Electronic supplementary information (ESI)

Enantioselective Friedel-Crafts reactions in water catalyzed by human telomeric G-quadruplex metalloenzyme

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Table of Contents

General remarks

Circular dichroism (CD) spectra were recorded on a dual beam DSM 1000 CD spectrophotometer (Olis, Bogart, GA) with a 10 mm quartz cell. Samples containing 10 μM oligomer were prepared and treated as described above before collecting CD spectra. Each measurement was recorded from 230 to 320 nm at room temperature (about 20 ^{o}C). The average scan for each sample was subtracted by a background CD spectrum of corresponding buffer solution. ^{1}H-NMR spectrum was recorded on a Bruker DRX 400 MHz type (^{1}H, 400 MHz) with an internal reference tetramethylsilane. Data for ^{1}H NMR spectra were recorded as follows: chemical shift (δ, ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), intergration, coupling constant (Hz). High-performance liquid chromatography (HPLC) analysis was performed on an Agilent 1100 Series instrument with the eluents of hexane and isopropanol (*i*-PrOH), using a Daicel Chiralpak AD Column (250 × 4.6 mm) and Daicel Chiralcel OD Column (250 × 4.6 mm).

Materials

DNA oligodeoxynucleotides: 5'-$G_3(TTAG_3)_3$-3' (ODN-**1**), 5'-$G_3(TTTG_3)_3$-3' (ODN-**2**), 5'-$G_3(ATAG_3)_3$-3' (ODN-**3**), 5'-$G_3(TATG_3)_3$-3' (ODN-**4**), 5'-$G_3(AAAG_3)_3$-3' (ODN-**5**), 5'-$G_3(AATG_3)_3$-3' (ODN-**6**), 5'-$T_3(TTAT_3)_3$-3' (ODN-**7**), 5'-$A_3(TTAA_3)_3$-3' (ODN-**8**), 5'-$(TTA)_7$-3' (ODN-**9**) and 3-(N-morpholino)propanesulfonic acid (MOPS) were purchased from Sangon (Shanghai, China), and the strand concentrations were determined by measuring the absorbance at 260 nm using the extinction coefficient values published in the literature.[1] $Cu(NO_3)_2 \cdot 3H_2O$ (>99%), $Zn(NO_3)_2 \cdot 6H_2O$ (>99%), $Co(NO_3)_2 \cdot 6H_2O$ (>99%), $Ni(NO_3)_2 \cdot 6H_2O$ (>99%), NaCl (>99%), KCl (>99%) and PEG200 were purchased from Alfa Aesar (Tianjin, China). 5-methoxyindole (98%), indole (99%), 5-chloroindole (98%), 1-methylindole (98%) and 1-methylindole (98%) were purchased from J&K (Beijing, China). Water was distilled and deionized using a Milli-Q A10 water purification system. Other reagents and solvents were obtained from commercial sources and used without further purification. α,β-unsaturated 2-acyl imidazoles **1a-e** were prepared according to the literature.[2,3]

Typical procedure

To a MOPS buffer (1 mL, 20 mM, pH 6.5) containing NaCl (50 mM), an aqueous solution of ODN-**1** (5'-$G_3(TTAG_3)_3$-3', final conc. 100 μM) was added. After stirred for a half hour at 4 °C, a solution of $Cu(NO_3)_2$ (2 μL of a 25 mM solution, final conc. 50 μM) was added. Then, 2-acyl imidazole **1a** in DMSO (10 μL of a 0.1 M solution) was added. The reaction was initiated by addition of nucleophile **2a** in DMSO (10 μL of a 0.5 M solution, 5 equiv.) and the mixture was stirred for 24 hours, followed by the extraction with ethyl acetate (3 × 5 mL), and the solvent was removed under reduced pressure. After a short flash chromatography, the residue was directly analyzed by ^{1}H-NMR and HPLC.[4,5]

Calculation the conversion of 1a[6]

Conversions of **1a** were calculated using the following formula:

Conversion of **1a** (%) = $PA_{3a}/(PA_{3a} + PA_{1a}/f)$ **Scheme S1**

Where PA_{1a} and PA_{3a} are the peak areas of **1a** and **3a**, respectively. And *f* is the correction factor determined to be 1.27 from a fitting curve (Fig. S1).

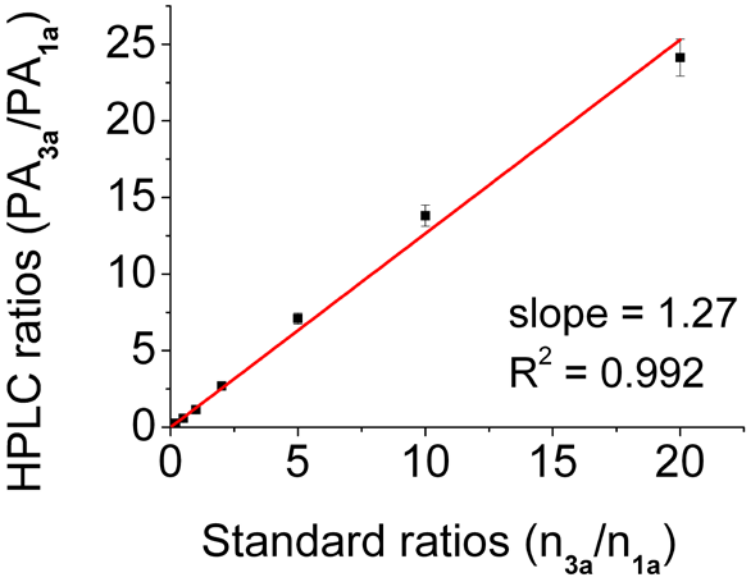


Fig. S1 Determination of the correction factor. The HPLC ratios of peak areas (PA_{3a}/PA_{1a}) were determined with the standard molar ratios (n_{3a}/n_{1a}) of 1/20, 1/10, 1/5, 1/2, 1, 2, 5, 10, 20. The correction factor (f = 1.27) was estimated from the fitting curve (R^2 = 0.992).

Table S1 Enantioselective Friedel-Crafts reactions catalyzed by ODN-**1**-Cu^{2+} by tuning the concentration of K^+ ions

[a] Unless otherwise noted, all reactions were carried out in a typical procedure. [b] Determined by chiral-phase HPLC for the crude product (Scheme S1, ESI†). [c] Determined by chiral-phase HPLC.

Table S2 Enantioselective Friedel-Crafts reactions catalyzed by ODN-**1**-Cu^{2+} by varying the amount of PEG200

[a] Unless otherwise noted, all reactions were carried out in a typical procedure. [b] Determined by chiral-phase HPLC for the crude product (Scheme S1, ESI†). [c] Determined by chiral-phase HPLC.

Table S3 Enantioselective Friedel-Crafts reactions catalyzed by various 21mer oligodeoxynucleotides combining with Cu^{2+} ions

[a] Unless otherwise noted, all reactions were carried out in a typical procedure. [b] Determined by chiral-phase HPLC for the crude product (Scheme S1, ESI†). [c] Determined by chiral-phase HPLC.

References

1 N. Kumar and S. Maiti, *Nucleic Acid Res.*, 2005, **33**, 6723.

2 D. A. Evans, K. R. Fandrick and H. J. Song, *J. Am. Chem. Soc.*, 2005, **127**, 8942.

3 M. C. Myers, A. R. Bharadwaj, B. C. Milgram and K. A. Scheidt, *J. Am. Chem. Soc.*, 2005, **127**, 14675.

4 A. J. Boersma, B. L. Feringa and G. Roelfes, *Angew. Chem., Int. Ed.*, 2009, **48**, 3346.

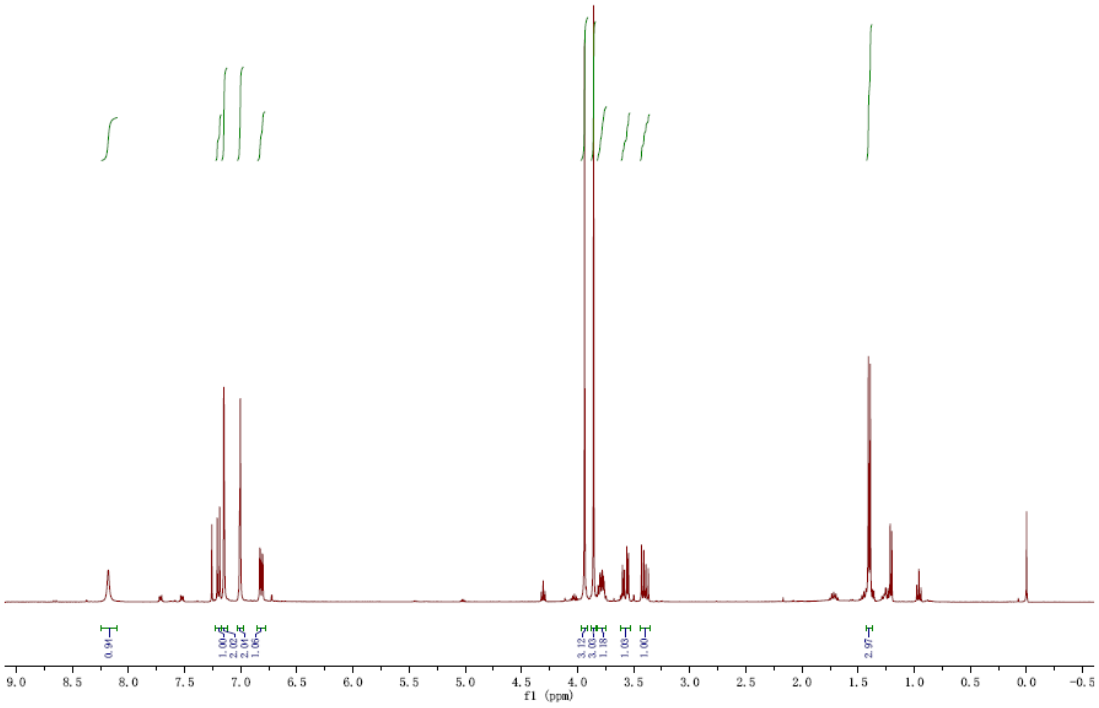
5 E. W. Dijk, A. J. Boersma, B. L. Feringa and G. Roelfes, *Org. Biomol. Chem.*, 2010, **8**, 3868.

6 N. S. Oltra and G. Roelfes, *Chem. Commun.*, 2008, 6039.

^{1}H-NMR spectra and HPLC traces

3-(5-methoxy-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (3a).

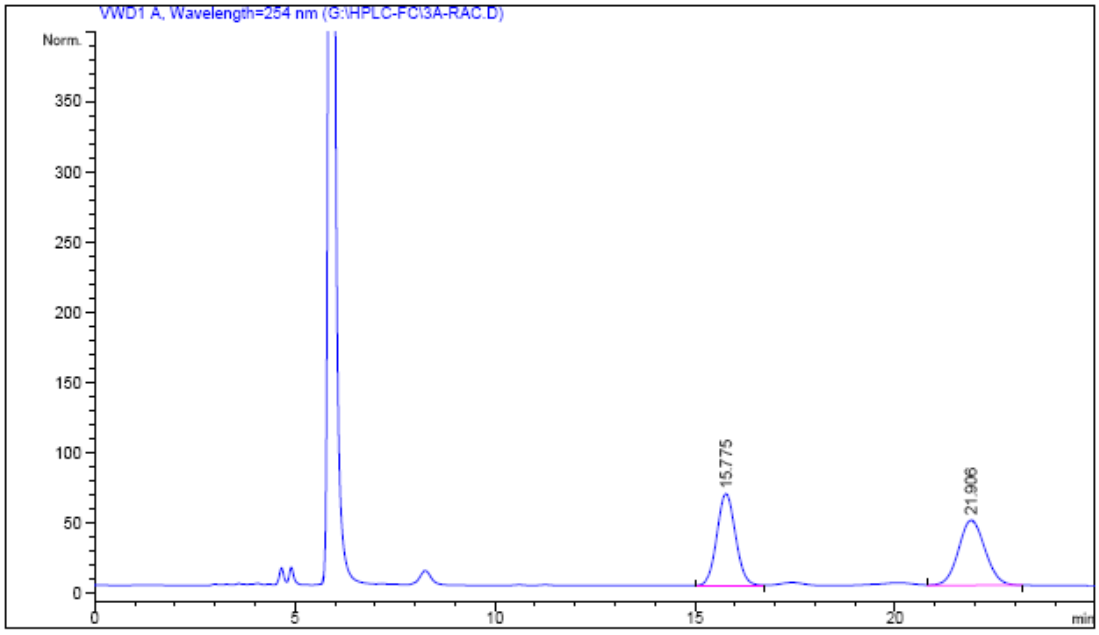
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.40 (d, *J* = 6.9 Hz, 3H), 3.40 (dd, *J* = 15.6, 8.4 Hz, 1H), 3.57 (dd, *J* = 15.6, 6.1 Hz, 1H), 3.77-3.82 (m, 1H), 3.86 (s, 3H), 3.94 (s, 3H), 6.82 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.01 (d, *J* = 2.7 Hz, 2H), 7.15 (s, 2H), 7.20 (d, *J* = 8.8 Hz, 1H), 8.18 (s, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 80:20, 1.0 mL/min, 254 nm.

Racemic **3a**.

Retention times: 15.8 (+) and 21.9 (-) mins.

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Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
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   1  15.775 BB    0.5048 2129.43652   65.44415  49.7794
   2  21.906 VB    0.7208 2148.31177   46.39069  50.2206

Totals :                  4277.74829  111.83483

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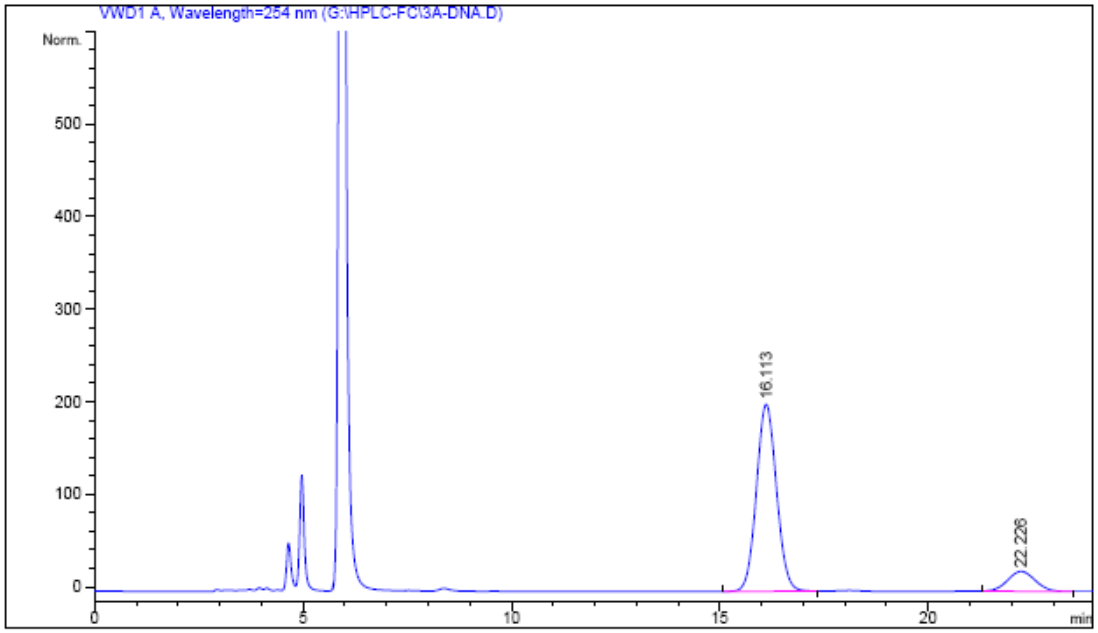
Product **3a** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (75% ee).

Retention times: 16.1 (+) and 22.2 (-) mins.

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Signal 1: VWD1 A, Wavelength=254 nm

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----|-------|----|-------|----------|----------|--------|
   1  16.113 BB    0.5219 6768.43994  202.01192  87.2538
   2  22.226 BB    0.7231  988.74414   21.49168  12.7462

Totals :                  7757.18408  223.50360

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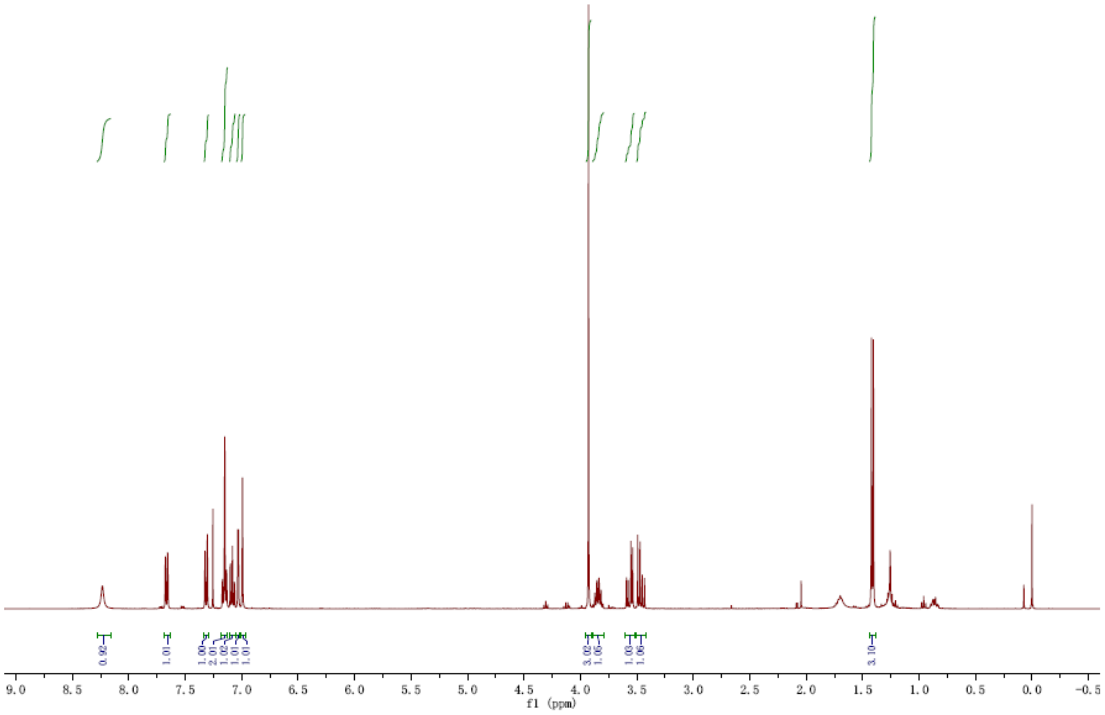
3-(1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (3b).

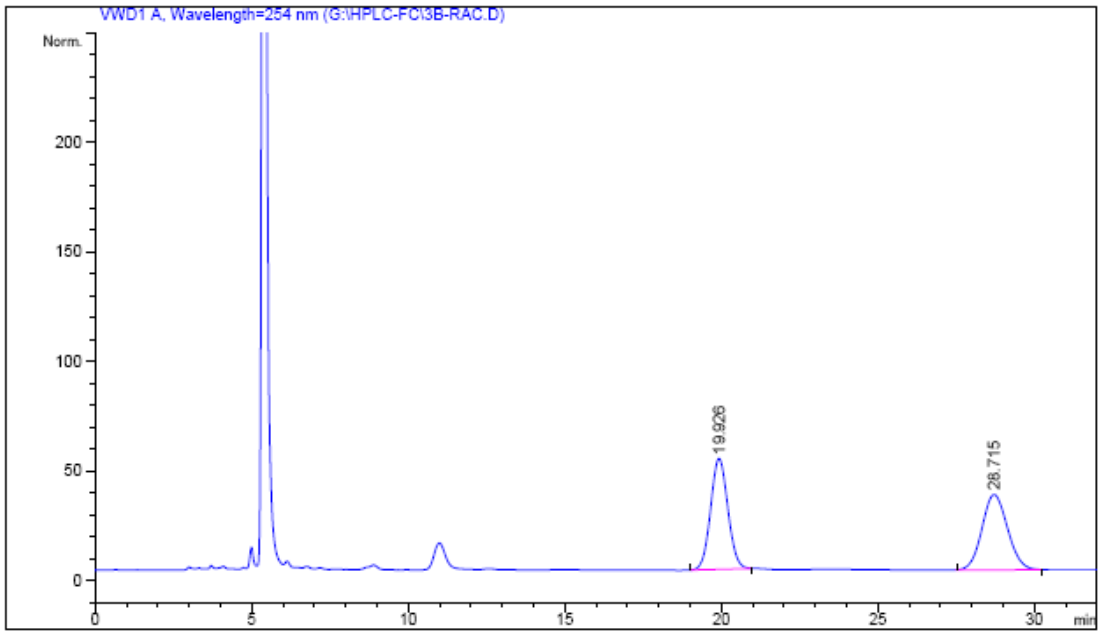
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.41 (d, *J* = 6.9 Hz, 3H), 3.46 (dd, *J* = 15.9, 8.2 Hz, 1H), 3.56 (dd, *J* = 15.9, 6.3 Hz, 1H), 3.93 (s, 3H), 6.99 (s, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.11–7.06 (m, 1H), 7.18–7.12 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 8.23 (s, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 85:15, 1.0 mL/min, 254 nm.

Racemic **3b**.

Retention times: 19.9 (+) and 28.7 (-) mins.

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Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  19.926 BB    0.5985 1941.53918   50.66333  49.7853
   2  28.715 BB    0.8849 1958.28259   34.42645  50.2147

Totals :                  3899.82178   85.08978

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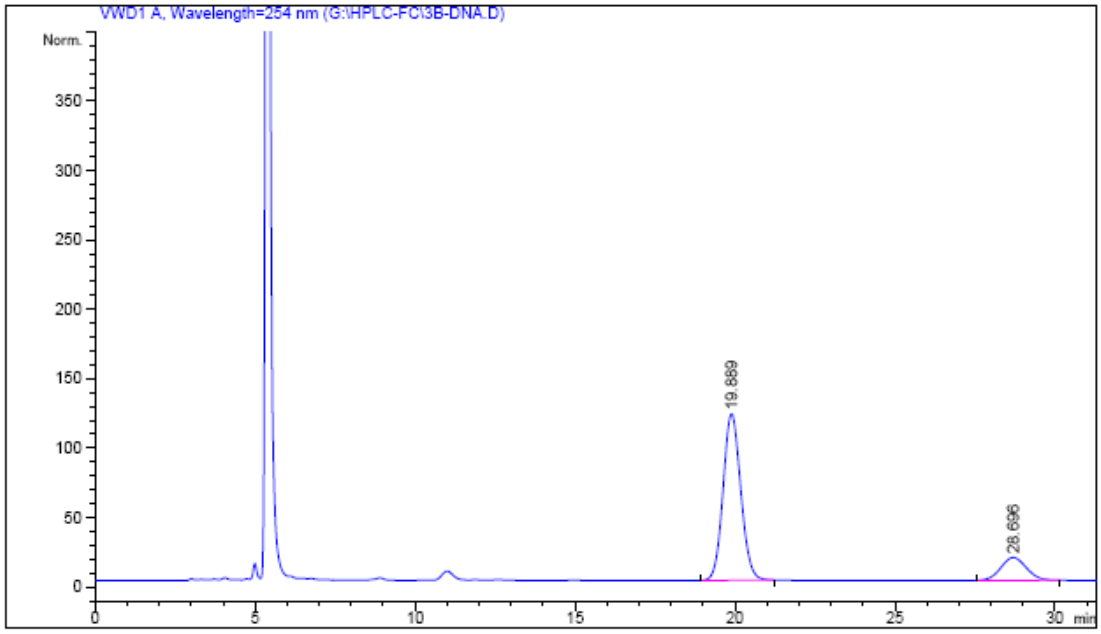
Product **3b** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (67% ee).

Retention times: 19.9 (+) and 28.7 (-) mins.

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Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  19.889 BB    0.5965 4619.33008  119.90215  83.4122
   2  28.696 BB    0.8477  918.62451   16.49621  16.5878

Totals :                  5537.95459  136.39836


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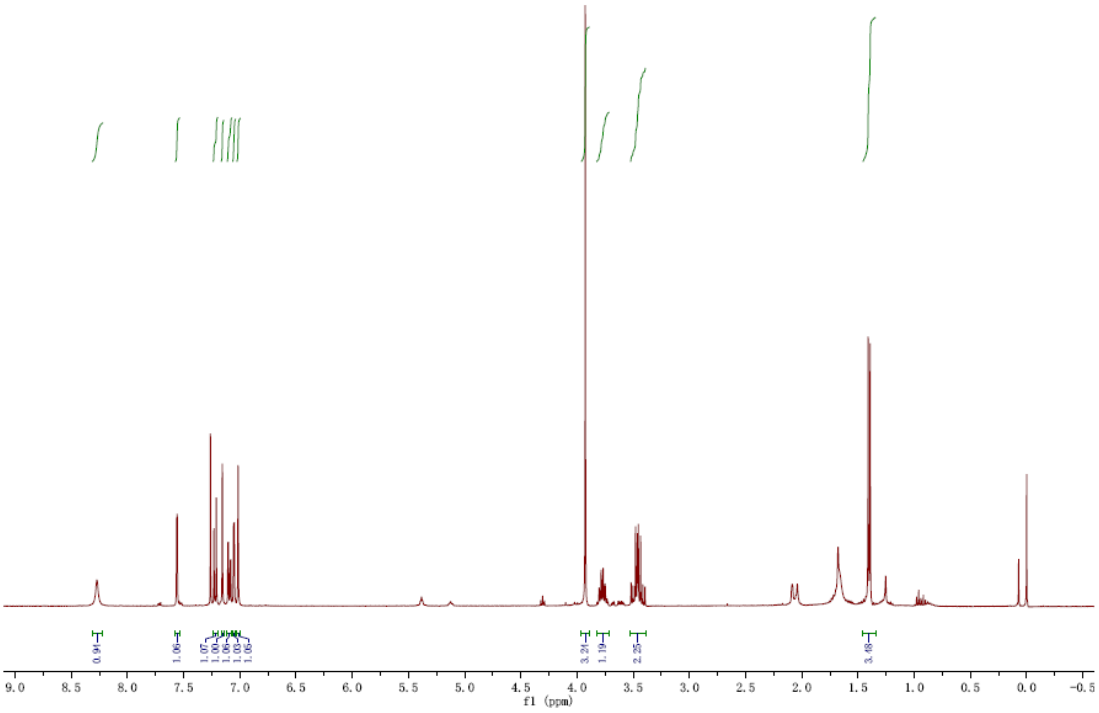
3-(5-chloro-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (3c).

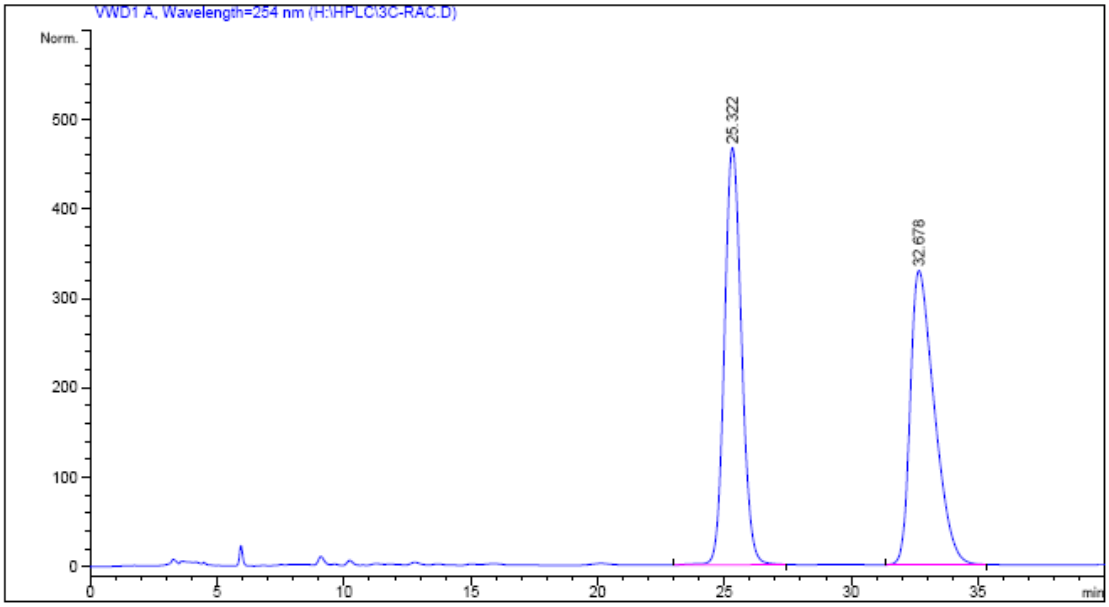
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.40 (d, *J* = 6.9 Hz, 3H), 3.46 (dd, *J* = 10.8, 7.3 Hz, 2H), 3.83–3.71 (m, 1H), 3.93 (s, 3H), 7.02 (s, 1H), 7.05 (d, *J* = 2.3 Hz, 1H), 7.10 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.16 (s, 1H), 7.22 (d, *J* = 8.6 Hz, 1H), 7.56 (d, *J* = 1.8 Hz, 1H), 8.31–8.22 (m, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 90:10, 1.0 mL/min, 254 nm.

Racemic **3c**.

Retention times: 25.3 (+) and 32.7 (-) mins.

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Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  25.322 BB    0.7256 2.17862e4   466.49615  50.0841
   2  32.678 BB    0.9897 2.17131e4   329.14279  49.9159

Totals :                  4.34993e4   795.63895

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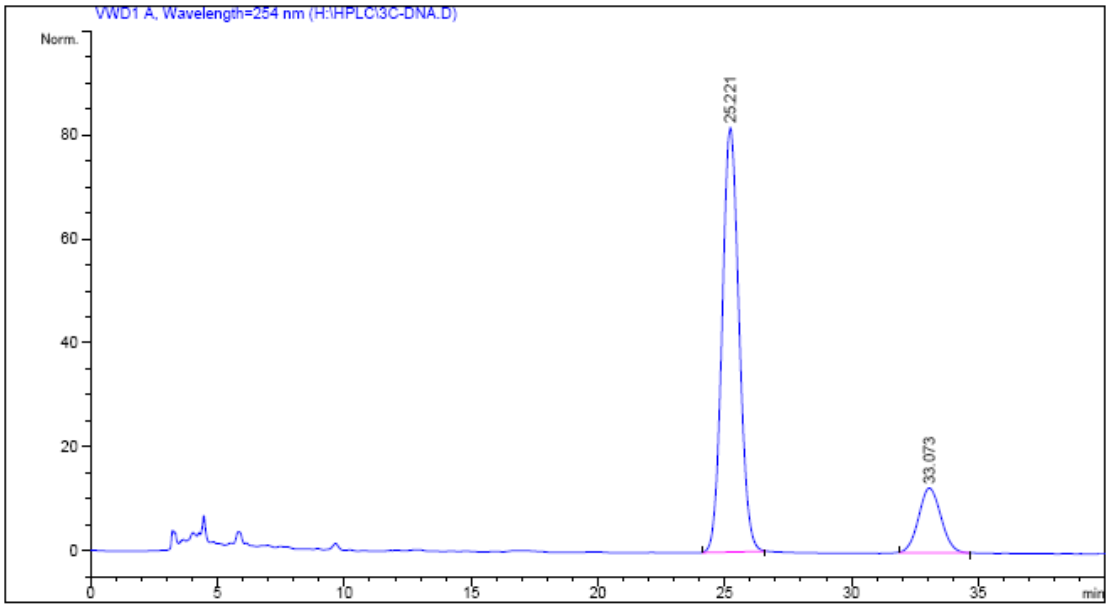
Product **3c** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (66% ee).

Retention times: 25.2 (+) and 33.1 (-) mins.

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Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  25.221 BB    0.7195 3786.17114   81.76723  83.2115
   2  33.073 BB    0.9421  763.88385   12.44414  16.7885

Totals :                  4550.05499   94.21137

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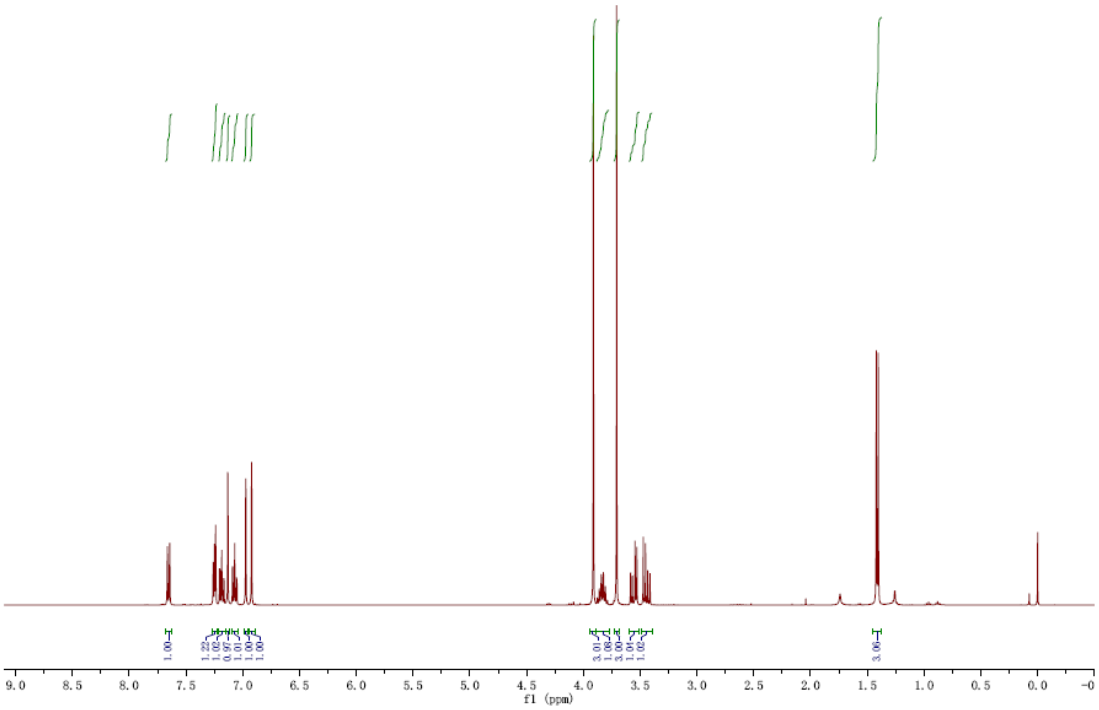
1-(1-methyl-1H-imidazol-2-yl)-3-(1-methyl-1H-indol-3-yl)butan-1-one (3d).

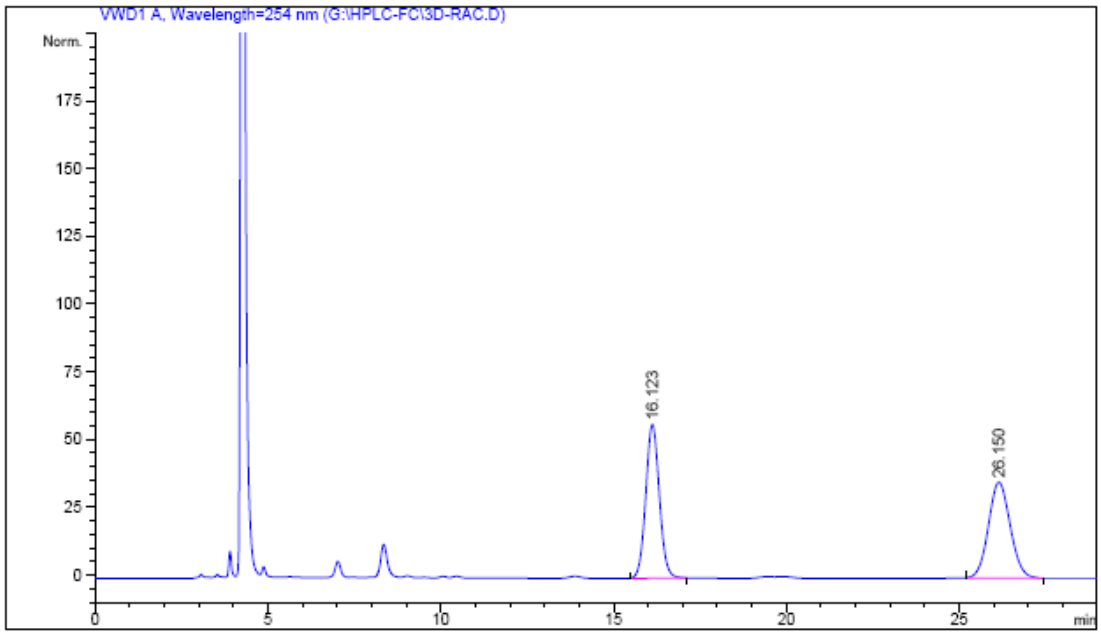
^{1}H-NMR ($CDCl_3$, 400 MHz) δ1.41 (d, *J* = 6.9 Hz, 3H), 3.44 (dd, *J* = 15.8, 8.0 Hz, 1H), 3.56 (dd, *J* = 15.8, 6.5 Hz, 1H), 3.71 (s, 3H), 3.83 (dd, *J* = 14.2, 7.0 Hz, 1H), 3.91 (s, 3H), 6.92 (s, 1H), 6.97 (s, 1H), 7.10–7.04 (m, 1H), 7.13 (d, *J* = 0.8 Hz, 1H), 7.21–7.15 (m, 1H), 7.27–7.23 (m, 1H), 7.65 (d, *J* = 7.9 Hz, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 95:5, 1.0 mL/min, 254 nm.

Racemic **3d**.

Retention times: 16.1 (-) and 26.2 (+) mins.

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Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  16.123 BB    0.4243 1553.19214   56.72754  50.1069
   2  26.150 BB    0.6796 1546.56458   35.33033  49.8931

Totals :                  3099.75671   92.05787

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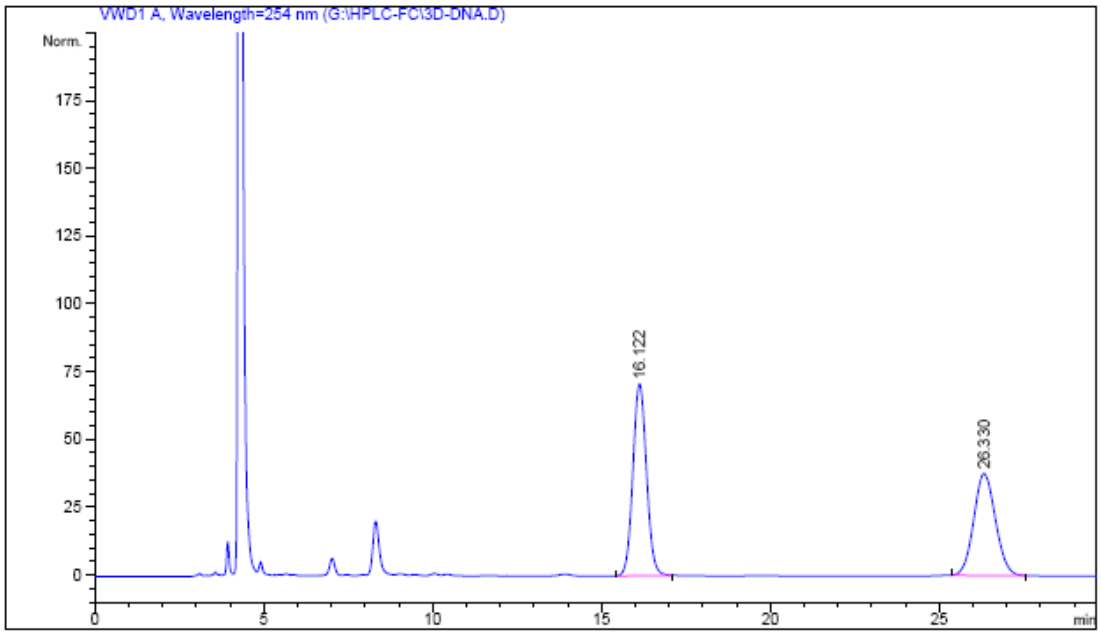
Product **3d** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (-8% ee).

Retention times: 16.1 (-) and 26.3 (+) mins.

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Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
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   1  16.122 BB    0.4374 1985.38806   70.88864  54.0762
   2  26.330 BB    0.6948 1686.07874   37.61511  45.9238

Totals :                  3671.46680  108.50375

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                        *** End of Report ***
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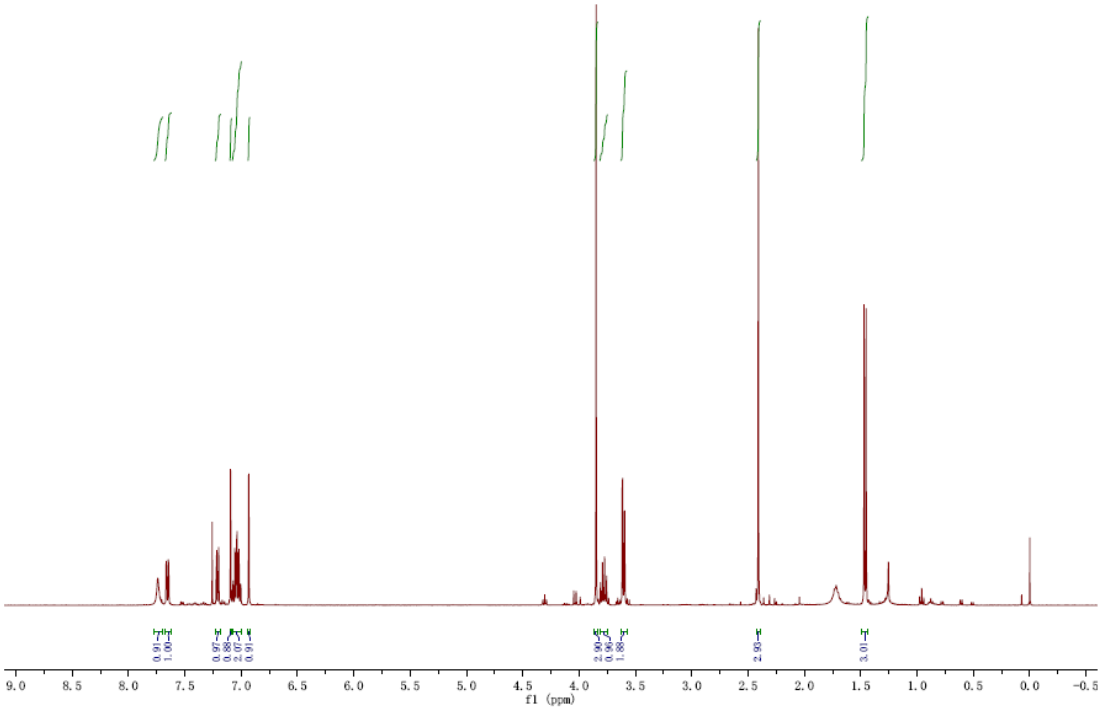
1-(1-methyl-1H-imidazol-2-yl)-3-(2-methyl-1H-indol-3-yl)butan-1-one (3e).

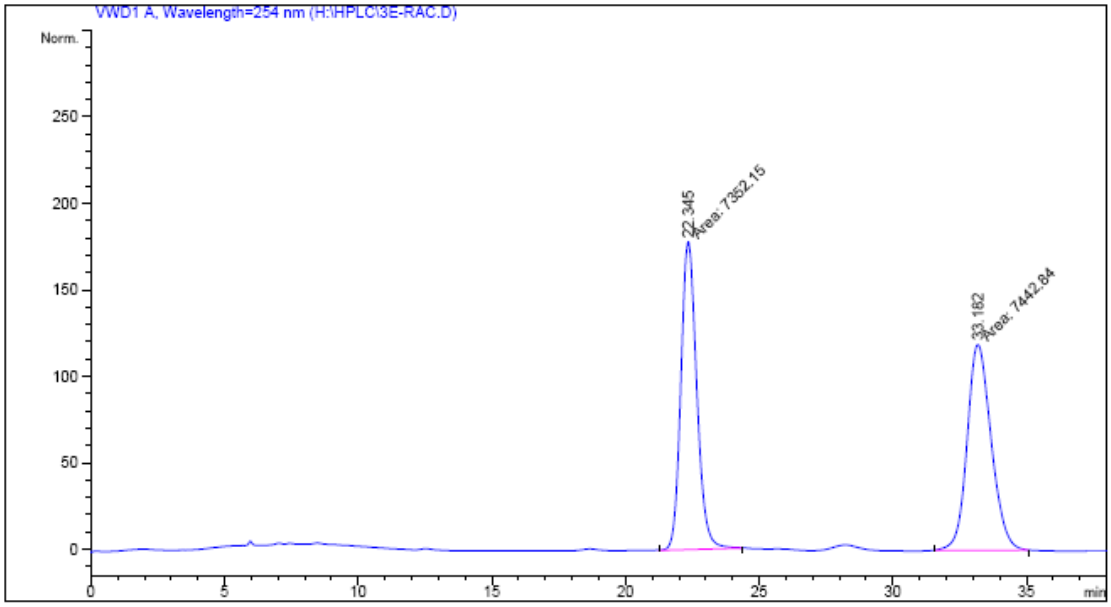
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.46 (d, *J* = 7.1 Hz, 3H), 2.41 (s, 3H), 3.61 (dd, *J* = 7.3, 1.7 Hz, 2H), 3.78 (dd, *J* = 14.7, 7.1 Hz, 1H), 3.85 (s, 3H), 6.93 (s, 1H), 7.08–7.00 (m, 2H), 7.09 (d, *J* = 0.8 Hz, 1H), 7.21 (dt, *J* = 8.1, 3.3 Hz, 1H), 7.65 (dd, *J* = 8.1, 6.7 Hz, 1H), 7.78–7.69 (m, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 85:15, 1.0 mL/min, 254 nm.

Racemic **3e**.

Retention times: 22.3 (-) and 33.2 (+) mins.

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Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  22.345 MM    0.6889 7352.15186  177.85948  49.6935
   2  33.182 MM    1.0436 7442.83643  118.86923  50.3065

Totals :                  1.47950e4   296.72871

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                      *** End of Report ***
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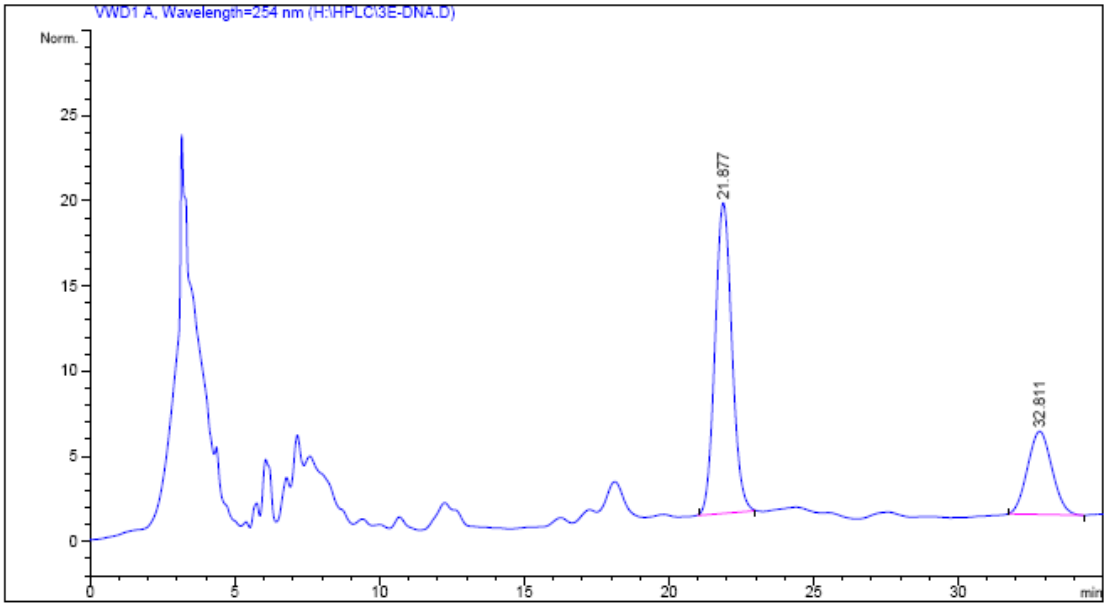
Product **3e** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (-44% ee).

Retention times: 21.9 (-) and 32.8 (+) mins.

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Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  21.877 BB    0.6299  742.38391   18.22075  72.1411
   2  32.811 BB    0.8585  286.68857    4.88252  27.8589

Totals :                  1029.07248   23.10326

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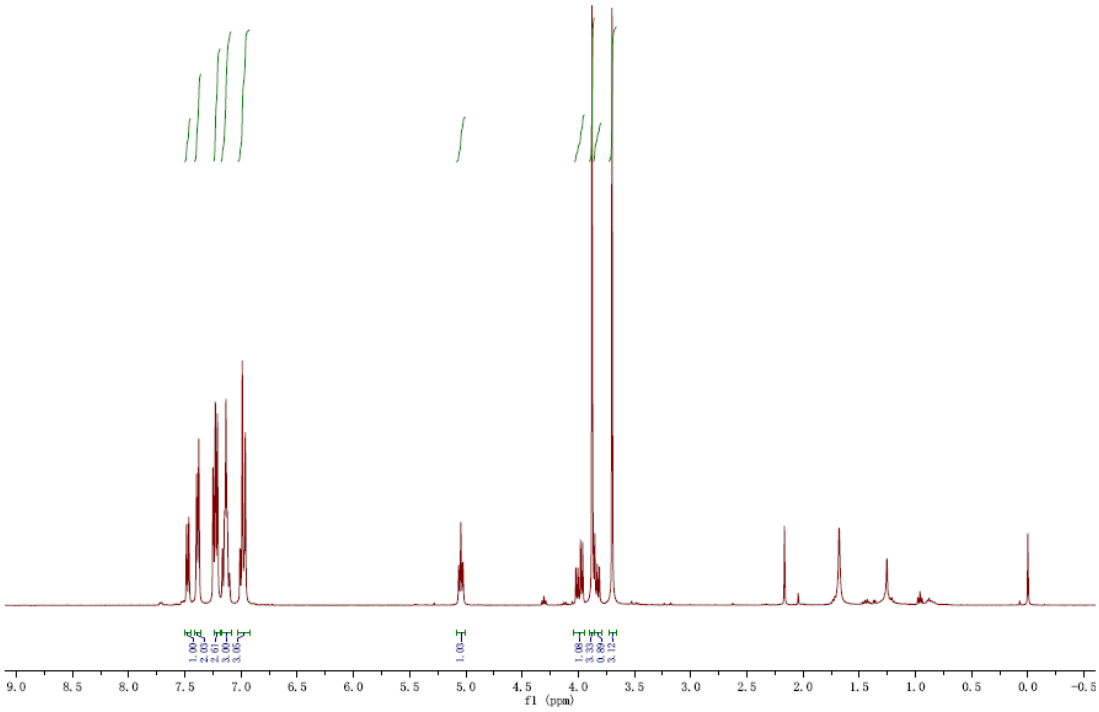
3-(5-methoxy-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)-3-phenyl-1-propanone (3f).

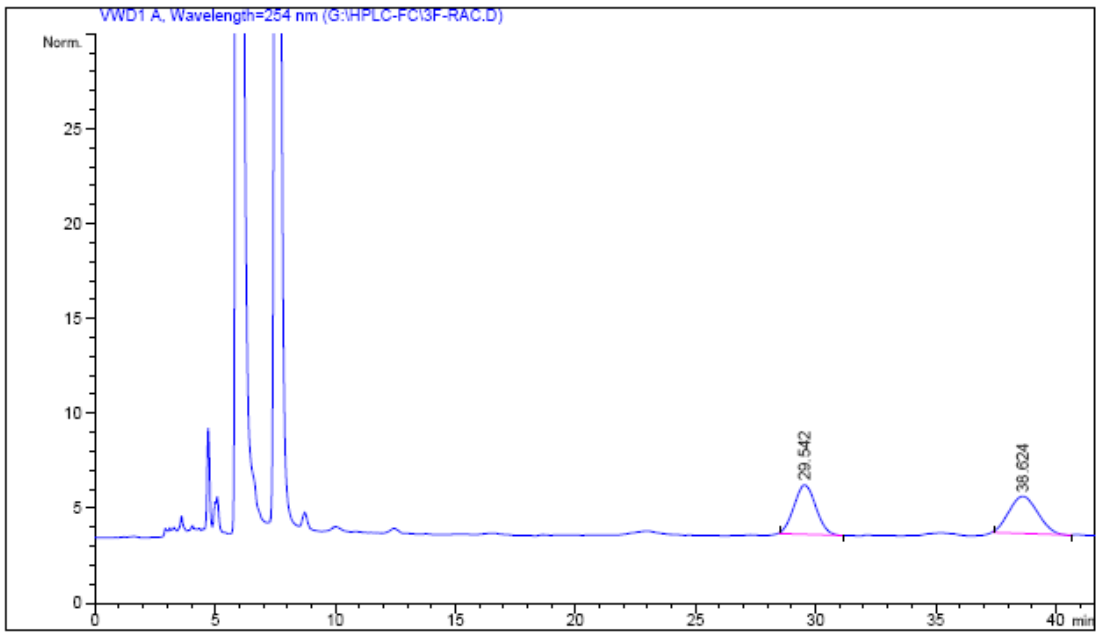
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.70 (s, 3H), 3.83 (dd, *J* = 16.4, 7.8 Hz, 1H), 3.88 (s, 3H), 3.99 (dd, *J* = 16.5, 7.5 Hz, 1H), 5.05 (t, *J* = 7.6 Hz, 1H), 6.98 (dd, *J* = 12.8, 6.2 Hz, 3H), 7.14 (dd, *J* = 11.2, 6.3 Hz, 3H), 7.22 (d, *J* = 7.4 Hz, 3H), 7.39 (d, *J* = 7.5 Hz, 2H), 7.48 (d, *J* = 7.9 Hz, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 80:20, 1.0 mL/min, 254 nm.

Racemic **3f**.

Retention times: 29.5 and 38.6 mins.

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=====================================================================
                      Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  29.542 BB    0.8192  164.92184    2.60316  50.3533
   2  38.624 BB    0.9805  162.60751    1.95514  49.6467

Totals :                   327.52936    4.55829

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                         *** End of Report ***
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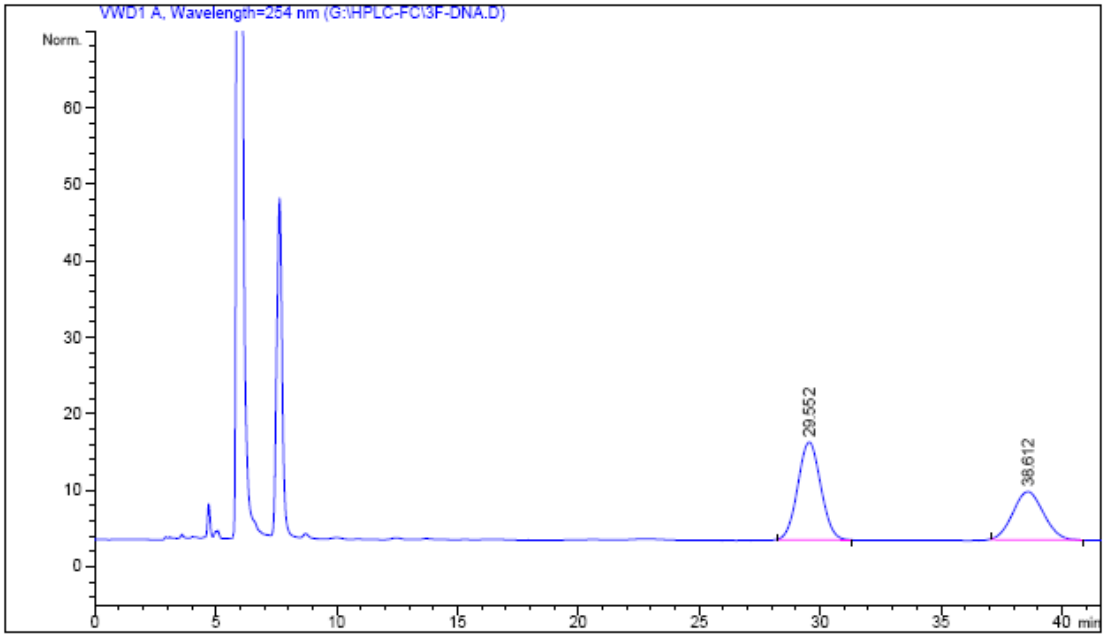
Product **3f** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (21% ee).

Retention times: 29.6 and 38.6 mins.

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                      Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  29.552 BB    1.0256  849.03088   12.80160  60.4565
   2  38.612 BB    1.2247  555.33667    6.29280  39.5435

Totals :                  1404.36755   19.09440


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                      *** End of Report ***
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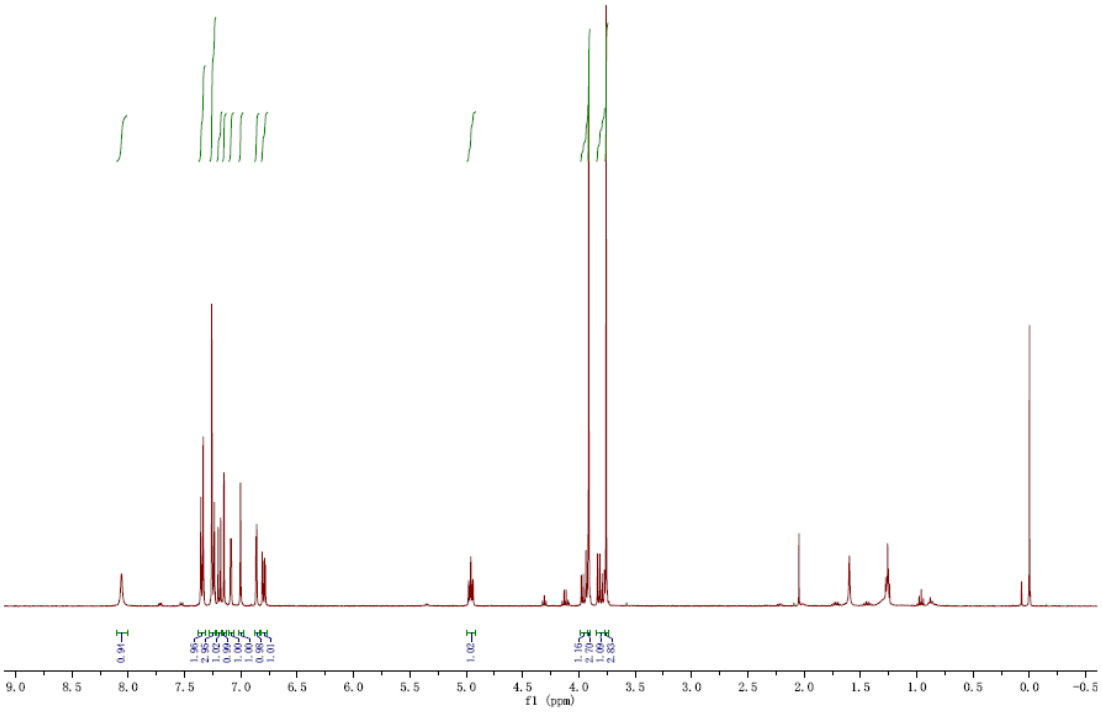
3-(4-bromophenyl)-3-(5-methoxy-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl) propan-1-one (3g).

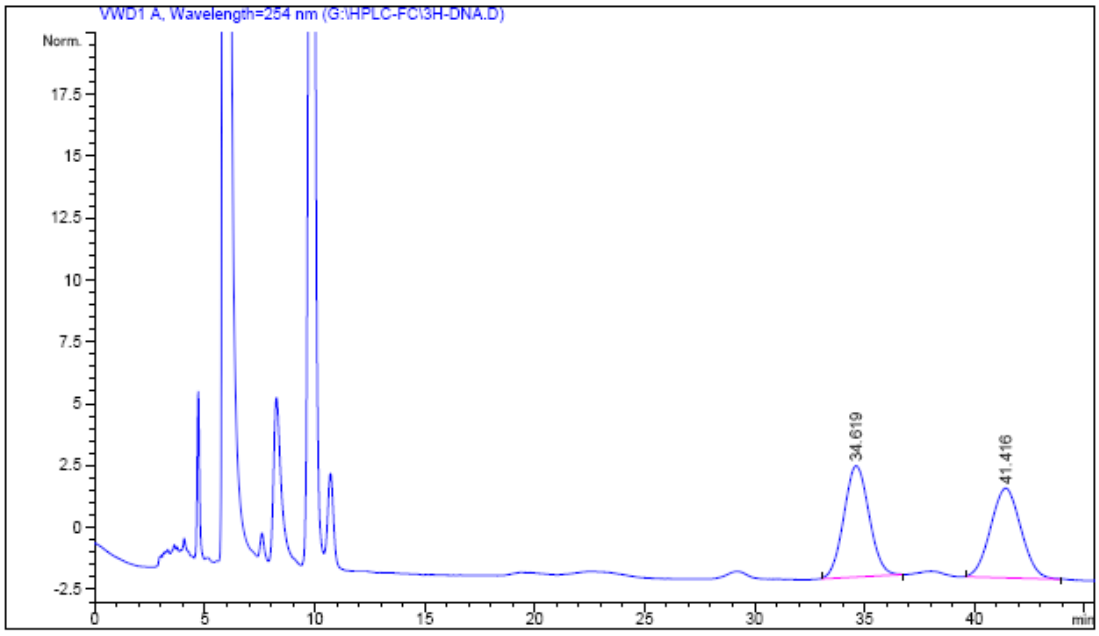
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.76 (s, 3H), 3.81 (dd, *J* = 16.8, 8.0 Hz, 1H), 3.91 (s, 3H), 3.95 (dd, *J* = 16.8, 7.2 Hz, 1H), 4.95 (t, *J* = 7.6 Hz, 1H), 6.79 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 7.00 (s, 1H), 7.09 (d, *J* = 2.1 Hz, 1H), 7.15 (d, *J* = 0.8 Hz, 1H), 7.19 (d, *J* = 8.8 Hz, 1H), 7.25 (d, *J* = 9.5 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 8.11–8.01 (m, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 80:20, 1.0 mL/min, 254 nm.

Racemic **3g**.

Retention times: 34.6 and 41.4 mins.

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                      Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  34.619 BB    1.2173  359.85638    4.49097  50.9060
   2  41.416 BB    1.4119  347.04718    3.62212  49.0940

Totals :                   706.90356    8.11310

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                         *** End of Report ***
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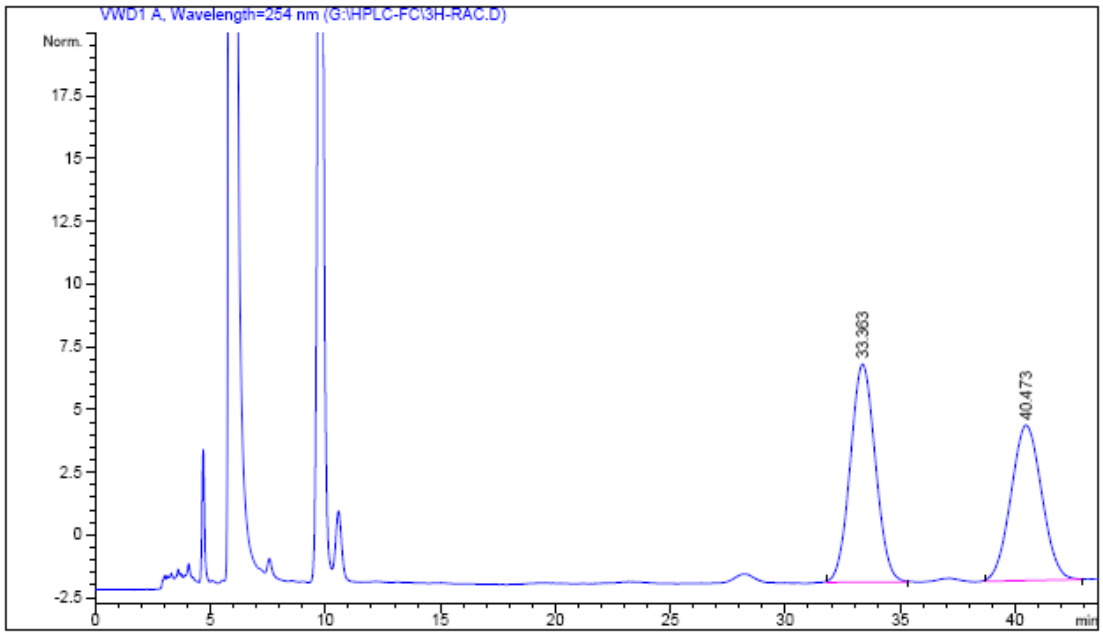
Product **3g** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (7% ee).

Retention times: 33.4 and 40.5 mins.

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                    Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  33.363 BB    1.1794  659.35144    8.68888  53.3143
   2  40.473 BB    1.4168  577.37415    6.19247  46.6857

Totals :                  1236.72559   14.88135


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                          *** End of Report ***
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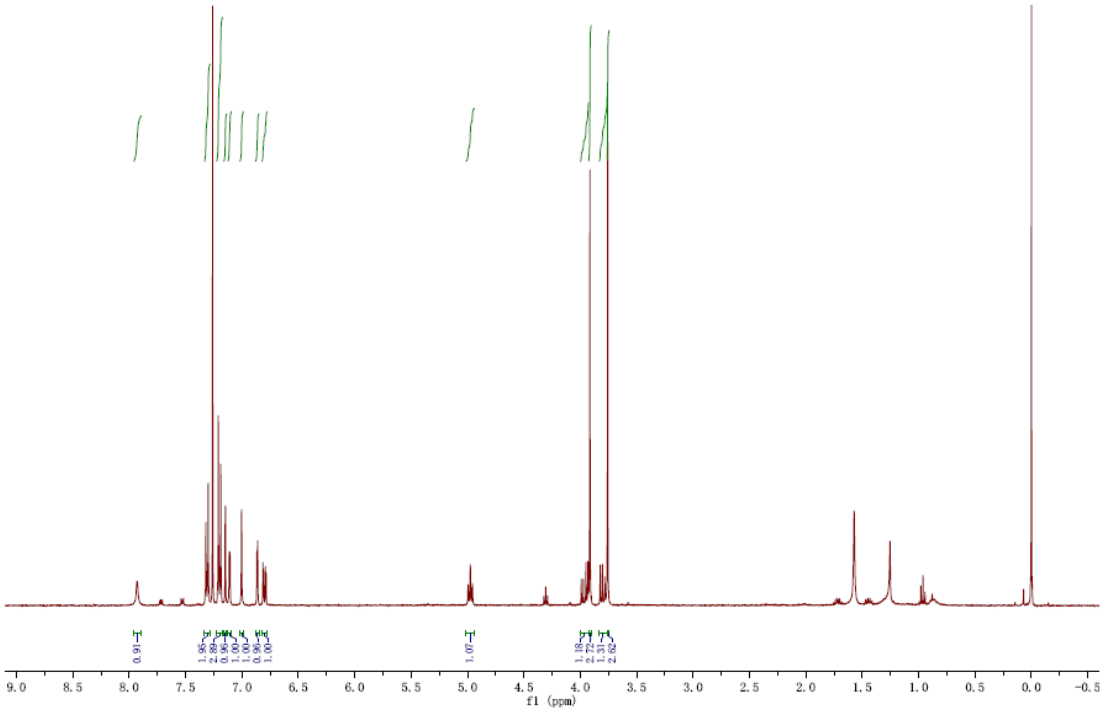
3-(4-chlorophenyl)-3-(5-methoxy-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)propan-1-one (3h).

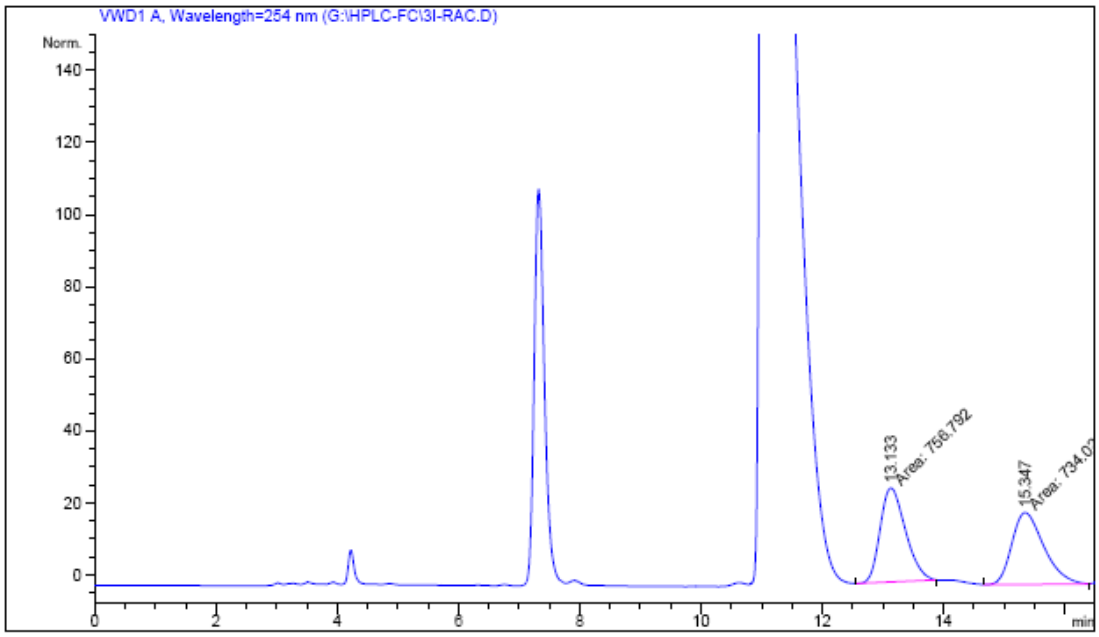
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.72 (s, 3H), 3.80 (dd, *J* = 16.4, 8.0 Hz, 1H), 3.92 (s, 3H), 3.96 (dd, *J* = 16.8, 7.6 Hz, 1H), 4.98 (t, *J* = 7.6 Hz, 1H)), 6.80 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 7.00 (s, 1H), 7.11 (d, *J* = 2.1 Hz, 1H), 7.15 (d, *J* = 0.8 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 3H), 7.25 (d, *J* = 8.8 Hz, 2H), 7.96–7.89 (m, 1H).



HPLC condition: Daicel chiralcel-OD, hexane/*i*-PrOH 80:20, 1.0 mL/min, 254 nm.

Racemic **3h**.

Retention times: 13.1 (+) and 15.3 (-) mins.

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                      Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  13.133 MM    0.4839  756.79150   26.06750  50.7634
   2  15.347 MM    0.6137  734.02838   19.93410  49.2366

Totals :                  1490.81989   46.00160

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                         *** End of Report ***
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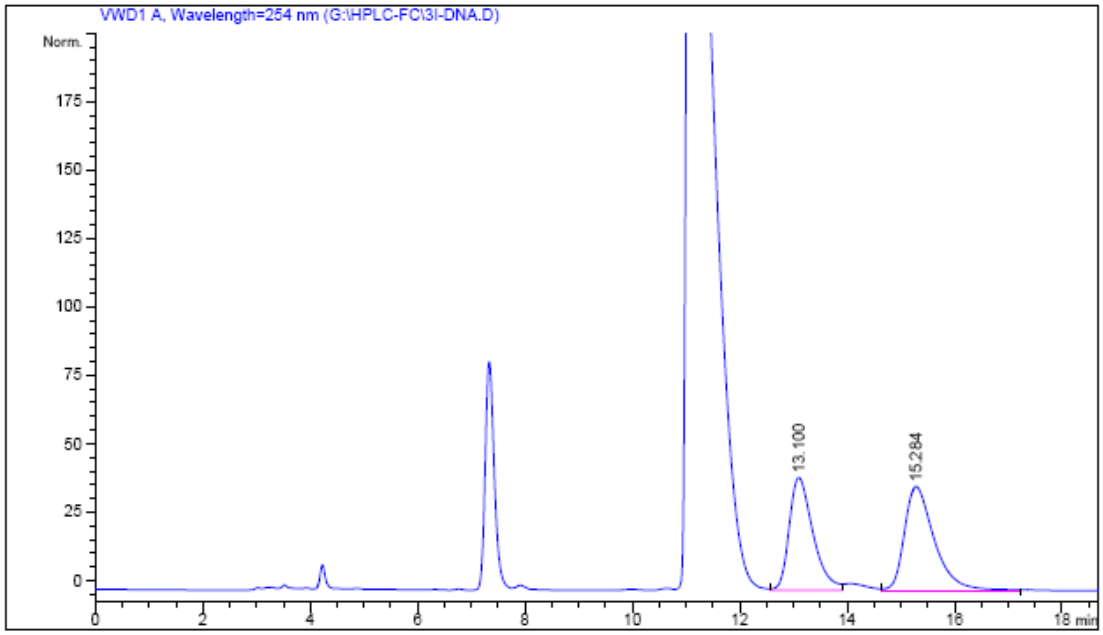
Product **3h** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (-7% ee).

Retention times: 13.1 (+) and 15.3 (-) mins.

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                          Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  13.100 VV    0.4704 1270.52747   41.20019  46.4244
   2  15.284 VB    0.5846 1466.23621   37.96003  53.5756

Totals :                  2736.76367   79.16022


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                          *** End of Report ***
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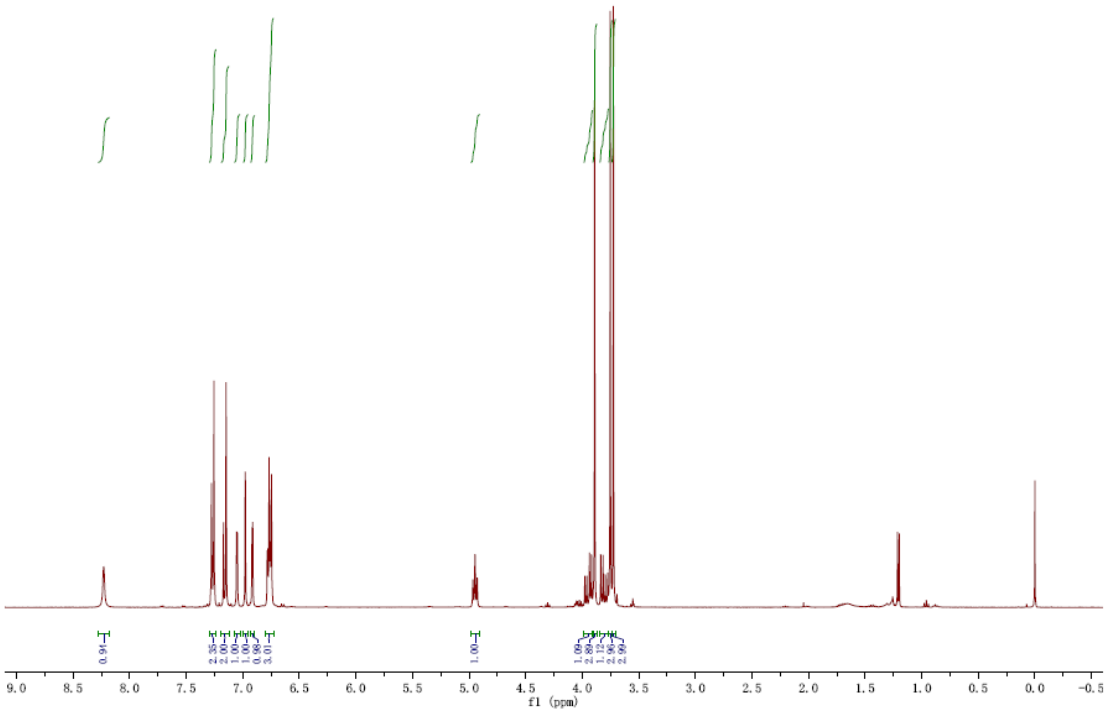
3-(5-methoxy-1H-indol-3-yl)-3-(4-methoxyphenyl)-1-(1-methyl-1H-imidazol-2-yl) propan-1-one (3i).

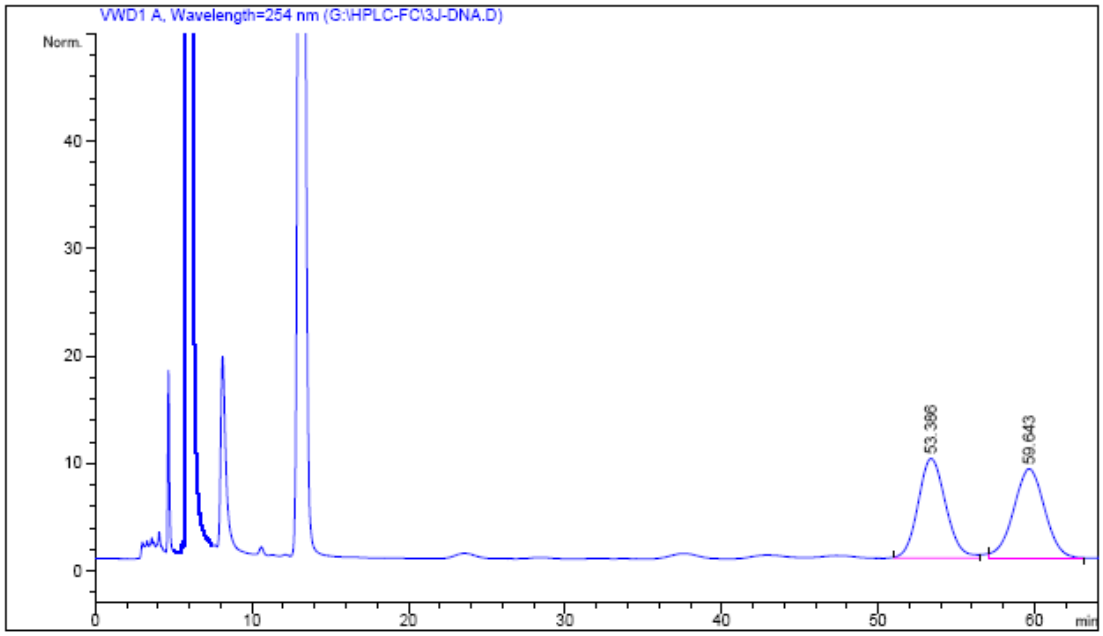
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 3.73 (s, 3H), 3.75 (s, 3H), 3.81 (dd, *J* = 16.3, 8.2 Hz, 1H), 3.89 (s, 3H), 3.95 (dd, *J* = 16.3, 7.1 Hz, 1H), 4.95 (t, *J* = 7.6 Hz, 1H), 6.80–6.73 (m, 3H), 6.92 (d, *J* = 2.3 Hz, 1H), 6.92 (d, *J* = 2.3 Hz, 1H), 6.98 (s, 1H), 7.05 (d, *J* = 2.1 Hz, 1H), 7.16 (d, *J* = 9.0 Hz, 2H), 7.27 (d, *J* = 8.8 Hz, 2H), 8.23 (s, 1H).



HPLC condition: Daicel chiralpak-AD, hexane/*i*-PrOH 80:20, 1.0 mL/min, 254 nm.

Racemic **3i**.

Retention times: 53.4 (-) and 59.6 (+) mins.

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                    Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  53.386 BB    1.8069 1137.32800    9.25191  49.7609
   2  59.643 BB    1.9740 1148.25562    8.30557  50.2391

Totals :                  2285.58362   17.55748

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                          *** End of Report ***
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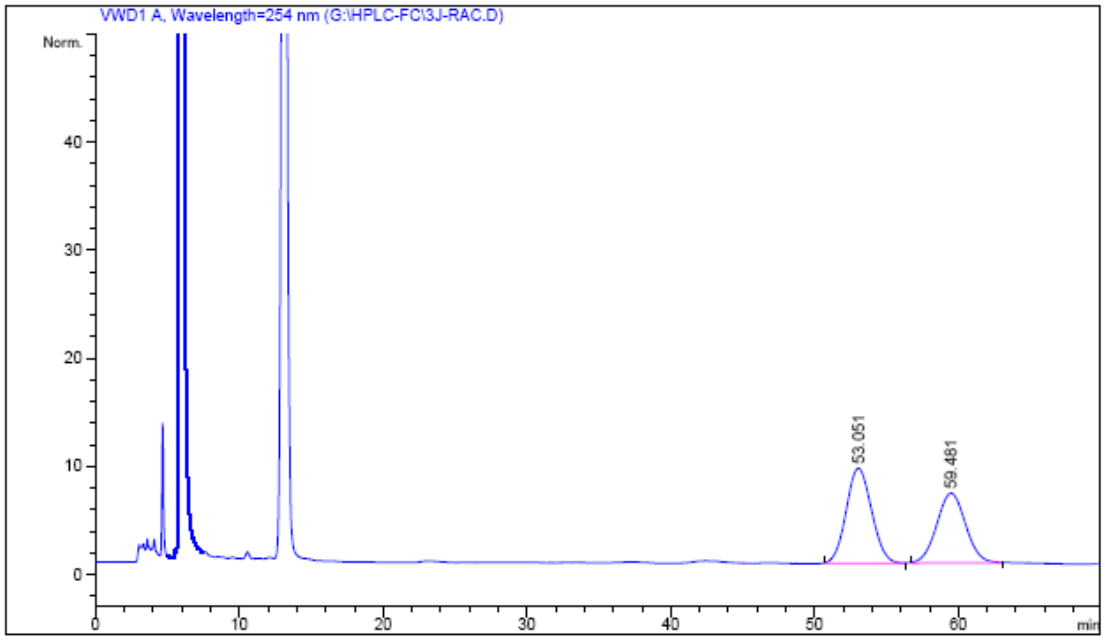
Product **3i** from the F-C reaction catalyzed by ODN-**1**-Cu^{2+} containing 50 mM NaCl (-9% ee).

Retention times: 53.1 (-) and 59.5 (+) mins.

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                        Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  53.051 BB    1.8493 1081.61475    8.78877  54.6586
   2  59.481 BB    1.8921  897.24005    6.45644  45.3414

Totals :                  1978.85480   15.24521

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                        *** End of Report ***
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