

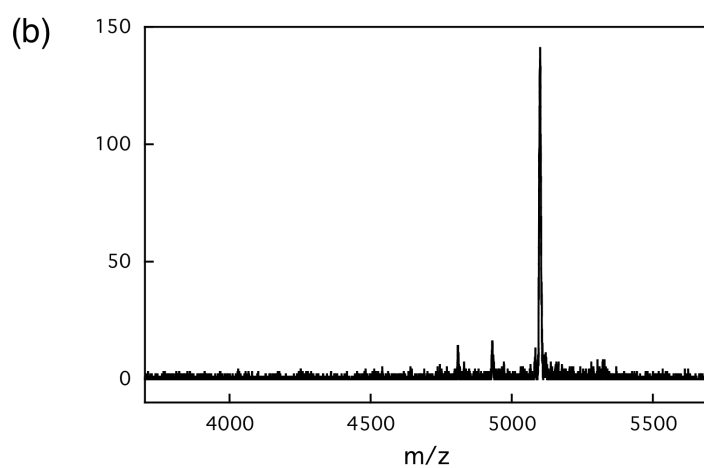
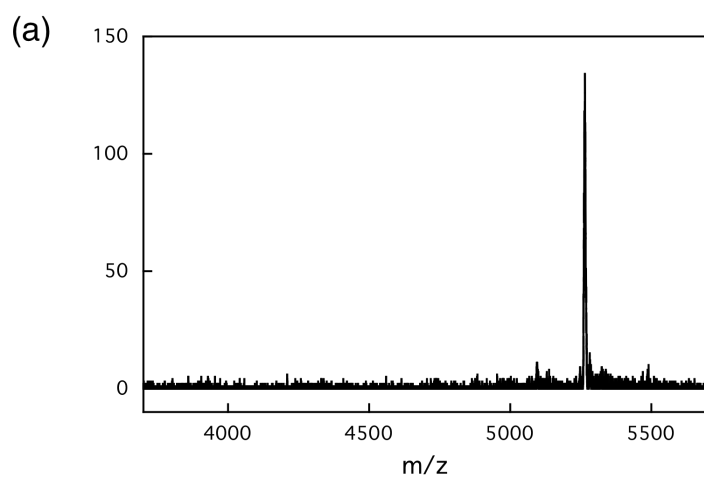
*Supporting Information*

**Thiazole orange-conjugated peptide nucleic acid for  
fluorescent detection of specific DNA sequence and  
site-selective photodamage**

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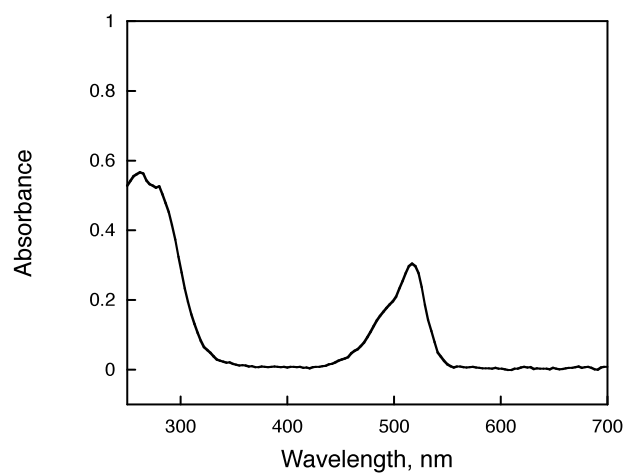
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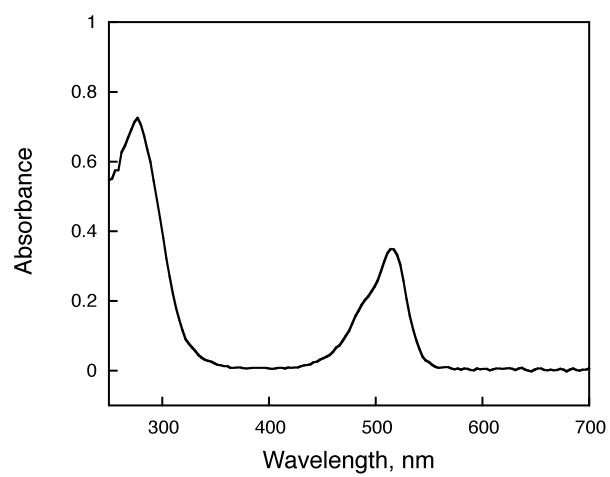


**Fig. S1** Mass spectra of TO-modified pcPNAs. (a) TO-pcPNA1;  $m/z = 5264.6$  (calculated  $[M-3H]^+$ : 5264.5) and (b) TO-pcPNA2;  $m/z = 5100.8$  (calculated  $[M-3H]^+$ : 5101.4).

(a)

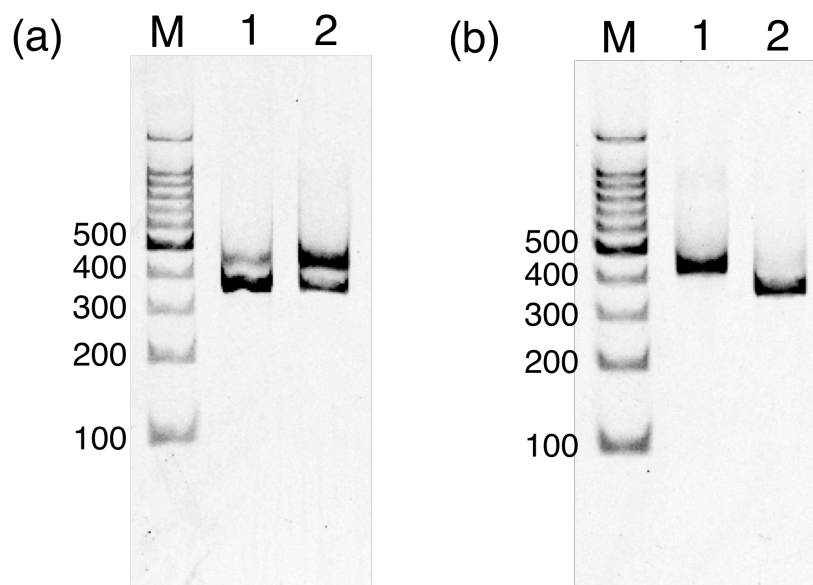


(b)



**Fig. S2** Absorption spectra of (a) TO-pcPNA1 and (b) TO-pcPNA2. These spectra were obtained using a NanoDrop 1000 (Thermo Fisher Scientific).

**Gel-Shift assay to assess the conditions for the formation and the decomposition of invasion complex of TO-conjugated pcPNA.**



**Fig. S3** (a) Assay of invasion complex formation of TO-pcPNA1/TO-pcPNA2 to dsDNA (381 bp) at [each TO-conjugated pcPNA] = 10 nM (lane 1) and 25 nM (lane 2). Lane M, 100 bp ladder marker. Invasion conditions: [381 bp DNA] = 5.0 nM, [HEPES (pH 7.0)] = 5.0 mM and [NaCl] = 20 mM at 50°C overnight. (b) Evaluation of the conditions for the removal of TO-conjugated pcPNAs from dsDNA (381 bp). The invasion complex was first prepared with [each TO-conjugated pcPNA] = 50 nM in lane 1. Then, it was incubated at 50°C for 3 h in the presence of 0.5 M NaCl (lane 2). The gel-shift assay was carried out using 5% nondenaturing PAGE. The bands were stained with GelStar and quantified with Typhoon FLA 7000 imaging analyzer.

## Sequence of pBFP-N1 and the scission sites of various enzymes

Recognition sites of the restriction enzymes are highlighted in yellow.

The sequence of 381 bp DNA coding a part of BFP is shown as blue characters.

TAGTTATTAATAGTAATCAATTACGGGGTCATTAGTTCATAGCCCATATATGGAGTTCCGCG  
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GTAACAACCTCCGCCCCATTGACGCAAATGGGCGGTAGGCGTGTACGGTGGGAGGTCTATAT  
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CCACCATGGTGAGCAAGGGCGAGGAGCTGTTACCGGGTGGTGCCCATCCTGGTTCGAGCT  
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