Table S1. Summary of calculation of the chemical reaction between deoxyadenosine or glutathione with bisphenol A-3,4-quinone. The B3LYP/6-31+G(d,p) level was applied and Langevin dipoles solvation model was considered.

		E_{gas} [a] [Hartrees]	G_{corr} [b] [Hartrees]	$\Delta G_{hydation}$ [c] [kcal/mol]	ω [d] [icm^{-1}]	r_c [e] [Å]
deoxyadenosine						
N3	N3-RC	-1694.099919	0.431432	-19.6	/	
	TS	-1694.034998	0.441454	-36.7	147.9	1.68
	i-3OHBPA-N3-dA	-1694.082342	0.444383	-32.2	/	
	TS	-1694.043715	0.440834	-30.6	103.3	2.34
	i-3OHBPA-N3-Ade	-1272.550974	0.303521	-73.1	/	
	Rib^+	-421.345183	0.109818	-62.6	/	
	p-3OHBPA-N3-dA	-1694.515487	0.454261	-58.8	/	
	TS	-1694.466631	0.445757	-64.8	49.3	2.86
	p-3OHBPA-N3-Ade	-1273.079574	0.316143	-20.5	/	
	Rib^+	-421.351739	0.109772	-59.6	/	
N7	N7-RC	-1694.095969	0.432947	-21.9	/	
	TS	-1694.042855	0.439017	-30.3	228.8	1.72
	i-3OHBPA-N7-dA	-1694.073972	0.438461	-42.5	/	
	TS	-1694.039444	0.438880	-39.9	21.1	2.60
	i-3OHBPA-N7-Ade	-1272.563496	0.303299	-72.2	/	
	Rib^+	-421.345183	0.109818	-62.6	/	
	p-3OHBPA-N7-dA	-1694.509117	0.451991	-63.2	15.5	2.87
	TS	-1694.471118	0.446083	-65.6	/	
	p-3OHBPA-N7-Ade	-1273.082772	0.316847	-24.2	/	
	Rib^+	-421.351739	0.109772	-59.6	/	
glutathione						
	RC	-2209.865760	0.448997	-164.1	/	
	TS	-2209.851788	0.456748	-167.7	118	2.20
	product	-2209.888724	0.458859	-165.0	/	

[a] *In vacuo* calculated energies on the B3LYP/6-31+G(d,p) level

[b] Thermal correction to Gibbs free energy using harmonic oscillator and rigid rotator approximation

[c] Hydration free energy calculated by Langevin dipoles method

[d] The calculated imaginary frequency of the transition state. Visualization of the corresponding eigenvector shows that it belongs to the reactive motion *i.e.* C6-N3, C6-N7 or C6-S stretching

[e] Reaction coordinate defined as a distance between the reactive C6 atom of bisphenol A-3,4-quinone and N3 or N7 of deoxyadenosine or S of glutathione

RC stands for reaction complex, TS is transition state, Rib^+ represents cationic deoxyribose fragment. See also Figs. 2 and 3

Table S2. Summary of calculation of the chemical reaction between deoxyadenosine or glutathione with bisphenol A-3,4-quinone The B3LYP/6-31+G(d,p) level was applied in conjunction with reaction field solvation model.

		G_{water} [a] [Hartrees]	G_{corr} [b] [Hartrees]	ω [c] [icm^{-1}]	r_c [d] [Å]
deoxyadenosine					
N3	N3-RC	-1694.133610	0.428321	/	
	TS	-1694.081036	0.440589	300.3	1.86
	i-3OHBPA-N3-dA	-1694.128538	0.44019	/	
	TS	-1694.081553	0.439131	102.0	2.35
	i-3OHBPA-N3-Ade	-1272.642117	0.303186	/	
	Rib^+	-421.433921	0.109683	/	
	p-3OHBPA-N3-dA	-1694.589684	0.452854	/	
	TS	-1694.549636	0.443425	30.3	2.99
	p-3OHBPA-N3-Ade	-1273.108885	0.316133	/	
	Rib^+	-421.435847	0.109278	/	
N7	N7-RC	-1694.129462	0.42817	/	
	TS	-1694.086598	0.439817	323.6	1.84
	i-3OHBPA-N7-dA	-1694.128235	0.439531	/	
	TS	-1694.096018	0.438180	14.0	2.50
	i-3OHBPA-N7-Ade	-1272.647615	0.303352	/	
	Rib^+	-421.433921	0.109683	/	
	p-3OHBPA-N7-dA	-1694.589688	0.452124		
	TS	-1694.554198	0.445878	17.7	2.70
	p-3OHBPA-N7-Ade	-1273.113421	0.315493	/	
	Rib^+	-421.435847	0.109278	/	
glutathione					
	RC	-2210.096900	0.447561	/	
	TS	-2210.074581	0.455322	168.6	2.22
	Product	-2210.104047	0.456891	/	

[a] Calculated free energy on the B3LYP/6-31+G(d,p) level in aqueous solution

[b] Thermal correction to Gibbs free energy using harmonic oscillator and rigid rotator approximation

[c] The calculated imaginary frequency of the transition state. Visualization of the corresponding eigenvector shows that it belongs to the reactive motion i.e. C6-N3, C6-N7 or C6-S stretching

[d] Reaction coordinate defined as a distance between the reactive C6 atom of bisphenol A-3,4-quinone and N3 or N7 of deoxyadenosine or S of glutathione

RC stands for reaction complex, TS is transition state, Rib^+ represents cationic deoxyribose fragment. See also Figs. 2 and 3