Novel insights into the effect of folate-albumin binding on the transport of ascorbic acid as an anticancer agent: Chemometric analysis based on combined spectroscopic and electrochemical studies

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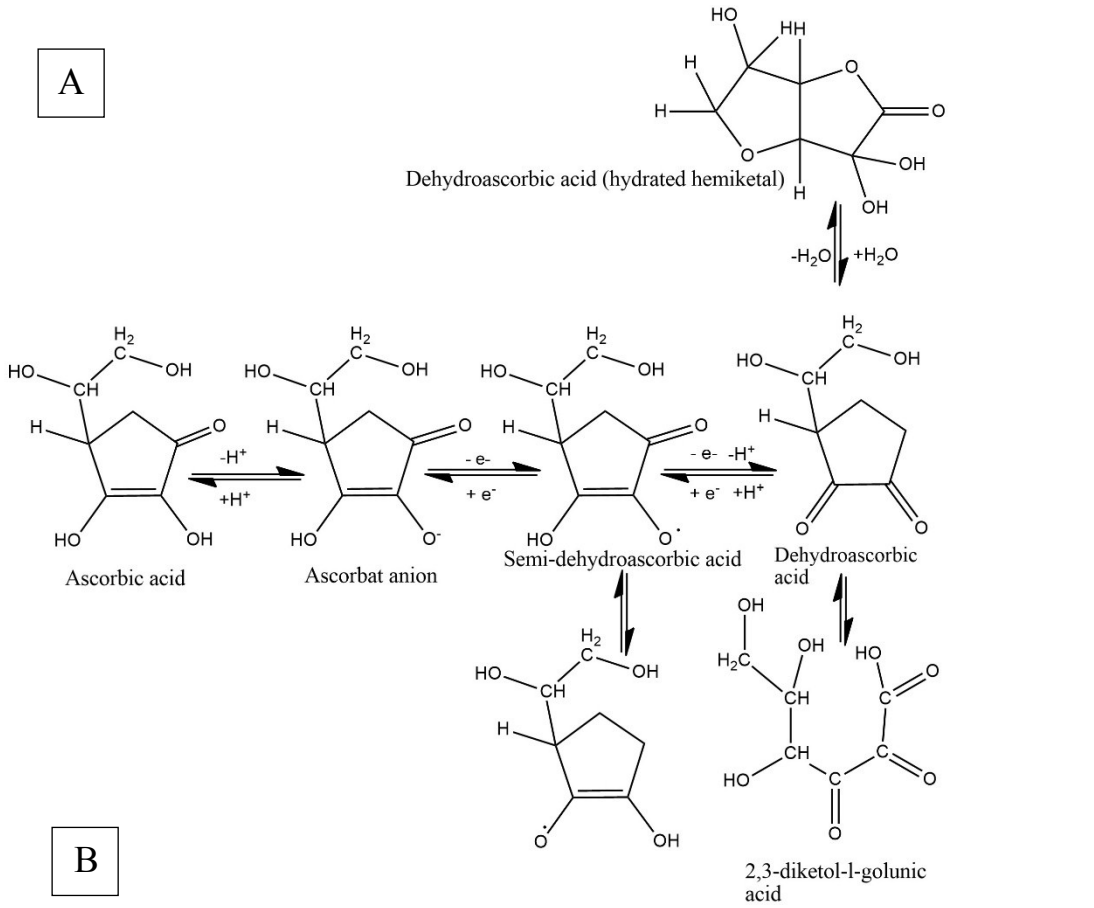

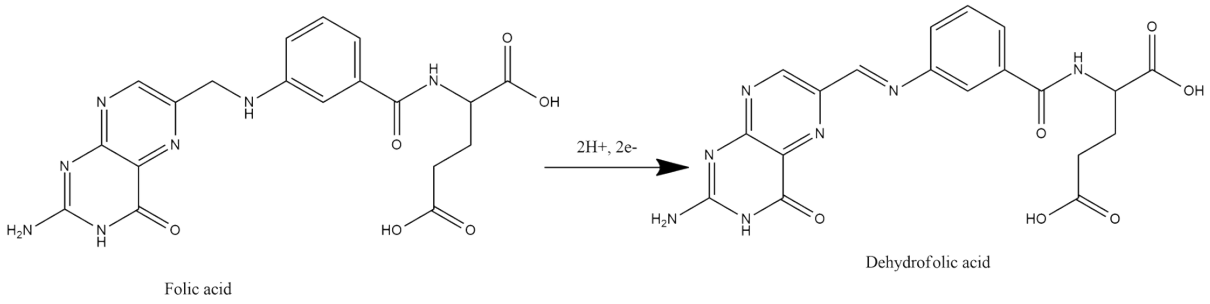

Scheme 1 (A) Oxidation of ascorbic acid at GCE (B) Oxidation of folic acid at GCE

Table S1. Amino acid residues involved in the interaction with the free binding energy for the best selected docking positions

Complex	$\Delta G_{binding}$ (KJ mol^{-1})	Amino acids in the vicinity of the ligands
BSA-FA	-24.57	Asp-111, Ser-109, Arg-144, Leu-189, His-145, Arg-185, Glu-140, Tyr-137, Tyr-160, Pro-117, Ile-181, Ile-141, Leu-114.
BSA-AA	-19.40	Lue-249, Lue-250, Lue-22, Lue-66, Val-23, Ala-26, Gly-247, His-67, Phe-70, Asp-248.

Figure captions

Fig. S1 Relationship between $\log[\Delta I/(\Delta I_{max}-\Delta I)]$ and log [AA].

Fig. S2 Relationship between $\log[\Delta I/(\Delta I_{max}-\Delta I)]$ and log [FA].

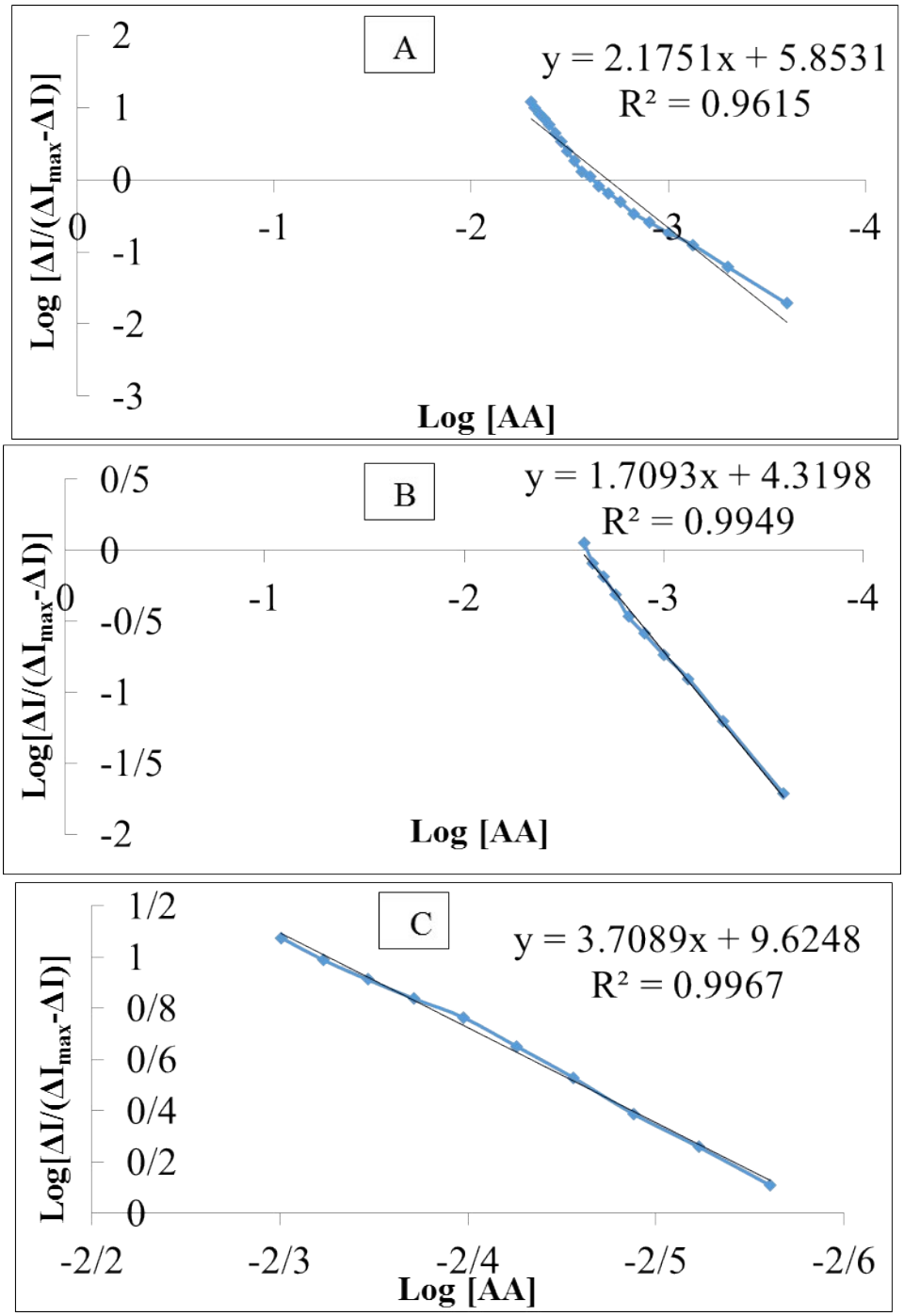
A
y = 2.1751x + 5.8531
R² = 0.9615
Log [ΔI/(ΔImax-ΔI)]
Log [AA]
2
1
0
-1
-2
-3
0
-1
-2
-3
-4
B
y = 1.7093x + 4.3198
R² = 0.9949
Log[ΔI/(ΔImax-ΔI)]
Log [AA]
0/5
0
-0/5
-1
-1/5
-2
0
-1
-2
-3
-4
C
y = 3.7089x + 9.6248
R² = 0.9967
Log[ΔI/(ΔImax-ΔI)]
Log [AA]
1/2
1
0/8
0/6
0/4
0/2
0
-2/2
-2/3
-2/4
-2/5
-2/6

Fig. S1

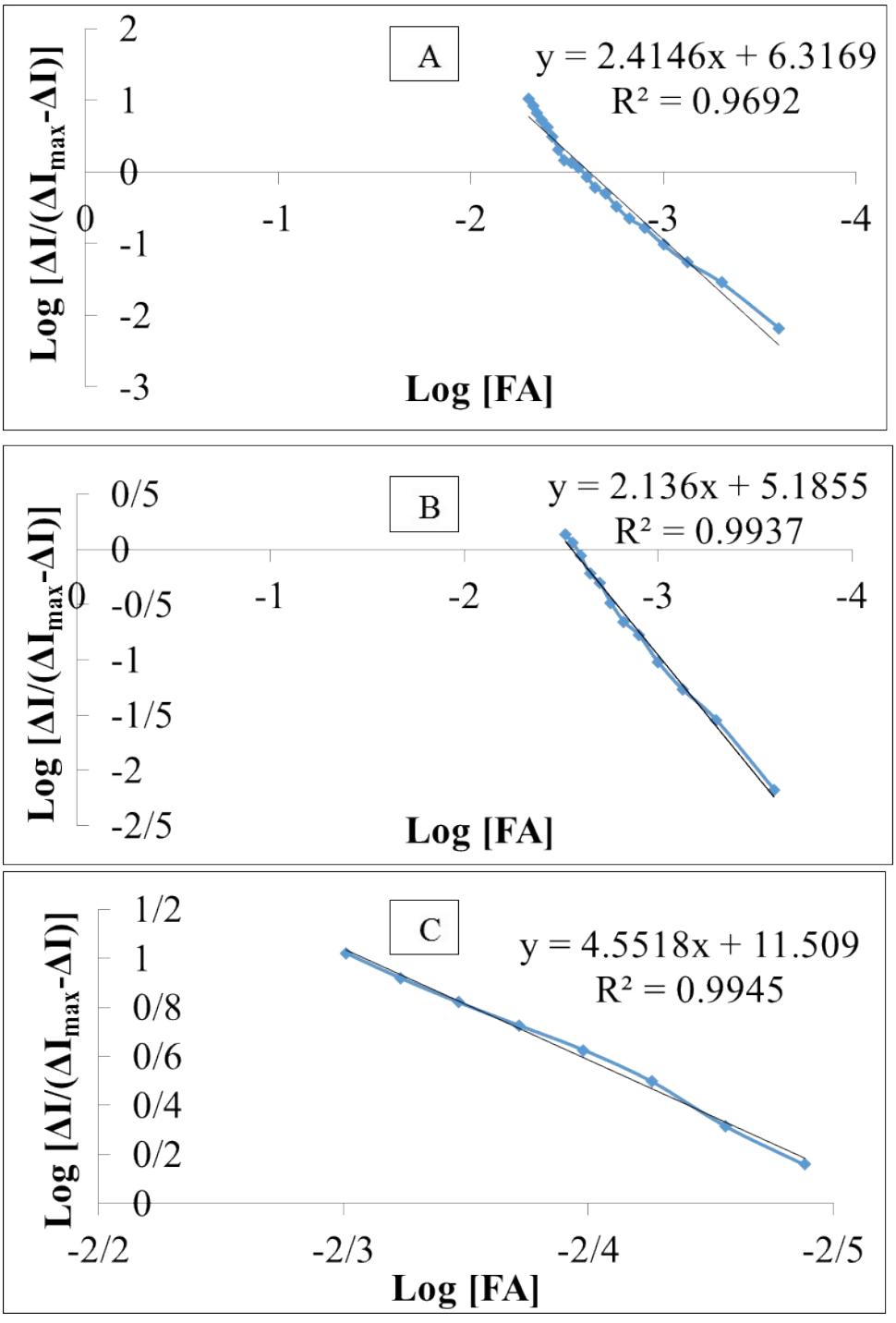
A
y = 2.4146x + 6.3169
R² = 0.9692
Log [ΔI/(ΔImax-ΔI)]
Log [FA]
2
1
0
-1
-2
-3
0
-1
-2
-3
-4
B
y = 2.136x + 5.1855
R² = 0.9937
Log [ΔI/(ΔImax-ΔI)]
Log [FA]
0/5
0
-0/5
-1
-1/5
-2
-2/5
0
-1
-2
-3
-4
C
y = 4.5518x + 11.509
R² = 0.9945
Log [ΔI/(ΔImax-ΔI)]
Log [FA]
1/2
1
0/8
0/6
0/4
0/2
0
-2/2
-2/3
-2/4
-2/5

Fig. S2