**Supplementary Material**

**Non-distorted visible-light absorbing thiol-PEGylated gold-coated superparamagnetic iron oxide nanoparticles porphyrin conjugates and their inhibitory effects against nosocomial pathogens.**

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## *Synthesis of 5,10,15, 20-tetrakis(4-hydroxyphenyl)porphyrin (m-THPP)*

m-THPP was prepared according to Adler-Longo’s method[1] with slight modification. A solution of 4-hydroxybenzaldehyde, (2.258 g, 18.490 mmol) in propionic acid (75 mL) was refluxed for 15 min. Freshly distilled pyrrole, (1.25 mL, 18.632 mmol) was added quickly. The resulting mixture was refluxed for additional 2 h. Propionic acid (50 mL) was removed under vacuum, and the remaining solution cooled to room temperature and neutralized with a saturated solution of 5% NaHCO3 (3 × 75 mL). The crude porphyrin was precipitated and washed with chloroform (3 × 75 mL) and finally re-dissolved in 100 mL of ethanol. The resulting crude m-THPP ethanol solution was left in the fume cupboard for 48 h. The as-synthesized crude THPP (1 g) was purified on silica gel (60 - 200 mesh) column with degassed EtOAC-Hexane mixture (2:1 v/v). The purple band was collected, evaporated on a rotary evaporator and the pure THPP was obtained as a dark violet solid.1H NMR (DMSO-d6) data (Chemical shifts (δ) in ppm): 2.898 (s, 2H, inner pyrrole N-H); 7.975 - 7.992 (d, 8H, J=8.0 Hz, ortho-Ar-H); 7.186 - 7.202 (d, 8H, J=8.0 Hz, meta-Ar-H); 8.851 (s, 8Hβ, pyrrole); 9.959 (s, 4H, Ar-OH).

*Synthesis of 5,10,15,20-tetrakis(3,5-dimethoxyphenyl)porphyrin (m-TdMPP)*

m-TdMPP was synthesized by the condensation of 3,5-dimethoxybenzaldehyde and pyrrole, using the Lindsey method with some modifications[2]. Briefly, 3,5-dimethoxybenzaldehyde (2.493 g, 15.000 mmol), and freshly distilled pyrrole (1.045 mL, 15.000 mmol) were dissolved in 100 mL of DCM. Next, 3 drops of each of trifluoro boron etherate, BF3.O(Et)2) and trifluoroacetic acid (TFA) (35 mL, 0.451 mmol) were added and the solution was stirred for 60 min at room temperature in argon atmosphere. Then 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (0.341 g, 1.501 mmol) was added and the mixture was stirred for additional 60 min, in open atmosphere. The solvent was removed under reduced pressure and the black tarry product was re-dissolved in hot methanol and filtered to give a purple crystalline crude product. The crude porphyrin m-TdMPP (1 g) was purified on silica gel (60 - 200 mesh) column with degassed hexane: ethyl acetate (2:1) mixture. The purple solution eluted from the column was concentrated to dryness in vacuo.1H NMR (CDCl3-d4) data (Chemical shifts (δ) in ppm): -2.844 (s, 2H, inner pyrrole N-H); 3.947 (s, 24H, Ar-OCH3), 7.385 - 7.390 (d, 8H, J=2.5, 5,10,15,20-Ar 2’,6’-H); 6.883 - 6.892 (t, 4H, J=2.0, 10,15,20-Ar 4’-H); 8.921 (s, 8Hβ, pyrrole).

*Synthesis of 5,10,15,20-tetrakis(3-pyridyl)porphyrin (m-T3-PyP)*

m-T3-PyP was prepared according to Adler-Longo’s method[1] with slight modification. Pyridine-3-carboxaldehyde, (2.30 mL, 2.574 g, 24.031 mmol) and 1.60 mL (24.031 mmol) of freshly distilled pyrrole, were added to 80 mL of refluxing propionic acid in a 100 mL round-bottomed flask. The mixture quickly turned black and was refluxed at 145°C for 1 h. After reaction time, propionic acid was reduced by heating (down to 10 mL), cooled to room temperature and treated with 5% NaHCO3 solution to neutralize the acid. The crude porphyrin (T3-PyP), was washed with acetone (50 mL) and filtered. The crude residue on the filter paper was dried in an oven for 12 hours at 60°C and weighed. The crude T3-PyP (0.3 g) was chromatographed on a silica gel (60 - 200 mesh) column and eluted with degassed CHCl3: acetone (3:7 v/v) mixture. The purple band was collected, evaporated on a rotary evaporator and the pure T3-PyP was obtained as a purple solid. 1H NMR (CDCl3-d4) data for m-T3-PyP. Chemical shifts (δ) in ppm: -2.833 (s, 2H, inner pyrrole N-H); 7.751 - 7.776 (dd, 4H, J=5.5 Hz, meta-Ar-H); 9.451 (s, 4H, ortho-Ar-H); 8.513 - 8.526 (d, 4H, J=6.5 Hz, ortho-Ar-H); 9.055 - 9.068 (dd, 4H, J=1.5 Hz, para-Ar-H); 8.852 (s, 8Hβ, pyrrole).

*Synthesis of 5,10,15,20-tetrakis(1-methylpyridinium-3-yl)porphyrin tetra-iodide (m-T3-Py+P4I-)*

5,10,15,20-Tetrakis(3′-pyridyl)porphyrin (m-T3-PyP) was cationized according to the modified method described by Vandressen *et al*.[3]. Neutral T3-PyP (50.301 mg) was dissolved in dry DMF (10 mL) in a 5 mL screw cap flask and a large excess of methyl iodide (600 µL) was then added to the solution. The reaction was stirred under room temperature for 18 h in the dark. The volume of the reaction mixture was then reduced to approximately 5 mL and methanol (6 mL) was added. The resulting mixture was added to 20 mL of diethyl ether to precipitate the cationic porphyrin. The purple solid was collected by filtration, washed with cold diethyl ether and dried in an oven for 12 h at 60°C and weighed. 1H-NMR (DMSO-d6) data for m-T3-Py+P4I- Chemical shifts (δ) in ppm: -3.125 (s, 2H, inner pyrrole N-H); 8.615-8.643 (dd, 4H, J=7.0 Hz, meta-Ar-H); 9.995 (s, 4H, ortho-Ar-H); 9.313 - 9.327 (d, 4H, J=7.0 Hz, ortho-Ar-H); 9.555 - 9.567 (d, 4H, J=6.0 Hz, para-Ar-H); 9.259 (s, 8Hβ, pyrrole).

**Table S1.** Preparation of 5.0 mg/mL of as-synthesized samples

|  |  |  |  |
| --- | --- | --- | --- |
| **Sample** | **Wt.****(mg)** | **Vol. solvent added (µL)** | **Solvent** |
| SPIONs@Au-TdMPPC | 13.2 | 2640 | WFI |
| SPIONs@Au-T3-PyPC | 11.2 | 2240 | WFI |
| SPIONs@Au-THPPCbr | 5.0 | 1000 | WFI |
| SPIONs@Au-THPPCgr | 13.6 | 2720 | WFI |
| SPIONs@Au-T3-Py+P4I-C | 6.5 | 1300 | WFI |
| THPP | 8.5 | 1700 | Acetone |
| TdMPP | 3.0 | 600 | Acetone |
| T-3PyP | 2.3 | 460 | Acetone |
| T-3Py+P4I- | 7.5 | 1500 | WFI |
| SPIONs@Au | 6.5 | 1300 | WFI |
| Ciprofloxacin (0.1 mg/mL) | 100 µL | 900 | WFI |
| Few drops of WFI | 15.5 | 3100 | Acetone |
| Culture control (TSB) | 100 µL | Distilled H2O |

WFI - Water for injection. Acetone - Negative control; Ciprofloxacin – positive control

*Bacterial culture conditions*

Bacteria cultures were inoculated in Tryptone Soya broth(TSB) and incubated at 37°C for 24 h. The overnight cultures (1 mL) was suspended in sterile TSB until turbidity was equal to a 0.5 McFarland Standard[4].

*Minimum Inhibition Concentration (MIC) of as-synthesized materials on bacterial pathogens*

Sterile 96-well micro titre plates were used for the assay (0.5 mL volume). All wells were filled with 100 µL of sterile TSB. Thereafter, test samples (100 µL) were added to the wells in the first row. This was followed by serial dilutions of the sample. The plates were inoculated with the test bacteria suspension (100 µL per well at a concentration of 1 x 106 colony forming units/mL) and incubated at 37°C overnight. A solution of *p*-Iodonitrotetrazolium violet solution(INT) (0.4 mg/ mL, 40 µL) was then added to each well and the plates were examined for pink colouration (signifying live bacterial growth) after approximately 6 h. The experiments were performed in triplicates.The MIC was determined as the lowest sample concentration at which no pink colour appeared.

**Table S2.** The Zeta potential of SPION Q, SPION Q@Au and SPION Q@Au -porphyrin conjugates

|  |  |
| --- | --- |
| Samples | Zeta potential (mV) |
| SPION Q | +5.6 |
| SPION Q@Au  | +24.1 |
| SPIONs@Au-THPPCgr | +13.8 |
| SPIONs@Au-THPPCbr | -19.6 |
| SPIONs@Au-TdMPPC | -22.5 |
| SPIONs@Au-T3-PyPC | -15.7 |
| SPIONs@Au-T3-Py+P4I-C | +3.3 |

**References**

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