SUPPLEMETARY MATERIAL

In Silico Approach for Assessment of Membrane Transporters Activities of Phenols: Case Study Based on Computational Models of Transport Activity for Transporter Bilitranslocase

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Table S1: List of 120 chemicals with BTL activity experimental values (target) and the classification predictions of separate models (NN-C, NN-D, Q-D) and consensus of models (A+B, NN-D+Q-C, A).

ID	Name	Target (exp.)	NN-D	NN-D	Q-C	AB prediction	A+B	NN-D + Q-D	A
1	Adenine	**0**	0	0	0	A	0	0	0
2	Adenosine	**0**	0	0	1	B	0	/	/
3	Adenosine 3′-monophoshate	**1**	0	1	1	B	1	1	/
4	Adenosine 5′-monophoshate	**1**	1	1	1	A	1	1	1
5	Adenosine 3′, 5′-cyclic monophosphate	**0**	0	0	0	A	0	0	0
6	Adenosine 5′-diphosphate	**1**	0	1	1	B	1	1	/
7	Adenosine 5′-triphosphate	**1**	1	0	1	B	1	/	/
8	Adenosine-5′-diphosphoglucose	**0**	0	0	0	A	0	0	0
9	Adenosine 5'-(α,β-methylene) diphosphate	**1**	1	1	1	A	1	1	1
10	Adenine 9-β-D-arabinofuranoside	**1**	1	0	1	B	1	/	/
11	Adenosine 3′-phosphate 5′-phosphosulfate	**1**	0	1	1	B	1	1	/
12	S-(5′-Adenosyl)-L-homocysteine	**1**	1	1	0	B	1	/	/
13	S-(5′-Adenosyl)-L-methionine chloride	**1**	1	1	0	B	1	/	/
14	Guanosine	**0**	1	0	1	B	1	/	/
15	Guanosine 5′-monophosphate	**1**	1	1	1	A	1	1	1
16	Guanosine 3′. 5′-cyclic monophosphate	**0**	0	0	0	A	0	0	0
17	Guanosine 5′-diphosphate	**1**	1	1	1	A	1	1	1
18	Guanosine 5′-triphosphate	**1**	1	1	1	A	1	1	1
19	Uracil	**0**	0	0	0	A	0	0	0
20	Uridine	**1**	0	0	1	B	0	/	/
21	Uridine 5′-monophosphate	**1**	1	0	1	B	1	/	/
22	Uridine 5′-diphosphate	**1**	1	1	1	A	1	1	1
23	Uridine 5′-triphosphate	**1**	1	1	1	A	1	1	1
24	Uridine 5'-diphosphoglucose	**0**	0	1x	0	B	0	/	/
25	Uridine 5'-diphosphogalactose	**1**	1	1x	0	B	1	/	/
26	Uridine 5′-diphosphoglucuronic acid	**0**	1	1	0	B	1	/	/
27	Thymine	**0**	1	0	0	B	0	0	/
28	Thymidine	**0**	0	0	0	A	0	0	0
29	Thymidine 5′-monophosphate	**1**	1	1	1	A	1	1	1
30	Thymidine 5′-diphosphate	**1**	1	1	1	A	1	1	1
31	Thymidine 5′-triphosphate	**1**	1	1	1	A	1	1	1
32	Cytosine	**0**	0	0	0	A	0	0	0
33	Cytidine	**0**	0	0	1	B	0	/	/
34	Cytidine 2′-monophosphate	**0**	1	0	0	B	0	0	/
35	Cytidine 5′-monophosphate	**0**	1	0	1	B	1	/	/
36	Uric acid	**1**	0	0	1	B	0	/	/
37	Ouabain	**0**	0	0	0	A	0	0	0
38	Aucubin	**0**	0	0	0	A	0	0	/
39	Loganin	**0**	1	0	1	B	1	/	/
40	Verbenalin	**0**	0	0	1	B	0	/	/
41	Isovitexin	**0**	0	0	0	A	0	0	0
42	Vitexin-2'-O-rhamnoside	**0**	0	0	0	A	0	0	0
43	Cibacron Blue F3G-A	**1**	1	1	1	A	1	1	1
44	Digoxin	**0**	0	0	0	A	0	0	0
45	Taurocholate	**0**	0	0	0	A	0	0	0
46	Pelargonidin	**1**	1	1	1	A	1	1	1
47	Cyanidin	**1**	0	1	1	B	1	1	/
48	Delphinidin	**1**	1	1	1	A	1	1	1
49	Peonidin	**1**	1	1	1	A	1	1	1

50	Petunidin	**1**	1	1	1	A	1	1	1
51	Malvidin	**1**	0	1	1	B	1	1	/
52	Pelargonidin 3-O-β-D-glucopyranoside	**1**	0	1	1	B	1	1	/
53	Cyanidin 3-O-β-D-glucopyranoside	**1**	1	1	1	A	1	1	1
54	Delphinidin 3-O-β-D-glucopyranoside	**1**	1	1	1	A	1	1	1
55	Peonidin 3-O-β-D-glucopyranoside	**1**	1	1	1	A	1	1	1
56	Petunidin 3-O-β-D-glucopyranoside	**1**	1	1	1	A	1	1	1
57	Malvidin 3-O-β-D-glucopyranoside	**1**	0	1	1	B	1	1	/
58	Pelargonidin 3,5-di-O-β-D-glucopyranoside	**1**	0	1	1	B	1	1	/
59	Cyanidin 3,5-di-O-β-D-glucopyranoside	**1**	1	1	1	A	1	1	1
60	Peonidin 3,5-di-O-β-D-glucopyranoside	**1**	0	1	1	B	1	1	/
61	Malvidin 3,5-di-O-β-D-glucopyranoside	**1**	1	1	1	A	1	1	1
62	Cyanidin 3-O-α-L-arabinopyranoside	**1**	1	1	1	A	1	1	1
63	Cyanidin 3-O-β-D-galactopyranoside	**1**	1	1	1	A	1	1	1
64	Malvidin 3-O-β-D-glucopyranoside	**1**	1	1	1	A	1	1	1
65	Galangin	**1**	1	1	0	B	1	/	/
66	Kaempferol	**1**	0	1	1	B	1	1	/
67	Quercetin	**1**	1	0	1	B	1	/	/
68	Myricetin	**0**	0	0	1	B	0	/	/
69	Syringetin	**0**	0	0	0	A	0	0	0
70	Rhamnetin	**0**	0	0	0	A	0	0	0
71	Quercetin 4'-glucopyranoside	**0**	1	0	0	B	0	0	/
72	Quercetin 3,4'-diglucopyranoside	**0**	0	0	0	A	0	0	0
73	Quercetin 3-glucopyranoside	**0**	0	0	0	A	0	0	0
74	Quercetin 3-xyloside	**0**	0	0	0	A	0	0	0
75	Quercetin 3-rhamnoside	**0**	0	0	0	A	0	0	0
76	Quercetin 3-galactoside	**0**	1	0	0	B	0	0	/
77	Quercetin 3-O-glucopyranosyl-6'-acetate	**0**	0	0	0	A	0	0	0
78	Quercetin 3-O-sulfate	**0**	0x	0	0	A	0	0	0
79	Isorhamnetin 3-glucoside	**0**	1	0	0	B	0	0	/
80	Isorhamnetin 3-O-rutinoside	**0**	0	0	0	A	0	0	0
81	Kaempferol 3-O-glucoside	**0**	0	0	0	A	0	0	0
82	Kaempferol 3-O-rutinoside	**0**	1	0	0	B	0	0	0
83	Syringetin 3-galactoside	**0**	0	0	0	A	0	0	0
84	Syringetin 3-glucoside	**0**	0	0	0	A	0	0	0
85	Nicotinic Acid	**0**	0	0	0	A	0	0	0
86	[D-Ala2]- Deltorphin II	**0**	1x	0x	1x	B	1x	/	/
87	[D-Pen2.5]-Enkephalin (DPDPE)	**0**	1	0	0	B	0	0	/
88	17β-Estradiol 3-glucuronide	**0**	0	0	0	A	0	0	0
89	5-Fluorouracil	**0**	0	0	0	A	0	0	0
90	Acetazolamide	**0**	0x	0x	0	A	0	0	0
91	Acycloguanosine (Acyclovir)	**0**	1	0	0	B	0	0	/
92	Etacrynic Acid	**0**	0	0x	0	A	0	0	0
93	Mefenamic Acid	**0**	0	0	0	A	0	0	0
94	Dehydroisoandrosterone 3-sulfate	**0**	0	0	0	A	0	0	0
95	Diclofenac	**0**	0	0	0	A	0	0	0
96	Dichlorofluorescein (DCFH)	**0**	0	0	0	A	0	0	0
97	Enalapril maleate	**0**	0	0	0x	A	0	0	0
98	Estrone 3-sulfate	**0**	0	0	0	A	0	0	0
99	Phenacitin	**0**	0	0	0	A	0	0	0
100	Furosemide	**0**	0	0	0	A	0	0	0
101	Glycocholate	**0**	1	0x	0	B	0	0	/
102	Ibuprofen	**0**	0	0x	0	A	0	0	0
103	Hydrochlorothiazide	**1**	1	1	1	A	1	1	1
104	Hydrocortisone	**0**	1	0	1	B	1	/	/
105	Indomethacin	**0**	0	1	0	B	0	/	/
106	Ketoprofen	**0**	1	0	0	B	0	0	/
107	L-Thyroxine (T4)	**0**	0	1	1x	B	1	1	/
108	Methotrexate	**0**	0	0x	1	B	0	/	/
109	Naproxene	**0**	0	0	0	A	0	0	0
110	Piroxicam	**0**	1	1x	1	A	1	1	1
111	Pravastatin	**0**	0	0	0	A	0	0	0
112	Probenecid	**0**	0	0	0	A	0	0	0
113	Progesterone	**0**	0	0	0	A	0	0	0

114	Prostaglandin E2	**0**	0	0	0	A	0	0	0
115	Sulindac	**1**	1	1	1	A	1	1	1
116	Triiodo-L-thyronine (T3)	**1**	1	1	1x	A	1	1	1
117	β-Estradiol	**0**	0	0	0	A	0	0	0
118	Sulfobromophtalein	**1**	1x	1	1	A	1	1	1
119	Bilirubin	**1**	0	1	1	B	1	1	/
120	Biliverdin	**1**	1	1	1	A	1	1	1
	∑ active	50	54	49	58		53	42	30
	∑ predictions in AD	120	116	111	116		119	97	75

1 – inhibitor, 0 – noninhibitor, x – out of AD

Table S2: List of 300 phenolic compounds and their BTL activity predictions with separate models (NN-C, NN-D, Q-D) and consensus of models (A+B, NN-D+Q-D, A).

ID	Name	Ref.	NN-C	NN-D	Q-D	AB prediction	A+B	NN-D + Q-D	A
FLAVONES									
1	acacetin	[11]	1	1	0	B	1	/	/
2	chrysin	[80,87]	1	1	0	B	1	/	/
3	apigenin	[27,87]	1	1	0	B	1	/	/
4	luteolin	[27,87]	1	1	1	A	1	1	1
5	tangeretin	[27]	0x	0	0x	A	0	0	0
6	diosmetin	[27]	0	1	0	B	0	/	/
7	diosmin	[27]	1	0	0	B	0	0	/
8	baicalein	[27]	0	1	1	B	1	1	/
9	7,3 dimethylhesperetin	[27]	0	0	0	A	0	0	0
10	rhoifolin	[27]	0	0	0	A	0	0	0
11	flavone	[80]	0	1	0	B	0	/	/
12	3-methylflavone-8-carboxylic acid	[80]	1	1	0	B	1	/	/
13	flavonoid 1	[25]	0	1	0	B	0	/	/
14	flavonoid 2	[25]	0	1	0x	B	0	/	/
15	flavonoid 3	[25]	0	0	0x	A	0	0	0
16	flavonoid 4	[25]	0x	0	0x	A	0	0	0
17	flavonoid 5	[25]	0	0	0x	B	0	0	/
18	flavonoid 9	[25]	0	0	0	A	0	0	0
19	wogonin	[25]	0	1x	0	B	0	/	/
20	flavopiridol	[25]	0	0x	0	A	0	0	0
21	tricetin	[85]	1	0	1	B	1	/	/
22	isoetin	[85]	1	0	1	B	1	/	/
23	nortangeretin	[85]	1	0	1	B	1	/	/
24	6-fluroflavone	[21]	0	1	0	B	0	/	/
25	6-chloroflavone	[21]	0	1	0	B	0	/	/
26	6-bromoflavone	[21]	0	1	0	B	0	/	/
27	6-nitroflavone	[21]	0	1	0	B	0	/	/
28	6-methylflavone	[21]	0	1	0	B	0	/	/
29	3'-bromo-6-methylflavone	[21]	0	0	0	A	0	0	0
30	3'methyl-6-bromoflavone	[21]	0	1	0	B	0	/	/
31	3'-bromoflavone	[21]	0	1	0	B	0	/	/
32	3'-nitroflavone	[21]	0	1	0	B	0	/	/
33	4'-bromoflavone	[21]	0	1	0	B	0	/	/
34	3-bromoflavone	[21]	0	1	0	B	0	/	/
35	3,6-dibromoflavone	[21]	0	1	0	B	0	/	/
36	2'-nitroflavone	[21]	0	0	1	B	0	/	/
37	2',6-dinitroflavone	[21]	0	0	1	B	0	/	/
38	2',6-dinitro-3'-bromoflavone	[21]	0	1	1	B	1	1	/
39	2',6-difluoroflavone	[21]	0	1	0	B	0	/	/
40	2'-fluoro-6-chloroflavone	[21]	0	1	0	B	0	/	/
41	2'-fluoro-6-bromoflavone	[21]	0	1	0	B	0	/	/
42	5,7-dimethoxyflavone	[21]	0	1	0	B	0	/	/
43	α-naphthoflavone	[21]	0x	1x	0	B	0	/	/
44	β-naphthoflavone	[21]	0	1x	0	B	0	/	/
45	4'-nitroflavone	[28]	1	0	0	B	0	0	/

46	2'-chlorochrysin	[28]	0	1	0	B	0	/	/
47	kaempferitrin	[26]	1	0	0	B	0	0	/
48	kaempferol glycoside 2	[26]	0	0	0	A	0	0	0
49	kaempferol glycoside 3	[26]	1	0	0	B	0	0	/
50	kaempferol glycoside 4	[26]	0	0	0	A	0	0	0
51	6-hydroxyflavone	[84]	1	1	0	B	1	/	/
52	3'-hydroxyflavone	[84]	0	0	0	A	0	0	0
53	4'-hydroxyflavone	[84]	0	1x	0	B	0	/	/
54	kaempferol-3,4'-dimethylether	[84]	0	1	0	B	0	/	/
55	flavone-8-acetic acid (FAA)	[13]	0	1	0	B	0	/	/
56	FAAD-8	[13]	0x	0	1	B	0	/	/
57	FAAD-9	[13]	0	1x	0	B	0	/	/
58	FAAD-10	[13]	0	0x	0	A	0	0	0
59	FAAD-11	[13]	0	0x	1	B	0	/	/
60	FAAD-12	[13]	0	0x	1	B	0	/	/
61	FAAD-13	[13]	0	0x	1	B	0	/	/
62	FAAD-18b	[13]	0	1x	1	B	1	1	/
63	FAAD-19a	[13]	0	0x	1	B	0	/	/
64	FAAD-19b	[13]	0	0x	1	B	0	/	/
65	FAAD-19c	[13]	1	0x	1	B	1	/	/
66	FAAD-19d	[13]	0	0x	1	B	0	/	/
67	FAAD-19e	[13]	0	0x	1	B	0	/	/
68	FAAD-19f	[13]	0	0x	1	B	0	/	/
69	FAAD-19g	[13]	0	0x	1	B	0	/	/
70	FAAD-19h	[13]	1	0x	1	B	1	/	/
71	FAAD-19i	[13]	1	0x	1	B	1	/	/
72	FAAD-19j	[13]	0	0x	1	B	0	/	/
73	FAAD-19k	[13]	0	0x	1	B	0	/	/
74	FAAD-19l	[13]	0	0x	1	B	0	/	/
75	FAAD-19m	[13]	0	0x	0	A	0	0	0
76	FAAD-20	[13]	0	0x	1	B	0	/	/
77	FAAD-21	[13]	0	1x	1	B	1	1	/
78	FAAD-22	[13]	0	0x	1	B	0	/	/
ISOFLAVONES									
79	daidzin	[80]	1	0	0	B	0	0	/
80	daidzein	[80,87]	1	0	0	B	0	0	/
81	genistein	[27,87]	1	1	0	B	1	/	/
82	glycitein	[6]	1	1	0	B	1	/	/
83	genistin	[80]	1	0	0	B	0	0	/
FLAVONOLS									
84	galangin	[80,7]	1	1	0	B	1	/	/
85	tamarixetin	[80]	0	0	0	A	0	0	0
86	kaempferol	[80,87]	1	1	1	A	1	1	1
87	fisetin	[80]	0	1	0	B	0	/	/
88	3,6-dihydroxyflavone	[80]	1	1	0	B	1	/	/
89	morin	[17]	1	0	1	B	1	/	/
90	robinetin	[85]	1	0	0	B	0	0	/
91	herbacetin	[85]	0	0	1	B	0	/	/
92	3-hydroxyflavone	[84]	1	1	0	B	1	/	/
93	kaempferol-7-neohesperidoside	[84]	0	0	0	A	0	0	0
FLAVANONES									
94	pinocembrin	[6]	1	1	0	B	1	/	/
95	eriodictyol	[27,87]	1	1	1	A	1	1	1
96	Naringenin	[27,87]	1	1	0	B	1	/	/
97	Naringin	[27,87]	0	0	0	A	0	0	0
98	hesperidin	[87]	0	0	0	A	0	0	0
99	hesperetin	[27]	1	1	0	B	1	/	/
100	naringenoxy phthalonitrile	[83]	0x	0x	0	A	0	0	0
101	naringenoxy benzylphthalonitrile	[83]	1x	0x	0	B	0	0	/
102	2-naringenin-7-O-phthalocyaninatozinc	[83]	1	1x	0	B	1	/	/
103	luteolin glucoside	[87]	0	0	0	A	0	0	0
104	biochanin A	[8]	0	0	0	A	0	0	0
105	formononetin	[8]	0	0	0	A	0	0	0
106	flavonoid 6	[25]	0	0	0	A	0	0	0

107	flavonoid 7	[25]	0	0	0x	A	0	0	0
108	flavonoid 8	[25]	0	0	0x	A	0	0	0
109	flavonoid 10	[25]	1	0	0	B	0	0	/
110	flavanone	[21]	0x	0	0	A	0	0	0
111	6-hydroxyflavanone	[84]	0	0	0	A	0	0	0
112	2'-hydroxyflavanone	[84]	0	0x	0	A	0	0	0
113	3'-hydroxyflavanone	[84]	0	0	0	A	0	0	0
114	4'-hydroxyflavanone	[84]	0	0x	0	A	0	0	0
115	7'-hydroxyflavanone	[84]	0	0x	0	A	0	0	0
116	narigin	[84]	1	0	0	B	0	0	/
FLAVANONOLS									
117	pinobanksin	[6]	1	1	1	A	1	1	1
118	taxifolin	[17]	1	0	0	B	0	0	/
119	isorhamnetin	[8]	1	0	0	B	0	0	/
120	dihydrokaempferol (aromadendrin)	[85]	0	1	0	B	0	/	/
121	dihydromyrcetin (ampeloptin)	[85]	1	0	0	B	0	0	/
122	silymarin	[7]	1	0	0	B	0	0	/
123	fustin	[84]	0	1	0	B	0	/	/
FLAVANES									
124	epicatechin gallate	[87]	0	1	1	B	1	1	/
125	epigallocatechin gallate	[87]	0	1	1	B	1	1	/
126	theaflavin	[6]	0	1x	1	B	1	1	/
127	catechin (cianidanol)	[87]	1	1	1	A	1	1	1
128	gallocatechin	[87]	0	1	1	B	1	1	/
FLAVANOLS									
129	leucopelargonidin	[85]	0	1	1	B	1	1	/
130	leucocyanidin	[85]	0	1	1	B	1	1	/
131	leucodelphinidin	[85]	1	1	1	A	1	1	1
132	mangiferin	[6]	0	0	0	A	0	0	0
XANTHONES									
133	1,5-Dihydroxyxanthone	[6]	1	1	0	B	1	/	/
134	euxanthone	[6]	1	1	0	B	1	/	/
CHROMONES									
135	chromone	[80]	0	0x	0	A	0	0	0
136	7-hydroxy chromone	[80]	0	1x	0	B	0	/	/
137	3-formyl chromone	[80]	0	1x	0	B	0	/	/
138	chromone 2-acid carboxylic	[80]	1	1x	0	B	1	/	/
139	chromone 3-acid carboxylic	[80]	1	1x	0	B	1	/	/
140	2-amino-3-formylchromone	[80]	0x	1x	0	B	0	/	/
141	rohitukine	[25]	1	0x	0	B	0	0	/
142	CD-2a	[22]	0	1	0	B	0	/	/
143	CD-2b	[22]	0	0	0	A	0	0	0
144	CD-2c	[22]	0	1	0	B	0	/	/
145	CD-2d	[22]	0	1	0	B	0	/	/
146	CD-2e	[22]	0	1	1	B	1	1	/
147	CD-9a	[22]	0	0	1	B	0	/	/
148	CD-9b	[22]	0	0	0	A	0	0	0
149	CD-9c	[22]	0	0x	0	A	0	0	0
150	CD-9d	[22]	0	1	0	B	0	/	/
151	FAAD-23	[13]	0	1x	1	B	1	1	/
152	FAAD-24	[13]	1	1x	0	B	1	/	/
153	FAAD-28	[13]	0	1x	0	B	0	/	/
154	FAAD-29	[13]	1	1x	0	B	1	/	/
COUMARINS									
155	mammeigin	[6]	0	1x	0	B	0	/	/
156	mesuagin	[6]	0	1x	0	B	0	/	/
157	mammeisin	[6]	0	1x	0	B	0	/	/
158	mesuol	[6]	0	1x	0	B	0	/	/
159	CD-70	[82]	0	1	0	B	0	/	/
160	CD-71	[82]	0	0x	0	A	0	0	0
161	CD-76	[82]	0	1	0	B	0	/	/
CHALCONES									
162	OCD-1	[24]	0	0	0	A	0	0	0
163	OCD-2	[24]	0	0	0x	A	0	0	0

164	OCD-3	[24]	0	0	0x	A	0	0	0
165	OCD-4	[24]	0x	0	0x	A	0	0	0
166	OCD-5	[24]	1	1	0	B	1	/	/
167	OCD-6	[24]	0	0	0	A	0	0	0
168	OCD-7	[24]	1	1	0	B	1	/	/
169	OCD-8	[24]	0	0	0	A	0	0	0
170	OCD-9	[24]	0	0	0	A	0	0	0
171	OCD-10	[24]	0	0	0x	A	0	0	0
PHENOLIC ACID DERIVATIVES									
172	caffeic acid phenethy ester (CAPE)	[23]	0	1	0	B	0	/	/
173	caffeic acid (dihydroxycinnamic acid)	[30]	1	1	0	B	1	/	/
174	methyl salicylate	[6]	0	0	0	A	0	0	0
175	salicylic acid	[6]	0	0	0	A	0	0	0
176	L-DOPA	[6]	0	0	0	A	0	0	0
177	cichoric acid	[6]	0	1	0x	B	0	/	/
178	chlorogenic acid	[6]	0	0	1	B	0	/	/
179	cinnamic acid	[6]	0	0x	0	A	0	0	0
180	ferulic acid	[6]	0	1	0	B	0	/	/
181	ellagic acid	[6]	1	1	1	A	1	1	1
182	rosmarinic acid	[6]	1	1	1	A	1	1	1
183	methyl caffeate	[12]	0	1	0	B	0	/	/
184	ethyl caffeate	[12]	0	1	0	A	0	0	0
185	propyl caffeate	[12]	0	0x	0	A	0	0	0
186	isopropyl caffeate	[12]	0	0	0	A	0	0	0
187	butyl caffeate	[12]	0	0	0	A	0	0	0
188	octyl caffeate	[12]	0	0	0	A	0	0	0
189	dodecyl caffeate	[12]	0	0	0x	A	0	0	0
190	trimethoxybenzoic acid	[27]	0	0	0	A	0	0	0
191	sinapic acid	[27]	0	1	0	B	0	/	/
192	isoferulic	[27]	0	1	0	B	0	/	/
193	hexyl caffeate	[30]	0	0	0	A	0	0	0
194	hexyl ferulate	[30]	0	0	0	A	0	0	0
195	dihydrocaffeic acid	[86,19]	0	0	0	A	0	0	0
196	methyl dihydrocaffeate	[86]	0	0	0	A	0	0	0
197	ethyl dihydrocaffeate	[86]	0	0x	0	A	0	0	0
198	propily dihydrocaffeate	[86]	1	0x	0	B	0	0	/
199	gallic acid	[17]	1	1x	1	A	1	1	1
200	methyl gallate	[17]	1	1x	1	A	1	1	1
201	ethyl gallate	[17]	0	0	1	B	0	/	/
202	butyl gallate	[17]	0	0x	1	B	0	/	/
203	octyl gallate	[17]	0	0	1	B	0	/	/
204	syringic acid	[9]	0	1x	0	B	0	/	/
205	propyl gallate	[9]	0	0	1	B	0	/	/
206	dodecyl gallate	[9]	0	0	1x	B	0	/	/
207	DOPAC, 3,4-dihydroxyphenylacetic acid	[8,81]	0	1	0	B	0	/	/
208	HVA, 3-methoxy-4-hydroxyphenylacetic acid	[8,81]	1	0	0	B	0	0	/
209	3-methoxy-4-hydroxybenzoic acid	[8]	1	1x	1	A	1	1	1
210	protocatechuic acid	[8]	0	1x	1	B	1	1	/
211	3-methoxy-4-hydroxyhippuric acid	[8]	1	1x	1	A	1	1	1
212	caftaric acid	[6]	0	1	0x	B	0	/	/
213	chicoric acid	[6]	1	1	0x	B	1	/	/
214	phenylmethyl caffeate	[20]	0	1	0	B	0	/	/
215	phenylpropyl caffeate	[20]	0	1	0	B	0	/	/
216	phenylbutyl caffeate	[20]	0	1	0	B	0	/	/
217	phenylpentyl caffeate	[20]	0	1	0	B	0	/	/
218	phenylhexyl caffeate	[20]	0	1	0	B	0	/	/
219	phenyloctyl caffeate	[20]	0	1	0	B	0	/	/
220	phenyldodecanyl caffeate	[20]	0	1x	0	B	0	/	/
221	cinnamyl caffeate	[20]	0	1	0	B	0	/	/
222	8-phenyl-7-octenyl caffeate	[20]	0	1x	0	B	0	/	/
223	12-phenyl-11-dodecenyl caffeate	[20]	0	1x	0	B	0	/	/
224	2-cyclohexylethyl caffeate	[20]	0	0	0	A	0	0	0
225	decanyl caffeate	[20]	1	1x	1	A	1	1	1
226	oleuropein	[81]	1	1	1	A	1	1	1

227	3,4-DHPEA-EA	[81]	0	0	0	A	0	0	0
228	3,4-DHPEA-EDA	[81]	1	0	1	B	1	/	/
229	THPE - 2(3,4,5-trihydroxyphenyl)ethanoic acid	[19]	1	0	0	B	0	0	/
230	THPP - 3(3,4,5-trihydroxyphenyl)propanoic acid	[19]	0	1x	0	B	0	/	/
231	PAD2	[23]	0	1	0	B	0	/	/
232	PAD3	[23]	0	1	0	B	0	/	/
233	PAD4	[23]	0	1	0	B	0	/	/
234	PAD5	[23]	0	0	0	A	0	0	0
235	PAD6	[23]	0	0	0	A	0	0	0
236	PAD7	[23]	0	0	0	A	0	0	0
237	PAD8	[23]	0	1	0	B	0	/	/
238	PAD9	[23]	0	1	0	B	0	/	/
239	PAD10	[23]	0	1	0	B	0	/	/
240	PAD11	[23]	0	1	0	B	0	/	/
241	PAD12	[23]	0	1	0	B	0	/	/
242	PAD13	[23]	0	1	0	B	0	/	/
243	PAD14	[23]	1	1	0	B	1	/	/
SIMPLE PHENOLS									
244	carvacrol	[6]	0	0	0	A	0	0	0
245	eugenol	[6]	0	0	0	A	0	0	0
246	guaiacol	[6]	0x	0	0	A	0	0	0
247	rheosmin (raspberry ketone)	[6]	0	0	0	A	0	0	0
248	butylated hydroxytoluene	[6]	0x	0	1x	B	0	/	/
249	2,6-xylenol	[6]	0	0	0	A	0	0	0
250	propofol (Diprivan)	[6]	0x	0	1x	B	0	/	/
251	butylhydroquinone	[18]	0	0x	1	B	0	/	/
252	3,5-dibutylcatechol	[18]	0	0x	0	A	0	0	0
253	gingerol	[6]	1	0	0	B	0	0	/
254	tyrosol	[81]	0	0x	0	A	0	0	0
255	hydroxytyrosol	[81]	0	0x	0	A	0	0	0
256	MOPET	[81]	0	0	0	A	0	0	0
257	tyramine	[6]	0	0	0	A	0	0	0
OTHERS									
258	α-tocopherol (vitamin E)	[86]	0x	0	0x	A	0	0	0
259	retinol (vitamin A)	[6]	0	0	0x	A	0	0	0
260	pterostilbene	[6]	0	0	0	A	0	0	0
261	silibinin	[6]	1	0	0	B	0	0	/
262	capsaicin	[6]	0x	0	0	A	0	0	0
263	cannabidiol	[6]	0	1x	0	B	0	/	/
264	thymol	[6]	0	0	0	A	0	0	0
265	sesamol	[6]	0x	0	0	A	0	0	0
266	sitosterol	[6]	0x	0x	0	A	0	0	0
267	bisphenol A (BPA)	[6]	0	0x	1x	B	0	/	/
268	2-phenylphenol	[6]	0x	0	0	A	0	0	0
269	caffeoylhexylamide	[30]	0	0x	0	A	0	0	0
270	feruloylhexylamide	[30]	1	0	0	B	0	0	/
271	apigenidin	[87]	0	1	0	B	0	/	/
272	caffeine	[7]	0x	0x	0	A	0	0	0
273	tamoxifen	[24]	0	0x	0	A	0	0	0
274	paradol	[12]	1	0	0	B	0	0	/
275	PAD15	[23]	0	1	0	B	0	/	/
276	PAD16	[23]	0	1	0	B	0	/	/
277	PAD17	[23]	0	1	0	B	0	/	/
278	PACD1	[88]	0	0x	1	B	0	/	/
279	PACD2	[88]	1	1x	0	B	1	/	/
280	PACD3	[88]	1	1x	1	A	1	1	1
281	PACD4	[88]	0	0x	0	A	0	0	0
282	PACD5	[88]	0	0x	0	A	0	0	0
283	PACD6	[88]	0	0	1	B	0	/	/
284	PACD7	[88]	0	0x	0	A	0	0	0
285	PACD8	[88]	0	1x	1	B	1	1	/
286	PACD9	[88]	0	0x	0	A	0	0	0
287	PACD10	[88]	0	0x	0	A	0	0	0
288	PACD11	[88]	1	0	0	B	0	0	/

289	PACD12	[88]	0	1x	0	B	0	/	/
290	PACD13	[88]	1	0x	0	B	0	0	/
291	PACD14	[88]	0	0x	1	B	0	/	/
292	PACD15	[88]	0	0	1	B	0	/	/
293	PACD16	[88]	1	1	0	B	1	/	/
294	PACD17	[88]	0	0x	0	A	0	0	0
295	PACD18	[88]	0	1	1	B	1	1	/
296	PACD19	[88]	0	0	0x	A	0	0	0
297	PACD20	[88]	0	1	0	B	0	/	/
298	PACD21	[88]	0	0x	0	A	0	0	0
299	gelastatin hydroxamate	[22]	0	0	0	A	0	0	0
300	bestatin	[13]	0	0x	1	B	0	/	/
		∑ active	75	138	72	/	65	31	15
		∑ predictions in AD	283	208	278	/	300	151	109

1 – inhibitor, 0 – noninhibitor, x – out of AD

Table S3: List of predictive QSAR models of 14 membrane transporters available at ChemBench platform.

Model	ID	Description	no. objects	ACC	CCR	SP	SE	Descriptors
MDR1	314a	Multidrug resistance protein 1 (MDR1, ABCB1, P-gp) inhibition at 10uM	1585	0.91	0.91	0.91	0.91	Dragon X-H
	313a	Multidrug resistance protein 1 (MDR1, ABCB1, P-gp) substrates vs. non-substrates	567	0.74	0.74	0.68	0.80	Dragon X-H
BSEP	243x	Bile Salt Export Pump (BSEP, ABCB11) inhibition at 10uM	725	0.84	0.84	0.87	0.80	Dragon X-H
	242x	Bile Salt Export Pump (BSEP, ABCB11) substrates vs. non-substrates	34	0.68	0.68	0.68	0.69	Dragon X-H
BCRP	241x	Breast cancer resistance protein (BCRP, ABCG2) inhibition at 10uM	395	0.83	0.82	0.87	0.77	Dragon X-H
	234q	Breast cancer resistance protein (BCRP, ABCG2) substrates vs. non-substrates	169	0.79	0.79	0.71	0.86	CDK
MRP1	322z	Multidrug resistance-associated protein 1 (MRP1, ABCC1) inhibition at 10uM	426	0.84	0.84	0.84	0.84	CDK
	321x	Multidrug resistance-associated protein 1 (MRP1, ABCC1) substrates vs. non-substrates	180	0.86	0.86	0.86	0.86	Dragon X-H
MRP2	324s_RF	Multidrug resistance-associated protein 2 (MRP2, ABCC2) inhibition at 10uM	104	0.83	0.83	0.79	0.87	Dragon X-H
	323x	Multidrug resistance-associated protein 2 (MRP2, ABCC2) substrates vs. non-substrates	222	0.80	0.80	0.79	0.81	Dragon X-H
MRP3	331x	Multidrug resistance-associated protein 3 (MRP3, ABCC3) inhibition at 10uM	36	0.64	0.62	0.74	0.53	Dragon X-H
	333a	Multidrug resistance-associated protein 3 (MRP3, ABCC3) substrate vs. non-substrates	100	0.92	0.92	0.94	0.90	Dragon X-H
MRP4	334q	Multidrug resistance-associated protein 4 (MRP4, ABCC4) inhibition at 10uM	67	0.78	0.78	0.78	0.77	CDK
	342z	Multidrug resistance-associated protein 4 (MRP4, ABCC4) substrates vs. non-substrates	122	0.76	0.76	0.74	0.79	CDK
MRP5	343z	Multidrug resistance-associated protein 5 (MRP5, ABCC5) inhibition at 50uM	37	0.84	0.79	0.62	0.96	CDK
	344q	Multidrug resistance-associated protein 5 (MRP5, ABCC5) substrates vs. non-substrates	58	0.76	0.76	0.76	0.76	CDK
MCT1	312z	Monocarboxylate transporter 1 (MCT1, SLC16A1) inhibition at 10uM	68	0.96	0.95	0.95	0.96	CDK
	311x	Monocarboxylate transporter 1 (MCT1, SLC16A1) substrates vs. non-substrates	36	0.78	0.78	0.89	0.67	Dragon X-H
NTCP	411x	Na+-taurocholate cotransporting polypeptide (NTCP, LBAT, SLC10A1) inhibition at 10uM	127	0.81	0.80	0.86	0.74	Dragon X-H
	412q	Na+-taurocholate cotransporting polypeptide (NTCP, LBAT, SLC10A1) substrates vs. non-substrates	70	0.89	0.89	0.87	0.89	CDK
ASBT	232z	Apical sodium-dependent bile acid transporter (ASBT, IBAT, SLC10A2) inhibition at 10uM	232	0.89	0.89	0.85	0.92	CDK
	233f_RF	Apical sodium-dependent bile acid transporter (ASBT, IBAT, SLC10A2) substrates vs. non-substrates	106	0.89	0.89	0.83	0.94	Dragon X-H
OCT1	421z	Organic cation transporter 1 (OCT1, SLC22A1) inhibition at 100uM	199	0.87	0.86	0.92	0.81	CDK
	422z	Organic cation transporter 1 (OCT1, SLC22A1) substrates vs. non-substrates	82	0.87	0.87	0.88	0.85	CDK

OATP2B1	414z	Organic anion transporting polypeptide 2B1 (OATP2B1, SLCO2B1, SLC21A9) inhibition at 100uM	114	0.83	0.83	0.79	0.88	CDK
	413x	Organic anion transporting polypeptide 2B1 (OATP2B1, SLCO2B1, SLC21A9) substrates vs. non-substrates	59	0.81	0.81	0.77	0.85	Dragon X-H
PEPT1	423z	Peptide transporter 1 (PEPT1, SLC15A1) inhibition at 100uM	82	0.74	0.74	0.73	0.76	CDK
	424z	Peptide transporter 1 (PEPT1, SLC15A1) substrates vs. non-substrates	292	0.86	0.86	0.83	0.89	CDK
BTL*	NN-2	Bilirubin membrane transporter (Bilitranslocase) inhibition	120	0.91	0.91	0.93	0.88	Dragon X-H

*new, not available in ChemBench, CCR=0.5 SE + 0.5 SP

Table S4: List of selected Dragon descriptors in NN-D and Q-D models.

NN-D model	Q-D model
nBM	ARR
nO	LOC
nP	VE3sign_Dz(p)
VE1_A	EE_B(s)
MATS7e	P_VSA_p_4
GATS5i	nArCO
P_VSA_LogP_2	nArOR
nArCO	H-052
nOHp	CATS2D_07_DA
nSO3OH	CATS2D_04_AN
nP(=O)O2R	B05[O-O]
SsssN	
CATS2D_03_LL	
T(Cl,,Cl)	
B03[N-O]	
B04[O-S]	
DLS_05	
LLS_01	

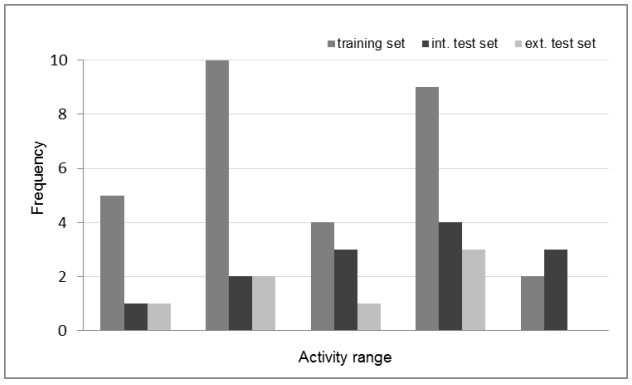


Figure S1: Frequency distribution of compounds for five ranges of BTL biological activity (< 2.5, 2.5 - 3.5, 3.5 – 4.5, 4.5 – 5.5, > 5.5) in datasets used for model building and validation.

Table S5: Hamming distances among the best four BTL regression models (M1-M4).

	M2	M3	M4
M1	8	15	9
M2	-	17	7
M3	-	-	10

Table S6: Summary of new compounds predictions with the best four BTL regression models.

		No. of compounds in the AD		
Model	No. of descriptors	Phenols ∑ = 205	Antioxidants* ∑ = 29	Antiprions* ∑ = 19
M1	12	152	0	2
M2	10	157	17	3
M3	9	97	5	1
M4	5	183	20	2

*results from study of Martinčič *et al.* [59]

Table S7: BTL activity predictions with regression models M1-M4 for phenolic compounds, which were classified as active in classification models. ID is the same as in Table S2.

ID	Active in classification models	M1	M2	M3	M4	$\bar{y}$ ± SD	$\bar{y}_w$
1	NN-C, NN-D	4.44	4.21	4.20	4.21	**4.27 ± 0.12**	**4.24**
2	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.14**
3	NN-C, NN-D	4.16	4.15	3.98	4.06	**4.09 ± 0.08**	**4.10**
4	NN-C, NN-D, Q-D	4.71	3.86	4.20	4.06	**4.21 ± 0.36**	**4.16**
6	NN-D	4.44	4.21	4.20	4.06	**4.23 ± 0.16**	**4.21**
7	NN-C	4.88	5.52	4.72	5.04	**5.04 ± 0.35**	**5.04**
8	NN-D, Q-D	3.94	4.15	4.20	4.06	**4.09 ± 0.12**	**4.09**
11x	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.13**
12	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.14**
13	NN-D	4.03	4.15	3.98	4.06	**4.06 ± 0.07**	**4.05**
14	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
19	NN-D	4.16	4.15	3.98	4.06	**4.09 ± 0.08**	**4.07**
21	NN-C, Q-D	4.71	4.70	4.66	4.71	**4.70 ± 0.02**	**4.70**
22	NN-C, Q-D	4.71	4.70	4.66	4.71	**4.70 ± 0.02**	**4.70**
23	NN-C, Q-D	4.71	4.70	4.66	3.80	**4.47 ± 0.45**	**4.38**
24	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.13**
25	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
26	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
27	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
28	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
30	NN-D	4.00	4.15	3.98	4.21	**4.08 ± 0.11**	**4.09**
31	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
32	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
33	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
34x	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.13**
35	NN-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
36	Q-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
37x	Q-D	4.16	4.15	3.98	4.21	**4.13 ± 0.10**	**4.12**
38x	NN-D,Q-D	4.00	3.78	3.98	4.21	**3.99 ± 0.17**	**4.02**

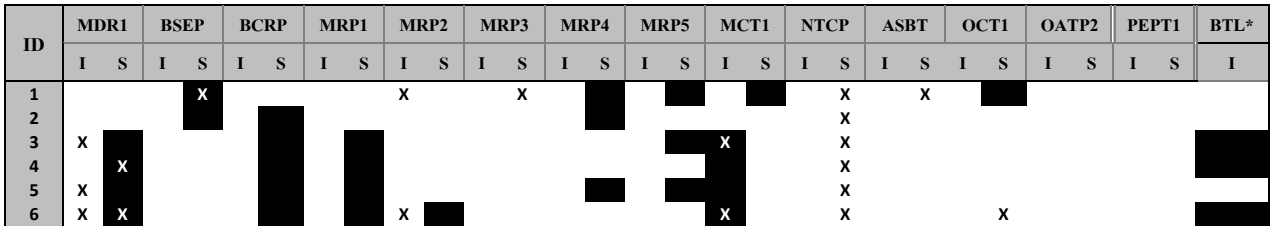
39	NN-D, Q-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.13**
40x	NN-D, Q-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.13**
41x	NN-D, Q-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.12**
42	NN-D, Q-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
43x	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
44x	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
45	NN-C	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.12**
46	NN-D	4.03	4.15	3.98	4.21	**4.09**	±	**0.10**	**4.12**
47	NN-C	4.81	5.52	5.48	5.04	**5.21**	±	**0.35**	**5.19**
49	NN-C	5.20	5.20	5.20	5.20	**5.20**	±	**0.00**	**5.20**
51	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.13**
53	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.13**
54	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
55	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.11**
56	Q-D	4.00	4.21	3.98	3.91	**4.03**	±	**0.13**	**4.01**
57	NN-D	4.16	4.15	3.98	3.91	**4.05**	±	**0.12**	**4.05**
59x	Q-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.12**
60	Q-D	4.16	4.15	3.98	3.82	**4.03**	±	**0.16**	**4.03**
61	Q-D	4.16	4.15	3.98	3.82	**4.03**	±	**0.16**	**4.01**
62x	NN-D, Q-D	4.00	4.15	3.98	4.21	**4.08**	±	**0.11**	**4.08**
63	NN-D	4.16	4.15	3.98	3.82	**4.03**	±	**0.16**	**4.02**
64	NN-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.89**
65	NN-C, Q-D	4.00	3.78	3.98	4.88	**4.16**	±	**0.49**	**4.27**
66	Q-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.88**
67	Q-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.88**
68	Q-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.89**
69	Q-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.89**
70	NN-C, Q-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.88**
71	NN-C, Q-D	4.00	3.78	3.98	4.88	**4.16**	±	**0.49**	**4.22**
72	Q-D	4.00	4.21	3.98	4.88	**4.27**	±	**0.42**	**4.28**
73	Q-D	4.00	3.78	3.98	4.88	**4.16**	±	**0.49**	**4.24**
74	Q-D	4.00	3.78	3.98	4.88	**4.16**	±	**0.49**	**4.24**
76	Q-D	4.16	3.78	3.98	4.88	**4.20**	±	**0.48**	**4.35**
77x	NN-D, Q-D	4.00	3.78	5.23	4.82	**4.45**	±	**0.68**	**4.57**
78	Q-D	2.30	4.21	3.98	3.91	**3.60**	±	**0.87**	**3.72**
79	NN-C	4.62	4.61	5.47	4.06	**4.69**	±	**0.58**	**4.62**
80	NN-C	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
81	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
82	NN-C, NN-D	4.44	3.86	4.20	4.21	**4.18**	±	**0.24**	**4.18**
83	NN-C	5.14	4.61	5.47	3.85	**4.77**	±	**0.71**	**4.69**
84	NN-C, NN-D	4.16	4.15	4.20	4.21	**4.18**	±	**0.03**	**4.18**
86	NN-C, NN-D, Q-D	3.94	4.15	4.20	4.21	**4.12**	±	**0.13**	**4.12**
87	NN-D	3.96	3.86	4.66	3.80	**4.07**	±	**0.40**	**4.16**
88	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
89	NN-C, Q-D	4.71	4.70	4.66	4.71	**4.70**	±	**0.02**	**4.69**
90	NN-C	4.74	4.99	4.66	5.05	**4.86**	±	**0.19**	**4.86**
91	Q-D	4.71	4.70	4.66	4.71	**4.70**	±	**0.02**	**4.68**
92	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
94	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.10**
95	NN-C, NN-D, Q-D	5.19	4.96	4.66	2.43	**4.31**	±	**1.27**	**4.30**
96	NN-C, NN-D	3.94	4.21	4.20	3.18	**3.88**	±	**0.48**	**3.90**
99	NN-C, NN-D	2.30	4.21	3.98	3.18	**3.42**	±	**0.86**	**3.39**
101x	NN-C	4.16	3.78	5.42	4.82	**4.54**	±	**0.72**	**4.65**
102x	NN-C, NN-D	5.45	5.45	5.46	5.46	**5.46**	±	**0.01**	**5.46**
109	NN-C	4.16	4.15	3.98	4.88	**4.30**	±	**0.40**	**4.34**
116	NN-C	5.25	5.52	4.72	5.04	**5.13**	±	**0.34**	**5.14**
117	NN-C, NN-D, Q-D	4.44	4.72	4.20	3.18	**4.14**	±	**0.67**	**4.13**
118	NN-C	5.19	5.25	4.66	4.06	**4.79**	±	**0.55**	**4.89**
119	NN-C	2.30	2.30	4.20	4.06	**3.22**	±	**1.06**	**3.11**
120	Q-D	5.19	5.25	4.66	4.06	**4.79**	±	**0.55**	**4.90**
121	NN-C	5.24	5.11	5.28	3.56	**4.80**	±	**0.83**	**4.71**
122	NN-C	5.68	5.70	5.23	5.62	**5.56**	±	**0.22**	**5.56**
123	NN-D	4.79	5.25	4.66	4.06	**4.69**	±	**0.49**	**4.86**
124	NN-D, Q-D	4.62	4.61	5.23	3.25	**4.43**	±	**0.84**	**4.18**

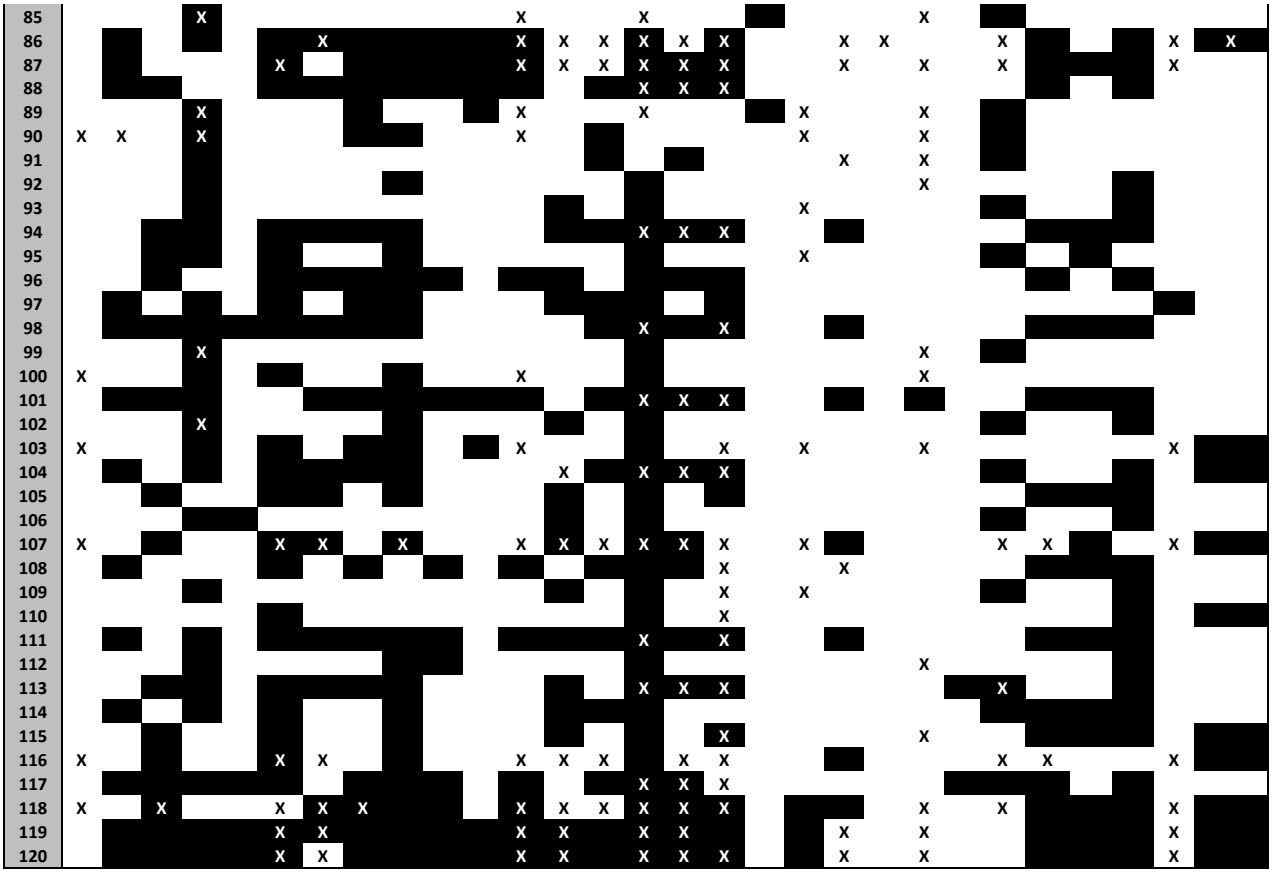
125	NN-D, Q-D	4.62	4.61	5.23	3.06	**4.38**	±	**0.92**	**4.03**
126	NN-D, Q-D	5.50	5.52	5.47	5.35	**5.46**	±	**0.08**	**5.44**
127x	NN-C, NN-D, Q-D	4.79	5.25	5.13	2.43	**4.40**	±	**1.32**	**4.40**
128x	NN-D, Q-D	5.19	5.25	5.13	4.64	**5.05**	±	**0.28**	**5.05**
129	NN-D, Q-D	5.19	5.25	5.13	2.43	**4.50**	±	**1.38**	**4.50**
130x	NN-D, Q-D	5.19	4.93	5.13	4.64	**4.97**	±	**0.25**	**4.96**
131x	NN-C, NN-D, Q-D	5.24	5.11	5.13	2.95	**4.61**	±	**1.11**	**4.48**
133	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
134	NN-C, NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.14**
136x	NN-D	4.00	4.24	4.25	4.21	**4.17**	±	**0.12**	**4.19**
137x	NN-D	4.16	4.15	4.23	4.21	**4.19**	±	**0.04**	**4.19**
138x	NN-C, NN-D	4.16	4.15	4.23	4.21	**4.19**	±	**0.04**	**4.19**
139x	NN-C, NN-D	4.16	4.15	4.23	4.21	**4.19**	±	**0.04**	**4.19**
140	NN-D	3.94	3.59	4.23	3.80	**3.89**	±	**0.27**	**3.91**
141	NN-C	2.30	2.30	3.69	3.91	**3.05**	±	**0.87**	**3.17**
142	NN-D	4.03	4.24	3.27	4.21	**3.94**	±	**0.45**	**3.90**
144	NN-D	4.00	4.24	3.27	4.21	**3.93**	±	**0.45**	**3.91**
145	NN-D	4.00	4.24	3.27	4.21	**3.93**	±	**0.45**	**3.91**
146	NN-D, Q-D	3.50	3.59	2.21	3.91	**3.30**	±	**0.75**	**3.31**
147	Q-D	3.50	3.59	2.21	3.82	**3.28**	±	**0.73**	**3.29**
150	NN-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.89**
151x	NN-D, Q-D	4.00	3.78	3.98	4.88	**4.16**	±	**0.49**	**4.25**
152	NN-C, NN-D	4.03	3.86	4.20	4.88	**4.24**	±	**0.45**	**4.28**
153	NN-D	4.03	3.86	4.20	4.73	**4.21**	±	**0.38**	**4.21**
154	NN-C, NN-D	4.44	3.86	4.66	4.73	**4.42**	±	**0.40**	**4.41**
155x	NN-D	4.00	4.15	3.98	4.88	**4.25**	±	**0.43**	**4.38**
156	NN-D	4.16	4.15	3.98	3.82	**4.03**	±	**0.16**	**4.00**
157x	NN-D	3.50	3.78	5.47	4.88	**4.41**	±	**0.93**	**4.51**
158x	NN-D	3.50	3.78	3.98	3.82	**3.77**	±	**0.20**	**3.79**
159	NN-D	4.00	3.78	3.98	4.21	**3.99**	±	**0.17**	**4.03**
161	NN-D	4.00	3.78	3.98	3.82	**3.90**	±	**0.11**	**3.89**
166	NN-C, NN-D	4.16	4.15	4.20	4.21	**4.18**	±	**0.03**	**4.18**
168	NN-C, NN-D	4.44	3.86	4.66	3.85	**4.20**	±	**0.41**	**4.24**
172	NN-D	4.16	4.21	3.98	4.21	**4.14**	±	**0.11**	**4.13**
173	NN-C, NN-D	3.94	3.86	4.23	3.80	**3.96**	±	**0.19**	**3.96**
177	NN-D	5.46	5.87	5.23	3.85	**5.10**	±	**0.88**	**4.82**
178	Q-D	4.62	5.11	5.13	5.22	**5.02**	±	**0.27**	**5.01**
180	NN-D	4.03	4.24	4.23	4.06	**4.14**	±	**0.11**	**4.13**
181	NN-C, NN-D, Q-D	3.96	3.59	4.66	4.25	**4.12**	±	**0.45**	**4.13**
182	NN-C, NN-D, Q-D	5.24	4.23	4.66	3.85	**4.50**	±	**0.60**	**4.52**
183	NN-D	3.94	4.15	4.23	4.21	**4.13**	±	**0.13**	**4.16**
184	NN-D	4.03	4.21	3.27	4.21	**3.93**	±	**0.45**	**3.97**
191	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.15**
192	NN-D	4.03	4.24	4.23	4.06	**4.14**	±	**0.11**	**4.13**
198	NN-C	4.03	4.21	2.21	4.21	**3.66**	±	**0.97**	**3.64**
199	NN-C, NN-D, Q-D	3.49	2.89	3.79	4.25	**3.61**	±	**0.57**	**3.67**
200	NN-C, NN-D, Q-D	3.49	3.59	3.79	3.80	**3.67**	±	**0.15**	**3.66**
201	Q-D	3.94	3.59	3.79	3.80	**3.78**	±	**0.14**	**3.78**
202	Q-D	3.94	3.86	5.08	3.80	**4.17**	±	**0.61**	**4.10**
203	Q-D	4.16	4.21	5.08	4.21	**4.42**	±	**0.45**	**4.32**
204	NN-D	4.16	4.15	3.79	4.21	**4.08**	±	**0.19**	**4.11**
205	Q-D	3.94	3.86	3.79	3.80	**3.85**	±	**0.07**	**3.85**
206x	Q-D	4.16	5.87	5.95	4.88	**5.22**	±	**0.85**	**5.05**
207	NN-D	3.94	3.59	4.73	3.80	**4.02**	±	**0.50**	**4.13**
208	NN-C	4.03	3.59	4.23	4.21	**4.01**	±	**0.29**	**4.08**
209	NN-C, NN-D, Q-D	3.94	3.59	4.23	4.06	**3.96**	±	**0.27**	**4.00**
210	NN-D, Q-D	3.49	3.59	3.79	4.25	**3.78**	±	**0.34**	**3.79**
211	NN-C, NN-D, Q-D	2.30	3.59	3.27	3.18	**3.09**	±	**0.55**	**3.11**
212	NN-D	3.32	4.23	3.79	3.85	**3.80**	±	**0.38**	**3.75**
213	NN-C, NN-D	5.46	5.87	5.23	3.85	**5.10**	±	**0.88**	**4.70**
214	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.12**
215	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.07**
216	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.08**
217	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.09**

218	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.10**
219	NN-D	4.16	3.78	5.47	4.88	**4.57**	±	**0.75**	**4.69**
220x	NN-D	4.16	5.87	5.86	4.88	**5.20**	±	**0.83**	**5.01**
221	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.11**
222	NN-D	4.16	3.78	5.47	4.88	**4.57**	±	**0.75**	**4.70**
223x	NN-D	4.16	5.87	5.23	4.88	**5.04**	±	**0.71**	**4.92**
225	NN-C, NN-D, Q-D	4.16	3.78	5.85	4.21	**4.50**	±	**0.92**	**4.37**
226	NN-C, NN-D, Q-D	4.34	4.32	4.23	4.38	**4.32**	±	**0.06**	**4.32**
228	NN-C, Q-D	2.30	3.78	3.69	3.18	**3.24**	±	**0.68**	**3.22**
229	NN-C	3.82	3.59	5.08	5.05	**4.39**	±	**0.79**	**4.48**
230	NN-D	3.96	3.86	5.08	5.05	**4.49**	±	**0.67**	**4.59**
231	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.06**
232	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.05**
233	NN-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.12**
237	NN-D	4.44	4.21	4.20	4.21	**4.27**	±	**0.12**	**4.25**
238	NN-D	3.50	3.78	3.98	4.21	**3.87**	±	**0.30**	**3.93**
239	NN-D	4.03	3.78	3.98	4.21	**4.00**	±	**0.18**	**4.03**
240	NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.06**
241	NN-D	4.16	4.21	3.98	4.21	**4.14**	±	**0.11**	**4.14**
242	NN-D	4.03	3.78	3.98	4.21	**4.00**	±	**0.18**	**4.03**
243	NN-C, NN-D	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.06**
248x	Q-D	4.16	4.15	5.28	2.43	**4.01**	±	**1.17**	**3.81**
250x	Q-D	4.16	4.15	5.28	2.43	**4.01**	±	**1.17**	**3.90**
251x	Q-D	4.16	2.30	2.21	2.43	**2.78**	±	**0.93**	**2.73**
253	NN-C	2.30	3.78	3.71	2.43	**3.06**	±	**0.80**	**2.93**
261	NN-C	5.68	5.70	5.47	5.62	**5.62**	±	**0.11**	**5.62**
263x	NN-D	3.50	3.78	5.74	3.18	**4.05**	±	**1.15**	**4.02**
267x	Q-D	4.16	4.15	3.98	2.43	**3.68**	±	**0.84**	**3.59**
270	NN-C	3.50	3.78	2.48	4.21	**3.49**	±	**0.73**	**3.74**
271	NN-D	4.16	3.95	4.20	3.74	**4.01**	±	**0.21**	**4.02**
274x	NN-C	4.16	3.78	3.98	4.21	**4.03**	±	**0.20**	**4.07**
275	NN-D	4.74	4.96	4.66	3.80	**4.54**	±	**0.51**	**4.49**
276	NN-D	3.87	3.78	4.20	3.91	**3.94**	±	**0.18**	**3.95**
277	NN-D	3.87	3.78	4.20	3.91	**3.94**	±	**0.18**	**3.95**
278x	Q-D	4.00	4.15	3.98	4.21	**4.08**	±	**0.11**	**4.10**
279x	NN-C, NN-D	3.50	3.86	3.79	4.88	**4.01**	±	**0.60**	**4.06**
280	NN-C, NN-D, Q-D	5.14	4.23	4.79	3.85	**4.50**	±	**0.58**	**4.32**
283	Q-D	4.03	3.86	2.48	3.91	**3.57**	±	**0.73**	**3.65**
285	NN-D, Q-D	4.03	4.21	3.71	3.82	**3.94**	±	**0.22**	**3.98**
288	NN-C	4.00	4.15	4.23	4.21	**4.15**	±	**0.10**	**4.16**
289x	NN-D	3.32	3.86	3.78	4.88	**3.96**	±	**0.66**	**4.03**
290	NN-C	3.32	2.44	3.78	2.53	**3.02**	±	**0.65**	**2.91**
291	Q-D	2.99	3.38	3.71	3.84	**3.48**	±	**0.38**	**3.56**
292x	Q-D	4.16	4.15	4.71	4.88	**4.48**	±	**0.38**	**4.51**
293	NN-C, NN-D	3.50	4.15	2.48	4.88	**3.75**	±	**1.02**	**3.97**
295x	NN-D, Q-D	4.16	4.15	3.98	4.21	**4.13**	±	**0.10**	**4.13**
297	NN-D	4.16	4.15	3.98	3.91	**4.05**	±	**0.12**	**4.06**
300	Q-D	2.30	4.23	3.71	4.06	**3.58**	±	**0.88**	**3.39**

x or red colour – out of AD

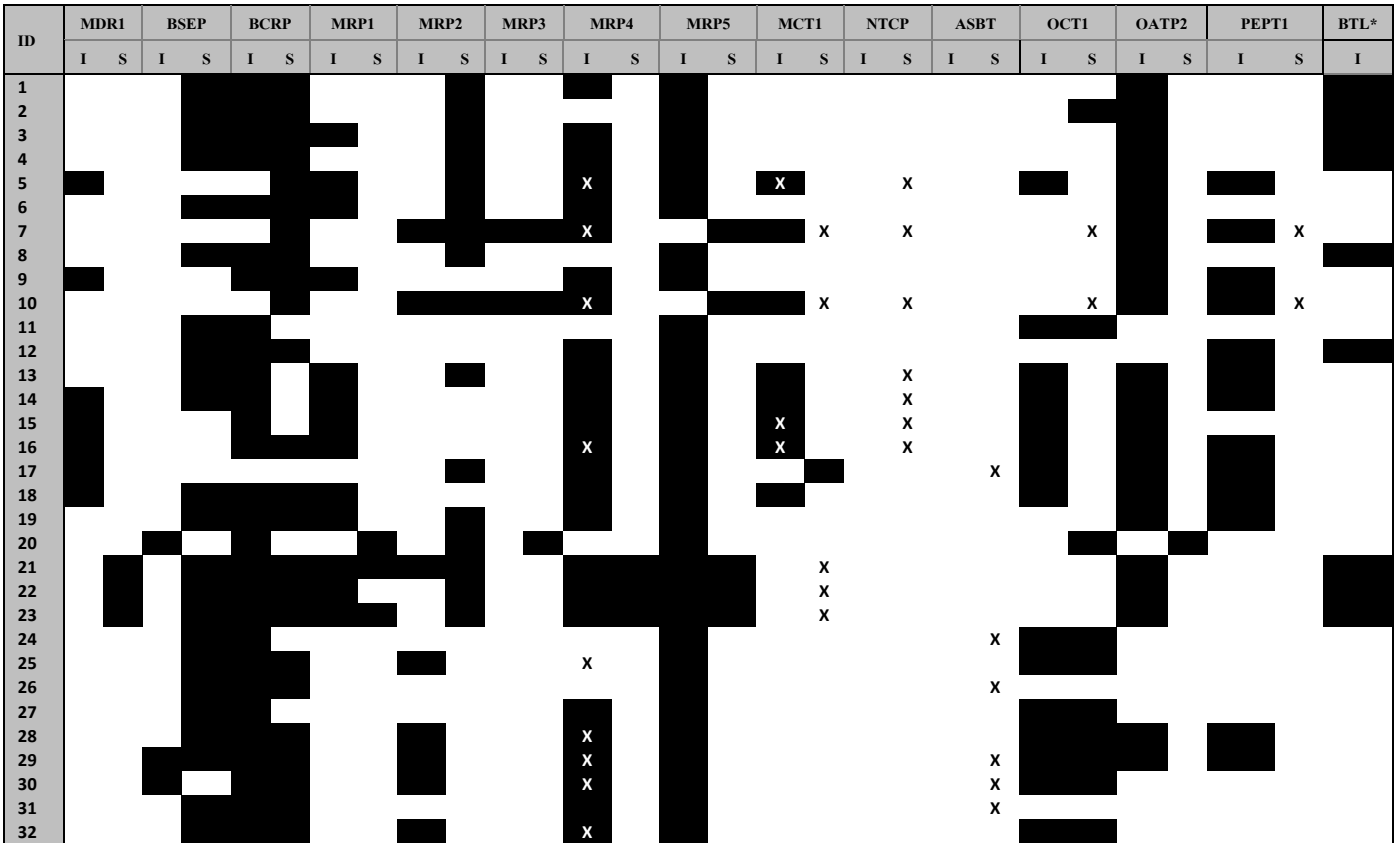
Table S8: Membrane transporters activity predictions with classification models from ChemBench for BTL dataset. ID is the same as in Table S1.

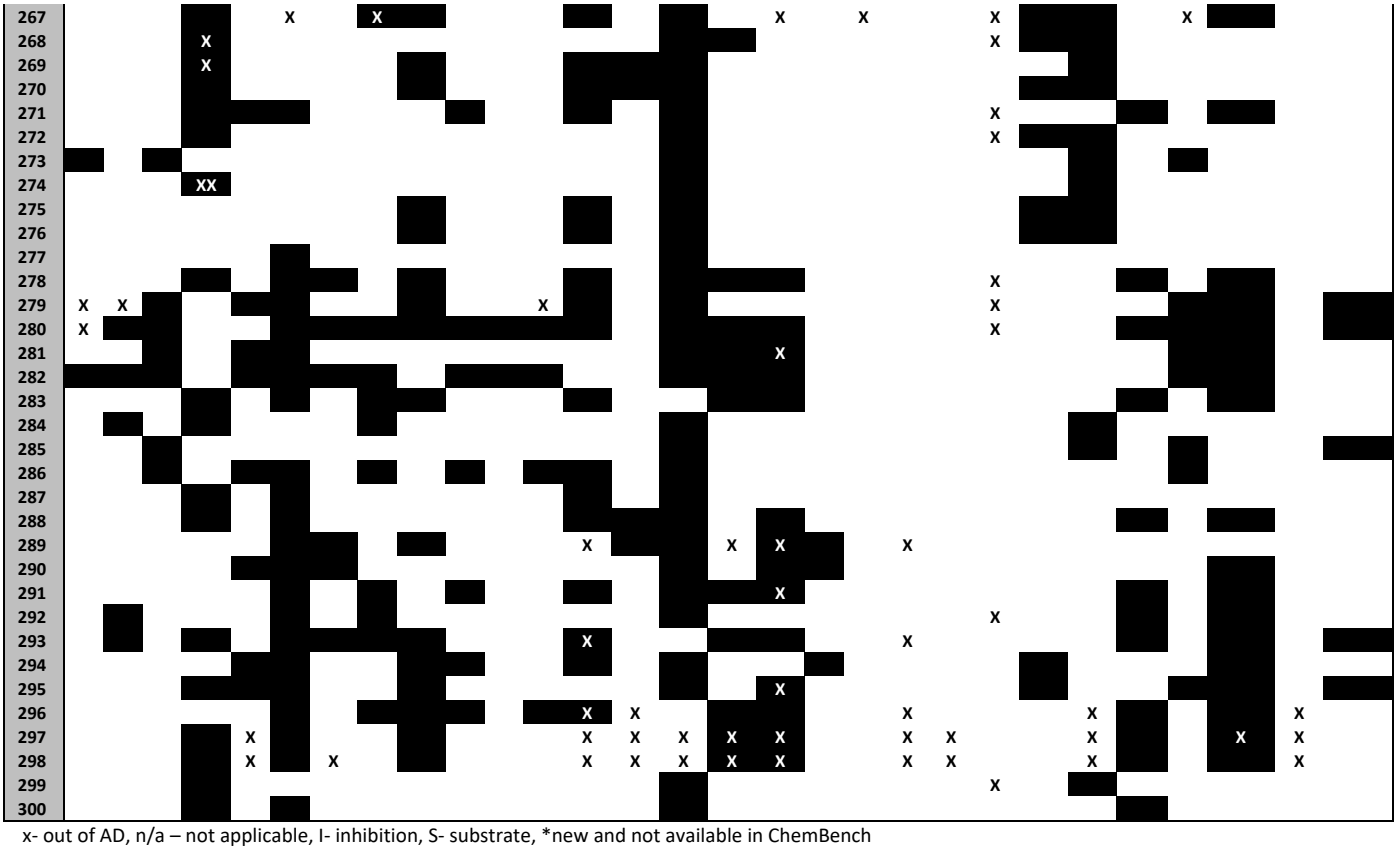




x- out of AD, n/a – not applicable, I- inhibition, S- substrate, *new and not available in ChemBench

Table S9: Membrane transporters activity predictions with classification models from ChemBench for phenolic dataset. ID is the same as in Table S2.





x- out of AD, n/a – not applicable, I- inhibition, S- substrate, *new and not available in ChemBench