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Supporting Information

Efficacious and sustained release of an anticancer drug mitoxantrone from new covalent organic frameworks using protein corona

Subhajit Bhunia,[b,‡] Pranay Saha,[c,‡] Parikshit Moitra,[d] Matthew A. Addicoat,[e] and Santanu Bhattacharya*[ac]

[a]Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560012, India, E-mail: sb@iisc.ac.in, sb23in@yahoo.com

[b]Department of Chemistry & Biochemistry, University of Texas at El Paso, El Paso, Texas 79968, United States

[c]School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Kolkata, West Bengal 700032, India

[d]Department of Pediatrics, Center for Blood Oxygen Transport and Hemostasis, University of Maryland Baltimore School of Medicine, Health Sciences Facility III, Baltimore, Maryland 21201, United States

[e]School of Science and Technology, Nottingham Trent University, Nottingham, NG11 8NS, UK.

‡These authors contributed equally to this work.

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Section S1: Methods

1.1. Characterization of Materials

^{1}H and ^{13}C NMR spectra were recorded using Bruker DPX-300 NMR spectrometer. The chemical shift (δ in ppm) was recorded with respect to the residual proton of the solvent as standard. Multiplicities are written as s (singlet), d (doublet), t (triplet), m (multiplet) and br (broad). X-Ray diffraction patterns of the powder samples were obtained with a Panalytical X'Part^{3} powder diffractometer using Cu-Kα (0.15406 nm) radiation. The solid state cross-polarization magic angle spinning (CP-MAS) ^{13}C NMR spectrum was recorded using a 100 MHz Bruker Avance II spectrometer at mass frequency of 8 kHz. FT-IR spectra were recorded using a Nicolet MAGNA-FT IR 750 Spectrometer Series II. Porosity measurement using volumetric N_2 adsorption/desorption was carried out by using Autosorb 1 (quantachrome, USA) instrument. The activation of the sample , the sample cell was outgassed at 130°C for 12 h under vacuum to remove all the entrapped solvent impurities. NLDFT pore size distribution was obtained by applying slit/cylindrical pore model on the N_2 adsorption/desorption isotherm. Thermo gravimetric (TGA) and differential thermal analyses (DTA) of the samples have been done by TGA Instruments thermal analyzer (TA-SDT Q-600). Elemental mapping and morphological analysis have been done using Hitachi S-5200 field-emission scanning electron microscope. The ultra-high resolution transmission electron microscopy (UHR-TEM) of the sample was done using a JEOL JEM 2010 transmission electron microscope operating at 200 kV. For the electron microscopy analysis the sample was dispersed in absolute ethanol and then drop coated on the carbon coated copper grid.

1.2. UV-Visible Spectroscopy

Loading of mitoxantrone into PER@PDA-COF-1 was measured by UV-visible absorption spectroscopy. Optical absorption spectra were recorded using Shimadzu UV-2600 UV-Vis spectrophotometer. For measuring the generation of reactive oxygen species (ROS) inside the cells, UV-vis spectra were measured in 96 well plates in Biotek epoch 2 microplate reader instrument.

1. 3. Fluorescence Spectroscopy

Fluorescence spectra of various samples were recorded in Horiba Fluromax-4 spectrofluorometer. Mitoxantrone concentrations released inside the cells in different culture conditions were measured. For larger number of samples Horiba Fluoromax-4 was used along with MicroMax 384 plate reader.

1. 4. Fluorescent lifetime analysis of PER@PDA-COF-1 with HSA

Fluorescence lifetime spectra were recorded in Horiba Jobin Yvon IBH with JY-IBH 5000M monochromator. Time-resolved fluorescence measurements were achieved with an excitation wavelength of 440 nm using a source of NaboLED-440L (pd<200ps). Instrumental response function (IRF) of the time correlated single-photon counting (TCSPC) of HSA-MXT-PER@PDA-CON-1 complex was 45 ps. Emission wavelength was set at 473 nm for MXT-PER@PDA-CON-1. The pico-timing amplifier and discriminator employed was Ortec 9327. The sample solutions were taken in cuvette separately and the detection was done using a MCP PMT Hamamatsu R3809 multichannel plate multiplier. For data acquisition and overall controlling DataStation v2.3 and for fluorescence decay analyses DAS6 softwares were used. Time calibrations were calculated using bi-exponentials against the IRF with FWHM ~2.7475E^{-02} ns/ch.

1. 5. Atomic Force Microscopy

AFM images were taken in Veeco diCP II AP0100 atomic force microscope with 0.01-0.025 ohm-cm-antimony-doped-silicon cantilever having a thickness × length × width of 3.75 μm × 125 μm × 35 μm and having a frequency of 300 KHz and Young's modulus of 40 N/m^2. PER@PDA-COF-1 (0.25 mg/ml) in PBS was drop coated over 0.8 cm^2 freshly cleaved mica sheets.

1.5.1. Bare PER@PDA-COF-1 nanosheet preparation

2 mg of PER@PDA-COF-1 was dispersed in 1 mL mili-Q water via bath sonication during 30 min. Then the solution was centrifuged at 4000 rpm and collected the supernatant solution. Then the supernatant phase was transferred and diluted to 4 mL. Then, the whole dispersion was subjected to 2 hr low frequency sonication (keeping the temperature constant) and centrifuged at 7000 rpm. Again, the supernatant phase was transferred to round bottom flask. The clear dispersion was drop cased on the precleaned mica sheet for AFM.

1.5.2. HSA-PER@PDA-COF-1 preparation

2 mg of PER@PDA-COF-1 was dispersed in 1 mL mili-Q water via bath sonication during 30 min. Then the solution was centrifuged at 4000 rpm and collected the supernatant solution.

Then the supernatant phase was transferred and diluted to 4 mL. Then, the whole aqueous dispersion was subjected to 1 hr low frequency sonication (keeping the temperature constant) and centrifuged at 7000 rpm. Again, the supernatant phase was transferred to round bottom flask. Then, HSA (10-30 µL, 0.3 mM) was added to the faint yellow aqueous solution of PER@PDA-COF-1. The whole solution was vortexed for 60 min. Then the solution was centrifuged at 3000 rpm and the supernatant layer was discarded (to remove the unbounded HSA). The yellow mass was again dissolved in 2 ml water and sonicated for 2 h. Then the solution was drop casted for AFM.

1.6 Electrochemical Measurement

Adsorption affinity of various Proteins (HSA, BSA, Concanavalin A, Cytochrome, Trypsin) on PER@PDA-COF-1 surface were examined by using CHI 760D electrochemical workstation in 0.1 M KCl solution as an electrolyte. Electrochemical analysis was carried out in three-electrode configuration with protein corona modified glass carbon electrode as working electrode, platinum as counter electrode, and Ag/AgCl as reference electrodes. Each sample was prepared by using same amount of COF adsorbed with same equivalent of proteins.

3 mg PER@PDA-COF-1 was suspended in 3 ml water and sonicated for 10 minutes. Then the suspended solution was divided into six portions. 50 µL of 0.3 mM solution of various proteins (HSA, BSA, Concanavalin A, Cytochrome, Trypsin) was added to each portion and sonicated for 30 minutes. Then each solution was centrifuged at 8000 rpm and precipitate was collected for catalytic ink preparation. For ink preparation, the precipitate was redissolved in 200 µL water and 5 µL of Nafion solution (0.5 wt%) was added into it. Then, 30 µL of each solution was drop casted on glassy working electrode (GCE) two times. After dried the (GCE) at 45 °C for 2 h, the working electrode was placed into electrolyte for measuring cyclic voltammetry (CV) between -1V and +1V at scan rate of 50 mV/s.

1. 7. Cell Culture

Cultures of the cell line (HeLa) were maintained in Dulbecco's modified Eagle's medium (DMEM) containing 10% fetal bovine serum (FBS) and 1X pen strep (100 units/ml penicillin and 100µg/ml streptomycin). The cells were incubated at 37 °C under 5% CO_2 environment with relative humidity >95%. The cells were maintained by passaging 3-4 times a week using 0.5% trypsin–EDTA.

1. 8. Cell Cytotoxicity Assay

Cytotoxicity of PER@PDA-COF-1, MXT-PER@PDA-COF-1and HSA-MXT-PER@PDA-CON-1 were measured in HeLa cell line using MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide) assay. Cells were seeded at a density of 1×10^4 cells/well in a 96-well plate and after 24 h of incubation, various concentrations of mitoxantrone (10-70 μM), PER@PDA-COF-1 (0.2 mg/ml) were added to the cells in triplicate by the method of half dilution. After an incubation of 12, 24, 36 and 48 h, 20 μL of MTT solution (5 mg/mL in 50 mM PBS, pH 7.4) was added to each well and further incubated at 37 °C for 3.5 h for complete settling of the formazan crystals. Thereafter the supernatant media were removeand 200 μL of DMSO was added to each well to dissolve formazan. The absorbance of the DMSO solution was measured at a wavelength of 570 nm on a microwell plate reader (BioTek Epoch 2 Microplate Reader). The variation in cell viability with concentration was plotted using the obtained absorbance values. The % cell viability was calculated as:

% Cell viability = $[(A_{590}$ Sample $- A_{590}$ DMSO)/ $(A_{590}$ control $- A_{590}$ DMSO)] x 100)

1. 9. Microscopy and determination of released mitoxantrone inside cells

Cells were **s**eeded at a density of 5×10^4 cells/well in a 24 well plate and after 24 h of incubation, media were aspirated and new media were added in different wells. Dulbecco's modified Eagle's medium (DMEM) containing 10% Fetal Bovine Serum (FBS) and 1 × pen strep (100 units/mL penicillin and 100 μg/mL streptomycin) were added to the cell culture wells. Mitoxantrone was added at a final concentration of 50 μM adsorbed in PER@PDA-COF-1 (0.2 mg/mL). HSA was added to a final concentration of 350 μM for making the corona complex with mitoxantrone adsorbed onto COF. Fluorescence microscopic images were taken using an Olympus CX81 fluorescence microscope. For the determination of release of mitoxantrone inside the cells, Radioimmunoprecipitation assay buffer (RIPA buffer) was added to culture wells and pipetted carefully to lyse the cells. These cell lysates were collected in different vials for centrifugation at 6000 rpm for 10 min. The cell debris were precipitated and the supernatants were collected for further fluorescence spectroscopic measurements for the released mitoxantrone at 600 nm. Cell lysates were prepared in a similar fashion for the ethidium bromide-acridine orange assay.

1. 10. Determination of intracellular ROS generation

Conjugated systems were investigated for probing the reactive oxygen species (ROS) generation inside cells. 1,3-Diphenylisobenzofuran (DPBF) was used to detect $^1O_2$. 1 mL of the cell lysates were taken from 5×10^4 cells treated with MXT-PER@PDA-CON-1and HSA-MXT-PER@PDA-CON-1at different time points. 10 μL (10 mM) DPBF solution was added

to the 1 mL cell lysate suspensions. The solution mixture was then irradiated with 635 nm laser for 15 min. Absorption intensity was measured at 420 nm. For control, the absorbance of water was measured. Comparative data were plotted at 1 h and 3 h time points.

1.11. Hemocompatibility

Human blood was collected from unmedicated healthy volunteers and was stored in trisodium citrate (anti-coagulant) treated tubes. All the blood compatibility experiments were performed according to standard ISO protocol (10993-4). Experiments were carried out within 2 hours of blood collection. Hemocompatibility of PER@PDA-COF-1, MXT-PER@PDA-COF-1, HSA_MXT-PER@PDA-COF-1 was evaluated by studying hemolysis, the morphology of blood cells, and coagulation activation, both through the extrinsic pathway (prothrombin time, PT assay) and the intrinsic pathway (activated partial thromboplastin time, APTT assay).

1.11.1Micrographs of blood smear:

After blood incubation with the systems, 10 µL of the blood was withdrawn and spread on a cleaned microscopy glass slide. Blood cells were observed with an Olympus CKX41 fluorescence microscope at 20× magnification in transmission mode.

1.11.2. Clotting time

Whole human blood was used for determining the blood clot time. Collected blood was recalcified to reverse the effect of citrate anticoagulant and supplied with the specific activators of coagulation. Prothrombin time (PT) to evaluate the extrinsic pathway was carried out using thromboplastin reagent (Uniplastin from Tulip diagnostics), and activated partial thromboplastin time (APTT) to evaluate the intrinsic pathway was measured using cephaloplastin reagent (Liquicelin-e from Tulip diagnostics) as per kit protocol. For PT and APTT assay, plasma was isolated by centrifuging at 2000g for 5 minutes and the supernatant is used. In brief 50 µL of human plasma was incubated with samples (PER@PDA-COF-1, MXT-PER@PDA-COF-1, HSA_MXT-PER@PDA-COF-1) on a cleaned glass slide. The very first visible sign of the clot was taken as the clotting of blood. PEI was used as a positive control and PBS served as the control experiment.

1.11.3. Hemolysis assay

Whole blood was incubated with different concentrations of liposomes (PER@PDA-COF-1, MXT-PER@PDA-COF-1, HSA_MXT-PER@PDA-COF-1), the samples were centrifuged at 600g for 5 minutes at room temperature, and supernatants were collected. The hemoglobin released was measured by the absorbance of 100-fold dilution of whole blood in Drabkin's

reagent at 540 nm in a microplate reader (Genetix epoch 2). A standard calibration curve was made using hemoglobin as the standard. PEI and PBS were used as positive and negative controls, respectively. The experiments were done in triplicate. The % of hemolysis was calculated by the relative method based on the Optical density (OD).

% of hemolysis = $(OD_{Sample}-OD_{Negative}/OD_{Positive}-OD_{Negative}) \times 100$.

Section S2: Materials and Synthetic scheme

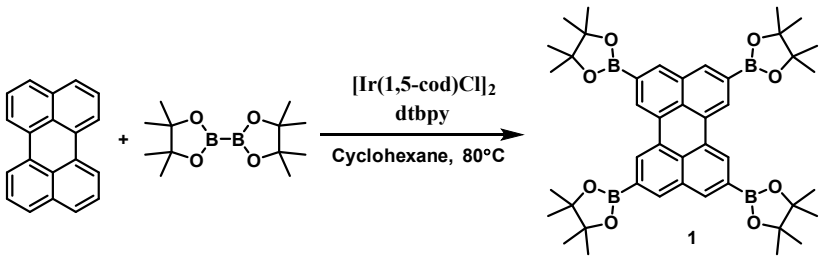
2.1. Materials

Perylene, Bis(1,5-cyclooctadiene)diiridium(I) dichloride, *p*-phenylenediamine and 4,4′-Di-tert-butyl-2,2′-dipyridyl were purchased from Aldrich, while bis(pinacolato)diboron, 4-bromo-benzaldehyde, tetrakis- (triphenylphosphine) palladium(0), were purchased from spectrochem, India. Dioxane, acetone, cyclohexane, o-dichlorobenzene, N,N' dimethyl acetamide etc. were purchased from Merck chemicals. These materials were used for synthesis without further purification.

2.2. Synthetic scheme

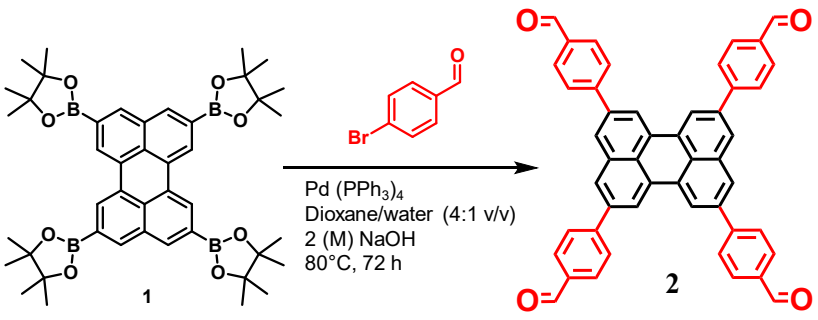
2.2.1. Synthesis of 2,5,8,11-tetrakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)perylene ($P\text{-}bpin_4$) (1)

Perylene (0. 5 g, 1.98 mmol) and 3 g bis-(pinacolato)-diboron (11.88 mmol) were mixed together in anhydrous cyclohexane in a 50 mL Schlenk flask. Then 132 mg of $[Ir(COD)OMe]_2$ (10 mol%) and 40 mg of 4,4′-di-tert-butyl-2,2′-dipyridyl (10 mol%) were added to the solution under extremely inert condition (argon environment). Then the mixture was degassed with 5/6 consecutive freeze-pump-thaw cycles to exclude dissolved oxygen completely. The colour of the solution turned from yellow to green gradually which was further heated under reflux at 80°C for 72 hrs. During the reaction the flask was anchored by Al-foil to keep the mixture away from visible light. After reflux, the mixture was extracted with dichloromethane and the combined organic layer was evaporated off to get the crude product as a yellow semi-solid. The crude was further purified by silica gel column chromatography using DCM-ethyl-acetate (5:1) mixture to get the pure product as a bright yellow solid (1.3 g, 90 %).



2.2.2. Synthesis of 4,4',4'',4'''-(perylene-2,5,8,11-tetrayl) tetrabenzaldehyde (TFPPe) (2)

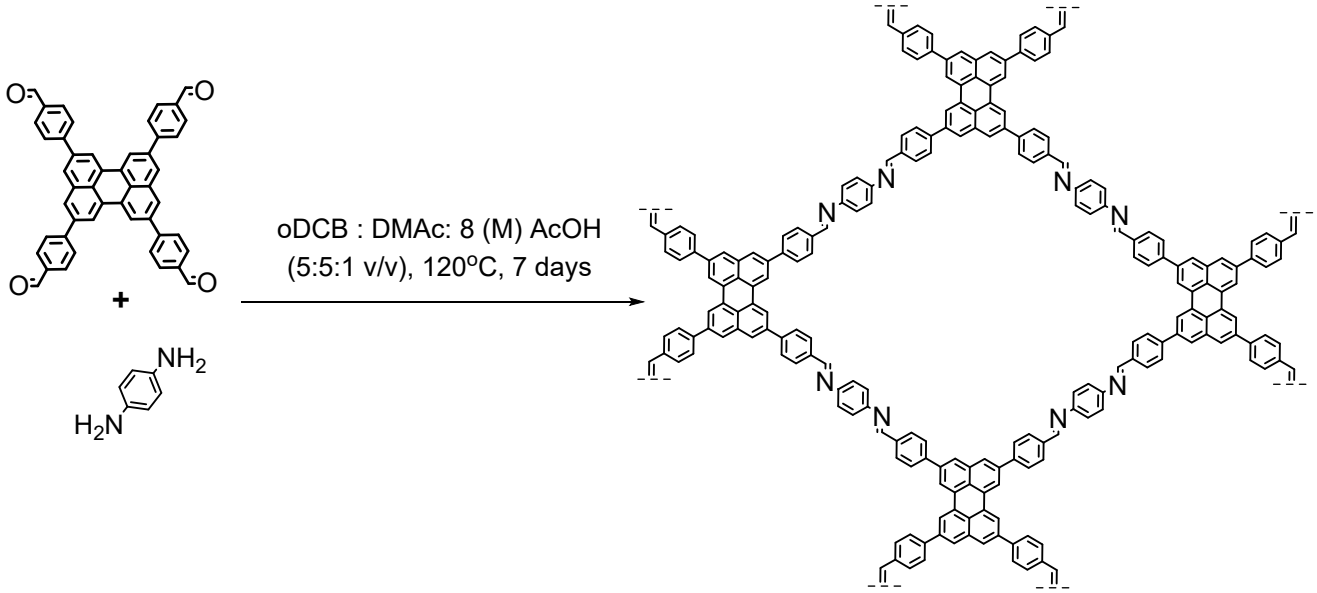
Compound **1** 0.5 g (0.659 mmol) of and 0.731g (3.954 mmol) 4-bromobenzaldehyde were dissolved in 20 ml dioxane/aqueous 2M K_2CO_3 mixture (4:1 v/v). Then 200 mg (5 mol%) $Pd(PPh_3)_4$ was added to the mixture under N_2 atmosphere. The mixture was degassed by 3/4 consecutive freeze-thaw cycles and the mixture was refluxed at 80 ºC for 3 days. The pure compound was obtained by simple filtration and successive washing with diethyl ether (5 x 100 mL) and was isolated as a deep orange solid TFPPe (0.4 g, 90 % yield). ^{1}H NMR (400 MHz, DMSO-d_6): 10.14 (s, 4H, Ar H), 8.95 (s, 4H, Ar H), 8.39 (s, 4H, Ar H), 8.27 (d, 8H, J= 8 Hz, Ar H), 8.12 (d, 8H, J= 8 Hz, Ar H); IR (KBr): ν (cm^{-1}) = 2806 (w), 2722 (w), 1697 (s), 1595 (s), 1566 (w), 1435 (w), 1385 (w), 1339 (w),1308 (w), 1216 (m), 1172 (m), 1109 (w), 1013 (w), 884 (m), 824 (s), 734 (w). Calculated C, H, N analysis for $C_{48}H_{28}O_4$: C 86.21, H 4.22; found: C 86.31, H 4.27%. Mp > 300°C.



2.2.3. Synthesis of 2D PER@PDA-COF-1

A glass seal tube (20 cm x 8 mm) was charged with 33 mg of TFPPe **(2,**50 µmol) and 10 mg (100 µmol) of p-phenylenediamine (**3**). The solid mixture was dissolved in DMAc/o-DCB (1:1 v/v, 1 ml) using 100 µL 8 (M) acetic acid. The mixture was sonicated for 5 min and frozen in

a liquid N_2 bath and degassed through 3/4 freeze-pump-thaw cycles and flame sealed under vacuum which was kept inside oven for 7 days under static heating at 120 °C. The PER@PDA-COF-1 material was obtained as a yellowish-orange insoluble powder which was activated by repeated washing with THF, acetone, water and methanol, n-hexane (25 mg, yield 58%). C, H, N calculated: C 90.93, H 4.99, N 4.08; found: C 91.2, H 5.5, N 3.8 %.



2.2.4. ^{1}H NMR spectra

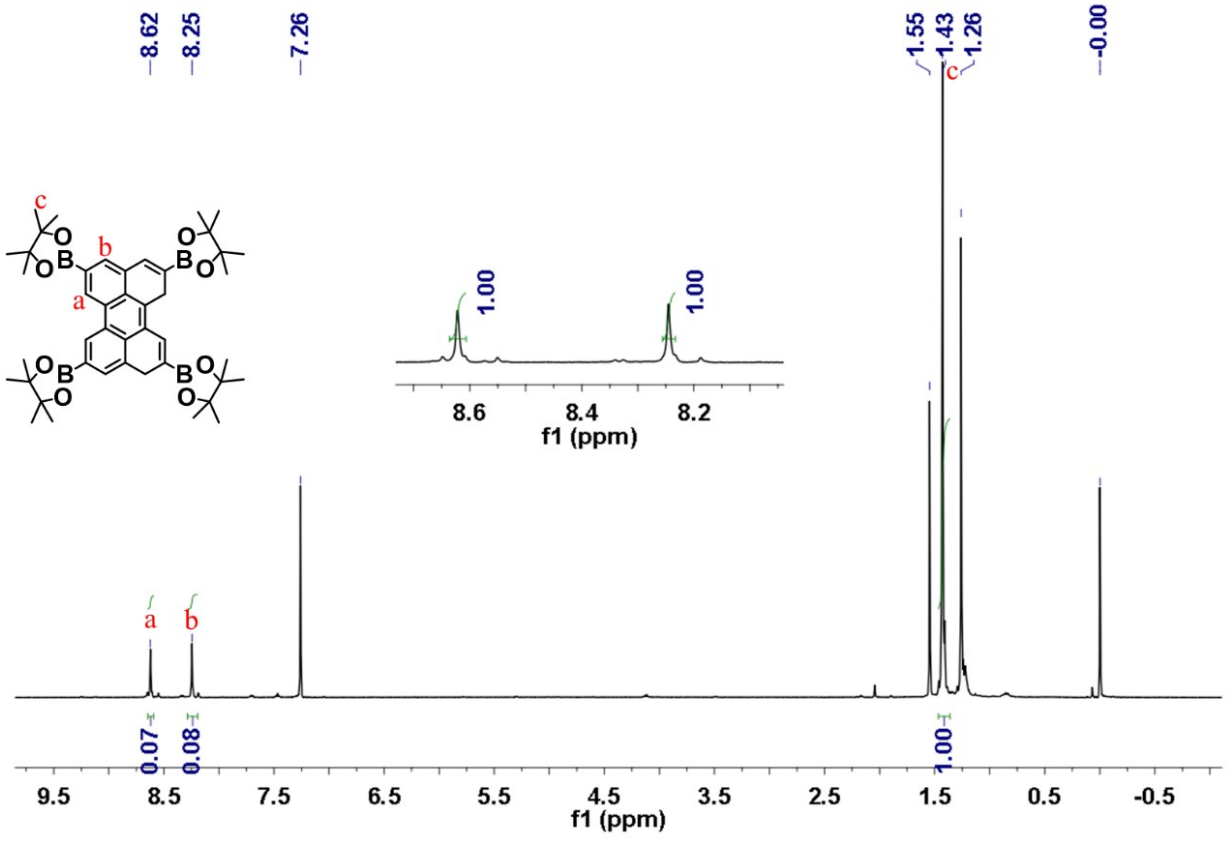


Figure S1. ^{1}H-NMR (in $CDCl_3$) spectrum of 2,5,8,11-tetrakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)perylene (P-bpin$_4$)

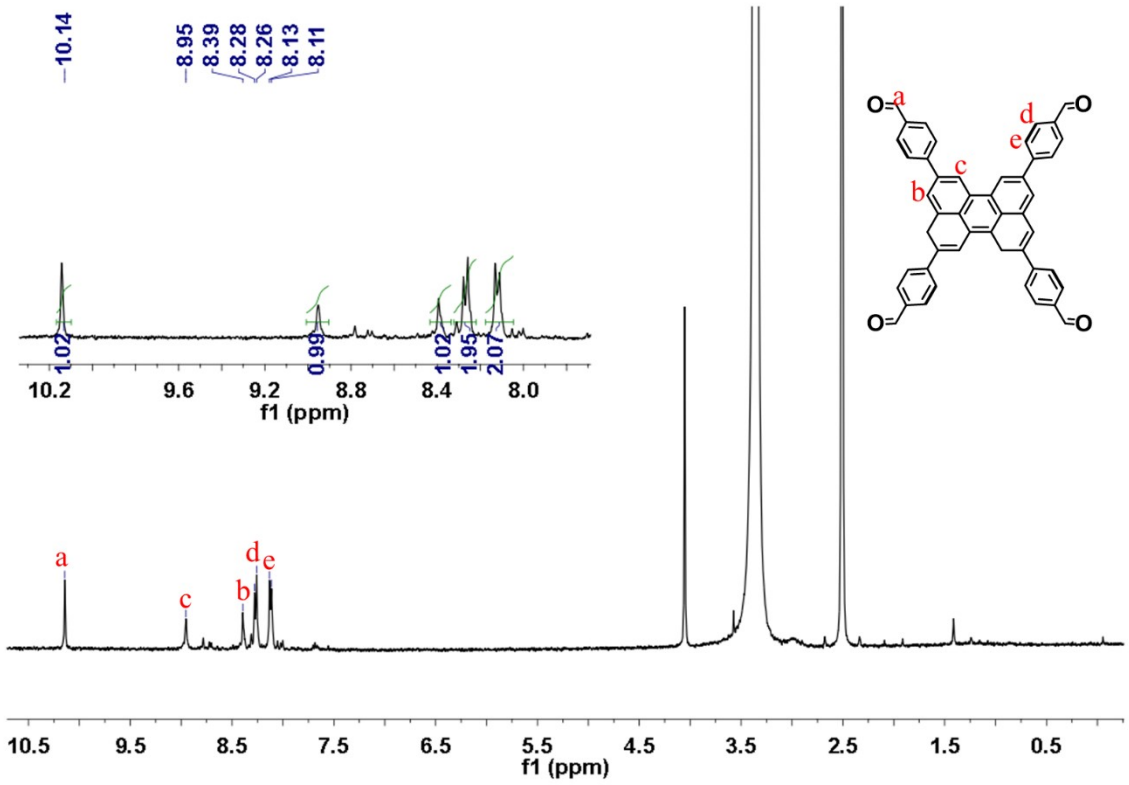


Figure S2. ^{1}H NMR (in D_6-DMSO) spectrum of 2,5,8,11-tetrakis(4-formylphenyl) perylene (TFPPe) (note that ^{13}C NMR spectra could not be recorded due to low solubility of TFPPe).

Section S3: Computational Details

The crystalline structure of PER@PDA-COF-1 was determined by building square lattice (**sql**) and kagome (**kgm**) structures using AuToGraFS.[1] Structures were optimized using the density-functional tight-binding (DFTB+) method as implemented in DFTB+ program package version 1.3.[2] The Coulombic interaction between partial atomic charges was determined using

the self-consistent charge (SCC) formalism. Lennard-Jones type dispersion was employed in all calculations to describe van der Waals (vdW) and π-stacking interactions. The lattice dimensions were optimized simultaneously with the geometry. Standard DFTB parameters for X-Y element pair interactions were employed from the mio-0-1 set.[3] To determine the optimal binding site of mitoxantrone to a PER@PDA-COF monolayer, 500 random geometries of mitoxantrone and a 2x2 supercell of the optimized **sql** monolayer were generated using the conformationally flexible Kick3 program[4] and optimised using DFTB as above.

Rhombus_PER@PDA-COF-1_AA (Space Group- P1)
a = 25.6839 Å, b = 26.1672 Å, c = 7.17259 Å; α = 89.8612°, β = 89.8726°, γ = 109.829°

atom	*x*	*y*	*z*	*atom*	*x*	*y*	*z*	*atom*	*x*	*y*	*z*
C1	0.4806	0.6580	0.0055	C44	0.30111	0.70839	0.98389	H46	0.53385	0.50442	0.59549
C2	0.5360	0.6580	0.0065	H23	0.33532	0.7889	0.10566	C86	0.63565	0.45739	0.4426
C3	0.5811	0.7084	0.0186	H24	0.28117	0.62735	0.86566	H47	0.71475	0.50848	0.32634
C4	0.5695	0.7581	0.0257	C45	0.62276	0.31219	0.98788	H48	0.55359	0.4191	0.56126
C5	0.5144	0.7560	0.0179	C46	0.57582	0.26426	0.99268	C87	0.84079	0.81074	0.53089
C6	0.4691	0.7064	0.0096	C47	0.67607	0.3075	0.99422	C88	0.88439	0.85576	0.46067
C7	0.6366	0.7076	0.02169	C48	0.58151	0.21323	0.998	C89	0.85373	0.76497	0.59109
C8	0.6158	0.8099	0.0363	H25	0.53429	0.26765	0.9897	C90	0.93819	0.8548	0.44844
C9	0.6713	0.8091	0.0378	C49	0.68173	0.25649	0.00301	H49	0.87615	0.89188	0.40874
C10	0.6829	0.7593	0.0304	H26	0.71343	0.34402	0.99745	C91	0.90744	0.7639	0.57853
C11	0.7165	0.8595	0.0446	C50	0.63484	0.20851	0.00232	H50	0.82152	0.72962	0.65276
C12	0.7058	0.9094	0.0419	H27	0.54406	0.17683	0.00399	C92	0.95073	0.8087	0.50583
C13	0.6519	0.9104	0.0387	H28	0.72327	0.25316	0.00823	H51	0.97103	0.89027	0.39002
C14	0.6074	0.8599	0.0414	C51	0.17825	0.75157	0.03691	H52	0.9165	0.72782	0.62658
H1	0.4469	0.6184	0.0019	C52	0.17331	0.80359	0.05367	C93	0.64076	0.96229	0.52562
H2	0.7415	0.9474	0.0372	C53	0.12938	0.70545	0.02951	C94	0.59028	0.96382	0.45223
C15	0.5469	0.6084	0.9926	C54	0.12166	0.80997	0.05497	C95	0.68054	0.01213	0.5806
C16	0.6009	0.6075	0.9957	H29	0.2111	0.83947	0.06332	C96	0.58036	0.01268	0.43276
C17	0.6451	0.6577	0.0144	C55	0.0777	0.71173	0.03433	H53	0.55833	0.92643	0.40339
H3	0.5116	0.5705	0.9752	H30	0.1316	0.66419	0.02438	C97	0.67078	0.06105	0.56066
C18	0.7380	0.7615	0.0263	C56	0.07288	0.76393	0.04289	H54	0.71985	0.01293	0.64379
C19	0.77185	0.8595	0.0482	H31	0.1192	0.85094	0.07074	C98	0.6205	0.06237	0.48537
H4	0.8056	0.8988	0.0602	H32	0.03987	0.67579	0.02803	H55	0.54087	0.01236	0.37215
C20	0.7832	0.8111	0.03695	N1	0.61341	0.36183	0.99162	H56	0.70253	0.09918	0.60494
H5	0.5650	0.8608	0.0467	N2	0.64401	0.15892	0.01932	C99	0.41155	0.70685	0.50317
H6	0.5054	0.7942	0.016	N3	0.23173	0.74886	0.04095	C100	0.39827	0.75224	0.56527
H7	0.74735	0.7237	0.0116	N4	0.01953	0.76686	0.05215	C101	0.36789	0.66206	0.43295
H8	0.6874	0.6566	0.0240	C57	0.60989	0.11357	0.95854	C102	0.34444	0.7531	0.55552
C21	0.6127	0.55614	0.97769	H33	0.57115	0.11067	0.87968	H57	0.43026	0.78757	0.62676
C22	0.6636	0.5556	0.90373	C58	0.64748	0.40655	0.92505	C103	0.31396	0.66276	0.42366
C23	0.5735	0.5059	0.0330	H34	0.6868	0.40902	0.84999	H58	0.376	0.62612	0.37906
C24	0.6748	0.5074	0.8865	C59	0.24447	0.70934	0.9702	C104	0.30111	0.70839	0.48389
H9	0.6949	0.5935	0.8535	H35	0.21395	0.67462	0.8931	H59	0.33532	0.7889	0.60566
C25	0.5846	0.4576	0.0157	C60	0.00712	0.80728	0.98744	H60	0.28117	0.62735	0.36566
H10	0.5338	0.50442	0.0954	H36	0.03778	0.84237	0.91127	C105	0.62276	0.31219	0.48788
C26	0.6356	0.45739	0.9426	C61	0.48067	0.65801	0.50555	C106	0.57582	0.26426	0.49268
H11	0.7147	0.5084	0.8263	C62	0.53606	0.65807	0.50654	C107	0.67607	0.3075	0.49422
H12	0.5535	0.4191	0.0612	C63	0.58112	0.7084	0.51861	C108	0.58151	0.21323	0.498
C27	0.8407	0.8107	0.0308	C64	0.56951	0.75817	0.52576	H61	0.53429	0.26765	0.4897
C28	0.8843	0.8557	0.9606	C65	0.51445	0.75608	0.51792	C109	0.68173	0.25649	0.50301
C29	0.8537	0.7649	0.0910	C66	0.46912	0.70643	0.50963	H62	0.71343	0.34402	0.49745
C30	0.9381	0.8548	0.9484	C67	0.63661	0.70765	0.52169	C110	0.63484	0.20851	0.50232
H13	0.8761	0.8918	0.9087	C68	0.61585	0.80991	0.53631	H63	0.54406	0.17683	0.50399
C31	0.9074	0.7639	0.07853	C69	0.67135	0.80915	0.53789	H64	0.72327	0.25316	0.50823
H14	0.8215	0.7296	0.15276	C70	0.68293	0.75938	0.5304	C111	0.17825	0.75157	0.53691
C32	0.9507	0.8087	0.00583	C71	0.7165	0.85953	0.54461	C112	0.17331	0.80359	0.55367
H15	0.9710	0.8902	0.89002	C72	0.70588	0.90942	0.54198	C113	0.12938	0.70545	0.52951
H16	0.9165	0.7278	0.12658	C73	0.6519	0.9104	0.53877	C114	0.12166	0.80997	0.55497
C33	0.6407	0.9622	0.02562	C74	0.60749	0.85997	0.54146	H65	0.2111	0.83947	0.56332
C34	0.5902	0.9638	0.95223	H37	0.44695	0.61849	0.5019	C115	0.0777	0.71173	0.53433

C1	0.4806	0.6580	0.00555	H38	0.74154	0.94747	0.53726	H66	0.1316	0.66419	0.52438
C2	0.5360	0.6580	0.00654	C75	0.54694	0.60841	0.4926	C116	0.07288	0.76393	0.54289
C3	0.5811	0.7084	0.01861	C76	0.60096	0.60757	0.49573	H67	0.1192	0.85094	0.57074
C4	0.5695	0.7581	0.02576	C77	0.64513	0.65771	0.51447	H68	0.03987	0.67579	0.52803
C5	0.5144	0.7560	0.01792	H39	0.5116	0.57052	0.47523	N5	0.61341	0.36183	0.49162
C6	0.4691	0.7064	0.00963	C78	0.73805	0.76154	0.52639	N6	0.64401	0.15892	0.51932
C7	0.6366	0.7076	0.02169	C79	0.77185	0.85953	0.54822	N7	0.23173	0.74886	0.54095
C8	0.6158	0.8099	0.03631	H40	0.80566	0.89882	0.56024	N8	0.01953	0.76686	0.55215
C9	0.6713	0.8091	0.03789	C80	0.78326	0.81116	0.53695	C117	0.60989	0.11357	0.45854
C10	0.6829	0.7593	0.0304	H41	0.56502	0.8608	0.54674	H69	0.57115	0.11067	0.37968
C11	0.7165	0.8595	0.04461	H42	0.50544	0.79423	0.51624	C118	0.64748	0.40655	0.42505
C12	0.7058	0.9094	0.04198	H43	0.74735	0.72374	0.51163	H70	0.6868	0.40902	0.34999
C13	0.6519	0.9104	0.03877	H44	0.68746	0.65664	0.52405	C119	0.24447	0.70934	0.4702
C14	0.6074	0.8599	0.04146	C81	0.61278	0.55614	0.47769	H71	0.21395	0.67462	0.3931
H1	0.4469	0.61849	0.0019	C82	0.66367	0.55568	0.40373	C120	0.00712	0.80728	0.48744
H2	0.7415	0.9474	0.03726	C83	0.57354	0.50591	0.53302	H72	0.03778	0.84237	0.41127
C15	0.5469	0.6084	0.9926	C84	0.67488	0.5074	0.38657				

Rhombus_PER@PDA-COF-1_AB (Space Group- P1)
a = 25.1071 Å, b = 26.0982 Å, c = 6.5741 Å; α = 92.198°, β = 90.567°, γ = 114.632°

atom	*x*	*y*	*z*	*atom*	*x*	*y*	*z*	*atom*	*x*	*y*	*z*
C1	0.473	0.643	0.018	H23	0.327	0.768	0.158	C85	0.099	0.461	0.580
C2	0.532	0.649	0.013	H24	0.259	0.603	0.844	H46	0.054	0.510	0.710
C3	0.579	0.704	0.016	C45	0.625	0.313	0.010	C86	0.140	0.459	0.440
C4	0.566	0.752	0.019	C46	0.574	0.262	0.017	H47	0.202	0.505	0.211
C5	0.508	0.744	0.018	C47	0.681	0.311	0.015	H48	0.076	0.425	0.675
C6	0.460	0.690	0.019	C48	0.577	0.210	0.020	C87	0.353	0.831	0.540
C7	0.638	0.709	0.012	H25	0.531	0.264	0.016	C88	0.400	0.877	0.459
C8	0.615	0.809	0.023	C49	0.684	0.259	0.025	C89	0.364	0.787	0.616
C9	0.674	0.814	0.030	H26	0.721	0.350	0.017	C90	0.456	0.877	0.447
C10	0.687	0.766	0.022	C50	0.633	0.208	0.023	H49	0.394	0.912	0.397
C11	0.721	0.869	0.041	H27	0.537	0.171	0.025	C91	0.419	0.786	0.604
C12	0.709	0.918	0.041	H28	0.727	0.257	0.030	H50	0.329	0.751	0.684
C13	0.651	0.912	0.026	C51	0.175	0.745	0.021	C92	0.466	0.831	0.516
C14	0.605	0.858	0.019	C52	0.183	0.802	0.029	H51	0.492	0.912	0.379
H1	0.437	0.600	0.022	C53	0.118	0.702	0.015	H52	0.427	0.750	0.658
H2	0.746	0.960	0.045	C54	0.135	0.816	0.029	C93	0.138	0.963	0.512
C15	0.544	0.600	0.004	H29	0.227	0.836	0.035	C94	0.096	0.963	0.367
C16	0.602	0.605	0.994	C55	0.070	0.715	0.018	C95	0.167	0.011	0.640
C17	0.648	0.660	0.998	H30	0.110	0.657	0.015	C96	0.085	0.010	0.346
H3	0.507	0.558	0.999	C56	0.077	0.772	0.023	H53	0.073	0.925	0.265
C18	0.745	0.773	0.024	H31	0.142	0.860	0.039	C97	0.156	0.059	0.619
C19	0.780	0.875	0.049	H32	0.025	0.681	0.016	H54	0.199	0.012	0.758
H4	0.816	0.918	0.062	N1	0.619	0.364	0.017	C98	0.115	0.060	0.470
C20	0.793	0.828	0.039	N2	0.639	0.157	0.040	H55	0.053	0.009	0.229
H5	0.559	0.855	0.011	N3	0.226	0.736	0.033	H56	0.179	0.097	0.719
H6	0.497	0.781	0.012	N4	0.026	0.781	0.039	C99	0.900	0.687	0.520
H7	0.755	0.736	0.009	C57	0.606	0.111	0.941	C100	0.889	0.732	0.605
H8	0.693	0.663	0.994	H33	0.572	0.108	0.825	C101	0.851	0.640	0.429
C21	0.615	0.555	0.977	C58	0.650	0.407	0.917	C102	0.834	0.732	0.595
C22	0.657	0.553	0.840	H34	0.684	0.407	0.806	H57	0.925	0.769	0.680
C23	0.586	0.509	0.098	C59	0.229	0.690	0.976	C103	0.796	0.640	0.419
C24	0.669	0.506	0.821	H35	0.192	0.652	0.903	H58	0.857	0.604	0.359
H9	0.680	0.589	0.743	C60	0.022	0.827	0.990	C104	0.786	0.686	0.499
C25	0.599	0.461	0.080	H36	0.059	0.864	0.921	H59	0.827	0.768	0.658
H10	0.554	0.510	0.210	C61	0.973	0.643	0.518	H60	0.759	0.603	0.344
C26	0.640	0.459	0.940	C62	0.032	0.649	0.513	C105	0.125	0.313	0.510
H11	0.702	0.505	0.711	C63	0.079	0.704	0.516	C106	0.074	0.262	0.517
H12	0.576	0.425	0.175	C64	0.066	0.752	0.519	C107	0.181	0.311	0.515
C27	0.853	0.831	0.040	C65	0.008	0.744	0.518	C108	0.077	0.210	0.520
C28	0.900	0.877	0.959	C66	0.960	0.690	0.519	H61	0.031	0.264	0.516
C29	0.864	0.787	0.116	C67	0.138	0.709	0.512	C109	0.184	0.259	0.525
C30	0.956	0.877	0.947	C68	0.115	0.809	0.523	H62	0.221	0.350	0.517
H13	0.894	0.912	0.897	C69	0.174	0.814	0.530	C110	0.133	0.208	0.523
C31	0.919	0.786	0.104	C70	0.187	0.766	0.522	H63	0.037	0.171	0.525
H14	0.829	0.751	0.184	C71	0.221	0.869	0.541	H64	0.227	0.257	0.530
C32	0.966	0.831	0.016	C72	0.209	0.918	0.541	C111	0.675	0.745	0.521
H15	0.992	0.912	0.879	C73	0.151	0.912	0.526	C112	0.683	0.802	0.529
H16	0.927	0.750	0.158	C74	0.105	0.858	0.519	C113	0.618	0.702	0.515
C33	0.638	0.963	0.012	H37	0.937	0.600	0.522	C114	0.635	0.816	0.529

C34	0.596	0.963	0.867	H38	0.246	0.960	0.545	H65	0.727	0.836	0.535
C35	0.667	0.011	0.140	C75	0.044	0.600	0.504	C115	0.570	0.715	0.518
C36	0.585	0.010	0.846	C76	0.102	0.605	0.494	H66	0.610	0.657	0.515
H17	0.573	0.925	0.765	C77	0.148	0.660	0.498	C116	0.577	0.772	0.523
C37	0.656	0.059	0.119	H39	0.007	0.558	0.499	H67	0.642	0.860	0.539
H18	0.699	0.012	0.258	C78	0.245	0.773	0.524	H68	0.525	0.681	0.516
C38	0.615	0.060	0.970	C79	0.280	0.875	0.549	N5	0.119	0.364	0.517
H19	0.553	0.009	0.729	H40	0.316	0.918	0.562	N6	0.139	0.157	0.540
H20	0.679	0.097	0.219	C80	0.293	0.828	0.539	N7	0.726	0.736	0.533
C39	0.400	0.687	0.020	H41	0.059	0.855	0.511	N8	0.526	0.781	0.539
C40	0.389	0.732	0.105	H42	0.997	0.781	0.512	C117	0.106	0.111	0.441
C41	0.351	0.640	0.929	H43	0.255	0.736	0.509	H69	0.072	0.108	0.325
C42	0.334	0.732	0.095	H44	0.193	0.663	0.494	C118	0.150	0.407	0.417
H21	0.425	0.769	0.180	C81	0.115	0.555	0.477	H70	0.184	0.407	0.306
C43	0.296	0.640	0.919	C82	0.157	0.553	0.340	C119	0.729	0.690	0.476
H22	0.357	0.604	0.859	C83	0.086	0.509	0.598	H71	0.692	0.652	0.403
C44	0.286	0.686	0.999	C84	0.169	0.506	0.321	C120	0.522	0.827	0.490
H23	0.327	0.768	0.158	H45	0.180	0.589	0.243	H72	0.559	0.864	0.421

Kagome_PER@PDA-COF-1_AA (Space Group- P1)
a = 51.6678 Å, b = 51.6429Å, c = 7.20576 Å; α = 90.648 °, b = 89.9154 °, g = 59.9827 °

atom	*x*	*y*	*z*	*atom*	*x*	*y*	*z*	*atom*	*x*	*y*	*z*
C1	0.08787	0.96648	0.97996	C122	0.01803	0.3441	0.96686	C242	0.36129	0.61874	0.41002
C2	0.05923	0.99277	0.97951	C123	0.06738	0.32336	0.82963	C243	0.38123	0.64815	0.54635
C3	0.03284	0.99033	0.98408	C124	0.01537	0.37231	0.97115	C244	0.38929	0.59309	0.42274
C4	0.03581	0.96123	0.98753	H73	0.99972	0.34121	0.02123	H145	0.34261	0.61709	0.34896
C5	0.06442	0.93603	0.98061	C125	0.06468	0.35158	0.83396	C245	0.40918	0.6225	0.55912
C6	0.09085	0.93807	0.97833	H74	0.08791	0.30426	0.77165	H146	0.37803	0.66978	0.59666
C7	0.00418	0.01704	0.98379	C126	0.03858	0.37678	0.90439	C246	0.41392	0.59437	0.49729
C8	0.00868	0.95876	0.99504	H75	0.99496	0.3911	0.03244	H147	0.392	0.57186	0.36812
C9	0.98003	0.98547	0.991	H76	0.08307	0.35405	0.7764	H148	0.42755	0.62437	0.62279
C10	0.97705	0.01454	0.98337	C127	0.03578	0.40679	0.90789	C247	0.44378	0.56715	0.50878
C11	0.95364	0.98303	0.99324	C128	0.06096	0.41013	0.9145	C248	0.46996	0.56875	0.50783
C12	0.95614	0.95435	0.997	C129	0.00714	0.43301	0.90502	C249	0.44632	0.53851	0.51856
C13	0.98399	0.9283	0.00242	C130	0.05822	0.43893	0.91614	C250	0.49854	0.54245	0.51471
C14	0.00999	0.93111	0.00455	H77	0.08356	0.39043	0.9208	H149	0.46902	0.59046	0.49764
H1	0.10774	0.96912	0.98233	C131	0.00331	0.4618	0.91289	C251	0.4739	0.51201	0.5198
H2	0.93546	0.95316	0.9914	H78	0.98743	0.43025	0.89477	H150	0.42561	0.53746	0.52573
C15	0.05669	0.02147	0.97173	C132	0.02921	0.46513	0.91617	C252	0.50073	0.51372	0.51818
C16	0.0288	0.04754	0.97284	C133	0.08417	0.44182	0.91777	C253	0.52497	0.54451	0.5153
C17	0.00283	0.04475	0.98245	C134	0.97352	0.48874	0.91676	C254	0.47615	0.4825	0.52141
H3	0.07738	0.02258	0.96093	C135	0.02684	0.49398	0.9195	C255	0.5297	0.48743	0.51863
C18	0.94846	0.03965	0.97253	C136	0.08193	0.46989	0.92426	C256	0.55325	0.51893	0.51269
C19	0.92501	0.00928	0.98837	H79	0.1062	0.42128	0.91151	H151	0.52252	0.56696	0.51868
H4	0.90512	0.00672	0.99574	C137	0.97111	0.51761	0.9167	C257	0.5051	0.45619	0.5221
C20	0.92205	0.03758	0.97576	C138	0.94738	0.48705	0.92136	C258	0.45083	0.47933	0.5191
H5	0.03187	0.91058	0.01426	C139	0.99704	0.5209	0.91627	C259	0.53191	0.45794	0.52134
H6	0.06685	0.91364	0.97488	C140	0.05297	0.49569	0.92707	C260	0.55504	0.49057	0.51261
H7	0.94603	0.06194	0.9587	C141	0.10889	0.47305	0.92689	C261	0.58088	0.52093	0.5072
H8	0.98093	0.06536	0.98938	C142	0.94208	0.54381	0.91727	C262	0.50732	0.42743	0.52259
C21	0.02589	0.07752	0.96082	C143	0.91841	0.51279	0.91748	C263	0.45261	0.45099	0.52394
C22	0.99996	0.10194	0.88675	H80	0.94903	0.46503	0.92945	H152	0.42855	0.49936	0.51121
C23	0.04897	0.08264	0.02137	C144	0.99322	0.54965	0.91232	C264	0.55947	0.43146	0.52155
C24	0.99735	0.13003	0.8732	H81	0.05134	0.51772	0.93691	H153	0.57733	0.47047	0.50564
H9	0.98167	0.09899	0.83284	C145	0.10804	0.49906	0.85968	C265	0.60853	0.49733	0.56949
C25	0.0464	0.11071	0.00792	C146	0.13635	0.45012	0.9959	C266	0.58048	0.54656	0.43718
H10	0.0692	0.06446	0.08474	C147	0.91613	0.54088	0.91509	C267	0.48087	0.42539	0.52685
C26	0.0205	0.135	0.9332	C148	0.93936	0.57263	0.91989	C268	0.53594	0.40108	0.51541
H11	0.97704	0.1485	0.81219	C149	0.89173	0.50913	0.91461	C269	0.42483	0.44923	0.52182
H12	0.06465	0.11408	0.05762	C150	0.96459	0.57591	0.91686	C270	0.56208	0.40274	0.51349
C27	0.89224	0.06492	0.96539	H82	0.013	0.55233	0.90422	H154	0.58013	0.43261	0.52804
C28	0.8675	0.06378	0.89176	C151	0.1334	0.50202	0.86146	C271	0.63455	0.49905	0.55954
C29	0.8876	0.09297	0.02843	H83	0.08744	0.51714	0.79918	H155	0.60986	0.47731	0.63134
C30	0.8395	0.08946	0.88107	C152	0.16171	0.45303	0.99769	C272	0.60643	0.54841	0.42822
H13	0.87015	0.0426	0.83678	H84	0.1379	0.42978	0.05412	H156	0.55968	0.56526	0.38322
C31	0.85962	0.11867	0.01795	H85	0.8941	0.56138	0.90905	H157	0.48325	0.40301	0.53362
H14	0.90602	0.09477	0.09193	H86	0.91676	0.59239	0.92665	H158	0.53697	0.37927	0.50729

C32	0.835	0.1174	0.94382	C153	0.89376	0.48259	0.84273	C273	0.39735	0.47322	0.58781
H15	0.8207	0.08793	0.82091	C154	0.86365	0.53167	0.98327	C274	0.42484	0.42365	0.45002
H16	0.85653	0.14019	0.06971	C155	0.96223	0.60573	0.91936	C275	0.59214	0.37574	0.49946
C33	0.98667	0.89835	0.9994	C156	0.16074	0.47907	0.93069	C276	0.63404	0.5246	0.48776
C34	0.0126	0.87316	0.92727	H87	0.13202	0.52244	0.80574	H159	0.65572	0.48042	0.61003
C35	0.9632	0.8941	0.06355	H88	0.18275	0.435	0.05399	H160	0.60536	0.56856	0.37023
C36	0.0148	0.84517	0.91736	C157	0.86904	0.47858	0.84187	C277	0.37106	0.47199	0.57891
H17	0.03121	0.87544	0.87161	H89	0.91484	0.46486	0.7812	H161	0.39641	0.49319	0.65122
C37	0.96534	0.86614	0.05355	C158	0.83889	0.5277	0.98244	C278	0.39858	0.42235	0.44129
H18	0.94293	0.9129	0.12601	H90	0.86117	0.55251	0.04336	H162	0.44558	0.40462	0.39408
C38	0.99115	0.84111	0.97918	C159	0.93667	0.63132	0.85205	C279	0.59767	0.34748	0.55965
H19	0.03514	0.82611	0.85727	C160	0.98576	0.60945	0.98893	C280	0.61638	0.3776	0.42337
H20	0.94678	0.8634	0.10481	C161	0.84115	0.50096	0.91278	C281	0.37111	0.44658	0.50396
C39	0.12061	0.91055	0.97265	H91	0.87133	0.45771	0.78347	H163	0.34997	0.49094	0.63158
C40	0.12473	0.883	0.03766	H92	0.81734	0.54541	0.03882	H164	0.39927	0.40228	0.38143
C41	0.14585	0.91088	0.90007	C162	0.93495	0.65912	0.85212	C282	0.62607	0.32234	0.54515
C42	0.15259	0.85708	0.02886	H93	0.91797	0.62955	0.79299	H165	0.57964	0.34507	0.62373
H21	0.10602	0.88173	0.10121	C163	0.9841	0.63719	0.98895	C283	0.64479	0.35251	0.40896
C43	0.17376	0.88497	0.89137	H94	0.00566	0.5904	0.04909	H166	0.61301	0.39887	0.36871
H22	0.14366	0.93161	0.84382	C164	0.95865	0.66262	0.91964	C284	0.65022	0.32437	0.46981
C44	0.17768	0.8575	0.95498	H95	0.91492	0.67856	0.79594	H167	0.62992	0.30063	0.59481
H23	0.15526	0.83597	0.08169	H96	0.0027	0.6394	0.04527	H168	0.66306	0.35474	0.34688
H24	0.19284	0.886	0.83128	C165	0.81548	0.49616	0.91209	C285	0.99344	0.8117	0.46173
C45	0.03376	0.19915	0.97681	N9	0.79089	0.51456	0.99696	N17	0.97329	0.8068	0.53132
C46	0.06016	0.20097	0.97964	H97	0.81871	0.47578	0.83351	H169	0.01331	0.79418	0.38092
C47	0.00577	0.22597	0.97608	C166	0.76583	0.51083	0.00245	C286	0.97503	0.77888	0.519
C48	0.05887	0.22853	0.97214	C167	0.73866	0.53584	0.06316	C287	0.00234	0.75133	0.51667
H25	0.08196	0.18023	0.98405	C168	0.76615	0.48385	0.95801	C288	0.94787	0.77845	0.51994
C49	0.00447	0.25354	0.97234	C169	0.71234	0.53464	0.07037	C289	0.00227	0.72442	0.50932
H26	0.98482	0.22529	0.98292	H98	0.73844	0.55656	0.10347	H170	0.02384	0.75089	0.52492
C50	0.03089	0.25532	0.9654	C170	0.73997	0.48243	0.96858	C290	0.9478	0.75155	0.50875
H27	0.07981	0.22923	0.97589	H99	0.78703	0.46363	0.91544	H171	0.92657	0.79975	0.52563
H28	0.98264	0.27427	0.9709	C171	0.71257	0.50798	0.01939	C291	0.97512	0.72405	0.50006
C51	0.23945	0.77953	0.01672	H100	0.69157	0.55426	0.12083	H172	0.02356	0.70308	0.50661
C52	0.23996	0.75194	0.02655	H101	0.74032	0.46155	0.93063	H173	0.92631	0.75191	0.5109
C53	0.2669	0.77945	0.01796	N10	0.68676	0.50557	0.02825	N18	0.97673	0.69616	0.49485
C54	0.26693	0.72499	0.02716	C172	0.66124	0.52669	0.97256	C292	0.95669	0.69194	0.41641
H29	0.21871	0.75184	0.03	H102	0.65861	0.54746	0.90575	H174	0.93716	0.71007	0.34005
C55	0.29386	0.75254	0.02243	C173	0.34352	0.44521	0.98739	C293	0.80534	0.14419	0.43191
H30	0.26718	0.80063	0.01971	N11	0.31851	0.46593	0.05634	N19	0.79982	0.16917	0.50814
C56	0.29436	0.72492	0.02195	H103	0.34545	0.42542	0.90773	H175	0.788	0.14165	0.35212
H31	0.26671	0.70382	0.03628	C174	0.29218	0.46449	0.0446	C294	0.7713	0.19461	0.50732
H32	0.31515	0.75256	0.02228	C175	0.26468	0.49166	0.03689	C295	0.74471	0.19311	0.51762
N1	0.0367	0.17072	0.98666	C176	0.29188	0.43724	0.05091	C296	0.76927	0.22294	0.50971
N2	0.02787	0.28384	0.96468	C177	0.23777	0.4917	0.02426	C297	0.71701	0.21925	0.52398
N3	0.21154	0.80577	0.01873	H104	0.2647	0.51295	0.0361	H176	0.74574	0.17133	0.52531
N4	0.32229	0.69879	0.02847	C178	0.26493	0.43732	0.04199	C298	0.74155	0.24907	0.51233
C57	0.04733	0.28913	0.88824	H105	0.31284	0.41586	0.06712	H177	0.7899	0.2242	0.50537
H33	0.06746	0.27144	0.8102	C179	0.23755	0.46438	0.02259	C299	0.71491	0.24759	0.51641
C58	0.01742	0.16467	0.91532	H106	0.21667	0.5132	0.01904	H178	0.69642	0.21795	0.53144
H34	0.99762	0.18146	0.83417	H107	0.26486	0.41606	0.04604	H179	0.74063	0.27083	0.51561
C59	0.20704	0.83022	0.94328	N12	0.21146	0.46255	0.01366	N20	0.68633	0.27292	0.52511
H35	0.22487	0.83189	0.86343	C180	0.18749	0.48208	0.93174	C300	0.68019	0.29807	0.45249
C60	0.32729	0.67375	0.95576	H108	0.18592	0.50172	0.85577	H180	0.69703	0.30115	0.3709
H36	0.30988	0.6714	0.87548	C181	0.08787	0.96648	0.47996	C301	0.04411	0.31902	0.39564
C61	0.35672	0.64676	0.97137	C182	0.05923	0.99277	0.47951	C302	0.01803	0.3441	0.46686
C62	0.36129	0.61874	0.91002	C183	0.03284	0.99033	0.48408	C303	0.06738	0.32336	0.32963
C63	0.38123	0.64815	0.04635	C184	0.03581	0.96123	0.48753	C304	0.01537	0.37231	0.47115
C64	0.38929	0.59309	0.92274	C185	0.06442	0.93603	0.48061	H181	0.99972	0.34121	0.52123
H37	0.34261	0.61709	0.84896	C186	0.09085	0.93807	0.47833	C305	0.06468	0.35158	0.33396
C65	0.40918	0.6225	0.05912	C187	0.00418	0.01704	0.48379	H182	0.08791	0.30426	0.27165
H38	0.37803	0.66978	0.09666	C188	0.00868	0.95876	0.49504	C306	0.03858	0.37678	0.40439
C66	0.41392	0.59437	0.99729	C189	0.98003	0.98547	0.491	H183	0.99496	0.3911	0.53244
H39	0.392	0.57186	0.86812	C190	0.97705	0.01454	0.48337	H184	0.08307	0.35405	0.2764
H40	0.42755	0.62437	0.12279	C191	0.95364	0.98303	0.49324	C307	0.03578	0.40679	0.40789
C67	0.44378	0.56715	0.00878	C192	0.95614	0.95435	0.497	C308	0.06096	0.41013	0.4145
C68	0.46996	0.56875	0.00783	C193	0.98399	0.9283	0.50242	C309	0.00714	0.43301	0.40502
C69	0.44632	0.53851	0.01856	C194	0.00999	0.93111	0.50455	C310	0.05822	0.43893	0.41614
C70	0.49854	0.54245	0.01471	H109	0.10774	0.96912	0.48233	H185	0.08356	0.39043	0.4208
H41	0.46902	0.59046	0.99764	H110	0.93546	0.95316	0.4914	C311	0.00331	0.4618	0.41289
C71	0.4739	0.51201	0.0198	C195	0.05669	0.02147	0.47173	H186	0.98743	0.43025	0.39477

H42	0.42561	0.53746	0.02573	C196	0.0288	0.04754	0.47284	C312	0.02921	0.46513	0.41617
C72	0.50073	0.51372	0.01818	C197	0.00283	0.04475	0.48245	C313	0.08417	0.44182	0.41777
C73	0.52497	0.54451	0.0153	H111	0.07738	0.02258	0.46093	C314	0.97352	0.48874	0.41676
C74	0.47615	0.4825	0.02141	C198	0.94846	0.03965	0.47253	C315	0.02684	0.49398	0.4195
C75	0.5297	0.48743	0.01863	C199	0.92501	0.00928	0.48837	C316	0.08193	0.46989	0.42426
C76	0.55325	0.51893	0.01269	H112	0.90512	0.00672	0.49574	H187	0.1062	0.42128	0.41151
H43	0.52252	0.56696	0.01868	C200	0.92205	0.03758	0.47576	C317	0.97111	0.51761	0.4167
C77	0.5051	0.45619	0.0221	H113	0.03187	0.91058	0.51426	C318	0.94738	0.48705	0.42136
C78	0.45083	0.47933	0.0191	H114	0.06685	0.91364	0.47488	C319	0.99704	0.5209	0.41627
C79	0.53191	0.45794	0.02134	H115	0.94603	0.06194	0.4587	C320	0.05297	0.49569	0.42707
C80	0.55504	0.49057	0.01261	H116	0.98093	0.06536	0.48938	C321	0.10889	0.47305	0.42689
C81	0.58088	0.52093	0.0072	C201	0.02589	0.07752	0.46082	C322	0.94208	0.54381	0.41727
C82	0.50732	0.42743	0.02259	C202	0.99996	0.10194	0.38675	C323	0.91841	0.51279	0.41748
C83	0.45261	0.45099	0.02394	C203	0.04897	0.08264	0.52137	H188	0.94903	0.46503	0.42945
H44	0.42855	0.49936	0.01121	C204	0.99735	0.13003	0.3732	C324	0.99322	0.54965	0.41232
C84	0.55947	0.43146	0.02155	H117	0.98167	0.09899	0.33284	H189	0.05134	0.51772	0.43691
H45	0.57733	0.47047	0.00564	C205	0.0464	0.11071	0.50792	C325	0.10804	0.49906	0.35968
C85	0.60853	0.49733	0.06949	H118	0.0692	0.06446	0.58474	C326	0.13635	0.45012	0.4959
C86	0.58048	0.54656	0.93718	C206	0.0205	0.135	0.4332	C327	0.91613	0.54088	0.41509
C87	0.48087	0.42539	0.02685	H119	0.97704	0.1485	0.31219	C328	0.93936	0.57263	0.41989
C88	0.53594	0.40108	0.01541	H120	0.06465	0.11408	0.55762	C329	0.89173	0.50913	0.41461
C89	0.42483	0.44923	0.02182	C207	0.89224	0.06492	0.46539	C330	0.96459	0.57591	0.41686
C90	0.56208	0.40274	0.01349	C208	0.8675	0.06378	0.39176	H190	0.013	0.55233	0.40422
H46	0.58013	0.43261	0.02804	C209	0.8876	0.09297	0.52843	C331	0.1334	0.50202	0.36146
C91	0.63455	0.49905	0.05954	C210	0.8395	0.08946	0.38107	H191	0.08744	0.51714	0.29918
H47	0.60986	0.47731	0.13134	H121	0.87015	0.0426	0.33678	C332	0.16171	0.45303	0.49769
C92	0.60643	0.54841	0.92822	C211	0.85962	0.11867	0.51795	H192	0.1379	0.42978	0.55412
H48	0.55968	0.56526	0.88322	H122	0.90602	0.09477	0.59193	H193	0.8941	0.56138	0.40905
H49	0.48325	0.40301	0.03362	C212	0.835	0.1174	0.44382	H194	0.91676	0.59239	0.42665
H50	0.53697	0.37927	0.00729	H123	0.8207	0.08793	0.32091	C333	0.89376	0.48259	0.34273
C93	0.39735	0.47322	0.08781	H124	0.85653	0.14019	0.56971	C334	0.86365	0.53167	0.48327
C94	0.42484	0.42365	0.95002	C213	0.98667	0.89835	0.4994	C335	0.96223	0.60573	0.41936
C95	0.59214	0.37574	0.99946	C214	0.0126	0.87316	0.42727	C336	0.16074	0.47907	0.43069
C96	0.63404	0.5246	0.98776	C215	0.9632	0.8941	0.56355	H195	0.13202	0.52244	0.30574
H51	0.65572	0.48042	0.11003	C216	0.0148	0.84517	0.41736	H196	0.18275	0.435	0.55399
H52	0.60536	0.56856	0.87023	H125	0.03121	0.87544	0.37161	C337	0.86904	0.47858	0.34187
C97	0.37106	0.47199	0.07891	C217	0.96534	0.86614	0.55355	H197	0.91484	0.46486	0.2812
H53	0.39641	0.49319	0.15122	H126	0.94293	0.9129	0.62601	C338	0.83889	0.5277	0.48244
C98	0.39858	0.42235	0.94129	C218	0.99115	0.84111	0.47918	H198	0.86117	0.55251	0.54336
H54	0.44558	0.40462	0.89408	H127	0.03514	0.82611	0.35727	C339	0.93667	0.63132	0.35205
C99	0.59767	0.34748	0.05965	H128	0.94678	0.8634	0.60481	C340	0.98576	0.60945	0.48893
C100	0.61638	0.3776	0.92337	C219	0.12061	0.91055	0.47265	C341	0.84115	0.50096	0.41278
C101	0.37111	0.44658	0.00396	C220	0.12473	0.883	0.53766	H199	0.87133	0.45771	0.28347
H55	0.34997	0.49094	0.13158	C221	0.14585	0.91088	0.40007	H200	0.81734	0.54541	0.53882
H56	0.39927	0.40228	0.88143	C222	0.15259	0.85708	0.52886	C342	0.93495	0.65912	0.35212
C102	0.62607	0.32234	0.04515	H129	0.10602	0.88173	0.60121	H201	0.91797	0.62955	0.29299
H57	0.57964	0.34507	0.12373	C223	0.17376	0.88497	0.39137	C343	0.9841	0.63719	0.48895
C103	0.64479	0.35251	0.90896	H130	0.14366	0.93161	0.34382	H202	0.00566	0.5904	0.54909
H58	0.61301	0.39887	0.86871	C224	0.17768	0.8575	0.45498	C344	0.95865	0.66262	0.41964
C104	0.65022	0.32437	0.96981	H131	0.15526	0.83597	0.58169	H203	0.91492	0.67856	0.29594
H59	0.62992	0.30063	0.09481	H132	0.19284	0.886	0.33128	H204	0.0027	0.6394	0.54527
H60	0.66306	0.35474	0.84688	C225	0.03376	0.19915	0.47681	C345	0.81548	0.49616	0.41209
C105	0.99344	0.8117	0.96173	C226	0.06016	0.20097	0.47964	N21	0.79089	0.51456	0.49696
N5	0.97329	0.8068	0.03132	C227	0.00577	0.22597	0.47608	H205	0.81871	0.47578	0.33351
H61	0.01331	0.79418	0.88092	C228	0.05887	0.22853	0.47214	C346	0.76583	0.51083	0.50245
C106	0.97503	0.77888	0.019	H133	0.08196	0.18023	0.48405	C347	0.73866	0.53584	0.56316
C107	0.00234	0.75133	0.01667	C229	0.00447	0.25354	0.47234	C348	0.76615	0.48385	0.45801
C108	0.94787	0.77845	0.01994	H134	0.98482	0.22529	0.48292	C349	0.71234	0.53464	0.57037
C109	0.00227	0.72442	0.00932	C230	0.03089	0.25532	0.4654	H206	0.73844	0.55656	0.60347
H62	0.02384	0.75089	0.02492	H135	0.07981	0.22923	0.47589	C350	0.73997	0.48243	0.46858
C110	0.9478	0.75155	0.00875	H136	0.98264	0.27427	0.4709	H207	0.78703	0.46363	0.41544
H63	0.92657	0.79975	0.02563	C231	0.23945	0.77953	0.51672	C351	0.71257	0.50798	0.51939
C111	0.97512	0.72405	0.00006	C232	0.23996	0.75194	0.52655	H208	0.69157	0.55426	0.62083
H64	0.02356	0.70308	0.00661	C233	0.2669	0.77945	0.51796	H209	0.74032	0.46155	0.43063
H65	0.92631	0.75191	0.0109	C234	0.26693	0.72499	0.52716	N22	0.68676	0.50557	0.52825
N6	0.97673	0.69616	0.99485	H137	0.21871	0.75184	0.53	C352	0.66124	0.52669	0.47256
C112	0.95669	0.69194	0.91641	C235	0.29386	0.75254	0.52243	H210	0.65861	0.54746	0.40575
H66	0.93716	0.71007	0.84005	H138	0.26718	0.80063	0.51971	C353	0.34352	0.44521	0.48739
C113	0.80534	0.14419	0.93191	C236	0.29436	0.72492	0.52195	N23	0.31851	0.46593	0.55634
N7	0.79982	0.16917	0.00814	H139	0.26671	0.70382	0.53628	H211	0.34545	0.42542	0.40773
H67	0.788	0.14165	0.85212	H140	0.31515	0.75256	0.52228	C354	0.29218	0.46449	0.5446

C114	0.7713	0.19461	0.00732	N13	0.0367	0.17072	0.48666	C355	0.26468	0.49166	0.53689
C115	0.74471	0.19311	0.01762	N14	0.02787	0.28384	0.46468	C356	0.29188	0.43724	0.55091
C116	0.76927	0.22294	0.00971	N15	0.21154	0.80577	0.51873	C357	0.23777	0.4917	0.52426
C117	0.71701	0.21925	0.02398	N16	0.32229	0.69879	0.52847	H212	0.2647	0.51295	0.5361
H68	0.74574	0.17133	0.02531	C237	0.04733	0.28913	0.38824	C358	0.26493	0.43732	0.54199
C118	0.74155	0.24907	0.01233	H141	0.06746	0.27144	0.3102	H213	0.31284	0.41586	0.56712
H69	0.7899	0.2242	0.00537	C238	0.01742	0.16467	0.41532	C359	0.23755	0.46438	0.52259
C119	0.71491	0.24759	0.01641	H142	0.99762	0.18146	0.33417	H214	0.21667	0.5132	0.51904
H70	0.69642	0.21795	0.03144	C239	0.20704	0.83022	0.44328	H215	0.26486	0.41606	0.54604
H71	0.74063	0.27083	0.01561	H143	0.22487	0.83189	0.36343	N24	0.21146	0.46255	0.51366
N8	0.68633	0.27292	0.02511	C240	0.32729	0.67375	0.45576	C360	0.18749	0.48208	0.43174
C120	0.68019	0.29807	0.95249	H144	0.30988	0.6714	0.37548	H216	0.18592	0.50172	0.35577
C1	0.08787	0.96648	0.97996	C122	0.01803	0.3441	0.96686	C242	0.36129	0.61874	0.41002
C2	0.05923	0.99277	0.97951	C123	0.06738	0.32336	0.82963	C243	0.38123	0.64815	0.54635

Kagome_PER@PDA-COF-1_AB (Space Group- P1)
a = 51.6378 Å, b = 51.5727 Å, c = 6.27591 Å; α = 89.9595 °, b = 89.9062 °, g = 59.8107 °

atom	*x*	*y*	*z*	*atom*	*x*	*y*	*z*	*atom*	*x*	*y*	*z*
C1	0.08734	0.96819	0.98231	C121	0.04396	0.31905	0.8653	C241	0.69006	0.98236	0.49197
C2	0.05837	0.9941	0.98929	C122	0.0259	0.34032	0.02062	C242	0.69833	0.95812	0.35122
C3	0.03236	0.99101	0.98432	C123	0.05968	0.32692	0.71931	C243	0.71019	0.97922	0.65544
C4	0.0362	0.96144	0.97788	C124	0.02345	0.36848	0.02816	C244	0.72592	0.93179	0.37169
C5	0.06521	0.93668	0.9624	H73	0.01357	0.3345	0.13633	H145	0.68305	0.96002	0.22185
C6	0.09131	0.93944	0.96208	C125	0.05737	0.35505	0.72772	C245	0.73781	0.95295	0.6754
C7	0.00335	0.01754	0.98167	H74	0.07384	0.31075	0.59592	H146	0.70392	0.99795	0.76702
C8	0.00939	0.95824	0.98061	C126	0.03907	0.37641	0.8816	C246	0.74624	0.92882	0.53309
C9	0.9804	0.98483	0.97244	H75	0.0094	0.38447	0.15252	H147	0.73202	0.91349	0.25655
C10	0.97667	0.01432	0.97281	H76	0.06966	0.36064	0.61007	H148	0.75299	0.95114	0.80499
C11	0.95439	0.98174	0.96393	C127	0.03603	0.40668	0.88941	C247	0.77625	0.90126	0.54376
C12	0.95756	0.95276	0.96552	C128	0.06105	0.41021	0.8828	C248	0.8021	0.90319	0.56302
C13	0.9856	0.92675	0.9814	C129	0.00715	0.43258	0.90634	C249	0.77909	0.87253	0.52323
C14	0.01126	0.93022	0.99063	C130	0.05786	0.43925	0.89584	C250	0.83094	0.87704	0.5474
H1	0.10666	0.97167	0.9901	H77	0.08372	0.39042	0.87324	H149	0.80054	0.92521	0.57909
H2	0.93691	0.9516	0.95439	C131	0.00293	0.46158	0.91556	C251	0.80702	0.84617	0.51412
C15	0.05527	0.02313	0.99391	H78	0.98772	0.42923	0.90958	H150	0.75837	0.87146	0.51577
C16	0.02706	0.04885	0.98634	C132	0.02865	0.46529	0.91087	C252	0.83368	0.84823	0.51945
C17	0.00132	0.04566	0.98133	C133	0.08367	0.44236	0.89893	C253	0.857	0.87966	0.55095
H3	0.07561	0.02499	0.9945	C134	0.973	0.48832	0.9346	C254	0.80985	0.81647	0.49512
C18	0.9477	0.03923	0.96475	C135	0.0261	0.49427	0.9226	C255	0.86299	0.82245	0.49323
C19	0.92534	0.0077	0.95315	C136	0.08147	0.4704	0.91755	C256	0.88544	0.85505	0.51209
H4	0.90557	0.00488	0.94829	H79	0.10562	0.42166	0.88932	H151	0.85391	0.90206	0.58127
C20	0.92184	0.03629	0.95435	C137	0.97045	0.51726	0.9505	C257	0.83915	0.79047	0.47992
H5	0.03344	0.90998	0.0058	C138	0.94687	0.48646	0.93573	C258	0.78478	0.8128	0.49412
H6	0.06805	0.91414	0.94844	C139	0.99606	0.52113	0.93825	C259	0.8658	0.79261	0.47752
H7	0.94437	0.06204	0.96245	C140	0.05222	0.49611	0.9259	C260	0.88781	0.82654	0.48306
H8	0.97924	0.06627	0.9786	C141	0.10865	0.47321	0.93319	C261	0.91197	0.85902	0.50196
C21	0.02409	0.07905	0.97341	C142	0.94141	0.54324	0.97629	C262	0.84191	0.76147	0.46658
C22	0.0054	0.09992	0.8185	C143	0.91799	0.51219	0.95883	C263	0.78732	0.78418	0.47623
C23	0.04069	0.08714	0.10878	H80	0.94821	0.46455	0.92088	H152	0.76212	0.83251	0.50379
C24	0.00378	0.12763	0.79754	C144	0.99169	0.55021	0.94073	C264	0.89369	0.76622	0.46756
H9	0.99238	0.09419	0.70902	H81	0.05016	0.51833	0.93719	H153	0.91007	0.80708	0.45057
C25	0.03893	0.1149	0.08866	C145	0.10686	0.50133	0.95789	C265	0.94169	0.83457	0.50822
H10	0.05508	0.07152	0.23354	C146	0.13769	0.44754	0.92719	C266	0.90818	0.88811	0.4853
C26	0.02063	0.13557	0.93133	C147	0.91553	0.54017	0.98363	C267	0.81575	0.75882	0.46285
H11	0.98935	0.14334	0.67314	C148	0.93834	0.57215	0.98927	C268	0.87078	0.73536	0.46
H12	0.05209	0.12082	0.19534	C149	0.89076	0.50929	0.95034	C269	0.75967	0.78198	0.47039
C27	0.89164	0.06363	0.94617	C150	0.96293	0.57629	0.96635	C270	0.89692	0.73711	0.46342
C28	0.87019	0.06632	0.79554	H82	0.01119	0.5532	0.92117	H154	0.91402	0.76798	0.46509
C29	0.88394	0.08757	0.08895	C151	0.1325	0.50366	0.97855	C271	0.96612	0.83904	0.49984
C30	0.84202	0.09218	0.7869	H83	0.08507	0.52223	0.96272	H155	0.94618	0.81138	0.52049
H13	0.87574	0.04812	0.68061	C152	0.16332	0.44981	0.94573	C272	0.93253	0.89267	0.48195
C31	0.85575	0.1133	0.08126	H84	0.14085	0.42494	0.90679	H156	0.88569	0.90802	0.47311
H14	0.90009	0.08592	0.21026	H85	0.89331	0.56045	0.00037	H157	0.8183	0.73632	0.45296
C32	0.83434	0.1161	0.92955	H86	0.91565	0.59132	0.01494	H158	0.87175	0.71357	0.45389
H15	0.8257	0.09391	0.66651	C153	0.887	0.4932	0.78328	C273	0.73607	0.79822	0.6161
H16	0.84994	0.13181	0.19398	C154	0.86785	0.5231	0.10447	C274	0.75611	0.76419	0.31574
C33	0.98824	0.89671	0.9845	C155	0.95906	0.60684	0.96716	C275	0.92696	0.70961	0.46608
C34	0.01626	0.8698	0.97976	C156	0.16127	0.47793	0.97273	C276	0.9621	0.86819	0.4894
C35	0.9623	0.89397	0.99007	H87	0.13002	0.52601	0.99951	H159	0.98901	0.81956	0.50304

C36	0.01818	0.84184	0.97923	H88	0.18557	0.4294	0.94121	H160	0.92861	0.91571	0.47077
H17	0.03735	0.8702	0.97513	C157	0.86107	0.49126	0.76927	C277	0.70979	0.79692	0.6061
C37	0.96414	0.86613	0.99223	H89	0.90438	0.4825	0.65956	H161	0.73837	0.8119	0.74117
H18	0.93976	0.91391	0.99415	C158	0.84208	0.5209	0.09172	C278	0.72976	0.76298	0.30518
C38	0.9922	0.83942	0.98746	H90	0.87036	0.53554	0.23782	H162	0.77402	0.75151	0.19863
H19	0.04042	0.8214	0.97462	C159	0.93018	0.63271	0.95715	C279	0.93008	0.68071	0.46491
H20	0.94352	0.86481	0.9965	C160	0.98382	0.61146	0.97581	C280	0.95364	0.71097	0.47251
C39	0.12187	0.9129	0.94563	C161	0.83814	0.50511	0.92312	C281	0.70605	0.77946	0.44936
C40	0.12732	0.88327	0.96776	H91	0.8585	0.47885	0.63584	H163	0.69157	0.80974	0.72083
C41	0.14701	0.91647	0.91096	H92	0.82441	0.53171	0.21342	H164	0.7274	0.74918	0.18114
C42	0.15635	0.85882	0.96477	C162	0.92623	0.66147	0.95838	C282	0.95808	0.65477	0.468
H21	0.10879	0.87885	0.99206	H93	0.90995	0.63075	0.94757	H165	0.91033	0.6779	0.46081
C43	0.1761	0.89211	0.91291	C163	0.97996	0.64018	0.97318	C283	0.98173	0.68504	0.47297
H22	0.14418	0.93878	0.88176	H94	0.00685	0.59237	0.98595	H166	0.95299	0.73261	0.47513
C44	0.18137	0.86275	0.94299	C164	0.95107	0.66582	0.96576	C284	0.98453	0.65641	0.47034
H23	0.16006	0.83597	0.98472	H95	0.90339	0.68106	0.95175	H167	0.95969	0.63266	0.46651
H24	0.19511	0.89587	0.88883	H96	0.99969	0.64306	0.97858	H168	0.00194	0.68712	0.4765
C45	0.03398	0.19944	0.00156	C165	0.81074	0.50321	0.90688	C285	0.3243	0.14517	0.43829
C46	0.06087	0.20035	0.99991	N9	0.78955	0.51613	0.04525	N17	0.30709	0.1392	0.55122
C47	0.00625	0.22669	0.00136	H97	0.80918	0.4905	0.76636	H169	0.33954	0.12958	0.31087
C48	0.06021	0.22767	0.98573	C166	0.76351	0.51401	0.03772	C286	0.30734	0.11196	0.53329
H25	0.08249	0.17921	0.00276	C167	0.7357	0.53996	0.08159	C287	0.33438	0.08404	0.53096
C49	0.0056	0.25403	0.99677	C168	0.76447	0.48646	0.00159	C288	0.27972	0.11249	0.53289
H26	0.98507	0.22644	0.0108	C169	0.70926	0.53891	0.07571	C289	0.33363	0.05742	0.526
C50	0.03247	0.25489	0.98259	H98	0.73491	0.56134	0.11298	H170	0.35609	0.08321	0.53913
H27	0.08139	0.22796	0.98273	C170	0.73816	0.48513	0.00524	C290	0.27898	0.08589	0.51836
H28	0.98399	0.27519	0.99701	H99	0.78608	0.46578	0.97555	H171	0.25867	0.13419	0.53705
C51	0.24374	0.78416	0.98472	C171	0.71018	0.51148	0.03539	C291	0.30603	0.05799	0.51357
C52	0.24327	0.75763	0.03485	H100	0.68769	0.55939	0.10774	H172	0.35467	0.0357	0.52475
C53	0.27175	0.78221	0.94687	H101	0.739	0.46367	0.97675	H173	0.25726	0.0867	0.51656
C54	0.26954	0.72995	0.04248	N10	0.68412	0.50933	0.03846	N18	0.30665	0.0305	0.51231
H29	0.2216	0.75915	0.06809	C172	0.66049	0.52754	0.93311	C292	0.28996	0.02506	0.38978
C55	0.29807	0.75448	0.95415	H102	0.65981	0.54532	0.8251	H174	0.27436	0.04164	0.26846
H30	0.27312	0.80235	0.90963	C173	0.35017	0.43338	0.98051	C293	0.13301	0.46884	0.44914
C56	0.2974	0.72785	0.99639	N11	0.32346	0.4565	0.98516	N19	0.12807	0.49595	0.46252
H31	0.26829	0.70987	0.08428	H103	0.35486	0.40964	0.9686	H175	0.11475	0.46301	0.44504
H32	0.31974	0.75303	0.92222	C174	0.29724	0.45484	0.97972	C294	0.09953	0.52151	0.47244
N1	0.03568	0.17147	0.01816	C175	0.27044	0.482	0.93619	C295	0.0721	0.52232	0.43277
N2	0.03059	0.283	0.98161	C176	0.29558	0.42861	0.01834	C296	0.09877	0.54859	0.52436
N3	0.21576	0.81034	0.973	C177	0.24292	0.4832	0.93101	C297	0.04512	0.54944	0.44184
N4	0.32472	0.70081	0.99431	H104	0.27161	0.50237	0.90351	H176	0.07171	0.50176	0.39231
C57	0.04623	0.28948	0.85558	C178	0.26804	0.42979	0.0134	C298	0.07183	0.57563	0.53534
H33	0.06168	0.27339	0.7311	H105	0.3159	0.40708	0.0535	H177	0.11997	0.54798	0.55879
C58	0.01913	0.16463	0.90564	C179	0.24123	0.45711	0.9731	C299	0.04453	0.57658	0.48882
H34	0.0033	0.18009	0.78025	H106	0.22261	0.50456	0.89204	H178	0.02393	0.54998	0.40801
C59	0.21188	0.83702	0.95409	H107	0.26691	0.40936	0.04417	H179	0.07209	0.5961	0.58103
H35	0.23074	0.84198	0.94875	N12	0.21446	0.45653	0.96351	N20	0.01664	0.60305	0.49254
C60	0.32652	0.67507	0.96967	C180	0.18846	0.47987	0.99678	C300	0.01398	0.62911	0.46513
H36	0.30637	0.67245	0.94443	H108	0.18534	0.50221	0.0474	H180	0.03366	0.63225	0.43136
C61	0.35576	0.64752	0.96713	C181	0.42022	0.30137	0.43556	C301	0.38436	0.64898	0.45598
C62	0.35831	0.619	0.96866	C182	0.39111	0.32724	0.44918	C302	0.35542	0.67436	0.47456
C63	0.38232	0.64893	0.95856	C183	0.36533	0.32385	0.4678	C303	0.40887	0.65373	0.43735
C64	0.3863	0.59293	0.96231	C184	0.36928	0.29429	0.47585	C304	0.35125	0.70321	0.47789
H37	0.33802	0.61709	0.97609	C185	0.39832	0.26953	0.46618	H181	0.33592	0.67121	0.48918
C65	0.4102	0.62288	0.95092	C186	0.42398	0.27269	0.44603	C305	0.40456	0.68262	0.43471
H38	0.38084	0.67098	0.95641	C187	0.33625	0.35025	0.47986	H182	0.43172	0.63436	0.42111
C66	0.41308	0.59408	0.95313	C188	0.3428	0.29088	0.49698	C306	0.37568	0.70821	0.45692
H39	0.38679	0.57137	0.96401	C189	0.3137	0.31727	0.50368	H183	0.32828	0.72212	0.49832
H40	0.43002	0.62553	0.94259	C190	0.30959	0.34686	0.4868	H184	0.42448	0.68491	0.41398
C67	0.44305	0.56649	0.95044	C191	0.28785	0.31404	0.52267	C307	0.37165	0.73882	0.45732
C68	0.46925	0.56814	0.94928	C192	0.29122	0.28496	0.53589	C308	0.39632	0.74286	0.47802
C69	0.44617	0.53744	0.95465	C193	0.31945	0.25934	0.52136	C309	0.34284	0.76495	0.43676
C70	0.49806	0.54197	0.95616	C194	0.34504	0.26267	0.50378	C310	0.39323	0.77178	0.46956
H41	0.46839	0.58989	0.9445	H109	0.43987	0.30433	0.42282	H185	0.41904	0.7236	0.50025
C71	0.47401	0.51099	0.9645	H110	0.27101	0.28295	0.54651	C311	0.3385	0.79403	0.43802
H42	0.42578	0.53579	0.95214	C195	0.38759	0.35639	0.44738	H186	0.32332	0.76197	0.41888
C72	0.50073	0.51301	0.96696	C196	0.35949	0.38217	0.47179	C312	0.36415	0.79785	0.45
C73	0.52425	0.54456	0.95492	C197	0.33409	0.37837	0.48807	C313	0.41914	0.77477	0.47798
C74	0.47672	0.4812	0.97966	H111	0.40797	0.35794	0.42884	C314	0.30845	0.82098	0.42964
C75	0.53	0.48695	0.97979	C198	0.28049	0.37143	0.47024	C315	0.36164	0.82682	0.44156
C76	0.55269	0.51915	0.96553	C199	0.25878	0.33983	0.51809	C316	0.41668	0.80287	0.4628

H43	0.52167	0.56709	0.94889	H112	0.23952	0.33642	0.53867	H187	0.44135	0.75437	0.48927
C77	0.506	0.45528	0.0023	C200	0.25458	0.36843	0.48266	C317	0.30591	0.85	0.42747
C78	0.45178	0.4773	0.97268	H113	0.36714	0.24214	0.49644	C318	0.28232	0.81916	0.42979
C79	0.5327	0.45727	0.99595	H114	0.40186	0.24665	0.47104	C319	0.33167	0.85364	0.43002
C80	0.55512	0.49053	0.97904	H115	0.27738	0.39391	0.44446	C320	0.38777	0.82869	0.44557
C81	0.5802	0.52155	0.96095	H116	0.31187	0.3984	0.50848	C321	0.44401	0.80562	0.46057
C82	0.50862	0.42649	0.02803	C201	0.35624	0.41244	0.47911	C322	0.27667	0.87614	0.42319
C83	0.45401	0.44883	0.00021	C202	0.32785	0.43894	0.48135	C323	0.25308	0.84492	0.43242
H44	0.42951	0.49692	0.94401	C203	0.38176	0.41588	0.4841	H188	0.28434	0.79691	0.42911
C84	0.56058	0.43084	0.00258	C204	0.32517	0.46721	0.48502	C324	0.32748	0.88265	0.42556
H45	0.57775	0.47072	0.98582	H117	0.30706	0.43799	0.47837	H189	0.38637	0.85068	0.43846
C85	0.60472	0.50384	0.096	C205	0.37917	0.44405	0.48967	C325	0.44771	0.82326	0.30497
C86	0.5826	0.54144	0.81857	H118	0.40451	0.39623	0.48433	C326	0.46723	0.78998	0.60964
C87	0.48247	0.42399	0.03352	C206	0.35076	0.47034	0.48956	C327	0.25084	0.87307	0.42809
C88	0.53743	0.40025	0.04079	H119	0.30266	0.48731	0.48565	C328	0.27347	0.90521	0.41696
C89	0.42719	0.44532	0.9939	H120	0.39947	0.44595	0.49274	C329	0.22593	0.84201	0.44247
C90	0.5633	0.40215	0.02142	C207	0.22387	0.39458	0.46116	C330	0.29856	0.90863	0.41801
H46	0.58135	0.43182	0.99471	C208	0.19951	0.39019	0.41533	H190	0.34693	0.88596	0.42502
C91	0.63065	0.5058	0.0878	C209	0.21757	0.42442	0.48764	C331	0.4739	0.8248	0.29629
H47	0.60343	0.48845	0.21179	C210	0.17017	0.41408	0.41072	H191	0.4301	0.83548	0.18536
C92	0.60853	0.54344	0.81047	H121	0.20326	0.36761	0.38225	C332	0.49331	0.79166	0.60177
H48	0.56406	0.55528	0.70901	C211	0.18832	0.44841	0.47659	H192	0.46476	0.77642	0.73511
H49	0.48548	0.40157	0.06157	H122	0.23558	0.4293	0.5219	H193	0.22886	0.89381	0.43022
H50	0.53897	0.37823	0.05555	C212	0.16395	0.4437	0.44375	H194	0.25079	0.92507	0.41516
C93	0.39772	0.47017	0.00527	H123	0.15171	0.40973	0.37834	C333	0.22784	0.81389	0.47127
C94	0.43033	0.41651	0.97573	H124	0.18388	0.47146	0.49967	C334	0.19688	0.86749	0.42602
C95	0.59336	0.37465	0.01079	C213	0.32229	0.22921	0.511	C335	0.29562	0.93885	0.41321
C96	0.6331	0.52555	0.94422	C214	0.34006	0.20857	0.35161	C336	0.49725	0.80888	0.44371
H51	0.64956	0.49181	0.19431	C215	0.30602	0.22121	0.65085	H195	0.4764	0.83842	0.17134
H52	0.60987	0.559	0.69656	C216	0.34092	0.18124	0.32952	H196	0.51125	0.77931	0.71904
C97	0.37291	0.46632	0.99896	H125	0.35286	0.21423	0.23911	C337	0.20225	0.81134	0.48308
H53	0.39372	0.49315	0.02054	C217	0.30696	0.19386	0.62927	H197	0.24967	0.79322	0.48678
C98	0.40558	0.41256	0.97458	H126	0.29245	0.23659	0.77961	C338	0.1713	0.86503	0.43792
H54	0.45262	0.39637	0.96049	C218	0.32412	0.17355	0.4664	H198	0.19372	0.89003	0.40184
C99	0.602	0.35077	0.1558	H127	0.35453	0.16573	0.20131	C339	0.27679	0.96073	0.26429
C100	0.61361	0.37167	0.84843	H128	0.29395	0.18802	0.7386	C340	0.31202	0.94611	0.55686
C101	0.37628	0.43745	0.98583	C219	0.45417	0.24529	0.43967	C341	0.17346	0.83688	0.46657
H55	0.3502	0.48605	0.00584	C220	0.46185	0.22207	0.58921	H199	0.20476	0.78902	0.50656
H56	0.409	0.38973	0.96182	C221	0.47552	0.24157	0.28413	H200	0.14903	0.88531	0.42627
C102	0.62993	0.3248	0.13847	C222	0.48975	0.19598	0.58194	C342	0.27482	0.98871	0.25699
H57	0.58678	0.35261	0.28562	H129	0.44587	0.22455	0.71508	H201	0.26386	0.95563	0.14933
C103	0.64148	0.34563	0.83037	C223	0.50343	0.21534	0.27618	C343	0.3099	0.97411	0.55051
H58	0.60728	0.38977	0.73113	H130	0.47005	0.25921	0.16447	H202	0.32645	0.92969	0.67761
C104	0.65008	0.32172	0.97492	C224	0.51095	0.19204	0.42428	C344	0.29143	0.99585	0.39933
H59	0.63645	0.3063	0.2526	H131	0.49546	0.17802	0.69943	H203	0.2603	0.00529	0.13714
H60	0.65677	0.3437	0.70067	H132	0.51961	0.2128	0.15144	H204	0.32288	0.97945	0.66341
C105	0.99382	0.81025	0.98681	C225	0.37	0.5305	0.50594	C345	0.1464	0.83455	0.48227
N5	0.96991	0.80861	0.01622	C226	0.3962	0.53104	0.44712	N21	0.12034	0.85741	0.44217
H61	0.01641	0.79	0.95429	C227	0.34391	0.55781	0.56038	H205	0.1496	0.81222	0.53416
C106	0.97019	0.78133	0.01451	C228	0.39621	0.55801	0.43419	C346	0.09417	0.85564	0.44925
C107	0.99534	0.75371	0.07604	H133	0.41662	0.50982	0.40693	C347	0.06686	0.88188	0.50009
C108	0.94359	0.78185	0.9527	C229	0.34385	0.58474	0.54466	C348	0.09379	0.8291	0.39809
C109	0.99424	0.72736	0.06249	H134	0.32355	0.55806	0.61597	C349	0.04017	0.88136	0.50993
H62	0.01586	0.75279	0.13519	C230	0.36978	0.58548	0.48102	H206	0.06692	0.90272	0.53671
C110	0.94247	0.75546	0.94042	H135	0.4169	0.55756	0.38503	C350	0.06716	0.82856	0.4097
H63	0.92383	0.8034	0.90878	H136	0.32348	0.60598	0.58576	H207	0.11445	0.80877	0.34755
C111	0.96806	0.72761	0.99279	C231	0.57303	0.11531	0.54575	C351	0.03993	0.85448	0.46699
H64	0.01388	0.70583	0.10868	C232	0.57285	0.08806	0.55859	H208	0.01945	0.90204	0.55398
H65	0.92159	0.75662	0.88783	C233	0.60064	0.11482	0.55201	H209	0.06702	0.80781	0.37081
N6	0.96993	0.69963	0.97976	C234	0.5997	0.06075	0.56446	N22	0.01468	0.85111	0.47876
C112	0.94688	0.6961	0.97166	H137	0.55135	0.08843	0.55619	C352	0.9875	0.8734	0.48139
H66	0.9231	0.71527	0.9751	C235	0.62744	0.08758	0.56786	H210	0.98174	0.89751	0.47281
C113	0.80478	0.14347	0.92142	H138	0.60106	0.13596	0.54977	C353	0.67806	0.77859	0.43547
N7	0.7986	0.16565	0.04623	C236	0.62733	0.06025	0.56772	N23	0.65551	0.79541	0.5555
H67	0.78842	0.14412	0.80008	H139	0.59924	0.03965	0.57198	H211	0.6773	0.76311	0.31243
C114	0.7704	0.19183	0.04901	H140	0.64892	0.08721	0.57273	C354	0.62876	0.79457	0.55026
C115	0.74355	0.19083	0.05897	N13	0.37158	0.5026	0.51113	C355	0.60124	0.82196	0.55056
C116	0.76913	0.21981	0.0563	N14	0.36681	0.61398	0.46968	C356	0.62857	0.76726	0.55931
C117	0.71603	0.21737	0.07212	N15	0.54548	0.14225	0.54244	C357	0.57419	0.82209	0.54589
H68	0.74431	0.16911	0.06135	N16	0.65481	0.03336	0.58438	H212	0.60129	0.84327	0.54659
C118	0.74155	0.24638	0.05952	C237	0.38929	0.6184	0.46061	C358	0.60149	0.76744	0.56441

H69	0.79003	0.22058	0.0512	H141	0.41331	0.5997	0.46037	H213	0.64983	0.74577	0.56762
C119	0.71468	0.24539	0.06558	C238	0.34815	0.49994	0.48781	C359	0.57401	0.79476	0.55071
H70	0.69514	0.2166	0.07942	H142	0.32511	0.51968	0.45888	H214	0.55293	0.84362	0.54375
H71	0.74083	0.26808	0.06239	C239	0.54002	0.16403	0.41551	H215	0.60144	0.74614	0.57142
N8	0.68655	0.27161	0.07801	H143	0.55652	0.16251	0.29151	N24	0.54728	0.79388	0.55614
C120	0.67933	0.29418	0.95458	C240	0.66132	0.01039	0.46709	C360	0.52516	0.8099	0.43077
H72	0.69455	0.29374	0.82421	H144	0.64596	0.01083	0.33817	H216	0.52632	0.82465	0.30322

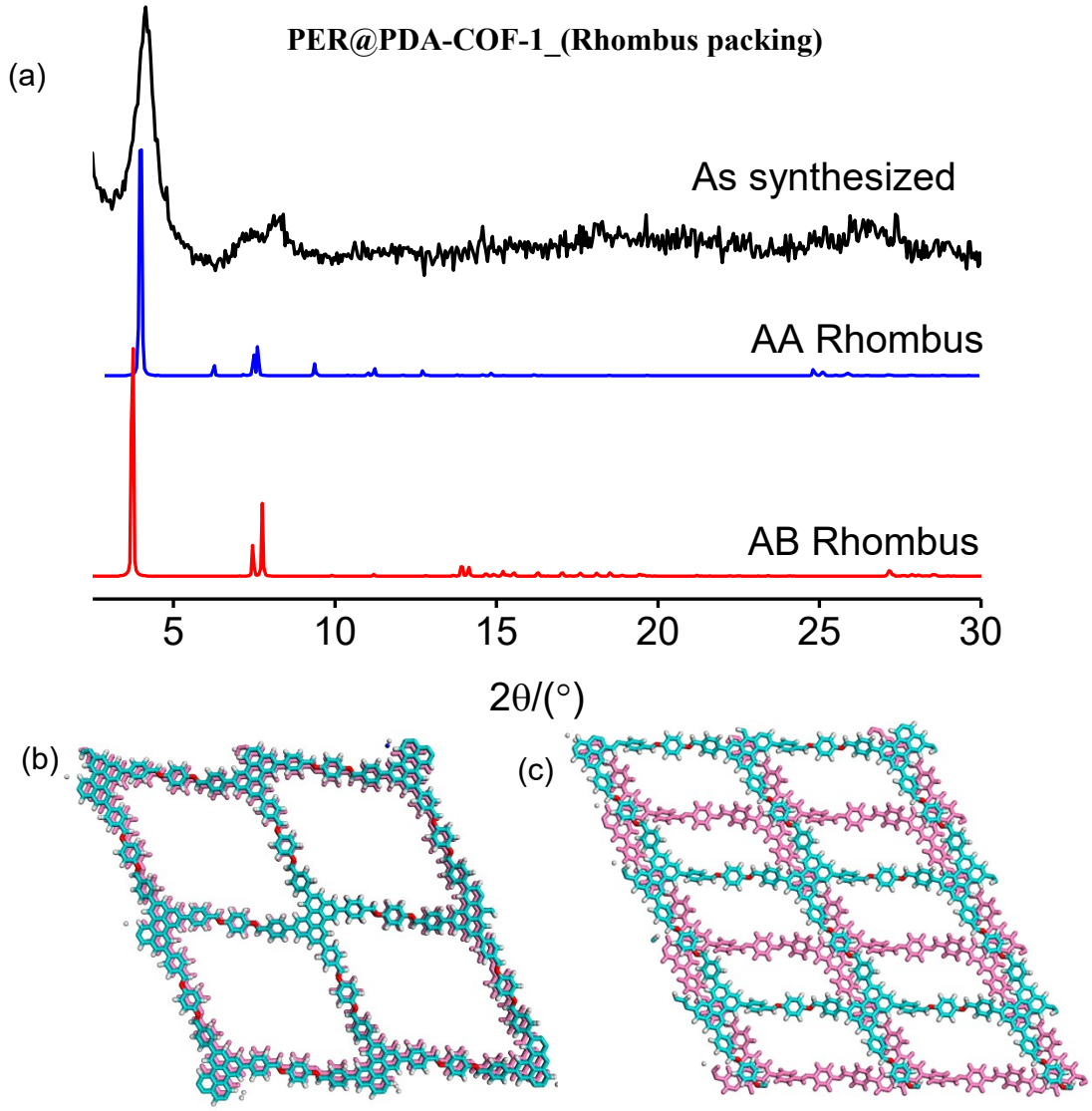


Figure S3. (a) Experimental powder X-ray diffraction pattern (PXRD) of PER@PDA-COF-1 (black plot), theoretical PXRD pattern for eclipse (AA) stacking of rhombus net of PER@PDA-COF-1 (blue plot) and Staggered (AB) stacking of rhombus net of PER@PDA-COF-1 (red plot); (b) Atomistic model of AA stacking of rhombus PER@PDA-COF-1 structure; (c) Atomistic model of AB stacking of rhombus PER@PDA-COF-1 structure.

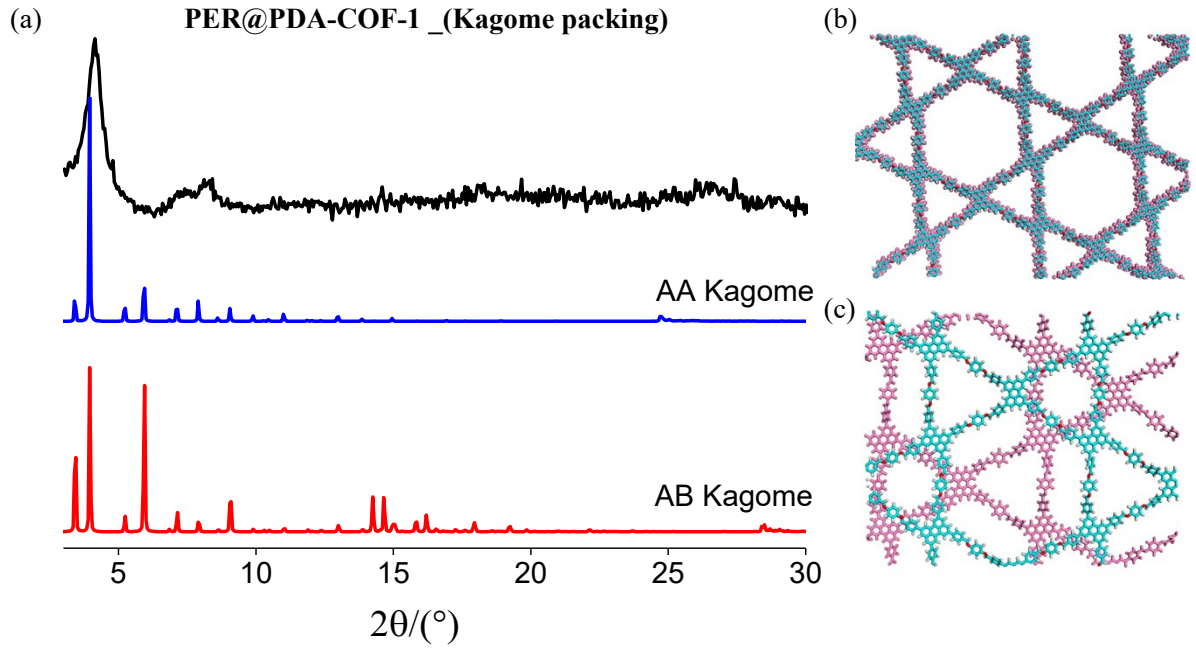


Figure S4. (a) Experimental powder X-ray diffraction pattern (PXRD) of PER@PDA-COF-1 (black plot), theoretical PXRD pattern for eclipse (AA) stacking of kagome net of PER@PDA-COF-1 (blue plot) and Staggered (AB) stacking of kagome net of PER@PDA-COF-1 (red plot); (b) Atomistic model of AA stacking of kagome PER@PDA-COF-1 structure; (c) Atomistic model of AB stacking of kagome PER@PDA-COF-1 structure.

Rhombus_PER@PDA-COF-1_AA + Mitoxantrone (Space group - *P*1) **a = 25.6974 Å, b = 26.1652 Å, c = 20.000 Å; α = 90 °, β= 90 °, λ= 110 °**											
Atom	***x***	***y***	***z***	***Atom***	***x***	***y***	***z***	***Atom***	***x***	***y***	***z***
C1	0.4774	0.67776	0.95252	C37	0.67232	0.07893	0.99676	C68	0.62913	0.73727	0.82297
C2	0.53208	0.67668	0.95957	H18	0.71959	0.02834	0.02401	C69	0.60134	0.77725	0.82284
C3	0.57741	0.72647	0.96763	C38	0.62295	0.08193	0.96945	C70	0.5419	0.75989	0.81784
C4	0.56682	0.77669	0.97085	H19	0.54372	0.03421	0.92537	C71	0.51511	0.79924	0.8242
C5	0.51219	0.77559	0.96662	H20	0.70382	0.11638	0.01497	C72	0.5474	0.85501	0.83519
C6	0.46704	0.72651	0.95704	C39	0.41045	0.72856	0.95082	C73	0.60421	0.87197	0.83605
C7	0.63238	0.72483	0.97194	C40	0.39488	0.76717	0.98721	C74	0.63251	0.83389	0.82893
C8	0.61355	0.82783	0.97744	C41	0.37151	0.6937	0.90676	H37	0.50916	0.52348	0.80989
C9	0.66861	0.82619	0.9796	C42	0.34262	0.77131	0.97946	H38	0.61236	0.55368	0.82179
C10	0.67927	0.77606	0.97598	H21	0.42427	0.79411	0.02263	H39	0.52691	0.88513	0.84226
C11	0.71418	0.87608	0.98467	C43	0.31943	0.69833	0.89839	H40	0.62816	0.91509	0.84371

C12	0.70442	0.9264	0.98568	H22	0.38311	0.66394	0.87712	O1	0.68176	0.75158	0.82839
C13	0.65087	0.92822	0.98194	C44	0.304	0.73724	0.93443	O2	0.45732	0.68591	0.80222
C14	0.60588	0.87821	0.97889	H23	0.33094	0.8015	0.00812	O3	0.67832	0.65383	0.82951
H1	0.44316	0.63927	0.94487	H24	0.29001	0.67147	0.86282	H41	0.69356	0.69487	0.8309
H2	0.74034	0.96414	0.98797	C45	0.61843	0.32832	0.97589	O4	0.45123	0.58681	0.8027
C15	0.54193	0.62642	0.95803	C46	0.58024	0.28154	0.00567	H42	0.43925	0.61952	0.7994
C16	0.59529	0.62468	0.9649	C47	0.66687	0.32397	0.94678	N5	0.6886	0.85203	0.82976
C17	0.64	0.67451	0.97196	C48	0.58968	0.23219	0.00629	H43	0.70812	0.82367	0.82066
H3	0.50659	0.58885	0.95022	H25	0.54274	0.28447	0.02907	N6	0.45885	0.78477	0.81955
C18	0.73404	0.77727	0.97475	C49	0.67692	0.27495	0.94848	H44	0.43717	0.7434	0.8139
C19	0.7692	0.87523	0.98614	H26	0.6971	0.35915	0.92218	C75	0.7238	0.90811	0.82658
H4	0.80353	0.91408	0.99074	C50	0.63813	0.22816	0.97723	H45	0.71676	0.93162	0.87
C20	0.77962	0.82647	0.98024	H27	0.55989	0.19642	0.03044	H46	0.71525	0.92808	0.78054
H5	0.56375	0.87963	0.97737	H28	0.71458	0.27214	0.9254	C76	0.78318	0.90816	0.82671
H6	0.50327	0.81368	0.96883	C51	0.18086	0.77982	0.95333	H47	0.79254	0.89596	0.87697
H7	0.7427	0.73918	0.97032	C52	0.17321	0.83054	0.95958	H48	0.81294	0.94964	0.81687
H8	0.68187	0.67299	0.97771	C53	0.13364	0.73234	0.94875	C77	0.42907	0.81863	0.84422
C21	0.60606	0.57265	0.96357	C54	0.12029	0.83401	0.96047	H49	0.44914	0.84034	0.89038
C22	0.65869	0.57137	0.94572	H29	0.20965	0.86776	0.96235	H50	0.3871	0.79182	0.85876
C23	0.56441	0.52293	0.97963	C55	0.08075	0.73581	0.94973	C78	0.42356	0.86005	0.79355
C24	0.6692	0.52263	0.94482	H30	0.13858	0.69238	0.94536	H51	0.40141	0.83881	0.74806
H9	0.69155	0.60892	0.93047	C56	0.07301	0.78648	0.95622	H52	0.46483	0.88714	0.77709
C25	0.5749	0.4741	0.97869	H31	0.11558	0.87407	0.96397	N7	0.39425	0.89211	0.82584
H10	0.52307	0.52263	0.99399	H32	0.04434	0.69861	0.94699	H53	0.35214	0.87103	0.82759
C26	0.62774	0.47306	0.96168	N1	0.60497	0.37606	0.97583	N8	0.78782	0.86859	0.77806
H11	0.7105	0.52263	0.93062	N2	0.64991	0.17957	0.97944	H54	0.7992	0.88593	0.73152
H12	0.54208	0.43582	0.99179	N3	0.23474	0.77797	0.95689	C79	0.40676	0.94721	0.80083
C27	0.837	0.82586	0.97981	N4	0.01854	0.78694	0.95466	H55	0.40487	0.94895	0.74515
C28	0.87999	0.86728	0.01194	C57	0.61259	0.13357	0.9649	H56	0.37482	0.96268	0.82075
C29	0.85081	0.78435	0.94725	H33	0.57053	0.13109	0.94663	C80	0.46348	0.98238	0.82593
C30	0.93399	0.86669	0.01253	C58	0.64116	0.42299	0.96187	H57	0.4971	0.97335	0.79826
H13	0.87076	0.90012	0.03793	H34	0.68542	0.42848	0.95001	H58	0.47021	0.02626	0.81959
C31	0.90493	0.78405	0.94728	C59	0.24889	0.74144	0.92593	C81	0.82141	0.83641	0.79832
H14	0.81853	0.75185	0.92096	H35	0.21999	0.71146	0.89091	H59	0.81536	0.80342	0.76114
C32	0.94759	0.82496	0.98047	C60	0.00449	0.8245	0.98335	H60	0.80578	0.81668	0.84687
H15	0.96646	0.89917	0.03863	H36	0.03456	0.85798	0.01325	C82	0.883	0.86907	0.80366
H16	0.91494	0.75144	0.92175	C61	0.5341	0.56678	0.81206	H61	0.90683	0.84089	0.81019
C33	0.64108	0.9807	0.97841	C62	0.50733	0.60567	0.80863	H62	0.89812	0.89337	0.75782
C34	0.59193	0.98405	0.95065	C63	0.53779	0.66218	0.81186	O5	0.89449	0.90663	0.85919
C35	0.68105	0.02936	0.00135	C64	0.59667	0.6794	0.81829	H63	0.88526	0.8853	0.90062
C36	0.58287	0.03349	0.94661	C65	0.62248	0.63952	0.82193	O6	0.46717	0.97123	0.89609
H17	0.55987	0.9475	0.93116	C66	0.59115	0.58348	0.81859	H64	0.4418	0.93351	0.9026
C37	0.67232	0.07893	0.99676	C67	0.50991	0.70236	0.81026				

Kagome_PER@PDA-COF-1_AA + Mitoxantrone (Space group - *P*1) **a = 51.6964 Å, b = 51.669 Å, c = 20.000 Å; α = 90.0067 °,β = 89.9971°, λ= 60.0359°**											
Atom	***x***	**y**	**z**	***Atom***	***x***	**y**	**z**	***Atom***	***x***	**y**	**z**
C1	0.09019	0.96498	0.02077	C73	0.5307	0.54621	0.02751	H82	0.02134	0.54863	0.02021
C2	0.06184	0.99145	0.0201	C74	0.48171	0.48446	0.02719	C151	0.14126	0.49603	0.96759
C3	0.03531	0.98939	0.02062	C75	0.53528	0.48927	0.02705	H83	0.09473	0.51134	0.94975
C4	0.03782	0.96053	0.02097	C76	0.55878	0.52067	0.02379	C152	0.16929	0.44876	0.02486
C5	0.06616	0.93511	0.01888	H43	0.52854	0.56847	0.02818	H84	0.14477	0.42685	0.05319
C6	0.09272	0.9368	0.01903	C77	0.5106	0.45818	0.02586	H85	0.90183	0.55909	0.01357
C7	0.00699	0.01631	0.02089	C78	0.45632	0.48145	0.02453	H86	0.92531	0.58953	0.02094
C8	0.01057	0.95845	0.02462	C79	0.53741	0.45987	0.02618	C153	0.89814	0.48568	0.96372
C9	0.98222	0.98537	0.02564	C80	0.56062	0.49234	0.0245	C154	0.87213	0.52852	0.03638
C10	0.97973	0.01422	0.02271	C81	0.5862	0.52277	0.01779	C155	0.97067	0.60214	0.02489
C11	0.95566	0.98338	0.03001	C82	0.51272	0.42953	0.02353	C156	0.16859	0.47363	0.99413
C12	0.9578	0.95493	0.03493	C83	0.45812	0.45318	0.02041	H87	0.14022	0.51558	0.94322
C13	0.98541	0.92869	0.03365	H44	0.43407	0.50146	0.024	H88	0.19043	0.43123	0.046
C14	0.01159	0.93093	0.02826	C84	0.56497	0.43345	0.02478	C157	0.87236	0.4836	0.9587
H1	0.11018	0.96725	0.02279	H45	0.58284	0.47239	0.02134	H89	0.91822	0.46983	0.93608
H2	0.93709	0.95396	0.03813	C85	0.61385	0.50001	0.04228	C158	0.84648	0.52619	0.0322
C15	0.05982	0.0199	0.01924	C86	0.58544	0.5475	0.98619	H90	0.87199	0.54612	0.06744
C16	0.03224	0.0462	0.01817	C87	0.48626	0.42758	0.02042	C159	0.94596	0.62731	0.9966
C17	0.00606	0.04379	0.01988	C88	0.54127	0.40321	0.02334	C160	0.99296	0.60619	0.05549
H3	0.08068	0.02063	0.01825	C89	0.43056	0.45127	0.01525	C161	0.84608	0.50378	0.99287

C18	0.95139	0.03965	0.0218	C90	0.56734	0.4049	0.0236	H91	0.87243	0.46603	0.92764
C19	0.92726	0.00989	0.02862	H46	0.5857	0.43439	0.02563	H92	0.82618	0.54189	0.05941
H4	0.9071	0.00796	0.03208	C91	0.63971	0.50182	0.03526	C162	0.94385	0.65524	0.99805
C20	0.92488	0.03792	0.024	H47	0.61503	0.48073	0.06822	H93	0.92834	0.62486	0.97193
H5	0.03327	0.91021	0.02845	C92	0.61132	0.54924	0.97874	C163	0.99075	0.63418	0.05747
H6	0.06814	0.91299	0.01679	H48	0.5643	0.56548	0.96612	H94	0.01225	0.58708	0.07893
H7	0.94918	0.06185	0.01813	H49	0.48838	0.40536	0.01841	C164	0.96622	0.65924	0.02832
H8	0.98433	0.06437	0.02108	H50	0.54254	0.38136	0.02128	H95	0.92453	0.67448	0.97496
C21	0.03002	0.07585	0.01499	C93	0.40347	0.47317	0.04397	H96	0.00826	0.637	0.08161
C22	0.0031	0.10142	0.99608	C94	0.43051	0.42759	0.98042	C165	0.8192	0.50124	0.98646
C23	0.05464	0.07963	0.0295	C95	0.59717	0.3777	0.02095	N9	0.79482	0.51889	0.01789
C24	0.00078	0.1294	0.99306	C96	0.63896	0.5264	0.00295	H97	0.82094	0.48336	0.95182
H9	0.98357	0.09949	0.98254	H51	0.66108	0.48403	0.05489	C166	0.76947	0.51573	0.01321
C25	0.05233	0.10764	0.02688	H52	0.61025	0.56862	0.95338	C167	0.74119	0.54124	0.02353
H10	0.07607	0.06028	0.04414	C97	0.37745	0.47156	0.03808	C168	0.77112	0.48789	0.00292
C26	0.02524	0.13317	0.00895	H53	0.40287	0.49166	0.07232	C169	0.71531	0.53926	0.02181
H11	0.97953	0.14892	0.97801	C98	0.40447	0.42609	0.97401	H98	0.73968	0.56292	0.03218
H12	0.07171	0.11014	0.03864	H54	0.45114	0.4103	0.95688	C170	0.74531	0.48575	0.00322
C27	0.89543	0.06555	0.02112	C99	0.60295	0.35104	0.05288	H99	0.79295	0.46763	0.99668
C28	0.87085	0.06564	0.99053	C100	0.62061	0.37787	0.98543	C171	0.71699	0.51141	0.01175
C29	0.89124	0.09256	0.04818	C101	0.37739	0.44804	0.00257	H100	0.69353	0.5593	0.03049
C30	0.84325	0.09177	0.98686	H55	0.3566	0.48873	0.06106	H101	0.74688	0.46398	0.99574
H13	0.87352	0.045	0.9684	H56	0.40493	0.40757	0.94596	N10	0.69171	0.50808	0.01547
C31	0.86357	0.11864	0.04514	C102	0.63109	0.32554	0.04964	C172	0.66589	0.52875	0.99495
H14	0.90995	0.09296	0.07318	H57	0.58513	0.35046	0.08157	H102	0.66282	0.54945	0.9695
C32	0.83903	0.11874	0.01423	C103	0.64863	0.35227	0.98135	C173	0.35032	0.44589	0.99464
H15	0.82441	0.09144	0.96227	H58	0.61663	0.39823	0.95937	N11	0.32489	0.46552	0.01927
H16	0.86057	0.13946	0.06697	C104	0.65443	0.32563	0.01347	H103	0.35302	0.42623	0.96505
C33	0.98752	0.89905	0.03602	H59	0.63543	0.30495	0.07515	C174	0.29938	0.46262	0.01372
C34	0.01148	0.87402	0.00521	H60	0.66646	0.35277	0.95249	C175	0.27106	0.48875	0.01621
C35	0.96543	0.89499	0.06769	C105	0.99277	0.81308	0.03347	C176	0.3007	0.43466	0.0105
C36	0.01293	0.84638	0.00505	N5	0.97304	0.80786	0.05982	C177	0.24494	0.4872	0.01383
H17	0.02903	0.87631	0.97968	H61	0.01258	0.79534	0.00569	H104	0.26972	0.51059	0.01932
C37	0.96694	0.86729	0.06793	C106	0.97618	0.77925	0.05715	C178	0.27459	0.43308	0.00978
H18	0.9468	0.91393	0.09325	C107	0.00425	0.75276	0.05708	H105	0.32242	0.41396	0.01055
C38	0.99065	0.84244	0.03606	C108	0.95017	0.77682	0.05811	C179	0.24628	0.45925	0.01052
H19	0.03162	0.82728	0.97993	C109	0.00608	0.72495	0.05666	H106	0.2232	0.50781	0.01658
H20	0.94951	0.86461	0.09283	H62	0.02481	0.75403	0.05904	H107	0.2759	0.41123	0.00783
C39	0.12229	0.90937	0.01776	C110	0.95199	0.74902	0.05587	N12	0.22082	0.45618	0.01264
C40	0.12592	0.8813	0.03538	H63	0.92822	0.79722	0.05934	C180	0.19538	0.47644	0.98936
C41	0.14792	0.91039	0.99784	C111	0.98007	0.72254	0.05446	H108	0.19253	0.49699	0.96358
C42	0.15382	0.8555	0.0337	H64	0.02801	0.70452	0.05679	C181	0.08216	0.04914	0.16851
H21	0.1065	0.87961	0.05131	H65	0.93143	0.74772	0.05679	C182	0.05547	0.04789	0.17094
C43	0.17579	0.88461	0.99567	N6	0.98333	0.69388	0.05469	C183	0.05617	0.02011	0.16929
H22	0.146	0.93169	0.98269	C112	0.96358	0.68883	0.02777	C184	0.08437	0.99319	0.16479
C44	0.17934	0.85666	0.01365	H66	0.94351	0.7068	0.00119	C185	0.1107	0.99515	0.16077
H23	0.15618	0.83385	0.04748	C113	0.8096	0.14575	0.01037	C186	0.10947	0.02306	0.16337
H24	0.19538	0.88601	0.97964	N7	0.80441	0.17101	0.03492	C187	0.02867	0.01871	0.17072
C45	0.03934	0.19686	0.02097	H67	0.7918	0.14317	0.9843	C188	0.08584	0.96425	0.16352
C46	0.06507	0.19976	0.01777	C114	0.77573	0.19629	0.03293	C189	0.0585	0.96278	0.16553
C47	0.0112	0.22305	0.02728	C115	0.7494	0.19444	0.03558	C190	0.03001	0.98994	0.16827
C48	0.06283	0.22774	0.01892	C116	0.77314	0.22481	0.03221	C191	0.00331	0.98819	0.17143
H25	0.08711	0.1796	0.01388	C117	0.72152	0.22029	0.03671	C192	0.00537	0.95968	0.17648
C49	0.00898	0.25102	0.02929	H68	0.75085	0.17254	0.03859	C193	0.03254	0.93382	0.1733
H26	0.99089	0.22147	0.03219	C118	0.74524	0.25066	0.03145	C194	0.05954	0.93467	0.16577
C50	0.03464	0.25393	0.02418	H69	0.79347	0.22649	0.03107	H109	0.08088	0.07094	0.17047
H27	0.08321	0.22935	0.01743	C119	0.7189	0.2488	0.03341	H110	0.13035	0.02366	0.16203
H28	0.98698	0.27117	0.03419	H70	0.70121	0.2186	0.03892	H111	0.98499	0.95833	0.18145
C51	0.24263	0.77913	0.0316	H71	0.74375	0.27261	0.03106	H112	0.03333	0.91225	0.17473
C52	0.24552	0.75046	0.03182	N8	0.69027	0.27405	0.03669	O1	0.11151	0.9405	0.16266
C53	0.26875	0.78127	0.03695	C120	0.68407	0.29894	0.0083	O2	0.00375	0.04322	0.17471
C54	0.27349	0.72481	0.03548	H72	0.70089	0.30127	0.97732	O3	0.13798	0.97038	0.15384
H29	0.22539	0.74849	0.02851	C121	0.04815	0.3178	0.00758	H113	0.13483	0.95266	0.15479
C55	0.29667	0.75563	0.04172	C122	0.02415	0.34208	0.04027	O4	0.02943	0.07415	0.17466
H30	0.26706	0.80328	0.03911	C123	0.07039	0.3223	0.97836	H114	0.01279	0.06941	0.17546
C56	0.29962	0.72697	0.04014	C124	0.02218	0.36997	0.04203	N13	0.086	0.90851	0.15808
H31	0.27508	0.70282	0.03663	H73	0.00689	0.33876	0.06406	H115	0.10483	0.91069	0.15253
H32	0.31675	0.75764	0.04614	C125	0.06851	0.3501	0.98064	N14	0.97619	0.01333	0.16624
N1	0.0433	0.16793	0.02152	H74	0.08938	0.30356	0.9531	H116	0.97656	0.0332	0.16322
N2	0.03116	0.28261	0.02855	C126	0.04416	0.37461	0.01178	C195	0.0904	0.87961	0.17716

N3	0.2138	0.80415	0.0309	H75	0.00334	0.38851	0.06808	H117	0.11334	0.86268	0.16227
N4	0.32827	0.70192	0.04696	H76	0.08597	0.35303	0.95661	H118	0.07489	0.8744	0.14963
C57	0.05053	0.28844	0.00233	C127	0.04178	0.40432	0.01148	C196	0.08688	0.87819	0.25247
H33	0.07012	0.27134	0.97294	C128	0.06718	0.40716	0.00928	H119	0.09086	0.85568	0.26692
C58	0.02184	0.16302	0.00623	C129	0.01333	0.43061	0.0117	H120	0.06343	0.89434	0.26685
H34	0.99934	0.18139	0.98984	C130	0.0649	0.43573	0.0087	C197	0.94788	0.01547	0.18107
C59	0.20898	0.82997	0.01096	H77	0.08951	0.38721	0.0091	H121	0.94647	0.99672	0.15792
H35	0.22723	0.8334	0.99039	C131	0.01004	0.45913	0.01025	H122	0.9303	0.0363	0.1576
C60	0.33435	0.67632	0.02271	H78	0.9935	0.42805	0.01194	C198	0.94316	0.01633	0.25631
H36	0.31745	0.67339	0.99352	C132	0.03614	0.46206	0.00991	H123	0.96084	0.99518	0.2787
C61	0.36364	0.64936	0.02937	C133	0.09103	0.43824	0.0067	H124	0.92131	0.01775	0.26685
C62	0.36806	0.62259	0.00046	C134	0.98054	0.48619	0.00921	N15	0.94379	0.04208	0.28441
C63	0.38789	0.64899	0.06246	C135	0.03424	0.49066	0.0106	H125	0.95509	0.04898	0.25293
C64	0.39567	0.59651	0.00359	C136	0.08914	0.4661	0.00552	N16	0.1079	0.88496	0.28578
H37	0.34938	0.62247	0.97455	H79	0.11288	0.41771	0.00467	H126	0.11594	0.89463	0.25246
C65	0.41561	0.62293	0.06501	C137	0.97863	0.51476	0.01295	C199	0.95706	0.0367	0.35095
H38	0.38475	0.66957	0.08592	C138	0.95427	0.48483	0.00491	H127	0.95161	0.05855	0.37322
C66	0.42013	0.59624	0.03532	C139	0.00475	0.51767	0.01448	H128	0.94685	0.02684	0.38311
H39	0.39849	0.57617	0.97955	C140	0.06049	0.4921	0.00779	C200	0.99079	0.01642	0.34937
H40	0.4342	0.62315	0.09106	C141	0.1163	0.46874	0.00198	H129	0.00054	0.02213	0.30576
C67	0.44977	0.56882	0.03519	C142	0.94989	0.5411	0.0149	H130	0.00109	0.01943	0.39556
C68	0.47586	0.57045	0.03427	C143	0.92565	0.51085	0.00662	C201	0.09607	0.90375	0.34482
C69	0.45207	0.54029	0.03323	H80	0.95542	0.46309	0.0012	H131	0.11492	0.90278	0.37362
C70	0.50433	0.54415	0.03094	C144	0.00148	0.54613	0.01926	H132	0.08521	0.89473	0.37757
H41	0.47469	0.59226	0.03438	H81	0.05927	0.51391	0.00822	C202	0.07395	0.93595	0.3264
C71	0.47958	0.51385	0.03035	C145	0.1156	0.49368	0.97162	H133	0.08532	0.94697	0.30207
H42	0.43137	0.5393	0.03478	C146	0.14368	0.44635	0.02848	H134	0.05679	0.93733	0.29115
C72	0.50641	0.51552	0.02963	C147	0.92374	0.53862	0.01246	O5	0.05829	0.95264	0.3857
				C148	0.94764	0.56961	0.01895	H135	0.07305	0.94963	0.41998
				C149	0.89844	0.50831	0.00233	O6	0.99815	0.98557	0.34489
				C150	0.97306	0.57242	0.02147	H136	0.01921	0.97293	0.35842

Molecular dynamics simulation

Molecular dynamics was undertaken for a total of 500ps using a model of PER@PDA-COF-1 as follows: From the lowest energy rhombus AA structure (a bilayer), a 1x1x4 supercell was created, resulting in an 8-layer model COF containing 800 atoms. As the MXT molecule will only interact with some of those layers, the top four layers had their coordinates frozen. The four remaining layers were entirely unconstrained. The MXT molecule was added to the pore near the unconstrained layers. After 100ps of equilibration, 500ps of MD was undertaken in the NVT ensemble using a timestep of 0.25 fs. A Nose-Hoover chain thermostat was used to maintain a temperature of 300K.

Snapshots were extracted every 10000 steps and the binding energy of MXT-PER@PDA-COF-1 was calculated using Density Functional Tight Binding (DFTB). All atoms were described using the 3ob-3-1 parameter set with D3-BJ dispersion.

All calculations were undertaken using AMS 2022.101. Analysis was undertaken using VMD and a self-written python script. Using cutoffs of 3.5 Å for D-A distance and 140^{o} for the hydrogen bond angle, on average one hydrogen bond was maintained between the MXT molecule and the PDA-COF-1. The most frequent hydrogen bond donors were the MXT amine groups.

Extending the definition to include all close contacts, rather than just hydrogen bonds involving polar atoms, showed an average of 26 MXT—PER@PDA-COF-1 contacts maintained throughout the trajectory, indicating that less specific intermolecular interactions dominate over hydrogen bonding. Supporting this, the average DFTB MXT@ PDA-COF-1 binding energy over the trajectory was 145 kJ/mol.

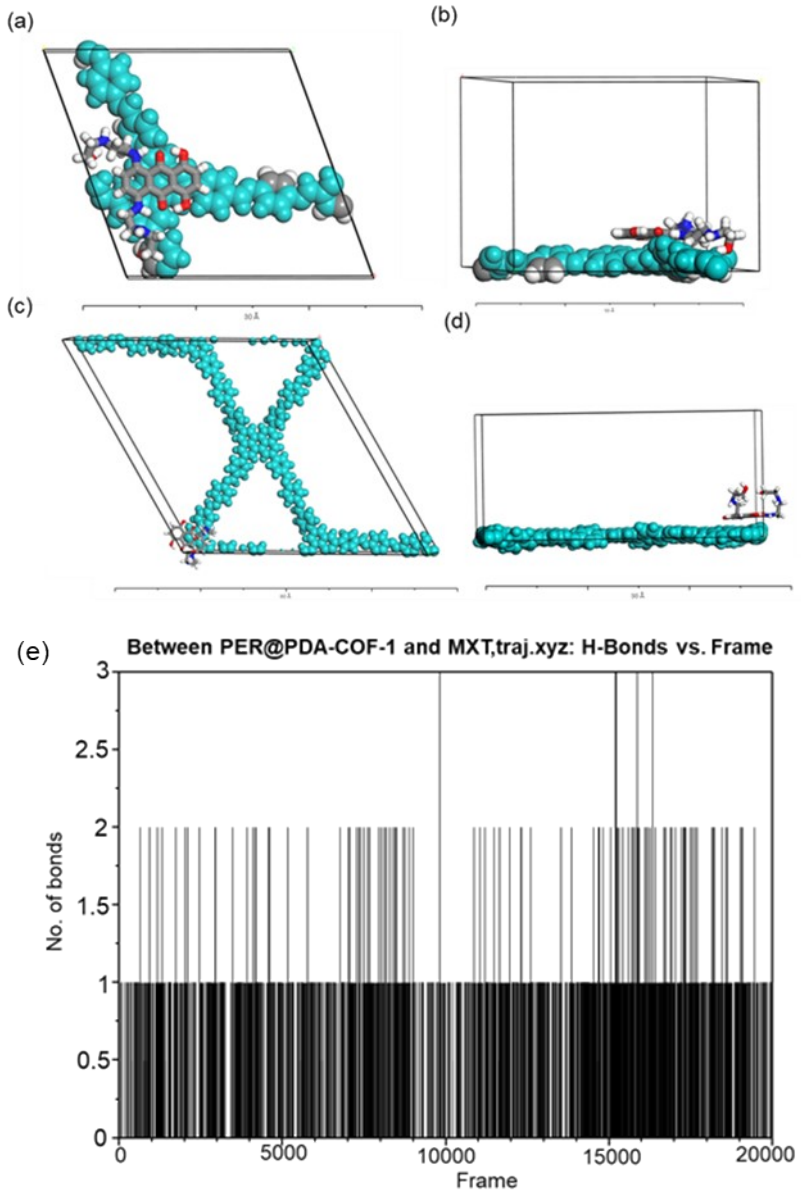


Figure S5. (a) Top view of the unit cell for MXT-PER@PDA-COF-1; (b) Side view of the unit for MXT-PER@PDA-COF-1 (Rhombus lattice); (c) Top view of the unit cell for MXT-PER@PDA-COF-1; (b) Side view of the unit for MXT-PER@PDA-COF-1 (Kagome lattice). where PER@PDA-COF-1 is depicted as cyan colour and the MXT molecule (Carbon in grey colour, Nitrogen in red colour, Hydrogen in white colour); (e) Number of hydrogen bond involved in the MXT-PER@PDA-COF-1 system with 200 ns time frame

Section S4: FT-IR spectra

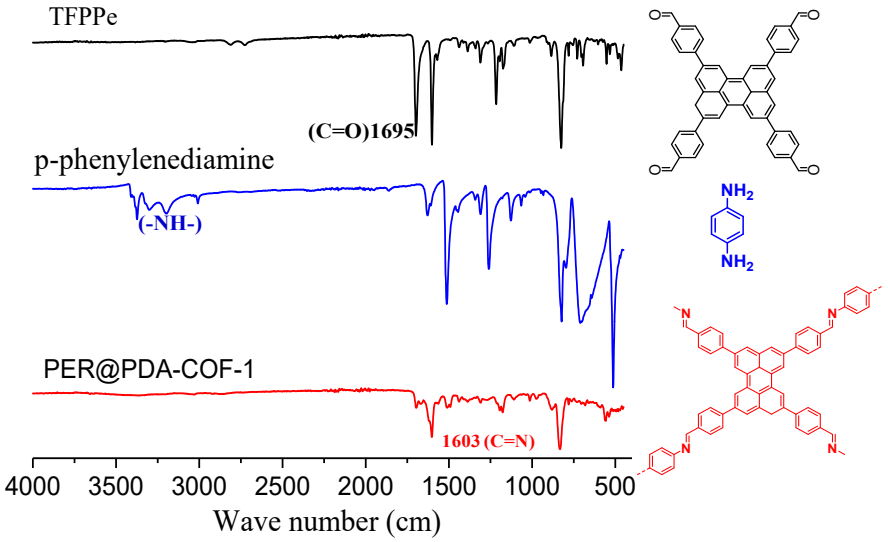


Figure S6. FTIR spectra of 4,4',4",4"'-(perylene-2,5,8,11-tetrayl) tetrabenzaldehyde (TFPPe, black plot), p-Phenylenediamine (blue plot) and PER@PDA-COF-1 (red plot).

Section S5: Solid state ^{13}C CP/MAS NMR

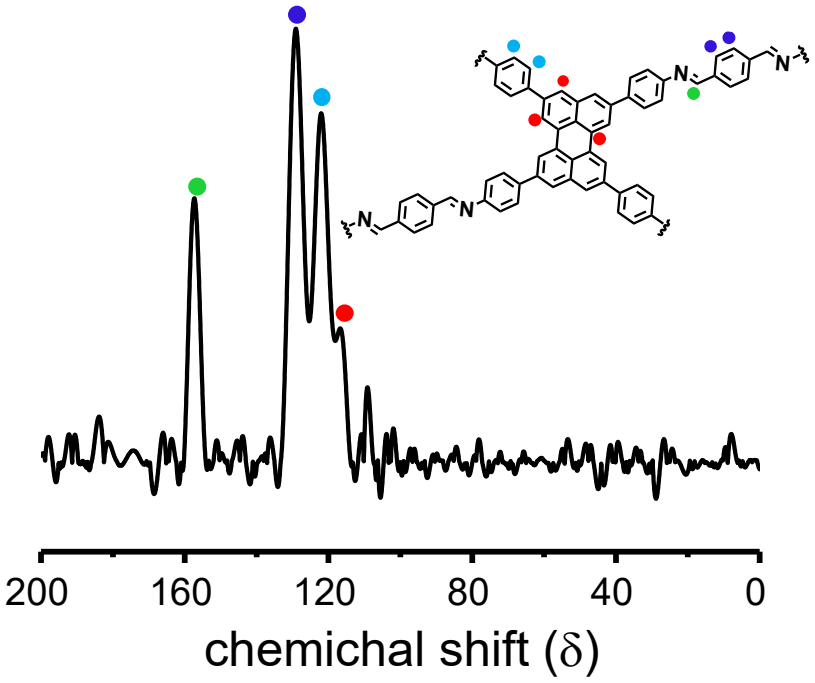


Figure S7. ^{13}C solid state CP/MAS NMR of PER@PDA-COF-1

Section S6: Thermo-gravimetric (TGA) analysis

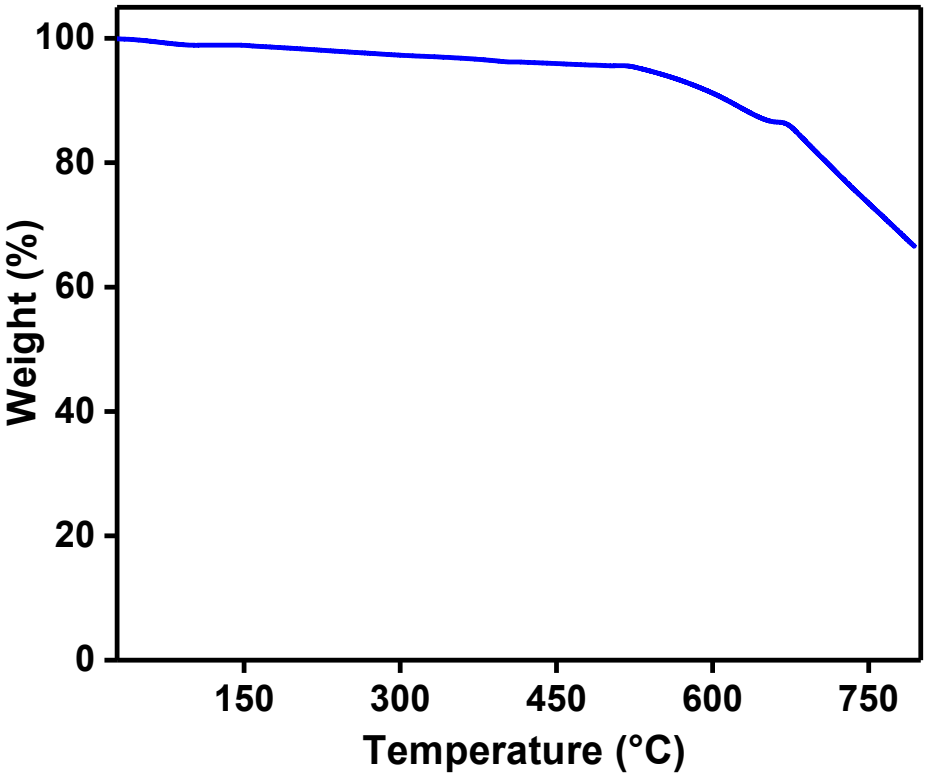


Figure S8. TGA plot of PER@PDA-COF-1 under N_2

Section S7: Ultra-high resolution transmission electron microscopy (UHR-TEM) analysis

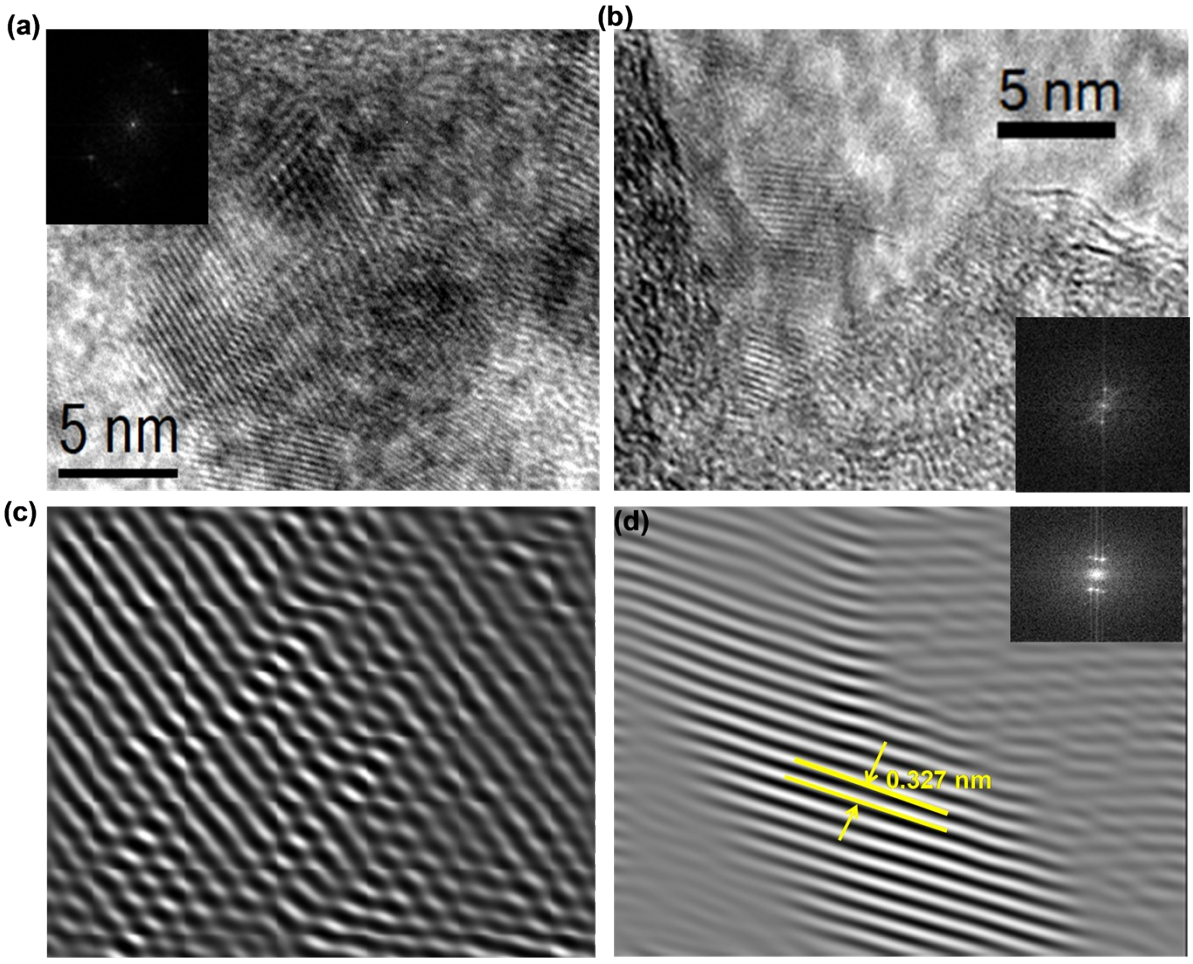


Figure S9. UHR-TEM image of the crystalline domain (a),(b) and the FFT pattern (inset); (c) Inverse FFT pattern; (d) distance between the two successive layers of the crystallite.

Section S8: FT-IR spectra of Mitoxantrone (MXT) and MXT loaded COF

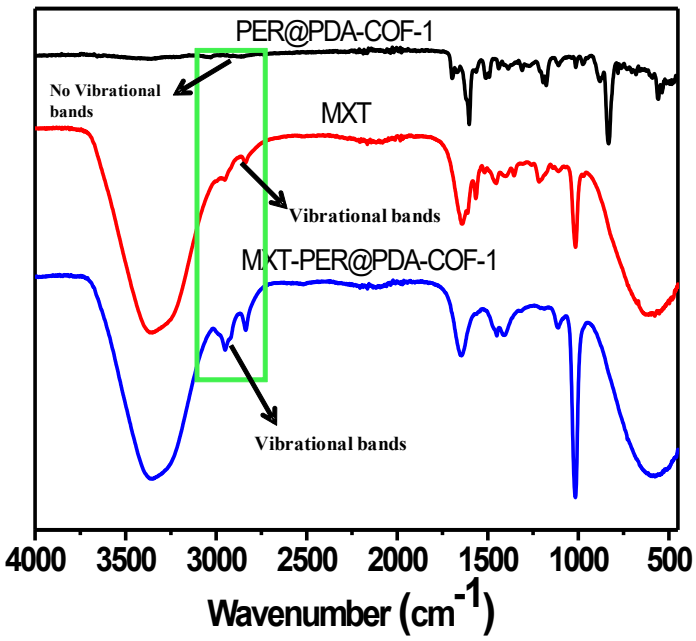


Figure S10. FTIR spectra of PER@PDA-COF-1 (black), MXT only (red) and MXT-PER@PDA-COF-1 (blue).

Section S9: Change of absorption of MXT upon binding with PER@PDA-COF-1

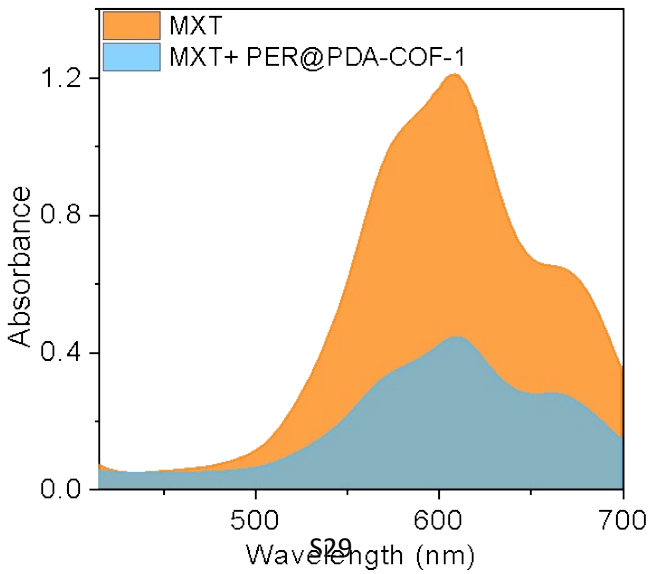


Figure S11. UV-Vis spectra of MXT before (orange) and after immobilization (blue) inside PER@PDA-COF-1.

Section S10: Change of fluorescent spectra of COF upon binding with MXT and the linear regression plot

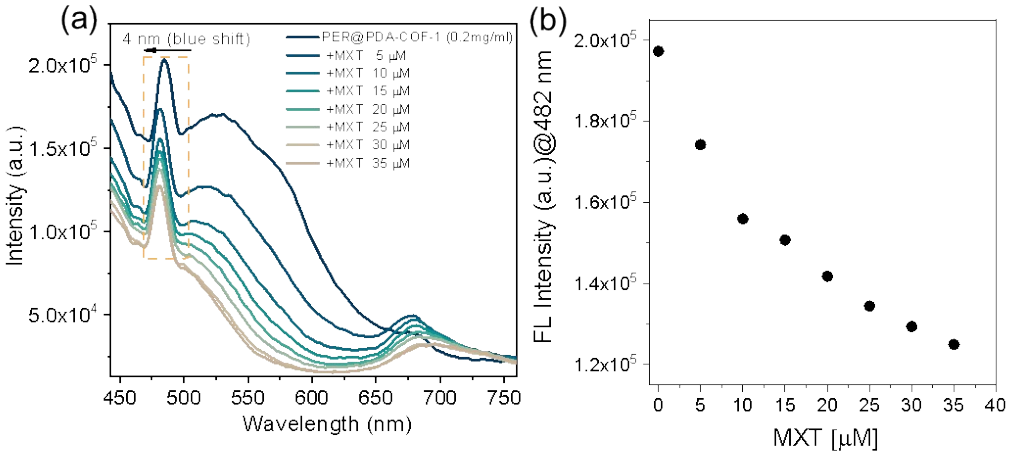


Figure S12. (a) Quenching of fluorescence emission of PER@PDA-COF-1 upon binding with mitoxantrone and (b) linear decrease in emission PER@PDA-COF-1.

Section S11: Binding constant calculation (K_{sv}) for the MXT binding with COF

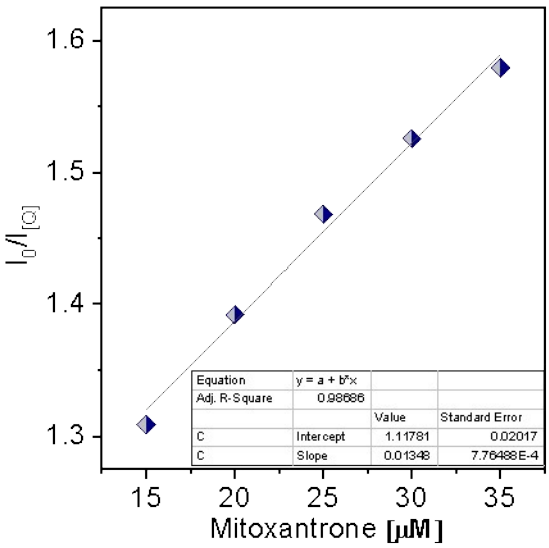


Figure S13. K_{sv} plot of MXT-PER@PDA-COF-1.

Section S12: Job's plot analysis of binding of proteins

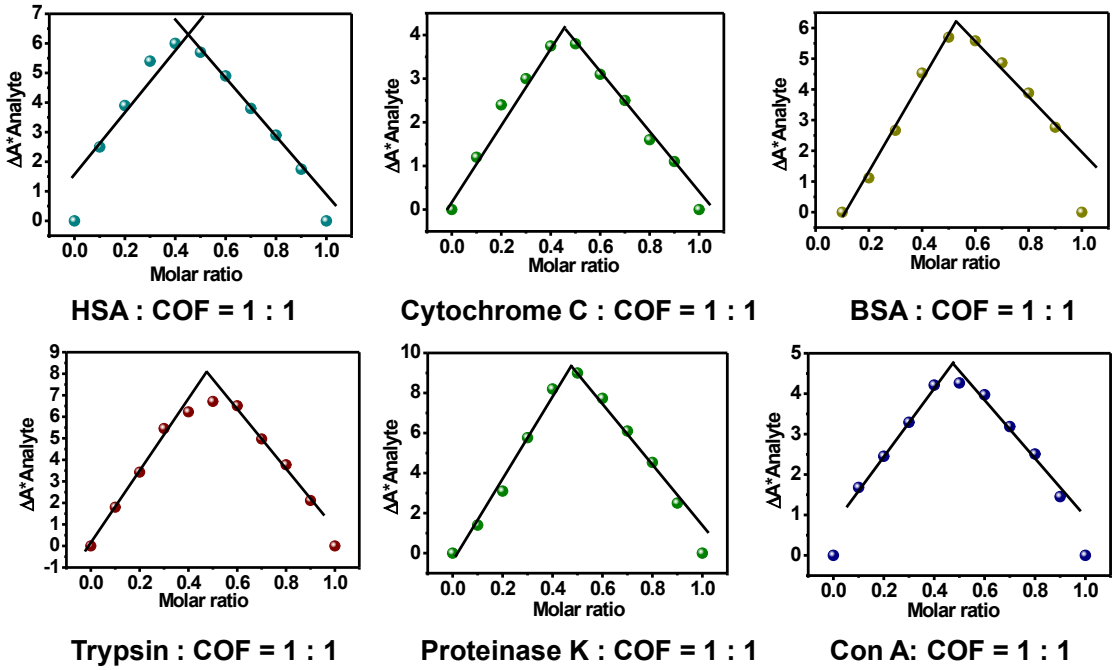


Figure S14. Job's plot analysis of binding of towards different proteins with the PER@PDA-COF-1 (COF).

Section S13: Comparative study of the "Turn-ON" response of PER@PDA-COF-1 towards various proteins

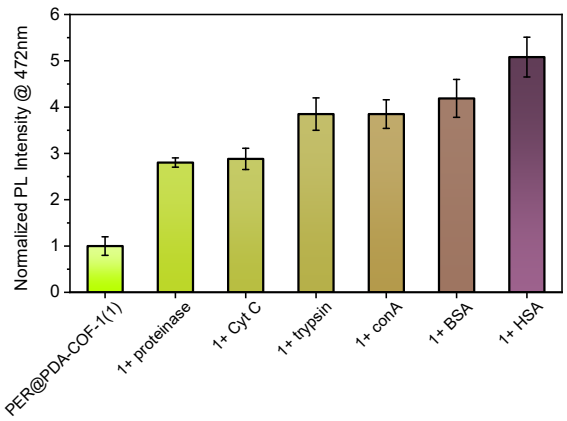


Figure S15. Turn-ON response of PER@PDA-COF-1 towards various proteins (Cyt C represents Cytochrome C, con A represents concanavalin A, BSA represents bovine serum albumin and HSA represents human serum albumin).

Section S14: Cyclic voltammetry

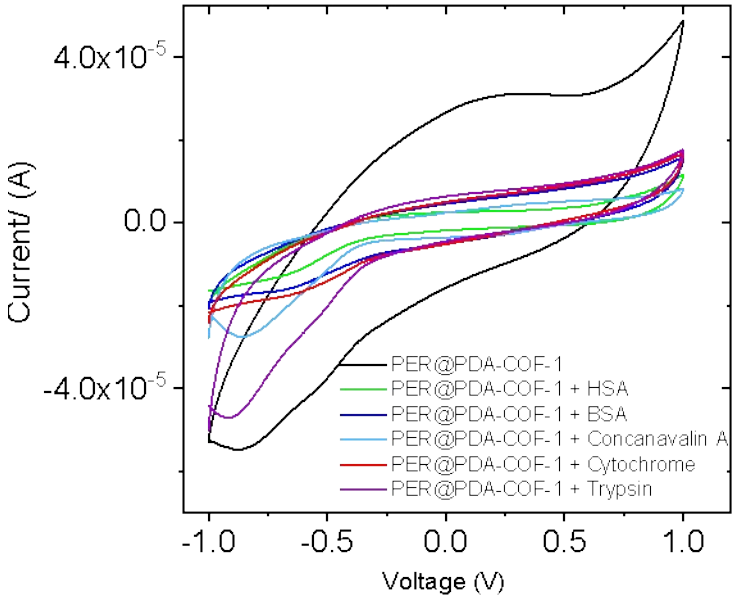


Figure S16. Cyclic voltammetry study of PER@PDA-COF-1 (black) only and the protein corona using HSA (green), BSA (blue), Concanavalin A (cyan), Cytochrome (red) and trypsin (purple).

Section S15: Effect of urea and temperature on the stability of albumin/COF nano assembly

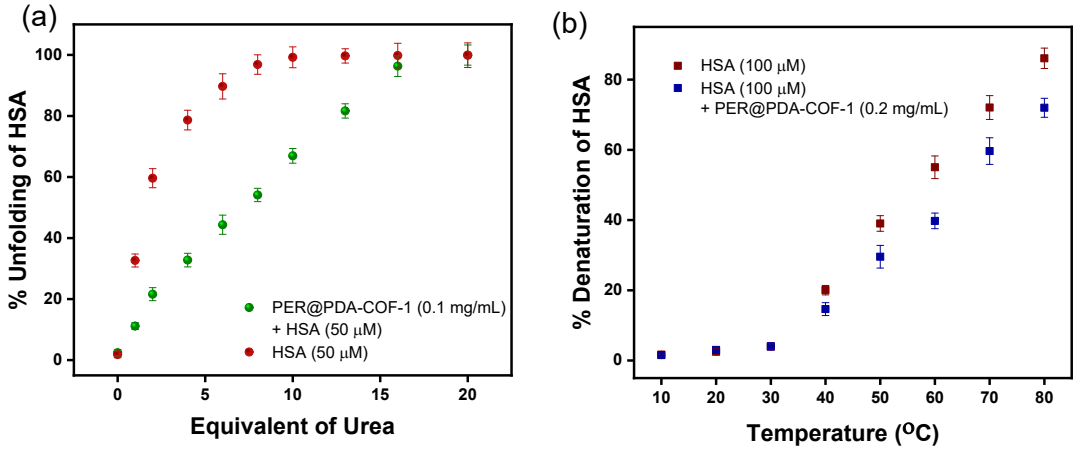


Figure S17. (a) Urea and (b) temperature dependent stability of albumin/COF nano-assembly.

Section S16: Effect of pH on the stability of of albumin/COF nano assembly

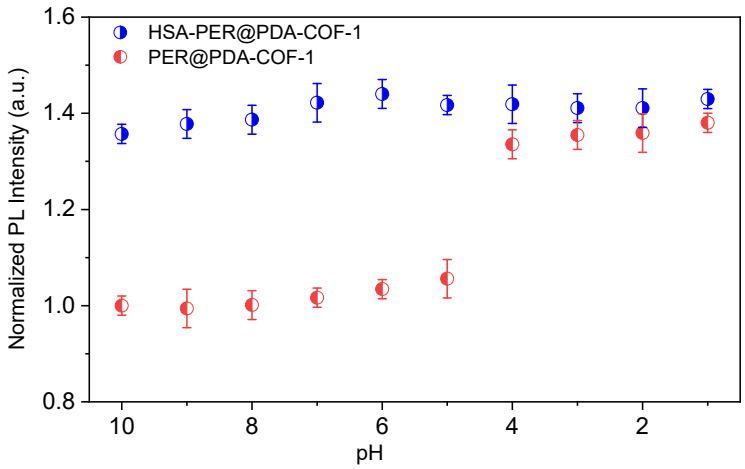


Figure S18. pH dependent stability of albumin/COF nano-assembly.

Section S17: Effect of temperature and urea on MXT release by system I, system II and system III.

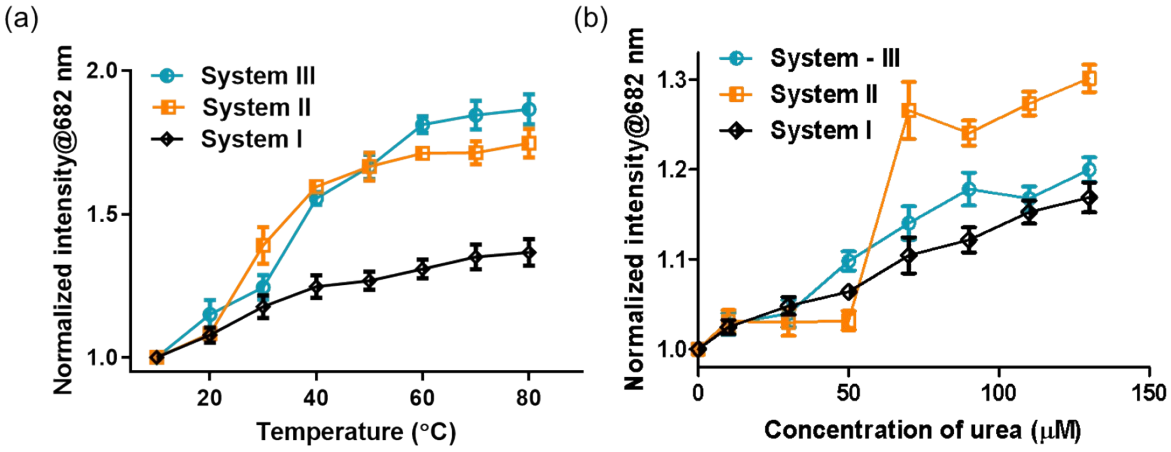


Figure S19. (a) Effect of temperature on release of Mitoxantrone release; (b) effect of urea concentration on MXT release from system-I, system-II & system-III.

Section S18: Comparison of Proteinase-K stability of System-II and System-III

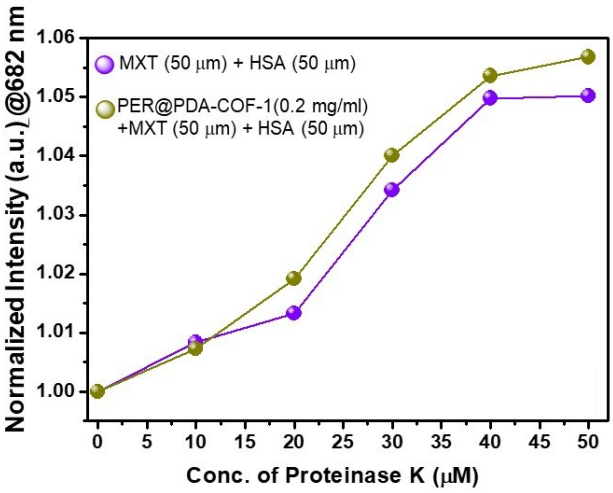


Figure S20. Proteinase-K stability of HSA-MXT-PER@PDA-CON-1.

Section S19: Comparative time dependent cellular release profile of MXT from system-I, system-II, system-III and MXT only

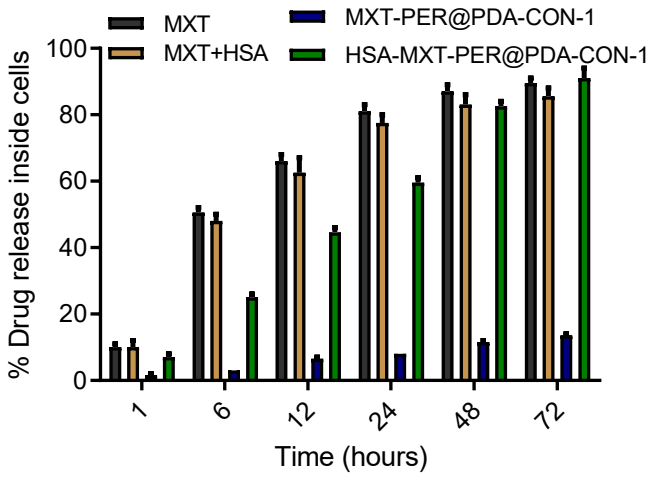


Figure S21. Comparative time dependent drug release studies among the different systems

Section S20: Extracellular and intracellular distribution of Time dependent released MXT by MXT-PER@PDA-COF and HSA-PER@PDA-COF-1.

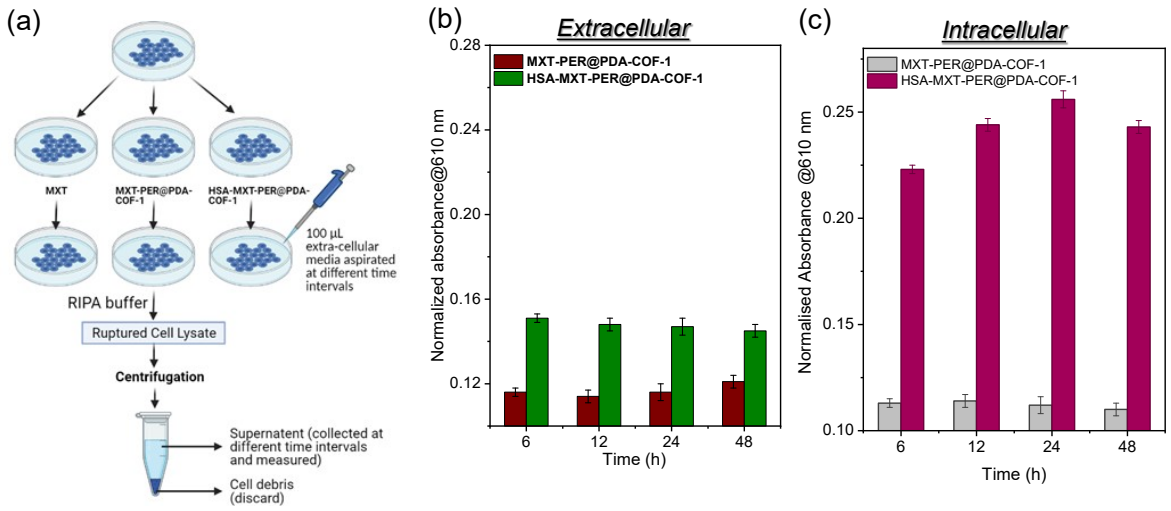


Figure S22. (a) Schematic demonstration for estimation of released MXT in extracellular and intracellular environment at different time interval; Comparison of (b) Extracellular and (c) intracellular release of MXT by MXT-PER@PDA-COF and HSA-PER@PDA-COF-1. The study was conducted using CT-26 cell line.

Section S21: Fluorescent microscopy study of cellular internalization of MXT.

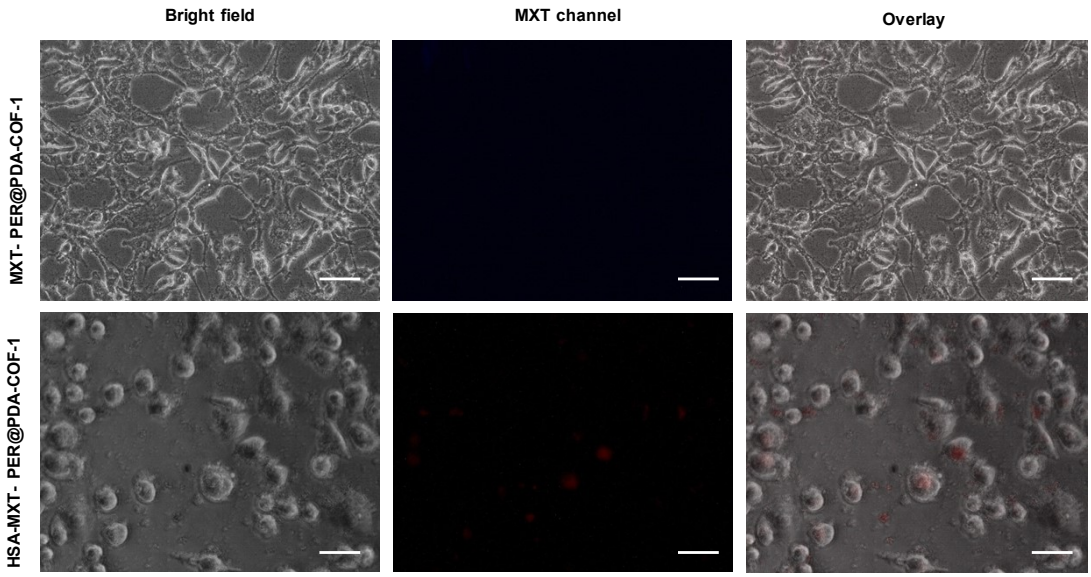


Figure S23. Comparative internalization of MXT inside cells (scale bar indicates 200 μm)

Section S22: Visualization of extracellular and intracellular MXT (CT-26 cell line).

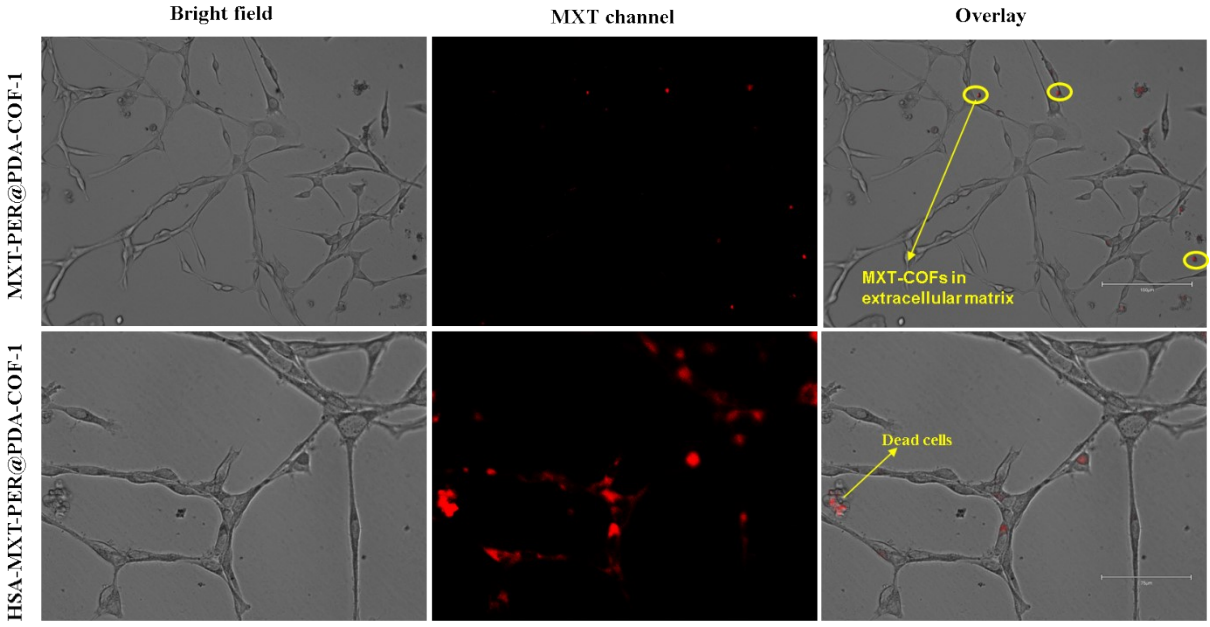


Figure S24. HSA induced improved internalization of MXT inside cells (scale bar indicates 200 μm)

(a)

Compounds	**Percentage of hemolysis**
Normal Saline (Negative control)	**0**
TritonX (Positive control)	**100**
PER@PDA-COF-1	**1.9%**
MXT-PER@PDA-COF-1	**1.7%**
HSA_MXT-PER@PDA-COF-1	**0.9%**

(b)

Compounds	**Clotting time (min)**
Normal Saline (Negative control)	6 mins
PEI (Positive control)	30 seconds
PER@PDA-COF-1	5.2 mins
MXT-PER@PDA-COF-1	5.5 mins
HSA-MXT-PER@PDA-COF-1	5.6 mins

Table S1. (a) Comparative percentage of hemolysis; (b) clotting time using different biosystem along with system I, system II and PER@PDA-COF-1 only. (% hemolysis was negligible and blood clotting time was not affected)

Section S23: Mice tumor Models and *In vivo* Studies.

The murine colon carcinoma cell line CT26 was purchased from ATCC and cultured in RPMI 1640 (Gibco) supplemented with 10% fetal bovine serum (Himedia) at 37 °C in a humidified atmosphere containing 5% CO2 and 95% humidity. All Balb/c mice were maintained under the environment, providing sterilized food pellets and distilled water throughout 12 h light/dark cycle in the Institute Animal Facility room in Indian Association for the Cultivation of Science (IACS). The temperature of the room was maintained at ~24 °C and the humidity was maintained at ~50%. All the experiments were performed in accordance with the ethical guidelines as prescribed under IACS/IAEC/2018/04. Balb/c mice (8 weeks old, male) were subcutaneously injected with 100 µL of CT26 (mouse colon carcinoma) cell suspension on the right flank maintaining an inoculum of 3 million cells/mouse. Clear tumors were observed after 9/10 days of injection. When the tumors were reached at the volume of ~100 mm^3, mices were divided into three groups (four mice per group). One group was kept as control and other two groups were given intra-tumoral injections of MXT-PER@PDA-COF-1 and HSA-MXT-PER@PDA-CON-1 respectively where final concentration of Mitoxantrone in stock formulation was maintained at 1.25 mg/mL and injected (4µL/gm body) weight on the 9^{th} day from the carcinoma cell injection. During treatment, tumor volume was measured every 3 days by using a calliper and calculated as

Tumor volume = $4\pi/3 \times (\text{tumor length}/2) \times (\text{tumor width}/2)^2$

After 24 days from the chemotherapeutic (MXT-PER@PDA-COF-1, HSA-MXT-PER@PDA-COF-1) injections, the mice were subjected for euthanasia and tumors were excised.

The tissues from various organs were collected, sliced and dehydrated successively and embedded in liquid paraffin and then were sliced into 3–5 mm for H&E staining Histological experiments were performed using the excised for tumors, kidneys, hearts, livers, lungs.

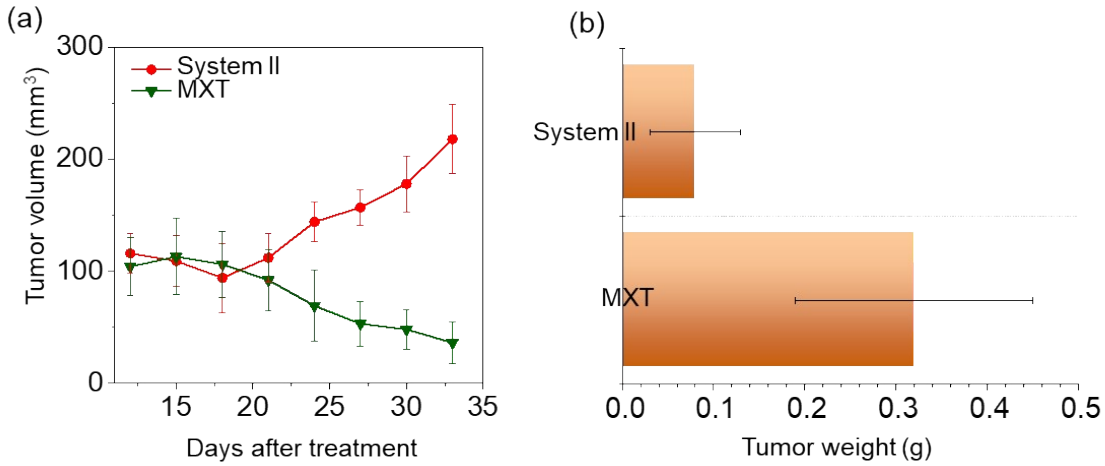


Figure S25. (a) Corresponding growth curves of tumors for MXT only (red) and System II (green plot); (b) Final tumor weights of the mice treated with MXT only and System II.

	7 days	**15 days**	**30 days**	**Ideal range**
Haemoglobin	12.1±1.6g/dL	12.4±2.1 g/dL	11.8±1.9 g/dL	11-19.2 g/dL
RBC	$7.9\times10^6\pm1.1$/mL	$8.1\times10^6\pm1.3$/mL	$7.6\times10^6\pm1.8$/mL	$6.36\text{-}9.42\times10^6$/mL
WBC	$8.8\times10^3\pm0.7$/mL	$7.1\times10^3\pm0.8$/mL	$6.2\times10^3\pm0.4$/mL	$0.8\text{-}6.8\times10^3$/mL
Platelet Count	$366\times10^3\pm34$/mL	$520\times10^3\pm25$/mL	$666\times10^3\pm42$/mL	$450\text{-}1590\times10^3$/mL
RDW	~15%	~16%	~16%	13-17%

Section S24:Blood biochemistry study:

Table S2. Haematology

Test	**Test value**	**Ideal range**
Neutrophils	~20%	10-30%
Lymphocytes	~76%	65-85%
Monocytes	~3%	0-5%
Eosinophils	~1%	0-6%
Basophils	0%	0-1%
Mean Corpuscular Volume (MCV)	47.6±3 fL	48.2-58.3 fL
Mean Corpuscular Haemoglobin	15.4±1.5 pg	15-19 pg

Mean Corpuscular Haemoglobin Conc. (MCHC)	32.4 ±2.2g/dL	30.2-35.3 g/dL
Packed Cell Volume (PCV)	~36.4%	34.6-44.6%

Table S3. Differential count

	System-I (7 day)	**System-II (7 day)**	**System-I (15 day)**	**System-II (15 day)**	**System-I (30 day)**	**System-II (30 day)**	**Ideal Range**
BUN	44 mg/dL	30.8 mg/dL	41.5 mg/dL	27.8 mg/dL	37 mg/dL	24.4 mg/dL	Upto 45 mg/dL
Creatinine	0.7 mg/dL	0.28 mg/dL	0.51 mg/dL	0.22 mg/dL	0.42 mg/dL	0.17 mg/dL	0.097-0.184 mg/dL

Table S4. Kidney Index

	System-I (7 day)	**System-II (7 day)**	**System-I (15 day)**	**System-II (15 day)**	**System-I (30 day)**	**System-II (30 day)**	**Ideal Range**
AST	750 U/L	485 U/L	660 U/L	410 U/L	515 U/L	355 U/L	30-380 U/L
ALT	84 U/L	58 U/L	67 U/L	42 U/L	67 U/L	34 U/L	17.5-30.2 U/L

Table S5. Liver Index

Section S25: Preparation of tissue lysate and bio-distribution studies

After treatments, mice were properly euthanized and its organs (spleen, kidneys, liver, lungs, and heart) and tumors (for tumor bearing mice) were extracted. Then, those were washed with 0.9% NaCl solution at 4 °C and conserved at -80 °C after immersion in liquid nitrogen. The organs were homogenized in PBS buffer (pH 7.4) and the resulting solution was collected for further spectroscopic studies. Same amount of each tissue was homogenized for preparing the lysates. Fluorescence of MXT (λ_{max} = 685 nm) was measured in each tissue lysate to check the distribution profile

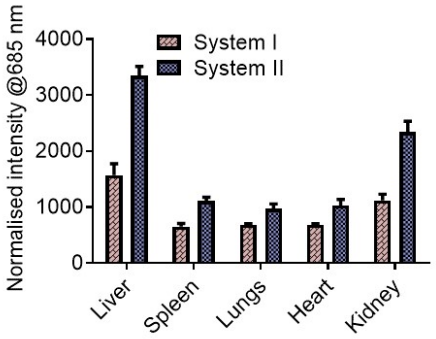


Figure S26. Distribution of MXT in major organs upon intravenous administration non-tumor bearing mice.

Section S26 Clearence Pathway

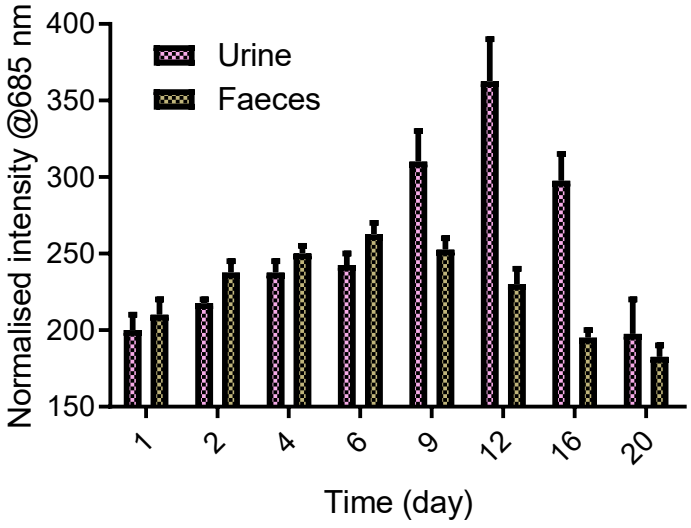


Figure S27. Detection of MXT in urine and faeces at various time intervals after injection of HSA-MXT-PER@PDA-COF-1

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