

## Electronic Supplementary Information for New Journal of Chemistry

### Effect of substituent and chain length in amino-1,4-naphthoquinones on glutathione-S-transferase inhibition: molecular docking and electrochemical perspectives: A structure-activity study.

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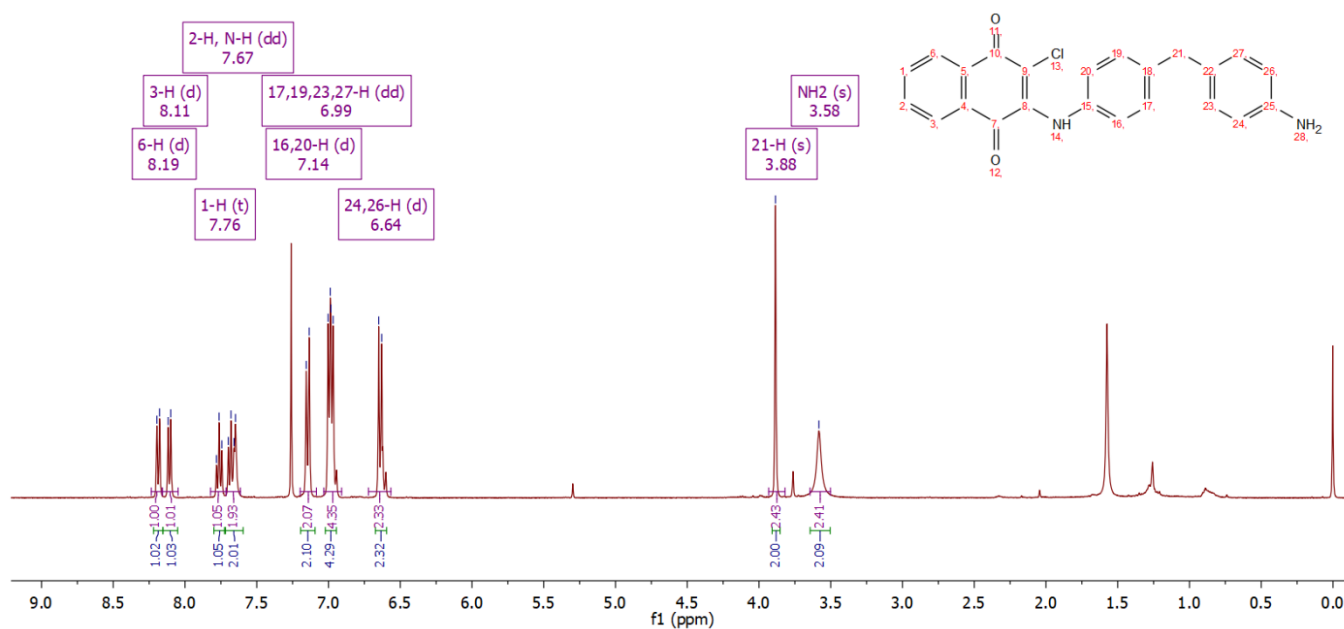
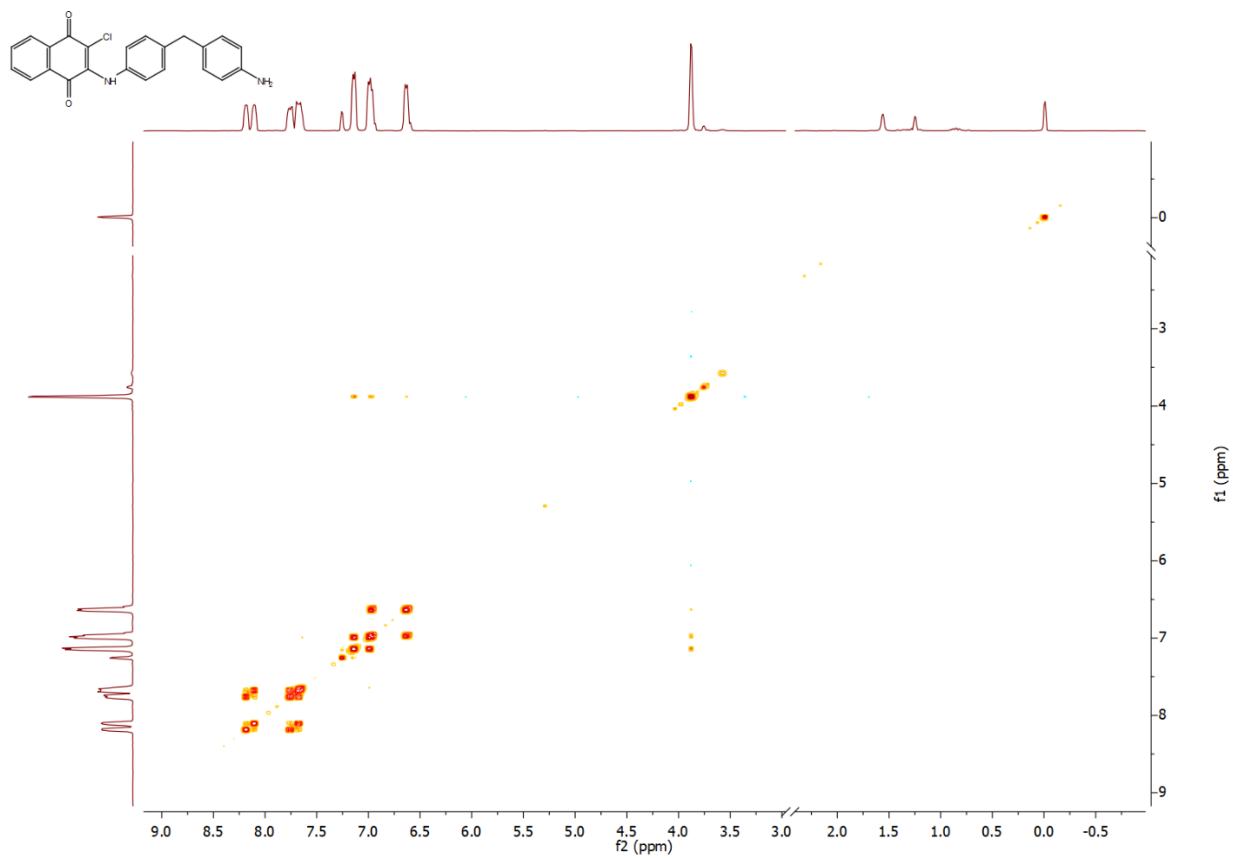
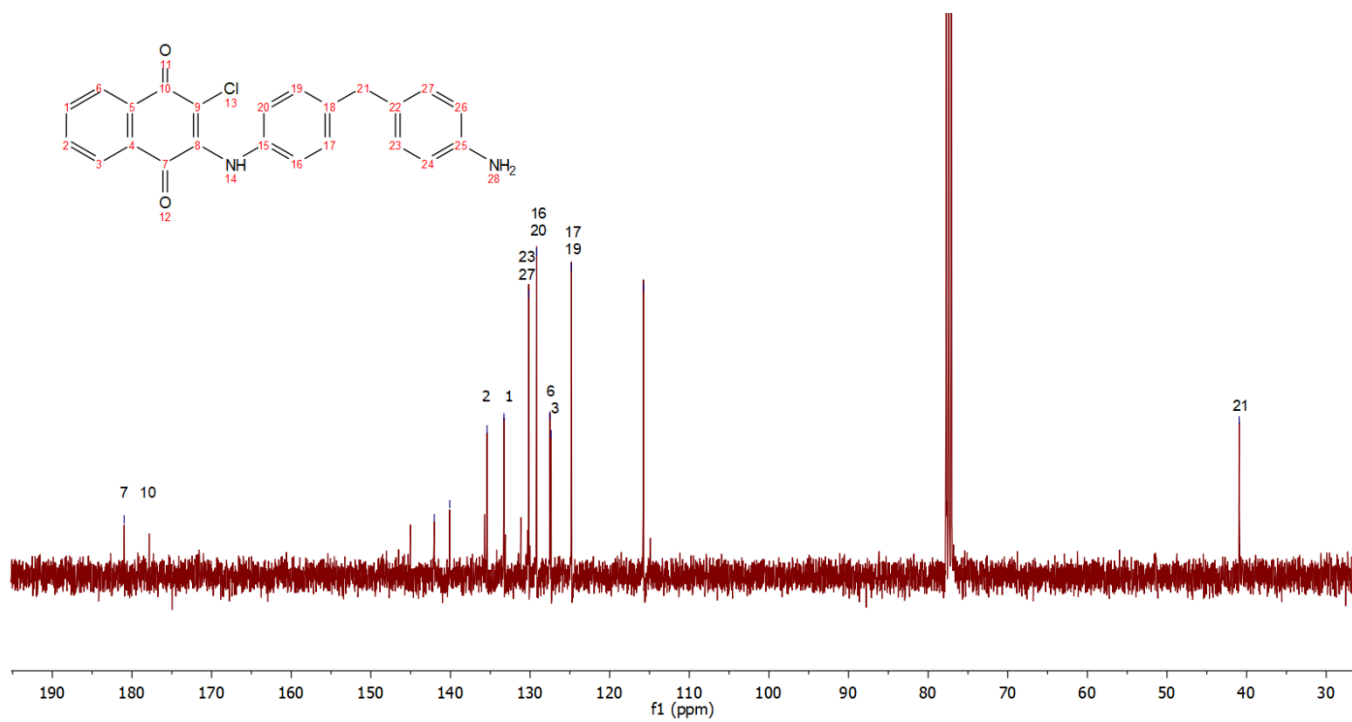


Figure S1. <sup>1</sup>H-NMR monoamination product **8** in CDCl<sub>3</sub>.



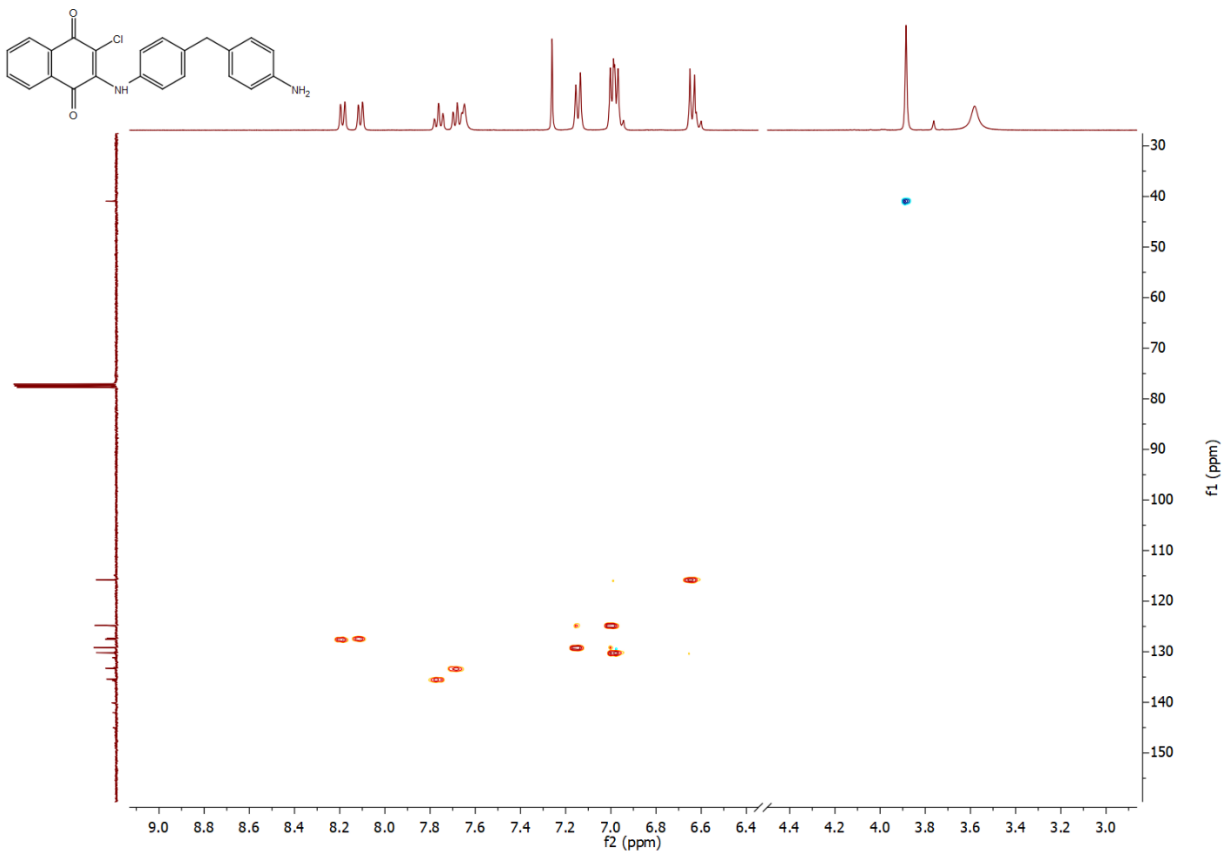


Figure S4. HSQC-NMR monoamination product **8** in  $\text{CDCl}_3$ .

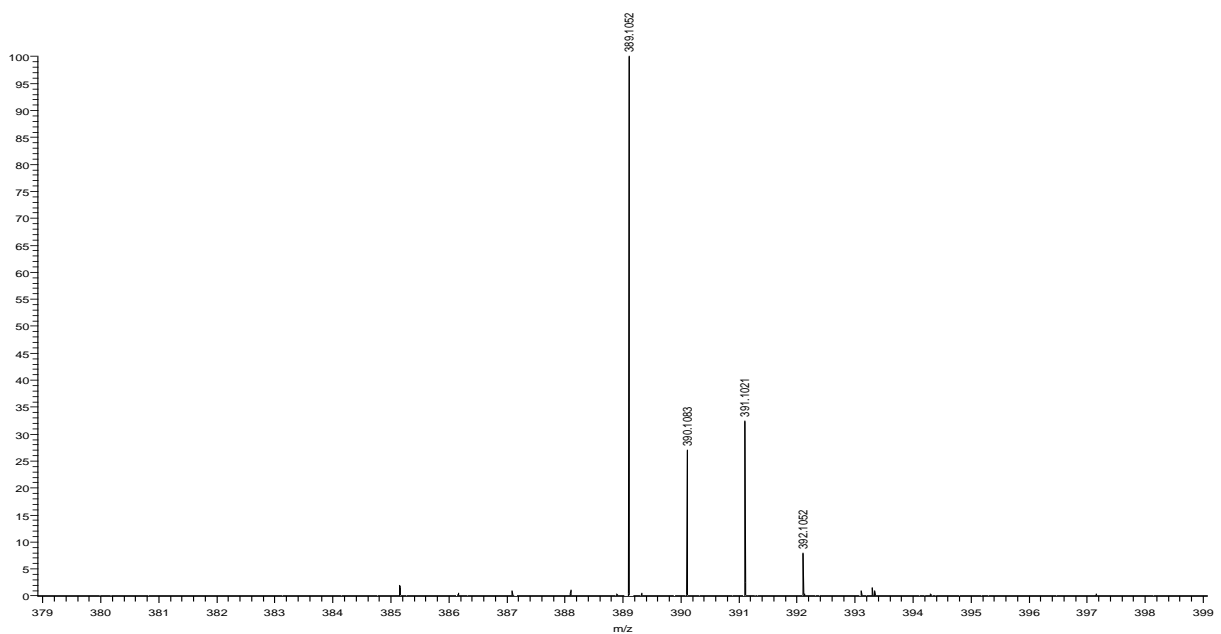


Figure S5. HRMS- $[\text{H}]^+$  monoamination product **8**.

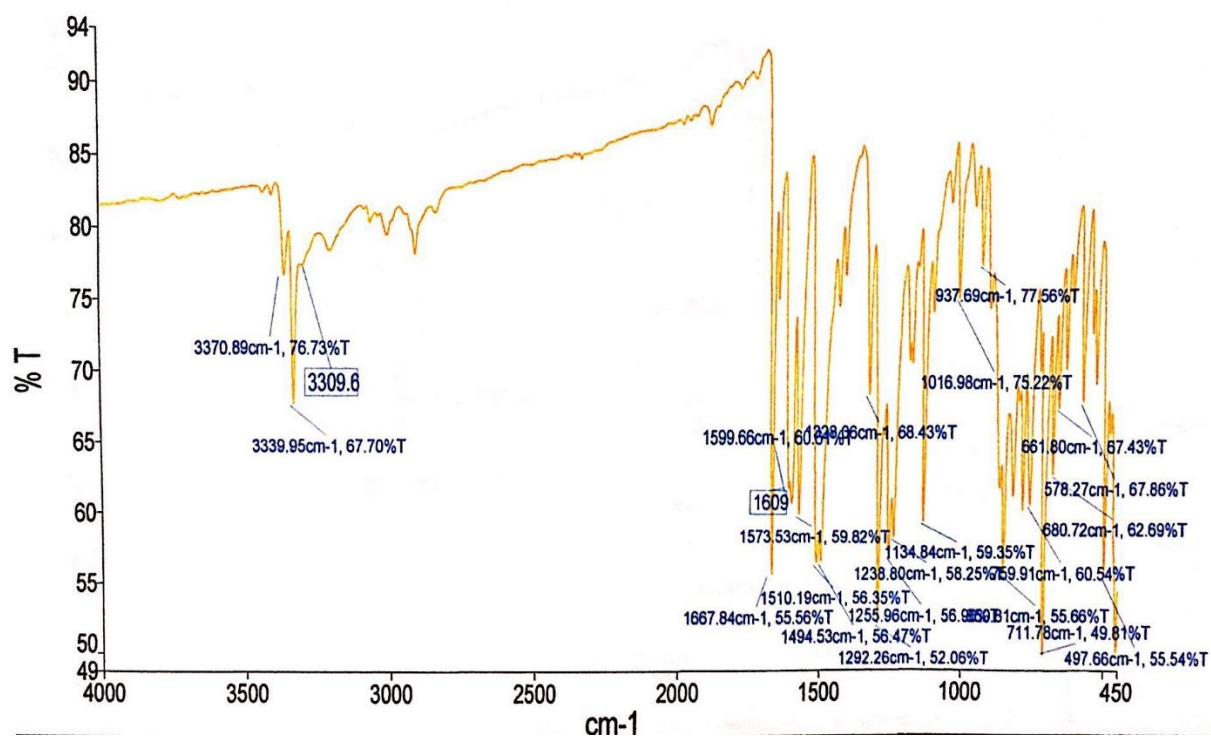


Figure S6. FT-IR product 8 in solid.

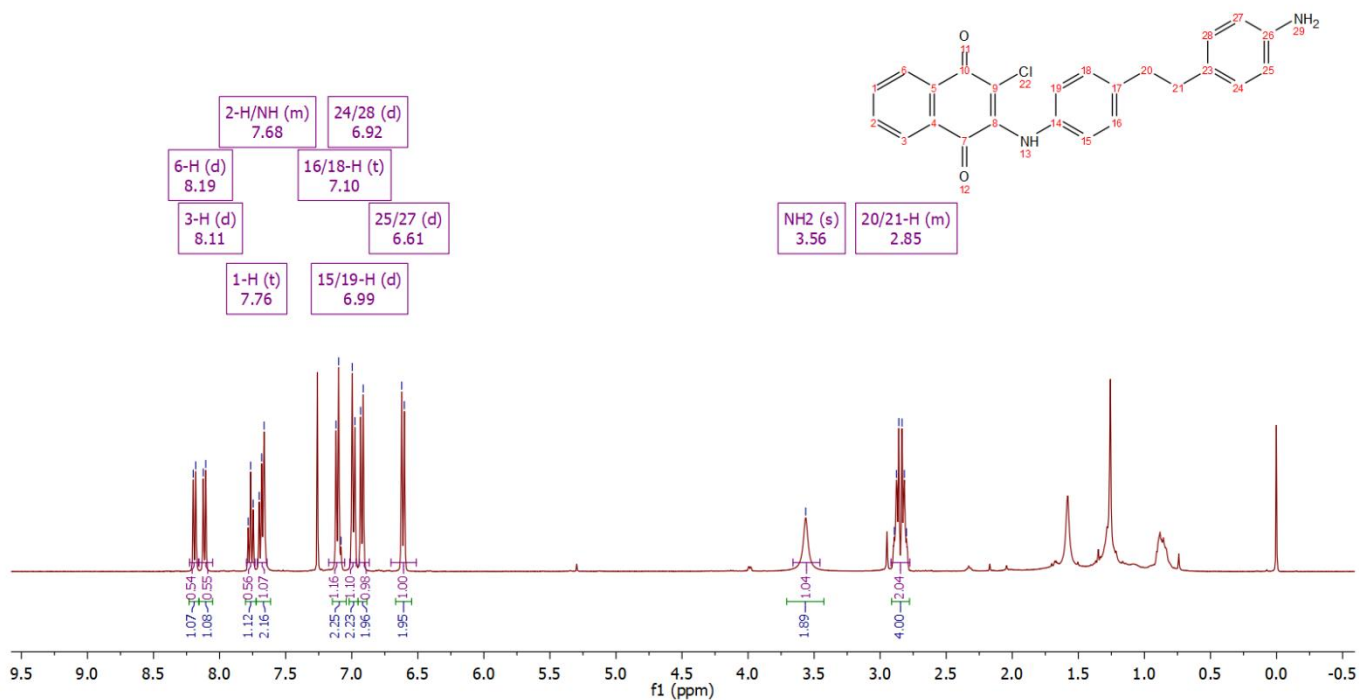


Figure S7.  $^1\text{H-NMR}$  monoamination product 9 in  $\text{CDCl}_3$ .

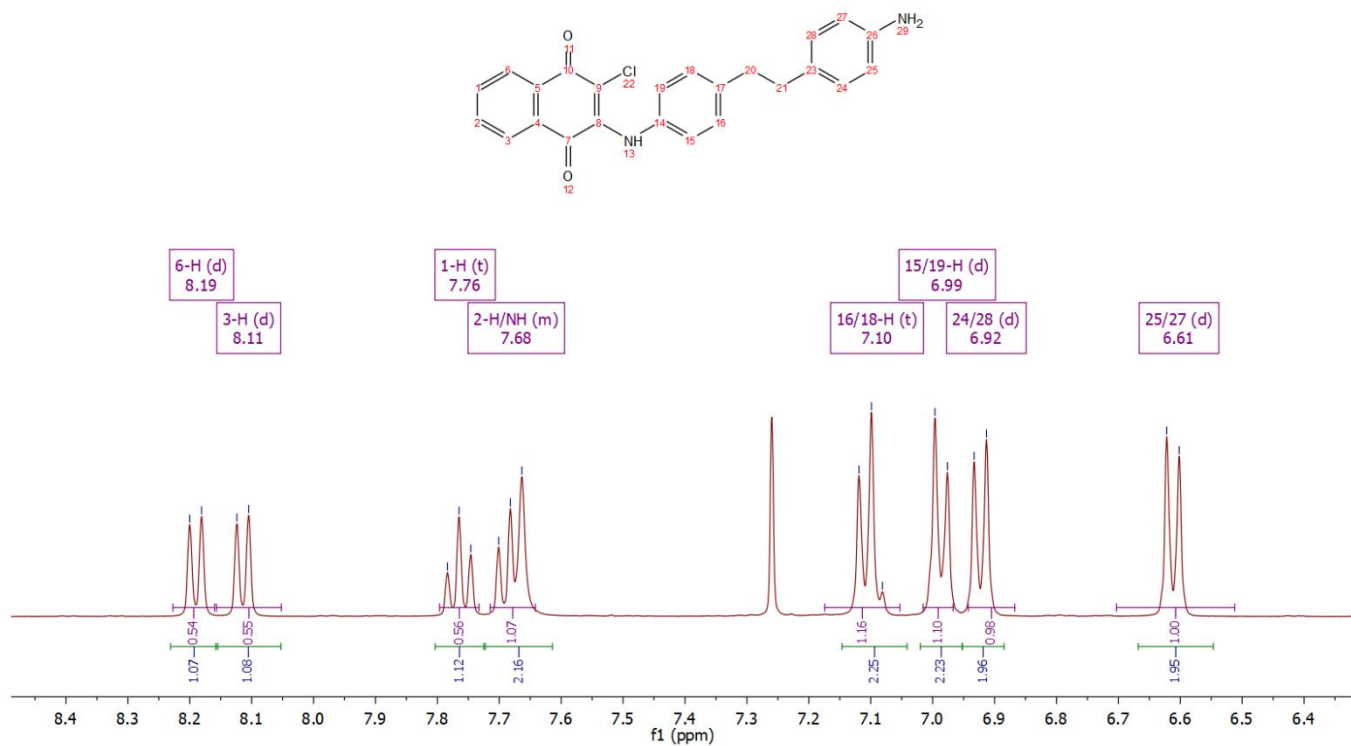


Figure S7A. Extended <sup>1</sup>H-NMR monoamination product 9 in CDCl<sub>3</sub>.

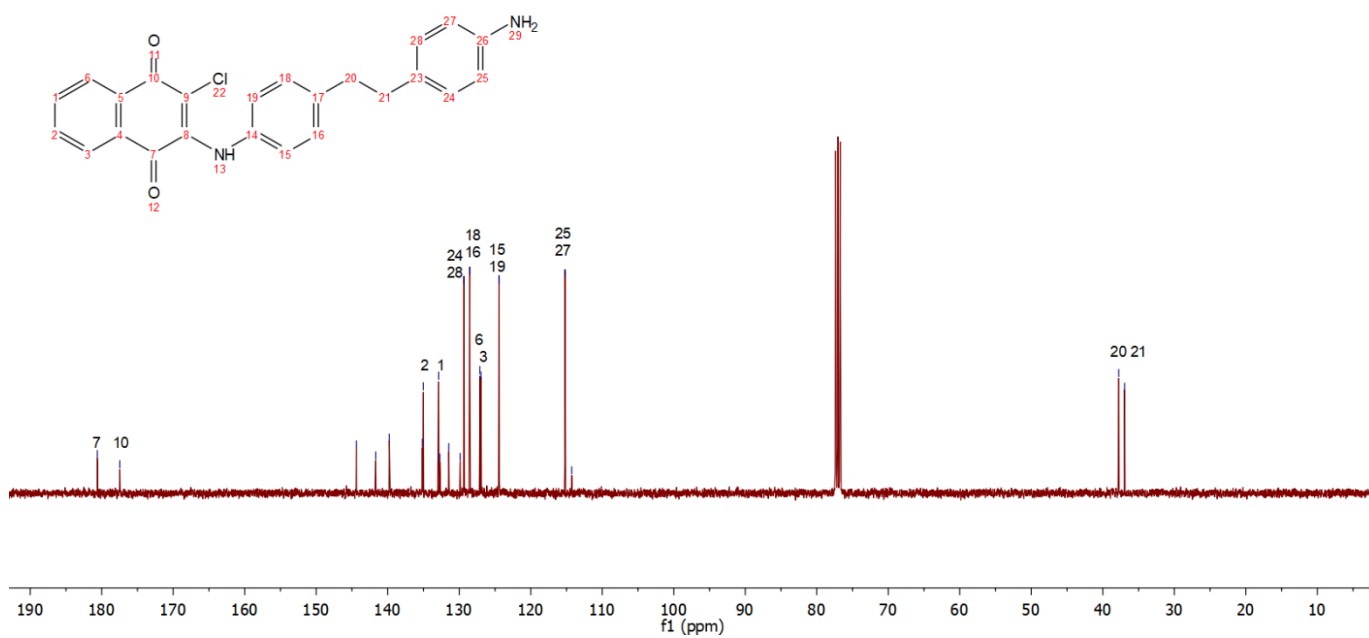


Figure S7B. <sup>13</sup>C-NMR monoamination product 9 in CDCl<sub>3</sub>.

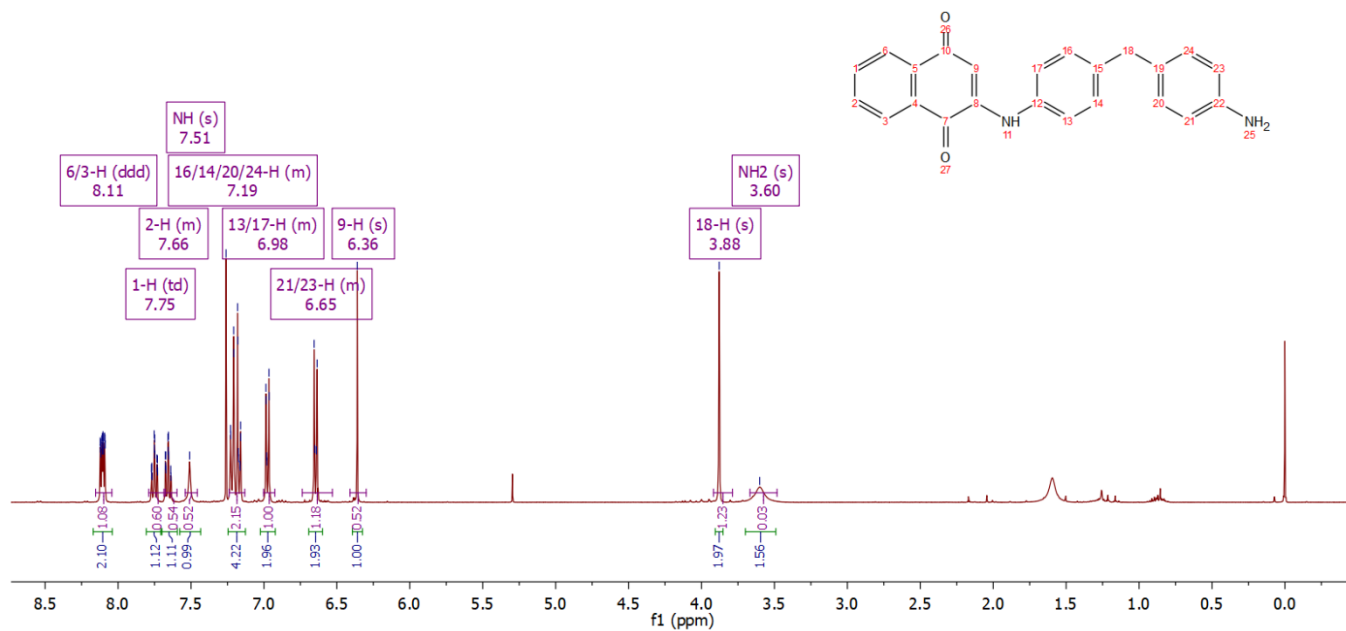


Figure S8. <sup>1</sup>H-NMR monoamination product **10** in CDCl<sub>3</sub>.

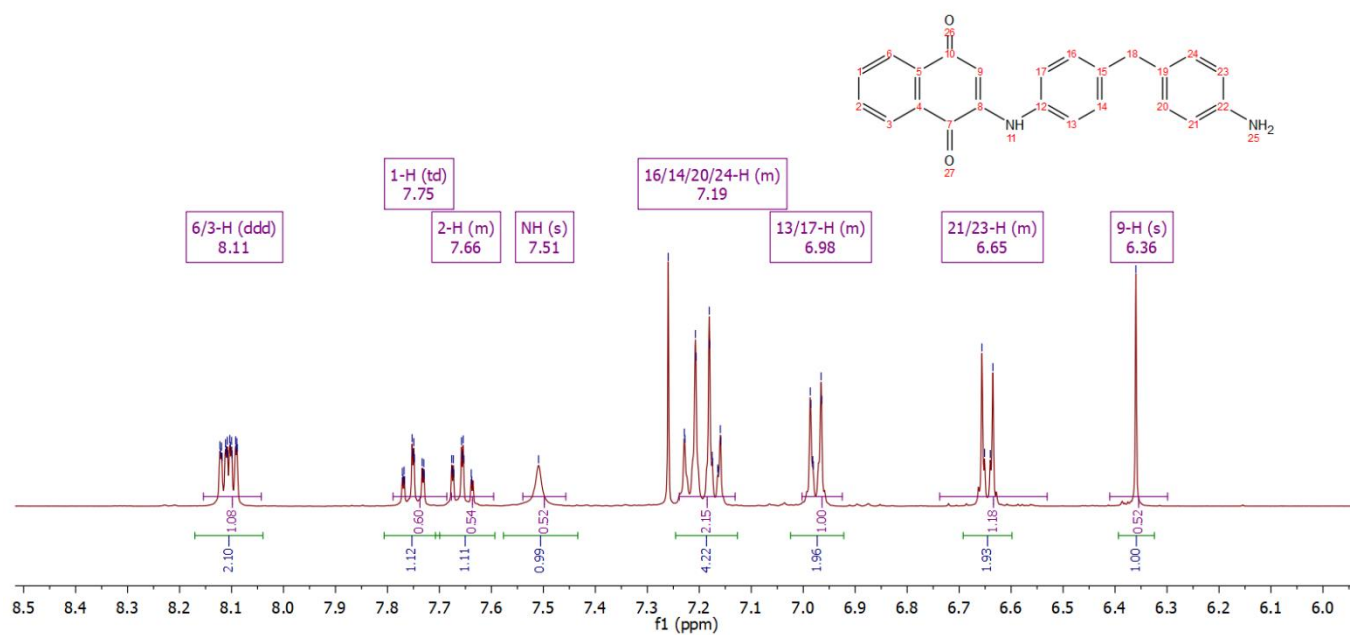


Figure S8A. Extended <sup>1</sup>H-NMR monoamination product **10** in CDCl<sub>3</sub>.

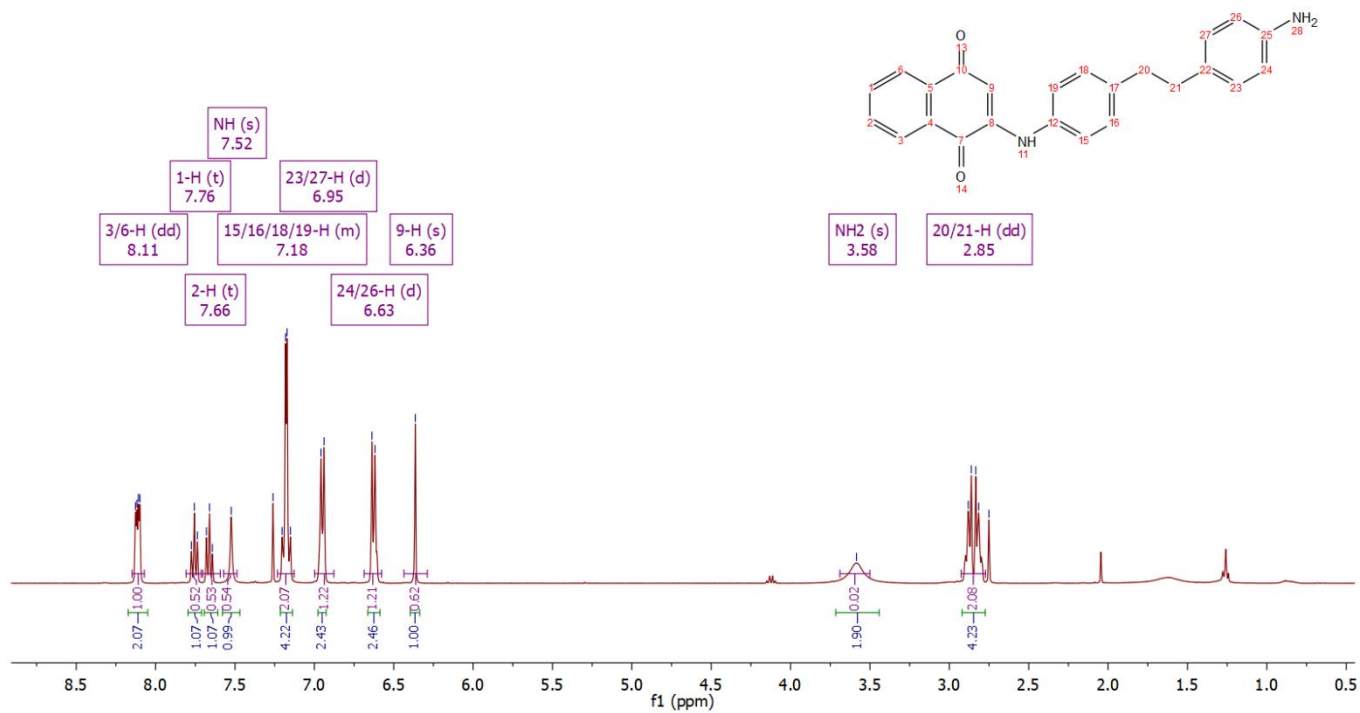


Figure S9. <sup>1</sup>H-NMR monoamination product **11** in CDCl<sub>3</sub>.

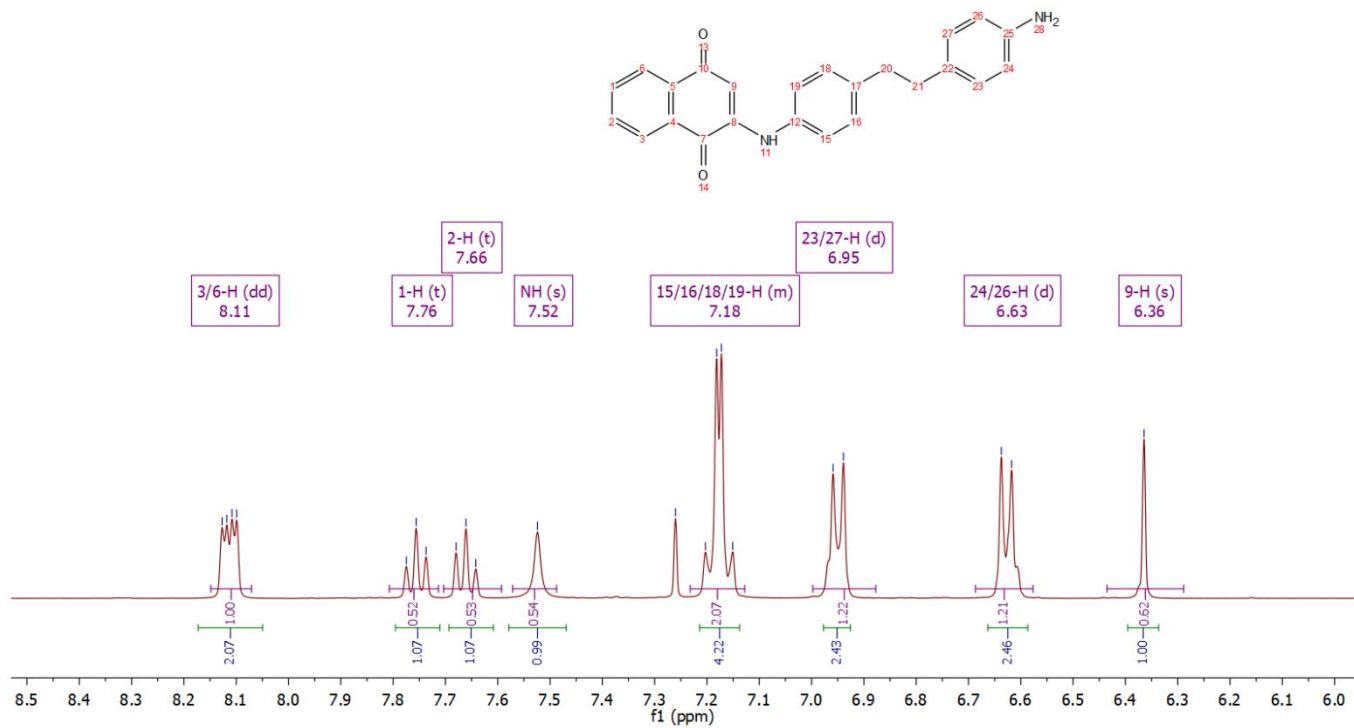
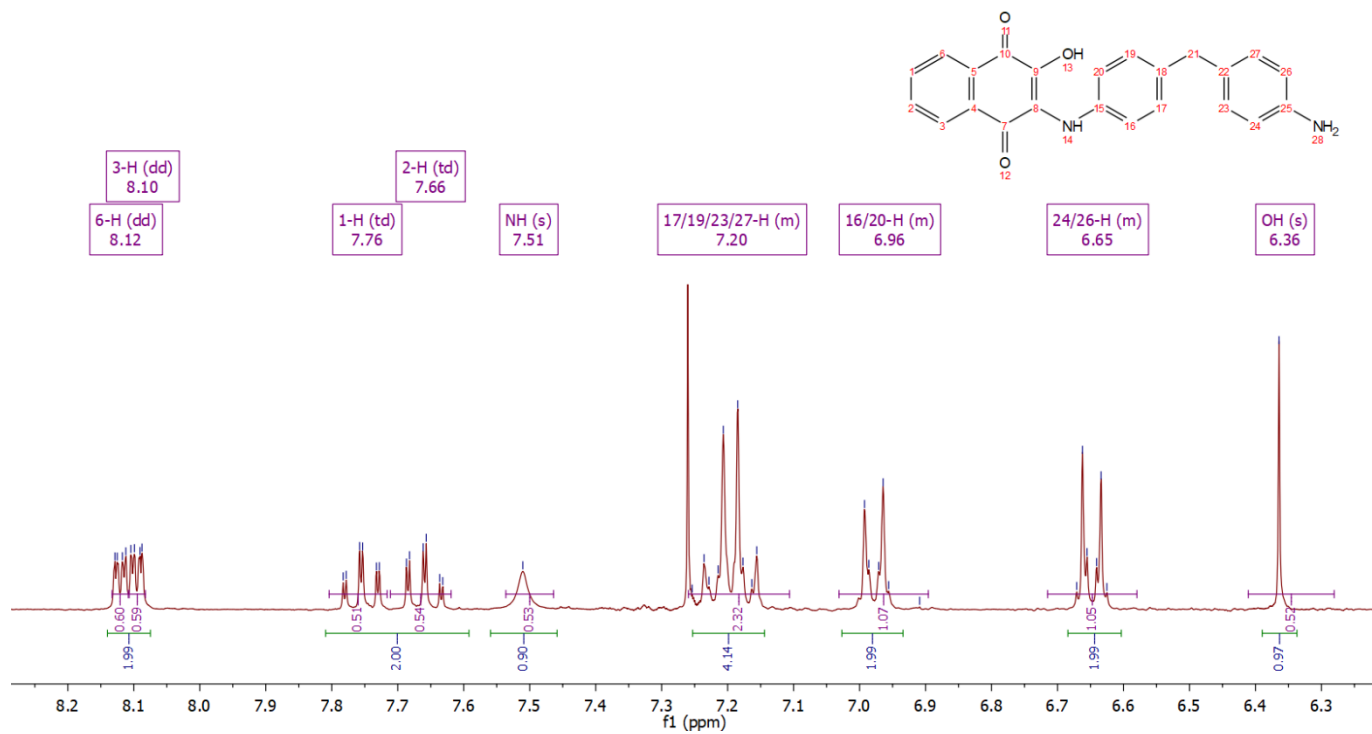
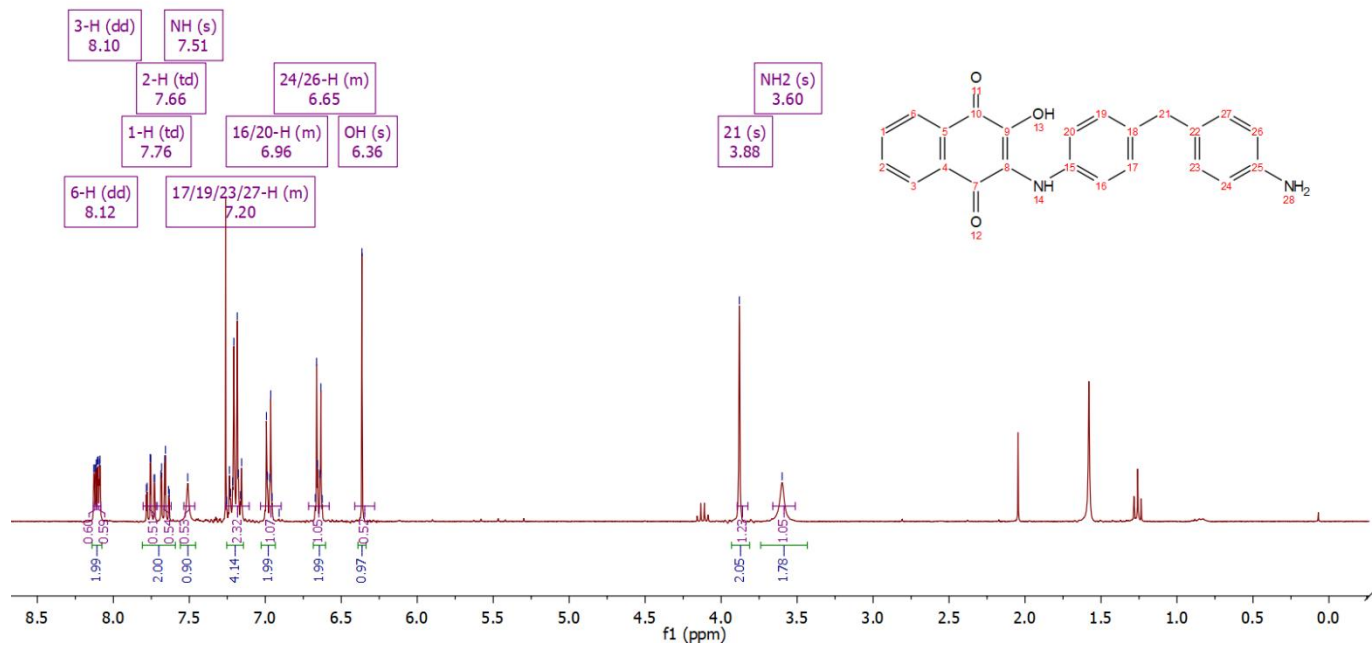


Figure S9A. Extended <sup>1</sup>H-NMR monoamination product **11** in CDCl<sub>3</sub>.





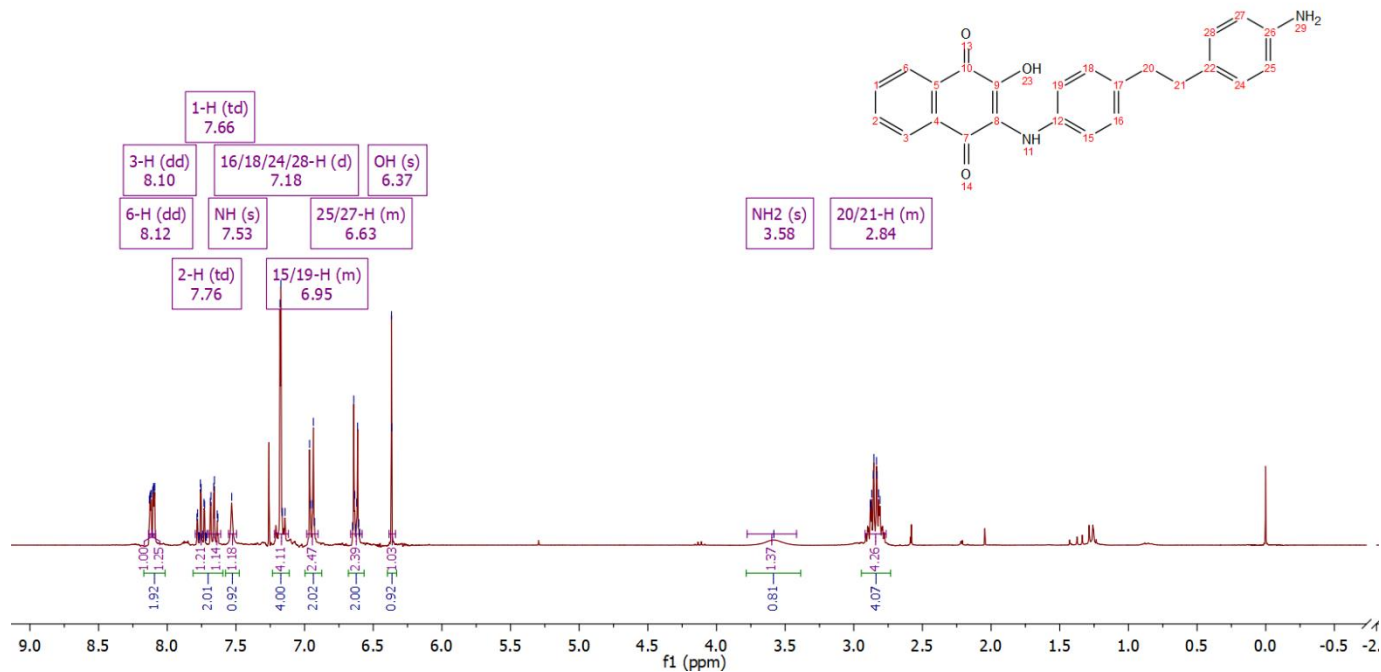


Figure S11. <sup>1</sup>H-NMR monoamination product **13** in CDCl<sub>3</sub>.

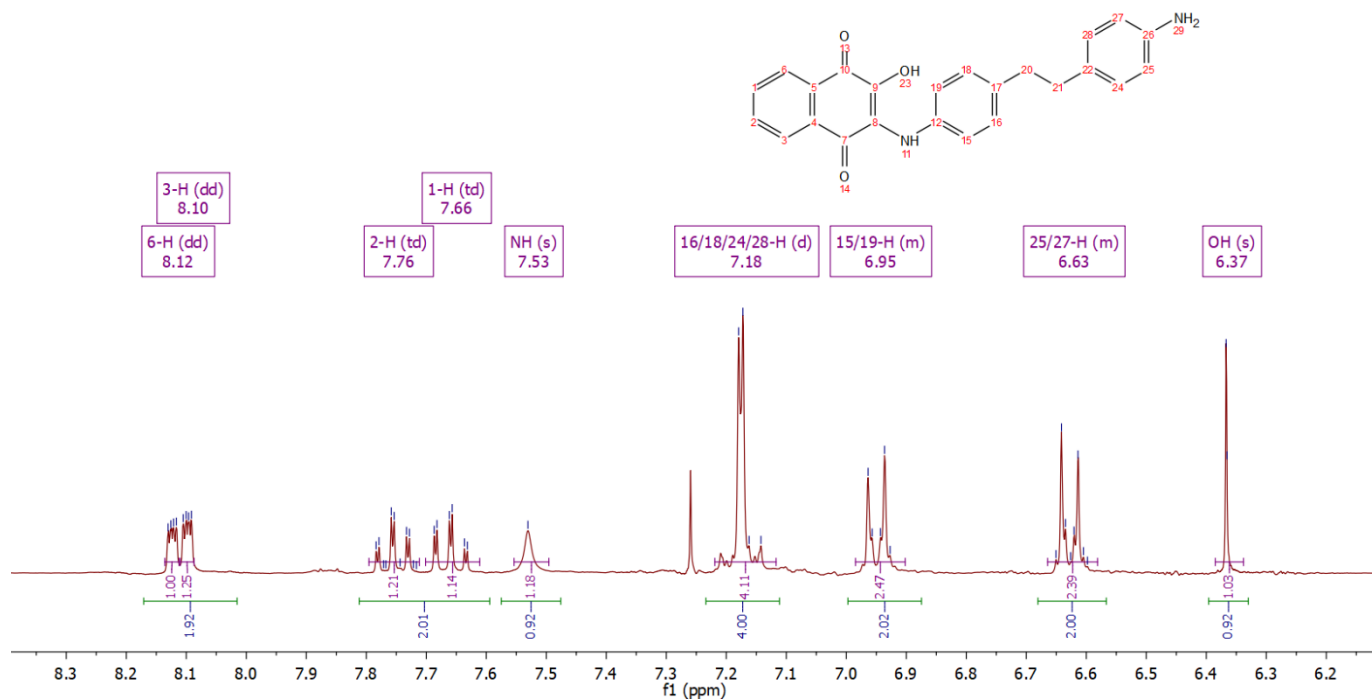


Figure S11A. Extended <sup>1</sup>H-NMR monoamination product **13** in CDCl<sub>3</sub>.

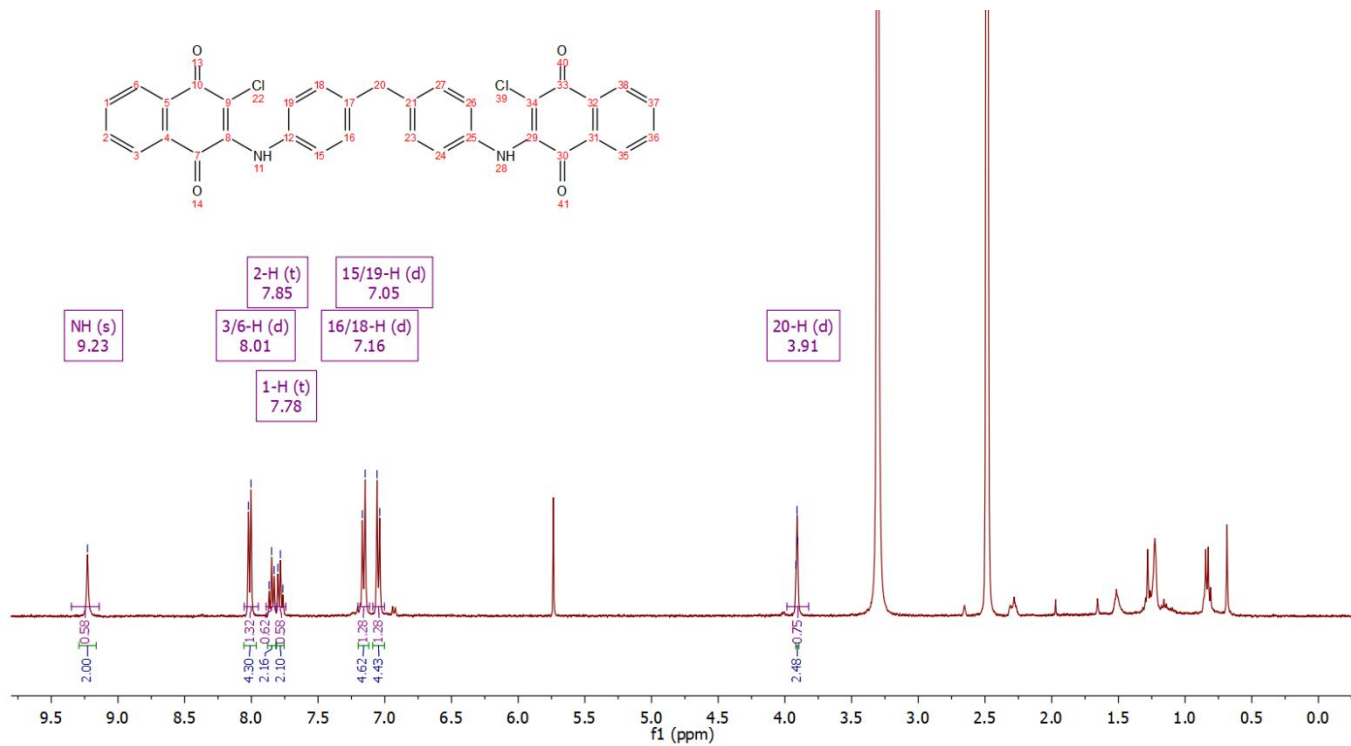


Figure S12. <sup>1</sup>H-NMR homodimer **14** in DMSO.

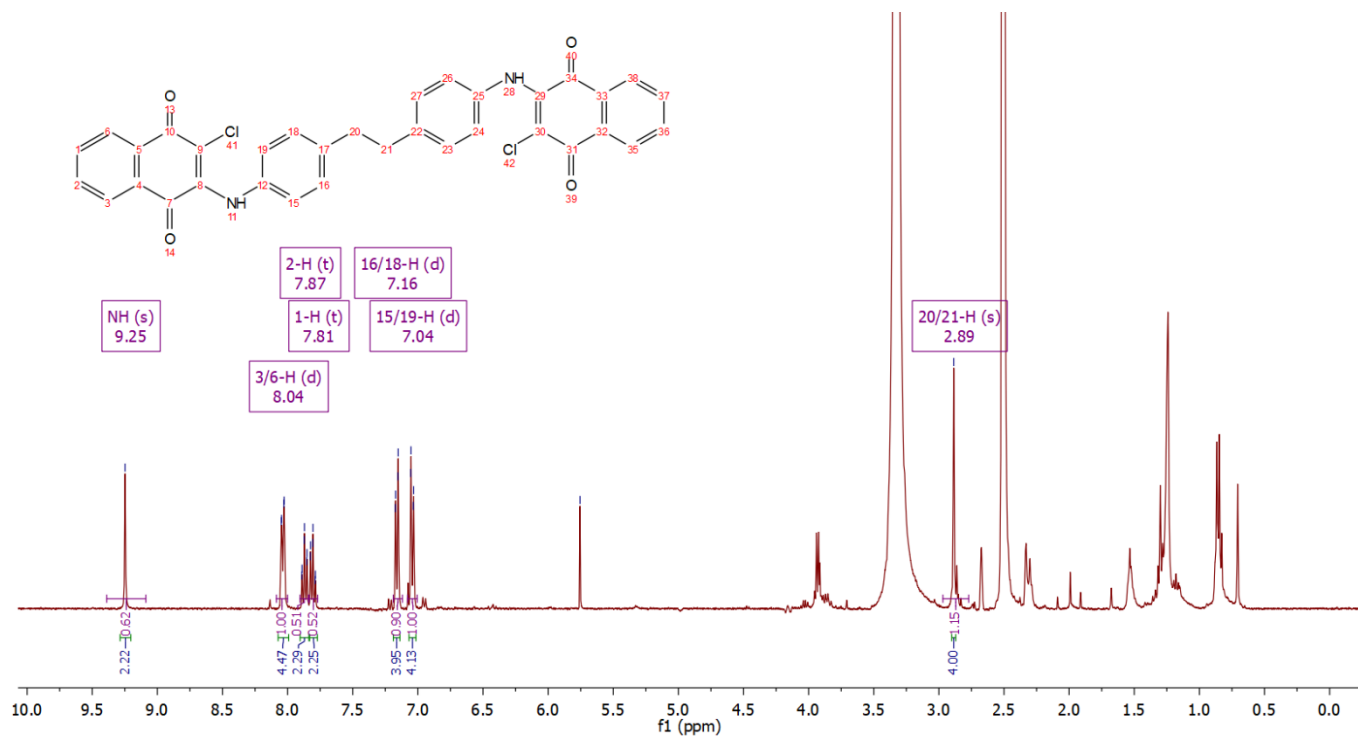


Figure S13. <sup>1</sup>H-NMR homodimer **15** in DMSO.

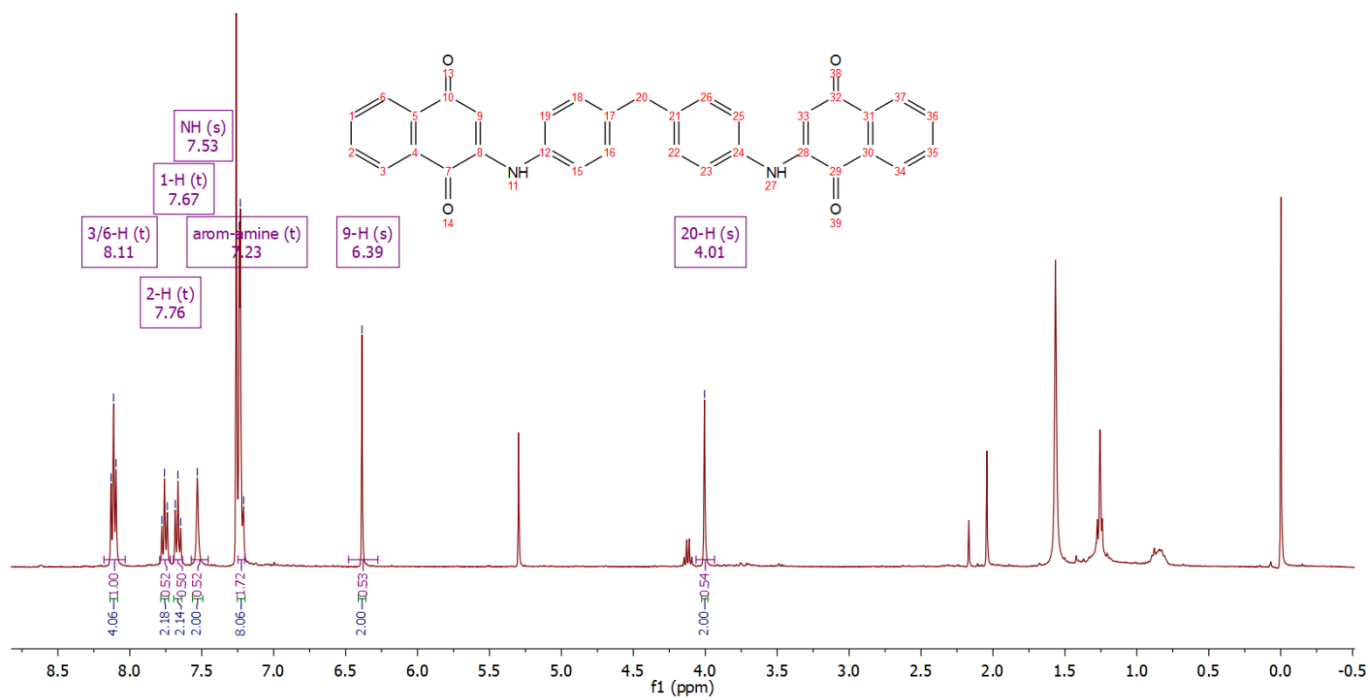


Figure S14.  $^1\text{H-NMR}$  homodimer **16** in  $\text{CDCl}_3$ .

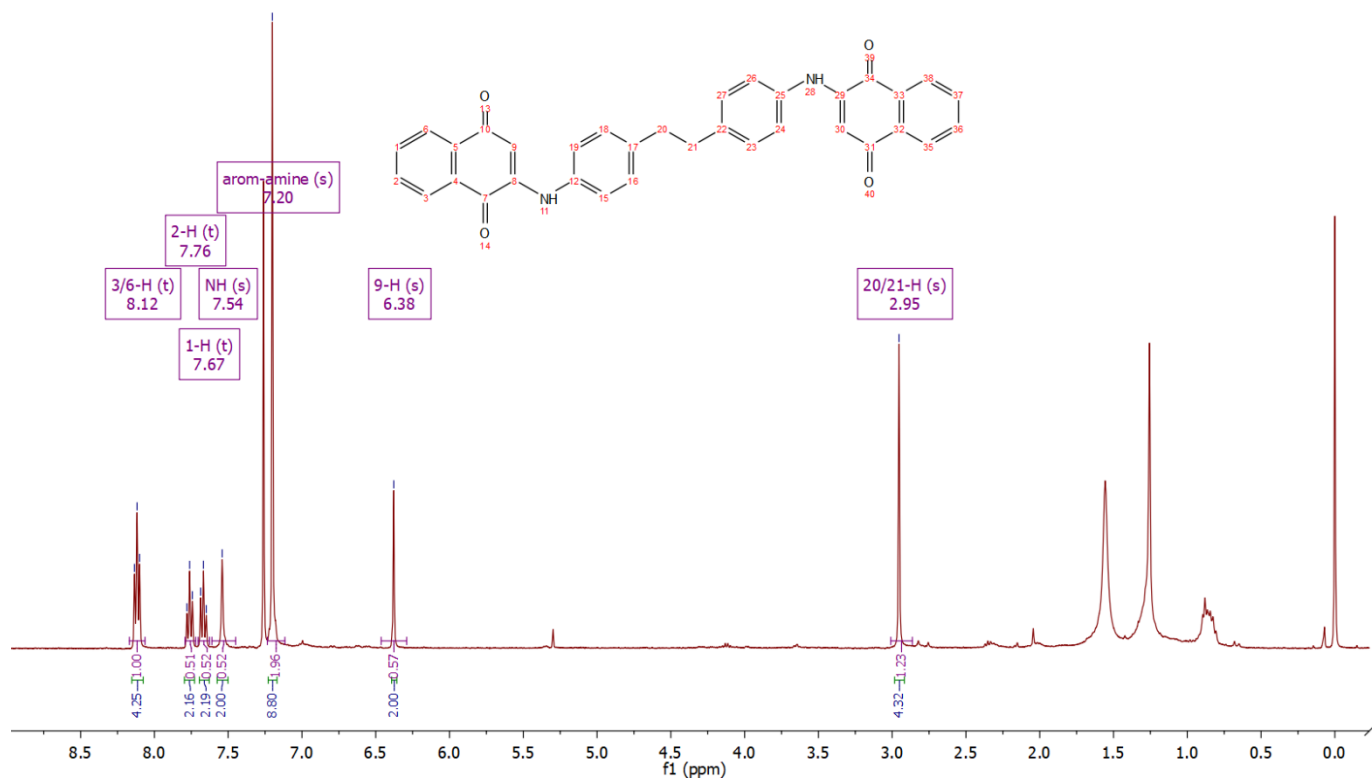


Figure S15.  $^1\text{H-NMR}$  homodimer **17** in  $\text{CDCl}_3$ .

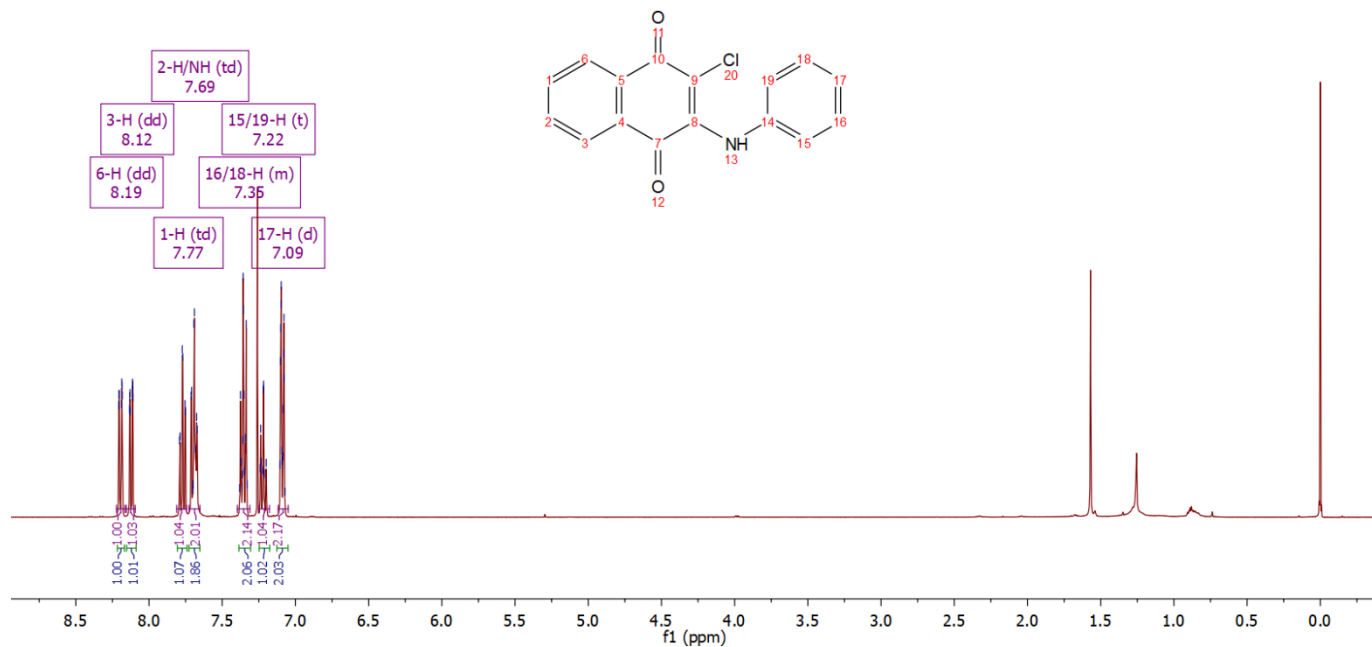


Figure S16.  $^1\text{H-NMR}$  pharmacophore **18** in  $\text{CDCl}_3$ .

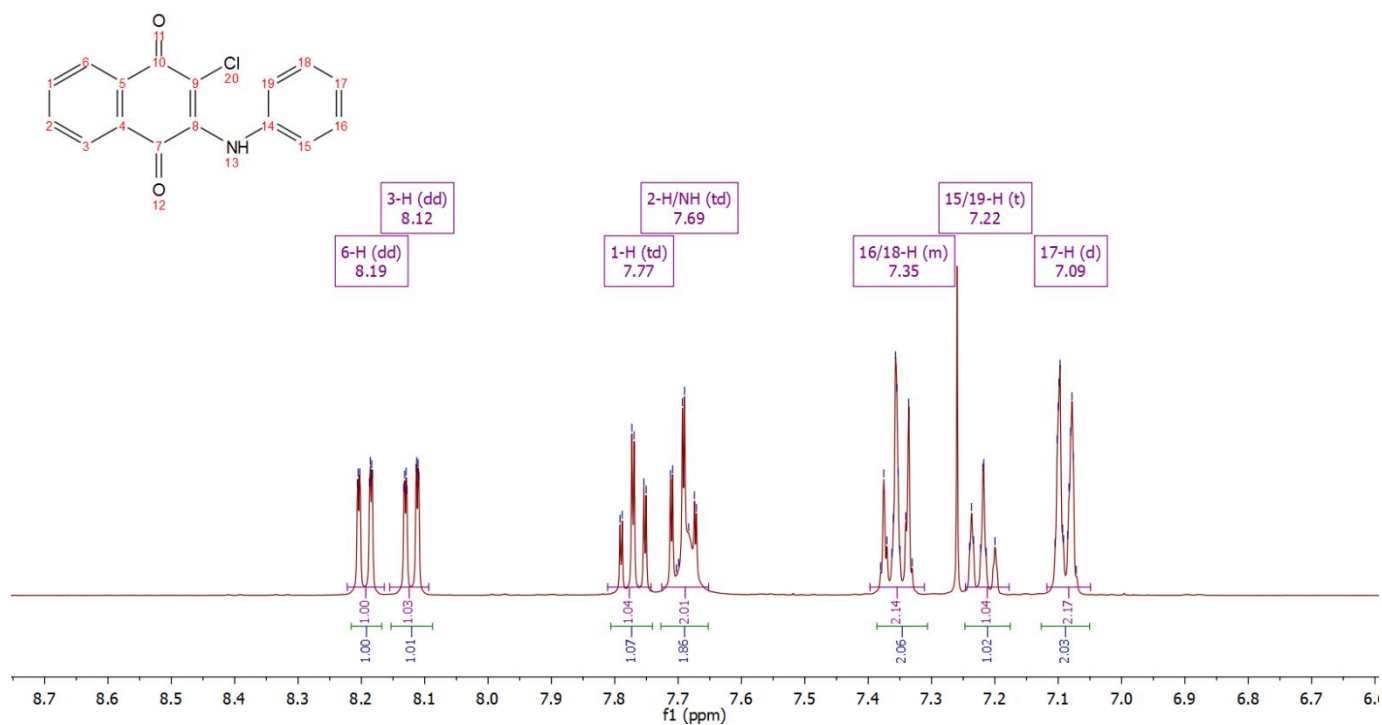


Figure S16A. Extended  $^1\text{H-NMR}$  pharmacophore **18** in  $\text{CDCl}_3$ .

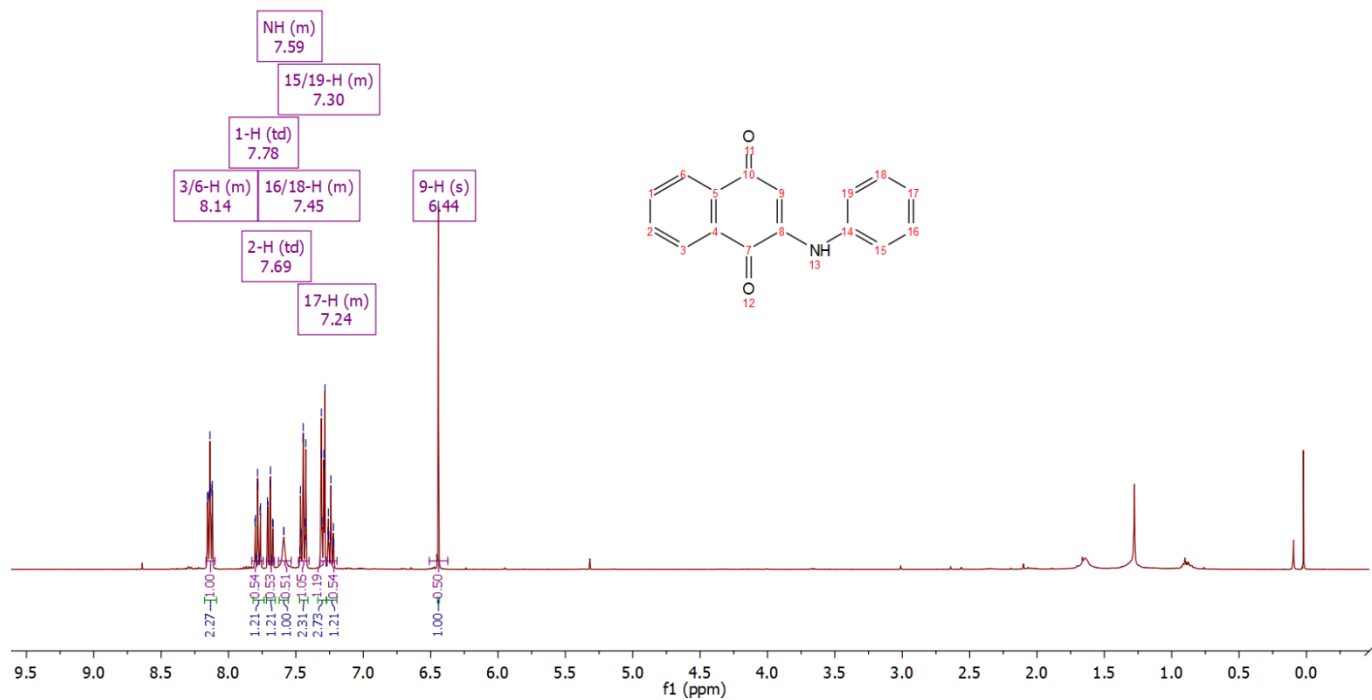


Figure S17.  $^1\text{H-NMR}$  pharmacophore 19 in  $\text{CDCl}_3$ .

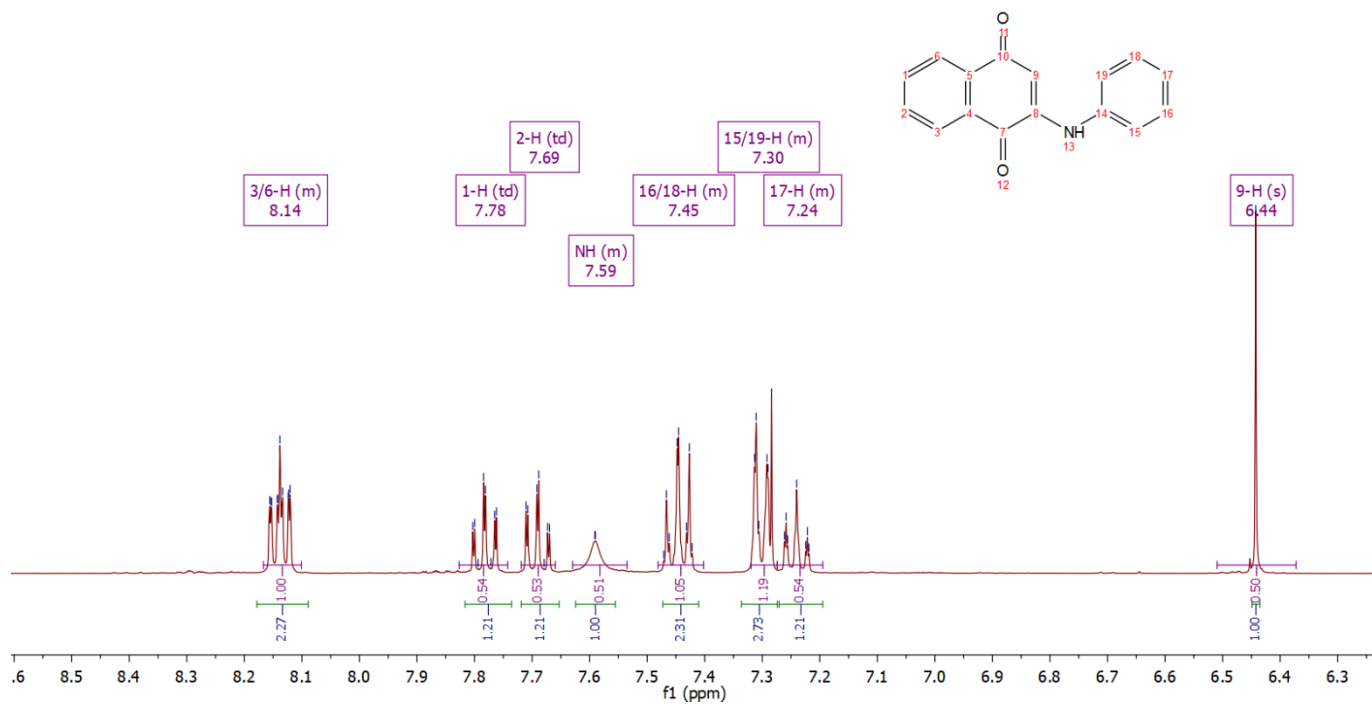


Figure S17A. Extended  $^1\text{H-NMR}$  pharmacophore 19 in  $\text{CDCl}_3$ .

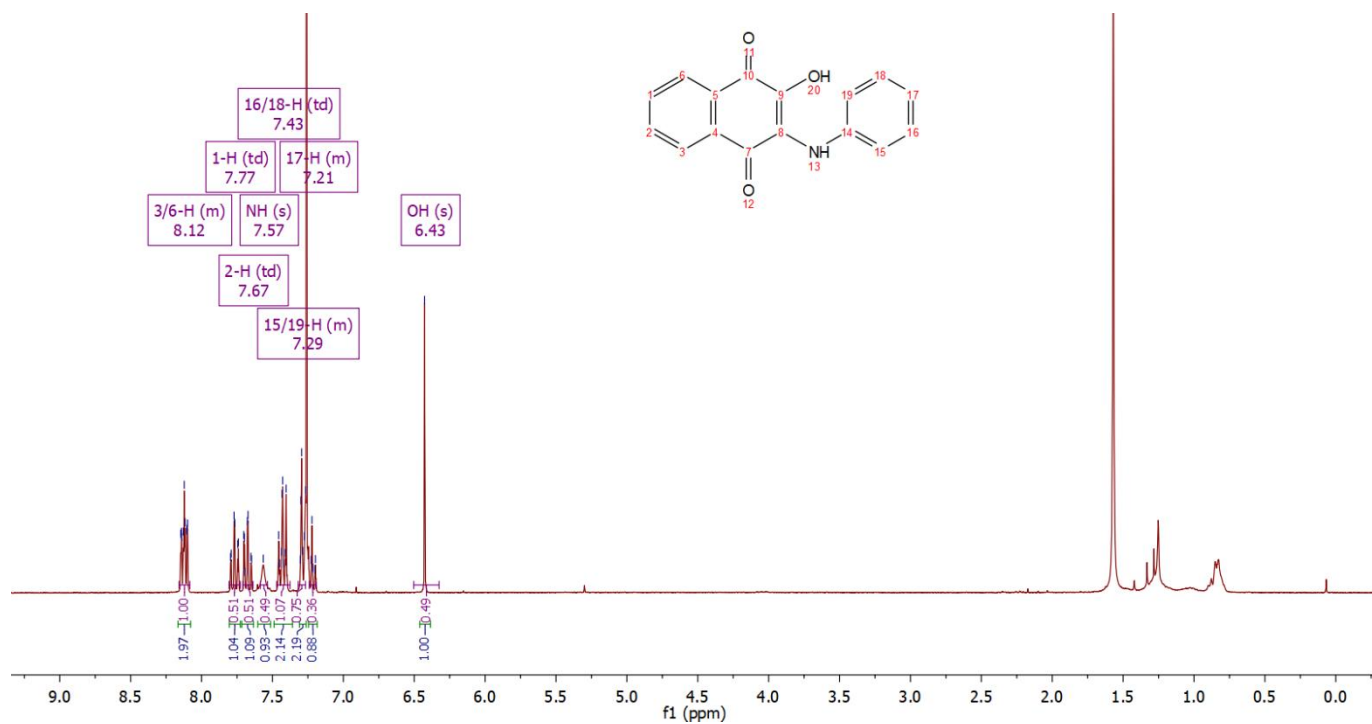


Figure S18.  $^1\text{H-NMR}$  pharmacophore **20** in  $\text{CDCl}_3$ .

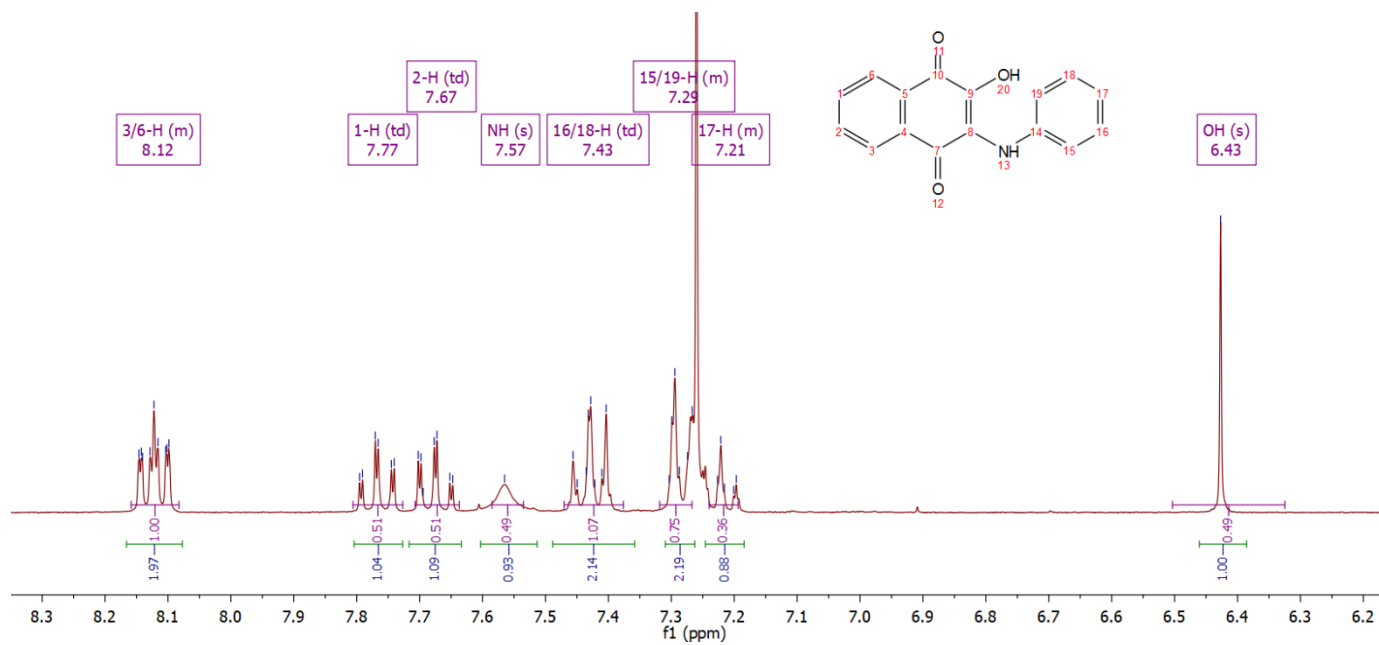


Figure S18A. Extended  $^1\text{H-NMR}$  pharmacophore **20** in  $\text{CDCl}_3$ .

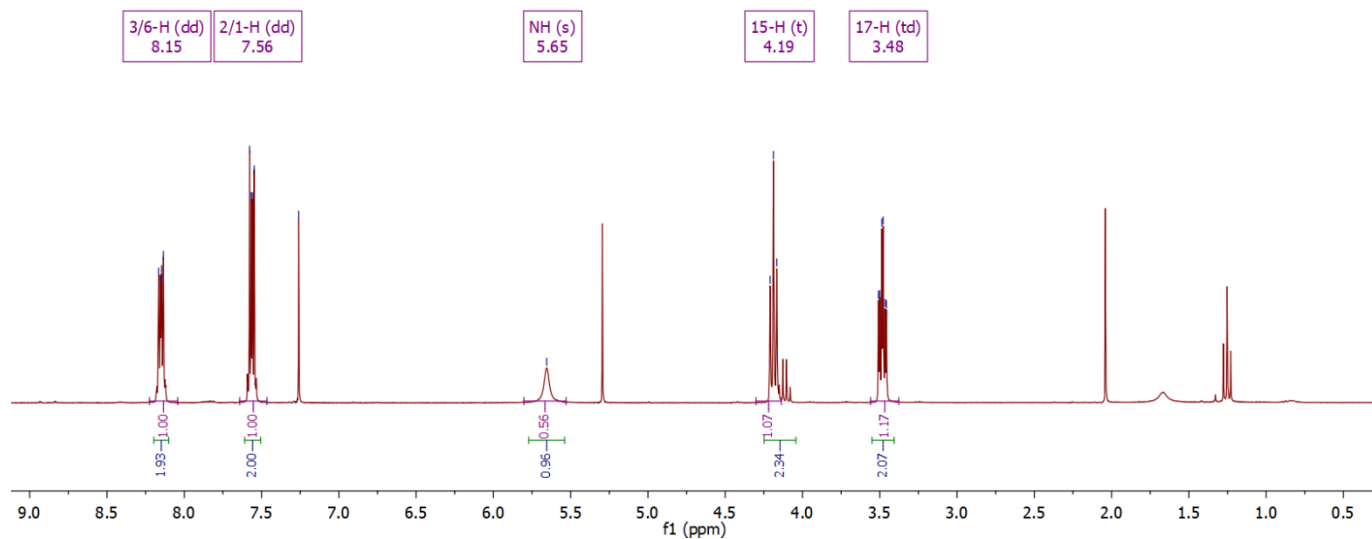
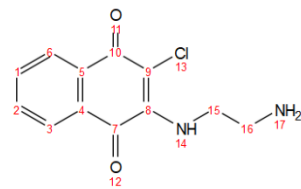


Figure S19. <sup>1</sup>H-NMR monoamination product **21** in CDCl<sub>3</sub>.

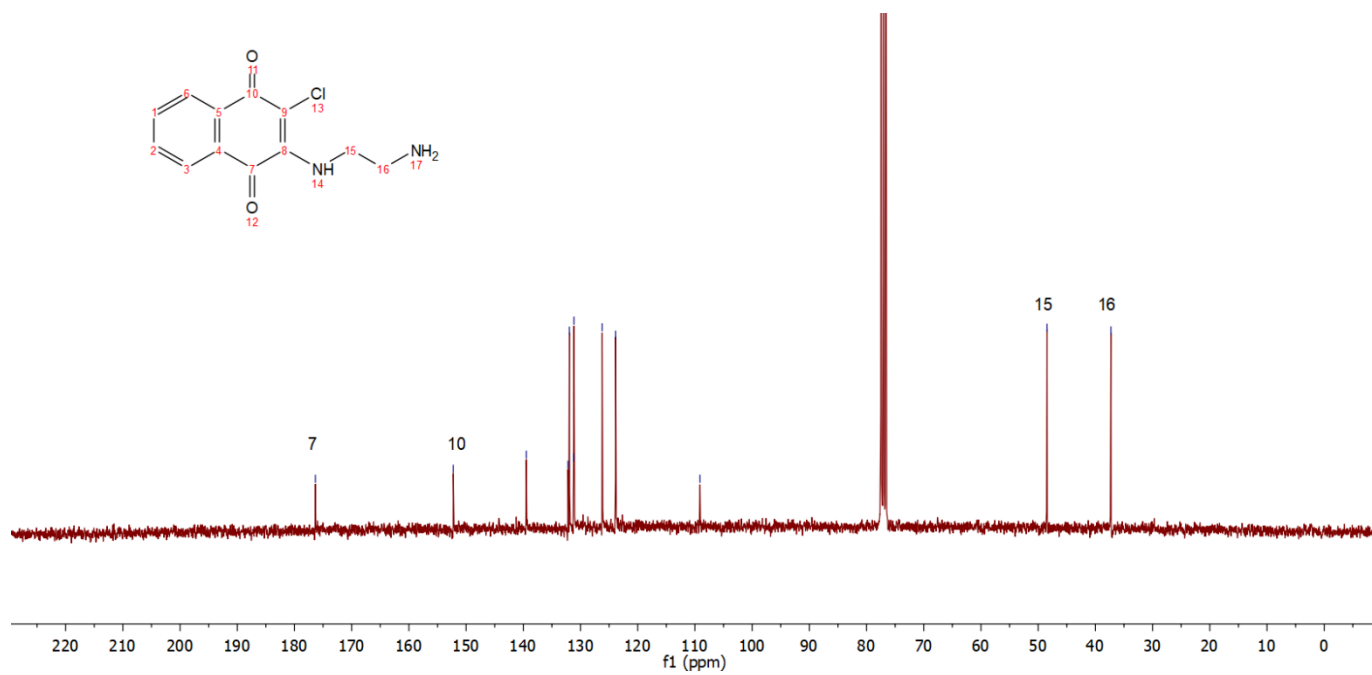


Figure S19A. <sup>13</sup>C-NMR monoamination product **21** in CDCl<sub>3</sub>.

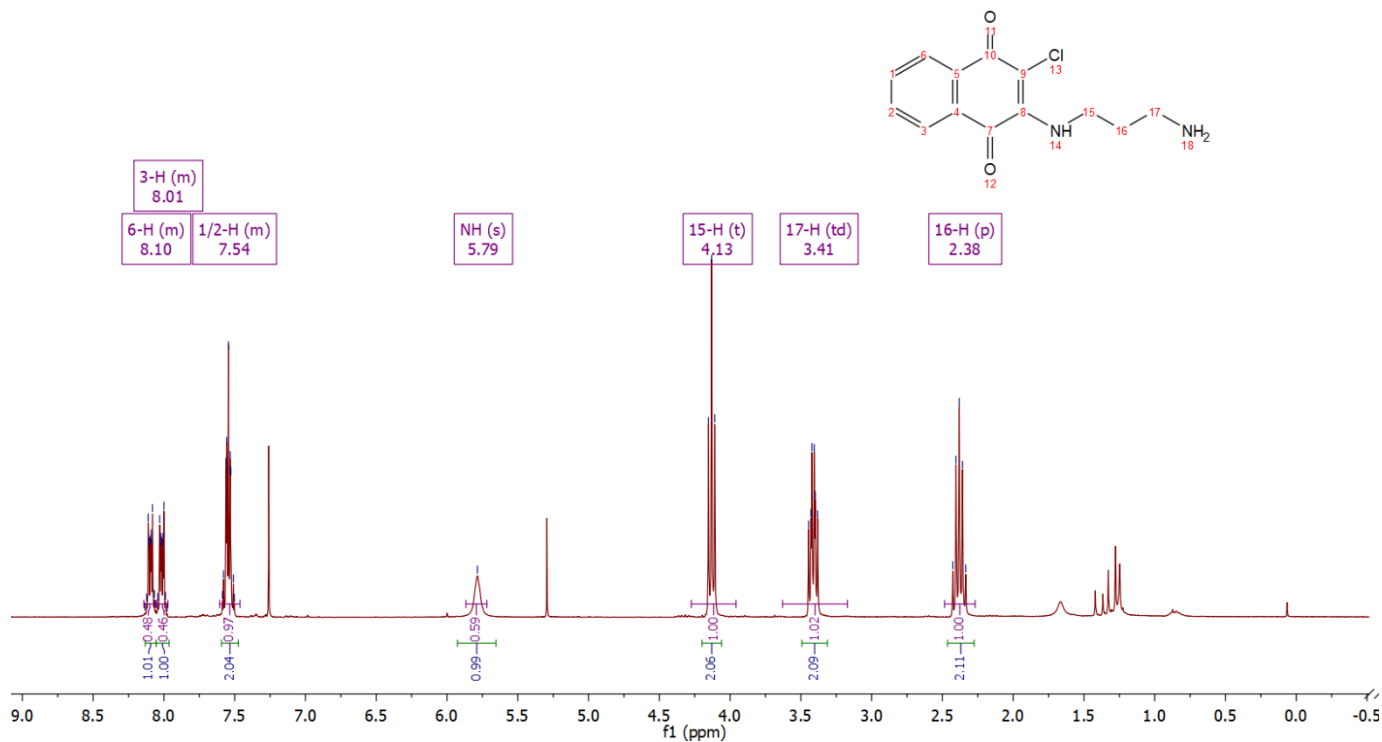


Figure S20. <sup>1</sup>H-NMR monoamination product **22** in CDCl<sub>3</sub>.

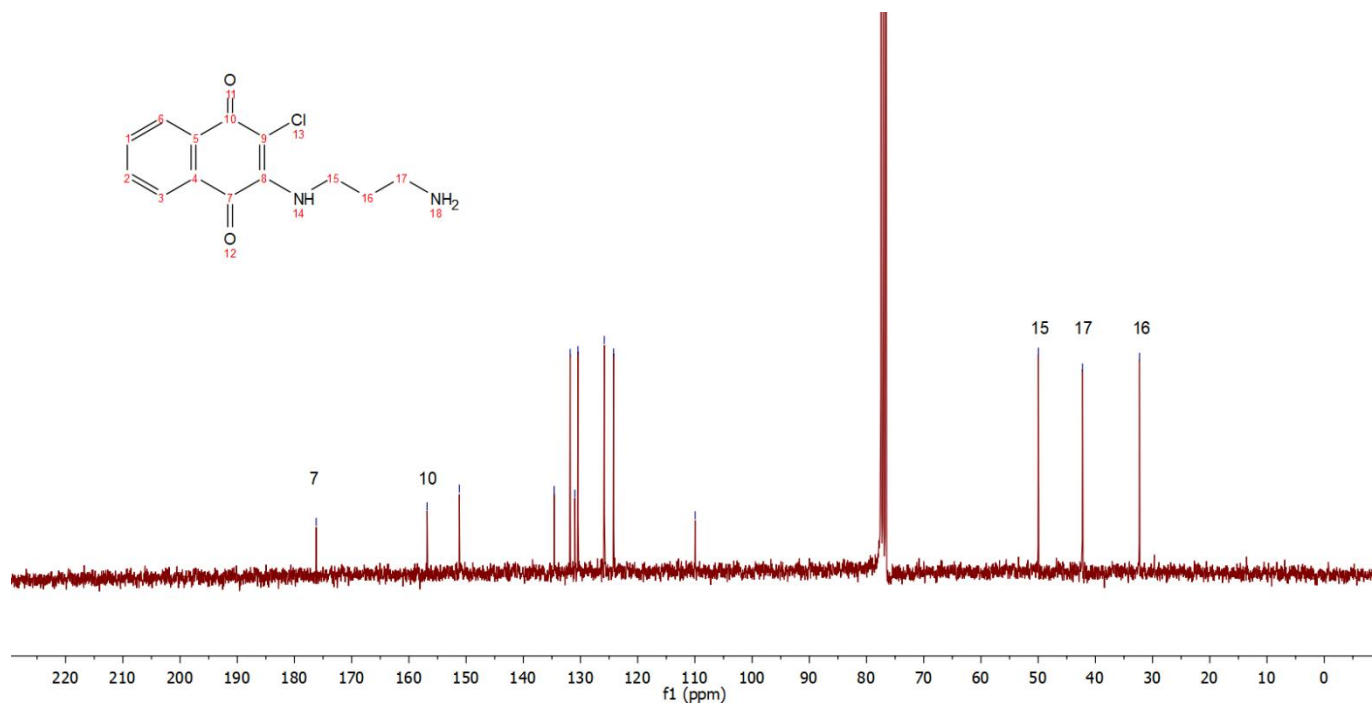
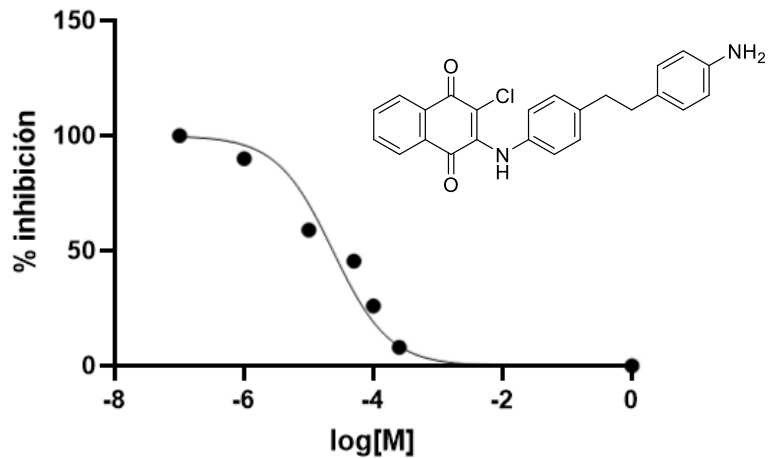
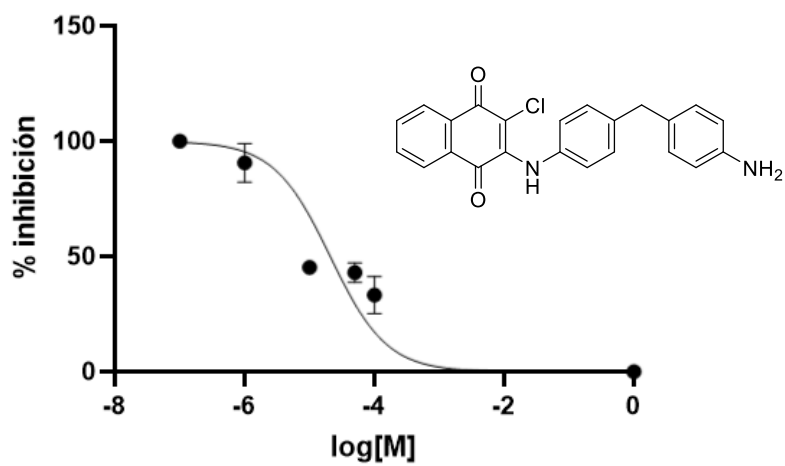
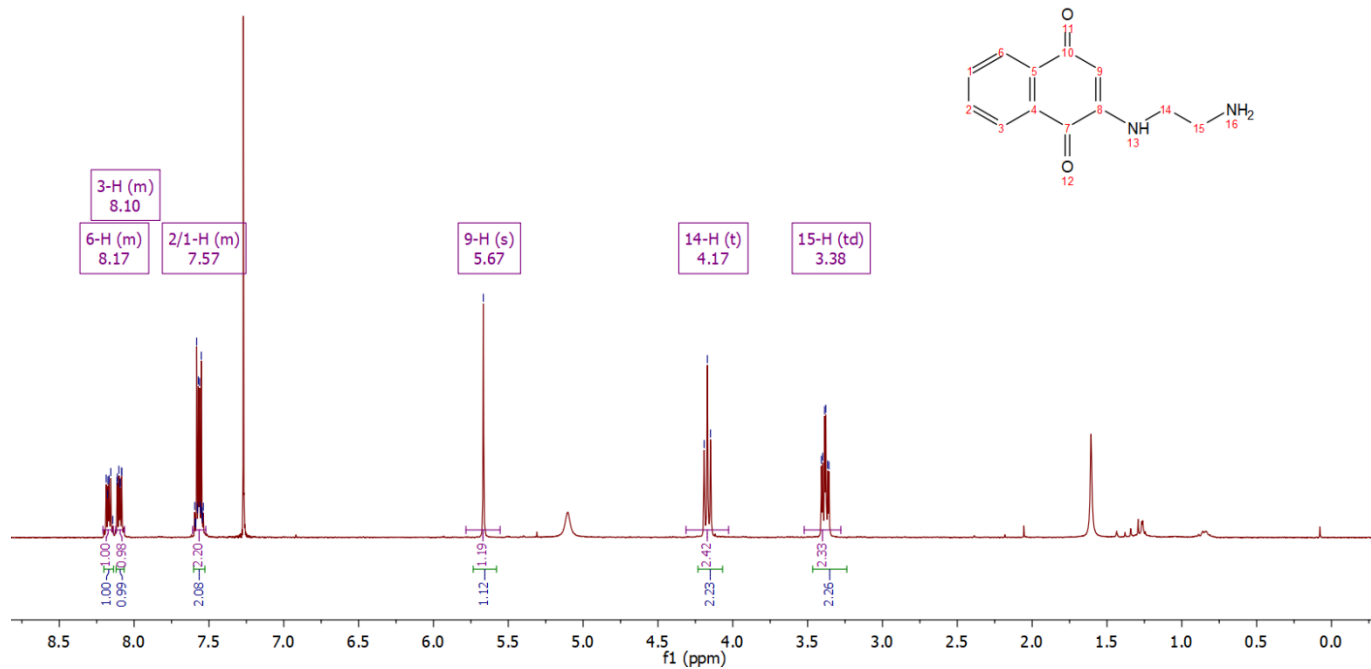


Figure S20A. <sup>13</sup>C-NMR monoamination product **22** in CDCl<sub>3</sub>.





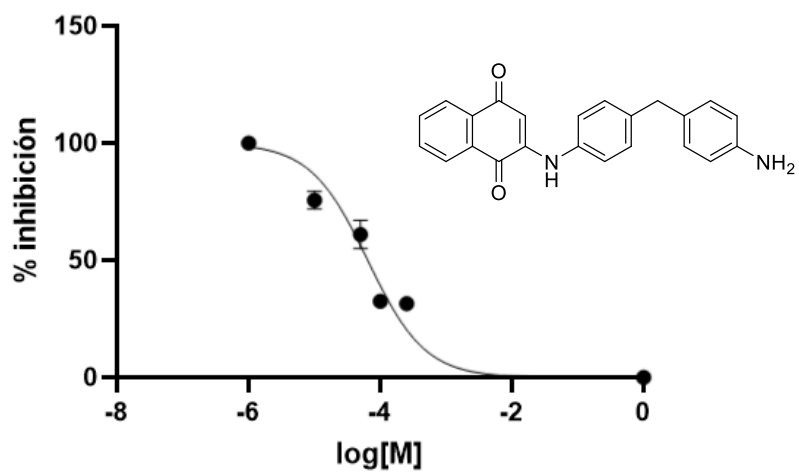


Figure S24. Curve dose-response monoamination product 10.

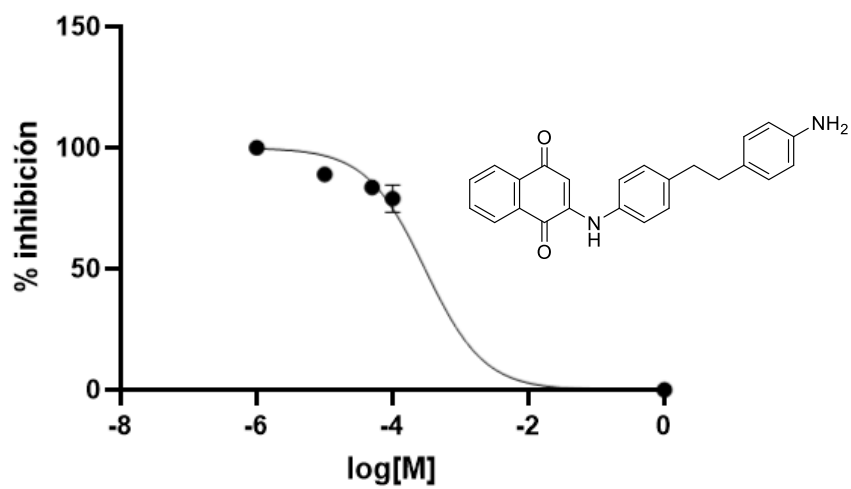


Figure S25. Curve dose-response monoamination product 11.

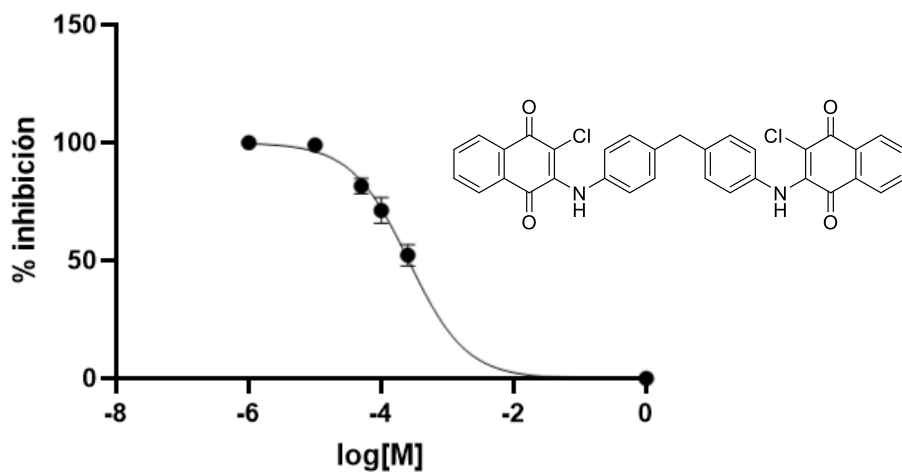


Figure S26. Curve dose-response homodimer 14.

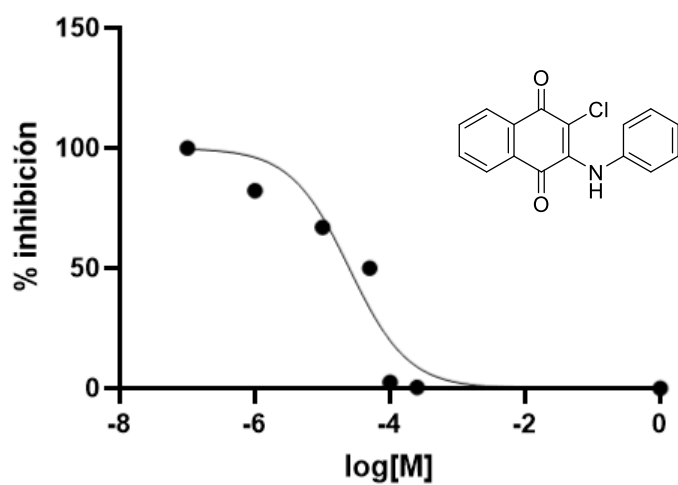


Figure S27. Curve dose-response pharmacophore 18.

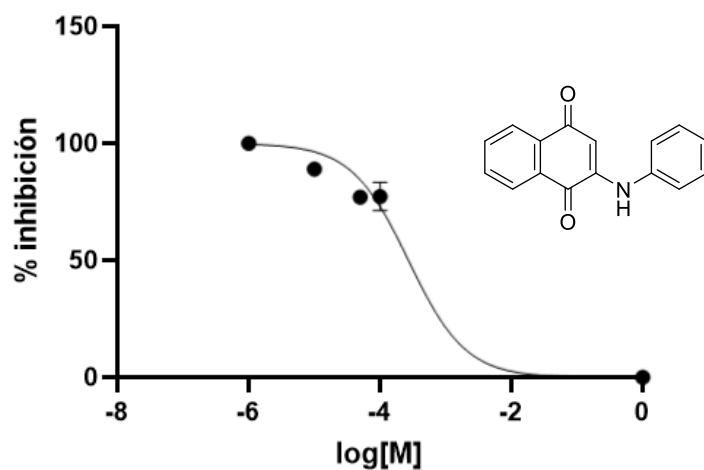


Figure S28. Curve dose-response pharmacophore 19.

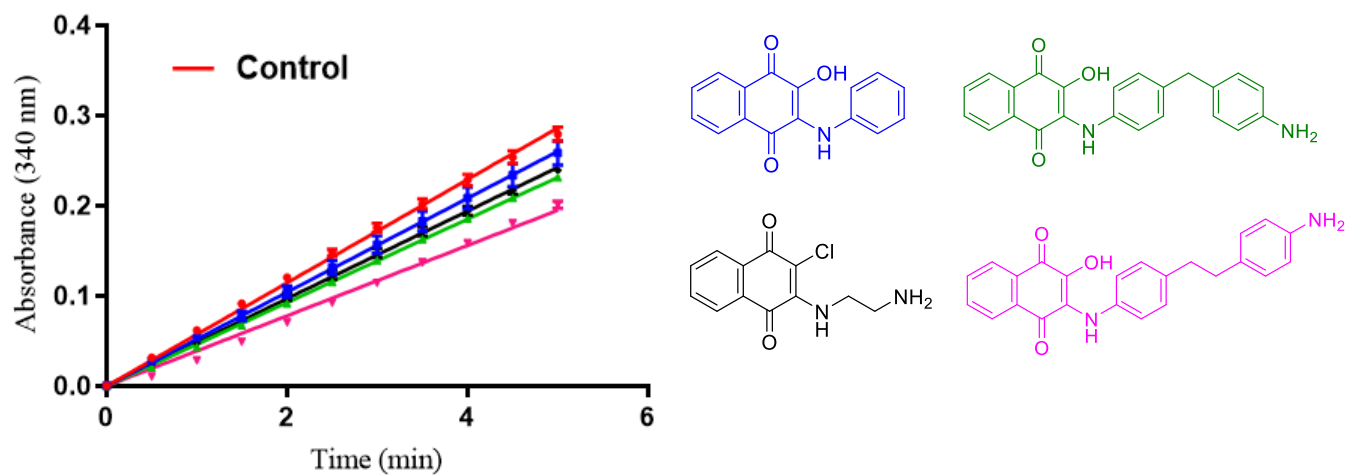
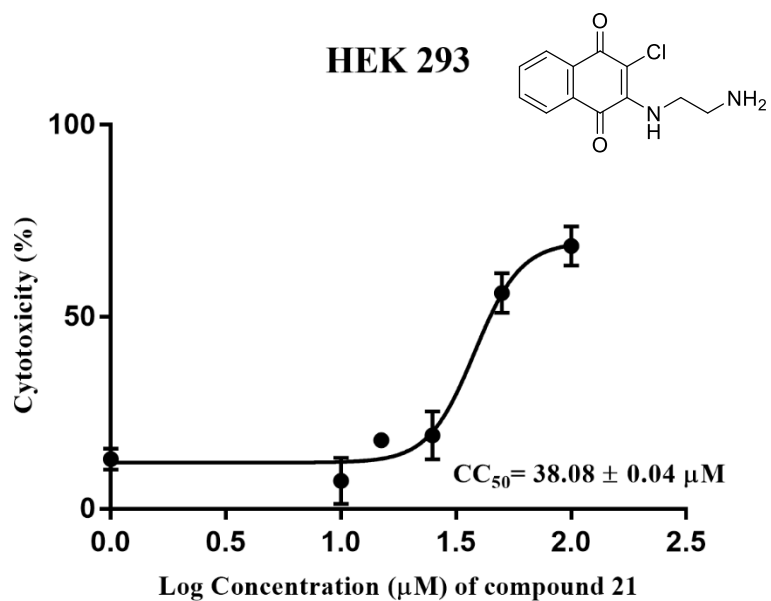
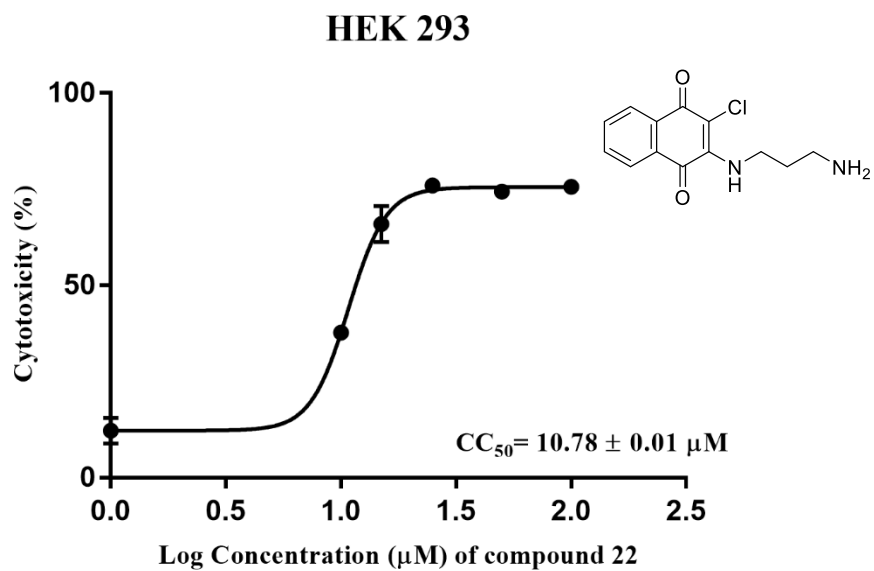


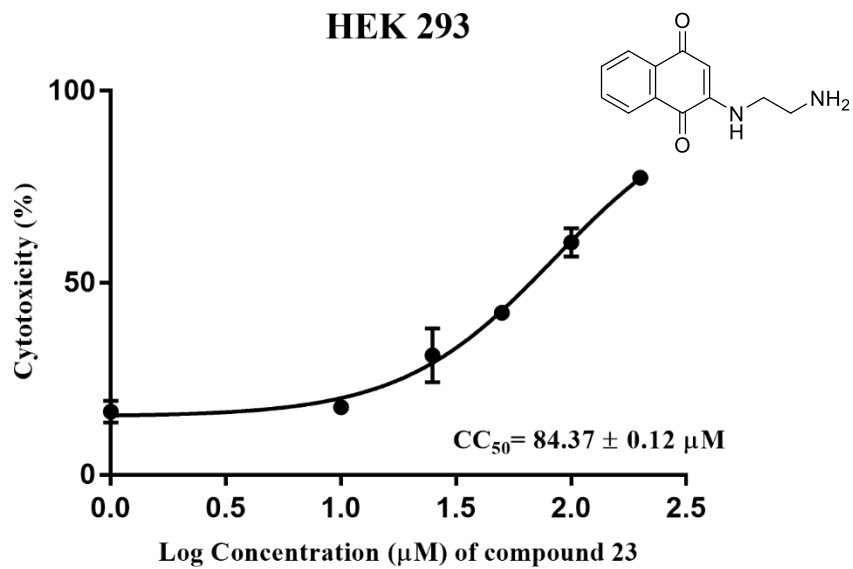
Figure S29. Screening GST activity monoamination products 12 (green), 13 (pink), 21 (black) and pharmacophore 20 (blue).



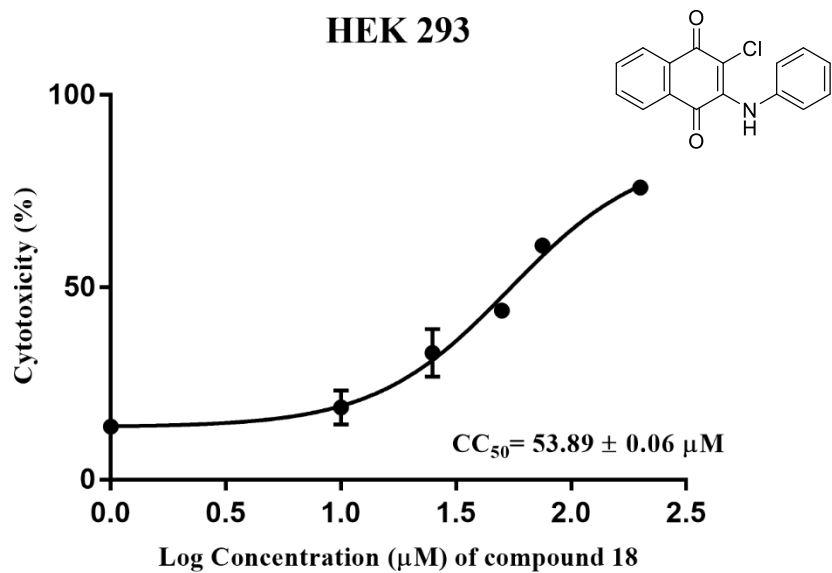
**Figure S30.**  $\text{CC}_{50}$  in HEK293 of monoamination product 21.



**Figure S31.**  $\text{CC}_{50}$  in HEK293 of monoamination product 22.



**Figure S32.**  $CC_{50}$  in HEK293 of monoamination product **23**.



**Figure S33.**  $CC_{50}$  in HEK293 of pharmacophore **18**.

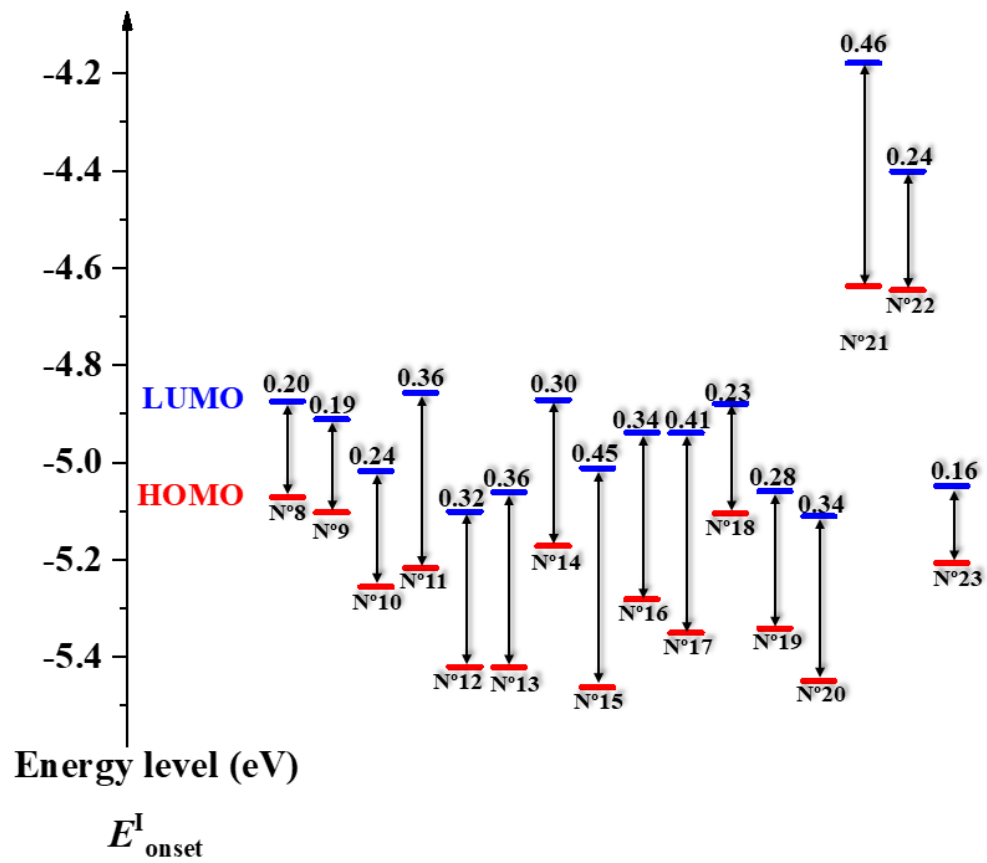


Figure S34. HOMO-LUMO bandgap determined from cyclic voltammetry of each synthesized molecule.