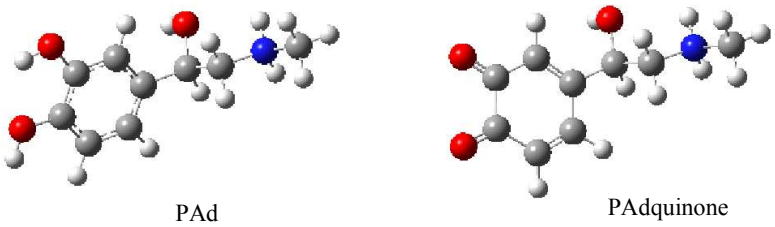

Figure S1. The most stable structures of PAd and PAdquinone in aqueous solution optimized at the G3MP2//B3LYP level.

TABLE S1: Calculated Gas Phase Gibbs Energies $G^{o}_{g,i}$ of H_2 at Different Levels of Theory

	G° (Hartree)
G3MP2// B3LYP	-1.1816
BMK/ TZVP	-1.1696
B3LYP/6-31G(d)	-1.1768
B3LYP/6-31G(d,p)	-1.1799
B3LYP/6-31+G(d)	-1.1768
B3LYP/6-31+G(d,p)	-1.1799
B3LYP/6-311G(d,p)	-1.1810
B3LYP/6-311+G(d,p)	-1.1810
B3LYP/6-311++G(2df,2p)	-1.1814

Table S2: Geometric Parameters[a,b] of the $O_{PAdquinone}H_{PAdquinone}\cdots N_{Gly}$ Parts in Complex PAdquinone-Gly in the Gas Phase and in Aqueous Solution[c], and the H-bond Interaction Energies (Δ*E*, in kcal/mol) in the Complexes

	R(N-H)	R($N_{Gly}\cdots H_{PAd}$)	□$N_{PAd}H\cdots N_{Gly}$	△*E*
B3LYP/6-31G(d,p)	1.074 (1.033)[d]	1.756	164.3	-28.80
	1.095 (1.037)	*1.653*	*172.8*	*-11.90*
B3LYP/6-31+G(d,p)	1.070(1.031)	1.787	167.7	-24.57
	1.083(1.037)	*1.710*	*171.3*	*-6.38*
B3LYP/6-311G(d,p)	1.065 (1.031)	1.808	163.5	-27.75
	1.081 (1.036)	*1.712*	*171.7*	*-10.69*
B3LYP/6-311+G(d,p)	1.064 (1.030)	1.830	165.9	-24.13
	1.075 (1.036)	*1.745*	*169.9*	*-5.98*

[a] For labelings, see Figure 2 (B). [b] Bond lengths are given in Å, and angles in degrees.
[c] The values in solution is denoted with italic. [d] Values in parentheses are the bond lengths in the free PAdquinone.