Supporting Information

A conjugated 2D covalent organic framework as a drug delivery vehicle towards triple negative breast cancer malignancy

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Section S1. Calculation of Cisplatin content in Drug loaded TRIPTA COF

Gravimetric analysis method:

Equation.

$$\textbf{\textit{LoadingParcentage}}\ \textbf{(\%)} = \frac{Mfinal - Minitial}{Mfinal} \times 100\%$$

Where M_{final}= 17.501 mg and $M_{initial}$= 12.042 mg denote the mass of material after and before cisplatin loading.

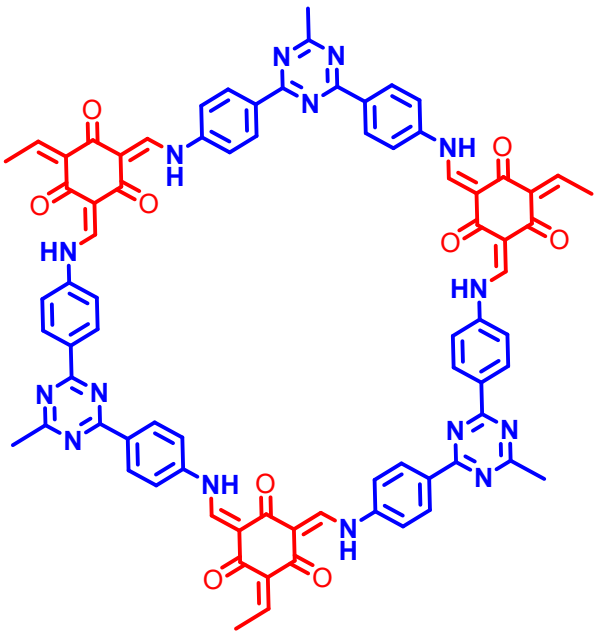
$$\text{Loading percentage} = \frac{17.501 - 12.042}{17.501} \times 100\%$$

$$= 31.19\%$$

Method using ICP-OES:

Number of cisplatin molecules per unit were done by analyzing the Pt content with the help of ICP-OES. For the measurement, in a typical experiment 5, 10, 15 mg of cisplatin loaded TRIPTA COF is dissolved in 10 ml of aqua regia, and the solutions were then subjected to ICP-OES analysis for measuring the platinum content in terms of ppm (mg/L).

Finally, from the platinum content and formula weight of the repeating unit, number of cisplatin moieties per repeating unit can be predicted approximately.



Repeating hexagonal unit of TRIPTA COF.

For the solution formed by dissolving 5 mg material in 10 ml of aqua regia, the platinum concentration is 153 ppm.

153 ppm 10 ml of Pt solution = 1.53 mg of platinum.

Thus, 5 mg material contains 1.53 mg Pt,

1347 mg would then contain 412.2 mg Platinum
(As the formula weight of the repeating unit is 1347 g/mol.)

Considering the atomic weight of platinum (195.084), 1347 mg of platinum is equivalent to 2.14 mmol of platinum.

Thus one repeating unit contains 2 unit of Pt (As number cannot be fraction thus the digit after decimal is rounded off)

Which further implies, it contains 2 unit of cisplatin

Calculations for the other set of solutions have been carried out in same procedure, results were listed in Table S1.

Table S1:

Serial no	Conc. of material (mg/ml)	Conc. Of Pt in ppm (mg/L)	Mol of platinum per Repeating unit	Approximate number of cisplatin per unit (Round figured)
1.	5	153	2.14	**2**
2.	10	301	2.07	**2**
3.	15	481	2.21	**2**

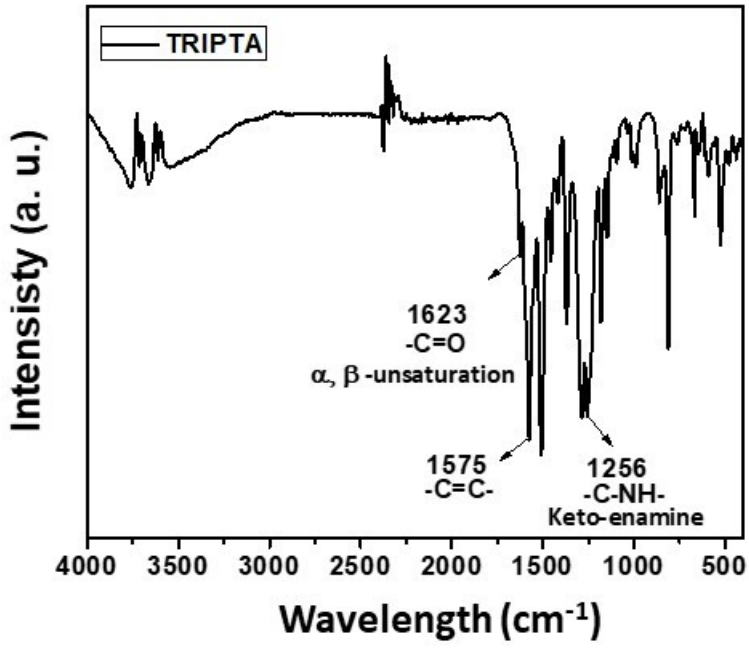


Figure S1:FTIR spectrum of as-synthesized TRIPTA COF.

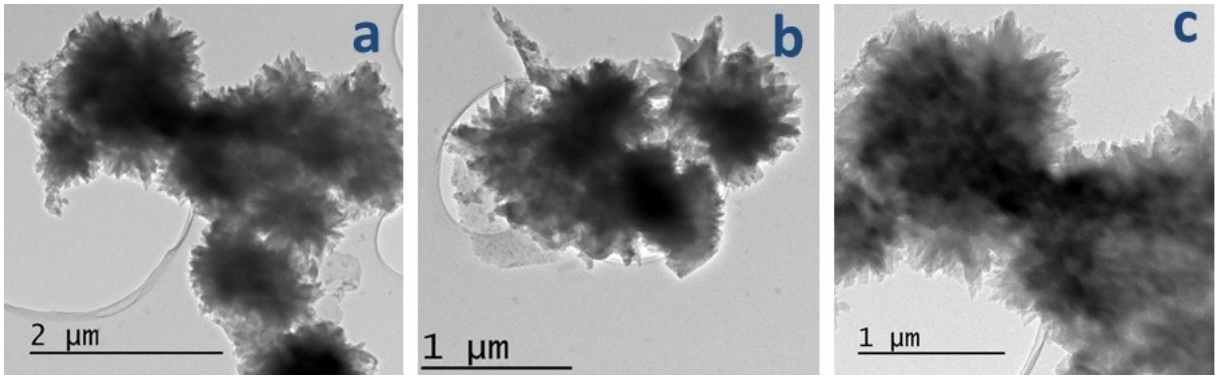


Figure S2: HRTEM images of TRIPTA after treatments with acidic solution pH = 5.0 (a), buffer pH=7.4 (using PBS solution, b) and neutral pH=7.0 for 48 h.

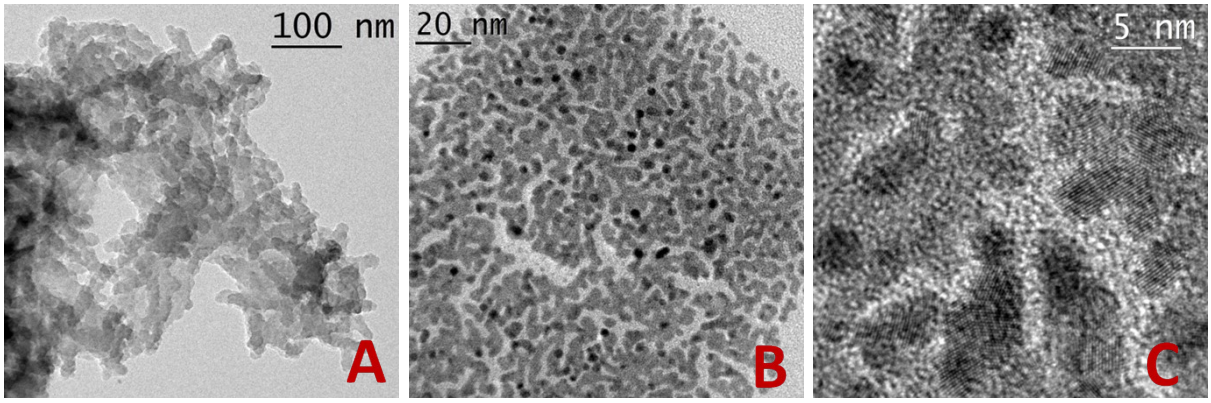


Figure S3. HRTEM images of TRIPTA COF after cisplatin loading at different magnification.

Drug binding assay:

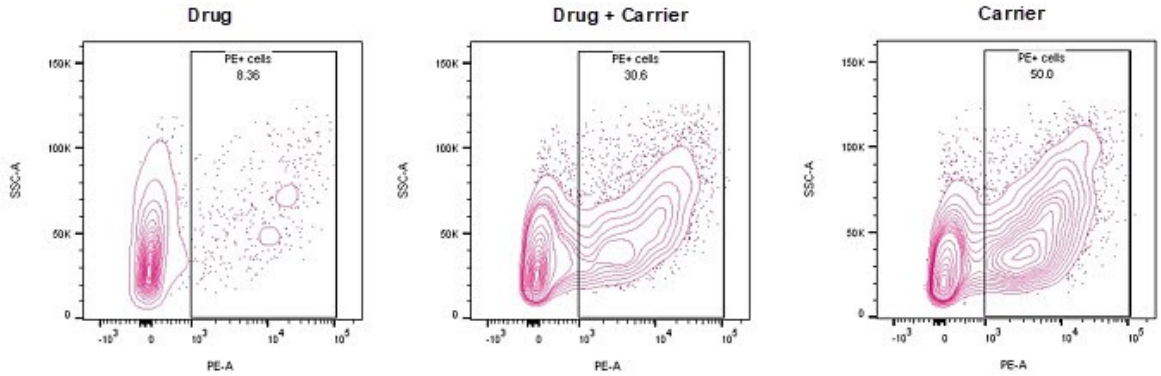


Figure S4: Drug binding assay of TRIPTA-COF-Cisplatin.

Drug binding study after 72 h incubation of cisplatin-TRIPTA-COF (drug + carrier) reveals that TRIPTA-COF (carrier)is binding viacovalent bond to form a uniform distribution of organic framework with cisplatin(drug).SSC provides us the information on the formed structural network with or without the carrier. As per Figure S4, the individual intensity of only drug is minimal than drug with carrier. The only carrier shows the highest intensity.

Drug release rate of Cisplatin loaded TRIPTA-COF in 24 h

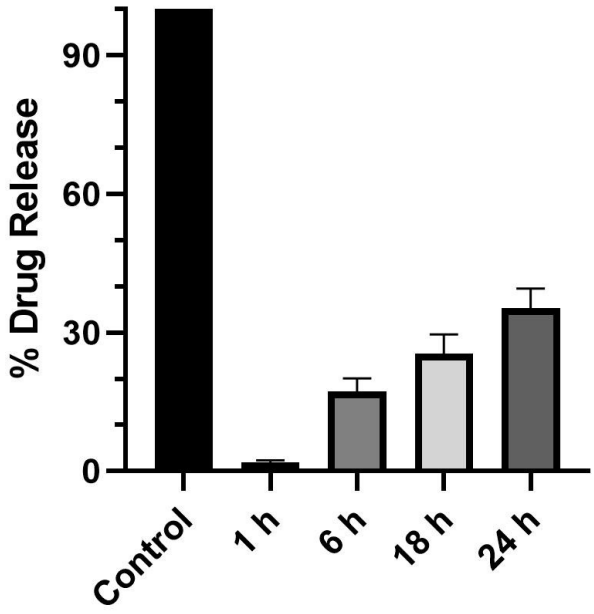


Figure S5: Drug release of Cisplatin loaded TRIPTA-COF

EMT with the involvement TRIPTA-COF-Cisplatin:

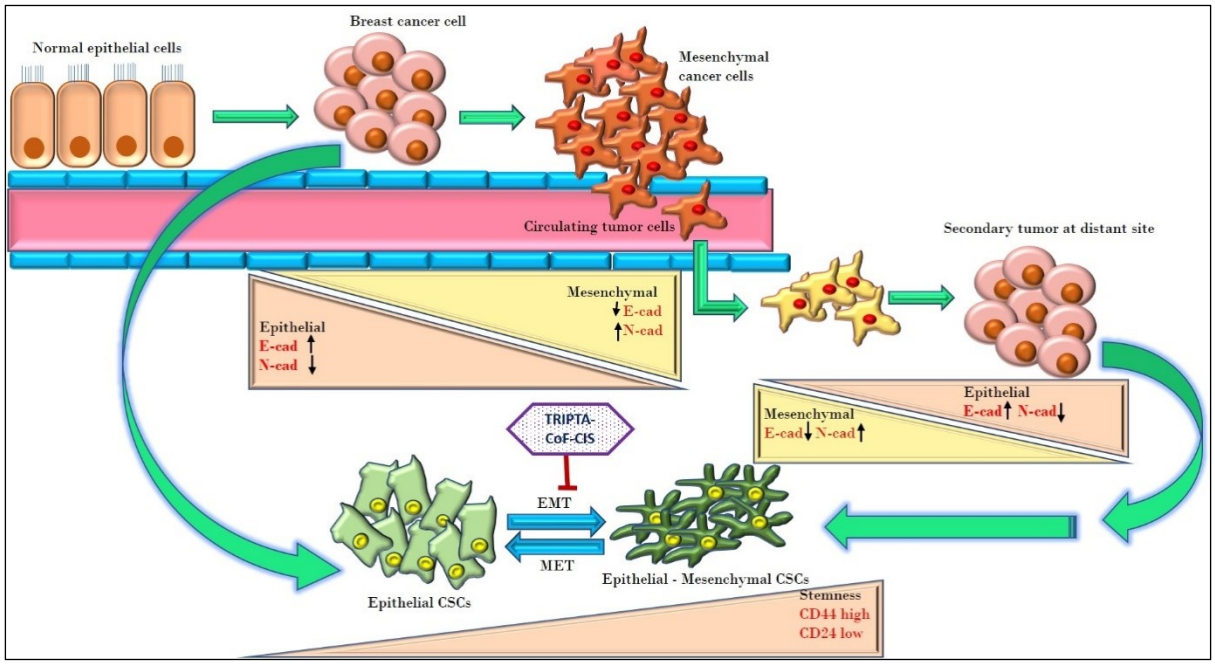


Figure S6: Epithelial-mesenchymal transition (EMT) has been minimized by the combinatorial treatment of cisplatin carried by the carrier material in comparison to cisplatin alone. Epithelial marker, E-cadherin is significantly increased in cisplatin together with carrier molecule and lower expression mesenchymal markers like N-cadherin.Transcriptional factor Snail has been observed under the same treatment.TRIPTA-CISPLATIN can serve as a potent drug carrier molecule for cisplatin showing higher detrimental effect on the proliferation and migration of breast cancer cells.

Cytotoxicity of TRIPTA-COF on peripheral blood mononuclear cells:

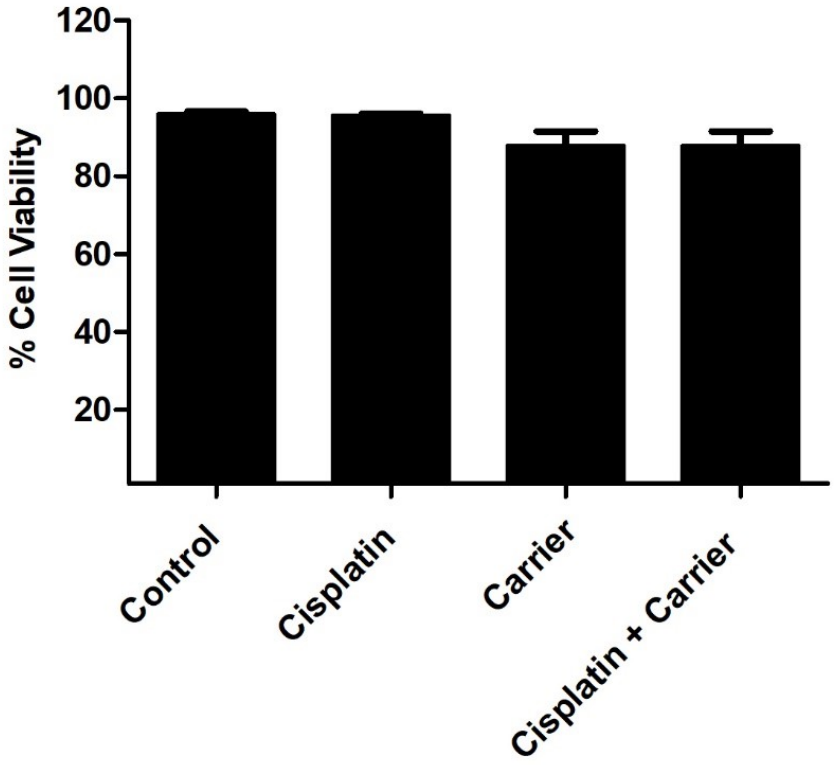


Figure S7: Cytotoxic effect of TRIPTA-COF-Cisplatin on peripheral blood mononuclear cells (PBMC): Cells were treated with concentration of IC50 of TRIPTA-COF-Cisplatin (carrier loaded drug), TRIPTA-COF (carrier) and cisplatin (drug) viability was measured by MTT assay. The data are represented as mean ± SD from triplicate independent experiments. No significant change was found.