Studies towards the synthesis of Epothilone A via organoboranes

P. Veeraraghavan Ramachandran, J. Subash Chandra, Bodhuri Prabhudas, Debarshi Pratihar, and M. Venkat Ram Reddy

Herbert C. Brown Center for Borane Research, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084.

Supporting Information
Table of Contents

<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 1: 300 MHz $^1$H NMR Spectrum of Compound <strong>2</strong> in CDCl$_3$</td>
<td>4</td>
</tr>
<tr>
<td>Figure 2: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>2</strong> in CDCl$_3$</td>
<td>4</td>
</tr>
<tr>
<td>Figure 3: 300 MHz $^1$H NMR Spectrum of Compound <strong>31</strong> in CDCl$_3$</td>
<td>5</td>
</tr>
<tr>
<td>Figure 4: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>31</strong> in CDCl$_3$</td>
<td>5</td>
</tr>
<tr>
<td>Figure 5: 300 MHz $^1$H NMR Spectrum of Compound <strong>OH-31</strong> in CDCl$_3$</td>
<td>6</td>
</tr>
<tr>
<td>Figure 6: 300 MHz $^1$H NMR Spectrum of Compound <strong>25</strong> in CDCl$_3$</td>
<td>7</td>
</tr>
<tr>
<td>Figure 7: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>25</strong> in CDCl$_3$</td>
<td>7</td>
</tr>
<tr>
<td>Figure 8: 300 MHz $^1$H NMR Spectrum of Compound <strong>37</strong> in CDCl$_3$</td>
<td>8</td>
</tr>
<tr>
<td>Figure 9: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>37</strong> in CDCl$_3$</td>
<td>8</td>
</tr>
<tr>
<td>Figure 10: 300 MHz $^1$H NMR Spectrum of Compound <strong>TBS-37</strong> in CDCl$_3$</td>
<td>9</td>
</tr>
<tr>
<td>Figure 11: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>TBS-37</strong> in CDCl$_3$</td>
<td>9</td>
</tr>
<tr>
<td>Figure 12: 300 MHz $^1$H NMR Spectrum of Compound <strong>38</strong> in CDCl$_3$</td>
<td>10</td>
</tr>
<tr>
<td>Figure 13: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>38</strong> in CDCl$_3$</td>
<td>10</td>
</tr>
<tr>
<td>Figure 14: 300 MHz $^1$H NMR Spectrum of Compound <strong>39</strong> in CDCl$_3$</td>
<td>11</td>
</tr>
<tr>
<td>Figure 15: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>39</strong> in CDCl$_3$</td>
<td>11</td>
</tr>
<tr>
<td>Figure 16: 300 MHz $^1$H NMR Spectrum of Compound <strong>40</strong> in CDCl$_3$</td>
<td>12</td>
</tr>
<tr>
<td>Figure 17: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>40</strong> in CDCl$_3$</td>
<td>12</td>
</tr>
<tr>
<td>Figure 18: 300 MHz $^1$H NMR Spectrum of Compound <strong>27</strong> in CDCl$_3$</td>
<td>13</td>
</tr>
<tr>
<td>Figure 19: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>27</strong> in CDCl$_3$</td>
<td>13</td>
</tr>
<tr>
<td>Figure 20: 300 MHz $^1$H NMR Spectrum of Compound <strong>45</strong> in CDCl$_3$</td>
<td>14</td>
</tr>
<tr>
<td>Figure 21: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>45</strong> in CDCl$_3$</td>
<td>14</td>
</tr>
<tr>
<td>Figure 22: 300 MHz $^1$H NMR Spectrum of Compound <strong>OH-45</strong> in CDCl$_3$</td>
<td>15</td>
</tr>
<tr>
<td>Figure 23: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>OH-45</strong> in CDCl$_3$</td>
<td>15</td>
</tr>
<tr>
<td>Figure 24: 300 MHz $^1$H NMR Spectrum of Compound <strong>46</strong> in CDCl$_3$</td>
<td>16</td>
</tr>
<tr>
<td>Figure 25: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>46</strong> in CDCl$_3$</td>
<td>16</td>
</tr>
<tr>
<td>Figure 26: 300 MHz $^1$H NMR Spectrum of Compound <strong>Bn-33</strong> in CDCl$_3$</td>
<td>17</td>
</tr>
<tr>
<td>Figure 27: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>Bn-33</strong> in CDCl$_3$</td>
<td>17</td>
</tr>
<tr>
<td>Figure 28: 300 MHz $^1$H NMR Spectrum of Compound <strong>Bn-OH-33</strong> in CDCl$_3$</td>
<td>18</td>
</tr>
<tr>
<td>Figure 29: 75.5 MHz $^{13}$C NMR Spectrum of Compound <strong>Bn-OH-33</strong> in CDCl$_3$</td>
<td>18</td>
</tr>
</tbody>
</table>
Figure 30: 300 MHz $^1$H NMR Spectrum of Compound 7 in CDCl$_3$  19
Figure 31: 75.5 MHz $^{13}$C NMR Spectrum of Compound 7 in CDCl$_3$  19
Figure 32: 300 MHz $^1$H NMR Spectrum of Compound 48 in CDCl$_3$  20
Figure 33: 75.5 MHz $^{13}$C NMR Spectrum of Compound 48 in CDCl$_3$  20
Figure 34: 300 MHz $^1$H NMR Spectrum of Compound OH-48 in CDCl$_3$  21
Figure 35: 75.5 MHz $^{13}$C NMR Spectrum of Compound OH-48 in CDCl$_3$  21
Figure 36: 300 MHz $^1$H NMR Spectrum of Compound 28 in CDCl$_3$  22
Figure 37: 75.5 MHz $^{13}$C NMR Spectrum of Compound 28 in CDCl$_3$  22
Figure 38: 300 MHz $^1$H NMR Spectrum of Compound 49 in CDCl$_3$  23
Figure 39: 75.5 MHz $^{13}$C NMR Spectrum of Compound 49 in CDCl$_3$  23
Figure 40: 300 MHz $^1$H NMR Spectrum of Compound OH-49 in CDCl$_3$  24
Figure 41: 75.5 MHz $^{13}$C NMR Spectrum of Compound OH-49 in CDCl$_3$  24
Figure 42: 300 MHz $^1$H NMR Spectrum of Compound 51 in CDCl$_3$  25
Figure 43: 75.5 MHz $^{13}$C NMR Spectrum of Compound 51 in CDCl$_3$  25
Figure 44: 300 MHz $^1$H NMR Spectrum of Compound TBS-51 in CDCl$_3$  26
Figure 45: 300 MHz $^1$H NMR Spectrum of Compound 52 in CDCl$_3$  26
Figure 46: 300 MHz $^1$H NMR Spectrum of Compound 53 in CDCl$_3$  27
Figure 47: 300 MHz $^1$H NMR Spectrum of Compound OH-53 in CDCl$_3$  27
Figure 48: 300 MHz $^1$H NMR Spectrum of Compound 6 in CDCl$_3$  28
Figure 49: 75.5 MHz $^{13}$C NMR Spectrum of Compound 6 in CDCl$_3$  28
Figure 50: 300 MHz $^1$H NMR Spectrum of Compound 54 in CDCl$_3$  29
Figure 51: 75.5 MHz $^{13}$C NMR Spectrum of Compound 54 in CDCl$_3$  29
Figure 52: 300 MHz $^1$H NMR Spectrum of Compound OH-54 in CDCl$_3$  30
Figure 53: 75.5 MHz $^{13}$C NMR Spectrum of Compound OH-54 in CDCl$_3$  30
Figure 54: 300 MHz $^1$H NMR Spectrum of Compound 4 in CDCl$_3$  31
Figure 55: 75.5 MHz $^{13}$C NMR Spectrum of Compound 4 in CDCl$_3$  31
Figure 56: 300 MHz $^1$H NMR Spectrum of Compound 55 in CDCl$_3$  32
Figure 57: 75.5 MHz $^{13}$C NMR Spectrum of Compound 55 in CDCl$_3$  32
Figure 58: 300 MHz $^1$H NMR Spectrum of Compound 3 in CDCl$_3$  33
Figure 59: 75.5 MHz $^{13}$C NMR Spectrum of Compound 3 in CDCl$_3$  33
Figure 1: 300 MHz $^1$H NMR Spectrum of Compound 2 in CDCl$_3$

Figure 2: 75.5 MHz $^{13}$C NMR Spectrum of Compound 2 in CDCl$_3$
Figure 3: 300 MHz $^1$H NMR Spectrum of Compound 31 in CDCl$_3$

Figure 4: 75.5 MHz $^{13}$C NMR Spectrum of Compound 31 in CDCl$_3$
Figure 5: 300 MHz $^1$H NMR Spectrum of Compound **OH-31** in CDCl$_3$
Figure 6: 300 MHz $^1$H NMR Spectrum of Compound 25 in CDCl$_3$

Figure 7: 75.5 MHz $^{13}$C NMR Spectrum of Compound 25 in CDCl$_3$
Figure 8: 300 MHz $^1$H NMR Spectrum of Compound 37 in CDCl$_3$

Figure 9: 75.5 MHz $^{13}$C NMR Spectrum of Compound 37 in CDCl$_3$
Figure 10: 300 MHz $^1$H NMR Spectrum of Compound TBS-37 in CDCl$_3$

Figure 11: 75.5 MHz $^{13}$C NMR Spectrum of Compound TBS-37 in CDCl$_3$
Figure 12: 300 MHz $^1$H NMR Spectrum of Compound 38 in CDCl$_3$

Figure 13: 75.5 MHz $^{13}$C NMR Spectrum of Compound 38 in CDCl$_3$
Figure 14: 300 MHz $^1$H NMR Spectrum of Compound 39 in CDCl$_3$

Figure 15: 75.5 MHz $^{13}$C NMR Spectrum of Compound 39 in CDCl$_3$
Figure 16: 300 MHz $^1$H NMR Spectrum of Compound 40 in CDCl$_3$

Figure 17: 75.5 MHz $^{13}$C NMR Spectrum of Compound 40 in CDCl$_3$
Figure 18: 300 MHz $^1$H NMR Spectrum of Compound 27 in CDCl$_3$

Figure 19: 75.5 MHz $^{13}$C NMR Spectrum of Compound 27 in CDCl$_3$
Figure 20: 300 MHz $^1$H NMR Spectrum of Compound 45 in CDCl$_3$

Figure 21: 75.5 MHz $^{13}$C NMR Spectrum of Compound 45 in CDCl$_3$
Figure 22: 300 MHz $^1$H NMR Spectrum of Compound OH-45 in CDCl$_3$

Figure 23: 75.5 MHz $^{13}$C NMR Spectrum of Compound OH-45 in CDCl$_3$
Figure 24: 300 MHz $^1$H NMR Spectrum of Compound 46 in CDCl$_3$

Figure 25: 75.5 MHz $^{13}$C NMR Spectrum of Compound 46 in CDCl$_3$
Figure 26: 300 MHz $^1$H NMR Spectrum of Compound Bn-33 in CDCl$_3$

Figure 27: 75.5 MHz $^{13}$C NMR Spectrum of Compound Bn-33 in CDCl$_3$
Figure 28: 300 MHz $^1$H NMR Spectrum of Compound Bn-OH-33 in CDCl$_3$

Figure 29: 75.5 MHz $^{13}$C NMR Spectrum of Compound Bn-OH-33 in CDCl$_3$
Figure 30: 300 MHz $^1$H NMR Spectrum of Compound 7 in CDCl$_3$

Figure 31: 75.5 MHz $^{13}$C NMR Spectrum of Compound 7 in CDCl$_3$
Figure 32: 300 MHz $^1$H NMR Spectrum of Compound $48$ in CDCl$_3$

Figure 33: 75.5 MHz $^{13}$C NMR Spectrum of Compound $48$ in CDCl$_3$
Figure 34: 300 MHz $^1$H NMR Spectrum of Compound OH-48 in CDCl$_3$

Figure 35: 75.5 MHz $^{13}$C NMR Spectrum of Compound OH-48 in CDCl$_3$
Figure 36: 300 MHz $^1$H NMR Spectrum of Compound 28 in CDCl$_3$

Figure 37: 75.5 MHz $^{13}$C NMR Spectrum of Compound 28 in CDCl$_3$
Figure 38: 300 MHz $^1$H NMR Spectrum of Compound 49 in CDCl$_3$

Figure 39: 75.5 MHz $^{13}$C NMR Spectrum of Compound 49 in CDCl$_3$
Figure 40: 300 MHz $^1$H NMR Spectrum of Compound **OH-49** in CDCl$_3$

Figure 41: 75.5 MHz $^{13}$C NMR Spectrum of Compound **OH-49** in CDCl$_3$
Figure 42: 300 MHz $^1$H NMR Spectrum of Compound 51 in CDCl$_3$

Figure 43: 75.5 MHz $^{13}$C NMR Spectrum of Compound 51 in CDCl$_3$
Figure 44: 300 MHz $^1$H NMR Spectrum of Compound TBS-51 in CDCl$_3$

Figure 45: 300 MHz $^1$H NMR Spectrum of Compound 52 in CDCl$_3$
Figure 46: 300 MHz $^1$H NMR Spectrum of Compound 53 in CDCl$_3$

Figure 47: 300 MHz $^1$H NMR Spectrum of Compound OH-53 in CDCl$_3$
Figure 48: 300 MHz $^1$H NMR Spectrum of Compound 6 in CDCl$_3$

Figure 49: 75.5 MHz $^{13}$C NMR Spectrum of Compound 6 in CDCl$_3$
Figure 50: 300 MHz $^1$H NMR Spectrum of Compound 54 in CDCl$_3$

Figure 51: 75.5 MHz $^{13}$C NMR Spectrum of Compound 54 in CDCl$_3$
Figure 52: 300 MHz $^1$H NMR Spectrum of Compound OH-54 in CDCl$_3$

Figure 53: 75.5 MHz $^{13}$C NMR Spectrum of Compound OH-54 in CDCl$_3$
Figure 54: 300 MHz $^1$H NMR Spectrum of Compound 4 in CDCl$_3$

Figure 55: 75.5 MHz $^{13}$C NMR Spectrum of Compound 4 in CDCl$_3$
Figure 56: 300 MHz $^1$H NMR Spectrum of Compound 55 in CDCl$_3$

Figure 57: 75.5 MHz $^{13}$C NMR Spectrum of Compound 55 in CDCl$_3$
Figure 58: 300 MHz $^1$H NMR Spectrum of Compound 3 in CDCl$_3$

Figure 59: 75.5 MHz $^{13}$C NMR Spectrum of Compound 3 in CDCl$_3$