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Theoretical and Experimental Studies on Some Anticancer Derivatives: Electrochemical investigation, erratum (Vol.4, Page 122, 2009)

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In one table some values were reported by error that we corrected by this errata.

The authors regret that an error occurred in previous published paper (Vol, 4, Page 122, 2009) [1]. This error is now corrected by the means of this erratum. The authors apologize for any inconvenience occurred for the readers.

Unfortunately, there was a mistake in the manuscript preparation. Some data was incorrectly transferred to the word table through a typographical error. Although the calculation methods and the results were absolutely correct, simply in reporting data some mistakes were occurred. For verification of the claim, an excel file is attached as a supplementary information. In this file detail of calculation has been shown. The corrected values which are now changed, are shown in Tables in bold.

Also, the authors report the same mistake in the manuscript [2-4].

Table 1. The Gibbs free energy of studied molecules for both reduced (red.) and oxidised (ox.) in the gas phase and solution phase, along with the change of Gibbs free energy, ΔG_1, in both gas and solution phases [1]

Mol.[a]	$\Delta G_{(gas)}$[b]		$\Delta G_{(sol.)}$[b]		ΔG_1(kJ/mol)	
	Red.	Ox.	Red.	Ox.	Gas	Solution
1[c]	-382.620818	-381.39224	-382.71608	-381.46134	0	0
2[c]	-648.56295	-647.3287	-648.71256	**-647.46212**	-14.8918	11.2896
3[c]	-648.55017	-647.31883	-648.69942	**-647.44571**	-7.2516	2.7042
4[c]	-539.78062	-538.55370	-539.98093	**-538.72583**	4.3530	-0.9451
5[c]	-495.940332	-494.70691	-496.04791	**-494.78891**	-12.7179	-11.1846
6[c]	-587.11008	-585.87597	-587.21809	**-585.95061**	-14.5242	-33.4488

[a] See Fig. 6 for the list of studied molecules.
[b] These energies are in atomic units, Hartree (1 Hartree =2625.49975 kJ mol^{-1}[1])
[c] These energies have been calculated at B3LYP level using 6-31G(d,p) basis set.

Table 2. The Gibbs free energy of the studied molecules for both reduced (red.) and oxidized (ox.) forms in the gas phase and the solution phase, along with the change of the Gibbs free energy in both gas and solution phases [a][2]

	Mol.[a]	$\Delta G_{(gas)}$[b]		$\Delta G_{(sol.)}$[b]		ΔG_1(kJ/mol)	
		Red.	Ox.	Red.	Ox.	Gas	Solution
DFT/6-31G	LD	-691.94277	-690.74601	-691.96865	**-690.80691**	-44.55473	**77.609773**
	CA	-380.95453	-379.77474	-380.98108	-379.78978	0	0

[a] Solution result was obtained with the PCM model
[b] These energies are in atomic units, Hartree (1 Hartree = 2625.49975 kJ mol^{-1})

Table 3. The Gibbs free energy of the studied molecules for both reduced (red.) and oxidized (ox.) forms in the gas phase and the solution phase, along with the change of the Gibbs free in both gas and solution phases [a][3]

	Mol.[a]	$\Delta G_{(gas)}$[b]		$\Delta G_{(sol.)}$[b]		ΔG_1	
		Red.	Ox.	Red.	Ox.	Gas	Solution
DFT/6-31G(d)	CAQ	-878.11509	-876.95047	-878.19358	-876.96237	0.06395	-0.00253
	CA	**-382.620818**	**-381.39224**	**-382.620908**	**-381.39224**	0	0

[a] Solution result was obtained with the PCM model
[b] These energies are in atomic units, Hartree (1 Hartree = 2625.49975 kJ mol^{-1})

Table 4. The Gibbs free energy of the studied molecules for both reduced (red.) and oxidized (ox.) forms in the gas phase and the solution phase, along with the change of the Gibbs free energy in both gas and solution phases [a][4]

	Mol.[a]	$\Delta G^{o}_{i,gas}$[b]		$\Delta G^{o}_{i,solv}$[b]		ΔG_i°	
		Red.	Ox.	Red.	Ox.	Gas	Solution
DFT/6-31G	AQS	-1313.16770	-1311.99694	-1313.23529	**-1312.06685**	**0.0090**	**0.0228**
	CA	-380.95453	-379.77474	-380.98108	-379.78978	0	0
HF/6-31G	AQS	-1306.981862	-1305.854934	-1307.195537	**-1305.948959**	**0.0689**	**-0.0366**
	CA	-380.270371	-379.074527	-380.366967	-379.15704	0	0

[a] Solution result was obtained with the PCM model
[b] These energies are in atomic units, Hartree (1 Hartree = 2625.49975 kJ mol^{-1})

References

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