Supporting Information

Incorporation of oxidized guanine nucleosides 5'-triphosphates in DNA with DNA polymerases and preparation of single-lesion carrying DNA.

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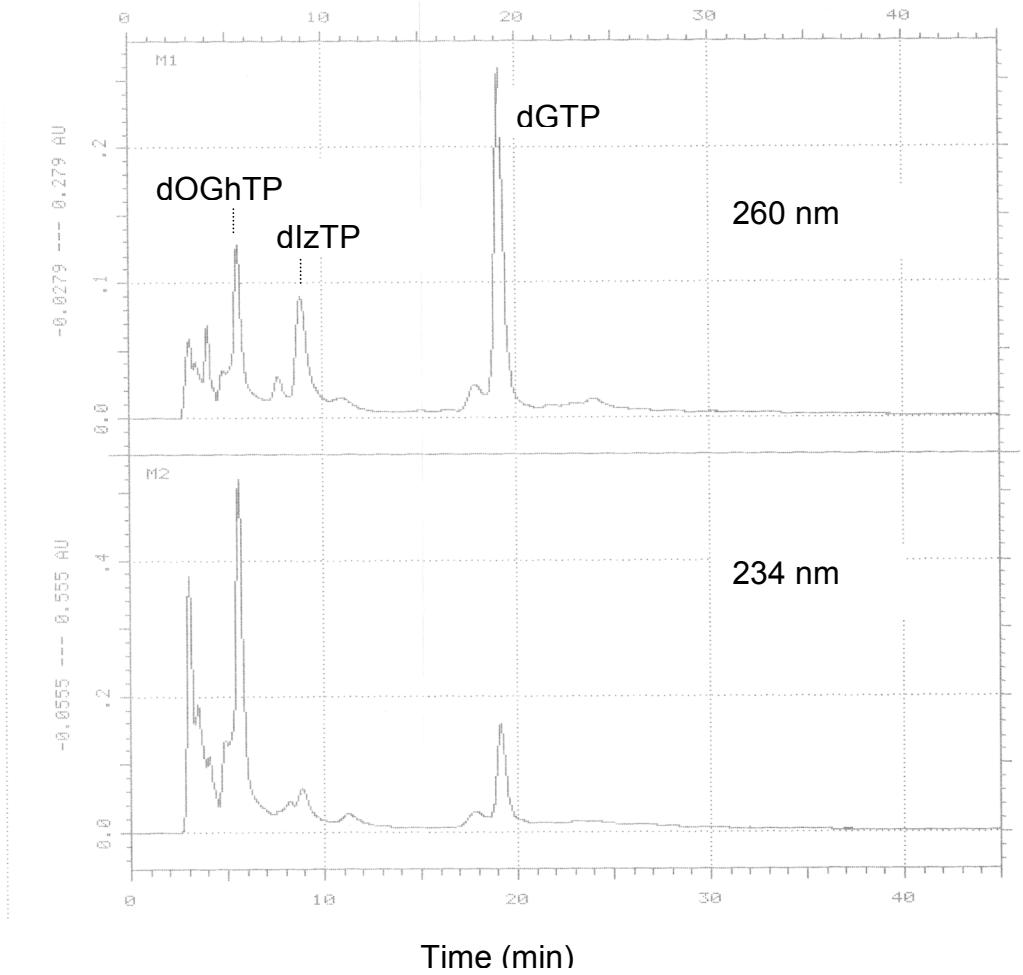
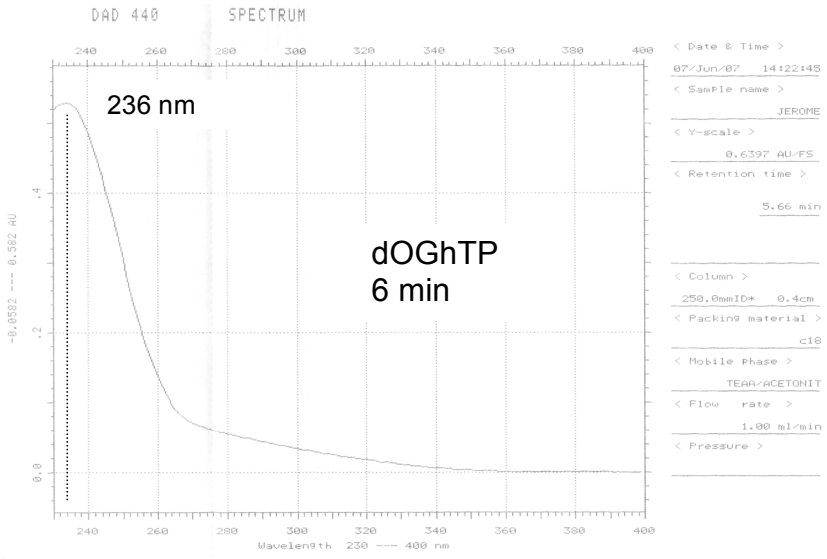
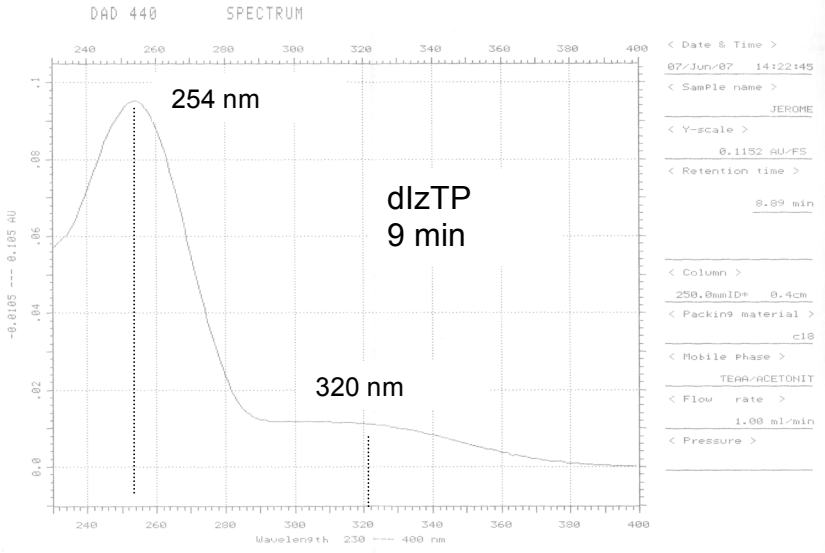
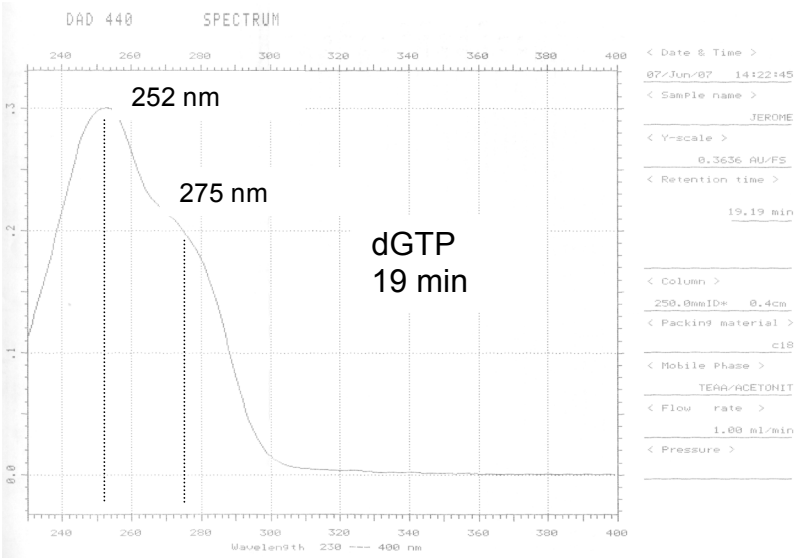


Figure S1. Example of a reverse phase HPLC chromatogram of the reaction medium for the isolation of the dN^{ox}TPs used in the present study. In this example the reaction was not allowed to go to completion to show the separation of the dIzTP and dOGhTP products from dGTP. The corresponding in-line UV-visible spectra are shown below.







HPLC in-line UV-visible spectra of Fig. S1

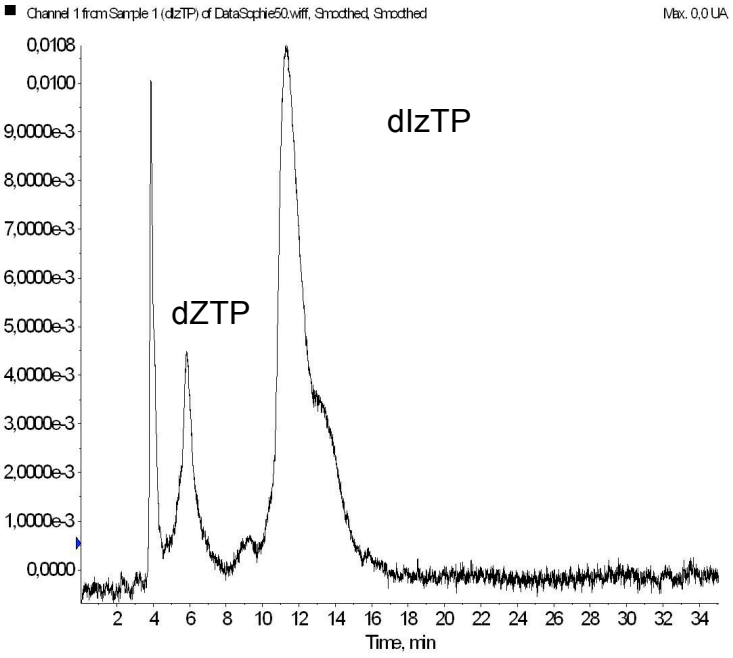


Fig. S2 A

dIzTP/dZTP mixture

260 nm

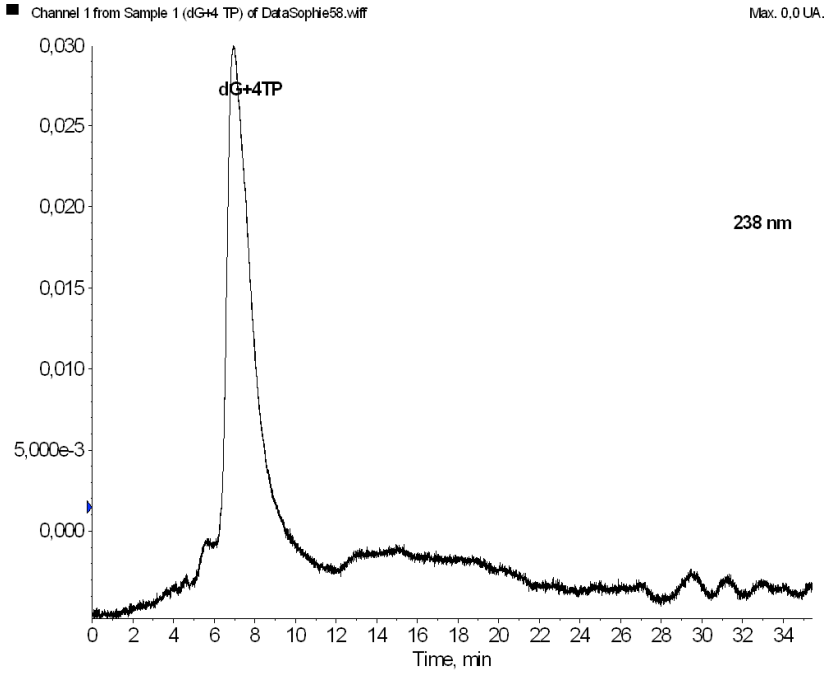


Fig. S2 B

dOGhTP

238 nm

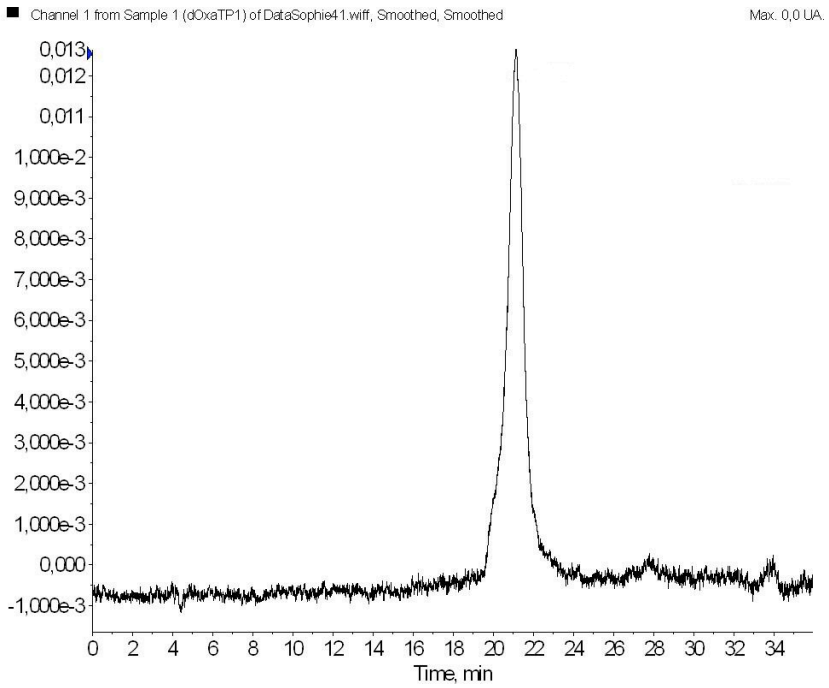


Fig. S2 C

dOxaTP

238 nm

Figure S2, Examples of reverse phase HPLC chromatograms of the isolated $dN^{ox}TPs$ used in this study. A, dIzTP/dZTP mixture; B, dOGhTP, C, dOxaTP (the latter was obtained from the hydrolysis of the purified dOGhTP for 30 min at 37 °C).

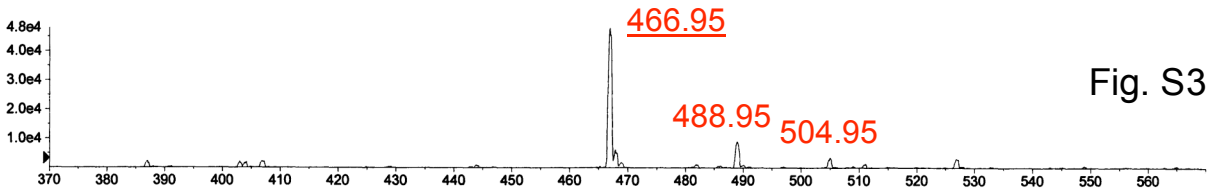


Fig. S3 A

In-line mass spectrum of dIzTP (retention time 12 min under the used LC/ESI-MS conditions)

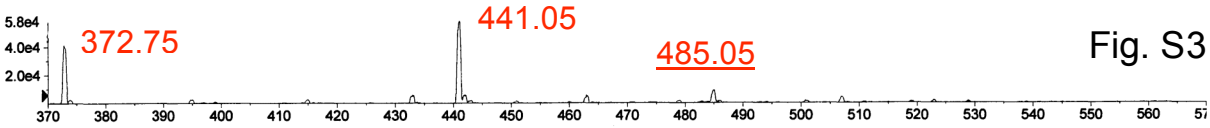


Fig. S3 B

In-line mass spectrum of dZTP (retention time 6 min under the used LC/ESI-MS conditions)

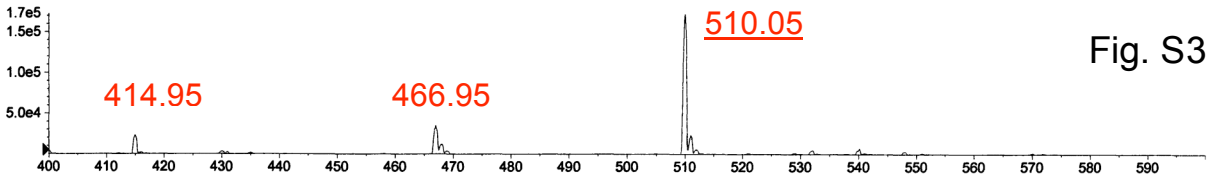


Fig. S3 C

In-line mass spectrum of dOGhTP (retention time 8 min under the used LC/ESI-MS conditions)

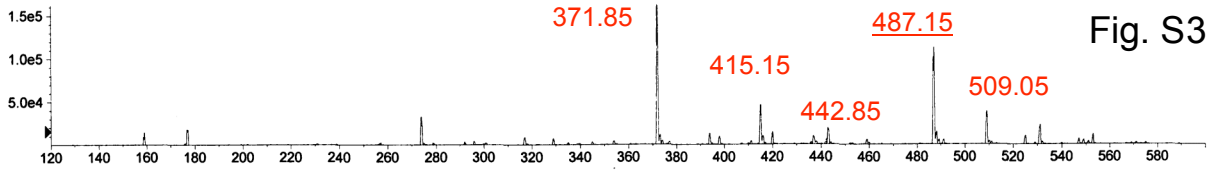


Fig. S3 D

In-line mass spectrum of dOxaTP (retention time 21 min under the used LC/ESI-MS conditions).

Figure S3. LC/ESI-MS analysis of the purified nucleosides 5'-triphosphate used for single-nucleotide primer extension. In-line mass spectra correspond to the chromatograms shown in Figure S2. A and B, dIzTP/dZTP mixture; C, dOGhTP, D, dOxaTP. Underlined *m/z* values correspond to the molecular masses (z = 1). Usual fragmentations leading for instance to abasic site (*m/z* = 372.75 amu), urea residue (*m/z* = 414.95 amu), 1'-aminosugar residue (*m/z* = 371.85 amu) are also indicated. Some sodium and potassium adducts can be observed at *m/z* = 488.95, 509.05 and, 504.95, respectively.

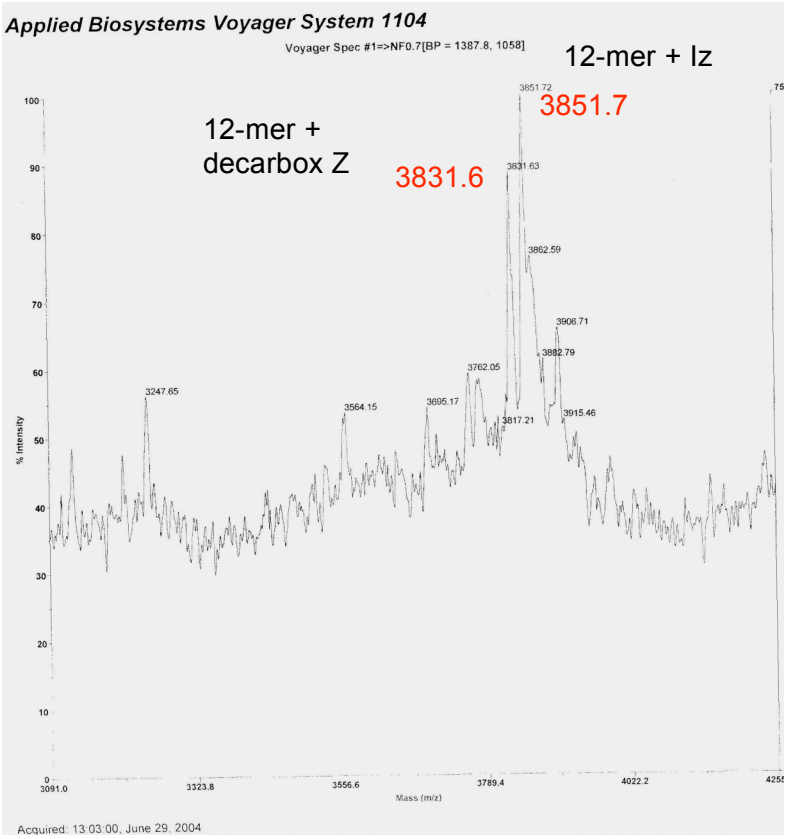


Fig. S4 **a**

dIzTP/dZTP opposite G

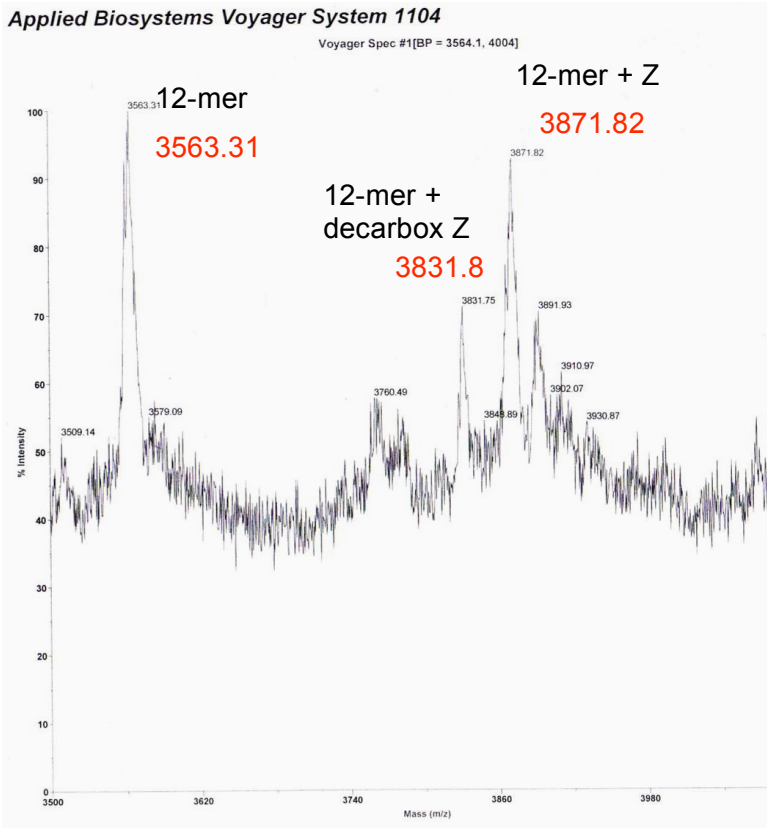


Fig. S4 **b**

dIzTP/dZTP opposite C

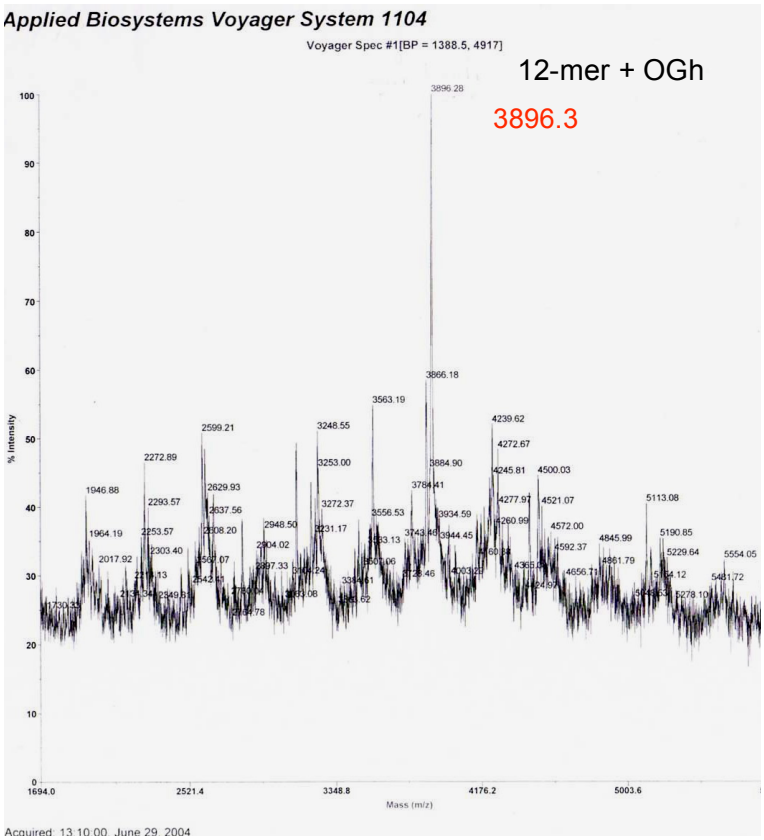


Fig. S4 **c**

dOGhTP opposite C

Figure S4. Maldi MS analysis of the 13-mer oligonucleotides after the incorporation of one lesion dIzTP/dZTP opposite G (**a**), dIzTP/dZTP opposite C (**b**), dOGhTP opposite C (**c**). See text for details. The calculated *m/z* for the mono-charged ion of the 12-mer primer is 3562.4 amu. The calculated *m/z* value for the 13-mer after the incorporation of one Iz residue is 3853.4 amu. The calculated *m/z* value for the 13-mer after the incorporation of one Z residue is 3871.4 amu (or after decarboxylation of Z, 3827.4). The calculated *m/z* value for the 13-mer after the incorporation of one OGh residue is 3896.6 amu. The observed *m/z* values are attributed within a 0.05% error.

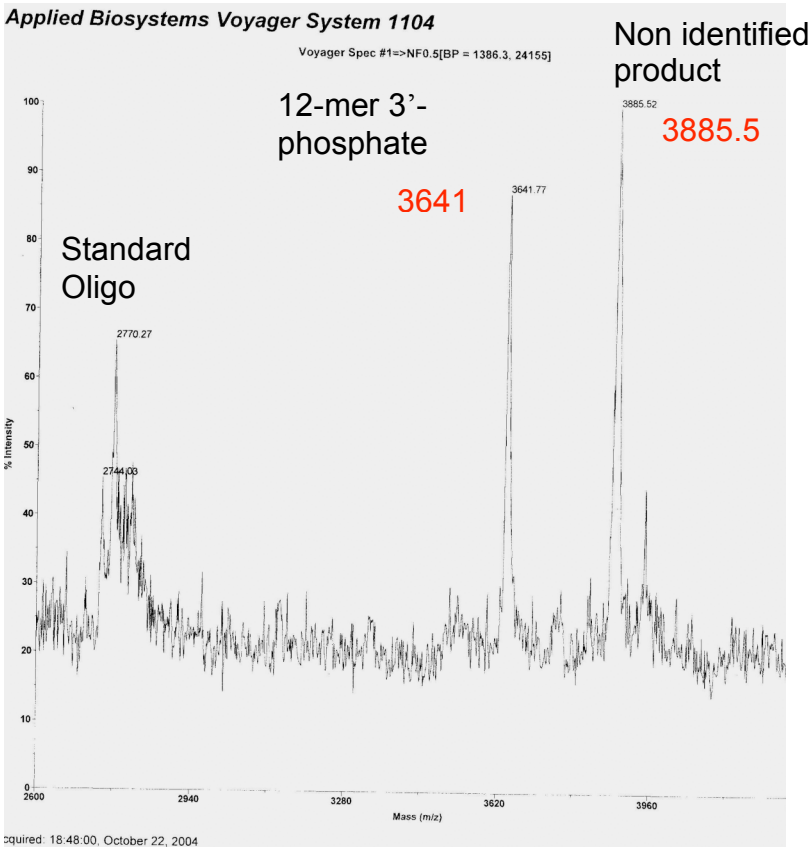


Figure S5. Maldi MS analysis of the 13-mer oligonucleotides containing one lesion dOGhTP opposite C after piperidine treatment. The calculated *m/z* value for the 12-mer-3'-phosphate mono-charged species is 3643 amu. A non identified product is observed. Whether this product corresponds to the non identified band observed on the electrophoresis gel of Figure 6) is not known.

A

12-mer primer 5'-TCCATATCACAT

25-mer-X template 3'-AGGTATAGTGTA**X**TTCTGATCATCT

X = A,C,G or T

B

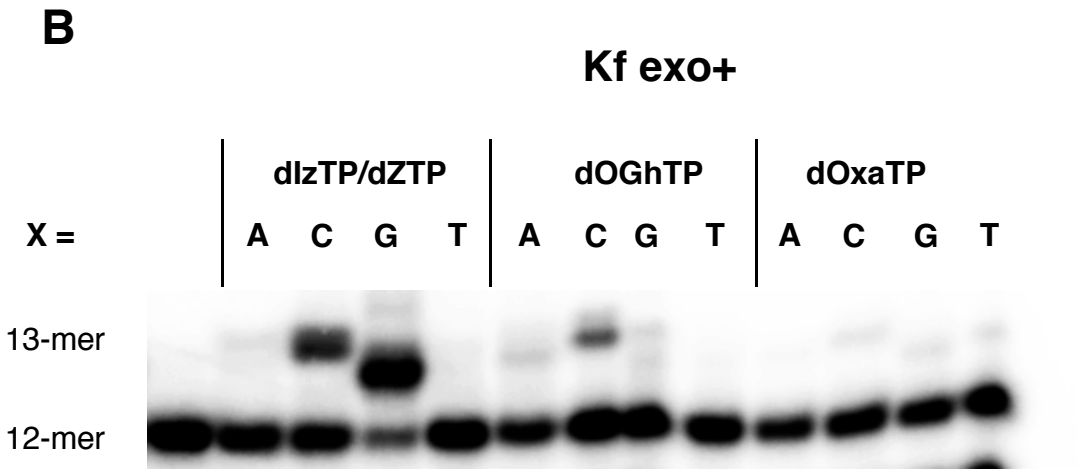


Figure S6, Single-nucleotide insertion opposite A, C, G or T of the modified nucleoside 5'-triphosphates with Kf exo+ (A) the template/primer duplexes used in this study, (B) PAGE analysis of the incorporation of a single modified dNTP, dIzTP/dZTP, dOGhTP or dOxaTP using 0.5 unit Kf exo+. The concentration of the added dNTP was 50 μM in the case of dIzTP/dZTP and dOGhTP and 100 μM in the case of dOxaTP. The reactions were performed at 37 °C for 10 min in the appropriate enzyme buffer (see Experimental Part).