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SUPPLEMENTARY MATERIAL TO

Quantitative structure–activity relationship modelling of influenza M2 ion channels inhibitors

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Fig. S-1 depicts the example showing how, using vertexes differentiation by atomic charges, the simplexes descriptors are generated at 2D level.

The contribution of each of nine SiRMS descriptors used in the Model A1 is represented in Table S-I.

The distribution of prediction errors (ΔY = mod($Y_{predicted} - Y_{observed}$)) demonstrates that a greater accuracy of prediction is observed for compounds with medium (Fig. S-3).

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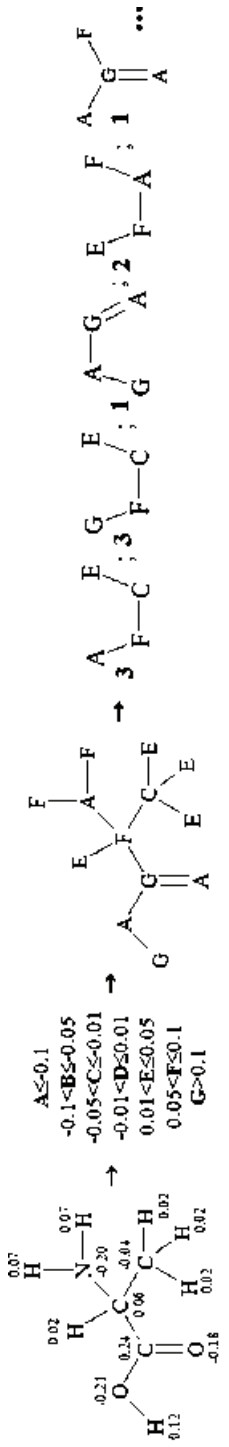
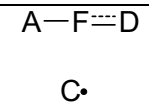
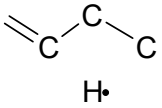
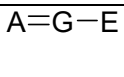
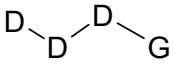
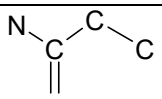
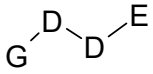
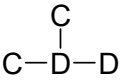
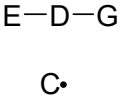


Fig. S-1. Depiction of the development of simplex descriptors at 2D level.

TABLE S-1. Structural parameters and their VIP scores

No.	Type differentiation vertexes simplexes	Structural fragment	VIP scores
1	Atom charge		0.78
2	Type		0.45
3	Atom charge		0.44
4	lipophilicity		0.41
5	type		0.41
6	lipophilicity		0.39
7	lipophilicity		0.33
8	Atom charge		0.30
9	lipophilicity		0.23

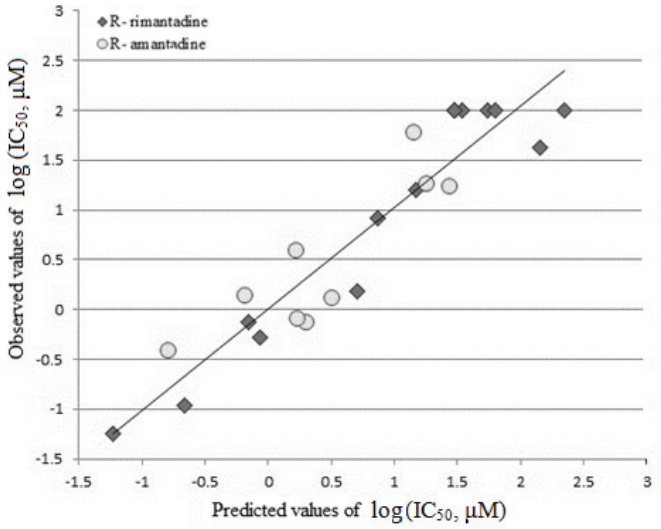


Fig. S-2. Observed *vs.* predicted diagram of antiviral activity (log IC_{50}) for 22 molecules (Model A1).

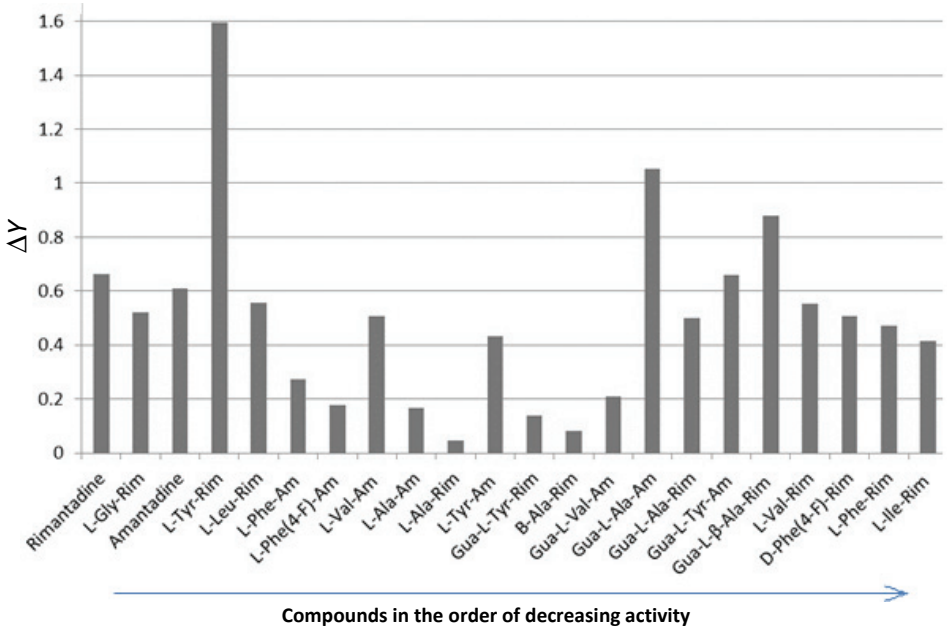


Fig. S-3. The distribution of activity prediction errors (Δ*Y*) by Model A2.

TABLE S-II. Predicted classes of activity by models B1 – B3 for "out-of-bag" set

Compound name	CC_{50} class			*HNTC* class	
	Observed	Predicted (Model B1)	Predicted (Model B2)	Observed	Predicted (Model B3)
L-Val-Rim	1	0	1	1	1
L-Phe-Am	1	1	1	1	1
L-Phe(4-F)-Am	1	0	1	1	0
L-Val-Am	0	0	1	0	0
Gua-L-Val-Am	0	0	0	0	0
L-Tyr-Am	0	0	0	0	1
Gua-L-Tyr-Am	0	0	0	0	0
L-Gly-Rim	0	0	0	1	1
L-Ile-Rim	1	1	1	1	1
L-Leu-Rim	0	0	0	1	1
L-Phe-Rim	1	1	1	1	1
β-Ala-Rim	0	0	0	1	1
D-Phe(4-F)-Rim	1	1	1	1	1
Amantadine	0	0	0	0	0
Gua-L-β-Ala-Rim	0	0	0	0	0
L-Tyr-Rim	0	0	0	1	1
Gua-L-Tyr-Rim	0	0	0	1	1
L-Ala-Rim	0	0	0	1	1
Gua-L-Ala-Rim	0	0	0	0	0
L-Ala-Am	0	0	0	0	0
Gua-L-Ala-Am	0	0	0	0	0