Construction of benzothiophene fused pyrrolidone in water via
catalyst-free process and mechanism study

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1. General information and materials

All reactions were performed under Ar atmospheres in oven-dried glassware with magnetic stirring. Unless otherwise stated, all reagents were purchased from commercial suppliers (Aldrich, TCI or Alfa Aesar) and used without further purification. All solvents were purified and dried according to standard methods prior to use. TLC monitored all reactions with silica gel-coated plates. Flash column chromatography was performed using 200-300 mesh silica gel. \(^1\)H- and \(^{13}\)C NMR spectra were recorded at ambient temperature on Bruker 400 instruments. All spectra were referenced to CDCl\(_3\) (\(^1\)H \(\delta\) 7.26 ppm and \(^{13}\)C NMR \(\delta\) 77.00 ppm). \(^{19}\)F NMR spectrum was recorded on Bruker 400 (376 MHz) spectrometers with CFCl\(_3\) as external standard. HRMS were obtained on Waters Xevo Q-TOF MS with ESI resource. Melting points were measured on a RY-I apparatus and are reported uncorrected. IR were measured on a Perkin-Elmer 983G apparatus. Compound 1 was synthesized according to the reported method\(^{[1]}\) [2].

2. The structure of thioisatin 1 substituted amine 3

\[
\begin{align*}
1a & \quad 1b & \quad 1c & \quad 1d & \quad 1e \\
\quad & \quad & \quad & \quad & \\
1f & \quad 1g & \quad 1h & \quad 1i & \quad 1j
\end{align*}
\]

Substituted amine 3

\[
\begin{align*}
3a & \quad 3b & \quad 3c & \quad 3d & \quad 3e \\
3f & \quad & \quad & \quad & \\
3g & \quad 3h & \quad 3i & \quad 3j & \quad 3k \\
3l & \quad & \quad & \quad & \\
3m & \quad 3n & \quad 3o & \quad 3p & \quad 3q \\
3r & \quad & \quad & \quad & \\
3s & \quad 3t & \quad 3u & \quad 3v & \\
& \quad & \quad & \quad & 
\end{align*}
\]

3. Synthetic procedure of 1g
To a NaOH (10%) (15 mL) solution of S-I (1.56 g, 8.12 mmol) was added \(N,N\)-dimethyl-4-nitrosoaniline (1.00 g, 6.66 mmol) in 5% aqueous hydrochloric acid (6 mL) at 60 °C. The reaction mixture was stirred at 60 °C for 1 h. After the reaction complete, the resulting purple black S-II was filtered off and washed successively with cold water, dilute hydrochloric acid, and water. It was used in the next stage without further purification.

S-II (obtained in the above step) was added to a HCl (15%) (40 mL). The resulting mixture was refluxed for 4 h. After cooling to room temperature, the mixture was filtered off. The resulting solid was added to \(Na_2CO_3\) (50%) (50 mL) solution. The mixture was refluxed for 0.5 h. The solution was filtered off, acidified with HCl. The resulting precipitate was filtered off, washed with water. The desired product was obtained as yellow solid (40 mg, 2%).

### 4. Table S1 Results of screening the reaction time

<table>
<thead>
<tr>
<th>Entry</th>
<th>Solvent</th>
<th>t/°C</th>
<th>Time/h</th>
<th>Yield 4a/%</th>
<th>Yield 5a/%</th>
</tr>
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<tr>
<td>1</td>
<td>H2O</td>
<td>80</td>
<td>8</td>
<td>55</td>
<td>28</td>
</tr>
<tr>
<td>2</td>
<td>H2O</td>
<td>80</td>
<td>12</td>
<td>60</td>
<td>24</td>
</tr>
<tr>
<td>3</td>
<td>H2O</td>
<td>80</td>
<td>16</td>
<td>55</td>
<td>24</td>
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<tr>
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<td>H2O</td>
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<td>8</td>
<td>76</td>
<td>0</td>
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<tr>
<td>5</td>
<td>H2O</td>
<td>100</td>
<td>12</td>
<td>80</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>H2O</td>
<td>100</td>
<td>16</td>
<td>72</td>
<td>0</td>
</tr>
</tbody>
</table>

### 5. General procedure for the synthesis of 4 and 6

**4a as an example**

Under Ar atmosphere, 1a (53.46 mg, 0.30 mmol) and 2a (123.44 mg, 0.75 mmol) were dissolved in H2O 2 mL. To the above reaction mixture, 3a (96.44 mg, 0.90 mmol) was added. The resulting reaction mixture was stirred at 120 °C for 4 h. After the reaction complete (monitored by TLC), the reaction mixture was extracted with ethyl acetate (2 × 10 mL). The combined organic layers were dried over anhydrous MgSO4 and evaporated under vacuum. The reside was purified by column chromatography (ethyl acetate: petroleum ether = 1:3) to give 4a (103 mg, 89%) as white solid.

**6d as an example**

Under Ar atmosphere, to a H2O (2 mL) solution of 1a (53.46 mg, 0.30 mmol) and 2a (123.44 mg, 0.75 mmol) was added 3p (65.83 mg, 0.90 mmol). The resulting reaction mixture was stirred at 120 °C for 5 h. After the reaction complete (monitored by TLC), the reaction mixture was extracted with ethylacetate (2 × 10 mL). The combined organic layers were dried over anhydrous MgSO4 and evaporated under vacuum. The reside was purified by column chromatography (ethyl acetate: petroleum ether = 1:3) to give 6d (50 mg, 58%) as white solid.

### 6. Synthetic procedure for 5a, 7 and 8

Under Ar atmosphere, to a H2O (2 mL) solution of 1a (53.46 mg, 0.30 mmol) and 2a (123.44 mg, 0.75 mmol) was added 3a (96.44 mg, 0.90 mmol). The resulting reaction mixture was stirred at 120 °C for 20 min. After the reaction complete (monitored by TLC), the reaction mixture was extracted with ethyl acetate (2 × 10 mL). The combined organic layers were dried over anhydrous MgSO4 and evaporated under vacuum. The reside was purified by column chromatography (ethyl acetate: petroleum ether = 1:3) to give 5a (63 mg, 50%) as white solid.

Under Ar atmosphere, 4a (79.09 mg, 0.20 mmol) and PTSA-H2O (57.06 mg, 0.30 mmol) were dissolved in toluene 2 mL. The resulting reaction mixture was stirred at 110 °C for 27 min. After the
reaction complete (monitored by TLC), the reaction mixture was extracted with ethyl acetate (2 × 10 mL). The combined organic layers were dried over anhydrous Mg\(_2\)SO\(_4\) and evaporated under vacuum. The residue was purified by column chromatography (ethyl acetate: petroleum ether = 1:5) to give 7 (53 mg, 50%) as yellow solid.

Under Ar atmosphere, 4a (79.09 mg, 0.20 mmol) and \(m\)-CPBA (75.93 mg 0.44 mmol) were dissolved in CH\(_2\)Cl\(_2\) 2 mL. The resulting reaction mixture was stirred for 17 min at room temperature. After the reaction complete (monitored by TLC), the reaction mixture was extracted with ethyl acetate (2 × 10 mL). The combined organic layers were dried over anhydrous Mg\(_2\)SO\(_4\) and evaporated under vacuum. The residue was purified by column chromatography (ethyl acetate: petroleum ether = 1:5) to give 8 (62 mg, 73%) as white solid.

7. Characterization of all new compounds

5-acetylbenzo[b]thiophene-2,3-dione (1g)
Yellow solid: 40 mg (yield 2%); mp 103-105 °C; IR (KBr) 1735, 1713, 1669 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.35 (d, \(J = 1.6\) Hz, 1H), 8.30 (dd, \(J = 8.4, 2.0\) Hz, 1H), 7.57 (d, \(J = 8.2\) Hz, 1H), 2.65 (s, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 195.5, 184.6, 181.3, 147.4, 137.3, 136.4, 127.9, 126.2, 124.4, 26.6 ppm. HRMS (ESI-TOF) \(m/z\) [M + Na]\(^+\) calcd for C\(_{10}\)H\(_6\)O\(_3\)SNa 228.9930, found 228.9932.

Ethyl (E)-2-(2-benzyl-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4a)
White solid: 103 mg (yield 89%); mp 183-185 °C; IR (KBr) 3364, 2962, 1745, 1680, 1611, 1030, 956, 811, 734 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.50 (s, 1H), 7.26 – 7.35 (m, 3H), 7.08 – 7.19 (m, 3H), 6.99 (d, \(J = 8.0\) Hz, 1H), 5.45 (d, \(J = 1.6\) Hz, 1H), 5.25 (d, \(J = 1.2\) Hz, 1H), 4.67 – 4.83 (q, \(J = 14.8\) Hz 2H), 3.99 – 4.16 (m, 2H), 2.33 (s, 3H), 1.23 (t, \(J = 7.0\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 173.5, 166.7, 157.3, 137.8, 136.2, 135.2, 133.7, 132.2, 132.0, 126.9, 126.3, 121.1, 95.5, 85.3, 76.7, 60.5, 54.7, 44.9, 21.0, 14.2 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{22}\)H\(_{22}\)NO\(_4\)S 396.1264, found 396.1268.

Ethyl (E)-2-(8b-hydroxy-7-methyl-2-(4-methylbenzyl)-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4b)
White solid: 80 mg (yield 65%); mp 180-182 °C; IR (KBr) 3413, 2953, 1748, 1680, 1622, 1155, 829, 813, 662 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.50 (s, 1H), 7.08 – 7.16 (m, 3H), 7.03 (d, \(J = 8.0\) Hz, 2H), 6.98 (d, \(J = 8.0\) Hz, 1H), 5.46 (d, \(J = 1.6\) Hz, 1H), 5.25 (d, \(J = 1.2\) Hz, 1H), 4.71 (q, \(J = 14.3\) Hz 2H), 3.99 – 4.16 (m, 2H), 2.33 (s, 3H), 2.33 (s, 3H), 1.23 (t, \(J = 7.0\) Hz, 3H) ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{22}\)H\(_{22}\)NO\(_4\)S 396.1264, found 396.1268.
3.98 – 4.14 (m, 2H), 3.80 (s, 1H), 2.33 (s, 3H), 2.30 (s, 3H), 1.23 (t, \(J = 7.2\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 173.6, 166.9, 157.6, 137.69, 137.66, 136.3, 135.1, 132.1, 130.7, 129.6, 126.9, 126.4, 121.1, 95.3, 85.3, 60.5, 54.7, 44.7, 21.1, 21.0, 14.2 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{23}\)H\(_{24}\)NO\(_4\)S 410.1421, found 410.1423.

![Chemical Structure of Ethyl (E)-2-(8b-hydroxy-2-(4-methoxybenzyl)-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4c)](image)

**Ethyl (E)-2-(8b-hydroxy-2-(4-methoxybenzyl)-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4c)**

White solid: 70 mg (yield 55%); mp 155-157 °C; IR (KBr) 3392, 2958, 1754, 1679, 1620, 1075, 814, 769, 664 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.50 (s, 1H), 7.12 (d, \(J = 8.0\) Hz, 1H), 7.08 (d, \(J = 8.8\) Hz, 2H), 6.97 (d, \(J = 8.0\) Hz, 1H), 6.81 (d, \(J = 8.4\) Hz, 2H), 5.43 (d, \(J = 1.2\) Hz, 1H), 5.27 (d, \(J = 1.2\) Hz, 1H), 4.67 (q, \(J = 14.9\) Hz, 2H), 3.99 – 4.15 (m, 2H), 3.87 – 3.96 (m, 1H), 3.76 (s, 2H), 2.33 (s, 3H), 1.23 (t, \(J = 7.0\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 173.6, 166.8, 159.2, 157.5, 137.7, 136.3, 135.1, 132.1, 128.4, 126.3, 125.8, 121.1, 114.3, 95.3, 85.3, 60.5, 55.3, 54.7, 44.4, 21.0, 14.2 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{23}\)H\(_{24}\)NO\(_5\)S 426.1370, found 426.1370.

![Chemical Structure of Ethyl (E)-2-(2-(4-fluorobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4d)](image)

**Ethyl (E)-2-(2-(4-fluorobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4d)**

White solid: 96 mg (yield 77%); mp 181-183 °C; IR (KBr) 3404, 2985, 1746, 1667, 1619, 1381, 839, 811, 664 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.49 (s, 1H), 7.08 – 7.17 (m, 3H), 6.92 – 7.03 (m, 3H), 5.46 (d, \(J = 1.6\) Hz, 1H), 5.22 (d, \(J = 1.2\) Hz, 1H), 4.70 (q, \(J = 11.5\) Hz, 2H), 3.98 – 4.15 (m, 3H), 3.88 (s, 1H), 2.33 (s, 3H), 1.23 (t, \(J = 7.2\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 171.22, 164.42, 160.07 (d, \(J = 245.2\)Hz), 155.0, 135.4, 129.9, 127.23, 127.19, 126.5, 126.4, 124.1, 118.9, 113.7 (d, \(J = 21.6\)Hz), 113.8, 113.6, 93.1, 83.1, 58.3, 52.4, 41.9, 18.7 ppm. \(^{19}\)F NMR (376 MHz, CDCl\(_3\)) \(\delta\) -113.88 – -113.97 (m) ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{22}\)H\(_{21}\)FNO\(_4\)S 414.1170, found 414.1172.

![Chemical Structure of Ethyl (E)-2-(2-(4-chlorobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4e)](image)

**Ethyl (E)-2-(2-(4-chlorobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3\(H\)-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4e)**

White solid: 106 mg (yield 82%); mp 180-182 °C; IR (KBr) 3387, 2982, 1749, 1680, 1625, 1091, 953, 832, 655 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.49 (s, 1H), 7.27 (s, 1H), 7.25 (s, 1H), 7.10 – 7.16 (m, 2H), 7.07 (d, \(J = 8.4\) Hz, 2H), 6.97 (d, \(J = 8.0\) Hz, 1H), 5.47 (d, \(J = 1.2\) Hz, 1H), 5.18 (d, \(J = 1.2\) Hz, 1H), 4.70 (s, 2H), 3.94 – 4.12 (m, 3H), 2.32 (s, 3H), 1.22 (t, \(J = 7.0\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100
SNOCOEt
HO
Br

Ethyl (E)-2-(2-(4-bromobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4f)

White solid: 91 mg (yield 64%); mp 181-183 °C; IR (KBr) 3392, 2980, 1749, 1680, 1623, 1071, 831, 806, 666 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.49 (s, 1H), 7.36 – 7.44 (m, 2H), 7.09 – 7.15 (m, 1H), 7.01 (d, J = 7.6 Hz, 2H), 6.97 (d, J = 8.0 Hz, 1H), 5.48 (d, J = 1.6 Hz, 1H), 5.18 (d, J = 1.6 Hz, 1H), 4.68 (s, 2H), 4.11 (s, 1H), 3.93 – 4.10 (m, 2H), 2.32 (s, 2H), 1.22 (t, J = 7.2 Hz, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.5, 166.7, 157.3, 137.6, 136.1, 135.2, 132.8, 132.2, 132.1, 128.6, 126.4, 122.0, 121.1, 95.4, 85.3, 60.6, 54.7, 44.2, 21.0, 14.2. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₂H₂₁BrNO₄S 430.0874, found 430.0879.

Ethyl (E)-2-(2-(4-cyanobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4g)

White solid: 56 mg (yield 44%); mp 190-192 °C; IR (KBr) 3341, 2980, 1752, 1677, 1621, 1091, 945, 827, 817 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.59 (d, J = 8.0 Hz, 2H), 7.48 (s, 1H), 7.23 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.0 Hz, 1H), 6.98 (d, J = 8.0 Hz, 1H), 5.50 (d, J = 1.2 Hz, 1H), 5.12 (d, J = 1.2 Hz, 1H), 4.77 (q, J = 14.9 Hz, 2H), 3.94 – 4.14 (m, 3H), 2.32 (s, 3H), 1.22 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.4, 166.5, 157.1, 139.0, 137.5, 135.9, 135.3, 132.9, 132.3, 127.4, 126.4, 121.2, 118.3, 112.0, 95.5, 85.4, 60.7, 54.6, 44.3, 21.0, 14.1 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₃H₂₁N₂O₄S 421.1217, found 421.1223.

Methyl (E)-4-((3-(2-ethoxy-2-oxoethylidene)-8b-hydroxy-7-methyl-1-oxo-1,3,3a,8b-tetrahydro-2H-benzo[4,5]thieno[2,3-c]pyrrol-2-yl)methyl)benzoate (4h)

White solid: 52 mg (yield 38%); mp 130-132 °C; IR (KBr) 3432, 1719, 1701, 1628, 1149, 949, 816, 752 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.95 (d, J = 8.0 Hz, 2H), 7.49 (s, 1H), 7.18 (d, J = 8.0 Hz, 2H), 7.13 (dd, J = 8.0, 0.8 Hz, 1H), 6.98 (d, J = 8.0 Hz, 1H), 5.47 (d, J = 1.2 Hz, 1H), 5.16 (d, J = 1.2 Hz, 1H), 4.79 (q, J = 12.0 Hz, 2H), 3.98 – 4.14 (m, 3H), 3.88 (s, 3H), 2.32 (s, 3H), 1.22 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.5, 166.61, 166.59, 157.3, 138.8, 137.6, 136.1, 135.2, 132.2, 130.3, 129.8, 126.7, 126.4, 121.2, 95.5, 85.4, 60.6, 54.6, 52.2, 44.5, 21.0, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₃H₂₁N₂O₄S 421.1217, found 421.1223.
Ethyl (E)-2-(8b-hydroxy-2-(3-methoxybenzyl)-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4i)

White solid: 85 mg (yield 67%); mp 188-189 °C; IR (KBr) 3403, 2952, 1750, 1677, 1616, 1034, 958, 794, 663 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.50 (s, 1H), 7.20 (t, \(J = 7.8\) Hz, 1H), 7.12 (d, \(J = 8.0\) Hz, 1H), 6.98 (d, \(J = 8.0\) Hz, 1H), 6.78 (dd, \(J = 8.2, 2.2\) Hz, 1H), 6.73 (d, \(J = 7.6\) Hz, 1H), 6.56 (s, 1H), 5.45 (d, \(J = 1.6\) Hz, 1H), 5.24 (d, \(J = 1.2\) Hz, 1H), 4.73 (q, \(J = 19.7\) Hz, 2H), 4.01 – 4.17 (m, 2H), 3.70 (s, 1H), 3.63 (s, 3H), 2.33 (s, 3H), 1.24 (t, \(J = 7.2\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 173.5, 166.7, 160.0, 157.2, 137.8, 136.3, 135.19, 135.18, 132.2, 130.0, 126.3, 121.1, 119.0, 113.8, 111.5, 95.6, 85.3, 77.3, 60.5, 55.0, 54.7, 44.6, 20.9, 14.2 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{23}\)H\(_{24}\)NO\(_5\)S 454.1370, found 454.1373.

Ethyl (E)-2-(2-(3-chlorobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4j)

White solid: 97 mg (yield 75%); mp 177-179 °C; IR (KBr) 3394, 2979, 1750, 1679, 1621, 1178, 953, 831, 664 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.49 (s, 1H), 7.19 – 7.25 (m, 2H), 7.14 (d, \(J = 8.0\) Hz, 2H), 6.91 – 7.06 (m, 2H), 5.46 (s, 1H), 5.20 (s, 1H), 4.73 (q, \(J = 13.9\) Hz 2H), 4.00 – 4.19 (m, 2H), 3.68 – 3.89 (m, 1H), 2.33 (s, 3H), 1.24 (t, \(J = 7.2\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 173.5, 166.7, 160.0, 157.2, 137.8, 136.3, 135.19, 135.18, 132.2, 130.0, 126.3, 121.1, 119.0, 113.8, 111.5, 95.6, 85.3, 77.3, 60.5, 55.0, 54.7, 44.6, 22.0, 14.2 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{22}\)H\(_{21}\)ClNO\(_4\)S 430.0874, found 430.0876.

Ethyl (E)-2-(2-(2-fluorobenzyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4k)

White solid: 103 mg (yield 81%); mp 158-160 °C; IR (KBr) 3412, 2968, 1747, 1668, 1035, 839, 744, 664 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.40 (s, 1H), 7.10 – 7.15 (m, 1H), 7.03 (dd, \(J = 8.0, 2.4\)Hz, 1H), 6.90 – 7.00 (m, 3H), 6.88 (d, \(J = 8.0\) Hz, 1H), 5.38 (d, \(J = 1.2\) Hz, 1H), 5.17 (d, \(J = 1.2\) Hz, 1H), 4.71 (q, \(J = 15.3\) Hz, 2H), 3.89 – 4.04 (m, 2H), 3.77 (s, 1H), 2.23 (s, 3H), 1.13 (t, \(J = 7.2\) Hz, 3H) ppm. \(^{13}\)C\{\(^1\)H\} NMR (100 MHz, CDCl\(_3\)) \(\delta\) 173.5, 160.3 (d, \(J = 244.9\) Hz), 157.1, 137.7, 136.1, 135.2, 132.2, 129.7 (d, \(J = 8.2\) Hz), 128.3 (d, \(J = 3.4\) Hz), 126.3, 124.7, 121.1, 120.9, 120.7, 115.6 (d, \(J = 21.1\) Hz), 95.2,
S8

85.3, 60.5, 54.7, 38.4, 21.0, 14.2 ppm. $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -118.01 – -118.09 (m). HRMS (ESI-TOF) m/z [M + H]$^+$ calculated for C$_{22}$H$_{21}$FNO$_4$S 414.1170, found 414.1173.

**Ethyl (E)-2-(8b-hydroxy-7-methyl-1-oxo-2-(pyridin-2-ylmethyl)-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4l)**

White solid: 50 mg (yield 42%); mp 171-172 °C; IR (KBr) 3360, 2957, 1745, 1680, 1609, 951, 813, 664 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.44 (d, $J = 4.4$ Hz, 1H), 7.64 (td, $J = 7.5$, 1.6 Hz, 1H), 7.17 – 7.23 (m, 1H), 7.11 (t, $J = 8.2$ Hz, 2H), 6.99 (d, $J = 8.0$ Hz, 1H), 5.45 (d, $J = 1.2$ Hz, 1H), 5.27 (d, $J = 1.2$ Hz, 1H), 5.04 (d, $J = 16.2$ Hz, 1H), 4.87 (s, 1H), 4.70 (d, $J = 16.2$ Hz, 1H), 4.03 – 4.17 (m, 2H), 2.32 (s, 3H), 1.24 (t, $J = 7.2$ Hz, 3H) ppm. $^{13}$C{$_1^H$} NMR (100 MHz, CDCl$_3$) $\delta$ 173.6, 166.7, 157.4, 153.6, 149.3, 137.6, 137.5, 136.2, 135.1, 132.0, 126.7, 123.0, 121.3, 121.0, 95.7, 85.5, 60.4, 54.8, 46.4, 21.0, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]$^+$ calculated for C$_{22}$H$_{21}$FNO$_4$S 414.1173, found 414.1173.

**Ethyl (E)-2-(8b-hydroxy-7-methyl-1-oxo-2-(thiophen-2-ylmethyl)-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4m)**

White solid: 94 mg (yield 78%); mp 176-178 °C; IR (KBr) 3370, 2960, 1743, 1681, 1615, 1029, 949, 824, 811 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.49 (s, 1H), 7.19 (dd, $J = 5.2$, 1.2 Hz, 1H), 7.06 – 7.14 (m, 1H), 6.94 – 7.05 (m, 2H), 6.82 – 6.93 (m, 1H), 5.43 (d, $J = 1.2$ Hz, 1H), 5.41 (d, $J = 1.2$ Hz, 1H), 4.92 (d, $J = 16.0$ Hz, 1H), 4.81 (d, $J = 16.0$ Hz, 1H), 4.00 – 4.18 (m, 2H), 3.84 (s, 1H), 2.32 (s, 3H), 1.26 (t, $J = 7.2$ Hz, 3H) ppm. $^{13}$C{$_1^H$} NMR (100 MHz, CDCl$_3$) $\delta$ 172.9, 166.8, 157.0, 137.7, 136.1, 135.8, 135.1, 132.1, 127.1, 126.0, 126.3, 125.9, 121.1, 95.1, 85.1, 60.6, 54.7, 40.0, 21.0, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]$^+$ calculated for C$_{20}$H$_{20}$NO$_4$S 397.1217, found 397.1219.

**Ethyl (E)-2-(2-benzyl-8b-hydroxy-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4n)**

White solid: 90 mg (yield 79%); mp 111-113 °C; IR (KBr) 3385, 2965, 1751, 1679, 1621, 1070, 832, 743, 701 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.68 (d, $J = 8.0$ Hz, 1H), 7.26 – 7.37 (m, 4H), 7.04 – 7.21 (m, 4H), 5.47 (d, $J = 1.2$ Hz 1H), 5.26 (d, $J = 1.2$ Hz 1H), 4.74 (q, $J = 15.9$ Hz, 2H), 3.99 – 4.15 (m, 2H), 3.89 (s, 1H), 1.23 (t, $J = 7.2$ Hz, 3H) ppm. $^{13}$C{$_1^H$} NMR (100 MHz, CDCl$_3$) $\delta$ 173.5, 166.8, 157.0, 137.7, 136.1, 141.3, 136.2, 133.7 131.1, 129.0, 1287.0, 126.9, 125.8, 125.2, 121.4, 95.6, 85.4, 60.5, 54.4, 44.9, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]$^+$ calculated for C$_{21}$H$_{20}$NO$_4$S 382.1108, found 382.1111.
Ethyl (E)-2-(2-benzyl-7-(tert-butyl)-8b-hydroxy-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4o)

White solid: 103 mg (yield 78%); mp 135-137 °C; IR (KBr) 3430, 2958, 1754, 1682, 1615, 1152, 950, 825, 696 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, J = 1.8 Hz, 1H), 7.36 (dd, J = 8.4, 2.0 Hz, 1H), 7.26 – 7.33 (m, 3H), 7.20 – 7.26 (m, 1H), 7.09 – 7.20 (m, 2H), 7.03 (d, J = 8.4 Hz, 1H), 5.50 (d, J = 1.2 Hz, 1H), 5.24 (d, J = 1.2 Hz, 1H), 4.74 (q, J = 23.2 Hz 2H), 3.92 – 4.13 (m, 3H), 1.32 (s, 9H), 1.22 ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.6, 166.8, 157.6, 148.8, 137.91, 137.87, 136.04, 136.02, 133. 8, 129.0, 128.6, 127.9, 126.9, 122.8, 120.9, 95.34, 95.28, 85.4, 60.5, 54.8, 44.9, 34.7, 31.4, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₅H₂₈NO₄S 438.1734, found 438.1735.

Ethyl (E)-2-(2-benzyl-7-chloro-8b-hydroxy-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4p)

White solid: 73 mg (yield 59%); mp 178-180 °C; IR (KBr) 3347, 2962, 1748, 1677, 1608, 1027, 814, 732, 659 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, J = 2.0 Hz, 1H), 7.27 – 7.34 (m, 3H), 7.22 – 7.25 (m, 1H), 7.08 – 7.19 (m, 2H), 7.00 (d, J = 8.4 Hz, 1H), 5.53 (d, J = 1.2 Hz, 1H), 5.26 (d, J = 1.2 Hz, 1H), 4.75 (q, J = 11.6 Hz, 2H), 4.21 (s, 1H), 3.93 – 4.12 (m, 2H), 1.22 ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.6, 166.9, 157.0, 139.6, 137.9, 133.5, 131.2, 130.9, 129.0, 128.1, 126.9, 126.2, 122.3, 95.7, 85.0, 60.7, 54.9, 45.0, 14.1 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₁H₁₉ClNO₄S 416.0718, found 416.0719.

Ethyl (E)-2-(2-benzyl-7-bromo-8b-hydroxy-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4q)

White solid: 119 mg (yield 80%); mp 178-180 °C; IR (KBr) 3348, 2962, 1749, 1678, 1609, 1027, 813, 732, 658 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, J = 2.0 Hz, 1H), 7.40 (dd, J = 8.2, 2.0 Hz, 1H), 7.26 – 7.35 (m, 3H), 7.14 (d, J = 6.8 Hz, 2H), 6.95 (d, J = 8.2 Hz, 1H), 5.53 (d, J = 1.2 Hz, 1H), 5.26 (d, J = 1.6 Hz, 1H), 4.75 (q, J = 11.5 Hz, 2H), 4.18 – 4.28 (m, 1H), 3.92 – 4.11 (m, 2H), 1.22 ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.0, 166.9, 157.0, 139.6, 137.9, 133.5, 131.2, 130.9, 129.0, 128.1, 126.9, 126.2, 122.3, 95.7, 85.0, 60.7, 54.9, 45.0, 14.1 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₁H₁₉BrNO₄S 460.0213, found 460.0210.
Ethyl (E)-2-(2-benzyl-7-fluoro-8b-hydroxy-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4r)

White solid: 54 mg (yield 45%); mp 154-156 °C; IR (KBr) 3381, 2981, 1749, 1670, 1624, 1154, 837, 814, 702 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.41 (dd, J = 8.2, 1.8 Hz, 1H), 7.37 – 7.38 (m, 3H), 7.14 (d, J = 6.4 Hz, 2H), 6.95 – 7.07 (m, 2H), 5.54 (d, J = 1.2 Hz, 1H), 5.27 (d, J = 1.2 Hz, 1H), 4.77 (q, J = 13.3 Hz 2H), 4.20 (s, 1H), 3.97 – 4.14 (m, 2H), 1.22 (t, J = 7.2 Hz, 3H) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.1, 166.8, 161.1 (d, J = 243.1 Hz), 157.0, 137.8 (d, J = 7.4 Hz), 135.9, 133.5, 129.0, 128.1, 126.9, 122.3 (d, J = 8.0 Hz), 118.6 (d, J = 23.2 Hz), 113.3, (d, J = 23.7 Hz), 95.7, 85.1, 60.6, 55.1, 45.0, 14.2 ppm.

¹⁹F NMR (376 MHz, CDCl₃) δ -117.65 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₁H₁₉FNO₄S 400.1013, found 400.1011.

Ethyl (E)-2-(7-acetyl-2-benzyl-8b-hydroxy-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4s)

White solid: 55 mg (yield 43%); mp 147-149 °C; IR (KBr) 3422, 1729, 1655, 1624, 1177, 955, 832, 699 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.24 (d, J = 1.2 Hz, 1H), 7.91 (dd, J = 8.2, 1.8 Hz, 1H), 7.26 – 7.34 (m, 3H), 7.18 (d, J = 8.0 Hz, 1H), 7.08 – 7.16 (m, 2H), 5.51 (d, J = 1.2 Hz, 1H), 5.30 (d, J = 1.2 Hz, 1H), 4.74 (q, J = 12.8 Hz, 2H), 4.41 (s, 1H), 4.05 – 4.19 (m, 2H), 2.57 (s, 3H), 1.25 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 197.0, 173.2, 166.7, 156.5, 148.2, 136.8, 134.6, 133.5, 131.1, 129.0, 128.1, 126.8, 126.3, 121.4, 95.9, 84.7, 60.6, 55.1, 45.0, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₃H₂₁NO₅S 424.1213, found 422.1210.

Ethyl (E)-2-(2-benzyl-8b-hydroxy-6-methoxy-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4t)

White solid: 89 mg (yield 72%); mp 130-132 °C; IR (KBr) 3417, 2964, 1751, 1678, 1610, 1173, 921, 804, 627 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, J = 8.6 Hz, 1H), 7.27 – 7.32 (m, 2H), 7.17 (d, J = 8.0 Hz, 1H), 7.07 – 7.20 (m, 2H), 6.69 (dd, J = 8.6, 2.2 Hz, 1H), 6.60 (d, J = 2.0Hz, 1H), 5.44 (d, J = 1.2Hz 1H), 5.24 (d, J = 1.1 Hz, 1H), 4.73 (q, J = 13.1 Hz, 2H), 4.00 – 4.16 (m, 2H), 3.82 – 3.93 (m, 1H), 3.77 (s, 3H), 1.23 (t, J = 7.2 Hz, 4H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 197.0, 173.2, 166.7, 156.5, 148.2, 136.8, 134.6, 133.5, 131.1, 129.0, 128.1, 128.1, 126.3, 121.4, 95.9, 84.7, 60.6, 55.1, 45.0, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₂H₂₂NO₅S 412.1213, found 412.1215.
Ethyl (E)-2-(2-benzyl-8b-hydroxy-5-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4u)

White solid: 75 mg (yield 63%); mp 139-141 °C; IR (KBr) 3383, 2976, 1748, 1680, 1624, 1072, 828, 721, 675 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.49 – 7.54 (m, 1H), 7.28 – 7.34 (m, 3H), 7.08 – 7.20 (m, 4H), 5.42 (d, J = 1.6 Hz, 1H), 5.28 (d, J = 1.2 Hz, 1H), 4.82 (d, J = 15.6 Hz, 1H), 4.68 (d, J = 16.0 Hz, 1H), 4.08 – 4.23 (m, 2H), 3.41 (s, 1H), 2.21 (s, 2H), 1.27 (t, J = 7.0 Hz, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.7, 166.8, 157.3, 140.8, 135.9, 133.8, 131.6, 131.5, 131.3, 127.9, 126.90, 125.7, 123.2, 123.1, 95.5, 85.8, 60.5, 54.2, 44.9, 19.9, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₂H₂₂NO₄S 396.1264, found 396.1265.

Ethyl (E)-2-(9-benzyl-10a-hydroxy-10-oxo-7a,9,10,10a-tetrahydro-8H-naphtho[1',2':4,5]thieno[2,3-c]pyrrol-8-ylidene)acetate (4v)

White solid: 32 mg (yield 23%); mp 200-202 °C; IR (KBr) 3398, 2992, 1748, 1669, 1626, 1185, 934, 820, 699 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 9.00 (d, J = 8.6 Hz, 1H), 7.77 (dd, J = 8.2, 3.4 Hz, 2H), 7.53 – 7.61 (m, 1H), 7.38– 7.44 (m, 1H), 7.26 – 7.38 (m, 4H), 7.23 – 7.26 (m, 1H), 7.07 – 7.23 (m, 3H), 5.69 (d, J = 1.2 Hz, 1H), 5.22 (d, J = 1.2 Hz, 1H), 4.76 (t, J = 16.4 Hz 2H), 4.46 – 4.51 (m, 1H), 3.80 – 3.91 (m, 1H), 3.56 – 3.68 (m, 1H), 1.00 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 172.5, 167.2, 157.6, 140.0, 133.8, 132.3, 132.2, 131.0, 129.0, 128.8, 128.5, 127.96, 127.9, 127.3, 125.1, 125.0, 119.9, 94.6, 89.3, 60.5, 55.3, 14.0 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₅H₂₂NO₄S 432.1264, found 432.1261.

Ethyl (E)-2-(8b-hydroxy-7-methyl-1-oxo-2-phenethyl-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4w)

White solid: 80 mg (yield 65%); mp 128-130 °C; IR (KBr) 3431, 2980, 1746, 1682, 1619, 1027, 818, 749, 663 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.32 (s, 1H), 7.02 – 7.15 (m, 6H), 6.98 (d, J = 8.0 Hz, 1H), 5.43 (d, J = 1.2 Hz, 1H), 5.34 (d, J = 1.2 Hz, 1H), 4.04 – 4.20 (m, 2H), 3.82 – 3.93 (m, 2H), 3.63 (dt, J = 13.8, 6.8 Hz, 1H), 2.77 – 2.90 (m, 2H), 2.30 (s, 3H), 1.28 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 172.5, 167.2, 157.6, 140.0, 133.8, 132.3, 132.2, 131.0, 129.0, 128.8, 128.5, 127.96, 127.9, 127.3, 125.1, 125.0, 119.9, 94.6, 89.3, 60.5, 55.3, 14.0 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₃H₂₄NO₄S 410.1421, found 410.1426.
**Ethyl (E)-2-(2-butyl-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4x)**

White solid: 66 mg (yield 61%); mp 132-134 °C; IR (KBr) 3420, 2941, 1751, 1683, 1619, 1049, 829, 804, 666 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.45 (s, 1H), 7.10 (d, J = 8.0 Hz, 1H), 6.96 (d, J = 8.0 Hz, 1H), 5.44 (d, J = 8.0 Hz, 1H), 5.30 (d, J = 1.2 Hz, 1H), 4.03 – 4.20 (m, 2H), 3.79 – 3.99 (m, 1H), 3.44 – 3.61 (m, 2H), 2.31 (s, 3H), 1.45 – 1.63 (m, 2H), 1.20 – 1.37 (m, 5H), 0.89 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.3, 167.0, 158.2, 137.7, 136.4, 135.0, 132.0, 126.3, 121.0, 93.9, 85.1, 54.6, 41.2, 28.2, 20.9, 20.0, 14.2, 13.6 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₁₉H₂₄NO₄S 362.1421, found 362.1426.

**Ethyl (E)-2-(2-cyclopentyl-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4y)**

White solid: 20 mg (yield 18%); mp 125-127 °C; IR (KBr) 3421, 2960, 1748, 1681, 1613, 1142, 807, 738, 666 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.44 (s, 1H), 7.09 (d, J = 8.0 Hz, 1H), 6.95 (d, J = 8.0 Hz, 1H), 5.48 (s, 1H), 5.35 (s, 1H), 4.42 (p, J = 8.4 Hz, 1H), 3.94 – 4.15 (m, 3H), 2.31 (s, 3H), 1.92 – 2.07 (m, 2H), 1.72 – 1.91 (m, 4H), 1.55 – 1.67 (m, 2H), 1.24 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 173.4, 167.1, 158.0, 137.8, 136.6, 134.9, 131.9, 126.2, 123.0, 94.7, 84.8, 60.4, 54.5, 54.4, 27.8, 27.3, 25.5, 25.4, 20.9, 14.3 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₀H₂₄NO₄S 374.1421, found 374.1426.

**Ethyl (E)-2-(8b-hydroxy-7-methyl-1-oxo-2-phenyl-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4z)**

White solid: 20 mg (yield 17%); mp 205-207 °C; IR (KBr) 3399, 2969, 1753, 1679, 1664, 1086, 808, 695, 664 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.56 (m, 4H), 7.22 (d, J = 7.2 Hz, 2H), 7.15 (d, J = 8.0 Hz, 1H), 7.04 (d, J = 8.0 Hz, 1H), 5.56 (d, J = 1.2 Hz, 1H), 5.12 (d, J = 1.2 Hz, 1H), 4.07 – 4.20 (m, 2H), 3.58 (s, 1H), 2.32 (s, 3H), 1.25 (t, J = 7.0 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 172.8, 166.8, 159.2, 138.0, 136.3, 135.2, 133.4, 132.2, 130.0, 129.5, 127.4, 126.2, 121.1, 96.1, 85.4, 60.4, 54.6, 21.0, 14.2 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₁H₂₃NO₄S 382.1105, found 382.1105.
**Ethyl (E)-2-(8b-hydroxy-7-methyl-1-oxo-2-(p-tolyl)-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4aa)**

White solid: 45 mg (yield 38%); mp 204-206 °C; IR (KBr) 3422, 2974, 1753, 1680, 1665, 1155, 836, 800, 717 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.48 (s, 1H), 7.27 (d, \(J = 8.4\) Hz, 2H), 7.14 (dd, \(J = 8.0, 0.8\) Hz, 1H), 7.09 (d, \(J = 8.0\) Hz, 2H), 7.02 (d, \(J = 8.0\) Hz, 1H), 5.59 (d, \(J = 1.2\) Hz, 1H), 5.11 (d, \(J = 1.6\) Hz, 1H), 3.98 – 4.16 (m, 2H), 3.81 – 3.96 (m, 1H), 2.38 (s, 3H), 2.31 (s, 3H), 1.21 (t, \(J = 7.0\) Hz, 3H) ppm. \(^13\)C\({}^{1}\)H NMR (100 MHz, CDCl\(_3\)) \(\delta\) 172.9, 167.0, 159.7, 139.7, 137.9, 136.4, 135.1, 132.1, 130.5, 127.1, 126.4, 121.1, 95.8, 85.3, 77.0, 60.4, 54.6, 21.3, 20.9, 14.2 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{22}\)H\(_{22}\)NO\(_4\)S 396.1264, found 396.1267.

**Ethyl (E)-2-(2-(4-bromophenyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4ab)**

White solid: 47 mg (yield 38%); mp 190-192 °C; IR (KBr) 3430, 2950, 1755, 1677, 1620, 1146, 844, 802, 757 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.48 (s, 1H), 7.08 – 7.19 (m, 3H), 7.02 (d, \(J = 8.0\) Hz, 1H), 6.97 (d, \(J = 8.4\) Hz, 2H), 5.58 (d, \(J = 1.2\) Hz 1H), 5.10 (d, \(J = 0.8\) Hz 1H), 3.98 – 4.15 (m, 3H), 3.82 (s, 2H), 2.31 (s, 3H), 1.21 (t, \(J = 7.0\) Hz, 3H) ppm. \(^13\)C\({}^{1}\)H NMR (100 MHz, CDCl\(_3\)) \(\delta\) 173.0, 167.0, 160.1, 159.9, 137.9, 136.4, 135.1, 132.1, 128.6, 126.4, 121.1, 115.2, 95.8, 85.3, 60.4, 55.6, 54.5 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{22}\)H\(_{22}\)NO\(_5\)S 412.1213, found 412.1212.

**Ethyl (E)-2-(2-(4-bromophenyl)-8b-hydroxy-7-methyl-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (4ac)**

Red solid: 40 mg (yield 29%); mp 190-192 °C; IR (KBr) 3449, 2922, 1751, 1685, 1623, 1155, 837, 806, 661 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.63 (d, \(J = 8.8\) Hz, 2H), 7.46 (s, 1H), 7.08 – 7.20 (m, 3H), 7.03 (d, \(J = 8.0\) Hz, 1H), 5.56 (d, \(J = 0.8\) Hz, 1H), 5.11 (d, \(J = 1.2\) Hz, 1H), 4.05 – 4.19 (m, 2H), 3.60 (s, 1H), 2.32 (s, 3H), 1.24 (t, \(J = 7.0\) Hz, 3H) ppm. \(^13\)C\({}^{1}\)H NMR (100 MHz, CDCl\(_3\)) \(\delta\) 172.5, 166.7, 158.8, 138.0, 136.1, 135.3, 132.3, 129.2, 126.3, 123.6, 121.2, 96.2, 85.4, 60.5, 54.6, 20.9, 14.2 ppm. HRMS (ESI-TOF) \(m/z\) [M + H]\(^+\) calcd for C\(_{21}\)H\(_{19}\)BrNO\(_4\)S 460.0213, found 460.0215.
Ethyl 2-(2-benzyl-3,8b-dihydroxy-7-methyl-1-oxo-2,3,3a,8b-tetrahydro-1H-benzo[4,5]thieno[2,3-c]pyrrol-3-yl)acetate (5a)

White solid: 62 mg (yield 50%); mp 122-124 °C; IR (KBr) 3381, 3056, 2984, 1734, 1662, 1451, 1371, 809, 737, 701 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.54 (s, 1H), 7.26 – 7.39 (m, 5H), 7.04 – 7.20 (m, 2H), 4.86 (d, J = 15.6 Hz, 1H), 4.53 (s, 1H), 4.26 (d, J = 15.6 Hz, 1H), 4.14 (s, 1H), 3.91 – 4.08 (m, 2H), 3.81 – 3.90 (m, 1H), 2.80 (d, J = 16.4 Hz, 1H), 2.60 (d, J = 16.4 Hz, 1H), 2.33 (s, 3H), 1.17 (t, J = 7.2 Hz, 2H) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃) δ 172.1, 169.7, 137.7, 137.4, 136.3, 136.1, 132.0, 128.7, 128.0, 127.6, 126.5, 121.7, 87.0, 86.4, 63.4, 61.5, 44.7, 43.8, 21.0, 13.9 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂ₓH₂₂NO₄S 414.1370, found 414.1269.

2-acetyl-N-(4-cyanobenzyl)-5-methylbenzo[b]thiophene-3-carboxamide (6a)

White solid: 14 mg (yield 13%); mp 170-172 °C; IR (KBr) 3267, 2922, 1776, 1637, 1637, 844, 827, 697 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.76 (s, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.63 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.0 Hz, 2H), 7.41 – 7.50 (m, 1H), 7.30 – 7.36 (m, 1H), 4.71 (d, J = 6.0 Hz, 2H), 2.57 (s, 2H), 2.44 (s, 3H) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃) δ 192.7, 165.0, 143.3, 138.9, 138.6, 137.5, 136.0, 134.9, 132.5, 130.1, 128.5, 125.1, 122.1, 118.7, 111.4, 43.7, 29.6, 21.5 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂ₒH₁₇N₂O₂S 348.1005, found 348.1008.

Methyl 4-((2-acetyl-5-methylbenzo[b]thiophene-3-carboxamido)methyl)benzoate (6b)

White solid: 20 mg (yield 17%); mp 183-185 °C; IR (KBr) 3448, 3262, 1684, 1280, 811, 750, 698 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (d, J = 8.4 Hz, 2H), 7.84 (s, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.55 (d, J = 8.2 Hz, 2H), 7.37 (dd, J = 8.2, 1.4 Hz, 1H), 7.10 (s, 1H), 4.82 (d, J = 5.9 Hz, 2H), 3.95 (s, 3H), 2.64 (s, 3H), 2.49 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 192.7, 166.8, 164.9, 142.8, 139.2, 138.6, 135.9, 135.2, 130.1, 129.6, 128.0, 125.1, 122.1, 52.2, 43.9, 29.6, 21.5 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₂₁H₂₆NO₄S 382.1108, found 382.1103.

2,5-diacetyl-N-benzylbenzo[b]thiophene-3-carboxamide (6c)

White solid: 33 mg (yield 31%); mp 148-150 °C; IR (KBr) 3259, 1681, 1665, 1245, 949, 829, 698 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.51 (s, 1H), 8.05 (dd, J = 8.4, 1.2 Hz, 1H), 7.87 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 7.2 Hz, 2H), 7.39 (t, J = 7.2 Hz, 2H), 7.33 (t, J = 7.2 Hz, 1H), 7.13 (s, 1H), 4.75 (d, J = 5.6
Hz, 2H), 2.62 (s, 3H), 2.60 (s, 3H) ppm. $^{13}$C $^1$H NMR (100 MHz, CDCl$_3$) $\delta$ 197.3, 192.3, 163.9, 144.3, 141.1, 138.1, 137.4, 136.3, 134.9, 129.0, 128.3, 128.0, 126.7, 126.5, 122.8, 44.5, 29.4, 26.6 ppm. HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for C$_{20}$H$_{18}$NO$_3$S 352.1002, found 352.1000.

2-acetyl-N-(sec-butyl)-5-methylbenzo[b]thiophene-3-carboxamide (6d)

White solid: 50mg (yield 58%); mp 101-103 °C; IR (KBr) 3444, 2970, 1665, 1620, 1014, 922, 806, 701 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.69 (d, $J = 8.8$ Hz, 2H), 7.31 (d, $J = 8.0$ Hz, 1H), 6.27 (s, 1H), 4.17 – 4.28 (m, 1H), 2.63 (s, 3H), 2.46 (s, 3H), 1.55 – 1.72 (m, 2H), 1.31 (d, $J = 6.4$ Hz, 3H), 1.03 (t, $J = 7.4$ Hz, 3H) ppm. $^{13}$C $^1$H NMR (100 MHz, CDCl$_3$) $\delta$ 192.4, 164.4, 139.5, 138.6, 137.9, 136.4, 135.6, 129.9, 124.7, 122.2, 47.6, 29.5, 29.1, 21.5, 20.2, 10.5 ppm. HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for C$_{16}$H$_{20}$NO$_2$S 290.1209, found 290.1211.

2-acetyl-N-cyclopentyl-5-methylbenzo[b]thiophene-3-carboxamide (6e)

White solid: 39 mg (yield 43%); mp 167-169 °C; IR (KBr) 3443, 2959, 1630, 1557, 1014, 911, 803, 697 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.58 – 7.79 (m, 2H), 7.30 (d, $J = 8.4$ Hz, 1H), 6.55 (d, $J = 5.6$ Hz, 1H), 4.50 (h, $J = 6.9$ Hz, 1H), 2.61 (s, 3H), 2.46 (s, 3H), 2.06 – 2.22 (m, 2H), 1.54 – 1.80 (m, 6H) ppm. $^{13}$C $^1$H NMR (100 MHz, CDCl$_3$) $\delta$ 192.5, 164.5, 139.6, 138.6, 137.8, 136.3, 135.6, 129.9, 124.8, 122.1, 51.9, 32.9, 29.1, 23.8, 21.5 ppm. HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for C$_{17}$H$_{20}$NO$_2$S 302.1207.

2-acetyl-5-methyl-N-phenylbenzo[b]thiophene-3-carboxamide (6f)

White solid: 35 mg (yield 38%); mp 178-180 °C; IR (KBr) 3448, 2920, 1667, 1643, 1216, 809, 742, 686 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.84 (s, 1H), 7.96 (s, 1H), 7.73 (dd, $J = 8.0, 5.6$ Hz, 3H), 7.41 (t, $J = 7.8$ Hz, 1H), 7.33 – 7.37 (m, 1H), 7.20 (t, $J = 7.4$ Hz, 1H), 2.67 (s, 3H), 2.47 (s, 3H) ppm. $^{13}$C $^1$H NMR (100 MHz, CDCl$_3$) $\delta$ 193.4, 162.5, 139.7, 138.8, 137.7, 137.5, 136.0, 135.5, 130.1, 129.2, 125.4, 125.0, 122.1, 120.3, 29.7, 21.5 ppm. HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for C$_{18}$H$_{12}$NO$_2$S 310.0896, found 310.0893.
2-acetyl-5-methyl-N-(p-tolyl)benzo[b]thiophene-3-carboxamide (6g)

White solid: 26 mg (yield 27%); mp 175-177 °C; IR (KBr) 3257, 2921, 1667, 1640, 1236, 809, 793, 754 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.73 (s, 1H), 7.93 (s, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 8.4 Hz, 2H), 7.34 (dd, J = 8.4, 1.2 Hz, 1H), 7.21 (d, J = 8.2 Hz, 2H), 2.66 (s, 3H), 2.46 (s, 3H), 2.37 (s, 3H) ppm. ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 193.3, 162.4, 139.8, 138.8, 137.6, 135.9, 135.6, 135.1, 134.7, 130.1, 129.8, 129.7, 125.4, 122.1, 120.3, 119.8, 29.6, 21.5, 21.0 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₁₉H₁₈NO₂S 324.1053, found 324.1057.

2-acetyl-N-(4-methoxyphenyl)-5-methylbenzo[b]thiophene-3-carboxamide (6h)

Yellow solid: 20 mg (yield 20%); mp 191-193 °C; IR (KBr) 3273, 2915, 1685, 1641, 1242, 825, 700, 704 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.74 (s, 1H), 7.93 (s, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.64 (d, J = 9.2 Hz, 2H), 7.34 (dd, J = 8.2, 0.6 Hz, 1H), 6.94 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H), 2.66 (s, 3H), 2.46 (s, 3H) ppm. ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 193.4, 162.4, 156.9, 139.7, 138.8, 137.6, 135.9, 135.7, 130.1, 129.8, 129.7, 125.4, 122.1, 120.3, 119.8, 29.6, 21.5 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₁₉H₁₈NO₃S 340.1002, found 340.1004.

2-acetyl-N-(4-bromophenyl)-5-methylbenzo[b]thiophene-3-carboxamide (6i)

Yellow solid: 35 mg (yield 30%); mp 198-200 °C; IR (KBr) 3256, 2920, 1667, 1647, 1236, 810, 782, 668 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 9.29 (s, 1H), 8.00 (s, 1H), 7.71 (d, J = 8.2 Hz, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.35 (dd, J = 8.4, 1.2 Hz, 1H), 2.65 (s, 3H), 2.47 (s, 3H) ppm. ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 193.9, 162.3, 139.4, 138.8, 137.3, 136.9, 136.2, 135.0, 132.1, 130.2, 125.7, 122.0, 121.8, 117.5, 30.0, 21.6 ppm. HRMS (ESI-TOF) m/z [M + H]⁺ calcd for C₁₈H₁₄BrNO₃S 388.0001, found 388.0007.
2-acetyl-5-methyl-N-(4-nitrophenyl)benzo[b]thiophene-3-carboxamide (6j)

Red solid: 5 mg (yield 5%); mp 225-227 °C; IR (KBr) 3315, 2918, 1689, 1660, 1242, 865, 853, 802 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 10.24 (s, 1H), 8.28 (d, J = 8.8 Hz, 2H), 8.19 (s, 1H), 7.95 (d, J = 9.2 Hz, 2H), 7.77 (d, J = 8.4 Hz, 1H), 7.41 (dd, J = 8.4, 0.8 Hz, 1H), 2.74 (s, 3H), 2.51 (s, 3H). ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 194.8, 162.1, 143.81, 143.80, 139.4, 139.1, 137.0, 136.5, 134.0, 130.5, 126.2, 125.1, 121.9, 119.8, 30.6, 21.7 ppm. HRMS (ESI-TOF) m/z [M + H]+ calcd for C₁₈H₁₅N₂O₄S 355.0747, found 355.0747.

Ethyl (E)-2-(2-benzyl-7-methyl-1-oxo-1,2-dihydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (7)

Yellow solid: 53 mg (yield 70%); mp 196-198 °C; IR (KBr) 3419, 1713, 1630, 1071, 811, 705, 647 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.10 (s, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.27 – 7.37 (m, 5H), 5.63 (s, 1H), 5.00 (s, 2H), 4.27 (q, J = 7.2 Hz, 2H), 2.52 (s, 3H), 1.32 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 166.5, 163.9, 145.8, 144.4, 144.2, 136.2, 132.1, 131.3, 128.9, 128.4, 127.6, 126.9, 122.7, 122.7, 98.0, 60.8, 43.4, 21.5, 14.3 ppm. HRMS (ESI-TOF) m/z [M + H]+ calcd for C₂₂H₂₀NO₃ 378.1158, found 378.1157.

Ethyl (E)-2-(2-benzyl-8b-hydroxy-7-methyl-4,4-dioxido-1-oxo-1,2,3a,8b-tetrahydro-3H-benzo[4,5]thieno[2,3-c]pyrrol-3-ylidene)acetate (8)

White solid: 62 mg (yield 73%); mp 197-199 °C; IR (KBr) 3441, 2994, 1737, 1700, 1637, 1072, 837, 732, 666 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.87 (s, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.26 – 7.32 (m, 2H), 7.21 – 7.26 (m, 1H), 7.13 (d, J = 7.2 Hz, 2H), 5.68 (d, J = 1.2 Hz, 1H), 5.55 (d, J = 1.2 Hz, 1H), 5.04 (s, 1H), 4.70 (q, J = 8.0 Hz, 2H), 4.03 – 4.16 (m, 1H), 3.84 – 3.99 (m, 1H), 2.49 (s, 3H), 1.19 (t, J = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 171.7, 166.6, 146.2, 145.9, 136.9, 134.7, 133.1, 133.0, 129.0, 128.1, 126.8, 126.7, 121.2, 100.6, 77.7, 68.2, 61.1, 45.25, 21.8, 14.1 ppm. HRMS (ESI-TOF) m/z [M + H]+ calcd for C₂₂H₂₂NO₅S 428.1162, found 428.1166.

8. NMR spectra of all new compounds
1g, $^1$H NMR 400 MHz, CDCl$_3$

1g, $^1$C NMR 100 MHz, CDCl$_3$
4a, $^1$H NMR 400 MHz, CDCl$_3$

4a, $^1$C NMR 100 MHz, CDCl$_3$
**4b, $^1$H NMR 400 MHz, CDCl$_3$**

**4b, $^{13}$C NMR 100 MHz, CDCl$_3$**
$\textbf{4c,}^{1}\text{H NMR 400 MHz, CDCl}_3$

$\textbf{4c}^{13}\text{C NMR 100 MHz, CDCl}_3$
**4d, $^1$H NMR 400 MHz, CDCl$_3$**

![NMR spectrum](image)

**4d, $^{13}$C NMR 100 MHz, CDCl$_3$**

![NMR spectrum](image)
4d, $^{19}$F NMR 376 MHz, CDCl$_3$

4e, $^1$H NMR 400 MHz, CDCl$_3$
$4e$, $^{13}$C NMR 100 MHz, CDCl$_3$

$4f$, $^1$H NMR 400 MHz, CDCl$_3$
$4f$, $^{13}$C NMR 100 MHz, CDCl$_3$

$4g$, $^1$H NMR 400 MHz, CDCl$_3$
**4g, $^1$C NMR 100 MHz, CDCl$_3$**

**4h, $^1$H NMR 400 MHz, CDCl$_3$**
$4h$, $^1C$ NMR 100 MHz, CDCl$_3$

$4i$, $^1H$ NMR 400 MHz, CDCl$_3$
$4i$, $^{13}$C NMR 100 MHz, CDCl$_3$

$4j$, $^1$H NMR 400 MHz, CDCl$_3$
$4j$, $^{13}$C NMR 100 MHz, CDCl$_3$

$4k$, $^1$H NMR 400 MHz, CDCl$_3$
4k, $^{13}$C NMR 100 MHz, CDCl$_3$

4k, $^{19}$F NMR 376 MHz, CDCl$_3$
$4l$, $^1H$ NMR 400 MHz, CDCl$_3$

$4l$, $^{13}C$ NMR 100 MHz, CDCl$_3$
4m, $^1$H NMR 400 MHz, CDCl$_3$

$^1$C NMR 100 MHz, CDCl$_3$
4n, $^1$H NMR 400 MHz, CDCl$_3$

4n, $^{13}$C NMR 100 MHz, CDCl$_3$
$4o$, $^1$H NMR 400 MHz, CDCl$_3$

$4o$, $^{13}$C NMR 100 MHz, CDCl$_3$
$^{1}H$ NMR 400 MHz, CDCl$_3$

$^{13}$C NMR 100 MHz, CDCl$_3$
$4q$, $^1$H NMR 400 MHz, CDCl$_3$

$4q$, $^{13}$C NMR 100 MHz, CDCl$_3$
$\textbf{4r, }^1\text{H NMR 400 MHz, CDCl}_3$

$\textbf{4r, }^1\text{C NMR 100 MHz, CDCl}_3$
$4r$, $^{19}$F NMR 376 MHz, CDCl$_3$

$4s$, $^1$H NMR 400 MHz, CDCl$_3$
4s, $^1$C NMR 100 MHz, CDCl$_3$

4t, $^1$H NMR 400 MHz, CDCl$_3$
\[ \text{4t, }^{13}\text{C NMR 100 MHz, CDCl}_3 \]

\[ \text{4u, }^1\text{H NMR 400 MHz, CDCl}_3 \]

\[ \text{HO} \]
\[ \text{N} \]
\[ \text{COEt} \]
\[ \text{H}_3\text{CO} \]
\[ \text{H}_3\text{CO} \]

\[ \text{SN} \]
\[ \text{COOEt} \]
\[ \text{HO} \]
\[ \text{H}_3\text{CO} \]
\[ \text{H}_3\text{CO} \]
$4u$, $^{13}$C NMR 100 MHz, CDCl$_3$

$4v$, $^1$H NMR 400 MHz, CDCl$_3$
\[4v, ^{13}\text{C} \text{NMR} 100 \text{ MHz}, \text{CDCl}_3\]

\[4w, ^1\text{H} \text{NMR} 400 \text{ MHz}, \text{CDCl}_3\]
**4w, $^{13}$C NMR 100 MHz, CDCl$_3$**

**4x, $^1$H NMR 400 MHz, CDCl$_3$**
$4x$, $^{13}$C NMR 100 MHz, CDCl$_3$

$4y$, $^1$H NMR 400 MHz, CDCl$_3$
$4y$, $^{13}$C NMR 100 MHz, CDCl$_3$

$4z$, $^1$H NMR 400 MHz, CDCl$_3$
$4z$, $^{13}C$ NMR 100 MHz, CDCl$_3$

$4aa$, $^1H$ NMR 400 MHz, CDCl$_3$
4aa, $^1$C NMR 100 MHz, CDCl$_3$

4ab, $^1$H NMR 400 MHz, CDCl$_3$
**4ab, $^1$C NMR 100 MHz, CDCl$_3$**

**4ac, $^1$H NMR 400 MHz, CDCl$_3$**
4ac, $^1$C NMR 100 MHz, CDCl$_3$

5a, $^1$H NMR 400 MHz, CDCl$_3$
5a, $^{13}$C NMR 100 MHz, CDCl$_3$

6a, $^1$H NMR 400 MHz, CDCl$_3$
6a. $^{13}$C NMR 100 MHz, CDCl$_3$

6b. $^1$H NMR 400 MHz, CDCl$_3$
$6b$, $^{13}$C NMR 100 MHz, CDCl$_3$

$6c$, $^1$H NMR 400 MHz, CDCl$_3$
$6c$, $^{13}$C NMR 100 MHz, CDCl$_3$

$6d$, $^1$H NMR 400 MHz, CDCl$_3$
6d, $^{13}$C NMR 100 MHz, CDCl$_3$

6e, $^1$H NMR 400 MHz, CDCl$_3$
$\text{6e, }^{13}\text{C NMR 100 MHz, CDCl}_3$

$\text{6f, }^1\text{H NMR 400 MHz, CDCl}_3$
6f, $^{13}$C NMR 100 MHz, CDCl$_3$

6g, $^1$H NMR 400 MHz, CDCl$_3$
$6g$, $^{13}$C NMR 100 MHz, CDCl$_3$

$6h$, $^1$H NMR 400 MHz, CDCl$_3$
6h, $^{13}$C NMR 100 MHz, CDCl$_3$

6i, $^1$H NMR 400 MHz, CDCl$_3$
**6i, \(^{13}\text{C} \text{NMR 100 MHz, CDCl}_3**

**6j, \(^1\text{H} \text{NMR 400 MHz, CDCl}_3**
$\textbf{6j, }^{13}\text{C NMR 100 MHz, CDCl}_3$

$\textbf{7, }^1\text{H NMR 400 MHz, CDCl}_3$
7. $^{13}$C NMR 100 MHz, CDCl$_3$

8. $^1$H NMR 400 MHz, CDCl$_3$
8, $^{13}$C NMR 100 MHz, CDCl$_3$
9. Computational details and archive entries

Table S2. Cartesian coordinates of some stationary points, optimized at the B3LYP-PCM/6-31+G* level of theory in water.

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<td>6</td>
<td>4.440953000</td>
<td>4.544552000</td>
<td>-0.181925000</td>
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</tbody>
</table>
### Table S3. Imaginary frequencies (I. F., $i \text{ cm}^{-1}$) of the transition states optimized at the B3LYP-PCM/6-31+G* level of theory in water. All of the minima structures do not have any imaginary frequencies.

<table>
<thead>
<tr>
<th>Species Name</th>
<th>I. F.</th>
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</thead>
<tbody>
<tr>
<td>TS-1</td>
<td>-39.8</td>
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<tr>
<td>TS-3</td>
<td>-1075.6</td>
</tr>
<tr>
<td>TS-5</td>
<td>-1292.3</td>
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<tr>
<td>TS-7</td>
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<tr>
<td>TS-2</td>
<td>-390.5</td>
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<tr>
<td>TS-4</td>
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<tr>
<td>TS-6</td>
<td>-88.2</td>
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</table>

### Table S4. Electronic energies ($E$, a.u.), entropies ($S$, cal/mol·K), and Gibbs free energies ($G$, a.u.) at the B3LYP/6-31+G* level of theory, and electronic energies ($E_{\text{m06}}$) by the m06/6-311++G** single point computations.

<table>
<thead>
<tr>
<th>Species Name</th>
<th>$E$</th>
<th>$S$</th>
<th>$G$</th>
<th>$E_{\text{m06}}$</th>
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</thead>
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</table>
Computational Methods

All calculations were finished using the Gaussian 09 computational program. Geometrical optimizations were performed by the B3LYP density functional method with the 6-31+g* basis set for all elements. The default self-consistent reaction field polarizable continuum model (PCM) was used to consider the solvation effects of water. All of the resultant stationary point geometries were characterized by vibrational analyses, from which zero-point energies and Gibbs free-energies were obtained, in addition to confirming whether all of the structures resided at minima or first-order saddle points on the potential energy surfaces. The contributions of small-frequency vibrations to the computed entropies were corrected by the quasi-RRHO approach.

Considering the default entropic data obtained from the Gaussian output files are the idea-gas-phase entropies, which would exaggerate the activation entropies for the bimolecular reaction in solution. Hence, the default entropies are scaled by a factor of 0.5 in Gibbs free-energy determinations.

To refined the electronic energies, the m06 density functional method and 6-311++G** basis set for all elements were used in singlet point calculations, in which the SMD solvation method was used.

10. References

(3) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji,


11. X-ray crystal structures

4a

4w