Supplementary Information

Evaluation of a Novel Platinum(II)Based AIE Compound-Encapsulated MesoporousSilica Nanoparticles for Cancer Theranostic Application

Sheik Saleem Pasha[1#], Leena Fageria[2#], Clàudia Climent[3], Nigam P. Rath[4], Pere Alemany[5], Rajdeep Chowdhury[2*], Aniruddha Roy[6*] and Inamur Rahaman Laskar[1*]

[1]Department of Chemistry, Pilani Campus, BITS, Pilani, Rajasthan 333031, India; [2]Department of Biological Sciences, Pilani Campus, BITS, Pilani, Rajasthan 333031, India; [3]Departamento de Física Teórica de la Materia, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

[4]Department of Chemistry and Biochemistry, University of Missouri-St Louis, University Blvd, St Louis, MO 63121, USA; [5]Departament de Ciència de Materials iQuímicaFísica and Institut de QuímicaTeòrica (IQTCUB), Universitat de Barcelona, MartíiFranquès 1, E-08028, Barcelona, Spain, [6]Department of Pharmacy, Pilani Campus, BITS, Pilani,Rajasthan 333031, India;

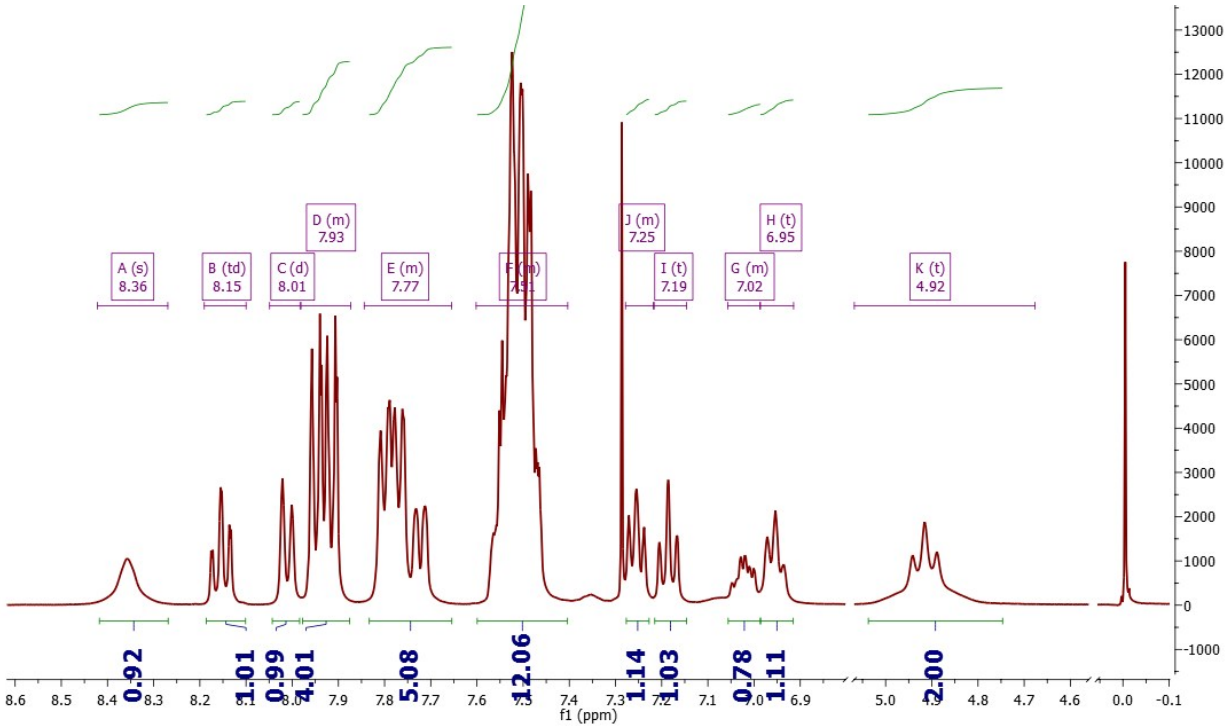

Fig.S1 ^{1}H NMR spectra of BMPP-Pt

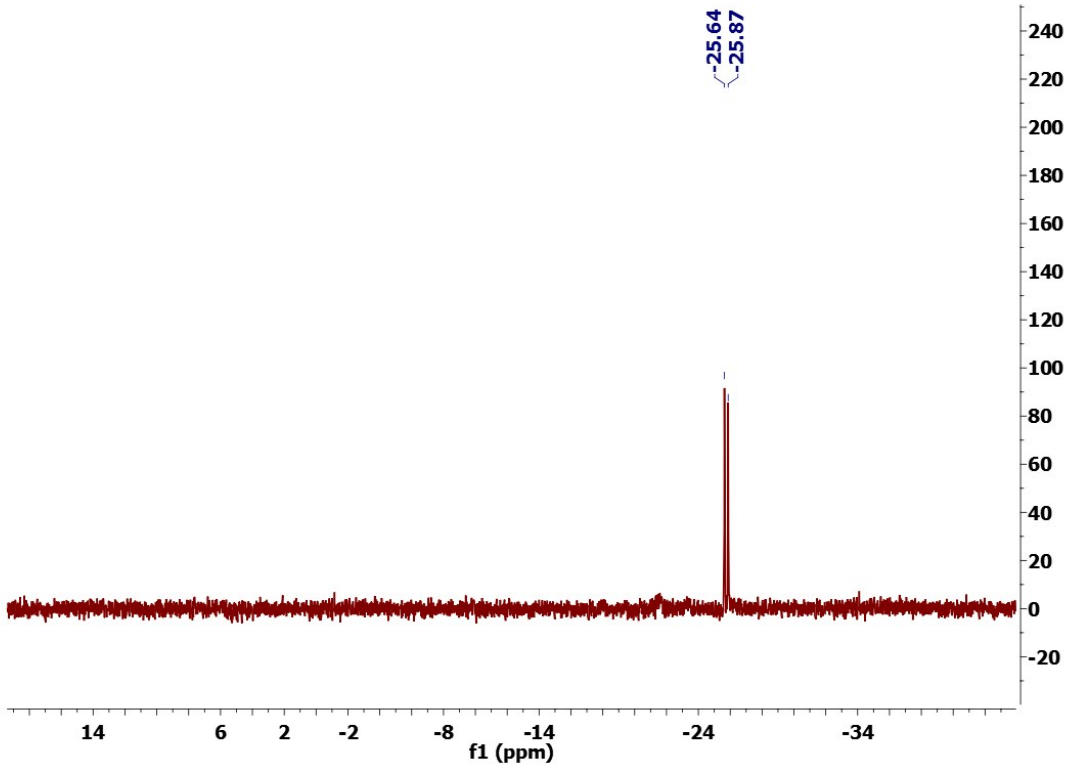

Fig. S2 ^{31}P NMR spectra of BMPP-Pt

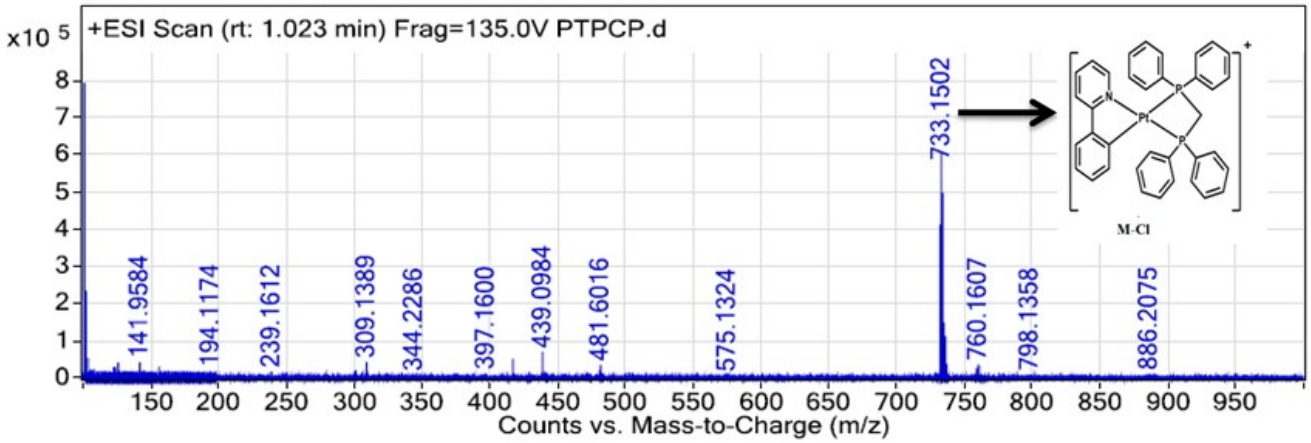

Fig. S3 Mass spectrum of BMPP-Pt

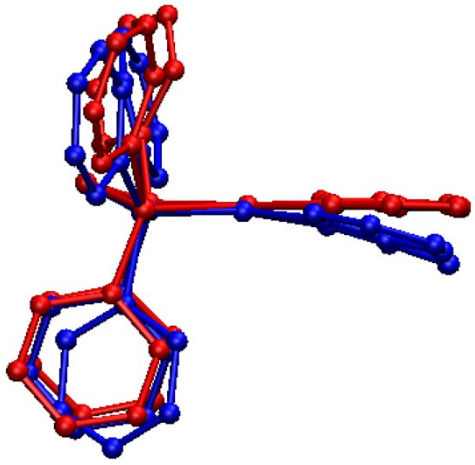

Fig. S4 OptimizedBMPP-Pt ground state structure (in red) overlapped with the crystal's monomer structure (blue) showing the loss of planarity in the latter between the phenylpyridine ligand and the $Pt(P)_2$ fragment. Hydrogen atoms are omitted for the sake of clarity.

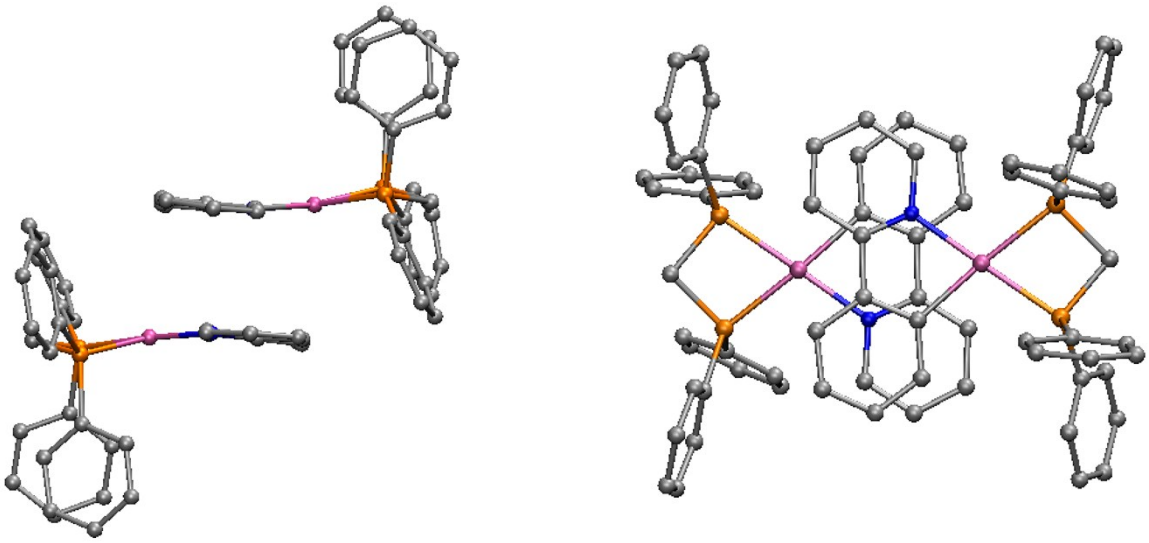

Fig. S5 Dimers of the BMPP-Pt complex present in the crystal structure. Side view on the left and top view on the right.Hydrogen atoms are omitted for the sake of clarity.

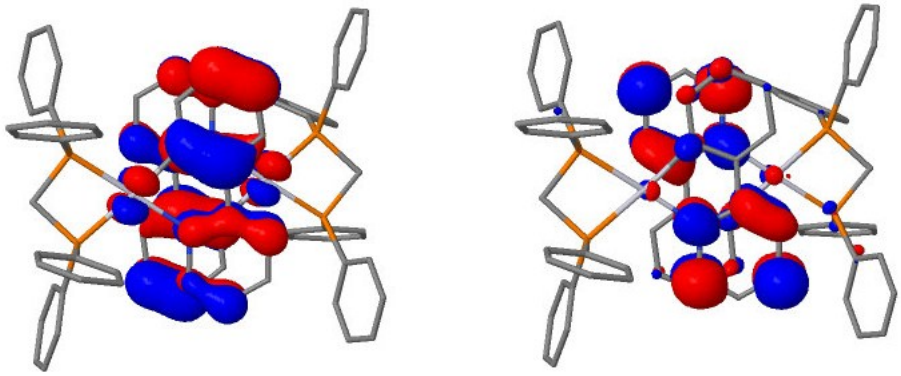

Fig. S6 Top view of the HOMO (left) and LUMO (right) of the BMPP-Pt dimers present in the crystal structure. Hydrogen atoms are omitted for the sake of clarity.

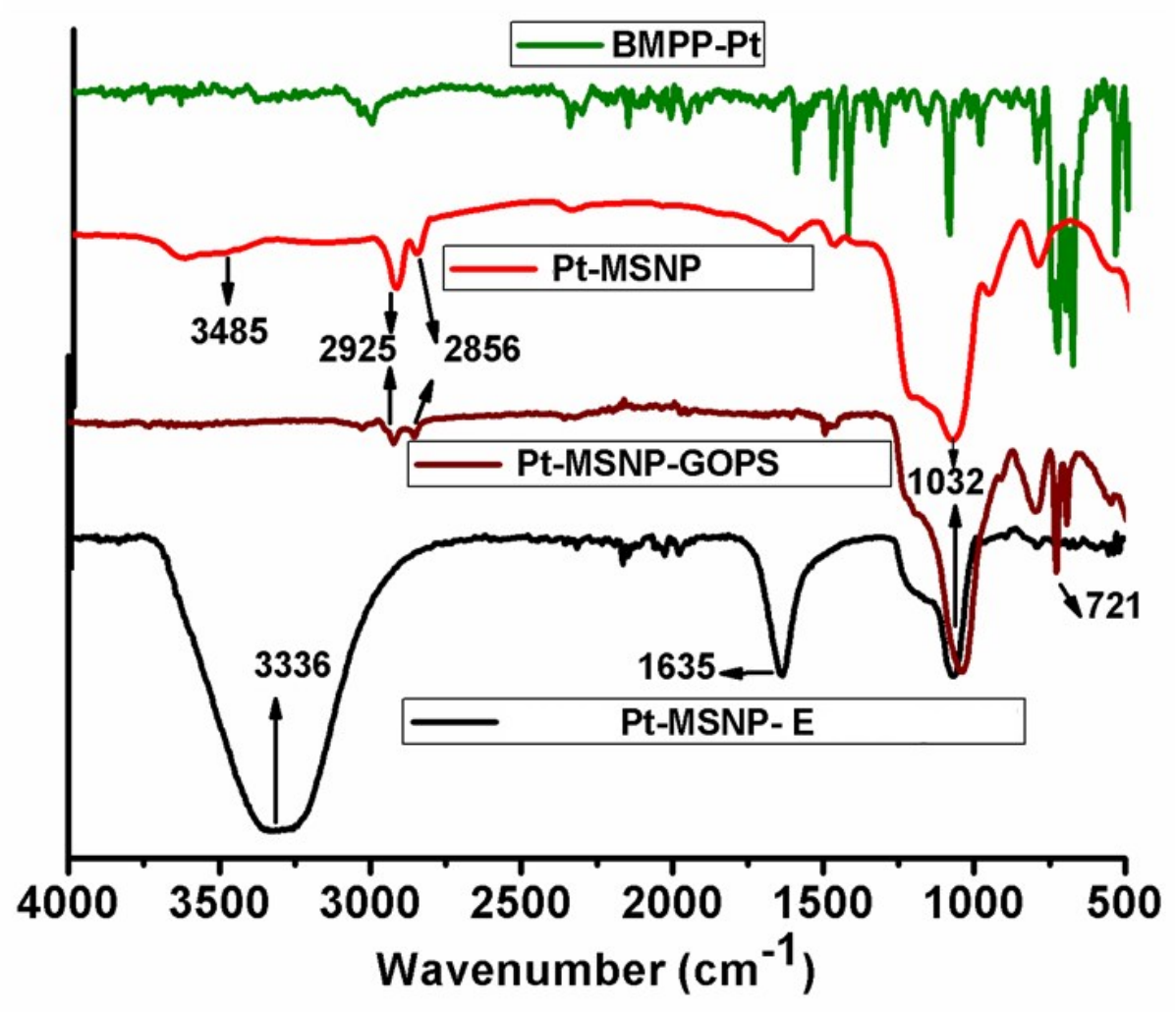

Fig. S7 FTIR spectra of free BMPP-Pt, Pt-MSNPs, Pt-MSNP-GOPSand Pt-MSNP-E

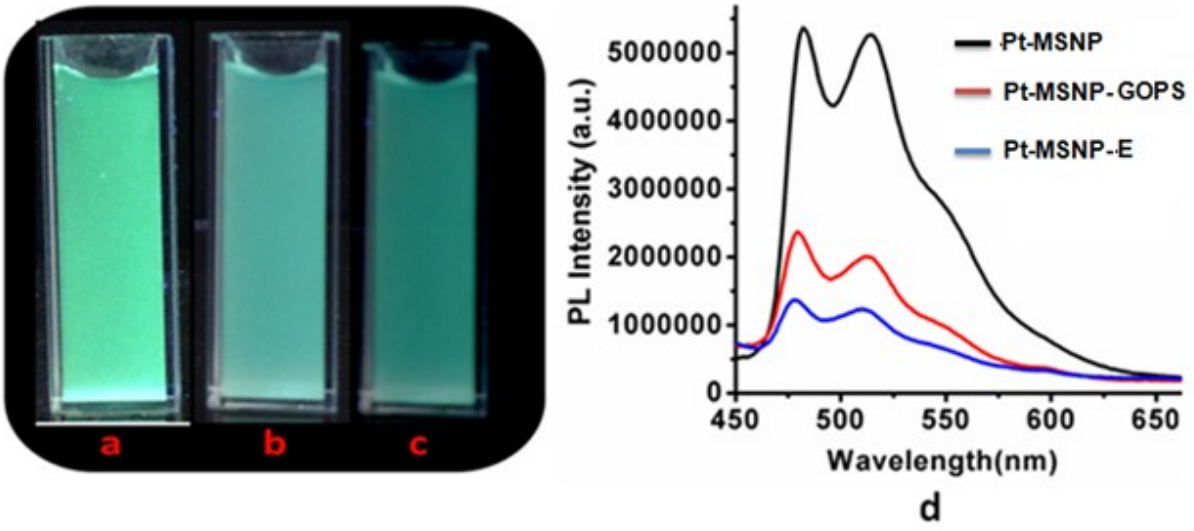

Fig. S8 Luminescent images(left) and PL spectra (right) of Pt-MSNPs **(a)**,Pt-MSNP-GOPS **(b)** and Pt-MSNP-E **(c)** (λ_{ex} = 365nm) in water (c= 2mg/ml).

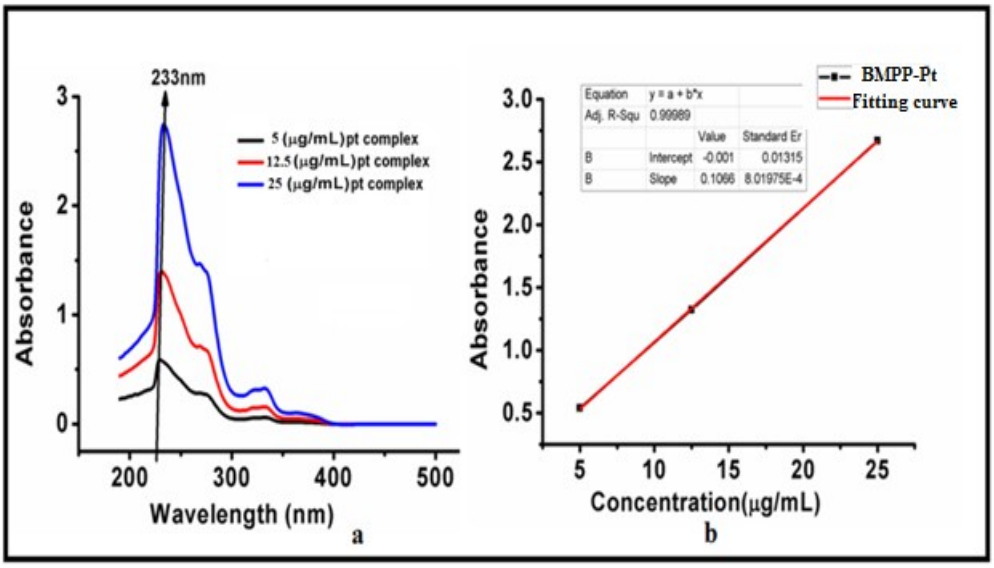

Fig. S9(a) Absorbance spectra of BMPP-Pt at different concentrations; (b) shows linear fitting of absorbance vs concentration graph

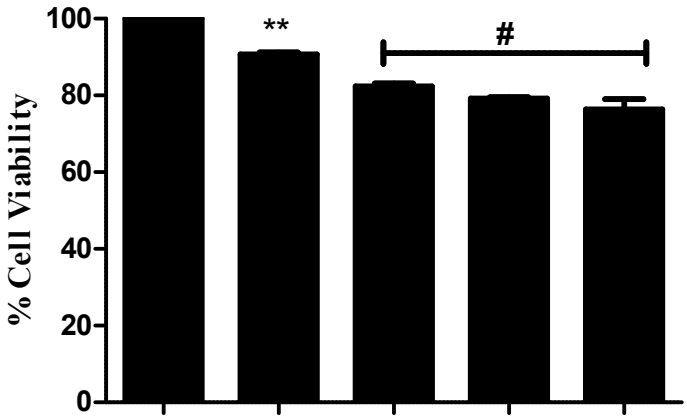

Fig. S10 Effect of blank MSNP on viability of Huh7 cells, analyzed by MTT assay after 24 h treatment of each.(Symbol (**) represents significant difference ($p<0.05$) as compared to un-treated cells; Symbol (#) represents no significant difference)

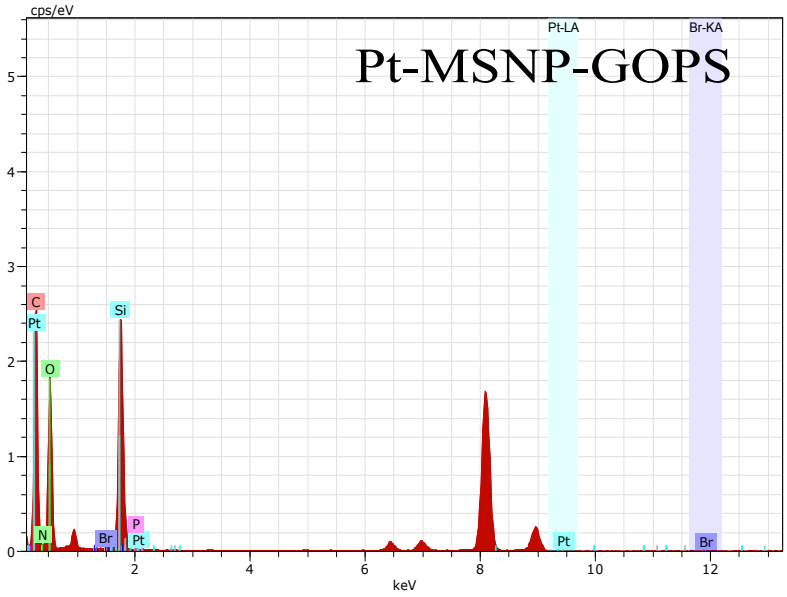

Fig. S11 S10 EDX spectra of Pt-MSNP-GOPS

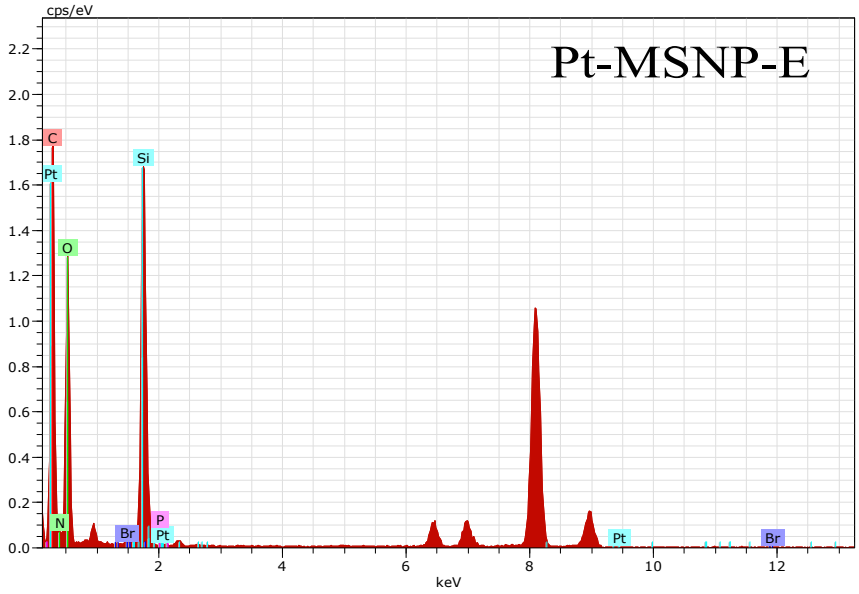

Fig. S12EDX spectra of Pt-MSNP-E

Table. S1 Relevant bond lengths and dihedral angles of the BMPP-Pt complex in the crystal's monomer geometry and the optimized ground state structure.

geometry	Pt-P (Å)	Pt-P (Å)	Pt-N (Å)	Pt-C (Å)	P-Pt-N-C (º)	P-Pt-C-C (º)
crystalmonomer	2.272	2.301	2.041	2.026	161	167
optimised S_0	2.451	2.312	2.113	2.039	178	179

Table. S2 Releasing study of BMPP-Pt from **3** (at λ_{max}, 233nm)

Time (in h)	**Absorbance (a.u.)**
0	0.01637
6	0.01216
48	0.0178
72	0.0135
96	0.0132
120	0.0139
144	0.0142
168	0.0131
192	0.0134
216	0.0132

Table. S3 Concentration of Elements present in Pt-MSNP-GOPS from EDX analysis

El	AN	Series	unn. C[wt.%]	norm. C[wt.%]	Atom. C[at.%]	Error (1 Sigma)[wt.%]
C	6	K-series	81.36	81.36	88.04	2.50
Si	8	K-series	8.79	8.79	7.14	0.29
O	14	K-series	8.52	8.52	3.94	0.06
N	7	K-series	**0.90**	**0.90**	**0.84**	**0.06**
Pt	78	L-series	0.39	0.39	0.03	0.07
P	15	K-series	0.02	0.02	0.01	0.03
Total			100.00	100.00	100.00	

Table. S4 Concentration of elements present in Pt-MSNP-E

El	AN	Series	unn. C[wt.%]	norm. C[wt.%]	Atom. C[at.%]	Error (1 Sigma)[wt.%]
C	6	K-series	81.36	81.36	88.04	2.50
Si	8	K-series	8.86	8.86	7.17	0.29
O	14	K-series	7.08	7.08	4.73	0.10
N	7	K-series	**2.13**	**2.13**	**2.04**	**0.08**
Pt	78	L-series	0.37	0.37	0.02	0.08
P	15	K-series	0.01	0.01	0.00	0.03
Total			100.00	100.00	100.00	