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Supplementary Information

Efficient Access to 1,3,4-Trisubstituted Pyrroles via Gold-Catalysed Cycloisomerization of 1,5-Diynes

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Table of Content

General information	
General Procedure for the Synthesis of diynes	
General procedure for the synthesis of pyrrol	
Crystal structure	
References	
NMR Spectra	

General information

Unless otherwise indicated, all reagents were used as received from commercial suppliers without further purification. Reaction progress was monitored by thin layer chromatography (TLC). Visualization was achieved by ultraviolet light (254 nm). Flash column chromatography was performed using silica gel 60 (200-300 mesh, Merck and co.). All ¹ H NMR, ¹³C NMR spectra were recorded on Bruker AV-III 400 in CDC13. Chemical shifts were given in parts per million (ppm, δ), referenced to the peak of tetramethylsilane, defined at $\delta = 0.00$ (¹H NMR), or the solvent peak of CDC13, defined at $\delta = 77.16$ (¹³C NMR). Coupling constants were quoted in Hz (*J*). ¹H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), septet (se), octet (o). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m). Mass spectra were recorded on a high resolution mass spectrometer ESI-QTOF.

General Procedure for the Synthesis of diynes

Compounds diynes (1a, 1c, 1d, 1e, 1f, 1n) were prepared according to the known procedure. The data of new compounds are described below.¹⁻⁹



N-((4-bromophenyl)ethynyl)-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1b) Compound **1b** was obtained as white solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.90 (d, J = 8.4 Hz, 2H), 7.43-7.40 (m, 2H), 7.32-7.23 (m, 7H), 7.17-7.15 (m, 2H), 4.56 (s, 2H), 2.36 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 134.4, 133.1, 131.8, 131.7, 129.8, 128.8, 128.4, 128.3, 122.2, 122.1, 121.8, 86.7, 83.2, 81.1, 70.5, 43.0, 21.7; HRMS (ESI) m/z calcd for C₂₄H₁₈BrNO₂SNa⁺ (M+Na)⁺ 486.0134, found 486.0139.



N-((2-chlorophenyl)ethynyl)-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1g)

Compound **1g** was obtained as white solid; $R_f = 0.55$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.96 (d, J = 8.4 Hz, 2H), 7.43-7.41 (m, 1H), 7.37-7.34 (m, 1H), 7.28-7.22 (m, 5H), 7.20 -7.15 (m, 4H), 4.59 (s, 2H), 2.33 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.1, 135.7, 134.4, 133.0, 131.8, 129.8, 129.3, 128.9, 128.7, 128.4, 128.2, 126.5, 122.8, 122.1, 87.1, 86.7, 81.1, 68.6, 43.1, 21.7; HRMS (ESI) m/z calcd for C₂₄H₁₈CINO₂SNa⁺ (M+Na)⁺ 442.0639, found 442.0639.



4-methyl-N-(3-phenylprop-2-yn-1-yl)-N-(o-tolylethynyl)benzenesulfonamide (1h)

Compound **1h** was obtained as white solid; $R_f = 0.57$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.91 (d, J = 8.0 Hz, 2H), 7.37 (d, J = 7.6 Hz, 1H), 7.27-7.22 (m, 5H), 7.18-7.10 (m, 5H), 4.57 (s, 2H), 2.35 (s, 3H), 2.33 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.0, 140.2, 134.4, 131.8, 131.7, 129.7, 129.4, 128.7, 128.4, 128.2, 128.1, 125.6, 122.5, 122.1, 86.5, 85.8, 81.3, 70.1, 43.1, 21.7, 20.8; HRMS (ESI) m/z calcd for C₂₅H₂₁NO₂SNa+ (M+Na)+ 422.1185, found 422.1187.



N-((3-chlorophenyl)ethynyl)-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1i) Compound **1i** was obtained as white solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.90 (d, J = 8.0 Hz, 2H), 7.357-7.353 (m, 1H), 7.31-7.21 (m, 8H), 7.19-7.16 (m, 2H), 4.56 (s, 2H), 2.37 (s, 3H).; ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 134.4, 134.2, 131.8, 131.3, 129.8, 129.64, 129.62, 128.8, 128.4, 128.33, 128.26, 124.6 122.1, 86.8, 83.4, 81.1, 70.3, 43.0, 21.7. HRMS (ESI) m/z calcd for C₂₄H₁₈ClNO₂SNa⁺ (M+Na)⁺ 442.0639, found 442.0641.



4-methyl-N-(3-phenylprop-2-yn-1-yl)-N-(m-tolylethynyl)benzenesulfonamide (1j)

Compound **1j** was obtained as white solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.91 (d, J = 8.0 Hz, 2H), 7.29-7.21 (m, 6H), 7.19-7.16 (m, 4H), 7.10-7.08 (m, 1H), 4.55 (s, 2H), 2.34 (s, 3H), 2.30 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.0, 138.1, 134.4, 132.3, 131.8, 129.7, 129.0, 128.73, 128.72, 128.4, 128.29, 128.27, 122.6, 122.2, 86.6, 81.8, 81.3, 71.4, 43.1, 21.7, 21.3; HRMS (ESI) m/z calcd for C₂₅H₂₁NO₂SNa+ (M+Na)+ 422.1185, found 422.1187.



N-((3-bromophenyl)ethynyl)-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1k) Compound 1k was obtained as pale yellow solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.52-7.51 (m, 1H), 7.42-7.39 (m 1H), 7.31-7.24 (m, 6H), 7.19-7.13 (m, 3H), 4.56 (s, 2H), 2.36 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 134.3, 134.2, 131.8, 131.1, 130.0, 129.8, 128.8, 128.33, 128.32, 124.8, 122.2, 122.0, 86.8, 83.5, 81.1, 70.1, 43.0, 21.7; HRMS (ESI) m/z calcd for C₂₄H₁₈BrNO₂SNa+ (M+Na)+ 486.0134, found 486.0139.



N-((3-fluorophenyl)ethynyl)-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (11)

Compound **11** was obtained as white solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.90 (d, J = 7.6 Hz, 2H), 7.30-7.22 (m, 6H), 7.17-7.16 (m, 3H), 7.07 (d, J = 9.2 Hz, 1H), 6.98 (t, J = 8.0 Hz, 1H), 4.56 (s, 2H), 2.35 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 162.4 (d, J = 247.2 Hz), 145.2, 134.3, 131.7, 130.0 (d, J = 8.8 Hz), 129.8, 128.8, 128.32, 128.29, 127.4 (d, J = 2.9 Hz), 124.6 (d, J = 9.8 Hz), 122.0, 118.2 (d, J = 22.8 Hz), 115.3 (d, J = 21.2 Hz) , 86.7, 83.1, 81.1, 70.4, 42.9, 21.7; ¹⁹F NMR (376 MHz, CDCl₃) δ -113.09; HRMS (ESI) m/z calcd for C₂₄H₁₈FNO₂SNa+ (M+Na)⁺ 426.0935, found 426.0935.



N-(cyclopropylethynyl)-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1m) Compound **1m** was obtained as yellow solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1);¹H NMR (400 MHz, CDCl₃, TMS) δ 7.85 (d, J = 8.0 Hz, 2H), 7.31-7.23 (m, 5H), 7.15-7.13 (m, 2H), 4.41 (s, 2H), 2.35 (s, 3H), 1.35-1.29 (m, 1H), 0.81- 0.76 (m, 2H), 0.67-0.63 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 144.7, 134.3, 131.7, 129.5, 128.6, 128.3, 128.2, 122.2, 86.2, 81.5, 75.5, 68.4, 42.9, 21.7, 9.0, -0.6; HRMS (ESI) m/z calcd for C₂₁H₁₉NO₂SNa⁺ (M+Na)+ 372.1029, found 372.1029.



N-((4-bromophenyl)ethynyl)-N-(3-(4-bromophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (10)

Compound **10** was obtained as pale yellow solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.89 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 8.8 Hz, 2H), 7.39 (d, J = 8.8 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.8 Hz, 2H), 4.53 (s, 2H), 2.38 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 134.3, 133.2, 133.0, 131.7, 131.6, 129.8, 128.4, 123.2 122.3, 121.7, 121.0, 85.6, 83.1, 82.4, 70.5, 42.9, 21.8; HRMS (ESI) m/z calcd for $C_{24}H_{17}Br_2NO_2SNa^+$ (M+Na)+ 565.9219, found 565.9222.



N-((4-bromophenyl)ethynyl)-N-(3-(4-iodophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (1p)

Compound **1p** was obtained as white solid; $R_f = 0.57$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.88 (d, J = 8.0 Hz, 2H), 7.59 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 8.0 Hz, 2H), 7.30-7.22 (m, 4H), 6.88 (d, J = 8.0 Hz, 2H), 4.53 (s, 2H), 2.38 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 137.5, 134.3, 133.2, 133.0, 131.7, 129.8, 128.3, 122.3, 121.6, 121.5, 94.9, 85.8, 83.1, 82.7, 70.5, 42.9, 21.8; HRMS (ESI) m/z calcd for C₂₄H₁₇BrINO₂SNa⁺ (M+Na)⁺ 611.9100, found 611.9101.



methy 4-(3-((N-((4-bromophenyl)ethynyl)-4-methylphenyl)sulfonamido)prop-1-yn-1yl)benzoate (1q)

Compound **1q** was obtained as pale yellow solid; $R_f = 0.55$ (petroleum ether : ethyl acetate = 5 : 1);¹H NMR (400 MHz, CDCl3, TMS) δ 7.94-7.89 (m, 4H), 7.42 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 7.26-7.20 (m, 4H), 4.57 (s, 2H), 3.91 (s, 3H), 2.36 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 166.4, 145.3, 134.2, 133.0, 131.7, 131.6, 130.1, 129.8, 129.4, 128.3, 126.6, 122.3, 121.6, 85.8, 84.2, 83.1, 70.5, 52.4, 42.8, 21.7; HRMS (ESI) m/z calcd for C₂₆H₂₀BrNO₄SNa⁺ (M+Na)⁺ 544.0189, found 544.0190.



N-((4-bromophenyl)ethynyl)-N-(3-(3-fluorophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (1r)

Compound **1r** was obtained as yellow solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.90 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.25-7.19 (m, 3H), 7.00 (td, $J_I = 8.4$, $J_2 = 2.4$ Hz, 1H), 6.95 (d, J = 8.0 Hz, 1H), 6.78 (d, J = 8.8 Hz, 1H), 4.55 (s, 2H), 2.38 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 162.2 (d, J = 247.7 Hz), 145.3, 134.3, 133.0, 131.6, 129.9 (d, J = 8.6 Hz), 129.8, 128.3, 127.6 (d, J = 3.1 Hz), 123.8 (d, J = 9.5 Hz), 122.3, 121.6, 118.6 (d, J = 23.1 Hz), 116.2 (d, J = 21.2 Hz), 85.4 (d, J = 3.4 Hz), 83.1, 82.1, 70.4, 42.8, 21.6; ¹⁹F NMR (376 MHz, CDCl₃) δ -112.70; HRMS (ESI) m/z calcd for C₂₄H₁₇BrFNO₂SNa+ (M+Na)⁺ 504.00340, found 504.0045.



N-((4-bromophenyl)ethynyl)-N-(3-(2-chlorophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (1s)

Compound **1s** was obtained as yellow solid; $R_f = 0.6$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.90 (d, J = 7.6 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 7.6 Hz, 2H), 7.24-7.22 (m, 3H), 7.16 (t, J = 7.6 Hz, 1H), 7.05-7.02 (m, 2H), 4.55 (s, 2H), 2.36 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 134.1, 133.8, 132.9, 131.5, 131.4, 129.68, 129.65, 129.5, 128.9, 128.1, 123.5, 122.1, 121.4, 85.0, 83.1, 82.4, 70.3, 42.6, 21.6. HRMS (ESI) m/z calcd for C₂₄H₁₇BrClNO₂SNa⁺ (M+Na)⁺ 519.9744, found 519.9747.



N-((4-bromophenyl)ethynyl)-N-(3-(3-iodophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (1t)

Compound **1t** was obtained as yellow solid; $R_f = 0.57$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.89 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.0 Hz, 1H), 7.45-7.41 (m, 3H), 7.32 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 7.14 (d, J = 7.6 Hz, 1H), 6.98 (t, J = 7.6 Hz, 1H), 4.55 (s, 2H), 2.41 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.3, 140.3, 137.8, 134.3, 133.1, 131.7, 130.8, 129.84, 129.79, 128.3, 124.0, 122.3, 121.6, 93.5, 84.9, 83.1, 82.6, 70.5, 42.8, 21.9; HRMS (ESI) m/z calcd for C₂₄H₁₇BrINO₂SNa⁺ (M+Na)⁺ 611.9100, found 611.9103.



N-((4-bromophenyl)ethynyl)-N-(3-(2-bromophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (1u)

Compound **1u** was obtained as yellow solid; $R_f = 0.61$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.89 (d, J = 8.0 Hz, 2H), 7.52 (d, J = 7.6 Hz, 1H), 7.42 (d, J = 8.4 Hz, 2H), 7.27-7.24 (m, 4H), 7.22 -7.13 (m, 3H), 4.61 (s, 2H), 2.31 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.2, 134.2, 133.7, 133.1, 132.5, 131.7, 130.0, 129.8, 128.4, 127.0, 125.5, 124.3, 122.3, 121.8, 85.8, 85.1, 83.2, 70.6, 42.9, 21.7; HRMS (ESI) m/z calcd for C₂₄H₁₇Br₂NO₂SNa+ (M+Na)+ 565.9219, found 565.9222.



N-((4-bromophenyl)ethynyl)-N-(3-(2-fluorophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (1v)

Compound **1v** was obtained as yellow solid; $R_f = 0.61$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.89 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.32-7.24 (m, 5H), 7.17-7.13 (m, 1H), 7.06-7.01 (m, 2H), 4.59 (s, 2H), 2.33 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 162.9 (d, J = 253.5 Hz), 145.2, 134.2, 133.7 (d, J = 1.0 Hz), 133.1, 131.6, 130.7 (d, J = 8.0 Hz), 129.8, 128.3, 124.0 (d, J = 3.7 Hz), 122.3, 121.7, 115.6 (d, J = 20.8 Hz),110.7(d, J = 15.8 Hz), 86.3 (d, J = 3.2 Hz), 83.1, 80.2, 70.6, 42.9, 21.7; ¹⁹F NMR (376 MHz, CDCl₃) δ -109.63; HRMS (ESI) m/z calcd for C₂₄H₁₇BrFNO₂SNa+ (M+Na)+ 504.0040, found 504.0045.



N-((4-bromophenyl)ethynyl)-N-(3-(2-iodophenyl)prop-2-yn-1-yl)-4-

methylbenzenesulfonamide (1w)

Compound **1w** was obtained as yellow solid; $R_f = 0.62$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.89 (d, J = 8.0 Hz, 2H), 7.72 (d, J = 8.0 Hz, 1H), 7.37 (d, J = 8.0 Hz, 2H), 7.25-7.18 (m, 5H), 7.11 (d, J = 7.6 Hz, 1H), 6.93 (t, J = 7.6 Hz, 1H), 4.61 (s, 2H), 2.25 (s, 3H);¹³C NMR (101 MHz, CDCl₃) δ 145.2, 138.7, 134.1, 133.0, 132.9, 131.5, 129.9, 129.7, 128.6, 128.2, 127.7, 122.1, 121.7, 100.4, 88.3, 84.9, 83.3, 70.6, 42.8, 21.6; HRMS (ESI) m/z calcd for C₂₄H₁₇BrINO₂SNa⁺ (M+Na)⁺ 611.9100, found 611.9105.



N-((4-bromophenyl)ethynyl)-4-chloro-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1x) Compound **1x** was obtained as yellow solid; $R_f = 0.62$ (petroleum ether : ethyl acetate = 5 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.95 (d, J = 8.8 Hz, 2H), 7.47-7.41 (m, 4H), 7.34-7.23 (m, 5H), 7.15 (d, J = 7.2 Hz, 2H), 4.58 (s, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 140.8, 135.7, 133.1, 131.71, 131.68, 129.7, 129.5, 129.0, 128.5, 122.5, 121.7, 121.4, 87.1, 82.7, 80.8, 70.7, 43.2; HRMS (ESI) m/z calcd for C₂₃H₁₅BrClNO₂SNa⁺ (M+Na)⁺ 505.9588, found 505.9594.

General procedure for the synthesis of pyrrol

To a sealed Schlenk tube was added diyne (0.2 mmol), $Cy_3PAuNTf_2$ (7.6mg, 0.01 mmol), H_2O (0.6 mmol, 10.8 mg) and this mixture was treated with dry CH_3NO_2 (2 mL) under air. The solution was heated at 50 °C for 1h. The resulting solution was cooled to room temperature, and filtered through Celite with ethyl acetate as the eluent. The solvents were evaporated under reduced pressure and the residue was purified by column chromatography on silica gel to afford the products.



phenyl(4-phenyl-1-tosyl-1H-pyrrol-3-yl)methanone (2a)

Compound **2a** was obtained as yellow solid, 44.3 mg, in 55% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.79 (m, 4H), 7.55 (d, J = 2.0 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 7.38 (t, J = 7.6 Hz, 2H), 7.34-7.21 (m, 8H), 2.42 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.8, 146.2, 138.4, 135.2, 132.9, 132.7, 130.55, 130.52, 129.8, 128.6, 128.5, 128.3, 127.52, 127.46, 126.7, 126.0, 119.3, 21.9.; HRMS (ESI) m/z calcd for C₂₄H₁₉NO₃SNa⁺ (M+Na)⁺ 424.0978, found 424.0978.



(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2b)

Compound **2b** was obtained as pale yellow solid, 68.6 mg, in 71% yield; $R_f = 0.41$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.79 (m, 4H), 7.57-7.54 (m, 2H), 7.44-7.33 (m, 6H), 7.27-7.26 (m, 1H), 7.19 (d, J = 8.0 Hz, 2H), 2.42 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.5, 146.3, 138.3, 134.9, 133.0, 131.6, 131.4, 130.5, 130.2, 129.7, 129.3, 128.5, 127.4, 127.0, 125.5, 121.6, 119.4, 21.8; HRMS (ESI) m/z calcd for C₂₄H₁₈BrNO₃SNa⁺ (M+Na)⁺ 502.0083, found 502.0086.



(4-(4-chlorophenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2c)

Compound **2c** was obtained as pale yellow solid, 53.8 mg, in 62% yield; $R_f = 0.41$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.79 (m, 4H), 7.57-7.54 (m, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.26-7.21 (m, 5H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.6, 146.3, 138.3, 135.0, 133.4, 133.0, 131.2, 130.5, 129.9, 129.7, 129.3, 128.55, 128.47, 127.4, 127.0, 125.6, 119.5, 21.8; HRMS (ESI) m/z calcd for C₂₄H₁₈ClNO₃SNa⁺ (M+Na)⁺ 458.0588, found 458.0589.



(4-(4-fluorophenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2d)

Compound **2d** was obtained as pale yellow solid, 54.5 mg, in 65% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.78 (m, 4H), 7.56-7.53 (m, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.30-7.27 (m, 2H), 7.24 (d, J = 2.4 Hz, 1H), 6.97-6.93 (m, 2H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.7, 162.3(d, J = 247.6 Hz), 146.3, 138.4, 135.0, 132.9, 130.5, 130.3 (d, J = 8.2 Hz), 129.7, 129.5, 128.7(d, J = 3.4 Hz), 128.5, 127.4, 126.9, 125.7, 119.3, 115.2 (d, J = 21.6 Hz), 21.8; ¹⁹F NMR (376 MHz, CDCl₃) δ -114.8; HRMS (ESI) m/z calcd for C₂₄H₁₈FNO₃SNa⁺ (M+Na)⁺ 442.0884, found 442.0884.



phenyl(4-(p-tolyl)-1-tosyl-1H-pyrrol-3-yl)methanone (2e)

Compound **2e** was obtained as yellow solid, 44.0 mg, in 53% yield; $R_f = 0.3$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.82-7.80 (m, 4H), 7.55-7.51 (m,

2H), 7.41 (t, J = 7.6 Hz, 2H), 7.33 (d, J = 8.4 Hz, 2H), 7.25-7.24 (m, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 2.43 (s, 3H), 2.30 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.8, 146.1, 138.5, 137.3, 135.2, 132.8, 130.6, 130.5, 129.8, 129.7, 129.1, 128.5, 127.4, 126.7, 126.0, 119.1, 21.8, 21.3. HRMS (ESI) m/z calcd for C₂₅H₂₁NO₃SNa⁺ (M+Na)⁺ 438.1134, found 438.1136. H₃CQ



(4-(4-methoxyphenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2f)

Compound **2f** was obtained as yellow solid, 45.1 mg, in 52% yield; $R_f = 0.25$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.82-7.79 (m, 4H), 7.55-7.52 (m, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.33 (d, J = 8.4 Hz, 2H), 7.26-7.21 (m, 3H), 6.80 (d, J = 8.4 Hz, 2H), 3.76 (s, 3H), 2.42 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.9, 159.1, 146.1, 138.5, 135.1, 132.8, 130.5, 130.2, 129.8, 129.7, 128.4, 127.4, 126.7, 125.8, 125.0, 118.8, 113.8, 55.3, 21.8; HRMS (ESI) m/z calcd for C₂₅H₂₁NO₄SNa⁺ (M+Na)⁺ 454.1084, found 454.1085.



(4-(2-chlorophenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2g)

Compound **2g** was obtained as yellow solid, 49.4 mg, in 57% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1);¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.78 (m, 4H), 7.56-7.50 (m, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 7.32-7.30 (m, 1H), 7.28-7.25 (m, 2H), 7.22-7.19 (m, 2H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.2, 146.2, 138.0, 135.1, 133.4, 132.7, 132.2, 131.4, 130.5, 129.64, 129.62, 129.0, 128.4, 127.4, 127.3, 127.1, 126.7, 125.9, 120.7, 21.8; HRMS (ESI) m/z calcd for C₂₄H₁₈CINO₃SNa⁺ (M+Na)⁺ 458.0588, found 458.0590.



phenyl(4-(o-tolyl)-1-tosyl-1H-pyrrol-3-yl)methanone (2h)

Compound **2h** was obtained as pale yellow solid, 49.3 mg, in 59% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.81 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 7.6 Hz, 2H), 7.58 (d, *J* = 2.0 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.41-7.34 (m, 4H), 7.20-7.11 (m, 5H), 2.44 (s, 3H), 2.10 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.4, 146.1, 138.3, 136.5, 135.3, 132.7, 132.6, 130.5, 130.2, 130.0, 129.7, 129.5, 128.4, 127.9, 127.4, 127.1, 126.3, 125.6, 120.1, 21.9, 20.4; HRMS (ESI) m/z calcd for C₂₅H₂₁NO₃SNa⁺ (M+Na)⁺ 438.1134, found 438.1134.



(4-(3-chlorophenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2i)

Compound **2i** was obtained as yellow solid, 50.0 mg, in 57% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.79 (m, 4H), 7.56-7.52 (m, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.36-7.32 (m, 3H), 7.27 (d, J = 2.4 Hz, 1H), 7.21-7.18 (m, 3H), 2.42 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.5, 146.3, 138.3, 134.9, 134.5, 134.1, 132.9, 130.5, 129.6, 129.5, 129.1, 128.53, 128.51, 127.5, 127.4, 126.99, 126.98, 125.6, 119.7, 21.8; HRMS (ESI) m/z calcd for C₂₄H₁₈ClNO₃SNa⁺ (M+Na)⁺ 458.0588, found 458.0590.



phenyl(4-(m-tolyl)-1-tosyl-1H-pyrrol-3-yl)methanone (2j)

Compound **2j** was obtained as yellow solid, 42.7 mg, in 51% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.78 (m, 4H), 7.54-7.51 (m, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 2.8 Hz, 1H), 7.16-7.13 (m, 1H), 7.10-7.08 (m, 2H), 7.03 (d, J = 7.2 Hz, 1H), 2.44 (s, 3H), 2.27 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.9, 146.2, 138.5, 137.9, 135.2, 132.8, 132.5, 130.7, 130.5, 129.8, 129.3, 128.4, 128.29, 128.25, 127.4, 126.7, 126.1, 125.8, 119.3, 21.9, 21.5; HRMS (ESI) m/z calcd for C₂₅H₂₁NO₃SNa⁺ (M+Na)⁺ 438.1134, found 438.1134.



(4-(3-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2k)

Compound **2k** was obtained as yellow solid, 60.7 mg, in 63% yield; $R_f = 0.41$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.78 (m, 4H), 7.56-7.53 (m, 2H), 7.47 (s, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 3H), 7.27-7.22 (m, 2H), 7.12 (t, *J* = 8.0 Hz, 1H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.5, 146.4, 138.3, 134.9, 134.8, 133.0, 131.4, 130.6, 130.4, 129.74, 129.66, 129.0, 128.53, 127.48, 127.45, 127.0, 125.6, 122.3, 119.7, 21.8; HRMS (ESI) m/z calcd for C₂₄H₁₈BrNO₃SNa⁺ (M+Na)⁺ 502.0083, found 502.0087.



(4-(3-fluorophenyl)-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2l)

Compound **21** was obtained as yellow solid, 47.5 mg, in 57% yield; $R_f = 0.41$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83-7.79 (m, 4H), 7.57-7.53 (m, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 2.4 Hz, 1H), 7.25-7.18 (m, 1H), 7.08-7.03 (m, 2H), 6.94-6.90 (m, 1H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.5, 162.6 (d, J = 246.3 Hz), 146.3, 138.3, 135.0, 134.9 (d, J = 8.4 Hz), 133.0, 130.5, 129.8, 129.7, 129.3 (d, J = 2.3 Hz), 128.5, 127.5, 126.9, 125.7, 124.4 (d, J = 2.8 Hz), 119.7, 115.6 (d, J = 22.4 Hz), 114.3 (d, J = 21.1 Hz), 21.8; ¹⁹F NMR (376 MHz, CDCl₃) δ -113.5; HRMS (ESI) m/z calcd for C₂₄H₁₈FNO₃SNa⁺ (M+Na)⁺ 442.0884, found 442.0882.



(4-cyclopropyl-1-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (2m)

Compound **2m** was obtained as yellow oil 46.5 mg, in 64% yield; $R_f = 0.55$ (petroleum ether : dichloromethane = 1 : 1)¹H NMR (400 MHz, CDCl₃, TMS) δ 7.81-7.79 (m, 2H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.50-7.46 (m, 2H), 7.50-7.50 (m, 2H), 7

2H), 6.79 (d, J = 1.6 Hz, 1H), 2.41 (s, 3H), 2.23-2.16 (m, 1H), 0.90-0.85 (m, 2H), 0.54- 0.50 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 191.3, 145.9, 139.3, 135.2, 133.6, 132.4, 130.4, 129.4, 128.5, 127.2, 127.1, 116.6, 21.8, 8.5, 7.2. HRMS (ESI) m/z calcd for C₂₁H₁₉NO₃SNa⁺ (M+Na)⁺ 388.0978, found 388.0978.



(4-bromophenyl)(4-phenyl-1-tosyl-1H-pyrrol-3-yl)methanone (2n)

Compound **2n** was obtained as yellow solid, 34.0mg, in 35% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.54-7.51 (m, 3H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.27-7.22 (m, 6H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 189.7, 146.3, 137.1, 135.0, 132.5, 131.7, 131.2, 130.5, 130.3, 128.6, 128.4, 127.9, 127.6, 127.5, 126.5, 125.6, 119.4, 21.8; HRMS (ESI) m/z calcd for C₂₄H₁₈BrNO₃SNa⁺ (M+Na)⁺ 502.0083, found 502.0085.



(4-bromophenyl)(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)methanone (20)

Compound **20** was obtained as yellow solid, 66.8 mg, in 60% yield; $R_f = 0.4$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 2.0 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 2.4 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 189.5, 146.5, 137.1, 134.9, 131.9, 131.55, 131.51, 131.2, 130.6, 130.2, 129.3, 128.2, 127.5, 126.9, 125.3, 121.8, 119.6, 21.9; HRMS (ESI) m/z calcd for C₂₄H₁₇Br₂NO₃SNa⁺ (M+Na)⁺ 581.9168, found 581.9168.



(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(4-iodophenyl)methanone (2p)

Compound **2p** was obtained as yellow solid, 81.0 mg, in 67% yield; $R_f = 0.40$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 3H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.26 (s, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H);¹³C NMR (101 MHz, CDCl₃) δ 189.7, 146.4, 137.9, 137.6, 134.9, 131.52, 131.49, 131.1, 130.6, 130.2, 129.3, 127.5, 127.0, 125.2, 121.8, 119.6, 100.8, 21.9; HRMS (ESI) m/z calcd for C₂₄H₁₇BrINO₃SNa⁺ (M+Na)⁺ 627.9049, found 627.9050.



methyl 4-(4-(4-bromophenyl)-1-tosyl-1H-pyrrole-3-carbonyl)benzoate (2q)

Compound **2q** was obtained as yellow solid, 58.6 mg, in 54% yield; $R_f = 0.38$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 8.08 (d, J = 8.0 Hz, 2H), 7.83 (d, J = 2.0 Hz, 2H), 7.81 (d, J = 2.0 Hz, 2H), 7.54 (d, J = 2.4 Hz, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 7.27 (d, J = 2.4 Hz, 1H), 7.19 (d, J = 8.0 Hz, 2H), 3.95 (s, 3H), 2.44 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 189.9, 166.3, 146.5, 141.9, 134.8, 133.7, 131.5, 130.6, 130.3, 129.7, 129.4, 129.2, 127.5, 127.4, 125.2, 121.8, 119.7, 52.6, 21.9; HRMS (ESI) m/z calcd for C₂₆H₂₀BrNO₅SNa⁺ (M+Na)⁺ 560.0138, found 560.0140.



(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(3-fluorophenyl)methanone (2r)

Compound **2r** was obtained as yellow solid, 53.8 mg, in 55% yield; $R_f = 0.41$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83 (d, J = 8.4 Hz, 2H), 7.58-7.56 (m, 2H), 7.47 (d, J = 9.2 Hz, 1H), 7.42-7.35 (m, 5H), 7.27- 7.23 (m, 2H), 7.17 (d, J = 8.4 Hz, 2H), 2.44 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 189.1, 162.6 (d, J = 249.4Hz), 146.5, 140.4 (d, J = 6.3 Hz), 134.8, 131.49, 131.46, 130.6, 130.25 (d, J = 7.6 Hz), 130.24, 129.3, 127.5, 127.1, 125.5 (d, J = 2.9 Hz), 125.1, 121.8, 120.0 (d, J = 21.4 Hz), 119.6, 116.3 (d, J = 22.5 Hz), 21.8; ¹⁹F NMR (376 MHz, CDCl₃) δ -111.7; HRMS (ESI) m/z calcd for C₂₄H₁₇BrFNO₃SNa⁺ (M+Na)⁺ 519.9990, found 519.9992.



(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(3-chlorophenyl)methanone (2s)

Compound **2s** was obtained as yellow solid, 47.6mg, in 46% yield; $R_f = 0.42$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.83 (d, J = 8.4 Hz, 2H), 7.72 (s, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.55 (d, J = 2.4 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.41-7.34 (m, 5H), 7.26 (d, J = 2.4 Hz, 1H), 7.17 (d, J = 8.4 Hz, 2H), 2.44 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 189.1, 146.5, 139.9, 134.9, 134.8, 132.9, 131.51, 131.48, 130.6, 130.3, 129.9, 129.6, 129.3, 127.8, 127.5, 127.2, 125.2, 121.8, 119.6, 21.9; HRMS (ESI) m/z calcd for C₂₄H₁₇BrClNO₃SNa⁺ (M+Na)⁺ 535.9693, found 535.9697.



(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(3-iodophenyl)methanone (2t)

Compound **2t** was obtained as yellow solid, 59.4 mg, in 50% yield; $R_f = 0.45$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 8.05 (s, 1H), 7.86-7.82 (m, 3H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 2.0 Hz, 1H), 7.40-7.36 (m, 4H), 7.26 (d, *J* = 2.0 Hz, 1H), 7.17-7.14 (m, 3H), 2.44 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 188.9, 146.4, 141.6, 140.1, 138.5, 134.8, 131.5, 131.4, 130.6, 130.25, 130.22, 129.2, 128.7, 127.5, 127.2, 125.1, 121.8, 119.6, 94.2, 21.9; HRMS (ESI) m/z calcd for C₂₄H₁₇BrINO₃SNa⁺ (M+Na)⁺ 627.9049, found 627.9051.



(2-bromophenyl)(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)methanone (2u)

Compound **2u** was obtained as yellow solid,54.6 mg, in 49% yield; $R_f = 0.38$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.79 (d, J = 8.4 Hz, 2H), 7.57 (d, J

= 7.2 Hz, 1H), 7.42-7.40 (m, 3H), 7.36-7.32 (m, 4H), 7.31-7.26 (m, 3H), 7.17 (d, J = 2.4 Hz, 1H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 190.0, 146.5, 141.1, 134.8, 133.5, 131.6, 131.3, 131.2, 130.61, 130.58, 129.39, 129.37, 129.0, 127.5, 127.4, 125.7, 121.8, 120.1, 119.9, 21.9; HRMS (ESI) m/z calcd for C₂₄H₁₇Br₂NO₃SNa⁺ (M+Na)⁺ 581.9168, found 581.9169.



(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(2-fluorophenyl)methanone (2v)

Compound **2v** was obtained as pale yellow solid, 49.8 mg, in 50% yield; $R_f = 0.43$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.80 (d, J = 8.4 Hz, 2H), 7.567-7.565 (m, 1H), 7.52-7.43 (m, 2H), 7.39-7.34 (m, 4H), 7.22-7.16 (m, 4H), 7.04 (t, J = 9.2 Hz, 1H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 187.1, 161.1 (d, J = 254.3 Hz), 146.4, 134.8, 133.5 (d, J = 8.5Hz), 131.5, 131.2, 130.7 (d, J = 2.3 Hz), 130.59, 130.57, 129.0, 128.4 (d, J = 2.6 Hz), 127.9 (d, J = 13.8 Hz), 127.5 126.5, 124.3 (d, J = 3.6 Hz), 121.7, 119.7, 116.5 (d, J = 21.9 Hz), 21.8; ¹⁹F NMR (376 MHz, CDCl₃) δ -112.0; HRMS (ESI) m/z calcd for C₂₄H₁₇BrFNO₃SNa⁺ (M+Na)⁺ 519.9990, found 519.9993.



(4-(4-bromophenyl)-1-tosyl-1H-pyrrol-3-yl)(2-iodophenyl)methanone (2w)

Compound **2w** was obtained as yellow solid, 51.0 mg, in 42% yield; $R_f = 0.45$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.86 (d, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.43-7.41 (m, 2H), 7.39-7.34 (m, 4H), 7.32-7.26 (m, 3H), 7.18 (d, *J* = 2.4 Hz, 1H), 7.14 (td, *J*₁ = 8.0 Hz, *J*₂ = 2.0 Hz, 1H), 2.43 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 191.5, 146.5, 144.5, 140.1, 134.8, 131.7, 131.4, 131.3, 130.59, 130.57, 129.5, 129.1, 129.0, 128.0, 127.5, 125.1, 121.8, 120.2, 92.9, 21.9; HRMS (ESI) m/z calcd for C₂₄H₁₇BrINO₃SNa⁺ (M+Na)⁺ 627.9049, found 627.9050.



(4-(4-bromophenyl)-1-((4-chlorophenyl)sulfonyl)-1H-pyrrol-3-yl)(phenyl)methanone (2x)

Compound **2x** was obtained as yellow solid, 71.3 mg, in 71% yield; $R_f = 0.42$ (petroleum ether : dichloromethane = 1 : 1); ¹H NMR (400 MHz, CDCl3, TMS) δ 7.87 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 7.2 Hz, 2H), 7.57-7.51 (m, 4H), 7.44-7.37 (m, 4H), 7.26 (d, J = 2.0 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 190.4, 141.8, 138.1, 136.3, 133.1, 131.5, 131.4, 130.3, 130.2, 129.8, 129.7, 128.8, 128.6, 126.7, 126.1, 121.8, 119.3; HRMS (ESI) m/z calcd for $C_{23}H_{15}BrCINO_3SNa^+$ (M+Na)⁺ 521.9537, found 521.9540.

Crystal structure



2a, CDCC 2127108

Bond precision:	C-C = 0.0017 A	Wavelength=1.34150	
Cell:	a=8.25955(8) alpha=90	b=10.43795(9	c=22.5124(2)
Temperature:	100 K	2000 20	ganana yo
	Calculated	Rep	orted
Volume	1940.86(3)	194	0.86(3)
Space group	P c a 21	Pca	2(1)
Hall group	P 2c -2ac	?	
Moiety formula	C24 H19 N O3 S	?	
Sum formula	C24 H19 N O3 S	C24	H19 N O3 S
Mr	401.46	401	.46
Dx,g cm-3	1.374	1.3	74
Z	4	4	
Mu (mm-1)	1.106	1.0	96
F000	840.0	840	.0
F000'	842.94		
h,k,lmax	10,13,29	10,	13,29
Nref	4457[2289]	440	8
Tmin, Tmax	0.769,0.896	0.4	83,1.000
Tmin'	0.760		
Correction metho AbsCorr = MULTI-	d= # Reported T Lim SCAN	nits: Tmin=0.	483 Tmax=1.000
Data completenes	s= 1.93/0.99	Theta(max) =	60.600
R(reflections)=	0.0221(4392)		wR2(reflections)= 0.0611(4408)
S = 1.048	Npar= 26	4	

References

- 1. Y. C. Hsu, S. A. Hsieh and R. S. Liu, Chem. Eur. J., 2019, 25, 5288.
- 2. N. Ghosh, S. Nayak and A. K. Sahoo, Chem. Eur. J., 2013, 19, 9428
- 3. S. Dutta, B. Prabagar, R. Vanjari, V. Gandon and A. K. Sahoo, Green Chem., 2020, 22, 1113.
- J. Febvay, Y. Sanogo, P. Retailleau, M. P. Gogoi, A. K. Sahoo, A. Marinetti and A. Voituriez, *Org. Lett.*, 2019, 21, 9281.
- 5. B. H. Zhu, C. M. Wang, H. Y. Su and L. W. Ye, Chin. J. Chem., 2018, 37, 58.
- S. Dutta, R. K. Mallick, R. Prasad, V. Gandon and A. K. Sahoo, *Angew. Chem. Int. Ed*, 2019, 58, 2289.
- 7. R. Liu, G. N. Winston-McPherson, Z. Y. Yang, X. Zhou, W. Song, I. A. Guzei, X. Xu and W. Tang, J. Am. Chem. Soc., 2013, 135, 8201.
- 8. B. Prabagar, S. Nayak, R. Prasad and A. K. Sahoo, Org. Lett., 2016, 18, 3066.
- 9. F. L. Hong, Z. S. Wang, D. D. Wei, T. Y. Zhai, G. C. Deng, X. Lu, R. S. Liu and L. W. Ye, J. Am. Chem. Soc., 2019, 141, 169

NMR Spectra



S22



90 80 fl (ppm)



















10 0 -10 -20 -30 -40 -50 -80 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -200 -200 -210 fl (ppm)

Ts ∖Ņ́













S32





























1w















210 200 190 180 170 180 150 140 130 120 110 100 90 80 70 80 50 40 30 20 10 0 -10 fl (ppm)













S47



S48



H₃CO

0















210 200 130 180 170 180 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 fl (ppm)





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)





210 200 150 150 150 150 150 150 140 130 120 110 100 50 80 70 60 50 40 30 20 10 0 -10 fl (ppm)







210 200 190 180 170 160 150 140 130 120 110 100 90 60 70 60 50 40 30 20 10 0 -10 fl(ppm)



21

wq1-6-1-a1

	Parameter	Value	
1	Data File Name	D:/ pt/ 2021/ wql-6-1- al/ 3/ fid	
2	Title	wql=6-1-al	
3	Comment		
4	Origin	Bruker BioSpin GmbH	
5	Owner	nmrsu	
6	Site		
7	Spectrometer	spect	
8	Author		
9	Solvent	CDC13	
10	Temperature	296.4	
11	Pulse Sequence	zgfhigqn.2	
12	Number of Scans	16	
13	Receiver Gain	197	
14	Relaxation Delay	1.0000	
15	Pulse Width	18.0000	
16	Acquisition Time	0.7340	
17	Acquisition Date	2021-06-11712:45:00	
18	Modification Date	2021-06-11712:45:00	
19	Spectrometer Frequency	376, 50	
20	Spectral Width	89285.7	
21	Lowest Frequency	-82292.7	
22	Nucleus	19F	
23	Acquired Size	65536	
24	Spectral Size	131072	



-113,460







210 200 190 180 170 160 180 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 fl (ppm)







210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 fl (grav)









alteria bala





210 200 190 150 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 fl (ppa)







210 200 190 180 170 180 180 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppa)





210 200 190 180 170 180 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 fl (ppm)























-0.000





















S69



