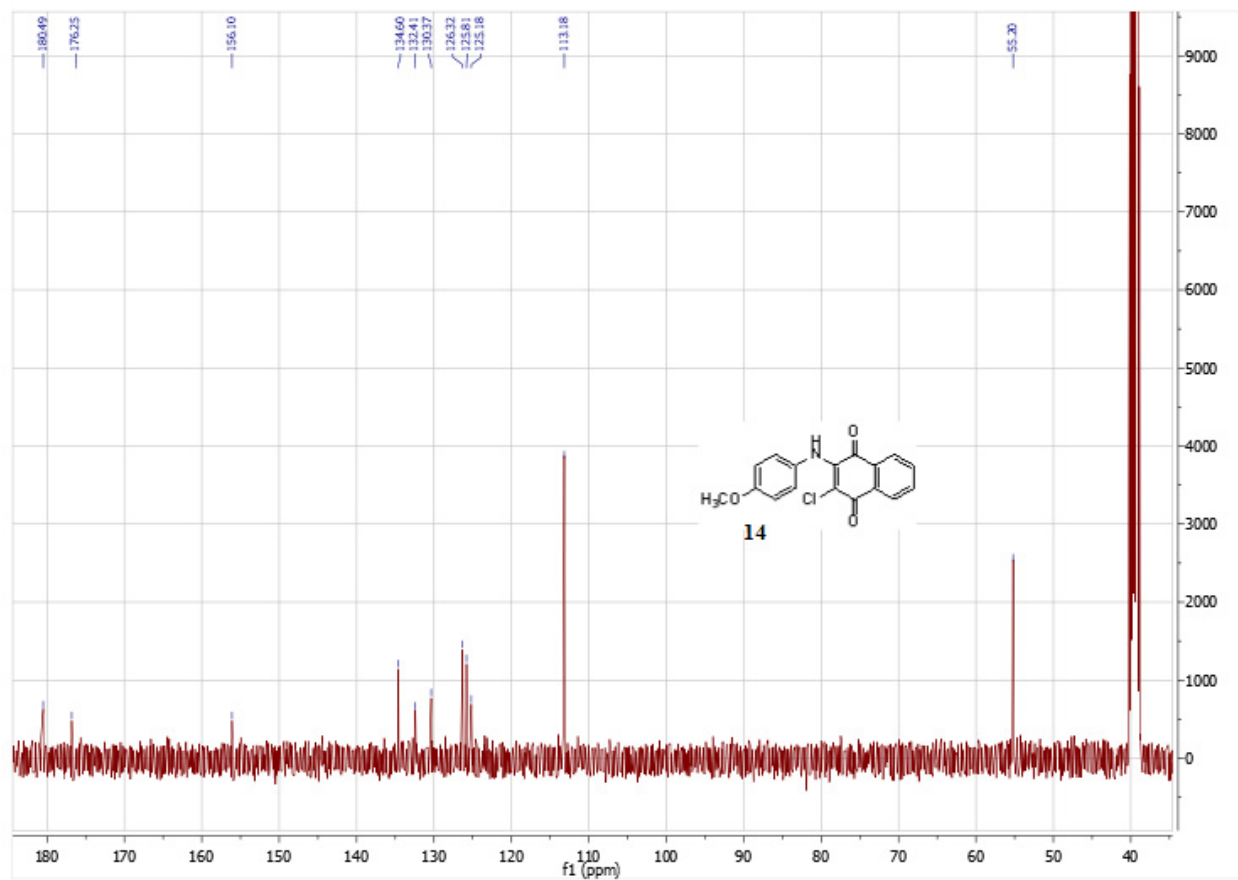


Figure S12:  $^{13}\text{C}$ -NMR spectrum of compound 14.

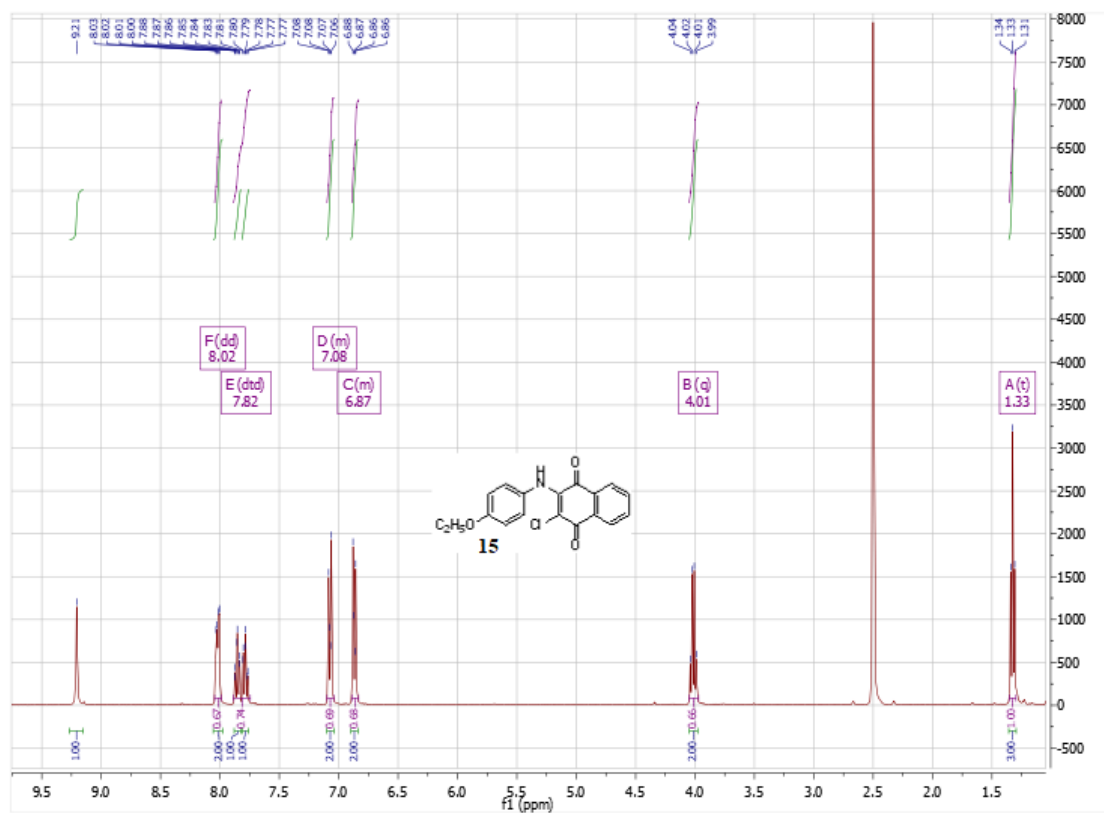


Figure S13:  $^1\text{H}$ -NMR spectrum of compound 15.



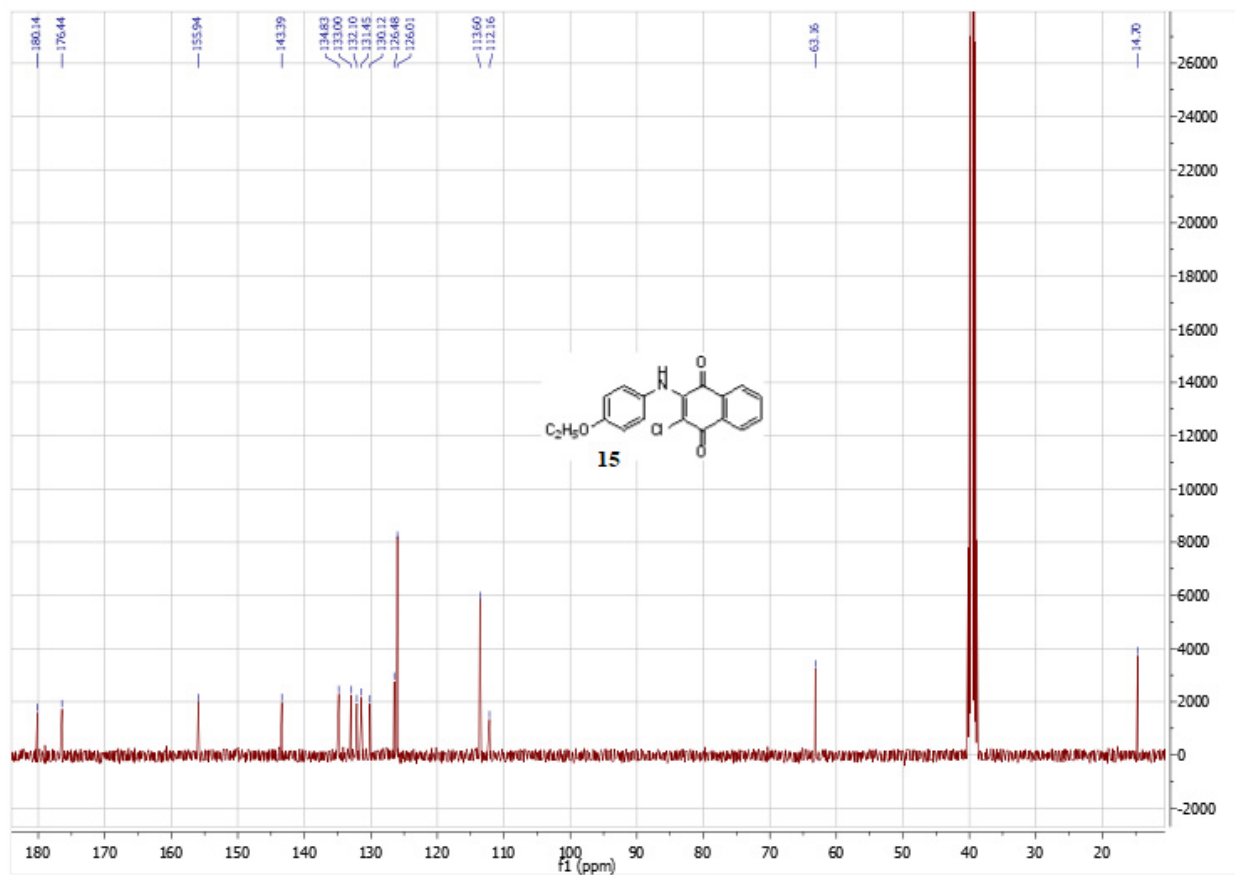


Figure S14: <sup>13</sup>C-NMR spectrum of compound 15.

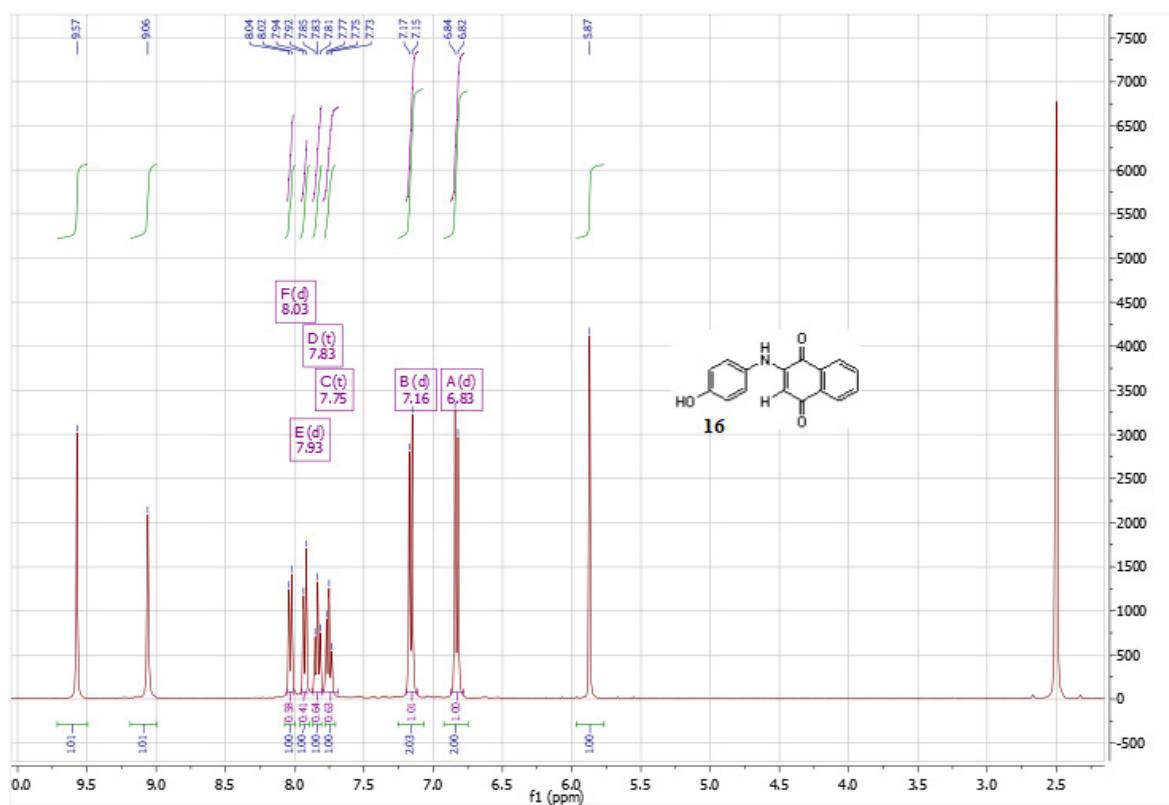
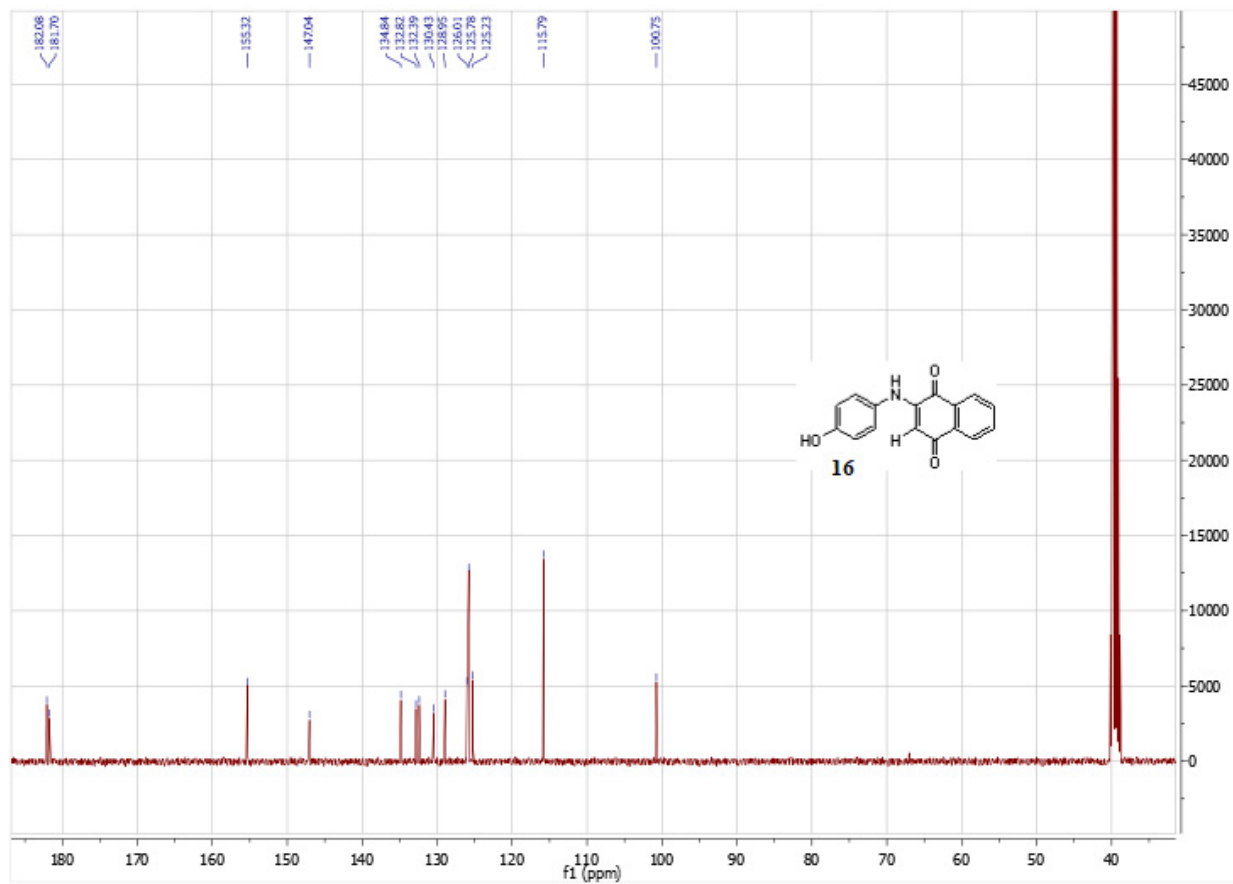


Figure S15: <sup>1</sup>H-NMR spectrum of compound 16.



**Figure S16:**  $^{13}\text{C}$ -NMR spectrum of compound **16**.