Supporting Information

Design, Molecular Modeling, Synthesis and anti-HIV-1 Activity of New Indolyl Aryl Sulfones. Novel Derivatives of the Indole-2-Carboxamide

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Compd	Calculated					Found				
	С	Н	Ν	Cl	S	С	Н	Ν	Cl	S
6	51.49	3.36	10.01	8.44	7.60	51.20	3.19	9.87	8.32	7.42
7	53.63	4.05	9.38	7.92	7.16	53.51	3.98	9.21	7.76	7.02
8	55.17	4.63	10.72	9.05	8.18	54.05	4.60	10.61	8.87	8.02
9	57.20	5.28	10.01	8.44	7.64	57.07	5.22	9.94	8.27	7.42
10	60.05	5.70	9.14	7.71	6.97	59.75	5.56	8.91	7.40	6.59
11	54.35	4.32	10.1	8.44	7.64	54.21	4.28	9.90	8.28	7.47
12	53.39	4.48	9.34	7.88	7.13	53.20	4.91	9.27	7.65	6.97
13	49.60	4.16	16.07	8.13	7.36	49.41	4.12	15.92	8.01	7.16

Appendix. Elemental Analyses of Compounds 6-13.

PLS coefficients, Present Fields, Activity Contribution and T-U Scores Plots for the Interpretation of the 3-D QSAR Model S2-S5.



Figure A. PLS Coefficient Plot Focalized on the Phenyl Groups of Compounds 4 (yellow) and 94 (red).

Figure B. Present Fields Plots Focalized on the Phenyl Groups of Compounds 4 (A, left) and 94 (B, right).



Figure C. Activity Contribution Plots Focalized on the Phenyl Groups of Compounds 4 (A, left) and 94 (B, right). A B







Figure D. PLS Coefficient Plots for the old (A) and the new (B) Models.

Figure E. PLS Coefficient Plot focalized on the Hydroxyethyl Groups of Compounds **4** (yellow) and **94** (red).



Figure F. Present Fields Plots Focalized on the Hydroxyethyl Groups of Compounds 4 (A, left) and 94 (B, right).



Figure G. Activity Contribution Plots Focalized on the Hydroxyethyl Groups of Compounds 4 (A, left) and 94 (B, right).





Figure H. T-U Scores Plots of the New Model. A: First Principal Component; B: Second Principal Components; C: Third Principal Component.

