

Supplementary material

Reverse screening of boronic acid derivatives: Analysis of potential antiproliferative effects on a triple-negative breast cancer model *in vitro*.

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Table S1. UniProt entries of the therapeutic targets predicted in the different employed servers.

UniProt Entry	Protein name
P22303	Acetylcholinesterase
Q13085	Acetyl-CoA carboxylase 1
O00763	Acetyl-CoA carboxylase 2
P29274	Adenosine A2a receptor
P15144	Aminopeptidase N
P09917	Arachidonate 5-lipoxygenase
P05067	Beta amyloid A4 protein
P08588	Beta-1 adrenergic receptor
P13945	Beta-3 adrenergic receptor
P06276	Butyrylcholinesterase
Q16566	CaM kinase IV
P00915	Carbonic anhydrase I
P00918	Carbonic anhydrase II
P22748	Carbonic anhydrase IV
Q16790	Carbonic anhydrase IX
O43570	Carbonic anhydrase XII
P07339	Cathepsin D
P08311	Cathepsin G
P11511	Cytochrome P450 19A1
P05177	Cytochrome P450 1A2
P20813	Cytochrome P450 2B6
P08684	Cytochrome P450 3A4
Q02127	Dihydroorotate dehydrogenase
Q9UHL4	Dipeptidyl peptidase II
Q86TI2	Dipeptidyl peptidase IX
Q6V1X1	Dipeptidyl peptidase VIII
E5KPS3	DNA-(apurinic or apyrimidinic site) lyase
P14416	Dopamine D2 receptor
P35462	Dopamine D3 receptor
P21917	Dopamine D4 receptor
Q01959	Dopamine transporter
O14733	Dual specificity mitogen-activated protein kinase kinase 7
Q9HAZ1	Dual specificity protein kinase CLK4
P51452	Dual specificity protein phosphatase 3
Q13627	Dual-specificity tyrosine-phosphorylation regulated kinase 1A
Q99714	Endoplasmic reticulum-associated amyloid beta-peptide-binding protein
P25101	Endothelin receptor ET-A
P00533	Epidermal growth factor receptor erbB1
P14061	Estradiol 17-beta-dehydrogenase 1
P37059	Estradiol 17-beta-dehydrogenase 2
P11474	Estrogen receptor alpha

Q92731	Estrogen receptor beta
P11166	Glucose transporter
P42262	Glutamate receptor ionotropic, AMPA 2
P09211	Glutathione S-transferase Pi
Q9Y2T6	G-protein coupled receptor 55
P35367	Histamine H1 receptor
Q9Y5N1	Histamine H3 receptor
Q13547	Histone deacetylase 1
Q9UBN7	Histone deacetylase 6
Q8TDS4	Hydroxycarboxylic acid receptor 2
Q07820	Induced myeloid leukemia cell differentiation protein Mcl-1
Q13887	Kruppel-like factor 5
P03956	Matrix metalloproteinase 1
P45452	Matrix metalloproteinase 13
P50281	Matrix metalloproteinase 14
P08253	Matrix metalloproteinase 2
P14780	Matrix metalloproteinase 9
P21397	Monoamine oxidase A
P27338	Monoamine oxidase B
P11229	Muscarinic acetylcholine receptor M1
P20309	Muscarinic acetylcholine receptor M3
P08473	Neprilysin
P19838	Nuclear factor NF-kappa-B p105 subunit
Q07869	Peroxisome proliferator-activated receptor alpha
P37231	Peroxisome proliferator-activated receptor gamma
P09874	Poly [ADP-ribose] polymerase-1
P06401	Progesterone receptor
P48147	Prolyl endopeptidase
P20618	Proteasome component C5
P16083	Quinone reductase 2
Q9BQF6	Sentrin-specific protease 7
P37023	Serine/threonine-protein kinase receptor R3
P08908	Serotonin 1a (5-HT1a) receptor
P28223	Serotonin 2a (5-HT2a) receptor
P41595	Serotonin 2b (5-HT2b) receptor
P28335	Serotonin 2c (5-HT2c) receptor
P50406	Serotonin 6 (5-HT6) receptor
P31645	Serotonin transporter
P40763	Signal transducer and activator of transcription 3
P21453	Sphingosine 1-phosphate receptor Edg-1
P40238	Thrombopoietin receptor
P04818	Thymidylate synthase
P10827	Thyroid hormone receptor alpha
Q64127	Transcription intermediary factor 1-alpha
P02766	Transthyretin
P36888	Tyrosine-protein kinase receptor FLT3
P35968	Vascular endothelial growth factor receptor 2
P47989	Xanthine dehydrogenase

Table S2. CLogP and LogS values of the five tested compounds. Calculated by using ChemDraw Ver18.0.

Compound	ClogP	LogS
1	2.102	-2.526
2	4.240	-4.112
3	4.403	-2.260
4	3.943	-4.085
5	2.442	-2.304