

Supplementary Material

Table S2. The outliers (here defined as the abstract of the (HIA-pre – HIA-exp) are larger 20%) of the training set and test set for the Model 3B (based on nine combined descriptors by SVM).

HIA-exp (%): the experimental HIA values in Model 3B

HIA-pre (%): the predicted HIA values in Model 3B by SVM method

MAE (%): MAE is the mean absolute error of HIA-exp and HIA-pre

No.	Name	HIA-exp (%)	HIA-pre (%)	MAE (%)
Training set				
2	Azlocillin	0	40	40
6	Meropenem	0	69	69
7	Mezlocillin	0	25	25
9	Pentamidine	0	63	63
11	Streptozocin	0	37	37
23	Nedocromil	3	81	78
28	Diatrizoate	5	45	40
32	Imipenem	5	63	58
36	Moexipril_diacid	5	72	67
38	Phthalylsulfathiazole	5	71	66
39	Succinylsulfathiazole	5	54	49
40	Sulbactam	5	81	76
41	Ticarcillin	5	48	43
43	Acamprosate	11	75	64
44	Cilazapril	20	79	59
45	Lincomycin	28	64	36
46	Netivudine	28	64	36
48	AAFC	32	72	40
49	Nadolol	32	79	47
50	Dihydroergotamine	35	62	27
51	Sulpiride	40	78	38
53	Metaproterenol	43	78	35
58	Guanoxan	50	83	33
59	Trandolapril	50	78	28
60	Metformin	54	82	28
62	Valsartan	55	84	29
71	Ziprasidone	60	86	26
77	Hydroflumethiazide	67	91	24

87	Moxisylyte	70	90	20
131	Riboflavin	80	46	34
241	Cephadrine	95	70	25
304	Glyburide	98	75	23
336	Amosulalol	100	75	25
353	Cicaprost	100	75	25
358	Cyclopenthiazide	100	80	20
363	Ergotamine	100	64	36
374	Genaconazole	100	80	20
424	Polythiazide	100	78	22
441	Tesaglitazar	100	78	22
450	Trofosfamide	100	68	32
464	Capecitabine	96	50	46
466	Chloramphenicol	89	68	21
492	Guanfacine	100	74	26
506	Methocarbamol	100	74	26
537	Stavudine	100	79	21
Test set				
4	Gentamicin_C1a	0	26	26
22	Clodronate	3	28	25
55	Rimiterol	48	85	37
64	Oxytetracycline	58	18	40
65	Cilazapril	59	79	20
68	Oxycodone	60	89	29
375	Glimepiride	100	76	24
376	Glipizide	100	79	21
393	Lornoxicam	100	80	20
461	Bicalutamide	90	70	20
491	Gliquidone	95	73	22
536	Sorivudine	82	52	30
547	Tranexamic_acid	55	84	29