

Supplementary material to:

PREDICTION OF AROMATASE INHIBITORY ACTIVITY USING THE EFFICIENT LINEAR METHOD (ELM)

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<http://dx.doi.org/10.17179/excli2015-140>

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Supplementary Table S1: Initial and 10 optimal parameter sets of ELM for predicting steroidal AIs

Feature	Initial	1	2	3	4	5	6	7*	8	9	10
C-025	0.13	-0.21	0.08	0.36	0.19	0.19	0.17	0.13	0.11	0.33	-0.06
ESpm13r	6.70	-13.48	-7.93	-15.55	-11.25	-11.25	-9.18	-15.24	-11.07	-9.62	-9.77
ESpm14u	2.95	7.30	7.12	11.57	6.33	6.33	9.18	9.23	9.71	8.05	4.53
ESpm10r	5.84	2.57	-0.90	5.65	4.32	4.32	2.34	5.30	3.99	0.00	5.23
ESpm12x	5.49	-0.54	-2.72	-6.68	-6.27	-6.27	-8.32	-5.94	-3.09	-8.67	-3.46
ESpm15d	0.12	0.13	0.09	0.21	0.12	0.12	0.19	0.15	0.13	0.32	0.26
ESpm10x	6.33	1.01	2.12	3.74	6.76	6.76	3.79	5.43	-2.69	9.73	1.85
H-050	0.07	0.03	0.05	0.06	0.09	0.09	0.05	0.13	0.03	0.07	0.09
nBM	0.04	0.03	0.00	-0.02	-0.03	-0.03	0.03	0.00	0.10	-0.04	0.03
MATS6p	1.52	3.93	3.18	3.88	3.34	3.34	3.84	3.85	2.37	3.08	4.48
MATS6e	1.52	-2.46	-2.44	-2.63	-1.88	-1.88	-3.24	-3.15	-1.80	-2.29	-4.02
GATS6m	0.94	-2.44	-1.92	-2.27	-1.69	-1.69	-1.99	-2.32	-1.48	-2.12	-2.58
GATS6p	1.03	2.62	1.35	2.41	1.89	1.89	1.40	1.58	1.01	1.86	1.72
piPC07	0.29	0.62	0.64	0.74	0.26	0.26	0.72	0.23	0.46	0.02	0.41
GGI1	0.08	0.02	-0.01	-0.02	-0.02	-0.02	-0.06	-0.03	0.03	-0.11	-0.09

* Experiment 7 provided the highest performance for predicting steroidal AIs

Supplementary Table S2: Initial and 10 optimal parameter sets of ELM for predicting non-steroidal AIs

Feature	Initial	1	2	3	4*	5	6	7	8	9	10
nAB	0.01	-0.02	-0.03	-0.02	-0.02	-0.02	-0.03	-0.02	-0.02	-0.02	-0.02
piPC05	0.31	2.17	1.94	1.83	2.10	1.81	2.16	2.21	1.92	2.06	1.96
BEHp4	0.37	-1.92	-2.30	-2.23	-2.19	-2.01	-1.97	-1.83	-1.93	-2.18	-1.79
Yindex	0.24	0.88	1.00	0.96	1.08	0.95	0.96	0.96	1.06	1.04	1.09
F04[O-O]	0.02	0.13	0.11	0.12	0.13	0.13	0.11	0.13	0.12	0.12	0.11
EEig09x	0.09	0.25	0.20	0.22	0.23	0.21	0.21	0.22	0.21	0.24	0.19
GATS5e	0.08	0.17	0.17	0.14	0.15	0.12	0.13	0.13	0.13	0.15	0.11
nCp	0.03	0.11	0.10	0.10	0.11	0.11	0.11	0.14	0.10	0.10	0.12
ATS5p	0.16	-0.51	-0.43	-0.41	-0.46	-0.46	-0.48	-0.48	-0.54	-0.49	-0.54
piPC08	0.16	0.90	0.94	1.05	0.95	1.03	0.89	0.98	0.95	1.03	0.90
EEig04x	0.14	-0.37	-0.51	-0.33	-0.40	-0.34	-0.37	-0.35	-0.49	-0.30	-0.35
piPC06	0.31	-2.92	-2.88	-2.97	-3.00	-2.92	-2.85	-3.11	-2.85	-3.02	-2.79
ESpm01x	0.53	1.06	1.88	1.24	1.25	1.22	1.06	1.24	1.68	1.03	1.33
F04[C-O]	0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01
BEHe4	0.38	1.89	2.05	2.15	2.14	1.94	2.05	1.66	1.92	2.21	1.73

* Experiment 4 provided the highest performance for predicting non-steroidal AIs