ERRATA

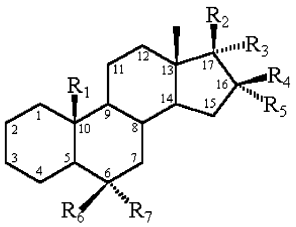
Molecular Quantum Similarity-Based QSARs for Binding Affinities of Several Steroid Sets [*J. Chem. Inf. Comput. Sci. 42*, 1185−1193 (2002)] by X. Gironés and R. Carbó-Dorca*. Institute of Computational Chemistry, University of Girona, E-17071 Girona, Catalonia, Spain

Pages 1185−1193. Two members of the first steroid set (21 and 32) were quoted as being the same structure, but different biological activity values were reported for binding activity to aromatase enzyme. Since we were unable to contact the authors nor to find the correct structures, these molecules have been removed, and a molecular set consisting of 48 structures remains. The QSAR model has been recalculated, yielding to the following equation and associated statistical parameters:

$$\text{binding activity} = 0.137\cdot\mathbf{f}_1 + 6.252\cdot\mathbf{f}_2 + 6.131\cdot\mathbf{f}_3 + 4.514\cdot\mathbf{f}_4 + 7.301\cdot\mathbf{f}_5$$

$$r^2 = 0.844 \quad q^2 = 0.737 \quad s = 0.716$$

Table 1. Structures and Binding Activities to Aromatase for a Set of 50 Steroids[1]



no.	R_1	R_2	R_3	R_4	R_5	R_6	R_7	=O in 3	=O in 7	other	activity
1	CH_2OH	=O	H	H	H			no	yes	Δ^5	−2.92
2	CH_2OH	OH	H	H	H	H		no	yes	Δ^5	−3.54
3	CHO	=O	H	H	H			no	yes	Δ^5	−3.00
4	H	=O	H	H	H			no	yes	Δ^5	−3.26
5	CH_3	OH	H	H	H	H		no	yes	Δ^5	−2.62
6	CH_2OH	=O	H	H	H			no	yes	Δ^3, Δ^5	−3.06
7	CHO	=O	H	H	H			no	yes	Δ^3, Δ^5	−2.14
8	H	=O	H	H	H			no	yes	Δ^3, Δ^5	−2.36
9	CH_2OH	=O	H	H	H			no	no	Δ^5	−1.89
10	CH_2OH	OH	H	H	H	H		no	no	Δ^5	−2.88
11	CHO	=O	H	H	H			no	no	Δ^5	−2.03
12	CH_3	=O	H	H	H			no	no	Δ^5	−0.97
13	CH_3	=O	H	Br	H			no	no	Δ^5	−2.93
14	CH_3	=O	H	H	H			no	yes	Δ^5	−1.28
15	CH_3	=O	H	H	H			no	yes	Δ^3, Δ^5	−1.23
16	CH_3	OH	H	H	H	H		no	yes	Δ^3, Δ^5	−2.61
17	CH_3	OH	H	H	H	H		no	no	Δ^5	−2.36
18	CH_3	=O	H	H	H			no	no	Δ^3, Δ^5	−0.65
19	CH_3	OH	H	H	H	H		no	no	Δ^3, Δ^5	−2.19
20	H	=O	H	H	H	H		yes	no	Δ^4	−1.03
21	CH_2OH	=O	H	H	H	H		no	no	Δ^4	0.46
22	CH_2OH	=O	H	H	H	H		yes	no	Δ^4	−0.84
23	CH_3	=O	H	H	=O			yes	no	Δ^4	0.15
24	CH_3	=O	H	H	see other			yes	no	Δ^4, 6,7-α-CF_2	−0.13
25	CH_3	=O	H	H	see other			no	no	Δ^4, 6,7-α-CH_2	0.87
26	CH_3	OH	H	H	H	see other		no	no	Δ^4, 6,7-α-CH_2	−0.51
27	CH_3	OH	H	H	H	H	H	no	no	Δ^4	−1.35
28	CH_2OH	OH	H	H	H	H	H	no	no	Δ^4	−0.67
29	$CH_2OC(O)CH_3$	=O	H	H	H	H		no	no	Δ^4	−0.89
30	CH_3	=O	H	Br	H	H		no	no	Δ^4	−0.79
31	CF_3	=O	H	H	H	H		no	no	Δ^4	−1.08
32	CH_3	=O	H	H	CH_3	H		yes	no	Δ^4	0.56
33	CH_3	=O	H	H	H	CH_3		yes	no	Δ^4	0.87
34	CH_3	=O	H	H	CH_2CH_3	H		yes	no	Δ^4	1.56
35	CH_3	=O	H	H	H	CH_2CH_3		yes	no	Δ^4	0.94
36	CH_3	=O	H	H	$(CH_2)_2CH_3$	H		yes	no	Δ^4	0.94
37	CH_3	=O	H	H	H	$(CH_2)_2CH_3$		yes	no	Δ^4	0.78
38	CH_3	=O	H	H	$(CH_2)_3CH_3$	H		yes	no	Δ^4	0.65
39	CH_3	=O	H	H	H	$(CH_2)_3CH_3$		yes	no	Δ^4	0.53
40	CH_3	=O	H	H	$CH(CH_3)_2$	H		yes	no	Δ^4	0.21
41	CH_3	=O	H	H	H	$CH(CH_3)_2$		yes	no	Δ^4	0.04
42	CH_3	=O	H	H	C_6H_5	H		yes	no	Δ^4	−0.04
43	CH_3	=O	H	H	H	C_6H_5		yes	no	Δ^4	0.24
44	CH_3	=O	H	H	$CH_2C_6H_5$	H		yes	no	Δ^4	−0.24
45	CH_3	=O	H	H	H	$CH_2C_6H_5$		yes	no	Δ^4	0.61
46	CH_3	=O	H	H	CH=CH_2	H		yes	no	Δ^4	0.91
47	CH_3	=O	H	H	H	CH=CH_2		yes	no	Δ^4	−0.32
48	CH_3	=O	H	H	=$CHCH_3$			yes	no	Δ^4	0.96

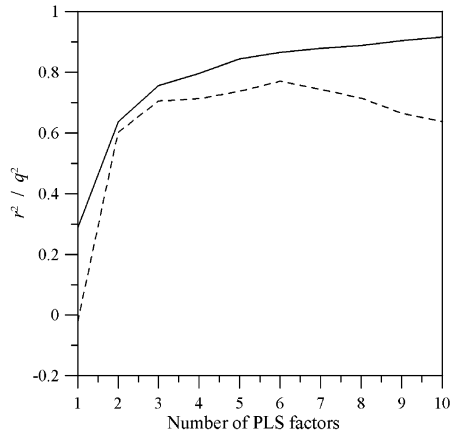


Figure 2. Evolution of r^2 (continuous line) and q^2 (dashed line) versus the number of PLS factors involved in the construction of the QSAR model for a set of 48 steroids.

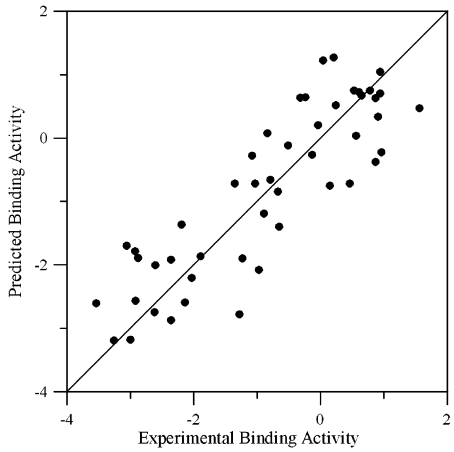


Figure 3. Experimental versus predicted binding activity for a set of 48 steroids.

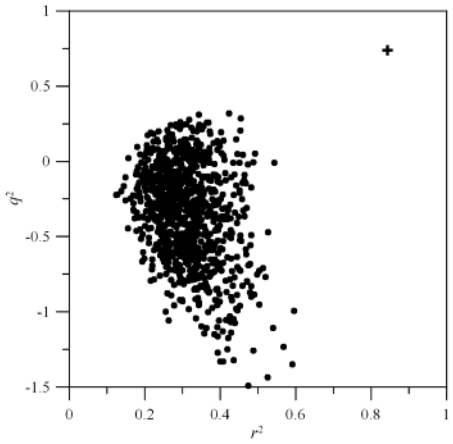


Figure 4. Random test results after permuting the binding activity values for a set of 48 steroids 1000 times. The real value is labeled with a cross.

Also, the recalculated plots associated with the model are presented in Figures 2−4. As shown, the corrected QSAR model does not significantly deviate from the previous reported one, being that the methodology is quite stable. Many thanks to N. S. Zefirov, who told us about the errata.

REFERENCES AND NOTES

(1) Beger, R. D.; Buzatu, D. A.; Wilkes, J. G.; Lay, J. O., Jr. ^{13}C NMR Quantitative Spectrometric Data-Activity Relationship (QSDAR) Models of Steroids Binding the Aromatase Enzyme. *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 1360−1366.

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