



Supporting Information

for

AgNTf₂-catalyzed formal [3 + 2] cycloaddition of ynamides with unprotected isoxazol-5-amines: efficient access to functionalized 5-amino-1*H*-pyrrole-3-carboxamide derivatives

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Beilstein J. Org. Chem. **2019**, *15*, 2623–2630. doi:10.3762/bjoc.15.255

Characterization data and ¹H and ¹³C NMR spectra for all new compounds

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General information.

Reactions were carried out in open flask and monitored by thin-layer chromatography (TLC) carried out on silica plates, visualized by irradiation with UV light. Commercially available reagents were used without further purification. ^1H and ^{13}C NMR spectra were recorded at 500 MHz for ^1H nuclei, 125.8 MHz for ^{13}C nuclei. Chemical shifts (δ) are reported in units of parts per million (ppm); signals are referenced to TMS (0.00 ppm) or solvent residual peak (DMSO- d_6 , 2.5 ppm for ^1H and 39.5 ppm for ^{13}C) as an internal standard. Coupling constants (J) are given in Hz, and multiplicity is abbreviated as: s (singlet), d (doublet), dd (doublet of doublets), t (triplet), q (quartet), and m (multiplet). All melting points are uncorrected and determined on a X-4 digital microscopic melting point apparatus. HRMS were measured using electrospray ionization (ESI).

Synthesis of substrates

Ynamide compounds **4a–q** were prepared according to the known literatures [1]. The isoxazol-5-amines **8a–e** are commercially available reagents.

Ref: [1] (a) Zhu, J.; Wang, Q.; Meng, X.; Zhao, C.; Sun, X.; Tian L.; Cao, Z. *Eur. J. Org. Chem.* **2019**, 2019, 4066–4070; doi:10.1002/ejoc.201900604 (b) Saito, N.; Saito, K.; Shiro M.; Sato, Y. *Org. Lett.* **2011**, 13, 2718–2721. doi: [10.1021/ol200812y](https://doi.org/10.1021/ol200812y)

Characterization data for all new compounds

N-(4-Acetyl-5-methyl-3-phenyl-1*H*-pyrrol-2-yl)-*N*,4-dimethylbenzenesulfonamide (**6**): white solid, m.p. 157.8-159.0 °C, yield 32.0 mg, 42%; R_f = 0.32 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*₆, 500MHz): δ 11.62 (s, 1H), 7.35 (d, J = 8.3 Hz, 2H), 7.26 (d, J = 8.1 Hz, 2H), 7.22 (d, J = 7.4 Hz, 1H), 7.17 (dd, J = 7.1, 7.1 Hz, 2H), 6.92 (d, J = 7.0 Hz, 2H), 2.91 (s, 3H), 2.40 (s, 3H), 2.38 (s, 3H), 1.70 (s, 3H); ^{13}C NMR (DMSO-*d*₆, 125.8MHz): δ 194.1, 143.5, 135.0, 134.7, 132.7, 130.0, 129.6, 127.6, 127.3, 126.7, 123.0, 121.3, 119.9, 38.5, 30.3, 21.0, 13.7. HRMS (ESI) m/z calcd for C₂₁H₂₃N₂O₃S (M+H)⁺ 383.1424, found 383.1426.

5-((*N*,4-Dimethylphenyl)sulfonamido)-2-methyl-4-phenyl-1*H*-pyrrole-3-carboxamide (**10aa**): white solid, m.p. 176.5-178.5 °C, yield 75.9 mg, 99%; R_f = 0.16 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*₆, 500MHz): δ 11.22 (s, 1H), 7.37 (d, J = 8.2 Hz, 2H), 7.25 (d, J = 8.1 Hz, 2H), 7.23-7.13 (m, 3H), 6.99 (d, J = 6.4 Hz, 2H), 6.76 (s, 1H), 5.87 (s, 1H), 2.96 (s, 3H), 2.39 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (DMSO-*d*₆, 125.8MHz): δ 166.7, 143.3, 135.1, 134.0, 129.57, 129.52, 128.8, 127.7, 127.3, 126.3, 122.3, 119.4, 114.4, 38.6, 21.0, 14.5. HRMS (ESI) m/z calcd for C₂₀H₂₂N₃O₃S (M+H)⁺ 384.1376, found 384.1375.

5-((*N*,4-Dimethylphenyl)sulfonamido)-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carboxamide (**10ba**): white solid, m.p. 196.0-198.0 °C, yield 81.9 mg, 99%; R_f = 0.17 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*₆, 500MHz): δ 11.21 (s, 1H), 7.38 (d, J = 8.3 Hz, 2H), 7.25 (d, J = 8.1 Hz, 2H), 6.89 (d, J = 8.7 Hz, 2H), 6.72 (d, J = 8.7 Hz, 2H+1H), 5.89 (b, 1H), 3.74 (s, 3H), 2.97 (s, 3H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (DMSO-*d*₆, 125.8MHz): δ 166.7, 158.0, 143.2, 135.3, 130.8, 129.5, 129.1, 127.2, 125.9, 122.3, 118.9, 114.0, 113.2, 54.9, 38.7, 21.0, 12.6. HRMS (ESI) m/z calcd for C₂₁H₂₄N₃O₄S (M+H)⁺ 414.1482, found 414.1486.

5-((*N*,4-Dimethylphenyl)sulfonamido)-2-methyl-4-(*p*-tolyl)-1*H*-pyrrole-3-carboxamide (**10ca**): white solid, m.p. 182.6-184.6 °C, yield 78.6 mg, 99%; R_f = 0.18 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*₆, 500MHz): δ 11.22 (s, 1H), 7.37 (d, J = 8.2 Hz, 2H), 7.25 (d, J = 8.1 Hz, 2H), 6.97 (d, J = 7.8 Hz, 2H), 6.86 (d, J = 7.9 Hz, 2H), 6.74 (b, 1H), 5.74 (b, 1H), 2.97 (s, 3H), 2.39 (s, 3H), 2.33 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (DMSO-*d*₆, 125.8MHz): δ 166.7, 143.2, 135.6, 135.3, 130.9, 129.5, 129.4, 129.1, 128.4, 127.2, 122.3, 119.3, 114.1, 38.7, 21.0, 20.7, 12.5. HRMS (ESI) m/z calcd for C₂₁H₂₄N₃O₃S (M+H)⁺ 398.1533, found 398.1530.

4-(4-(*tert*-Butyl)phenyl)-5-((*N*,4-dimethylphenyl)sulfonamido)-2-methyl-1*H*-pyrrole-3-carboxamide (**10da**): white solid, m.p. 195.7-197.6 °C, yield 74.7 mg, 85%; R_f = 0.16 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*₆, 500MHz): δ 11.23 (s, 1H), 7.35 (d, J = 8.1 Hz, 2H), 7.22 (d, J = 8.2 Hz, 2H), 7.19 (d, J = 8.2 Hz, 2H), 6.95 (d, J = 8.1 Hz, 2H), 6.74 (b, 1H), 5.84 (b, 1H), 2.98 (s, 3H), 2.37 (s, 3H), 2.32 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (DMSO-*d*₆, 125.8MHz): δ 166.8, 148.6, 143.1, 135.2, 130.9, 129.4, 129.3, 128.9, 127.3, 124.4, 122.2, 119.3, 114.2, 38.7, 34.1, 31.2, 21.0, 12.5. HRMS (ESI) m/z calcd for C₂₄H₃₀N₃O₃S (M+H)⁺ 440.2002, found 440.2006.

5-((*N*,4-Dimethylphenyl)sulfonamido)-4-(4-fluorophenyl)-2-methyl-1*H*-pyrrole-3-carboxamide (**10ea**): white solid, m.p. 185.9-187.9 °C, yield 79.5 mg, 99%; R_f = 0.15 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*₆, 500MHz): δ 11.23 (s, 1H), 7.28 (d, J = 8.2 Hz, 2H), 7.25 (d, J = 8.1 Hz, 2H), 7.04-6.93 (m, 4H), 6.79 (b, 1H), 6.11 (b, 1H), 3.03 (s, 3H), 2.38 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (DMSO-*d*₆, 125.8MHz): δ 166.7, 161.0 (d, J = 242.7 Hz), 143.3, 135.3, 131.3 (d, J = 8.0 Hz), 130.2 (d, J = 3.3 Hz), 129.5, 128.3, 127.2, 122.4, 118.5, 114.7, 114.4 (d, J = 21.2 Hz), 38.8, 21.0, 12.4. HRMS (ESI) m/z calcd for C₂₀H₂₁FN₃O₃S (M+H)⁺ 402.1282, found 402.1286.

4-(4-Chlorophenyl)-5-((N,4-dimethylphenyl)sulfonamido)-2-methyl-1H-pyrrole-3-carboxamide (10fa): white solid, m.p. 192.2-194.0 °C, yield 82.8 mg, 99%; R_f = 0.14 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO- d_6 , 500MHz): δ 11.26 (s, 1H), 7.35 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.1 Hz, 2H), 6.98 (d, J = 8.2 Hz, 2H), 6.82 (b, 1H), 6.32 (b, 1H), 3.07 (s, 3H), 2.39 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 166.7, 143.3, 135.4, 132.9, 131.0, 130.8, 129.4, 128.1, 127.5, 127.1, 122.5, 118.4, 114.9, 38.9, 21.0, 12.3. HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{21}\text{ClN}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 418.0987, found 418.0985.

4-(4-Bromophenyl)-5-((N,4-dimethylphenyl)sulfonamido)-2-methyl-1H-pyrrole-3-carboxamide (10ga): white solid, m.p. 210.9-212.5 °C, yield 91.3 mg, 99%; R_f = 0.16 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO- d_6 , 500MHz): δ 11.27 (s, 1H), 7.34 (d, J = 8.1 Hz, 2H), 7.30 (d, J = 8.3 Hz, 2H), 7.22 (d, J = 8.1 Hz, 2H), 6.92 (d, J = 8.3 Hz, 2H), 6.83 (b, 1H), 6.34 (b, 1H), 3.08 (s, 3H), 2.40 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 166.7, 143.3, 135.4, 133.3, 131.3, 130.4, 129.4, 128.1, 127.1, 122.4, 119.4, 118.5, 114.9, 39.0, 21.1, 12.3. HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{21}\text{BrN}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 462.0482, found 462.0478.

5-((N,4-Dimethylphenyl)sulfonamido)-2-methyl-4-(m-tolyl)-1H-pyrrole-3-carboxamide (10ha): white solid, m.p. 183.4-185.4 °C, yield 78.6 mg, 99%; R_f = 0.16 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO- d_6 , 500MHz): δ 11.24 (s, 1H), 7.37 (d, J = 8.1 Hz, 2H), 7.25 (d, J = 8.1 Hz, 2H), 7.07 (dd, J = 7.5, 7.5 Hz, 1H), 7.00 (d, J = 7.5 Hz, 1H), 6.80 (d, J = 7.5 Hz, 1H), 6.74 (b, 1H), 6.71 (s, 1H), 5.78 (b, 1H), 2.96 (s, 3H), 2.38 (s, 3H), 2.33 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 166.7, 143.2, 136.7, 135.2, 133.9, 130.1, 129.5, 128.9, 127.7, 127.2, 127.1, 126.8, 122.2, 119.2, 114.2, 38.6, 21.0, 20.9, 12.5. HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{24}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 398.1533, found 398.1536.

4-(3-Chlorophenyl)-5-((N,4-dimethylphenyl)sulfonamido)-2-methyl-1H-pyrrole-3-carboxamide (10ia): white solid, m.p. 193.2-194.9 °C, yield 82.8 mg, 99%; R_f = 0.16 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO- d_6 , 500MHz): δ 11.29 (s, 1H), 7.37 (d, J = 8.2 Hz, 2H), 7.24 (d, J = 8.1 Hz, 2H), 7.22-7.13 (m, 2H), 6.99 (ddd, J = 6.6, 1.4, 2.0 Hz, 1H), 6.95 (s, 1H), 6.87 (b, 1H), 6.43 (b, 1H), 3.06 (s, 3H), 2.34 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 166.7, 143.4, 136.2, 135.1, 132.2, 129.5, 129.2, 128.8, 127.94, 127.93, 127.1, 125.8, 122.5, 118.1, 115.1, 38.7, 21.1, 12.2. HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{21}\text{ClN}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 418.0987, found 418.0985.

5-((N-isopropyl-4-methylphenyl)sulfonamido)-2-methyl-4-phenyl-1H-pyrrole-3-carboxamide (10ka): white solid, m.p. 158.7-160.3 °C, yield 41.2 mg, 50%; R_f = 0.22 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO- d_6 , 500MHz): δ 10.93 (s, 1H), 7.64 (d, J = 8.1 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.27 (s, 5H), 6.78 (b, 1H), 5.83 (b, 1H), 3.85 (sept, J = 6.3 Hz, 1H), 2.41 (s, 3H), 2.38 (s, 3H), 0.88 (d, J = 6.3 Hz, 3H), 0.48 (d, J = 6.2 Hz, 3H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 166.8, 143.2, 137.4, 134.5, 130.2, 129.7, 127.6, 127.4, 126.6, 123.1, 116.5, 114.6, 51.9, 21.4, 21.2, 21.0, 12.5. HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{26}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 412.1689, found 412.1685.

5-((N-Butyl-4-methylphenyl)sulfonamido)-2-methyl-4-phenyl-1H-pyrrole-3-carboxamide (10la): white solid, m.p. 169.5-171.5 °C, yield 68.1 mg, 80%; R_f = 0.19 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO- d_6 , 500MHz): δ 11.12 (s, 1H), 7.50 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 8.1 Hz, 2H), 7.24-7.12 (m, 3H), 6.97 (d, J = 6.9 Hz, 2H), 6.73 (b, 1H), 5.73 (b, 1H), 3.13 (b, 2H), 2.41 (s, 3H), 2.34 (s, 3H), 1.22-1.14 (m, 2H), 1.03 (dq, J = 7.4, 7.3 Hz, 2H), 0.67 (t, J = 7.3 Hz, 3H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 166.7, 143.3, 135.9, 134.0, 129.6 (2C), 129.4, 127.7, 127.4, 126.5, 120.4, 119.8, 114.3, 49.7, 29.8, 21.0, 18.9, 13.4, 12.5. HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{28}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 426.1846, found 426.1845.

2-Methyl-5-((4-methyl-N-phenylphenyl)sulfonamido)-4-phenyl-1H-pyrrole-3-carboxamide (10ma): white solid, m.p. 189.0-191.0 °C, yield 83.8 mg, 94%; R_f = 0.21 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*6, 500MHz): δ 11.57 (s, 1H), 7.38 (d, J = 3.6 Hz, 2H), 7.33-7.14 (m, 8H), 7.12-6.99 (m, 4H), 6.80 (b, 1H), 6.00 (b, 1H), 2.39 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (DMSO-*d*6, 125.8MHz): δ 166.6, 143.7, 141.2, 136.1, 133.9, 129.6, 129.53, 129.51, 129.0, 127.7, 127.5, 126.8, 126.6, 126.2, 121.0, 120.9, 114.8, 21.0, 12.5. HRMS (ESI) m/z calcd for $\text{C}_{25}\text{H}_{24}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 446.1533, found 446.1529.

5-(N-Benzylmethylsulfonamido)-2-methyl-4-phenyl-1H-pyrrole-3-carboxamide (10na): white solid, m.p. 180.9-182.4 °C, yield 75.2 mg, 98%; R_f = 0.20 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*6, 500MHz): δ 11.31 (s, 1H), 7.34-7.26 (m, 3H), 7.26-7.17 (m, 3H), 7.14-7.00 (m, 4H), 6.73 (b, 1H), 5.67 (b, 1H), 4.47 (s, 2H), 2.97 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (DMSO-*d*6, 125.8MHz): δ 166.6, 135.9, 134.1, 129.9, 129.4, 128.5, 128.1, 127.8, 127.5, 126.7, 120.8, 120.7, 114.1, 54.1, 39.3, 12.6. HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{22}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 384.1376, found 384.1380.

2-Methyl-5-((N-methyl-2-nitrophenyl)sulfonamido)-4-phenyl-1H-pyrrole-3-carboxamide (10oa): white solid, m.p. 200.6-202.6 °C, yield 82.1 mg, 99%; R_f = 0.16 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*6, 500MHz): δ 11.47 (s, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.74 (dd, J = 7.9, 7.4 Hz, 1H), 7.56 (dd, J = 7.6, 7.6 Hz, 1H), 7.45 (d, J = 7.9 Hz, 1H), 7.14-7.07 (m, 3H), 7.04-6.97 (m, 2H), 6.80 (b, 1H), 5.94 (b, 1H), 3.24 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (DMSO-*d*6, 125.8MHz): δ 166.6, 147.1, 134.6, 133.4, 132.2, 130.9, 130.5, 129.4, 129.3, 127.7, 126.4, 124.2, 121.1, 120.1, 114.5, 40.2, 12.5. HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{19}\text{N}_4\text{O}_5\text{S}$ ($\text{M}+\text{H}$) $^+$ 415.1071, found 415.1072.

2-Methyl-5-((N-methyl-4-nitrophenyl)sulfonamido)-4-phenyl-1H-pyrrole-3-carboxamide (10pa): white solid, m.p. 198.6-200.1 °C, yield 82.1 mg, 99%; R_f = 0.17 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*6, 500MHz): δ 11.34 (s, 1H), 8.15 (d, J = 8.9 Hz, 2H), 7.69 (d, J = 8.8 Hz, 2H), 7.08-6.98 (m, 3H), 7.04-7.67 (m, 2H), 6.80 (b, 1H), 5.99 (b, 1H), 3.21 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (DMSO-*d*6, 125.8MHz): δ 166.6, 149.6, 143.9, 133.7, 129.4, 128.9, 128.5, 127.7, 126.2, 124.2, 121.5, 119.8, 114.7, 45.1, 12.4. HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{19}\text{N}_4\text{O}_5\text{S}$ ($\text{M}+\text{H}$) $^+$ 415.1071, found 415.1075.

5-((N,4-Dimethylphenyl)sulfonamido)-2,4-diphenyl-1H-pyrrole-3-carboxamide (10ab): white solid, m.p. 195.1-197.8 °C, yield 87.3 mg, 98%; R_f = 0.22 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*6, 500MHz): δ 11.50 (s, 1H), 7.62 (d, J = 7.5 Hz, 2H), 7.48-7.38 (m, 4H), 7.32-7.16 (m, 9H), 7.11 (b, 1H), 3.15 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (DMSO-*d*6, 125.8MHz): δ 168.3, 143.3, 135.4, 133.7, 131.8, 129.5, 128.9, 128.3, 127.7, 127.3, 126.9, 126.8, 126.7, 126.0, 124.5, 120.2, 117.9, 38.6, 21.0. HRMS (ESI) m/z calcd for $\text{C}_{25}\text{H}_{24}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 446.1533, found 446.1531.

5-((N,4-Dimethylphenyl)sulfonamido)-4-phenyl-2-(p-tolyl)-1H-pyrrole-3-carboxamide (10ac): white solid, m.p. 189.5-191.7 °C, yield 88.2 mg, 96%; R_f = 0.18 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*6, 500MHz): δ 11.41 (s, 1H), 7.49 (d, J = 8.1 Hz, 2H), 7.42 (d, J = 8.2 Hz, 2H), 7.25 (d, J = 8.1 Hz, 2H), 7.21 (d, J = 8.0 Hz, 2H), 7.20-7.14 (m, 6H), 7.07 (b, 1H), 3.13 (s, 3H), 2.38 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (DMSO-*d*6, 125.8MHz): δ 168.4, 143.3, 136.2, 135.5, 133.7, 129.5, 129.0, 128.88, 128.87, 127.7, 127.3, 126.9, 126.7, 126.0, 124.2, 120.2, 117.4, 38.7, 21.0, 20.8. HRMS (ESI) m/z calcd for $\text{C}_{26}\text{H}_{26}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 460.1689, found 460.1685.

5-((N,4-Dimethylphenyl)sulfonamido)-2-isopropyl-4-phenyl-1H-pyrrole-3-carboxamide (10ad): white solid, m.p. 176.3-178.1 °C, yield 80.7 mg, 98%; R_f = 0.20 (hexanes/EtOAc = 1/1); ^1H NMR (DMSO-*d*6, 500MHz): δ 10.90 (s, 1H), 7.33 (d, J = 8.3 Hz, 2H), 7.23 (d, J = 8.3 Hz, 2H), 7.20-7.14 (m, 3H), 7.12-7.06 (m, 2H),

6.82 (b, 1H), 6.09 (b, 1H), 3.48 (sept, $J = 7.0$ Hz, 1H), 3.06 (s, 3H), 2.37 (s, 3H), 1.20 (d, $J = 7.0$ Hz, 6H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 167.3, 143.1, 137.6, 135.4, 134.1, 129.41, 129.37, 127.7, 127.3, 126.0, 122.5, 118.8, 113.6, 38.6, 25.3, 22.3, 21.0. HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{26}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 412.1689, found 412.1688.

2-(*tert*-Butyl)-5-((*N*,4-dimethylphenyl)sulfonamido)-4-phenyl-1*H*-pyrrole-3-carboxamide (**10ae**): white solid, m.p. 198.1-200.7 °C, yield 32.3 mg, 38%; $R_f = 0.56$ (hexanes/EtOAc = 1/1); ^1H NMR (DMSO- d_6 , 500MHz): δ 10.41 (s, 1H), 7.35 (d, $J = 8.1$ Hz, 2H), 7.21 (d, $J = 8.0$ Hz, 2H), 7.18-7.10 (m, 6H), 6.95 (b, 1H), 3.10 (s, 3H), 2.36 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (DMSO- d_6 , 125.8MHz): δ 169.9, 142.9, 135.8, 134.31, 134.26, 129.3, 128.7, 127.5, 127.2, 125.5, 121.3, 118.5, 115.8, 38.8, 32.7, 30.1, 21.0. HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{28}\text{N}_3\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 426.1846, found 426.1845.

X-ray structure and data of 10ad

X-ray diffraction data were collected on a Bruker SMART APEX diffractometer. Diffraction experiments employed graphite-monochromated Mo K α radiation ($\lambda=0.71073$ Å). Colorless blocks were obtained by slow evaporation of a EtOAc/hexanes (v/v: 1:5) solution of **10ad** at room temperature. CCDC 1916501 (**10ad**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

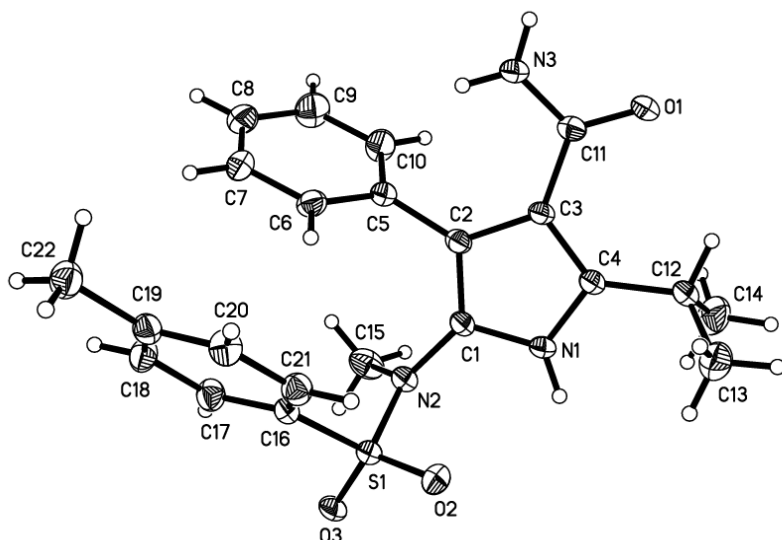


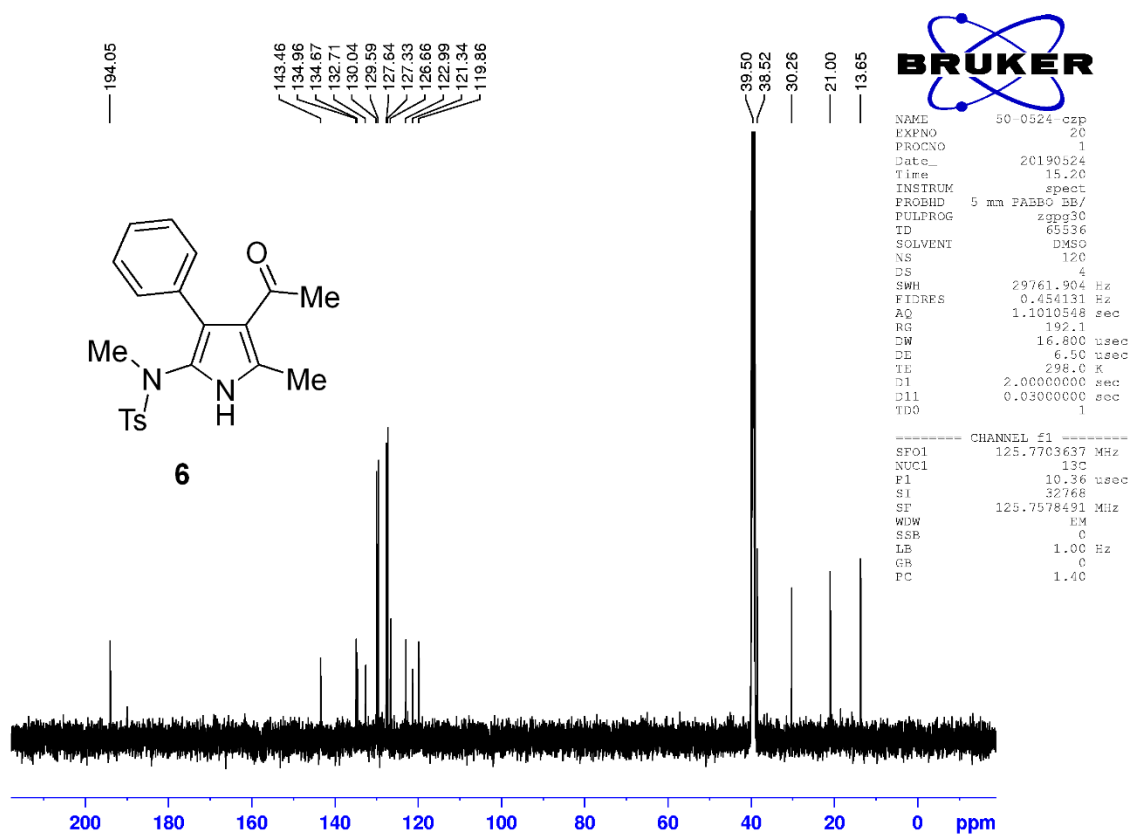
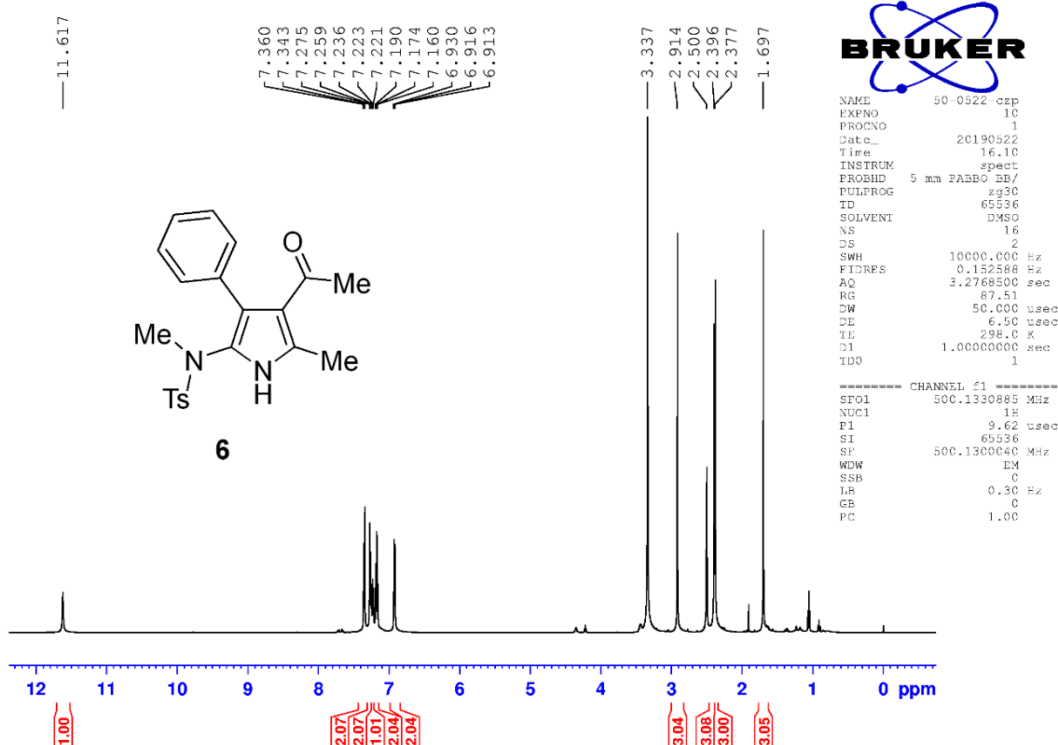
Figure 1 X-ray structure of **10ad**.

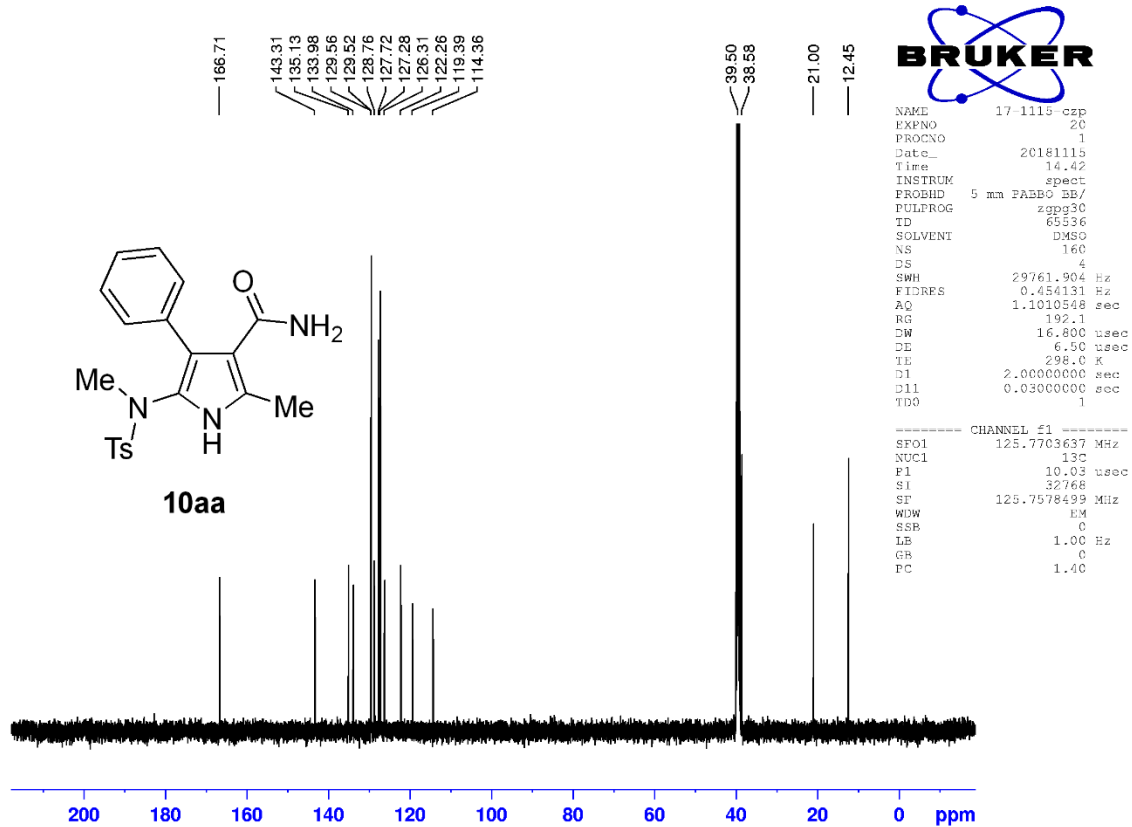
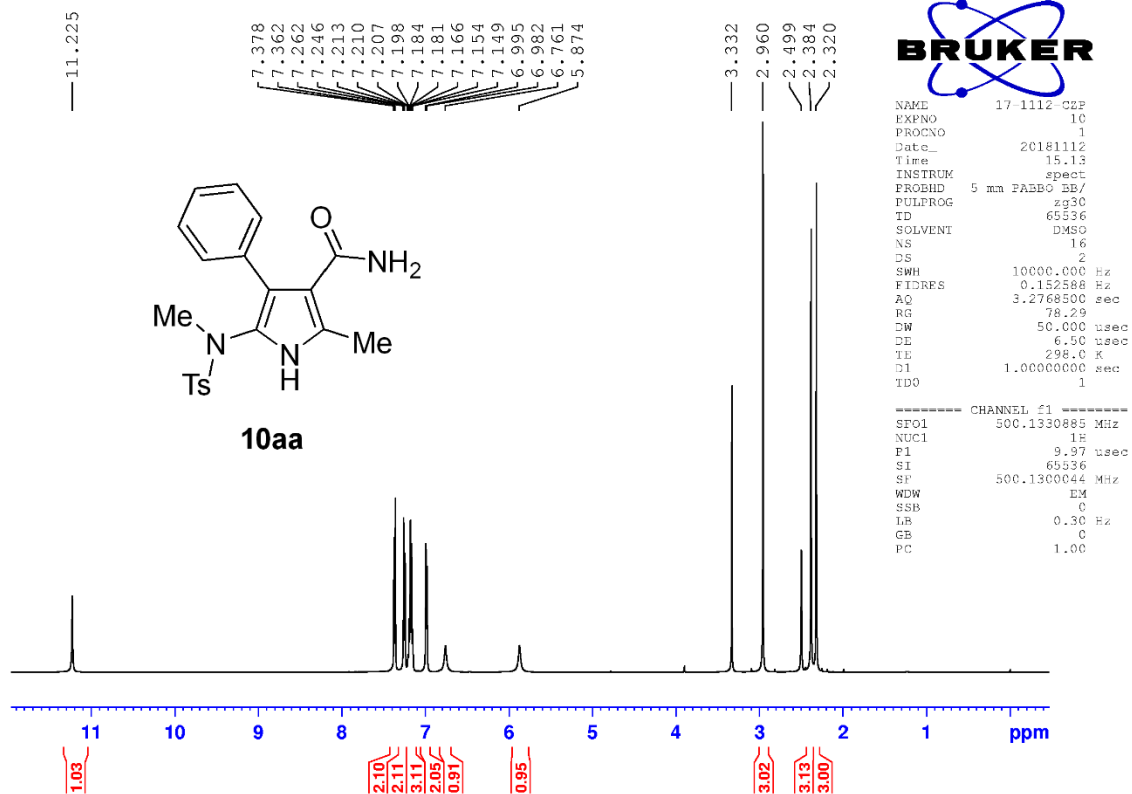
Table 1 crystal data and structure refinement for **10ad**.

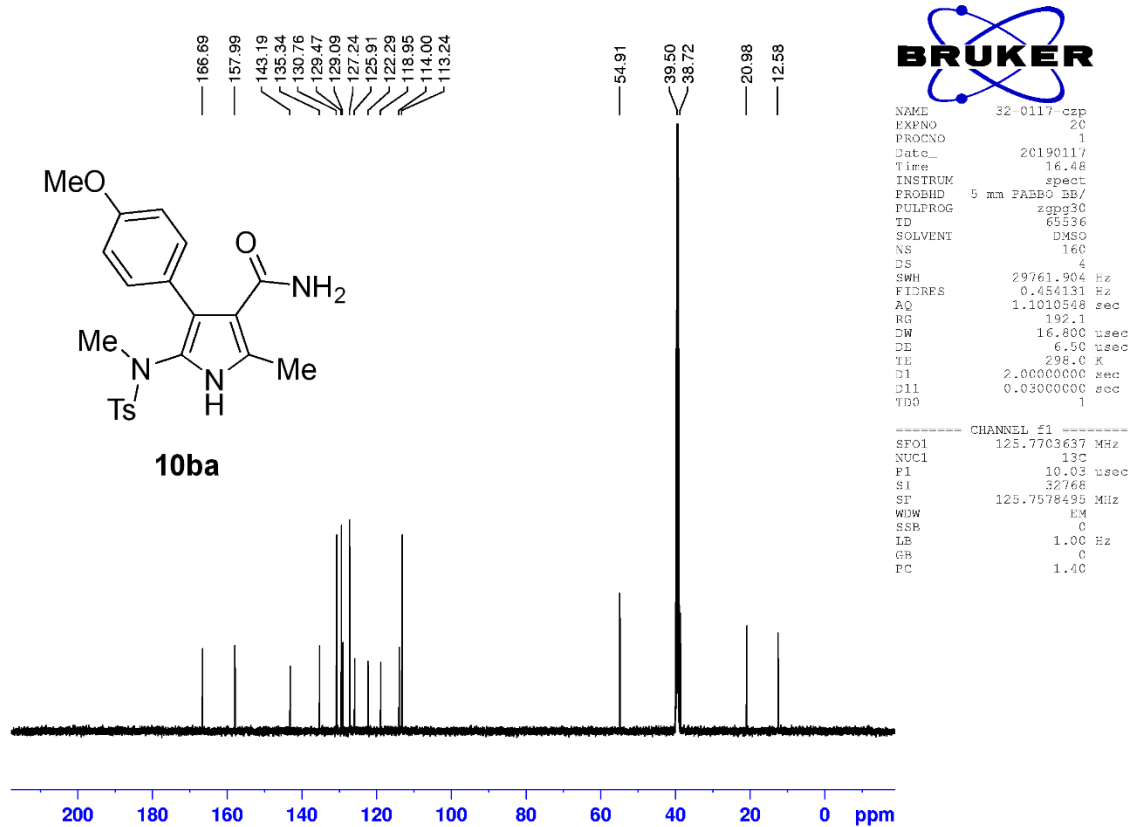
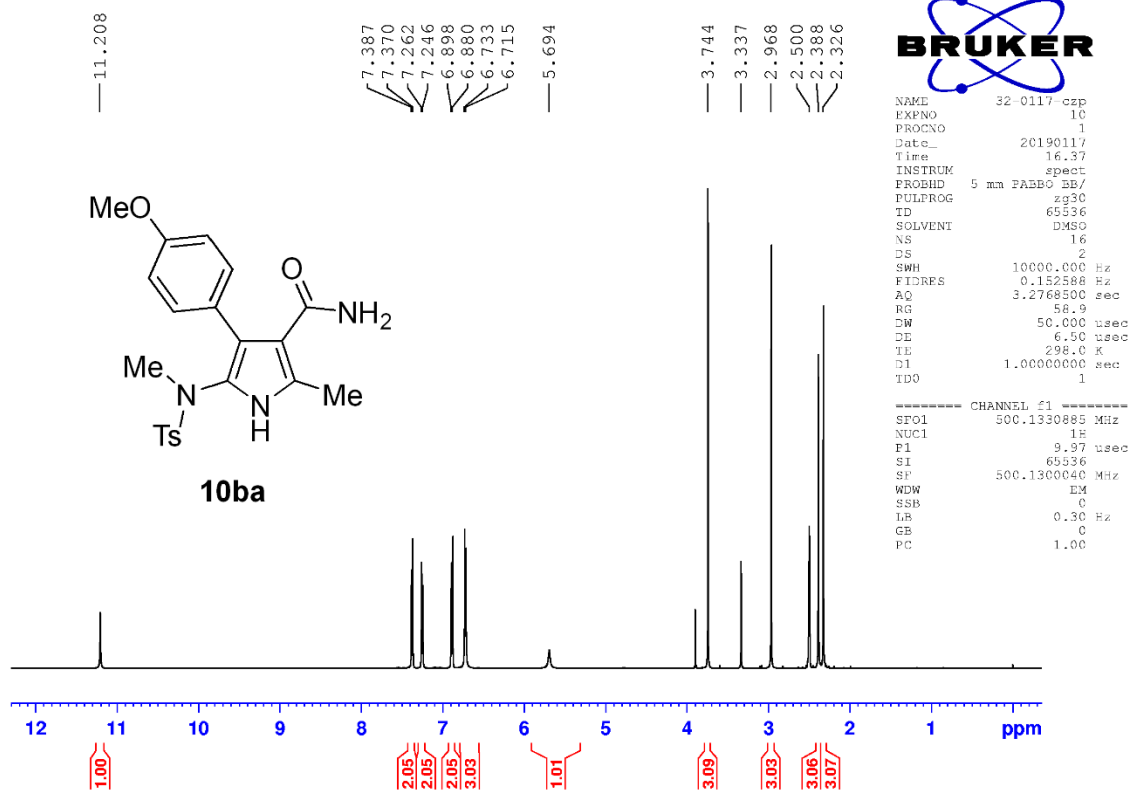
	<u>Compound 10ad</u>
Identification code	190410i
Empirical formula	C ₂₂ H ₂₅ N ₃ O ₃ S
Formula weight	411.51
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 17.4461(15) Å alpha = 90 deg. b = 6.7560(6) Å beta = 119.320(4) deg. c = 21.3479(19) Å gamma = 90 deg.
Volume	2193.9(3) Å ³
Z, Calculated density	4, 1.246 Mg/m ³
Absorption coefficient	0.174 mm ⁻¹
F(000)	872
Crystal size	0.27 x 0.18 x 0.10 mm
Theta range for data collection	2.19 to 25.02 deg.
Limiting indices	-18<=h<=20, -8<=k<=8, -25<=l<=13

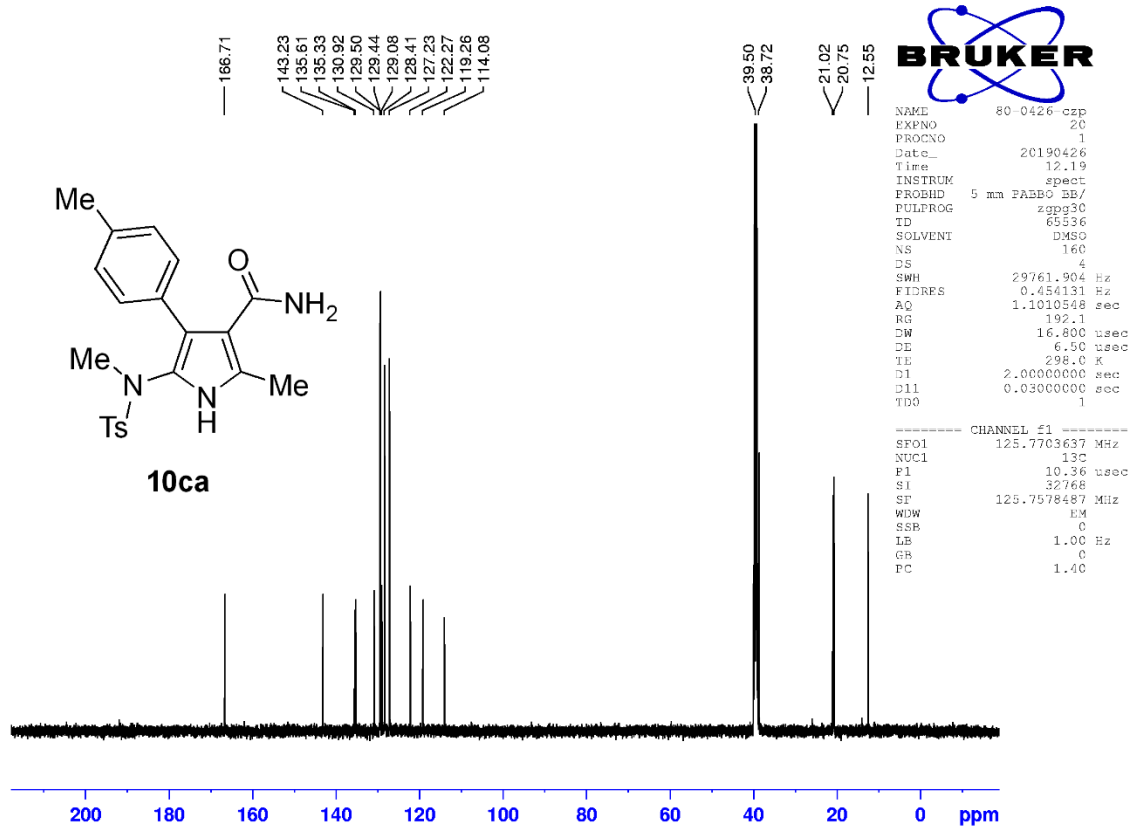
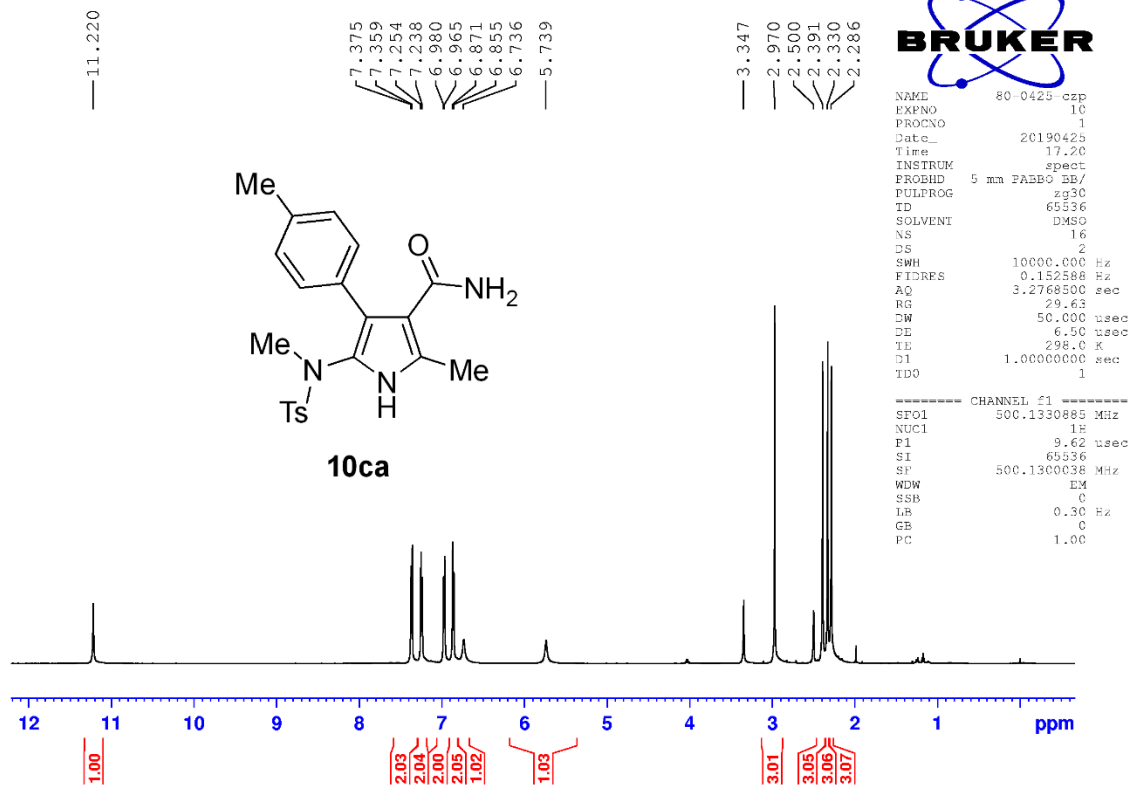
Reflections collected / unique	10595 / 3857 [R(int) = 0.0716]
Completeness to theta = 25.02	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9828 and 0.9544
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3857 / 1 / 262
Goodness-of-fit on F ²	0.868
Final R indices [I>2sigma(I)]	R1 = 0.0583, wR2 = 0.1379
R indices (all data)	R1 = 0.1088, wR2 = 0.1596
Largest diff. peak and hole	0.408 and -0.361 e.A ⁻³

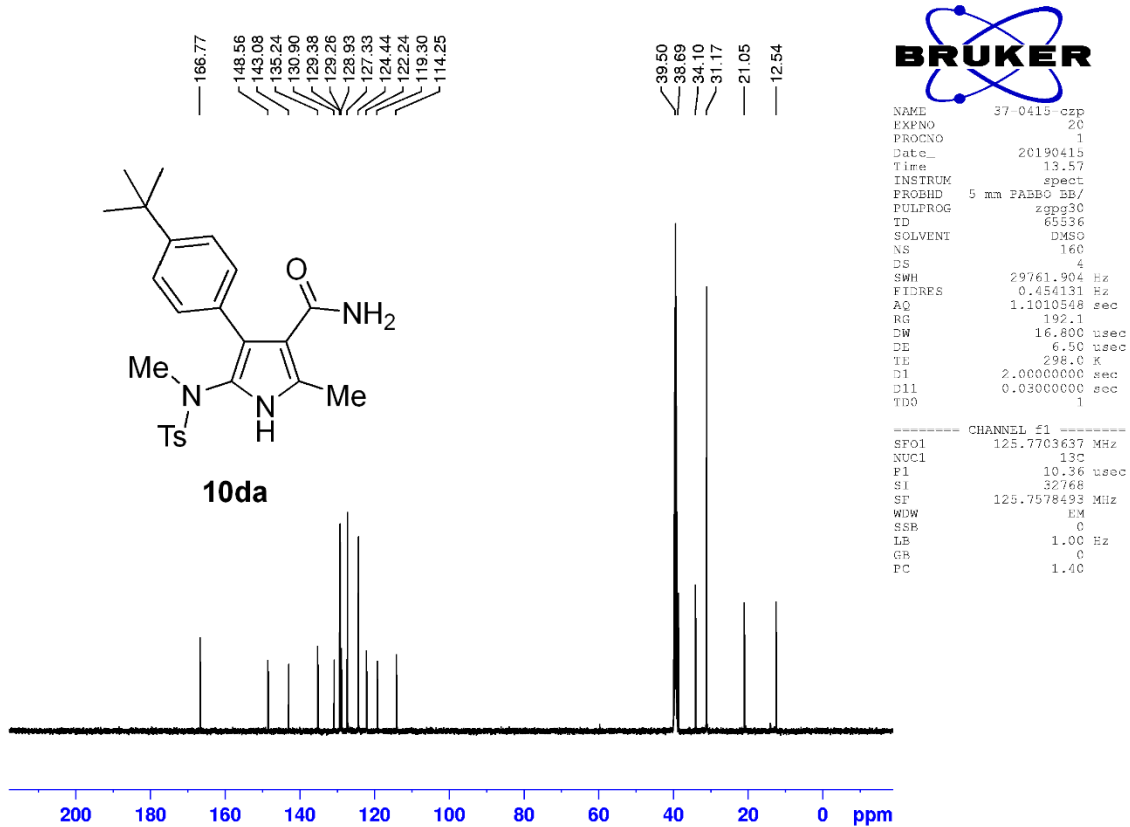
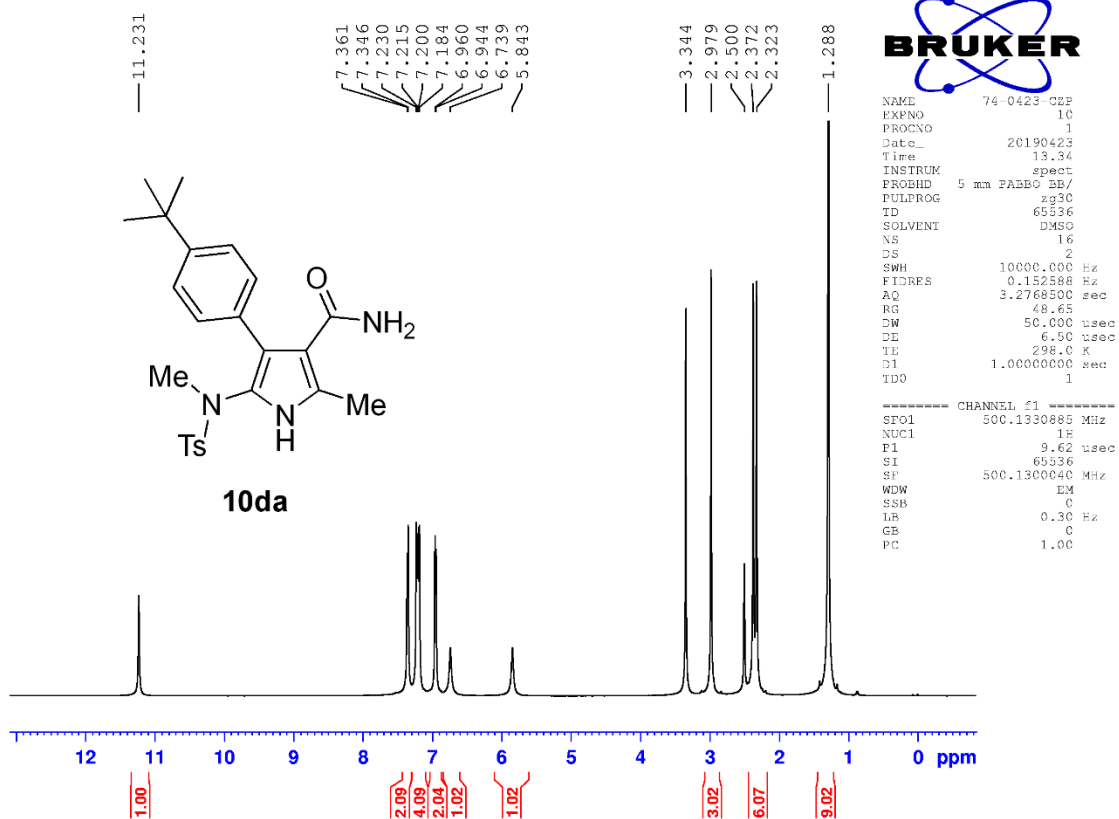
Copies of NMR spectra

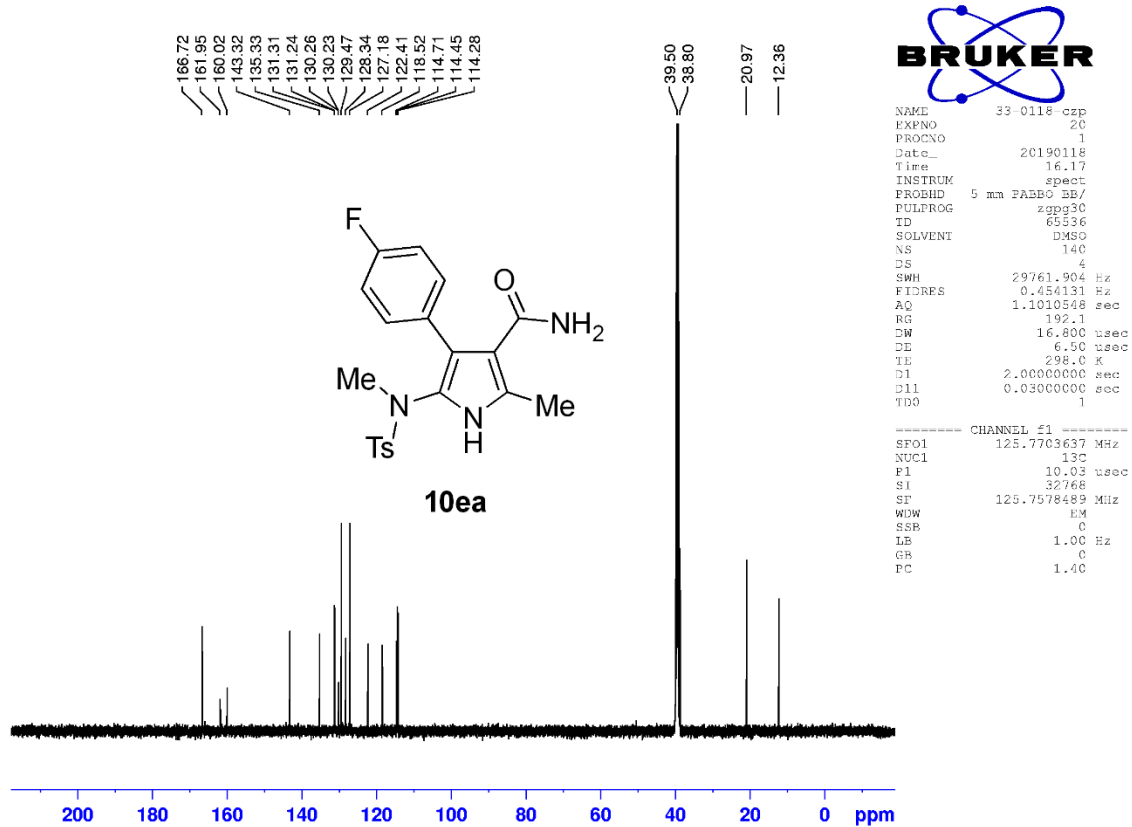
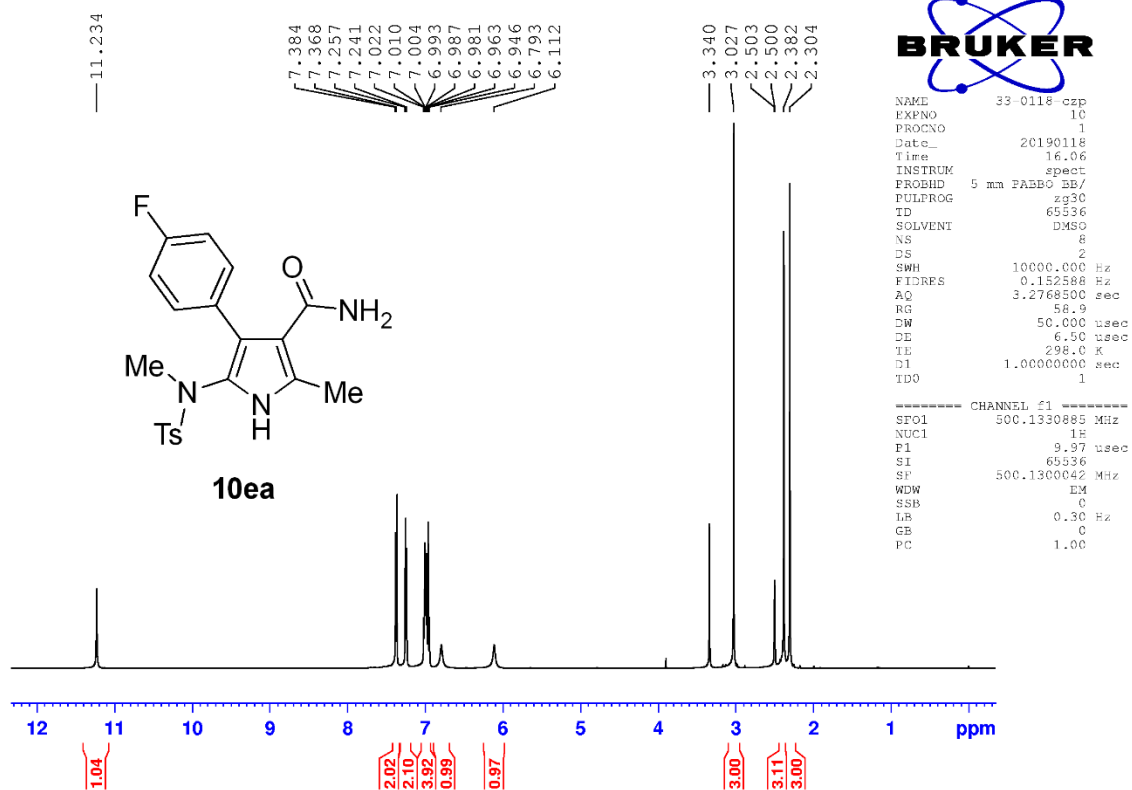


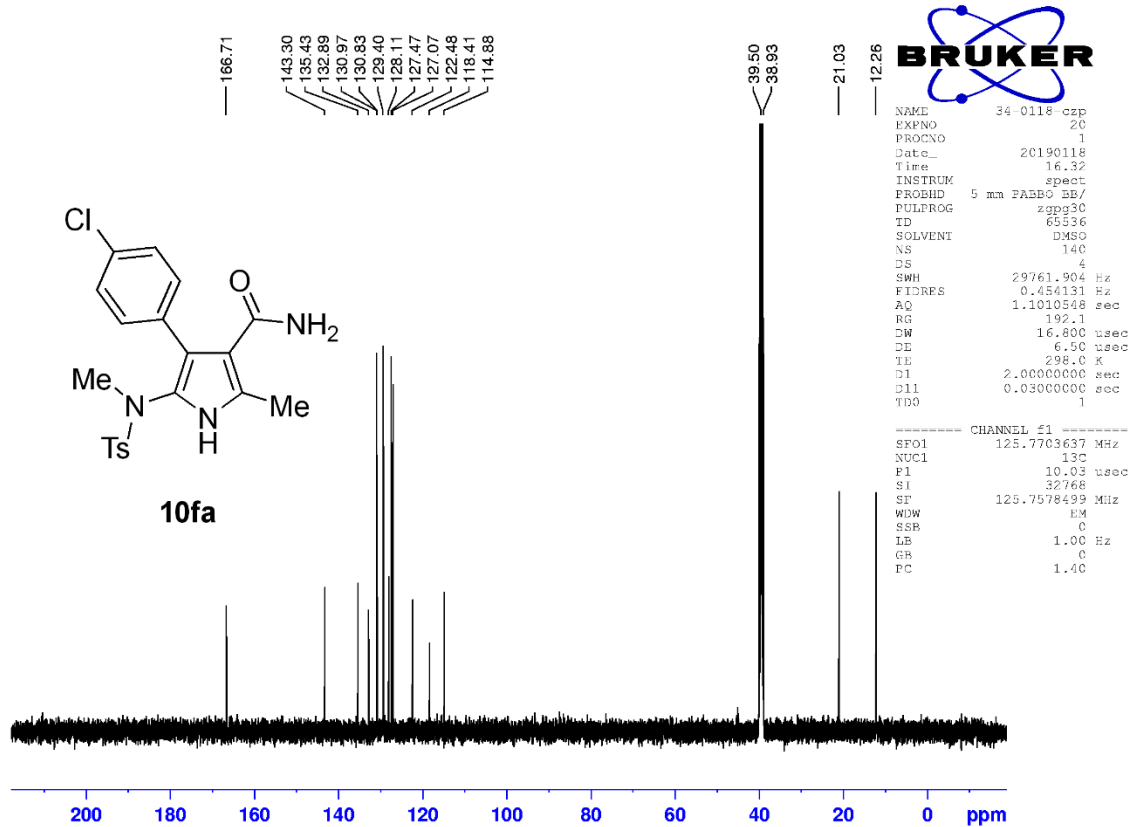
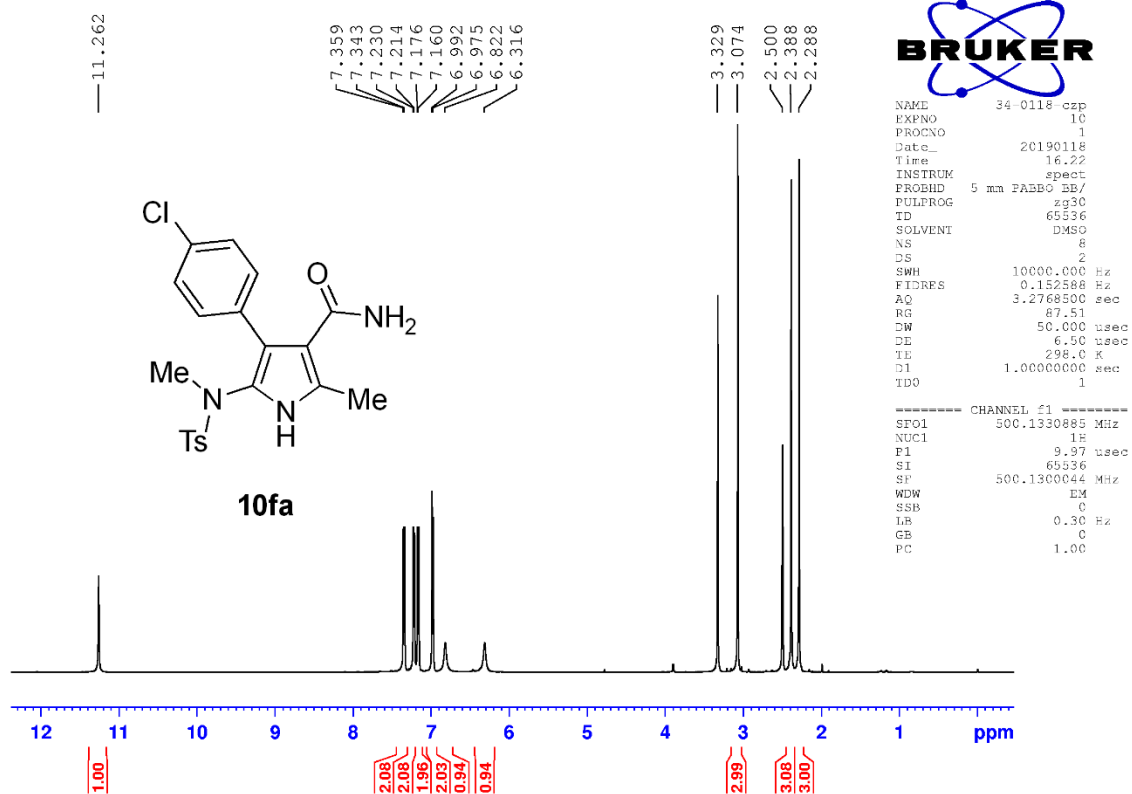


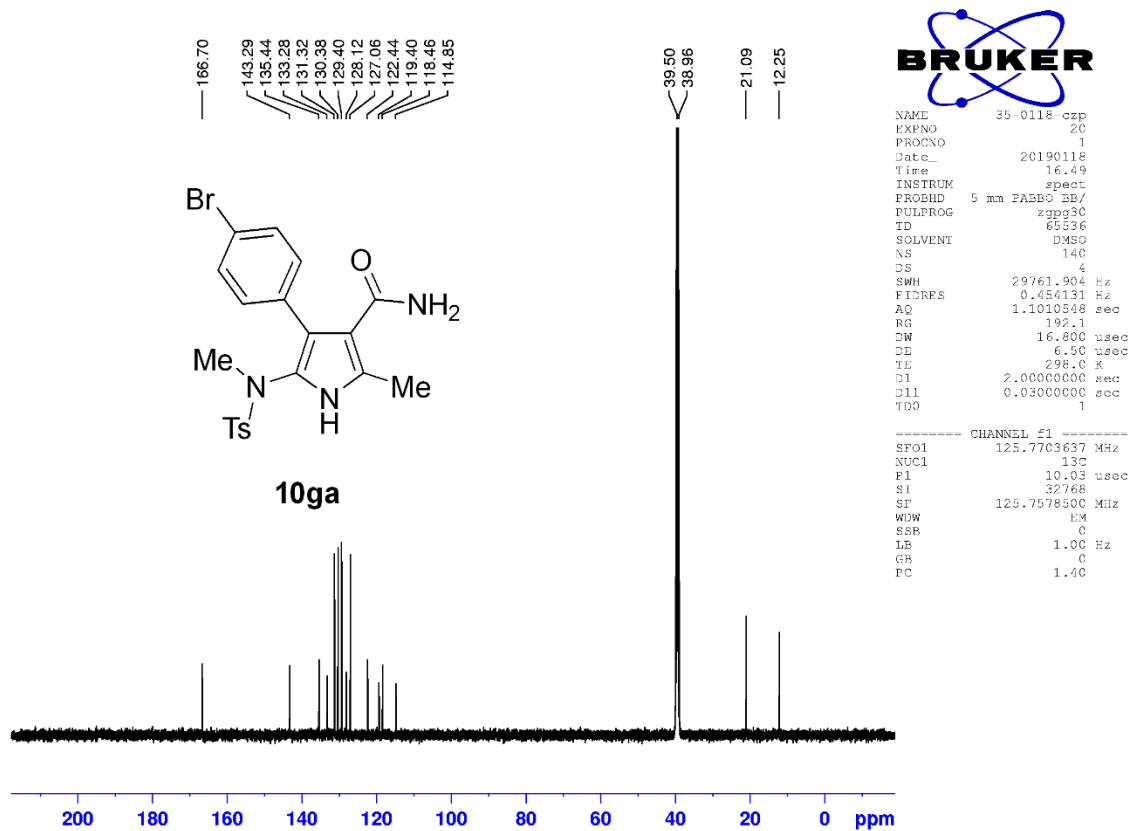
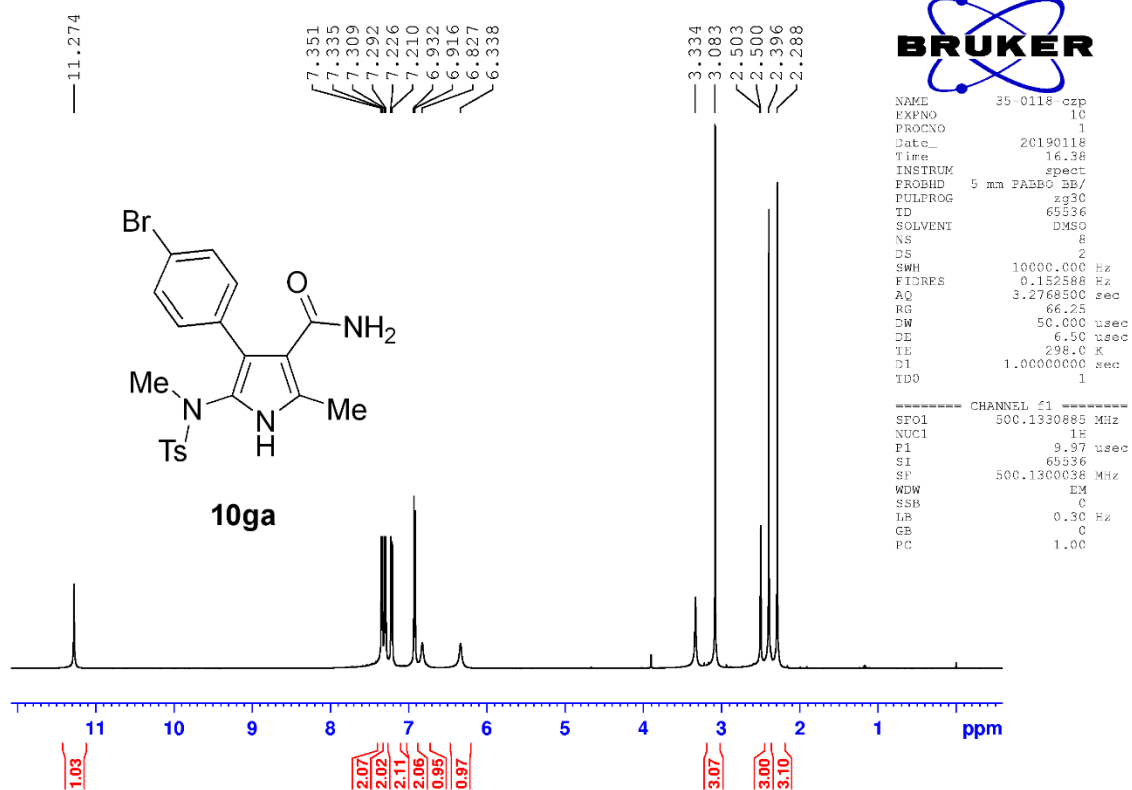


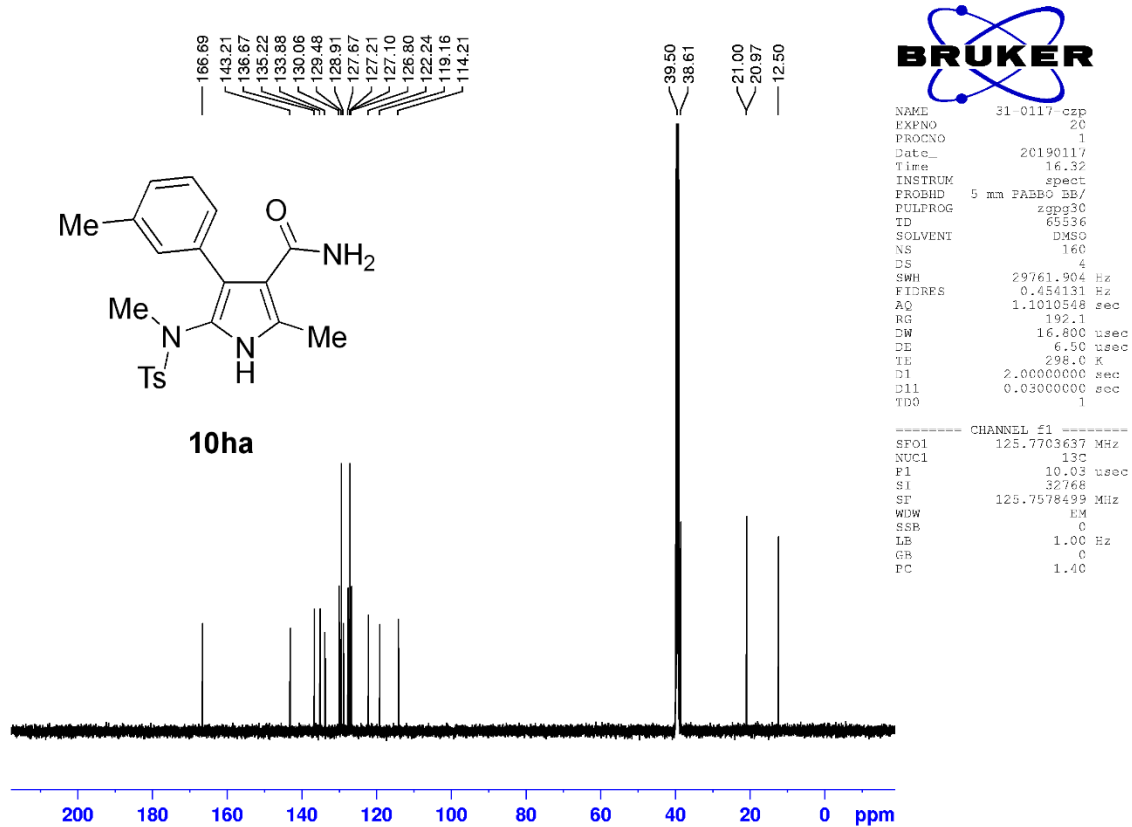
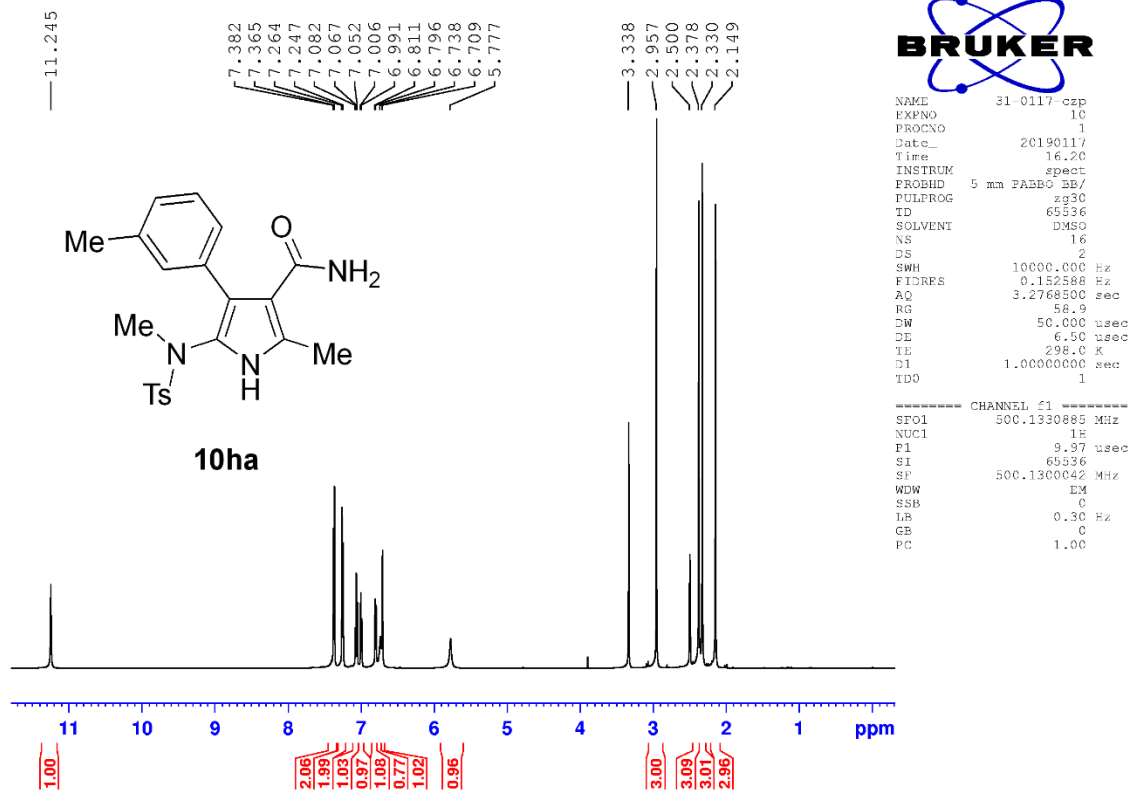


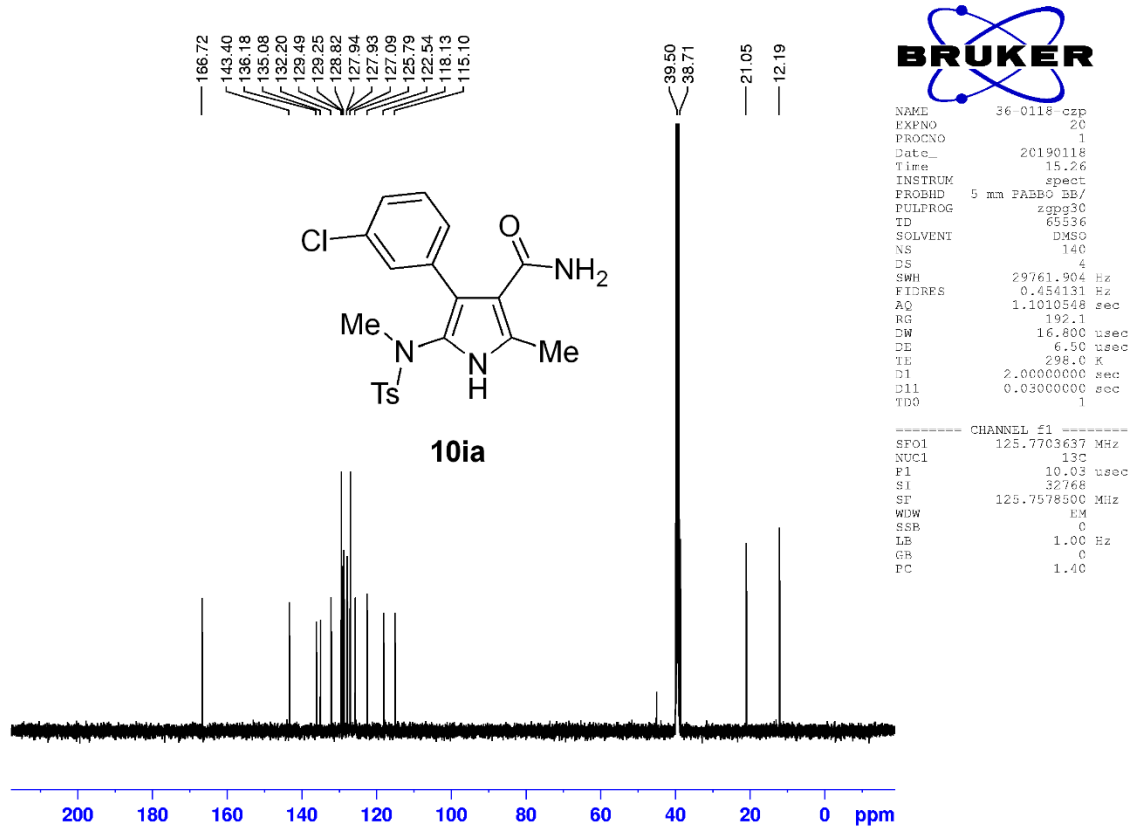
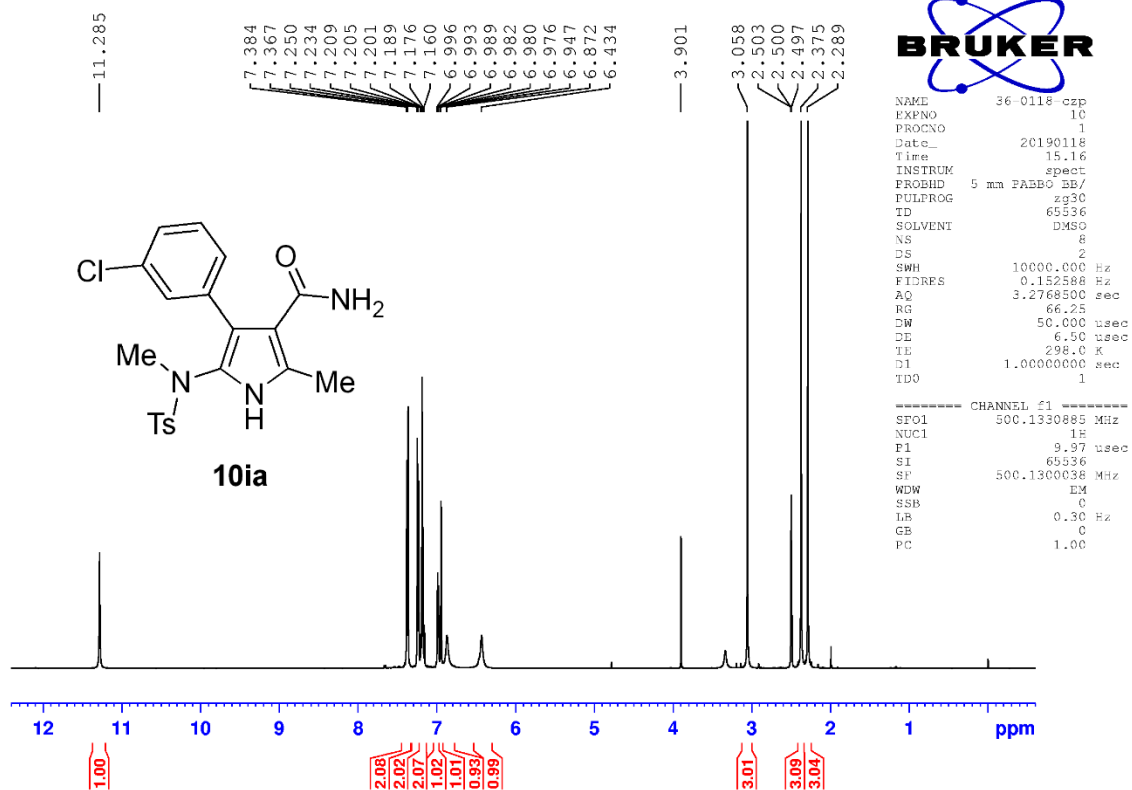


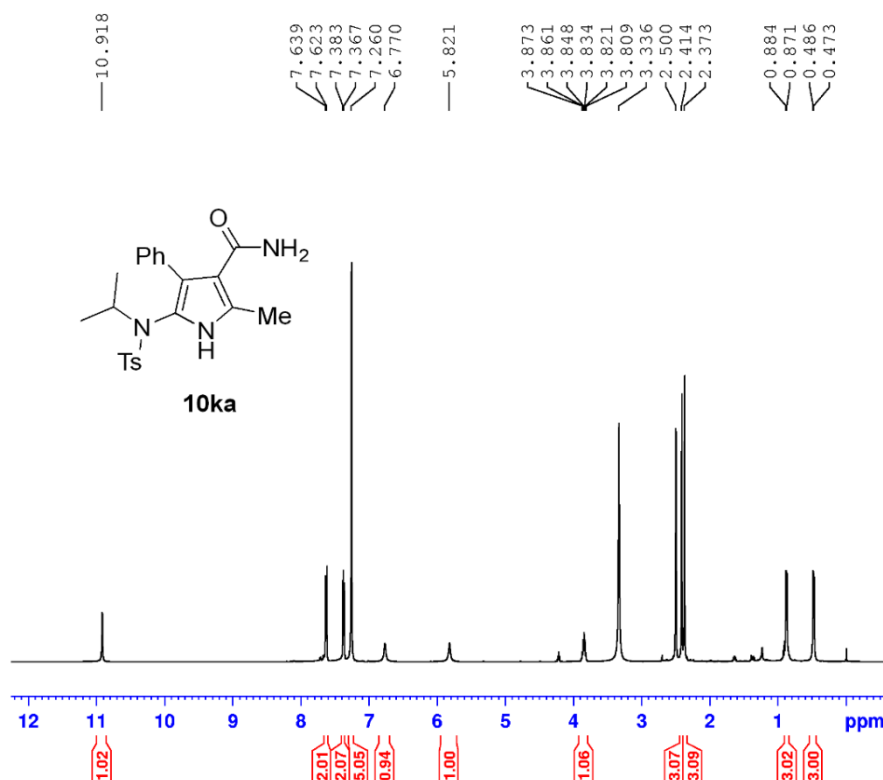










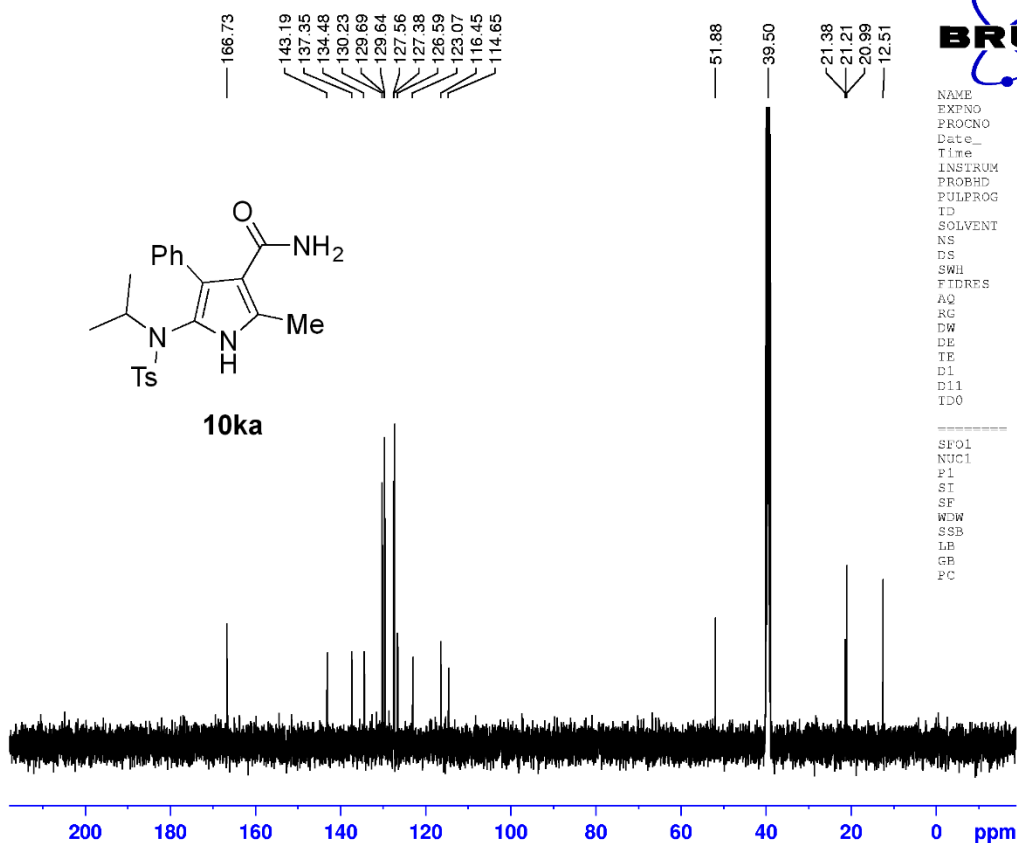


BRUKER

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DS        2
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AQ        3.2768500 sec
RG        106.4
DW        50.000 usec
DE        6.30 usec
TE        298.0 K
D1        1.00000000 sec
TD0       1

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P1        9.62 usec
SI        65536
SF        500.1300045 MHz
WDW       EM
SSB       0
LB        0.30 Hz
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BRUKER

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AQ        1.1010548 sec
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TD0       1

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NUC1      13C
P1        10.36 usec
SI        32768
SF        125.7578504 MHz
WDW       EM
SSB       0
LB        1.00 Hz
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PC        1.40
  
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