The activation of N-glycosidic bond cleavage operated by base-excision repair enzyme hOGG1; theoretical study of the role of Lys 249 residue in activation of G, OxoG and FapyG

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The supplementary information includes Tables S1-S15, Figures S1-S6 and xyz coordinates of optimized structures.
Table S1. The interatomic distances (Å) and angles (degrees) of G calculated employing small model and B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with G are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from Ne-ammonium to N3 nitrogen (N3H). The numbering of atoms can be found in Figure 1.

<table>
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<th>G (N3)</th>
<th>G (N3H)</th>
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Table S3. The interatomic distances (Å) and angles (degrees) of FapyG calculated employing small model and B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with FapyG are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from Nε-ammonium to N9 nitrogen (N9H). The numbering of atoms can be found in Figure 1.

<table>
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1κ’ for torsional angle C4-N9-C1´-C8 - 180°

2κ’ for torsional angle C4-N9-C1´-H9 - 180°
Table S4. The calculated and experimental interatomic distances (Å) and angles (degrees) of G, OxoG and FapyG.

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<th>Calc. Large Model b)</th>
<th>Experiment c)</th>
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a) Calculations employing medium structural model and ONIOM method (see Computational details).
b) Calculations employing large structural model and AM1/OPLS_2005 QM/MM method (left column) and B3LYP/OPLS_2005 QM/MM method (right column) (see Computational details).
c) X-ray structures with PDB ID 3IH7, 1YQK, 1N3C, 2NOZ (from left to right).
Table S5. The Wiberg bond orders calculated for pairs of atoms of G, OxoG, and FapyG employing B3LYP-D2/6-31G**/PCM. The interactions of Lys 249 with nucleosides are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from Nε-ammonium to N9 nitrogen (N9H).

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<tr>
<td>N9-C8</td>
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<td>N9-C4</td>
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<td>1.1589</td>
<td>1.1902</td>
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<tr>
<td>N9-H’(Nε)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>N3-H’(Nε)</td>
<td>-</td>
<td>-</td>
<td>0.1639</td>
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<tr>
<td>Nε-H’(Nε)</td>
<td>-</td>
<td>-</td>
<td>0.5938</td>
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</tr>
<tr>
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</tr>
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<td>OxoG (C1’)</td>
<td>0.9241</td>
<td>0.9224</td>
<td>0.9231</td>
<td>0.9119</td>
<td>0.9052</td>
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</tr>
<tr>
<td>OxoG (N3)</td>
<td>1.0265</td>
<td>1.0285</td>
<td>1.0031</td>
<td>0.9867</td>
<td>0.9734</td>
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</tr>
<tr>
<td>OxoG (N3H)</td>
<td>1.1050</td>
<td>1.1154</td>
<td>1.1180</td>
<td>1.1522</td>
<td>1.0507</td>
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</tr>
<tr>
<td>OxoG (N9)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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<td>OxoG (N9H)</td>
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<td>-</td>
<td>0.1394</td>
<td>0.5098</td>
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<tr>
<td>FapyG</td>
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</tr>
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<td>FapyG (C1’)</td>
<td>0.9713</td>
<td>0.9687</td>
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<td>0.7039</td>
<td>0.7073</td>
<td>0.6998</td>
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<td>0.6986</td>
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<td>FapyG (N3H)</td>
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<td>1.2071</td>
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<td>1.0421</td>
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<td>FapyG (N9)</td>
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Table S6. The NBO atomic charges in e calculated for G employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with G are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from Ne-ammonium to N3 nitrogen (N3H).

<table>
<thead>
<tr>
<th>Atom</th>
<th>G</th>
<th>G (C1’)</th>
<th>G (N3)</th>
<th>G (N3H)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1’</td>
<td>0.279</td>
<td>0.269</td>
<td>0.280</td>
<td>0.278</td>
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<td>-0.419</td>
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<td>C8</td>
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<td>0.211</td>
<td>0.220</td>
</tr>
<tr>
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<td>0.359</td>
<td>0.366</td>
<td>0.375</td>
<td>0.378</td>
</tr>
<tr>
<td>N3</td>
<td>-0.598</td>
<td>-0.595</td>
<td>-0.655</td>
<td>-0.612</td>
</tr>
<tr>
<td>N7</td>
<td>-0.486</td>
<td>-0.484</td>
<td>-0.461</td>
<td>-0.453</td>
</tr>
<tr>
<td>C5</td>
<td>-0.056</td>
<td>-0.058</td>
<td>-0.046</td>
<td>-0.036</td>
</tr>
<tr>
<td>O4’</td>
<td>-0.597</td>
<td>-0.603</td>
<td>-0.591</td>
<td>-0.590</td>
</tr>
<tr>
<td>C2’</td>
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<td>-0.495</td>
<td>-0.496</td>
<td>-0.498</td>
</tr>
<tr>
<td>Ne</td>
<td>-</td>
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<td>-0.822</td>
<td>-0.922</td>
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Table S7. The NBO atomic charges in e calculated for OxoG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with OxoG are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9).

<table>
<thead>
<tr>
<th>Atom</th>
<th>OxoG</th>
<th>OxoG (C1’)</th>
<th>OxoG (N3)</th>
<th>OxoG (N3H)</th>
<th>OxoG (N9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1´</td>
<td>0.264</td>
<td>0.273</td>
<td>0.279</td>
<td>0.276</td>
<td>0.261</td>
</tr>
<tr>
<td>N9</td>
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<td>-0.460</td>
<td>-0.474</td>
<td>-0.465</td>
<td>-0.544</td>
</tr>
<tr>
<td>C8</td>
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<td>0.821</td>
<td>0.826</td>
<td>0.830</td>
<td>0.828</td>
</tr>
<tr>
<td>C4</td>
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<td>0.404</td>
<td>0.402</td>
<td>0.412</td>
<td>0.380</td>
</tr>
<tr>
<td>N3</td>
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<td>-0.596</td>
<td>-0.651</td>
<td>-0.616</td>
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</tr>
<tr>
<td>N7</td>
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<td>-0.621</td>
<td>-0.614</td>
<td>-0.613</td>
<td>-0.615</td>
</tr>
<tr>
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<td>-0.040</td>
<td>-0.026</td>
<td>-0.015</td>
<td>-0.029</td>
</tr>
<tr>
<td>O4´</td>
<td>-0.605</td>
<td>-0.608</td>
<td>-0.598</td>
<td>-0.596</td>
<td>-0.595</td>
</tr>
<tr>
<td>C2´</td>
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<td>-0.502</td>
<td>-0.500</td>
<td>-0.500</td>
<td>-0.512</td>
</tr>
<tr>
<td>Nε</td>
<td>-</td>
<td>-0.922</td>
<td>-0.818</td>
<td>-0.912</td>
<td>-0.799</td>
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Table S8. The NBO atomic charges in e calculated for FapyG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with FapyG are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from $\text{N}_\varepsilon$-ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from $\text{N}_\varepsilon$-ammonium to N9 nitrogen (N9H).

<table>
<thead>
<tr>
<th>Atoms</th>
<th>FapyG</th>
<th>FapyG (C1’)</th>
<th>FapyG (N3)</th>
<th>FapyG (N3H)</th>
<th>FapyG (N9)</th>
<th>FapyG (N9H)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1’</td>
<td>0.244</td>
<td>0.239</td>
<td>0.251</td>
<td>0.253</td>
<td>0.250</td>
<td>0.275</td>
</tr>
<tr>
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<td>-0.645</td>
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<td>-0.672</td>
<td>-0.745</td>
<td>-0.707</td>
</tr>
<tr>
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<td>0.507</td>
<td>0.520</td>
<td>0.525</td>
<td>0.521</td>
<td>0.527</td>
</tr>
<tr>
<td>C4</td>
<td>0.431</td>
<td>0.433</td>
<td>0.424</td>
<td>0.438</td>
<td>0.405</td>
<td>0.383</td>
</tr>
<tr>
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<td>-0.599</td>
<td>-0.657</td>
<td>-0.614</td>
<td>-0.620</td>
<td>-0.598</td>
</tr>
<tr>
<td>N7</td>
<td>-0.622</td>
<td>-0.622</td>
<td>-0.626</td>
<td>-0.627</td>
<td>-0.626</td>
<td>-0.617</td>
</tr>
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<td>-0.604</td>
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<td>-0.595</td>
</tr>
<tr>
<td>C2’</td>
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<td>-0.505</td>
<td>-0.502</td>
<td>-0.511</td>
<td>-0.512</td>
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<td>$\text{N}_\varepsilon$</td>
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<td>-0.923</td>
<td>-0.814</td>
<td>-0.910</td>
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Table S9. The $f,f^+,f^2$ Fukui indices calculated for G employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with G are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H).

<table>
<thead>
<tr>
<th>Atoms</th>
<th>G</th>
<th>G (C1’)</th>
<th>G (N3)</th>
<th>G (N3H)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f$</td>
<td></td>
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<td></td>
</tr>
<tr>
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<td>-0.008</td>
<td>-0.007</td>
<td>-0.004</td>
</tr>
<tr>
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<td>0.011</td>
<td>0.006</td>
<td>0.004</td>
</tr>
<tr>
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<td>0.039</td>
</tr>
<tr>
<td>Nε</td>
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<td>0.002</td>
<td>-0.001</td>
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<tr>
<td>$f^+$</td>
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<td></td>
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<td></td>
</tr>
<tr>
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<td>-0.001</td>
<td>-0.003</td>
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<td>0.023</td>
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Table S10. The Fukui indices $f, f^+, f^2$ calculated for OxoG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with OxoG are indicated in parenthesis as follows: C1’-pathway (C1’), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9).

<table>
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<th>OxoG</th>
<th>OxoG (C1’)</th>
<th>OxoG (N3)</th>
<th>OxoG (N3H)</th>
<th>OxoG (N9)</th>
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<tbody>
<tr>
<td></td>
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<td>-0.008</td>
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<td>-0.001</td>
<td>-0.002</td>
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Table S11. The Fukui indices $f^-$, $f^+$, $f^2$ calculated for FapyG employing B3LYP-D2/6-31G**/PCM method. The interactions of Lys 249 with FapyG are indicated in parenthesis as follows: C1'-pathway (C1'), N3-pathway (N3), N3-pathway with proton transferred from Nε-ammonium to N3 nitrogen (N3H), N9-pathway (N9), N9-pathway with proton transferred from Nε-ammonium to N9 nitrogen (N9H).

<table>
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<th>FapyG (C1')</th>
<th>FapyG (N3)</th>
<th>FapyG (N3H)</th>
<th>FapyG (N9)</th>
<th>FapyG (N9H)</th>
</tr>
</thead>
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<td>-0.011</td>
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<td>0.008</td>
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<td>$f^+$</td>
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<td>0.008</td>
<td>0.022</td>
</tr>
<tr>
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<td>0.000</td>
<td>-0.006</td>
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<td>-0.005</td>
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<tr>
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<td>$f^2$</td>
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</tr>
<tr>
<td>C1'</td>
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<td>0.010</td>
<td>0.008</td>
<td>0.008</td>
<td>0.004</td>
<td>0.005</td>
</tr>
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Table S12. The Hardness $\eta$ a) in (eV) calculated for G, OxoG and FapyG. The numbering of atoms is according to IUPAC.

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a) The global reactivity descriptor of a molecule called chemical hardness $\eta = \frac{1}{2}(\varepsilon_{LUMO} - \varepsilon_{HOMO})$ was calculated employing the B3LYP-D2/6-31G**/PCM method. $\varepsilon_{LUMO}$ and $\varepsilon_{HOMO}$ are electronic energies of lowest unoccupied and highest occupied molecular orbital.
Table S13. The interaction energies in kcal/mol of G, OxoG and FapyG interacting with Lys 249 calculated employing small model and B3LYP-D2/PCM method including the BSSE correction that was calculated in gas phase. a)

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a) The interaction energy for Lys249 and nucleoside employing small model was computed using the following protocol: (i) the geometry optimization of complexes and monomers using the B3LYP-D2/6-31G(d,p)/PCM=diethylether method keeping the constraint defined for small model, (ii) the energy calculation for the complex ($E_{\text{complex}}$) and the monomers ($E_1, E_2$) employing the B3LYP-D2/6-311++G(d,p)/PCM=diethylether method, (iii) the BSSE calculation employing the B3LYP-D2/6-311++G(d,p) method, (iv) the interaction energy calculation: $\Delta E_{\text{int}} = E_{\text{complex}} - (E_1+E_2)$, $\Delta E_{\text{int}}$ (BSSE) = $\Delta E_{\text{int}} + E_{\text{BSSE}}$. b) Calculated with 6-311++G(d,p) basis set. c) Calculated with aug-cc-pVDZ basis set.
Table S14. The reaction energies $\Delta E_r$, the activation energies $\Delta E^\#$, the Gibbs free reaction energies $\Delta G_r$, and the Gibbs free activation energies $\Delta G^\#$ in kcal/mol calculated employing small model and B3LYP-D2/6-31G**/PCM method for proton transfer from Lys 249 to nucleobase owing to N3-pathway and N9-pathway.

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$^b$) The N3-pathway and N9-pathway depicted in Figure S4 and Figure S5 are indicated in parenthesis.  
$^b$) The energy of complex with proton at nucleobase minus energy of complex with proton at Lys 249.  
$^c$) The energy of transition state of proton transfer minus energy of complex with proton at Lys 249.
Table S15. The electronic and Gibbs free activation and reaction energies in kcal/mol calculated for cleavage of N-glycosidic bond with $S_N^2$ reaction mechanism initiated by C1’-pathway as depicted in Figure S3. The calculations employing B3LYP-D2/6-31G**/PCM method.

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**Figure S1.** The NICSs were calculated at the centre of mass of 5 and 6-membered ring of G, OxoG and FapyG indicated by purple ball.
Figure S2. The NLMO of lone-pair electrons at N9 nitrogen calculated for G, OxoG and FapyG.
Figure S3. The reactant (R), transition state (TS) and product (P) of N-glycosidic bond cleavage of G, OxoG and FapyG employing C1-pathway. The C1’-N9 and C1’-Nε distances between atoms indicated by dashed lines are in Å.
Figure S4. The reactant (R), transition state (TS), and product (P) calculated for proton addition to nitrogen N3 of G, OxoG and FapyG employing Lys 249. The N3-Nε distances between atoms indicated by dashed line are in Å.
Figure S5. The reactant (R), transition state (TS), and product (P) calculated for proton addition to glycosidic nitrogen N9 of FapyG owing to deprotonation of Lys 249. The N9-Ne distances between atoms indicated by dashed lines are in Å.
Figure S6. The NLMO of lone-pair electrons at N9 nitrogen calculated for N9-pathway of OxoG and FapyG.
Optimized Geometries (Small model)

**G**

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N  23.30502600 21.96082000 33.39133100
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* The atoms indicated by star were fixed during geometry optimizations. The initial geometries were derived from the 1N3C PDB x-ray structure.