Corrigendum

Hajduk P.J., Mendoza R., Petros A.M., Huth J.R., Bures M., Fesik S.W. and Martin Y.C. Ligand binding to domain-3 of human serum albumin: a chemometric analysis. *Journal of Computer-Aided Molecular Design*, **17** (2-4): 93–102.

In Table 4 of this paper, calculated binding affinities for certain compounds were incorrect, due to a slight difference in the weighting coefficients used in the calculation and the final (published) ones. The Table reproduced below contains the correct values.
The authors also wish to remark that the weighting coefficient for a sulfonylurea moiety is identical to that of an acylsulfonamide moiety.

Table 4. Comparison of drug molecule binding affinities for full-length and domain-3 of human serum albumin.

Name	Log K'hsa[a]	Log(K_D-3A) (pred.)[b]	Log(K_D-3A) (expt.)[c]
Naproxen	0.25	−4.38	−5.00
Clotrimazole	1.34	−7.00[d]	−4.92
Ketoprofen	0.03	−5.16	−4.74
Chlorpropamide	−0.44	−3.29	−4.14
Tolbutamide	−0.22	−3.19	−4.09
Indomethacin	0.47	−3.90	−3.93
Clofibrate	0.27	−3.89	−3.70
Salicylicacid	−0.66	−2.70[e]	−3.58
Acetylsalicylicacid	−1.39	−2.70	−3.52
Lidocaine	−0.23	−2.70	−2.70[f]
Pindolol	−0.13	−2.70	−2.70
Atenolol	−0.48	−2.70	−2.70
Captopril	−2.69	−2.70	−2.70
Norfloxacin	0.14	−2.70	−2.70
Phenytoin	0	−2.70	−2.70
Trimethoprim	−0.26	−2.70	−2.70

[a]Taken from Ref. 15. More positive values indicate longer retention times on an HSA affinity column and thus higher affinity for albumin.

[b]Predicted binding affinity (in log units) for domain-3A of albumin using group contributions model as described in the text.

[c]Experimental binding affinity (in log units) for domain-3A of albumin determined using NMR.

[d]Lower limit of group contributions model.

[e]Upper limit of group contributions model.

[f]Upper limit of NMR estimate.