Supporting Information,

**Urea-modified tryptophan based in situ reducing and stabilizing agent for fabrication of gold nanoparticles as Suzuki-Miyaura cross-coupling catalyst in water**

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</thead>
<tbody>
<tr>
<td>ESI-Figure S1</td>
<td>2</td>
<td>Figure S18</td>
<td>17</td>
<td>Figure S38</td>
<td>27</td>
</tr>
<tr>
<td>ESI-Figure S2</td>
<td>2</td>
<td>Figure S19</td>
<td>18</td>
<td>Figure S39</td>
<td>28</td>
</tr>
<tr>
<td>ESI-Figure S3</td>
<td>3</td>
<td>Figure S20</td>
<td>18</td>
<td>Figure S40</td>
<td>28</td>
</tr>
<tr>
<td>Figure S4</td>
<td>4</td>
<td>Figure S21</td>
<td>19</td>
<td>Figure S41</td>
<td>29</td>
</tr>
<tr>
<td>Scheme 1</td>
<td>4</td>
<td>Figure S22</td>
<td>19</td>
<td>Figure S42</td>
<td>29</td>
</tr>
<tr>
<td>Figure S5</td>
<td>6</td>
<td>Figure S23</td>
<td>20</td>
<td>Figure S43</td>
<td>30</td>
</tr>
<tr>
<td>Figure S6</td>
<td>6</td>
<td>Figure S24</td>
<td>20</td>
<td>Figure S44</td>
<td>30</td>
</tr>
<tr>
<td>Figure S7</td>
<td>7</td>
<td>Figure S25</td>
<td>21</td>
<td>Figure S45</td>
<td>31</td>
</tr>
<tr>
<td>Figure S8</td>
<td>7</td>
<td>Figure S26</td>
<td>21</td>
<td>Figure S46</td>
<td>31</td>
</tr>
<tr>
<td>Figure S9</td>
<td>8</td>
<td>Figure S27</td>
<td>22</td>
<td>Figure S47</td>
<td>32</td>
</tr>
<tr>
<td>Figure S10</td>
<td>8</td>
<td>Figure S28</td>
<td>22</td>
<td>Figure S48</td>
<td>32</td>
</tr>
<tr>
<td>Figure S11</td>
<td>9</td>
<td>Figure S29</td>
<td>23</td>
<td>Figure S49</td>
<td>33</td>
</tr>
<tr>
<td>Figure S12</td>
<td>9</td>
<td>Figure S30</td>
<td>23</td>
<td>Figure S50</td>
<td>33</td>
</tr>
<tr>
<td>Scheme 2</td>
<td>10</td>
<td>Figure S31</td>
<td>24</td>
<td>Figure S51</td>
<td>34</td>
</tr>
<tr>
<td>Figure S13</td>
<td>15</td>
<td>Figure S32</td>
<td>24</td>
<td>Figure S52</td>
<td>34</td>
</tr>
<tr>
<td>Figure S14</td>
<td>15</td>
<td>Figure S33</td>
<td>25</td>
<td>ESI Table 1</td>
<td>35</td>
</tr>
<tr>
<td>Figure S15</td>
<td>16</td>
<td>Figure S34</td>
<td>25</td>
<td>Table 2</td>
<td>36</td>
</tr>
<tr>
<td>Figure S16</td>
<td>16</td>
<td>Figure S35</td>
<td>26</td>
<td>Table 3</td>
<td>37</td>
</tr>
<tr>
<td>Figure S17</td>
<td>17</td>
<td>Figure S36</td>
<td>26</td>
<td>Figure S53</td>
<td>37</td>
</tr>
<tr>
<td>Figure S37</td>
<td>27</td>
<td>Figure S37</td>
<td>26</td>
<td>Figure S54</td>
<td>38</td>
</tr>
</tbody>
</table>
**ESI-Figure S1.** The water solution of urea modified tryptophan 1, HAuCl$_4$ and gold nanoparticles.

**ESI-Figure S2.** The proposed mechanism of gold nanoparticle from urea modified tryptophan 1 and HAuCl$_4$. 
ESI-Figure S3. Absorption spectra of gold nanoparticle a) compound 1:HAuCl$_4$ = 10:1 and b) compound 1:HAuCl$_4$ = 1:10.
Figure S4. The mechanism of gold nanoparticle catalyzed cross-coupling reaction.

Experimental Section

\[
\begin{align*}
\text{H}_2\text{N} & \quad \text{R} \quad \text{COOH} \\
\xrightarrow{\text{KCNO}} \\
\text{R} & \quad \text{H}_2\text{N} \quad \text{O} \\
\xrightarrow{4 \text{ hr.}, \text{RT}} \\
\text{O} & \quad \text{R} \quad \text{HO}_2\text{B(OH)}_2 \\
\end{align*}
\]

\( R = \text{Leu, Trp} \)

Scheme 1: Synthesis of Urea derivative Amino Acid
Materials: L-Tryptophan, L-Leucine KCNO are purchased from SRL and HAuCl₄ are purchased from Sigma-Aldrich.

Synthesis of Urea derivative: L-Amino Acid (1 mmol) was dissolved in hot H₂O. Then cooled it to 5°C and KCNO (6 mmol) was added to it slowly. After complete addition it was stirred for another 4 hours. Then cooled it to 5°C and acidified it to pH = 1. A white precipitation was observed. Filtered the precipitate and dried it in vacuum desiccator.

(a) Urea modified tryptophan

¹H NMR (400MHz, DMSO-d₆, δ in ppm): 10.84 (s, 1H, -ArNH), 7.49 (d, 1H, -ArNH J = 7.63), 7.32(d, 1H, -ArH, J = 8.39), 7.09 (d, 2H, -ArH, J = 7.59), 6.95 (d, 1H, -ArH, J = 7.63), 6.09 (d, 1H, -NH, J = 8.39), 5.59 (s, 2H, -NH₂), 4.36 (m, 1H, -CH), 3.07 (m, 2H, -CH₂);

¹³C NMR (100MHz, DMSO-d₆, δ in ppm): 174.29, 163.27, 136.07, 127.60, 124.20, 123.71, 120.97, 118.33, 111.32, 109.58, 106.55, 53.0876, 27.73.

FT-IR (KBr): 3430, 3388, 3221, 1709, 1651, 1540, 1241 and 740 cm⁻¹.

ESI-MS: m/z 175.1202 [M+H]+; Mcalcd: 175.1224, 213.0808 [M+K]+; Mcalcd: 213.1002, 349.2479 [2M+H]+; Mcalcd: 349.2411,

(a) Urea modified leucine

¹H NMR (400MHz, DMSO-d₆, δ in ppm) (Figure 7): 6.19 (d, 1H, -NH, J = 6.8), 5.54 (s, 2H, -NH₂), 4.05 (t, 1H, -CH₂JCH₂, J = 4.04), 1.44 - 1.4 (m, 2H, -CH₂), 0.87 (m, 6H, -CH₃).

¹³C NMR (100MHz, DMSO-d₆, δ in ppm) (Figure 8): 172.46, 162.77, 47.93, 38.17, 21.39, 19.93, 18.69.

FT-IR (KBr): 3460, 3293, 2959, 1691, 1640, 1571, 1311, 1017 and 719 cm⁻¹,

ESI-MS: m/z 247.527 [M]+; Mcalcd: 247.4987,
Figure S5: $^1$HNMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 1.

Figure S6: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 1.
Figure S7: FT-IR Spectra of Compound 1

Figure S8: ESI-MS Spectra of Compound 1
Figure S9: $^1$H NMR (400 MHz, DMSO-$d_6$) spectra of Compound 2.

Figure S10: $^{13}$C NMR (100 MHz, DMSO-$d_6$) spectra of Compound 2.
Figure S11: FT-IR Spectra of Compound 2

Figure S12: ESI-MS Spectra of Compound 2
Suzuki–Miyaura cross-coupling reaction:
A mixture of aryl halide (1 mmol), Phenylboronic acid (1.5 mmol) and K₂CO₃ (3 mmol) was dissolved in H₂O in a 15 mL round bottomed flask. Aqueous compound 1-gold nanoparticles (0.01 mol %) catalytic solution was added to it and the mixture was stirred for a time period and temperature as mentioned in Table 1. The progress of the reaction was monitored by TLC. After completion of the reaction and acidified it with 2(N) HCl product was precipitated out for 3a-c, 3f-h, 3k and separate layer separated out for 3d,e,i,j. The products were characterized by IR, ¹H NMR, ¹³C NMR and ESI–MS.

Biphenyl-4-carboxylic Acid (3a).
White solid, 198 mg, 98.37 % yield; m.p.: 185°C.

¹H NMR (400 MHz, DMSO-d₆, δppm, 298 K): 12.93 [s, 1H, -CO₂H], 8.02 [d, 2H, J = 8.54, -Ar¹H], 7.79 [d, 2H, J = 7.93, -Ar¹H], 7.72 [d, 2H, J = 7.93, -Ar²H], 7.49 [d, 2H, J = 7.32, -Ar²H], 7.41 [t, 1H, J = 7.32, -Ar²H];

¹³C NMR (100 MHz, DMSO-d₆, δppm, 298 K): 144.33, 139.05, 130.01, 129.67, 129.32, 126.99, 126.85;

FT-IR (KBr): 2984, 2840, 2667, 2552, 1682, 1608, 1423, 1292, 936, 863, 752, 698 cm⁻¹;

ESI-MS: m/z 236.86 [M+K]⁺;  M_calcd:198.22.
Biphenyl-4-Carboxylic Acid (3b).
White solid, 325 mg, 78 % yield; m.p: 187°C.

$^1$H NMR (400 MHz, DMSO-δ$_6$, δ$_{ppm}$ 298 K): 12.91 [s, 1H, -CO$_2$H], 8.03 [d, 2H, J = 8.51, -Ar$_1$H], 7.79 [d, 2H, J = 7.95, -Ar$_1$H], 7.71 [d, 2H, J = 7.98, -Ar$_2$H], 7.49 [d, 2H, J = 7.30, -Ar$_2$H], 7.42 [t, 1H, J = 7.35, -Ar$_2$H];

$^{13}$C NMR (100 MHz, DMSO-δ$_6$, δ$_{ppm}$ 298 K): 144.34, 139.05, 130.08, 129.67, 129.32, 126.99, 126.85; 126.85;

FT-IR (KBr): 2987, 2837, 2670, 2542, 1688, 1612, 1428, 1295, 938, 869, 755, 698 cm$^{-1}$

ESI-MS: m/z 235.96 [M+K]$^+$; $M_{calc}$:198.22.

Biphenyl-2,4-diol (3c).
Light brown solid, 287 mg, 89.64 % yield; m.p: 285°C.

$^1$H NMR (400 MHz, CDCl$_3$, δ$_{ppm}$ 298 K): 8.25 [d, 1H, J = 6.71, -Ar$_2$H], 7.75 [d, 1H, J = 6.71, -Ar$_2$H], 7.61 [t, 1H, J = 7.32, -Ar$_2$H], 7.52 [t, 1H, J = 7.32, -Ar$_2$H], 7.42 [m, 1H, -Ar$_2$H], 7.14 [d, 1H, J = 9.16, -Ar$_1$H], 6.53 [d, 1H, J = 7.22, -Ar$_1$H], 6.38 [dd, 1H, J = 8.54, -Ar$_1$H], 5.6 [s, 1H, -OH], 5.3 [s, 1H, -OH];

$^{13}$C NMR (100 MHz, CDCl$_3$, δ$_{ppm}$ 298 K): 156.13, 152.40, 135.99, 133.80, 133.05, 129.67, 128.33, 111.96, 109.17, 103.87; 126.85;

FT-IR (KBr): 3442, 3315, 3074, 2927, 2851, 2362, 1603, 1442, 1342, 1310, 1159, 1084, 1023, 966, 834, 697, 579 cm$^{-1}$;

ESI-MS: m/z 225.14 [M+K]$^+$; $M_{calc}$:186.07.

1-(biphenyl-4-yl)ethanone (3d).
Light brown liquid, 288 mg, 88 % yield;

$^1$H NMR (400 MHz, DMSO-δ$_6$, δ$_{ppm}$ 298 K): 7.92 [d, 2H, J = 8.39, -Ar$_1$H], 7.79 [d, 2H, J = 6.87, -Ar$_1$H], 7.53 [d, 2H, J = 8.39, -Ar$_2$H], 7.36 [d, 2H, J = 6.87, -Ar$_2$H], 7.30 [t, 1H, J = 7.25, -Ar$_2$H], 2.54 [s, 3H, -CH$_3$];

$^{13}$C NMR (100 MHz, DMSO-δ$_6$, δ$_{ppm}$ 298 K): 197.16, 138.31, 135.25, 130.19, 128.90, 127.51, 26.80; 126.85;

FT-IR (KBr): 1680, 1585, 1446, 1395, 1359, 1260, 1093, 1010, 952, 825, 761, 697 cm$^{-1}$;

ESI-MS: m/z 219.91 [M+Na]$^+$; $M_{calc}$:196.09.
Biphenyl-2-carbaldehyde (3e).
Brown liquid, 270 mg, 96 % yield;

\(^1\text{H NMR (500 MHz, DMSO-d}_6, \delta_{\text{ppm}} 298 \text{ K}):\)
\[\begin{align*}
\text{10.34} & \text{[s, 1H, } -\text{CHO}], \\
\text{8.01} & \text{[d, 1H, } J = 6.62, -\text{Ar}^1\text{H}], \\
\text{7.86} & \text{[t, 1H, } J = 5.99, -\text{Ar}^1\text{H}], \\
\text{7.83} & \text{[d, 1H, } J = 7.25, -\text{Ar}^1\text{H}], \\
\text{7.67} & \text{[t, 2H, } J = 7.25, -\text{Ar}^1\text{H}], \\
\text{7.58} & \text{[d, 2H, } J = 7.25, -\text{Ar}^2\text{H}], \\
\text{7.50} & \text{[d, 2H, } J = 7.57, -\text{Ar}^2\text{H}], \\
\text{7.43} & \text{[m, 1H, } -\text{Ar}^2\text{H}].
\end{align*}\]

\(^{13}\text{C NMR (125 MHz, DMSO-d}_6, \delta_{\text{ppm}} 298 \text{ K}):\)
\[\begin{align*}
\text{189.86, 135.82, 134.42, 134.17, 130.78, 129.73,} \\
\text{127.92, 127.40 ; 126.85;}
\end{align*}\]

\(^\text{FT-IR (KBr)}:\)
\[\text{3646, 3050, 1780, 1690, 1591, 1443, 1302, 1271, 1182, 1111, 1069, 1051, 1028} \text{ cm}^{-1};
\]

\(^\text{ESI-MS:}\)
\[\text{m/z 221.02 [M+K]+;}\]
\[\text{M_{calcd}: 182.22.}\]
\[\text{\lambda = 193 nm (} \varepsilon = 2.67 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}), \]
\[\text{210 nm (} \varepsilon = 1.5 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}), \]
\[\text{249 nm (} \varepsilon = 4.17 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}).}\]

2,4-dimethoxy-6-phenyl-1,3,5-triazine (3f).

Light brown semisolid, 255 mg, 97 % yield;

\(^1\text{H NMR (400 MHz, DMSO-d}_6, \delta_{\text{ppm}} 298 \text{ K}):\)
\[\begin{align*}
\text{8.01} & \text{[d, 2H, } J = 7.63, -\text{Ar}^2\text{H}], \\
\text{7.85} & \text{[d, 2H, } J = 7.63, -\text{Ar}^2\text{H}], \\
\text{7.81} & \text{[t, 1H, } J = 6.10, -\text{Ar}^2\text{H}], \\
\text{3.91} & \text{[s, 6H, } -\text{OC}_3\text{H}_3].
\end{align*}\]

\(^{13}\text{C NMR (100 MHz, DMSO-d}_6, \delta_{\text{ppm}} 298 \text{ K}):\)
\[\begin{align*}
\text{173.17, 134.16, 130.88, 130.05, 127.42, 126.53} \\
\text{; 126.85;}
\end{align*}\]

\(^\text{FT-IR (KBr)}:\)
\[\text{3480, 3256, 3090, 2254, 2128, 1655, 1440, 1367, 1024, 996, 824, 767, 704, 643} \text{ cm}^{-1}\]

\(^\text{ESI-MS:}\)
\[\text{m/z 242.22 [M+Na]+;}\]
\[\text{M_{calcd}: 218.22.}\]

2-methoxy-4,6-diphenyl-1,3,5-triazine (3g).
Brown semisolid, 315 mg, 95 % yield;

\(^1\text{H NMR (400 MHz, DMSO-d}_6, \delta_{\text{ppm}} 298 \text{ K}):\)
\[\begin{align*}
\text{8.01} & \text{[d, 4H, } J = 7.63, -\text{Ar}^2\text{H}], \\
\text{7.85} & \text{[d, 4H, } J = 7.63, -\text{Ar}^2\text{H}], \\
\text{7.82} & \text{[t, 2H, } J = 6.10, -\text{Ar}^2\text{H}], \\
\text{3.92} & \text{[s, 3H, } -\text{OCH}_3].
\end{align*}\]

\(^{13}\text{C NMR (100 MHz, DMSO-d}_6, \delta_{\text{ppm}} 298 \text{ K}):\)
\[\begin{align*}
\text{173.16, 134.16, 130.88, 130.06, 127.42, 126.53} \\
\text{; 126.85;}
\end{align*}\]

\(^\text{FT-IR (KBr)}:\)
\[\text{301.07 [M+K]+;}\]
\[\text{M_{calcd}: 263.29.}\]

2,4,6-triphenyl-1,3,5-triazine (3h).
Brown semisolid, 375 mg, 94 % yield;

$^1$H NMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K): 8.20-7.26 [m, 15H, -Ar$_2$H];

$^{13}$C NMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K): 177.88, 135.33, 133.33, 132.24, 128.04;

ESI-MS: m/z 310.36 [M+H]$^+$; $M_{calc}$: 309.22.

4-vinylbiphenyl (3i).

White liquid, 346 mg, 75 % yield;

$^1$H NMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K): 7.74 [d, 2H, $J = 8.24$, -Ar$_1$H], 7.66 [d, 2H, $J = 8.17$, -Ar$_1$H], 7.48 [d, 2H, $J = 8.11$, -Ar$_2$H], 7.38 [d, 2H, $J = 8.25$, -Ar$_2$H], 6.66 [t, 1H, $J = 17.92$, -CH$_2$], 5.84 [d, 1H, $J = 18.32$, -CH$_2$], 5.29 [d, 1H, $J = 8.44$, -CH$_2$];

$^{13}$C NMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K): 134.42, 134.26, 134.16, 130.88, 130.85, 127.59, 127.42, 126.53 ; 126.85;

FT-IR (KBr): 3490, 3370, 3252, 3107, 2382, 2258, 2127, 1649, 1025, 997, 824, 767, 474 cm$^{-1}$ ;

ESI-MS: m/z 181.25 [M+H]$^+$; $M_{calc}$: 180.25

5-nitrobiphenyl-3-carbaldehyde (3j).

Light brown solid, 243 mg, 81 % yield, m.p. 130°C;

$^1$H NMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K): 10.12 [s, 1H, -CHO], 8.66 [s, 1H, -Ar$_1$H], 8.49 [dd, 1H, $J = 8.77$, -Ar$_1$H], 8.30 [d, 1H, $J = 7.63$, - Ar$_1$H], 7.86 [t, 2H, $J = 8.01$, - Ar$_2$H], 7.77 [d, 1H, $J = 6.87$, - Ar$_2$H], 7.36 [d, 1H, $J = 5.34$, - Ar$_2$H], 7.30 [t, 1H, $J = 7.25$, - Ar$_2$H];

$^{13}$C NMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K): 191.79, 148.25, 137.17, 134.92, 134.10, 133.46, 130.95, 130.01, 128.54, 127.35, 124.05;

ESI-MS: m/z 225.16 [M]$^+$; $M_{calc}$: 225.22

4-phenylpyridine-2,6-dicarboxylic acid (3k).

White solid, 254.33 mg, 78 % yield, m.p. 281°C;

$^1$H NMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K): 11.95 [br, 2H, -CO$_2$H], 8.05 [s, 2H, -Ar$_1$H], 7.8 [t, 2H, $J = 8.77$, -Ar$_2$H], 7.32 [t, 2H, $J = 7.43$, - Ar$_2$H], 7.39 [t, 1H, $J = 7.25$, - Ar$_2$H];
\[^{13}\text{C NMR (100 MHz, DMSO-d}_6, \delta_{\text{ppm}, 298\text{ K})}: 172.09, 134.39, 134.14, 133.46, 130.06, 127.57, 127.39;\]

**ESI-MS:** m/z 522.37 [2M+K]\(^+\); \(M_{\text{calc}} = 243.05\).

**NMR experiments**

All NMR studies were carried out on a Brüker AVANCE 500 MHz spectrometer and Jeol 400 MHz at 278 K. Compound concentrations were in the range 1–10 mM in CDCl\(_3\) and (CD\(_3\))\(_2\)SO.

**FT-IR spectroscopy.**

All reported solid-state FTIR spectra were obtained with a Perkin Elmer Spectrum RX1 spectrophotometer with the KBr disk technique.

**Mass spectrometry.**

Mass spectra were recorded on a Q-Tof Micro YA263 high-resolution (Waters Corporation) mass spectrometer by positive-mode electrospray ionization.
Figure S13: $^1$HNMR (400 MHz, DMSO-d$_6$, $\delta$ ppm, 298 K) spectra of Compound 3a.

Figure S14: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta$ ppm, 298 K) spectra of Compound 3a.
Figure S15: FT-IR Spectra of Compound 3a

Figure S16: ESI-MS Spectra of Compound 3a
Figure S17: $^1$HNMR (400 MHz, DMSO-d$_6$, $\delta$ppm, 298 K) spectra of Compound 3b.

Figure S18: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta$ppm, 298 K) spectra of Compound 3b.
Figure S19: FT-IR Spectra of Compound 3b.

Figure S20: ESI-MS Spectra of Compound 3b.
Figure S20: $^1$HNMR (400 MHz, CDCl$_3$, $\delta_{\text{ppm}}$, 298 K) spectra of Compound 3c.

Figure S22: $^{13}$CNMR (100 MHz, CDCl$_3$, $\delta_{\text{ppm}}$, 298 K) spectra of Compound 3c.
Figure S23: FT-IR Spectra of Compound 3c.

Figure S24: ESI-MS Spectra of Compound 3c.
ESI Figure S25: $^1$HNMR (400 MHz, DMSO-$d_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3d.

Figure S26: $^{13}$CNMR (100 MHz, DMSO-$d_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3d.
Figure S27: FT-IR Spectra of Compound 3d.

ESI Figure S28: ESI-MS Spectra of Compound 3d.
**ESI Figure S29:** $^1$HNMR (500 MHz, DMSO-$d_6$, $\delta_{\text{ppm}}$, 298 K) spectra of Compound 3e.

**Figure S30:** $^{13}$CNMR (125 MHz, DMSO-$d_6$, $\delta_{\text{ppm}}$, 298 K) spectra of Compound 3e.
Figure S31: FT-IR Spectra of Compound 3e.

Figure S32: ESI-MS Spectra of Compound 3e.
Figure S33: $^1$HNMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3f.

Figure S34: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3f.
Figure S35: FT-IR Spectra of Compound 3f.

Figure S36: ESI-MS Spectra of Compound 3f.
Figure S37: $^1$HNMR (500 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3g.

Figure S38: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3g.
Figure S39: ESI-MS Spectra of Compound 3g.

Figure S40: $^1$HNMR (400 MHz, DMSO-$d_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3h.
Figure S41: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta$ppm, 298 K) spectra of Compound 3h.

Figure S42: ESI-MS Spectra of Compound 3h.
Figure S43: $^1$HNMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3i.

Figure S44: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3i.
Figure S45: FT-IR Spectra of Compound 3i.

Figure S46: ESI-MS Spectra of Compound 3i.
Figure S47: $^1$HNMR (400 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3j.

Figure S48: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3j.
Figure S49: ESI-MS Spectra of Compound 3j.
DMSO-d$_6$, $\delta_{ppm}$, 298 K) spectra of Compound 3k.

**Figure S50:** $^1$HNMR (400 MHz,
Figure S51: $^{13}$CNMR (100 MHz, DMSO-d$_6$, $\delta$ppm, 298 K) spectra of Compound 3k.

Figure S52: ESI-MS Spectra of Compound 3k.
ESI-Table 1: Hydrogen bonding parameters in crystal structure of urea modified leucine.

<table>
<thead>
<tr>
<th>D-H....A</th>
<th>D-H</th>
<th>H.....A</th>
<th>D........A</th>
<th>D-H..A(°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N(1) --H(1A) ..O(2) a</td>
<td>0.86</td>
<td>2.24</td>
<td>3.1</td>
<td>175</td>
</tr>
<tr>
<td>N(2) --H(2) ..O(2) c</td>
<td>0.86</td>
<td>2.27</td>
<td>2.905</td>
<td>131</td>
</tr>
<tr>
<td>O(3) --H(3) ..O(1) b</td>
<td>0.82</td>
<td>1.73</td>
<td>2.523</td>
<td>162</td>
</tr>
</tbody>
</table>

Symmetry equivalent:  
a = 1-x,-1/2+y,3/2-z,  
b = 1-x,1/2+y,3/2-z,  
c = -1+x,y,z

Table 2: Torsional angle parameter of urea modified leucine.

<table>
<thead>
<tr>
<th>C1-N2-C2-C3</th>
<th>φ(°)</th>
<th>ψ(°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-65.49</td>
<td>N2-C2-C3-O3</td>
<td>-35.91</td>
</tr>
</tbody>
</table>

Table 3: Crystallographic Parameters of Compound 2.

<table>
<thead>
<tr>
<th>Empirical formula</th>
<th>C_7H_{14}N_2O_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula weight</td>
<td>174.20</td>
</tr>
<tr>
<td>Temperature/K</td>
<td>198(140)</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Orthorhombic</td>
</tr>
<tr>
<td>Space group</td>
<td>P2₁2₁2₁</td>
</tr>
<tr>
<td>a/Å</td>
<td>5.2432(9)</td>
</tr>
<tr>
<td>b/Å</td>
<td>10.3449(19)</td>
</tr>
<tr>
<td>c/Å</td>
<td>17.386(4)</td>
</tr>
<tr>
<td>α/°</td>
<td>90</td>
</tr>
<tr>
<td>β/°</td>
<td>90</td>
</tr>
<tr>
<td>γ/°</td>
<td>90</td>
</tr>
<tr>
<td>Volume/Å³</td>
<td>943.0(3)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>ρ(calc) g/cm³</td>
<td>1.227</td>
</tr>
<tr>
<td>μ/mm⁻¹</td>
<td>0.096</td>
</tr>
<tr>
<td>F(000)</td>
<td>376.0</td>
</tr>
<tr>
<td>Crystal size/mm³</td>
<td>0.2589 × 0.2489 × 0.2209</td>
</tr>
<tr>
<td>---------------------------</td>
<td>--------------------------</td>
</tr>
<tr>
<td>Radiation</td>
<td>MoKα (λ = 0.71073)</td>
</tr>
<tr>
<td>2Θ range for data collection/°</td>
<td>4.582 to 50.014</td>
</tr>
<tr>
<td>Index ranges</td>
<td>-6 ≤ h ≤ 6, -12 ≤ k ≤ 12, -17 ≤ l ≤ 20</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>3782</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>1659 [R_{int} = 0.0788, R_{sigma} = 0.0906]</td>
</tr>
<tr>
<td>Data/restraints/parameters</td>
<td>1659/0/113</td>
</tr>
<tr>
<td>Goodness-of-fit on F²</td>
<td>1.073</td>
</tr>
<tr>
<td>Final R indexes [I&gt;=2σ (I)]</td>
<td>R₁ = 0.0676, wR₂ = 0.1787</td>
</tr>
<tr>
<td>Final R indexes [all data]</td>
<td>R₁ = 0.0774, wR₂ = 0.1915</td>
</tr>
<tr>
<td>Largest diff. peak/hole / e Å⁻³</td>
<td>0.40/-0.43</td>
</tr>
<tr>
<td>Flack parameter</td>
<td>-2.7(10)</td>
</tr>
</tbody>
</table>

**Fig. S53:** ¹H NMR Spectra of a) 4-Bromo Benzoic Acid, b) Phenyl Boronic Acid, c) After 1ˢᵗ catalytic Cycle, d) After 2ⁿᵈ catalytic Cycle, e) After 3ʳᵈ catalytic Cycle, f) compound 5.
Figure S54: AFM image and height profile diagram of the gold nanoparticles.