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Supporting Information for

A bifunctional imidazolium functionalized ionic porous organic polymer in water remediation.

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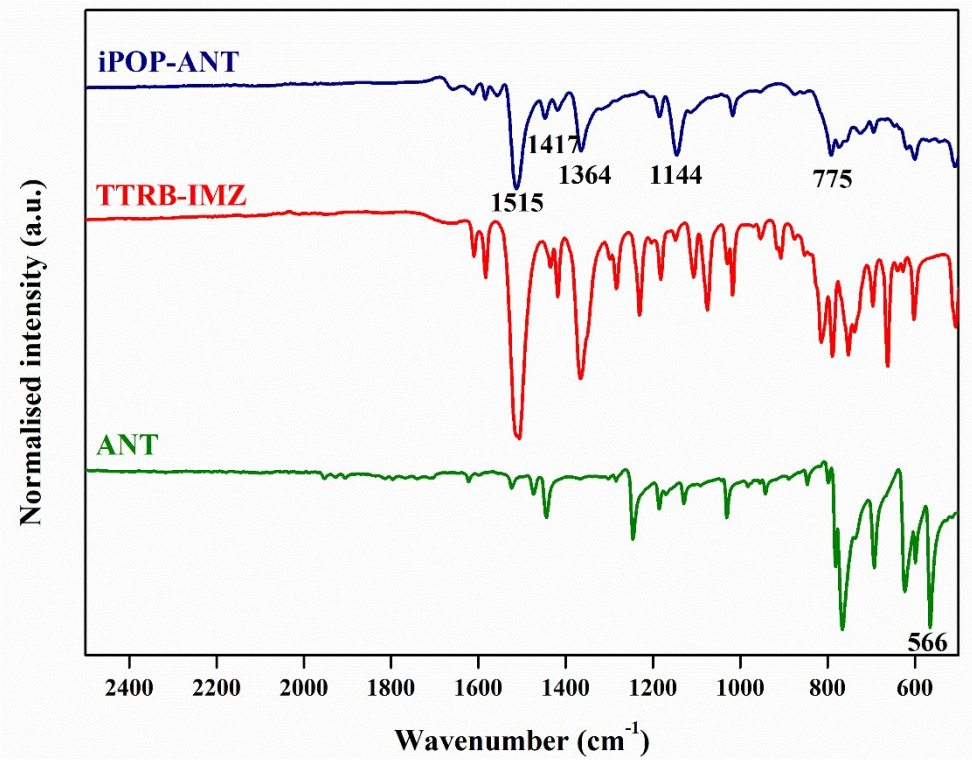


Figure S1. FTIR spectra of iPOP-ANT (Blue), TTRB-IMZ (Red), ANT (Green)

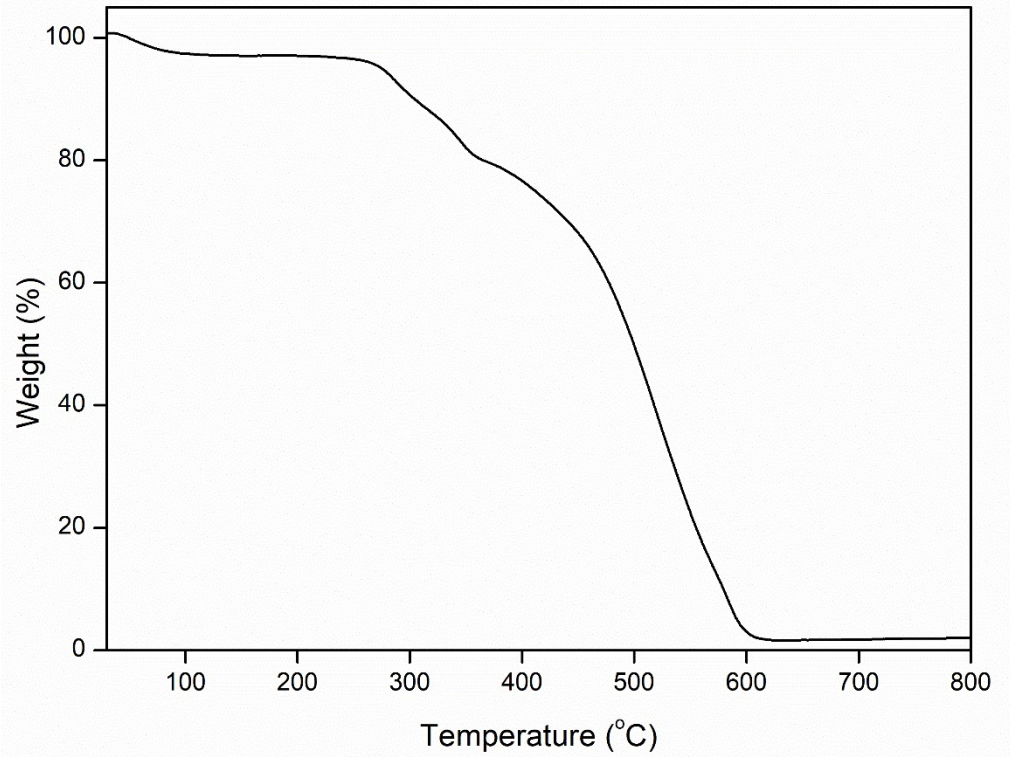


Figure S2. TGA curve for iPOP-ANT

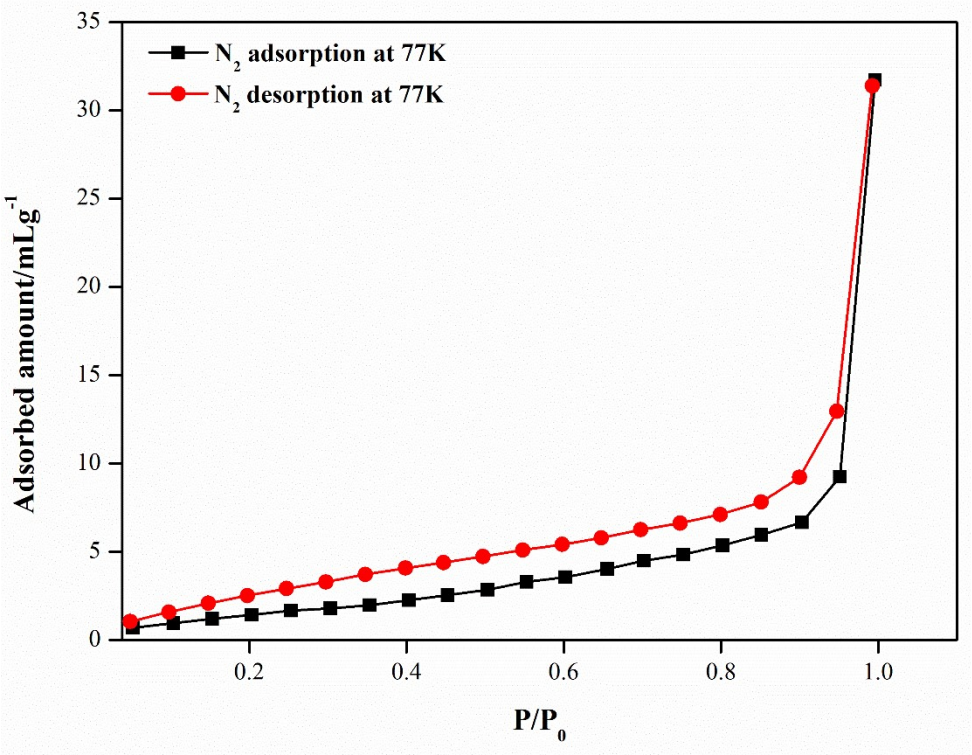


Figure S3. N_2 adsorption and desorption profile at 77K

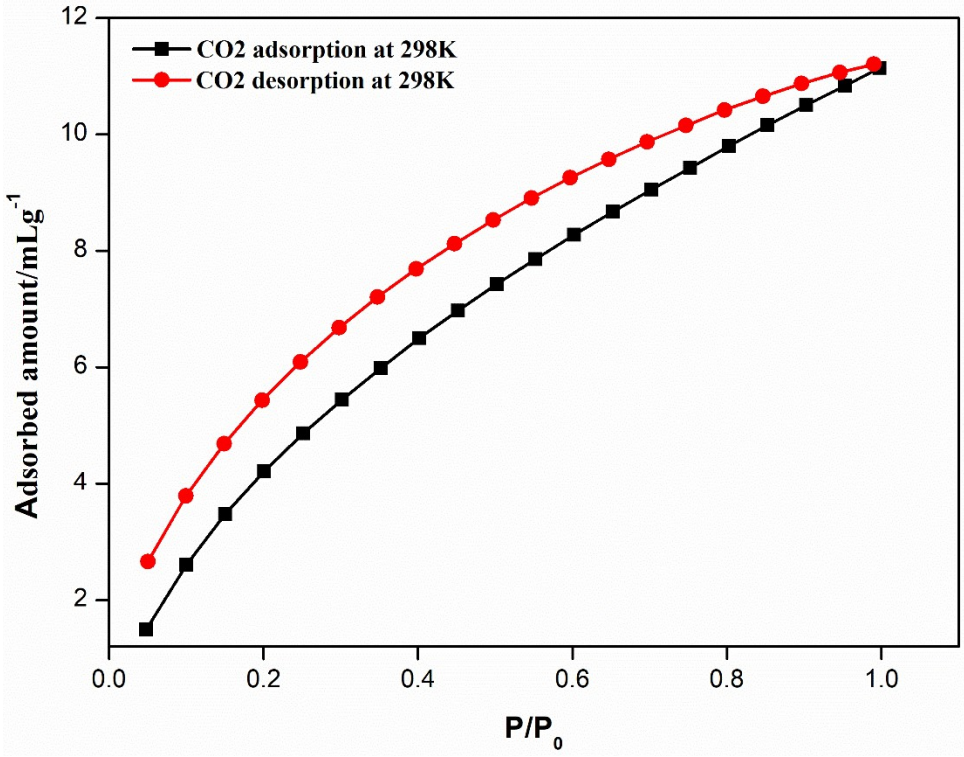


Figure S4. CO_2 adsorption and desorption profile at 298K

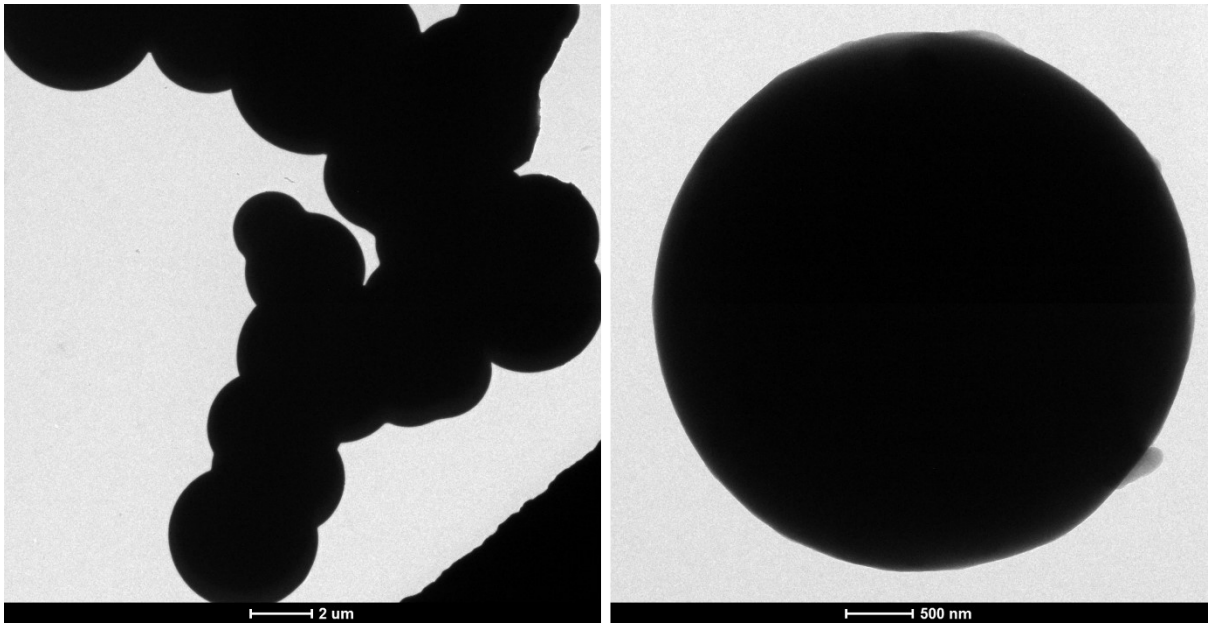


Figure S5. TEM images of iPOP-ANT

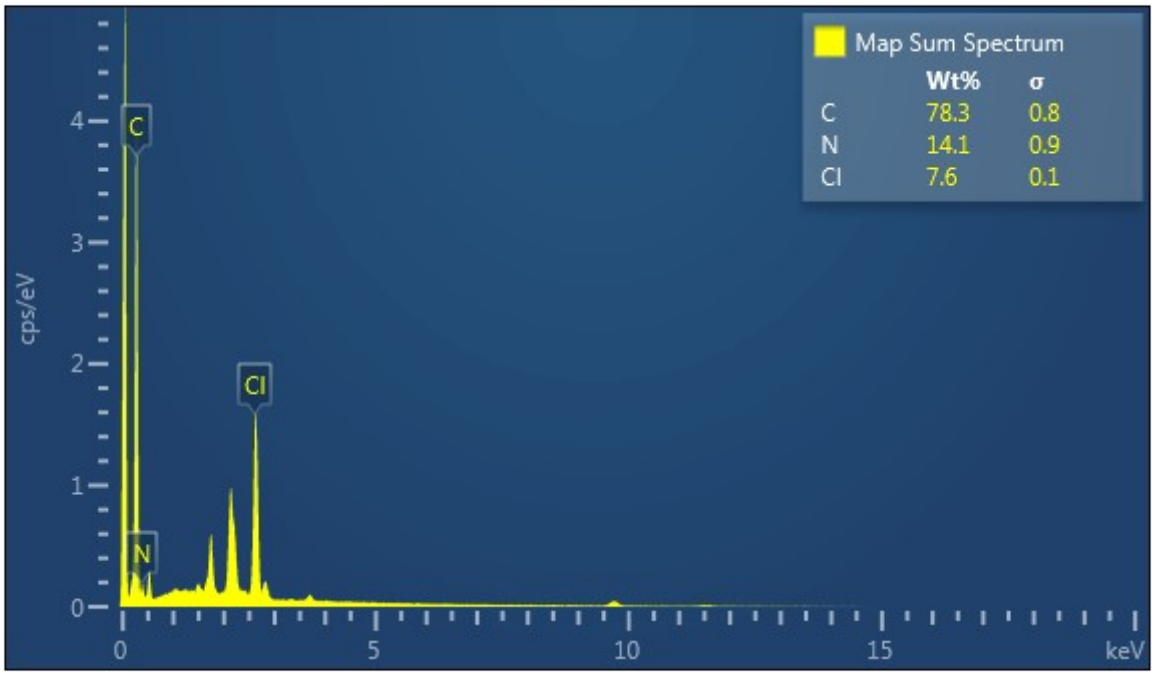


Figure S6. EDX analysis of iPOP-ANT

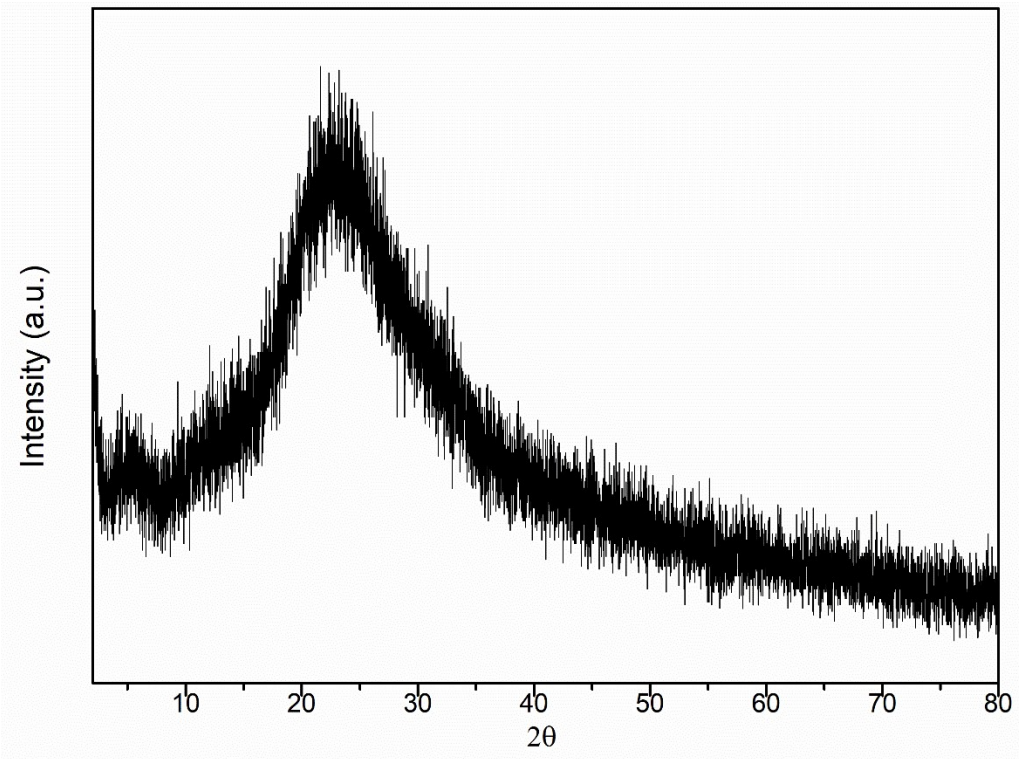


Figure S7. PXRD of iPOP-ANT

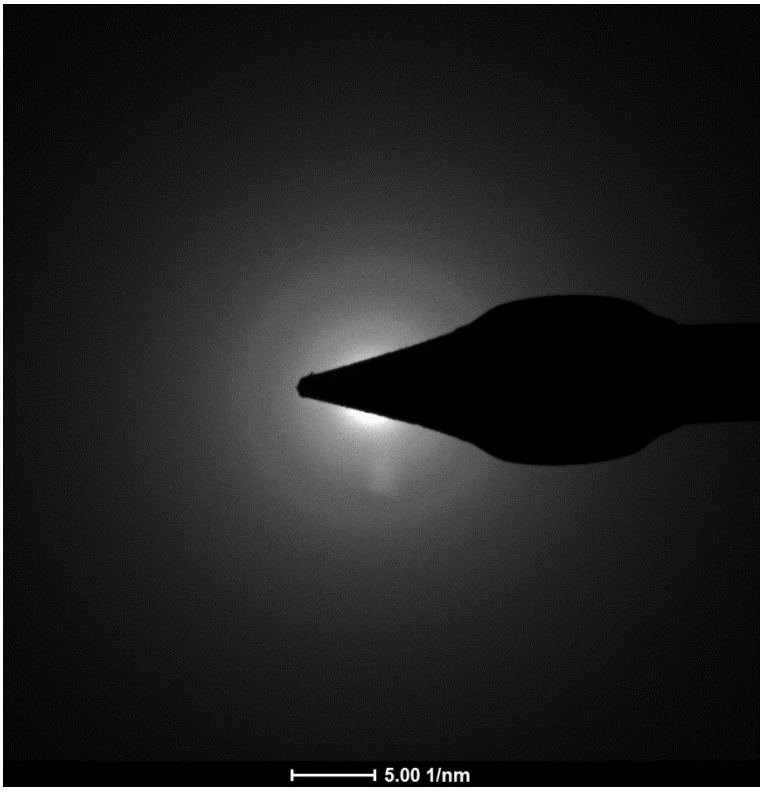


Figure S8. The electron diffraction pattern of iPOP-ANT.

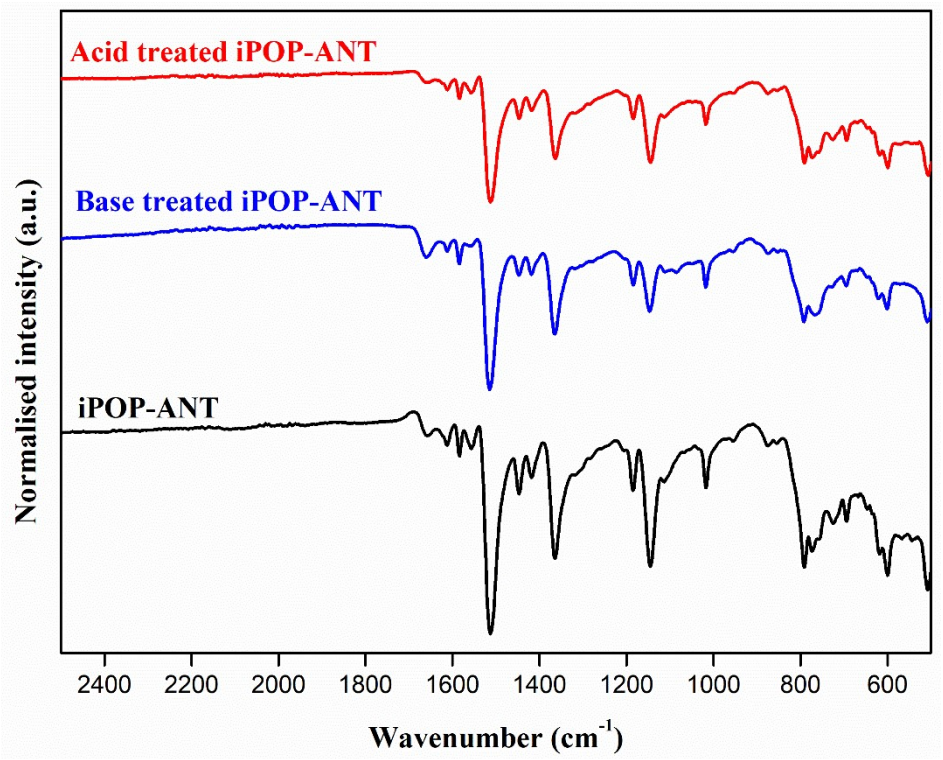


Figure S9. FTIR profile of acid and base treated iPOP-ANT

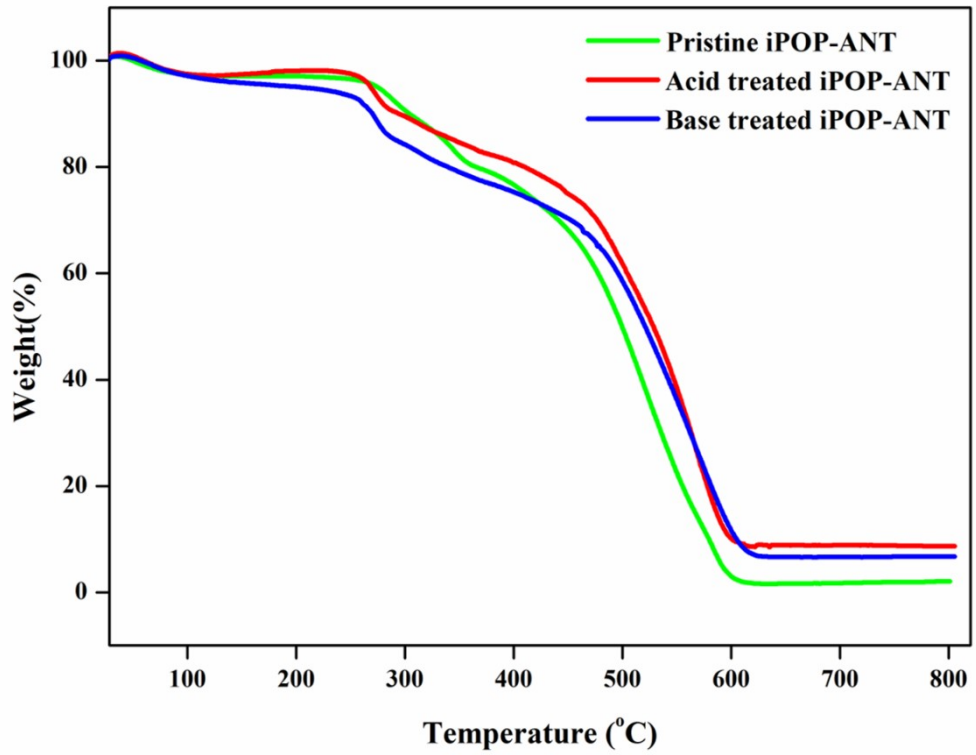


Figure S10. TGA profile of acid and base treated iPOP-ANT

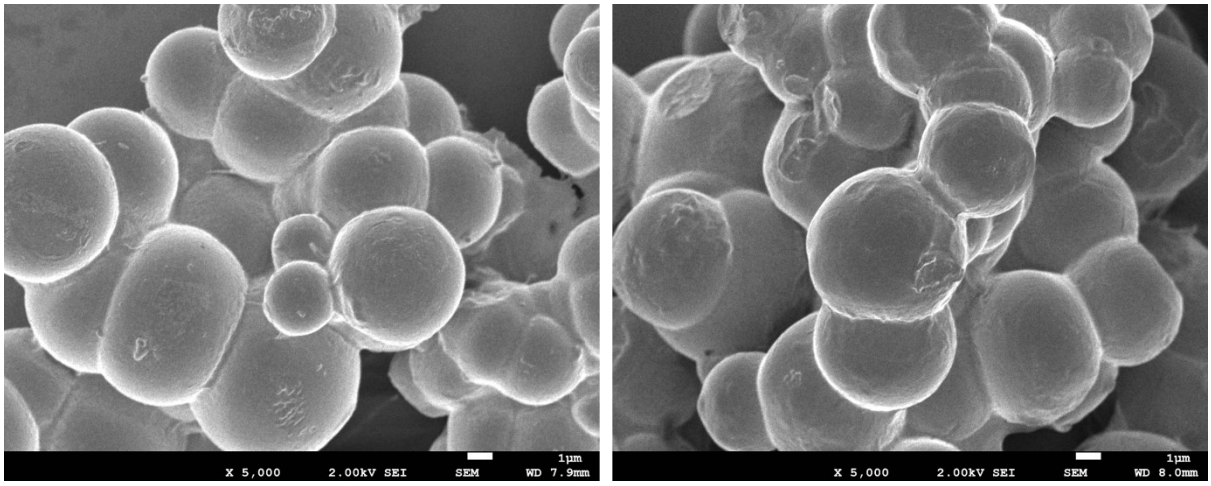


Figure S11. SEM images of acid and base treated iPOP-ANT

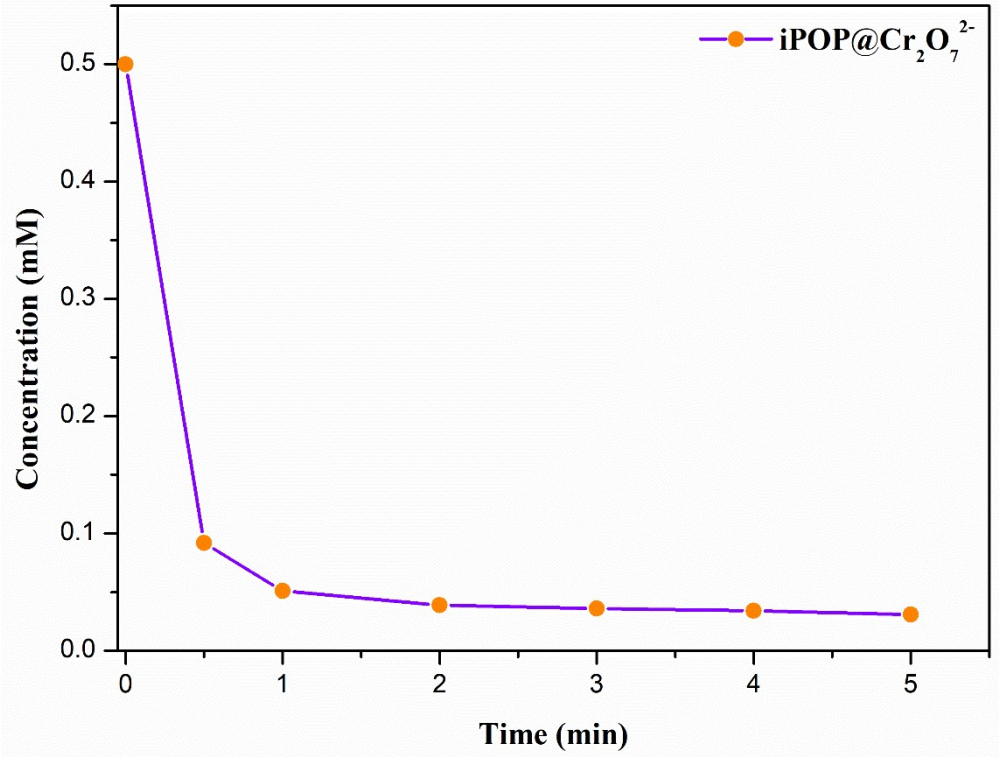


Figure S12. Decrease in the concentration of the $Cr_2O_7^{2-}$ ion from water after addition of iPOP-ANT.

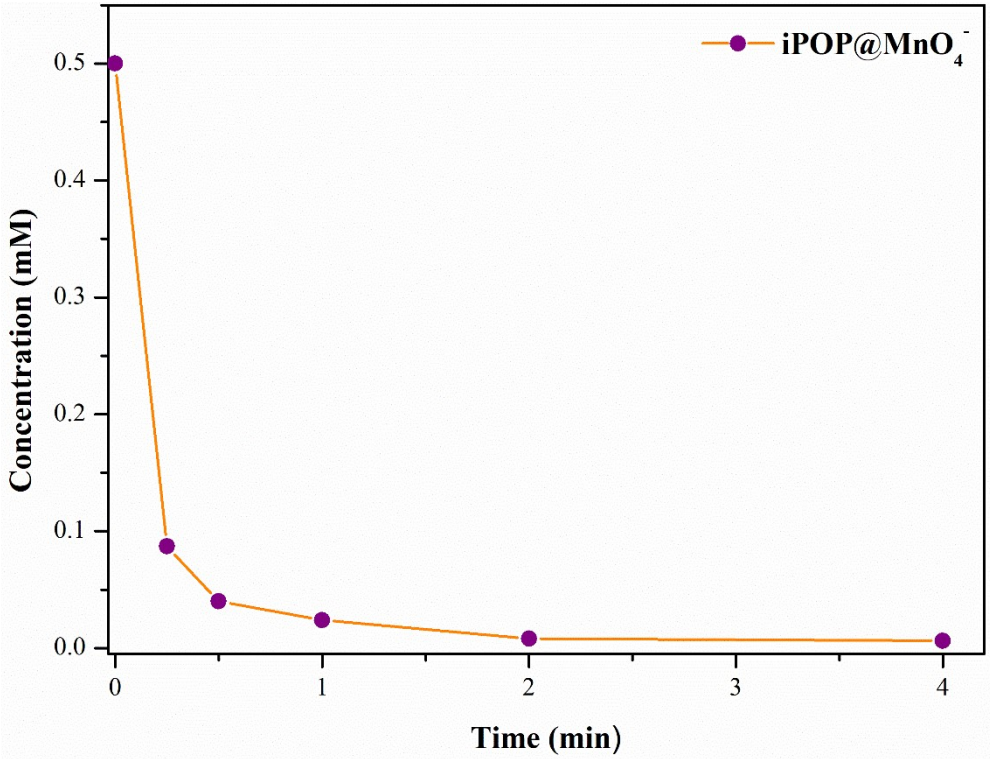


Figure S13. Decrease in the concentration of the MnO_4^- ion from water after addition of iPOP-ANT.

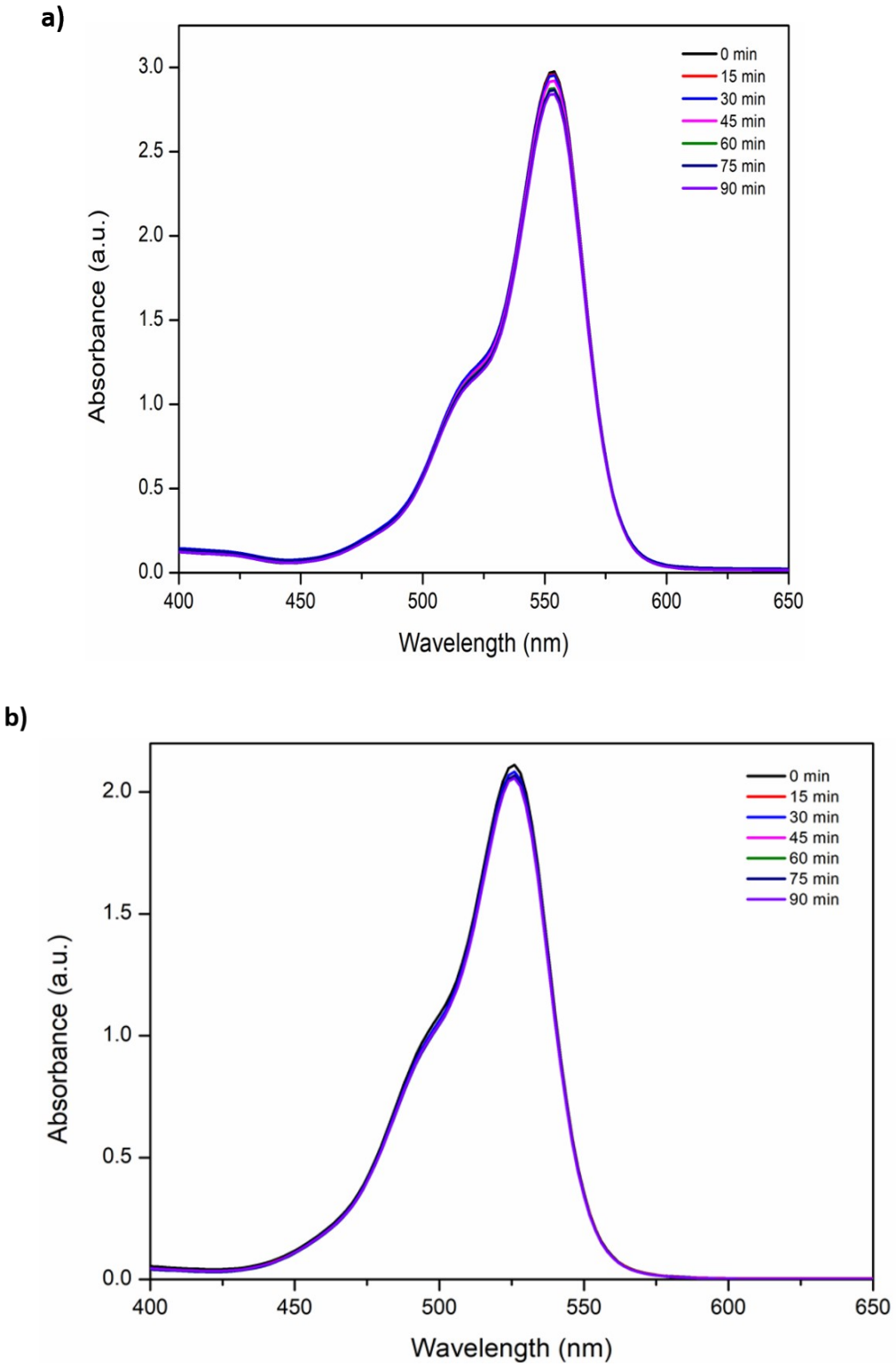


Figure S14. UV-vis spectrum in the presence of iPOP-ANT at different times for the aqueous solution of (a) RhB (b) Rh6G

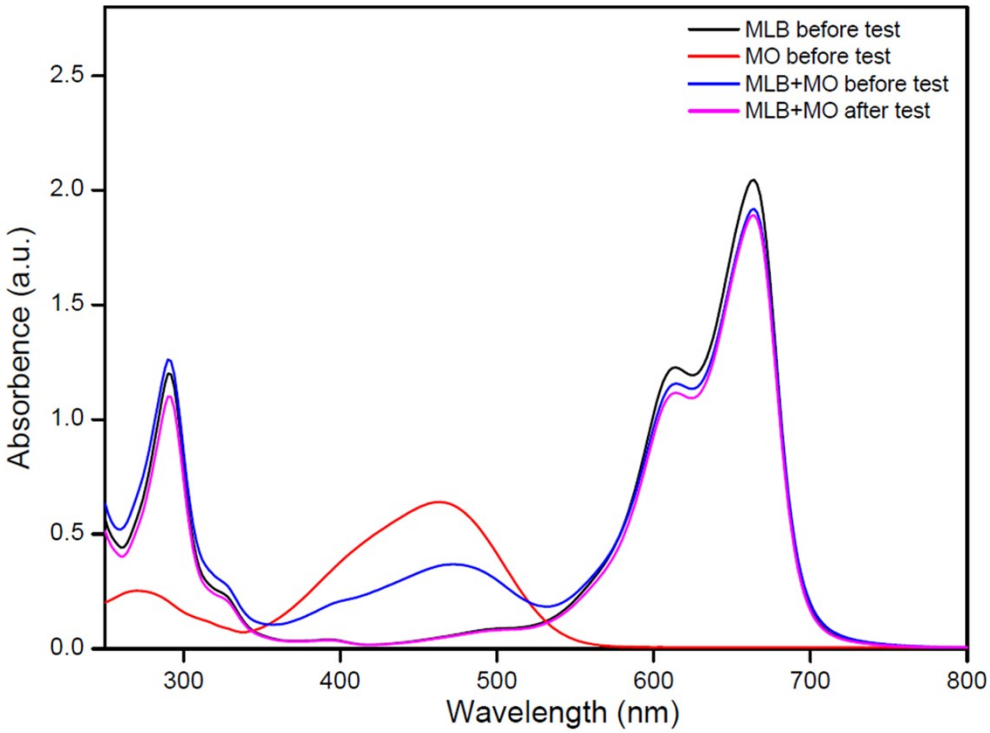


Figure S15. Selective capture of anionic dyes over cationic dyes

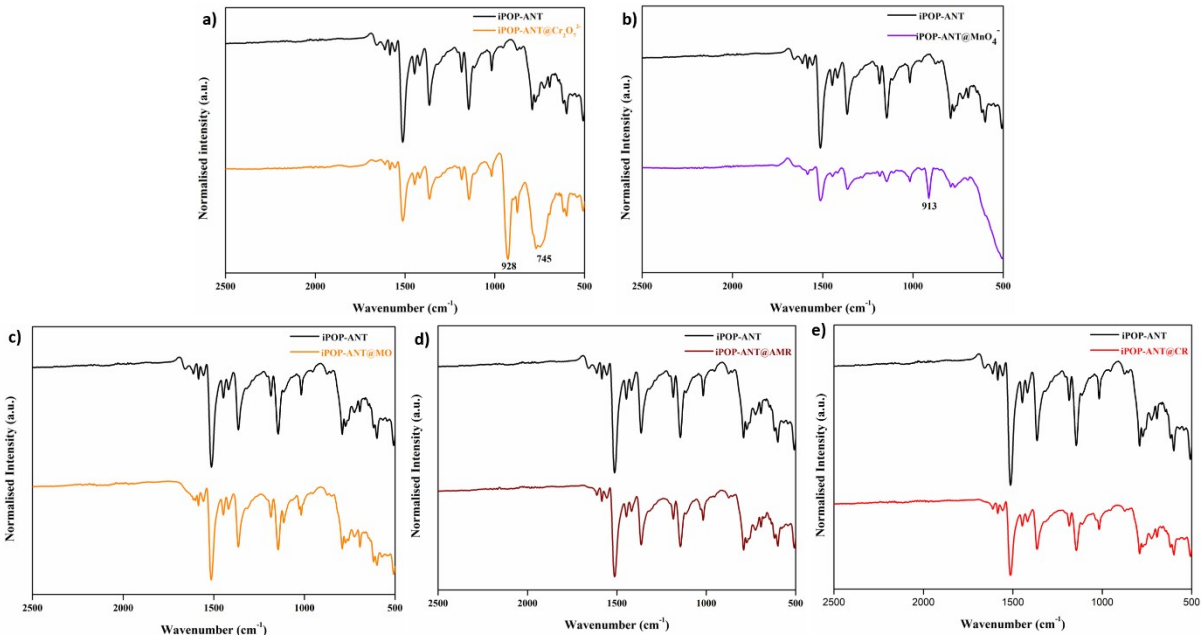


Figure S16. FTIR spectra of (a) iPOP-ANT@$Cr_2O_7^{2-}$ (b) iPOP-ANT@MnO_4^- (c) iPOP-ANT@MO (d) iPOP-ANT@AMR (e) iPOP-ANT@CR

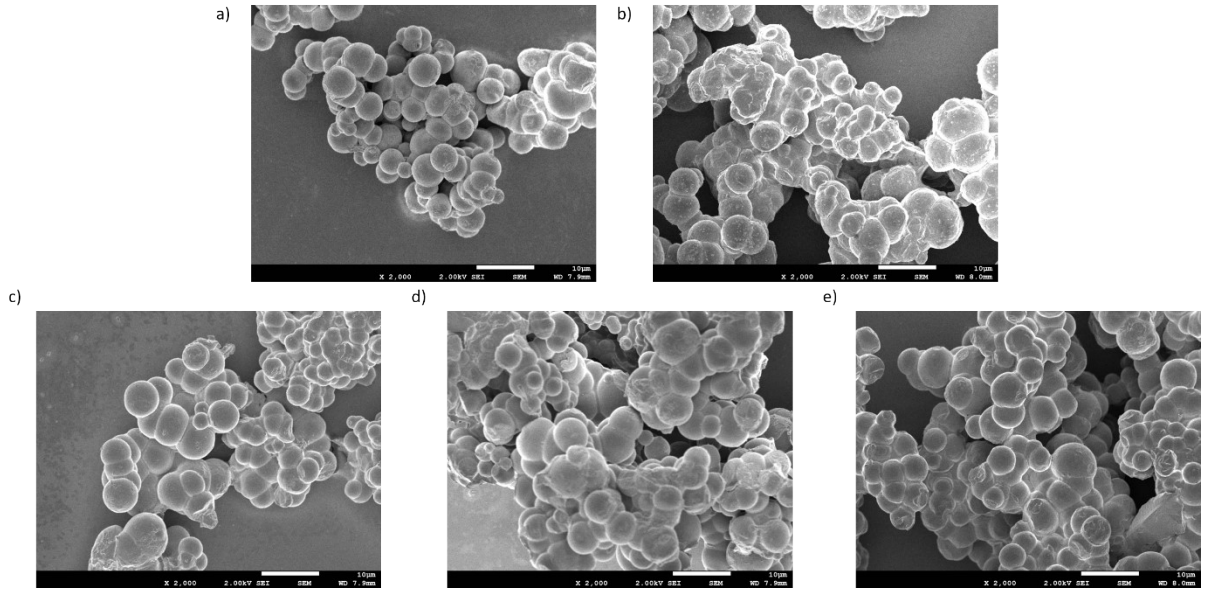
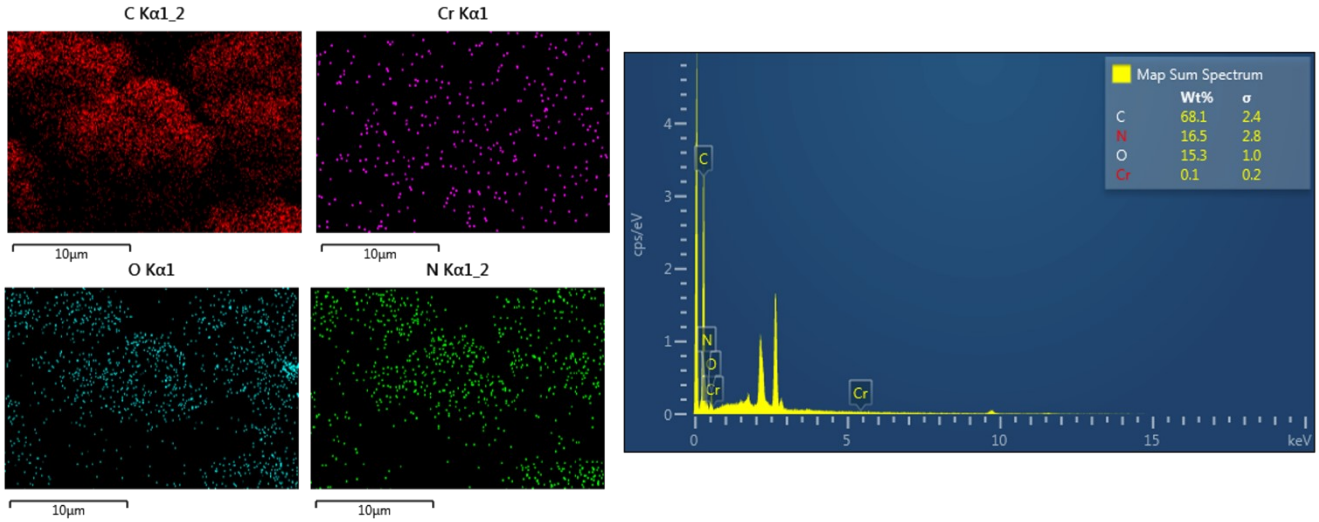
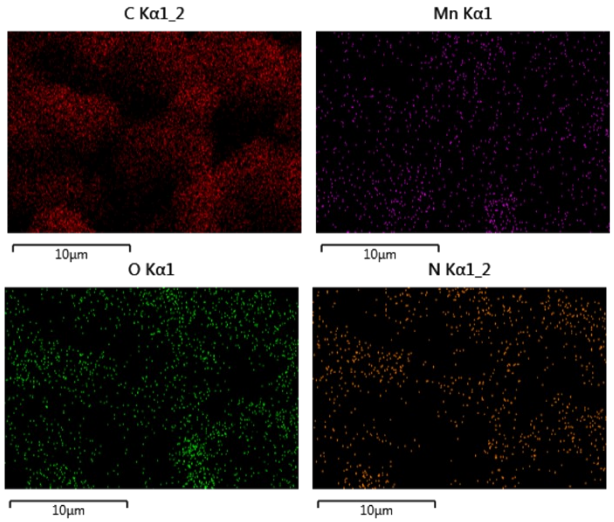


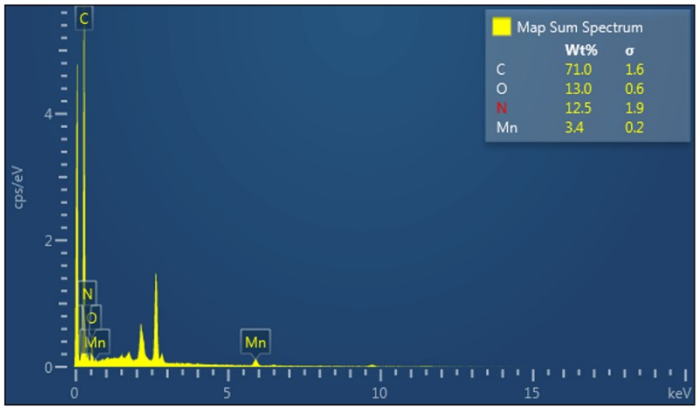
Figure S17. SEM images of (a) iPOP-ANT@$Cr_2O_7^{2-}$ (b) iPOP-ANT@MnO_4^- (c) iPOP-ANT@MO (d) iPOP-ANT@AMR (e) iPOP-ANT@CR

a)



b)


C Kα1_2
Mn Kα1
O Kα1
N Kα1_2
10µm


Map Sum Spectrum
Wt% σ
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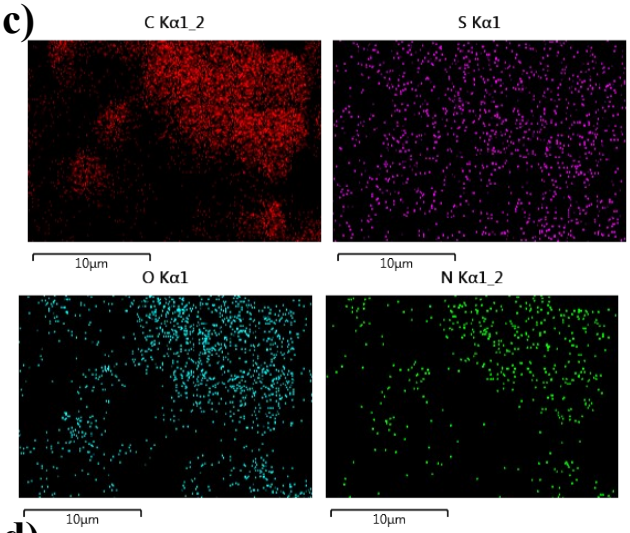
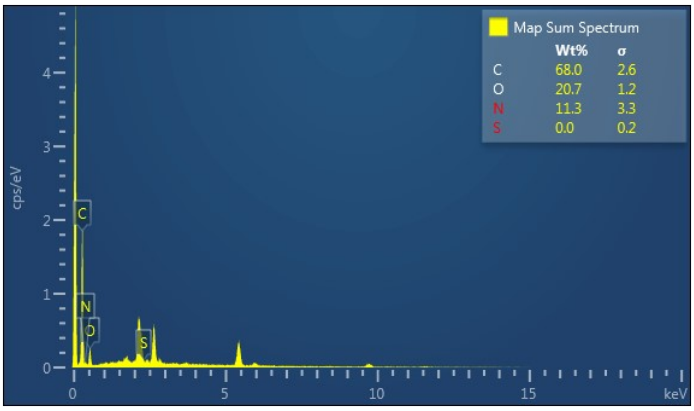
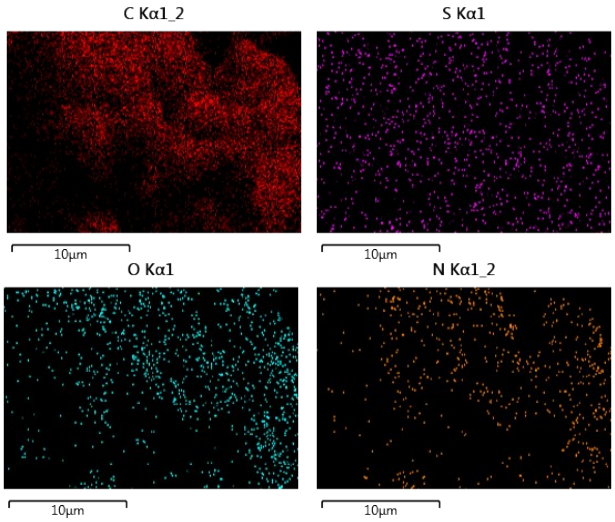
O 13.0 0.6
N 12.5 1.9
Mn 3.4 0.2
cps/eV
keV

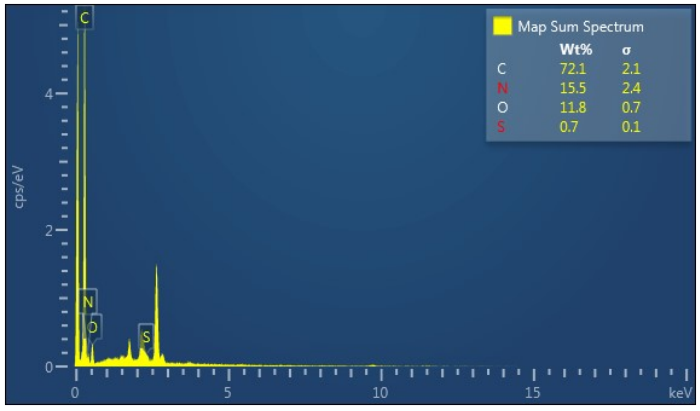
c)


C Kα1_2
S Kα1
O Kα1
N Kα1_2
10µm


Map Sum Spectrum
Wt% σ
C 68.0 2.6
O 20.7 1.2
N 11.3 3.3
S 0.0 0.2
cps/eV
keV

d)


C Kα1_2
S Kα1
O Kα1
N Kα1_2
10µm


Map Sum Spectrum
Wt% σ
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N 15.5 2.4
O 11.8 0.7
S 0.7 0.1
cps/eV
keV

e)

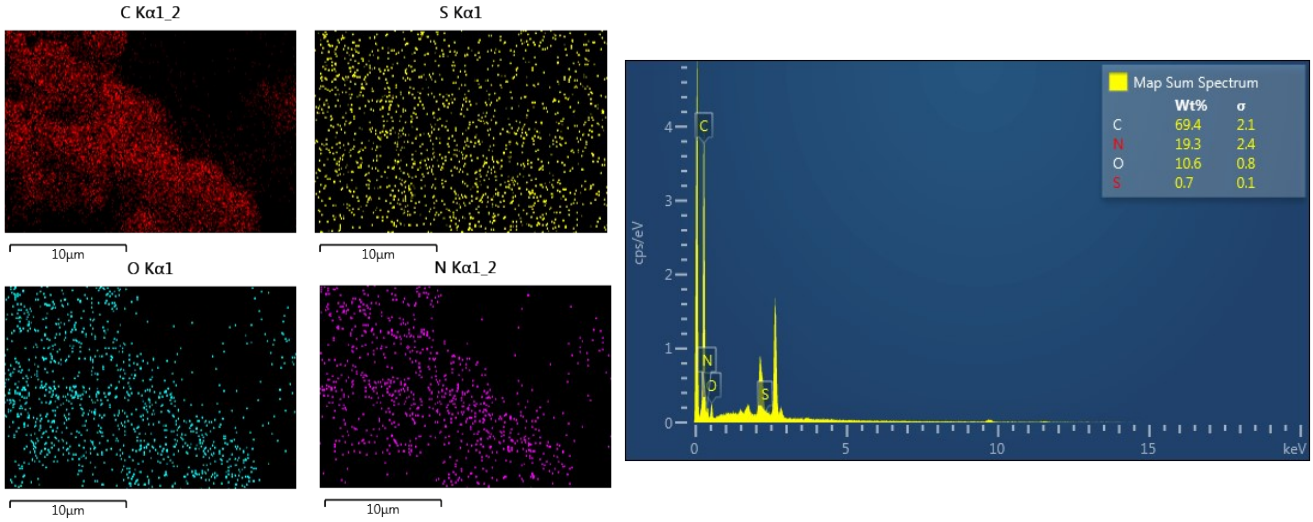

Figure S18. EDX analysis and Elemental mapping of (a) iPOP ANT@$Cr_2O_7^{2-}$ (b) iPOP ANT@MnO_4^- (c) iPOP ANT@MO (d) iPOP ANT@AMR (e) iPOP ANT@CR

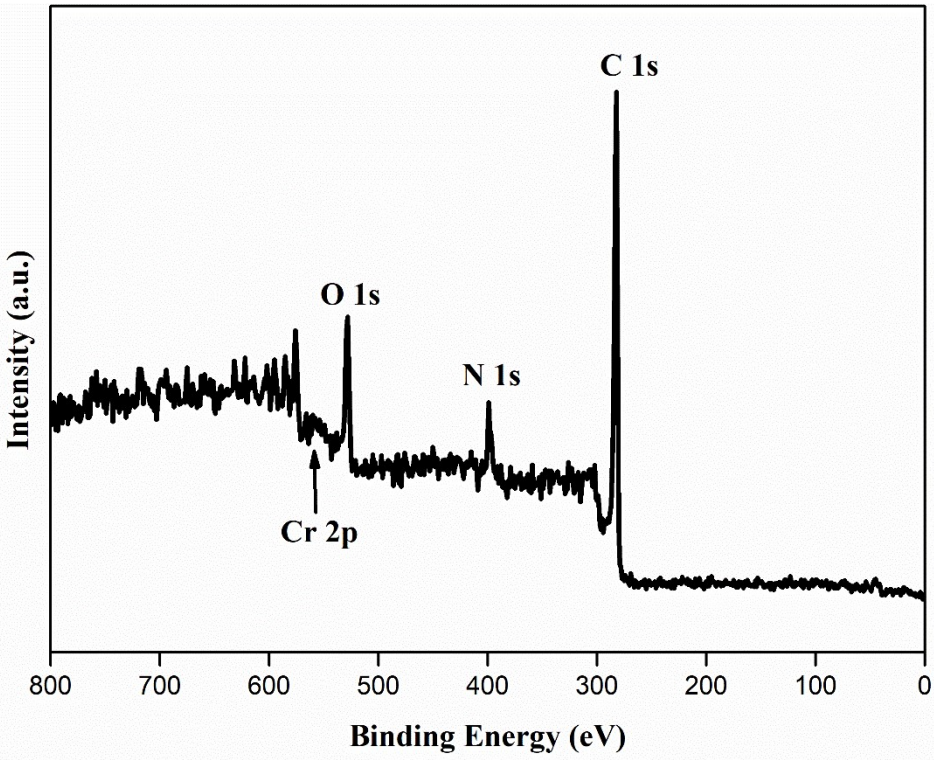

Figure S19. XPS survey spectra of iPOP@ $Cr_2O_7^{2-}$

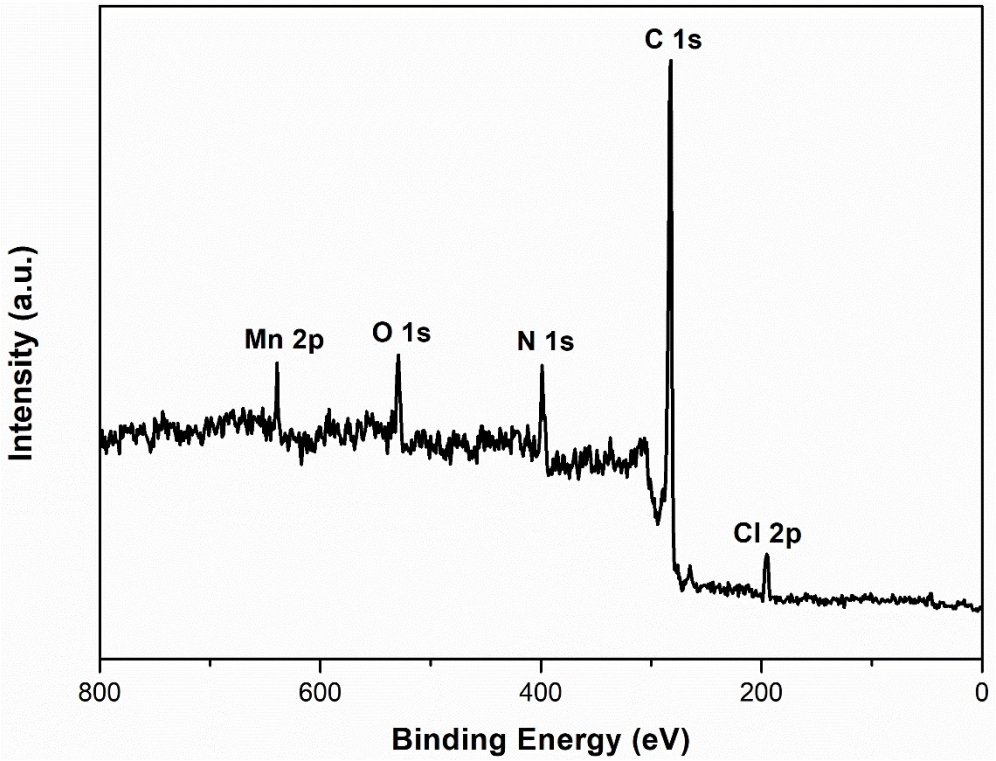

Figure-S20. XPS survey spectra of iPOP@MnO_4^-

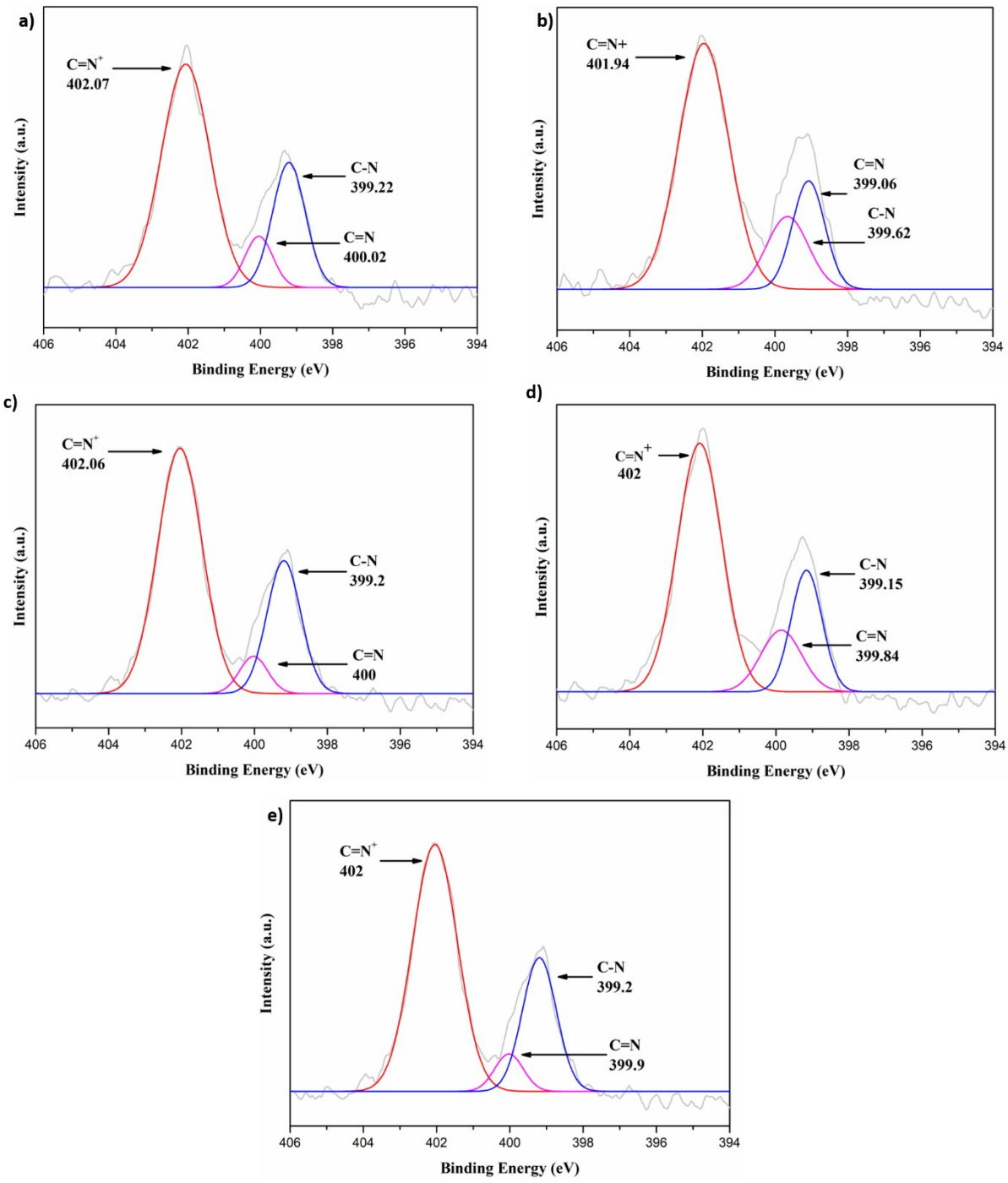

Figure S21. XPS N1s spectra for (a) iPOP-ANT@$Cr_2O_7^{2-}$ (b) iPOP-ANT@MnO_4^- (c) iPOP-ANT@MO (d) iPOP-ANT@AMR (e) iPOP-ANT@CR

The pseudo-second-order kinetic model

The linear form of pseudo second order kinetic model is expressed as

$$\frac{t}{Q_t} = \frac{1}{k_2 Q_e^2} + \frac{t}{Q_e}$$

Where Q_t and Q_e are the amount of pollutants adsorbed at time t and equilibrium (mg g^{-1}), k_2 is the pseudo-second-order rate constant of adsorption process (g mg^{-1} min^{-1}).[1]

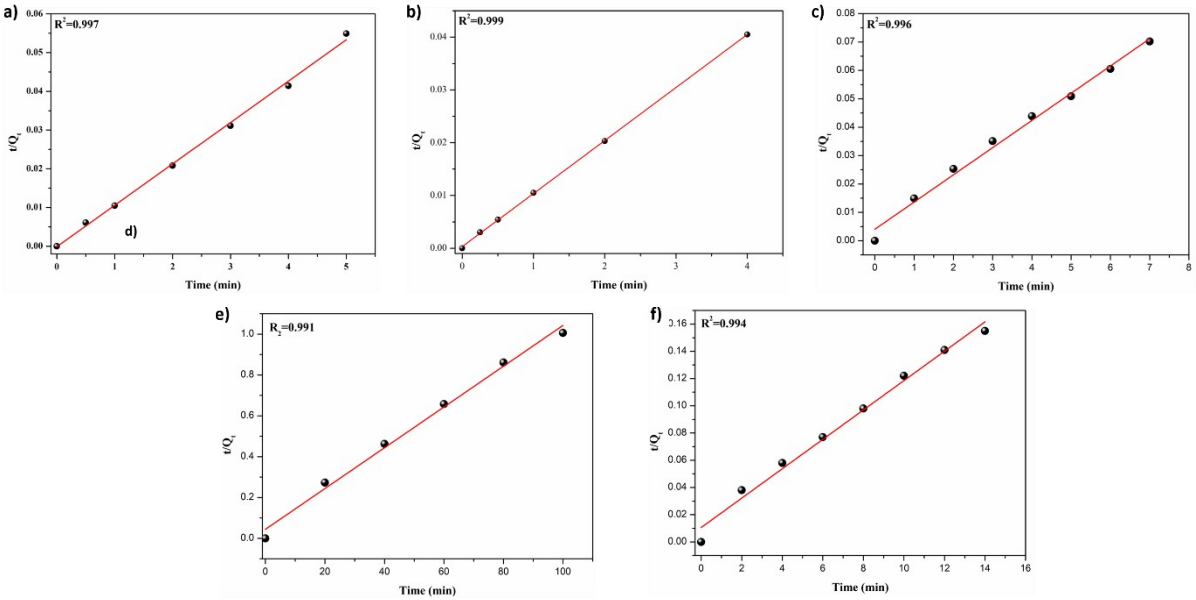

Figure S22. The pseudo-second-order kinetics model for (a) iPOP-ANT@$Cr_2O_7^{2-}$ (b) iPOP-ANT@MnO_4^- (c) iPOP-ANT@MO (d) iPOP-ANT@AMR (e) iPOP-ANT@CR

Adsorption isotherm experiment

2.5mg of iPOP-ANT was immersed in 5 mL aqueous solution of oxo-anion and dyes having different concentration. After 12hours the supernatant was collected and UV-Visible spectroscopy was carried out. The obtained data were fitted further with the following equation

Langmuir model

$$Q_e = \frac{Q_m C_e}{K_d + C_e}$$

where, Ce (mM) and Qe (mg g^{-1}) are the concentration at equilibrium and amount of oxo-anion adsorbed at equilibrium respectively. Qm (mg g^{-1}) is the maximum amount of pollutant per unit mass of adsorbent to form a completemonolayer. K_d (mg/L) is a constant related to the affinity of the binding sites.[2]

Freundlich model

$$Q_e = K_F C_e^{\frac{1}{n}}$$

where, K_F and 1/n are the Freundlich model constants, indicating capacity and intensity of adsorption, respectively.[2]

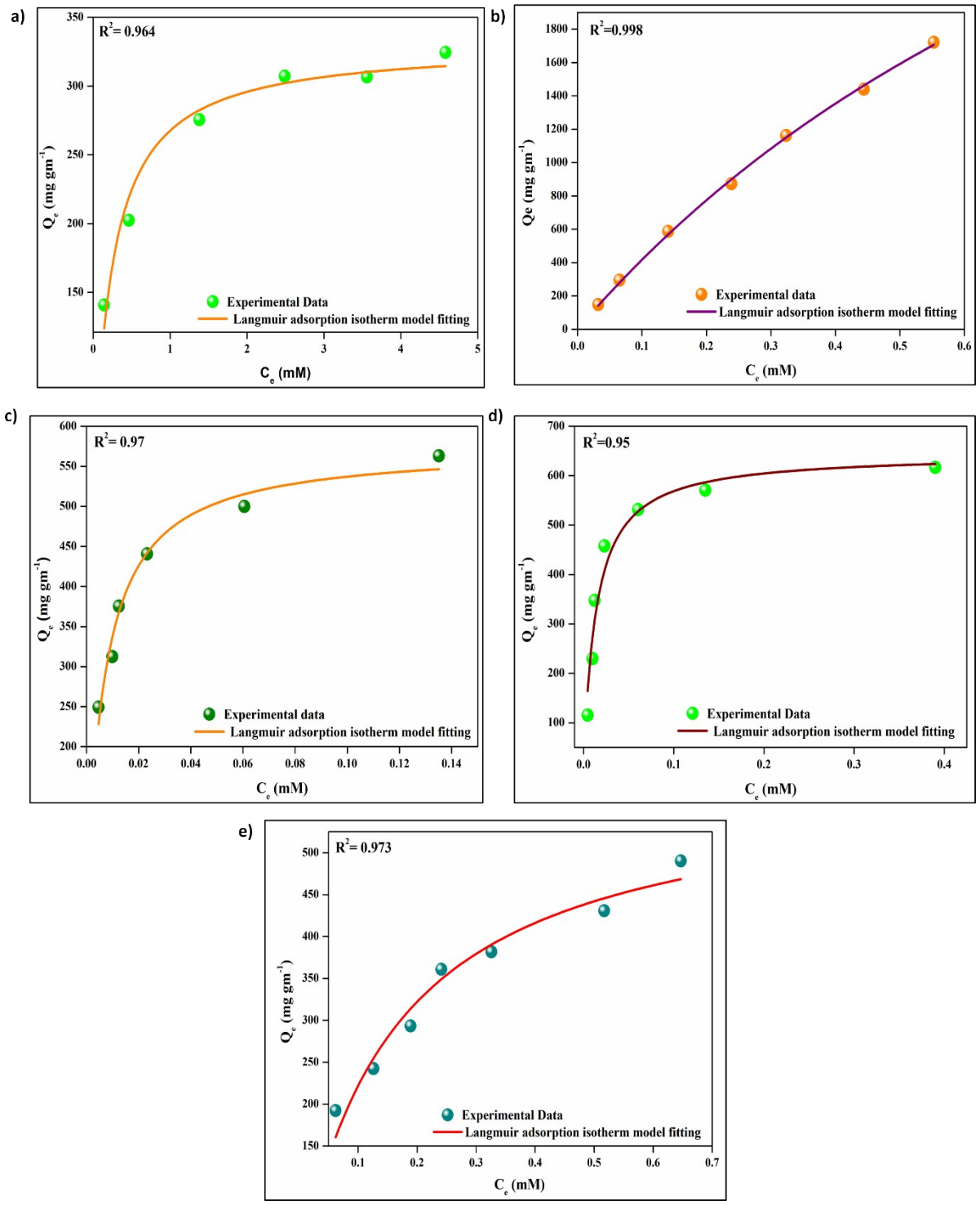

Figure S23. The Langmuir model fitting for (a) $Cr_2O_7^{2-}$ (b) MnO_4^- (c)MO (d)AMR (e)CR

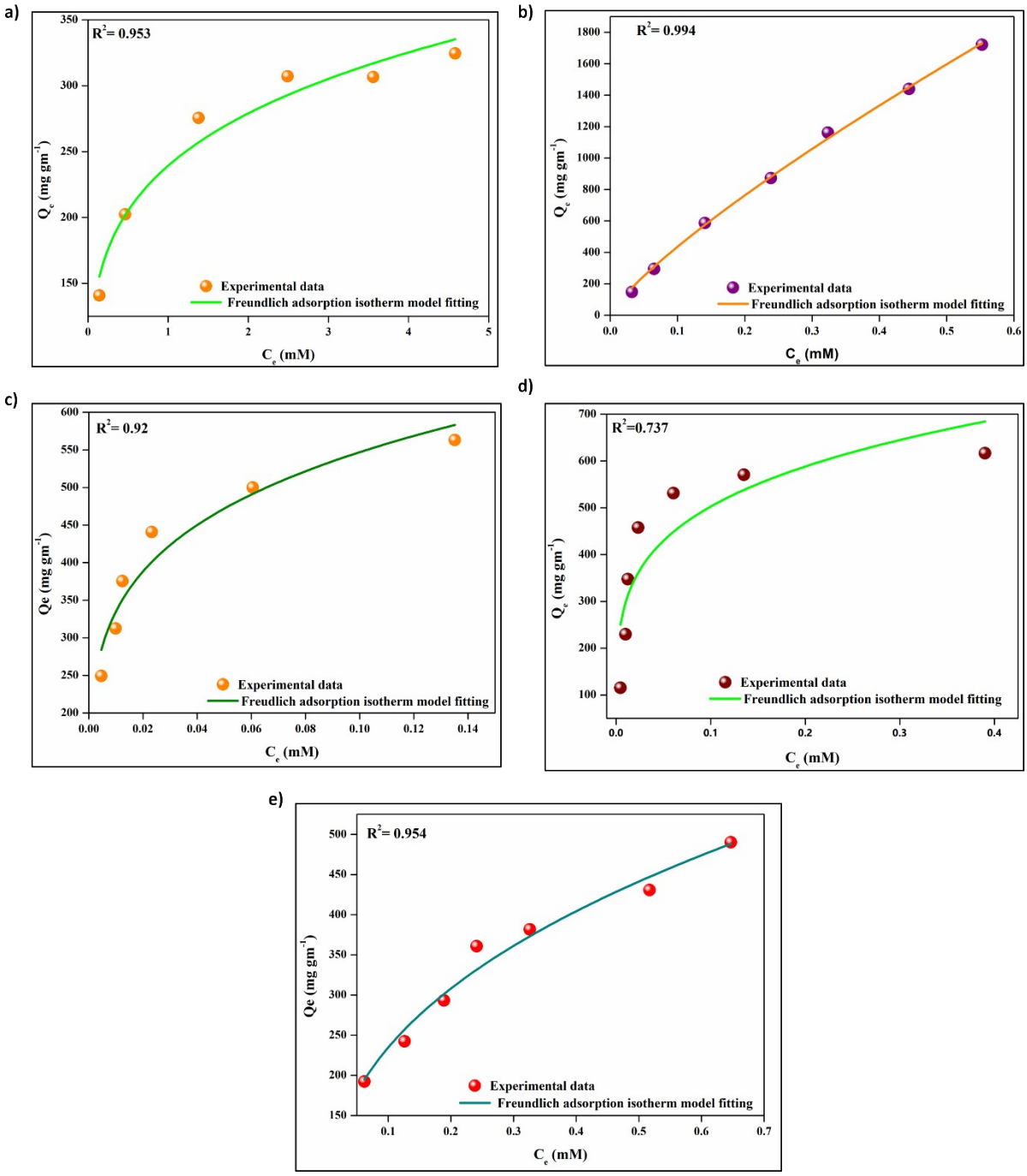

Figure S24. The Freundlich model fitting for (a) $Cr_2O_7^{2-}$ (b) MnO_4^- (c)MO (d)AMR (e)CR

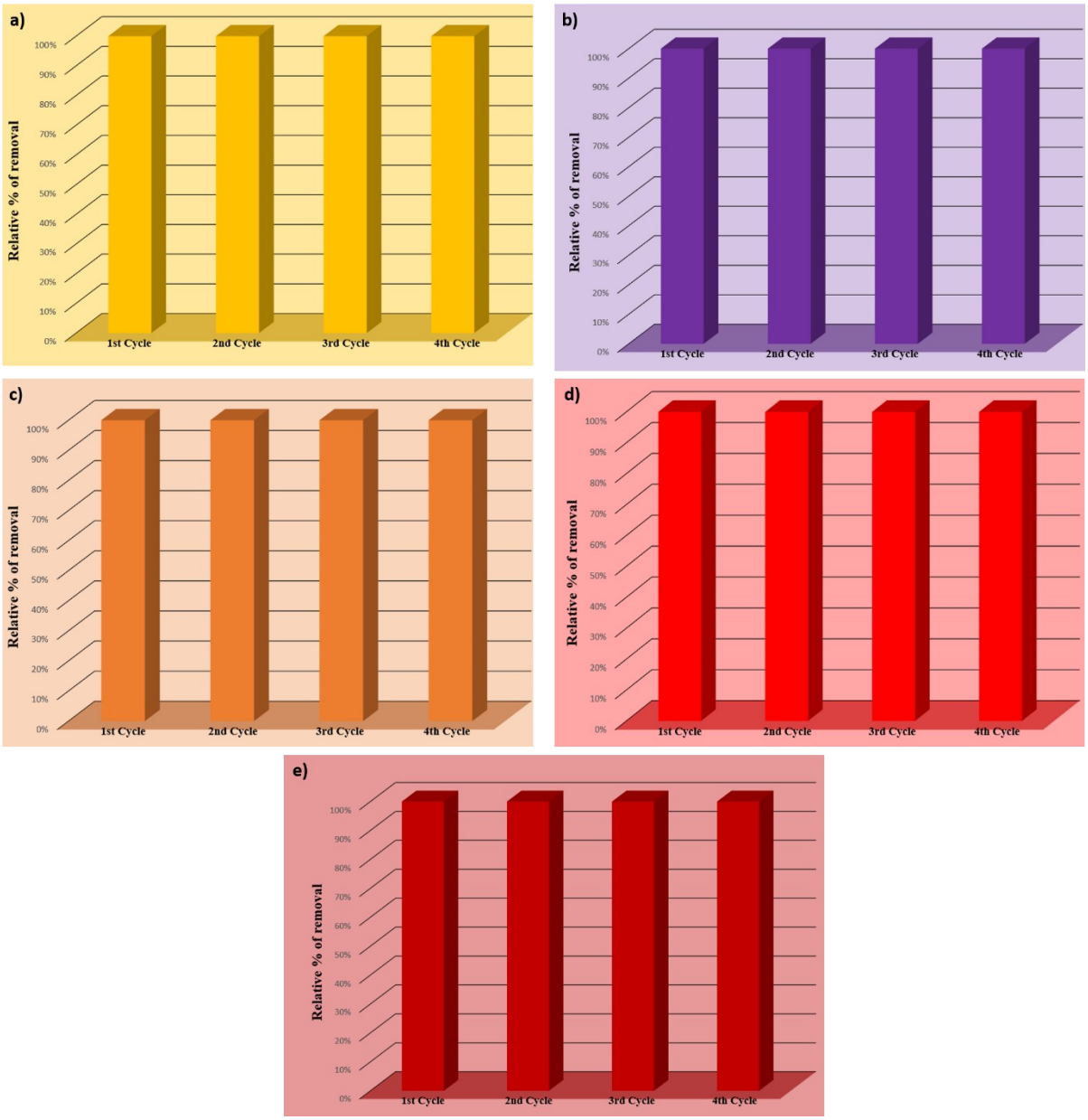

Figure S25. Reusability test of iPOP-ANT for (a) $Cr_2O_7^{2-}$ (b) MnO_4^- (c) MO (d) AMR (e) CR

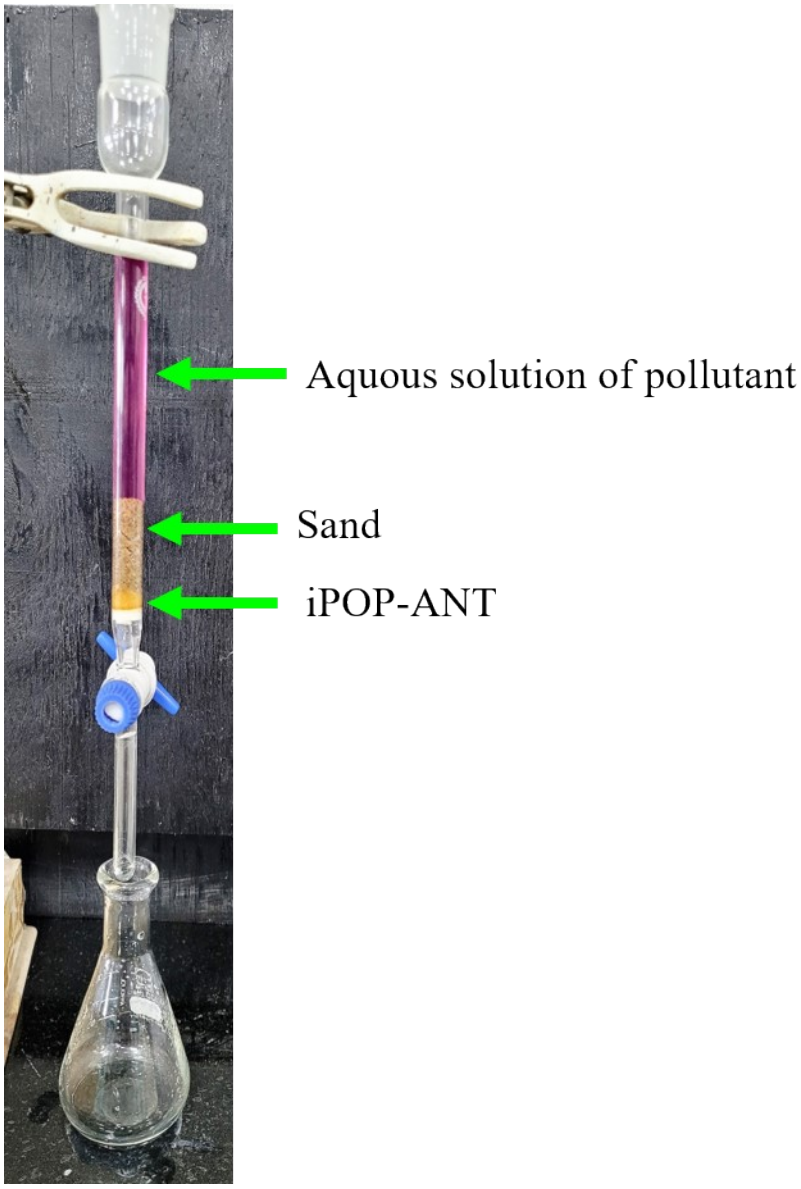

Figure S26. Representation of compound-loaded column for the separation if polluting anions

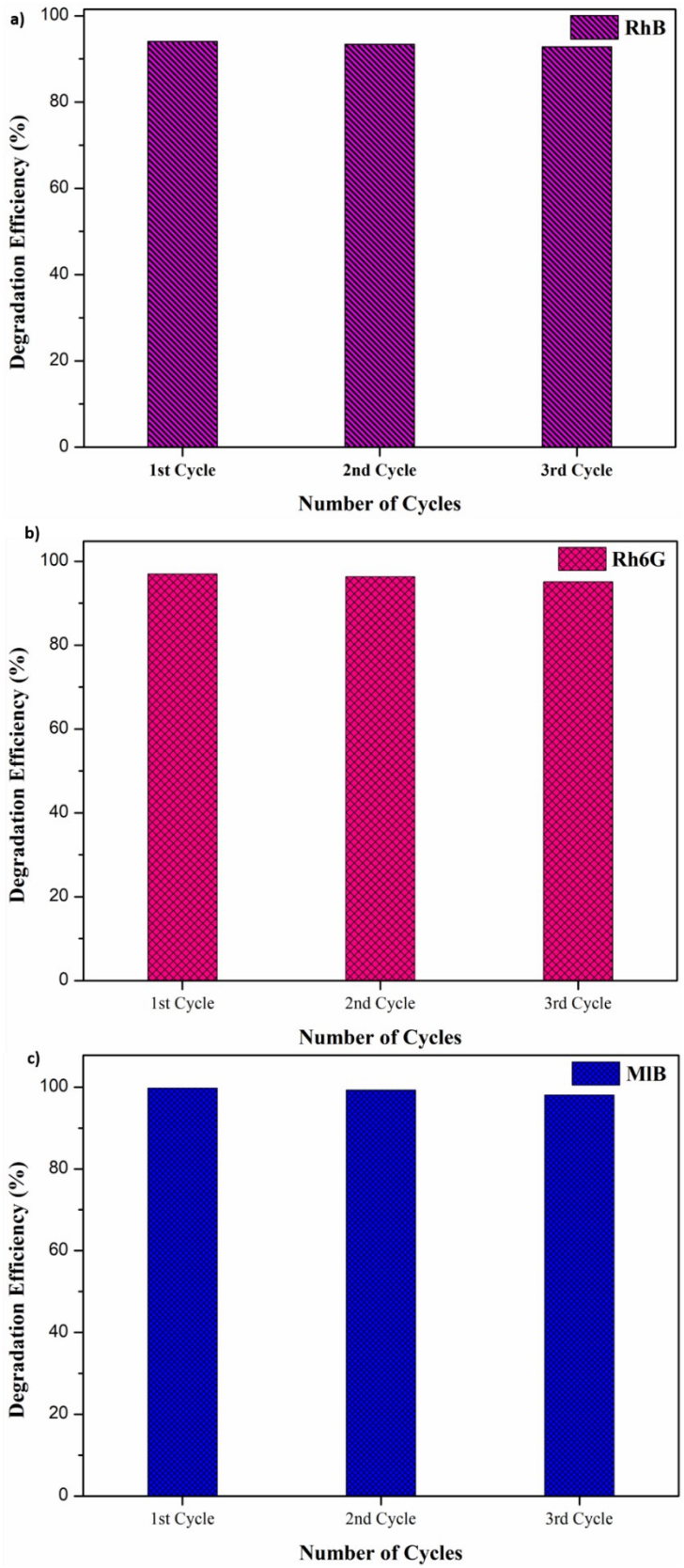

Figure S27. % Degradation efficiency of observed recyclability

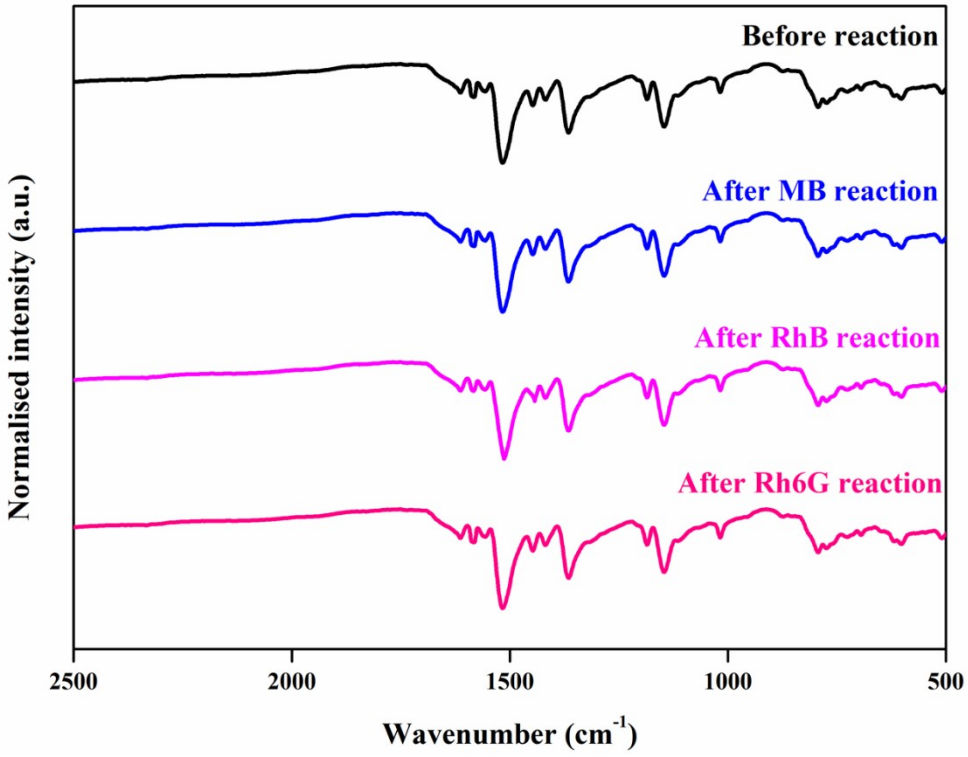

Figure S28. FT-IR spectra of COP-NT before and after reaction.

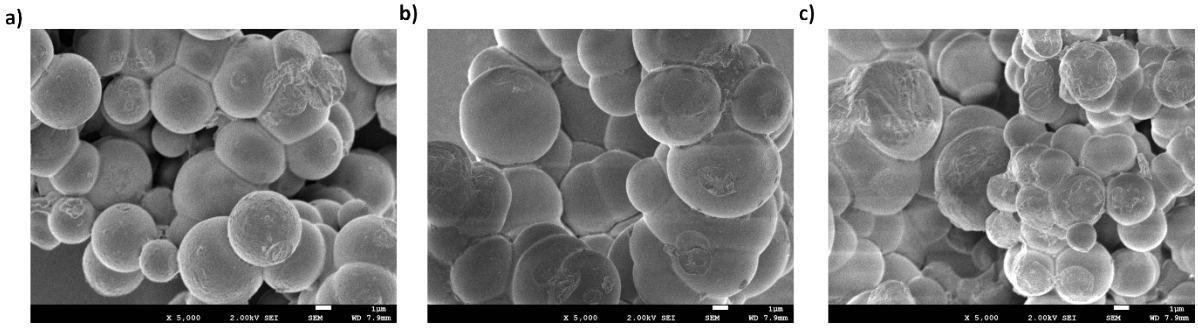

Figure S29. SEM images of iPOP-ANT after photodegradation of (a) RhB (b) Rh6G (c)MB

Compound	Capacity(mg/g)	Selectivity	Reference
iPOP-ANT	**330.75**	**Cl^-, Br^-, NO_3^-**	**This work**
FIR-53	100	ND	3[3]
1-Br	128	ND	[4]
CON-LDU-2	325	Cl^-, Br^-, NO_3^-, SO_4^{2-}	[5]
CON-1	293	ND	[6]
UiO-66-NH_2@silica	277.4	Cl^-, Br^-, NO_3^-, SO_4^{2-}	[7]
FJI-C11	321	ND	[8]
1-NO_3-OH	154.8	ClO_4^-, NO_3^-, Cl^-, BF_4^-, SO_4^{2-}	[9]
1-SO_4	116	ND	[10]
COP-NH_2	304.9	ND	[11]
1-Cl	28.7	ClO_4^-, BF_4^-, $CF_3SO_3^-$	[12]
ZJU-101	245	Cl^-, Br^-, NO_3^-, SO_4^{2-} I^-, F^-	[13]
DUT-52	120.68	Cl^-, Br^-, NO_3^-, SO_4^{2-} , PO_4^{3-}, CO_3^{2-}	[14]
QUST-iPOP-1	396	Cl^-, Br^-, NO_3^-, SO_4^{2-}	[15]
$\{Zn_{1.5}L\}_n$	469	Cl^-, Br^-, NO_3^-	[16]
C-NSA_{Naph}-HCP@Br	745	F^-, Cl^-, Br^-, ClO_3^-, NO_3^- , OAc^-, CO_3^{2-} PO_4^{3-}	[17]

Table S1. A comparison table of $Cr_2O_7^{2-}$capture (mg g^{-1}) with some well-studied examples in the literature (ND-Not done)

Compound	**Surrogate ion used**	**Capacity(mg/g)**	**Selectivity**	**Reference**
iPOP-ANT	MnO_4^-	**5372**	**Cl^-, Br^-, NO_3^-**	**This work**
Ox-FVESP	MnO_4^-	1428.57	ND	[18]
$[Cu_3Cl(L)(H_2O)_2]\cdot Cl\cdot 4DMA\cdot 8H_2O$	MnO_4^-	106	ClO_4^-, NO_3^- PF_6^-, $H_2PO_4^-$	[19]
ZrIT-1	MnO_4^-	276.6	ClO_4^-, NO_3^-, $H_2PO_4^-$, SO_4^{2-}, BF_4^-	[20]
SLUG-21	MnO_4^-	283	NO_3^-, CO_3^{2-}	[21]
SCNU-Z1-Cl	MnO_4^-	313.5	Cl^-, $ClO_4^-NO_3^-$, N_3^-,SO_4^{2-}	[22]
Compound-1	MnO_4^-	297.3	Cl^-, Br^-, NO_3^-, SO_4^{2-}	[2]
$Ag(btr)\cdot PF_6\cdot 0.5CH_3CN$	MnO_4^-	163	NO_3^-, BF_4^-, ClO_4^-	[23]
QUST-iPOP-1	MnO_4^-	514.86	Cl^-, Br^-, NO_3^-, SO_4^{2-}	[15]
	ReO_4^-	441.6		
SCU-CPN-1	ReO_4^-	876	NO_3^-, SO_4^{2-}	[24]
SCU-CPN-4	ReO_4^-	437	NO_3^-, SO_4^{2-}	[25]
SCU-COF-1	ReO_4^-	367.65	NO_3^-, CO_3^{2-}, SO_4^{2-}, PO_4^{3-}	[26]
SCU-CPN-2	ReO_4^-	1467	NO_3^-, SO_4^{2-}	[27]
iPOP-3	ReO_4^-	515.5	Cl^-, Br^-, NO_3^-, SO_4^{2-}	[28]
iPOP-3	ReO_4^-	350.3	Cl^-, Br^-, NO_3^-, SO_4^{2-}	[28]

Table S2. A comparison table of MnO_4^- capture (mg g^{-1}) with some well-studied examples in the literature (ND-Not done)

Compound	Capacity(mg/g)	Recycling	Reference
iPOP-ANT	**574.63**	**4**	**This work**
Fe_3O_4-PEI/β-CD	192.2	4	[29]
MWCNTs@Fe_3O_4/PEI	1727.6	6	[30]
CANEX1000	180.25	10	[31]
CANEX300	160.2	10	[31]
Fe/MCM-41	500.	-	[32]
4Czpyz-poly	204	-	[33]
QUST-iPOP-1	300	3	[15]
NH_2-MWCNTs	160	-	[34]
$[Cd(INA)_2 \cdot (H_2O)]$.ISB	384	-	[35]
SCNU-Z1-Cl	285	-	[22]

Table S3. A comparison table of MO capture (mg g-1) with some well-studied examples in the literature

Compound	Capacity(mg/g)	Recycling	Reference
iPOP-ANT	**645.084**	**4**	**This work**
MIL-100(Fe)	386.05	5	[36]
MCB	404.18	-	[37]

Table S4. A comparison table of AMR capture (mg g-1) with some well-studied examples in the literature

Compound	Capacity(mg/g)	Recycling	Reference
iPOP-ANT	**587.82**	**4**	**This work**
Fe_3O_4/PEG	133.3	-	[38]
MCB {[Tb(L)(H_2O)(DMF)]·DMF}$_n$	636.94	-	[39]
SCNU-Z1-Cl	585	-	[22]
Fe_3O_4@Carbon@ZIF-8	806.45	-	[40]
AmMAC1.35	319.49	-	[41]
QUST-iPOP-1	1074.9	3	[15]
Co-MOF	996.7	-	[42]
ZIF-67	998.5	-	[42]
ZIF-8@CS sponge	987	5	[43]

Table S5. A comparison table of CR capture (mg g-1) with some well-studied examples in the literature

Material	Dye used	Source of irradiation	Degradation time	% of degradation	Reference
iPOP-ANT	**RhB**	**Solar Light**	**140 min**	**94 %**	**This work**
	Rh6G		**160 min**	**97 %**	
	MB		**210 min**	**99.8 %**	
TP-COP	RhB	Solar Light	160 min	95 %	[44]
POP-1	RhB	LED Light	180 min	93 %	[45]
sp2c-CTP-4.	MB	Vis Light	90 min	98 %	[46]
PDA-COP 1	MO	Vis-light	120 min	92 %	[47]
CON-TP	MO	Vis-Light	600 min	67 %	[48]
	Rh		240 min	78 %	
	MB		100 min	57 %	
TpSD	RhB	Vis-Light (Xe arc lamp)	30	>99 %	[49]
	Rh6G		60	99.2 %	
	MB		60	95.8 %	

Table S6. Comparative studies of our designed TP-COP with the reported COPs in terms of photocatalytic dye degradation.

Experimental Section

Materials

4-Bromomethylbenzonitrile, tri-fluoromethanesulfonic acid, and anthracene were purchased from Sigma-Aldrich; other reagents and solvents were purchased locally and were used without further purification.

Synthesis of 2,4,6-tris(4-((1H-imidazol-1-yl)methyl)phenyl)-1,3,5-triazine (Precursor-1)

Precursor-1 was synthesized according to a reported procedure[45]

9,10-Bis(chloromethyl)anthracene (Precursor-2)

Precursor-2 was also synthesized following a reported literature method[51].

Physical measurements

Fourier transform infrared (FTIR) analysis was carried out on PerkinElmer's spectrum II spectrometer. NMR spectra were obtained by an AVANCE III 500 Ascend Bruker Biospin machine at an ambient temperature using $CDCl_3$. ^{13}C CP/MAS NMR was carried out by ECZR series 600MHz NMR by JEOL. Thermogravimetric analysis (TGA) was analyzed using Mettler Toledo Thermal Analyzer with heating rate of 10 °C/min. Morphological data of the polymer were recorded in JEOL JSM-7400F field emission scanning electron microscopy (FE-SEM) and FEI Tecnai G2, F30 HR-TEM (300 kV). Gas adsorption measurements were carried out using Quantachrome, Autosorb iQ2 Brunauer−Emmett−Teller (BET) surface area analyzer was used. PXRD of the polymer was done on Empyrean, Malvern Panalytical, with Cu-Kα radiation with 2θ range from 2^o to 80^o and a step size of 0.02^o. UV-DRS was obtained from Cary 5000 UV-Vis NIR Spectrometer. X-ray photoelectron spectroscopy (XPS) were performed through a Physical Electronics make PHI 5000 VersaProbe III (Mg Kα X-rays, hν = 1253.6 eV).

Synthesis of iPOP-ANT

Precursor-1 was reacted with Precursor-2 in 20 ml DMF under an inert atmosphere at 373K for 24 hr. After being cooled to room temperature,the obtained precipitate was collected by centrifugation; washed successively with DMSO, DMF, water, MeCN, THF, DCM, and diethyl ether to remove the small chain oligomers and unreacted precursors. Furthermore, the obtained solid was dipped in a 1:1:1 mixture of MeOH, THF, and DCM solution for 72 hrs

for solvent exchange. The yellow-colored compound was then collected by filtration, heated at 80°C for 24 hrs to obtain the guest-free desolvated compound.

Procedures for the time-dependent study of oxo-Anion exchange

An aqueous solution of 3 mL of $K_2Cr_2O_7$ (0.5mM) was taken in a cuvette, and the initial absorption was recorded using UV- spectroscopy. 1.5mg of the desolvated iPOP-ANT was added to the cuvette and shaken gently. The absorbance of the supernatant solution was monitored by liquid UV-vis spectroscopy with different adsorption times. UV-vis spectroscopy of the $KMnO_4$ solution was also recorded similarly. From the time-dependent study, the percentage of oxo-anion removal and decrease of concentration with time was calculated using the following equation[47]

$$Dt = \frac{C_o - C_t}{C_0} \times 100\% = \frac{A_{0-A_t}}{A_0} \times 100\%$$

where D_t is the exchange capacity, C_0 and A_0 are the initial concentration and absorbance of the oxo-anion solution respectively, and C_t and A_t is the concentration and absorbance of the oxo-anion solution at specific times, respectively.

Kinetics data for removing $Cr_2O_7^{2-}$ and MnO_4^- were fitted in the pseudo-second-order model using the following equation

$$Q_t = \frac{k_2 Q_e^2 t}{1 + k_2 Q_e t}$$

Where t is the time in minutes, and Q_t and Q_e are the amounts of adsorbate (mg g^{-1}) on the adsorbent at different time intervals and equilibrium, respectively.

Selective adsorption of oxo-anions in the presence of competitive anions

In this study, Cl^-, Br^-, NO_3^- ions were taken as competing anions, commonly present in ordinary water and wastewater sources. An equimolar (5 mM,1:1) aqueous solution of both the targeted oxo-anions and the competing anions was taken. 2 mg of the desolvated iPOP-ANT was added to the solution and allowed to stir for 24 hours. The solid particles were separated through filtration, the obtained supernatant was diluted ten times, and the UV-VIS spectra were recorded. The capture efficiency of iPOP-ANT in the presence of competing

ions was determined by comparison with a blank solution (0.5 mM aqueous of the oxo-anion).

In order to check the effect of excess competing ions on the adsorption of the targeted ions adsorption experiments were also carried out taking the excess concentrations of the competing ions in a ratio of 1:10 (5mM:50mM), 1:50 (5mM:250mM), 1:100 (5mM:500mM) and 1:1000 (5mM:5000mM).

Procedures for the time-dependent study of anionic dye exchange

For this experiment, three common anionic dyes, methyl orange (MO), congo red (CR), and amaranth (AMR), and two common cationic dyes, rhodamine B (RhB) and rhodamine 6G (Rh6G), were taken.

In the case of anion exchange study, in a typical experiment, an aqueous of 3 mL of MO (60 mgL^{-1}) was taken in a cuvette, and the initial absorption was recorded using UV-VIS spectroscopy. 1.5mg of the desolvated iPOP-ANT was added to the cuvette and shaken gently. The corresponding absorbance of the supernatant solution was monitored by liquid UV-Vis spectroscopy with different adsorption times. UV-VIS spectra of the other dye solutions were recorded similarly. From the time-dependent study, the percentage of dye removal and decrease of concentration with time was calculated.

Calculation of capacity

5 mg of the desolvated iPOP-ANT was added to 2.5 mL of 5 mM of the oxo-anion solution or 60 mgL^{-1} anionic dye solution. The mixture was stirred for 24 hours, after one day, the solid particles were removed by filtration and the filtrate was used for UV-vis by diluting the solution. The uptake capacity was calculated from the solutions' initial and final absorbance values using the following equation[47]

$$Q_t = \frac{(C_0 - C_t) \times V}{m}$$

Where Q_t is the capacity of the adsorbent, C_0 and C_t are the initial concentration and concentration at time t , V is the volume of the solution, and m is the mass used for the adsorbent, respectively.

Recyclability test of iPOP-ANT

The material after capturing the pollutants were regenerated by treating them with saturated KCl solution for 24 hours. The reusability of the regenerated material was examined with 5ml

of 0.5mM of the oxo-anion solution and 60 mgL^{-1} of anionic dye solution. The concentration of the anionic solutions was measured after 24 hours by UV-vis spectroscopy. These studies were repeated up to four cycles for each of the anions.

The same method was used for the column study, where the adsorbent was regenerated by passing saturated KCl solution through the column.

Photocatalytic degradation of the cationic dyes

The photocatalytic performance of iPOP-ANT was investigated by monitoring the degradation of cationic dyes- rhodamine B (RhB), rhodamine-6G, and methylene Blue (MB) under solar irradiation. The dye solutions (10 ppm) were prepared in deionized water, the pH of the solutions was regulated using 1N HCl or 0.1M KOH solution when required. A series of dye solutions were taken in 5 mL capacity glass vials, and 0.5 mg/mL iPOP-ANT were dispersed in the dye solutions. The vials were placed under solar light irradiation with occasional stirring. The solutions were centrifuged at different time intervals; the supernatant was analysed with the help of UV-vis spectroscopy to determine the concentration of the solution. After centrifugation, the solid iPOP-ANT was collected, washed with acetone, dried at 75 °C to regenerate the photocatalyst. The regenerated material was reused, keeping all the conditions similar.

Computational details

The structures of the pristine iPOP-ANT and various anionic and cationic binders was optimized at the B3LYP-D3 method, using 6-31G(d) basis set for elements till period 3, whereas SDD basis set was used for elements in the higher periods[48-51]. Confirmation of minimum geometry was performed by frequency analysis to obtain zero imaginary frequencies. For the iPOP-ANT and binders, electrostatic potential (ESP) maps were generated to understand the binding sites. Various sites were considered based on the relative electron density spread over the molecules, and the structures (complex after binding) with the lowest total energies are provided. The binding energy is then calculated by employing the formula:

$$\text{Binding energy (BE)} = E_{Complex} - E_{Binder} - E_{iPOP\text{-}ANT}$$

where $E_{Complex}$, E_{Binder} and $E_{iPOP-ANT}$ are the total energies of complex, binder and pristine iPOP-ANT, respectively. All calculations were performed using Gaussian 16 program package[51].

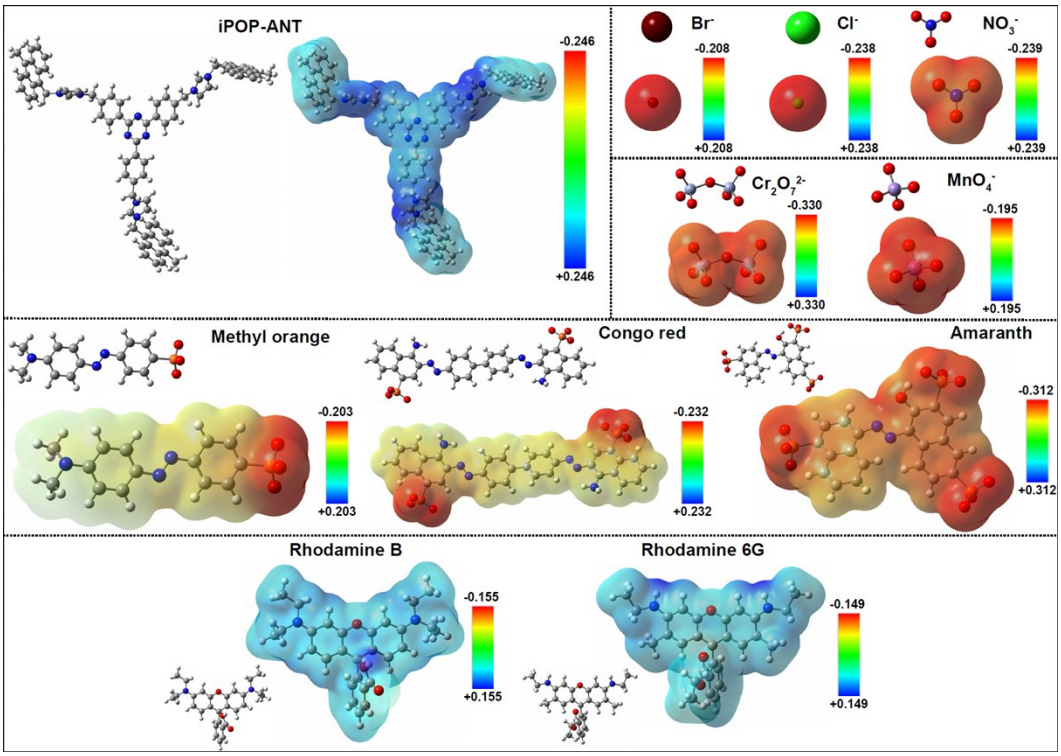

Figure S30. Electrostatic potential (ESP) distribution maps (isodensity=0.001 a.u.) of iPOP-ANT and various anionic and cationic binder.

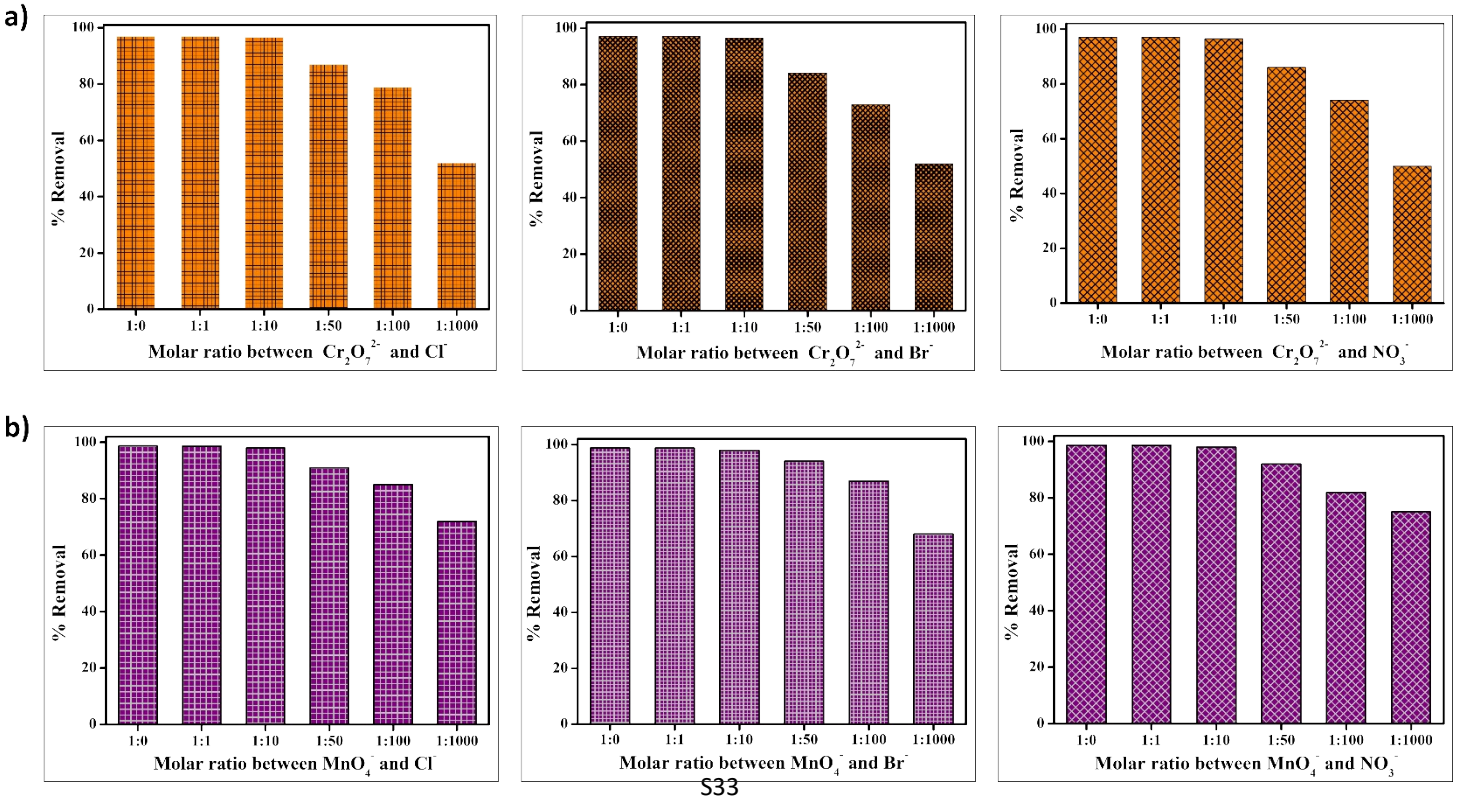

Figure S31. Effect of excess competing anions on targeted oxo-anions uptake by iPOP-ANT

Table S8. Total energies of the binders computed at B3LYP-D3/SDD-6-31G(d) level of theory. (Total energy of iPOP-ANT = -3618.6701969 Hartree)

Binder	**Energy in Hartree**
Br-	-13.4719946
Cl-	-460.2522334
NO_3-	-280.3362178
$Cr_2O_7^{2-}$	-700.7695611
MnO_4^-	-405.271683
Methyl orange	-1330.0319243
Congo red	-2808.92219816
Amaranth	-2824.98864711
Rhodamine B	-1420.7311829
Rhodamine 6G	-1420.7422623

Table S9. Total energies of the complex (iPOP-ANT with binders) computed at B3LYP-D3/SDD-6-31G(d) level of theory.

Complex	**Energy in Hartree**
Br^-	-3632.3181592
Cl^-	-4079.1934194
NO_3^-	-3899.2759295
$Cr_2O_7^{2-}$	-4319.9025258
MnO_4^-	-4024.1341171
Methyl orange	-4948.9846538
Congo red	-6428.0815432

Amaranth	-6444.387854
Rhodamine B	-5039.3502113
Rhodamine 6G	-5039.3475763

Table S10. Binding energies computed at B3LYP-D3/SDD-6-31G(d) level of theory.

Complex	**Energy in Hartree**	**Energy in kcal/mol**
Br^-	-0.1759677	-110.420259653101
Cl^-	-0.27098901	-170.04647321727
NO_3^-	-0.2695148	-169.121345544273
$Cr_2O_7^{2-}$	-0.4627678	-290.388182803504
MnO_4^-	-0.1922372	-120.629419711543
Methyl orange	-0.2825326	-177.290054097922
Congo red	-0.48914814	-306.941925294418
Amaranth	-0.72900999	-457.455955754761
Rhodamine B	+0.0511685	+32.1083872552967
Rhodamine 6G	+0.0648829	+40.7142143990838

Table S11. Cartesian coordinates of iPOP-ANT.

C	2.378746	-1.952677	0.053059
N	1.394356	-2.891438	0.004961
C	0.138173	-2.419278	-0.137297
C	0.956069	-0.163556	-0.168776
N	2.224221	-0.602706	-0.027036
N	-0.142688	-1.042373	-0.230670
C	3.819185	-2.472725	0.215188
C	4.357639	-2.649879	1.489513
C	4.585939	-2.766390	-0.913114
C	5.662337	-3.121776	1.636304
H	3.753518	-2.418891	2.378853
C	5.890480	-3.237720	-0.766288

H	4.161193	-2.626576	-1.917773
C	6.428610	-3.415809	0.508510
H	6.086520	-3.261800	2.641094
H	6.495030	-3.469244	-1.655327
C	0.768529	1.362228	-0.260496
C	0.798712	1.995381	-1.502843
C	0.568748	2.111478	0.899645
C	0.628006	3.377565	-1.585908
H	0.955763	1.405156	-2.417289
C	0.398564	3.493387	0.816566
H	0.545047	1.612046	1.879085
C	0.427798	4.126454	-0.426326
H	0.651391	3.876502	-2.565529
H	0.241102	4.084163	1.730712
C	-0.984354	-3.472100	-0.192969
C	-1.606627	-3.891239	0.982752
C	-1.378706	-4.007113	-1.419942
C	-2.624114	-4.844460	0.932136
H	-1.296325	-3.469536	1.949768
C	-2.395631	-4.960451	-1.470421
H	-0.887880	-3.676526	-2.346818
C	-3.018669	-5.378886	-0.294349
H	-3.114900	-5.174453	1.859162
H	-2.706648	-5.382299	-2.437265
C	-4.141592	-6.431262	-0.350449
H	-3.971881	-7.090261	-1.176172
H	-4.148675	-6.994143	0.559504
C	0.239595	5.652175	-0.517736
H	0.620730	6.112373	0.369875
H	0.768868	6.026465	-1.369016
C	7.868867	-3.936472	0.670281
H	8.109159	-4.581293	-0.149088
H	7.950500	-4.480437	1.588071

N	-5.436897	-5.757145	-0.519719
C	-6.037697	-5.450681	-1.737183
C	-6.264192	-5.320885	0.510998
C	-7.259282	-4.813061	-1.480134
H	-5.563539	-5.702569	-2.684934
H	-5.990752	-5.457915	1.556407
H	-7.964628	-4.449589	-2.219868
N	-1.190801	5.962097	-0.654905
C	-2.074567	6.190756	0.395701
C	-1.883780	6.075529	-1.856584
H	-1.746509	6.152281	1.433681
C	-3.221825	6.379186	-1.569173
H	-1.386376	5.935012	-2.815370
H	-4.017530	6.530784	-2.290760
N	8.801387	-2.800278	0.689486
C	9.211806	-2.108180	1.825117
C	9.419276	-2.240139	-0.424774
C	10.099497	-1.097418	1.431077
H	8.850699	-2.377379	2.816902
H	9.242110	-2.626558	-1.427629
H	10.594751	-0.384919	2.082154
N	-7.402902	-4.730684	-0.054847
N	-3.342701	6.452287	-0.141272
N	10.231019	-1.180984	0.004692
C	-4.567836	6.746474	0.615959
H	-5.359506	6.113338	0.273471
H	-4.394795	6.569742	1.656978
C	-8.533231	-4.138122	0.674623
H	-8.756144	-3.174884	0.265499
H	-8.276373	-4.035841	1.708287
C	11.061982	-0.317089	-0.846241
H	10.831843	0.708489	-0.645927
H	10.863393	-0.532776	-1.875290

C	-4.960949	8.220274	0.403884
C	-5.755838	8.570275	-0.692986
C	-4.519244	9.189162	1.311473
C	-6.217541	7.590796	-1.631328
C	-6.120767	9.937553	-0.889917
C	-4.882598	10.556663	1.113498
C	-3.706521	8.847878	2.441046
C	-6.996081	7.952825	-2.691992
H	-5.928611	6.541412	-1.469105
C	-6.938285	10.278146	-2.016280
C	-5.676911	10.906783	0.016196
C	-4.420994	11.536195	2.051766
H	-3.434329	7.791064	2.582842
C	-3.286502	9.808496	3.314576
C	-7.361949	9.316966	-2.887385
H	-7.354278	7.203232	-3.412960
H	-7.212083	11.334677	-2.156921
C	-3.648483	11.173243	3.116565
H	-4.707455	12.585979	1.887587
H	-2.663056	9.550179	4.183258
H	-7.989280	9.574356	-3.753522
H	-3.293041	11.922183	3.839601
C	-9.766241	-5.050894	0.539958
C	-10.052046	-5.976118	1.549784
C	-10.584803	-4.941820	-0.589478
C	-9.225062	-6.100251	2.713280
C	-11.195994	-6.823021	1.425122
C	-11.727654	-5.789998	-0.715027
C	-10.307957	-3.998495	-1.631794
C	-9.524428	-7.006091	3.689000
H	-8.346372	-5.443032	2.796778
C	-11.476186	-7.762428	2.470129
C	-12.013067	-6.715752	0.294483

C	-12.554704	-5.665936	-1.878429
H	-9.425287	-3.350384	-1.522726
C	-11.119509	-3.908112	-2.725171
C	-10.667144	-7.849826	3.565572
H	-8.893146	-7.102448	4.584649
H	-12.359967	-8.409134	2.361945
C	-12.259540	-4.755060	-2.850790
H	-13.431590	-6.325441	-1.963192
H	-10.910550	-3.184655	-3.527023
H	-10.878517	-8.569950	4.369766
H	-12.892639	-4.656129	-3.744898
C	12.549564	-0.577695	-0.544935
C	13.244735	-1.538631	-1.287102
C	13.186264	0.150773	0.465764
C	12.608448	-2.292740	-2.326088
C	14.624909	-1.780539	-1.007809
C	14.565905	-0.092462	0.746313
C	12.490024	1.139810	1.233867
C	13.306131	-3.222152	-3.041370
H	11.544878	-2.097814	-2.530603
C	15.322762	-2.765509	-1.779736
C	15.260915	-1.053936	0.004613
C	15.202287	0.661588	1.785223
H	11.428006	1.318360	1.007396
C	13.130017	1.839504	2.215241
C	14.683963	-3.462121	-2.764036
H	12.821501	-3.801195	-3.841266
H	16.385273	-2.942613	-1.554554
C	14.506582	1.596218	2.495693
H	16.265069	0.464266	1.991668
H	12.598975	2.600044	2.806505
H	15.215986	-4.219389	-3.358581
H	14.991911	2.177838	3.293317

C	16.748533	-1.314981	0.305361
H	16.983649	-2.334957	0.083394
H	17.352867	-0.670225	-0.297939
H	16.942687	-1.121136	1.339589
C	-6.070443	12.380394	-0.196421
H	-6.185931	12.571298	-1.242900
H	-6.993794	12.579095	0.306411
H	-5.305031	13.014659	0.199498
C	-13.245963	-7.628774	0.160474
H	-14.092994	-7.152284	0.608128
H	-13.444693	-7.810003	-0.875172
H	-13.056822	-8.558407	0.655355

Table S12. Cartesian coordinates of Br^-.

Br	-0.945297	0.940126	-0.012375

Table S13. Cartesian coordinates of Cl^-.

Cl	-0.945297	0.940126	-0.012375

Table S14. Cartesian coordinates of NO_3^-.

N	-1.857868	1.111675	0.000000
O	-0.658527	1.111675	0.000000
O	-2.514824	2.115078	0.000000
O	-2.504580	-0.084721	-0.000001

Table S15. Cartesian coordinates of $Cr_2O_7^{2-}$.

Cr	-2.835669	0.109604	-1.280594
O	-2.224808	-1.571146	-1.202951
O	-2.218108	0.901043	-2.762600
O	-4.625271	0.093065	-1.314497
O	-2.274489	1.015455	0.157673
Cr	-2.885350	2.696204	0.080030
O	-2.324170	3.602055	1.518297

O	-2.208165	3.511128	-1.362682
O	-4.671930	2.677296	-0.028946

Table S16. Cartesian coordinates of MnO_4^-.

Mn	-0.535714	1.790966	0.000000
O	0.074296	2.653629	1.494189
O	0.074265	0.065618	0.000000
O	-2.365714	1.790989	0.000000
O	0.074296	2.653629	-1.494189

Table S17. Cartesian coordinates of methyl orange.

C	-3.321643	-0.959469	0.853877
C	-1.926483	-0.960008	0.854185
C	-1.228426	-0.106599	0.000000
C	-1.925562	0.747037	-0.855876
C	-3.320387	0.747182	-0.856467
C	-4.018506	-0.105844	-0.001256
H	-3.871810	-1.632068	1.527724
H	-1.377383	-1.632559	1.529024
H	-1.374953	1.419790	-1.529323
H	-3.870100	1.419825	-1.530886
N	0.241573	-0.106492	0.000848
N	0.857954	0.647206	-0.754028
C	2.327954	0.647227	-0.753267
C	3.026010	1.500078	-1.608009
C	3.025089	-0.206492	0.102527
C	4.421169	1.500596	-1.606647
H	2.476911	2.173218	-2.282260
C	4.419914	-0.206258	0.103495
H	2.474480	-0.878888	0.776329
C	5.118033	0.647620	-0.750865
H	4.971337	2.173392	-2.280297
H	4.969627	-0.878977	0.777839

S	6.898032	0.647865	-0.749123
O	7.379090	0.156035	-1.963721
O	7.377198	1.864086	-0.259451
N	-5.488506	-0.105273	-0.001924
C	-5.978973	0.254844	1.336231
H	-7.017798	0.504999	1.279963
H	-5.847211	-0.574388	1.999491
H	-5.428917	1.096046	1.703269
C	-5.978863	-1.444115	-0.359629
H	-7.033064	-1.401982	-0.537914
H	-5.480724	-1.781792	-1.244350
H	-5.779728	-2.123101	0.443006
O	7.007598	-0.529097	0.430562

Table S18. Cartesian coordinates of congo red.

C	2.182371	12.046796	0.004074
C	1.001311	11.347029	0.001574
C	1.004695	9.925022	0.001481
C	2.246147	9.238018	0.004379
C	3.454059	9.987836	0.007092
C	3.421123	11.360781	0.006830
H	2.182397	13.146792	0.004071
H	0.034052	11.871564	-0.000624
C	-0.203397	9.174898	-0.001341
C	2.248631	7.815936	0.004400
H	4.411386	9.445638	0.009122
H	4.353732	11.943991	0.008908
C	1.067555	7.116080	0.001627
C	-0.171292	7.802333	-0.001355
H	-1.103843	7.219043	-0.003512
N	3.540596	7.114711	0.007378
H	3.607587	6.542834	0.824978
H	3.609785	6.539948	-0.808011

N	1.067555	5.646080	0.001286
N	0.000612	5.030080	0.001178
C	0.000612	3.560080	0.000571
C	1.208312	2.862454	0.000117
C	-1.207948	2.862514	0.000054
C	1.208211	1.467294	0.000345
H	2.160865	3.411893	0.000894
C	-1.207972	1.467688	-0.000197
H	-2.160051	3.412783	0.000353
C	0.000184	0.770000	0.000345
H	2.160488	0.917466	0.000438
H	-2.160293	0.917635	-0.000612
S	-1.752286	10.052016	-0.004461
O	-1.929654	10.716822	1.210091
O	-1.904769	10.752206	-1.202399
O	-2.669424	8.656716	-0.034379
C	-0.000184	-0.770000	0.000345
C	-1.208211	-1.467294	0.000345
C	1.207972	-1.467688	-0.000197
C	-1.208312	-2.862454	0.000117
H	-2.160488	-0.917466	0.000438
C	1.207948	-2.862514	0.000054
H	2.160293	-0.917635	-0.000612
C	-0.000612	-3.560080	0.000571
H	-2.160865	-3.411893	0.000894
H	2.160051	-3.412783	0.000353
N	-0.000612	-5.030080	0.001178
N	-1.067555	-5.646080	0.001286
C	-1.067555	-7.116080	0.001627
C	-2.248631	-7.815936	0.004400
C	0.171292	-7.802333	-0.001355
C	-2.246147	-9.238018	0.004379
N	-3.540596	-7.114711	0.007378

C	0.203397	-9.174898	-0.001341
H	1.103843	-7.219043	-0.003512
C	-1.004695	-9.925022	0.001481
C	-3.454059	-9.987836	0.007092
H	-3.607587	-6.542834	0.824978
H	-3.609785	-6.539948	-0.808011
S	1.752286	-10.052016	-0.004461
C	-1.001311	-11.347029	0.001574
C	-3.421123	-11.360781	0.006830
H	-4.411386	-9.445638	0.009122
O	1.929654	-10.716822	1.210091
O	1.904769	-10.752206	-1.202399
O	2.669424	-8.656716	-0.034379
C	-2.182371	-12.046796	0.004074
H	-0.034052	-11.871564	-0.000624
H	-4.353732	-11.943991	0.008908
H	-2.182397	-13.146792	0.004071

Table S19. Cartesian coordinates of amaranth.

C	3.414088	1.508218	0.783400
C	2.499366	0.635483	0.205690
C	2.996144	-0.583509	-0.397539
C	4.413283	-0.859818	-0.334754
C	5.298780	0.065388	0.309322
C	4.789164	1.226483	0.849076
H	1.101871	-1.297052	-1.138201
H	3.014652	2.428110	1.201231
C	2.159931	-1.509310	-1.081779
C	4.903419	-2.057709	-0.927578
H	5.476736	1.918958	1.322706
C	4.055615	-2.936006	-1.564241
C	2.675497	-2.655062	-1.650036
H	5.964796	-2.261244	-0.870655

H	4.454709	-3.846466	-2.008871
H	2.008047	-3.343066	-2.165596
N	1.176866	1.134347	0.278746
N	0.229102	0.317655	0.054194
C	-1.087928	0.793082	0.061628
C	-1.490364	2.142147	-0.083508
C	-2.095744	-0.246166	0.123327
C	-2.880537	2.456575	-0.155461
C	-3.481686	0.100368	0.033122
C	-1.772103	-1.622275	0.261806
C	-3.831551	1.470768	-0.105809
C	-4.472867	-0.914437	0.079815
H	-0.728036	-1.905334	0.336087
C	-2.759468	-2.588160	0.300880
H	-4.877415	1.754375	-0.183976
C	-4.127298	-2.242320	0.213422
H	-5.520766	-0.640674	-0.010414
H	-2.507107	-3.640406	0.389309
O	-0.590586	3.126932	-0.212152
H	-1.096264	3.930444	-0.526936
S	-3.402044	4.200263	-0.220992
O	-3.421887	4.671078	1.187637
O	-2.288637	4.818974	-1.037299
S	-5.413675	-3.531562	0.323968
O	-5.896055	-3.470826	1.733566
O	-6.436898	-3.119638	-0.679239
S	7.106669	-0.225490	0.426487
O	7.229547	-1.510093	1.173225
O	7.560824	-0.313572	-0.991267
O	-4.697518	-4.796867	-0.013581
O	-4.718771	4.202639	-0.906029
O	7.632148	0.959439	1.161216

Table S20. Cartesian coordinates of rhodamine B.

C	-3.629745	0.275333	-0.285864
C	-2.442349	0.945412	-0.343135
C	-1.197882	0.238754	-0.272635
C	-1.220857	-1.183237	-0.135454
C	-2.487541	-1.850457	-0.077463
C	-3.652677	-1.143896	-0.151019
C	1.213986	-1.221742	-0.125955
C	1.236966	0.200021	-0.265025
C	2.503688	0.866562	-0.328788
H	2.507798	1.961713	-0.436854
C	3.668833	0.159518	-0.259619
C	3.645868	-1.259204	-0.120076
C	2.458353	-1.928489	-0.055481
H	-4.586973	0.814354	-0.342086
H	-2.411046	2.040455	-0.447571
H	-2.491584	-2.945780	0.028614
H	4.643175	0.667696	-0.308940
H	2.426791	-3.023244	0.052108
N	4.868075	-1.900292	0.064892
N	-4.954897	-1.823287	-0.091430
C	-6.196607	-1.040692	-0.172676
H	-6.409097	-0.608685	0.782896
C	-5.015407	-3.285273	0.049406
H	-4.973795	-3.738885	-0.918790
H	-4.186688	-3.621613	0.636773
C	4.911402	-3.288636	0.233471
H	4.651609	-3.440337	1.260309
H	4.155145	-3.714357	-0.392417
C	5.976845	-1.029664	0.087529
H	6.044547	-0.563266	1.048148
C	6.262407	-3.967118	-0.059867
H	6.979111	-3.667737	0.676072

H	6.141988	-5.029867	-0.028836
H	6.604808	-3.675162	-1.030652
C	-6.331427	-3.679938	0.745059
H	-7.147740	-3.545854	0.066417
H	-6.282294	-4.705673	1.045647
H	-6.478624	-3.062501	1.606456
O	-0.014571	-1.888331	-0.063525
C	0.030640	0.905386	-0.334337
H	6.870948	-1.585786	-0.102757
C	5.803629	0.050423	-0.996449
H	5.012566	-0.232792	-1.658951
H	5.563944	0.984937	-0.533702
H	6.714024	0.149573	-1.549847
H	-7.003524	-1.681075	-0.461974
C	-6.030262	0.079078	-1.216729
H	-5.776752	0.993293	-0.721912
H	-5.250879	-0.184149	-1.900960
H	-6.947578	0.206111	-1.752726
C	0.055470	2.438213	-0.480709
C	0.084754	3.247090	0.655109
C	0.048275	3.017955	-1.749985
C	0.108052	4.635727	0.522393
C	0.071089	4.406276	-1.882586
H	0.025125	2.379983	-2.645391
C	0.101377	5.215240	-0.746334
H	0.131588	5.273271	1.418008
H	0.065418	4.863484	-2.882788
H	0.119556	6.309690	-0.851116
C	0.093223	2.607675	2.056065
O	0.125698	3.333502	3.083533
O	0.064083	1.184243	2.189834
H	0.073902	0.950052	3.120779

Table S21. Cartesian coordinates of rhodamine 6G.

C	-3.691449	-0.463807	-0.313078
C	-2.500516	0.102515	-0.664010
C	-1.263143	-0.569933	-0.399897
C	-1.296685	-1.844952	0.244001
C	-2.566705	-2.405846	0.598232
C	-3.725040	-1.737098	0.327643
C	1.134369	-1.954313	0.154270
C	1.167810	-0.680188	-0.491305
C	2.437546	-0.122013	-0.850664
H	2.449684	0.859504	-1.348186
C	3.595644	-0.792796	-0.583985
C	3.562282	-2.063916	0.060928
C	2.371640	-2.626849	0.418396
H	-2.461031	1.084383	-1.159370
H	-2.578887	-3.388244	1.093961
H	2.332072	-3.607303	0.916598
N	4.784504	-2.633215	0.408878
N	-5.030609	-2.307635	0.689413
C	-6.264850	-1.568382	0.387659
H	-6.485047	-0.898341	1.192307
H	-6.134394	-1.010125	-0.515795
C	5.979157	-2.018027	0.018823
H	6.108491	-2.311059	-1.002111
H	5.829878	-0.959727	0.069963
C	7.234661	-2.398905	0.825199
H	7.482374	-3.422701	0.637099
H	8.051518	-1.774190	0.529604
H	7.042422	-2.264461	1.869167
C	-7.428704	-2.561759	0.213743
H	-7.703946	-2.959321	1.168252
H	-8.267507	-2.056436	-0.217484
H	-7.123310	-3.359723	-0.430375

O	-0.097335	-2.514219	0.510642
C	-0.031434	-0.009722	-0.755606
C	0.004870	1.365218	-1.448297
C	0.106310	2.528308	-0.685306
C	-0.064134	1.447419	-2.839591
C	0.139993	3.773844	-1.312981
C	-0.030931	2.692716	-3.467021
H	-0.144172	0.530231	-3.440970
C	0.071536	3.856013	-2.703704
H	0.220422	4.690696	-0.711269
H	-0.085304	2.757832	-4.563505
H	0.097892	4.837618	-3.198563
C	0.183004	2.438003	0.850129
O	0.154506	1.316909	1.421012
O	0.286963	3.632218	1.629837
H	-5.079132	-3.198648	1.140790
H	4.808431	-3.481720	0.937523
C	4.962855	-0.197755	-0.969031
H	5.531815	-0.008508	-0.082820
H	5.490872	-0.890227	-1.590786
H	4.815823	0.718908	-1.501018
C	-5.024167	0.253408	-0.597794
H	-5.644274	-0.373598	-1.203791
H	-5.521910	0.461189	0.326316
H	-4.832297	1.170957	-1.113730
C	0.320495	3.293292	3.018687
H	1.169587	2.672115	3.213833
H	-0.573925	2.766867	3.279052
C	0.421846	4.579984	3.858778
H	-0.430258	5.198438	3.668165
H	0.453009	4.326062	4.897745
H	1.313205	5.109451	3.594123

Table S22. Cartesian coordinates of iPOP-ANT binded with Br^-.

C	0.348171	1.143687	-0.988263
N	-0.836794	1.119646	-0.359214
C	-1.325534	-0.098935	-0.083426
C	0.469728	-1.125924	-1.025681
N	1.039140	0.048222	-1.336200
N	-0.709155	-1.248433	-0.397529
C	0.925833	2.467103	-1.337363
C	2.123335	2.547245	-2.061861
C	0.267638	3.652879	-0.969732
C	2.643448	3.787387	-2.426286
H	2.631805	1.634013	-2.347487
C	0.790083	4.888655	-1.334436
H	-0.658697	3.590977	-0.410683
C	1.978376	4.967238	-2.074292
H	3.561938	3.833727	-3.006093
H	0.263904	5.798092	-1.054565
C	1.183467	-2.368238	-1.417885
C	2.409663	-2.297049	-2.093419
C	0.627271	-3.628581	-1.140210
C	3.059609	-3.461772	-2.496528
H	2.840645	-1.326385	-2.308333
C	1.276881	-4.788457	-1.546908
H	-0.321410	-3.683941	-0.619292
C	2.495468	-4.715540	-2.236615
H	4.001961	-3.390875	-3.033870
H	0.827997	-5.756650	-1.338715
C	-2.636135	-0.182201	0.611307
C	-3.345372	0.986072	0.937692
C	-3.177282	-1.428428	0.956662
C	-4.563182	0.906058	1.603582
H	-2.926468	1.949423	0.671496
C	-4.398069	-1.504737	1.623996

H	-2.631779	-2.330428	0.705662
C	-5.098415	-0.340186	1.958193
H	-5.097043	1.818331	1.858552
H	-4.798523	-2.477229	1.899499
C	-6.408493	-0.428994	2.706584
H	-6.567802	-1.436698	3.100765
H	-6.432706	0.269538	3.547726
C	3.181148	-5.971866	-2.722977
H	2.487553	-6.611388	-3.276536
H	4.017115	-5.730278	-3.385538
C	2.525124	6.306643	-2.511931
H	1.740833	6.929477	-2.951288
H	3.314205	6.182541	-3.259037
N	-7.573974	-0.095044	1.850824
C	-7.798682	-0.557259	0.566012
C	-8.641596	0.622094	2.233442
C	-9.027277	-0.101591	0.185144
H	-7.067530	-1.154555	0.045117
H	-8.764639	1.101349	3.192745
H	-9.589328	-0.232940	-0.726355
N	3.715239	-6.796967	-1.612013
C	3.682464	-8.137102	-1.552248
C	4.430124	-6.330596	-0.522855
H	3.206682	-8.785901	-2.271855
C	4.826919	-7.422261	0.193354
H	4.582081	-5.275982	-0.357426
H	5.405723	-7.513698	1.099227
N	3.096350	7.085382	-1.385480
C	3.945607	6.598210	-0.407604
C	2.965692	8.409074	-1.208940
C	4.323269	7.660650	0.360938
H	4.193433	5.550577	-0.346449
H	2.375168	9.069120	-1.825911

H	4.977925	7.730245	1.215737
N	-9.532881	0.634867	1.239186
N	4.346249	-8.537736	-0.465199
N	3.696582	8.779027	-0.154605
C	4.544831	-9.958810	-0.025210
H	3.804693	-10.153136	0.750589
H	4.279317	-10.579507	-0.882169
C	-10.862633	1.330807	1.254757
H	-10.730506	2.271584	0.720942
H	-11.058905	1.580928	2.298321
C	3.829878	10.173598	0.382692
H	3.181006	10.236489	1.255803
H	3.405649	10.831234	-0.377324
C	5.950206	-10.211334	0.446467
C	6.254244	-10.140030	1.825726
C	6.956850	-10.504001	-0.500476
C	5.295395	-9.751025	2.817881
C	7.593414	-10.458763	2.268953
C	8.297109	-10.820751	-0.048586
C	6.705383	-10.495768	-1.910100
C	5.618900	-9.684992	4.148674
H	4.282867	-9.491675	2.524532
C	7.879245	-10.381094	3.670409
C	8.592158	-10.831404	1.335892
C	9.287077	-11.110148	-1.044576
H	5.716722	-10.246992	-2.281862
C	7.686923	-10.781635	-2.821915
C	6.930077	-10.005843	4.584200
H	4.867052	-9.388427	4.874425
H	8.876677	-10.614062	4.021430
C	8.999638	-11.092533	-2.382984
H	10.299862	-11.338500	-0.739820
H	7.462737	-10.769506	-3.884731

H	7.177976	-9.953130	5.639683
H	9.774399	-11.315048	-3.109921
C	-11.951937	0.480685	0.661538
C	-12.603459	-0.473637	1.475943
C	-12.305708	0.631383	-0.698355
C	-12.217197	-0.724916	2.830882
C	-13.703263	-1.235251	0.931916
C	-13.407320	-0.143136	-1.239900
C	-11.607295	1.516059	-1.585428
C	-12.866729	-1.650005	3.606581
H	-11.383075	-0.184093	3.266434
C	-14.351898	-2.188521	1.781370
C	-14.120067	-1.039370	-0.408198
C	-13.728055	0.029876	-2.626898
H	-10.771737	2.104104	-1.218941
C	-11.954187	1.641874	-2.904927
C	-13.951323	-2.394047	3.075408
H	-12.551450	-1.816182	4.632741
H	-15.176630	-2.772206	1.392127
C	-13.031282	0.886653	-3.435742
H	-14.536120	-0.543366	-3.061802
H	-11.403908	2.323073	-3.547638
H	-14.460775	-3.124851	3.695624
H	-13.300327	0.988812	-4.482333
C	5.258361	10.518978	0.702051
C	6.108207	10.974397	-0.330478
C	5.741316	10.370373	2.022872
C	5.678813	11.054792	-1.694158
C	7.466139	11.374065	-0.018767
C	7.096941	10.772504	2.326234
C	4.951244	9.823980	3.087078
C	6.508862	11.498299	-2.689584
H	4.672775	10.750278	-1.963612

C	8.293482	11.828325	-1.098111
C	7.935324	11.302884	1.314917
C	7.565598	10.613858	3.670505
H	3.932274	9.500508	2.898367
C	5.447098	9.685834	4.357976
C	7.838478	11.890030	-2.387844
H	6.150980	11.550273	-3.713898
H	9.315630	12.122537	-0.899696
C	6.774187	10.087274	4.656954
H	8.578318	10.907361	3.916675
H	4.819970	9.270104	5.141440
H	8.493074	12.237639	-3.180856
H	7.158971	9.976583	5.665891
C	9.323237	11.767901	1.697992
H	9.835679	12.301221	0.900344
H	9.279451	12.450862	2.552330
H	9.957957	10.921728	1.988486
C	9.958745	-11.219125	1.856833
H	10.478333	-10.354261	2.287380
H	9.871600	-11.972893	2.645758
H	10.607522	-11.642773	1.093332
C	-15.318070	-1.814290	-0.911614
H	-16.163675	-1.705065	-0.225253
H	-15.666949	-1.485237	-1.888041
H	-15.093959	-2.885575	-0.985316
Br	-1.169118	-0.395591	-2.200936

Table S23. Cartesian coordinates of iPOP-ANT binded with Cl^-.

C	0.313915	1.133714	-1.049838
N	-0.871921	1.106691	-0.422553
C	-1.358367	-0.113126	-0.148180
C	0.440552	-1.135600	-1.088366
N	1.007820	0.039981	-1.397377

N	-0.738982	-1.261077	-0.462025
C	0.889160	2.458605	-1.397334
C	2.087549	2.541811	-2.120017
C	0.227799	3.642711	-1.030002
C	2.605452	3.783309	-2.482970
H	2.598461	1.629870	-2.405411
C	0.748044	4.879849	-1.393232
H	-0.699220	3.578439	-0.472357
C	1.937250	4.961483	-2.131288
H	3.524691	3.832013	-3.061394
H	0.219440	5.787958	-1.113622
C	1.157618	-2.376107	-1.480221
C	2.384649	-2.301818	-2.153903
C	0.603805	-3.637837	-1.204083
C	3.037766	-3.464870	-2.556714
H	2.813797	-1.330081	-2.367629
C	1.256581	-4.796040	-1.610480
H	-0.345519	-3.695594	-0.684598
C	2.476020	-4.720032	-2.298346
H	3.980750	-3.391581	-3.092623
H	0.809535	-5.765343	-1.403500
C	-2.669804	-0.199689	0.544571
C	-3.382107	0.966824	0.870571
C	-3.208699	-1.447308	0.888419
C	-4.600717	0.883736	1.534616
H	-2.964945	1.931252	0.605541
C	-4.430298	-1.526699	1.553905
H	-2.660831	-2.347955	0.637712
C	-5.133713	-0.363893	1.887730
H	-5.136973	1.794679	1.789316
H	-4.829003	-2.500233	1.828265
C	-6.444693	-0.456027	2.634135
H	-6.602352	-1.464307	3.027508

H	-6.471694	0.241968	3.475637
C	3.165197	-5.974559	-2.784408
H	2.473837	-6.615299	-3.339353
H	4.001603	-5.730743	-3.445596
C	2.481676	6.302345	-2.567359
H	1.696658	6.923693	-3.007520
H	3.272131	6.180417	-3.313370
N	-7.609647	-0.124169	1.776845
C	-7.831436	-0.586147	0.491441
C	-8.679418	0.590385	2.158293
C	-9.060473	-0.132982	0.109017
H	-7.098196	-1.181526	-0.028714
H	-8.804937	1.068819	3.117686
H	-9.620887	-0.265054	-0.803385
N	3.699473	-6.799110	-1.673125
C	3.669578	-8.139349	-1.614169
C	4.411716	-6.331780	-0.582648
H	3.196296	-8.788788	-2.334846
C	4.809871	-7.422973	0.133526
H	4.561094	-5.276927	-0.416397
H	5.387539	-7.513646	1.040200
N	3.049514	7.081703	-1.439625
C	3.898405	6.595854	-0.460772
C	2.915666	8.405002	-1.262525
C	4.272578	7.658688	0.308929
H	4.148459	5.548737	-0.399846
H	2.324592	9.064092	-1.879993
H	4.925817	7.729243	1.164734
N	-9.569261	0.601753	1.162730
N	4.332644	-8.539133	-0.526369
N	3.644178	8.775969	-0.206903
C	4.533723	-9.960015	-0.086895
H	3.792873	-10.156422	0.687701

H	4.270848	-10.580808	-0.944597
C	-10.900572	1.294739	1.176733
H	-10.769741	2.236112	0.643648
H	-11.098937	1.543829	2.220148
C	3.773593	10.170525	0.331382
H	3.123297	10.231481	1.203570
H	3.349031	10.827654	-0.428886
C	5.938956	-10.209697	0.386713
C	6.240801	-10.138508	1.766460
C	6.947641	-10.499594	-0.558908
C	5.279630	-9.752193	2.757419
C	7.580017	-10.454529	2.211483
C	8.287931	-10.813635	-0.105220
C	6.698237	-10.491113	-1.968897
C	5.601024	-9.686203	4.088726
H	4.266964	-9.494917	2.462722
C	7.863608	-10.377028	3.613403
C	8.580959	-10.824425	1.279686
C	9.280005	-11.100271	-1.099911
H	5.709577	-10.244313	-2.341977
C	7.681751	-10.774286	-2.879424
C	6.912265	-10.004400	4.526005
H	4.847452	-9.391718	4.813534
H	8.861035	-10.607988	3.965764
C	8.994502	-11.082528	-2.438732
H	10.292843	-11.326555	-0.793790
H	7.459107	-10.762046	-3.942563
H	7.158489	-9.951742	5.581882
H	9.770826	-11.302913	-3.164650
C	-11.987115	0.442548	0.581423
C	-12.637723	-0.513680	1.394324
C	-12.339213	0.593238	-0.778905
C	-12.252904	-0.764877	2.749688

C	-13.735035	-1.277415	0.848241
C	-13.438307	-0.183408	-1.322515
C	-11.641452	1.479965	-1.664443
C	-12.901531	-1.691844	3.523902
H	-11.420625	-0.222458	3.186779
C	-14.382809	-2.232604	1.696196
C	-14.150294	-1.081691	-0.492375
C	-13.757377	-0.010314	-2.709886
H	-10.807740	2.069648	-1.296388
C	-11.986675	1.605765	-2.984381
C	-13.983690	-2.437981	2.990707
H	-12.587398	-1.857909	4.550433
H	-15.205672	-2.817890	1.305404
C	-13.061311	0.848465	-3.517215
H	-14.563529	-0.585094	-3.146308
H	-11.436958	2.288547	-3.625892
H	-14.492437	-3.170265	3.609754
H	-13.329037	0.950626	-4.564143
C	5.200836	10.518884	0.653046
C	6.051193	10.976772	-0.377968
C	5.682170	10.370594	1.974493
C	5.623635	11.056996	-1.742236
C	7.407776	11.379266	-0.064026
C	7.036452	10.775551	2.280085
C	4.891741	9.821846	3.037222
C	6.454167	11.502906	-2.736183
H	4.618671	10.750409	-2.013347
C	8.235702	11.835972	-1.141889
C	7.875149	11.308362	1.270308
C	7.503476	10.617175	3.624956
H	3.873769	9.496227	2.846823
C	5.386024	9.684072	4.308772
C	7.782466	11.897408	-2.432258

H	6.097682	11.554674	-3.760995
H	9.256903	12.132333	-0.941798
C	6.711778	10.088277	4.609937
H	8.515178	10.912778	3.872788
H	4.758662	9.266507	5.091073
H	8.437460	12.246917	-3.224105
H	7.095318	9.977863	5.619377
C	9.261463	11.776232	1.655696
H	9.773899	12.311140	0.859109
H	9.214904	12.458606	2.510356
H	9.897626	10.931300	1.946646
C	9.947632	-11.209418	1.802424
H	10.464668	-10.343652	2.234228
H	9.860992	-11.963828	2.590791
H	10.598471	-11.631193	1.039641
C	-15.345833	-1.858974	-0.997999
H	-16.192690	-1.752013	-0.312826
H	-15.694000	-1.530136	-1.974754
H	-15.119243	-2.929718	-1.071978
Cl	-1.198171	-0.408226	-2.265624

Table S24. Cartesian coordinates of iPOP-ANT binded with NO_3^-.

C	-0.804999	1.383201	-0.985767
N	-1.783702	0.700042	-0.372693
C	-1.497678	-0.572553	-0.058754
C	0.592011	-0.409377	-0.937438
N	0.398664	0.872127	-1.283322
N	-0.325441	-1.169829	-0.321530
C	-1.075568	2.790967	-1.375615
C	-0.115515	3.525155	-2.085967
C	-2.304561	3.395286	-1.061273
C	-0.385237	4.831378	-2.488839
H	0.832359	3.060570	-2.330529

C	-2.569868	4.699256	-1.464230
H	-3.047223	2.827394	-0.513169
C	-1.615980	5.426554	-2.189998
H	0.360551	5.381555	-3.057218
H	-3.529914	5.150473	-1.225523
C	1.899652	-1.028853	-1.273473
C	2.886761	-0.284498	-1.934171
C	2.154131	-2.374226	-0.957033
C	4.098119	-0.877066	-2.284857
H	2.692957	0.753128	-2.178903
C	3.362562	-2.963092	-1.311489
H	1.390643	-2.950387	-0.447581
C	4.342904	-2.221990	-1.986519
H	4.848076	-0.292152	-2.811382
H	3.540489	-4.009080	-1.073812
C	-2.547749	-1.374644	0.620410
C	-3.807274	-0.814792	0.893481
C	-2.291187	-2.698313	1.004162
C	-4.782153	-1.561805	1.544985
H	-4.005142	0.208778	0.597610
C	-3.270670	-3.443958	1.656930
H	-1.320475	-3.131733	0.794295
C	-4.521031	-2.881900	1.938069
H	-5.749311	-1.113215	1.758599
H	-3.052750	-4.464265	1.962694
C	-5.569252	-3.687030	2.671060
H	-5.137280	-4.595655	3.100044
H	-6.015358	-3.109119	3.485346
C	5.638590	-2.871117	-2.416507
H	5.452859	-3.804627	-2.955538
H	6.207879	-2.209872	-3.075944
C	-1.918158	6.827764	-2.669335
H	-2.902879	6.880185	-3.142248

H	-1.175749	7.160407	-3.400359
N	-6.688143	-4.098849	1.787498
C	-6.566747	-4.635275	0.517700
C	-7.985842	-4.112628	2.128511
C	-7.822353	-4.972690	0.103280
H	-5.608986	-4.718726	0.029431
H	-8.391635	-3.768396	3.067619
H	-8.178747	-5.422288	-0.810410
N	6.511757	-3.217382	-1.268479
C	7.248228	-4.333787	-1.159592
C	6.796421	-2.401653	-0.187562
H	7.251856	-5.154087	-1.861187
C	7.722025	-3.053901	0.573992
H	6.313441	-1.446183	-0.059213
H	8.219568	-2.777551	1.490541
N	-1.930925	7.818348	-1.564706
C	-0.987891	7.926438	-0.557819
C	-2.799746	8.833128	-1.439122
C	-1.309808	9.030946	0.176001
H	-0.188334	7.210388	-0.454497
H	-3.641003	9.022871	-2.088211
H	-0.840345	9.481580	1.036601
N	-8.691906	-4.634159	1.122243
N	7.986159	-4.258333	-0.049385
N	-2.445760	9.578155	-0.389209
C	8.946267	-5.300272	0.445623
H	8.424913	-5.865417	1.217784
H	9.110786	-5.980379	-0.391352
C	-10.180584	-4.823464	1.093658
H	-10.592094	-3.988406	0.527251
H	-10.518334	-4.707118	2.124433
C	-3.150272	10.810104	0.097872
H	-3.746813	10.510271	0.959006

H	-3.849097	11.089746	-0.691763
C	10.227920	-4.693136	0.945701
C	10.391760	-4.429800	2.325444
C	11.251545	-4.378816	0.024245
C	9.350854	-4.636770	3.289171
C	11.657841	-3.915458	2.798632
C	12.517105	-3.862030	0.506031
C	11.086394	-4.547548	-1.388056
C	9.535247	-4.367714	4.620949
H	8.381745	-5.009661	2.972456
C	11.802390	-3.656814	4.200067
C	12.720204	-3.670927	1.893899
C	13.526778	-3.555666	-0.464785
H	10.145448	-4.917225	-1.782401
C	12.084402	-4.241216	-2.275011
C	10.779827	-3.871289	5.086134
H	8.725587	-4.538114	5.324763
H	12.742176	-3.269623	4.573223
C	13.324448	-3.735672	-1.806771
H	14.478027	-3.156951	-0.137817
H	11.928130	-4.383356	-3.340544
H	10.918759	-3.662579	6.142266
H	14.110656	-3.491470	-2.514196
C	-10.569347	-6.156845	0.517328
C	-10.585263	-7.293702	1.357430
C	-10.901387	-6.266127	-0.851971
C	-10.168973	-7.248436	2.725952
C	-11.034782	-8.559399	0.826831
C	-11.345099	-7.543386	-1.379637
C	-10.804873	-5.161206	-1.761457
C	-10.198693	-8.361051	3.526323
H	-9.807773	-6.318164	3.152665
C	-11.050069	-9.692954	1.701956

C	-11.444970	-8.667225	-0.525248
C	-11.661902	-7.616086	-2.776389
H	-10.467217	-4.192940	-1.405484
C	-11.118374	-5.286051	-3.089378
C	-10.646187	-9.603352	3.008129
H	-9.878539	-8.293977	4.562192
H	-11.380596	-10.651964	1.323233
C	-11.553345	-6.533224	-3.606698
H	-11.983237	-8.558030	-3.200894
H	-11.035115	-4.427209	-3.749206
H	-10.666899	-10.480034	3.647880
H	-11.798352	-6.626820	-4.659971
C	-2.186153	11.917354	0.423932
C	-1.715564	12.753575	-0.612910
C	-1.748073	12.101343	1.755896
C	-2.069365	12.543312	-1.984435
C	-0.840068	13.864829	-0.297477
C	-0.875605	13.213111	2.062864
C	-2.118709	11.225408	2.828586
C	-1.609418	13.359278	-2.984035
H	-2.711927	11.712260	-2.256305
C	-0.385755	14.686180	-1.381365
C	-0.457915	14.104727	1.044283
C	-0.444281	13.381217	3.418435
H	-2.763677	10.373230	2.637919
C	-1.674398	11.424229	4.110458
C	-0.752293	14.447608	-2.678663
H	-1.899361	13.174229	-4.014419
H	0.278214	15.516399	-1.179875
C	-0.824800	12.519013	4.412676
H	0.210806	14.206536	3.667540
H	-1.976869	10.742309	4.900038
H	-0.388080	15.089154	-3.474881

H	-0.478760	12.670948	5.430240
C	0.402535	15.288321	1.429019
H	0.544242	16.000774	0.619328
H	-0.051165	15.842567	2.256797
H	1.396947	14.963873	1.759389
C	14.045646	-3.195735	2.447673
H	13.963960	-2.179695	2.853039
H	14.378967	-3.845975	3.262688
H	14.844560	-3.189339	1.709420
C	-11.968758	-9.999074	-1.016131
H	-12.747062	-10.377603	-0.346036
H	-12.411103	-9.950673	-2.008801
H	-11.170764	-10.751111	-1.047012
N	8.569321	-6.502014	-3.262698
O	7.309415	-6.604259	-3.300011
O	9.111889	-5.359799	-3.275819
O	9.286825	-7.542161	-3.215631

Table S25. Cartesian coordinates of iPOP-ANT binded with $Cr_2O_7^{2-}$.

C	2.358154	-0.863593	-0.824366
N	2.809776	0.244215	-0.216728
C	1.873126	1.135436	0.141430
C	0.200654	-0.160781	-0.688133
N	1.064329	-1.110943	-1.076111
N	0.558437	0.976757	-0.073846
C	3.354734	-1.874711	-1.261930
C	2.943446	-3.013393	-1.968738
C	4.722300	-1.690609	-0.996779
C	3.882064	-3.940718	-2.416329
H	1.889456	-3.156607	-2.175403
C	5.655999	-2.618538	-1.444276
H	5.040433	-0.809793	-0.451417
C	5.245387	-3.747907	-2.166444

H	3.550678	-4.808404	-2.981354
H	6.712377	-2.457376	-1.243381
C	-1.241339	-0.376132	-0.972515
C	-1.667493	-1.538878	-1.629314
C	-2.192459	0.593025	-0.610535
C	-3.015245	-1.722482	-1.931575
H	-0.936004	-2.287718	-1.909105
C	-3.535858	0.408029	-0.916746
H	-1.863148	1.492735	-0.104085
C	-3.958762	-0.748091	-1.587944
H	-3.329095	-2.621701	-2.455686
H	-4.259136	1.172755	-0.644165
C	2.319839	2.381082	0.816764
C	3.686286	2.619530	1.041196
C	1.381650	3.330420	1.245424
C	4.100480	3.777723	1.689197
H	4.411368	1.885121	0.710612
C	1.800469	4.490045	1.894531
H	0.327469	3.148254	1.073099
C	3.160862	4.721454	2.127194
H	5.160340	3.945293	1.864914
H	1.060975	5.210428	2.235416
C	3.606360	5.968047	2.856451
H	2.756633	6.474845	3.322654
H	4.329458	5.730815	3.641882
C	-5.410951	-0.931247	-1.965647
H	-5.799233	-0.048424	-2.481738
H	-5.537463	-1.791257	-2.629401
C	6.261131	-4.735009	-2.694044
H	7.088325	-4.222517	-3.193215
H	5.804829	-5.418939	-3.415324
N	4.269744	6.944392	1.957081
C	3.821722	7.333547	0.706996

C	5.349636	7.678835	2.265186
C	4.657511	8.320104	0.270760
H	2.963507	6.871421	0.245927
H	5.913370	7.611418	3.183198
H	4.667102	8.901226	-0.638190
N	-6.284751	-1.144537	-0.786127
C	-7.514841	-0.632841	-0.625955
C	-6.023967	-1.990540	0.277404
H	-8.002754	0.051798	-1.302972
C	-7.126750	-1.975804	1.081013
H	-5.084925	-2.513146	0.365447
H	-7.350004	-2.492416	2.001475
N	6.866915	-5.559637	-1.619502
C	6.183989	-6.187103	-0.592509
C	8.158586	-5.915374	-1.545781
C	7.095634	-6.929383	0.100301
H	5.125280	-6.042394	-0.447984
H	8.937135	-5.595219	-2.221353
H	6.990984	-7.574128	0.959051
N	5.605159	8.516217	1.256922
N	-8.042266	-1.119483	0.500010
N	8.321266	-6.741291	-0.509402
C	-9.401487	-0.798516	1.049534
H	-9.256725	-0.046088	1.824342
H	-9.949347	-0.318755	0.237242
C	6.731251	9.506680	1.195968
H	7.517752	9.050753	0.595116
H	7.114650	9.589085	2.213968
C	9.611807	-7.372545	-0.076613
H	9.970511	-6.798748	0.777437
H	10.317383	-7.205211	-0.891623
C	-10.104840	-2.023992	1.564149
C	-10.041632	-2.347631	2.939337

C	-10.811437	-2.848264	0.660278
C	-9.259119	-1.603055	3.881871
C	-10.784976	-3.487235	3.429396
C	-11.552662	-3.989687	1.158843
C	-10.821886	-2.601955	-0.750241
C	-9.211533	-1.942461	5.209488
H	-8.676798	-0.748449	3.551601
C	-10.707601	-3.796402	4.825905
C	-11.562051	-4.275531	2.545260
C	-12.254000	-4.799065	0.205526
H	-10.264002	-1.765005	-1.157460
C	-11.510440	-3.405611	-1.620056
C	-9.947386	-3.055104	5.691525
H	-8.609838	-1.355045	5.897127
H	-11.255527	-4.647004	5.211410
C	-12.237326	-4.523302	-1.135348
H	-12.806707	-5.665173	0.544833
H	-11.500387	-3.189758	-2.684618
H	-9.906209	-3.316317	6.744306
H	-12.778467	-5.158704	-1.829348
C	6.286164	10.834855	0.649113
C	5.695195	11.777387	1.521384
C	6.448791	11.124896	-0.724422
C	5.426967	11.493236	2.898159
C	5.339986	13.083034	1.016702
C	6.082418	12.436843	-1.225688
C	6.952551	10.164398	-1.663039
C	4.859497	12.423805	3.729669
H	5.663901	10.515990	3.306581
C	4.751655	14.022131	1.923888
C	5.568798	13.415444	-0.341661
C	6.251850	12.688317	-2.627337
H	7.227577	9.169554	-1.327013

C	7.092671	10.456546	-2.994301
C	4.516157	13.708809	3.236750
H	4.670628	12.178707	4.770955
H	4.475046	15.005542	1.565041
C	6.736266	11.738568	-3.485885
H	5.975455	13.652897	-3.032196
H	7.479176	9.704881	-3.676597
H	4.067119	14.440444	3.901098
H	6.847415	11.963749	-4.541874
C	9.444548	-8.832930	0.241420
C	9.483478	-9.778917	-0.807081
C	9.234463	-9.243859	1.578168
C	9.607587	-9.393001	-2.180446
C	9.391463	-11.192905	-0.502041
C	9.144926	-10.656493	1.874656
C	9.091886	-8.321274	2.666195
C	9.645401	-10.316619	-3.191412
H	9.664966	-8.342008	-2.444206
C	9.433796	-12.116992	-1.597533
C	9.259325	-11.618950	0.841438
C	8.932442	-11.050716	3.235285
H	9.142489	-7.252238	2.484133
C	8.883057	-8.747481	3.952614
C	9.555408	-11.701229	-2.896225
H	9.743494	-9.990735	-4.223003
H	9.355585	-13.178577	-1.403530
C	8.802788	-10.133194	4.244270
H	8.860629	-12.103743	3.476784
H	8.781891	-8.020994	4.753814
H	9.582614	-12.428759	-3.701305
H	8.639239	-10.462914	5.265446
C	9.222813	-13.085145	1.213232
H	9.473449	-13.746740	0.386950

H	9.939474	-13.298653	2.012643
H	8.230162	-13.376246	1.578159
C	-12.373432	-5.416726	3.118500
H	-11.722524	-6.216911	3.491805
H	-12.982530	-5.072642	3.960384
H	-13.059210	-5.861892	2.400964
C	5.239605	14.817081	-0.806617
H	5.697700	15.559733	-0.145794
H	5.595859	15.034467	-1.811222
H	4.157042	14.993819	-0.795183
Cr	-10.422516	1.201082	-1.426317
O	-11.659877	2.142883	-1.846415
O	-10.017484	1.469312	0.103533
O	-10.809418	-0.343556	-1.628495
O	-9.057007	1.619891	-2.489989
Cr	-7.358073	1.306893	-2.922748
O	-7.000407	2.261788	-4.169886
O	-6.411354	1.651530	-1.672758
O	-7.180748	-0.233839	-3.336714

Table S26. Cartesian coordinates of iPOP-ANT binded with MnO_4^-.

C	0.396108	1.145582	-0.870490
N	-0.786687	1.123087	-0.237313
C	-1.275766	-0.094847	0.040718
C	0.515109	-1.124174	-0.907315
N	1.084691	0.049224	-1.220338
N	-0.661712	-1.245144	-0.275011
C	0.973966	2.468224	-1.222190
C	2.169026	2.546762	-1.950884
C	0.318321	3.654866	-0.852803
C	2.689192	3.786185	-2.317671
H	2.675523	1.632860	-2.237868
C	0.840814	4.889921	-1.219874

H	-0.606130	3.594203	-0.290508
C	2.026609	4.966903	-1.963894
H	3.605709	3.831285	-2.900691
H	0.316584	5.800044	-0.938582
C	1.226152	-2.367426	-1.301443
C	2.450066	-2.297848	-1.981269
C	0.669578	-3.627050	-1.021271
C	3.097361	-3.463445	-2.386116
H	2.881334	-1.327742	-2.198116
C	1.316530	-4.787801	-1.429707
H	-0.277343	-3.681163	-0.497032
C	2.532788	-4.716494	-2.123681
H	4.037913	-3.393795	-2.926764
H	0.867339	-5.755420	-1.219521
C	-2.584030	-0.176403	0.740044
C	-3.290879	0.992773	1.068371
C	-3.125304	-1.421896	1.087837
C	-4.506450	0.914359	1.738528
H	-2.871874	1.955558	0.800288
C	-4.343843	-1.496602	1.759446
H	-2.581642	-2.324591	0.835345
C	-5.041778	-0.331155	2.095557
H	-5.038446	1.827315	1.994945
H	-4.744375	-2.468543	2.036776
C	-6.349338	-0.418228	2.848540
H	-6.508352	-1.425587	3.243723
H	-6.369878	0.280702	3.689448
C	3.215429	-5.973768	-2.611863
H	2.519230	-6.612793	-3.162720
H	4.049344	-5.733369	-3.277435
C	2.573263	6.305528	-2.404032
H	1.788114	6.929006	-2.840937
H	3.359607	6.180251	-3.153823

N	-7.517431	-0.083412	1.996689
C	-7.747101	-0.545956	0.712874
C	-8.582950	0.635038	2.382697
C	-8.976526	-0.089143	0.336077
H	-7.018405	-1.144265	0.189706
H	-8.702142	1.114850	3.342208
H	-9.541885	-0.220295	-0.573403
N	3.752499	-6.798947	-1.502394
C	3.718500	-8.139020	-1.441915
C	4.471667	-6.332858	-0.415938
H	3.239526	-8.787628	-2.159572
C	4.869785	-7.424629	0.299376
H	4.625326	-5.278334	-0.251511
H	5.451638	-7.516283	1.203270
N	3.149236	7.084155	-1.279924
C	4.001369	6.596510	-0.304789
C	3.020607	8.408064	-1.103522
C	4.382836	7.658885	0.461959
H	4.248286	5.548639	-0.244028
H	2.428646	9.068469	-1.718731
H	5.040536	7.728159	1.314444
N	-9.477673	0.648323	1.391542
N	4.385635	-8.539881	-0.357003
N	3.755555	8.777703	-0.051901
C	4.584228	-9.960971	0.082929
H	3.846586	-10.154161	0.861385
H	4.315071	-10.581764	-0.772823
C	-10.806619	1.345693	1.411426
H	-10.675345	2.286091	0.876734
H	-10.998992	1.596487	2.455555
C	3.892209	10.172369	0.484304
H	3.246446	10.236342	1.359639
H	3.466042	10.830121	-0.274526

C	5.990965	-10.214789	0.549828
C	6.299875	-10.143199	1.927989
C	6.993995	-10.508954	-0.400480
C	5.344899	-9.752727	2.923299
C	7.640237	-10.463168	2.366698
C	8.335479	-10.826937	0.046888
C	6.737635	-10.501078	-1.809223
C	5.673102	-9.686450	4.252929
H	4.331635	-9.492425	2.633357
C	7.931024	-10.385183	3.767117
C	8.635330	-10.837291	1.430336
C	9.321666	-11.117835	-0.952410
H	5.747953	-10.251408	-2.177656
C	7.715691	-10.788399	-2.724319
C	6.985443	-10.008510	4.684036
H	4.924101	-9.388759	4.981158
H	8.929422	-10.619062	4.114771
C	9.029592	-11.100507	-2.289817
H	10.335261	-11.347136	-0.651076
H	7.487822	-10.776502	-3.786355
H	7.237068	-9.955594	5.738626
H	9.801581	-11.324173	-3.019345
C	-11.898888	0.496474	0.822380
C	-12.548592	-0.456789	1.639474
C	-12.257226	0.646946	-0.536341
C	-12.157887	-0.707880	2.993173
C	-13.651095	-1.217468	1.099616
C	-13.361543	-0.126634	-1.073705
C	-11.560958	1.530481	-1.426234
C	-12.805705	-1.631929	3.771541
H	-11.321678	-0.167757	3.425580
C	-14.297789	-2.169666	1.951748
C	-14.072349	-1.021735	-0.239127

C	-13.686915	0.046106	-2.459655
H	-10.723503	2.117794	-1.062918
C	-11.912303	1.656082	-2.744575
C	-13.892935	-2.375046	3.244477
H	-12.487036	-1.797988	4.796673
H	-15.124493	-2.752640	1.565637
C	-12.992045	0.901777	-3.271302
H	-14.497100	-0.526464	-2.891490
H	-11.363537	2.336405	-3.389501
H	-14.401007	-3.105029	3.866788
H	-13.264620	1.003760	-4.316996
C	5.322163	10.516363	0.798538
C	6.168898	10.970414	-0.237144
C	5.809551	10.367827	2.117737
C	5.734849	11.050663	-1.599359
C	7.528333	11.368766	0.069663
C	7.166652	10.768642	2.416202
C	5.022603	9.822752	3.184930
C	6.561904	11.492839	-2.597864
H	4.727555	10.747106	-1.865175
C	8.352400	11.821661	-1.012756
C	8.002078	11.297675	1.401738
C	7.639813	10.610091	3.758906
H	4.002637	9.500287	2.999909
C	5.522727	9.684640	4.454157
C	7.892979	11.883282	-2.300926
H	6.200516	11.544742	-3.620951
H	9.375547	12.114868	-0.818029
C	6.851276	10.084792	4.748337
H	8.653696	10.902619	4.001421
H	4.897884	9.269929	5.239984
H	8.545183	12.229837	-3.096365
H	7.239449	9.974138	5.755979

C	9.391811	11.761378	1.779775
H	9.902045	12.293795	0.980111
H	9.351727	12.444764	2.633954
H	10.026634	10.914654	2.068438
C	10.003306	-11.226243	1.946694
H	10.525313	-10.361744	2.375043
H	9.918101	-11.979567	2.736254
H	10.648970	-11.650923	1.181130
C	-15.272923	-1.795597	-0.738026
H	-16.116018	-1.685162	-0.048778
H	-15.624845	-1.466603	-1.713382
H	-15.050215	-2.867154	-0.812028
Mn	-1.263984	-0.271939	-2.638067
O	-2.440656	-0.365670	-1.565121
O	-0.232688	-1.465757	-2.401881
O	-1.874687	-0.379785	-4.107750
O	-0.507906	1.123455	-2.477516

Table S27. Cartesian coordinates of iPOP-ANT binded with methyl orange.

C	4.026504	-0.276125	-0.759913
N	4.211309	0.904927	-0.150497
C	3.119907	1.449443	0.408260
C	1.811750	-0.289375	-0.248056
N	2.847865	-0.912153	-0.829334
N	1.900603	0.890290	0.384277
C	5.197608	-0.914016	-1.414591
C	5.043561	-2.109698	-2.130095
C	6.466977	-0.315135	-1.347654
C	6.132989	-2.686055	-2.779890
H	4.065274	-2.572470	-2.184058
C	7.551996	-0.893612	-1.996652
H	6.585895	0.609796	-0.795542
C	7.393171	-2.079931	-2.726738

H	5.994354	-3.602287	-3.348438
H	8.526058	-0.412937	-1.947461
C	0.479008	-0.940903	-0.324882
C	0.326729	-2.165108	-0.990543
C	-0.649210	-0.327033	0.245392
C	-0.930399	-2.756542	-1.097037
H	1.195254	-2.640498	-1.430758
C	-1.902490	-0.918342	0.134244
H	-0.532086	0.620130	0.758791
C	-2.056151	-2.134945	-0.545634
H	-1.036125	-3.698026	-1.630159
H	-2.769390	-0.425148	0.567236
C	3.269127	2.758416	1.094980
C	4.514009	3.409355	1.125817
C	2.170201	3.356186	1.727615
C	4.655010	4.625660	1.784297
H	5.363652	2.946678	0.637530
C	2.315283	4.575279	2.386585
H	1.209392	2.855685	1.704760
C	3.558019	5.217469	2.425953
H	5.626181	5.114020	1.808594
H	1.458147	5.019907	2.886216
C	3.714785	6.525868	3.166085
H	2.840672	6.730607	3.790773
H	4.595922	6.511888	3.813737
C	-3.423851	-2.757227	-0.710618
H	-4.144273	-2.030759	-1.097565
H	-3.389268	-3.599830	-1.407047
C	8.559887	-2.687184	-3.471375
H	9.094937	-1.930837	-4.052520
H	8.221843	-3.465066	-4.161913
N	3.887509	7.679154	2.248320
C	3.140257	7.933136	1.111665

C	4.725718	8.709194	2.440480
C	3.548516	9.140885	0.625037
H	2.400864	7.234294	0.754462
H	5.427514	8.803665	3.255125
H	3.228072	9.713892	-0.231095
N	-3.981055	-3.257987	0.569636
C	-5.264079	-3.161861	0.950709
C	-3.300288	-4.000631	1.518248
H	-6.043908	-2.651541	0.406115
C	-4.204562	-4.349257	2.478917
H	-2.245372	-4.203545	1.425277
H	-4.102220	-4.928369	3.383425
N	9.559263	-3.301410	-2.562750
C	9.282521	-4.132266	-1.491345
C	10.891125	-3.234897	-2.711476
C	10.479765	-4.564540	-0.999607
H	8.270006	-4.330339	-1.177859
H	11.410183	-2.672819	-3.472845
H	10.722269	-5.226777	-0.183068
N	4.540672	9.604688	1.467370
N	-5.421783	-3.812216	2.106114
N	11.469271	-3.988737	-1.773309
C	-6.702554	-3.945566	2.877037
H	-6.668570	-3.201593	3.672513
H	-7.498277	-3.645800	2.193586
C	5.282268	10.899720	1.306925
H	6.059119	10.726136	0.562715
H	5.785771	11.077740	2.258189
C	12.944299	-4.191364	-1.587510
H	13.246735	-3.551359	-0.759115
H	13.418604	-3.794437	-2.486154
C	-6.900410	-5.340087	3.403811
C	-6.513062	-5.655270	4.726876

C	-7.460399	-6.326091	2.561258
C	-5.851060	-4.721853	5.590342
C	-6.778808	-6.980345	5.241628
C	-7.722186	-7.652399	3.083946
C	-7.780477	-6.067022	1.189845
C	-5.481438	-5.055946	6.867757
H	-5.622261	-3.721101	5.237251
C	-6.379071	-7.277776	6.584594
C	-7.412593	-7.954736	4.431793
C	-8.290043	-8.621614	2.192911
H	-7.581976	-5.089146	0.763345
C	-8.324207	-7.028481	0.379597
C	-5.749763	-6.352915	7.375385
H	-4.983147	-4.323331	7.496185
H	-6.567668	-8.265044	6.987202
C	-8.582137	-8.327480	0.888138
H	-8.486057	-9.624165	2.549596
H	-8.558151	-6.798886	-0.656039
H	-5.455864	-6.609238	8.388400
H	-9.010027	-9.086497	0.240829
C	4.366970	12.031692	0.930003
C	3.669382	12.723069	1.946780
C	4.201847	12.385878	-0.428106
C	3.734270	12.341242	3.324530
C	2.852240	13.861030	1.596186
C	3.372881	13.526244	-0.773188
C	4.812168	11.651402	-1.498332
C	3.055587	13.029470	4.296704
H	4.323872	11.479797	3.621578
C	2.163989	14.549268	2.646739
C	2.738684	14.275912	0.246009
C	3.221279	13.846530	-2.162793
H	5.430814	10.786683	-1.279692

C	4.632342	11.999664	-2.811199
C	2.257855	14.151326	3.954434
H	3.127036	12.716427	5.334452
H	1.543565	15.403100	2.405025
C	3.823503	13.114560	-3.150382
H	2.599170	14.683486	-2.451241
H	5.111422	11.421395	-3.596057
H	1.723324	14.691307	4.729663
H	3.682874	13.384586	-4.192247
C	13.288153	-5.636510	-1.352644
C	13.440102	-6.500974	-2.459611
C	13.439734	-6.119602	-0.032213
C	13.209519	-6.067885	-3.804874
C	13.838089	-7.878186	-2.245670
C	13.838205	-7.494578	0.173018
C	13.204400	-5.310703	1.127785
C	13.359813	-6.912226	-4.873074
H	12.897217	-5.046936	-3.998725
C	13.978693	-8.719842	-3.397919
C	14.068475	-8.351282	-0.931511
C	13.986389	-7.963049	1.518547
H	12.893814	-4.276410	1.016789
C	13.353464	-5.806884	2.397321
C	13.749049	-8.260719	-4.667060
H	13.180139	-6.551209	-5.881729
H	14.263108	-9.755975	-3.270429
C	13.751564	-7.153297	2.598299
H	14.282084	-8.990011	1.692498
H	13.169311	-5.165306	3.254295
H	13.863561	-8.926436	-5.516708
H	13.869336	-7.538302	3.606350
C	14.545594	-9.761968	-0.663905
H	14.845761	-10.294501	-1.563670

H	15.415753	-9.755734	0.000197
H	13.765269	-10.357420	-0.174216
C	-7.727768	-9.304373	5.038763
H	-6.810316	-9.867029	5.250971
H	-8.263954	-9.186113	5.985696
H	-8.353444	-9.927770	4.403759
C	1.923112	15.512352	-0.062532
H	2.234773	16.347759	0.572317
H	2.023135	15.850918	-1.091499
H	0.856270	15.339885	0.125650
C	-17.147378	-0.116406	-3.199505
C	-15.922856	-0.584232	-2.724790
C	-14.753621	0.170172	-2.860631
C	-14.843703	1.434034	-3.477266
C	-16.059706	1.907680	-3.937196
C	-17.243012	1.142062	-3.818646
H	-18.022445	-0.747889	-3.094769
H	-15.849801	-1.557818	-2.248375
H	-13.941696	2.029468	-3.567321
H	-16.109606	2.902382	-4.371112
N	-13.570257	-0.410212	-2.350667
N	-12.530662	0.294886	-2.518929
C	-11.334002	-0.248513	-2.021297
C	-10.186449	0.538877	-2.219659
C	-11.216116	-1.493621	-1.367373
C	-8.944301	0.101930	-1.771997
H	-10.302674	1.489375	-2.734246
C	-9.975161	-1.922603	-0.924002
H	-12.106948	-2.097291	-1.229032
C	-8.832942	-1.127677	-1.116892
H	-8.043492	0.685668	-1.930952
H	-9.853120	-2.885437	-0.437665
S	-7.223982	-1.679214	-0.461099

O	-6.230322	-0.983763	-1.321256
O	-7.258607	-1.209604	0.949938
N	-18.471871	1.676036	-4.274433
C	-19.681781	0.949259	-3.935817
H	-20.548707	1.570021	-4.187212
H	-19.786119	-0.011095	-4.474988
H	-19.709843	0.746386	-2.861337
C	-18.503496	2.191312	-5.639934
H	-19.383943	2.831717	-5.767469
H	-17.618287	2.792030	-5.851092
H	-18.552458	1.382508	-6.391908
O	-7.271074	-3.157027	-0.620486

Table S28. Cartesian coordinates of iPOP-ANT binded with congo red.

C	0.230016	1.714325	-0.703780
N	-0.755754	1.047245	-0.099963
C	-0.427220	-0.139162	0.432176
C	1.758405	0.144721	-0.131034
N	1.505951	1.315549	-0.748758
N	0.820426	-0.627693	0.445324
C	-0.169407	2.951716	-1.423865
C	0.776357	3.788344	-2.028646
C	-1.534538	3.272627	-1.521112
C	0.363506	4.932789	-2.710866
H	1.828949	3.537674	-1.952453
C	-1.941787	4.403077	-2.214619
H	-2.262929	2.624974	-1.048528
C	-0.996681	5.244346	-2.812693
H	1.106118	5.579973	-3.171851
H	-3.003766	4.631006	-2.270748
C	3.160569	-0.321484	-0.075616
C	4.123459	0.234081	-0.929779
C	3.541662	-1.331247	0.823709

C	5.435353	-0.228643	-0.898149
H	3.826813	1.000736	-1.635584
C	4.859068	-1.773047	0.864910
H	2.793199	-1.763382	1.478268
C	5.816914	-1.237882	-0.006181
H	6.164089	0.168909	-1.598862
H	5.145232	-2.558227	1.560295
C	-1.534893	-0.952202	0.980272
C	-2.791241	-0.359125	1.194249
C	-1.356242	-2.311523	1.268389
C	-3.841555	-1.097490	1.724177
H	-2.939431	0.686154	0.955733
C	-2.417970	-3.058972	1.774086
H	-0.389934	-2.769016	1.086103
C	-3.656676	-2.453079	2.015103
H	-4.798699	-0.605463	1.890971
H	-2.274649	-4.113471	1.998855
C	-4.776932	-3.226886	2.663658
H	-4.454955	-4.232871	2.952079
H	-5.113543	-2.720697	3.572639
C	7.228041	-1.767555	-0.037243
H	7.265528	-2.857439	-0.089562
H	7.750365	-1.394995	-0.920330
C	-1.442625	6.468816	-3.582363
H	-1.933278	6.209623	-4.526040
H	-0.598126	7.120992	-3.820516
N	-5.978304	-3.380143	1.819435
C	-6.082817	-4.090248	0.631345
C	-7.186496	-2.894674	2.131371
C	-7.392432	-4.037511	0.255767
H	-5.223094	-4.535775	0.157499
H	-7.402347	-2.229186	2.948188
H	-7.905368	-4.451013	-0.597652

N	8.031524	-1.369997	1.138434
C	9.100850	-2.060100	1.556292
C	8.018747	-0.134632	1.768951
H	9.389676	-3.031429	1.155932
C	9.100522	-0.104260	2.595917
H	7.247457	0.592221	1.573154
H	9.468884	0.656732	3.263260
N	-2.418001	7.267353	-2.811118
C	-2.109728	8.081795	-1.735952
C	-3.753474	7.179117	-2.901728
C	-3.288545	8.497316	-1.193115
H	-1.088333	8.281800	-1.453087
H	-4.295100	6.603855	-3.636695
H	-3.506042	9.135565	-0.351221
N	-8.060330	-3.282986	1.204275
N	9.759877	-1.314121	2.447629
N	-4.301004	7.915413	-1.931647
C	11.068152	-1.706575	3.041075
H	10.866917	-2.463296	3.801161
H	11.616547	-2.191199	2.232141
C	-9.527385	-3.056031	1.271804
H	-9.815063	-2.575026	0.341490
H	-9.676076	-2.298634	2.038308
C	-5.765359	8.084240	-1.664908
H	-6.275273	7.324596	-2.259190
H	-6.046376	9.055013	-2.072885
C	11.819160	-0.535179	3.629795
C	11.623381	-0.198341	4.986499
C	12.689362	0.234809	2.823662
C	10.653684	-0.862062	5.806920
C	12.402562	0.865518	5.580017
C	13.462529	1.307517	3.421968
C	12.824591	-0.004342	1.416730

C	10.464718	-0.520818	7.120158
H	10.032449	-1.640710	5.377078
C	12.174949	1.178451	6.959698
C	13.347187	1.577946	4.804992
C	14.319979	2.070911	2.561920
H	12.252407	-0.784965	0.930482
C	13.656834	0.759696	0.642228
C	11.239971	0.513136	7.708212
H	9.716795	-1.039808	7.713346
H	12.742938	1.976731	7.422324
C	14.414102	1.811851	1.221096
H	14.895047	2.891293	2.973145
H	13.727610	0.556400	-0.422968
H	11.085141	0.779244	8.749933
H	15.069014	2.414883	0.597850
C	-10.247618	-4.358359	1.544305
C	-10.195008	-4.919231	2.839790
C	-10.901343	-5.047691	0.501464
C	-9.613232	-4.226422	3.950437
C	-10.737613	-6.237783	3.073810
C	-11.469959	-6.362949	0.744606
C	-11.045614	-4.485467	-0.807642
C	-9.545388	-4.787721	5.198704
H	-9.250301	-3.214051	3.820815
C	-10.634798	-6.786511	4.393184
C	-11.349774	-6.959659	2.020735
C	-12.135195	-7.013430	-0.349067
H	-10.635663	-3.509189	-1.025757
C	-11.720398	-5.133236	-1.804292
C	-10.054508	-6.092988	5.422698
H	-9.113932	-4.226779	6.023153
H	-11.036318	-7.772898	4.590266
C	-12.258005	-6.427919	-1.580195

H	-12.572832	-7.992007	-0.200276
H	-11.808321	-4.651029	-2.772705
H	-9.996898	-6.533827	6.413560
H	-12.779680	-6.945829	-2.379720
C	-6.071582	7.960619	-0.199908
C	-6.132337	9.122471	0.601443
C	-6.260172	6.676432	0.361779
C	-5.851028	10.431202	0.087711
C	-6.470395	9.002247	2.006189
C	-6.604805	6.566819	1.761484
C	-6.139043	5.466021	-0.397629
C	-5.893337	11.547650	0.881071
H	-5.582329	10.557610	-0.956786
C	-6.502987	10.202755	2.789264
C	-6.741343	7.727055	2.559944
C	-6.804699	5.257186	2.306545
H	-5.880884	5.511636	-1.451313
C	-6.359717	4.235273	0.164922
C	-6.223810	11.432695	2.255434
H	-5.671700	12.522716	0.456389
H	-6.736714	10.142760	3.844230
C	-6.691982	4.128380	1.540634
H	-7.061404	5.153974	3.353978
H	-6.305656	3.321568	-0.417469
H	-6.251693	12.318884	2.882120
H	-6.866736	3.139846	1.944760
C	-7.169898	7.559994	4.002261
H	-7.435907	8.498023	4.485857
H	-8.049261	6.912016	4.069206
H	-6.376804	7.092770	4.599416
C	14.198459	2.633509	5.479127
H	13.615924	3.535007	5.710137
H	14.607144	2.260437	6.423403

H	15.050142	2.938789	4.872767
C	-11.859540	-8.356556	2.308809
H	-12.684111	-8.335237	3.031882
H	-12.218403	-8.878360	1.424209
H	-11.066940	-8.977915	2.740216
C	-10.659228	-1.085019	-2.161407
C	-9.669229	-0.587556	-1.335471
C	-8.308418	-0.965670	-1.502661
C	-7.990286	-1.906059	-2.541649
C	-9.036413	-2.412071	-3.353612
C	-10.341230	-1.999644	-3.186370
H	-11.687717	-0.763965	-2.023626
H	-9.915641	0.134958	-0.567207
C	-7.242143	-0.428812	-0.698493
C	-6.620458	-2.281457	-2.774151
H	-8.819552	-3.140969	-4.128757
H	-11.112443	-2.377980	-3.850281
C	-5.613541	-1.616339	-2.059842
C	-5.943746	-0.712298	-1.019227
H	-5.135668	-0.259093	-0.462986
N	-6.287321	-3.273775	-3.671420
H	-6.876587	-3.396640	-4.482310
H	-5.295339	-3.315670	-3.874689
N	-4.299728	-1.914321	-2.439567
N	-3.437014	-1.042470	-2.125888
C	-2.111521	-1.388164	-2.450931
C	-1.598993	-2.693643	-2.377799
C	-1.257348	-0.335345	-2.802552
C	-0.252484	-2.924003	-2.623943
H	-2.265974	-3.504262	-2.102830
C	0.081489	-0.575982	-3.077476
H	-1.662675	0.669740	-2.838747
C	0.620014	-1.871665	-2.968725

H	0.135779	-3.936364	-2.560957
H	0.735820	0.257459	-3.314413
S	-7.555090	0.587452	0.779452
O	-8.335240	1.756930	0.314121
O	-8.319503	-0.316914	1.695521
O	-6.193745	0.936623	1.294873
C	2.068032	-2.102034	-3.144233
C	2.821678	-1.361160	-4.077735
C	2.748781	-3.027245	-2.332744
C	4.197423	-1.507061	-4.176530
H	2.311691	-0.666299	-4.739824
C	4.124711	-3.176731	-2.425673
H	2.201552	-3.584975	-1.578904
C	4.871932	-2.406721	-3.331233
H	4.771034	-0.917244	-4.883149
H	4.659711	-3.855382	-1.769542
N	6.265494	-2.547857	-3.224207
N	6.953910	-1.872759	-4.055955
C	8.328422	-1.868327	-3.831538
C	9.090808	-0.995475	-4.630396
C	8.956227	-2.626037	-2.804338
C	10.499013	-0.842907	-4.352633
N	8.473985	-0.246755	-5.606756
C	10.276837	-2.479834	-2.509051
H	8.354361	-3.322588	-2.240278
C	11.099436	-1.590235	-3.285436
C	11.302227	0.065561	-5.088105
H	9.016775	-0.015436	-6.426334
H	7.523366	-0.536775	-5.801972
S	10.900376	-3.297116	-1.014495
C	12.482288	-1.418081	-3.030022
C	12.644627	0.218804	-4.809588
H	10.856956	0.679184	-5.865583

O	12.039043	-4.142704	-1.413154
O	11.270040	-2.133503	-0.136775
O	9.713892	-4.032366	-0.461803
C	13.237726	-0.536925	-3.778475
H	12.945274	-2.004206	-2.245895
H	13.241343	0.922313	-5.383359
H	14.298436	-0.427155	-3.569492

Table S29. Cartesian coordinates of iPOP-ANT binded with amaranth.

C	0.351517	-0.960613	3.487420
N	1.569683	-1.320329	3.064083
C	1.724242	-2.617652	2.758283
C	-0.422925	-3.083891	3.321598
N	-0.666867	-1.817007	3.676522
N	0.748425	-3.537716	2.856461
C	0.084807	0.480913	3.690639
C	-0.975765	0.888729	4.509941
C	0.853339	1.446391	3.016778
C	-1.251072	2.242573	4.670229
H	-1.577830	0.139046	5.010404
C	0.551241	2.799392	3.150750
H	1.660975	1.128502	2.365799
C	-0.495126	3.205270	3.990622
H	-2.065453	2.555087	5.320433
H	1.117980	3.537855	2.590127
C	-1.574456	-4.021270	3.332253
C	-2.778288	-3.659447	3.952431
C	-1.504182	-5.224992	2.616031
C	-3.903691	-4.465388	3.815093
H	-2.828947	-2.728311	4.503914
C	-2.642476	-6.004796	2.444288
H	-0.564566	-5.504607	2.152521
C	-3.857505	-5.617978	3.020265

H	-4.835832	-4.170506	4.292913
H	-2.592426	-6.906494	1.837565
C	3.021755	-3.028937	2.181272
C	4.108466	-2.140236	2.199610
C	3.142218	-4.244991	1.493366
C	5.264549	-2.423745	1.484513
H	4.015146	-1.198054	2.726204
C	4.297021	-4.521491	0.764447
H	2.307875	-4.938289	1.491590
C	5.348871	-3.598328	0.721635
H	6.048731	-1.679251	1.426825
H	4.355734	-5.439793	0.183203
C	6.442641	-3.760247	-0.314622
H	6.368907	-4.724200	-0.827239
H	6.332660	-2.965247	-1.056817
C	-5.129028	-6.359766	2.690535
H	-4.933590	-7.404125	2.431052
H	-5.836778	-6.341447	3.524870
C	-0.868639	4.664066	4.103774
H	0.018787	5.303127	4.148862
H	-1.475145	4.844716	4.995734
N	7.827604	-3.625192	0.184138
C	8.646702	-4.601900	0.729007
C	8.523488	-2.484003	0.077575
C	9.862311	-4.021061	0.947391
H	8.301282	-5.609902	0.897970
H	8.050793	-1.546071	-0.261228
H	10.786824	-4.425511	1.326950
N	-5.808627	-5.743839	1.523047
C	-6.166769	-6.377500	0.395341
C	-6.201985	-4.417631	1.426811
H	-5.987610	-7.420097	0.175747
C	-6.833310	-4.276160	0.232668

H	-5.963657	-3.663174	2.157126
H	-7.202075	-3.386212	-0.244831
N	-1.633049	5.101282	2.916699
C	-2.561547	4.354296	2.213084
C	-1.490610	6.293151	2.323330
C	-2.963819	5.120535	1.161995
H	-2.806088	3.338150	2.475407
H	-0.736481	7.028101	2.555390
H	-3.650795	4.907964	0.360885
N	9.753902	-2.695628	0.549093
N	-6.785300	-5.499944	-0.405499
N	-2.280776	6.318147	1.242349
C	-7.295140	-5.748776	-1.782763
H	-6.789677	-5.026698	-2.430862
H	-6.939856	-6.747657	-2.069431
C	10.810648	-1.651011	0.568654
H	11.250041	-1.646569	1.563667
H	10.291271	-0.699461	0.454748
C	-2.199651	7.347871	0.172089
H	-1.427828	7.005328	-0.526852
H	-1.801171	8.253304	0.622314
C	-8.806419	-5.642519	-1.867754
C	-9.410592	-4.390315	-2.170524
C	-9.604255	-6.786136	-1.607288
C	-8.650413	-3.180706	-2.339220
C	-10.857772	-4.305170	-2.265921
C	-11.051319	-6.700934	-1.737133
C	-9.041596	-8.051546	-1.204288
C	-9.259628	-1.953973	-2.503987
H	-7.566768	-3.163239	-2.262690
C	-11.445224	-3.010945	-2.507134
C	-11.659014	-5.466063	-2.097513
C	-11.818538	-7.890797	-1.466488

H	-7.966185	-8.144968	-1.074462
C	-9.819180	-9.158300	-0.953606
C	-10.678109	-1.872147	-2.601347
H	-8.641432	-1.056444	-2.514069
H	-12.526434	-2.921810	-2.578445
C	-11.233443	-9.078026	-1.088880
H	-12.901229	-7.853804	-1.543715
H	-9.353845	-10.099495	-0.648277
H	-11.156757	-0.899190	-2.743930
H	-11.849999	-9.956471	-0.887255
C	11.817552	-1.881255	-0.535542
C	11.530530	-1.394396	-1.833227
C	12.976679	-2.648749	-0.293111
C	10.354349	-0.633510	-2.130605
C	12.447472	-1.681308	-2.915320
C	13.893965	-2.930849	-1.383920
C	13.295363	-3.180407	1.003347
C	10.068930	-0.202634	-3.400815
H	9.648731	-0.355583	-1.358893
C	12.113831	-1.203478	-4.224987
C	13.628076	-2.426253	-2.678910
C	15.041580	-3.743647	-1.096908
H	12.649637	-2.964046	1.848287
C	14.408350	-3.947568	1.224341
C	10.962597	-0.497313	-4.463489
H	9.152302	0.356596	-3.559728
H	12.780208	-1.414577	-5.053444
C	15.293251	-4.241887	0.153459
H	15.731811	-3.988480	-1.895139
H	14.617739	-4.326203	2.221738
H	10.734184	-0.156050	-5.470081
H	16.171249	-4.857795	0.328944
C	-3.525326	7.543569	-0.518932

C	-4.468627	8.463913	-0.006941
C	-3.829695	6.766012	-1.658286
C	-4.230418	9.202480	1.201307
C	-5.724825	8.674833	-0.704387
C	-5.085147	6.975056	-2.348664
C	-2.950690	5.737347	-2.139980
C	-5.148062	10.089362	1.699859
H	-3.304739	9.049478	1.747247
C	-6.649857	9.616806	-0.138375
C	-6.004506	7.950076	-1.888833
C	-5.371354	6.152549	-3.489726
H	-2.019905	5.522184	-1.622337
C	-3.279129	4.965315	-3.224850
C	-6.378347	10.299280	1.018583
H	-4.938107	10.632334	2.618974
H	-7.603523	9.787234	-0.625489
C	-4.504122	5.178247	-3.913872
H	-6.308962	6.285798	-4.018917
H	-2.602618	4.179810	-3.547875
H	-7.106602	10.999941	1.421091
H	-4.755153	4.557200	-4.770577
C	-7.283222	8.167091	-2.674834
H	-7.848477	9.038434	-2.344238
H	-7.064392	8.319027	-3.738603
H	-7.948295	7.297044	-2.601598
C	-13.160850	-5.338373	-2.281627
H	-13.619781	-4.744531	-1.471618
H	-13.388491	-4.823817	-3.225684
H	-13.675301	-6.303559	-2.310040
C	14.569744	-2.670501	-3.840742
H	14.806675	-1.730345	-4.350583
H	15.519464	-3.112156	-3.542373
H	14.116930	-3.336932	-4.586245

C	-3.188911	2.018058	-0.760691
C	-1.938121	1.476794	-0.488461
C	-1.832929	0.059598	-0.216551
C	-3.037965	-0.737386	-0.242871
C	-4.294967	-0.110845	-0.528897
C	-4.354494	1.238177	-0.797445
H	0.300481	-0.001565	0.104792
H	-3.233091	3.076689	-0.989779
C	-0.601996	-0.593288	0.069144
C	-2.936970	-2.139121	-0.013096
H	-5.315552	1.688825	-1.024264
C	-1.717552	-2.736950	0.205952
C	-0.542532	-1.958018	0.251030
H	-3.839225	-2.735379	-0.047449
H	-1.662319	-3.812403	0.349537
H	0.416867	-2.434899	0.426987
N	-0.930187	2.468727	-0.485372
N	0.274791	2.072412	-0.549820
C	1.298007	3.022621	-0.476188
C	1.155613	4.385314	-0.150144
C	2.624342	2.486164	-0.685920
C	2.318566	5.198980	0.036872
C	3.770079	3.321010	-0.490700
C	2.841723	1.136568	-1.073962
C	3.577403	4.675638	-0.117206
C	5.075376	2.786085	-0.652891
H	1.983049	0.497197	-1.242160
C	4.115366	0.644026	-1.235958
H	4.436762	5.318626	0.052512
C	5.243706	1.471862	-1.024534
H	5.946345	3.407690	-0.467909
H	4.271246	-0.392047	-1.522475
O	-0.061871	4.923020	0.058109

H	0.120869	5.804535	0.507154
S	2.140087	6.978105	0.387533
O	1.849039	7.628448	-0.903147
O	0.897102	6.966606	1.289716
S	6.886832	0.738566	-1.110928
O	7.186675	0.421476	-2.532108
O	7.830781	1.672245	-0.457383
S	-5.867738	-1.029568	-0.548749
O	-5.668264	-2.146477	-1.531549
O	-6.042653	-1.539572	0.848364
O	6.674311	-0.547689	-0.329379
O	3.362169	7.383553	1.100713
O	-6.891994	-0.041079	-0.977080

Table S30. Cartesian coordinates of iPOP-ANT binded with rhodamine B.

C	4.663064	-0.378585	-0.575168
N	4.774522	0.805863	0.045383
C	3.639943	1.302701	0.560890
C	2.431681	-0.484461	-0.154422
N	3.515177	-1.061626	-0.694964
N	2.446470	0.694585	0.485096
C	5.884933	-0.964989	-1.183577
C	5.809103	-2.162261	-1.908919
C	7.125017	-0.315364	-1.062678
C	6.946720	-2.690528	-2.515579
H	4.853532	-2.664129	-2.004471
C	8.258286	-0.845932	-1.668730
H	7.183486	0.610794	-0.502966
C	8.177897	-2.033968	-2.408805
H	6.868880	-3.608712	-3.092491
H	9.209103	-0.326324	-1.578056
C	1.130882	-1.189214	-0.287976
C	1.055950	-2.415168	-0.963544

C	-0.043752	-0.624635	0.237771
C	-0.170606	-3.056653	-1.123439
H	1.960371	-2.852604	-1.369490
C	-1.266281	-1.265814	0.073384
H	0.013597	0.323863	0.758808
C	-1.342324	-2.484156	-0.616418
H	-0.216002	-3.998911	-1.663696
H	-2.169512	-0.810486	0.472242
C	3.707503	2.613121	1.257667
C	4.922487	3.313951	1.341674
C	2.560229	3.162483	1.846866
C	4.986775	4.531590	2.009576
H	5.809497	2.888695	0.886966
C	2.628457	4.383073	2.515435
H	1.622380	2.623470	1.782980
C	3.841308	5.075029	2.607848
H	5.935405	5.058887	2.075285
H	1.734241	4.789931	2.981107
C	3.914249	6.384908	3.358298
H	3.007780	6.550748	3.947397
H	4.768100	6.403432	4.041414
C	-2.675624	-3.160657	-0.839386
H	-3.408732	-2.462096	-1.252974
H	-2.578328	-3.997578	-1.536728
C	9.397800	-2.589477	-3.107169
H	9.924767	-1.809041	-3.663311
H	9.120208	-3.376907	-3.813650
N	4.077007	7.548950	2.452367
C	3.366948	7.778174	1.286970
C	4.863947	8.611207	2.682230
C	3.745058	9.003995	0.821638
H	2.671866	7.051698	0.897393
H	5.527524	8.729946	3.525234

H	3.436644	9.567886	-0.044902
N	-3.263628	-3.690204	0.415253
C	-4.563968	-3.648257	0.743832
C	-2.592335	-4.409418	1.388354
H	-5.341137	-3.167268	0.169552
C	-3.520018	-4.799427	2.310000
H	-1.527103	-4.568812	1.337928
H	-3.431064	-5.378529	3.215930
N	10.383560	-3.167228	-2.160540
C	10.097535	-4.014125	-1.104239
C	11.716550	-3.045878	-2.254408
C	11.290394	-4.399897	-0.565417
H	9.082017	-4.254788	-0.833137
H	12.242825	-2.459275	-2.991948
H	11.526253	-5.055906	0.258065
N	4.682309	9.503416	1.705467
N	-4.741943	-4.310396	1.889559
N	12.286276	-3.780396	-1.295981
C	-6.046551	-4.499639	2.606958
H	-6.075405	-3.758987	3.405728
H	-6.825336	-4.228962	1.892558
C	5.376347	10.828324	1.579987
H	6.189315	10.690273	0.867595
H	5.832985	11.021782	2.551669
C	13.759548	-3.923857	-1.050679
H	14.001603	-3.276343	-0.208392
H	14.253480	-3.503380	-1.927782
C	-6.208621	-5.903731	3.120365
C	-5.862965	-6.209687	4.457075
C	-6.693100	-6.907348	2.252196
C	-5.275348	-5.254574	5.350133
C	-6.095157	-7.547089	4.955933
C	-6.921612	-8.245862	2.759140

C	-6.967339	-6.654478	0.869737
C	-4.944756	-5.579910	6.640440
H	-5.073391	-4.243553	5.010165
C	-5.738666	-7.834906	6.313094
C	-6.655115	-8.542270	4.117473
C	-7.412655	-9.232775	1.842265
H	-6.791704	-5.667168	0.455105
C	-7.437904	-7.633075	0.034595
C	-5.180379	-6.889298	7.132171
H	-4.502805	-4.830879	7.291264
H	-5.903057	-8.831074	6.704229
C	-7.663103	-8.944072	0.527657
H	-7.581955	-10.244280	2.187159
H	-7.638630	-7.407873	-1.008946
H	-4.917785	-7.138652	8.155472
H	-8.032924	-9.716525	-0.139242
C	4.431727	11.924077	1.169843
C	3.665648	12.581311	2.159608
C	4.307761	12.278215	-0.192651
C	3.689874	12.195381	3.537530
C	2.817704	13.686904	1.779808
C	3.447689	13.385701	-0.567419
C	4.990654	11.574645	-1.239540
C	2.944616	12.850466	4.483492
H	4.301553	11.357099	3.855474
C	2.059698	14.341208	2.803692
C	2.742418	14.103741	0.427559
C	3.339888	13.706678	-1.960947
H	5.634658	10.734675	-0.998760
C	4.850409	11.922035	-2.557453
C	2.116367	13.940713	4.112748
H	2.986438	12.535271	5.522205
H	1.415305	15.170346	2.539748

C	4.011229	13.004861	-2.925591
H	2.696406	14.519127	-2.271714
H	5.384275	11.367744	-3.324045
H	1.529096	14.454543	4.867317
H	3.902265	13.274284	-3.971398
C	14.152248	-5.355019	-0.806941
C	14.384335	-6.206908	-1.909747
C	14.269491	-5.838312	0.516908
C	14.191274	-5.776660	-3.261812
C	14.829157	-7.567885	-1.684465
C	14.715059	-7.196990	0.733514
C	13.954265	-5.045601	1.669096
C	14.419308	-6.608709	-4.325882
H	13.845718	-4.768267	-3.464747
C	15.050832	-8.397215	-2.832901
C	15.024922	-8.037956	-0.363624
C	14.827293	-7.665941	2.082352
H	13.606501	-4.024230	1.549063
C	14.071603	-5.541813	2.941944
C	14.854544	-7.941306	-4.108779
H	14.266297	-6.250128	-5.339790
H	15.371871	-9.421573	-2.697465
C	14.515809	-6.871947	3.154385
H	15.157325	-8.680915	2.264703
H	13.826650	-4.912650	3.792879
H	15.030659	-8.597457	-4.955328
H	14.608024	-7.257008	4.165072
C	15.547924	-9.429438	-0.081600
H	15.905991	-9.944713	-0.970166
H	16.389319	-9.391247	0.617571
H	14.773249	-10.058614	0.373683
C	-6.939409	-9.906694	4.706363
H	-6.009164	-10.432678	4.953989

H	-7.518115	-9.815178	5.630964
H	-7.512723	-10.551742	4.044134
C	1.890307	15.307578	0.090182
H	2.141482	16.151697	0.740140
H	2.018272	15.655198	-0.932652
H	0.824613	15.090933	0.233951
C	-6.765173	1.872114	-2.759761
C	-7.392994	0.658927	-2.817467
C	-8.736389	0.483895	-2.378021
C	-9.390276	1.653217	-1.897730
C	-8.778819	2.889117	-1.833968
C	-7.429902	3.043144	-2.247155
C	-11.379896	0.430521	-1.489077
C	-10.769816	-0.770766	-1.950788
C	-11.580835	-1.940918	-1.897314
H	-11.155689	-2.882140	-2.227356
C	-12.870845	-1.906791	-1.446236
C	-13.478353	-0.683508	-0.986776
C	-12.680951	0.489729	-1.032741
H	-5.749308	1.938631	-3.122856
H	-6.858136	-0.196980	-3.213931
H	-9.368390	3.713102	-1.459566
H	-13.435440	-2.828511	-1.442969
H	-13.048565	1.453491	-0.712256
N	-14.756027	-0.653361	-0.522115
N	-6.795594	4.243521	-2.164456
C	-5.435063	4.417215	-2.698827
H	-4.832347	3.552813	-2.409747
C	-7.575074	5.428302	-1.738473
H	-8.403297	5.573364	-2.446214
H	-8.021689	5.200942	-0.763210
C	-15.350168	0.656562	-0.168850
H	-14.704828	1.124738	0.584109

H	-15.325576	1.300024	-1.059274
C	-15.605846	-1.854270	-0.569433
H	-15.016063	-2.714175	-0.242463
C	-16.773610	0.617501	0.379630
H	-16.841508	0.058458	1.317807
H	-17.079439	1.647311	0.589220
H	-17.489914	0.201850	-0.335129
C	-6.791282	6.731458	-1.611558
H	-6.353689	7.055161	-2.560437
H	-7.488496	7.511166	-1.289190
H	-6.000255	6.667068	-0.858219
O	-10.684317	1.600452	-1.476575
C	-9.434284	-0.740380	-2.394755
H	-16.387947	-1.741391	0.179655
C	-16.224789	-2.099307	-1.949028
H	-16.859951	-1.258462	-2.246409
H	-15.452294	-2.224676	-2.714674
H	-16.842090	-3.003626	-1.930663
H	-4.980964	5.266350	-2.190432
C	-5.407154	4.630154	-4.215480
H	-5.851680	3.780824	-4.744397
H	-5.966353	5.529618	-4.493390
H	-4.374964	4.749657	-4.561116
C	-8.787133	-1.969444	-2.934147
C	-7.757145	-2.666971	-2.265944
C	-9.189920	-2.404933	-4.204422
C	-7.144777	-3.760087	-2.893944
C	-8.580847	-3.502862	-4.812296
H	-9.976265	-1.863866	-4.722645
C	-7.551585	-4.180141	-4.157262
H	-6.349576	-4.273163	-2.363755
H	-8.907560	-3.821221	-5.797775
H	-7.070001	-5.032558	-4.626135

C	-7.260913	-2.338232	-0.894533
O	-6.201316	-2.719991	-0.447849
O	-8.129736	-1.590074	-0.169461
H	-7.706089	-1.448566	0.698597

Table S31. Cartesian coordinates of iPOP-ANT binded with rhodamine 6G.

C	3.784524	-0.648586	-0.720486
N	3.979819	0.521523	-0.093485
C	2.869337	1.172928	0.283830
C	1.525259	-0.451281	-0.565238
N	2.577674	-1.175989	-0.973270
N	1.622483	0.726580	0.069224
C	4.979799	-1.401931	-1.179598
C	4.830062	-2.591306	-1.906438
C	6.272808	-0.919806	-0.914794
C	5.949961	-3.275870	-2.373851
H	3.833816	-2.964133	-2.112860
C	7.388049	-1.606066	-1.382111
H	6.388611	0.000244	-0.353936
C	7.236773	-2.785945	-2.124137
H	5.818159	-4.185761	-2.954087
H	8.382549	-1.215114	-1.181129
C	0.166620	-0.980243	-0.849649
C	0.008148	-2.197284	-1.526899
C	-0.975449	-0.256229	-0.467017
C	-1.265920	-2.673817	-1.828851
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C	-2.244990	-0.733069	-0.772956
H	-0.853267	0.685427	0.055259
C	-2.401882	-1.942671	-1.464487
H	-1.373268	-3.611207	-2.368817
H	-3.119724	-0.155428	-0.484150
C	3.029340	2.475030	0.981105

C	4.308766	3.010566	1.206216
C	1.904783	3.181468	1.430000
C	4.456546	4.220638	1.874617
H	5.178047	2.463887	0.859980
C	2.056756	4.393955	2.099521
H	0.917340	2.770045	1.257185
C	3.331921	4.921128	2.332746
H	5.452826	4.619057	2.050535
H	1.176654	4.923547	2.455834
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H	2.552240	6.517452	3.561873
H	4.254187	6.140539	3.862834
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H	-3.712909	-3.295537	-2.520938
C	8.444706	-3.509999	-2.672872
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H	8.148820	-4.266200	-3.405559
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H	3.841363	9.380524	-0.358137
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C	9.770140	-5.509438	0.077674
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