

New estrone oxime derivatives: synthesis, cytotoxic evaluation and docking studies

Catarina Canário ¹, Mariana Matias ¹, Vanessa de Brito ¹, Adriana O. Santos ¹, Amílcar Falcão ^{2,3}, Samuel Silvestre ^{1,4,*} and Gilberto Alves ¹

¹ CICS-UBI – Health Sciences Research Centre, University of Beira Interior, Covilhã, Portugal;

² Laboratory of Pharmacology, Faculty of Pharmacy, University of Coimbra, Coimbra, Portugal;

³ CIBIT - Coimbra Institute for Biomedical Imaging and Translational Research, University of Coimbra, Coimbra, Portugal;

⁴ CNC – Center for Neuroscience and Cell Biology, University of Coimbra, Coimbra, Portugal.

* Correspondence: sms@ubi.pt

NMR Data of Compounds

1. Spectra of compound 5

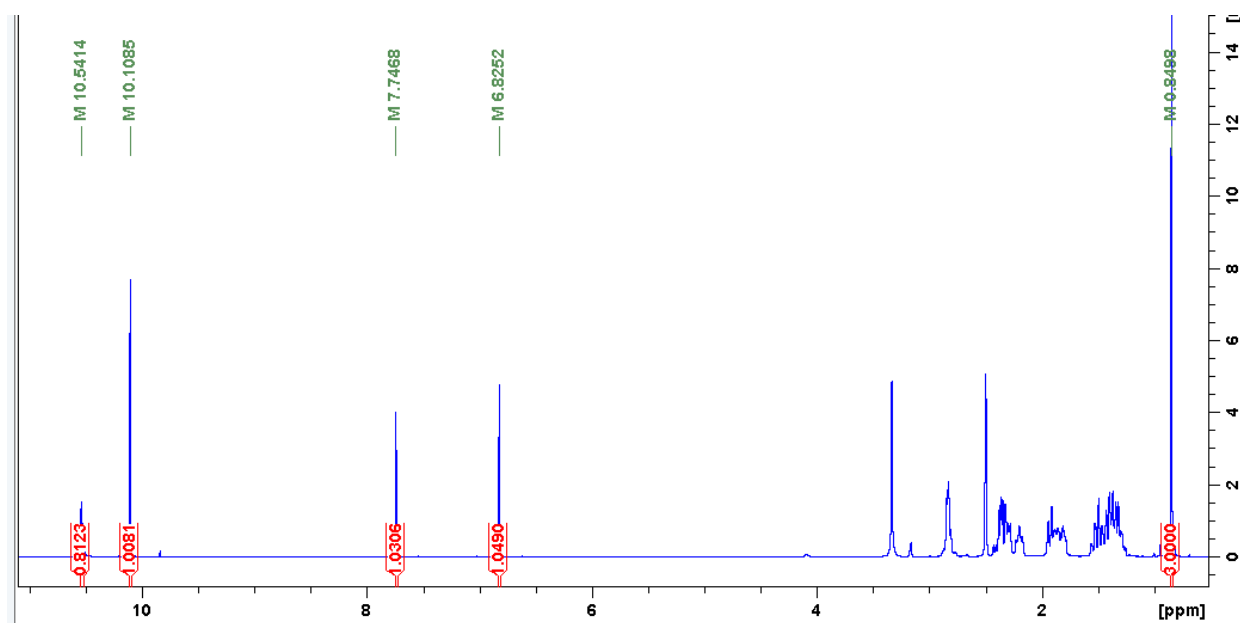
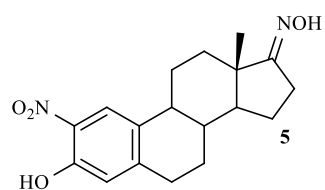


Figure S1. ¹H-NMR spectrum of compound 5 in DMSO-d₆.

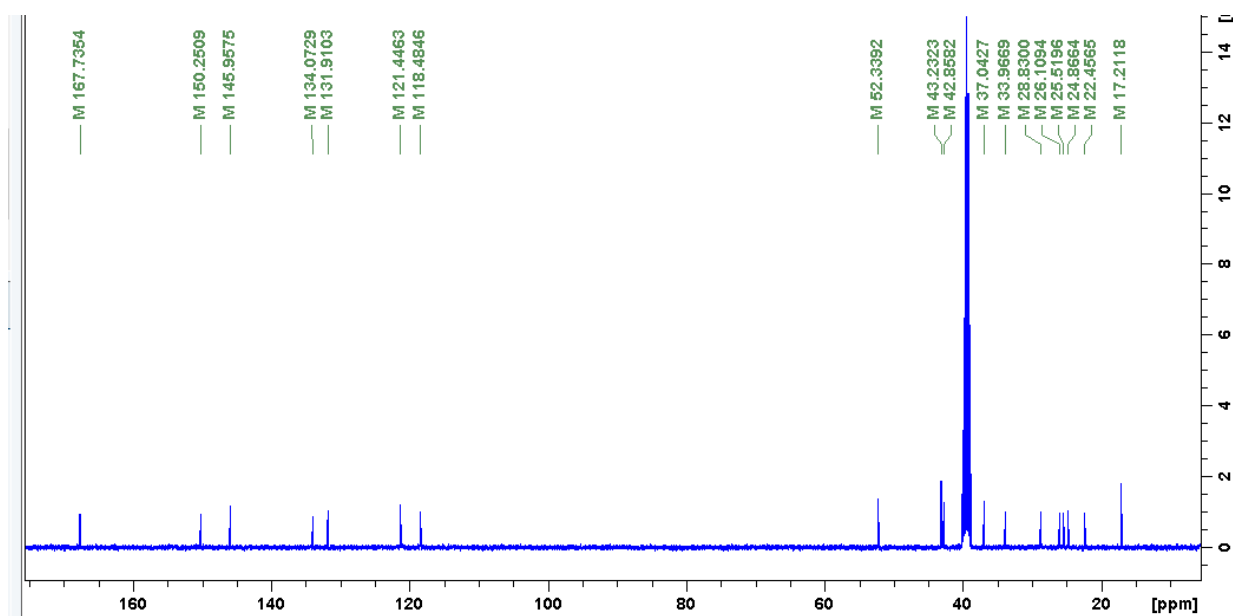


Figure S2. ¹³C-NMR spectrum of compound **5** in DMSO-d₆.

2. Spectra of compound 6

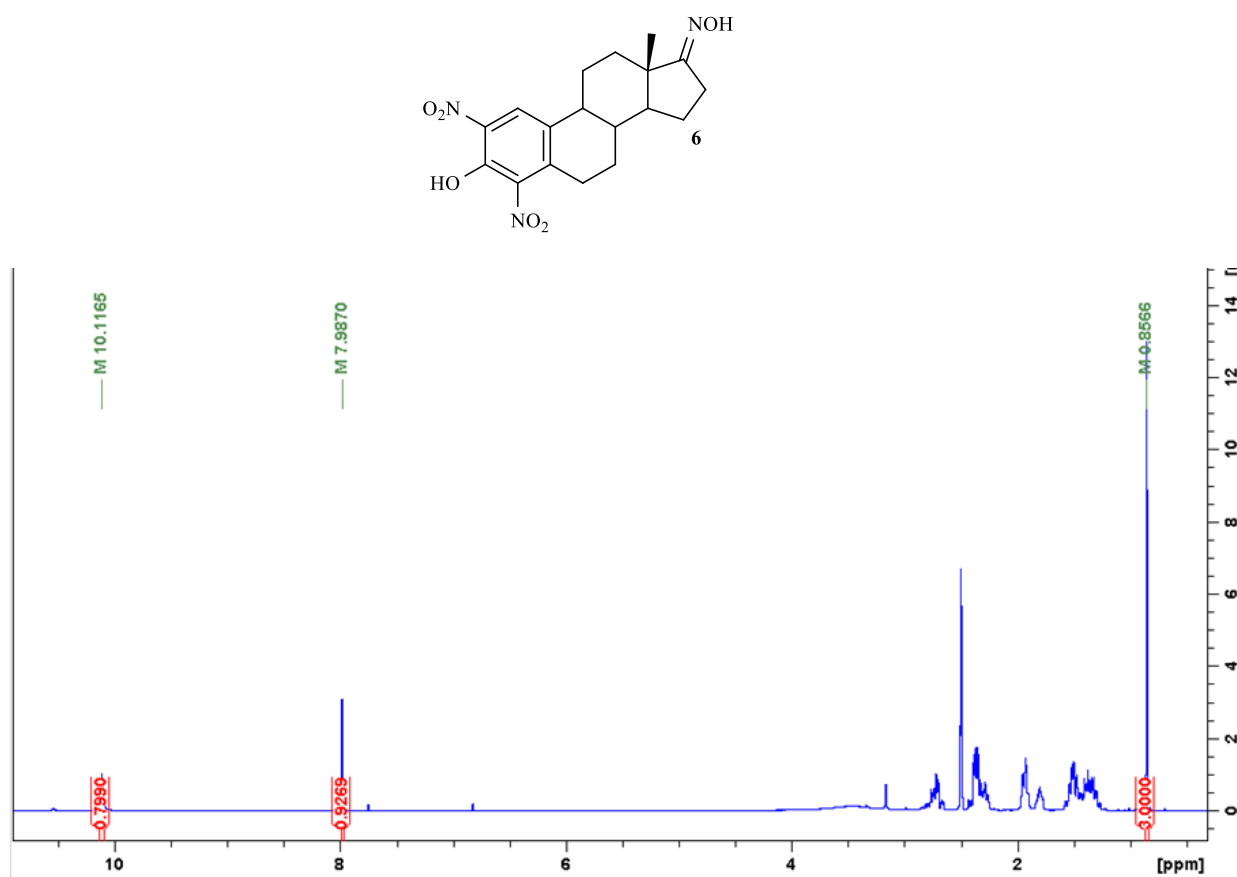


Figure S3. ¹H-NMR spectrum of compound 6 in DMSO-d₆.

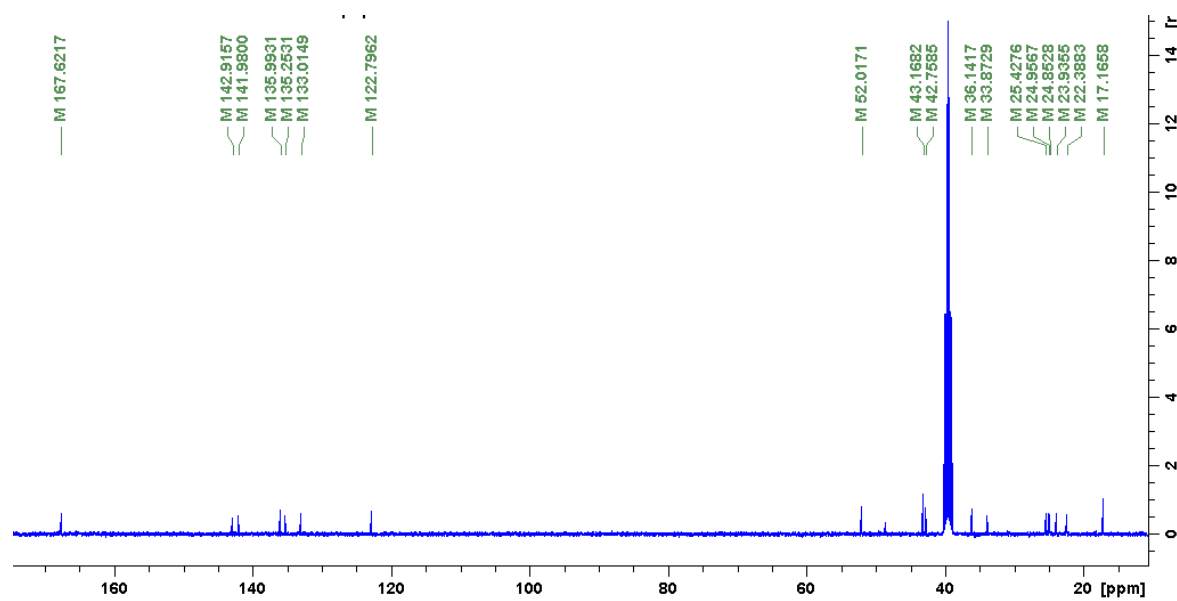


Figure S4. ¹³C-NMR spectrum of compound 6 in DMSO-d₆.

3. Spectra of compound 10

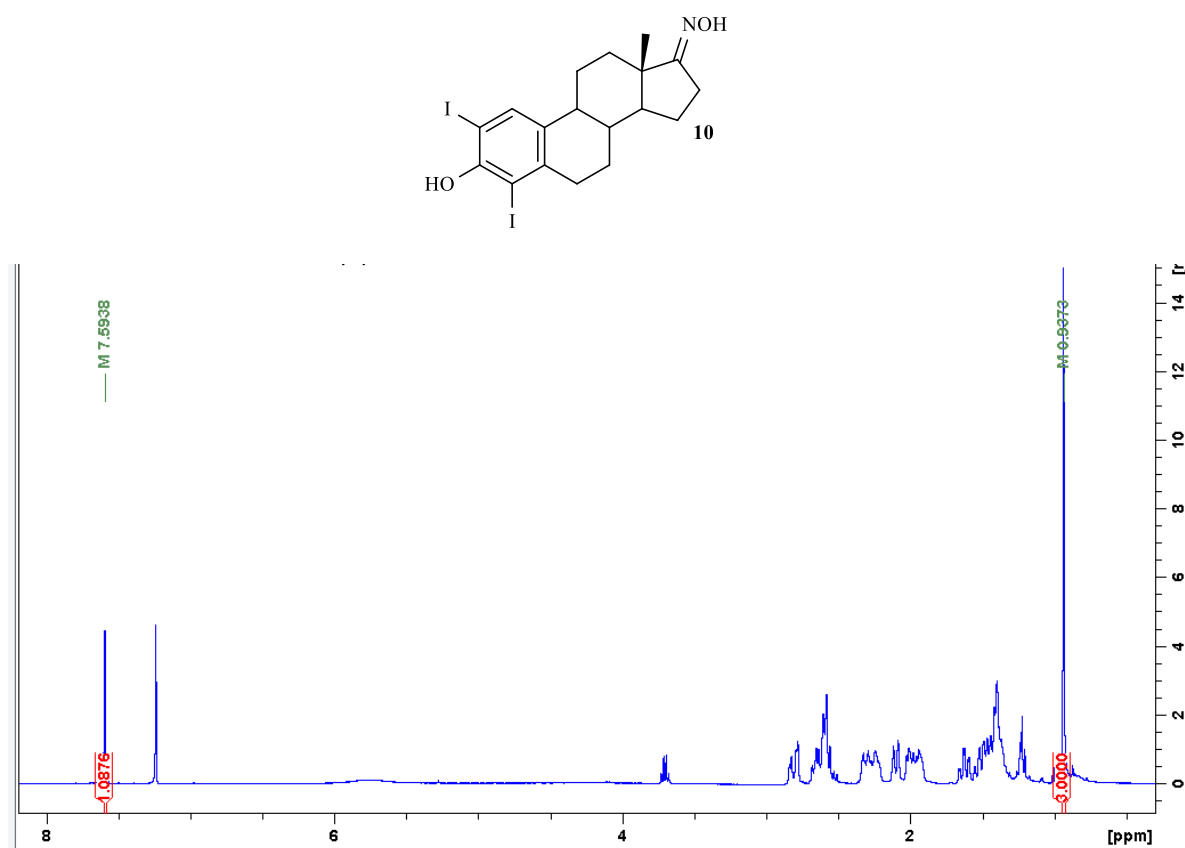


Figure S5. ¹H-NMR spectrum of compound 10 in in CDCl₃.

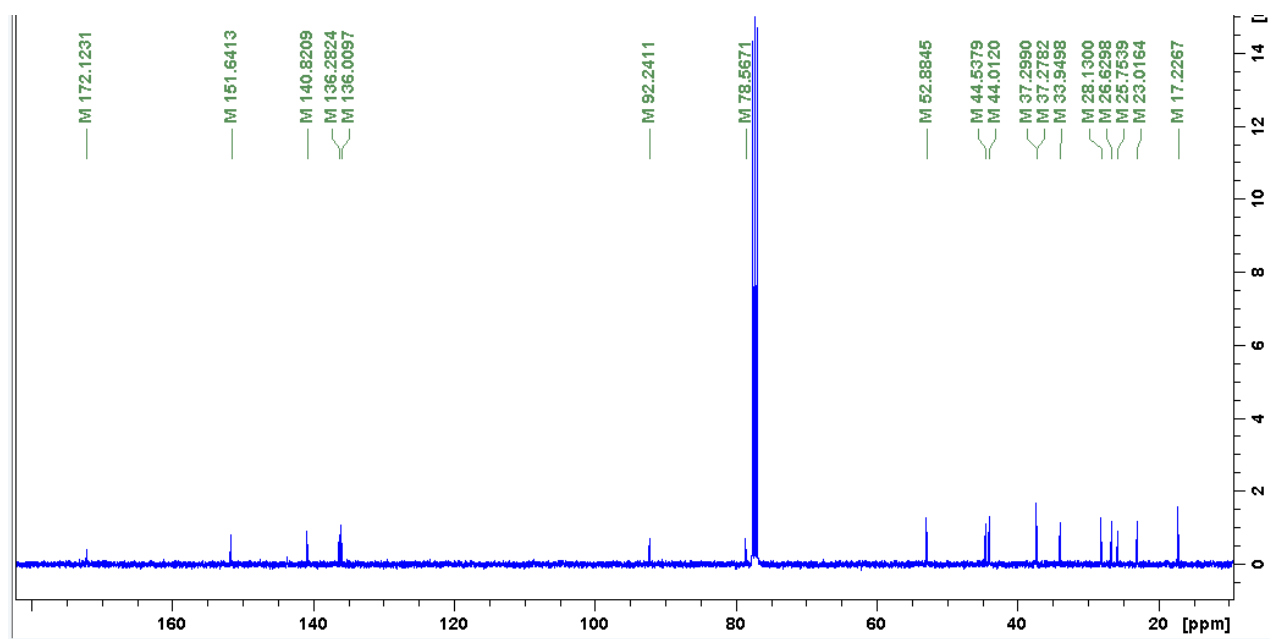


Figure S6. ¹³C-NMR spectrum of compound 10 in in CDCl₃.

4. Spectra of compound 11

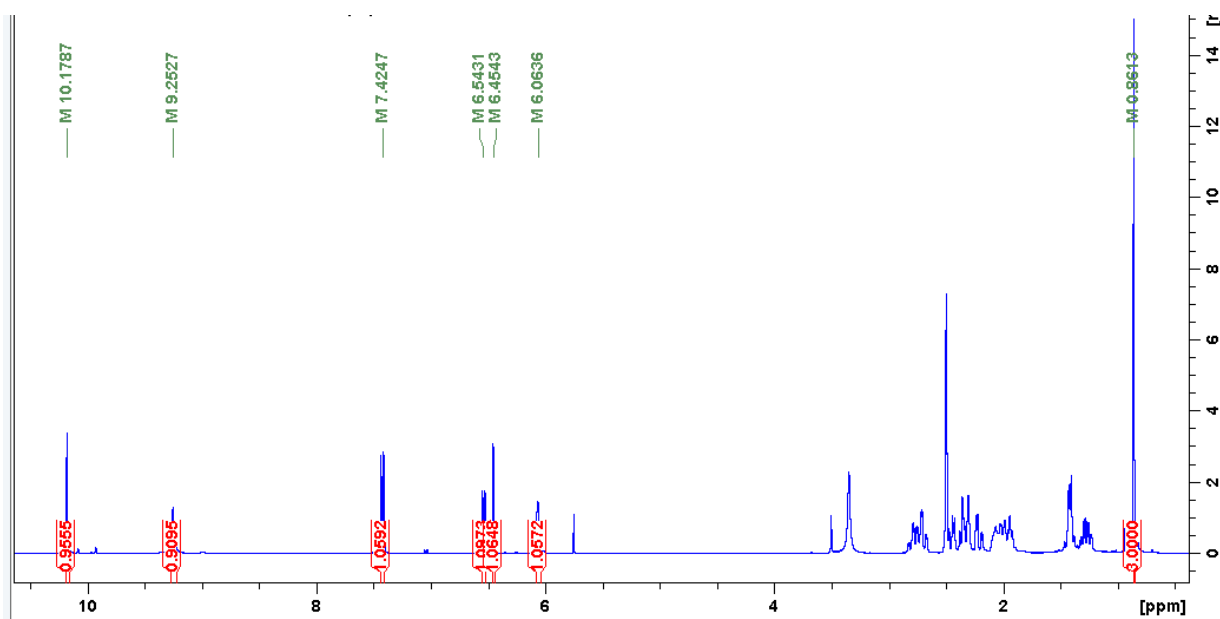
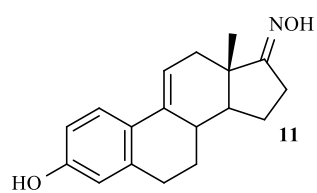


Figure S7. ¹H-NMR spectrum of compound 11 in DMSO-d₆.

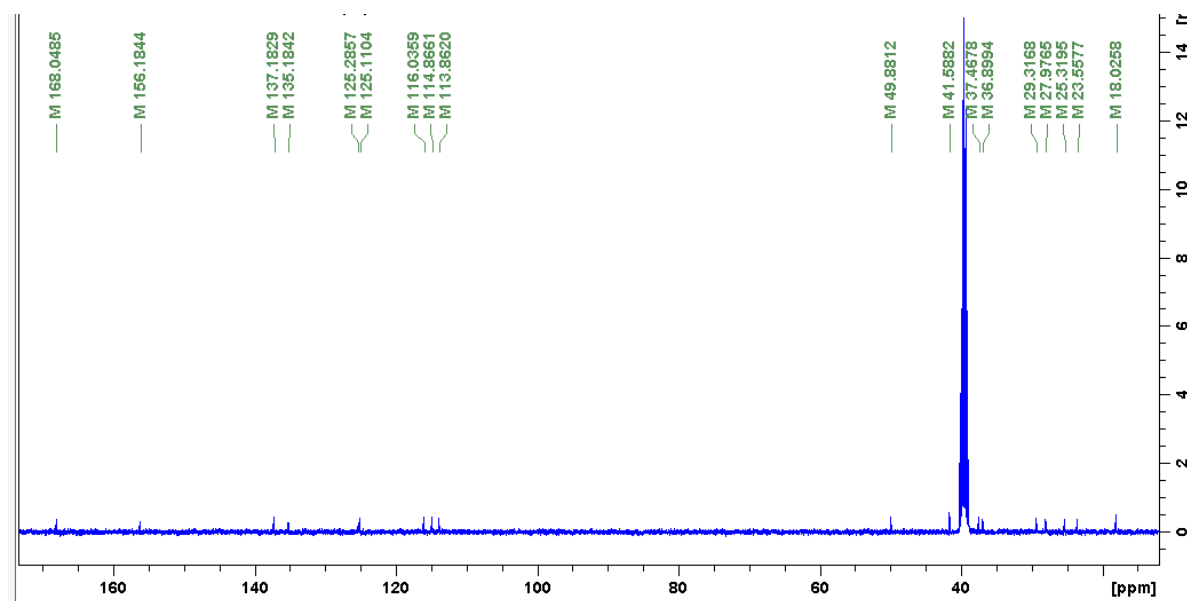


Figure S8. ¹³C-NMR spectrum of compound 11 in DMSO-d₆.

5. Spectra of compound 12

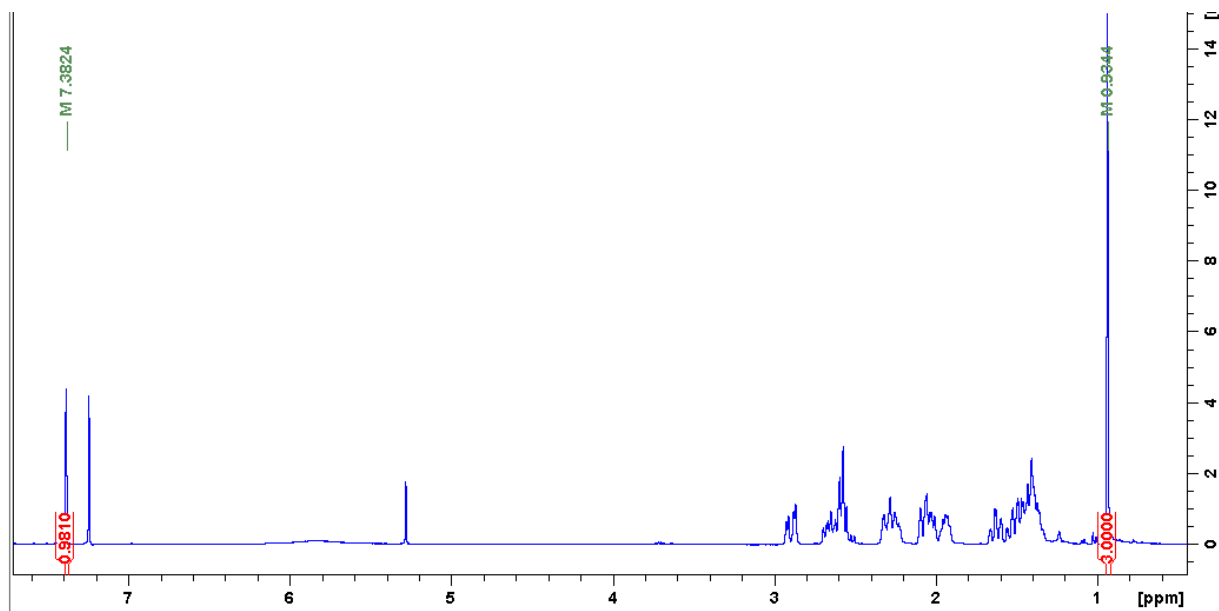
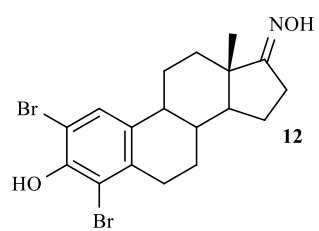


Figure S9. ¹H-NMR spectrum of compound 12 in in CDCl₃.

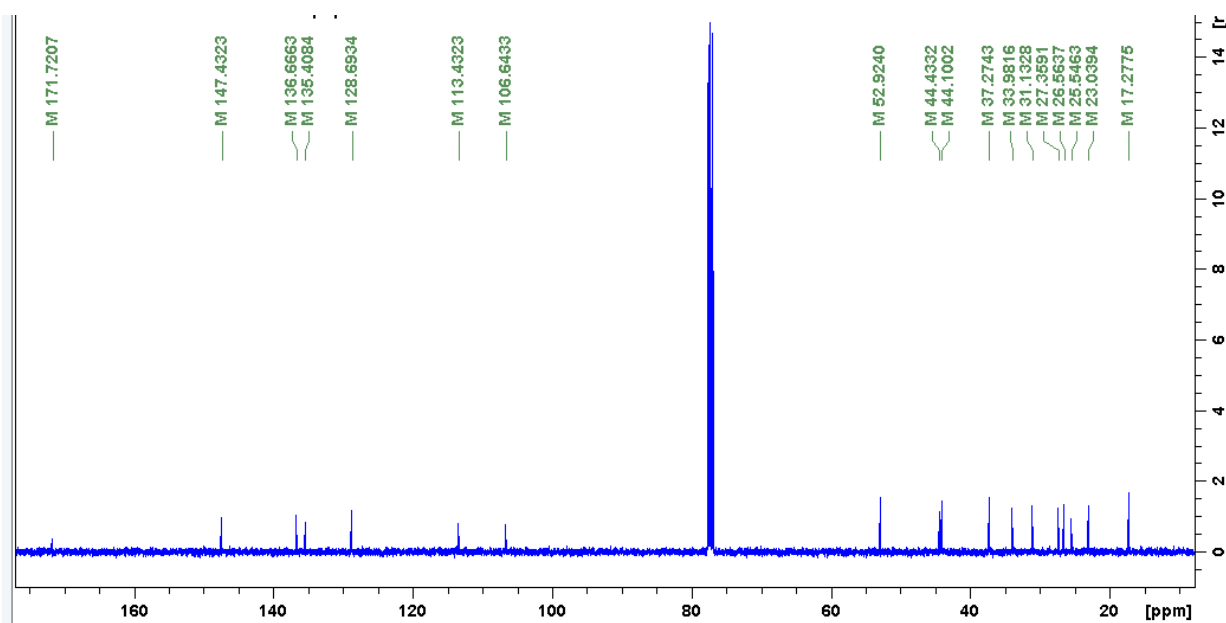


Figure S10. ¹³C-NMR spectrum of compound **12** in CDCl₃.