Development of a Chirality-Sensitive Flexibility Descriptor for 3+3D-QSAR

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Table S1. The best PLS models optimized by a Monte Carlo Annealing protocol in the descriptor space

Model #1		Model #2		Model #3	
Descriptors	PLS coeff.	Descriptors	PLS coeff.	Descriptors	PLS coeff.
b_a_c_h	1.6506	b_a_c_h	1.4879	b_a_c_h	1.9692
b_a_d_h	0.9283	b_a_d_h	0.5925	d_f_h_i	1.4901
d_f_h_i	1.4519	d_f_h_i	1.6826	Constant	11.6021
Constant	14.8839	Constant	13.5173		
rank	2	rank	2	rank	2
r²	0.74	r²	0.73	r²	0.70
LOO-q²	0.69	LOO-q²	0.67	LOO-q²	0.65
L50%O-q²	0.65	L50%O-q²	0.63	L50%O-q²	0.62

Figure S1. Dependence of the endomorphin L50%O q^2 values on the rejection factor utilized for filtering out descriptors from PPQs where the Pearson correlogram calculated for PPQ point-plane distance distributions showed multiple peaks.

Figure S2. Probability distribution of a chance correlation by using PLS for endomorphin analogs.

Figure S3. Relative importance (PLS coeff * stddev) of the descriptors calculated from the PLS model without MCA for endomorphin analogs.

Figure S4. Training set of prostaglandin PGF2 α analogs.

Figure S5. Dependence of the prostaglandin L50%O q^2 values on the rejection factor utilized for filtering out descriptors from PPQs where the Pearson correlogram calculated for PPQ point-plane distance distributions showed multiple peaks.

Figure S6. Probability distribution of a chance correlation by using PLS for prostaglandin analogs.

Figure S7. Relative importance (PLS coeff * stdev) of the descriptors calculated from the PLS model without MCA for prostaglandin analogs.