

Supporting information materials for

Development of targeted photodynamic therapy by combining a zinc phthalocyanine sensitizer with TSPO or EGFR binding groups : impact of the number of targeting agents on the biological activity

Isabelle Toubia,^{ad#} Christophe Nguyen,^{b#} Stéphane Diring,^a Mélanie Onofre,^b Morgane Daurat,^c Corentin Gauthier,^c Magali Gary-Bobo,^{*b} Marwan Kobeissi,^{*d} Fabrice Odobel^{*a}

^aCEISAM, Chimie Et Interdisciplinarité, Synthèse, Analyse, Modélisation, CNRS, UMR CNRS 6230, UFR des Sciences et des Techniques ; 2, rue de la Houssinière - BP 92208; 44322 NANTES Cedex 3 (France). E-mail:Fabrice.Odobel@univ-nantes.fr

^bIBMM, Univ Montpellier, CNRS, ENSCM, Montpellier, France. E-mail : magali.gary-bobo@inserm.fr

^cNanoMedSyn, 15 avenue Charles Flahault, 34293 Montpellier cedex 5

^dLaboratoire RammalRammal, Equipe de Synthèse Organique Appliquée SOA, Université Libanaise, Faculté des Sciences 5, Nabatieh, Liban. E-mail: mkobeissi@ul.edu.lb

#These authors contributed equally to this study.

Contents

1. ¹ H NMR spectra	2
2. ¹³ C NMR spectra	8
3. ES-MS spectra	12
4. UV absorption spectra of targeting moieties	19
5. HPLC analyses	20

1. ^1H NMR spectra

^{13}C NMR spectra are not included because a suitable signal-to-noise ratio could not be recorded due to solubility issues.

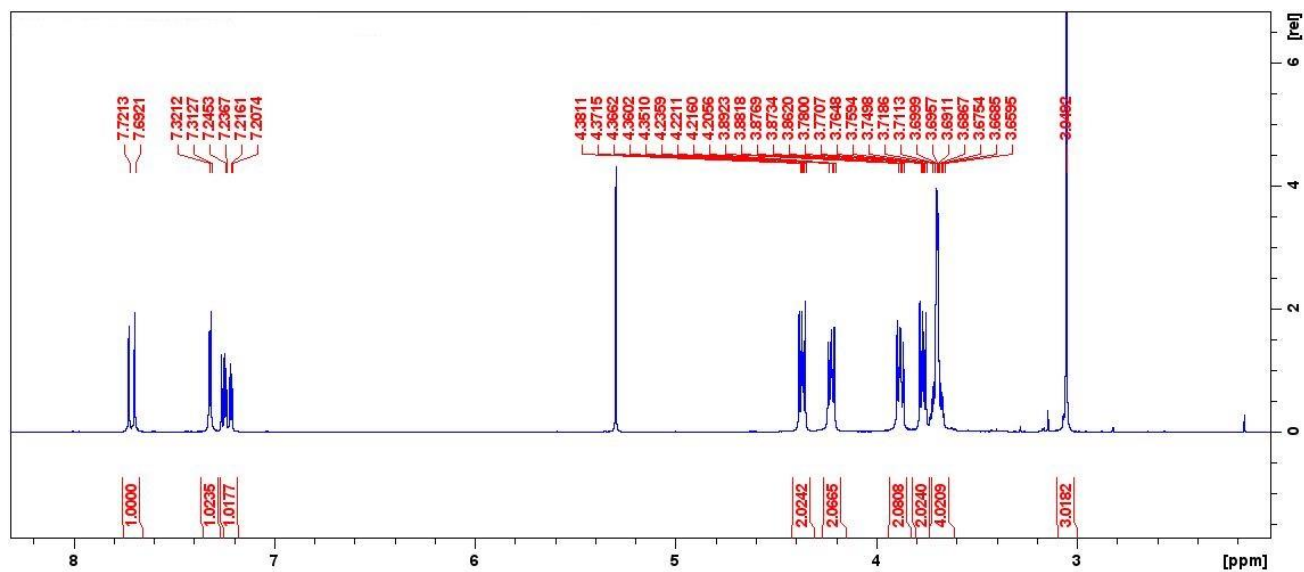


Figure S1. ^1H NMR spectrum of phthalonitrile **2** recorded in CDCl_3 .

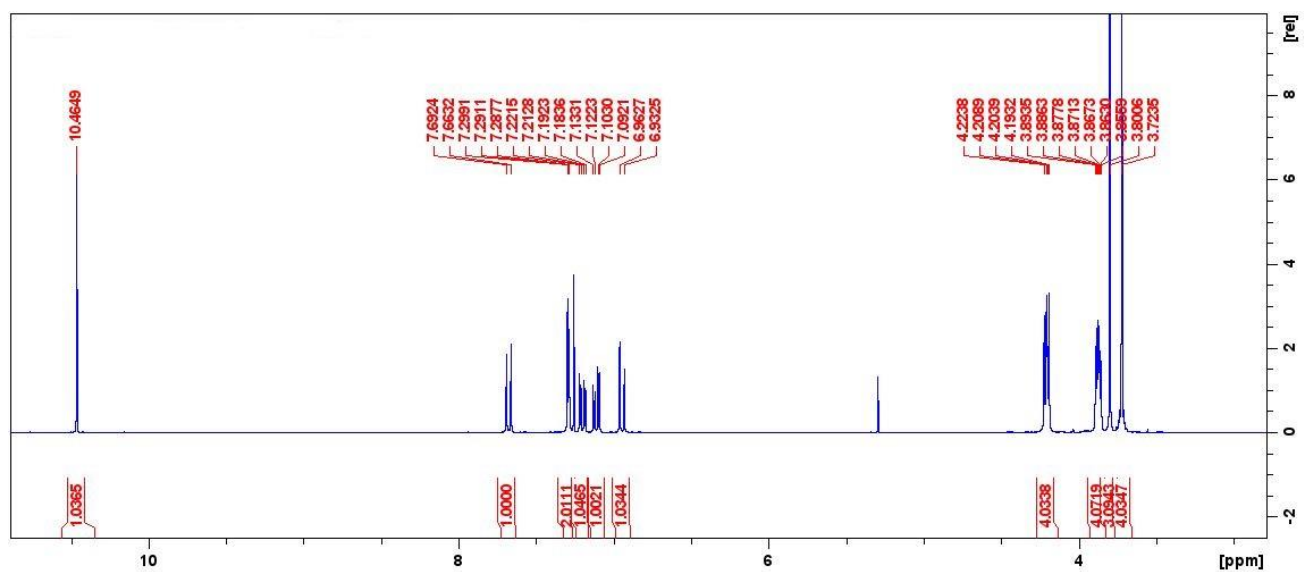


Figure S2. ^1H NMR spectrum of phthalonitrile **3** recorded in CDCl_3 .

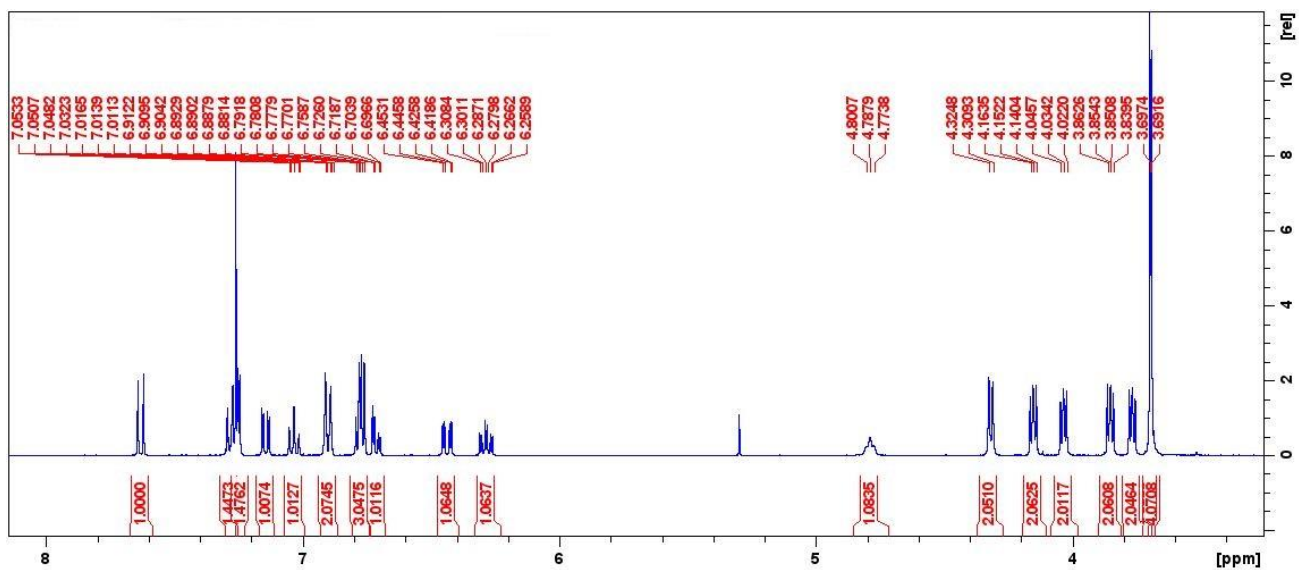


Figure S3. ¹H NMR spectrum of phthalonitrile 5 recorded in CDCl₃.

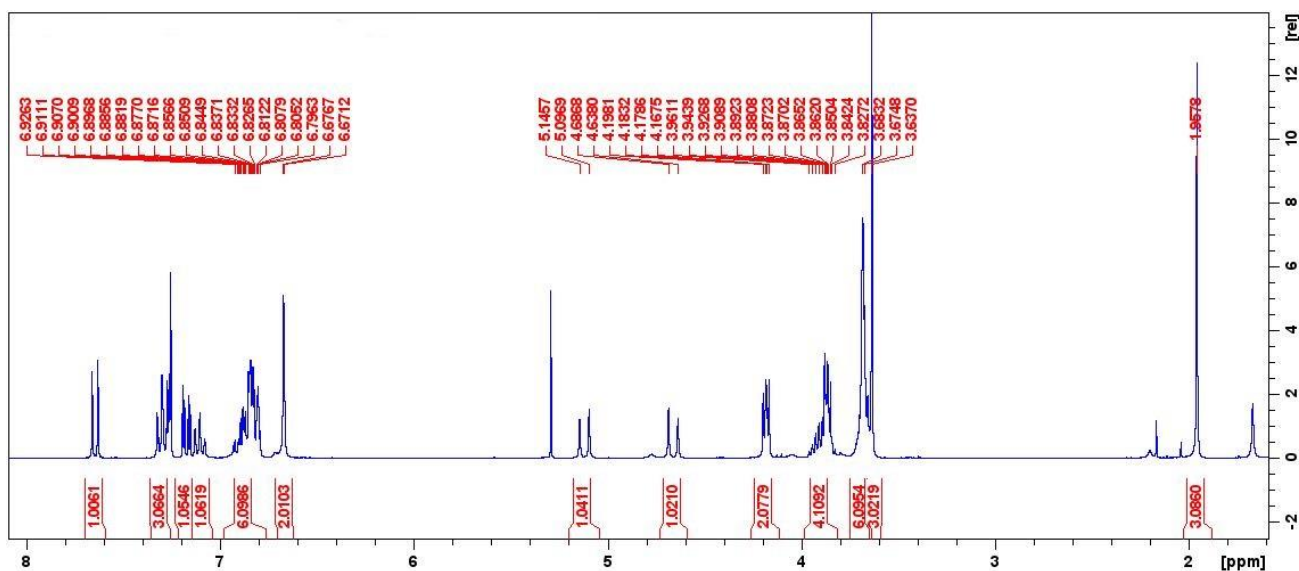


Figure S4. ¹H NMR spectrum of phthalonitrile 6 recorded in CDCl₃.

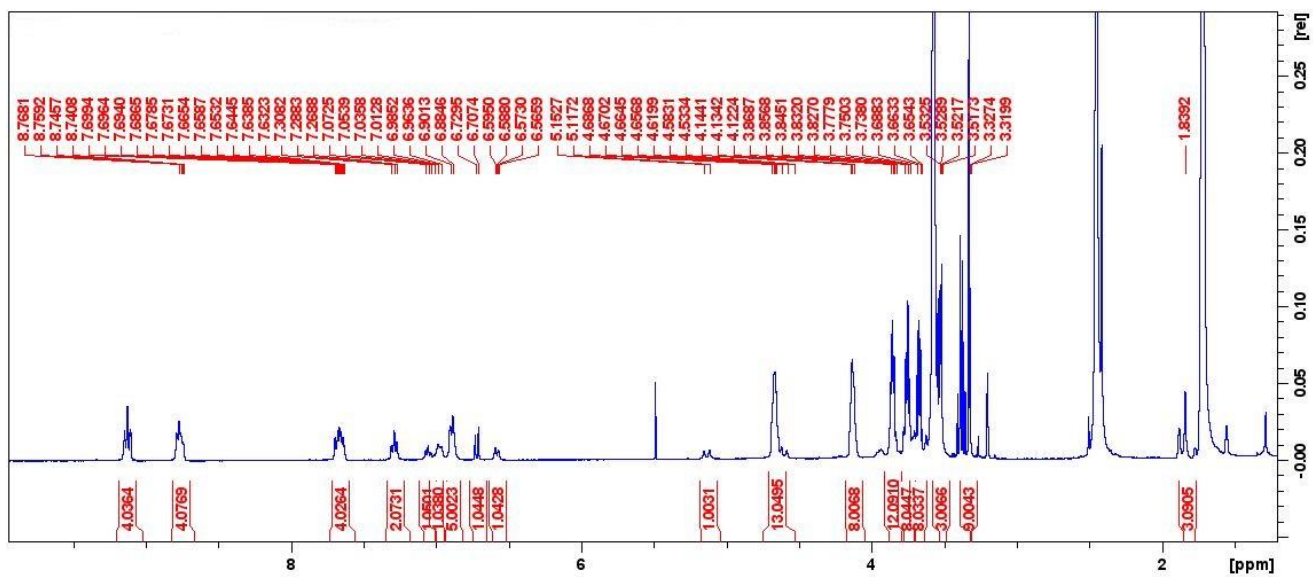


Figure S5. ^1H NMR spectrum of ZnPc-[DAA1106]_1 recorded in THF-d_8 .

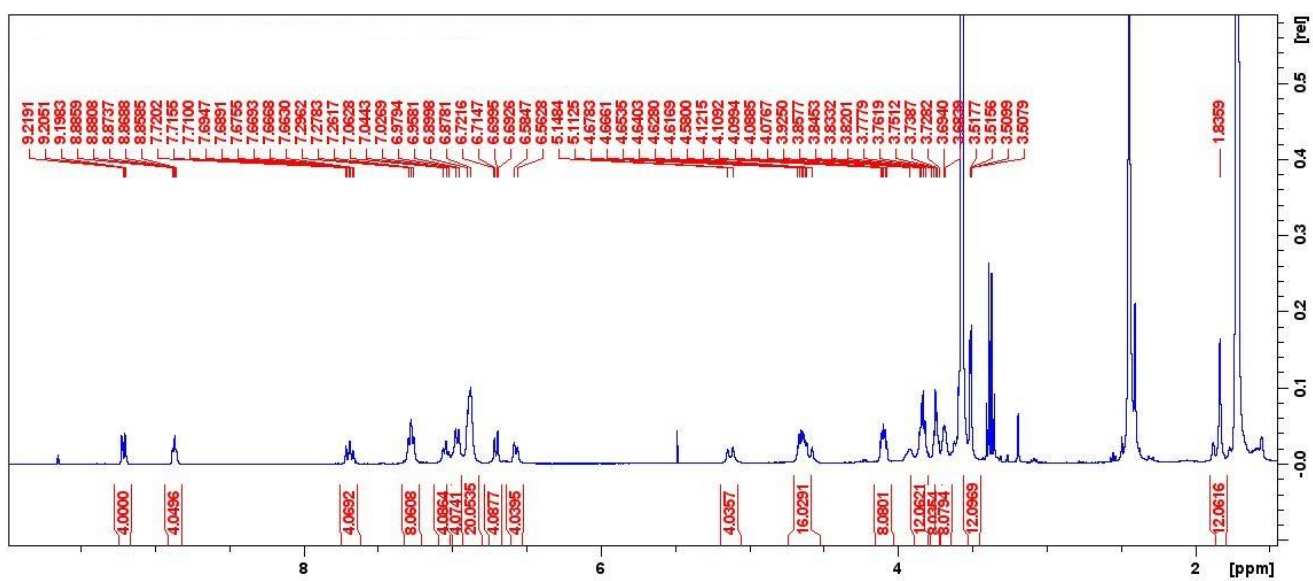


Figure S6. ^1H NMR spectrum of ZnPc-[DAA1106]_4 recorded in THF-d_8 .

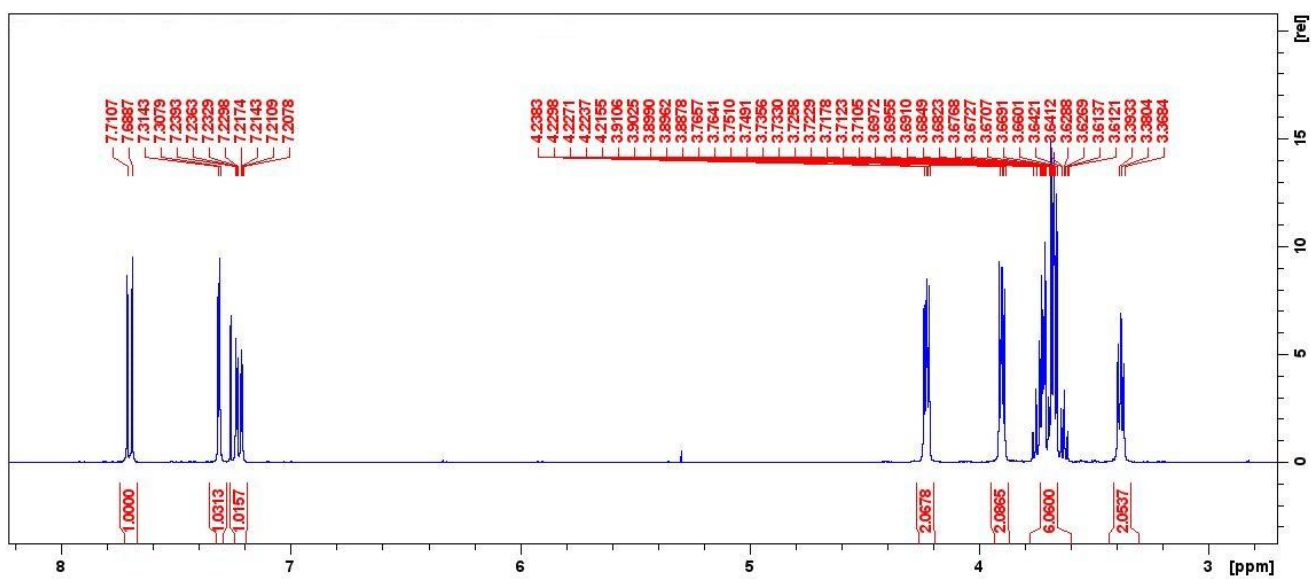


Figure S7. ^1H NMR spectrum of phthalonitrile **8** recorded in CDCl_3 .

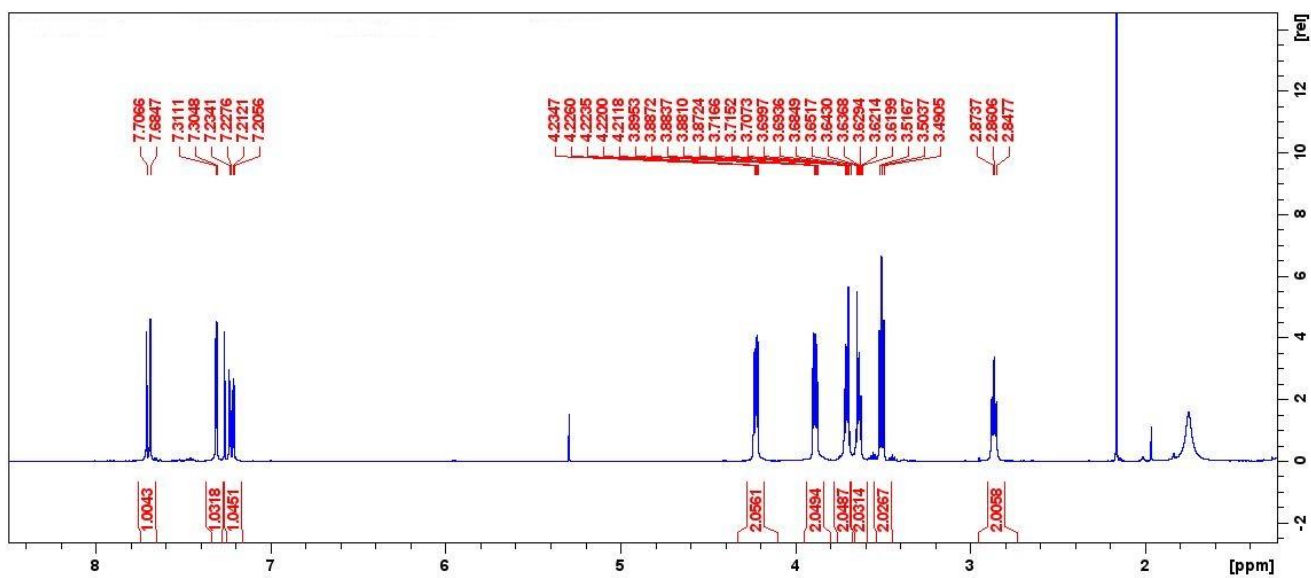


Figure S8. ^1H NMR spectrum of phthalonitrile **9** recorded in CDCl_3 .

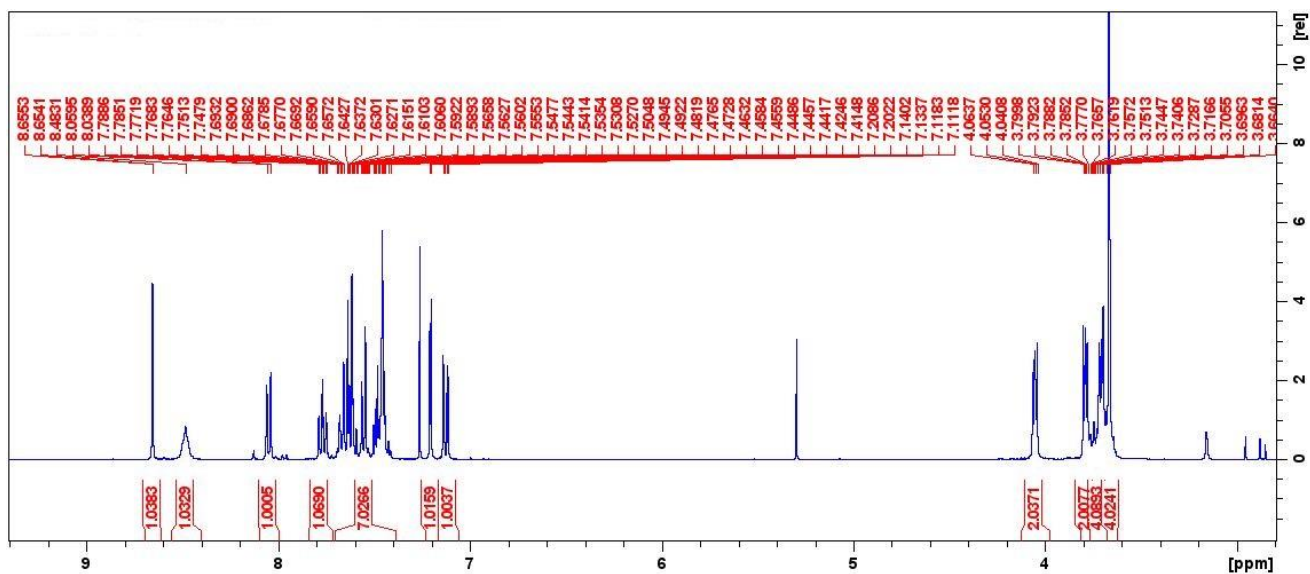


Figure S9. ^1H NMR spectrum of phthalonitrile **10** recorded in CDCl_3 .

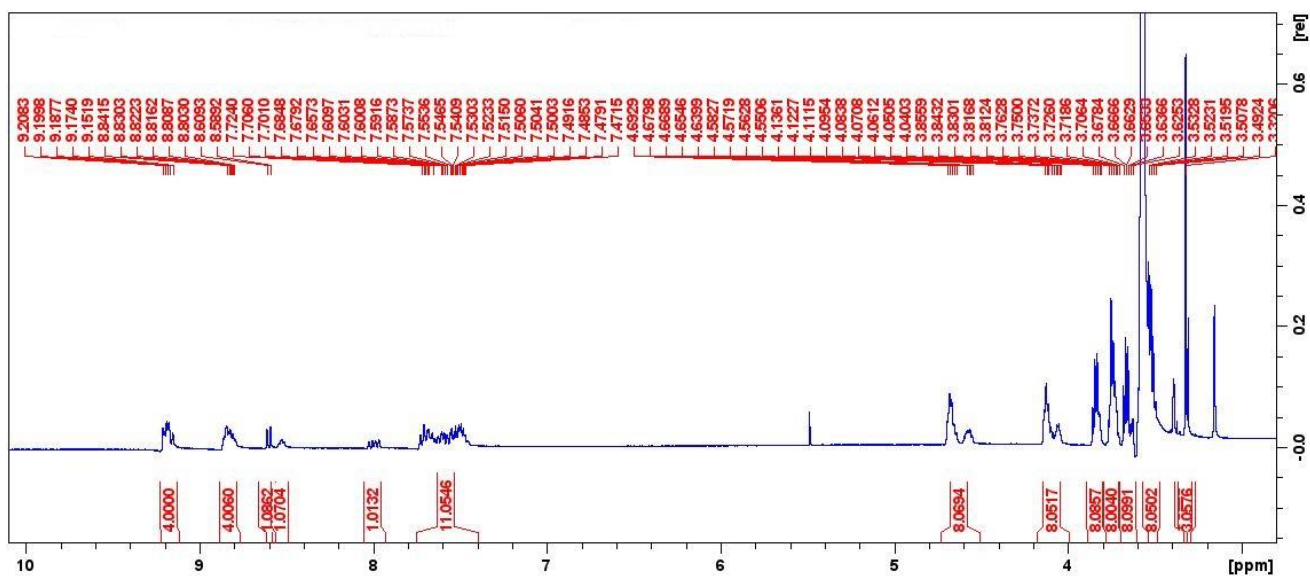


Figure S10. ^1H NMR spectrum of ZnPc -[PK11195]₁ recorded in THF-d_8 .

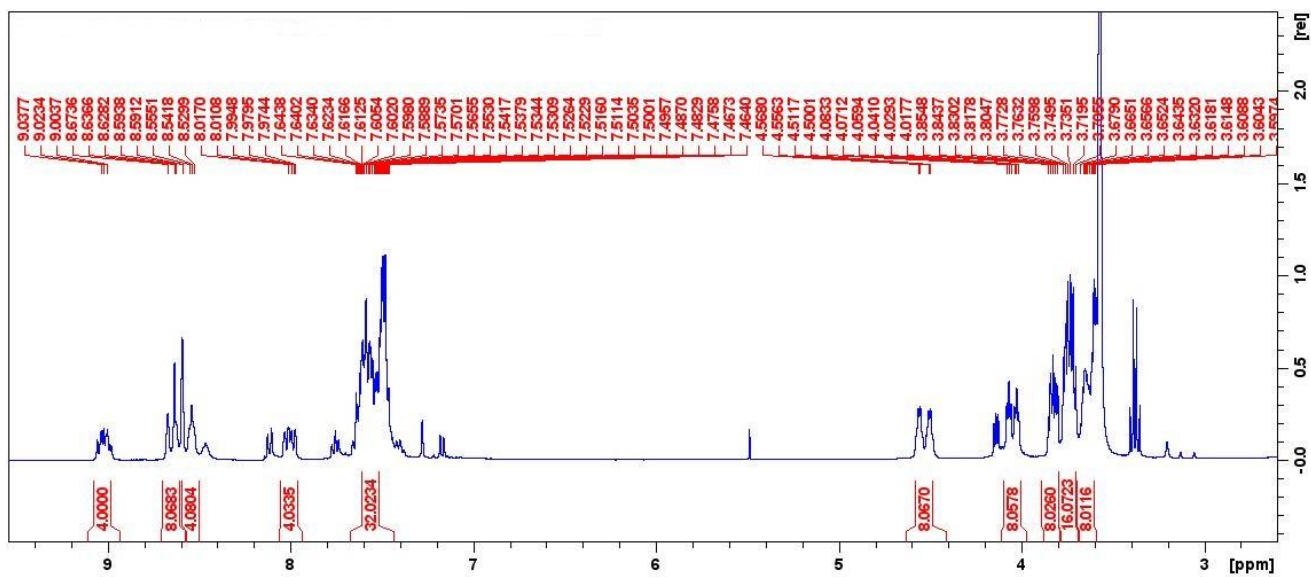


Figure S11. ^1H NMR spectrum of $\text{ZnPc-}[\text{PK11195}]_4$ recorded in $\text{THF-}d_8$.

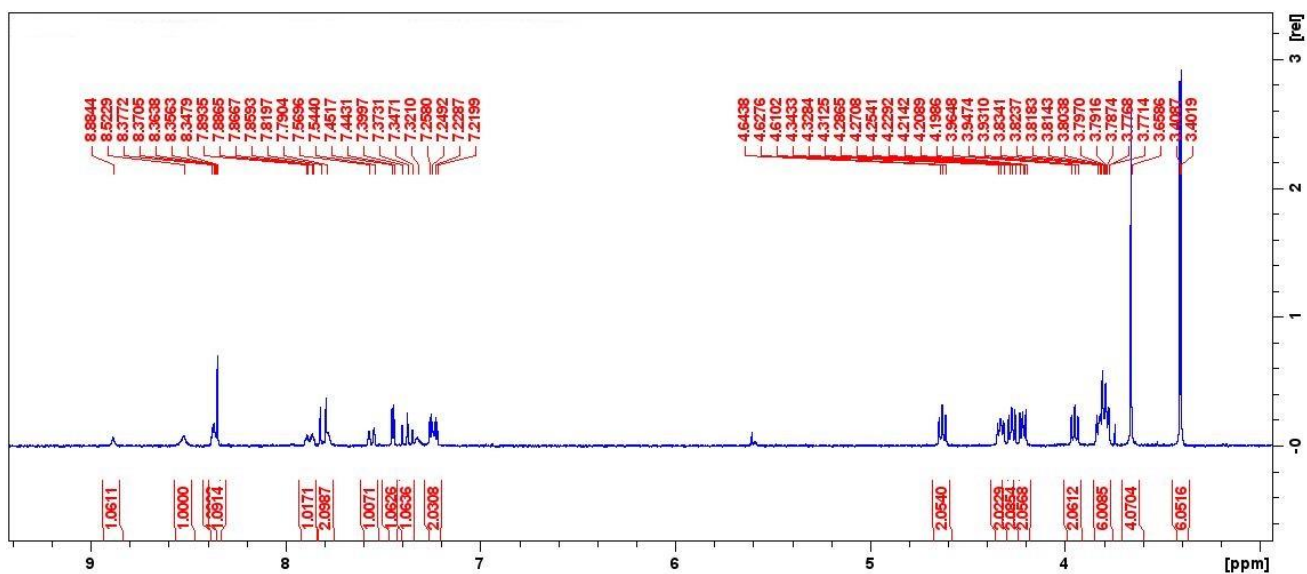


Figure S12. ^1H NMR spectrum of phthalonitrile **11** recorded in $\text{Acetone-}d_6$.

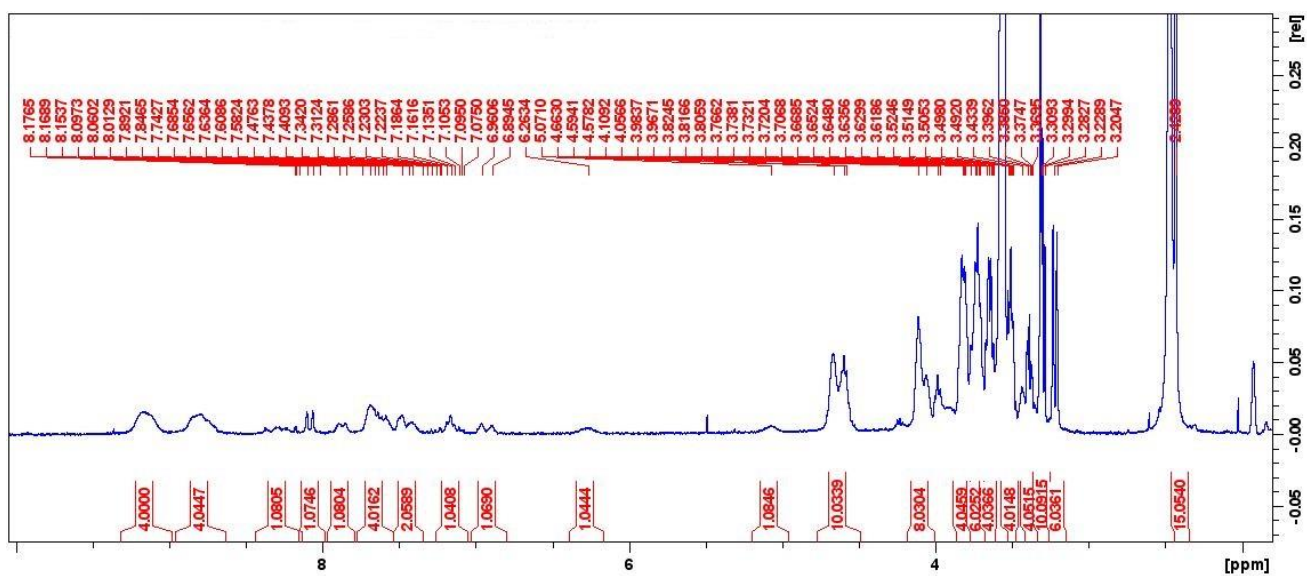


Figure S13. ^1H NMR spectrum of $\text{ZnPc-}[\text{Erlø}]_1$ recorded in THF-d_8 .

2. ^{13}C NMR spectra

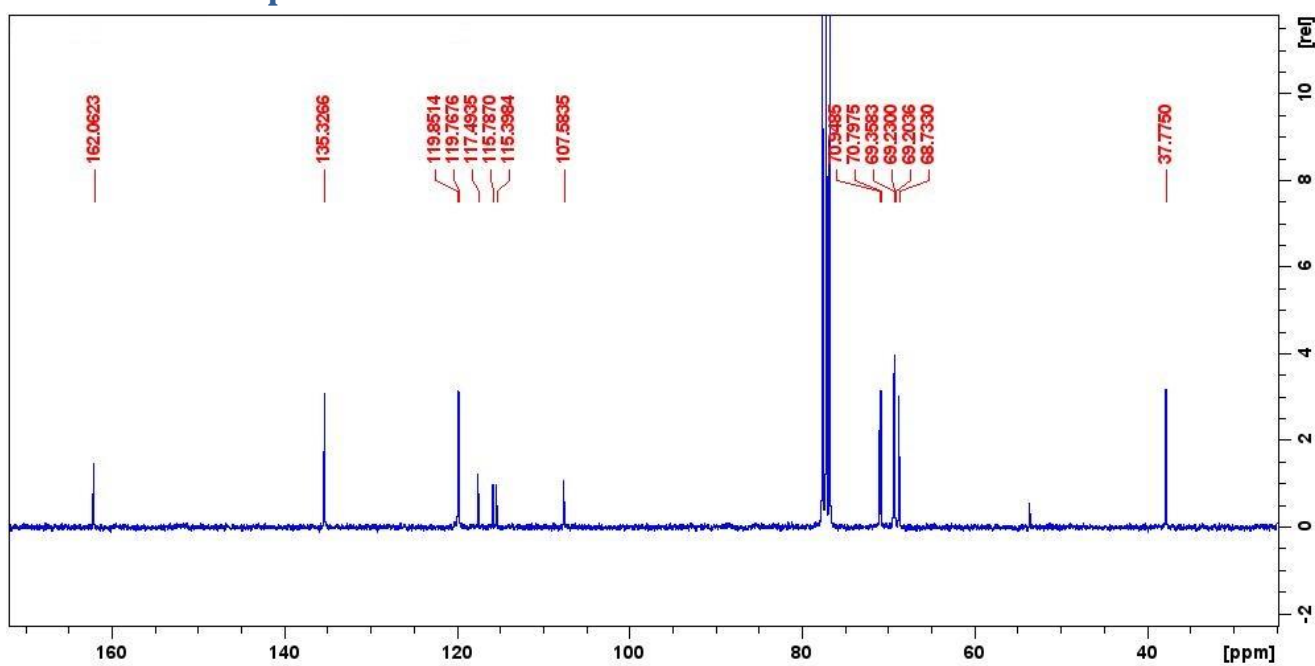


Figure S14. ^{13}C NMR spectrum of **phthalonitrile 2** recorded in CDCl_3 .

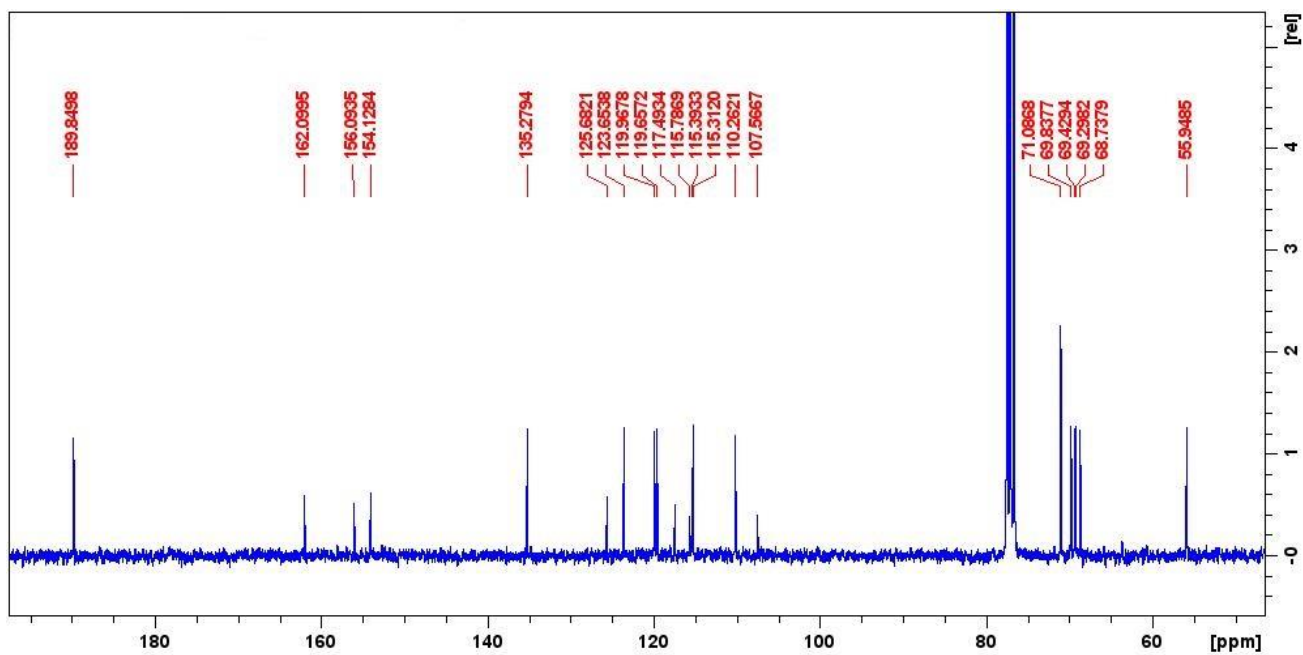


Figure S15. ^{13}C NMR spectrum of phthalonitrile **3** recorded in CDCl_3 .

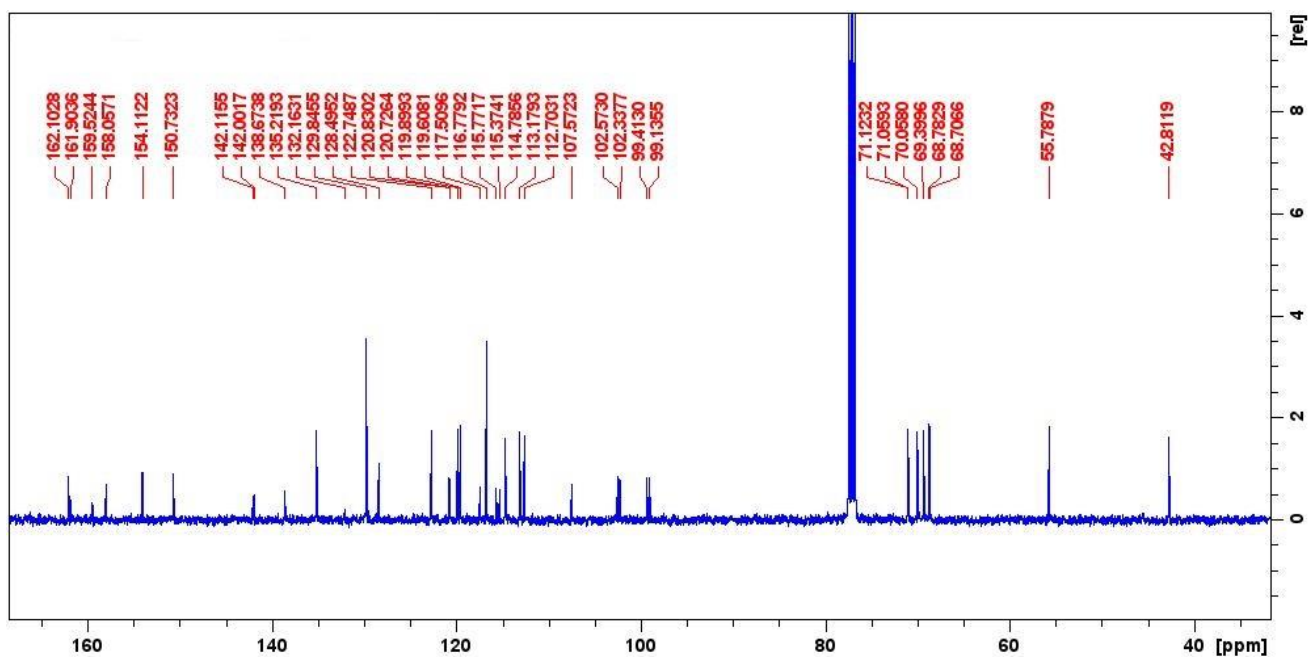


Figure S16. ^{13}C NMR spectrum of phthalonitrile **5** recorded in CDCl_3 .

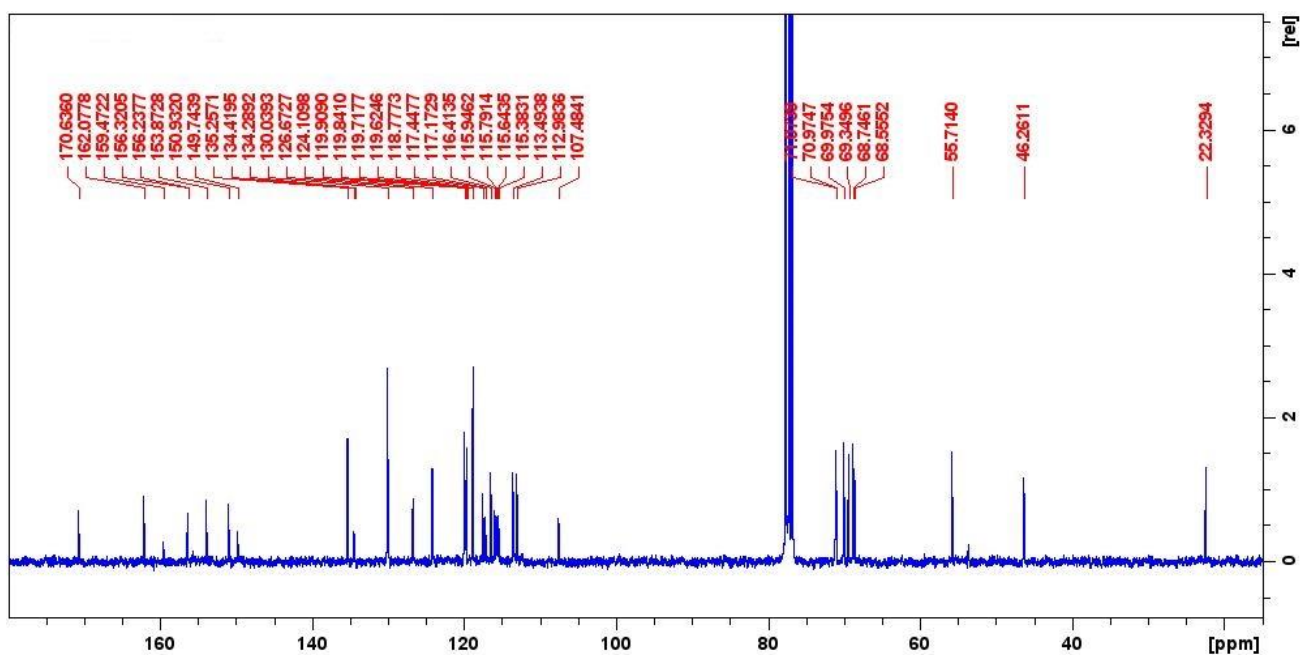


Figure S17. ^{13}C NMR spectrum of phthalonitrile **6** recorded in CDCl_3 .

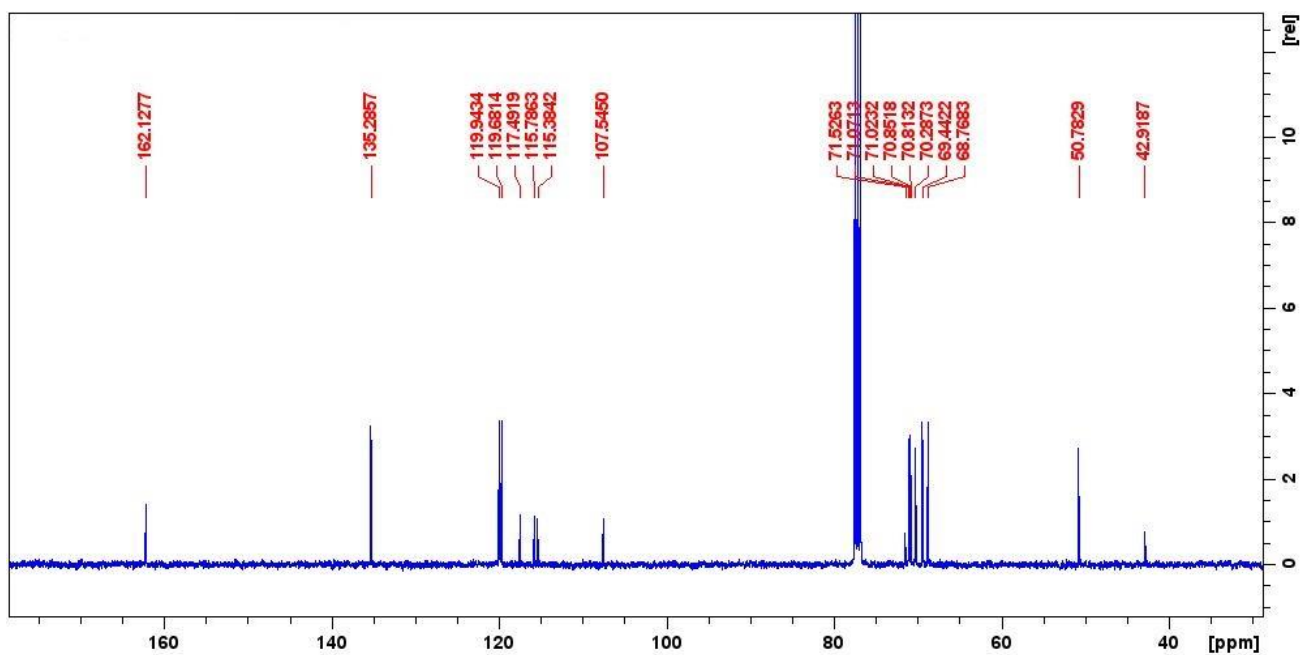


Figure S18. ^{13}C NMR spectrum of phthalonitrile **8** recorded in CDCl_3 .

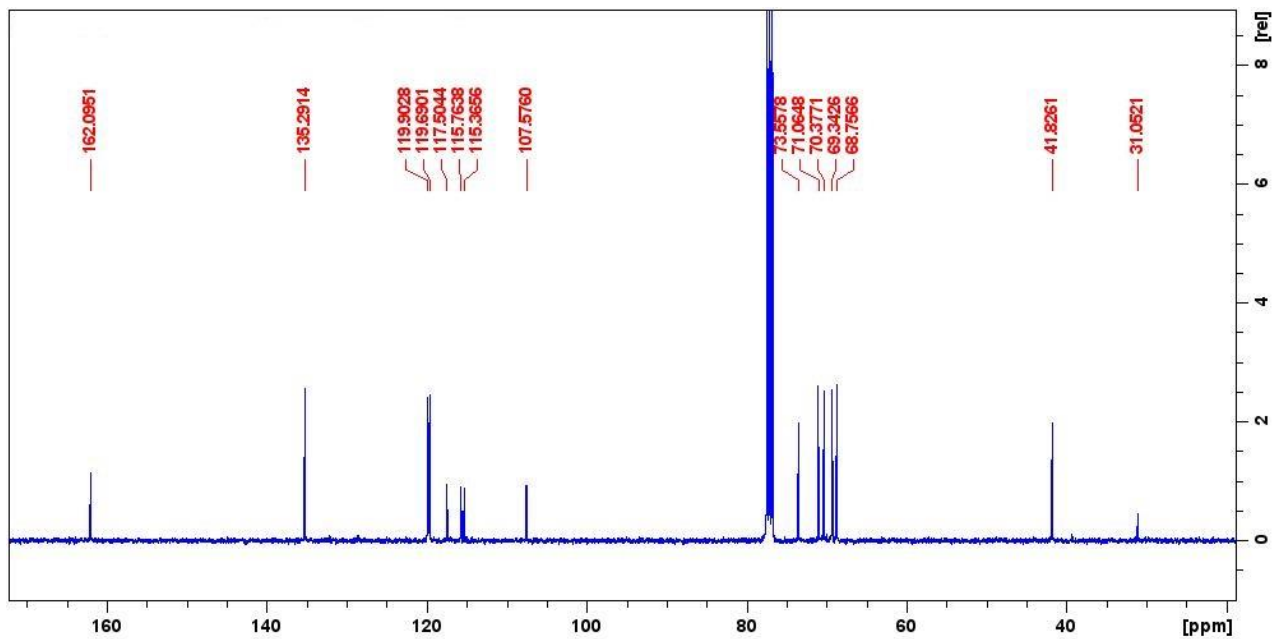


Figure S19. ^{13}C NMR spectrum of **phthalonitrile 9** recorded in CDCl_3 .

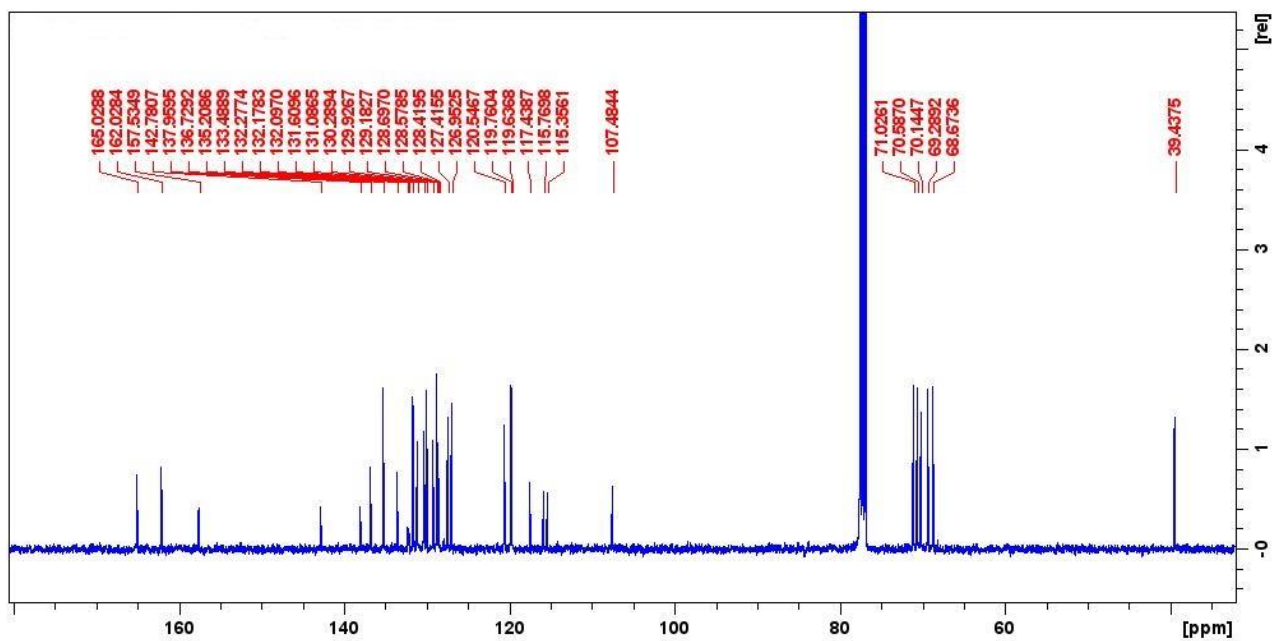


Figure S20. ^{13}C NMR spectrum of **phthalonitrile 10** recorded in CDCl_3 .

3. ES-MS spectra

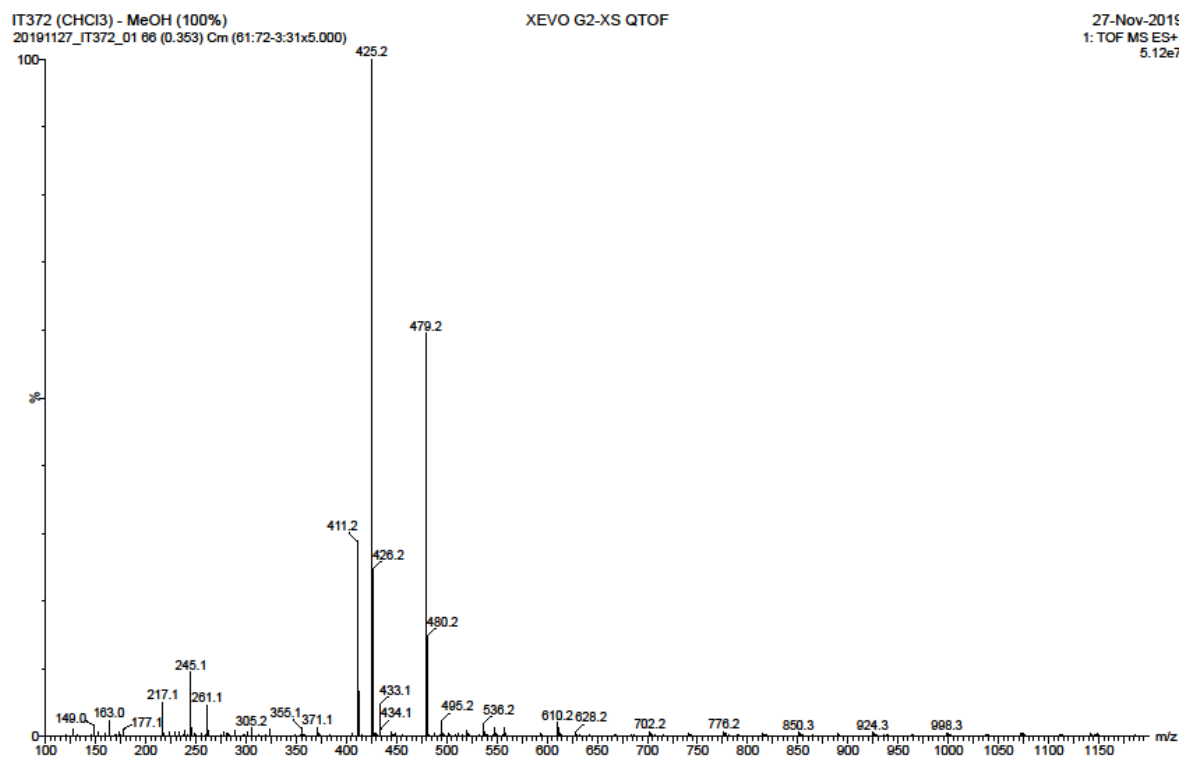


Figure S21. ES-MS spectra of phthalonitrile 3.

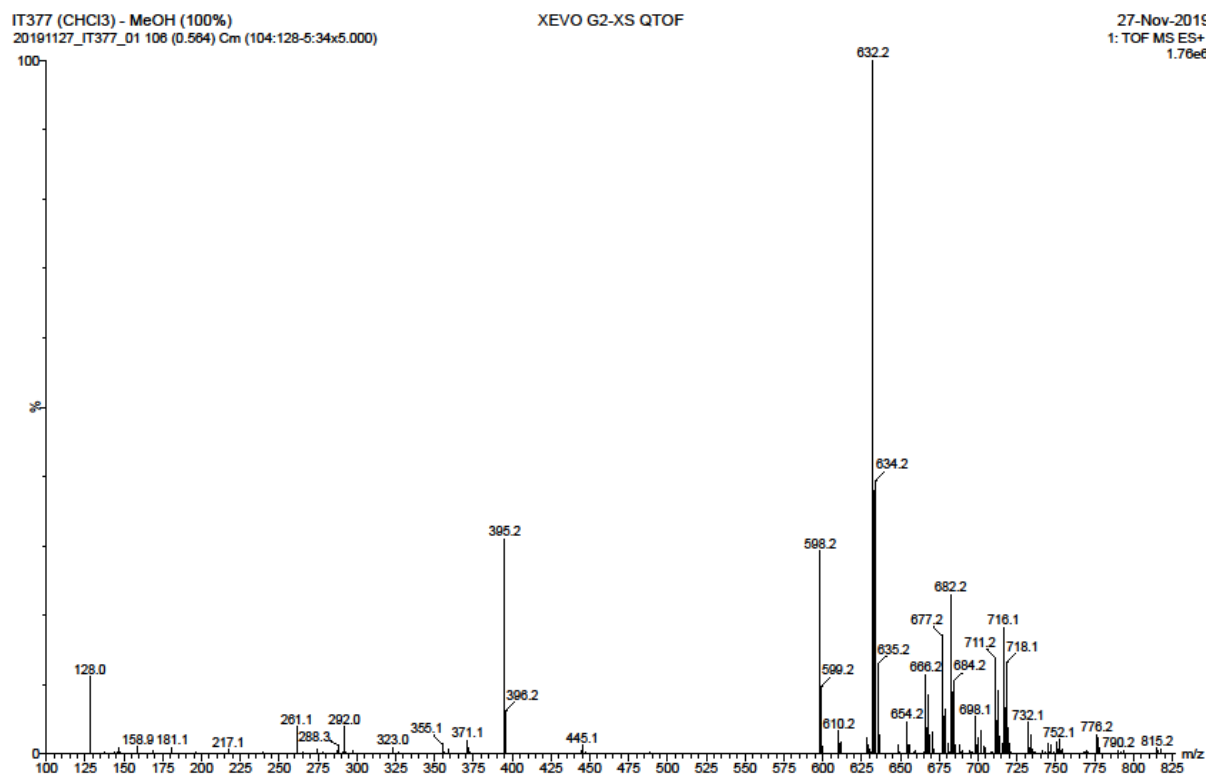


Figure S22. ES-MS spectra of phthalonitrile 5.

IT378 (CHCl3) - MeOH (100%)
20191125_IT378_01 62 (0.640) Cm (54:74)

XEVO G2-XS QTOF

25-Nov-2019
1: TOF MS ES+
1.38e8

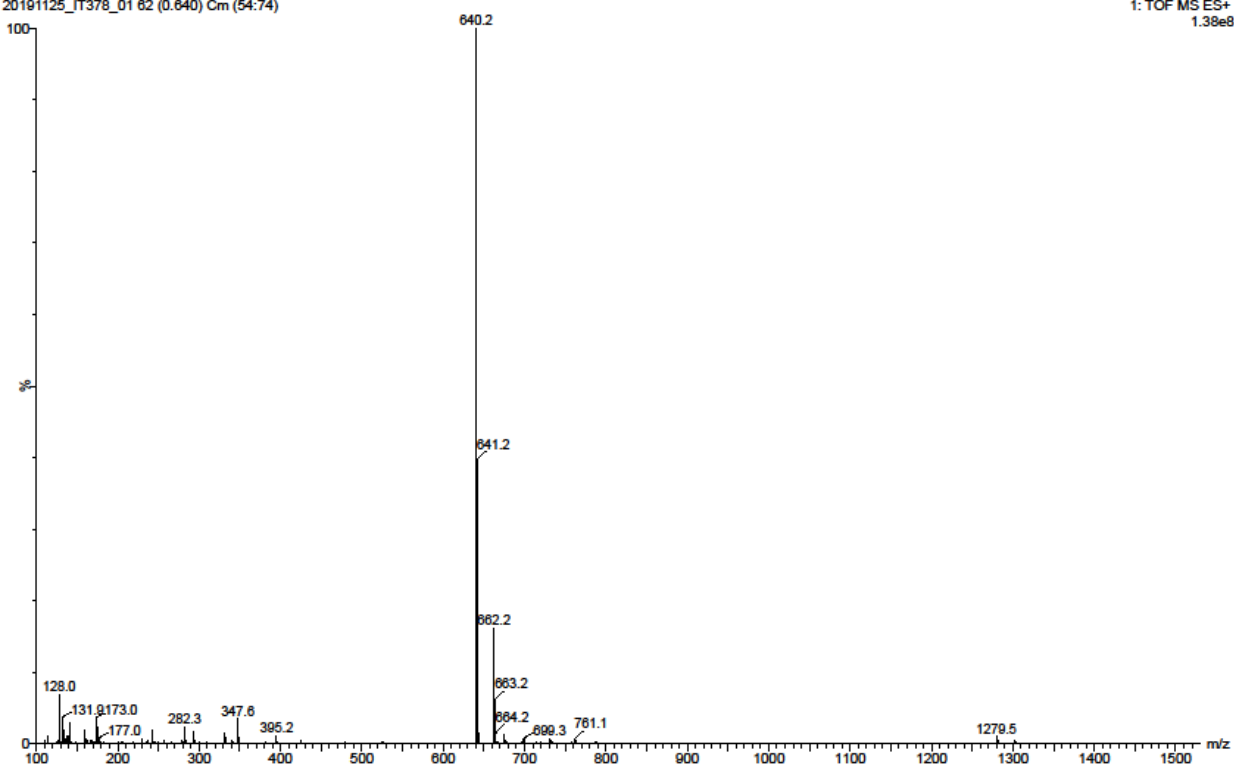


Figure S23. ES-MS spectra of phthalonitrile 6.

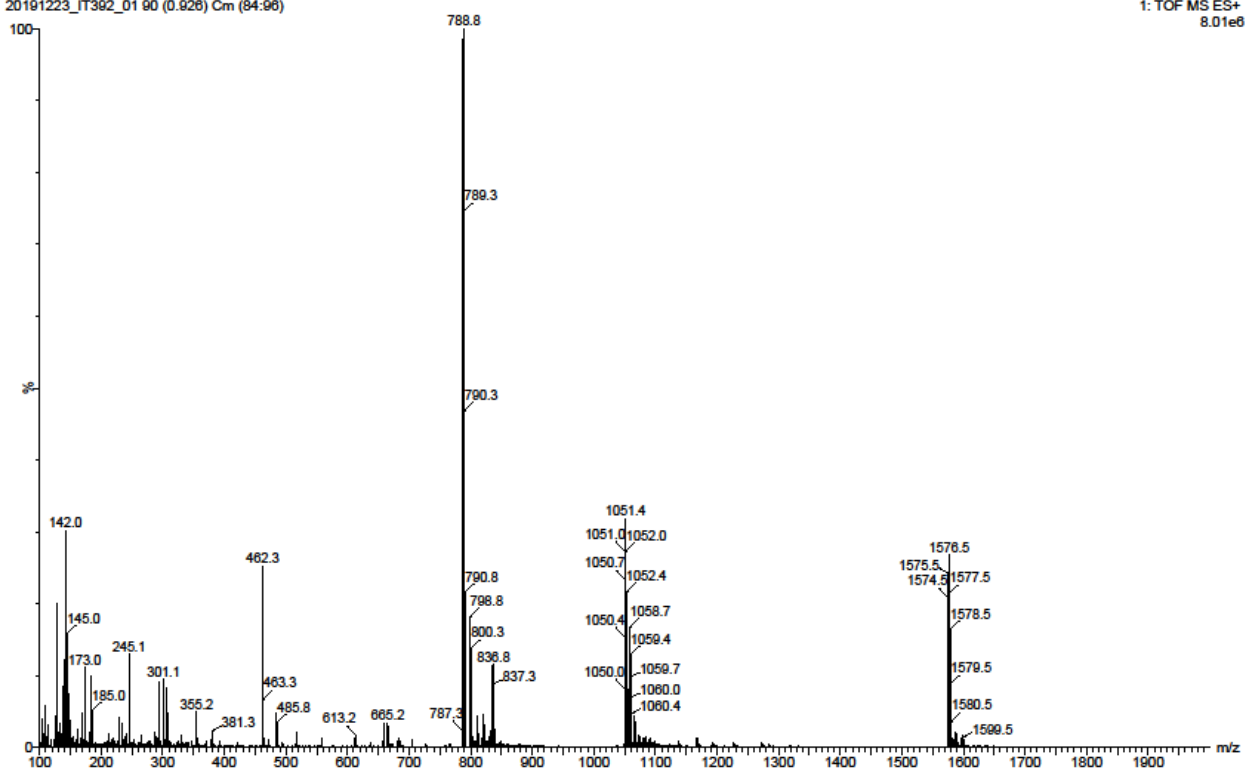


Figure S24. ES-MS spectra of ZnPc-[DAA1106]₁.

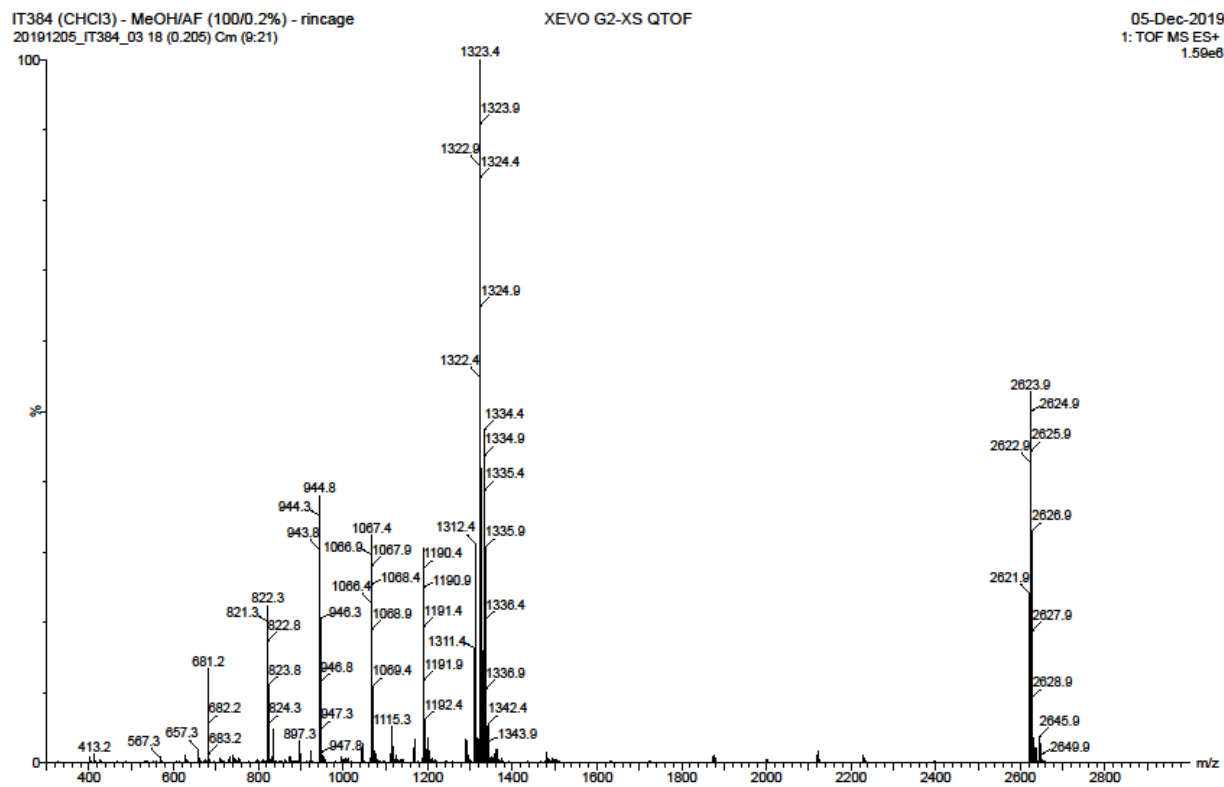


Figure S25. ES-MS spectra of ZnPc-[DAA1106]₄.

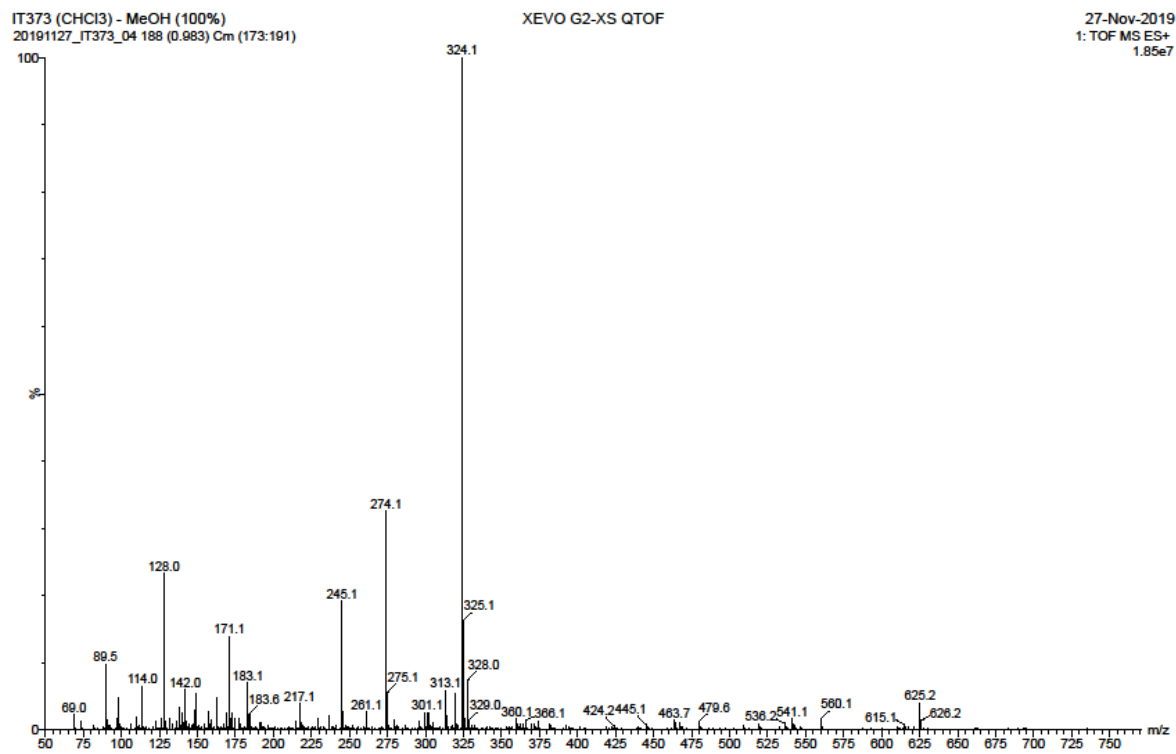


Figure S26. ES-MS spectra of phthalonitrile 8.

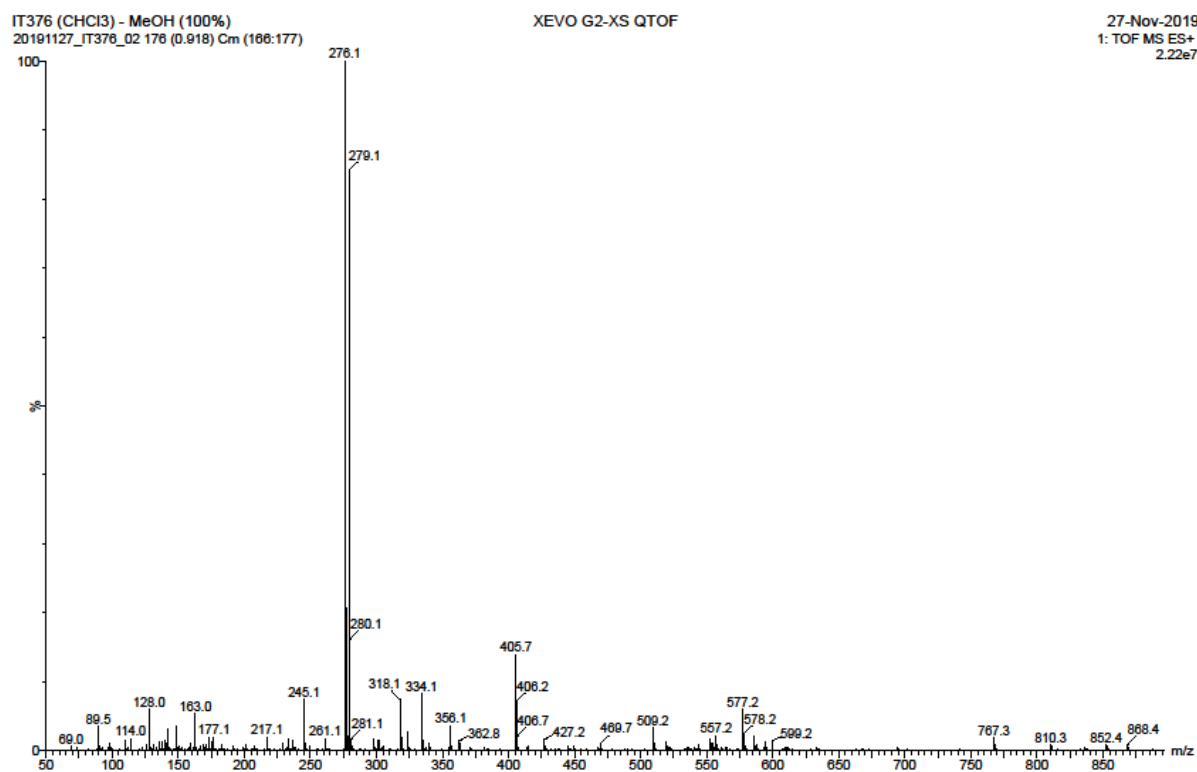


Figure S27. ES-MS spectra of phthalonitrile 9.

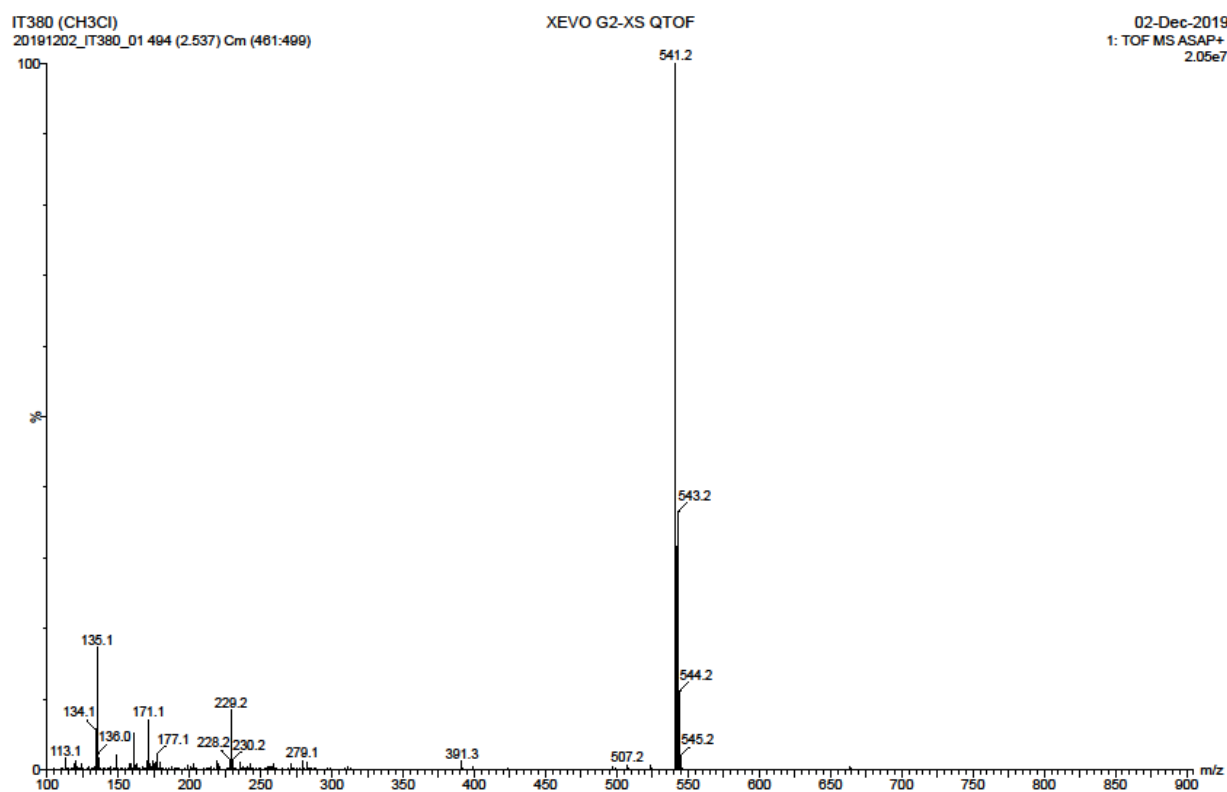


Figure S28. ES-MS spectra of phthalonitrile 10.

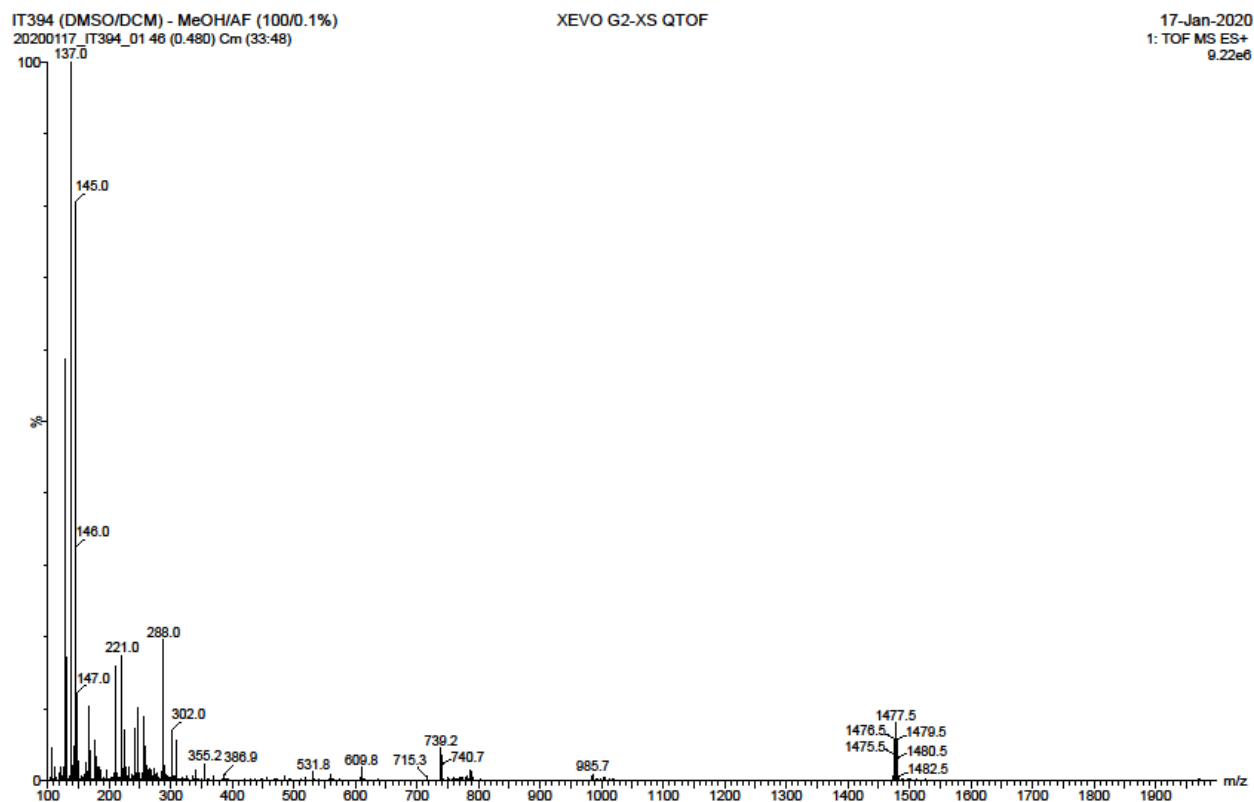


Figure S29. ES-MS spectra of ZnPc[PK11195]₁.

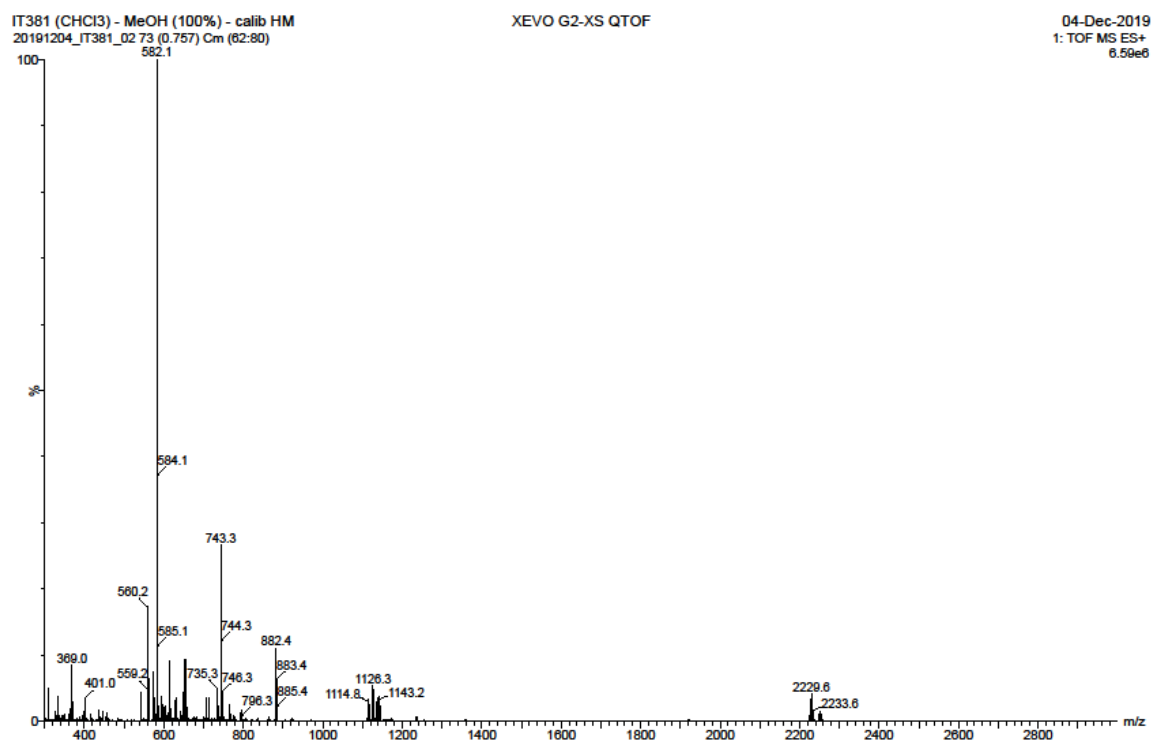


Figure S30. ES-MS spectra of ZnPc[PK11195]₄.

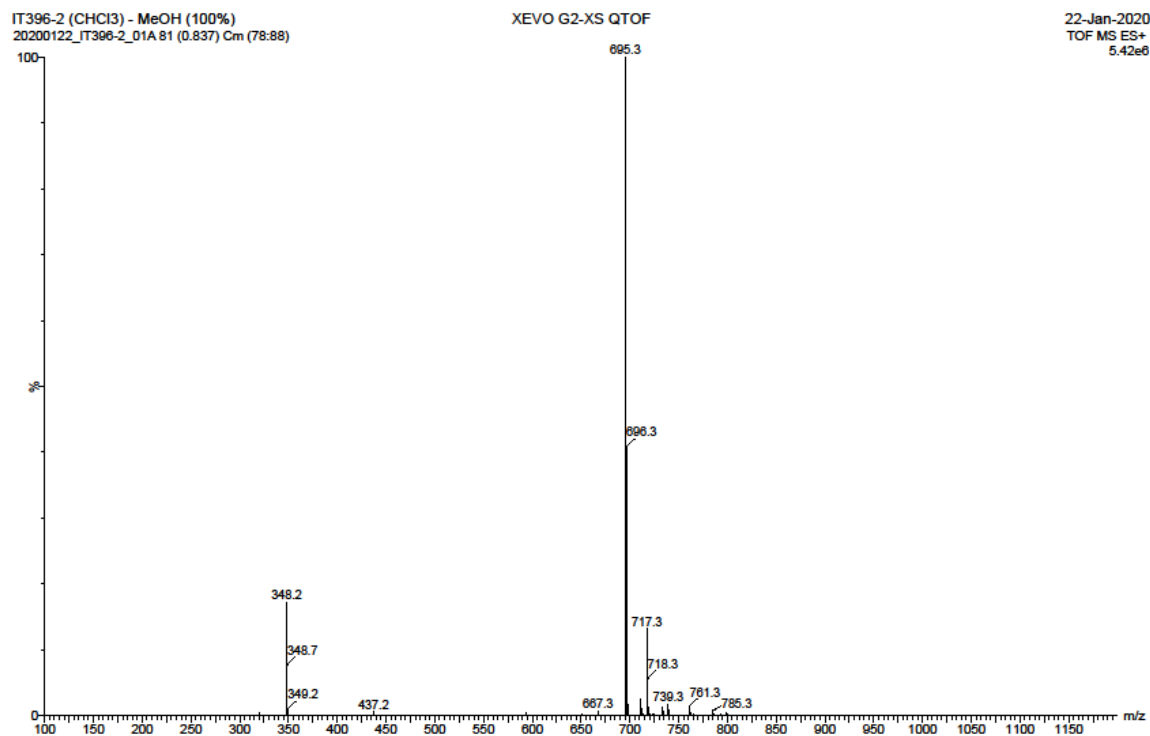


Figure S31. ES-MS spectra of **phthalonitrile 11**.

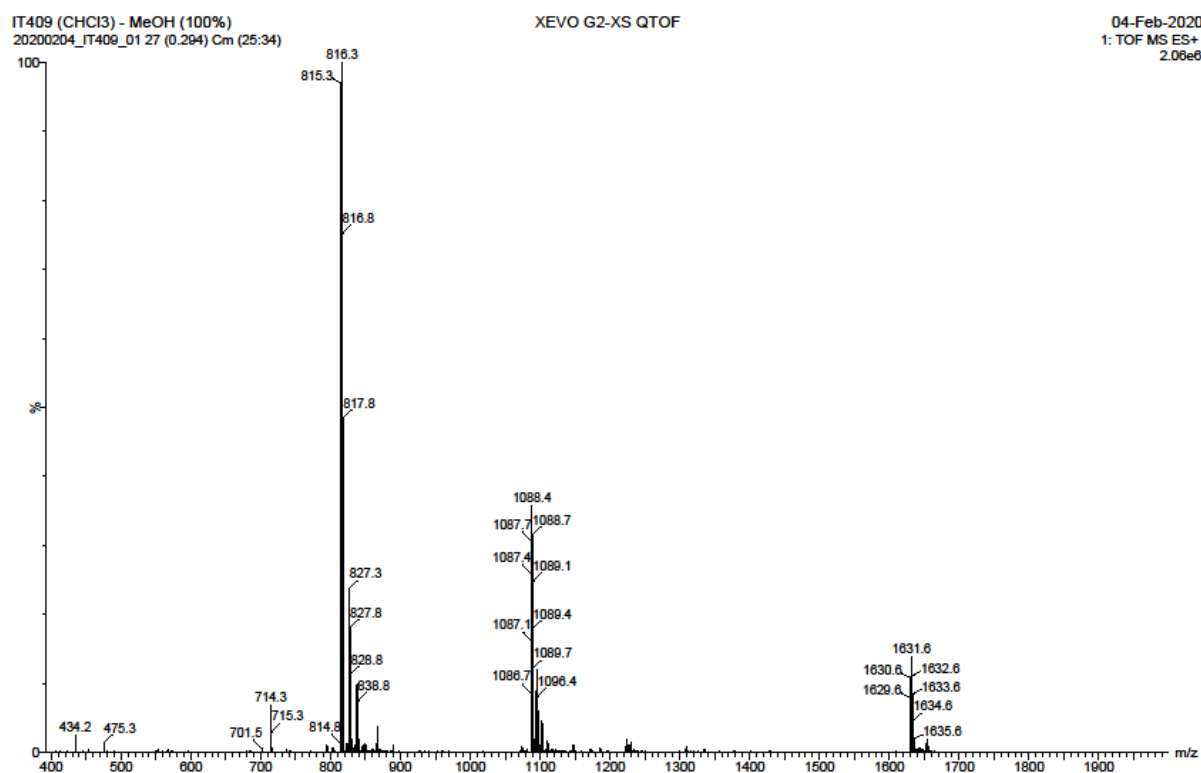


Figure S32. ES-MS spectra of **ZnPc-[Erl]₁**.

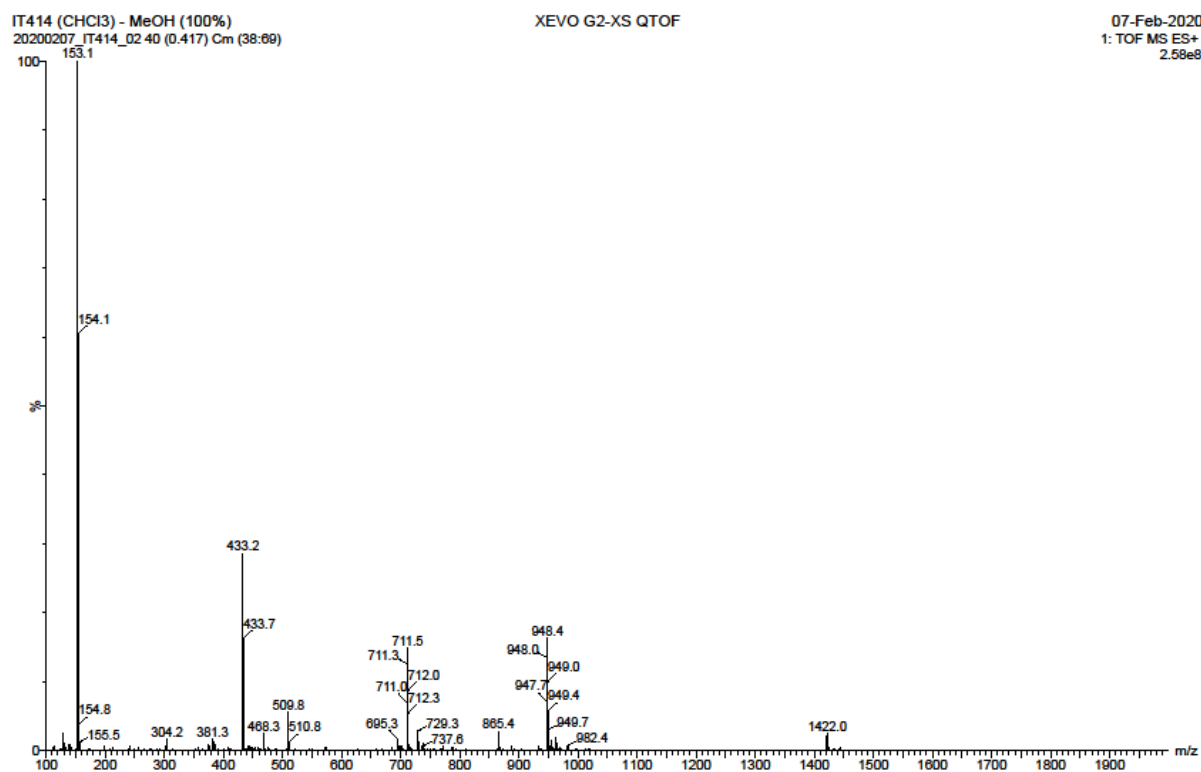


Figure S33. ES-MS spectra of ZnPc-[Erl]₄.

4. UV absorption spectra of targeting moieties

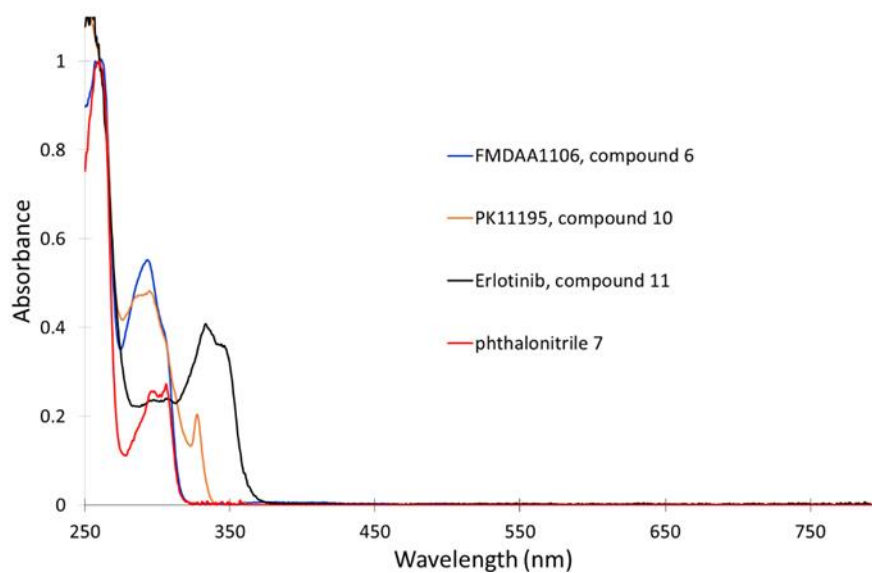


Figure S34. Normalized absorption spectra of targeting moieties recorded in CHCl₃.

4. HPLC analyses.

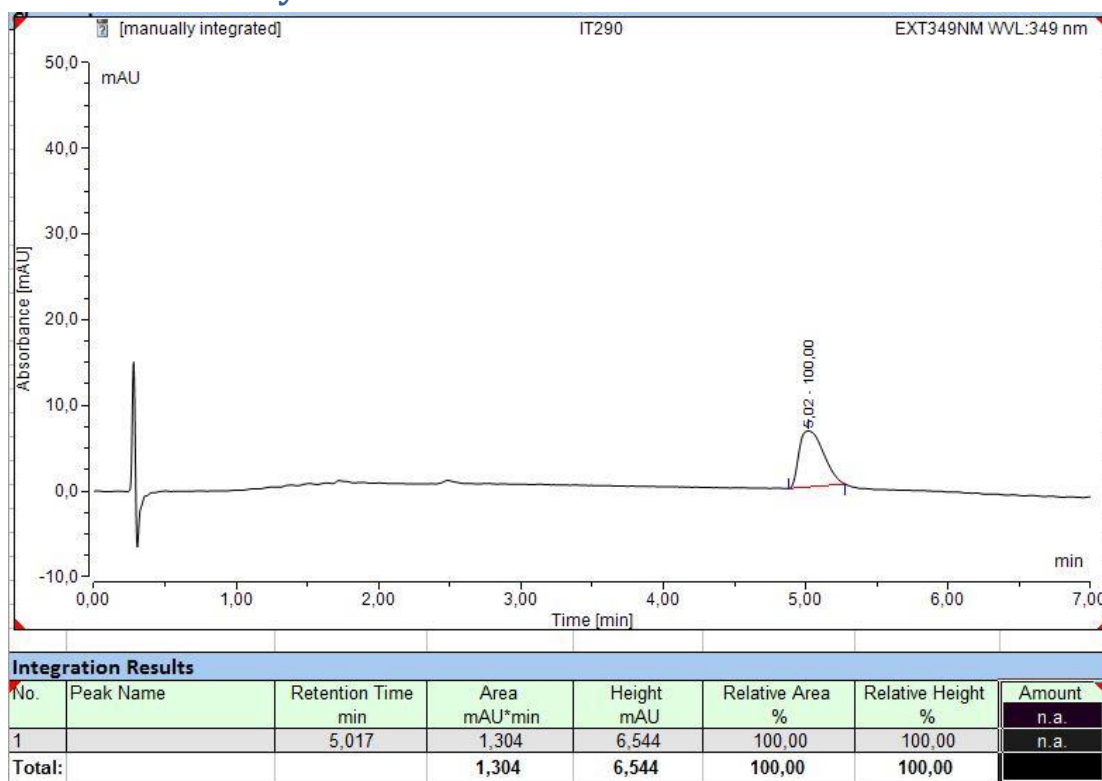


Figure S35. HPLC chromatogram of ZnPc(EG₃)₄.

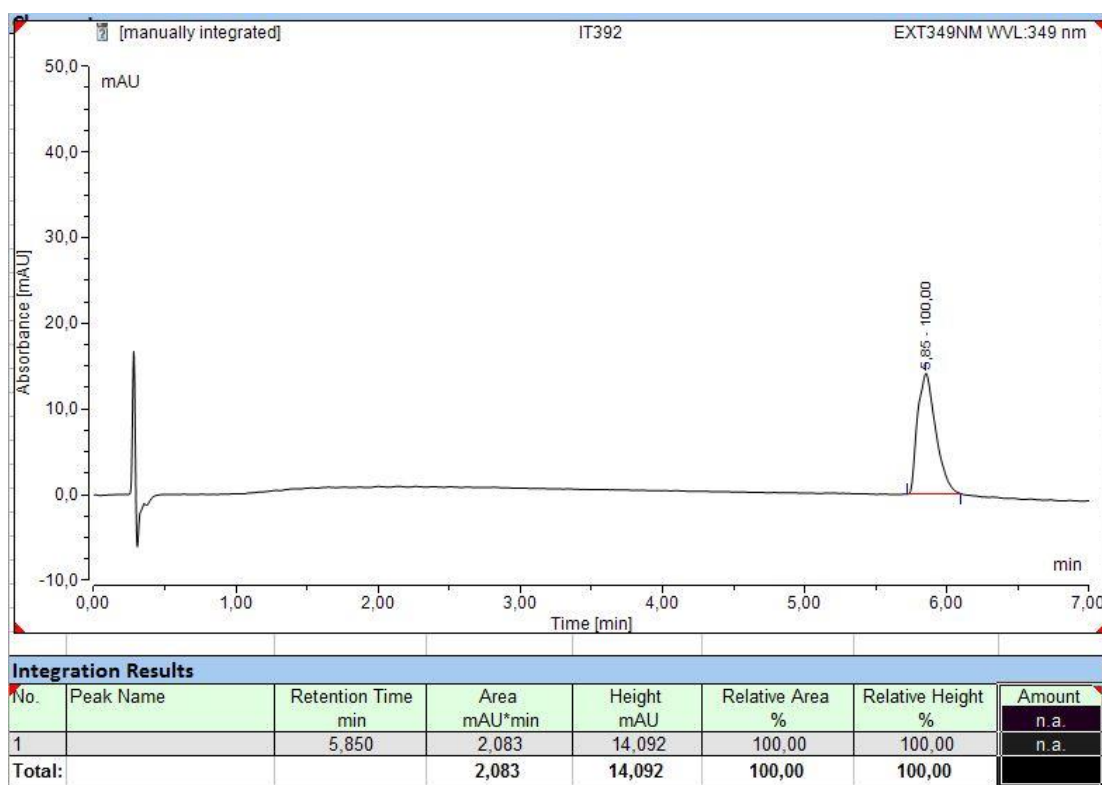


Figure S36. HPLC chromatogram of ZnPc-[DAA1106]₁.

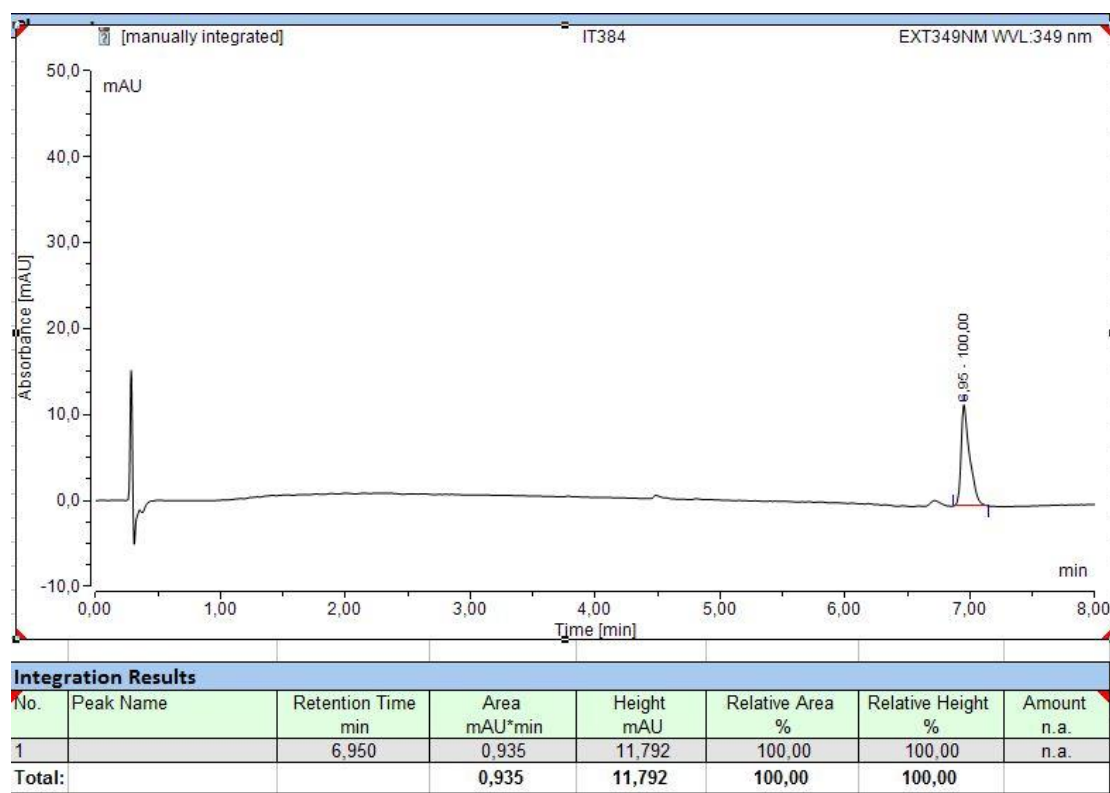


Figure S37. HPLC chromatogram of ZnPc-[DAA1106]₄.

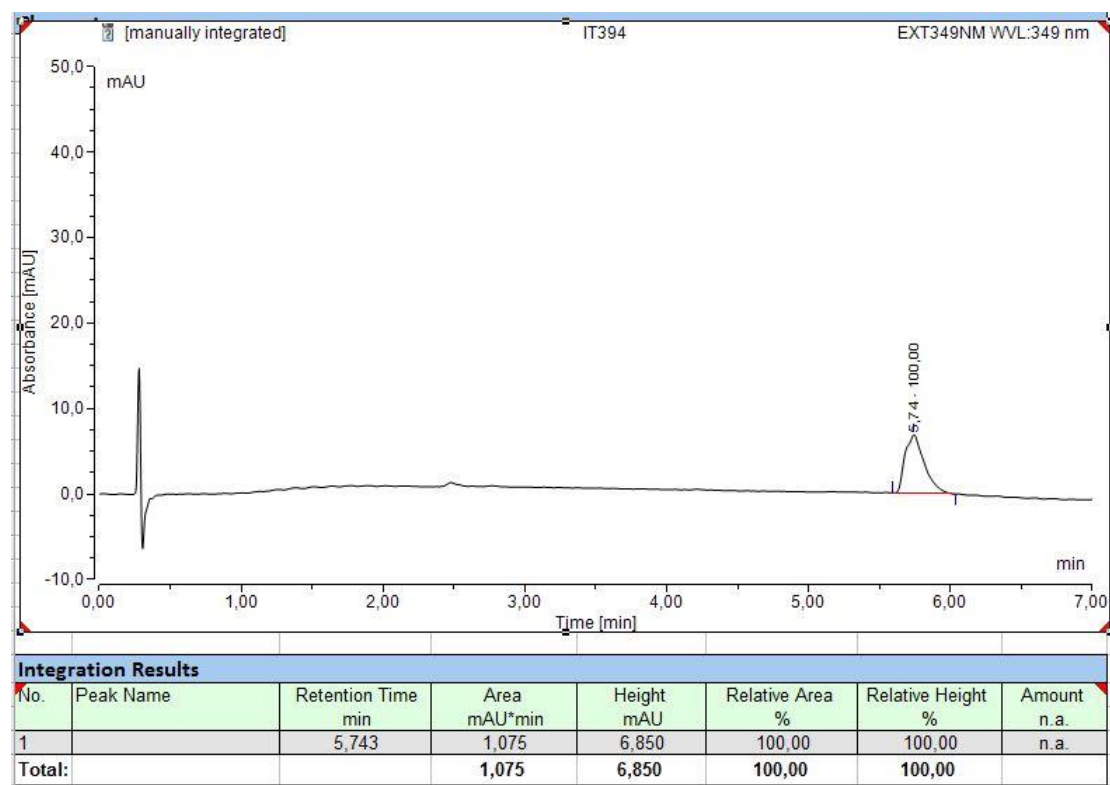


Figure S38. HPLC chromatogram of ZnPc-[PK11195]₁.

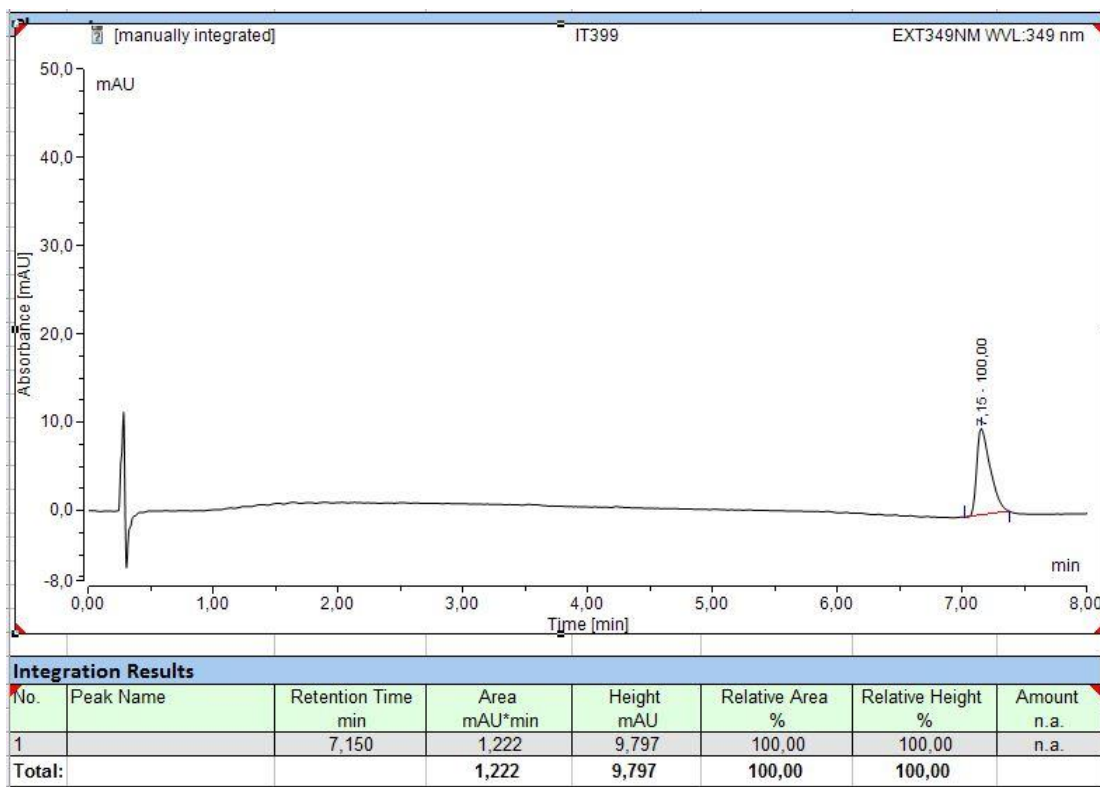


Figure S39. HPLC chromatogram of ZnPc-[PK11195]₄.

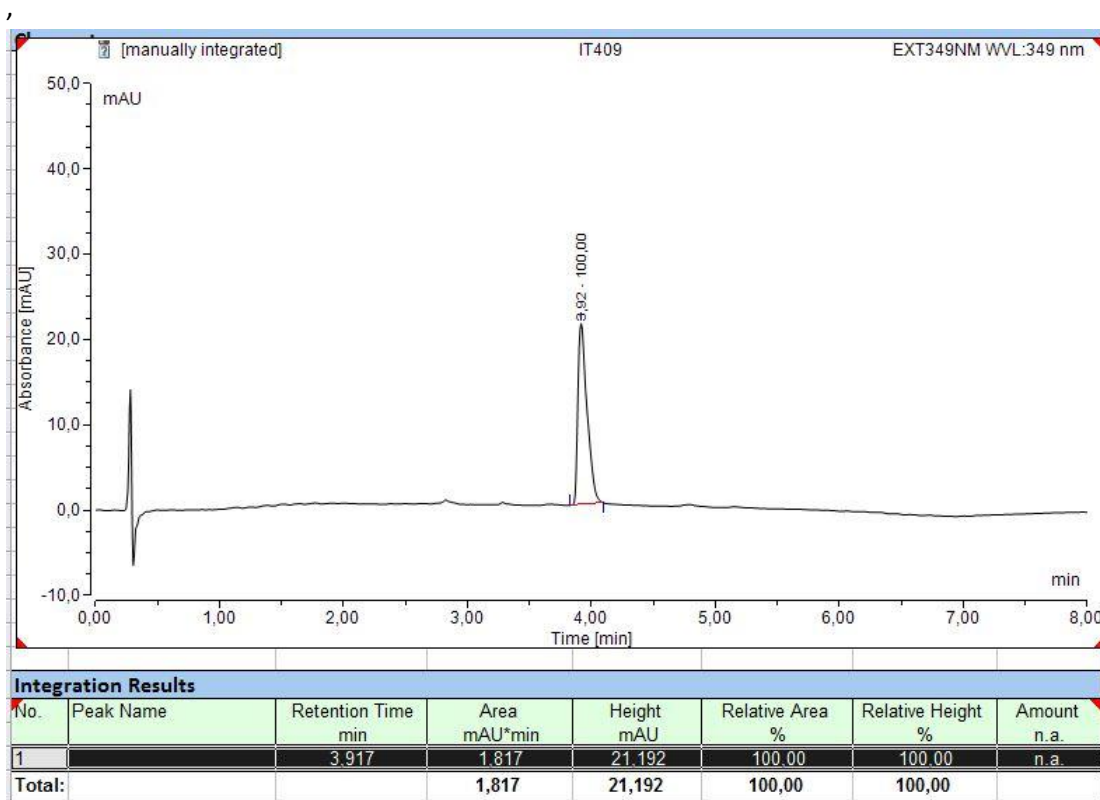


Figure S40. HPLC chromatogram of ZnPc-[Erlo]₁.

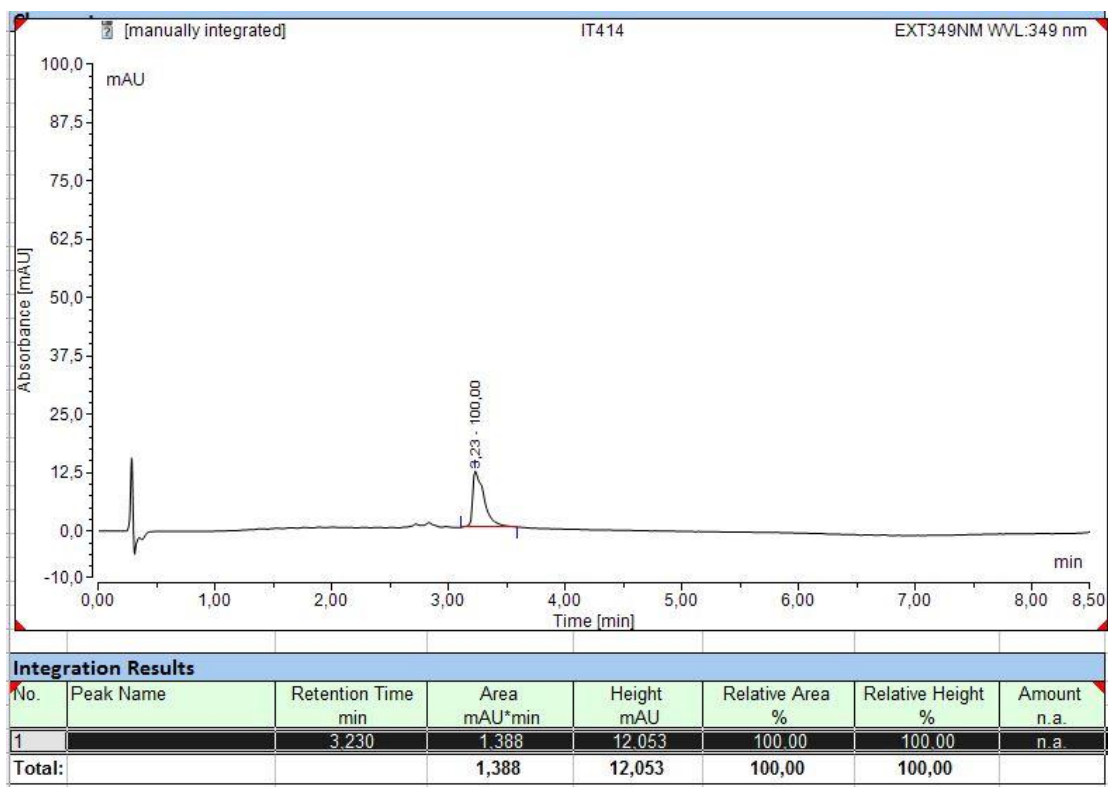


Figure S41. HPLC chromatogram of ZnPc-[Erl]₄.