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Synthesis, properties and singlet oxygen generation of thiazolidinone double bond linked porphyrin at *meso* and *β*-position†

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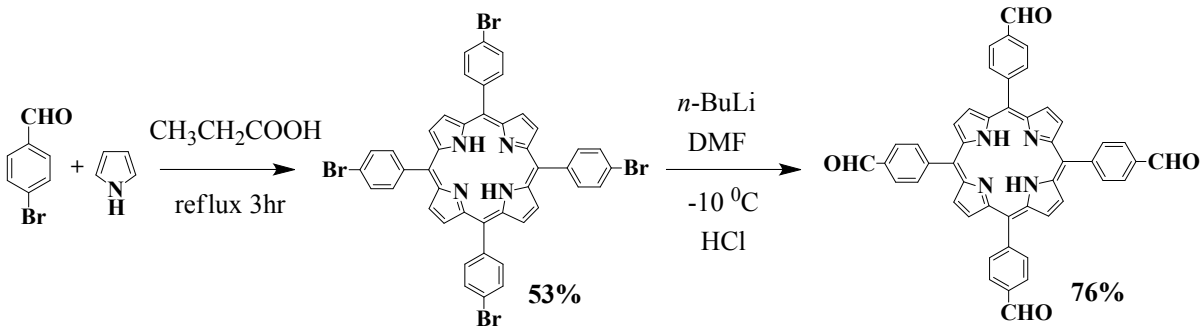
Synthesis of porphyrin aldehyde (1a)

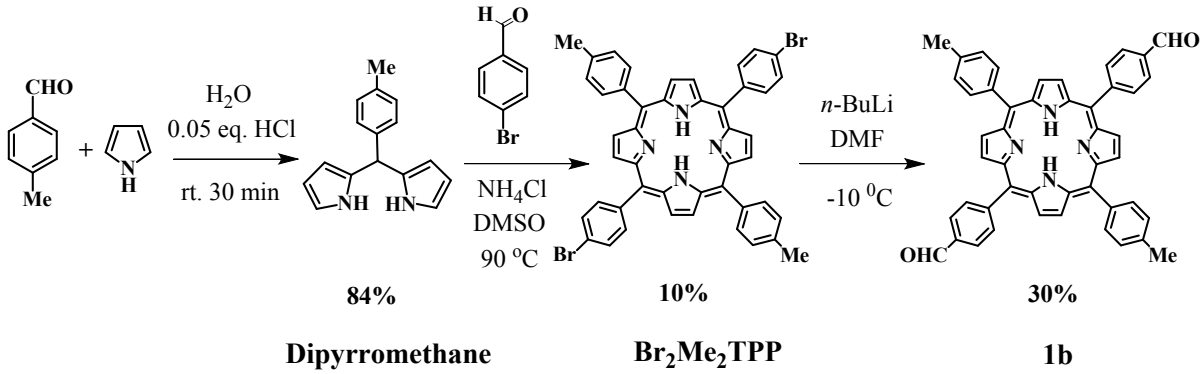


Br_4TPP **1a**

Synthesis of 5,10,15,20-Tetrakis(4'-bromophenyl)porphyrine **(Br_4TPP)*:*** A solution of *p*-bromobenzaldehyde (20 mmol) in propionic acid (150 mL) was refluxed at 140 °C, freshly distilled pyrrole (20 mmol) was added drop wise. The reaction mixture was allowed to refluxed for 2 h. Completion of reaction was monitored by TLC and LCMS. Reaction mixture cooled to room temperature. The resulted dark violet precipitate was collected by filtration and washed with hot water then with methanol (50 mL×3). The product was further purified by recrystallization from chloroform and methanol twice. Yield: 33% yield; IR (KBr) ν/cm^{-1}: 3317, 1597, 1473, 1441, 1350, 1219, 1095, 968, 835, 800, 729, 701; MS: *m*/*z* calcd 925.8891; found, 925.8893 $[M]^+$, 927.8911 [M+2] 929.8813, [M+4] 931.8961, [M+6] 933.8914 and [M+8] 935.8989; UV-Vis (λnm; $CHCl_3$ solution): 371, 419, 450, 515, 550, 595 and 666; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.82 (s, 8H, *β*-pyrrolic H), 8.06-8.04 (d, J = 8.2 Hz, 8H, *meso*-ArH), 7.89-7.87 (d, J = 8.0 Hz, 8H, *meso*-ArH), -2.89 (s, 2H, internal NH) ppm.

Synthesis of 5,10,15,20-tetrakis(4'-formylphenyl)porphyrin **(1a):** The 5,10,15,20-tetrakis(4'-bromophenyl)porphyrine **Br_4TPP** (0.21 mmol) was dispersed in dry diethyl ether (200 mL), cooled to -15°C and *n*-buthyllithium (2.5 M solution in hexane, 1.26 mmol) was added by syringe. The resulting green mixture was stirred at -10°C to -15°C for 2h then dry *N*,*N*-dimethylformamide (0.5 mL) was added. The cooling bath was removed and the reaction was stirred for additional 30 minutes at room temperature then poured into diluted hydrochloric acid (150 mL, 5%). The resulting two-phase mixture was vigorously stirred for 10 minutes and neutralized by concentrated aqueous ammonia. The resulting emulsion was extracted twice with chloroform. The organic phase was separated, dried over magnesium sulphate and evaporated to dryness at 40°C under reduced pressure. The purple remaining was purified on silica (25% ethylacetate/Hexane) and recrystallized from dichloromethane-methanol to give 5,10,15,20-tetrakis(4'-formylphenyl)porphyrin as a fine purple powder. Appearance: Purple; Yield: 50 mg (32%); IR (KBr) ν/cm^{-1}: 3321, 1681, 1589, 1489, 1471, 1321, 1254, 1074, 941, 821, 810, 750; MS: *m*/*z* calcd 726.2267; found, 726.2254; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.38 (s, 4H, CHO), 8.82 (s, 8H, β-pyrrolic H), 8.39-8.37 (d, J = 8.5 Hz, 8H, meso-ArH), 8.29-8.27 (d, J = 8.3 Hz, 8H, meso-ArH), -2.81 (s, 2H, internal NH) ppm.

Synthesis of porphyrin aldehyde (1b)



5-(4-Methylphenyl)dipyrromethane **(Dipyrromethane):** To 100 mL of 0.18 M aqueous HCl (1.5:98.5), pyrrole (3 equiv.) was added, followed by the addition of the 4-methylbenzaldehyde (1 equiv.). The reaction mixture was stirred at room temperature and the reaction progress was monitored by both TLC. After 30 min, the precipitated (semi-) solid product, which often sticks to the walls of the flask and the stirring bar and might hamper the

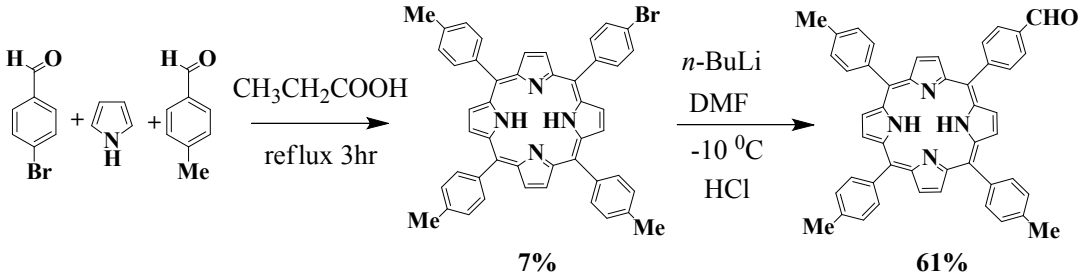
stirring, was filtered off and washed with water (and petroleum ether) to afford dipyrromethanes in high yields. Appearance: White solid; Yield: 68% yield; IR (KBr) ν/cm^{-1}: 3381, 3018, 1611, 1481, 1402, 1341, 1299, 1051, 991, 851, 741, 651; MS: *m*/*z* calcd 236.1313; found, 237.1352 [M+H]; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.79 (bs. 2 H. NH), 7.12 (dd, ArH), 6.69 (q. 2 H), 6.16 (q. 2 H), 5.92 (1, 2 H), 5.45 (s. 1 H. *meso*-H), 2.33 (s, 3 H, $ArCH_3$) ppm.

Synthesis of 5,15-di-(4'-bromophenyl)-10,20-di(4''-methylphenyl)porphyrin **(Br_2Me_2TPP):** 5-(4-Methylphenyl)dipyrromethane (8.8 mmols) and 4-bromobenzaldehyde 2 (8.8 mmol) were dissolved in dimethylsulfoxide (90 mL) then ammonium chloride (27.7 mmol) was added. The resulting mixture was stirred at 90^{o}C for 24 h. The mixture was cooled down and the porphyrin was filtered off. The solid was washed a few times by methanol and dried to give the 5,15-di-(4'-bromophenyl)-10,20-di(4''-methylphenyl)porphyrin. Appearance: Purple Yield: 3.8% yield; IR (KBr) ν/cm^{-1}: 3351, 3041, 2851, 2801, 1681, 1451, 1351, 1001, 998, 801, 751, 510; MS: *m*/*z* calcd 798.0994; found, 798.0992 $[M]^+$, 800.0914 [M+2] and 802.1114 [M+4]; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.81-8.78 (dd, 8H, β-pyrrolic H), 8.07 (m, 8H, meso-ArH), 7.87 (m, 4H, meso-ArH), 7.85 (m, 4H, meso-ArH), 2.69 (s, 6H, CH_3), -2.82 (s, 2H, internal NH) ppm.

Synthesis of 5,15-di-(4'-formyl)-10,20-di(4''-methylphenyl)porphyrin **(1b):** The 5,15-di-(4'-bromophenyl)-10,20-di(4''-methylphenyl)porphyrin **(Br_2Me_2TPP)** (0.25 mmol) was dispersed in dry diethyl ether (200 mL), cooled to -15°C and *n*-buthyllithium (2.5 M solution in hexane, 1 mmol) was added by syringe. The resulting green mixture was stirred at -10°C to -15°C for 2h then dry *N*,*N*-dimethylformamide (0.5 mL) was added. The cooling bath was removed and the reaction was stirred for additional 30 minutes at room temperature then poured into diluted hydrochloric acid (150 mL, 5%). The resulting two-phase mixture was vigorously stirred for 10 minutes and neutralized by concentrated aqueous ammonia. The resulting emulsion was extracted twice with chloroform. The organic phase was separated, dried over magnesium sulphate and evaporated to dryness at 40°C under reduced pressure. The purple remaining was purified on silica (10% ethylacetate/Hexane) and recrystallized from dichloromethane-methanol to give 5,15-di-(4'-formyl)-10,20-di(4''-methylphenyl)porphyrin **(1b)** as a fine purple powder. Appearance: Purple; Yield: 80 mg (45%); IR (KBr) ν/cm^{-1}: 3356, 3011, 2868, 1676, 1654, 1530, 1411, 1354, 1255, 1001, 944, 854, 831, 710. MS: *m*/*z* calcd 698.2682; found, 698.2694; ^{1}H NMR (400 MHz, $CDCl_3$): δ =

10.32 (s, 2H, CHO), 8.83-8.76 (dd, 8H, *β*-pyrrolic H), 8.32-8.25 (m, 8H, meso-ArH), 7.93-7.86 (m, 8H, meso-ArH), 2.68 (s, 6H, CH_3), -2.87 (s, 2H, internal NH) ppm.

Synthesis of porphyrin aldehyde (1c)

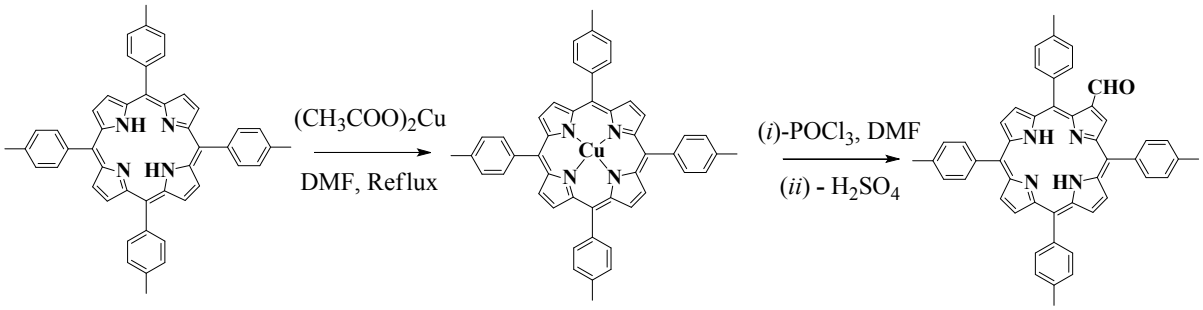


5-(4'-bromophenyl)-10,15,20-tri(4''-methylphenyl)porphyrin (**$BrMe_3TPP$**): A solution of *p*-bromobenzaldehyde (2.7 mmol) and tolualdehyde (8.15 mmol) in propionic acid (200 mL) was heated to refluxed at 140 °C, and added with freshly distilled pyrrole (10.8 mmol). The reaction mixture was refluxed for 2 h. The mixture was cooled to room temperature, resulted dark violet precipitate was collected by filtration and washed with hot water then with methanol (50×3 mL). The product was further purified by coloum chromotography chloroform and hexan 5%-10%. Yield: 200 mg (10.5%); IR (KBr) ν/cm^{-1}: 3354, 2836 1543, 1503, 1414, 1336, 1199, 1093, 973, 821, 811, 712; MS: *m*/*z* calcd 734.2045; found, 734.2048 $[M]^+$ and 736.2111 $[M+2]^+$; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.88-8.79 (s, 8H, *β*-pyrrolic H), 8.12 (d, *J* = 8.2 Hz, 8H, *meso*-ArH), 7.89 (d, 2H, *meso*-ArH), 7.55 (d, 6H, *meso*-ArH), 2.70 (s, 9 H, CH_3) -2.75 (s, 2H, internal NH) ppm.

5-(4'-formylphenyl)-10,15,20-tri(4''-methylphenyl)porphyrin **(1c):** The 5-(4'-bromophenyl)-10,15,20-tri(4''-methylphenyl)porphyrin (**$BrMe_3TPP$**) (0.272 mmol) was dispersed in dry diethyl ether (200 mL), cooled to -15°C and *n*-buthyllithium (2.5 M solution in hexane, 0.816 mmol) was added by syringe. The resulting green mixture was stirred at -10°C to -15°C for 2h then dry *N*,*N*-dimethylformamide (0.5 mL) was added. The cooling bath was removed and the reaction was stirred for additional 30 minutes at room temperature then

poured into diluted hydrochloric acid (150 mL, 5%). The resulting two-phase mixture was vigorously stirred for 10 minutes and neutralized by concentrated aqueous ammonia. The resulting emulsion was extracted twice with chloroform. The organic phase was separated, dried over magnesium sulphate and evaporated to dryness at 40°C under reduced pressure. The purple remaining was purified on silica (5% ethylacetate/Hexane) to give -(4'-formylphenyl)-10,15,20-tri(4''-methylphenyl)porphyrin **(1c)** as a fine purple powder. Appearance: Purple; Yield: 41 mg (22%); IR (KBr) ν/cm^{-1}: 3431, 3054, 2814, 1631, 1501, 1447, 1431, 1377, 1210, 961, 854, 720, 531. MS: *m*/*z* calcd 684.2889; found, 684.2881 $[M]^+$; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.38 (s, 1H, CHO), 8.97-8.88 (s, 8H, β-pyrrolic H), 8.11 (d, J = 8.2 Hz, 8H, *meso*-ArH), 7.91 (d, 2H, *meso*-ArH), 7.53 (d, 6H, *meso*-ArH), 2.71 (s, 9 H, CH_3) -2.78 (s, 2H, internal NH) ppm.

Synthesis of porphyrin aldehyde (1d)



89% **13%**

Me_4TPP **Me_4CuTPP** **1d**

Synthesis of (5, 10, 15, 20-tetra(4''-methylphenyl)porphyrin)copper(II) **(Me_4CuTPP):** A DMF solution (150 mL) of Me_4TPP (2.5 mmol) and cupric acetate (4 mmol) was placed to a round bottom flask. The mixture was heated at reflux for 2 h and the progress of the reaction was monitored by TLC. After removal of the most of DMF, the mixture was poured into ice water (300 mL), crude product was obtained by vacuum filtration. And then, the powder was washed with water and methanol, dried under vacuum to get 1.42 g product and used for the following synthesis without further purity.

***Synthesis of 2-formyl-5,10,15,20-tetra(4''-methylphenyl)porphyrin (*1d):** **Me_4CuTPP** (1.92 mmol) in 1, 2-dichloroethane (120 mL) and the Vilsmeier complex, prepared from dry DMF (14 mL) and phosphorus oxychloride (11 mL) were heated at efflux for 7h, then left

overnight. The mixture was vigorously stirred, and concentrated sulfuric acid (25 mL) was added. Stirring was continued for 10 mins, and then the mixture was poured into an ice-cold solution of sodium hydroxide (36 g) in water (1.25 L). The organic layer was diluted with chloroform (700 mL), separated and washed with a saturated solution of sodium bicarbonate (2×300 mL). The organic layer was dried over anhydrous sodium sulfate and the solvent removed. The resultant residue was purified by column chromatography. Appearance: dark purple; Yield: 45% yield; IR (KBr) ν/cm^{-1}: 3511, 3041, 1680, 1531, 1476, 1465, 1314, 1232, 1015, 951, 832, 815, 621, 521. MS: *m*/*z* calcd 698.3046; found, 698.3048; ^{1}H NMR (400 MHz, $CDCl_3$): δ = -2.54 (s, 2H, inner NH), 7.73-7.81 (m, 12H, *m*- and *p*-PhH), 8.17- 8.23 (m, 8H, *o*-PhH), 8.77 (d, 2H, β- pyrrolic H), 8.85- 8.92 (m, 4H, pyrrolic H), 9.22 (s, 1H, H-3), 9.41 (s, 1H, CHO).

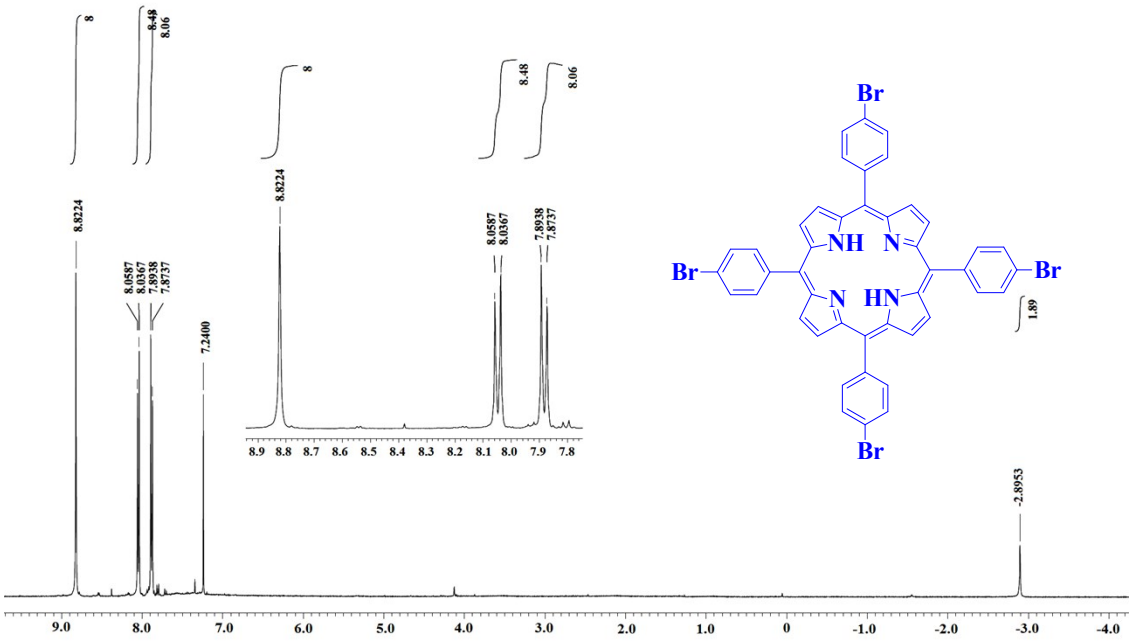


Figure S1: ^{1}H NMR spectrum of 5,10,15,20-tetrakis(4'-bromophenyl)porphyrin (**Br_4TPP**) in $CDCl_3$.

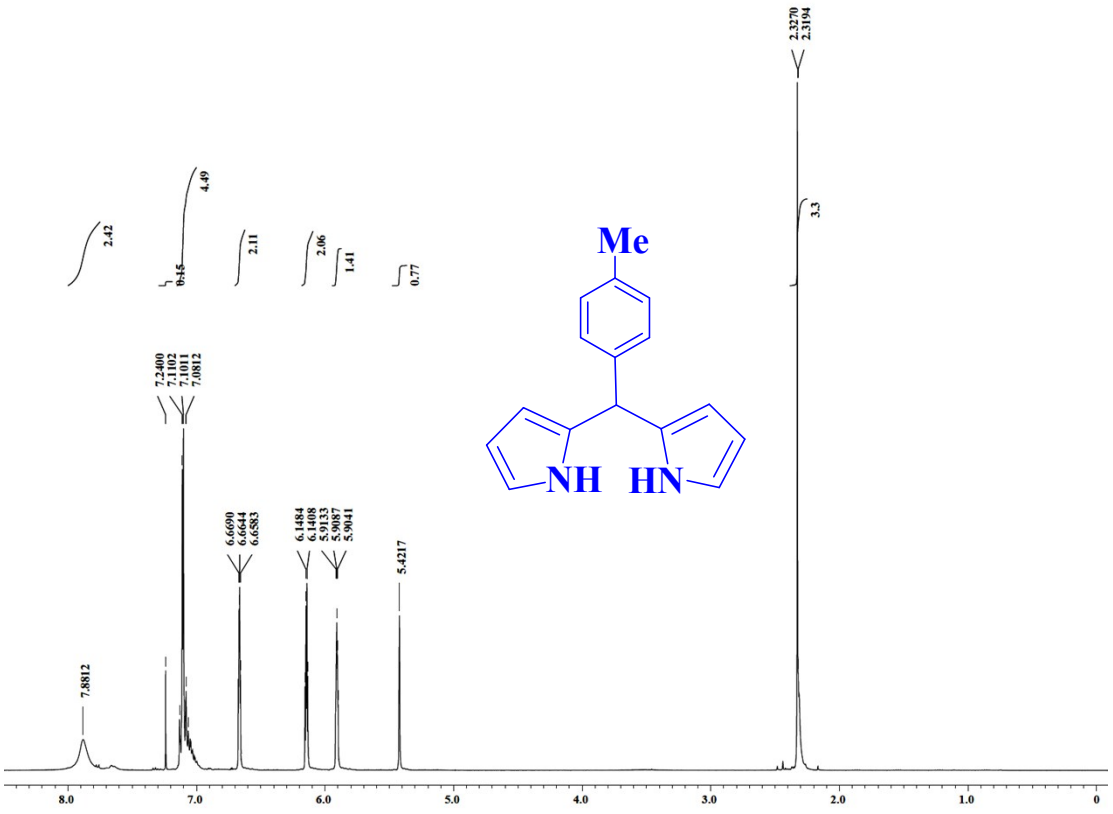


Figure S2: ^{1}H NMR spectrum of 5-(4-methylphenyl)dipyrromethane (**Dipyrromethane**) in $CDCl_3$.

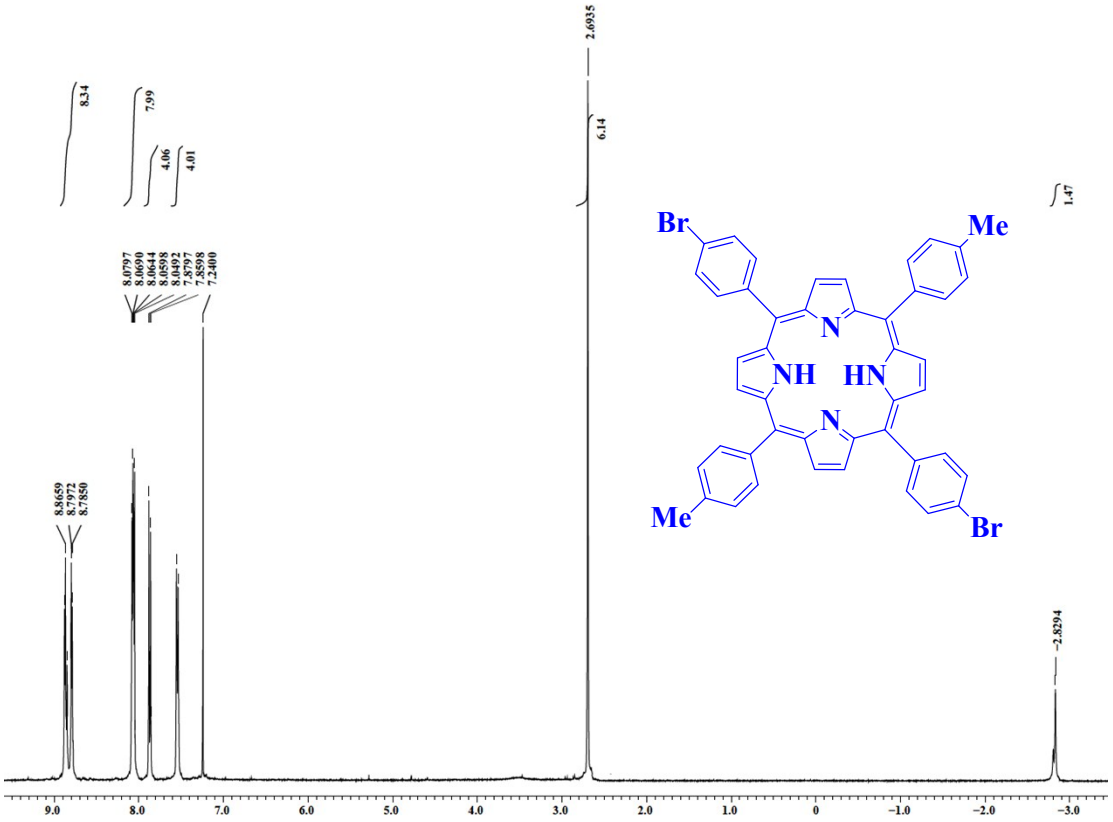


Figure S3: ^{1}H NMR spectrum of 5,15-di(4'-bromophenyl)-10,20-di(4''-methylphenyl)porphyrin (**Br_2Me_2TPP**) in $CDCl_3$.

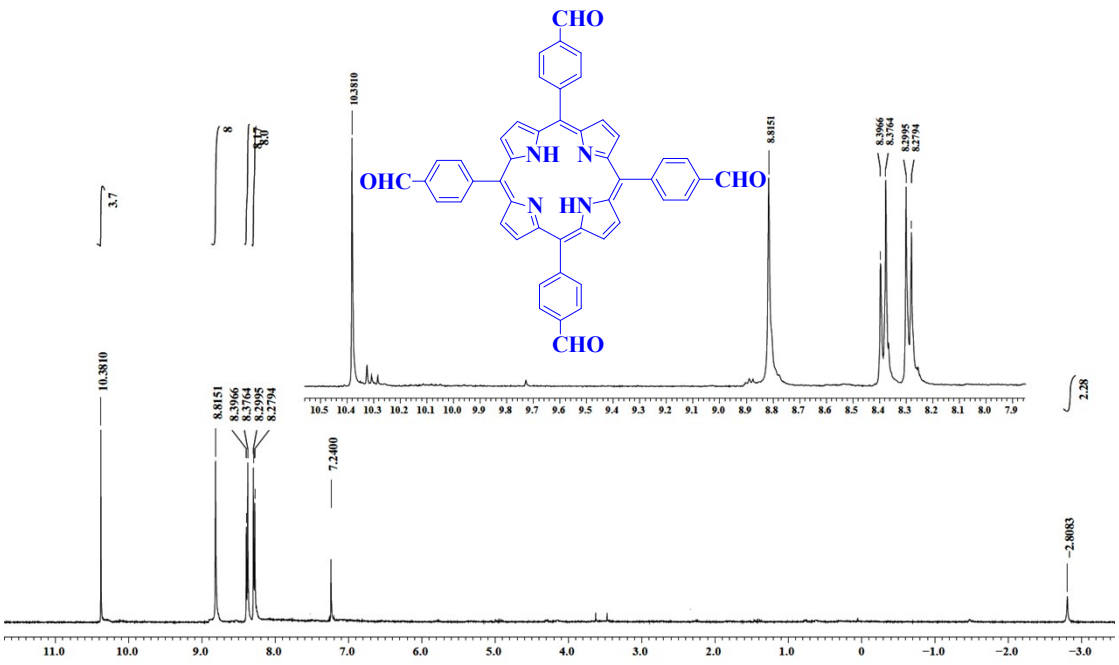


Figure S4: ^{1}H NMR spectrum of 5,10,15,20-tetrakis(4'-formylphenyl)porphyrin (**1a**) in $CDCl_3$.

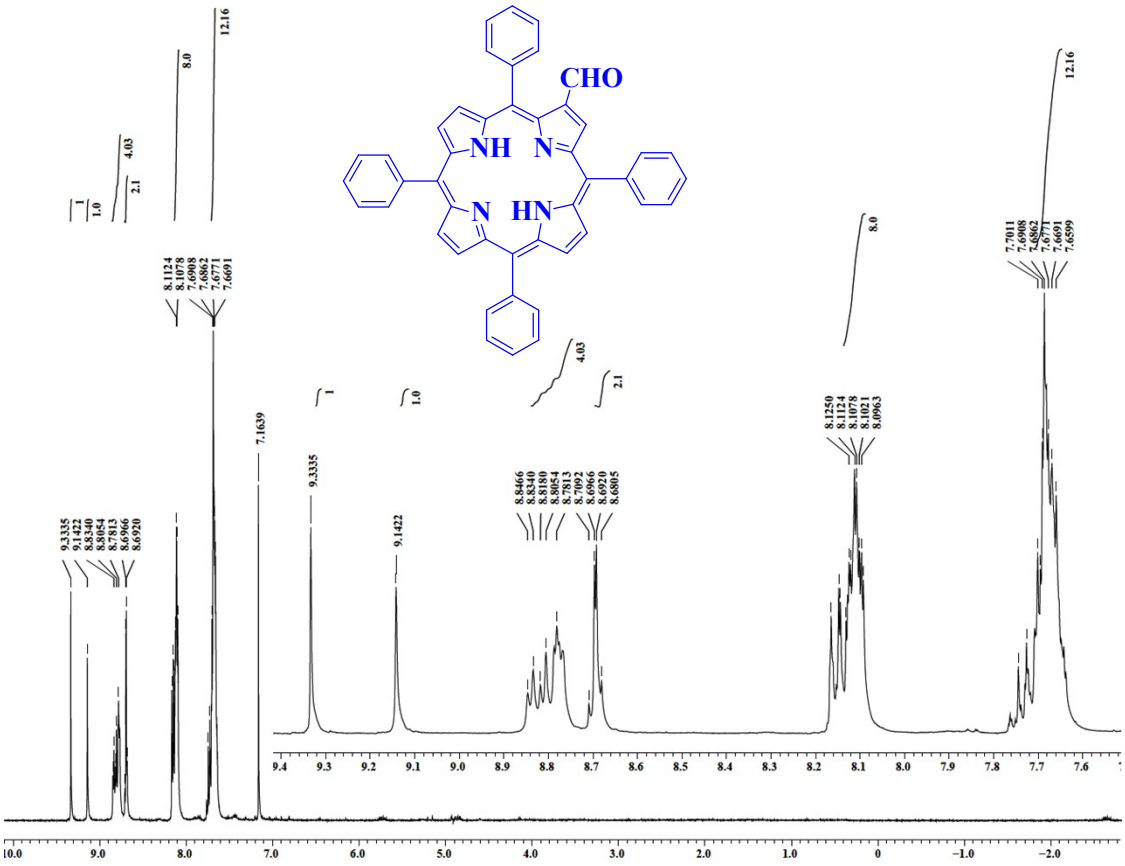


Figure S5: ^{1}H NMR spectrum of 2-formyl-5,10,15,20-tetraphenylporphyrin (**1d**) in $CDCl_3$.

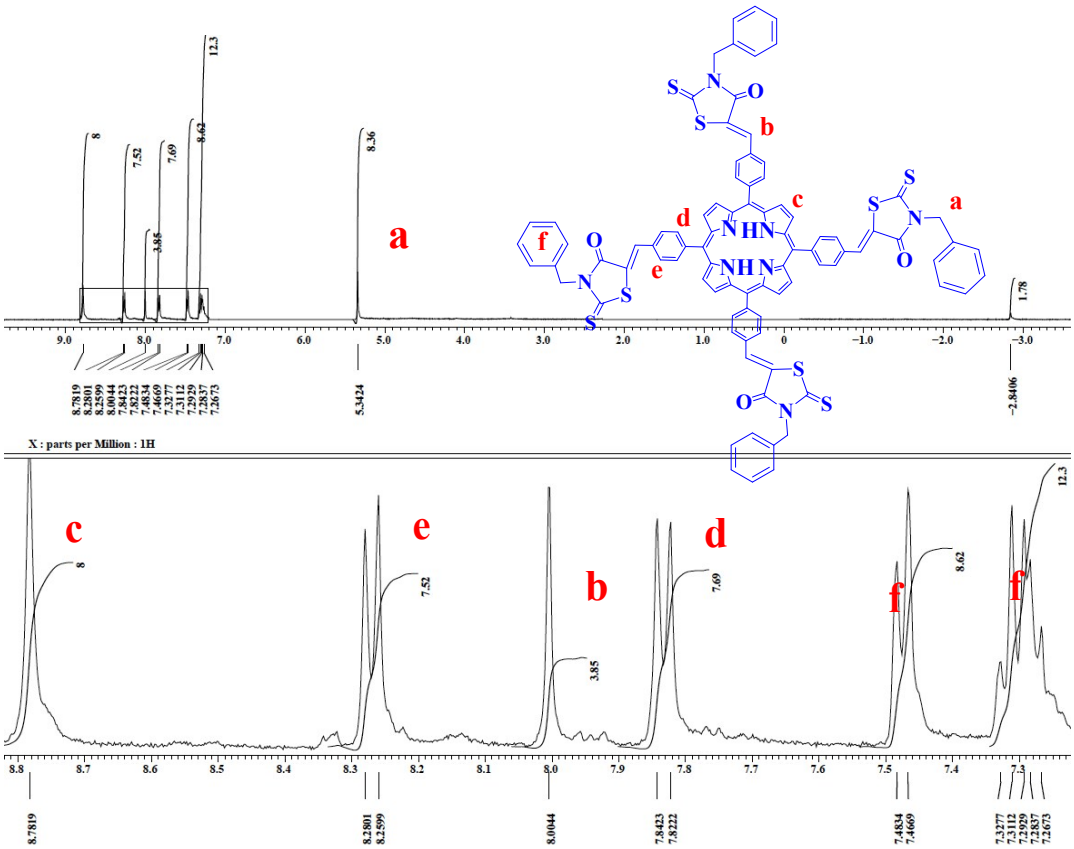


Figure S6: ^{1}H NMR spectrum of **3a** in $CDCl_3$.

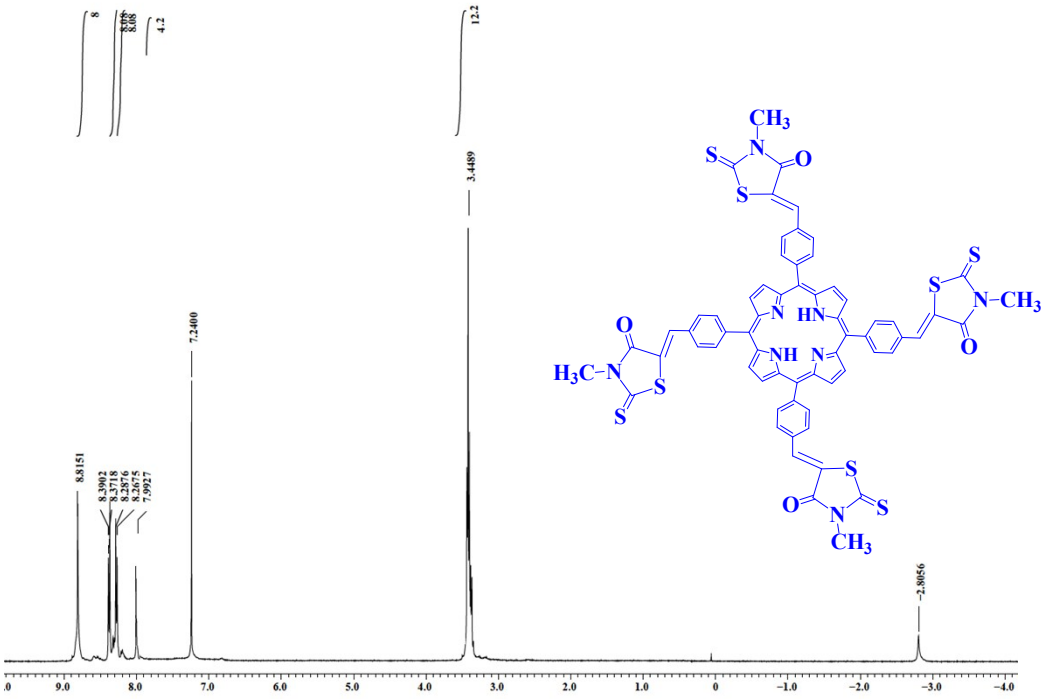


Figure S7: ^{1}H NMR spectrum of **3c** in $CDCl_3$.

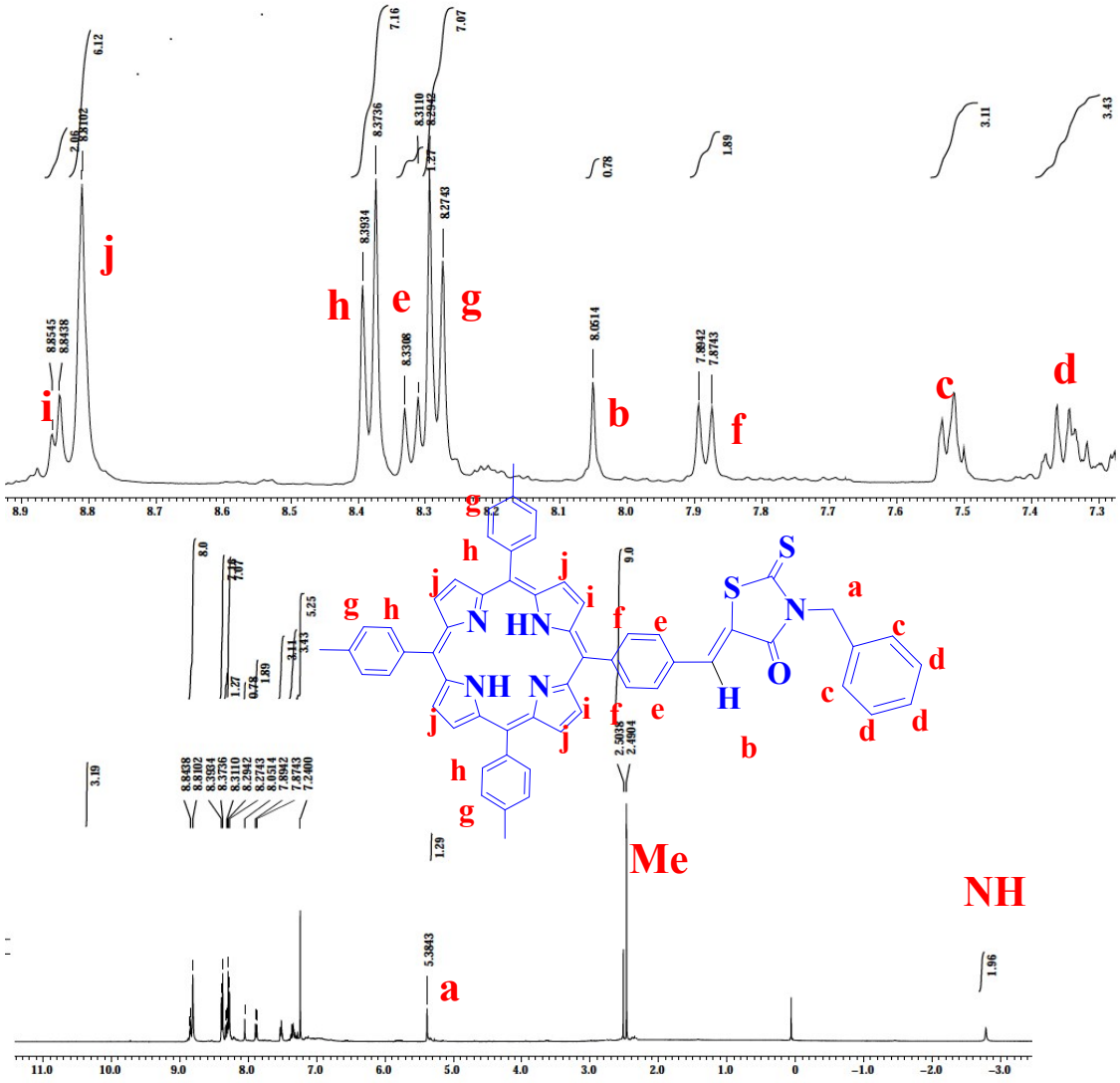


Figure S8: ^{1}H NMR spectrum of **5a** in $CDCl_3$.

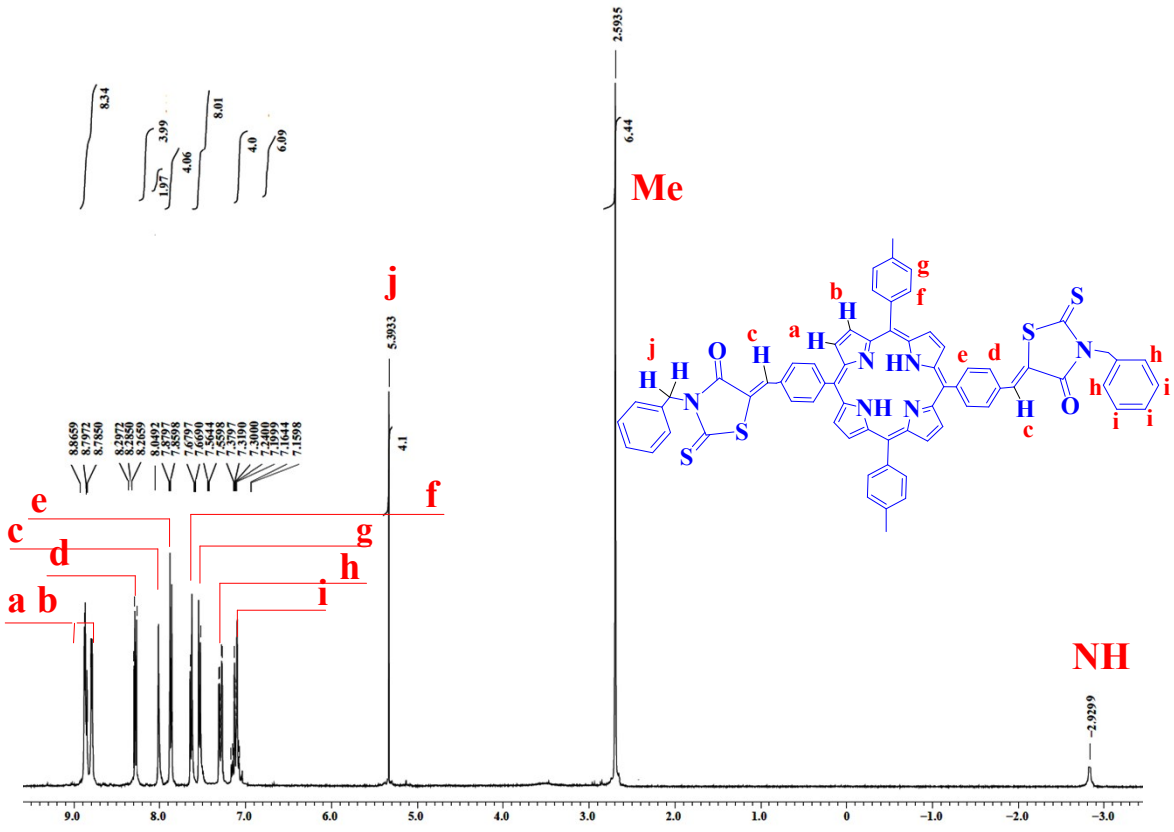


Figure S9: ^{1}H NMR spectrum of **4a** in $CDCl_3$.

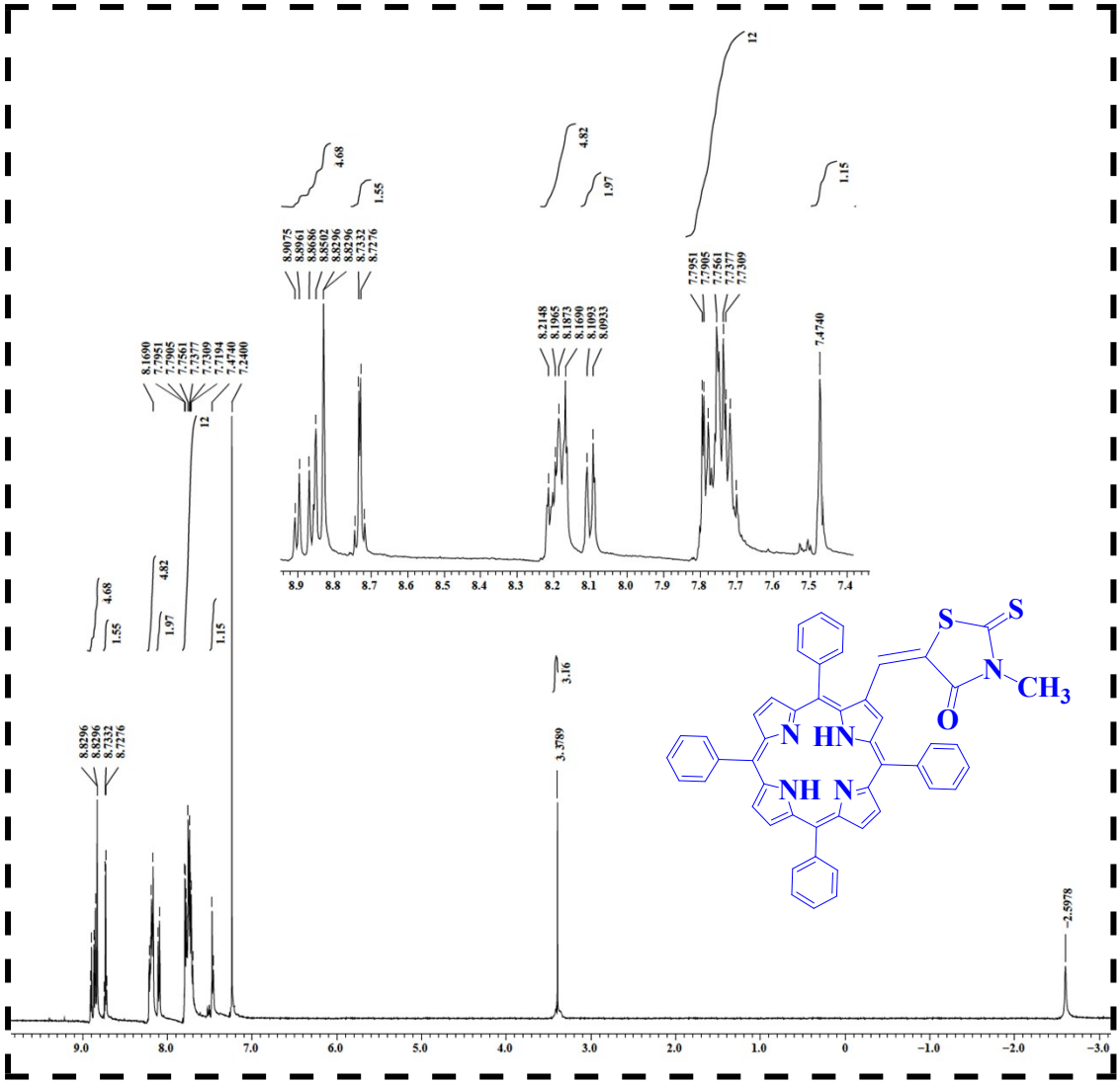


Figure S10: ^{1}H NMR spectrum of **6c** in $CDCl_3$.

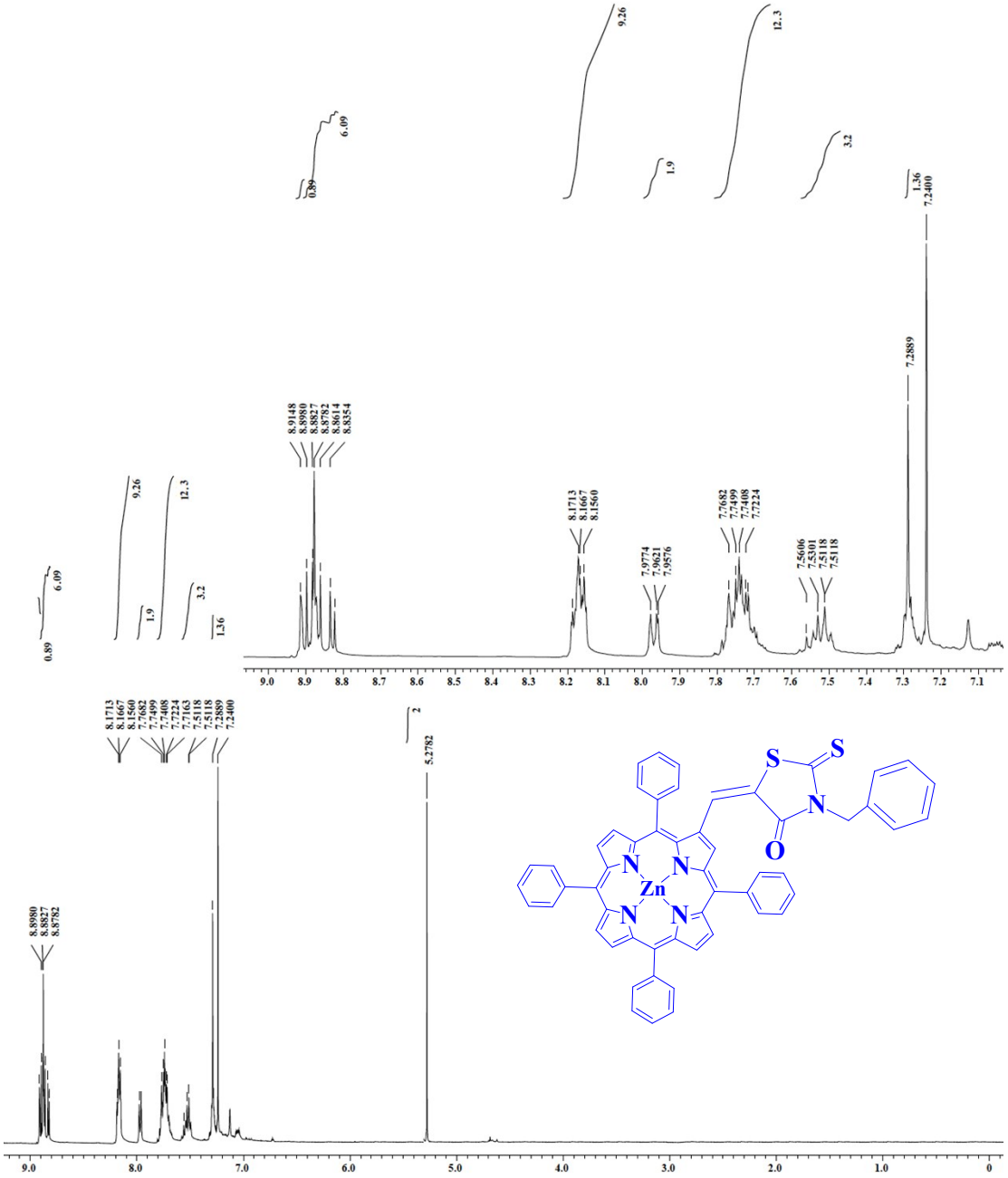


Figure S11: ^{1}H NMR spectrum of **6a** in $CDCl_3$.

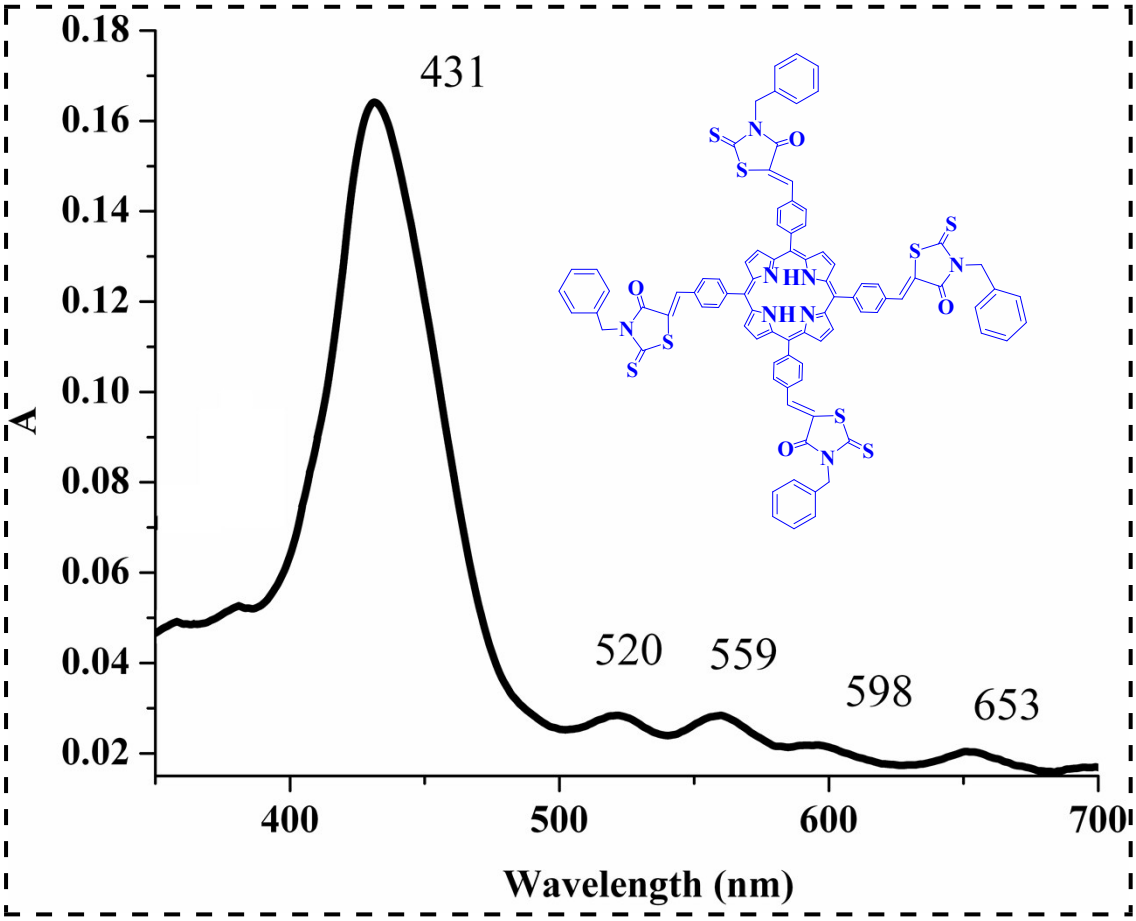


Figure S12: UV-Visible absorption spectra of **3a** in chloroform.

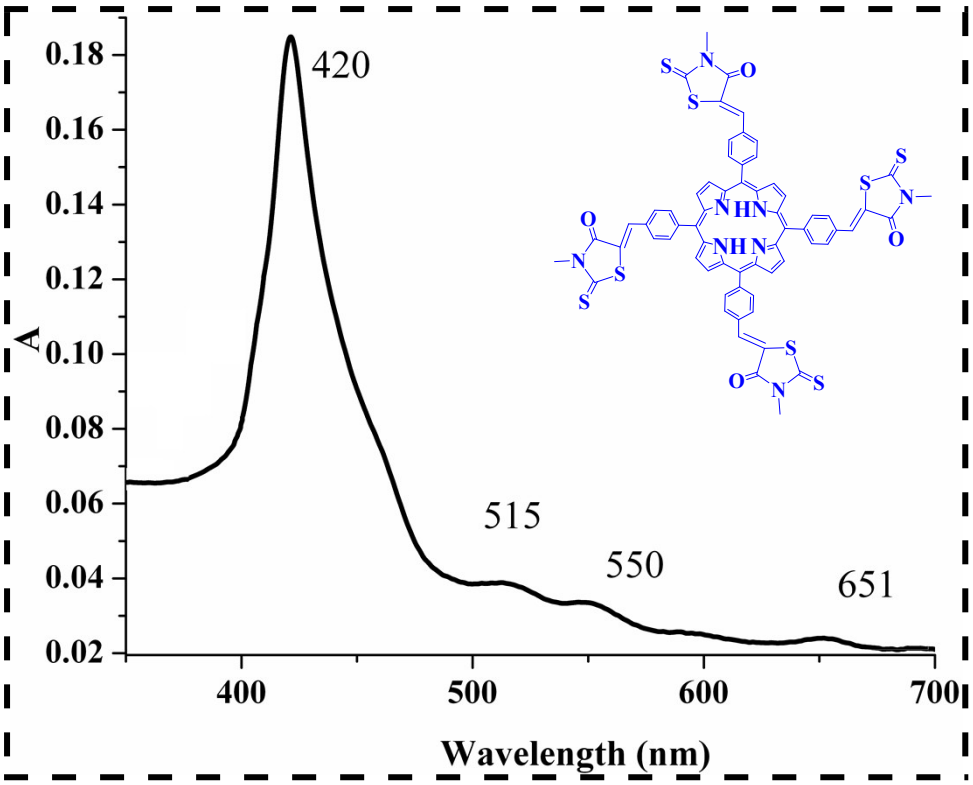


Figure S13: UV-Visible absorption spectra of **3c** in chloroform.

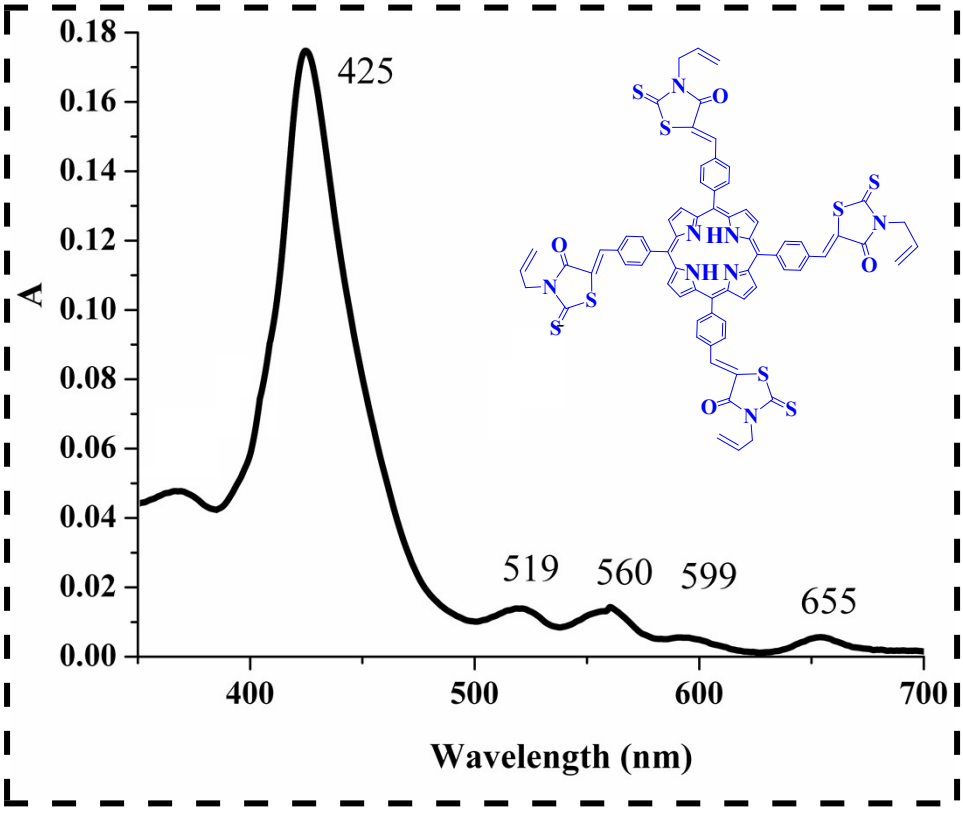


Figure S14: UV-Visible absorption spectra of **3b** in chloroform.

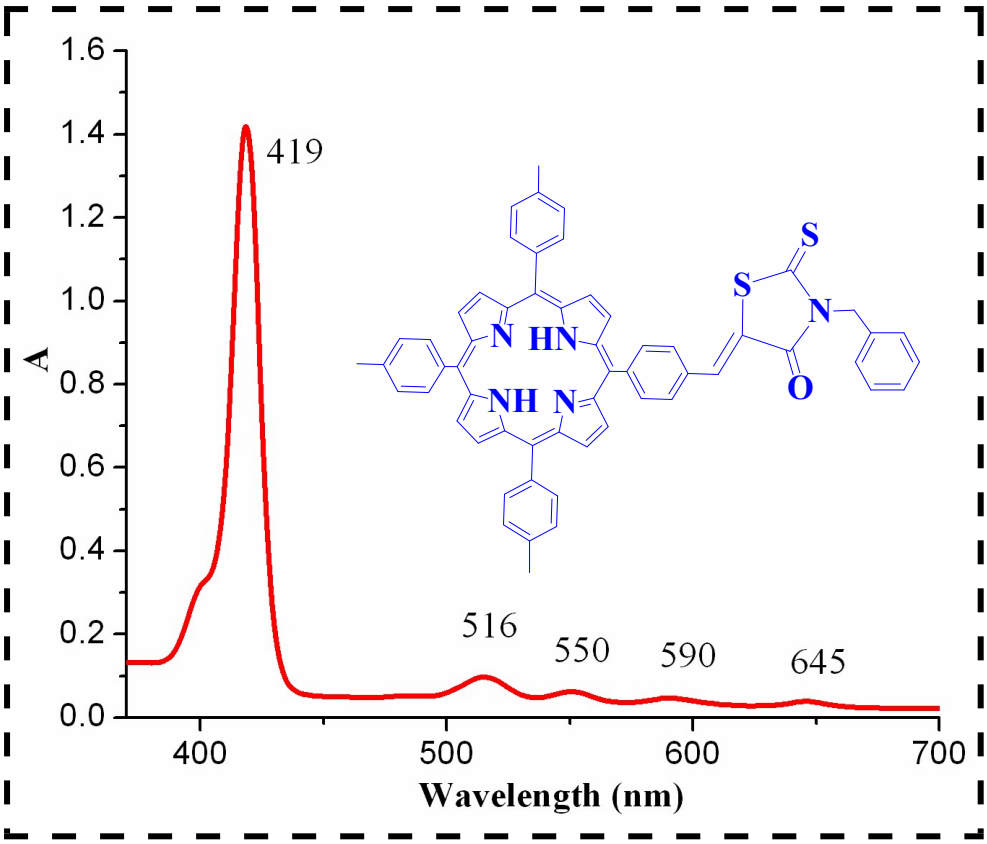


Figure S15: UV-Visible absorption spectra of **5a** in chloroform.

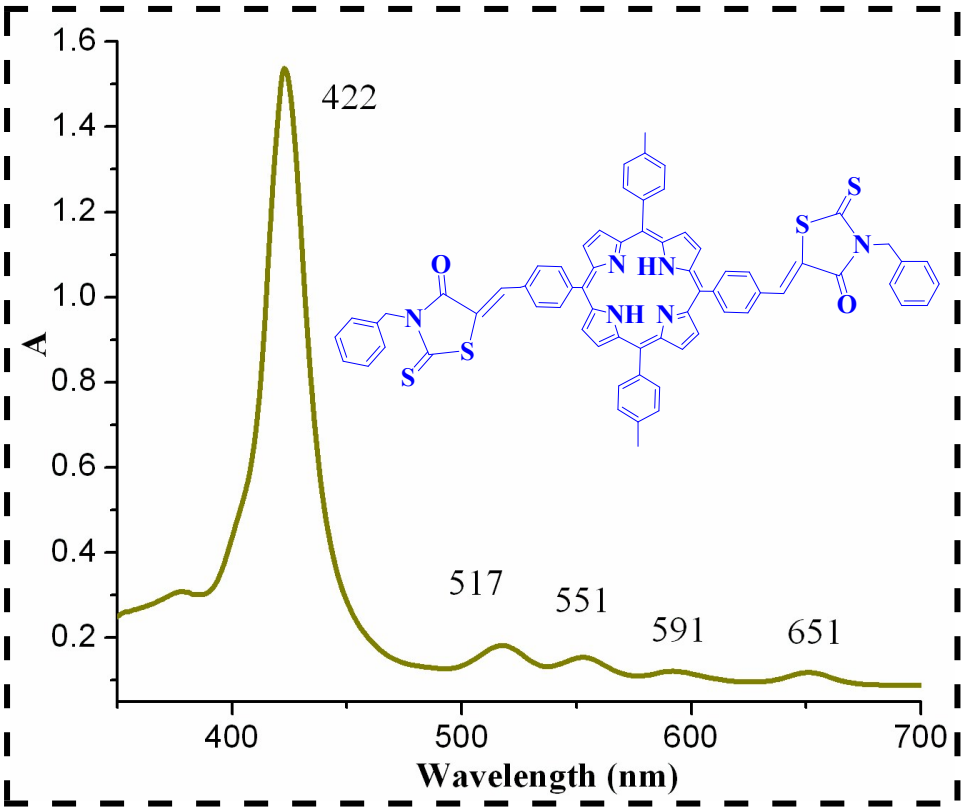


Figure S16: UV-Visible absorption spectra of **4a** in chloroform.

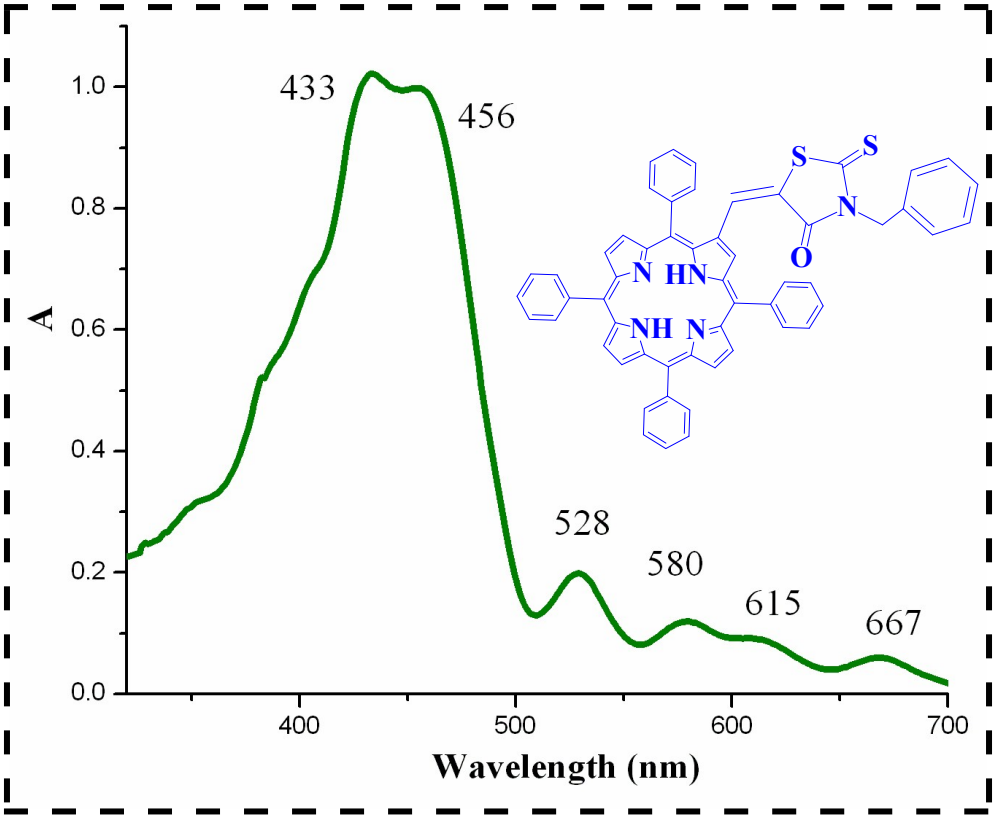


Figure S17: UV-Visible absorption spectra of **6a** in chloroform.

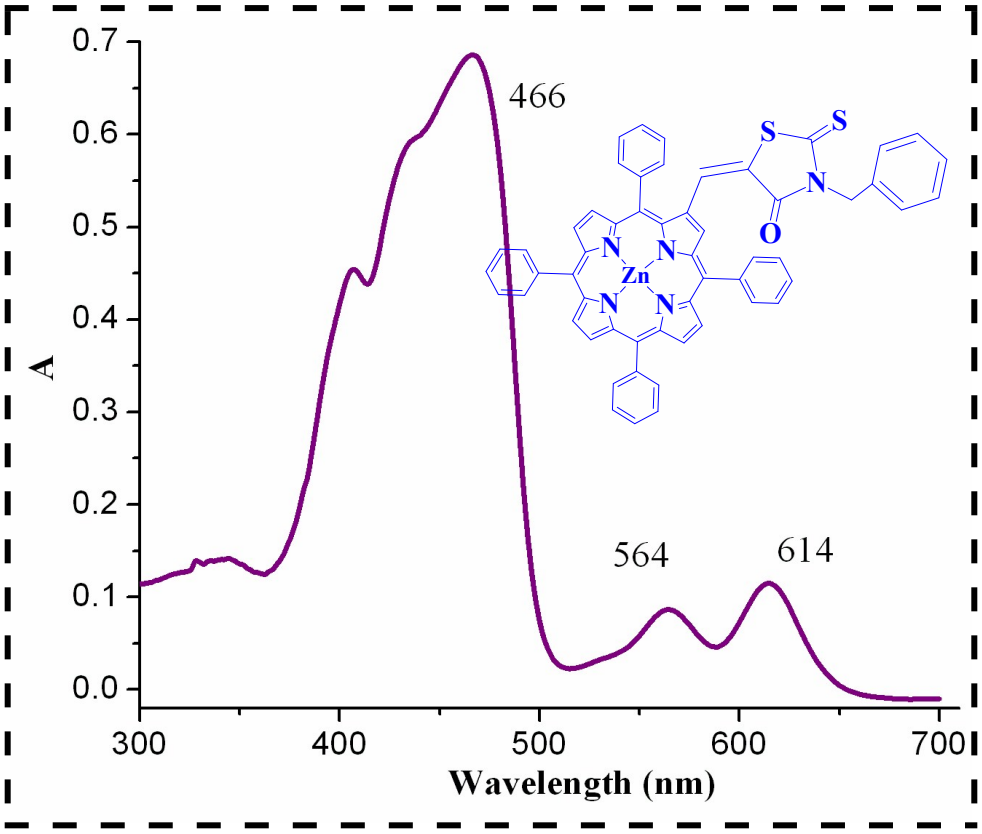


Figure S18: UV-Visible absorption spectra of **Zn6a** in chloroform.

Fluorescence

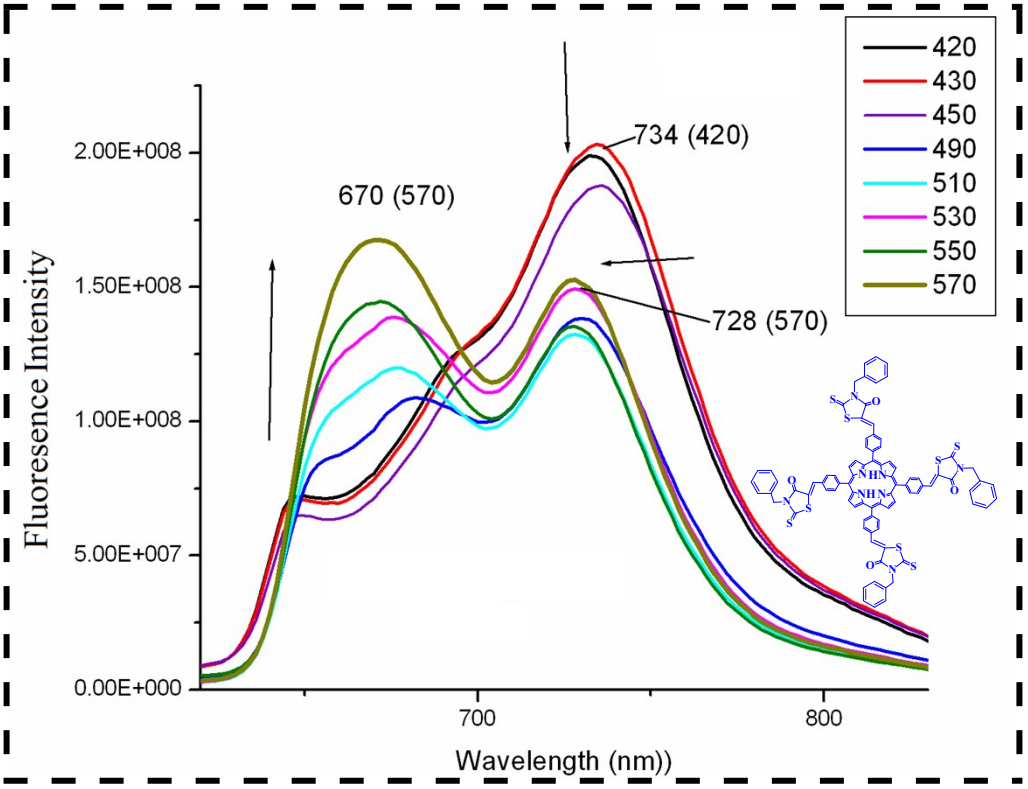


Figure S19: fluorescence emission spectra of **3a** in chloroform at different $\lambda_{excitation}$.

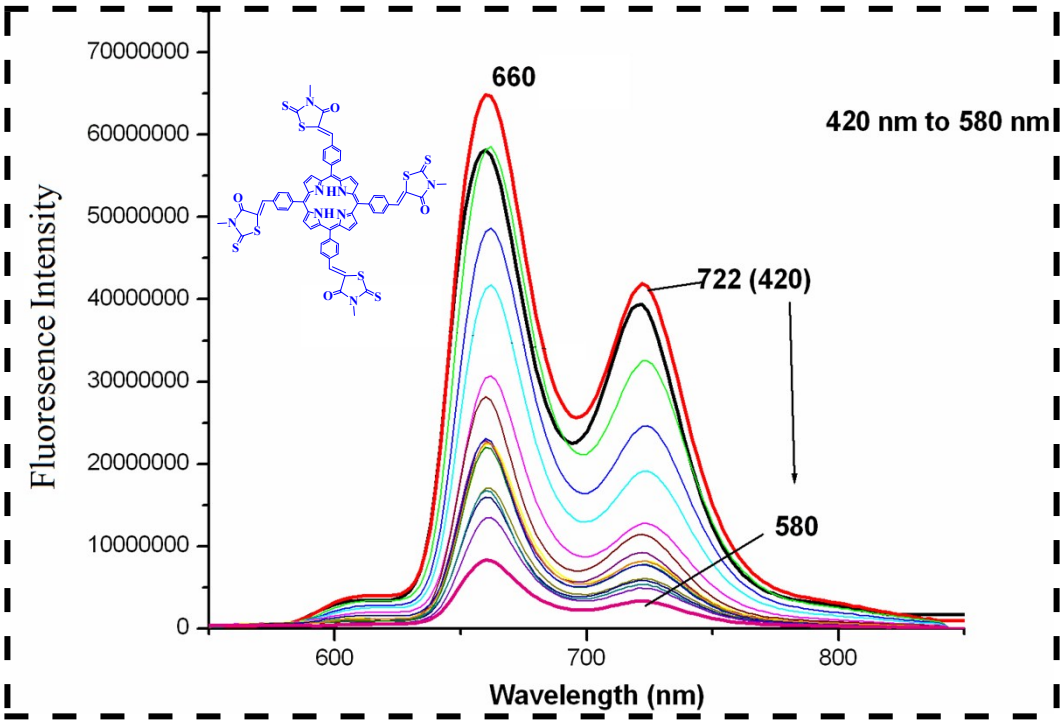


Figure S20: fluorescence emission spectra of **3c** in chloroform at different $\lambda_{excitation}$.

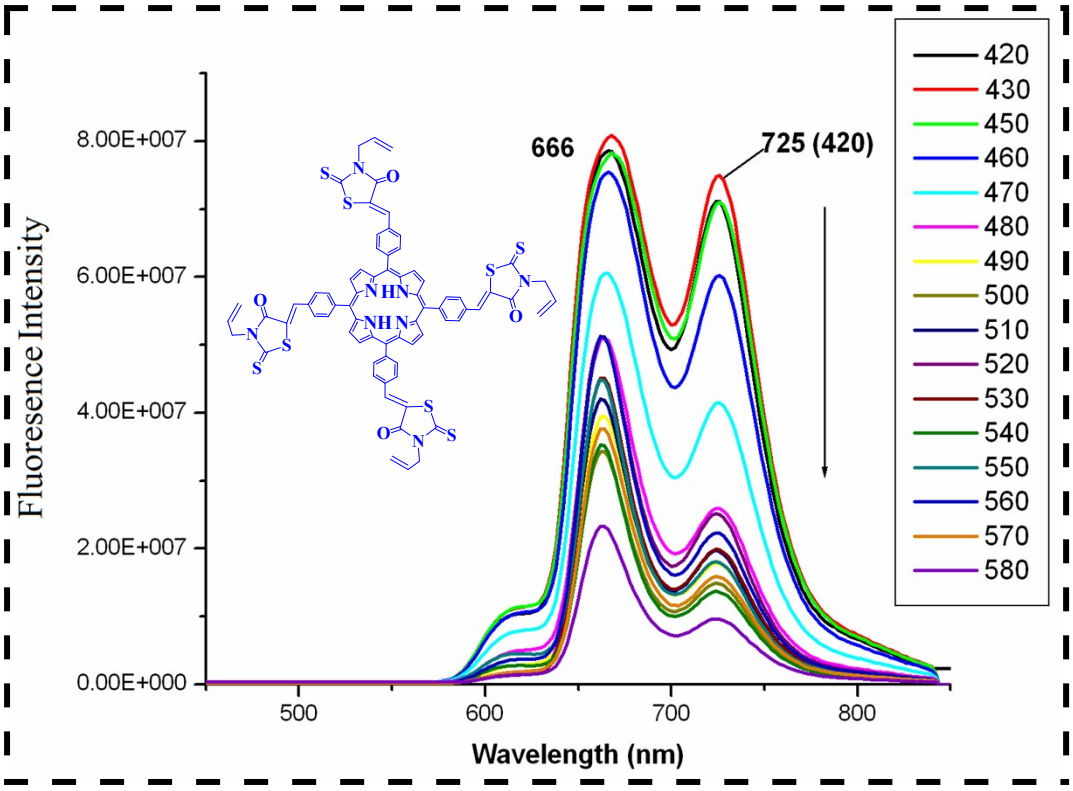


Figure S21: fluorescence emission spectra of **3b** in chloroform at different $\lambda_{excitation}$.

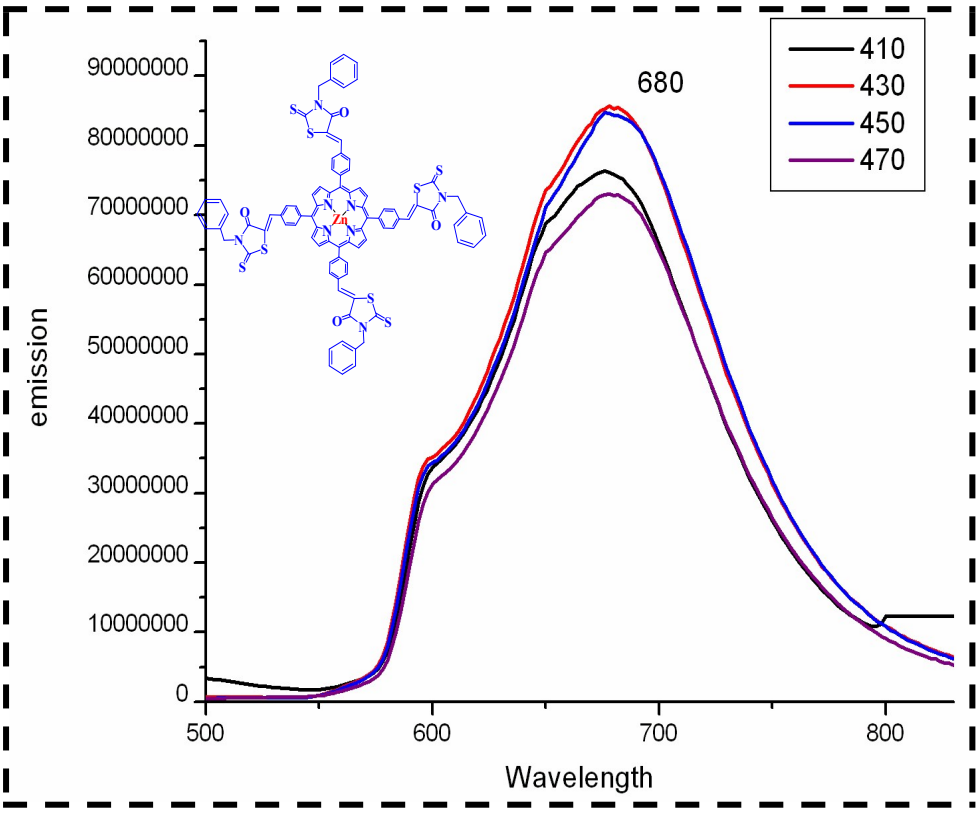


Figure S22: fluorescence emission spectra of **Zn3a** in chloroform at different $\lambda_{excitation}$.

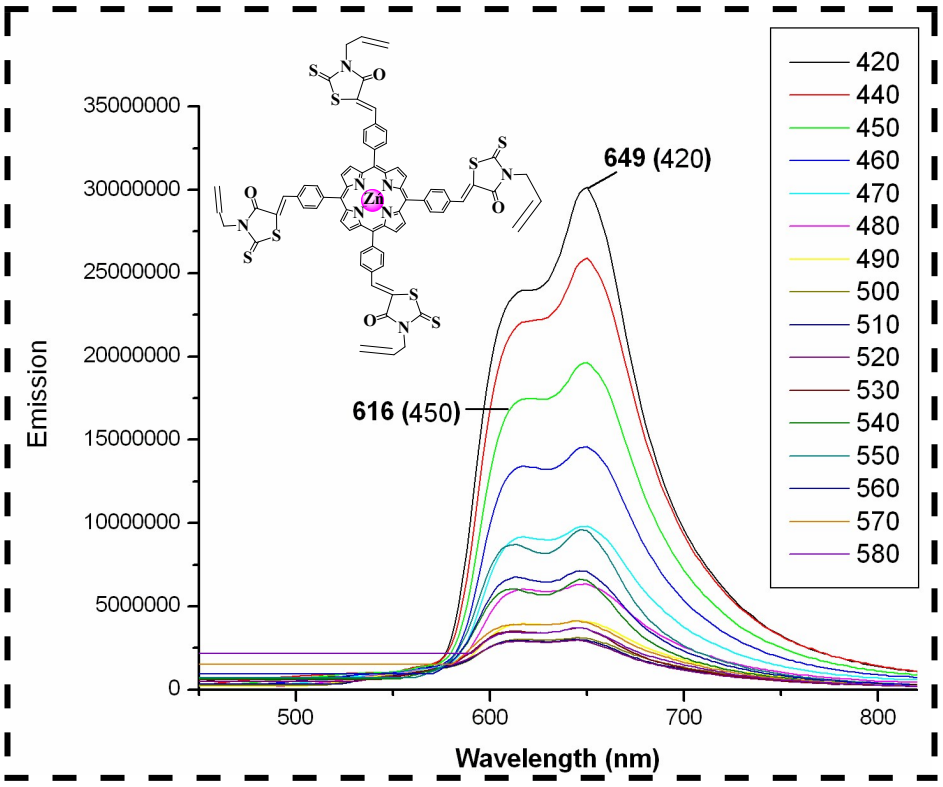


Figure S23: fluorescence emission spectra of **Zn3b** in chloroform at different $\lambda_{excitation}$.

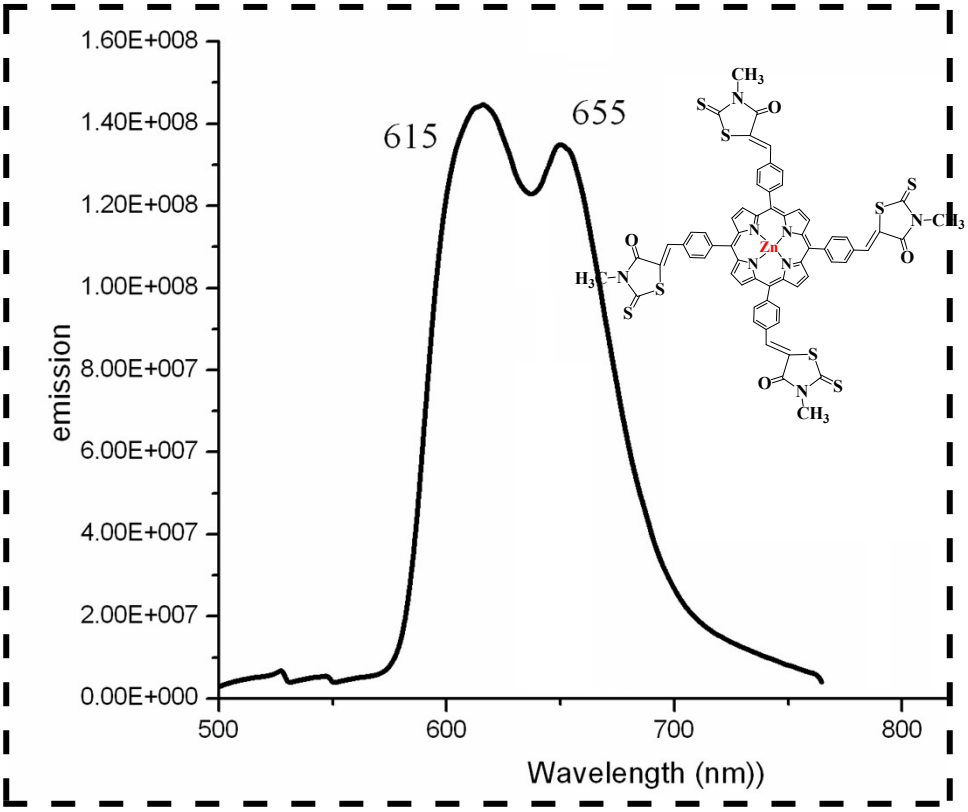


Figure S24: fluorescence emission spectra of **Zn3c** in chloroform at 420 nm $\lambda_{excitation}$.

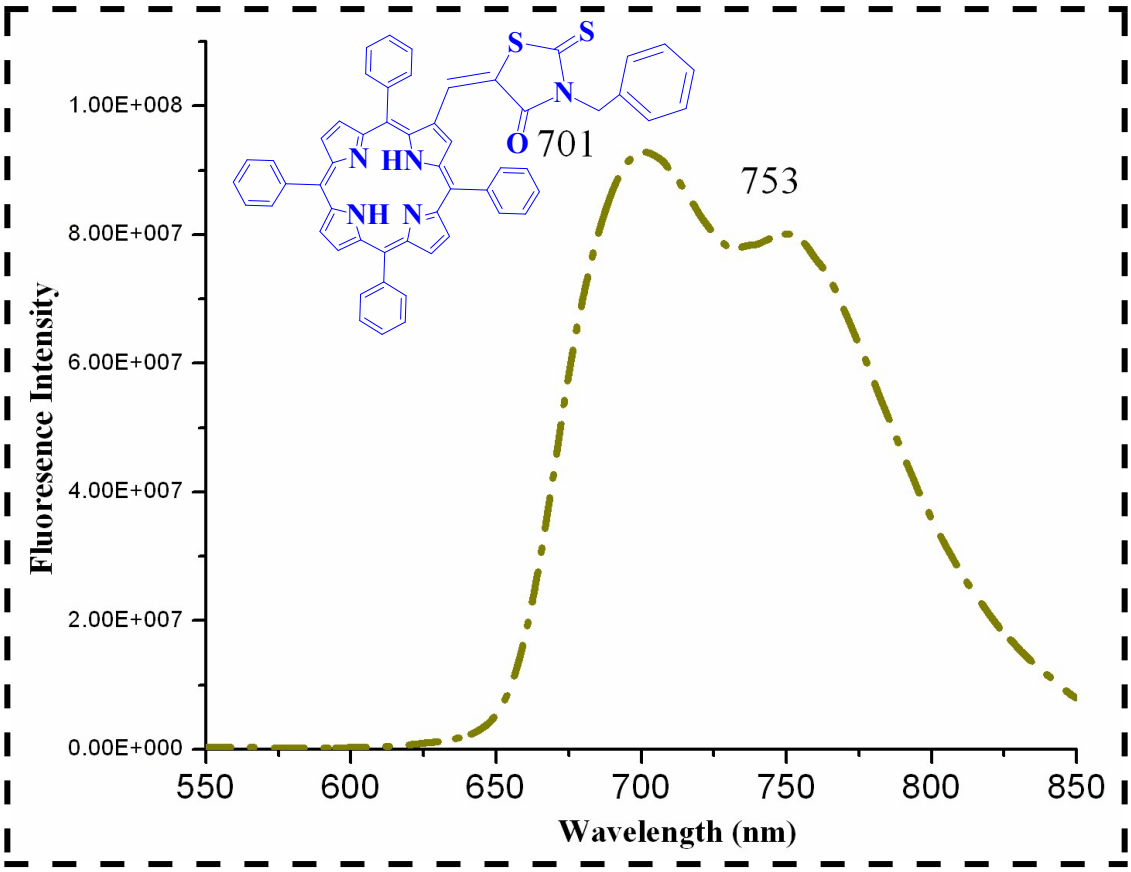


Figure S25: fluorescence emission spectra of **6a** in chloroform at 440 nm $\lambda_{excitation}$.

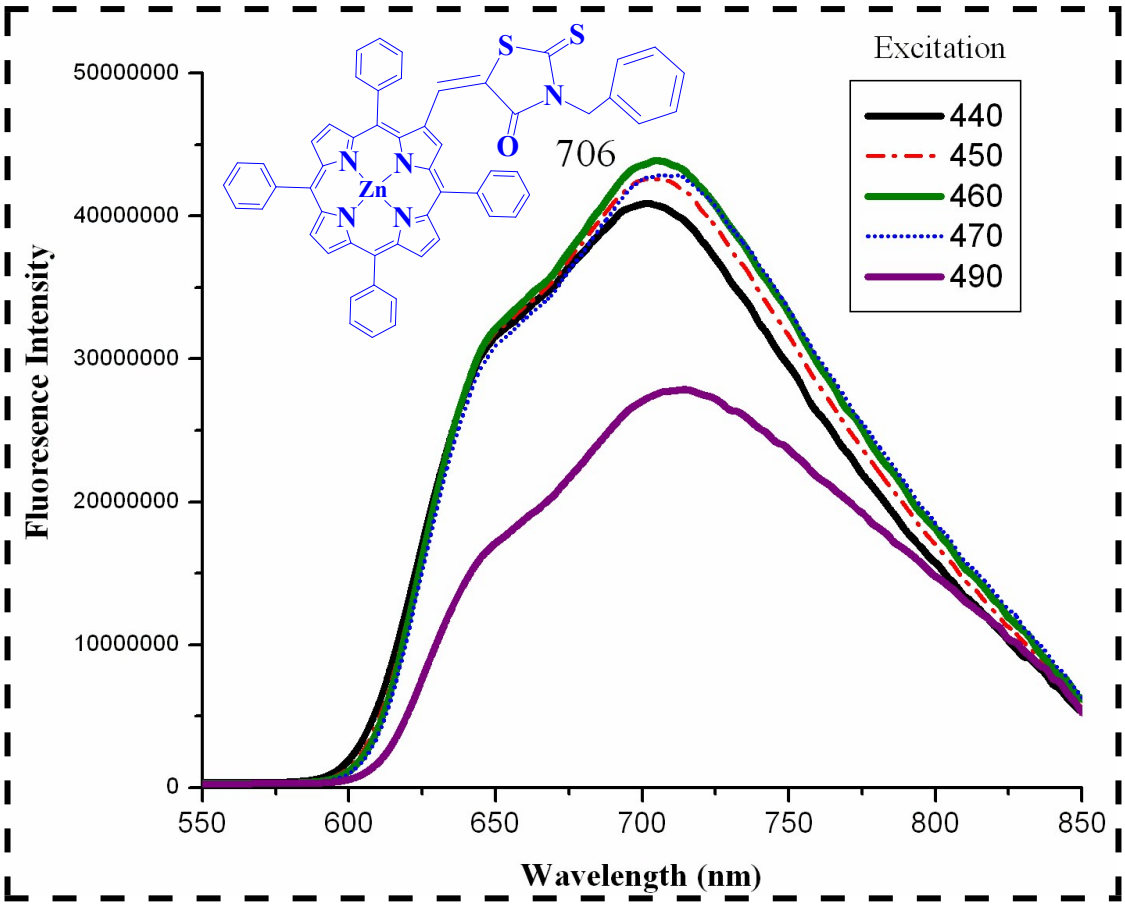


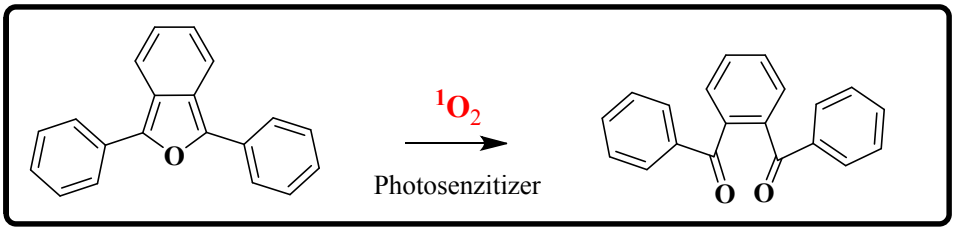
Figure S26: fluorescence emission spectra of **Zn6a** in chloroform at different $\lambda_{excitation}$.

Fluorescence quantum yields (ϕ_f)

The fluorescence quantum yields (ϕ_f) of porphyrin– thiazolidinone conjugates were estimated from the emission and absorption spectra by a comparative method[1,2] using the below equation, where [*F*(sample)] and [*F*(standard)] are the integrated fluorescence intensities of the porphyrin– thiazolidinone and the standard, [*A*(sample)] and [*A*(standard)] the absorbance of porphyrin– thiazolidinone and the standard at the excitation wavelength and ϕ_f (standard) is the quantum yield of the standard sample. Free-base tetraphenylporphyrin (TPP, $\phi_f = 0.11$)[2] was used as the standard for free-base porphyrins, and zinc(II) tetraphenylporphyrin (ZnTPP) was used as the standard ($\phi_f = 0.033$)[2] for the Zn^{2+} derivative of porphyrin– thiazolidinone.

$$\phi_f = \frac{[F(\text{sample})]}{[F(\text{standard})]} \frac{[A(\text{standard})]}{[A(\text{sample})]} \times \phi_f\,(\text{standard})$$

Singlet Oxygen Generation and singlet oxygen quantum yields ΦΔ



Singlet oxygen efficiency of the porphyrin conjugates quantify by using indirect method. In the case of the indirect method used 1,3-diphenylisobenzofuran (DPBF), singlet oxygen scavenger, was qualitatively evaluated by monitoring the photodecomposition of 1,3-diphenylisobenzofuran (DPiBF). To carry out experiments, irradiated methanolic solution of the porphyrin and DPiBF using a 200 W mercury lamp .The decrease in absorbance corresponding to DPiBF in the presence of porphyrin conjugates was monitored **Figure S27-S29**.

The results, summarized in **Figure S30**, show that the DPiBF photodegradation was highly enhanced in the presence of any photosensitizer. This means that all porphyrin derivatives are

able to produce singlet oxygen. The relationship between % decay absorbance of DPiBF and illumination time indirectly reflected $^1O_2$ yield of those porphyrins compared with H_2TPP/ZnTPP.[3]

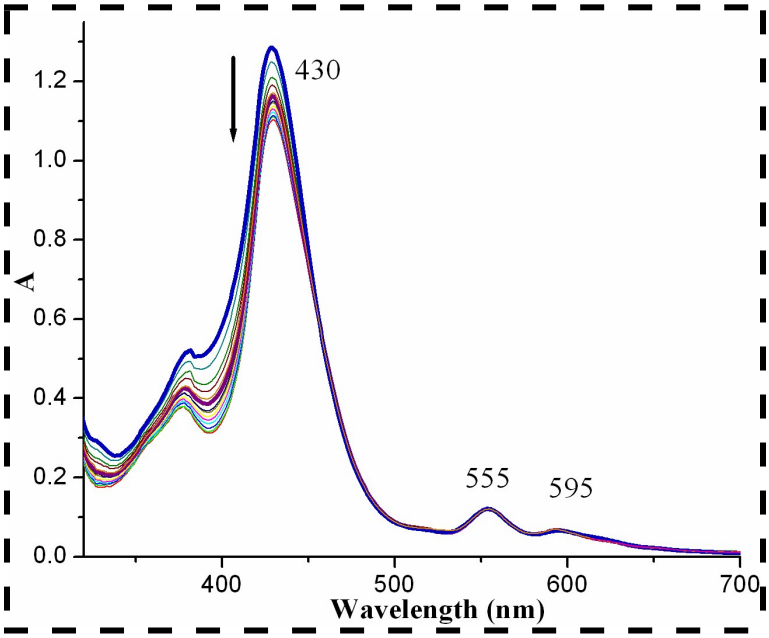


Figure S27: Changes in absorption spectra of DPiBF upon irradiation in the presence of **Zn3a** (3 μM) for 0−60 mins (recorded at 10 min intervals) in methanol.

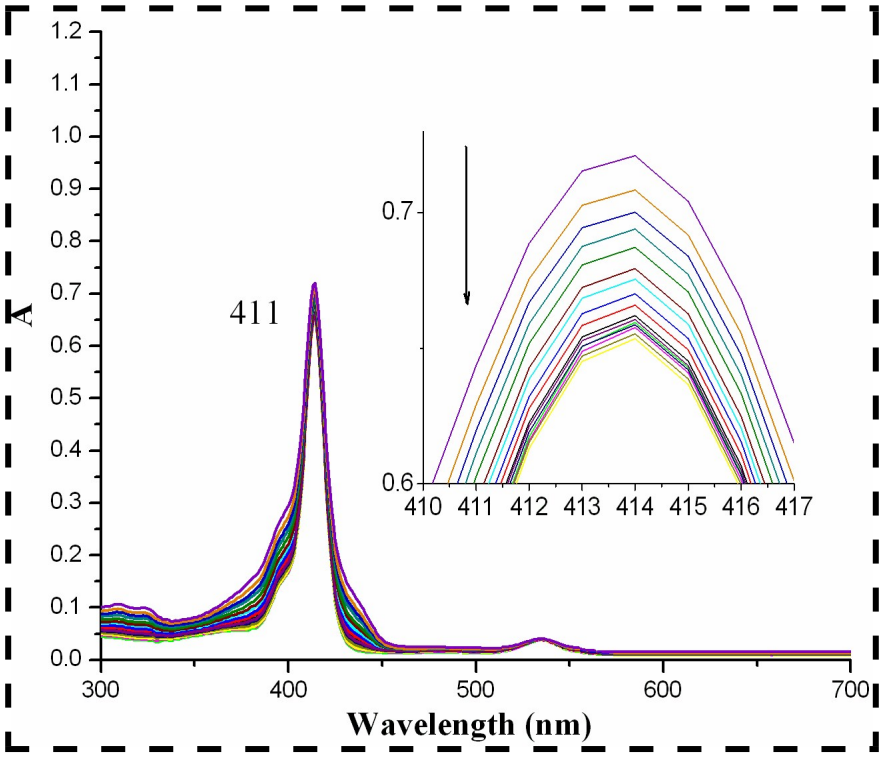


Figure S28: Changes in absorption spectra of DPiBF upon irradiation in the presence of **Zn5a** (2.2 μM) for 0−60 mins (recorded at 10 min intervals) in methanol.

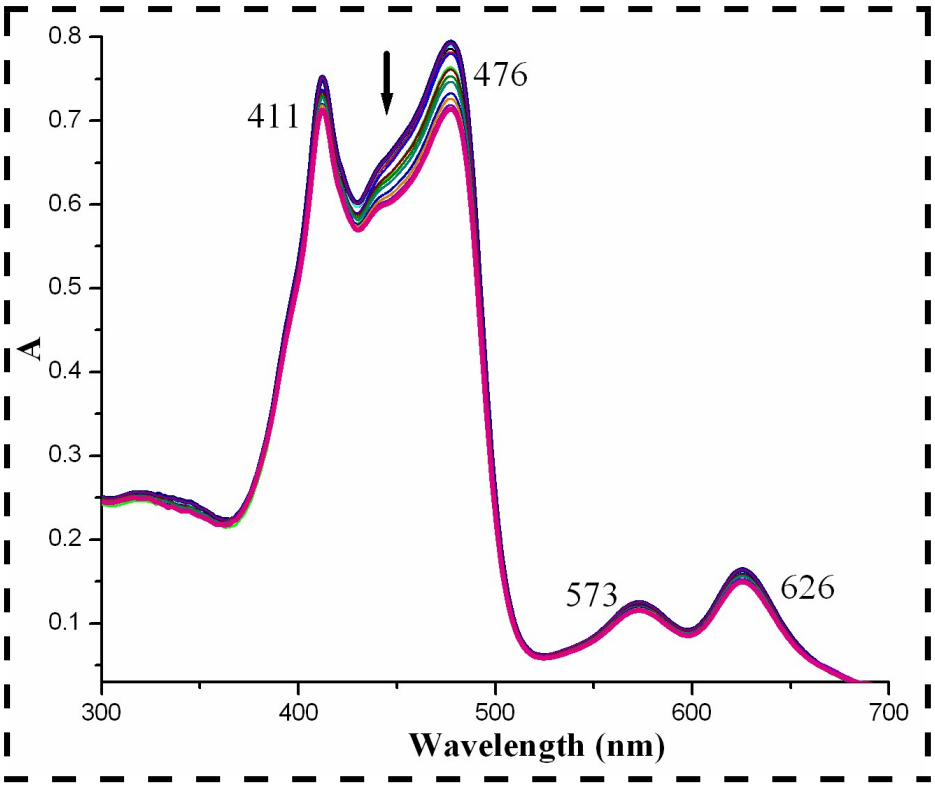


Figure S29: Changes in absorption spectra of DPiBF upon irradiation in the presence of **Zn6a** (2.6 μM) for 0−60 mins (recorded at 10 min intervals) in methanol.

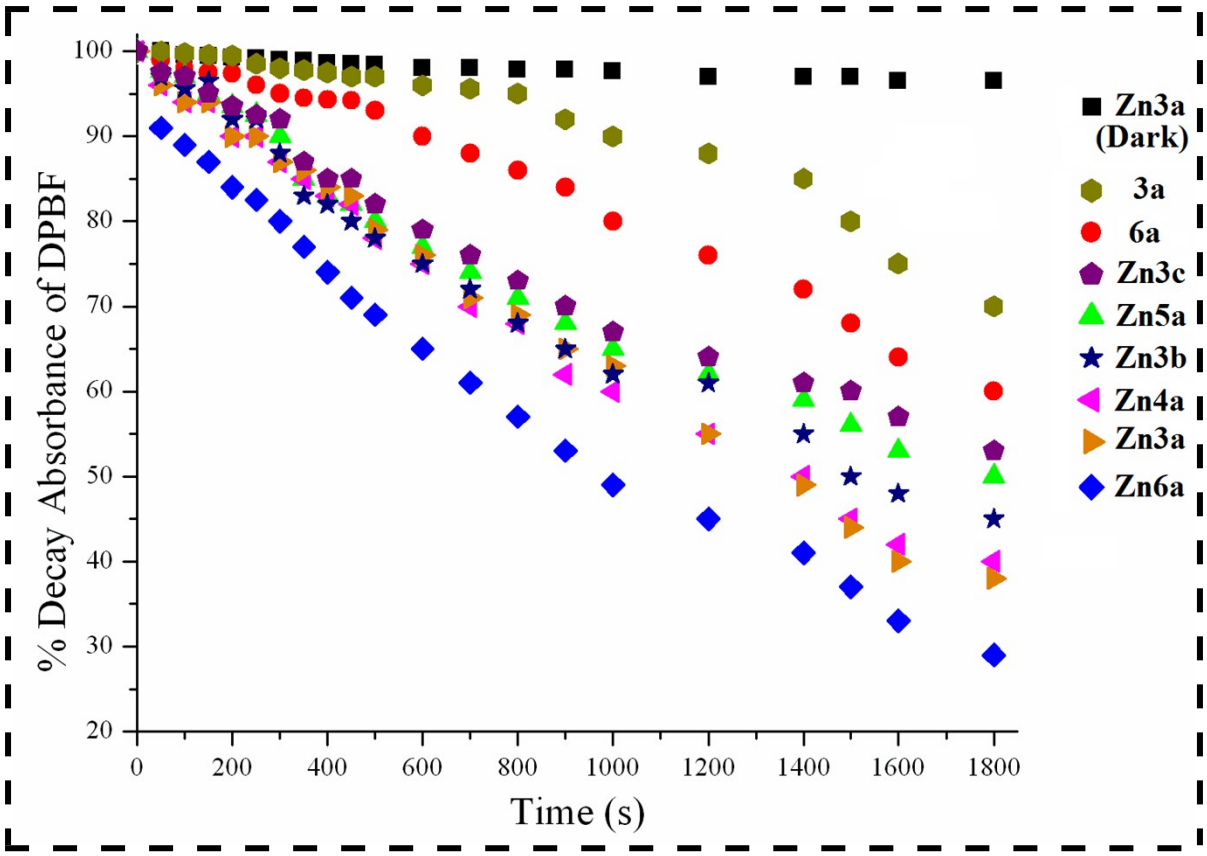


Figure S30: Photodecomposition of 1,3-diphenylisobenzofuran (DPiBF) by singlet oxygen generated by porphyrin-rhodanine derivatives after irradiation.

Singlet Oxygen quantum yields ΦΔ

Methanolic solution of zinc porphyrins and DPiBF irradiated using a 200 W mercury lamp over a time period of 0−60 min. The decrease in absorbance corresponding to DPiBF in the presence of zinc porphyrins was monitored. The singlet oxygen quantum yields were estimated by plotting the depletion in absorbance of DPiBF against the irradiation time. This plot followed linearity, as shown in **Figure S31**, and the experiment was done using optically matching solutions of the compound as well as the reference. The singlet oxygen quantum yields were calculated by a relative method by comparing the photooxidation of DPiBF sensitized by the zinc porphyrins conjugates to that of the reference, zinc porphyrin (ΦΔ = 0.7), using equation below,[4,5] wherein the superscripts "sample" and "ref" represent for the porphyrin derivatives and reference, respectively.

Equation $$\mathbf{\Phi\Delta} = \Phi(^1O_2)^{ref} \times [(m^{sample} \times F^{ref}) / (m^{ref} \times F^{sample})]$$

The term "*m*" is the slope of a plot of difference in change in absorbance of DPiBF with the irradiation time, and F is the absorption correction factor, $F = 1 - 10^{-OD}$, where OD is the optical density at the irradiation wavelength.

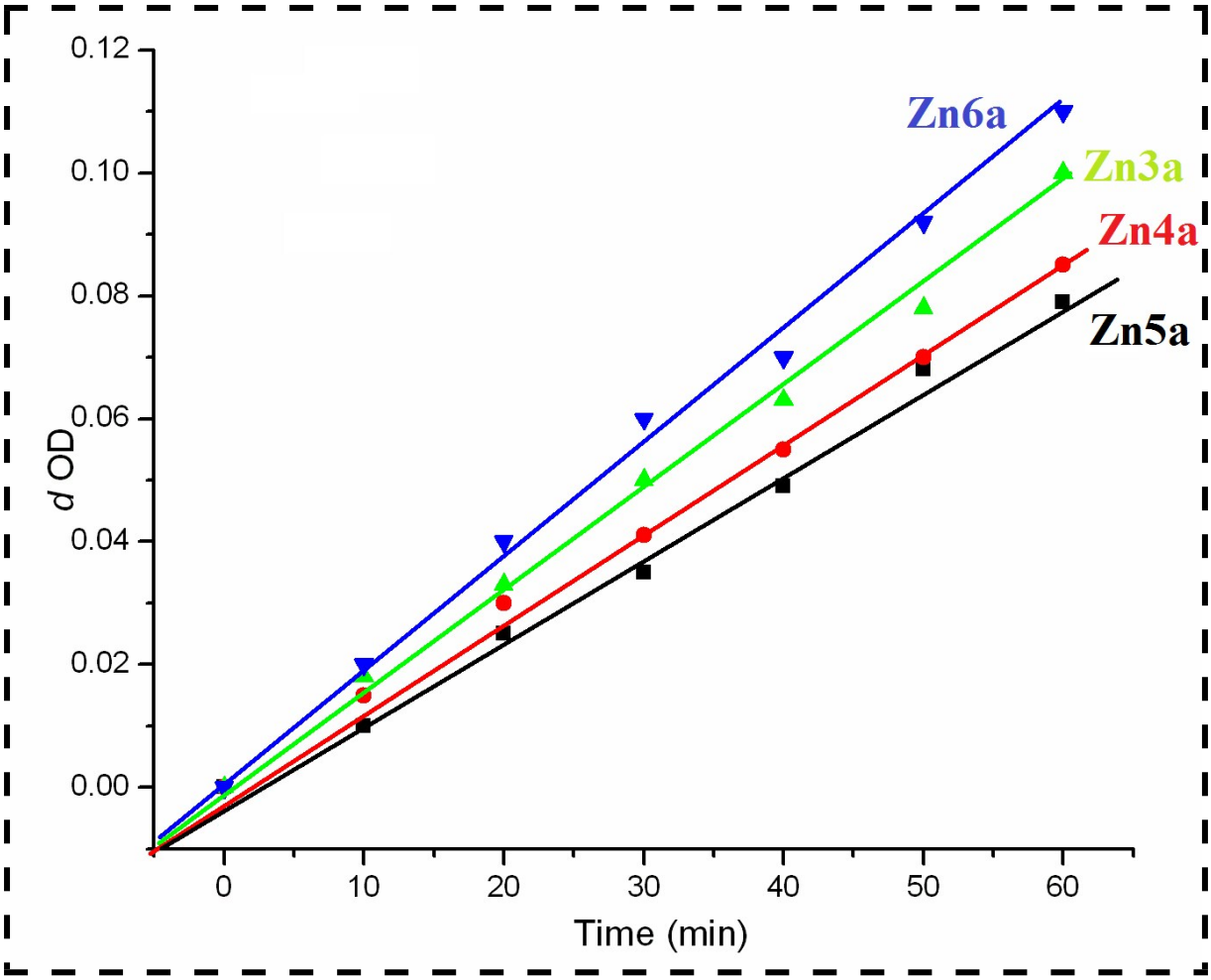


Figure S31: Relative plot of the singlet oxygen generation efficacy of the porphyrin conjugates **Zn6a, Zn3a, Zn4a** and **Zn5a**.

Reference

1) A. Lembo, P. Tagliatesta and M. D. Guldi, *J. Phys. Chem. A*, 2006, 110, 11424–11434

2) I. Gupta and M. Ravikanth, *J. Chem. Sci.* 2005, 117, 161–166.

3) Y. Zheng, K. Wang, T. Li, X. L. Zhang and Z. Y. Li, *Molecules* **2011**, 16, 3488-3498

4) W. Spiller, H. Kliesch, D. W. Hrle, S. Hackbarth, B. Der And G. Schnurpfeil, *Journal of Porphyrins and Phthalocyanines*, 1998, 2, 145–158.

5) B. Marydasan, A. K. Nair, and D. Ramaiah, *J. Phys. Chem. B* 2013, 117, 13515−13522.

Qualitative Analysis Report

Data Filename	C.d	**Sample Name**	C
Sample Type	Sample	**Position**	P1-F3
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Acq Method	DAILY MS.m	**Acquired Time**	15-04-2015 11:57:12
IRM Calibration Status	Success	**DA Method**	default.m
Comment			

Sample Group	**Info.**
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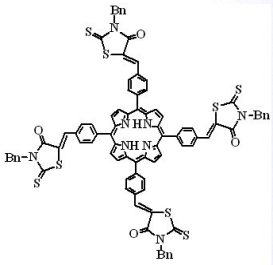

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User Spectra

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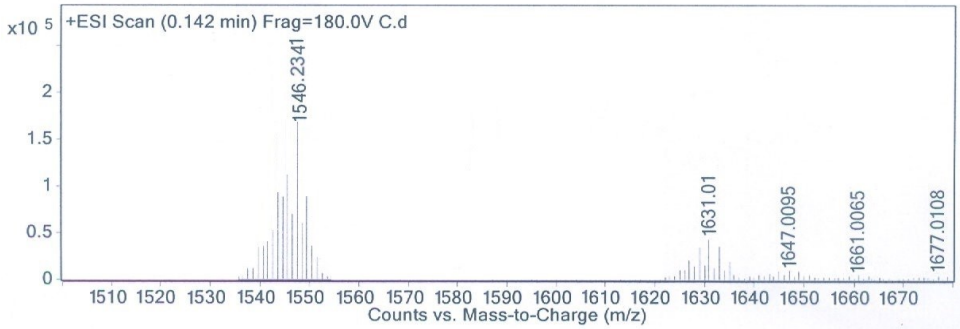

Peak List

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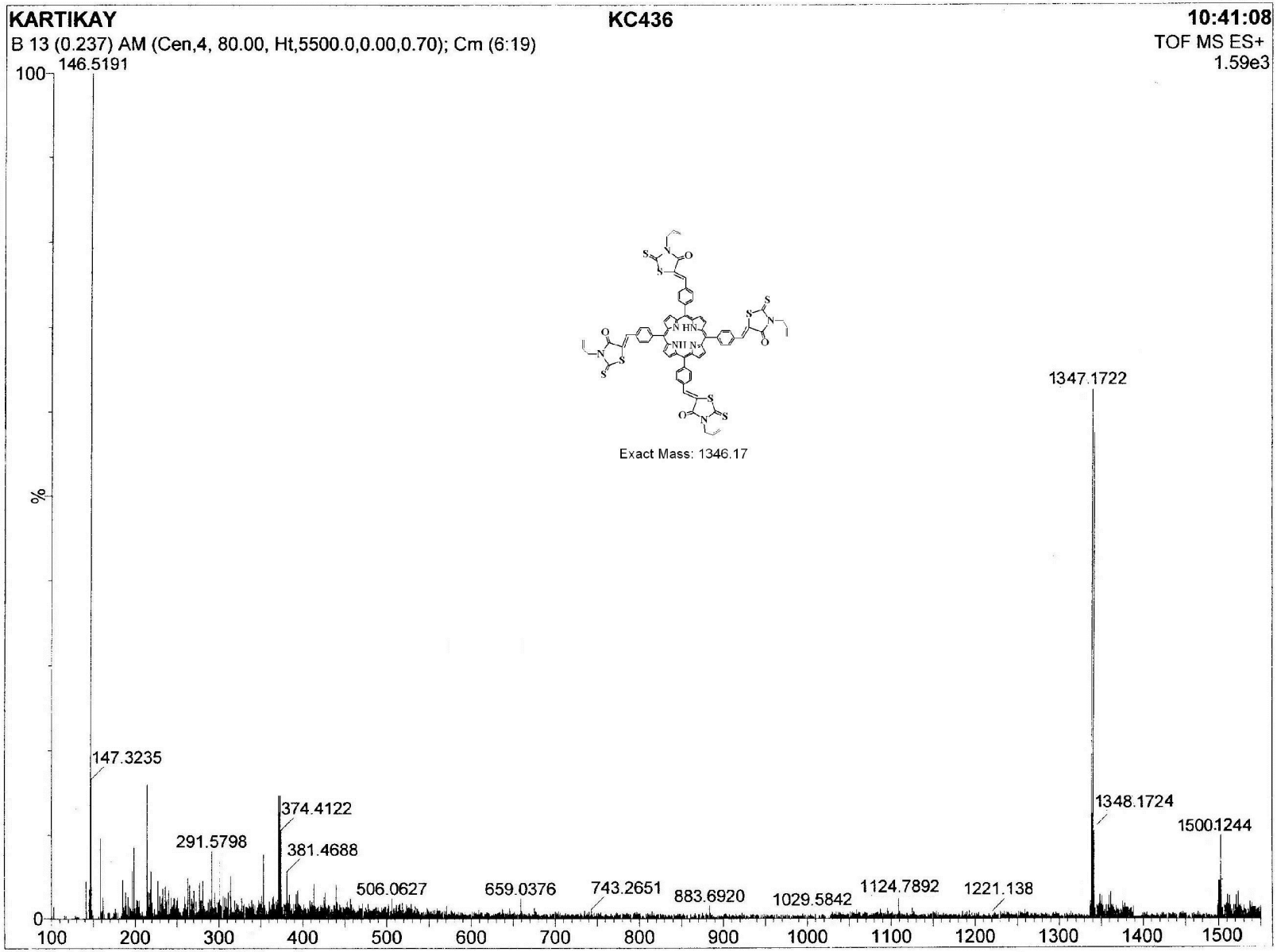
1546.2341	1	233012.94
1547.2348		35354.34
1550.0088		79388.07
1631.0100		67978.62
1647.0095	1	79318.33
1661.0065	1	87996.23
1677.0108	1	19989.58


KARTIKAY
KC436
10:41:08
B 13 (0.237) AM (Cen,4, 80.00, Ht,5500.0,0.00,0.70); Cm (6:19)
TOF MS ES+
1.59e3
100
%
0
146.5191
147.3235
291.5798
374.4122
381.4688
506.0627
659.0376
743.2651
883.6920
1029.5842
1124.7892
1221.138
1347.1722
1348.1724
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600
700
800
900
1000
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1500
Exact Mass: 1346.17

Qualitative Analysis Report

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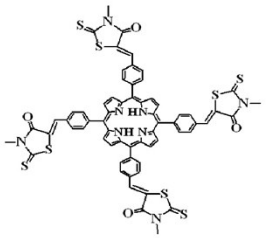
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	
Acq Method	DAILY MS.m	**Acquired Time**	
IRM Calibration Status	[redacted]	**DA Method**	
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)



Exact Mass: 1242.11

User Spectra

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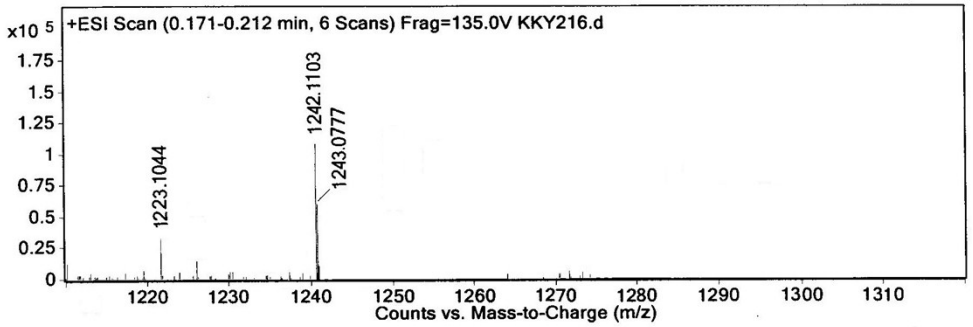

Peak List

m/z	z	Abund
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1242.1103	1	71547.54
1243.0777	1	32266.27

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Qualitative Analysis Report

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Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	
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IRM Calibration Status	[redacted]	**DA Method**	default.m
Comment			
Sample Group		**Info.**	
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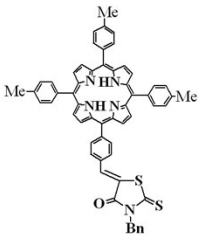

Exact Mass: 889.29

User Spectra

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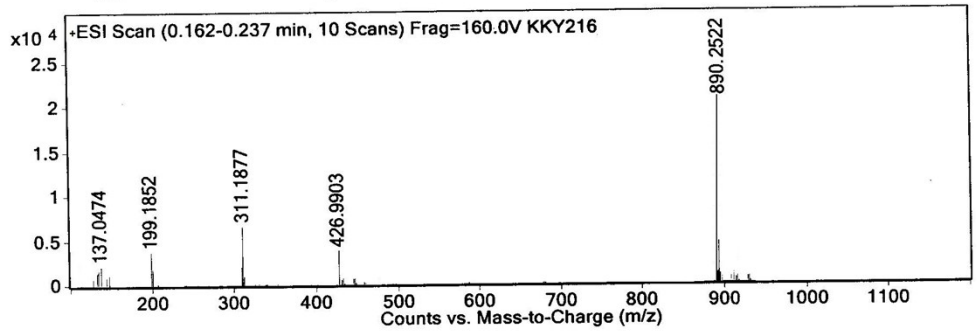

Peak List

m/z	z	Abund
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311.1877		6629.14
426.9903		3790.01
890.2522		24276.24

--- End Of Report ---

Qualitative Analysis Report

Data Filename	KKY213.d	**Sample Name**	KKY
Sample Type	Sample	**Position**	P1-E6
Instrument Name	Instrument 1	**User Name**	
Acq Method	DAILY MS.m	**Acquired Time**	
IRM Calibration Status	[redacted]	**DA Method**	
Comment			
Sample Group		**Info.**	
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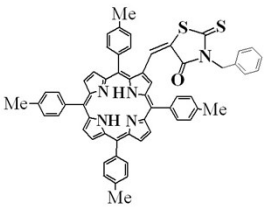

Exact Mass: 903.31

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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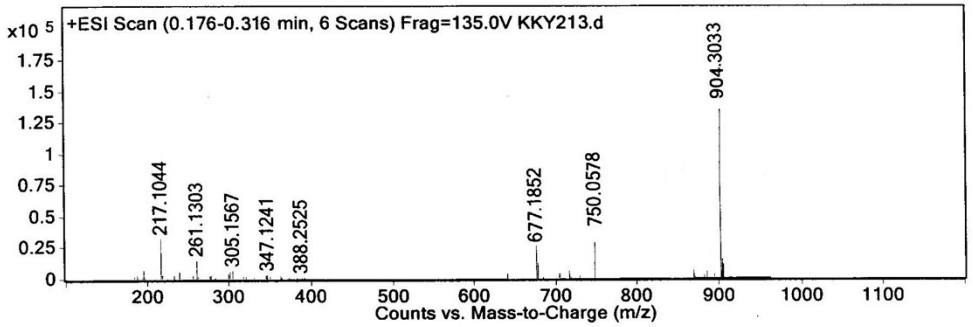

Peak List

m/z	z	Abund
217.1044		32266.27
261.1303		14948.37
305.1567		6463.43
347.1241	1	3148.3
388.2525	1	1005.6
677.3615		21187.3
750.0578	1	2937.71
904.3033	1	113114.55
905.3523		5497.98

--- End Of Report ---

Qualitative Analysis Report

Data Filename	D.d	**Sample Name**	D
Sample Type	Sample	**Position**	P1-F4
Instrument Name	Instrument 1	**User Name**	SANJAY PANDEY
Acq Method	DAILY MS.m	**Acquired Time**	
IRM Calibration Status	Success	**DA Method**	
Comment			
Sample Group		**Info.**	
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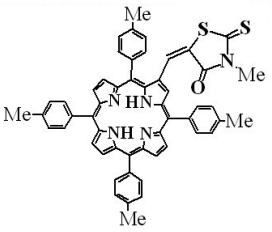

Exact Mass: 827.28

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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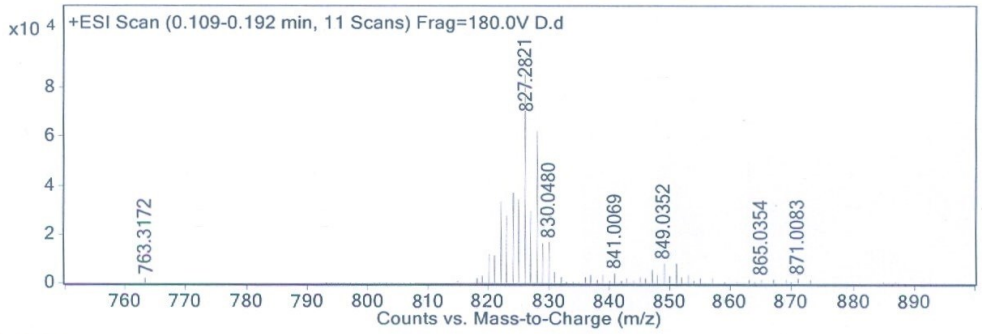

Peak List

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827.2821	1	90280.62
829.0403	1	68723.09
830.0480		24187.69
832.0406		33875.86
841.0069	1	9051.95
849.0352	1	9131.24
871.0083	1	8151.2