

Supplementary Material

Table S1. The 380 compounds used in the training set, the 172 compounds used in the test set, with their experimental and predicted human intestinal absorption (HIA) values in Model 3B (based on nine combined descriptors) by Support Vector Machine (SVM) method.

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

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

No.	Name	HIA-exp (%)	HIA-pre (%)
Training set			
2	Azlocillin	0	40
3	Cefodizime	0	-2
5	Lucifer_Yellow_CH	0	16
6	Meropenem	0	69
7	Mezlocillin	0	25
8	Netilmicin	0	16
9	Pentamidine	0	63
10	Raffinose	0	13
11	Streptozocin	0	37
12	Tobramycin	0	3
13	Vancomycin	0	6
14	Alendronic_acid	1	-13
15	Aztreonam	1	3
18	Risedronic_acid	1	8
19	Streptomycin	1	-15
21	Amphotericin B	3	-8
23	Nedocromil	3	81
24	Neomycin	3	13
25	Amygdalin	5	21
26	Cefotaxime	5	19
27	Chlorhexidine	5	21
28	Diatrizoate	5	45
29	Edetic_acid	5	-3
30	Etidronate	5	8
32	Imipenem	5	63
33	Iohexol	5	-11
34	Iotroxic_acid	5	21
35	Mitoxantrone	5	16
36	Moexipril_diacid	5	72
38	Phthalylsulfathiazole	5	71

39	Succinylsulfathiazole	5	54
40	Sulbactam	5	81
41	Ticarcillin	5	48
42	Cefmetazole	10	26
43	Acamprosate	11	75
44	Cilazapril	20	79
45	Lincomycin	28	64
46	Netivudine	28	64
47	Fosmidomycin	30	30
48	AAFC	32	72
49	Nadolol	32	79
50	Dihydroergotamine	35	62
51	Sulpiride	40	78
52	Famotidine	41	25
53	Metaproterenol	43	78
54	Cymarin	47	57
56	Atenolol	50	67
57	Cefpodoxime_proxetil	50	34
58	Guanoxan	50	83
59	Trandolapril	50	78
60	Metformin	54	82
61	Eflornithine	55	54
62	Valsartan	55	84
63	Dipyridamole	58	42
66	Fenoterol	60	76
69	Pirbuterol	60	76
70	Ramipril	60	76
71	Ziprasidone	60	86
72	Furosemide	61	75
73	Sulfasalazine	62	80
75	Chlorthalidone	65	75
76	Tolrestat	66	83
77	Hydroflumethiazide	67	91
79	Mibefradil	69	80
80	Anagrelide	70	86
81	Benserazide	70	52
82	Bromhexine	70	86
83	Etodolac	70	87
84	Famciclovir	70	60
85	Isocarboxazid	70	89
87	Moxisylyte	70	90
88	Pimozide	70	84
89	Recainam	71	84
90	Ceftizoxime	72	56
91	Cycloserine	72	88
92	Benzbromarone	73	77

93	Quetiapine	73	89
95	Clavulanic_acid	75	71
96	Ketoconazole	75	77
97	Mesna	75	90
98	Oseltamivir	75	73
99	Primidone	75	86
100	Ethylmorphine	77	87
101	Pantoprazole	77	79
102	Sibutramine	77	93
104	Guanabenz	78	86
105	Mefloquine	78	78
106	Urapidil	78	88
107	Zatebradin	79	94
109	Allopurinol	80	92
110	Carvedilol	80	86
111	Chlorpheniramine	80	94
112	Clonazepam	80	85
113	Dantrolene	80	86
114	Enoximone	80	91
115	Floxacillin	80	72
116	Flunarizine	80	88
119	Isoniazid	80	88
120	Itraconazole	80	89
121	Mesalamine	80	84
122	Methadone	80	93
124	Methylphenidate	80	87
125	Modafinil	80	85
126	Nabumetone	80	93
128	Oxamniquine	80	84
131	Riboflavin	80	46
132	Terbinafine	80	92
133	Ticlopidine	80	91
135	Trimipramine	80	89
137	Flecainide	81	76
138	Aspirin	82	90
141	Mifobate	82	80
143	Milrinone	83	88
145	Bromazepam	84	84
146	Acebutolol	85	73
149	Dolasetron	85	88
150	Isoproterenol	85	80
151	Lansoprazole	85	84
152	Molecule-618	85	89
153	Oxyfedrine	85	87
154	Piretanide	85	81
155	Sulfamethizole	85	89

156	Triazolam	85	87
157	Zalcitabine	85	79
158	Lamivudine	86	75
159	Benzydamine	87	88
161	Cimetidine	87	77
162	Clindamycin	87	71
163	Acrivastine	88	91
164	Disulfiram	88	88
165	Metoclopramide	88	82
166	Misoprostol	88	81
167	Moricizine	88	79
168	Moxonidine	88	86
170	Trovafloxacin	88	77
172	Sultopride	89	86
173	Tenidap	89	80
174	Almitrine	90	74
176	Amphetamine	90	84
178	Betaxolol	90	86
179	Bisoprolol	90	81
180	Chlorzoxazone	90	97
181	Dapsone	90	83
184	Diflunisal	90	87
185	Diloxanide	90	84
187	Felbamate	90	71
188	Feprazone	90	89
189	Flutamide	90	90
191		90	88
	Hydroxyprogesterone_caproate		
192	Isosorbide_dinitrate	90	89
193	Isotretinoin	90	92
195	Loratadine	90	87
196	Mebeverine	90	87
198	Meloxicam	90	85
199	Mifepristone	90	84
202	Nalidixic_acid	90	91
203	Nisoldipine	90	87
204	Papaverine	90	91
205	Phenazopyridine	90	86
206	Phenytoin	90	89
207	Protionamide	90	88
211	Sparfloxacin	90	82
212	Sulfisomidine	90	83
213	Sulindac	90	88
214	Telithromycin	90	75
215	Thiabendazole	90	93
216	Tiagabine	90	85

218	Tolazoline	90	84
219	Triamcinolone_acetonide	90	81
220	Diltiazem	91	87
221	Hydrocortisone	91	84
223	Terazosin	91	84
224	Isradipine	92	90
225	Alprenolol	93	88
226	Amrinone	93	85
227	Scopolamine	93	83
228	Tetrahydrocannabinol	93	91
230	Clozapine	94	88
231	Felodipine	94	86
232	Fluconazole	94	81
233	Nicotinic_acid	94	95
235	Amitriptyline	95	86
239	Carbimazole	95	100
241	Cephradine	95	70
243	Clomethiazole	95	93
245	Clonidine	95	88
246	Clopentixol	95	90
247	Diethylpropion	95	91
249	Domperidone	95	79
250	Dothiepin	95	91
255	Glymidine	95	84
256	Hexobarbital	95	89
257	Ketoprofen	95	91
258	Ketorolac	95	90
259	Levamisole	95	92
260	Lorazepam	95	84
261	Methimazole	95	93
262	Metronidazole	95	87
263	Nicardipine	95	85
264	Nitrazepam	95	85
266	Nizatidine	95	80
268	Pentazocine	95	89
269	Pentoxifylline	95	88
272	Practolol	95	76
275	Propranolol	95	87
277	Ritodrine	95	83
278	Sotalol	95	79
279	Sulfisoxazole	95	85
280	Tacrine	95	81
282	Timolol	95	80
283	Tropisetron	95	88
284	Venlafaxine	95	91
285	Zolpidem	95	89

286	Bumetanide	96	77
287	Clofibrate	96	92
291	Progesterone	96	88
292	Torseamide	96	85
293	Trapidil	96	93
294	Cotinine	97	89
296	Gliclazide	97	87
297	Oxazepam	97	86
298	Risperidone	97	90
300	Chlorpromazine	98	95
301	Cisapride	98	80
302	Cyproterone_acetate	98	86
303	Glibornuride	98	85
304	Glyburide	98	75
305	Ibuprofen	98	92
306	Imatinib	98	82
307	Isoxepac	98	88
308	Lacidipine	98	84
310	Lidocaine	98	88
314	Pelrinone	98	84
316	Ropinirole	98	91
317	Tolmesoxide	98	90
318	Valproic_acid	98	93
319	Zopiclone	98	86
320	Caffeine	99	91
321	Chlordiazepoxide	99	88
322	Ciprofibrate	99	86
323	Diazepam	99	86
324	Fluorescein	99	83
325	Lomefloxacin	99	86
329	Tiacrilast	99	85
330	Tianeptine	99	85
331	Viloxazine	99	89
332	Acetanilide	100	93
333	Acetazolamide	100	83
334	Alfacalcidol	100	94
335	Aminopyrine	100	84
336	Amosulalol	100	75
337	Anastrozole	100	93
338	Astemizole	100	89
339	Azimilide	100	87
340	Bendroflumethiazide	100	84
341	Benorylate	100	84
343	Bezafibrate	100	84
347	Camazepam	100	88
348	Carbamazepine	100	90

349	Carmustine	100	84
350	Chloral_hydrate	100	86
352	Chlorphenesin	100	84
353	Cicaprost	100	75
354	Cilomilast	100	90
356	Corticosterone	100	88
357	Coumarin	100	95
358	Cyclopentiazide	100	80
359	Diacetylmorphine	100	88
360	Dicyclomine	100	90
361	Dofetilide	100	84
363	Ergotamine	100	64
366	Ethynodiol_diacetate	100	92
367	Fenclofenac	100	87
368	Finasteride	100	87
369	Flucytosine	100	84
372	Fusidic_acid	100	84
374	Genaconazole	100	80
377	Glycine	100	84
378	Granisetron	100	87
379	Haloperidol	100	89
380	Hydralazine	100	86
381	Indobufen	100	90
382	Indomethacin	100	84
384	Isosorbide-2-mononitrate	100	84
385	Isoxicam	100	87
387	Letrozole	100	93
388	Levetiracetam	100	84
395	Meclofenamic_acid	100	87
398	Meptazinol	100	88
399	Methsuximide	100	90
400	Methylergonovine	100	83
401	Methysergide	100	85
404	Nefazodone	100	91
405	Nicorandil	100	86
408	Nitroxoline	100	89
409	Norethindrone	100	89
414	Orphenadrine	100	91
417	Oxyphenbutazone	100	92
419	Pentobarbital	100	89
422	Phenindione	100	89
424	Polythiazide	100	78
425	Probenecid	100	85
426	Procarbazine	100	84
428	Proxyphylline	100	84
429	Pseudoephedrine	100	86

434	Selegiline	100	92
435	Sudoxicam	100	84
437	Sulfinpyrazone	100	89
438	Tamoxifen	100	93
440	Terfenadine	100	94
441	Tesaglitazar	100	78
444	Tinidazole	100	91
445	Tocainide	100	91
446	Toremifene	100	95
447	Triamcinolone	100	81
448	Trifluoperazine	100	84
449	Trihexyphenidyl	100	89
450	Trofosfamide	100	68
451	Zileuton	100	86
453	Zonisamide	100	90
458	Aminoglutethimide	100	84
459	Azelastine	100	85
463	Buspirone	100	92
464	Capecitabine	96	50
466	Chloramphenicol	89	68
467	Cinchonine	100	88
469	Clobazam	87	88
470	Codeine	93	87
471	Cyproheptadine	80	80
473	Desipramine	98	87
479	Dienogest	94	90
480	Doxepin	100	85
482	Estramustine	75	81
483	Ethambutol	78	70
485	Etoricoxib	100	92
486	Fenfluramine	95	90
487	Fenoprofen	85	92
489	Flurazepam	100	91
492	Guanfacine	100	74
494	Hydroxychloroquine	90	87
500	Levosimendan	90	90
501	Linezolid	100	83
502	Losartan	80	87
503	Maprotiline	98	86
504	Mebendazole	100	93
505	Mestranol	90	83
506	Methocarbamol	100	74
507	Metolazone	64	82
509	Moclobemide	88	87
510	Moxalactam	0	16
511	Nafronyl	100	90

512	Naltrexone	95	89
514	Naratriptan	70	87
515	Nifedipine	90	87
516	Nilutamide	100	84
519	Oxprenolol	95	87
520	Penbutolol	100	90
521	Phenobarbital	100	87
522	Phenprocoumon	95	88
524	Pindolol	90	84
525	Piroximone	81	88
526	Pizotyline	80	87
527	Praziquantel	96	87
530	Propoxyphene	95	90
531	Propylthiouracil	76	89
532	Quinagolide	100	83
533	Reproterol	60	59
534	Rizatriptan	90	89
535	Saccharin	91	96
537	Stavudine	100	79
538	Sulfamethazine	95	85
539	Tamsulosin	100	81
541	Tetrabenazine	100	91
542	Tiludronic_acid	6	22
545	Topiramate	86	78
546	Tramadol	95	89
548	Trazodone	100	90
549	Trimethoprim	97	80
550	Ximoprofen	98	87
552	Zanamivir	2	-6
Test set			
1	Arbekacin	0	1
4	Gentamicin_C1a	0	26
16	Ceftriaxone	1	16
17	Lactulose	1	15
20	Acarbose	2	12
22	Clodronate	3	28
31	Gentamincin_C1	5	17
37	Pamidronic_acid	5	-9
55	Rimiterol	48	85
64	Oxytetracycline	58	18
65	Cilazapril	59	79
67	Ivermectin	60	48
68	Oxycodone	60	89
74	Terbutaline	63	79
78	Sumatriptan	67	85
86	Mianserin	70	81

94	Almotriptan	75	88
103	Tolterodine	77	92
108	Acetohexamide	80	85
117	Fluoxetine	80	88
118	Guanadrel	80	82
123	Methoxyamphetamine	80	86
127	Omeprazole	80	87
129	Pramipexole	80	83
130	Quinidine	80	89
134	Trimeprazine	80	92
136	Vitamin_A	80	90
139	Ibutilide	82	86
140	Methylprednisolone	82	85
142	Albuterol	83	79
144	Nateglinide	83	89
147	Acetaminophen	85	88
148	Chlorguanide	85	78
160	Bupropion	87	93
169	Nitrendipine	88	86
171	Dihydrocodeine	89	87
175	Amantadine	90	80
177	Azatadine	90	82
182	Dexamethasone	90	86
183	Diethylstilbestrol	90	89
186	Ethacrynic_acid	90	80
190	Fluvoxamine	90	84
194	Ketotifen	90	85
197	Mefenamic_acid	90	89
200	Morphine	90	87
201	Moxifloxacin	90	86
208	Quinalbarbitone	90	88
209	Rabeprazole	90	84
210	Riluzole	90	101
217	Tibolone	90	88
222	Naloxone	91	88
229	Atropine	94	86
234	Acipimox	95	86
236	Amobarbital	95	85
237	Amoxapine	95	88
238	Baclofen	95	81
240	Carteolol	95	83
242	Chorpropamide	95	86
244	Clomipramine	95	89
248	Disopyramide	95	91
251	Fludrocortisone_acetate	95	77
252	Flumazenil	95	90

253	Flurbiprofen	95	91
254	Galantamine	95	88
265	Nitrofurantoin	95	84
267	Pefloxacin	95	87
270	Perindopril	95	77
271	Phenylpropanolamine	95	84
273	Promethazine	95	93
274	Propafenone	95	88
276	Protriptyline	95	86
281	Temazepam	95	87
288	Gatifloxacin	96	86
289	Metoprolol	96	84
290	Minoxidil	96	83
295	Gallopamil	97	93
299	Antipyrine	98	88
309	Lamotrigine	98	87
311	Mexiletine	98	85
312	Nefopam	98	87
313	Oxaprozin	98	91
315	Rivastigmine	98	92
326	Miconazole	99	84
327	Pheniramine	99	90
328	Prednisolone	99	84
342	Bepiridil	100	93
344	Biperiden	100	89
345	Bornaprine	100	91
346	Budesonide	100	85
351	Chloroquine	100	96
355	Citalopram	100	92
362	Doxazosin	100	86
364	Ethinyl_Estradiol	100	89
365	Ethyl_alcohol	100	93
370	Flupentixol	100	81
371	Fluvastatin	100	81
373	Gemfibrozil	100	91
375	Glimepiride	100	76
376	Glipizide	100	79
383	Irbesartan	100	89
386	Ketanserin	100	86
389	Levobunolol	100	89
390	Levonorgestrel	100	90
391	Lisuride	100	86
392	Lormetazepam	100	86
393	Lornoxicam	100	80
394	Lynestrenol	100	82
396	Megestrol_acetate	100	89

397	Meperidine	100	88
402	Midazolam	100	87
403	Nalbuphine	100	87
406	Nicotine	100	88
407	Nilvadipine	100	83
410	Norgestimate	100	83
411	Nortriptyline	100	83
412	Ofloxacin	100	87
413	Ondansetron	100	89
415	Oxcarbazepine	100	89
416	Oxybutynin	100	86
418	Paroxetine	100	90
420	Perphenazine	100	89
421	Phenglutarimide	100	91
423	Piroxicam	100	88
427	Propofol	100	89
430	Pyrazinamide	100	93
431	Remoxipride	100	87
432	Repaglinide	100	90
433	Salsalate	100	88
436	Sulfamethoxazole	100	86
439	Tenoxicam	100	85
442	Testosterone	100	86
443	Tilidine	100	90
452	Zomepirac	100	87
454	Zotepine	100	92
455	Acitretin	95	91
456	Alprazolam	90	90
457	Amikacin	0	5
460	Betahistine	100	86
461	Bicalutamide	90	70
462	Bifemelane	95	90
465	Chlorambucil	100	83
468	Cinoxacin	95	87
472	Delmopinol	98	92
474	Desmethyldiazepam	99	86
475	Desogestrel	72	84
476	Dextromoramide	100	88
477	Diazoxide	90	87
478	Diclofenac	97	87
481	Erythromycin	35	34
484	Ethionamide	90	88
488	Flunisolide	80	79
490	Gestodene	100	90
491	Gliquidone	95	73
493	Hydrochlorothiazide	68	80

495	Imipramine	98	89
496	Indoprofen	100	89
497	Kanamycin	1	9
498	Ketazolam	100	86
499	Labetalol	95	76
508	Acetanilide	80	91
513	Naproxen	99	91
517	Norgestrel	100	90
518	Oxatomide	100	88
523	Phenylbutazone	98	91
528	Procyclidine	100	88
529	Propiverine	84	87
536	Sorivudine	82	52
540	Telmisartan	90	104
543	Tolbutamide	90	90
544	Tolmetin	99	90
547	Tranexamic_acid	55	84
551	Zaleplon	100	91
