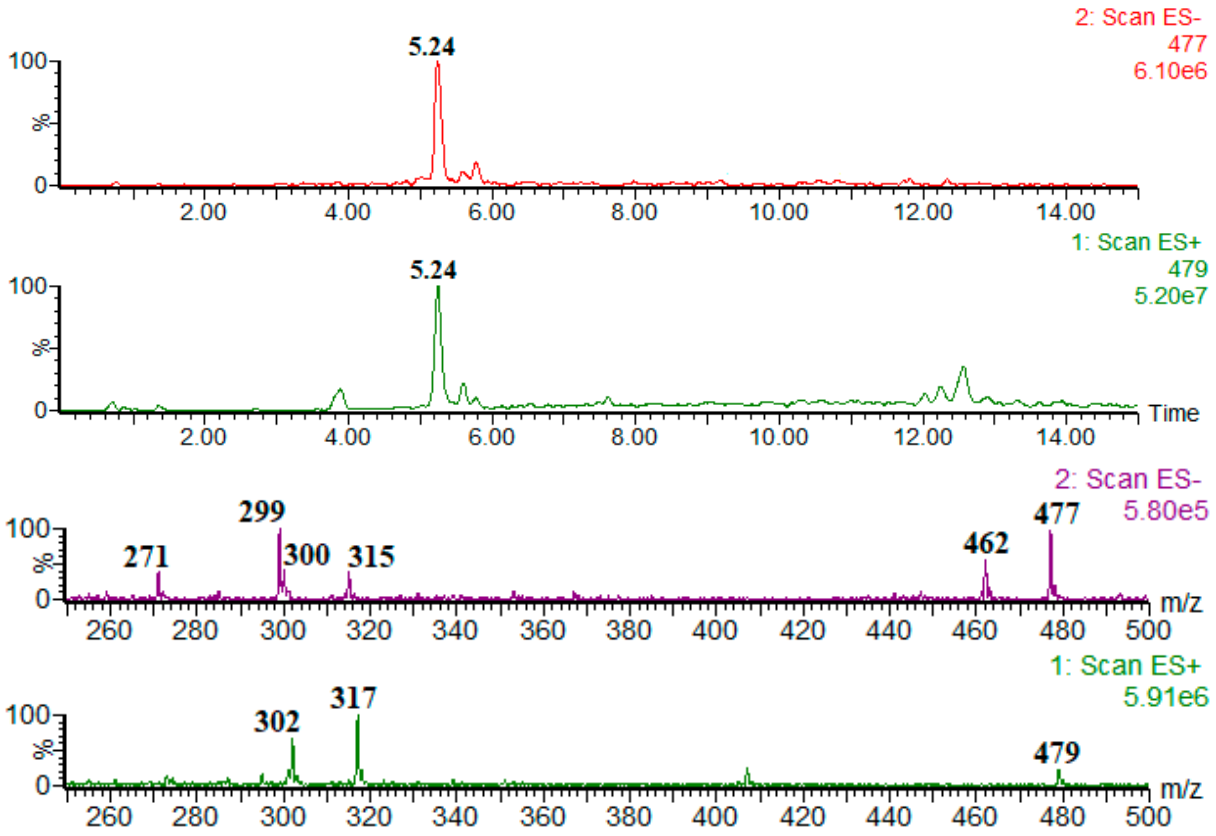


Figure S1. HPLC-MS data obtained for 3-*O*-methylquercetin-7-*O*–glucoside (**1**).

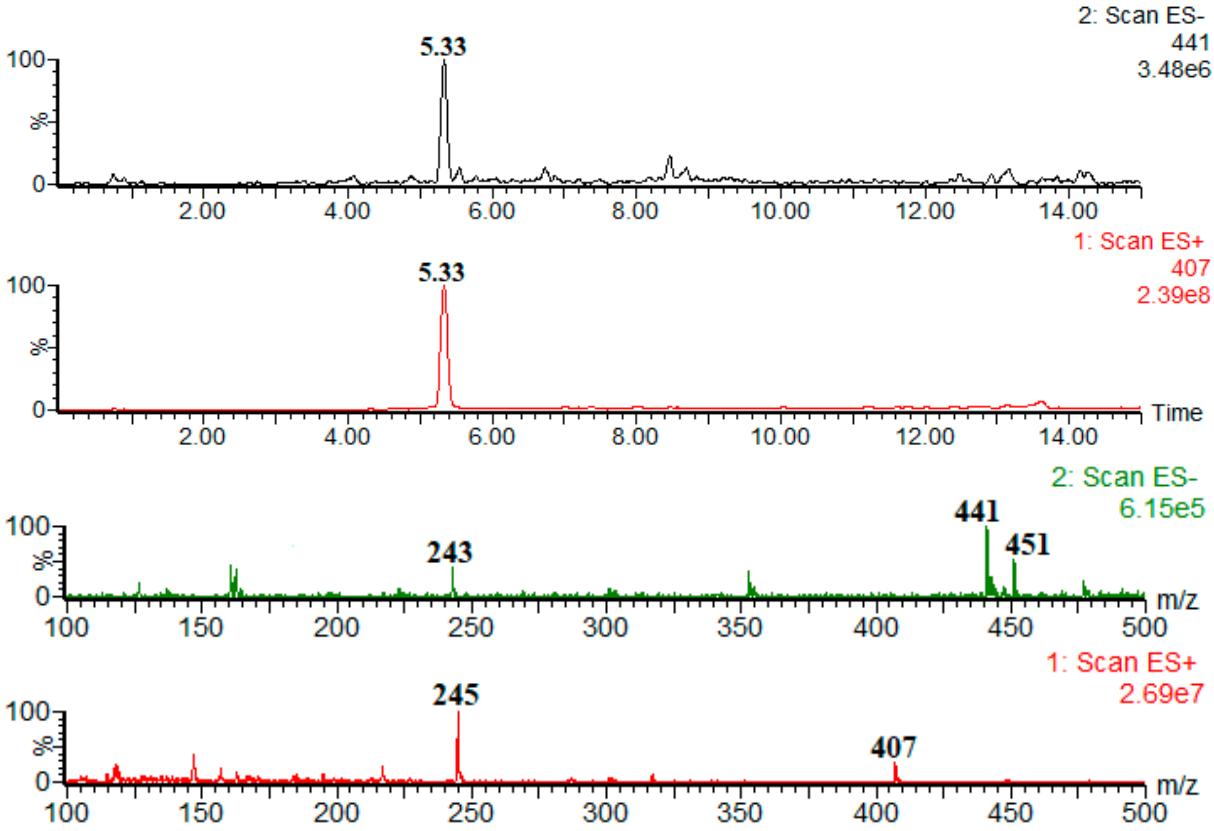


Figure S2. HPLC-MS data obtained for 4'-hydroxydehydrokawain-4'-*O*-glucoside (**2**).

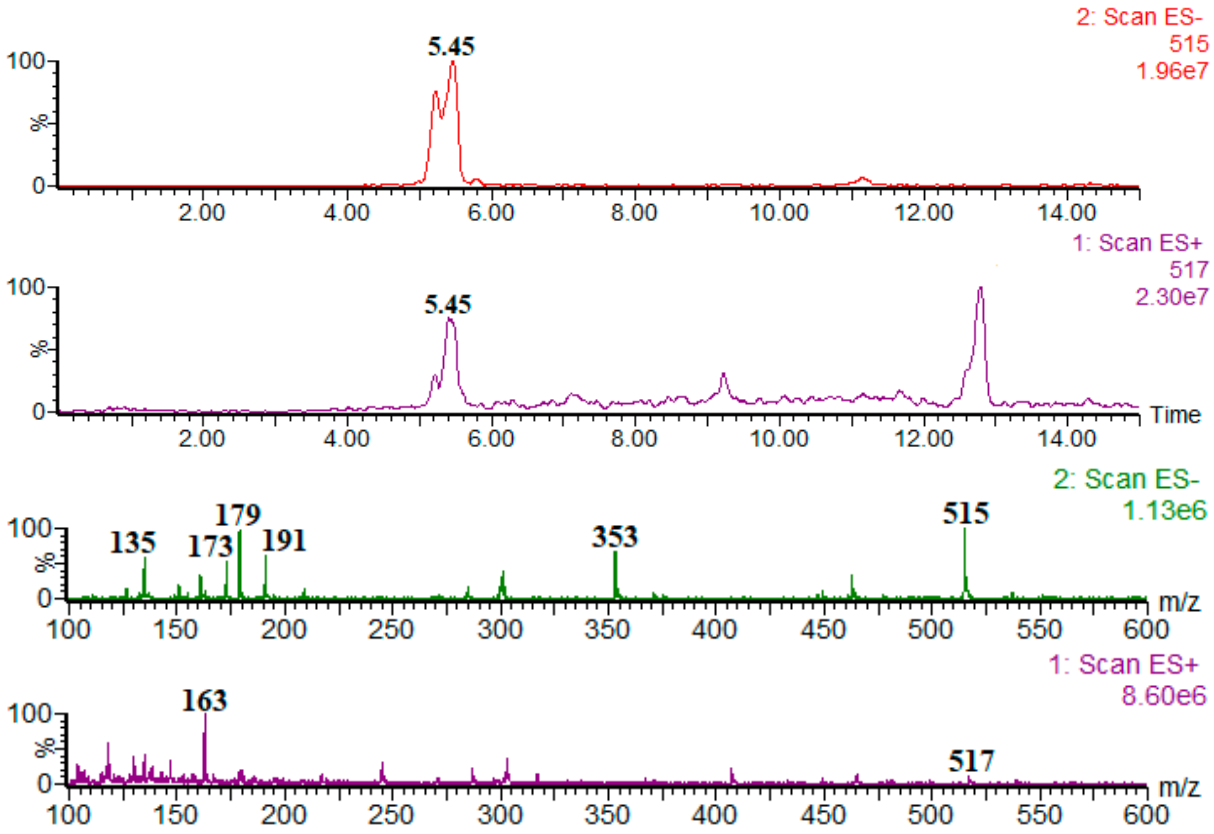


Figure S3. HPLC-MS data obtained for 3,5-di-*O*-caffeoylquinic acid (**3**).

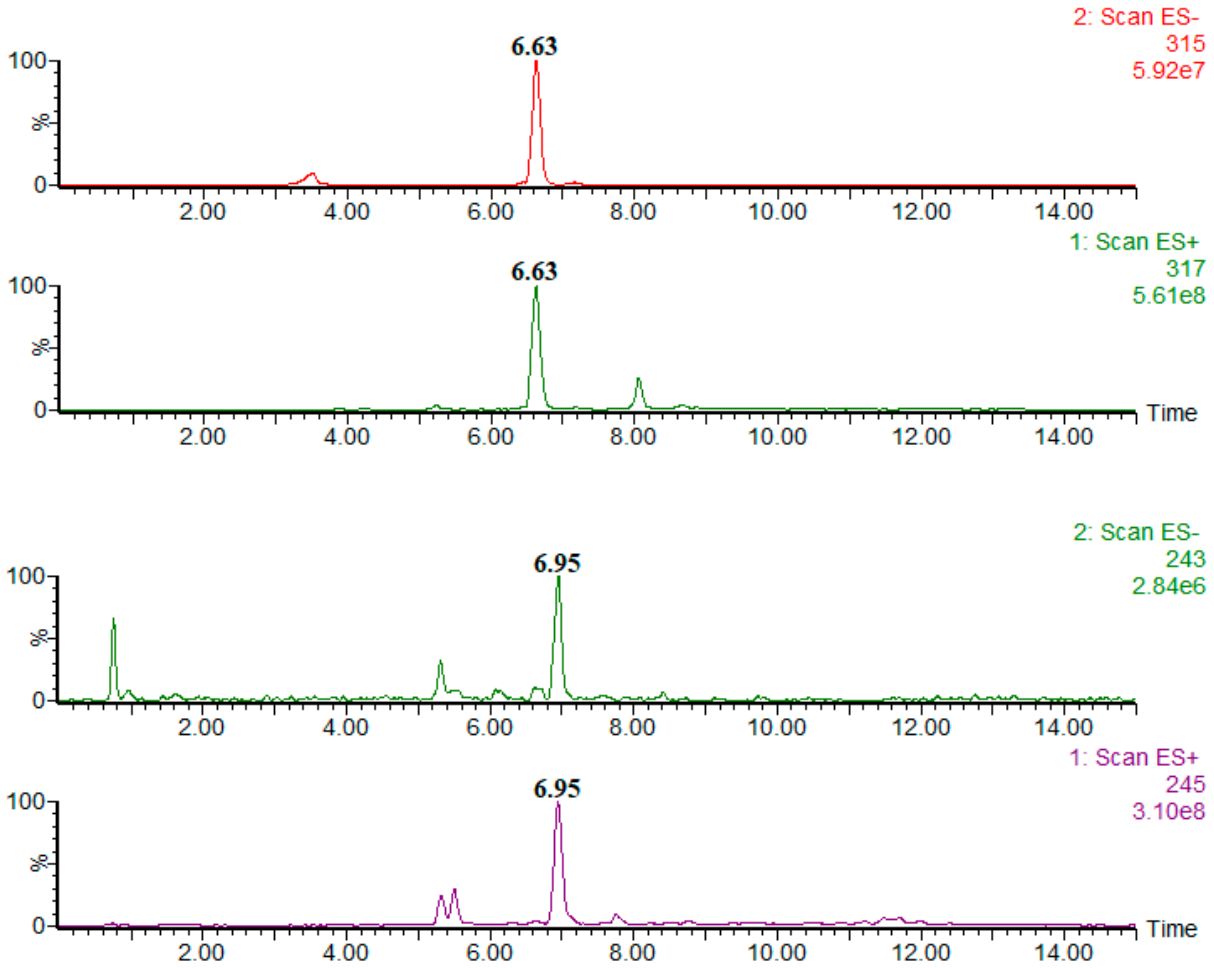
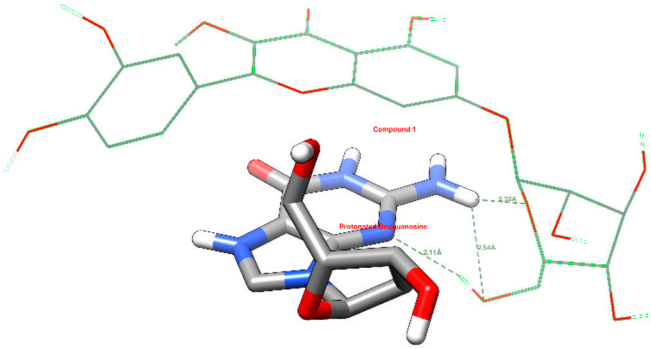
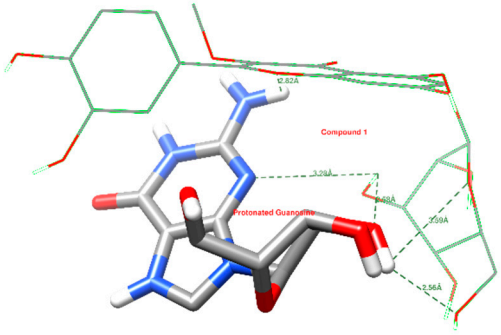


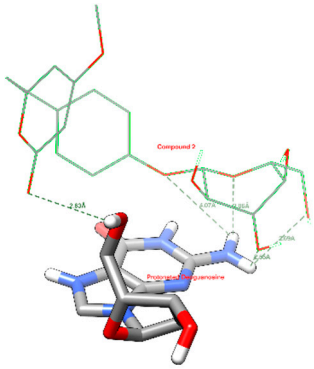
Figure S4. Single ion chromatograms of free aglycones of **1** and **2**, 3-*O*-methylquercetin at *m/z* 315 and 317, 4'-hydroxydehydrokawain at *m/z* 243 and 245.



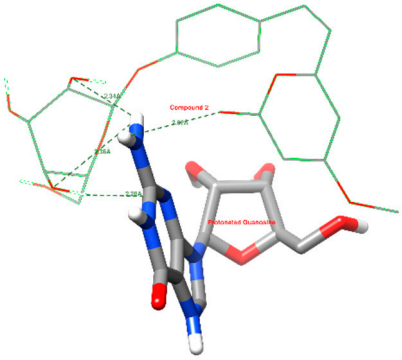
[**1**+dG+H]$^+$



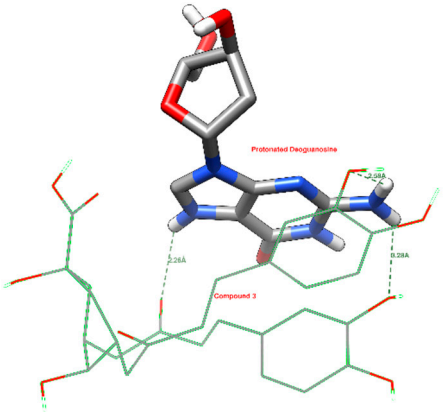
[**1**+G+H]$^+$



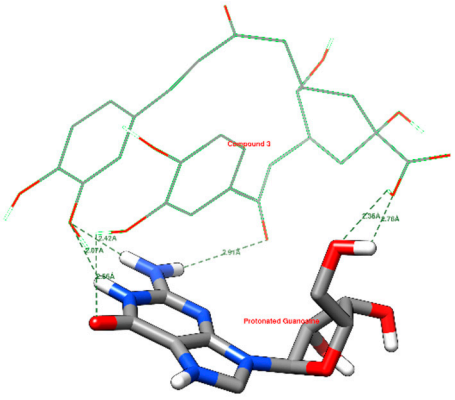
[**2**+dG+H]$^+$



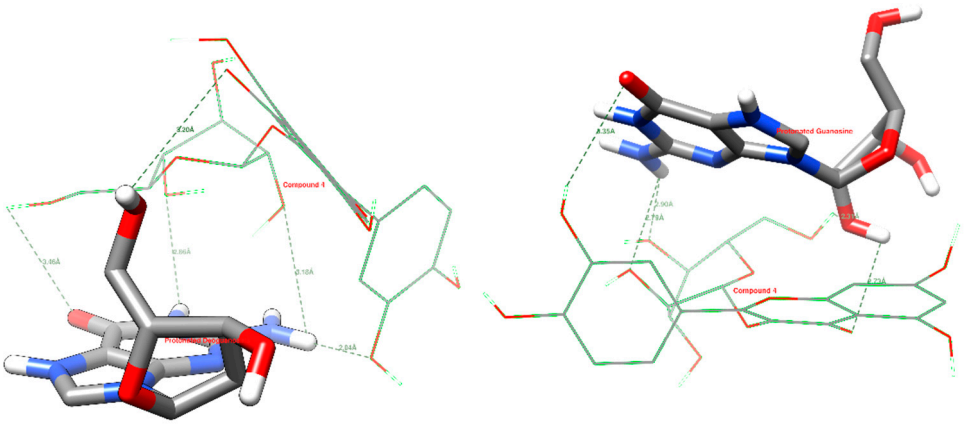
[**2**+G+H]$^+$



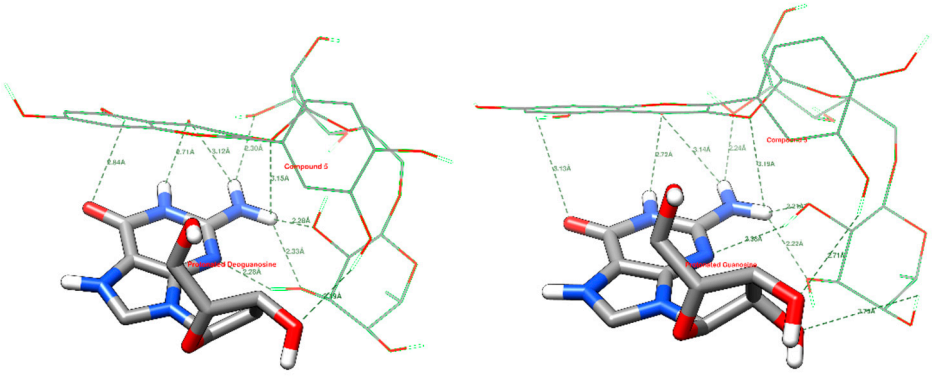
[**3**+dG+H]$^+$



[**3**+G+H]$^+$

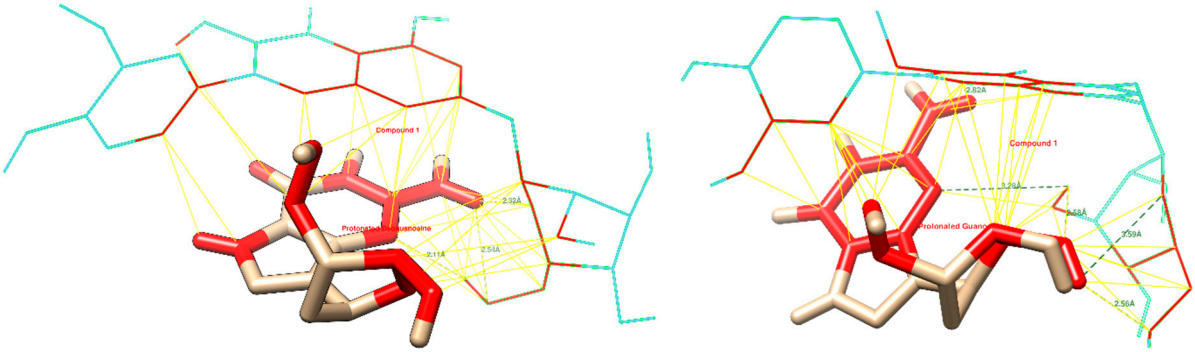


[**4**+dG+H]$^+$ [**4**+G+H]$^+$

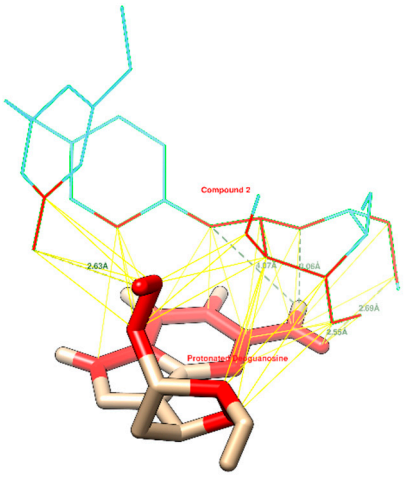


[**5**+dG+H]$^+$ [**5**+G+H]$^+$

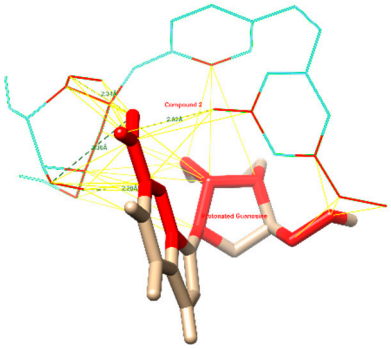
Figure S5. Potential hydrogen bonds formation (green dashed lines) of **1**-**5** with protonated deoxyguanosine and guanosine.



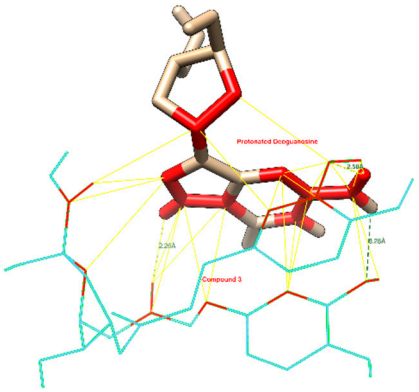
[**1**+dG+H]$^+$ [**1**+G+H]$^+$



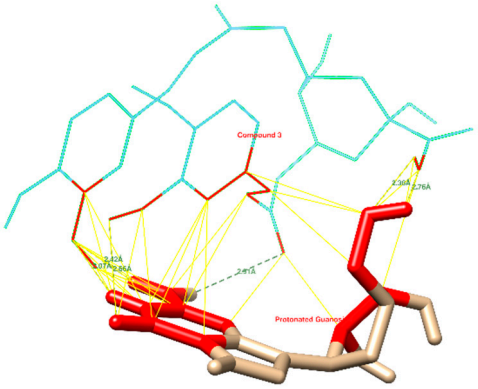
[**2**+dG+H]$^+$



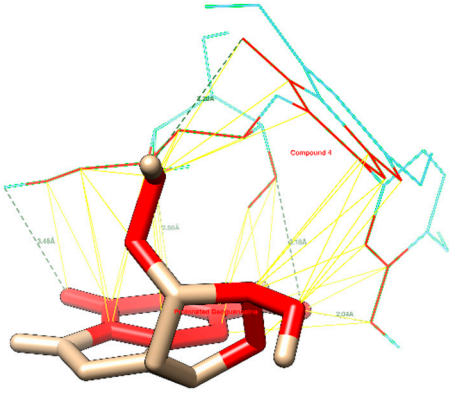
[**2**+G+H]$^+$



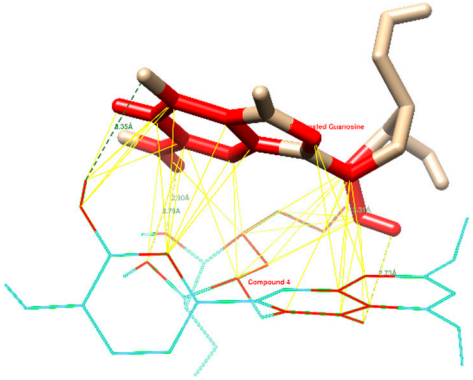
[**3**+dG+H]$^+$



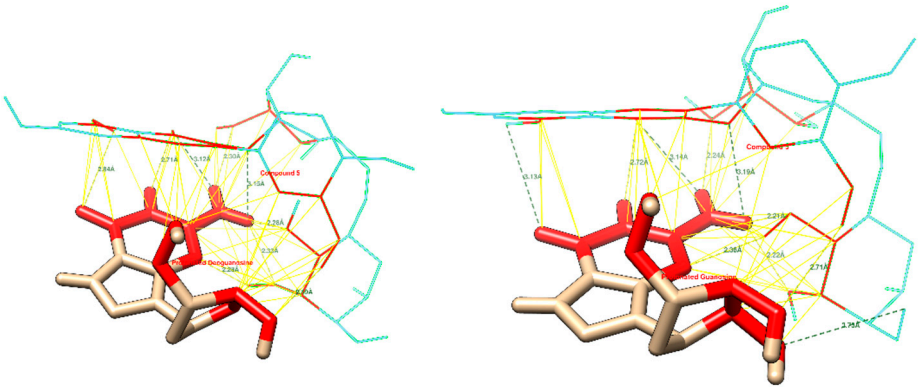
[**3**+G+H]$^+$



[**4**+dG+H]$^+$



[**4**+G+H]$^+$



[**5**+dG+H]$^+$ [**5**+G+H]$^+$

Figure S6. Potential interactions (especially pi-pi, yellow lines) of **1**-**5** with protonated deoxyguanosine and guanosine.