

**Supplementary material to:**

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

Watshara Shoombuatong<sup>1</sup>, Veda Prachayasittikul<sup>1,2</sup>, Virapong Prachayasittikul<sup>2</sup>,  
Chanin Nantasenamat<sup>1,2,\*</sup>

<sup>1</sup> Center of Data Mining and Biomedical Informatics, Faculty of Medical Technology,  
Mahidol University, Bangkok 10700, Thailand

<sup>2</sup> Department of Clinical Microbiology and Applied Technology, Faculty of Medical  
Technology, Mahidol University, Bangkok 10700, Thailand

\* Corresponding author: E-mail: chanin.nan@mahidol.ac.th (C.N.); Phone: +66 2 441 4371;  
Fax: +66 2 441 4380

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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