Supplement

Virtual Screening and Biochemical Testing of Borocycles as Immunoproteasome Inhibitors

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Table S1 Smiles of 5-membered borocycles subjected to covalent virtual screening

<table>
<thead>
<tr>
<th>Smiles</th>
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</thead>
<tbody>
<tr>
<td>OB1OCc2ccccc12</td>
</tr>
<tr>
<td>OB1OCc2ncnc12</td>
</tr>
<tr>
<td>OB1OCc2nnc12</td>
</tr>
<tr>
<td>Cc1cc2COB(O)c2c1</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2c1</td>
</tr>
<tr>
<td>Cc1cc2c1cc2COB(O)c12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2ccc12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2cc(F)cc12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2c1ccc(F)c12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2cc(cc12)C#N</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2cc(cc12)C#N</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2cccc(C=O)c12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2ccc(C=O)c12</td>
</tr>
<tr>
<td>CC1(C)=OB(O)c2ccccc12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2c1cccc2F</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2c1cccc2F</td>
</tr>
<tr>
<td>[2H]C1([2H])OB(O)c2ccccc12</td>
</tr>
<tr>
<td>OBIOCc2ccccc12</td>
</tr>
<tr>
<td>OBIOCc2nncnc12</td>
</tr>
<tr>
<td>OBIOCc2nnc12</td>
</tr>
<tr>
<td>Cc1cc2COB(O)c2c1</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2c1</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2ccc(O)cc12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2cc(O)ccc12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2ccccc12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2ccccc12</td>
</tr>
<tr>
<td>Cc1cc2B(O)OCc2ccccc12</td>
</tr>
</tbody>
</table>

(*) indicates the presence of deuterium.
<table>
<thead>
<tr>
<th>Smiles of 6-membered borocycles subjected to covalent virtual screening</th>
</tr>
</thead>
<tbody>
<tr>
<td>NC1CCCOB1O</td>
</tr>
<tr>
<td>OB1OCC2eecces12</td>
</tr>
<tr>
<td>CLNC1CCCOB1O</td>
</tr>
<tr>
<td>Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>OB1OCC2eece(F)ece12</td>
</tr>
<tr>
<td>CCICOB(O)e2ec(N)cc12</td>
</tr>
<tr>
<td>CCl(C)C2eece(N)cc2B(O)O1</td>
</tr>
<tr>
<td>OB1OCC2eeceC(O)=Oe12</td>
</tr>
<tr>
<td>OB1OCC2eecece12</td>
</tr>
<tr>
<td>OB1OCC2eecee12[N+][O-]=O</td>
</tr>
<tr>
<td>OC1(O)=O1eecc2CCOB(O)e12</td>
</tr>
<tr>
<td>OB1O[C=H][CC(O)=O]NC[=O]C1eecces1</td>
</tr>
<tr>
<td>OB1OCC(C(O)=O)CC1INC(=O)C1eecces1</td>
</tr>
<tr>
<td>OB1Oc2eecc2-e2eecces1</td>
</tr>
<tr>
<td>CCC(=O)C(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>CC=CC(O)C(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>CCC(=O)C(=O)Ne1ee2CC(O)))OB(O)e2c1</td>
</tr>
<tr>
<td>CC1CC(C)=CC1CC(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>CNI[CC]<a href="C">=O</a>C1e1ccCN(Cc1ccnc1CCC(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>OB1OCCe2eeceNC(=O)C3CCC03cc12</td>
</tr>
<tr>
<td>CC([=O]H)NC1cc(nn1)C(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>Cn1eecc(nn1)C(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>CCCC=CC(O)=ONe1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>CC=CC(O)=ONe1ee2CC(C)(C)OB(O)e2c1</td>
</tr>
<tr>
<td>CC(C)(C)NCCC(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>CO1(O)=OCC(O)=ONe1ee2CC(C)(C)OB(O)e2c1</td>
</tr>
<tr>
<td>CCL4HNe1C(=O)Ne1ee2CC(C)(C)OB(O)e2c1</td>
</tr>
<tr>
<td>Cn1eecc1CC(C)=ONe1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>OB1OCCe2eeccNC(=O)C34CC(C)CCC4cc12</td>
</tr>
<tr>
<td>OCl1eeccen1C(=O)Ne1ee2CCCOB(O)e2c1</td>
</tr>
<tr>
<td>CNI[CC]<a href="H">=O</a>C1e1ccNe1ee2CC(C)(C)OB(O)e2c1</td>
</tr>
<tr>
<td>CC1(C)Ce2eeccNC(=O)C3CCC03cc2B(O)O1</td>
</tr>
</tbody>
</table>