

**Table S1** List of compounds selected from commercial chemical libraries for the aptamer-based competitive drug screening assay designed in this study

Product name	Molecular weight	CAS number	Formula	Target
<b>Compounds containing at least one tertiary amino group</b>				
Methotrexate*	454.44	59-05-2	C <sub>20</sub> H <sub>22</sub> N <sub>8</sub> O <sub>5</sub>	Dihydrofolate reductase
Ketoconazole*	531.43	65277-42-1	C <sub>26</sub> H <sub>28</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>4</sub>	Cytochrome P450
Sildenafil citrate*	666.7	171599-83-0	C <sub>28</sub> H <sub>38</sub> N <sub>6</sub> O <sub>11</sub> S	Phosphodiesterase
Mycophenolate mofetil*	433.49	128794-94-5	C <sub>23</sub> H <sub>31</sub> NO <sub>7</sub>	Inosine monophosphate dehydrogenase
Dyphylline*	254.24	479-18-5	C <sub>10</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub>	Phosphodiesterase
Tadalafil*	389.4	171596-29-5	C <sub>22</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>	Phosphodiesterase
Apixaban*	459.5	503612-47-3	C <sub>25</sub> H <sub>25</sub> N <sub>5</sub> O <sub>4</sub>	Factor Xa
Aminophylline*	420.43	317-34-0	C <sub>16</sub> H <sub>24</sub> N <sub>10</sub> O <sub>4</sub>	Phosphodiesterase
Fluvastatin sodium*	433.45	93957-55-2	C <sub>24</sub> H <sub>25</sub> FNNaO <sub>4</sub>	HMG-CoA Reductase
Atorvastatin calcium*	1155.34	134523-03-8	C <sub>66</sub> H <sub>68</sub> CaF <sub>2</sub> N <sub>4</sub> O <sub>10</sub>	HMG-CoA Reductase
Ozagrel*	228.25	82571-53-7	C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	Factor Xa
Vardenafil HCl trihydrate*	579.11	224785-90-4	C <sub>23</sub> H <sub>39</sub> ClN <sub>6</sub> O <sub>7</sub> S	Phosphodiesterase
Clarithromycin*	747.95	81103-11-9	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>	Cytochrome P450
Cobicistat (GS-9350)*	776.02	1004316-88-4	C <sub>40</sub> H <sub>53</sub> N <sub>7</sub> O <sub>5</sub> S <sub>2</sub>	Cytochrome P450 (e.g. CYP17)
Rivaroxaban*	435.88	366789-02-8	C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>5</sub> S	Factor Xa
Anagrelide HCl*	292.55	58579-51-4	C <sub>10</sub> H <sub>8</sub> Cl <sub>3</sub> N <sub>3</sub> O	Phosphodiesterase
Moclobemide (Ro 111163)*	268.74	71320-77-9	C <sub>13</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>	Monoamine oxidase
Avanafil*	483.95	330784-47-9	C <sub>23</sub> H <sub>26</sub> ClN <sub>7</sub> O <sub>3</sub>	Phosphodiesterase
GSK256066	518.58	801312-28-7	C <sub>27</sub> H <sub>26</sub> N <sub>4</sub> O <sub>5</sub> S	Phosphodiesterase
PF-3845	456.46	1196109-52-0	C <sub>24</sub> H <sub>23</sub> F <sub>3</sub> N <sub>4</sub> O <sub>2</sub>	Fatty acid amide hydrolase
Nepicastat (SYN-117) HCl	331.81	170151-24-3	C <sub>14</sub> H <sub>16</sub> ClF <sub>2</sub> N <sub>3</sub> S	Hydroxylase
CP-91149	399.87	186392-40-5	C <sub>21</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>3</sub>	Phosphorylase
Torcetrapib	600.47	262352-17-0	C <sub>26</sub> H <sub>25</sub> F <sub>9</sub> N <sub>2</sub> O <sub>4</sub>	Cholesterol ester transfer protein
Lonafarnib	638.82	193275-84-2	C <sub>27</sub> H <sub>31</sub> Br <sub>2</sub> ClN <sub>4</sub> O <sub>2</sub>	Farnesyltransferase
JNJ-1661010	365.45	681136-29-8	C <sub>19</sub> H <sub>19</sub> N <sub>5</sub> OS	Fatty acid amide hydrolase
PF-4981517	456.59	1390637-82-7	C <sub>26</sub> H <sub>32</sub> N <sub>8</sub>	Cytochrome P450

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Evacetrapib (LY2484595)	638.65	1186486-62-3	C <sub>31</sub> H <sub>36</sub> F <sub>6</sub> N <sub>6</sub> O <sub>2</sub>	Cholesterol ester transfer protein
(R)-Nepicastat HCl	331.81	195881-94-8	C <sub>14</sub> H <sub>16</sub> ClF <sub>2</sub> N <sub>3</sub> S	Hydroxylase
NLG919	282.38	1402836-58-1	C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O	Indoleamine 2,3-dioxygenase
AGI-5198	462.56	1355326-35-0	C <sub>27</sub> H <sub>31</sub> FN <sub>4</sub> O <sub>2</sub>	Dehydrogenase
PF-04620110	396.44	1109276-89-2	C <sub>21</sub> H <sub>24</sub> N <sub>4</sub> O <sub>4</sub>	Transferase
Deltarasin	603.75	1440898-61-2	C <sub>40</sub> H <sub>37</sub> N <sub>5</sub> O	Phosphodiesterase
Erastin	547.04	571203-78-6	C <sub>30</sub> H <sub>31</sub> ClN <sub>4</sub> O <sub>4</sub>	Ferroptosis
Edoxaban	548.06	1229194-11-9	C <sub>31</sub> H <sub>40</sub> ClN <sub>7</sub> O <sub>8</sub> S <sub>2</sub>	Factor Xa
LB42708	555.46	226929-39-1	C <sub>30</sub> H <sub>27</sub> BrN <sub>4</sub> O <sub>2</sub>	Transferase
Darapladib (SB-480848)	666.77	356057-34-6	C <sub>36</sub> H <sub>38</sub> F <sub>4</sub> N <sub>4</sub> O <sub>2</sub> S	Phospholipase (e.g. PLA)
U73122	464.64	112648-68-7	C <sub>29</sub> H <sub>40</sub> N <sub>2</sub> O <sub>3</sub>	Phospholipase (e.g. PLA)
Apremilast (CC-10004)	460.5	608141-41-9	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>7</sub> S	Phosphodiesterase
Fostamatinib (R788)	580.46	901119-35-5	C <sub>23</sub> H <sub>26</sub> FN <sub>6</sub> O <sub>9</sub> P	Spleen tyrosine kinase
AP26113	529.01	1197958-12-5	C <sub>26</sub> H <sub>34</sub> ClN <sub>6</sub> O <sub>2</sub> P	Anaplastic lymphoma kinase
GDC-0941	513.64	957054-30-7	C <sub>23</sub> H <sub>27</sub> N <sub>7</sub> O <sub>3</sub> S <sub>2</sub>	Phosphoinositide 3-kinase
Tipifarnib	489.4	192185-72-1	C <sub>27</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>4</sub> O	Farnesyltransferase, Ras
<b>Compounds containing primary and/or secondary but without tertiary amino groups</b>				
Cilostazol*	369.46	73963-72-1	C <sub>20</sub> H <sub>27</sub> N <sub>5</sub> O <sub>2</sub>	Phosphodiesterase
Rolipram*	275.34	61413-54-5	C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>	Phosphodiesterase
Topiramate*	339.36	97240-79-4	C <sub>12</sub> H <sub>21</sub> NO <sub>8</sub> S	Carbonic anhydrase
Pralatrexate*	477.47	146464-95-1	C <sub>23</sub> H <sub>23</sub> N <sub>7</sub> O <sub>5</sub>	Dihydrofolate reductase
Pimobendan*	334.37	74150-27-9	C <sub>19</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	Phosphodiesterase
Irsogladine*	256.09	57381-26-7	C <sub>9</sub> H <sub>7</sub> Cl <sub>2</sub> N <sub>5</sub>	Phosphodiesterase
Pyrimethamine*	248.71	58-14-0	C <sub>12</sub> H <sub>13</sub> ClN <sub>4</sub>	Dihydrofolate reductase
Pioglitazone HCl*	392.9	112529-15-4	C <sub>19</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>3</sub> S	Peroxisome proliferator-activated receptor
Roflumilast*	403.21	162401-32-3	C <sub>17</sub> H <sub>14</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	Phosphodiesterase
Milrinone*	211.22	78415-72-2	C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O	ATPase
Brinzolamide*	383.51	138890-62-7	C <sub>12</sub> H <sub>21</sub> N <sub>3</sub> O <sub>5</sub> S <sub>3</sub>	Carbonic anhydrase
Methazolamide*	236.27	554-57-4	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	Carbonic anhydrase
Gimeracil*	145.54	103766-25-2	C <sub>5</sub> H <sub>4</sub> ClNO <sub>2</sub>	Dehydrogenase

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Rasagiline mesylate*	267.34	161735-79-1	C <sub>13</sub> H <sub>17</sub> NO <sub>3</sub> S	Monoamine oxidase
S-(+)-Rolipram*	275.34	85416-73-5	C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>	Phosphodiesterase
Phosphoramidon disodium salt	588.48	164204-38-0	C <sub>23</sub> H <sub>34</sub> N <sub>3</sub> Na <sub>2</sub> O <sub>10</sub> P	Metalloendopeptidase
Safinamide mesylate	398.45	202825-46-5	C <sub>18</sub> H <sub>23</sub> FN <sub>2</sub> O <sub>5</sub> S	Monoamine oxidase
Liproxstatin-1	340.85	950455-15-9	C <sub>19</sub> H <sub>21</sub> ClN <sub>4</sub>	Ferroptosis
Epacadostat (INCB024360)	438.23	1204669-58-8	C <sub>11</sub> H <sub>13</sub> BrFN <sub>7</sub> O <sub>4</sub> S	Indoleamine 2,3-dioxygenase
GSK3787	392.78	188591-46-0	C <sub>15</sub> H <sub>12</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>3</sub> S	Peroxisome proliferator-activated receptor
WY-14643 (Pirixinic acid)	323.8	50892-23-4	C <sub>14</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> S	Peroxisome proliferator-activated receptor
PluriSIn #1 (NSC 14613)	213.24	91396-88-2	C <sub>12</sub> H <sub>11</sub> N <sub>3</sub> O	Dehydrogenase
TAK-700 (Orteronel)	307.35	566939-85-3	C <sub>18</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>	Cytochrome P450
Telotristat etiprate (LX 1606 Hippurate)	754.15	11137608-69-5	C <sub>36</sub> H <sub>35</sub> ClF <sub>3</sub> N <sub>7</sub> O <sub>6</sub>	Hydroxylase
UK 383367	324.38	348622-88-8	C <sub>15</sub> H <sub>24</sub> N <sub>4</sub> O <sub>4</sub>	Procollagen C proteinase
INCB024360	271.64	914471-09-3	C <sub>9</sub> H <sub>7</sub> ClFN <sub>5</sub> O <sub>2</sub>	Indoleamine 2,3-dioxygenase
URB597	338.4	546141-08-6	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	Fatty acid amide hydrolase
A922500	428.48	959122-11-3	C <sub>26</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>	Diacylglycerol Acyltransferase 1
Dalcetrapib (JTT-705, RO4607381)	389.59	211513-37-0	C <sub>23</sub> H <sub>35</sub> NO <sub>2</sub> S	Cholesterol ester transfer protein
AGI-6780	481.51	1432660-47-3	C <sub>21</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> S <sub>2</sub>	Dehydrogenase
Ferrostatin-1 (Fer-1)	262.35	347174-05-4	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>	Ferroptosis
Vidofludimus	355.36	717824-30-1	C <sub>20</sub> H <sub>18</sub> FNO <sub>4</sub>	Dehydrogenase
FTI 277 HCl	484.07	180977-34-8	C <sub>22</sub> H <sub>30</sub> ClN <sub>3</sub> O <sub>3</sub> S <sub>2</sub>	Transferase
D4476	398.41	301836-43-1	C <sub>23</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>	Casein kinase 1
U-104	309.32	178606-66-1	C <sub>13</sub> H <sub>12</sub> FN <sub>3</sub> O <sub>3</sub> S	Carbonic anhydrase
<b>Compounds with no amino group</b>				
Voriconazole*	349.31	137234-62-9	C <sub>16</sub> H <sub>14</sub> F <sub>3</sub> N <sub>5</sub> O	Cytochrome P450
Isotretinoin*	300.44	4759-48-2	C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>	Hydroxylase
Trilostane*	329.43	13647-35-3	C <sub>20</sub> H <sub>27</sub> NO <sub>3</sub>	Dehydrogenase
Lovastatin*	404.54	75330-75-5	C <sub>24</sub> H <sub>36</sub> O <sub>5</sub>	HMG-CoA reductase

Product name	Molecular weight	CAS number	Formula	Target
Tioxolone*	168.17	4991-65-5	C <sub>7</sub> H <sub>4</sub> O <sub>3</sub> S	Carbonic anhydrase
Pravastatin sodium*	446.51	81131-70-6	C <sub>23</sub> H <sub>35</sub> NaO <sub>7</sub>	HMG-CoA reductase
Tolcapone*	273.24	134308-13-7	C <sub>14</sub> H <sub>11</sub> NO <sub>5</sub>	Transferase
Avasimibe	501.72	166518-60-1	C <sub>29</sub> H <sub>43</sub> NO <sub>4</sub> S	Cytochrome P450
PF-2545920	392.45	1292799-56-4	C <sub>25</sub> H <sub>20</sub> N <sub>4</sub> O	Phosphodiesterase
GW0742	471.49	317318-84-6	C <sub>21</sub> H <sub>17</sub> F <sub>4</sub> NO <sub>3</sub> S <sub>2</sub>	Peroxisome proliferator-activated receptor
Cilomilast	343.42	153259-65-5	C <sub>20</sub> H <sub>25</sub> NO <sub>4</sub>	Phosphodiesterase
Apigenin	270.24	520-36-5	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	Cytochrome P450
Baicalein	270.24	491-67-8	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	Cytochrome P450
Icariin	676.66	489-32-7	C <sub>33</sub> H <sub>40</sub> O <sub>15</sub>	Phosphodiesterase
Luteolin	286.24	491-70-3	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>	Phosphodiesterase
Naringenin	272.25	480-41-1	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	Cytochrome P450
Alizarin	240.21	72-48-0	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>	Cytochrome P450
CPI-613	388.59	95809-78-2	C <sub>22</sub> H <sub>28</sub> O <sub>2</sub> S <sub>2</sub>	Dehydrogenase
Xanthohumol	354.4	6754-58-1	C <sub>21</sub> H <sub>22</sub> O <sub>5</sub>	Cyclooxygenase

\*FDA approved drugs