Supporting Information

Enzyme-activatable charge transfer in gold nanoclusters

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Supplementary Methods

TA Measurement. The fs-TA measurements were performed on a Helios pump-probe system (Ultrafast Systems LLC) combined with an amplified femtosecond laser system (Coherent). Optical parametric amplifier (TOPAS-800-fs) provided a 350 nm pump pulse (~0.2μJ/pulse), which was excited by a Ti: sapphire regenerative amplifier (Legend Elite-1K-HE; 800 nm), 35 fs, 7 mJ/pulse, 1 kHz) and seeded with a mode-locked Ti: sapphire laser system (Micra 5) and an Nd: YLF laser (Evolution 30) pumped. Focusing the 800 nm beams (split from the regenerative amplifier with a tiny portion, ~400 nJ/pulse) onto a CaF_2 plate produced the white-light continuum (WLC) probe pulses (350-650nm). The pulse-to-pulse fluctuation of the WLC is corrected by a reference beam split from WLC. A motorized optical delay line was used to change the time delays (0-8 ns) between the pump and probe pulses. The instrument response function (IRF) was determined to be ~100 fs by a routine cross-correlation procedure. The instrument response function (IRF) was determined to be ~100 fs by a routine cross-correlation procedure. A mechanical chopper operated at a frequency of 500 Hz used to modulate the pump pulses such that the fs-TA spectra with and without the pump pulses can be recorded alternately.

DFT Calculations. All the geometries of MPR-AuNCs and MP-AuNCs were optimized without any constraints by using the M06-2X method in conjunction with 6-31G(d)&Def2-TZVP basis set.[1] Herein, the solvation model based on density (SMD) was used to take the effect of solvent (water) into account.[2] Vibrational frequency calculations have been performed for each optimized structure at the same level to ensure these structures without imaginary frequencies. And the isomers were ordered according to the zero-point energy (ZPE)-corrected electronic energies. Additionally, the natural population analysis (NPA) and electron density difference (EDD) were obtained at higher 6-31+g(d, p)&Def2-TZVP level.[3] All the above calculations were performed by using the Gaussian 09 program package.[4] Dimensional plots of molecular structures and molecular orbitals were generated with the GaussView program,[5] while EDD diagram was plotted by employing the Multiwfn software.[6]

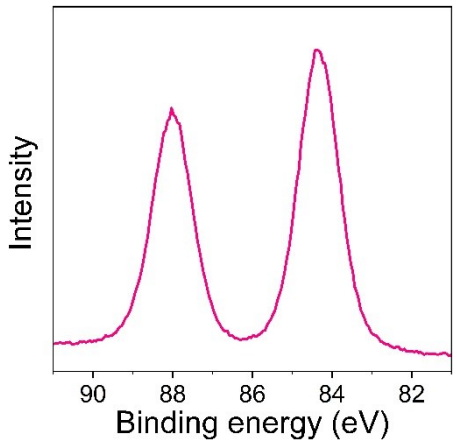

Fig. S1 | High resolution Au(4f) spectrum of MPR-AuNCs.

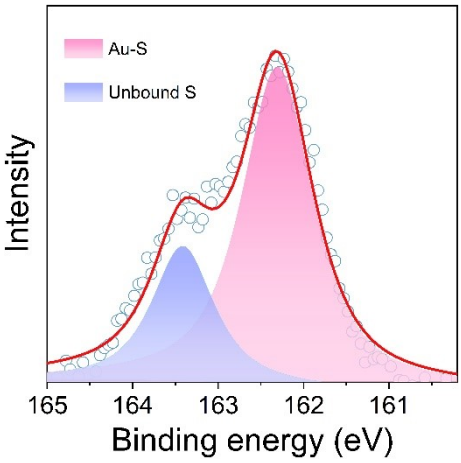

Fig. S2 | High resolution S(2p) spectrum of MPR-AuNCs.

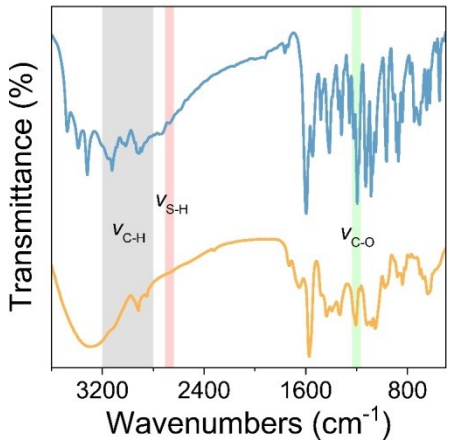

Fig. S3 | FTIR spectra of MPR (blue line) and MPR-AuNCs (orange line).

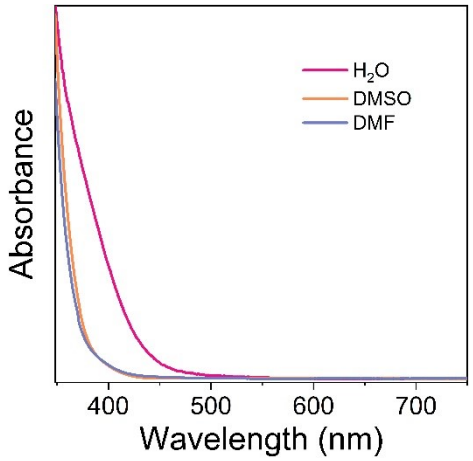

Fig. S4 | Comparison of the absorption spectra of MPR-AuNCs in water, DMSO, and DMF.

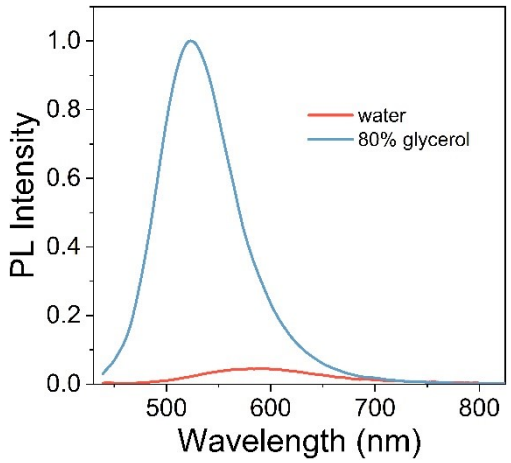

Fig. S5 | The emission spectra of MPR-AuNCs in water and 80% glycerol with the same absorbance at 420 nm (0.08).

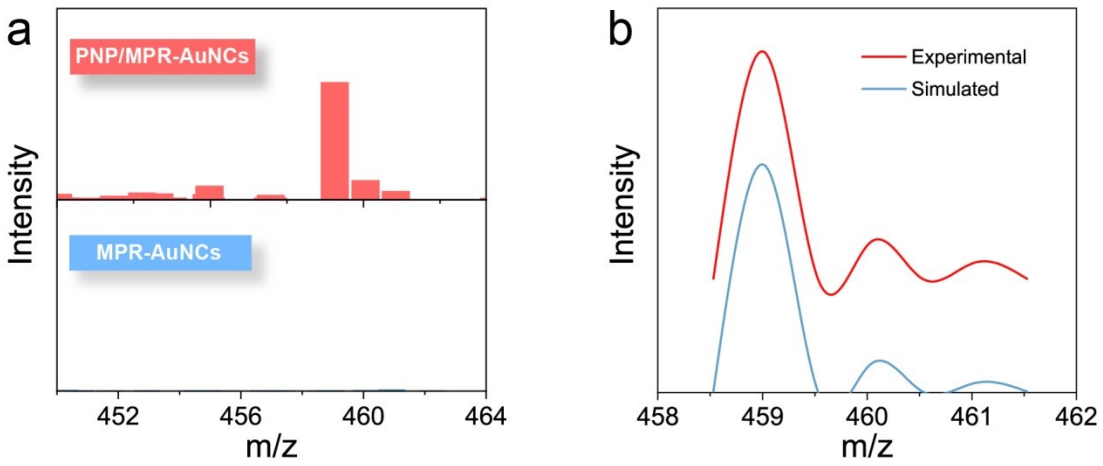

Fig. S6 | Observation of ribose-1-phosphate (RP) after PNP-catalyzed reaction. (a) ESI-MS spectra of MPR-AuNCs before and after the addition of PNP (50 U/L). (b) The experimental (red line) and simulated (blue line) isotope patterns of RP ($[2RP-H]^-$).

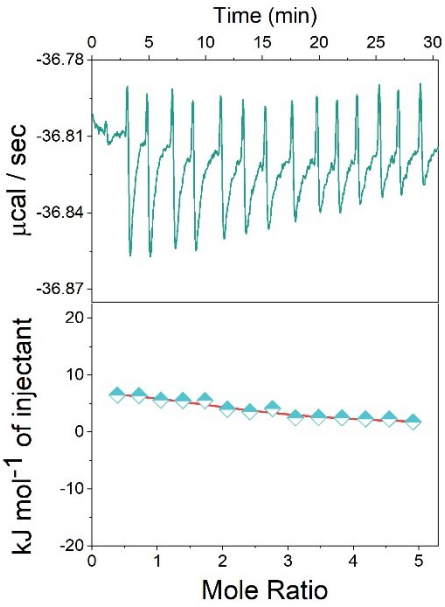

Fig. S7 | Typical data obtained from isothermal titration calorimetry (ITC) measurements of MPR titrated with PNP. Top: Corrected heat rate of the titration. Bottom: Integrated normalized heats from each titration step corrected by the heats of dilution (filled rhombus) together with a fit corresponding to an independent binding model (straight line).

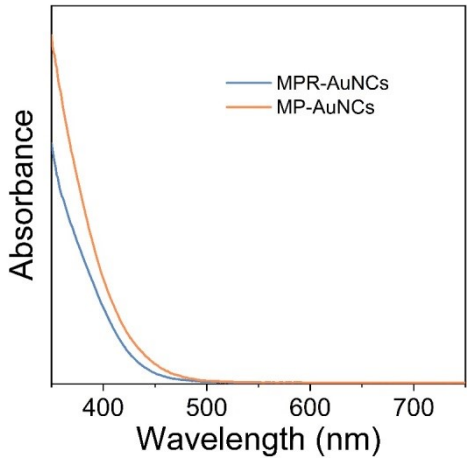

Fig. S8 | Absorption spectra of MPR-AuNCs and MP-AuNCs.

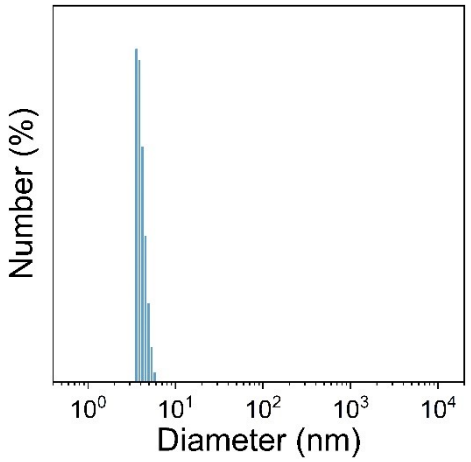

Fig. S9 | DLS measurement of MP-AuNCs.

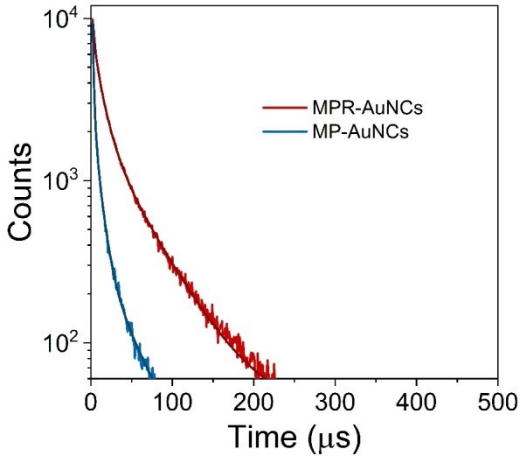

Fig. S10 | PL lifetime measurements of MPR-AuNCs and MP-AuNCs.

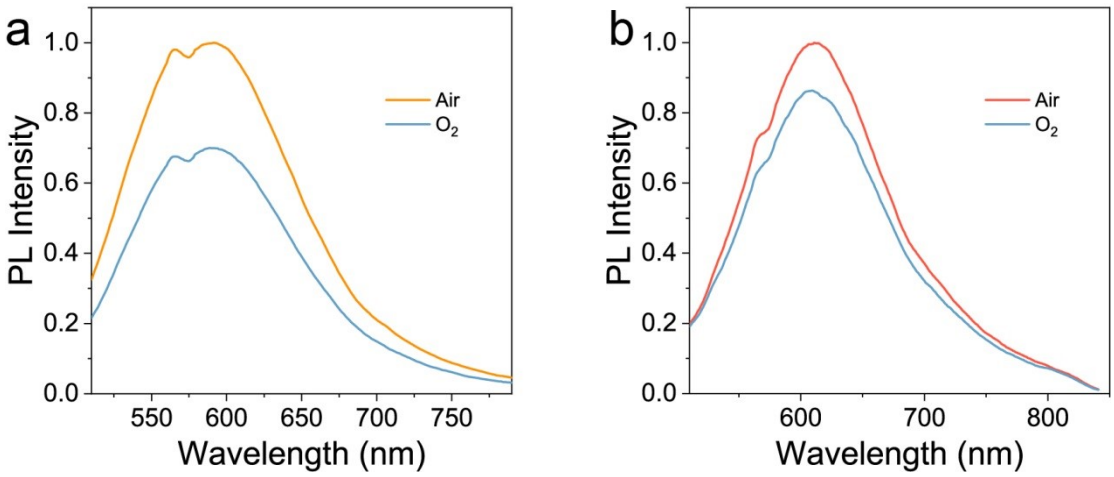

Fig. S11 | O_2 quenching experiments. Emission spectra of (a) MPR-AuNCs and (b) MP-AuNCs under air and pure O_2, respectively.

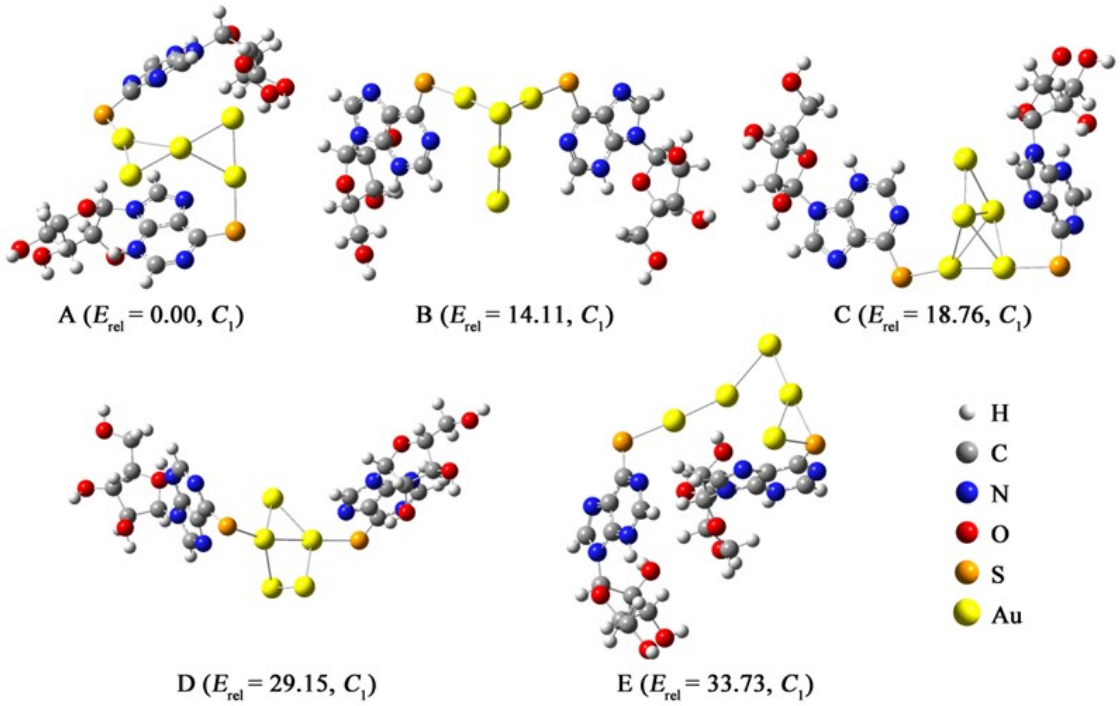

Fig. S12 | Low-lying A-E isomers of MPR-AuNC, and the relative energy (E_{rel}, in kcal/mol) and geometric symmetry are given in the parentheses.

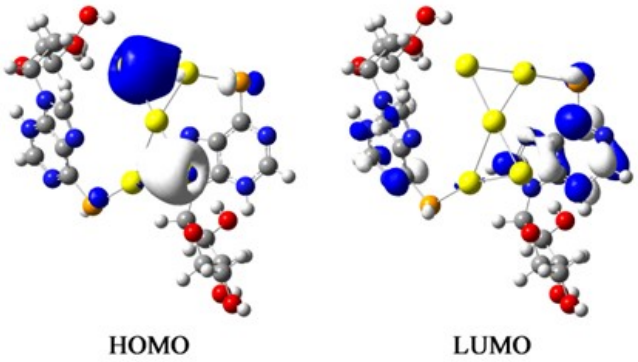

Fig. S13 | The HOMO and LUMO orbitals of the most stable MPR-AuNC with isovalue of 0.04 a.u.

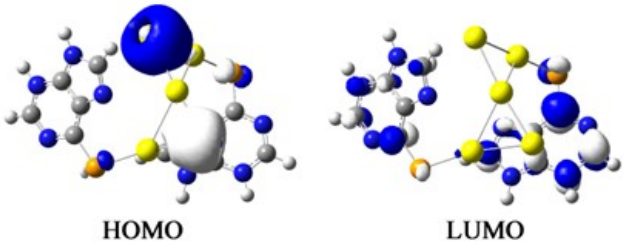

Fig. S14 | The HOMO and LUMO orbitals of the most stable MP-AuNC with isovalue of 0.04 a. u.

Table S1 | The NPA charges on the Au_5 moiety in the global minima of MPR-AuNC and MP-AuNC at the ground and excited state (Q_{GS} and Q_{ES}, in |e|), and the charge transfer from Au_5 core to the surrounding ligands (ΔQ, $\Delta Q = Q_{ES} - Q_{GS,}$ in |e|) during the light-excited process.

Complex	Q_{GS}	Q_{ES}	ΔQ
MPR-AuNC	0.227	0.317	0.091
MP-AuNC	0.288	0.984	0.696

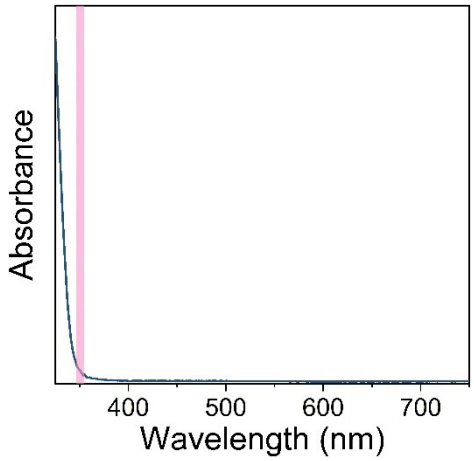

Fig. S15 | Absorption spectrum of MPR.

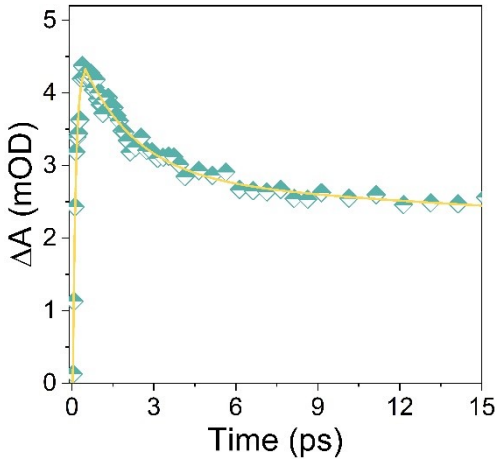

Fig. S16 | Kinetics trace of MPR-AuNCs monitored at 460 nm.

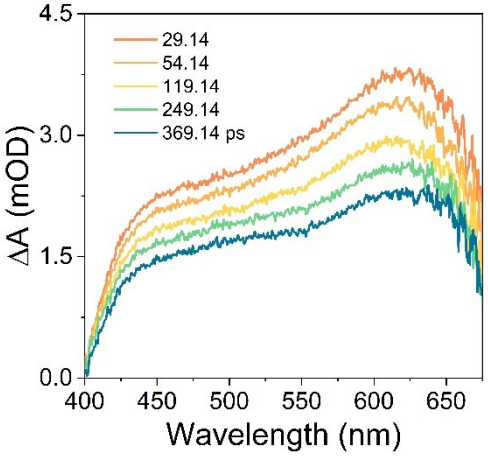

Fig. S17 | Long-time evolution of TA spectra of MPR-AuNCs.

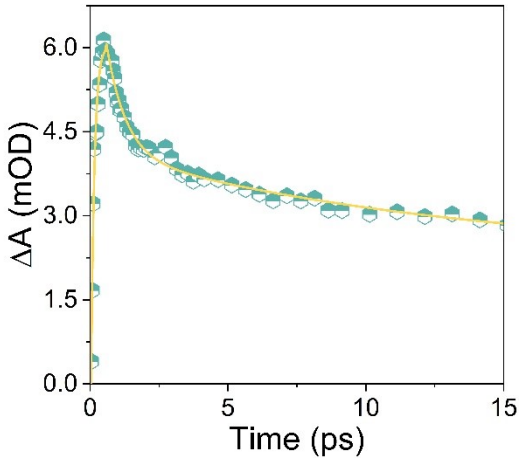

Fig. S18 | Kinetics trace of MP-AuNCs recorded at 460 nm.

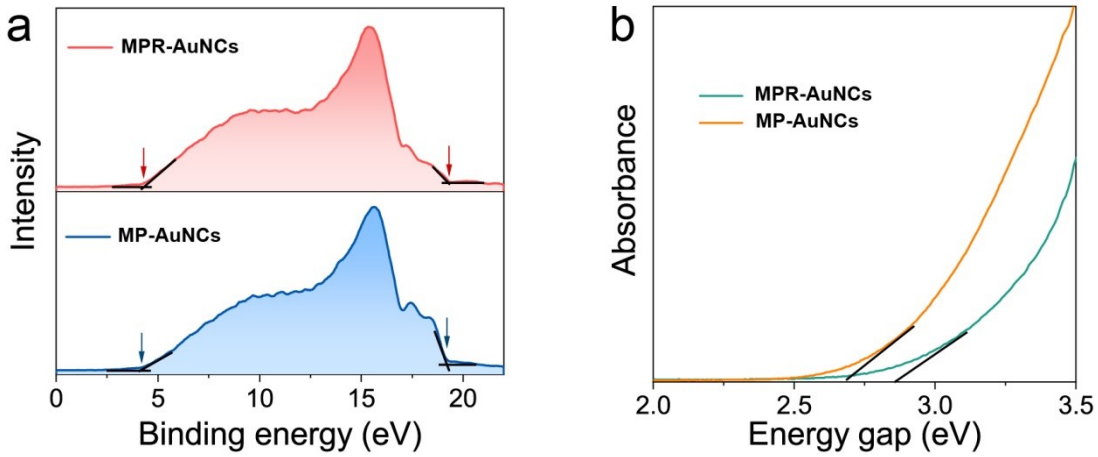

Fig. S19 | Determination of HOMO-LUMO energy levels of MPR-AuNCs and MP-AuNCs. (a) Ultraviolet photoelectron spectra of MPR-AuNCs and MP-AuNCs. (b) Optical energy gaps of MPR-AuNCs and MP-AuNCs.

Table S2 | The energy levels of ground state (E_{S_0}) and charge-transfer singlet state ($E_{1_{CT}}$)

Sample	$E_{cut\text{-}off}$ (eV)	E_{onset} (eV)	E_g (eV)	E_{S_0} (eV)[a]	$E_{1_{CT}}$ (eV)[b]
MPR-AuNCs	19.31	4.31	2.87	–6.22	–3.35
MP-AuNCs	19.18	4.16	2.67	–6.20	–3.53

[a] $E_{S_0} = -(21.22 - E_{cut\text{-}off} + E_{onset})$

[b] $E_{1_{CT}} = E_{S_0} + E_{onset}$

$E_{cut\text{-}off}$: cut-off binding energy; E_{onset}: onset binding energy; Eg: optical energy gap

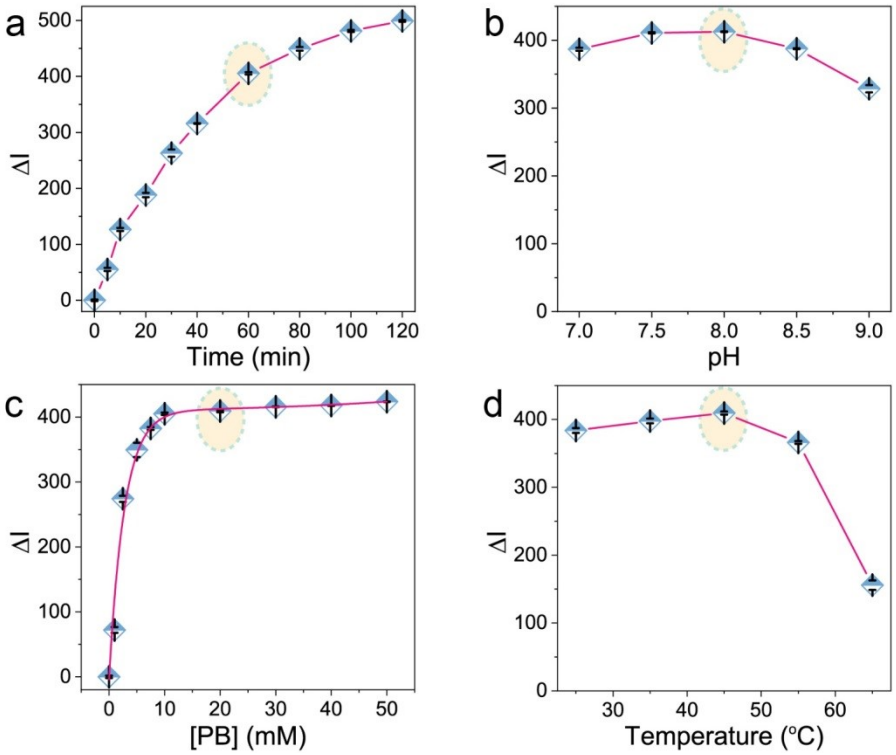

Fig. S20 | Optimization of the operating conditions for PNP sensing. ΔI as functions of (a) incubation time, (b) incubation pH, (c) concentration of phosphate buffer, and (d) incubation temperature. The activity of PNP was set at 25 U/L.

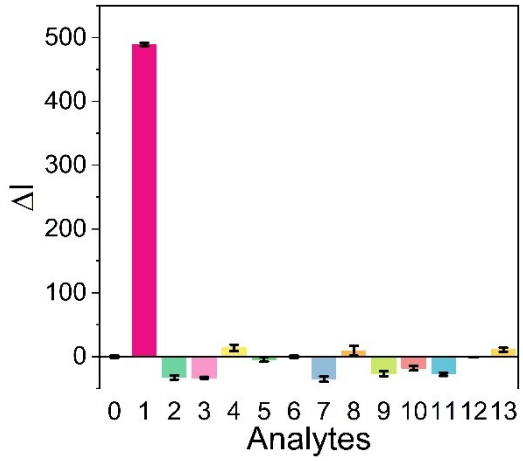

Fig. S21 | Selectivity of the proposed approach for PNP activity determination. Samples marked 0−13 correspond to blank, PNP (25 U/L), BSA (1 mg/mL), trypsin (1 mg/mL), alkaline phosphatase (1000 U/L), α-glucosidase (1000 U/L), β-glucuronidase (10000 U/L), xanthine oxidase (1000 U/L), glucose oxidase (1000 U/L), Zn^{2+} (100 μM), Fe^{3+} (100 μM), Fe^{2+} (100 μM), glucose (200 μM), and urea (1000 μM).

Cartesian Coordinates

1. The global minimum of MPR-AuNC (Isomer A)
Gibbs Free Energies= -3289.715064 a.u

Au	2.33414900	-0.49440200	-1.89385300
Au	-0.20182000	-0.80674300	-1.10066300
Au	-2.84218700	-1.27336300	-0.58281800
Au	-1.11914800	-2.79712000	0.66844000
Au	1.19080100	1.71499800	-0.94051100
N	2.82417000	0.26472900	1.73763700
C	1.51003700	0.30107100	2.15843900
N	0.94922400	-0.87366800	2.22729000
C	1.92629400	-1.75545400	1.80738800
C	1.92450300	-3.15419800	1.60358300
N	3.10742200	-3.73889400	1.24563600
C	4.17141400	-3.01186100	1.02118600
H	5.07001700	-1.15254600	0.88622600
N	4.21948400	-1.66540200	1.11981400
C	3.09435400	-1.04298900	1.52875900
S	0.54903500	-4.17393700	1.78719400
H	5.09675600	-3.49084200	0.72323000
H	1.04439400	1.24422800	2.41514900
N	-3.94365100	2.53385200	-0.70669200
C	-3.05534800	2.01266100	-1.63240700
N	-1.82555900	2.41546100	-1.46278900
C	-1.87245200	3.25014700	-0.36836900
C	-0.87308600	3.97748300	0.31424200
N	-1.27332800	4.82864100	1.30439500
C	-2.53617300	4.91380800	1.63430900
H	-4.49585900	4.28712300	1.38701300
N	-3.53038900	4.19529600	1.07226700
C	-3.19170400	3.34527700	0.07774900
S	0.81110000	3.89381500	-0.01033900
H	-2.84121400	5.59893200	2.41645600
H	-3.39506000	1.36515300	-2.42580200
C	-5.27918300	0.42667500	0.96989800
C	-5.64005300	0.70733800	-0.48134700
C	-5.38830900	2.22172500	-0.55346200
C	-5.91566300	1.62084600	1.66518800
H	-4.18338700	0.47662600	1.07854500
H	-6.71569300	0.55145100	-0.62176700
H	-6.97656400	1.41935100	1.85233900
O	-5.81600500	2.69880600	0.69791800
C	-5.23478900	2.04647700	2.95046300
H	-5.65893100	3.00022700	3.29281600
H	-4.16118300	2.18824100	2.76509500
O	-5.45935000	1.00776300	3.88555500
H	-4.97580800	1.23388300	4.69519300
O	-5.76855300	-0.80273400	1.44692700
H	-5.15297300	-1.48905700	1.13356900
O	-4.89786600	-0.11412500	-1.34366800
H	-5.29065700	-0.12532300	-2.23300300
H	-5.93229300	2.73455800	-1.34625700
C	6.11517500	1.43602800	2.00166000
C	4.77759700	1.47107000	2.75194100
C	3.71588000	1.40023500	1.61257600
C	5.73545000	1.79026700	0.56546000
H	6.49271500	0.40265800	2.03496000
H	4.67508700	2.42770300	3.27315000
H	5.71604100	2.88308800	0.45632000
O	4.42055900	1.25376000	0.39762600
C	6.61050000	1.16576200	-0.50149500
H	6.20798300	1.41013500	-1.49263900
H	6.59323400	0.07302500	-0.38015500
O	7.91552900	1.68539300	-0.32734900
H	8.47593900	1.30339900	-1.02010200
O	7.07342900	2.35067500	2.48246500
H	7.36316000	2.04075700	3.35546200
O	4.71066800	0.38531400	3.64756700
H	3.93370300	0.50783400	4.21853800
H	3.08113500	2.29205700	1.59519500

2. Isomer B

Gibbs Free Energies= -3289.692575 a.u

Au	-1.63569300	-2.66637300	0.62204700
Au	-0.06994400	1.20349900	-2.29271800
Au	0.00676100	-1.24158300	-1.47606400
Au	1.30766600	-2.47098400	0.87532000
Au	0.07497600	-4.00411500	-0.98160500
N	-6.49612500	2.01177600	1.42434900
C	-6.81074100	1.11691400	2.42827700
N	-5.99335100	0.10440300	2.50758300
C	-5.05944100	0.33641900	1.51944500
C	-3.93634700	-0.40308700	1.08922600
N	-3.19373700	0.11440000	0.06697000
C	-3.52765400	1.24870000	-0.49523000
H	-4.82134000	2.85898400	-0.63367700
N	-4.59907400	1.99126700	-0.14654900
C	-5.36077000	1.52989500	0.86783500
S	-3.52968800	-1.89258800	1.83178700
N	5.79284300	2.43618200	2.28150700
C	5.93023900	1.61567400	3.38518300
N	5.13126100	0.58596800	3.37958400
C	4.43179100	0.69770500	2.19585500
C	3.42823500	-0.10674800	1.61331800
N	2.92811600	0.28535800	0.40453200
C	3.37460700	1.36545400	-0.18506700
H	4.64230100	3.00326200	-0.19271200
N	4.33236200	2.17396800	0.31463400
C	4.86098400	1.83062200	1.50883700
S	2.86745200	-1.52080600	2.40101100
H	-2.91900600	1.64270400	-1.30387800
H	-7.67847400	1.28425000	3.05243100
H	6.64270000	1.86288800	4.16068700
H	2.96055300	1.65815000	-1.14456900
C	7.65905900	3.67598200	-0.35104000
C	7.85960700	2.88971900	0.94707200
C	6.74543800	3.45673000	1.88201600
C	6.91958800	4.92345100	0.12069300
H	6.99783000	3.09078000	-1.00843200
H	8.83638200	3.13938000	1.37250600
H	7.64211900	5.63423500	0.54560000
O	6.04641900	4.43665000	1.14547000
C	6.06222000	5.61073500	-0.92093500
H	5.49568400	6.42153800	-0.44684800
H	5.34762500	4.88554200	-1.33566100
O	6.93665500	6.10216100	-1.92013100
H	6.39447100	6.55812100	-2.58185100
O	8.85862300	4.02790000	-1.00106400
H	9.26754200	3.20976200	-1.32734700
O	7.74462700	1.50873100	0.69670700
H	8.11152900	1.02596100	1.45586500
H	7.16055900	3.87571500	2.80245500
C	-5.85557200	5.36764800	0.81144000
C	-6.28004300	4.45143500	1.96320800
C	-7.08827600	3.32594200	1.24593500
C	-6.85522900	5.02469400	-0.28828500
H	-4.84739900	5.06611900	0.48845300
H	-6.95398500	4.99802900	2.62990700
H	-7.79194300	5.57106900	-0.10987700
O	-7.06746800	3.61787600	-0.13499800
C	-6.37260100	5.26010200	-1.70490800
H	-7.11870800	4.87650200	-2.41143100
H	-5.43317800	4.71110900	-1.86183700
O	-6.18301300	6.65486300	-1.85446300
H	-5.91017400	6.81434700	-2.77092900
O	-5.91309900	6.74197200	1.11699500
H	-5.20423800	6.93075100	1.75270000
O	-5.14325600	3.98378400	2.65048300
H	-5.43179400	3.59726300	3.49415200
H	-8.11337800	3.26010500	1.62063400

3. Isomer C

Gibbs Free Energies= -3289.685171 a.u

Au	-0.54487500	-2.81831300	-0.27420700
Au	2.05235300	-2.88060300	0.14286100
Au	1.03787100	-0.35522600	-1.16795500
Au	0.33058500	1.77797300	0.40139600
Au	0.68096900	-0.74037600	1.48302300
N	-6.87285100	-0.22614400	-1.02542100
C	-7.10282800	-1.56423600	-1.27891800
N	-6.03194000	-2.30483000	-1.21390600
C	-5.02328800	-1.42667000	-0.87167600
C	-3.63901300	-1.61719000	-0.65008400
N	-2.90244000	-0.51287100	-0.31379700
C	-3.46515700	0.66302600	-0.20522800
H	-5.16354200	1.84826100	-0.31018400
N	-4.77748800	0.90917500	-0.40259600
C	-5.55280700	-0.14695100	-0.73361400
S	-2.91541400	-3.15591900	-0.79102600
C	-7.86793500	2.27813100	1.13034700
C	-8.26668600	0.84839000	0.75800900
C	-7.90414300	0.76132400	-0.75814000
C	-7.91076700	2.99622800	-0.21372500
H	-6.83128100	2.26347800	1.50041900
H	-9.35043000	0.73943000	0.86639800
H	-8.95436100	3.23735700	-0.45979400
O	-7.39955600	2.02511000	-1.13359000
C	-7.04799000	4.23449900	-0.33529200
H	-7.07532500	4.59052600	-1.37242300
H	-6.00843000	3.97791200	-0.08597900
O	-7.56919500	5.19980900	0.55960600
H	-7.05564600	6.01322400	0.44059500
O	-8.73878800	2.89430300	2.05092000
H	-8.64528800	2.42747800	2.89705700
O	-7.57418400	-0.07454400	1.56512900
H	-8.00604400	-0.94126900	1.48328200
H	-8.76936200	0.48543600	-1.36660900
H	-8.10015100	-1.90885800	-1.51873400
H	-2.85796200	1.52213500	0.06188500
N	3.69661100	1.93983700	1.04346200
C	3.68417100	1.13492700	2.16429300
N	3.97731000	-0.11339400	1.92027600
C	4.19068700	-0.16035700	0.55654800
C	4.46827000	-1.23563100	-0.32041800
N	4.58939300	-0.94009200	-1.65410400
C	4.42529000	0.28470000	-2.08349200
H	4.01823900	2.27823800	-1.70234300
N	4.14268500	1.34926800	-1.30148100
C	4.02799900	1.11832500	0.02349000
S	4.61892100	-2.86570500	0.20280800
C	4.95794900	4.84334000	-0.32566700
C	4.98577000	4.08615100	1.00405500
C	3.59066400	3.38695600	1.04944800
C	3.46569600	5.01282300	-0.58448600
H	5.38797000	4.19380600	-1.10380700
H	5.04180400	4.80848700	1.82491300
H	3.08914200	5.85724100	0.00958000
O	2.89685900	3.78514200	-0.11501800
C	3.06024200	5.17258000	-2.03505600
H	1.96524200	5.19234900	-2.10462200
H	3.42606100	4.31003100	-2.60998400
O	3.63123500	6.38208200	-2.49836100
H	3.34264500	6.50915800	-3.41504800
O	5.59914200	6.09735700	-0.28462900
H	6.55326300	5.93516700	-0.21025000
O	6.07323500	3.19254600	1.02780600
H	6.17892600	2.86136100	1.93535500
H	3.02959300	3.65213800	1.95002800
H	3.45946900	1.55739000	3.13533000
H	4.51835500	0.49921800	-3.14215700

4. Isomer D

Gibbs Free Energies= -3289.668606 a.u

Au	0.94198900	-0.89930700	-1.17468800
Au	-0.66846000	-0.56941300	1.04241600
Au	-1.00997100	-3.03685400	-0.46964800
Au	-0.84366000	1.21167200	-1.08685800
Au	1.17459800	-2.96261300	1.00084200
N	4.94874200	1.89532000	0.49531200
C	3.82744800	1.25092300	0.97463300
N	3.27170100	0.45339700	0.10533000
C	4.06952200	0.54140600	-1.01932800
C	3.99539500	-0.07359900	-2.29348300
N	5.00303000	0.20381500	-3.18164400
C	5.96439700	1.02889300	-2.86552600
H	6.83985900	2.31956100	-1.49803600
N	6.07293300	1.67388300	-1.68264200
C	5.12404400	1.41340400	-0.75822600
S	2.77004700	-1.14353100	-2.80753500
C	8.29040800	2.29689200	1.23593400
C	7.02821400	1.72722800	1.88586900
C	5.89416400	2.63470600	1.31625300
C	7.87879500	3.72830900	0.91065100
H	8.47312700	1.74998700	0.29801900
H	7.08547600	1.87747300	2.96846100
H	7.94438300	4.33947600	1.82173200
O	6.51243100	3.60453400	0.49884400
C	8.63676700	4.39256500	-0.21942100
H	8.18283400	5.36757400	-0.43538100
H	8.56074200	3.76854400	-1.12144100
O	9.98114700	4.52589600	0.20312000
H	10.46862600	4.96404500	-0.51119900
O	9.42296000	2.28401900	2.07422500
H	9.65149600	1.35517100	2.24139700
O	6.88707900	0.36484300	1.56135300
H	6.24825700	-0.03402000	2.17498600
H	5.31048500	3.10410400	2.11293400
H	3.47617800	1.43460800	1.98145200
H	6.74945300	1.24005000	-3.58193800
N	-5.41025000	0.71243600	-0.19970700
C	-4.82758300	-0.53830300	-0.13711100
N	-3.88807100	-0.63688600	0.76061800
C	-3.84110400	0.60815000	1.35906400
C	-3.02510200	1.13881100	2.38551800
N	-3.30265700	2.40789300	2.81436600
C	-4.23876600	3.11626200	2.23692700
H	-5.70091200	3.30301600	0.78008800
N	-5.00172500	2.69389600	1.20519700
C	-4.80992000	1.42709600	0.78261500
S	-1.73106200	0.28294400	3.11902200
C	-8.50195700	2.23572900	0.07023900
C	-7.90675800	0.82721300	-0.00086800
C	-6.64623200	1.01762100	-0.90101000
C	-7.93635500	2.90119700	-1.17996900
H	-8.09731300	2.73670800	0.96304200
H	-8.60977100	0.16632000	-0.51717800
H	-8.52866000	2.59081500	-2.05227000
O	-6.60728100	2.37759900	-1.27491800
C	-7.82726600	4.41091300	-1.13518600
H	-7.31445200	4.76229000	-2.03890900
H	-7.22825500	4.70395500	-0.26124000
O	-9.14515700	4.92134300	-1.05130800
H	-9.08409200	5.88878500	-1.05486200
O	-9.91050700	2.26513900	0.05159100
H	-10.22255300	1.88513600	0.88877700
O	-7.61552100	0.35751600	1.29414500
H	-7.47451600	-0.60276900	1.24905200
H	-6.67371300	0.36831400	-1.78008600
H	-5.15326800	-1.32536800	-0.80438600
H	-4.43808300	4.12446800	2.58051400

5. Isomer E

Gibbs Free Energies= -3289.661316 a.u

Au	2.02510700	-1.35326700	-0.29674900
Au	4.86871100	-1.52559300	0.16864000
Au	3.96520900	0.87600500	0.36978200
Au	-0.26984000	-2.21491900	-1.09637100
Au	2.54884300	3.00150700	-1.46986200
N	-6.86199900	-1.10632800	-1.16725300
C	-6.79938900	-2.43429100	-0.78623100
N	-5.63447000	-2.98466600	-0.98260600
C	-4.85305500	-1.97107500	-1.50199300
C	-3.48615600	-1.92312300	-1.86624600
N	-3.01194400	-0.72935700	-2.35165000
C	-3.78968200	0.31943900	-2.42842100
H	-5.64875600	1.19340200	-2.14532800
N	-5.09001100	0.34395500	-2.06698500
C	-5.61250800	-0.80867500	-1.59621100
S	-2.45303100	-3.26953400	-1.70991500
N	-1.27294900	0.78984200	0.97185500
C	-0.84252800	1.10447600	-0.30252400
N	0.24684300	1.82260100	-0.32362700
C	0.59268700	1.97877000	1.00057100
C	1.68989600	2.57073200	1.64278900
N	1.72921200	2.59237900	2.99475800
C	0.77266500	2.02237800	3.68865800
H	-0.97127300	0.92188600	3.74209400
N	-0.27687300	1.37502900	3.14434900
C	-0.35846100	1.33949700	1.80224300
S	3.07908100	3.25577200	0.82761300
H	-3.39563300	1.25379200	-2.81225000
H	-7.67391800	-2.92549900	-0.38072200
H	-1.40461100	0.77942600	-1.16810100
H	0.80238600	2.04643800	4.77107300
C	-7.43976600	1.99713700	0.25555400
C	-7.54005000	0.51254200	0.61631100
C	-7.88681700	-0.16627900	-0.74803600
C	-8.25259700	2.08487000	-1.03330900
H	-6.38522800	2.22561300	0.03578600
H	-8.37534200	0.36290100	1.30720900
H	-9.32180500	2.12473700	-0.78201200
O	-7.95209700	0.86123500	-1.71341700
C	-7.89208100	3.22374700	-1.96424100
H	-8.46215300	3.12408400	-2.89592900
H	-6.82096000	3.16557000	-2.20632600
O	-8.20336200	4.42833500	-1.28941800
H	-8.00235600	5.15931500	-1.89351100
O	-7.96650700	2.86407300	1.23314900
H	-7.40382500	2.79183800	2.02126900
O	-6.32528700	0.06905500	1.17644500
H	-6.47465300	-0.80134800	1.58218300
H	-8.82720700	-0.72158100	-0.69726200
C	-2.63700300	-1.55689400	3.26477100
C	-1.88244300	-1.45372700	1.92847300
C	-2.36874300	-0.09258300	1.33876800
C	-3.66800900	-0.43149800	3.20607300
H	-1.91638600	-1.35653300	4.07120800
H	-2.19483300	-2.25952400	1.25538900
H	-4.59280000	-0.82601400	2.76693700
O	-3.09859600	0.56099500	2.35310300
C	-3.95234100	0.23512900	4.53560800
H	-4.67146000	1.05101300	4.39080200
H	-3.01556900	0.66303600	4.92078500
O	-4.46162700	-0.76315100	5.40035300
H	-4.63684100	-0.34565200	6.25766000
O	-3.30268600	-2.78404300	3.46414800
H	-2.62788700	-3.46932100	3.59507700
O	-0.49631000	-1.49319900	2.17764100
H	-0.02693400	-1.59355800	1.31935100
H	-2.97777600	-0.23288700	0.43807900

6. The global minimum of MP-AuNC
Gibbs Free Energies= -2297.964114 a.u

Au	-1.39152100	-2.03863600	-1.35101600
Au	-0.11248200	0.27665700	-0.90611800
Au	0.99584400	2.72653400	-0.60715600
Au	-1.38373200	2.42077600	0.49510700
Au	0.95884700	-2.29624200	-0.14552700
N	-1.78139700	-2.49013500	2.27440100
C	-0.90443400	-1.47623600	2.58776300
N	-1.39214700	-0.28317600	2.37257900
C	-2.65652500	-0.50457900	1.86035700
C	-3.68842700	0.36438800	1.43847200
N	-4.87597200	-0.20206600	1.06251400
C	-5.02319800	-1.50316600	1.04340300
H	-4.24319300	-3.39135400	1.34013200
N	-4.06364000	-2.38895500	1.38632400
C	-2.88773000	-1.88120000	1.80749900
S	-3.58965700	2.08352300	1.40254000
H	-5.96797500	-1.93262800	0.73193600
H	0.07199000	-1.69627500	2.99603300
N	4.47074400	1.59494600	-0.23903400
C	3.66764800	0.98934400	-1.18010300
N	3.30583600	-0.22197200	-0.84737900
C	3.87812900	-0.43656400	0.38988600
C	3.83910300	-1.52695200	1.28867600
N	4.61936800	-1.44721600	2.41056000
C	5.31030800	-0.36636500	2.67141500
H	5.87300600	1.55548500	2.16878400
N	5.32665700	0.73939000	1.89596500
C	4.61442000	0.69225700	0.75154700
S	2.91563400	-2.95858400	1.08130100
H	5.91679800	-0.31908700	3.56812600
H	3.41160000	1.49771300	-2.09967000
H	-1.60369100	-3.48801300	2.34213800
H	4.87442400	2.52579100	-0.29188000

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