

Novel phenothiazine bridged porphyrin-(hetero)aryl dyads: synthesis, optical properties, *in vitro* cytotoxicity and staining of human ovarian tumor cell lines.

Eva Molnar¹, Emese Gal¹, Luiza Gaina¹, Castelia Cristea^{1*}, Luminita Silaghi-Dumitrescu¹, Eva Fischer-Fodor^{2,3}, Maria Perde-Schrepler², Patriciu Achimas-Cadariu^{4,5}, Monica Focsan⁶

Supplementary materials

Contents:

NMR spectra of *5,15-diphenyl-10,20-bis(7-bromo-10-methyl-10H-phenothiazin-3-yl)-21,23H-porphyrin 3a* (figure S1 and S2)

NMR spectra of *5,10,15-triphenyl-20-(8-chloro-10-methyl-10H-phenothiazin-3-yl)-21,23-Zn-porphyrin 5a* (figure S3 and S4)

NMR spectra of *5,15-diphenyl-15,20-bis(7-(3'-formyl-10'-methyl-10'H-phenothiazin-7yl)-10-methyl-10H-phenothiazin-3-yl)-21,23H-porphyrin 13* (figures S5-S8)

HRMS spectrum of *5,15-diphenyl-10,20-bis(7-bromo-10-methyl-10H-phenothiazin-3-yl)-21,23H-porphyrin 3a* (figure S9)

HRMS spectrum of *5,10,15-triphenyl-20-(7-bromo-10-methyl-10H-phenothiazin-3-yl)-21,23-Zn-porphyrin 4a* (figure S10)

HRMS spectrum of *5,10,15-triphenyl-20-(8-chloro-10-methyl-10H-phenothiazin-3-yl)-21,23-Pd-porphyrin 5b* (figure S11)

HRMS spectrum of *5,10,15-triphenyl-20-(8-chloro-10-methyl-10H-phenothiazin-3-yl)-21,23-Cu-porphyrin 5d* (figure S12)

HRMS spectrum of *5,15-diphenyl-10,20-bis(7-bromo-10-methyl-10H-phenothiazin-3-yl)-21,23-Cu-porphyrin 6d* (figure S13)

Correlations between fluorescence intensity and concentration for 9, 13, 15 fluorescent dyes against ovarian adenocarcinoma A2780cis and OVCAR3 cells (figure 14-15)

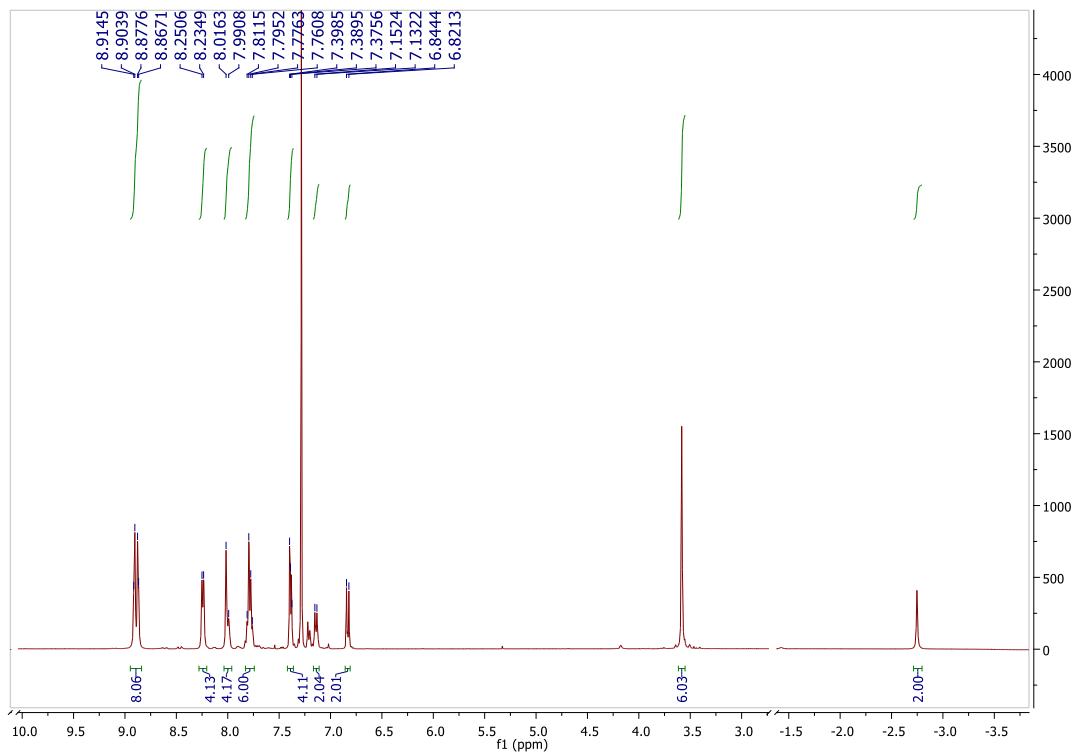


Figure S1. ^1H -NMR 400 MHz spectrum of **3a** (CDCl_3)

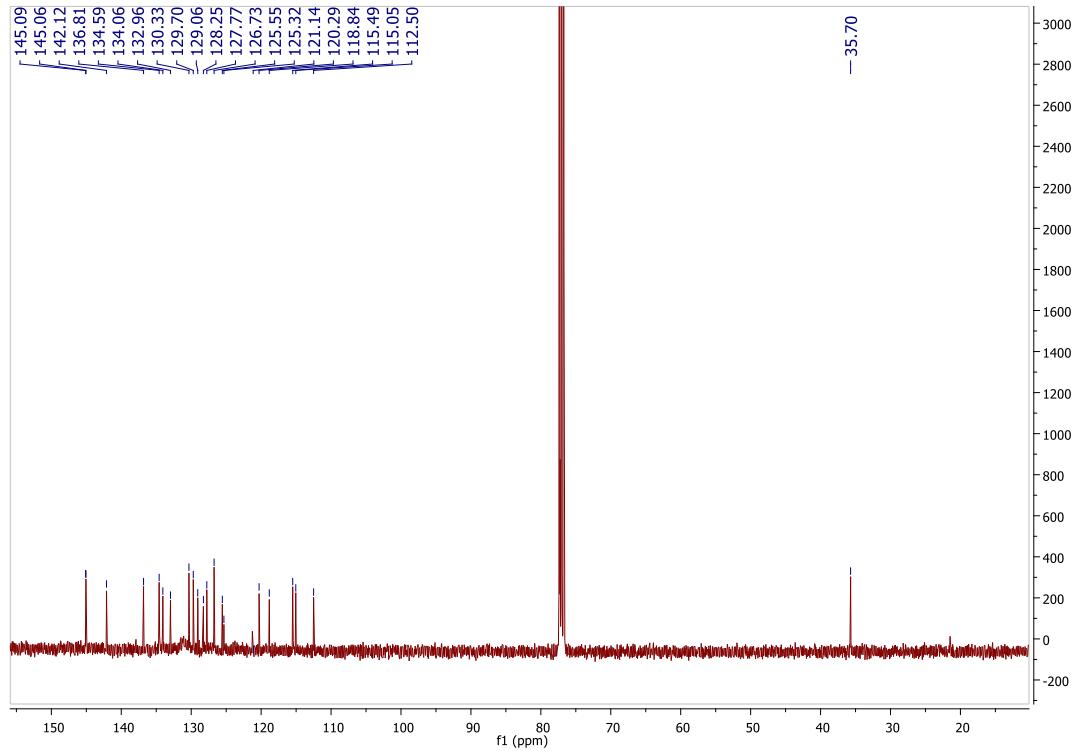


Figure S2. ^{13}C -NMR 100 MHz spectrum of compound **3a** (CDCl_3)

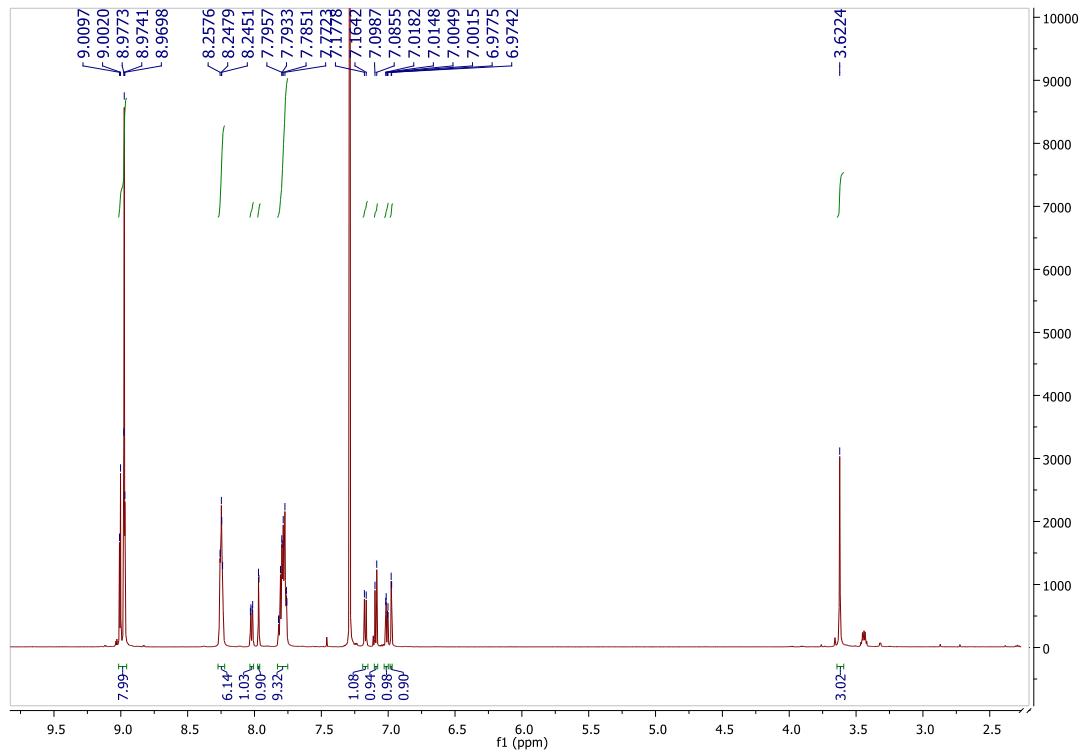


Figure S3. ^1H -NMR 600 MHz spectrum of **5a** (CDCl_3)

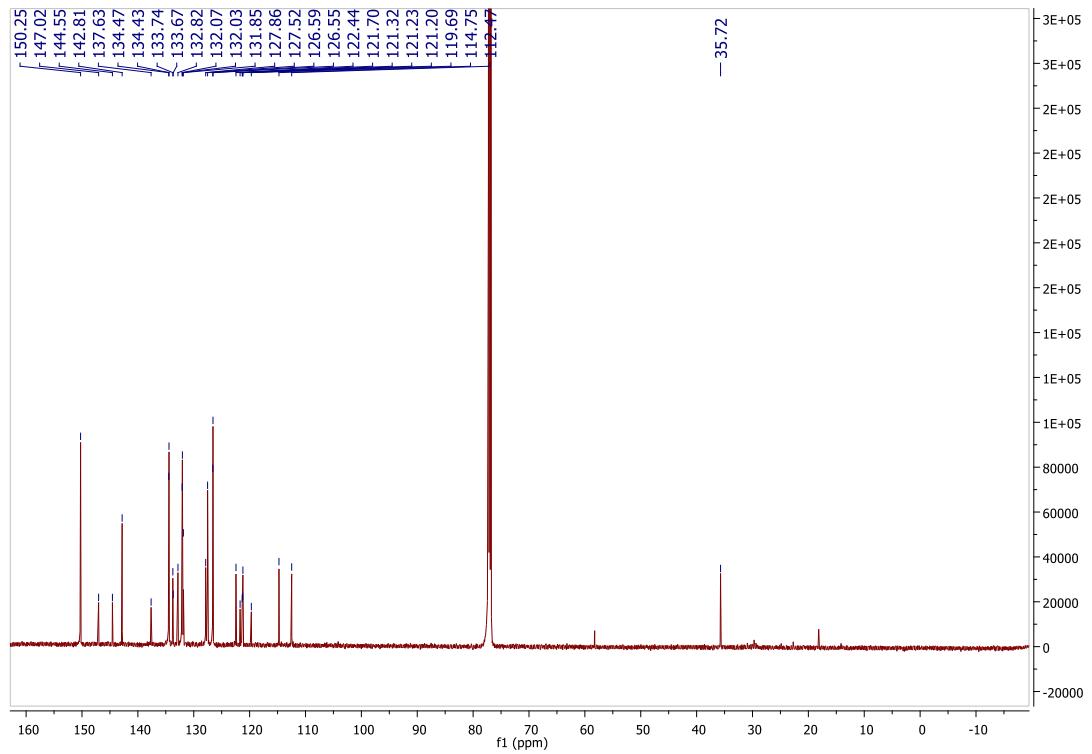


Figure S4. ^{13}C -NMR 150 MHz spectrum of **5a** (CDCl_3)

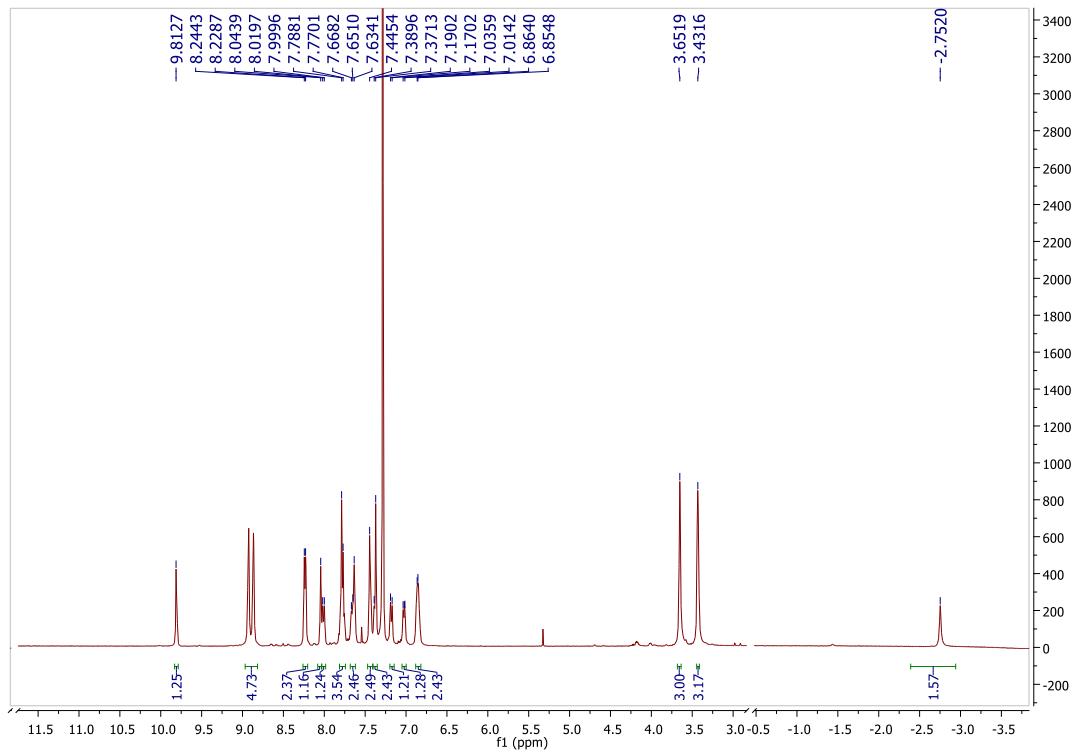


Figure S5. ^1H -NMR 400 MHz spectrum of compound **13** (CDCl_3)

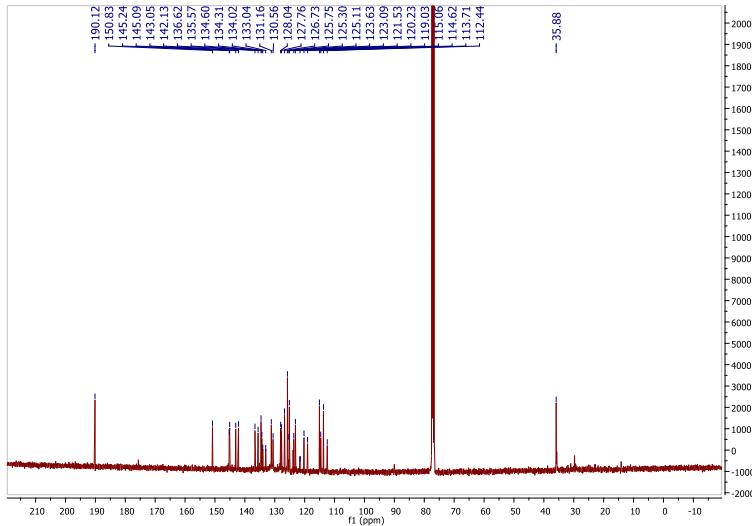


Figure S6. ^{13}C -NMR 100 MHz spectrum of compound **13** (CDCl_3)

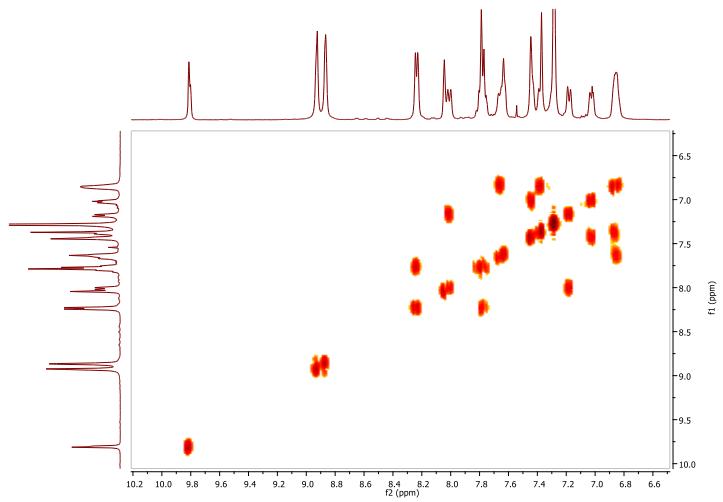


Figure S7. 2D-NMR(^1H - ^1H) COSY 400MHz spectrum of compound **13** (aromatic region, CDCl_3)

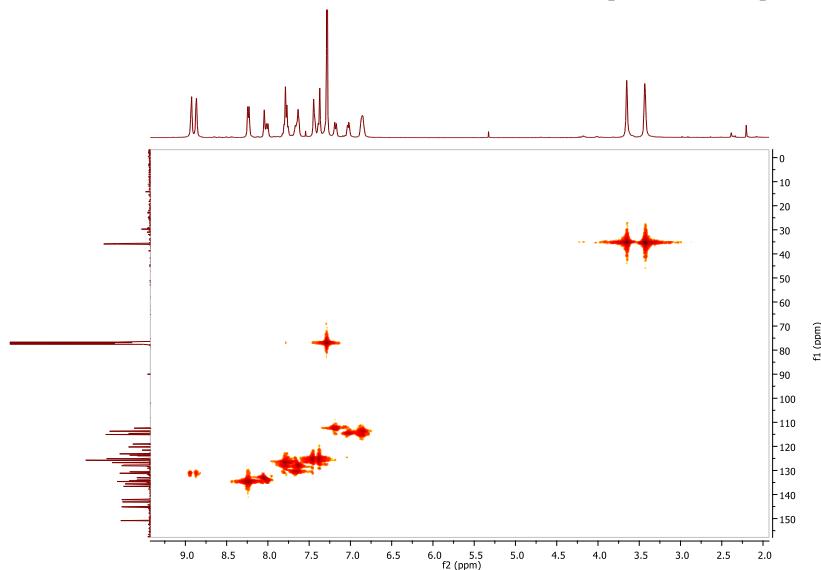


Figure S8. 2D-NMR (^1H - ^{13}C) HMQC 400MHz spectrum of compound **13** (CDCl_3 ,

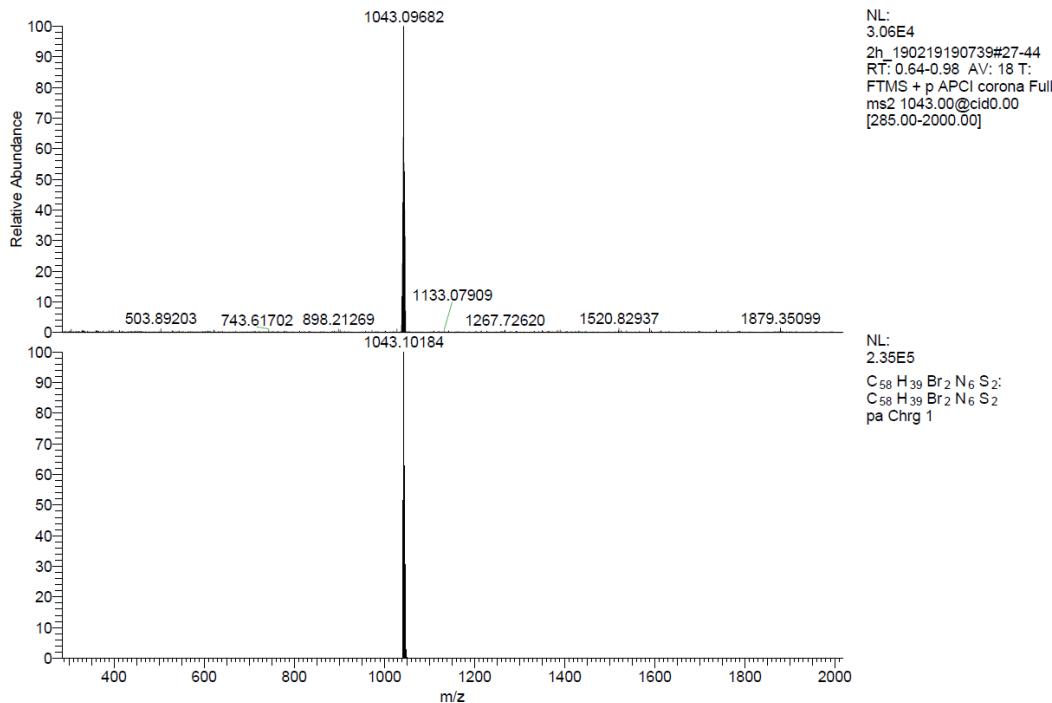


Figure S9. HRMS spectrum of 5,15-diphenyl-10,20-bis(7-bromo-10-methyl-10H-phenotheniazin-3-yl)-21,23H-porphyrin 3a

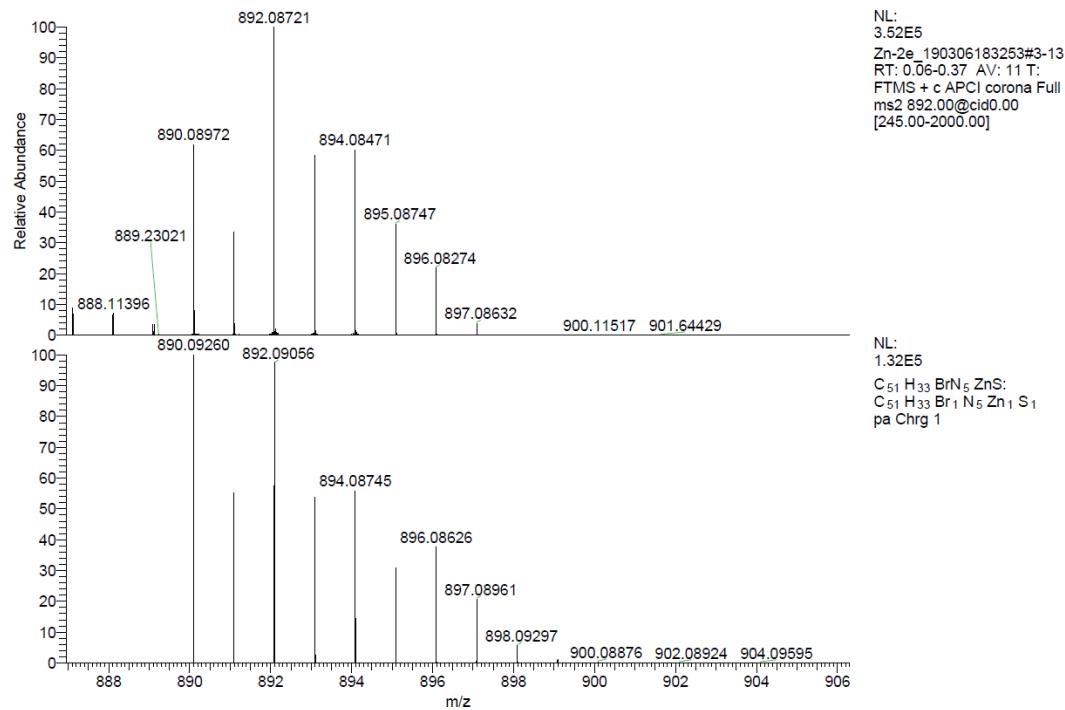


Figure S10. HRMS spectrum of 5,10,15-triphenyl-20-(7-bromo-10-methyl-10H-phenotheniazin-3-yl)-21,23-Zn-porphyrin 4a

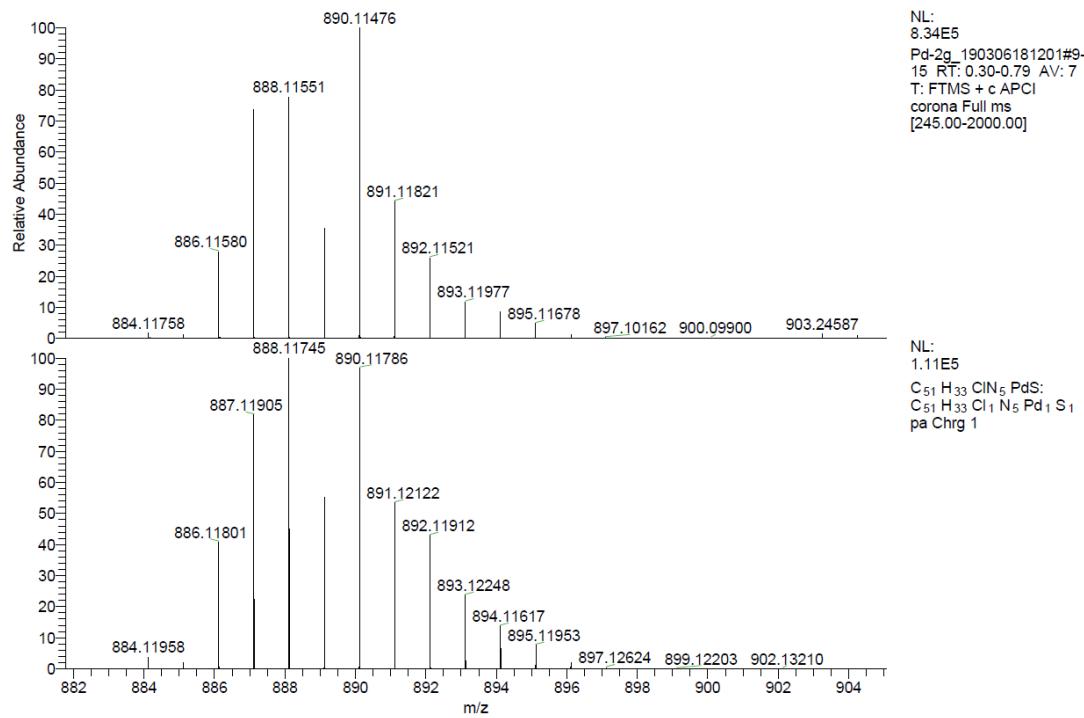


Figure S11. HRMS spectrum of 5,10,15-triphenyl-20-(8-chloro-10-methyl-10H-phenotheniazin-3-yl)-21,23-Pd-porphyrin 5b

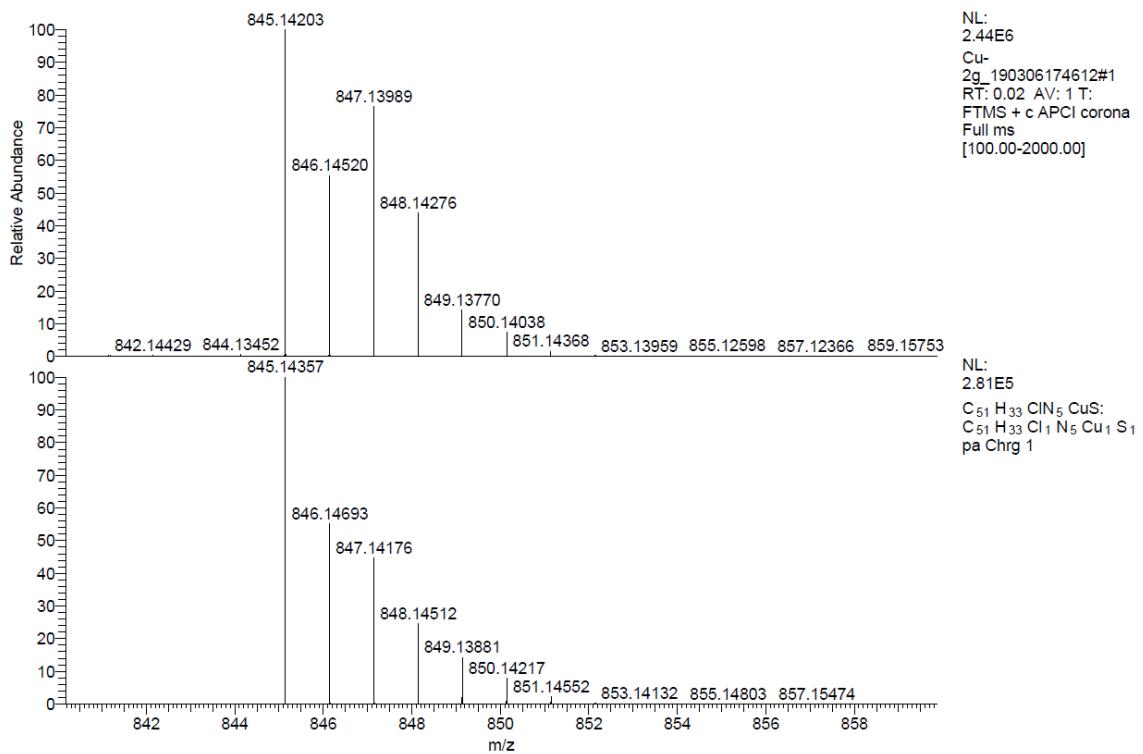


Figure S12. HRMS spectrum of 5,10,15-triphenyl-20-(8-chloro-10-methyl-10H-phenotheniazin-3-yl)-21,23-Cu-porphyrin 5d

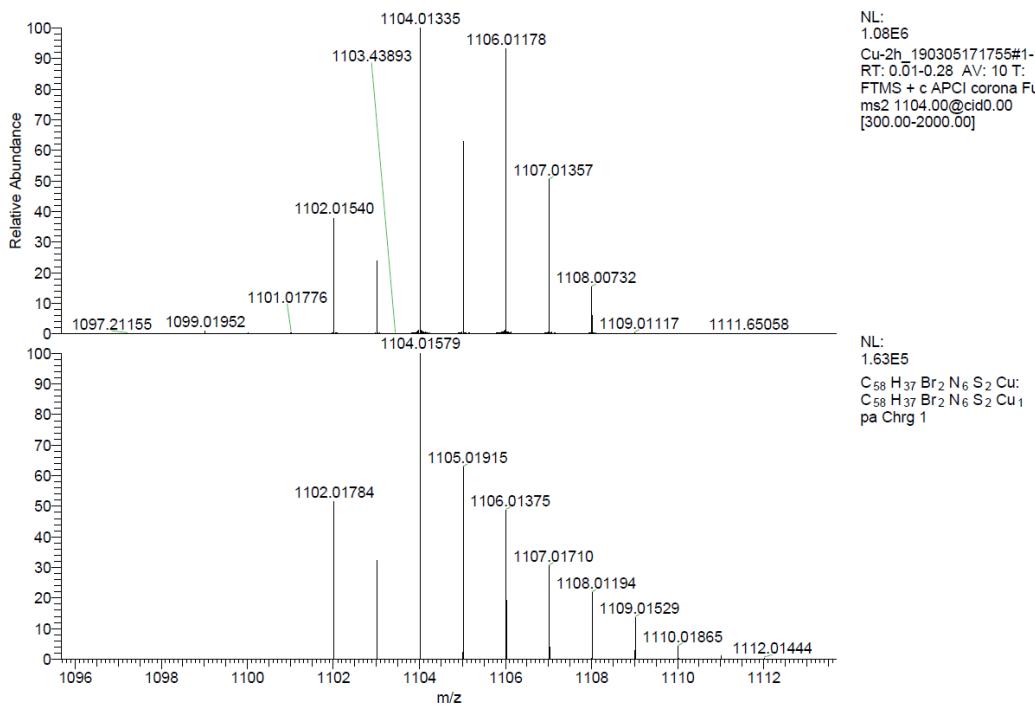


Figure S13. HRMS spectrum of 5,15-diphenyl-10,20-bis(7-bromo-10-methyl-10H-phenothiazin-3-yl)-21,23-Cu-porphyrin **6d**

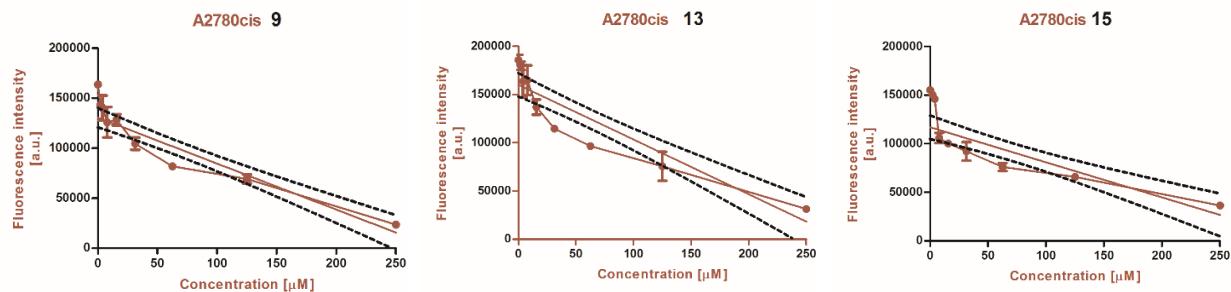


Figure S14. Linear regression of the metabolic rate of ovarian cancer cell line A2780cis *versus* the concentration of the fluorescent dyes: **9, 13, 15**.

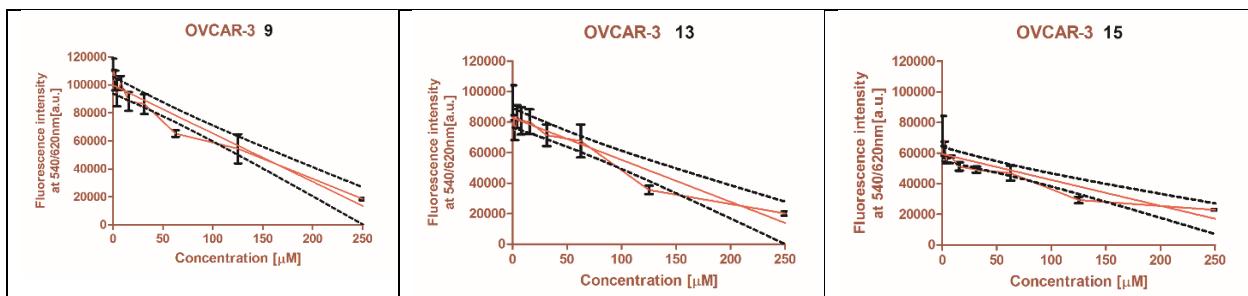


Figure S15. Linear regression of the metabolic rate of ovarian cancer cell line OVCAR-3 *versus* the concentration of the fluorescent dyes: **9, 13, 15**.