Supporting Information

Convenient Synthesis of Benzoxazolone Derivatives by Cross-Coupling of Benzoxazolone Boronates with Aryl Halides

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Table S1  TSPO binding activity and metabolic stability of benzoxazolone derivatives

<table>
<thead>
<tr>
<th>Compd</th>
<th>Ar</th>
<th>R</th>
<th>TPSO Inhibitiona (%)</th>
<th>Metabolic stability (remaining%)</th>
<th>(mL/min/mg)c</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-Py</td>
<td>Ph</td>
<td>79 (Ki = 23 nM)</td>
<td>24</td>
<td>0.125</td>
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<tr>
<td>8a</td>
<td>o-(HOCH2CH2O)-Ph</td>
<td>86</td>
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<td>0</td>
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<tr>
<td>8b</td>
<td>m-(HOCH2CH2O)-Ph</td>
<td>96</td>
<td></td>
<td>5</td>
<td>N.T.</td>
</tr>
<tr>
<td>8c</td>
<td>p-(HOCH2CH2O)-Ph</td>
<td>97</td>
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<td>4</td>
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<tr>
<td>8d</td>
<td>o-(Me2CH2)-Ph</td>
<td>35</td>
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<tr>
<td>8e</td>
<td>m-(Me2CH2)-Ph</td>
<td>63</td>
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<td>8f</td>
<td>p-(Me2CH2)-Ph</td>
<td>47</td>
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<td>2-Py</td>
<td>93</td>
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<tr>
<td>8h</td>
<td>Ph</td>
<td>87</td>
<td></td>
<td>0</td>
<td>N.T.</td>
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<tr>
<td>8i</td>
<td>Ph</td>
<td>97</td>
<td></td>
<td>0</td>
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<tr>
<td>8j</td>
<td>Ph</td>
<td>83d</td>
<td></td>
<td>34</td>
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<tr>
<td>8k</td>
<td>Ph</td>
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<td></td>
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<tr>
<td>8l</td>
<td>p-CF3Ph</td>
<td>91d</td>
<td></td>
<td>N.T.</td>
<td>0.483</td>
</tr>
</tbody>
</table>

aPercent inhibition of [3H]-PK11195 specific binding at 100 nM of the compound.

bMetabolic stability data refer to percent of compound remaining after incubation with rat liver S-9 fraction and NADPH for 30 min. The initial concentration of each compound was 1.0 μM.

cMetabolic stability data refer to clearance in rat liver microsomes fraction and NADPH. The initial concentration of each compound was 1.0 μM.

dExaminations were conducted at 30 nM of the compound.

fNot tested.

fThe anxiolytic effect in rat model of this compound was reported in reference 2b.
Compound 5

**1H NMR Spectra:***
- DFile: B05_CVB-4939_TG-241NON_E11_2.als
- Date: Sat Mar 17 13:37:12 2012
- NUC: 1H
- Frequency: 399.65 MHz
- Set Frequency: 124.00 KHz
- Final Frequency: 10500.00 Hz
- Points: 32768
- Frequency: 7992.01 Hz
- Scans: 32
- Acquisition Time: 4.1001 sec
- Pulse: 2.9000 sec
- Pulse Width: 6.00 usec
- Temperature: 21.9°C
- Solvent: DMSO
- Reference: 0.00 ppm
- Gain: 15

**13C NMR Spectra:***
- DFile: B05_CVB-4939_TG-242BCM_E11_2.als
- Date: Sat Mar 17 14:27:33 2012
- NUC: 13C
- Frequency: 100.40 MHz
- Set Frequency: 125.00 KHz
- Final Frequency: 10500.00 Hz
- Points: 32768
- Frequency: 27118.64 Hz
- Scans: 1000
- Acquisition Time: 1.2083 sec
- Pulse: 2.7920 sec
- Pulse Width: 5.50 usec
- Temperature: 21.4°C
- Solvent: DMSO
- Reference: 39.50 ppm
- Gain: 21

**Chemical Structures:**
- Compound 5
- Br
- O
- N
- O
- OH

**Data Analysis:**
- PPM values are listed below the spectra.

**Notes:**
- Data includes compound structure and experimental conditions for both 1H and 13C NMR analyses.