Supporting Information

Ultra-sensitive recognizing of AP-site in DNA at the Single-cell Level: 
One molecular rotor sequentially self-regulated to form multiple stable 
conformations

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1. **Procedures section**

A.R. grade of solvents and reagents were used in this work. Column chromatographic was used to purify compounds and silica gel (200-300 mesh) was used as fillers. DNA, RNA, Triacylglycerol Acylhydrolase, Lysozyme, Proteinase, Histone, Collagen, Hemoglobin, BSA, β-amylase, Trypsin and Chymotrypsin were obtained from Sigma Chemical Co. (USA). AP-sites in DNA were induced by nitrosamine 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) as reference method.\textsuperscript{51, 52} AP-sites Quantification Kit (DNA Damage counting kit) was purchased from Dojindo (Japan).

Doubly purified water was used in all experiments, which was prepared using by a Milli-Q system. BMN-Fluors and intermediate products as stock were used in spectrographic determination and cell experiments. NMR spectra were obtained from Avance 400 or 600 MHz spectrometer (Bruker Co., Switzerland). Lambd 950 spectrophotometer from PerkinElmer (USA) and a LS-55 spectrophotometer from PerkinElmer were used to detect the absorption spectra and fluorescence spectra in vitro. Ultra-high-resolution electro-spray time-of-flight mass spectrometry (Compact) was used to detect the molecular mass. BD FACSCanto II (USA) was used to sort cells in flow cytometer analysis.

The different sequences of DNA were used in the all spectrum measurements, which were synthesized by the Thermo Fisher Scientific. The sequences of DNA were listed as follow:

**DNA sequencing:** 5’-
D(*TP*TP*CP*TP*AP*GP*GP*TP*CP*TP*AP*GP*GP*AP*CP*CP*CP*C)-3’,

**2 AP sites in DNA sequencing:** 5’-D(*TP*TP*CP*TP*AP*GP*GP*(RDG)P*(RDG)P*CP*TP*AP*GP*GP*AP*CP*CP*CP*C)-3’,

**4 AP sites in DNA sequencing:** 5’-D(*TP*TP*CP*TP*AP*GP*(RDG)P*(RDG)P*(RDG)P*CP*TP*AP*GP*GP*AP*CP*CP*CP*C)-3’,

**6 AP sites in DNA sequencing:** 5’-D(*TP*TP*CP*TP*AP*(RDG)P*(RDG)P*(RDG)P*(RDG)P*CP*TP*AP*GP*GP*AP*CP*CP*CP*C)-3’,

**8 AP sites in DNA sequencing:** 5’-D(*TP*TP*CP*TP*(RDG)P*(RDG)P*(RDG)P*(RDG)P*(RDG)P*AP*GP*GP*AP*CP*CP*CP*C)-3’,

**10 AP sites in DNA sequencing:** 5’-D(*TP*TP*CP*(RDG)P*(RDG)P*(RDG)P*(RDG)P*(RDG)P*(RDG)P*(RDG)P*(RDG)P*
(RDG)P*(RDG)P*(RDG)P*(RDG)P*GP*GP*GP*AP*CP*CP*CP*C)-3',


Gel electrophosis of the different AP sites in DNA sequencing

5-formyl uracil in DNA sequencing: 5'-D(*TP*TP*CP*TP*AP*GP*GP*AP*GP*GP*AP*GP*CP*CP*CP*C)-3',

1.1 Spectrographic determination in vitro

A Lambda 950 spectrophotometer from PerkinElmer (USA) and a LS-55 spectrophotometer from PerkinElmer (USA) were used to measure absorption spectra and fluorescence spectra, respectively. In all spectral experiments, the final solutions contained < 5.0‰ DMSO. Each experiment was carried out in five replicates (n = 5). The relative fluorescence quantum yields were determined using Rhodamine B ($\Phi_F = 0.97$ in methanol) by the following equation:

$$\Phi_1 = \Phi_0 \left( \frac{F_1}{F_0} \right) \left( \frac{A_x}{A_s} \right) \left( \frac{\lambda_{ex}}{\lambda_{em}} \right) \left( \frac{n_x}{n_s} \right)^2$$

where $\Phi$ represents quantum yield; $F$ is the integrated area under the corrected emission spectrum; $A$ is absorbance at the excitation wavelength; $\lambda_{ex}$ is the excitation wavelength; $n$ is the refractive index of the solution (because of the low concentrations of the solutions, $10^{-7}$-$10^{-8}$ mol/L, the refractive indices of the solutions were replaced with those of the solvents); and the subscripts x and s refer to the unknown and the standard, respectively. The detection limit was
calculated by three times the standard deviation divided by the slope of the blank. The data were obtained from replicate experiments (n = 5).

1.2 $^1$H NMR Titration in D$_2$O

All $^1$H NMR titration spectra were obtained at 25 °C using a Bruker 600-MHz spectrometer equipped. Data were acquired and processed using Bruker TopSpin 2.1 software and the software package Sparky. d1-BMN (3.0 mM) and HDM (3.0 mM) in D$_2$O was used in $^1$H NMR titration.

1.3 Photostability in solution

d1-BMN (3.0 μM) in PBS buffer (pH 7.4) at 25 °C. The solutions were irradiated by a 500W iodine-tungsten lamp situated 250 mm away for 7 h. An aqueous solution of sodium nitrite (50 g/L) was placed between the samples and the lamp as a light filter (to cut off the light shorter than 400 nm) and as a heat filter. The photostabilities were expressed in terms of remaining absorption (%) calculated from the changes of absorbance at the absorption maximum before and after irradiation by iodine-tungsten lamp. The absorbance was determined. The data were obtained from replicate experiments (n = 5).

1.4 Quantum Calculations

All the quantum chemical calculations were done with the Gaussian 16 suite. The geometry optimizations of the dyes were performed using density functional theory (DFT) with Becke’s three-parameter hybrid exchange function with Lee-Yang-Parr gradient-corrected correlation functional (B3-LYP functional).

Gaussian 16 was used in quantum chemical, and the work of Han was as reference for setting up calculations parameter$^3$. The density functional theory (DFT)$^4$ with B3-LYP and B3LYP-D3 functional were used in the geometry optimizations of the dyes. And 6–31G* basis set was utilized. No constraints to bonds/angles/dihedral angles were applied in the calculations and all atoms were free to optimize. The time-dependent density functional
theory (TD-DFT)$^{55,56}$ at the B3LYP/6-31G** level was used to calculate electronic transition energies and corresponding oscillator strengths.

1.5 Molecular docking

All works of molecular docking were conducted in Yinfo Cloud Platform (http://cloud.yinfotek.com/). The UCSF DOCK 6.9 software was used for the molecular docking. The chemical structure of the small molecule d1-BMN was drawn by JSME and converted to 3D structure with energy minimization in MMFF94 force field. The crystal structure of DNA Polymerase- damaged DNA complex was taken from the RCSB Protein Data Bank. PDB encoding is 4Q45. NDB encoding is NA2985. DOI: 10.2210/pdb4Q45/pdb. The DMS tool$^{57}$ was employed to build molecular surface of the receptor using a probe atom with a 1.4 Å radius. The binding pocket was defined by the crystal ligand and spheres were generated filling the site by employing the Sphgen module in UCSF Chimera.$^{58}$ A box enclosing the spheres was set with center of (45.397, 58.906, 38.962) and sizes of (18.842, -23.879, 113.892), within which grids necessary for rapid score evaluation were created by the Grid module. Finally, DOCK 6.9$^{59}$ program was utilized to conduct semi-flexible docking where 10000 different orientations were produced. Clustering analysis were performed (RMSD threshold was set 2.0 Å) for candidate poses and the best scored ones were output.

DNA sequencing: 5'-D(*TP*CP*TP*AP*GP*GP*GP*TP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3',

Damaged DNA sequencing: 5'-D(*TP*CP*TP*AP*GP*GP*(RDG)P*TP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3'.

1.6 Molecular dynamics simulation

Molecular dynamics simulation (MD) was performed using the sander module implemented in the Amber 16 suite, with the BSC1 force field used for the DNA. Hydrogen atoms and sodium ions (to neutralize the negative charges) were added to the DNA with the tleap utility. The simulation system was immersed in a truncated octahedral box of TIP3P explicit water, extended 10 Å outside the DNA on all sides. To start the MD simulation, the simulation system was energy-minimized during 10,000 conjugate-gradient steps. After energy minimization, the system was heated in the NVT ensemble from 0 to 300 K over 50 ps. This procedure was followed by 50 ps of NPT simulation at 300 K
and 1 atm pressure using the Langevin dynamics algorithm. After equilibration, 20ns production MD simulation was performed. In all MD simulations, bonds involving hydrogen atoms were constrained using the SHAKE algorithm. Long range interactions were treated using the particle-mesh Ewald (PME) method and a non-bonded interaction cutoff of 10 Å was used. A time step of 2.0 fs was used and coordinates of the system were saved every 2ps.

1.7  Cell Culture

Hepg 2 cell lines were obtained from the Chinese Academy of Medical Sciences. The red-free Dulbecco’s Modified Eagle’s Medium (DMEM, WelGene) and eagle's minimum essential medium (MEM, WelGene) supplemented with penicillin/streptomycin and 10 % fetal bovine serum (FBS; Gibco) were used for culture cells in a CO₂ incubator at 37 °C. One day before imaging, the cells mentioned above were seeded into confocal dishes with well glass bottom (MatTek, 1# glass, 0.13-0.16 mm). They were incubated at 37 °C in 5.0 wt %/vol CO₂ for 24 h. And then, the cells were incubated with OPM at a certain concentration.

1.8  Single Cell Gel Electrophoresis Assay

Briefly, cells are mixed with 0.5% low-melting agarose at 37 °C and then placed on a microscope slide coated with 0.5% normal agarose. When the agarose has solidified, an additional layer of agarose is added. After the preparation of the three layers of this material, the cells are lysed in a detergent solution for at least 1.0 h and then the slides are put into a neutral buffer in a electrophoresis chamber, allowing the DNA unwinding, the electrophoresis is carried out, resulting in the migration of small pieces from the core of DNA, toward the electric field. After electrophoresis the slides are rinsed with PBS and cells are stained with a dye (EB). The method is also described in detail in the reference S10 and S11.

Sample Preparation: Cell samples (HepG 2 cell) should be prepared immediately before starting the assay. Cell samples should be handled under yellow light to prevent DNA damage from ultraviolet light. Buffers should be cooled to 4°C to inhibit endogenous damage occurring during sample preparation and to inhibit repair in cells. PBS must be calcium and magnesium free to inhibit endonuclease activities. The appropriate controls should also be included. Optimal results in the CometAssay® are usually obtained with 500-1000 cells per CometSlideTM sample
area. Using 50 µL of a cell suspension at $1 \times 10^5$ cells per ml combined with 500 µL of LMAgarose will provide the correct agarose concentration and cell density for optimal results when spreading 50 µL per well.

**Controls:** A sample of untreated cells should always be processed to control for endogenous levels of damage within cells, and for damage that may occur during sample preparation. Control cells and treated cells should be handled in an identical manner. Treatment will generate significant oxidative damage in the majority of cells, thereby providing a positive control for each step in the CometAssay.

**Neutral CometAssay:**

1. Prepare Lysis Solution and cool at 4°C for at least 20 minutes before use.

2. Melt LMAgarose in a beaker of boiling water for 5 minutes, with the cap loosened, and then cool in a 37°C water bath for at least 20 minutes.

3. Combine cells at 1×10⁵/mL with molten LMAgarose (at 37°C) at a ratio of 1:10 (v/v) and immediately pipette 50 µL onto CometSlide™. Use side of pipette tip to spread agarose/cells over sample area. Comet LMAgarose (molten and at 37°C from step 2) 500 µL Cells in 1X PBS (Ca²⁺ and Mg²⁺ free) at 1×10⁵/ml 50 µL.

4. Place slides flat at 4°C in the dark (*e.g.* place in refrigerator) for 10 minutes. A 0.5 mm clear ring appears at edge of CometSlide™ area. Increasing gelling time to 30 minutes improves adherence of samples in high humidity environments.

5. Immerse slides in 4°C Lysis Solution for 1 hour or overnight for added sensitivity.

6. Remove slides from Lysis Buffer, drain excess buffer from slide and gently immerse in 50 ml of 4°C 1× Neutral Electrophoresis Buffer for 30 minutes.

7. For the CometAssay® ES unit, add ~850 mL 4°C 1× Neutral Electrophoresis Buffer, place slides in electrophoresis slide tray and cover with Slide Tray Overlay. Set power supply to 21 volts and apply voltage for 45 min at 4°C. For other electrophoresis units, align slides equidistant from electrodes, add 1× Neutral Electrophoresis Buffer not to exceed 0.5 cm above slides, and apply voltage at 1 volt per cm (measured electrode to electrode).

8. Drain excess Neutral Electrophoresis Buffer and gently immerse slides in DNA Precipitation Solution for 30 minutes at room temperature.
9. Immerse slides in 70% ethanol for 30 minutes at room temperature.

10. Dry samples at 37°C for 10-15 minutes. Drying brings all the cells in a single plane to facilitate observation. Samples may be stored at room temperature, with desiccant prior to scoring at this stage.

11. Place 100 µL of diluted EB or d1-BMN onto each circle of dried agarose and stain 30 minutes (room temperature) in the dark. Gently tap slide to remove excess EB or d1-BMN solution and rinse briefly in water. Allow slides to dry completely at 37°C.

**Data Analysis:** In healthy cells the fluorescence is confined to the nucleoid (comprised of high molecular weight DNA): undamaged DNA is supercoiled and thus, does not migrate very far out of the nucleoid under the influence of an electric current. Whereas in cells that have accrued DNA damage, migrating fragments (comet tail) from the nucleoid (comet head) are observed. The negatively charged DNA migrates toward the anode and the extrusion length reflects increasing relaxation of supercoiling, which is indicative of damage. In neutral comet assays, Tail Moment is primarily used.

**Quantitative Analysis:** The DNA damage was assessed with percentage of DNA in the tail (TI %) and for this purpose one hundred cells were assessed per slide by using Comet assay IV image analysis system (Perceptive Instruments, UK). EB maximum excitation is 300 nm and 360 nm, EB maximum emission is 590 nm. d1-BMN maximum excitation is 354 and 400 nm, d1-BMN maximum emission is 414, 440, 468, 495, 524 or 562 nm. Fluorescein filter is adequate.

Gel electrophoresis was used to verify that DNA containing AP-sites not converted to single strand break during the assay in this work. Gel electrophoresis results indicated that DNA not converted to single strand break before (1), during (2), and after the assay (3) compare with the control group (C).
The DNA gel electrophoresis before (1), during (2), and after the assay (3) compare with the control group (C).

1.9 Cytotoxicity

Hepg 2 cell lines and NIH 3T3 cell lines were prepared for cell viability studies in 96-well plates (1 × 10^5 cells per well that were incubated in 100 μL). The cells were incubated for an additional 24 h with dyes d1-BMN in different concentrations. Subsequently, 100 μL of 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT, Sigma Chemical Co. U.S.A.) was added into each well, followed by further incubation for 4 h at 37 °C. The DMEM was remove and DMSO (200 μL/well) added to dissolve the reddish-blue crystals. Optical density (OD) was determined by a microplate reader (Spectra Max M5, Molecular Devices) at 570 nm with subtraction of the absorbance of the cell-free blank volume at 630 nm. The results from the six individual experiments were averaged. The relative cell viability (100%) was calculated using the following equation:

\[
\text{Cell viability (\%)} = \frac{(OD_{\text{dye}} - OD_{k-dye})}{(OD_{\text{ctrl}} - OD_{k-ctrl})} \times 100
\]
1.10 Flow cytometry

Hepg 2 cell lines with incubated by **d1-BMN** (3.0 μM) for 10 min, then the cells were washed. And they were dispersed into PBS solution at level of 10,000 cells/500 μL. Samples were analyzed with the laser (405 nm) on a flow cytometer (BD FACSCanto II, USA). The average fluorescence intensity in 10,000 cells was obtained and analyzed with BD FACSDiva software. Each individual cell should contain a mixture of AP-site with different sizes, thus, the same cell can give a mixture of fluorescence signals, for example red, orange, yellow, green and blue fluorescence. So, to sort the cell into different channels, we used the sorting function of flow cytometry to in succession and repeatedly sort the cell. Furthermore, in every control experiment for different fluorescence channels, they were added fluorescence compensation to obtain absolutely strong fluorescence signal for the target collection channel.

2. Derivative molecule and synthetic route.

![Recognition Reaction–Hydrolysis Reaction](image)

**Scheme S1.** Derivative molecules. The hydrolysis transformation of 2-(4-vinylbenzylidene)malononitrile derivatives.

The synthesis of 2d-1 ((E)-4-(2-(5-hydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde)

1d-1 (2-methyl-1H-benzo[d]imidazol-5-ol (2.6 mmol, 386 mg)), p-Phthalaldehyde (3.0 mmol, 400 mg) was added into acetic acid solution. Under stirring, they were heated to refluxed temperature (120 °C). After complete consumption of 1d-1 monitored by TLC, concentrated hydrochloric acid (1.0 mL) was added into the mixture solution, and was stood for 1.0 h. Then, there appeared brown solid in the mixture solution, and it were filtrated. The filter liquor was regulated by sodium hydroxide to neutral. Than, the crude product appeared, which was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (50:1 to 5:1, v/v) to obtain a yellow solid 2d-1 ((E)-4-(2-(5-hydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde). Yield 89%. ¹H NMR (400 MHz, CDCl₃), δ: 12.32 (s, 1H), 10.06 (s, 1H), 7.98 (d, 2H, J = 5.26 Hz), 7.89 (d, 2H, J = 5.27 Hz), 7.80 (d, 1H, J = 10.95 Hz), 7.60 (d, 1H, J = 10.95 Hz), 7.47 (d, 1H, J = 10.95 Hz), 7.36 (d, 1H, J = 10.95 Hz), 7.23 (d, 1H, J = 5.24 Hz), 5.35 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ: 190.7, 151.7, 143.3, 141.5, 140.9, 136.1, 133.4, 131.8, 129.7, 129.0, 124.0, 116.6, 114.6, 111.4, 102.6. HRMS: m/z calcd for C₁₆H₁₂N₂O₂: 264.0899, found: 264.0905.
The synthesis of 3d-1 ((E)-2-(4-(2-(5-hydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile)

2d-1 (2.0 mmol, 530 mg) and malononitrile (4.0 mmol, 265 mg) were suspended in DCM, and then they was at room temperature under stirring for 4.0 h. Than, the crude product appeared, which was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 1:1, v/v) to obtain a yellow solid 3d-1. Yield 73%. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 12.05 (s, 1H), 7.95 (s, 1H), 7.88 (d, 2H, \(J = 5.26\) Hz), 7.77 (d, 1H, \(J = 10.95\) Hz), 7.65 (d, 2H, \(J = 5.27\) Hz), 7.57 (d, 1H, \(J = 10.95\) Hz), 7.44 (d, 1H, \(J = 10.80\) Hz), 7.33 (d, 1H, \(J = 10.80\) Hz), 7.18 (d, 1H, \(J = 10.80\) Hz), 5.36 (s, 1H). \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 161.8, 151.6, 141.6, 140.1, 135.9, 133.2, 131.4, 130.6, 128.9, 124.0, 116.7, 113.5, 111.4, 102.5, 81.5. HRMS: m/z calcd for C\(_{19}\)H\(_{22}\)N\(_4\)O: 312.1011, found: 312.1019.

The synthesis of d1-BMN ((E)-2-(4-(2-(5-aminoxy)-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile)

3d-1 (2.76 mmol, 860 mg) was dissolved in 4 mL of methanol, and then potassium tert-butoxide (309 mg, 2.76 mmol) was added. The mixture was allowed to stir for 0.5 h under N\(_2\) atmosphere. Methanol was removed, and the residue was taken up in 2 mL of dichloromethane. The freshly prepared O-mesitylsulfonylhydroxylamine (378 mg, 1.76 mmol) in 2 mL of dichloromethane was then added under ice cooling. The mixture was allowed to stir for 1 h, and dichloromethane was then removed under reduce pressure to afford the corresponding product. It was purified by column chromatography on silica gel eluted with DCM/Methanol (100:1 to 10:1, v/v) to obtain a yellow solid d1-BMN. Yield 69%. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 12.07 (s, 1H), 7.98 (s, 1H), 7.90 (d, 2H, \(J = 5.26\) Hz), 7.79 (d, 1H, \(J = 10.95\) Hz), 7.67 (d, 2H, \(J = 5.27\) Hz), 7.59 (d, 1H, \(J = 10.95\) Hz), 7.46 (d, 1H, \(J = 10.80\) Hz), 7.35 (d, 1H, \(J = 10.80\) Hz), 7.20 (d, 1H, \(J = 10.80\) Hz), 6.85 (s, 2H). \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 161.8, 151.6, 141.6, 140.1, 136.9, 133.2, 131.4, 130.6, 128.9, 124.4, 116.7, 113.5, 111.4, 102.5, 81.5. HRMS: m/z calcd for C\(_{19}\)H\(_{13}\)N\(_4\)O: 327.1120, found: 327.1129.
The synthesis of 2d-2 (\((E)-4-(2-(5,6\text{-dihydroxy-1\text{-H}}\text{-benzo}[d]\text{imidazol-2-yl})\text{vinyl})\text{benzaldehyde}\))

\[
\begin{align*}
\text{HO} & \quad \text{N} & \quad \text{N} & \quad \text{CHO} \\
(\text{E})-4-(2-(5,6\text{-dihydroxy-1\text{-H}}\text{-benzo}[d]\text{imidazol-2-yl})\text{vinyl})\text{benzaldehyde}
\end{align*}
\]

The synthesis of 2d-2 was followed by the procedure described in previous method for 2d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (50:1 to 2:1, v/v) to obtain a yellow solid 2d-2 (\((E)-4-(2-(5,6\text{-dihydroxy-1\text{-H}}\text{-benzo}[d]\text{imidazol-2-yl})\text{vinyl})\text{benzaldehyde}\)). Yield 80%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\): 12.30 (s, 1H), 10.06 (s, 1H), 7.98 (d, 2H, \(J = 5.26\) Hz), 7.89 (d, 2H, \(J = 5.27\) Hz), 7.47 (d, 2H, \(J = 10.95\) Hz), 7.34 (d, 1H, \(J = 10.59\) Hz), 7.21 (d, 1H, \(J = 10.59\) Hz), 5.35 (s, 2H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 191.7, 143.9, 141.5, 138.9, 136.1, 133.4, 132.8, 129.7, 129.0, 124.0, 103.5. HRMS: m/z calcd for C\(_{16}\)H\(_{12}\)N\(_2\)O\(_3\): 280.0848, found: 280.0844.

The synthesis of 3d-2 (\((E)-2-(4-(2-(5,6\text{-dihydroxy-1\text{-H}}\text{-benzo}[d]\text{imidazol-2-yl})\text{vinyl})\text{benzyldiene})\text{malononitrile}\))

\[
\begin{align*}
\text{HO} & \quad \text{N} & \quad \text{N} & \quad \text{C} & \quad \text{CN} \\
(\text{E})-2-(4-(2-(5,6\text{-dihydroxy-1\text{-H}}\text{-benzo}[d]\text{imidazol-2-yl})\text{vinyl})\text{benzyldiene})\text{malononitrile}
\end{align*}
\]

The synthesis of 3d-2 was followed by the procedure described in previous method for 3d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 1:1, v/v) to obtain a yellow solid 3d-2. Yield 70%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\): 12.30 (s, 1H), 7.98 (d, 2H, \(J = 5.26\) Hz), 7.89 (d, 2H, \(J = 5.27\) Hz), 7.64 (s, 1H), 7.47 (d, 2H, \(J = 10.95\) Hz), 7.34 (d, 1H, \(J = 10.55\) Hz), 7.21 (d, 1H, \(J = 10.55\) Hz), 5.36 (s, 2H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 161.7, 141.5, 138.9, 136.7, 133.4, 132.8, 130.6, 129.0, 124.0, 113.6, 103.5, 81.4. HRMS: m/z calcd for C\(_{19}\)H\(_{13}\)N\(_4\)O\(_2\): 328.0960, found: 328.0962.
The synthesis of d2-BMN ((E)-2-(4-(2-(5,6-bis(aminooxy)-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile)

The synthesis of d2-BMN was followed by the procedure described in previous method for d1-BMN. It was purified by column chromatography on silica gel eluted with DCM/Methanol (100:1 to 10:1, v/v) to obtain a yellow solid d2-BMN. Yield 54%. 1H NMR (400 MHz, CDCl3), δ 12.32 (s, 1H), 7.98 (d, 2H, J = 5.26 Hz), 7.89 (d, 2H, J = 5.26 Hz), 7.64 (s, 1H), 7.47 (d, 2H, J = 10.95 Hz), 7.34 (d, 1H, J = 10.95 Hz), 7.21 (d, 1H, J = 10.95 Hz), 6.78 (s, 4H). 13C NMR (100 MHz, CDCl3): δ: 161.5, 141.5, 138.9, 136.5, 133.4, 132.8, 130.3, 129.0, 124.5, 113.6, 103.8, 81.8. HRMS: m/z calcd for C19H14N2O2: 358.1178, found: 358.1182.

The synthesis of 2a-1 ((E)-4-(2-(6-hydroxy-3H-indol-2-yl)vinyl)benzaldehyde)

The synthesis of 2a-1 was followed by the procedure described in previous method for 2d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 10:1, v/v) to obtain a yellow solid 2a-1 ((E)-4-(2-(6-hydroxy-3H-indol-2-yl)vinyl)benzaldehyde). Yield 80%. 1H NMR (400 MHz, CDCl3), δ: 10.06 (s, 1H), 7.98 (d, 2H, J = 5.26 Hz), 7.89 (d, 2H, J = 5.27 Hz), 7.80 (d, 1H, J = 10.95 Hz), 7.60 (d, 1H, J = 10.95 Hz), 7.47 (d, 1H, J = 10.95 Hz), 7.36 (d, 1H, J = 10.59 Hz), 7.21 (d, 1H, J = 10.59 Hz), 5.35 (s, 1H), 3.04 (s, 2H). 13C NMR (100 MHz, CDCl3): δ: 190.7, 164.6, 156.4, 140.9, 136.1, 131.8, 129.7, 129.8, 129.6, 129.0, 124.0, 120.1, 114.6, 109.4, 35.3. HRMS: m/z calcd for C17H13NO2: 263.0946, found: 263.0948.

The synthesis of 3a-1 ((E)-2-(4-(2-(5,6-dihydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile)

The synthesis of 3a-1 was followed by the procedure described in previous method for 3d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 1:1, v/v) to obtain a yellow solid 3a-1. Yield 73%. 1H NMR (400 MHz, CDCl3), δ 7.94 (s, 1H), 7.86 (d, 2H, J = 5.26 Hz), 7.75 (d, 1H, J = 10.95 Hz), 7.63 (d, 2H, J = 5.27 Hz), 7.55 (d, 1H, J = 10.95 Hz), 7.42 (d, 1H, J = 10.95 Hz), 7.31 (d, 1H, J = 10.85 Hz), 7.17 (d, 1H, J = 10.85 Hz), 7.09 (d, 1H, J = 10.85 Hz), 7.05 (d, 1H, J = 10.85 Hz), 6.64 (d, 1H, J = 10.85 Hz), 6.36 (d, 1H, J = 10.85 Hz), 5.94 (d, 1H, J = 10.85 Hz), 5.26 (d, 1H, J = 10.85 Hz).
= 10.95 Hz), 5.35 (s, 1H), 3.04 (s, 2H). 13C NMR (100 MHz, CDCl3): δ: 164.6, 161.8, 157.6, 156.8, 134.9, 131.2, 130.4, 129.6, 128.9, 123.4, 119.8, 116.7, 114.5, 113.4, 109.5, 81.6, 35.4. HRMS: m/z calcd for C20H13N3O: 311.1059, found: 311.1063.

The synthesis of a1-BMN (E)-2-(4-(6-(aminoxy)-3H-indol-2-yl)vinyl)benzylidene)malononitrile

The synthesis of a1-BMN was followed by the procedure described in previous method for d1-BMN. It was purified by column chromatography on silica gel eluted with DCM/Methanol (100:1 to 10:1, v/v) to obtain a yellow solid a1-BMN. Yield 63%. 1H NMR (400 MHz, CDCl3), δ7.99 (s, 1H), 7.91 (d, 2H, J = 5.26 Hz), 7.80 (d, 1H, J = 10.95 Hz), 7.68 (d, 2H, J = 5.27 Hz), 7.60 (d, 1H, J = 10.95 Hz), 7.47 (d, 1H, J = 10.95 Hz), 7.36 (d, 1H, J = 10.90 Hz), 7.22 (d, 1H, J = 10.95 Hz), 6.87(s, 2H), 3.04 (s, 2H). 13C NMR (100 MHz, CDCl3): δ: 164.6, 161.8, 157.6, 156.8, 134.9, 131.2, 130.4, 129.6, 128.9, 123.4, 119.8, 116.7, 114.5, 113.4, 109.5, 81.6, 35.4. HRMS: m/z calcd for C20H14N4O: 326.1168, found: 326.1165.

The synthesis of 2a-2 (E)-4-(2-(5,6-dihydroxy-3H-indol-2-yl)vinyl)benzaldehyde

The synthesis of 2a-2 was followed by the procedure described in previous method for 2d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 10:1, v/v) to obtain a yellow solid 2a-2. Yield 75%. 1H NMR (400 MHz, CDCl3), δ: 10.06 (s, 1H), 7.98 (d, 2H, J = 5.26 Hz), 7.89 (d, 2H, J = 5.27 Hz), 7.47 (d, 2H, J = 5.26 Hz), 7.34 (d, 1H, J = 10.59 Hz), 7.21 (d, 1H, J = 10.59 Hz), 5.34 (s, 2H), 3.04 (s, 2H); 13C NMR (100 MHz, CDCl3): δ: 191.7, 164.4, 148.6, 145.3, 144.0, 140.9, 136.1, 129.7, 129.0, 125.0, 120.0, 117.6, 111.4, 35.3. HRMS: m/z calcd for C17H13NO5: 279.0895, found: 279.0898.
The synthesis of 3a-2 ((E)-2-(4-(2-(5,6-dihydroxy-3H-indol-2-yl)vinyl)benzyldiene)malononitrile)

The synthesis of 3a-2 was followed by the procedure described in previous method for 3d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 1:1, v/v) to obtain a yellow solid 3a-2. Yield 56%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\) 7.98 (d, 2H, \(J = 5.26\) Hz), 7.89 (d, 2H, \(J = 5.27\) Hz), 7.64 (s, 1H), 7.47 (d, 2H, \(J = 10.95\) Hz), 7.34 (d, 1H, \(J = 10.55\) Hz), 7.21 (d, 1H, \(J = 10.55\) Hz), 5.34 (s, 2H), 3.04 (s, 2H). \(^1^3\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 164.8, 161.6, 148.3, 145.6, 144.1, 134.2, 130.4, 129.6, 128.9, 125.4, 120.4, 117.7, 113.5, 111.4, 102.5, 81.4, 35.2. HRMS: m/z calcd for C\(_{20}\)H\(_{13}\)N\(_2\): 327.1008, found: 327.1002.

The synthesis of a2-BMN ((E)-2-(4-(2-(5,6-bis(aminooxy)-3H-indol-2-yl)vinyl)benzyldiene)malononitrile)

The synthesis of a2-BMN was followed by the procedure described in previous method for d1-BMN. It was purified by column chromatography on silica gel eluted with DCM/Methanol (100:1 to 2:1, v/v) to obtain a yellow solid d2-BMN. Yield 54%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\) 7.98 (d, 2H, \(J = 5.26\) Hz), 7.89 (d, 2H, \(J = 5.27\) Hz), 7.65 (s, 1H), 7.47 (d, 2H, \(J = 10.95\) Hz), 7.34 (d, 1H, \(J = 10.95\) Hz), 7.21 (d, 1H, \(J = 10.95\) Hz), 6.78 (s, 4H), 3.04 (s, 2H). \(^1^3\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 164.7, 161.6, 148.3, 145.5, 144.1, 134.2, 130.4, 129.6, 128.8, 125.4, 120.4, 117.7, 113.5, 111.4, 102.5, 81.4, 35.2. HRMS: m/z calcd for C\(_{23}\)H\(_{15}\)N\(_5\): 357.1226, found: 357.1222.

The synthesis of 2b ((E)-4-(2-(6-hydroxy-3-methyl-3H-indol-2-yl)vinyl)benzaldehyde)

The synthesis of 2b was followed by the procedure described in previous method for 2d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 10:1, v/v) to obtain a yellow solid 2b. Yield 83%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\): 10.06 (s, 1H), 7.98 (d, 2H, \(J = 5.27\) Hz), 7.65 (s, 1H), 7.47 (d, 2H, \(J = 10.95\) Hz), 7.34 (d, 1H, \(J = 10.55\) Hz), 7.21 (d, 1H, \(J = 10.55\) Hz), 3.04 (s, 2H). \(^1^3\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 164.7, 161.6, 148.3, 145.5, 144.1, 134.2, 130.4, 129.6, 128.8, 125.4, 120.4, 117.7, 113.5, 111.4, 102.5, 81.4, 35.2. HRMS: m/z calcd for C\(_{24}\)H\(_{15}\)O\(_2\)N\(_2\): 367.1380, found: 367.1378.
The synthesis of 3b ((E)-2-(4-(6-hydroxy-3-methyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile)

(E)-2-(4-(6-hydroxy-3-methyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

The synthesis of 3b was followed by the procedure described in previous method for 3d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 1:1, v/v) to obtain a yellow solid 3b. Yield 78%. ¹H NMR (400 MHz, CDCl₃), δ 7.94 (s, 1H), 7.86 (d, 2H, J = 5.26 Hz), 7.75 (d, 1H, J = 10.95 Hz), 7.63 (d, 2H, J = 5.27 Hz), 7.55 (d, 1H, J = 10.95 Hz), 7.42 (d, 1H, J = 10.95 Hz), 7.31 (d, 1H, J = 10.85 Hz), 7.17 (d, 1H, J = 10.95 Hz), 5.35 (s, 1H), 3.23 (s, 1H), 1.31 (s,3H). ¹³C NMR (100 MHz, CDCl₃): δ: 164.7, 160.9, 157.1, 154.9, 134.9, 130.4, 129.6, 128.9, 126.4, 120.0, 114.7, 113.5, 109.4, 81.5, 35.8, 18.6. HRMS: m/z calcld for C₁₉H₁₃NO₅: 325.1215, found: 325.1209.

The synthesis of b-BMN ((E)-2-(4-(6-(aminoxy)-3-methyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile)

(E)-2-(4-(6-(aminoxy)-3-methyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

The synthesis of b-BMN was followed by the procedure described in previous method for d1-BMN. It was purified by column chromatography on silica gel eluted with DCM/Methanol (100:1 to 10:1, v/v) to obtain a yellow solid b-BMN. Yield 61%. ¹H NMR (400 MHz, CDCl₃), δ 7.99 (s, 1H), 7.91 (d, 2H, J = 5.26 Hz), 7.80 (d, 1H, J = 10.95 Hz), 7.68 (d, 2H, J = 5.27 Hz), 7.60 (d, 1H, J = 10.95 Hz), 7.47 (d, 1H, J = 10.95 Hz), 7.36 (d, 1H, J = 10.90 Hz), 7.22 (d, 1H, J = 10.95 Hz), 6.87(s, 2H), 3.23 (s, 1H) , 1.32 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ: 164.5, 161.2, 157.1, 154.9, 134.9, 130.4, 129.6, 128.9, 126.4, 120.3, 114.7, 113.5, 109.4, 81.5, 35.8, 18.6. HRMS: m/z calcld for C₂₃H₁₆N₅O: 340.1324, found: 340.1315.
The synthesis of 2c ((E)-4-(2-(6-hydroxy-3,3-dimethyl-3H-indol-2-yl)vinyl)benzaldehyde)

The synthesis of 2c was followed by the procedure described in previous method for 2d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 10:1, v/v) to obtain a yellow solid 2c. Yield 89%. 

$^1$H NMR (400 MHz, CDCl$_3$), $\delta$: 10.06 (s, 1H), 7.98 (d, 2H, $J = 5.26$ Hz), 7.89 (d, 2H, $J = 5.27$ Hz), 7.80 (d, 1H, $J = 10.95$ Hz), 7.60 (d, 1H, $J = 10.95$ Hz), 7.47 (d, 1H, $J = 10.95$ Hz), 7.36 (d, 1H, $J = 10.59$ Hz), 7.21 (d, 1H, $J = 10.59$ Hz), 5.35 (s, 1H), 1.17 (s, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$: 191.3, 157.1, 153.4, 145.4, 140.9, 136.1, 129.7, 129.0, 128.1, 120.0, 114.6, 109.4, 39.1, 30.3. HRMS: m/z calcd for C$_{19}$H$_{17}$NO$_2$: 291.1259, found: 291.1251.

The synthesis of 3c ((E)-2-(4-(2-(6-hydroxy-3,3-dimethyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile)

The synthesis of 3c was followed by the procedure described in previous method for 3d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 1:1, v/v) to obtain a yellow solid 3c. Yield 70%. 

$^1$H NMR (400 MHz, CDCl$_3$), $\delta$: 7.94 (s, 1H), 7.86 (d, 2H, $J = 5.26$ Hz), 7.75 (d, 1H, $J = 10.95$ Hz), 7.63 (d, 2H, $J = 5.27$ Hz), 7.55 (d, 1H, $J = 10.95$ Hz), 7.42 (d, 1H, $J = 10.95$ Hz), 7.31 (d, 1H, $J = 10.85$ Hz), 7.17 (d, 1H, $J = 10.95$ Hz), 5.35 (s, 1H), 1.20 (s, 6H). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$: 164.5, 161.3, 157.1, 153.4, 145.4, 134.1, 130.7, 129.7, 129.0, 128.1, 114.6, 113.6, 109.4, 81.4, 39.1, 30.3. HRMS: m/z calcd for C$_{20}$H$_{17}$N$_3$O: 339.1372, found: 339.1379.

The synthesis of c-BMN ((E)-2-(4-(2-(6-(aminoxy)-3,3-dimethyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile)

The synthesis of c-BMN was followed by the procedure described in previous method for d1-BMN. It was purified by column chromatography on silica gel eluted with
DCM/Methanol (100:1 to 10:1, v/v) to obtain a yellow solid **c-BMN**. Yield 67%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\) 7.99 (s, 1H), 7.91 (d, 2H, \(J = 5.26\) Hz), 7.80 (d, 1H, \(J = 10.95\) Hz), 7.68 (d, 2H, \(J = 5.27\) Hz), 7.60 (d, 1H, \(J = 10.95\) Hz), 7.47 (d, 1H, \(J = 10.95\) Hz), 7.36 (d, 1H, \(J = 10.90\) Hz), 7.22 (d, 1H, \(J = 10.95\) Hz), 6.87 (s, 2H), 1.19 (s, 6H). \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): \(\delta\) 164.5, 161.3, 157.1, 153.4, 145.4, 134.1, 130.7, 129.7, 129.0, 128.1, 114.6, 113.6, 109.4, 81.4, 39.1, 30.3. HRMS: m/z calcd for C\(_{22}\)H\(_{18}\)N\(_4\)O: 354.1481, found: 354.1485.

**The synthesis of 2e** (\((E)-4-(2-(5-hydroxy-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde\))

The synthesis of 2e was followed by the procedure described in previous method for 2d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 10:1, v/v) to obtain a yellow solid 2e. Yield 87%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\): 10.06 (s, 1H), 7.98 (d, 2H, \(J = 5.26\) Hz), 7.89 (d, 2H, \(J = 5.27\) Hz), 7.80 (d, 1H, \(J = 10.95\) Hz), 7.60 (d, 1H, \(J = 10.95\) Hz), 7.47 (d, 1H, \(J = 10.95\) Hz), 7.36 (d, 1H, \(J = 10.95\) Hz), 7.21 (d, 1H, \(J = 5.24\) Hz), 5.35 (s, 1H), 3.38 (s, 3H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 190.7, 151.7, 143.3, 141.5, 140.9, 136.1, 133.4, 131.8, 129.7, 129.0, 124.7, 116.6, 114.6, 111.4, 103.6, 34.1. HRMS: m/z calcd for C\(_{17}\)H\(_{14}\)N\(_2\)O: 278.1055, found: 278.1058.

**The synthesis of 3e** (\((E)-2-(4-(2-(5-hydroxy-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile\))

The synthesis of 3e was followed by the procedure described in previous method for 3d-1. It was purified by column chromatography on silica gel eluted with DCM/Ethyl Acetate (100:1 to 1:1, v/v) to obtain a yellow solid 3e. Yield 75%. \(^1\)H NMR (400 MHz, CDCl\(_3\)), \(\delta\) 7.95 (s, 1H), 7.88 (d, 2H, \(J = 5.26\) Hz), 7.77 (d, 1H, \(J = 10.95\) Hz), 7.65 (d, 2H, \(J = 5.27\) Hz), 7.57 (d, 1H, \(J = 10.95\) Hz), 7.44 (d, 1H, \(J = 10.95\) Hz), 7.33 (d, 1H, \(J = 10.85\) Hz), 7.18 (d, 1H, \(J = 10.95\) Hz), 5.36 (s, 1H), 3.38 (s, 3H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\): 161.8, 151.6, 141.6, 140.1, 135.9, 133.2, 131.4, 130.6, 128.9, 124.0, 116.7, 113.5, 111.4, 102.5, 81.5, 34.2. HRMS: m/z calcd for C\(_{20}\)H\(_{14}\)N\(_2\): 326.1168, found: 325.1159.
The synthesis of e-BMN ((E)-2-(4-(2-(aminooxy)-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile)

The synthesis of e-BMN was followed by the procedure described in previous method for d1-BMN. It was purified by column chromatography on silica gel eluted with DCM/Methanol (100:1 to 10:1, v/v) to obtain a yellow solid e-BMN. Yield 57 %. $^1$H NMR (400 MHz, CDCl$_3$), $\delta$ 7.99 (s, 1H), 7.91 (d, 2H, $J = 5.26$ Hz), 7.80 (d, 1H, $J = 10.95$ Hz), 7.68 (d, 2H, $J = 5.27$ Hz), 7.60 (d, 1H, $J = 10.95$ Hz), 7.47 (d, 1H, $J = 10.95$ Hz), 7.36 (d, 1H, $J = 10.90$ Hz), 7.23 (d, 1H, $J = 10.95$ Hz), 6.87 (s, 2H), 3.38 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$: 161.8, 151.6, 141.6, 140.1, 136.9, 133.2, 131.4, 130.6, 128.9, 124.4, 116.7, 113.5, 111.4, 102.5, 81.5, 34.1. HRMS: m/z calcd for C$_{20}$H$_{15}$N$_5$O: 341.1277, found: 341.1271.
### Table S1. The basic optical data of BMN-Fluors

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<th>a2-BMN</th>
<th>b-BMN</th>
<th>c-BMN</th>
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<td>181122</td>
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<tr>
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*Fluorescence enhancement fold; \(\phi\) fluorescence quantum yield; \(\varepsilon\) Molar extinction coefficient.*
Figure S1. Spectral data of BMN-Fluors (3.0 μM) for AP-sites (2, 4, 6, 8, 10 and 14 AP-sites/20 bp DNA) in PBS buffer (pH = 7.4) at the different reaction time (0, few seconds and 300 s). a. a1-BMN, b. a2-BMN, c. b-BMN, d. c-BMN, e. d2-BMN, f. e-BMN. The amount of AP-sites in DNA sequence was quantitatively detected by AP-sites Counting Kit (Dojindo, Japan, see Supporting Information).
Figure S2. (a) Selective experiment; 1. control; 2. AP-Site in DNA; 3. HSA; 4. RNA; 5. triacylglycerol acylhydrolase; 6. lysozyme; 7. proteinase k; 8. histone; 9. collagen; 10. hemoglobin; 11. BSA; 12. β-amylase; 13. trypsin; and 14. chymotrypsin; (b) The influence of protein. 1. Control, 2. AP-Site in DNA, 3. P-Beta Aminopropionaldehyde, 4. amino transferase, 5. NAT, 6. Cyclodextrin glucanotransferase, 7. Alpha-Cyclodextrin glucosyltransferase, 8. Dnmt3a(cytosine-5)-methyltransferase 3A), 9. α-Glucosyltransferasetreated stevia, 10. Kinase (phosphorylating), 11. Glutamic oxalacetic transaminase, 12. Acyltransferase, 13. lactose synthetase, 14. Phosphotransacetylase; (c) The influence of ions. 1. Control, 2. AP-Site in DNA 3. Al³⁺ (0.10 mM), 4. NO₃⁻ (0.30 mM), 5. Ni²⁺ (0.10 mM), 6. Cl⁻ (0.20 mM), 7. Mg²⁺ (0.10 mM), 8. SO₄²⁻ (0.10 mM), 9. CO₃²⁻ (0.050 mM), 10. Na⁺ (0.10 mM), 11. K⁺ (0.10 mM), 12. Ca²⁺ (0.10 mM), 14. H₂PO₄⁻ (0.10 mM). Excitation wavelength = 400 nm, emission wavelength = 552 nm. d1-BMN: 3.0 μM. Data were obtained from replicate experiments (n = 5). (d) Spectral data of d1-BMN (3.0 μM) for AP-sites (2 AP-sites/20 bp DNA) and 5-formyluracil in DNA in PBS buffer (pH =7.4) at the different reaction time (0, few seconds and 300 s). Excitation wavelength = 400 nm or 354 nm. (e) Spectral data of d1-BMN (3.0 μM) for AP-sites (2 AP-sites/20 bp DNA) and 5-formyluracil in DNA in PBS buffer (pH =7.4) at 300 s. Excitation wavelength = 400 nm or 354 nm. (f) NMR spectra between d1-BMN-NO (3.0 mM) and ROS in D₂O.
Molecular docking and molecular dynamics simulation

Figure S3. The molecular configuration of d1-BMN-CHO in different amount of AP-site in DNA (20 bp). The molecular twist angles are calculated and listed in the figure.

Molecular docking and simulated molecular conformation parameters

(1) Molecular docking parameter

d1-BMN gets the different best configuration parameters by molecular docking as follow:

**Configuration 1. (The angle between two planes is 17.9°)**

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4  C  33.0271  15.4868  128.7096  C.ar  1  UNL111  -0.1500  
5  C  34.2806  16.0418  129.0035  C.ar  1  UNL111  0.0825  
6  C  35.1172  16.4871  127.9708  C.ar  1  UNL111  -0.1500  
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8  C  34.4540  16.4183  124.5055  C.ar  1  UNL111  0.1415  
9  N  33.3074  15.8637  125.0252  N.ar  1  UNL111  0.0332  
10 C  34.6105  16.6238  125.4764  N.ar  1  UNL111  -0.1050  
11 C  35.6831  16.2329  123.4048  C.2  1  UNL111  -0.1784  
12 C  36.8351  15.5371  123.0010  C.ar  1  UNL111  0.0284  
13 C  36.9386  14.1464  122.8496  C.ar  1  UNL111  -0.1500  
14 C  37.9980  13.4409  123.4299  C.ar  1  UNL111  -0.1500  
15 C  38.9570  14.1266  124.1778  C.ar  1  UNL111  0.0862  
16 C  38.8594  15.5082  124.3499  C.ar  1  UNL111  -0.1500  
17 C  37.7983  16.2080  123.7683  C.ar  1  UNL111  -0.1500  
18 C  40.0708  13.3771  124.7924  C.2  1  UNL111  0.4238  
19 O  40.9908  12.9145  124.1292  O.2  1  UNL111  -0.5700  
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Configuration 6. (The angle between two planes is 77.6°)
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(2) Simulated molecular conformation parameters

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The molecular configuration parameters of conformation 3:

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| HETATM | 2  | OP2 | RDG | 7   | 30.324 | 55.505 | 45.965 | 1.00 | 0.00 | O      |
| HETATM | 3  | OP1 | RDG | 7   | 31.132 | 57.105 | 47.688 | 1.00 | 0.00 | O1-    |
| HETATM | 4  | O5' | RDG | 7   | 32.823 | 55.651 | 46.566 | 1.00 | 0.00 | O      |
| HETATM | 5  | C5' | RDG | 7   | 33.214 | 54.428 | 45.985 | 1.00 | 0.00 | C      |
| HETATM | 6  | 1H5'| RDG | 7   | 33.035 | 53.608 | 46.680 | 1.00 | 0.00 | H      |
| HETATM | 7  | 2H5'| RDG | 7   | 32.523 | 54.218 | 45.168 | 1.00 | 0.00 | H      |
| HETATM | 8  | C4' | RDG | 7   | 34.655 | 54.495 | 45.497 | 1.00 | 0.00 | C      |
| HETATM | 9  | O4' | RDG | 7   | 34.900 | 55.713 | 45.036 | 1.00 | 0.00 | O      |
| HETATM | 10 | 4HHO| RDG | 7   | 35.435 | 55.096 | 45.580 | 1.00 | 0.00 | H      |
| HETATM | 11 | H4' | RDG | 7   | 34.725 | 53.674 | 44.783 | 1.00 | 0.00 | H      |
| HETATM | 12 | C3' | RDG | 7   | 35.703 | 54.189 | 46.616 | 1.00 | 0.00 | C      |
| HETATM | 13 | C2' | RDG | 7   | 35.369 | 54.784 | 48.055 | 1.00 | 0.00 | C      |
| HETATM | 14 | C1' | RDG | 7   | 35.987 | 54.044 | 49.166 | 1.00 | 0.00 | C      |
| HETATM | 15 | H1' | RDG | 7   | 36.776 | 54.486 | 49.757 | 1.00 | 0.00 | H      |
| HETATM | 16 | N3  | RDG | 7   | 35.509 | 52.816 | 49.360 | 1.00 | 0.00 | N      |
| HETATM | 17 | O1  | RDG | 7   | 36.169 | 52.285 | 50.479 | 1.00 | 0.00 | O      |
| HETATM | 18 | C2  | RDG | 7   | 35.871 | 50.968 | 50.797 | 1.00 | 0.00 | C      |
| HETATM | 19 | C1  | RDG | 7   | 36.664 | 50.378 | 51.663 | 1.00 | 0.00 | C      |
| HETATM | 20 | C6  | RDG | 7   | 36.514 | 49.094 | 52.049 | 1.00 | 0.00 | C      |
| HETATM | 21 | C5  | RDG | 7   | 35.531 | 48.390 | 51.367 | 1.00 | 0.00 | C      |
| HETATM | 22 | C4  | RDG | 7   | 34.579 | 48.961 | 50.442 | 1.00 | 0.00 | C      |
| HETATM | 23 | C3  | RDG | 7   | 34.798 | 50.296 | 50.168 | 1.00 | 0.00 | C      |
| HETATM | 24 | H2  | RDG | 7   | 34.099 | 50.826 | 49.537 | 1.00 | 0.00 | H      |
| HETATM | 25 | N1  | RDG | 7   | 33.706 | 47.986 | 49.947 | 1.00 | 0.00 | N      |
| HETATM | 26 | C7  | RDG | 7   | 34.111 | 46.915 | 50.606 | 1.00 | 0.00 | C      |
| HETATM | 27 | N2  | RDG | 7   | 35.084 | 47.098 | 51.472 | 1.00 | 0.00 | N      |
| HETATM | 28 | H5  | RDG | 7   | 35.425 | 46.342 | 52.049 | 1.00 | 0.00 | H      |
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The molecular configuration parameters of conformation 1:

| HETATM | 1  | P   | RDG | 7  | 31.493 | 53.146 | 47.761 | 1.00  | 0.00  | P    |
| HETATM | 2  | OP2 | RDG | 7  | 32.341 | 52.699 | 46.679 | 1.00  | 0.00  | O    |
| HETATM | 3  | OP1 | RDG | 7  | 31.049 | 54.525 | 47.752 | 1.00  | 0.00  | O1-  |
| HETATM | 4  | O5' | RDG | 7  | 32.196 | 52.927 | 49.178 | 1.00  | 0.00  | O    |
| HETATM | 5  | C5' | RDG | 7  | 33.501 | 52.589 | 49.323 | 1.00  | 0.00  | C    |
| HETATM | 6  | 1H5' | RDG | 7  | 33.707 | 52.212 | 49.578 | 1.00  | 0.00  | C    |
| HETATM | 7  | 2H5' | RDG | 7  | 33.765 | 51.800 | 48.620 | 1.00  | 0.00  | C    |
| HETATM | 8  | C4' | RDG | 7  | 34.122 | 54.817 | 49.701 | 1.00  | 0.00  | O    |
| HETATM | 9  | C5' | RDG | 7  | 35.044 | 54.539 | 49.514 | 1.00  | 0.00  | H    |
| HETATM | 10 | 4HHO | RDG | 7  | 34.276 | 53.896 | 48.007 | 1.00  | 0.00  | H    |
| HETATM | 11 | C3' | RDG | 7  | 35.877 | 53.324 | 49.365 | 1.00  | 0.00  | C    |
| HETATM | 12 | C2' | RDG | 7  | 36.255 | 53.049 | 50.860 | 1.00  | 0.00  | C    |
| HETATM | 13 | C1' | RDG | 7  | 36.777 | 51.710 | 51.250 | 1.00  | 0.00  | C    |
| HETATM | 14 | H1' | RDG | 7  | 37.800 | 51.548 | 51.554 | 1.00  | 0.00  | C    |
| HETATM | 15 | H3 | RDG | 7  | 36.108 | 48.370 | 51.406 | 1.00  | 0.00  | C    |
| HETATM | 16 | C2 | RDG | 7  | 36.604 | 47.301 | 52.218 | 1.00  | 0.00  | C    |
| HETATM | 17 | C1 | RDG | 7  | 36.861 | 46.123 | 52.145 | 1.00  | 0.00  | C    |
| HETATM | 18 | C6 | RDG | 7  | 35.779 | 46.001 | 51.323 | 1.00  | 0.00  | C    |
| HETATM | 19 | C5 | RDG | 7  | 34.707 | 45.201 | 51.250 | 1.00  | 0.00  | C    |
| HETATM | 20 | C4 | RDG | 7  | 34.252 | 45.201 | 50.486 | 1.00  | 0.00  | C    |
| HETATM | 21 | C3 | RDG | 7  | 34.907 | 45.201 | 49.178 | 1.00  | 0.00  | C    |
| HETATM | 22 | H2 | RDG | 7  | 34.585 | 49.969 | 49.981 | 1.00  | 0.00  | C    |
| HETATM | 23 | N3 | RDG | 7  | 33.048 | 46.663 | 49.832 | 1.00  | 0.00  | C    |
| HETATM | 24 | C7 | RDG | 7  | 32.779 | 45.490 | 50.398 | 1.00  | 0.00  | C    |
| HETATM | 25 | N2 | RDG | 7  | 33.760 | 45.033 | 51.204 | 1.00  | 0.00  | C    |
| HETATM | 26 | H5 | RDG | 7  | 33.727 | 44.173 | 51.732 | 1.00  | 0.00  | C    |
| HETATM | 27 | C8 | RDG | 7  | 31.763 | 44.676 | 50.126 | 1.00  | 0.00  | C    |
| HETATM | 28 | C9 | RDG | 7  | 30.814 | 44.968 | 49.110 | 1.00  | 0.00  | C    |
| HETATM | 29 | C10| RDG | 7  | 29.583 | 44.170 | 48.844 | 1.00  | 0.00  | C    |
| HETATM | 30 | C11| RDG | 7  | 28.861 | 44.446 | 47.626 | 1.00  | 0.00  | C    |
| HETATM | 31 | C12| RDG | 7  | 27.683 | 43.765 | 47.367 | 1.00  | 0.00  | C    |
| HETATM | 32 | C13| RDG | 7  | 27.265 | 42.754 | 48.247 | 1.00  | 0.00  | C    |
| HETATM | 33 | C14| RDG | 7  | 27.965 | 42.449 | 49.481 | 1.00  | 0.00  | C    |
| HETATM | 34 | C15| RDG | 7  | 29.100 | 43.175 | 49.739 | 1.00  | 0.00  | C    |
| HETATM | 35 | C16| RDG | 7  | 25.967 | 42.192 | 47.954 | 1.00  | 0.00  | C    |
| HETATM | 36 | C17| RDG | 7  | 25.322 | 41.355 | 48.649 | 1.00  | 0.00  | O    |
| HETATM | 37 | C18| RDG | 7  | 25.564 | 42.475 | 46.993 | 1.00  | 0.00  | H    |
| HETATM | 38 | H12| RDG | 7  | 27.144 | 43.929 | 46.446 | 1.00  | 0.00  | H    |
| HETATM | 39 | H10| RDG | 7  | 29.256 | 45.245 | 47.017 | 1.00  | 0.00  | H    |
| HETATM | 40 | H9 | RDG | 7  | 31.036 | 45.775 | 48.427 | 1.00  | 0.00  | H    |
6. Gaussian result

**Figure S4.** The simulated fluorescence emission spectra by Gaussian 16.

7. Biocompatibility of d1-BMN

Prior to precede single cell gel electrophoresis assay, the biocompatibility of d1-BMN such as photostability, biological pH stability, cell toxicity, water solubility and so on, were evaluated by fluorescence intensity as the evaluation parameter, respectively.
7.1 The photostability of d1-BMN under irradiated by iodine-tungsten lamp in PBS buffer

d1-BMN (3.0 μM) retained more than 98% of fluorescence intensity in PBS buffer after they were continuously irradiated by an iodine-tungsten lamp for 6 h. Such kind of photostability of d1-BMN ensures that it can provide a stable response signal during single cell assay.

![Figure S5](image)

**Figure S5.** The photostability of d1-BMN (3.0 μM) in PBS buffer (pH 7.4) at 25 °C. Iodine-tungsten lamp: 500W. Excitation wavelength = 400 nm. Emission wavelength = 605 nm.

7.2 The biological stability of d1-BMN in cells

d1-BMN (3.0 μM) retained more than 98.5 % of fluorescence intensity in living cell after they were continuously irradiated by an laser at 405 nm (initial power = 2.6 mM) for 6 h. Such kind of biological stability of d1-BMN ensures that it can provide a stable response signal during single cell assay.
**Figure S6. The biological stability of d1-BMN (3.0 μM) in cell.** Excitation wavelength = 405 nm. Emission wavelength = 605 nm. The endogenic AP-site was inhibited by O-phenylhydroxylamine. $F_0$ is the fluorescence intensity at the reaction time of 0, $F$ is the fluorescence intensity at the reaction time of 1 to 6 h.

7.3 Cell toxicity of d1-BMN

The MTT assay results revealed that greater than 95% of cells survived after incubation with d1-BMN (5.0 μM) for 24 h. Even the incubation concentration of d1-BMN increased to 10 μM, greater than 95% of the cells still survived. Such high survival rate is of great significance for the single cell assay.

**Figure S7. Cell toxicity of d1-BMN (5.0 and 10.0 μM) for HepG2 cells and NIH 3T3 cells.** The cells were incubated for an additional 24 h with dyes d1-BMN in different concentrations Optical density (OD) was determined by a microplate reader (Spectra Max M5, Molecular Devices) at 570 nm with subtraction of the absorbance of the cell-free blank volume at 630 nm. The results from the six individual experiments were averaged.
7.4 The amount change of AP-site
Before the experiment, the endogenic AP-site was inhibited by O-phenylhydroxylamine, and then, the cells were incubated by d1-BMN for 6.0 h. During this process, whether any new sites are generated is detected in real time. The result indicated that there is no any new AP-site being created. This is of great significance for the single cell assay of damage site-AP-site.

Figure S8. The amount change of damage site. HepG2 cells were incubated by d1-BMN (5.0 μM) for different time. The endogenic AP-site was inhibited by O-phenylhydroxylamine.

7.5 The pH-stability of d1-BMN
There was no any influence on the fluorescent signals when the pH of phosphate buffer was at 3.7–10.7. Such kind of pH-stability of d1-BMN ensures that it can provide a stable response signal during single cell assay in cellular environment.

Figure S9. The pH-stability of d1-BMN (3.0 μM) in pH range from 3.7 to 11.7.
7.6 The water solubility of d1-BMN

The solubility of d1-BMN was 10 μM. Such kind of water solubility of d1-BMN ensures that it is suitable for the signal during single cell assay.

Figure S10. The water solubility of d1-BMN (3.0 μM) in PBS buffer (pH 7.4) at 25 °C.
8. Single cell gel electrophoresis assay

Table S2. Single cell gel electrophoresis assay results in Hepg 2 cells (n = 200).

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** P < 0.01; ★ Staining with d1-BMN; ☆ Staining with Ethidium Bromide (EB).

Figure SS-8. a and b. The single cell gel electrophoresis assay of d1-BMN (5.0 μM) in Hepg 2 cell by incubating with ROS (a no ROS and b with ROS).
9. Sort different degree of damaged cell by flow cytometry

a. Figure S11. Sort different degree of damaged cell by flow cytometry. d1-BMN (10.0 μM), Hepg 2 cell. a. Cell count scatter plot, 10000 cells. b-d. Cell count histogram at different fluorescence (red, orange, yellow, green and blue).
References.


S7. DMS, Conrad Huang, University of California, San Francisco.


Attached Spectra.

2d-1

(E)-4-(2-(5-hydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde

$^1$H NMR
(E)-4-(2-(5-hydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde

\(^{13}\text{C} \text{ NMR}\)
(E)-2-(4-(2-(5-hydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

\[ 3d-1 \]
(E)-2-((4-(2-(5-hydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

\[ ^{13}\text{C NMR} \]
(E)-2-((4-(2-(5-(aminoxy)-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

\( ^1H \text{ NMR} \)
d1-BMN

(E)-2-(4-(5-(aminooxy)-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
(E)-4-(2-(5,6-dihydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde

$^1$H NMR
(E)-4-(2-(5,6-dihydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde

$^{13}\text{C} \text{ NMR}$
(E)-2-(4-(2-(5,6-dihydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile
(E)-2-(4-(2-(5,6-dihydroxy-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
\((E)\)-2-\((4-(2-(5,6-bis(aminooxy)-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile\)

\(^1\text{H NMR}\)

\(\text{fl (ppm)}\)
d2-BMN

\[(E)-2-(4-(2-(5,6-bis(aminoxyl)-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile\]

$^{13}$C NMR
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$^1$H NMR
2a-1

(E)-4-((6-hydroxy-3H-indol-2-yl)vinyl)benzaldehyde

$^{13}$C NMR
(E)-2-((6-hydroxy-3H-indol-2-yl)vinyl)benzylidene)malononitrile

^1H NMR
3a-1

(E)-2-(4-(2-(6-hydroxy-3H-indol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
(E)-2-((4-(2-(6-(aminooxy)-3H-indol-2-yl)vinyl)benzylidene)malononitrile

\[ \text{\textsuperscript{1}H NMR} \]

\[ \text{f1 (ppm)} \]

S-72
(E)-2-(4-(2-(6-aminoxy)-3H-indol-2-yl)vinyl)benzylidene)malononitrile
2a-2

(E)-4-(2-(5,6-dihydroxy-3H-indol-2-yl)vinyl)benzaldehyde

$^1$H NMR
$2a-2$

$(E)-4-(2-(5,6\text{-dihydroxy}-3H\text{-indol-2-yl})\text{vinyl})\text{benzaldehyde}$

$^{13}\text{C NMR}$
$^{1}H$ NMR
(E)-2-(4-((2-(5,6-dihydroxy-3H-indol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
(E)-2-(4-(2-((5,6-bis(aminooxy)-3H-indol-2-yl)vinyl)benzylidene)malononitrile

\[^{1}H\text{ NMR}\]
a2-BMN

(E)-2-{4-{2,5-bis(aminooxy)-3H-indol-2-yl}vinyl}benzylidene)malononitrile

$^{13}$C NMR
(E)-4-(2-(6-hydroxy-3-methyl-3H-indol-2-yl)vinyl)benzaldehyde

\[ ^1H \text{ NMR} \]
(E)-4-(2-(6-hydroxy-3-methyl-3H-indol-2-yl)vinyl)benzaldehyde

$^{13}$C NMR
(E)-2-((4-(2-(6-hydroxy-3-methyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

^1H NMR
(E)-2-(4-((6-hydroxy-3-methyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
b-BMN

(E)-2-(4-(2-(6-(aminooxy)-3-methyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

$^1$H NMR
b-BMN

\( (E)-2-((4-(2-((aminooxy)-3-methyl-3H-indol-2-yl)vinyl)benzyldene)malononitrile \)

\( ^{13}C \) NMR
(E)-4-(2-(6-hydroxy-3,3-dimethyl-3H-indol-2-yl)vinyl)benzaldehyde

$^1$H NMR
(E)-4-((2-(6-hydroxy-3,3-dimethyl-3H-indol-2-yl)vinyl)benzaldehyde

$^{13}$C NMR

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(E)-2-((2-(6-hydroxy-3,3-dimethyl-3H-indol-2-yl)vinyl)benzyldene)malononitrile

\[ ^1\text{H NMR} \]
(E)-2-(4-(2-(6-hydroxy-3,3-dimethyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
(E)-2-(4-(2-(6-(aminoxy)-3,3-dimethyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

\[ \text{^1H NMR} \]
(E)-2-(4-(2-(6-(aminooxy)-3,3-dimethyl-3H-indol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
(E)-4-(2-(5-hydroxy-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde

$^1$H NMR
(E)-4-(2-(5-hydroxy-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzaldehyde

$^{13}$C NMR
(E)-2-(4-(2-(5-hydroxy-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

^1H NMR
(E)-2-(4-(2-(5-hydroxy-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

$^{13}$C NMR
(E)-2-(4-(2-(5-aminooxy)-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

\( ^1H \text{ NMR} \)
(E)-2-(4-(2-(5-(aminoxy)-1-methyl-1H-benzo[d]imidazol-2-yl)vinyl)benzylidene)malononitrile

\[ ^{13}C \text{ NMR} \]