Supporting Information
for
Regio- and stereoselective carbometalation reactions of \( N \)-alkynyl-amides and sulfonamides

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Full experimental procedures and detailed analytical data for the synthesis of all new compounds

Table of contents

General Methods ..........................................................S2
Reagents and Materials.......................................................S2
General Procedures ..........................................................S3
  1. Stoichiometric carbocupration reaction (Method A) ..............S3
  2. Copper-catalyzed carbomagnesiation reaction (Method B) ......S3
  3. Stoichiometric carbocupration reaction (Method C).............S4
Compound characterization..................................................S4
References ........................................................................S18
**General methods**

All reactions were carried out in flame-dried glassware under a positive pressure of argon in dry solvents using standard Schlenk techniques unless otherwise indicated. The progress of the reactions was monitored by analytical TLC using glass plates precoated with silica gel with F$_{254}$ indicator (Merck). Visualization of spots was done using UV light (254 nm), iodine, p-anisaldehyde, phosphomolybdic acid (PMA), and Hanessian's (cerium ammonium molybdate) stains. All organometallic compounds, dry solvents, and reagents were transferred using plastic single-use graduated syringes and oven-dried stainless-steel needles. Purification of crude mixtures was accomplished by preparative flash column chromatography on silica gel 60A (GraceResolv) using gradient mixtures of ethyl acetate–n-hexane. $^1$H and $^{13}$C NMR spectra were measured on a Bruker Avance 300 (300 MHz $^1$H, 75 MHz $^{13}$C) or Bruker Avance AV 400 (400 MHz $^1$H, 100 MHz $^{13}$C). Chemical shifts values ($\delta$) are reported in ppm (calibration of spectra to the residual peak of chloroform: $\delta$ = 7.26 ppm (s) for $^1$H NMR; $\delta$ = 77.00 ppm for $^{13}$C NMR). All the $^1$H NMR spectra are reported as follows: $\delta$ value (multiplicity, $J$ coupling constant (in Hz), number of nuclei). Multiplicity abbreviations used: (s) – singlet, (d) – doublet, (dd) – doublet of doublet, (t) – triplet, (q) – quartet, (m) – multiplet, and (br) – broad signal.

**Reagents and materials**

All solvents were purified and dried immediately prior to use: THF and diethyl ether (HPLC grade, non-stabilized, BioLab) were dried using Innovative Technology PureSolv PS-MD-2 solvent purifier (aluminum oxide columns) and kept under a positive pressure of nitrogen. Grignard reagents were prepared from the corresponding alkyl- or arylhalides and Mg(0) in diethyl ether, transferred to a Schlenk flask, and stored at room temperature under a positive pressure of argon. The concentration of the prepared Grignard reagents was determined by back titration with a 1.00 M solution of 2-butanol in dry toluene in the presence of 2,2'-biquinoline as indicator. Methyllithium solution in diethyl ether (1.60 M) and n-butyllithium solution in hexane (1.60 M) were purchased from Aldrich and used as received. All starting material precursors (1-bromoalkynes) and starting chiral ynamides were prepared by literature procedures [1-4] and purified by preparative silica-gel flash column chromatography.
General procedures

1. Stoichiometric carbocupration reaction (Method A)

To a solution of copper salt (2 equiv) in dry Et$_2$O (10 mL) at −60 °C was added dropwise alkylmagnesium bromide (2 equiv). The reaction mixture was allowed to warm to −20 °C and stirred for 30 min. Then, the reaction mixture was cooled to −50 °C and a solution of alkynyl carbamate (1 equiv) in dry Et$_2$O was added dropwise. The reaction solution was allowed to warm to the indicated temperature and stirred for an additional 90 min (monitored by TLC). The reaction was quenched by a 2:1 mixture of an aqueous saturated solution of NH$_4$Cl and NH$_4$OH (30%) and allowed to warm up to room temperature. The phases were separated and the aqueous phase was extracted three times with Et$_2$O. The combined organic layers were washed with an aqueous saturated solution of NH$_4$Cl, dried over anhydrous MgSO$_4$, and concentrated under reduced pressure. Purification was accomplished by silica-gel flash column chromatography.

2. Copper-catalyzed carbomagnesiation reaction (Method B)

To a solution of copper salt (0.1 equiv) in dry Et$_2$O (10 mL) at −60 °C was added dropwise alkylmagnesium bromide (2 equiv). A solution of alkynyl carbamate (1 equiv) in dry Et$_2$O was added dropwise. The reaction solution was allowed to warm to room temperature and stirred for an additional 2 h (monitored by TLC). The reaction was quenched by a 2:1 mixture of an aqueous saturated solution of NH$_4$Cl and NH$_4$OH (30%) and allowed to warm up to room temperature. The phases were separated, and the aqueous phase was extracted three times with Et$_2$O. The combined organic layers were washed with an aqueous saturated solution of NH$_4$Cl, dried over anhydrous MgSO$_4$, and concentrated under reduced pressure. Purification was accomplished by silica-gel flash column chromatography.
3. Stoichiometric carbocupration reaction (Method C)

To a solution of copper salt (1.2 equiv) in dry Et₂O (8 mL) at −50 °C was added dropwise a solution of methyllithium (1.60 M in diethyl ether, 2.40 mmol, 2.4 equiv). The reaction mixture was allowed to warm to −40 °C and stirred for 30 min to form a colourless or a pale yellow solution of dimethyl cuprate–lithium bromide dimethylsulfide complex. Then, the reaction mixture was cooled to −50 °C, and a solution of alkynyl carbamate (1 equiv) in 1.5 mL of dry Et₂O was added dropwise. The reaction solution was allowed to warm to −30 °C and stirred for an additional 90 min (monitored by TLC). The reaction was quenched by a 2:1 mixture of an aqueous saturated solution of NH₄Cl and NH₄OH (30%) and allowed to warm up to room temperature. The phases were separated and the aqueous phase was extracted three times with Et₂O. The combined organic layers were washed with an aqueous saturated solution of NH₄Cl, dried over anhydrous MgSO₄, and concentrated under reduced pressure. Purification was accomplished by silica-gel flash column chromatography.

**Compound characterization**

(Z)-N-Benzyl-N-(2-butyloct-1-en-1-yl)-4-methylbenzenesulfonamide (3a)

The title compound was prepared using the general procedure (Method A) with CuI as a copper source. The carbocupration reaction of alkynyl sulfonamide 2 was performed at −20 °C. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 3a in 93% yield (90% if Method B was applied). ¹H NMR (300 MHz, CDCl₃) δ 7.67 (d, J = 8.4 Hz, 2H); 7.31 (d, J = 8.4 Hz, 2H); 7.22 (m, 5H); 4.89 (s, 1H); 4.12 (s, 2H); 2.42 (s, 3H); 1.91 (t, J = 8.1 Hz, 2H); 1.85 (t, J = 8.1 Hz, 2H); 1.15 (m, 12H); 0.85 (t, J = 7.2 Hz, 6H). ¹³C NMR (75 MHz, CDCl₃) δ 149.1; 142.8; 135.1; 134.9; 129.0; 127.7; 127.2; 127.1; 119.3; 54.5; 32.0; 31.3; 29.2; 29.1; 28.9; 26.5; 22.2; 21.6; 21.1; 13.7; 13.4 (1 signal missing due to overlap). HRMS ESI (m/z): [MNa]⁺ calcd. for C₂₆H₃₇NO₂SNa 450.2443; found 450.2437.
(Z)-N-Benzyl-4-methyl-N-(2-methyloct-1-en-1-yl)benzenesulfonamide (3b)

The title compound was prepared using the general procedure (Method A) with Cul as a copper source. The carbocupration reaction of alkynyl sulfonamide 2 was performed at −20 °C. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 3b in 30% yield. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.74 (d, $J = 7.8$ Hz, 2H); 7.31 (d, $J = 7.8$ Hz, 2H); 7.29 (m, 5H); 5.04 (s, 1H); 4.11 (s, 2H); 2.48 (s, 3H); 1.94 (t, $J = 8.1$ Hz, 2H); 1.40 (s, 3H); 1.23−1.03 (m, 8H); 0.83 (t, $J = 7.2$ Hz, 3H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 146.3; 143.3; 136.2; 136.1; 135.3; 129.5; 128.2; 127.7; 124.7; 119.7; 54.9; 36.5; 31.9; 30.3; 29.7; 26.9; 22.7; 19.4; 14.1 (4 signals missing due to overlap).

(Z)-N-Benzyl-N-(5-butylundeca-1,4-dien-4-yl)-4-methylbenzenesulfonamide (3c)

The title compound was prepared using the general procedure (Method A) with Cul as a copper source. The carbocupration reaction of alkynyl amide 4 was performed at −20 °C. Allyl bromide (3.3 equiv) was added at −65 °C, and the reaction mixture was warmed to −30 °C and stirred for 30 min. Then the reaction was quenched and worked up as described in the general procedure. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 3c in 50% yield. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.74 (d, $J = 8.1$ Hz, 2H); 7.29−7.21 (m, 7H); 5.63 (m, 1H); 4.92 (d, $J = 8.1$ Hz, 1H); 4.88 (d, $J = 13.2$ Hz, 1H); 4.64 (d, $J = 14.4$ Hz, 1H); 4.10 (d, $J = 14.4$ Hz, 1H); 2.84 (m, 1H); 2.82 (m, 1H); 2.42 (s, 3H); 1.87 (m, 4H); 1.23−1.02 (m, 12H); 0.86-0.81 (m, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 147.4; 142.6; 137.6; 136.0; 129.1; 129.0; 128.8; 127.6; 127.2; 127.1; 125.4; 115.0; 51.7; 35.3; 31.2; 30.7; 29.8; 29.3; 29.2; 27.2; 22.2; 21.1; 13.7; 13.5 (4 signals missing due to overlap). HRMS ESI ($m/z$): [MNa]$^+$ calcd. for C$_{29}$H$_{41}$NO$_2$SNa 490.2756; found 490.2750.
(Z)-Ethyl benzyl(2-butyloct-1-en-1-yl)carbamate (6a)

The title compound was prepared using the general procedure (Method A) with CuBr-DMS as a copper source. The carbocupration reaction of alkynyl amide 4 was performed at −20 °C. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 6a in 94% yield (72% when CuI was used and 81% if Method B was applied). $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.23–7.12 (m, 5H); 5.53 (s, 1H); 4.43 (s, 2H); 4.07 (q, $J_1$ = 14 Hz, $J_2$ = 7.2 Hz, 2H); 1.89 (t, $J = 6.6$ Hz, 2H); 1.80 (m, 2H); 1.35–1.09 (m, 15H); 0.82–0.76 (m, 6H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 155.3; 140.2; 136.8; 128.9; 126.2; 125.7; 120.9; 113.1; 63.5; 52.0; 31.5; 30.7; 29.3; 28.8; 28.7; 27.9; 25.8; 21.6; 13.6; 12.9 (2 signals missing due to overlap). HRMS ESI (m/z): [MNa]$^+$ calcd. for C$_{22}$H$_{35}$NO$_2$Na 368.2565; found 368.2560.

(Z)-Methyl benzyl(5-butylundeca-1,4-dien-4-yl)carbamate (6b)

The title compound was prepared using the general procedure (Method A) with CuBr as a copper source. The carbocupration reaction of alkynyl amide 4 was performed at −20 °C. Allyl bromide (3.3 equiv) was added at −20 °C, the reaction mixture was warmed to −15 °C and stirred for 30 min. Then the reaction was quenched and worked up as described in the general procedure. Purification by preparative column chromatography on silica gel using 1% of ethyl acetate in hexane gave the product 6b in 55% yield. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.24 (m, 5H); 5.71 (m, 1H); 5.05 (d, $J = 5$ Hz, 1H); 5.03 (d, $J = 11$ Hz, 1H); 4.75 (d, $J = 14$ Hz, 1H); 4.46 (d, $J = 14$ Hz, 1H); 3.74 (s, 3H); 3.12 (m, 1H); 2.86 (m, 1H); 2.14 (m, 2H); 1.79 (m, 2H); 1.39–1.23 (m, 12H); 0.98 (m, 6H). $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 158.9; 141.5; 139.7; 137.5; 131.2; 131.1; 130.4; 129.0; 117.5; 54.5; 54.2; 53.6; 37.6; 33.5; 32.8; 32.1; 31.5; 31.3; 29.0; 24.5; 24.4; 15.9 (2 signals missing due to overlap). HRMS ESI (m/z): [MNa]$^+$ calcd. for C$_{24}$H$_{37}$NO$_2$Na 394.2722; found 394.2716.
The title compound was prepared using the general procedure (Method A) with Cul as a copper source. The carbocupration reaction of alkynyl amide 4 was performed at −20 °C. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 6c in 50% yield (81% if Method B was applied). $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.26–7.14 (m, 5H); 5.54 (s, 1H); 4.43 (s, 2H); 3.62 (s, 3H); 1.82–1.71 (m, 3H); 1.69–1.52 (m, 6H); 1.22–1.05 (m, 12H); 0.81 (t, J = 6.9 Hz, 3H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 148.1; 136.7; 129.9; 127.3; 126.2; 123.7; 120.3; 52.1; 51.7; 31.4; 30.9; 29.3; 28.7; 28.3; 28.2; 26.6; 25.8; 25.3; 21.7; 21.6; 13.1 (2 signals missing due to overlap). HRMS ESI (m/z): [MNa]$^+$ calcd. for C$_{23}$H$_{35}$NO$_2$Na 380.2565; found 380.2566.

The title compound was prepared using the general procedure (Method A) with Cul as a copper source. The carbocupration reaction of alkynyl amide 4 was performed at −20 °C. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 6d in 68% yield (60% if Method B was applied). $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.31–7.19 (m, 5H); 5.61 (s, 1H); 4.49 (s, 2H); 4.14 (q, $J^2 = 14.1$ Hz, $J^1 = 6.9$ Hz, 2H); 1.87 (brs, 2H); 1.61 (s, 3H); 1.26–1.06 (m, 11H); 0.86 (t, J = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 148.1; 137.2; 127.9; 126.8; 124.3; 121.3; 113.6; 52.7; 52.3; 36.0; 31.4; 29.8; 26.3; 22.2; 18.9; 13.6; 13.4 (2 signals missing due to overlap). HRMS ESI (m/z): [MNa]$^+$ calcd. for C$_{19}$H$_{29}$NO$_2$Na 326.2096; found 326.2110.
(E)-Ethyl benzyl(2-phenyloct-1-en-1-yl)carbamate (6e)

The title compound was prepared using the general procedure (Method A) with Cul as a copper source. The carbocupration reaction of alkynyl amide 4 was performed at −20 °C. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 6e in 84% yield (90% if Method B was applied). $^1$H NMR (300 MHz, CDCl$_3$) δ 7.30–7.23 (m, 10H); 6.03 (s, 1H); 4.62 (s, 2H); 4.17 (q, $J^1$ = 13.8 Hz, $J^2$ = 6.9 Hz, 2H); 2.33–2.25 (m, 2H); 1.55–1.14 (m, 11H); 0.81 (t, $J = 6.6$ Hz, 3H).

$^{13}$C NMR (75 MHz, CDCl$_3$) δ 158.1; 139.5; 137.2; 128.0; 127.8; 126.0; 125.1; 124.3; 113.6; 61.3; 52.6; 36.6; 33.8; 31.5; 29.0; 26.8; 22.2; 14.2; 13.7; 13.6 (4 signals missing due to overlap). HRMS ESI (m/z): [MNa]$^+$ calcd. for C$_{24}$H$_{31}$NO$_2$Na 388.2252; found 388.2247.

(S,Z)-4-Benzyl-3-(2-methyloct-1-en-1-yl)oxazolidin-2-one (9a)

The title compound was prepared using the general procedure (Method A) with Cul as a copper source. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 9a in 75% yield. $^1$H NMR (300 MHz, CDCl$_3$) δ 7.38–7.16 (m, 3H); 7.15–7.08 (m, 2H); 5.67–5.62 (m, 1H); 4.25–4.14 (m, 1H); 4.11–3.99 (m, 2H); 3.09 (dd, $J^1$ = 13.37 Hz, $J^2$ = 3.57 Hz, 1H); 2.68–2.54 (m, 1H); 2.10 (dd, $J^1$ = 8.48 Hz, $J^2$ = 6.97 Hz, 2H); 1.75 (d, $J = 1.46$ Hz, 3H); 1.53–1.37 (m, 2H); 1.36–1.23 (m, 6H); 0.87 (t, $J = 6.9$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 156.7; 138.9; 135.6; 128.9; 128.8; 127.0; 116.7; 66.6; 58.9; 38.4; 31.6; 29.4; 26.9; 22.5; 19.9; 14.0 (3 signals missing due to overlap). HRMS ESI (m/z): [MH]$^+$ calcd. for C$_{19}$H$_{28}$NO$_2$ 302.2120; found 302.2129.
(S,Z)-4-Benzyl-3-(2-methylhex-1-en-1-yl)oxazolidin-2-one (9b)

The title compound was prepared using the general procedure (Method C) with CuBr-DMS as a copper source. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 9b in 80% yield. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.23 (m, 3H); 7.09 (d, $J = 7.0$ Hz, 2H); 5.62 (s, 1H); 4.22–4.13 (m, 1H); 4.08–3.98 (m, 2H); 3.06 (dd, $J^1 = 13.4$ Hz, $J^2 = 3.4$ Hz, 1H); 2.59 (dd, $J^1 = 13.6$ Hz, $J = 9.1$ Hz, 1H); 2.09 (dd, $J^1 = 8.3$, $J^2 = 7.3$ Hz, 2H); 1.78–1.68 (m, 3H); 1.48–1.36 (m, 2H); 1.36–1.25 (m, 2H); 0.89 (t, $J = 7.2$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 156.7; 138.8; 135.5; 128.9; 128.7; 127.0; 116.7; 66.5; 58.9; 38.4; 31.3; 29.1; 22.8; 19.9; 13.9 (2 signals missing due to overlap). HRMS ESI (m/z): [M+H]$^+$ calcd. for C$_{17}$H$_{24}$NO$_2$ 274.1807; found 274.1809.

(S,Z)-4-Benzyl-3-(2-methyl-5-((triisopropylsilyl)oxy)pent-1-en-1-yl)oxazolidin-2-one (9c)

The title compound was prepared using the general procedure (Method B) with CuBr-DMS as a copper source. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 9c in 51% yield. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.36–7.20 (m, 3H); 7.17–7.10 (m, 2H); 5.73–5.69 (m, 1H); 4.24–4.10 (m, 2H); 4.08–4.02 (m, 1H); 3.73 (dt, $J^1 = 6.2$ Hz, $J^2 = 1.6$ Hz, 2H); 3.15–3.04 (m, 1H); 2.69–2.56 (m, 1H); 2.31–2.14 (m, 2H); 1.79 (d, $J = 1.4$ Hz, 3H); 1.77–1.65 (m, 2H); 1.20–0.92 (m, 21H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 156.7; 137.7; 135.5; 128.9; 128.7; 127.0; 116.9; 66.5; 63.1; 58.6; 38.2; 30.4; 28.2; 20.1; 17.9; 11.8 (9 signals missing due to overlap). HRMS ESI (m/z): [MNa]$^+$ calcd. for C$_{25}$H$_{42}$NO$_3$Si 432.2934; found 432.2933.
The title compound was prepared using the general procedure (Method B) using CuBr-DMS as a copper source. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 9d in 90% yield. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta 7.34–7.17\) (m, 3H); 7.15–7.07 (m, 2H); 5.64 (d, \(J = 1.1\) Hz, 1H); 4.27–3.98 (m, 5H); 3.07 (dd, \(J^1 = 13.4\) Hz, \(J^2 = 3.7\) Hz, 1H); 2.68–2.53 (m, 1H); 2.23–2.12 (m, 2H); 1.96 (s, 3H); 1.76 (m, 18H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta 177.5\); 156.6; 137.6; 135.4; 129.0; 128.9; 128.8; 127.1; 117.6; 66.7; 63.8; 58.9; 40.6; 38.8; 36.4; 28.3; 27.9; 26.2; 19.9 (7 signals missing due to overlap). HRMS ESI (m/z): [MNa]\(^+\) calcd. for C\(_{27}\)H\(_{35}\)NO\(_4\)Na 460.2464; found 460.2487.

The title compound was prepared using the general procedure (Method B) with CuBr-DMS as a copper source. A 1:1 mixture of Et\(_2\)O and THF was used to avoid precipitation of the starting material. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 9e in 50% yield. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta 7.47–7.33\) (m, 5H); 7.20–7.13 (m, 3H); 6.64–6.58 (m, 2H); 6.49–6.47 (m, 1H); 3.96–3.89 (m, 2H); 3.71–3.60 (m, 1H); 2.84 (dd, \(J^1 = 13.32\) Hz, \(J^2 = 3.59\) Hz, 1H); 2.28 (dd, \(J^1 = 13.31\) Hz, \(J^2 = 10.27\) Hz, 1H); 2.14 (d, \(J = 1.43\) Hz, 3H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta 156.7\); 139.7; 135.3; 128.8; 128.4; 128.0; 127.6; 126.7; 125.1; 118.4; 65.7; 55.5; 36.8; 23.0 (5 signals missing due to overlap). HRMS ESI (m/z): [MNa]\(^+\) calcd. for C\(_{19}\)H\(_{20}\)NO\(_2\) 294.1494; found 294.1498.
(S,Z)-4-Benzyl-3-(2-(4-fluorophenyl)prop-1-en-1-yl)oxazolidin-2-one (9f)

The title compound was prepared using the general procedure (Method B) with CuBr-DMS as a copper source. A 12:1 mixture of Et₂O and THF was used to avoid precipitation of the starting material. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 9f in 71% yield. Single crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of a saturated solution of the title compound in CHCl₃ at room temperature. 

\[ \text{\textsuperscript{1}H NMR (300 MHz, CDCl}_3 \delta 7.39–7.28 (m, 2H); 7.24–7.06 (m, 5H); 6.68 (dd, } J^1 = 7.3 \text{ Hz, } J^2 = 2.1 \text{ Hz, 2H); 6.46–6.43 (m, 1H); 3.98–3.91 (m, 2H); 3.70–3.57 (m, 1H); 2.82 (dd, } J^1 = 13.4 \text{ Hz, } J^2 = 3.7 \text{ Hz, 1H); 2.32 (dd, } J^1 = 13.4 \text{ Hz, } J^2 = 10.0 \text{ Hz, 1H); 2.09 (t, } J = 1.4 \text{ Hz, 3H).} \]

\[ \text{\textsuperscript{13}C NMR (75 MHz, CDCl}_3 \delta 163.6; 160.3; 156.7; 135.6; 135.2; 129.6; 128.8; 128.7; 128.6; 128.6; 118.9; 115.6; 115.3; 65.8; 55.6; 36.9; 22.9. HRMS ESI (m/z): } [\text{MNa}^+] \text{ calcd. for C}_{19}H_{19}FNO}_2 312.1400; \text{ found 312.1404.} \]

(S,Z)-4-Benzyl-3-(2-(4-methoxyphenyl)prop-1-en-1-yl)oxazolidin-2-one (9g)

The title compound was prepared using the general procedure (Method B) with CuBr-DMS as a copper source. A 12:1 mixture of Et₂O and THF was used to avoid precipitation of the starting material. Purification by preparative column chromatography on silica gel using 5% of ethyl acetate in hexane gave the product 9g in 60% yield. 

\[ \text{\textsuperscript{1}H NMR (300 MHz, CDCl}_3 \delta 7.32–7.25 (m, 2H); 7.22–7.13 (m, 3H); 6.98–6.92 (m, 2H); 6.72–6.63 (m, 2H); 6.42–6.39 (m, 1H); 4.01–3.89 (m, 2H); 3.85 (s, 3H); 3.69 (ddt, } J^1 = 10.9 \text{ Hz, } J^2 = 7.3 \text{ Hz, } J^3 = 3.7 \text{ Hz, 1H); 2.83 (dd, } J^1 = 13.4 \text{ Hz, } J^2 = 3.6 \text{ Hz, 1H); 2.30 (dd, } J^1 = 13.4 \text{ Hz, } J^2 = 10.0 \text{ Hz, 1H); 2.11 (d, } J = 1.4 \text{ Hz, 3H).} \]

\[ \text{\textsuperscript{13}C NMR (75 MHz, CDCl}_3 \delta 159.0; 156.8; 135.4; 131.8; 129.1; 128.9; 128.5; 126.7; } \]
125.4; 117.9; 113.8; 65.9; 55.6; 55.2; 36.9; 22.9 (4 signals missing due to overlap). HRMS ESI (m/z): [MNa]+ calcd. for C_{20}H_{22}NO_{3} 324.1600; found 324.1598.

X-ray data for compound 9f

Figure S1: Crystal structure of compound 9f (ORTEP plot, ellipsoid probability 25%).

Table 1. Crystal data and structure refinement for 9f.

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Completeness to theta = 24.50     96.8 %
Absorption correction             Semi-empirical from equivalents
Max. and min. transmission        0.9764 and 0.9561
Refinement method                 Full-matrix least-squares on F^2
Data / restraints / parameters    2637 / 0 / 209
Goodness-of-fit on F^2            1.012
Final R indices [I>2sigma(I)]     R1 = 0.0481, wR2 = 0.1338
R indices (all data)              R1 = 0.0679, wR2 = 0.1480
Absolute structure parameter      2(2)
Extinction coefficient            0.032(3)
Largest diff. peak and hole       0.145 and -0.146 e.Å^3

Atomic coordinates ( x 10^4) and equivalent isotropic
displacement parameters (Å^2 x 10^3) for 9f.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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**Bond lengths [Å] and angles [deg] for 9f.**

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Symmetry transformations used to generate equivalent atoms:

Hydrogen coordinates (\( \times 10^4 \)) and isotropic displacement parameters (\( \AA^2 \times 10^3 \)) for 9f.
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Torsion angles [deg] for 9f.

C(6)-C(1)-C(2)-C(3)  1.8(4)
C(7)-C(1)-C(2)-C(3)  178.5(3)
C(1)-C(2)-C(3)-C(4)  -1.2(5)
C(2)-C(3)-C(4)-C(5)  0.9(6)
C(2)-C(3)-C(4)-F(1)  -179.9(3)
F(1)-C(4)-C(5)-C(6)  179.6(3)
C(3)-C(4)-C(5)-C(6)  -1.2(6)
C(4)-C(5)-C(6)-C(1)  1.9(6)
C(2)-C(1)-C(6)-C(5)  -2.1(5)
C(7)-C(1)-C(6)-C(5)  -178.8(3)
C(2)-C(1)-C(7)-C(9)  57.5(4)
C(6)-C(1)-C(7)-C(9)  -125.9(3)
C(2)-C(1)-C(7)-C(8)  -120.1(3)
C(6)-C(1)-C(7)-C(8)  56.4(4)
C(1)-C(7)-C(9)-N(1)  7.7(5)
C(8)-C(7)-C(9)-N(1)  -174.7(3)
C(11)-N(1)-C(9)-C(7) -165.3(3)
C(10)-N(1)-C(9)-C(7) 36.3(5)
C(11)-N(1)-C(10)-C(13) -105.8(3)
C(9)-N(1)-C(10)-C(13) 54.3(3)
C(11)-N(1)-C(10)-C(12) 17.4(3)
C(9)-N(1)-C(10)-C(12) 177.6(3)
C(12)-O(2)-C(11)-O(1) 177.7(3)
C(12)-O(2)-C(11)-N(1)  -3.8(3)
C(9)-N(1)-C(11)-O(1)  7.1(5)
C(10)-N(1)-C(11)-O(1) 168.8(3)
C(9)-N(1)-C(11)-O(2)  -171.3(2)
C(10)-N(1)-C(11)-O(2)  -9.6(3)
C(12)-O(2)-C(12)-O(2) 14.9(3)
N(1)-C(10)-C(12)-O(2) -18.9(3)
C(13)–C(10)–C(12)–O(2)  103.3(3)
N(1)–C(10)–C(13)–C(14)  57.0(3)
C(12)–C(10)–C(13)–C(14)  57.6(3)
C(10)–C(13)–C(14)–C(15)  88.3(4)
C(10)–C(13)–C(14)–C(19)  94.0(4)
C(19)–C(14)–C(15)–C(16)  57.6(5)
C(13)–C(14)–C(15)–C(16)  179.6(3)
C(12)–C(10)–C(13)–C(14)  179.8(5)
C(10)–C(13)–C(14)–C(19)  88.3(5)
C(10)–C(13)–C(14)–C(19)  179.6(3)

References


