Supporting Information

Self-assembling Study of PNA-Porphyrin and PNA-BODIPY Hybrids in Mixed Solvent Systems

Emmanouil Nikoloudakis,[a] Kostas Karikis,[a] Jingjing Han,[b] Chrysoula Kokotidou,[c] Asterios Charisiadis,[a] Fotios Folias,[a] Antonios M. Douvas,[d] Anna Mitraki,[c]* Georgios Charalambidis,[a]* Xuehai Yan,[b]* Athanassios G. Coutsolelos[a]*

[a]Department of Chemistry, University of Crete, Laboratory of Bioinorganic Chemistry, Voutes Campus, 70013 Heraklion, Crete, Greece; E-mail: acoutsol@uoc.gr

[b]State Key Laboratory of Biochemical Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China. E-mail: yanxh@ipe.ac.cn

[c]University of Crete, Department of Materials Science and Technology and Institute of Electronic Structure and Laser (I.E.S.L.) Foundation for Research and Technology - Hellas (FO.R.T.H.), Vassilika Vouton, 70013, Heraklion, Crete, Greece. E-mail: mitraki@materials.uoc.gr

[d]Institute of Nanoscience and Nanotechnology (INN) National Center for Scientific Research (NCSR) "Demokritos" Patr. Gregoriou E' & 27, Neapoleos str., 153 41 Agia Paraskevi, Attica, Greece

Corresponding Authors

E-mail: acoutsol@uoc.gr (A.G.C.); yanxh@ipe.ac.cn (X.Y.); gcharal@uoc.gr (G.C.);

mitraki@materials.uoc.gr (A.M.);

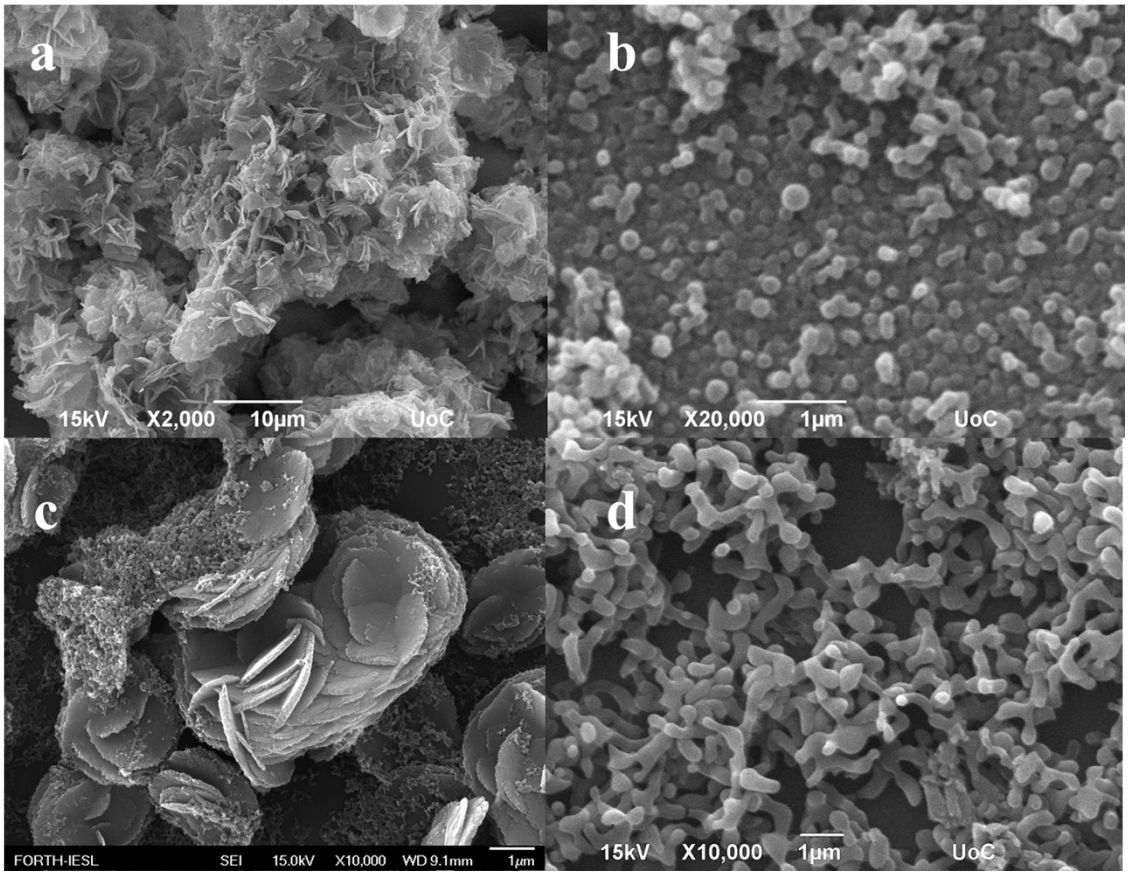

Fig. S1 Assembly pattern of **PNA-BDP** in a) DCM/ethanol 2:8 7mM, b) HFIP-EtOH 2:8 7mM, c) DCM/Heptane 1:1 1mM, d) MeCN-H_2O 2:8 1mM.

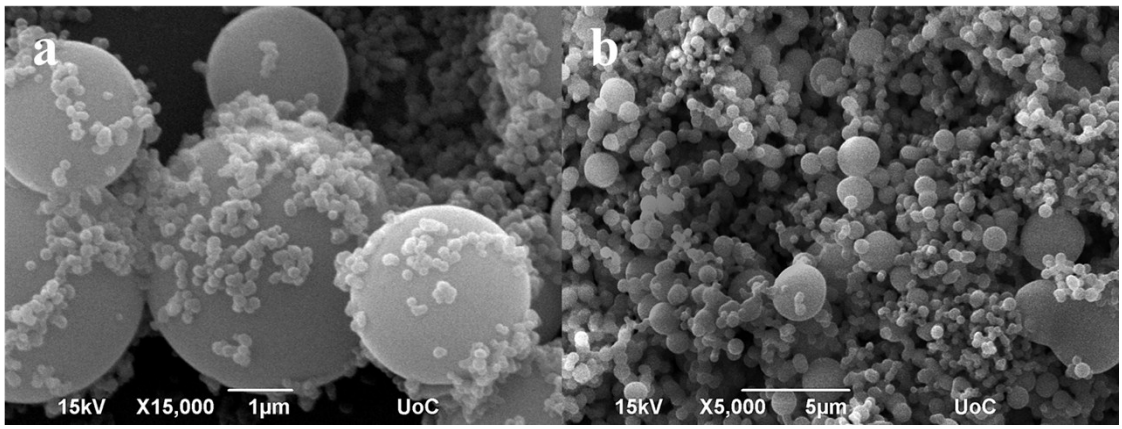

Fig. S2 Assembly pattern of **PNA-TPP** in 7mM: a) DCM/Heptane 1:1, b) DCM/ethanol 2:8.

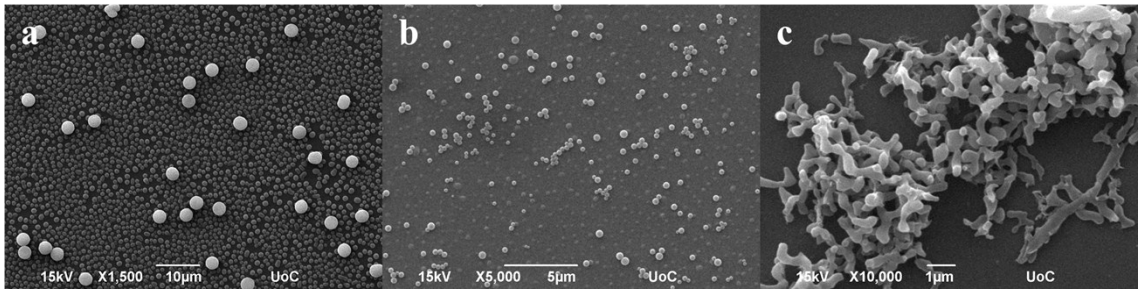

Fig. S3 Assembly pattern of **PNA** in a) DCM/EtOH 2:8 1 mM, b) HFIP/EtOH 2:8 1 mM, c) DCM/Heptane 1:1 1 mM.

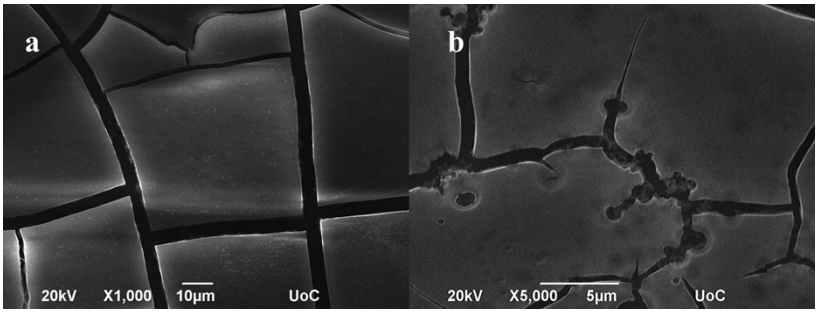

Fig. S4 SEM images in DCM of a) **PNA-BDP** and b) **PNA-TPP**.

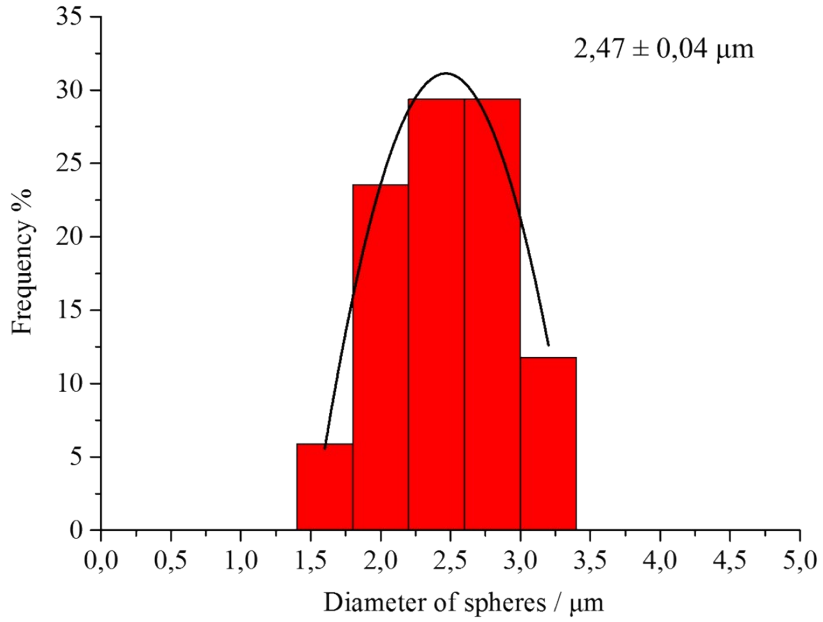

Fig. S5 Statistical diameter distribution of the PNA-BDP microspheres analyzed from SEM micrographs (Fig. 3a).

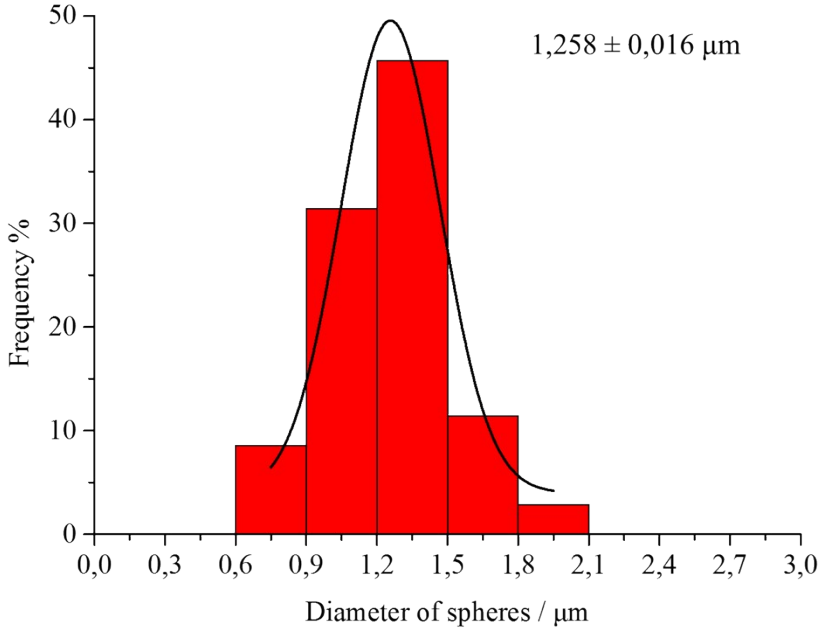

Fig. S6 Statistical diameter distribution of the PNA-TPP microspheres analyzed from SEM micrographs (Fig. 3b).

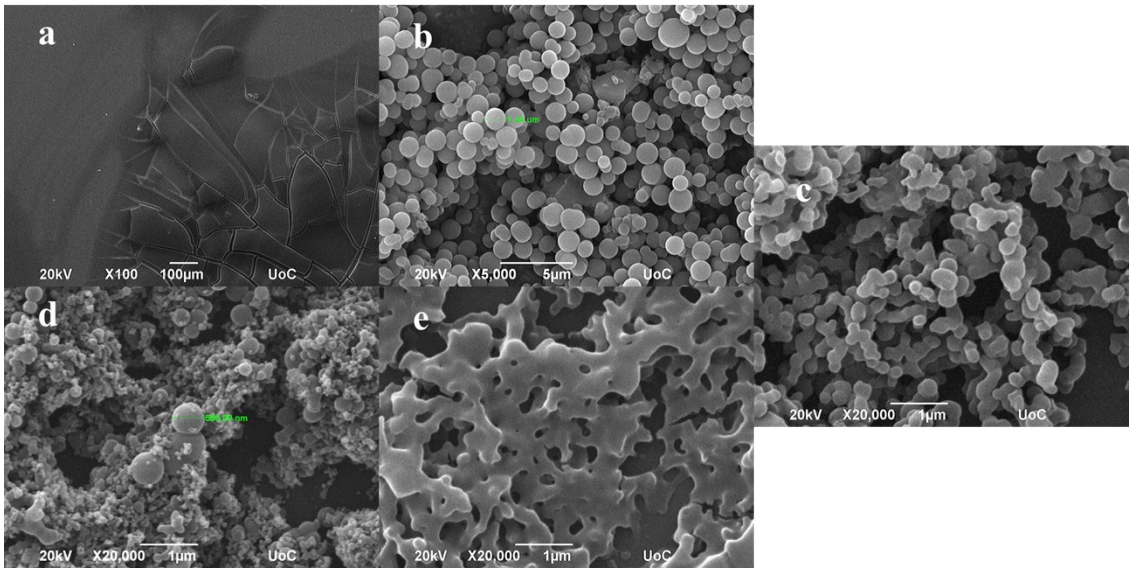

Fig. S7 Assembly pattern via spin coating of **PNA-TPP** in a) DCM 7mM, b) DCM-EtOH 2:8 7mM, c) DCM-Heptane 1:1 7mM, d) HFIP-EtOH 2:8 7mM, e) DCM-Heptane 2:8 7mM.

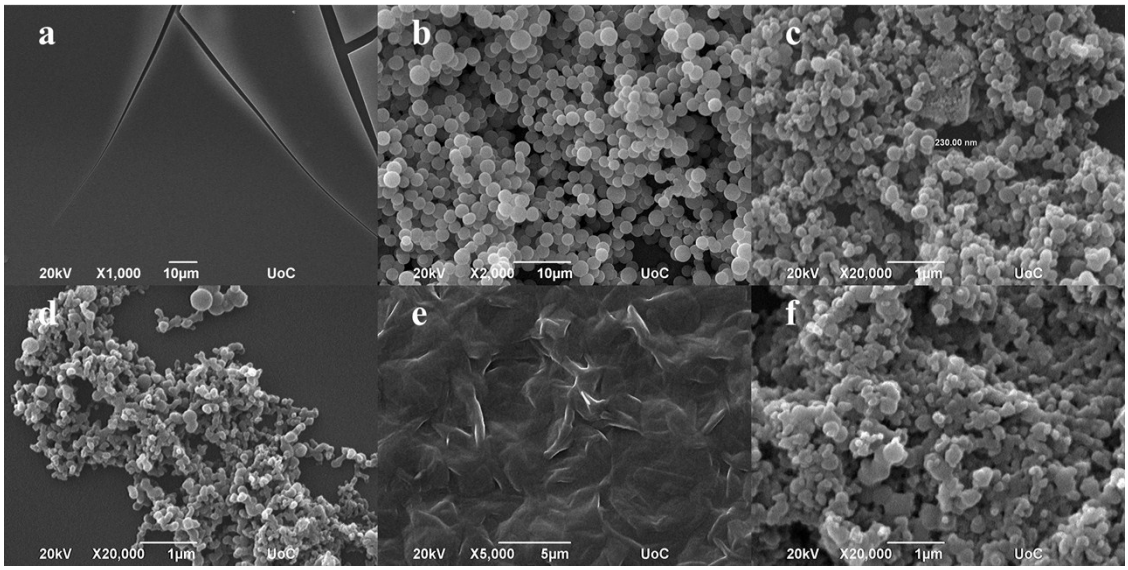

Fig. S8 Assembly pattern via spin coating of **PNA-BDP** in a) DCM 7mM, b) DCM-EtOH 2:8 7mM, c) HFIP-EtOH 2:8 7mM, d) HFIP-EtOH 2:8 1mM, e) DCM-Heptane 2:8 1mM, f) DCM-Heptane 1:1 1mM,

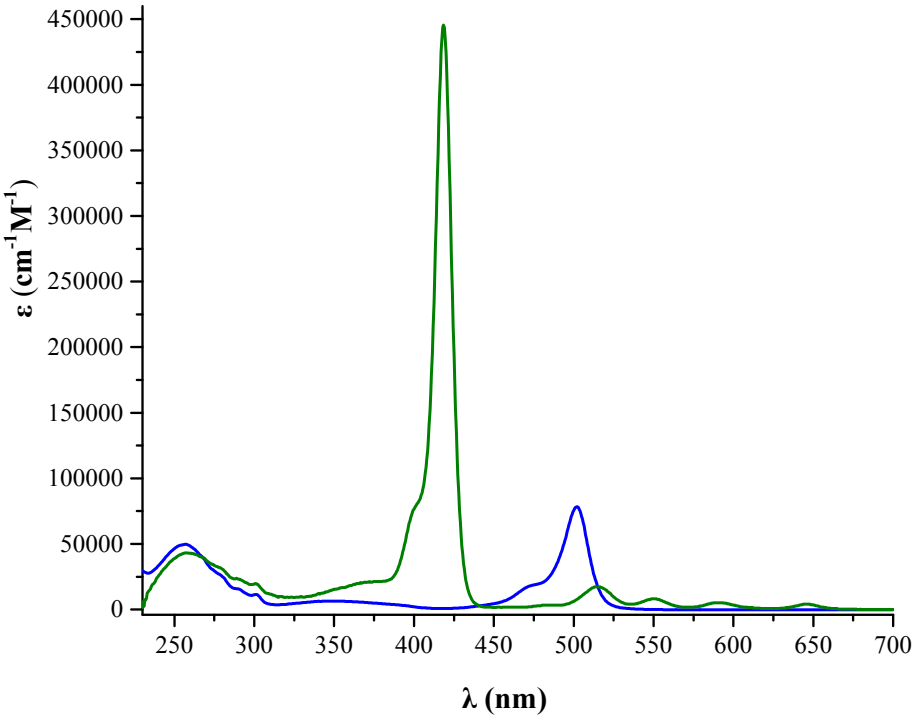

Fig. S9 UV-Vis spectra of **PNA-BDP** (blue) and **PNA-TPP** (green) in DCM.

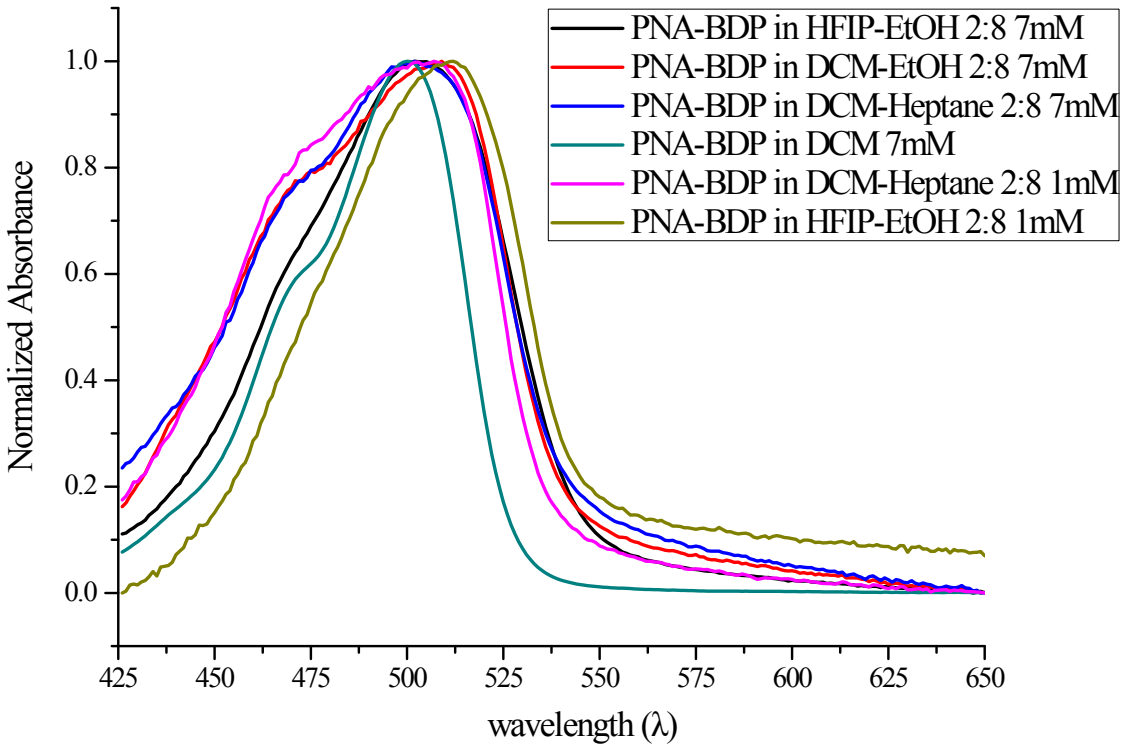

Fig. S10 Normalized solid absorbance spectra of **PNA-BDP** via drop casting method.

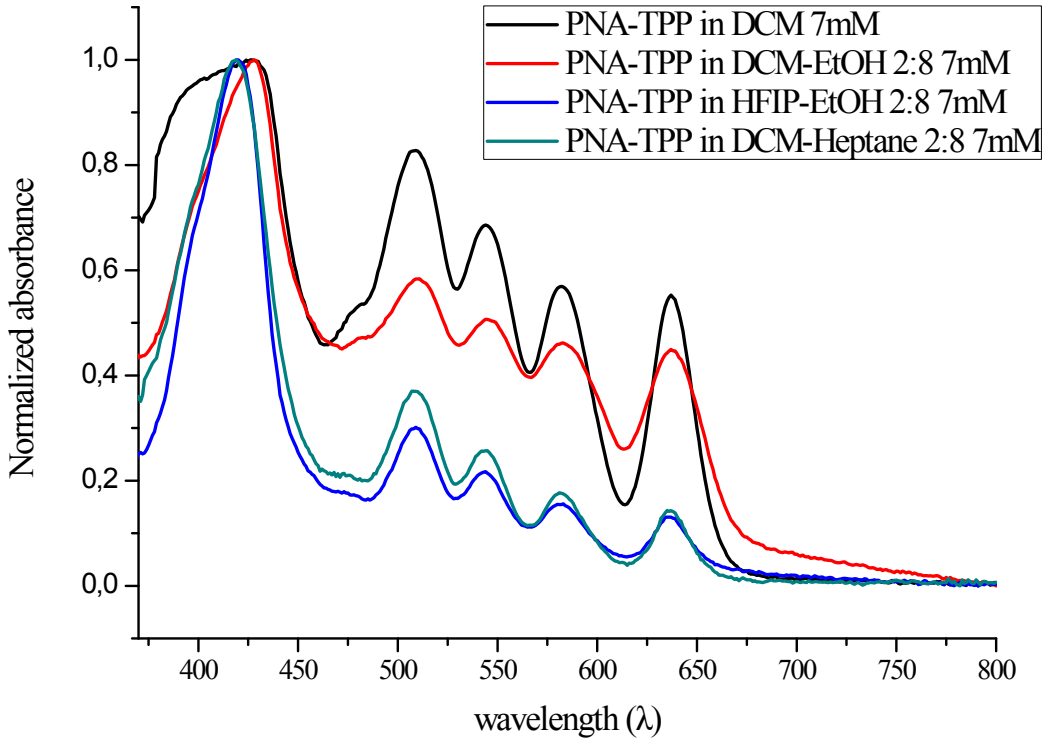

Fig. S11 Normalized solid absorbance spectra of **PNA-TPP** via drop casting method.

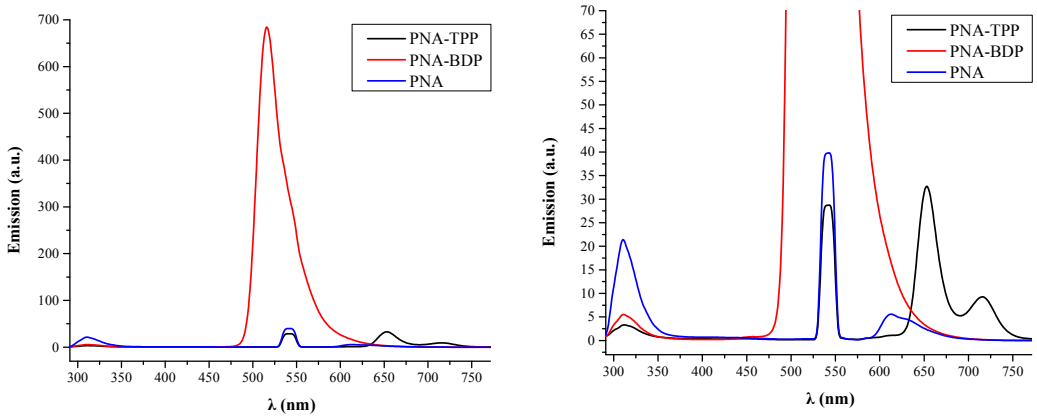

Fig. S12 Isoabsorbing emission spectra of: **PNA-TPP**, **PNA-BDP**, **PNA** and **BDP** in DCM, upon excitation at 270 nm (the right spectrum is a zoom of the left one). The peaks in 540 are due to the excitation-light (2·270 = 540 nm).

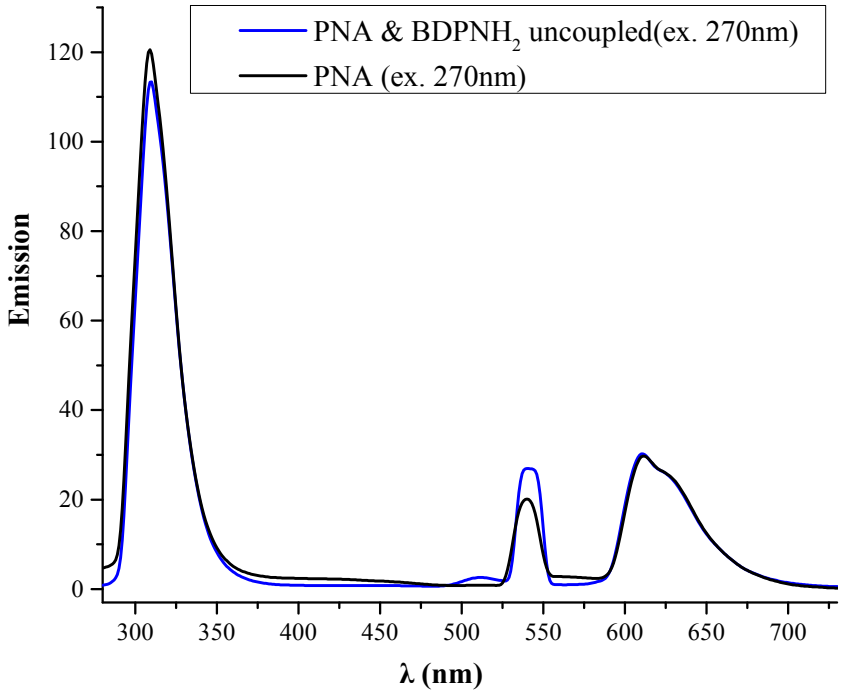

Fig. S13 Isoabsorbing emission spectra of a DCM solution of PNA and BDP uncoupled and a solution of BDP in DCM, upon excitation at 270 nm. The peaks in 540 are due to the excitation-light (2·270 = 540 nm).

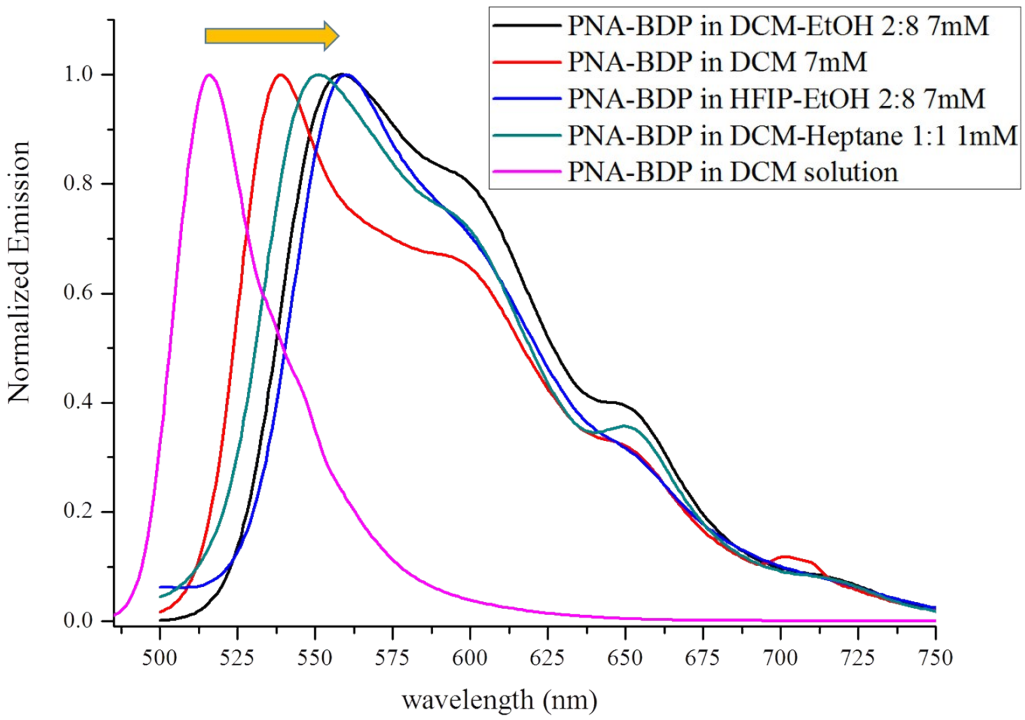

Fig. S14 Normalized solid state emission spectra (excitation at 470 nm) of **PNA-BDP**. Normalized emission spectrum of **PNA-BDP** in DCM solution after excitation at 470 nm (magenta line).

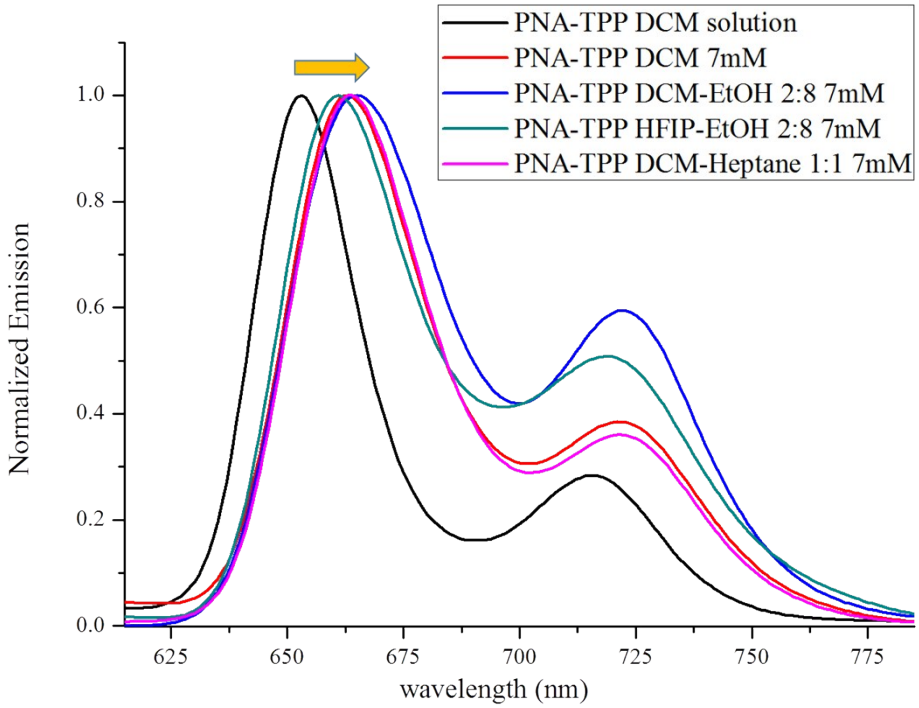

Fig. S15 Normalized solid emission spectra (excitation at 510 nm) of **PNA-TPP**. Normalized emission spectrum of **PNA-TPP** in DCM solution after excitation at 510 nm (black line).

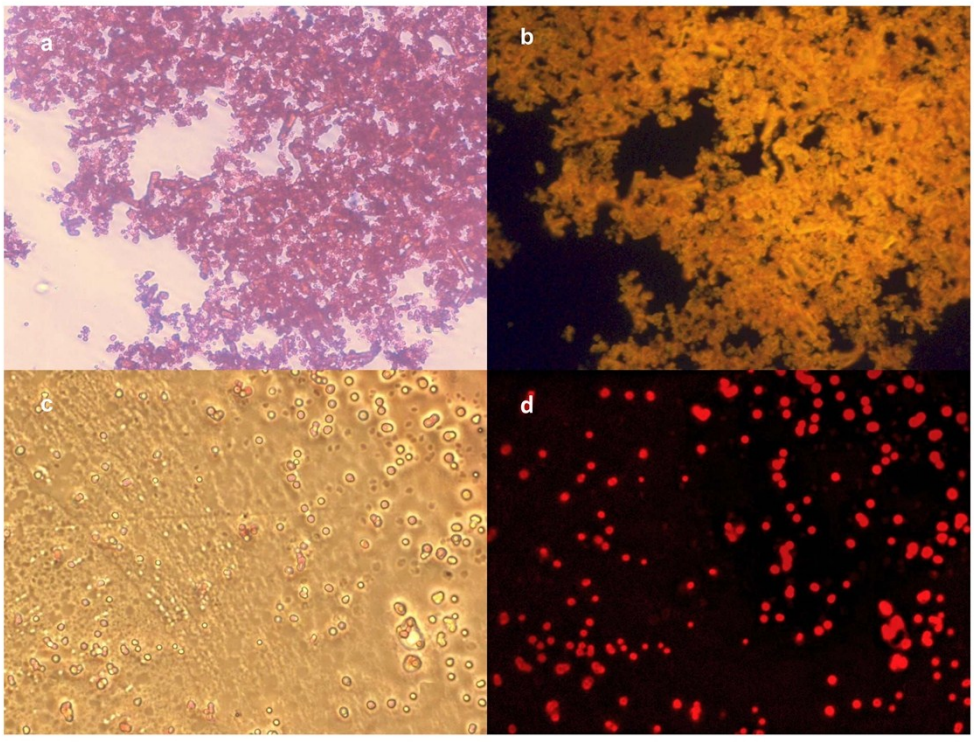

Fig. S16 Fluorescence microscopy of the nano-assemblies of PNA-BDP hybrids in HFIP/EtOH 2:8 a) before and b) after excitation. Fluorescence microscopy of the nano-assemblies of PNA-TPP hybrids in HFIP/EtOH 2:8. c) before and d) after excitation. The compounds were used at a concentration of 7 mM.

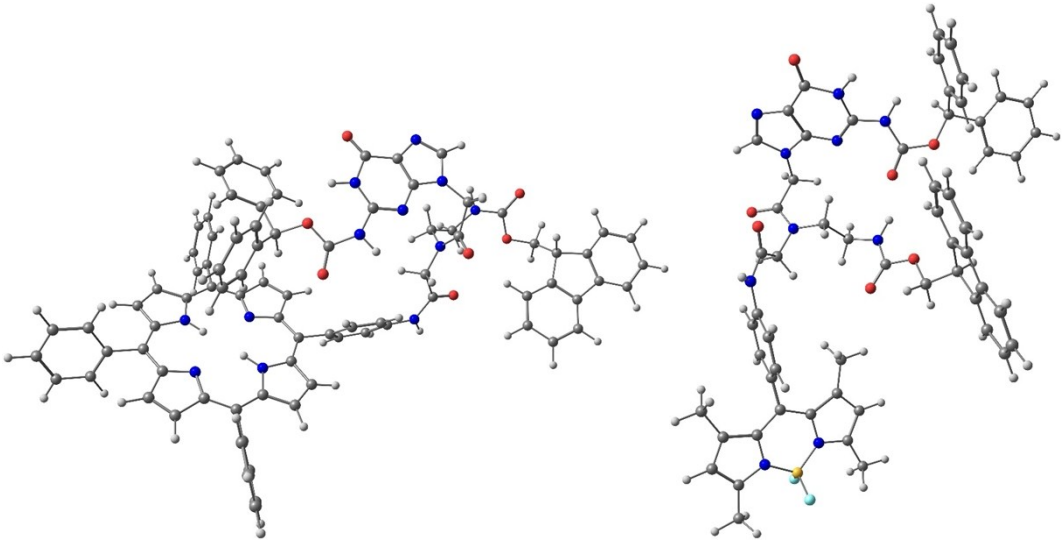

Fig. S17 Different views of the gas phase geometry optimized structures of **PNA-TPP** (left part) and **PNA-BDP** (right part). Carbon, nitrogen, hydrogen, oxygen, boron and fluoride correspond to grey, blue, white, red, yellow and cyan, respectively.

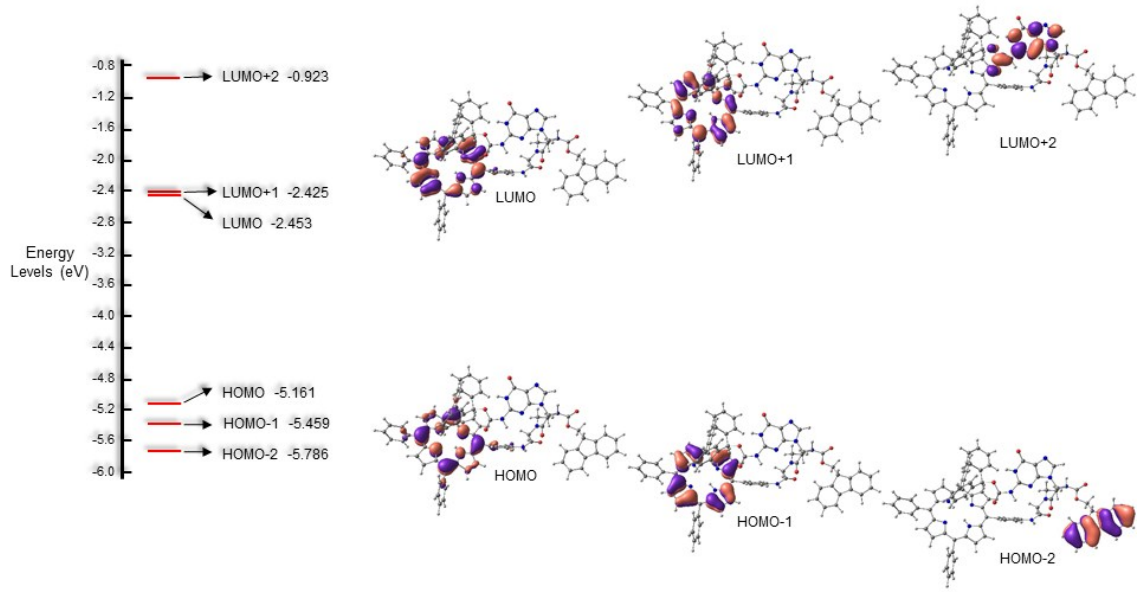

Fig. S18 Frontier molecular orbitals of **PNA-TPP** with the corresponding energy levels.

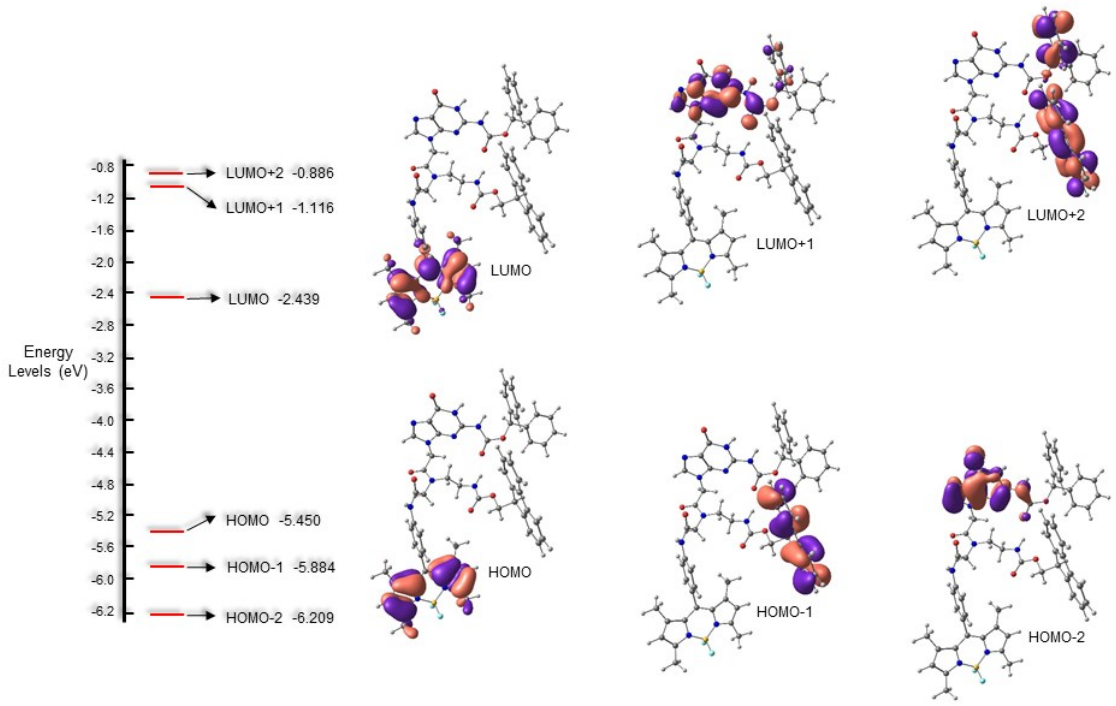

Fig. S19 Frontier molecular orbitals of **PNA-BDP** with the corresponding energy levels.

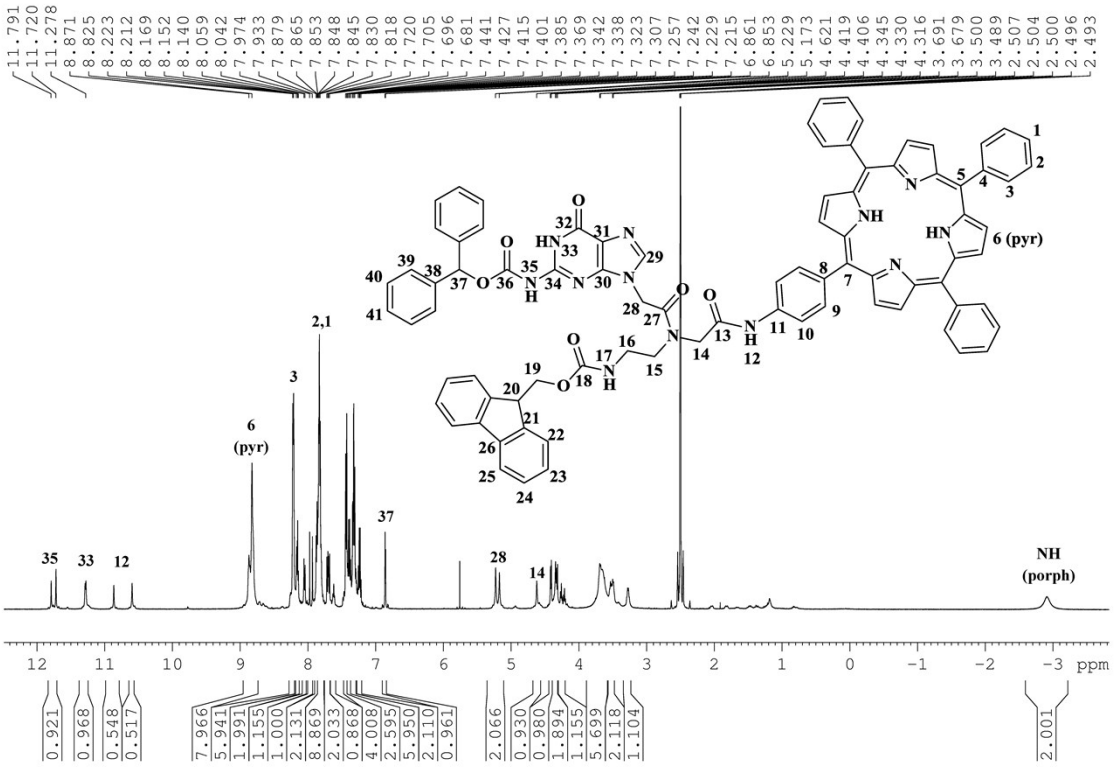

Fig. S20 ^{1}H NMR spectrum of **PNA-TPP** (500 MHz, DMSO).

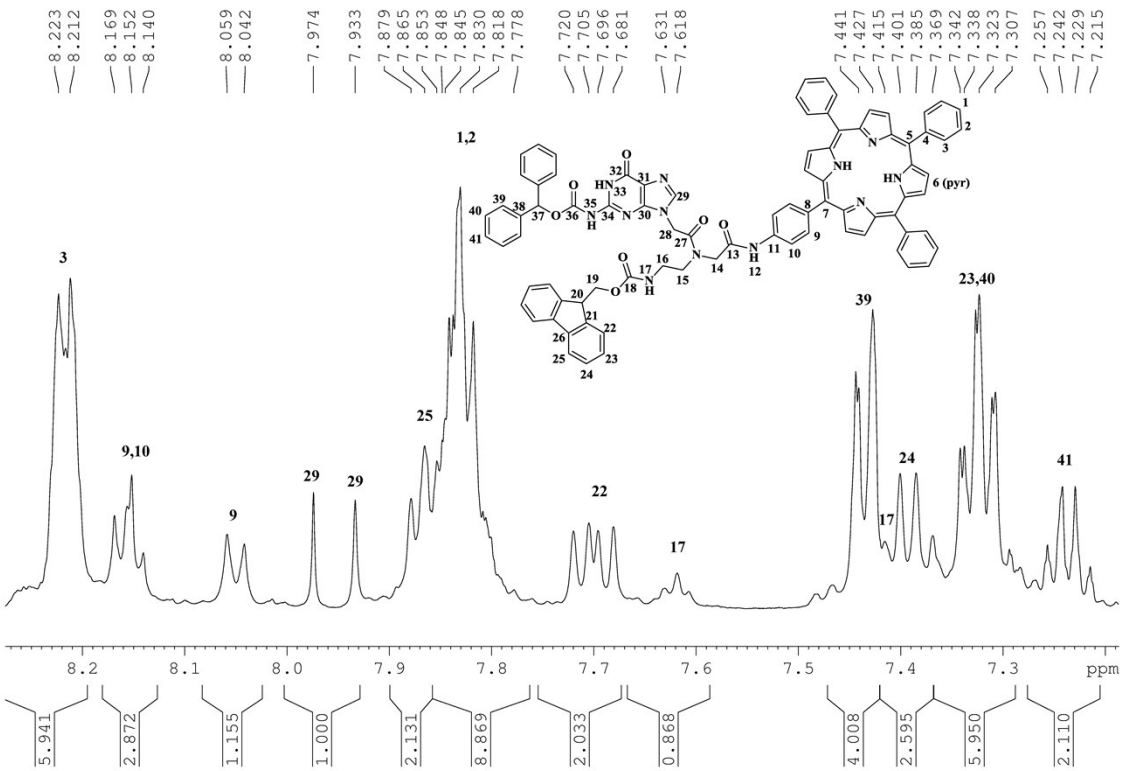

Fig. S21 [1]H NMR spectrum of **PNA-TPP** (500 MHz, DMSO).

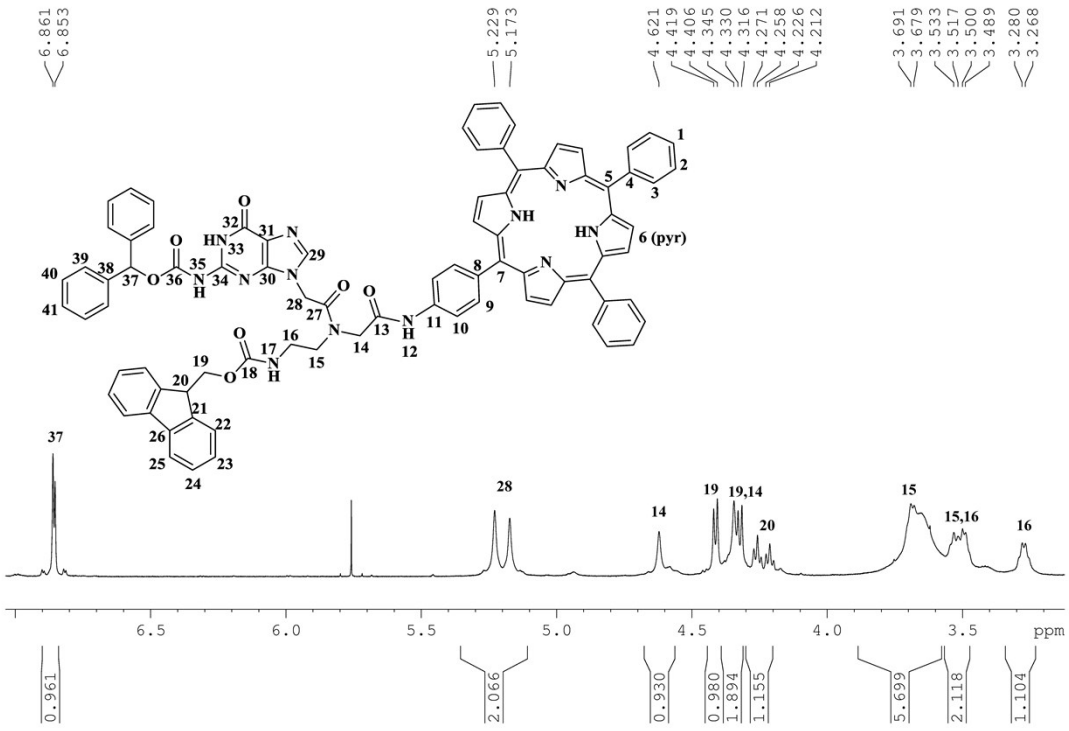

Fig. S22 [1]H NMR spectrum of **PNA-TPP** (500 MHz, DMSO).

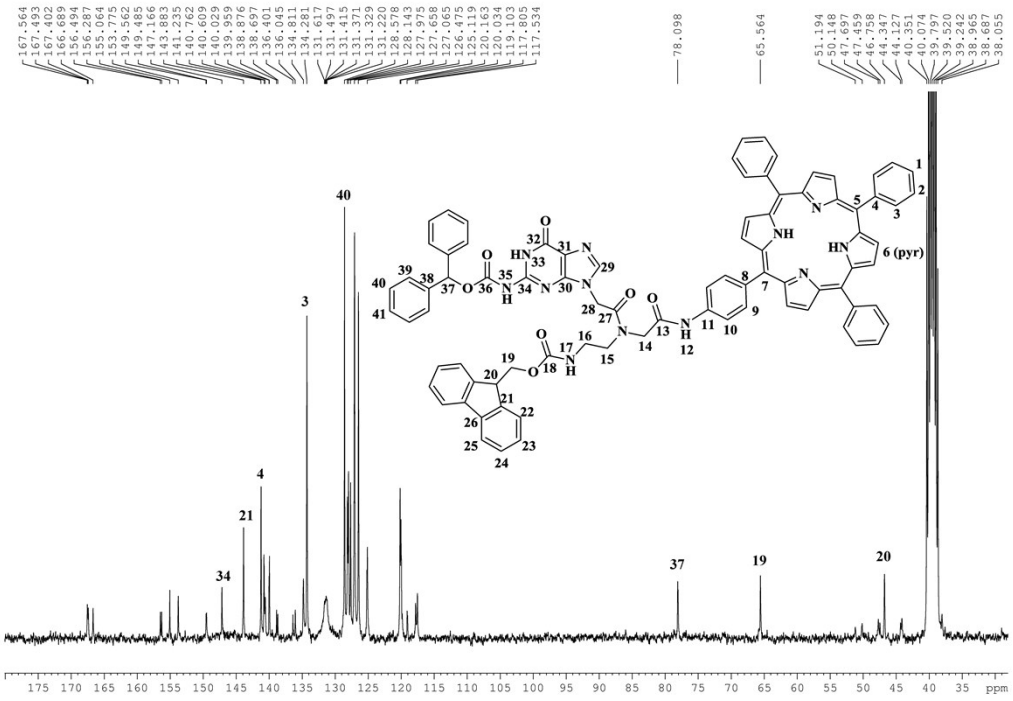

Fig. S23 ^{13}C NMR spectrum of **PNA-TPP** (75 MHz, DMSO).

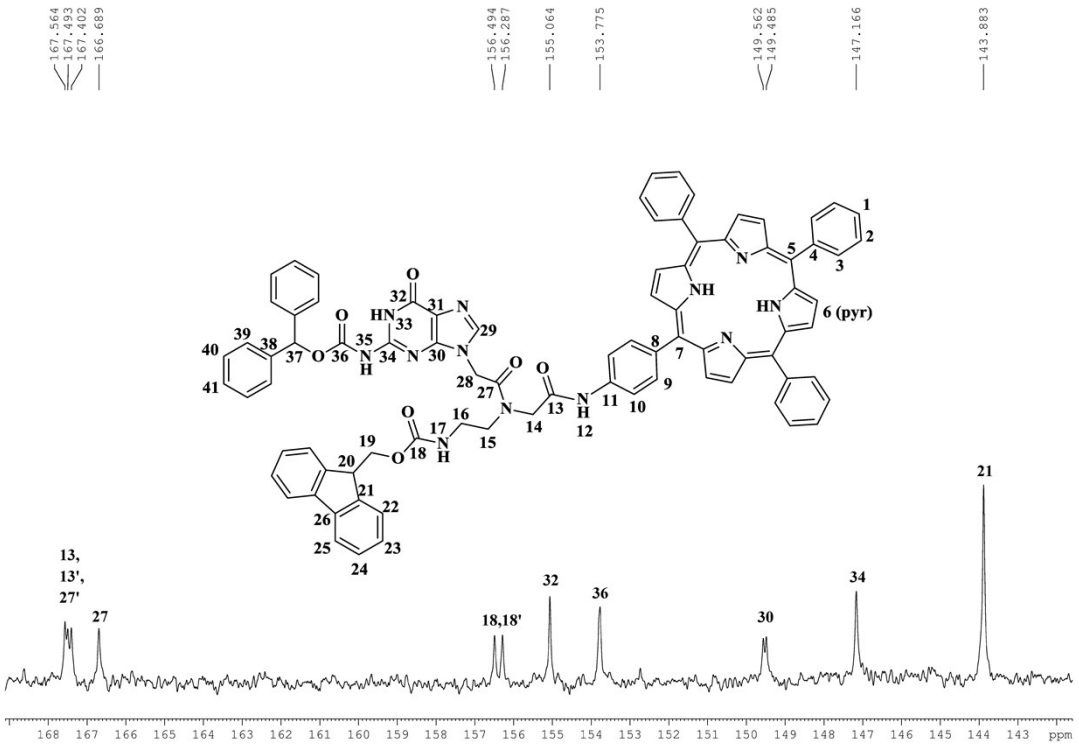

Fig. S24 ^{13}C NMR spectrum of **PNA-TPP** (75 MHz, DMSO).

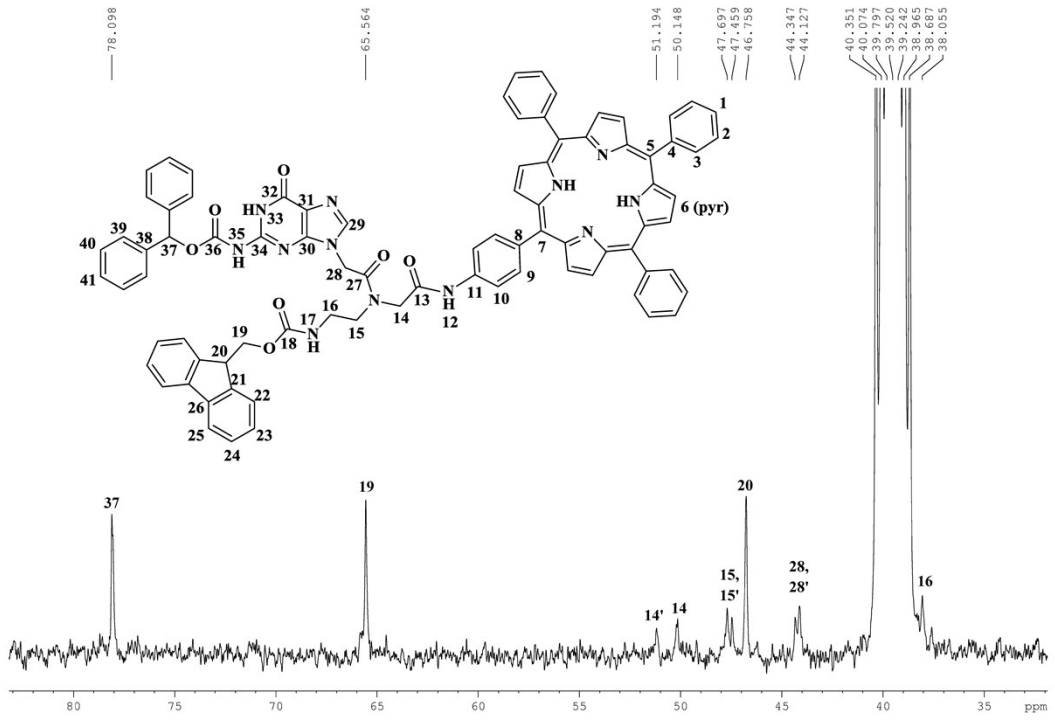

Fig. S25 ^{13}C NMR spectrum of **PNA-TPP** (75 MHz, DMSO).

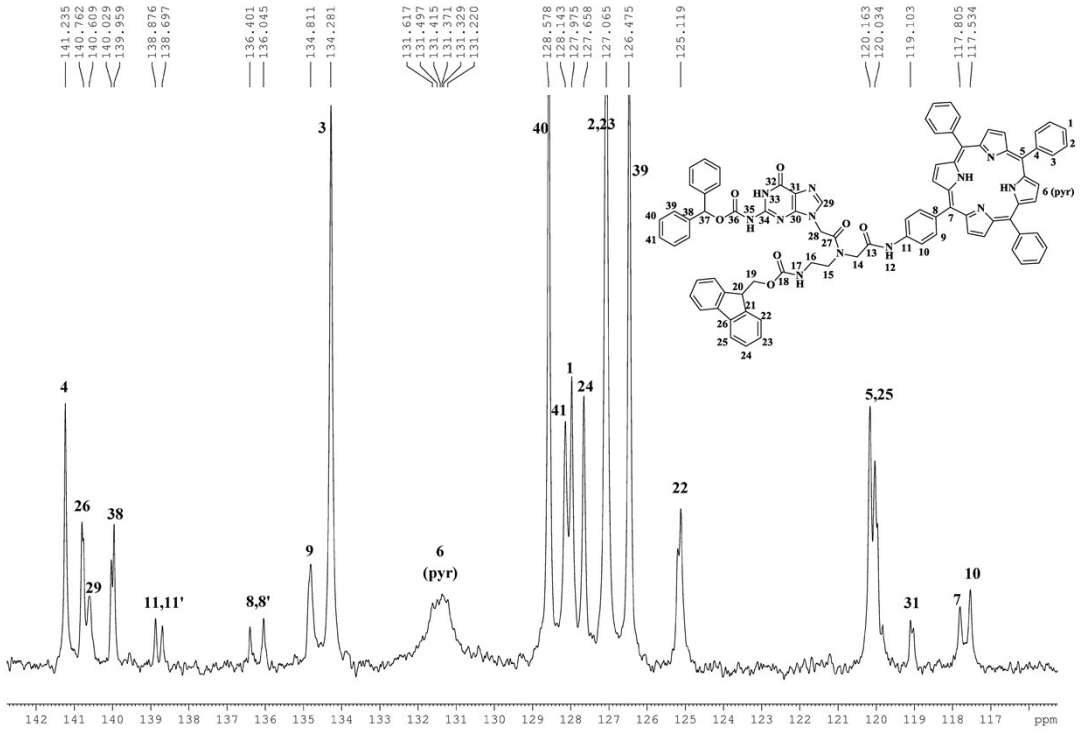

Fig. S26 ^{13}C NMR spectrum of **PNA-TPP** (75 MHz, DMSO).

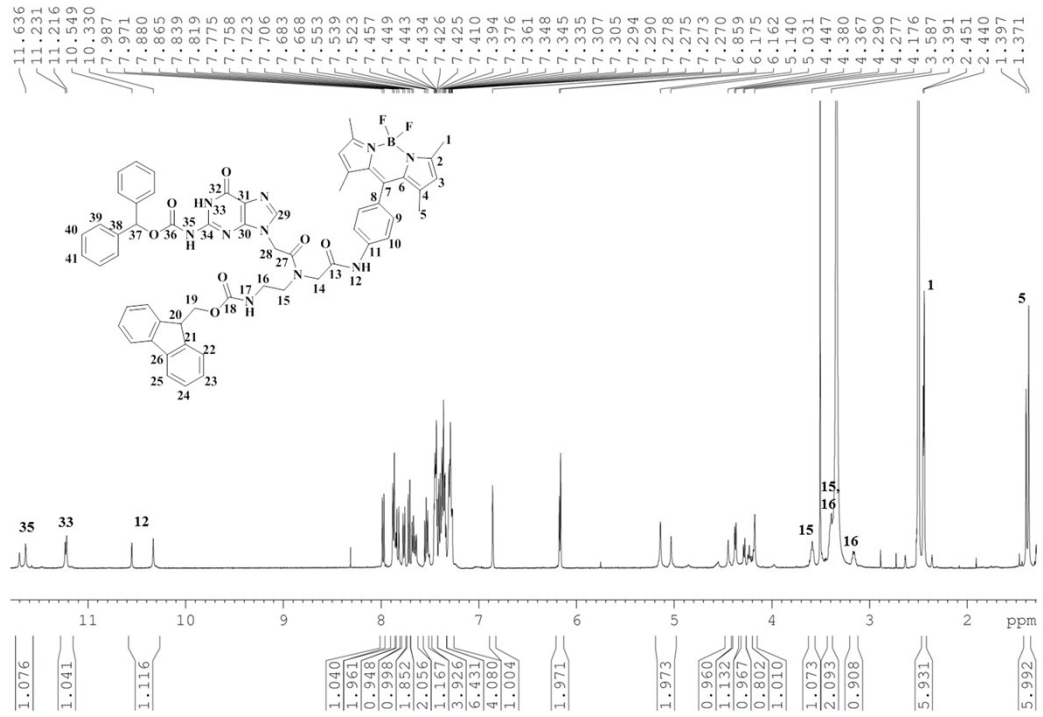

Fig. S27 [1]H NMR spectrum of **PNA-BDP** (500 MHz, DMSO).

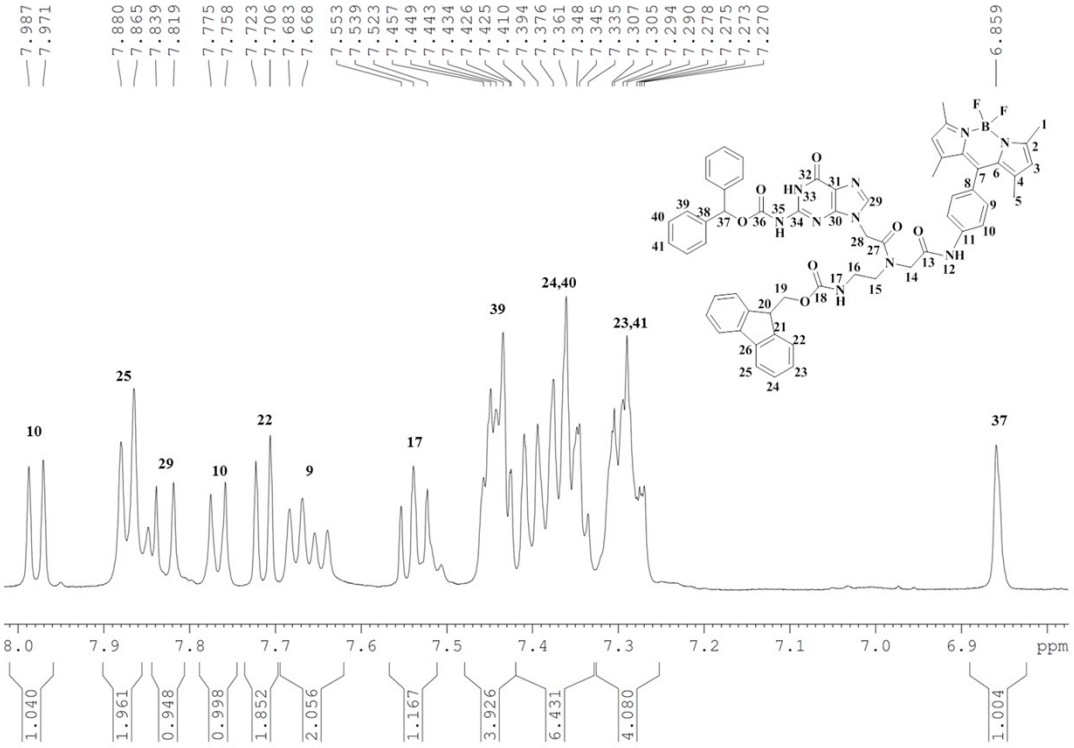

Fig. S28 [1]H NMR spectrum of **PNA-BDP** (500 MHz, DMSO).

Fig. S29 ^{1}H NMR spectrum of **PNA-BDP** (500 MHz, DMSO).

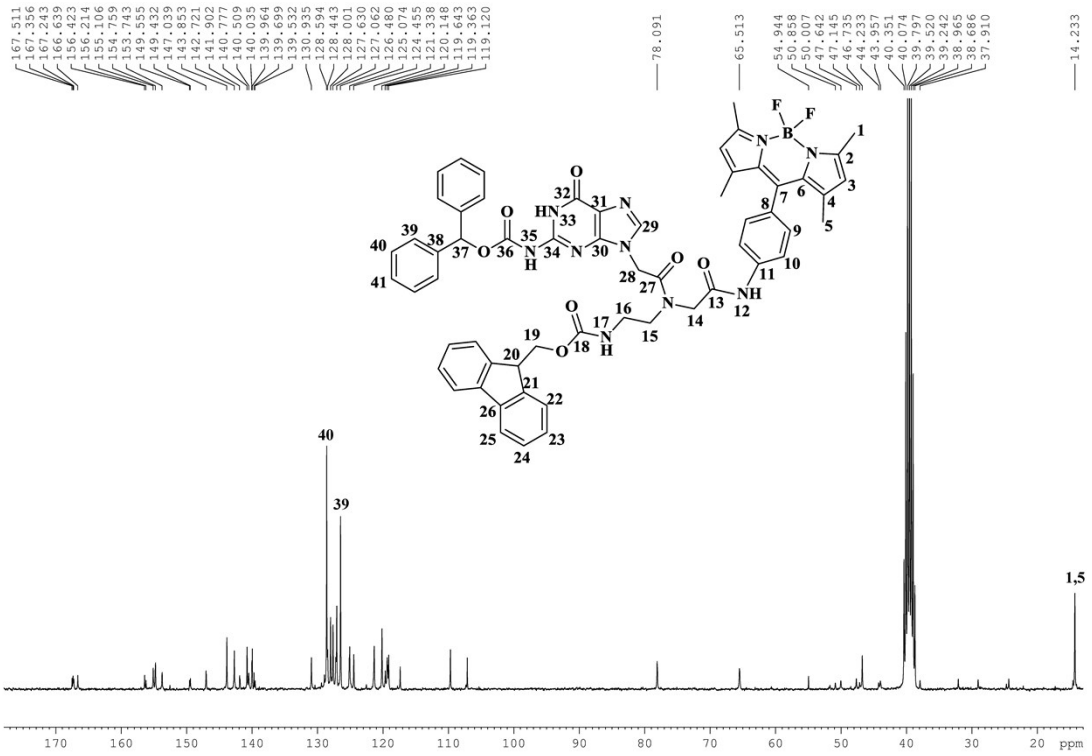

Fig. S30 ^{13}C NMR spectrum of **PNA-BDP** (75 MHz, DMSO).

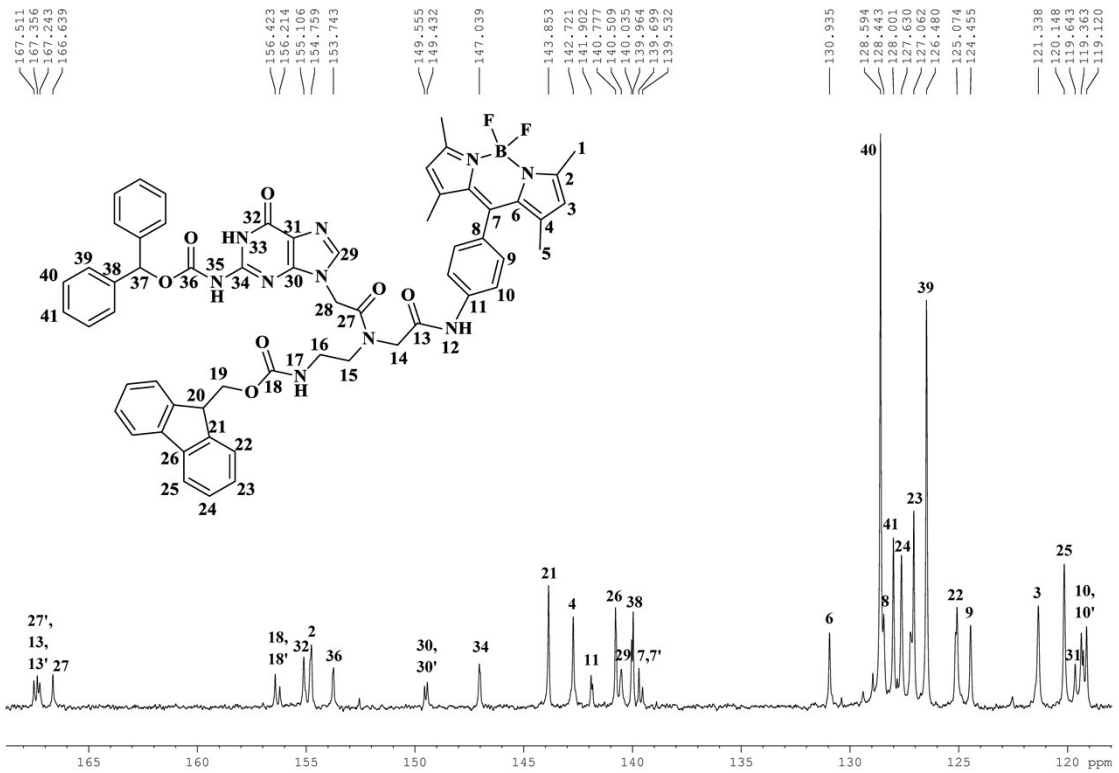

Fig. S31 ^{13}C NMR spectrum of **PNA-BDP** (75 MHz, DMSO).

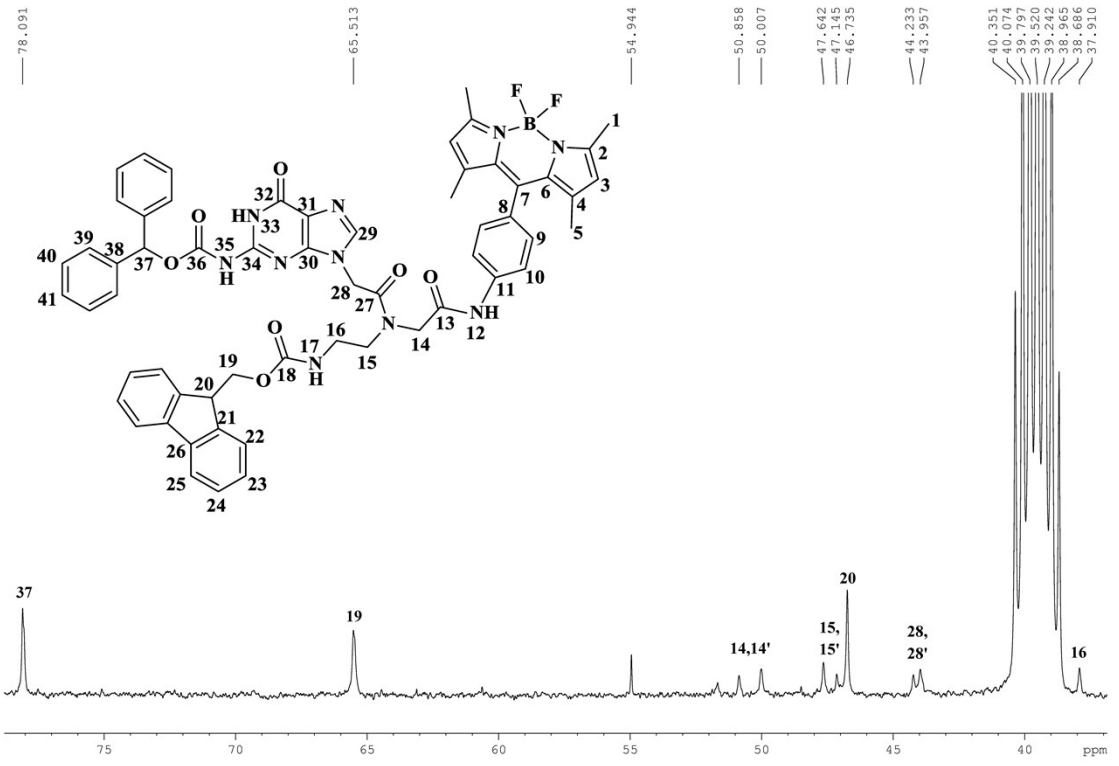

Fig. S32 ^{13}C NMR spectrum of **PNA-BDP** (75 MHz, DMSO).

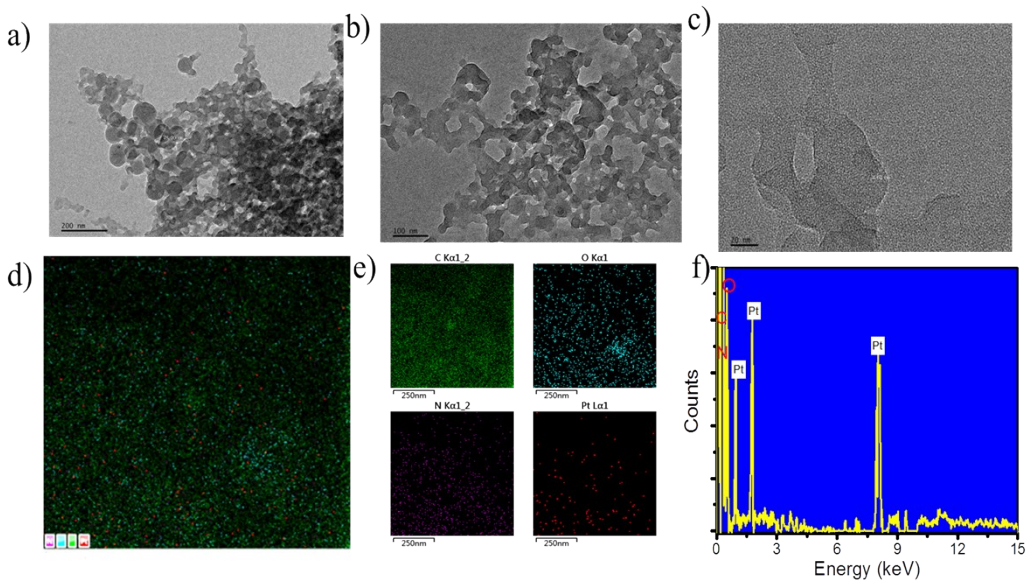

Fig.S33 a) HRTEM image of the PNA-TPP nanospheres before the mineralization with Pt. b) and c) HRTEM image of the mineralized Pt nanoparticles on the nanostructures. d–f) Elemental mapping of the hybrid spheres showing the C,O,N and Pt components, respectively.

Table S1 UV-Vis absorption bands of PNA-TPP and PNA-BDP conjugates in solution and in film deposited from various solvent systems. (For comparison, the bands of $TPPH_2$ and BDP in DCM solution are also given).

Compound	Solvent system	Solution	Spin coating self-assembly[a]	Drop casting self-assembly
		λ_{abs} (nm)	λ_{abs} (nm)	λ_{abs} (nm)
PNA-TPP	DCM	418.5, 515, 550, 590 646	432, 520, 556, 596, 651	426, 509, 544, 582, 637
	DCM/EtOH (2:8)		429, 521, 557, 594, 652	428, 511, 544, 583, 637
	DCM/Heptane (1:1)		426, 521, 551, 592, 650	419, 512, 545, 583, 638
	HFIP/EtOH (2:8)		422, 521, 550, 596, 654	420, 509, 544, 583, 637
	DMSO/H_2O (1:9)			425, 520, 555, 594, 650
TPP-NH_2	DCM	419, 514, 547, 592, 646[b]		
PNA-BDP	DCM	502	510	499
	DCM/EtOH (2:8)		511	509
	DCM/Heptane (1:1)		509	502
	HFIP/EtOH (2:8)		502	502
	DMSO/H_2O (1:9)			512
BDP-NH_2	DCM	500[c]		

[a] Deposited from solutions of various solvent systems by spin coating. (Compound concentration 1mM; film thickness ~10 nm.)

[b] Obtained from R. A. Krüger, A. S. Terpstra, T. C. Sutherland, Can. J. Chem. 2011, 89, 214–220.

[c] Obtained from M. Fioroni, K. Burger, A. E. Mark, D. Roccatano, J. Phys. Chem. B, 2001, 105, 10967–10975.

Table S2 Coordinates of gas phase geometry optimized structure of **PNA-TPP** calculated by DFT at the B3LYP/LANL2DG/6-31G* level with energy E = -4423.11275648 Hartree/particle.

	x	y	z
C	1.042989000	1.959797000	-4.836572000
C	1.297895000	0.630577000	-4.788217000
C	0.571042000	0.113970000	-3.632419000
N	-0.103933000	1.116486000	-2.991866000
C	0.177141000	2.253784000	-3.698646000
C	-2.336917000	5.076062000	-0.815044000
C	-1.570112000	5.194072000	-1.943644000
C	-1.103787000	3.886577000	-2.305927000
N	-1.605327000	3.017808000	-1.363870000
C	-2.363469000	3.693109000	-0.434053000
C	-0.283311000	3.553364000	-3.396607000
C	-3.676847000	-0.100320000	2.106361000
C	-3.876429000	1.240928000	2.096662000
C	-3.094146000	1.764606000	0.983705000
N	-2.425152000	0.756736000	0.341788000
C	-2.749092000	-0.388477000	1.016699000
C	-3.057505000	3.135699000	0.651640000
C	-0.046523000	-3.172653000	-1.736008000
C	-0.844584000	-3.297490000	-0.630442000
C	-1.390438000	-2.006421000	-0.323137000
N	-0.875741000	-1.135001000	-1.255571000
C	-0.058053000	-1.797245000	-2.142988000
C	0.610101000	-1.242871000	-3.246940000
C	-2.272098000	-1.687002000	0.724051000
C	-3.821877000	4.096398000	1.515836000
C	-2.762210000	-2.826489000	1.561651000
C	1.425981000	-2.191082000	-4.076190000
C	0.132586000	4.683387000	-4.290338000
C	-5.218987000	4.189281000	1.425999000

C	-5.924294000	5.085159000	2.231726000
C	-5.244075000	5.902342000	3.136795000
C	-3.853291000	5.819560000	3.232249000
C	-3.147454000	4.923460000	2.427403000
C	-2.479110000	-2.913544000	2.934914000
C	-3.014208000	-3.934291000	3.718164000
C	-3.830301000	-4.918765000	3.141759000
C	-4.051404000	-4.884875000	1.758718000
C	-3.547571000	-3.838645000	0.988424000
C	0.974844000	-2.608739000	-5.337726000
C	1.733312000	-3.490522000	-6.109527000
C	2.954846000	-3.969636000	-5.631525000
C	3.413311000	-3.561814000	-4.377296000
C	2.654331000	-2.680004000	-3.605566000
C	1.457430000	5.147471000	-4.291945000
C	1.842748000	6.200837000	-5.122717000
C	0.909238000	6.808114000	-5.965270000
C	-0.411743000	6.355781000	-5.972010000
C	-0.796901000	5.302520000	-5.140660000
N	-4.389390000	-5.926696000	3.971750000
C	-4.148240000	0.552883000	-4.030230000
C	-4.673170000	0.451143000	-2.740802000
C	-6.038159000	0.212240000	-2.548593000
C	-6.874794000	0.066017000	-3.663129000
C	-6.348151000	0.155928000	-4.951857000
C	-4.985050000	0.403499000	-5.137686000
C	-6.585667000	0.144037000	-1.140225000
O	-7.439322000	-1.052146000	-0.954985000
C	-7.460114000	1.313794000	-0.703398000
C	-7.590058000	2.473380000	-1.476517000
C	-8.388540000	3.532842000	-1.035887000
C	-9.072477000	3.443381000	0.176443000

C	-8.940168000	2.293712000	0.960354000
C	-8.130990000	1.244794000	0.528397000
C	-6.808232000	-2.240745000	-0.907182000
N	-7.670226000	-3.280237000	-0.563129000
O	-5.635749000	-2.435634000	-1.142208000
C	-8.871591000	-3.296048000	0.147263000
N	-9.163440000	-4.428454000	0.739492000
C	-10.332743000	-4.379260000	1.426738000
C	-11.211929000	-3.305619000	1.567362000
C	-10.896445000	-2.056222000	0.915474000
N	-9.657848000	-2.185355000	0.188512000
O	-11.484391000	-0.990550000	0.907319000
N	-10.858636000	-5.394372000	2.193037000
C	-12.030000000	-4.881122000	2.732493000
N	-12.269430000	-3.641654000	2.385887000
C	-10.328434000	-6.743677000	2.386948000
C	-8.791256000	-6.832026000	2.428663000
N	-8.077876000	-6.071966000	3.333285000
O	-8.240866000	-7.575409000	1.627112000
C	-8.633745000	-5.258868000	4.420564000
C	-6.672824000	-5.880422000	3.010844000
C	-5.686417000	-6.397065000	4.056743000
O	-5.994452000	-7.186649000	4.940403000
C	-8.882748000	-6.001698000	5.746179000
N	-10.135425000	-6.749118000	5.712376000
C	-10.401989000	-7.940642000	6.345771000
O	-9.278835000	-8.522090000	6.828982000
O	-11.525024000	-8.408184000	6.431641000
C	-9.467293000	-9.809798000	7.456634000
C	-9.368470000	-10.959665000	6.441074000
C	-9.763904000	-12.292180000	7.060395000
C	-8.708518000	-13.219458000	6.940846000

C	-7.587816000	-12.566305000	6.251123000
C	-7.955906000	-11.237870000	5.946549000
C	-10.959481000	-12.653950000	7.672132000
C	-11.098089000	-13.954080000	8.173593000
C	-10.050834000	-14.874837000	8.057980000
C	-8.850161000	-14.516211000	7.439704000
C	-6.326073000	-13.051126000	5.901278000
C	-5.432118000	-12.195168000	5.253057000
C	-5.794805000	-10.876018000	4.961172000
C	-7.061647000	-10.387692000	5.303700000
H	1.401483000	2.678574000	-5.559144000
H	1.912529000	0.047558000	-5.458758000
H	-2.846810000	5.864880000	-0.282579000
H	-1.340226000	6.097243000	-2.488674000
H	-1.418127000	2.020785000	-1.349110000
H	-4.104958000	-0.824946000	2.783432000
H	-4.492000000	1.825686000	2.764823000
H	0.507057000	-3.953039000	-2.236092000
H	-1.045111000	-4.197345000	-0.068952000
H	-1.076298000	-0.141021000	-1.285258000
H	-5.753202000	3.561922000	0.718656000
H	-7.005846000	5.141306000	2.145168000
H	-5.793500000	6.599606000	3.763744000
H	-3.315990000	6.450138000	3.935817000
H	-2.065755000	4.856193000	2.506738000
H	-1.851360000	-2.158360000	3.398779000
H	-2.813732000	-3.960473000	4.786469000
H	-4.619464000	-5.674114000	1.279694000
H	-3.788603000	-3.790159000	-0.067878000
H	0.022422000	-2.240825000	-5.709286000
H	1.367105000	-3.805430000	-7.083122000
H	3.545308000	-4.655995000	-6.232435000

H	4.364648000	-3.926570000	-3.998961000
H	3.016271000	-2.358766000	-2.632637000
H	2.183998000	4.679645000	-3.633464000
H	2.872210000	6.548919000	-5.108265000
H	1.209231000	7.628033000	-6.612246000
H	-1.143914000	6.819698000	-6.627692000
H	-1.823761000	4.947427000	-5.152780000
H	-3.826092000	-6.241105000	4.754862000
H	-3.084798000	0.735666000	-4.159470000
H	-4.014747000	0.546766000	-1.880926000
H	-7.935600000	-0.122909000	-3.520827000
H	-7.002569000	0.034656000	-5.811028000
H	-4.577684000	0.474401000	-6.142824000
H	-5.751936000	0.026124000	-0.441237000
H	-7.070679000	2.549350000	-2.425187000
H	-8.482043000	4.423796000	-1.650824000
H	-9.709090000	4.259455000	0.507457000
H	-9.472243000	2.209241000	1.903359000
H	-8.029479000	0.358425000	1.147772000
H	-7.200961000	-4.177378000	-0.522135000
H	-9.344490000	-1.345836000	-0.289746000
H	-12.663751000	-5.491415000	3.364432000
H	-10.759290000	-7.142077000	3.308755000
H	-10.619581000	-7.385700000	1.552831000
H	-9.553465000	-4.764777000	4.094103000
H	-7.912233000	-4.458061000	4.613583000
H	-6.486850000	-4.815810000	2.821170000
H	-6.499234000	-6.423122000	2.079156000
H	-8.904022000	-5.255567000	6.555472000
H	-8.064812000	-6.693616000	5.939441000
H	-10.982900000	-6.212188000	5.574172000
H	-10.441440000	-9.815414000	7.947934000

H	-8.672164000	-9.879784000	8.201530000
H	-10.043589000	-10.715134000	5.608921000
H	-11.779731000	-11.944671000	7.754869000
H	-12.027046000	-14.250674000	8.653124000
H	-10.173657000	-15.880921000	8.450599000
H	-8.042887000	-15.238723000	7.350170000
H	-6.039162000	-14.074686000	6.129621000
H	-4.445510000	-12.558065000	4.976038000
H	-5.089248000	-10.213597000	4.467800000
H	-7.317861000	-9.358452000	5.076827000

Table S3 Coordinates of gas phase geometry optimized structure of **PNA-BDP** calculated by DFT at the B3LYP/LANL2DG/6-31G* level with energy E = -3579.09481117 Hartree/particle.

	x	**y**	**z**
C	5.131286000	-2.365046000	-1.345109000
C	4.105715000	-2.694522000	-2.226748000
C	3.275633000	-1.696589000	-2.759274000
C	3.523664000	-0.358704000	-2.424144000
C	4.536378000	-0.038478000	-1.520366000
C	5.346621000	-1.034289000	-0.962221000
N	2.236053000	-2.074975000	-3.643875000
C	6.404519000	-0.687703000	0.034521000
C	7.700269000	-0.369374000	-0.407759000
C	6.080213000	-0.684145000	1.400404000
C	8.276617000	-0.305304000	-1.720471000
C	9.604093000	0.066227000	-1.536788000
C	9.837707000	0.225794000	-0.155429000
N	8.698818000	-0.036449000	0.514827000
N	7.052796000	-0.359200000	2.354403000
C	6.495673000	-0.425488000	3.578496000
C	5.141082000	-0.797250000	3.448101000
C	4.854500000	-0.965270000	2.098390000

C	7.645342000	-0.571089000	-3.056414000
C	11.104457000	0.621456000	0.531421000
C	3.512063000	-1.362020000	1.558157000
C	7.261568000	-0.133732000	4.827787000
B	8.534808000	0.019061000	2.062496000
F	9.391161000	-0.901095000	2.666948000
F	8.799584000	1.306609000	2.526491000
C	-9.536150000	-5.932238000	3.818164000
C	-9.099923000	-5.813395000	2.499554000
C	-7.837560000	-5.275297000	2.213891000
C	-7.017697000	-4.860394000	3.268550000
C	-7.455170000	-4.988272000	4.589259000
C	-8.713018000	-5.521305000	4.869225000
C	-7.415422000	-5.110312000	0.755584000
O	-6.014130000	-4.729914000	0.762717000
C	-7.633933000	-6.361804000	-0.083426000
C	-6.818436000	-7.488450000	0.101966000
C	-7.014200000	-8.628582000	-0.674644000
C	-8.025515000	-8.661067000	-1.641632000
C	-8.841236000	-7.546185000	-1.831113000
C	-8.643235000	-6.397958000	-1.055312000
C	-5.394114000	-4.112425000	-0.271242000
N	-6.071218000	-4.156361000	-1.482189000
O	-4.312821000	-3.596823000	-0.097982000
C	-5.651124000	-3.534633000	-2.666822000
N	-4.959529000	-2.434307000	-2.648200000
C	-4.654887000	-1.985877000	-3.895664000
C	-5.022948000	-2.507209000	-5.135114000
C	-5.818271000	-3.709210000	-5.170522000
N	-6.068783000	-4.154226000	-3.817173000
O	-6.264009000	-4.361134000	-6.096028000
N	-3.901966000	-0.872836000	-4.170487000

C	-3.847520000	-0.784796000	-5.551551000
N	-4.508953000	-1.741159000	-6.157899000
C	-3.306588000	0.024464000	-3.185456000
C	-1.774800000	0.073850000	-3.322634000
N	-1.018886000	-0.696600000	-2.484011000
O	-1.287225000	0.825511000	-4.162185000
C	-1.524592000	-1.723512000	-1.567478000
C	0.421268000	-0.654318000	-2.664936000
C	0.885556000	-1.766972000	-3.618868000
O	0.103488000	-2.374633000	-4.330039000
C	-1.594172000	-1.227192000	-0.109160000
N	-1.816769000	-2.309918000	0.830325000
C	-0.753806000	-3.030107000	1.288921000
O	-1.190211000	-4.121292000	1.976600000
O	0.424431000	-2.742973000	1.136336000
C	-0.165249000	-4.989443000	2.485435000
C	-0.857735000	-6.238329000	3.042548000
C	-1.479494000	-7.135346000	1.980471000
C	-0.909422000	-8.424914000	2.039377000
C	0.087928000	-8.450391000	3.117617000
C	0.129278000	-7.176783000	3.721290000
C	-2.461651000	-6.840607000	1.038849000
C	-2.866537000	-7.844858000	0.149786000
C	-2.302067000	-9.124254000	0.208252000
C	-1.320230000	-9.424698000	1.154909000
C	0.913198000	-9.478454000	3.578334000
C	1.779880000	-9.222360000	4.643632000
C	1.820325000	-7.958653000	5.242832000
C	0.991941000	-6.927463000	4.783462000
H	5.755555000	-3.150530000	-0.928722000
H	3.926033000	-3.734627000	-2.486362000
H	2.936227000	0.432928000	-2.875859000

H	4.705119000	1.000871000	-1.252954000
H	2.409508000	-2.894431000	-4.216570000
H	10.342648000	0.211495000	-2.314993000
H	4.448269000	-0.927274000	4.269763000
H	7.249608000	-1.589680000	-3.133375000
H	8.389295000	-0.438784000	-3.848361000
H	6.810161000	0.106807000	-3.263650000
H	11.910354000	0.751746000	-0.195523000
H	11.397554000	-0.137345000	1.264492000
H	10.965666000	1.556312000	1.085493000
H	2.798115000	-1.498690000	2.374560000
H	3.545555000	-2.300535000	0.996050000
H	3.099236000	-0.607970000	0.879245000
H	8.131615000	-0.794084000	4.907082000
H	6.626202000	-0.265562000	5.707400000
H	7.646880000	0.891519000	4.811318000
H	-10.517449000	-6.351055000	4.023688000
H	-9.743567000	-6.147780000	1.690368000
H	-6.040281000	-4.443679000	3.057289000
H	-6.806030000	-4.667639000	5.399510000
H	-9.050448000	-5.617995000	5.897429000
H	-7.984091000	-4.280135000	0.314933000
H	-6.028529000	-7.463191000	0.846955000
H	-6.376215000	-9.495061000	-0.525423000
H	-8.173216000	-9.552166000	-2.244934000
H	-9.629106000	-7.563776000	-2.578760000
H	-9.286014000	-5.530976000	-1.199885000
H	-6.800336000	-4.854235000	-1.573409000
H	-6.560531000	-5.040854000	-3.777334000
H	-3.286904000	0.005427000	-6.031848000
H	-3.663919000	-0.296191000	-2.206650000
H	-3.656203000	1.043362000	-3.371077000

H	-0.842322000	-2.577344000	-1.619681000
H	-2.500378000	-2.089749000	-1.889534000
H	0.916382000	-0.751096000	-1.693704000
H	0.677122000	0.316839000	-3.094466000
H	-2.398135000	-0.490962000	0.003303000
H	-0.655779000	-0.739791000	0.165669000
H	-2.719243000	-2.775522000	0.812054000
H	0.391433000	-4.467525000	3.271231000
H	0.536100000	-5.246102000	1.686446000
H	-1.622506000	-5.898246000	3.756169000
H	-2.899479000	-5.848914000	0.984903000
H	-3.624085000	-7.625335000	-0.598287000
H	-2.626418000	-9.890194000	-0.491646000
H	-0.884389000	-10.419665000	1.196881000
H	0.885680000	-10.463253000	3.119007000
H	2.428347000	-10.013000000	5.011586000
H	2.498548000	-7.776027000	6.071829000
H	1.026453000	-5.949628000	5.258210000

Table S4 Summary of the calculated HOMO and LUMO values, the HOMO-LUMO (H-L) gap and the dipole moment (μ) regarding **PNA-TPP** and **PNA-BDP**.

Compound	**HOMO (eV)**	**LUMO (eV)**	**H-L (eV)**	***μ* (D)**
PNA-TPP	-5.161	-2.453	2.708	10.15
PNA-BDP	-5.450	-2.439	3.011	11.91