# Utilizing Native Directing Groups: Synthesis of a Selective IKur Inhibitor, BMS-919373, via a Regioselective C-H Arylation

Steven R. Wisniewski, Jason M. Stevens, Miao Yu, Kenneth J. Fraunhoffer, Evan O. Romero, and Scott A. Savage*

Chemical and Synthetic Development, Bristol-Myers Squibb Company, One Squibb Drive, New Brunswick, New Jersey 08903,United States.

scott.savage@bms.com

Supporting Information

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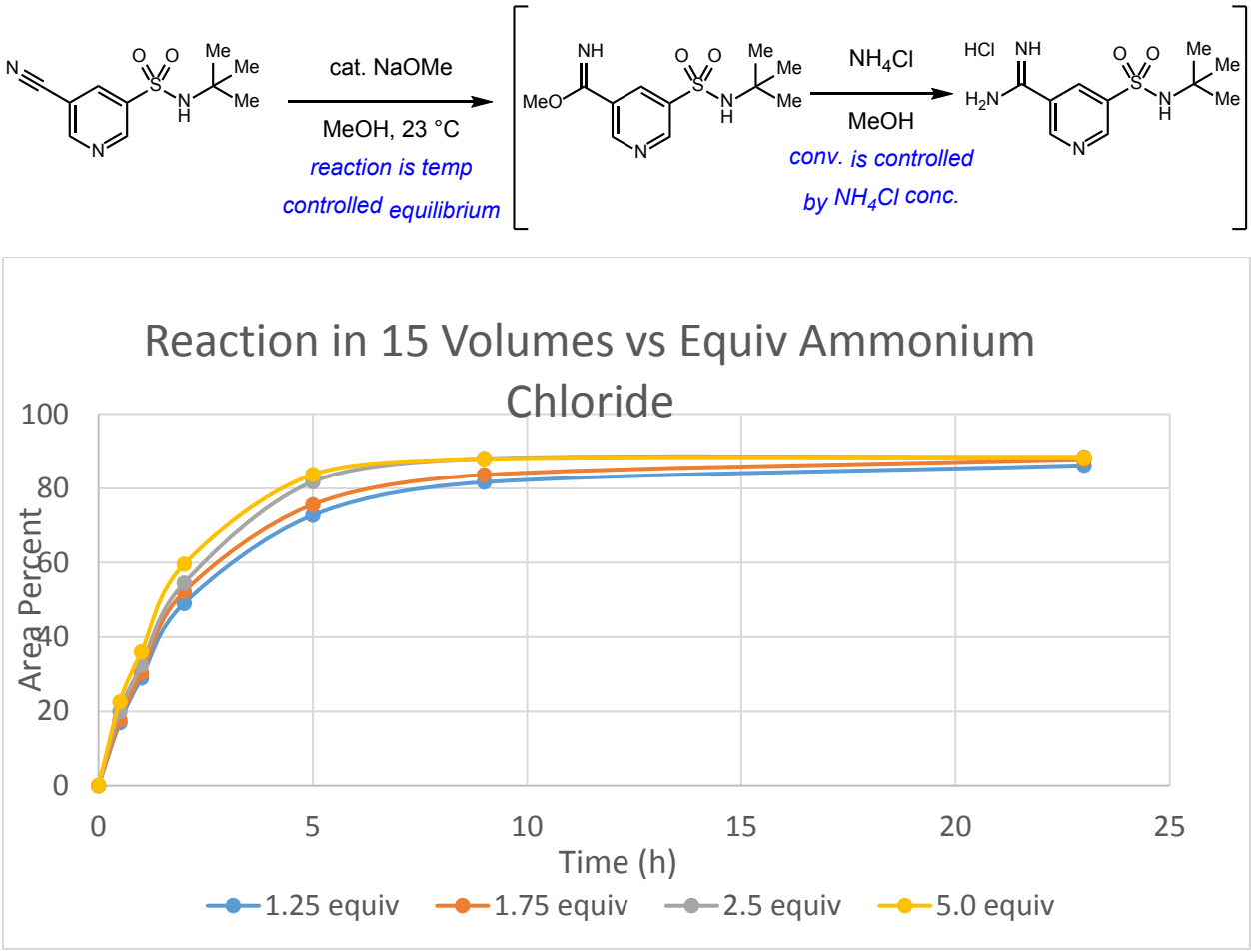



Figure S1. Condensation: Effect of Ammonium Chloride on the Amidine Formation

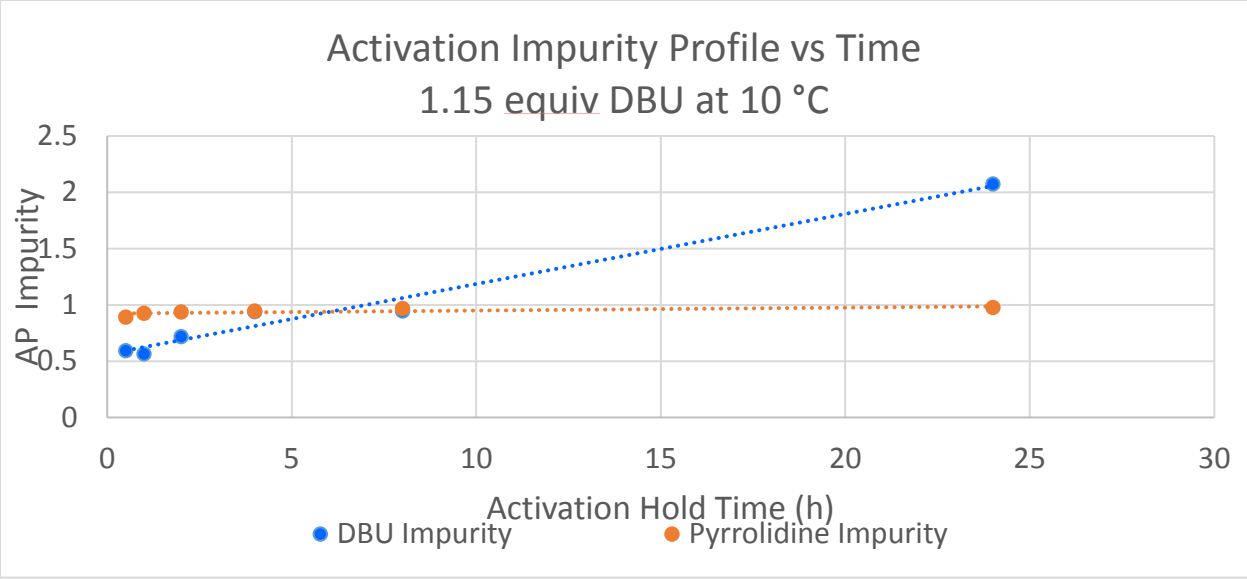
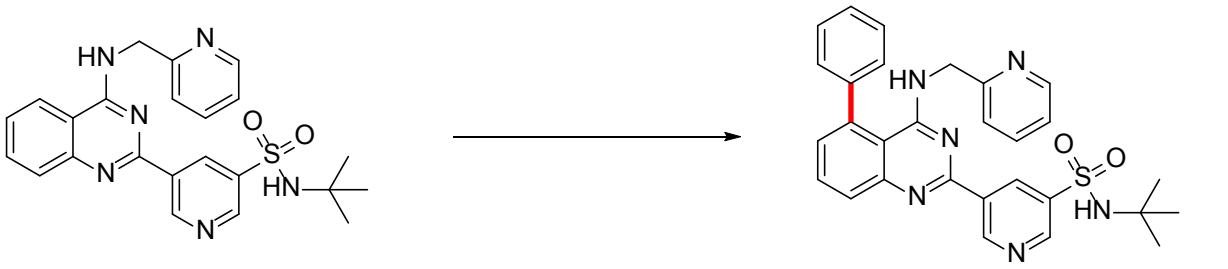



Figure S2. SnAr: Control Strategy for the DBU Impurity

Optimization of the C-H Activation:



| Solvents | Base (3 equiv) | Acid (equiv) | Pd source (5 mol %) | Ligands (5-10 mol %) | Substrate |
|---|---|---|---|---|---|
| Dioxane | KHCO3 | HOAc (0.005 - 3.0) | Pd(OAc)2 | monodentate phosphines | Iodobenzene |
| Anisole | Cs2CO3 | PivOH (0.1 - 0.3) | Pd(TFA)2 | bidentate phosphines | Phenyl Triflate |
| DMAc | K2CO3 | 2-Ph-Benzoic Acid (0.1 - 0.3) | Pd(OPiv)2 | diketocompounds | Bromobenzene |
| NMP | NaHCO3 | Dibenzyl phosphate (0.1 - 0.3) | (MeCN)2PdCl2 | subst. pyridines | |
| Toluene | Na2CO3 | | Pd2dba3 | Phosphites | |
| Xylene | K3PO4 | | | | |
| Trifluorotoluene | K2HPO4 | | | | |
| Chlorobenzene | KH2PO4 | | | | |
| t-AmylOH | CsF | | | | |
| Propylene Carbonate | KF | | | | |
| | NaOMe | | | | |
| | KOtBu | | | | |
| | KOPiv | | | | |
| | KOAc | | | | |
| | TMAOAc | | | | |
| | NEt3 | | | | |
| | 2,6-lutidene | | | | |
| | Cy2NMe | | | | |
| | DIPEA | | | | |
| | DBU | | | | |
| | DABCO | | | | |

General Procedure for High Throughput Screening. In the glovebox, pre-dosed ligand vials are added to the reaction plate (if applicable). A solution of catalyst (25 µL of a 0.02 M solution of $Pd(OAc)_2$ in THF) is then added, and the plate is aged at rt for 20 min. A solution of substrate (50 µL of a 0.2 M solution in tetrahydrofuran) is then added. Non-volatile additives or co-catalysts are then added as solutions in THF. The solvent is removed via the genevac. Stir bars are added to the plate followed by solid dispensing of the base. Solvent and iodobenzene are then added. Note: if a volatile ligand or additive is used, it is added a solution in the reaction solvent at this stage. The plate is sealed with a Teflon sheet and lid, removed from the glovebox and mixed at 95-120 °C overnight. After 16 h, the vials are diluted with 3:1 NMP/MeCN (500 µL). An aliquot (40 µL) is further diluted into MeCN (1 mL) and subjected to UPLC analysis.

Screen #1

| SM | PhI | Pd(OAc)2 | Ligand/Co-Catalyst | | Base | | | | Temp | | Pdt. | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | equiv | mol % | Name | mol % | Name | Equiv | Name | M | °C | h | AP | AP |
| 10 | 4.0 | 5.0% | CuBr | 10.0% | KOPiv | 3.00 | DMAc | 0.10 | 118 | 24.0 | 19.84% | 26.72% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | KOPiv | 3.00 | DMAc | 0.10 | 118 | 24.0 | 0.44% | 44.76% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | KOPiv | 2.86 | DMAc | 0.10 | 118 | 24.0 | 0.43% | 0.47347 |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | KOPiv | 3.21 | DMAc | 0.10 | 118 | 24.0 | 0.30% | 0.38679 |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | KOPiv | 3.00 | DMAc | 0.10 | 118 | 24.0 | 0.31% | 0.43695 |
| 10 | 4.0 | 5.0% | None | | KOPiv | 2.93 | DMAc | 0.10 | 118 | 24.0 | 0 | 11.11% |
| 10 | 4.0 | 5.0% | CuBr2 | 10.0% | TMAOAc | 3.08 | DMAc | 0.10 | 118 | 24.0 | 0 | 4.25% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | TMAOAc | 3.75 | DMAc | 0.10 | 118 | 24.0 | 0.25% | 52.07% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | TMAOAc | 3.75 | DMAc | 0.10 | 118 | 24.0 | 0.39% | 57.02% |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | TMAOAc | 3.45 | DMAc | 0.10 | 118 | 24.0 | 0.26% | 53.82% |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | TMAOAc | 3.38 | DMAc | 0.10 | 118 | 24.0 | 0.33% | 54.80% |
| 10 | 4.0 | 5.0% | None | | TMAOAc | 2.93 | DMAc | 0.10 | 118 | 24.0 | 0.12% | 54.89% |
| 10 | 4.0 | 5.0% | CuBr | 10.0% | KOPiv | 2.93 | p-Xylene | 0.10 | 118 | 24.0 | 14.78% | 37.50% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | KOPiv | 3.14 | p-Xylene | 0.10 | 118 | 24.0 | 10.78% | 46.01% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | KOPiv | 3.07 | p-Xylene | 0.10 | 118 | 24.0 | 23.17% | 35.38% |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | KOPiv | 3.00 | p-Xylene | 0.10 | 118 | 24.0 | 3.51% | 46.01% |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | KOPiv | 3.00 | p-Xylene | 0.10 | 118 | 24.0 | 26.93% | 30.37% |
| 10 | 4.0 | 5.0% | None | | KOPiv | 3.07 | p-Xylene | 0.10 | 118 | 24.0 | 31.73% | 33.05% |
| 10 | 4.0 | 5.0% | CuBr2 | 10.0% | TMAOAc | 3.30 | p-Xylene | 0.10 | 118 | 24.0 | 26.67% | 2.52% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | TMAOAc | 3.30 | p-Xylene | 0.10 | 118 | 24.0 | 0.60% | 44.76% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | TMAOAc | 3.15 | p-Xylene | 0.10 | 118 | 24.0 | 0.24% | 45.26% |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | TMAOAc | 3.08 | p-Xylene | 0.10 | 118 | 24.0 | 0.12% | 47.48% |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | TMAOAc | 3.38 | p-Xylene | 0.10 | 118 | 24.0 | 0.24% | 39.02% |
| 10 | 4.0 | 5.0% | None | | TMAOAc | 3.15 | p-Xylene | 0.10 | 118 | 24.0 | 0.20% | 24.99% |
| 10 | | 5.0% | CuBr | 10.0% | KOPiv | 3.28 | Iodobenzene | 0.10 | 118 | 24.0 | 64.96% | 0.12% |
| 10 | | 5.0% | PPh3 | 10.0% | KOPiv | 2.93 | Iodobenzene | 0.10 | 118 | 24.0 | 42.95% | 15.45% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | KOPiv | 2.93 | Iodobenzene | 0.10 | 118 | 24.0 | 66.23% | 0.09% |
| 10 | | 5.0% | PCy3 | 10.0% | KOPiv | 3.07 | Iodobenzene | 0.10 | 118 | 24.0 | 60.17% | 2.26% |
| 10 | | 5.0% | P(fur)3 | 10.0% | KOPiv | 3.00 | Iodobenzene | 0.10 | 118 | 24.0 | 65.58% | 0.07% |
| 10 | | 5.0% | None | | KOPiv | 3.21 | Iodobenzene | 0.10 | 118 | 24.0 | 64.17% | 0.00% |
| 10 | | 5.0% | CuBr | 10.0% | TMAOAc | 3.30 | Iodobenzene | 0.10 | 118 | 24.0 | 45.47% | 0.00% |
| 10 | | 5.0% | PPh3 | 10.0% | TMAOAc | 3.00 | Iodobenzene | 0.10 | 118 | 24.0 | 20.43% | 29.98% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | TMAOAc | 2.85 | Iodobenzene | 0.10 | 118 | 24.0 | 30.10% | 38.96% |
| 10 | | 5.0% | PCy3 | 10.0% | TMAOAc | 2.85 | Iodobenzene | 0.10 | 118 | 24.0 | 24.38% | 21.93% |
| 10 | | 5.0% | P(fur)3 | 10.0% | TMAOAc | 3.08 | Iodobenzene | 0.10 | 118 | 24.0 | 0.26% | 51.53% |
| 10 | | 5.0% | None | | TMAOAc | 3.00 | Iodobenzene | 0.10 | 118 | 24.0 | 18.06% | 28.59% |
| 10 | | 5.0% | CuBr | 10.0% | KOPiv | 3.00 | Bromobenzene | 0.10 | 118 | 24.0 | 35.32% | 14.08% |
| 10 | | 5.0% | PPh3 | 10.0% | KOPiv | 2.93 | Bromobenzene | 0.10 | 118 | 24.0 | 0.64% | 53.19% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | KOPiv | 3.66 | Bromobenzene | 0.10 | 118 | 24.0 | 0.00% | 26.26% |
| 10 | | 5.0% | PCy3 | 10.0% | KOPiv | 2.93 | Bromobenzene | 0.10 | 118 | 24.0 | 0.58% | 54.32% |
| 10 | | 5.0% | P(fur)3 | 10.0% | KOPiv | 2.93 | Bromobenzene | 0.10 | 118 | 24.0 | 1.28% | 44.88% |
| 10 | | 5.0% | None | | KOPiv | 3.07 | Bromobenzene | 0.10 | 118 | 24.0 | 2.24% | 47.25% |
| 10 | | 5.0% | CuBr | 10.0% | TMAOAc | 3.08 | Bromobenzene | 0.10 | 118 | 24.0 | 16.91% | 5.51% |
| 10 | | 5.0% | PPh3 | 10.0% | TMAOAc | 2.85 | Bromobenzene | 0.10 | 118 | 24.0 | 0.32% | 50.92% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | TMAOAc | 2.93 | Bromobenzene | 0.10 | 118 | 24.0 | 0.15% | 52.48% |
| 10 | | 5.0% | PCy3 | 10.0% | TMAOAc | 3.23 | Bromobenzene | 0.10 | 118 | 24.0 | 0.21% | 51.20% |
| 10 | | 5.0% | P(fur)3 | 10.0% | TMAOAc | 2.93 | Bromobenzene | 0.10 | 118 | 24.0 | 0.12% | 48.65% |
| 10 | | 5.0% | None | | TMAOAc | 2.93 | Bromobenzene | 0.10 | 118 | 24.0 | 0.18% | 53.96% |

creen #1, cont

| SM | PhI | Pd(OAc)2 | Ligand/Co-Catalyst | | Base | | | | Temp | | Pdt. | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | Name | µmol | Name | mol % | Name | Equiv | Name | M | °C | h | AP | AP |
| 10 | 4.0 | 5.0% | CuBr | 10.0% | KOAc | 2.85 | DMAc | 0.10 | 118 | 24.0 | 5.88% | 38.09% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | KOAc | 3.16 | DMAc | 0.10 | 118 | 24.0 | 1.08% | 19.91% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | KOAc | 3.36 | DMAc | 0.10 | 118 | 24.0 | 0.83% | 57.00% |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | KOAc | 3.06 | DMAc | 0.10 | 118 | 24.0 | 0.49% | 59.91% |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | KOAc | 3.16 | DMAc | 0.10 | 118 | 24.0 | 0.15% | 53.32% |
| 10 | 4.0 | 5.0% | None | | KOAc | 3.06 | DMAc | 0.10 | 118 | 24.0 | 0.34% | 58.18% |
| 10 | 4.0 | 5.0% | CuBr | 10.0% | Cs2CO3 | 3.07 | DMAc | 0.10 | 118 | 24.0 | 20.73% | 14.92% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | Cs2CO3 | 3.10 | DMAc | 0.10 | 118 | 24.0 | 2.47% | 23.94% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | Cs2CO3 | 3.10 | DMAc | 0.10 | 118 | 24.0 | 2.79% | 29.02% |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | Cs2CO3 | 3.38 | DMAc | 0.10 | 118 | 24.0 | 1.71% | 18.95% |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | Cs2CO3 | 3.10 | DMAc | 0.10 | 118 | 24.0 | 1.46% | 26.17% |
| 10 | 4.0 | 5.0% | None | | Cs2CO3 | 3.22 | DMAc | 0.10 | 118 | 24.0 | 1.18% | 17.36% |
| 10 | 4.0 | 5.0% | CuBr | 10.0% | KOAc | 2.96 | p-Xylene | 0.10 | 118 | 24.0 | 10.58% | 43.41% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | KOAc | 3.16 | p-Xylene | 0.10 | 118 | 24.0 | 0.37% | 35.56% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | KOAc | 3.06 | p-Xylene | 0.10 | 118 | 24.0 | 4.33% | 26.03% |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | KOAc | 4.08 | p-Xylene | 0.10 | 118 | 24.0 | 0.47% | 56.68% |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | KOAc | 3.06 | p-Xylene | 0.10 | 118 | 24.0 | 1.16% | 47.47% |
| 10 | 4.0 | 5.0% | None | | KOAc | 3.06 | p-Xylene | 0.10 | 118 | 24.0 | 14.02% | 46.57% |
| 10 | 4.0 | 5.0% | CuBr | 10.0% | Cs2CO3 | 2.97 | p-Xylene | 0.10 | 118 | 24.0 | 6.27% | 8.83% |
| 10 | 4.0 | 5.0% | PPh3 | 10.0% | Cs2CO3 | 2.97 | p-Xylene | 0.10 | 118 | 24.0 | 0.25% | 3.08% |
| 10 | 4.0 | 5.0% | PtBu3 HBF4 | 10.0% | Cs2CO3 | 3.35 | p-Xylene | 0.10 | 118 | 24.0 | 0.72% | 20.73% |
| 10 | 4.0 | 5.0% | PCy3 | 10.0% | Cs2CO3 | 3.16 | p-Xylene | 0.10 | 118 | 24.0 | 0.15% | 42.08% |
| 10 | 4.0 | 5.0% | P(fur)3 | 10.0% | Cs2CO3 | 2.85 | p-Xylene | 0.10 | 118 | 24.0 | 0.52% | 45.12% |
| 10 | 4.0 | 5.0% | None | | Cs2CO3 | 3.50 | p-Xylene | 0.10 | 118 | 24.0 | 0.33% | 28.40% |
| 10 | | 5.0% | CuBr | 10.0% | KOAc | 2.96 | odobenzen | 0.10 | 118 | 24.0 | 57.55% | 3.23% |
| 10 | | 5.0% | PPh3 | 10.0% | KOAc | 2.85 | odobenzen | 0.10 | 118 | 24.0 | 6.54% | 41.65% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | KOAc | 3.06 | odobenzen | 0.10 | 118 | 24.0 | 28.01% | 49.95% |
| 10 | | 5.0% | PCy3 | 10.0% | KOAc | 3.26 | odobenzen | 0.10 | 118 | 24.0 | 17.68% | 54.14% |
| 10 | | 5.0% | P(fur)3 | 10.0% | KOAc | 3.26 | odobenzen | 0.10 | 118 | 24.0 | 21.23% | 28.51% |
| 10 | | 5.0% | None | | KOAc | 2.85 | odobenzen | 0.10 | 118 | 24.0 | 76.90% | 0.76% |
| 10 | | 5.0% | CuBr | 10.0% | Cs2CO3 | 3.41 | odobenzen | 0.10 | 118 | 24.0 | 59.55% | 14.78% |
| 10 | | 5.0% | PPh3 | 10.0% | Cs2CO3 | 3.22 | odobenzen | 0.10 | 118 | 24.0 | 9.88% | 8.41% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | Cs2CO3 | 2.97 | odobenzen | 0.10 | 118 | 24.0 | 9.04% | 50.58% |
| 10 | | 5.0% | PCy3 | 10.0% | Cs2CO3 | 3.07 | odobenzen | 0.10 | 118 | 24.0 | 5.02% | 56.15% |
| 10 | | 5.0% | P(fur)3 | 10.0% | Cs2CO3 | 3.10 | odobenzen | 0.10 | 118 | 24.0 | 8.73% | 43.99% |
| 10 | | 5.0% | None | | Cs2CO3 | 3.07 | odobenzen | 0.10 | 118 | 24.0 | 19.10% | 41.39% |
| 10 | | 5.0% | CuBr | 10.0% | KOAc | 3.97 | romobenzer | 0.10 | 118 | 24.0 | 9.39% | 27.26% |
| 10 | | 5.0% | PPh3 | 10.0% | KOAc | 2.96 | romobenzer | 0.10 | 118 | 24.0 | 0.38% | 45.23% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | KOAc | 3.06 | romobenzer | 0.10 | 118 | 24.0 | 0.54% | 49.05% |
| 10 | | 5.0% | PCy3 | 10.0% | KOAc | 2.96 | romobenzer | 0.10 | 118 | 24.0 | 0.44% | 48.70% |
| 10 | | 5.0% | P(fur)3 | 10.0% | KOAc | 3.16 | romobenzer | 0.10 | 118 | 24.0 | 0.55% | 38.60% |
| 10 | | 5.0% | None | | KOAc | 3.26 | romobenzer | 0.10 | 118 | 24.0 | 0.26% | 50.01% |
| 10 | | 5.0% | CuBr | 10.0% | Cs2CO3 | 3.10 | romobenzer | 0.10 | 118 | 24.0 | 16.62% | 8.07% |
| 10 | | 5.0% | PPh3 | 10.0% | Cs2CO3 | 3.10 | romobenzer | 0.10 | 118 | 24.0 | 0.00% | 30.94% |
| 10 | | 5.0% | PtBu3 HBF4 | 10.0% | Cs2CO3 | 3.16 | romobenzer | 0.10 | 118 | 24.0 | 0.36% | 32.01% |
| 10 | | 5.0% | PCy3 | 10.0% | Cs2CO3 | 2.97 | romobenzer | 0.10 | 118 | 24.0 | 0.06% | 44.40% |
| 10 | | 5.0% | P(fur)3 | 10.0% | Cs2CO3 | 3.00 | romobenzer | 0.10 | 118 | 24.0 | 0.19% | 39.41% |
| 10 | | 5.0% | None | | Cs2CO3 | 3.10 | romobenzer | 0.10 | 118 | 24.0 | 0.05% | 42.13% |

Screen #2

| SM | PhI | Pd | Ligand | Base | | Additive | | | Temp | | Pdt. | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | equiv | 5 mol % | 5 mol % | Name | Equiv | 10 mol % | Name | vol | °C | h | AP | AP |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.28 | CuBr2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 55.94% | 30.16% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.14 | CuCl2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 49.31% | 26.80% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.07 | CuI | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 49.26% | 0.36226 |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.00 | CuCl | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 55.20% | 0.25413 |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 2.93 | Cu2O | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 44.29% | 0.3637 |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.00 | Cu(OAc)2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 0 | 40.19% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.14 | | 50:50 Toluene:Iodobenzene | 14.73 | 105 | 24.0 | 1 | 19.00% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.00 | | 50:50 Dioxane:Iodobenzene | 14.73 | 105 | 24.0 | 69.75% | 5.73% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.00 | | 50:50 CPME:Iodobenzene | 14.73 | 105 | 24.0 | 57.13% | 26.22% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.00 | | 50:50 t-AmOH:Iodobenzene | 14.73 | 105 | 24.0 | 55.47% | 34.73% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.57 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 72.15% | 14.59% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.07 | | 50:50 F3-toluene:Iodobenzene | 14.73 | 105 | 24.0 | 67.77% | 13.65% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.28 | CuBr2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 72.63% | 4.97% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 2.93 | CuCl2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 71.31% | 6.00% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 2.93 | CuI | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 66.48% | 12.74% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.07 | CuCl | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 59.17% | 16.35% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.00 | Cu2O | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 74.14% | 1.56% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 2.79 | Cu(OAc)2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 63.28% | 13.57% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.07 | | 50:50 Toluene:Iodobenzene | 14.73 | 105 | 24.0 | 74.12% | 0.00% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.14 | | 50:50 Dioxane:Iodobenzene | 14.73 | 105 | 24.0 | 68.91% | 1.65% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.07 | | 50:50 CPME:Iodobenzene | 14.73 | 105 | 24.0 | 76.83% | 0.51% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.00 | | 50:50 t-AmOH:Iodobenzene | 14.73 | 105 | 24.0 | 67.95% | 0.00% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 2.93 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 77.52% | 1.38% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.28 | | 50:50 F3-toluene:Iodobenzene | 14.73 | 105 | 24.0 | 72.99% | 0.13% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.36 | CuBr2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 33.16% | 60.64% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 2.85 | CuCl2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 46.75% | 40.01% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.26 | CuI | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 37.85% | 51.31% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 2.96 | CuCl | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 54.93% | 37.21% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 2.96 | Cu2O | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 58.99% | 28.80% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.16 | Cu(OAc)2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 50.76% | 36.87% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.06 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 52.12% | 31.62% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.16 | | 50:50 Dioxane:Iodobenzene | 14.73 | 105 | 24.0 | 12.57% | 82.48% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.16 | | 50:50 CPME:Iodobenzene | 14.73 | 105 | 24.0 | 36.62% | 49.42% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.06 | | 50:50 t-AmOH:Iodobenzene | 14.73 | 105 | 24.0 | 14.47% | 80.29% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.26 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 45.63% | 39.13% |
| 10 | | Pd(OAc)2 | PtBu3 HBF4 | KOAc | 3.06 | | 50:50 F3-toluene:Iodobenzene | 14.73 | 105 | 24.0 | 33.59% | 34.02% |

Screen #2, cont

| SM | PhI | Pd(OAc)2 | Ligand/Co-Catalyst | | Base | | | | Temp | | Pdt. | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | Name | µmol | Name | mol % | Name | Equiv | Name | M | °C | h | AP | AP |
| 10 | | Pd(OAc)2 | | KOAc | 2.75 | CuBr2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 57.66% | 30.30% |
| 10 | | Pd(OAc)2 | | KOAc | 2.96 | CuCl2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 52.21% | 34.80% |
| 10 | | Pd(OAc)2 | | KOAc | 3.06 | CuI | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 30.75% | 53.79% |
| 10 | | Pd(OAc)2 | | KOAc | 3.26 | CuCl | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 52.25% | 35.98% |
| 10 | | Pd(OAc)2 | | KOAc | 2.96 | Cu2O | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 59.69% | 28.18% |
| 10 | | Pd(OAc)2 | | KOAc | 3.06 | Cu(OAc)2 | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 47.40% | 34.45% |
| 10 | | Pd(OAc)2 | | KOAc | 2.96 | | 50:50 Toluene:Iodobenzene | 14.73 | 105 | 24.0 | 53.62% | 25.18% |
| 10 | | Pd(OAc)2 | | KOAc | 2.96 | | 50:50 Dioxane:Iodobenzene | 14.73 | 105 | 24.0 | 49.91% | 35.92% |
| 10 | | Pd(OAc)2 | | KOAc | 2.85 | | 50:50 CPME:Iodobenzene | 14.73 | 105 | 24.0 | 49.03% | 33.97% |
| 10 | | Pd(OAc)2 | | KOAc | 3.36 | | 50:50 t-AmOH:Iodobenzene | 14.73 | 105 | 24.0 | 54.70% | 22.61% |
| 10 | | Pd(OAc)2 | | KOAc | 2.96 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 57.04% | 25.30% |
| 10 | | Pd(OAc)2 | | KOAc | 3.06 | | 50:50 F3-toluene:Iodobenzene | 14.73 | 105 | 24.0 | 44.51% | 27.92% |
| 10 | 4.0 | Pd(OAc)2 | | KOPiv | 3.43 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 72.66% | 0.56% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KOPiv | 3.14 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 58.29% | 27.10% |
| 10 | 4.0 | Pd(OAc)2 | | KOAc | 3.16 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 50.75% | 37.93% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KHCO3 | 3.10 | TFA | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 55.77% | 30.38% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KHCO3 | 2.80 | PivOH | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 58.85% | 22.13% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | KHCO3 | 3.20 | AcOH | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 55.51% | 31.85% |
| 10 | 4.0 | Pd(OPiv)2 | | KOPiv | 3.00 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 89.03% | 0.38% |
| 10 | 4.0 | Pd(OPiv)2 | PtBu3 HBF4 | KOPiv | 3.00 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 74.55% | 4.10% |
| 10 | 4.0 | Pd(OPiv)2 | | KOAc | 3.06 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 53.75% | 32.93% |
| 10 | 4.0 | Pd(OAc)2 | | KHCO3 | 3.00 | TFA | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 77.41% | 0.27% |
| 10 | 4.0 | Pd(OAc)2 | | KHCO3 | 2.80 | PivOH | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 56.15% | 0.11% |
| 10 | 4.0 | Pd(OAc)2 | | KHCO3 | 3.40 | AcOH | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 75.32% | 0.00% |
| 10 | 4.0 | Pd(TFA)2 | PtBu3 HBF4 | KOPiv | 2.57 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 57.28% | 30.86% |
| 10 | 4.0 | Pd(TFA)2 | | KOPiv | 3.21 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 51.35% | 35.11% |
| 10 | 4.0 | Pd(TFA)2 | | KOAc | 3.06 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 51.29% | 30.61% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | K2CO3 | 13.39 | TFA | 67:33 p-Xylene:Iodobenzene | 22.10 | 105 | 24.0 | 39.78% | 36.22% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | K2CO3 | 9.91 | PivOH | 67:33 p-Xylene:Iodobenzene | 22.10 | 105 | 24.0 | 35.86% | 39.63% |
| 10 | 4.0 | Pd(OAc)2 | PtBu3 HBF4 | K2CO3 | 10.06 | AcOH | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 24.62% | 54.82% |
| 10 | 4.0 | PdCl2(MeCN)2 | | KOPiv | 3.00 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 78.19% | 2.13% |
| 10 | 4.0 | PdCl2(MeCN)2 | PtBu3 HBF4 | KOPiv | 3.43 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 47.59% | 41.59% |
| 10 | 4.0 | PdCl2(MeCN)2 | | KOAc | 2.85 | | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 48.97% | 36.44% |
| 10 | 4.0 | Pd(OAc)2 | | K2CO3 | 8.32 | TFA | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 51.83% | 0.04% |
| 10 | 4.0 | Pd(OAc)2 | | K2CO3 | 9.19 | PivOH | 50:50 p-Xylene:Iodobenzene | 14.73 | 105 | 24.0 | 34.51% | 0.03% |
| 10 | 4.0 | Pd(OAc)2 | | K2CO3 | 7.81 | AcOH | 50:50 p-Xylene:Iodobenzene | 0.10 | 105 | 24.0 | 34.08% | 0.18% |

Screen #3

| SM umol | PhI equiv | Pd(OAc)2 mol % | Additive/Co-Catalyst Name | mol % | Base Name | Equiv | Name | vol | Temp °C | h | Pdt. AP | SM AP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 10.0 | 5.0% | | | KOPiv | 3.43 | Dioxane | 12.28 | 118 | 24.0 | 48.68% | 45.89% |
| 10 | 10.0 | 5.0% | | | KOPiv | 3.07 | CPME | 12.28 | 118 | 24.0 | 37.46% | 59.22% |
| 10 | 10.0 | 5.0% | | | KOPiv | 2.93 | t-AmOH | 12.28 | 118 | 24.0 | 29.73% | 0.65455 |
| 10 | 10.0 | 5.0% | | | KOPiv | 3.64 | p-Xylene | 12.28 | 118 | 24.0 | 52.32% | 0.46198 |
| 10 | 10.0 | 5.0% | | | KOPiv | 3.07 | F3-toluene | 12.28 | 118 | 24.0 | 52.23% | 0.44475 |
| 10 | 10.0 | 5.0% | | | KOPiv | 2.93 | DMAc | 12.28 | 118 | 24.0 | 0 | 84.10% |
| 10 | | 5.0% | | | KOPiv | 3.64 | 50:50 Dioxane:Bromobenzene | 14.73 | 118 | 24.0 | 0 | 98.62% |
| 10 | | 5.0% | | | KOPiv | 2.93 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.79% | 96.38% |
| 10 | | 5.0% | | | KOPiv | 2.93 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.21% | 97.94% |
| 10 | | 5.0% | | | KOPiv | 3.07 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 2.29% | 93.42% |
| 10 | | 5.0% | | | KOPiv | 3.07 | 50:50 F3-toluene:Bromobenzene | 14.73 | 118 | 24.0 | 2.96% | 92.38% |
| 10 | | 5.0% | | | KOPiv | 3.07 | 50:50 DMAc:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 92.75% |
| 10 | 10.0 | 5.0% | PivOH | 10.0% | KHCO3 | 2.90 | Dioxane | 12.28 | 118 | 24.0 | 38.45% | 60.03% |
| 10 | 10.0 | 5.0% | PivOH | 10.0% | KHCO3 | 2.90 | CPME | 12.28 | 118 | 24.0 | 30.17% | 69.05% |
| 10 | 10.0 | 5.0% | PivOH | 10.0% | KHCO3 | 2.90 | t-AmOH | 12.28 | 118 | 24.0 | 65.53% | 32.14% |
| 10 | 10.0 | 5.0% | PivOH | 10.0% | KHCO3 | 3.40 | p-Xylene | 12.28 | 118 | 24.0 | 64.08% | 34.15% |
| 10 | 10.0 | 5.0% | PivOH | 10.0% | KHCO3 | 3.30 | F3-toluene | 12.28 | 118 | 24.0 | 61.65% | 36.88% |
| 10 | 10.0 | 5.0% | PivOH | 10.0% | KHCO3 | 3.10 | DMAc | 12.28 | 118 | 24.0 | 1.55% | 83.30% |
| 10 | | 5.0% | PivOH | 10.0% | KHCO3 | 2.90 | 50:50 Dioxane:Bromobenzene | 14.73 | 118 | 24.0 | 0.18% | 98.64% |
| 10 | | 5.0% | PivOH | 10.0% | KHCO3 | 2.80 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.10% | 99.12% |
| 10 | | 5.0% | PivOH | 10.0% | KHCO3 | 2.70 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.21% | 97.79% |
| 10 | | 5.0% | PivOH | 10.0% | KHCO3 | 3.10 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.27% | 97.73% |
| 10 | | 5.0% | PivOH | 10.0% | KHCO3 | 3.20 | 50:50 F3-toluene:Bromobenzene | 14.73 | 118 | 24.0 | 0.46% | 98.38% |
| 10 | | 5.0% | PivOH | 10.0% | KHCO3 | 3.00 | 50:50 DMAc:Bromobenzene | 14.73 | 118 | 24.0 | 0.07% | 95.78% |
| 10 | 10.0 | 5.0% | TFA | 10.0% | KHCO3 | 4.50 | Dioxane | 12.28 | 118 | 24.0 | 79.84% | 17.93% |
| 10 | 10.0 | 5.0% | TFA | 10.0% | KHCO3 | 2.90 | CPME | 12.28 | 118 | 24.0 | 48.37% | 50.63% |
| 10 | 10.0 | 5.0% | TFA | 10.0% | KHCO3 | 3.90 | t-AmOH | 12.28 | 118 | 24.0 | 51.19% | 47.05% |
| 10 | 10.0 | 5.0% | TFA | 10.0% | KHCO3 | 3.00 | p-Xylene | 12.28 | 118 | 24.0 | 62.74% | 34.54% |
| 10 | 10.0 | 5.0% | TFA | 10.0% | KHCO3 | 3.00 | F3-toluene | 12.28 | 118 | 24.0 | 63.35% | 35.20% |
| 10 | 10.0 | 5.0% | TFA | 10.0% | KHCO3 | 3.00 | DMAc | 12.28 | 118 | 24.0 | 1.33% | 80.37% |
| 10 | | 5.0% | TFA | 10.0% | KHCO3 | 3.20 | 50:50 Dioxane:Bromobenzene | 14.73 | 118 | 24.0 | 0.18% | 98.60% |
| 10 | | 5.0% | TFA | 10.0% | KHCO3 | 2.80 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.12% | 99.01% |
| 10 | | 5.0% | TFA | 10.0% | KHCO3 | 2.90 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.39% | 97.99% |
| 10 | | 5.0% | TFA | 10.0% | KHCO3 | 2.90 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.47% | 98.05% |
| 10 | | 5.0% | TFA | 10.0% | KHCO3 | 3.20 | 50:50 F3-toluene:Bromobenzene | 14.73 | 118 | 24.0 | 0.68% | 96.67% |
| 10 | | 5.0% | TFA | 10.0% | KHCO3 | 3.00 | 50:50 DMAc:Bromobenzene | 14.73 | 118 | 24.0 | 0.10% | 96.87% |
| 10 | 10.0 | 5.0% | AcOH | 10.0% | KHCO3 | 2.90 | Dioxane | 12.28 | 118 | 24.0 | 77.36% | 20.31% |
| 10 | 10.0 | 5.0% | AcOH | 10.0% | KHCO3 | 3.10 | CPME | 12.28 | 118 | 24.0 | 43.92% | 54.84% |
| 10 | 10.0 | 5.0% | AcOH | 10.0% | KHCO3 | 3.10 | t-AmOH | 12.28 | 118 | 24.0 | 57.39% | 39.77% |
| 10 | 10.0 | 5.0% | AcOH | 10.0% | KHCO3 | 2.90 | p-Xylene | 12.28 | 118 | 24.0 | 65.27% | 32.72% |
| 10 | 10.0 | 5.0% | AcOH | 10.0% | KHCO3 | 3.20 | F3-toluene | 12.28 | 118 | 24.0 | 66.21% | 32.36% |
| 10 | 10.0 | 5.0% | AcOH | 10.0% | KHCO3 | 3.00 | DMAc | 12.28 | 118 | 24.0 | 1.34% | 79.09% |
| 10 | | 5.0% | AcOH | 10.0% | KHCO3 | 3.00 | 50:50 Dioxane:Bromobenzene | 14.73 | 118 | 24.0 | 0.17% | 98.63% |
| 10 | | 5.0% | AcOH | 10.0% | KHCO3 | 3.30 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.16% | 98.55% |
| 10 | | 5.0% | AcOH | 10.0% | KHCO3 | 2.80 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.33% | 97.89% |
| 10 | | 5.0% | AcOH | 10.0% | KHCO3 | 2.90 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 1.18% | 95.80% |
| 10 | | 5.0% | AcOH | 10.0% | KHCO3 | 2.90 | 50:50 F3-toluene:Bromobenzene | 14.73 | 118 | 24.0 | 0.68% | 97.55% |
| 10 | | 5.0% | AcOH | 10.0% | KHCO3 | 3.20 | 50:50 DMAc:Bromobenzene | 14.73 | 118 | 24.0 | 0.08% | 96.05% |

reen #3, cont

| SM umol | PhI equiv | Pd(OAc)2 mol % | Additive/Co-Catalyst Name | mol % | Base Name | Equiv | Name | vol | Temp °C | h | Pdt. AP | SM AP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 10.0 | 5.0% | CuCl2 | 10.0% | KOPiv | 3.07 | p-Xylene | 12.28 | 118 | 24.0 | 27.23% | 67.55% |
| 10 | 10.0 | 5.0% | CuBr2 | 10.0% | KOPiv | 3.00 | p-Xylene | 12.28 | 118 | 24.0 | 51.44% | 38.49% |
| 10 | 10.0 | 5.0% | CuCl2 | 10.0% | KOPiv | 3.00 | CPME | 12.28 | 118 | 24.0 | 23.48% | 70.66% |
| 10 | 10.0 | 5.0% | CuBr2 | 10.0% | KOPiv | 3.07 | CPME | 12.28 | 118 | 24.0 | 21.64% | 72.66% |
| 10 | 10.0 | 5.0% | CuCl2 | 10.0% | KOPiv | 3.07 | t-AmOH | 12.28 | 118 | 24.0 | 18.39% | 68.10% |
| 10 | 10.0 | 5.0% | CuBr2 | 10.0% | KOPiv | 2.93 | t-AmOH | 12.28 | 118 | 24.0 | 20.04% | 70.05% |
| 10 |  | 5.0% | CuCl2 | 10.0% | KOPiv | 2.93 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.08% | 89.68% |
| 10 |  | 5.0% | CuBr2 | 10.0% | KOPiv | 3.07 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 73.12% |
| 10 |  | 5.0% | CuCl2 | 10.0% | KOPiv | 3.14 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.05% | 86.64% |
| 10 |  | 5.0% | CuBr2 | 10.0% | KOPiv | 2.93 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.08% | 68.97% |
| 10 |  | 5.0% | CuCl2 | 10.0% | KOPiv | 3.21 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 83.96% |
| 10 |  | 5.0% | CuBr2 | 10.0% | KOPiv | 3.14 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 73.37% |
| 10 | 10.0 | 5.0% | Cu2O | 10.0% | KOPiv | 3.14 | p-Xylene | 12.28 | 118 | 24.0 | 25.28% | 71.17% |
| 10 | 10.0 | 5.0% | Cu(OAc) | 10.0% | KOPiv | 2.93 | p-Xylene | 12.28 | 118 | 24.0 | 59.95% | 29.16% |
| 10 | 10.0 | 5.0% | Cu2O | 10.0% | KOPiv | 3.00 | CPME | 12.28 | 118 | 24.0 | 22.93% | 74.46% |
| 10 | 10.0 | 5.0% | Cu(OAc) | 10.0% | KOPiv | 2.93 | CPME | 12.28 | 118 | 24.0 | 16.13% | 79.22% |
| 10 | 10.0 | 5.0% | Cu2O | 10.0% | KOPiv | 2.93 | t-AmOH | 12.28 | 118 | 24.0 | 21.31% | 68.36% |
| 10 | 10.0 | 5.0% | Cu(OAc) | 10.0% | KOPiv | 3.00 | t-AmOH | 12.28 | 118 | 24.0 | 20.03% | 66.33% |
| 10 |  | 5.0% | Cu2O | 10.0% | KOPiv | 2.93 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.04% | 95.02% |
| 10 |  | 5.0% | Cu(OAc) | 10.0% | KOPiv | 3.86 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 87.73% |
| 10 |  | 5.0% | Cu2O | 10.0% | KOPiv | 3.00 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.08% | 87.85% |
| 10 |  | 5.0% | Cu(OAc) | 10.0% | KOPiv | 3.07 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 83.50% |
| 10 |  | 5.0% | Cu2O | 10.0% | KOPiv | 2.93 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.29% | 93.70% |
| 10 |  | 5.0% | Cu(OAc) | 10.0% | KOPiv | 3.28 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.04% | 85.09% |
| 10 | 10.0 | 5.0% | CuCl | 10.0% | KOPiv | 3.00 | p-Xylene | 12.28 | 118 | 24.0 | 43.01% | 46.39% |
| 10 | 10.0 | 5.0% | CuO | 10.0% | KOPiv | 2.86 | p-Xylene | 12.28 | 118 | 24.0 | 16.67% | 78.28% |
| 10 | 10.0 | 5.0% | CuCl | 10.0% | KOPiv | 3.21 | CPME | 12.28 | 118 | 24.0 | 21.62% | 75.00% |
| 10 | 10.0 | 5.0% | CuO | 10.0% | KOPiv | 2.93 | CPME | 12.28 | 118 | 24.0 | 21.45% | 69.34% |
| 10 | 10.0 | 5.0% | CuCl | 10.0% | KOPiv | 3.14 | t-AmOH | 12.28 | 118 | 24.0 | 16.38% | 71.24% |
| 10 | 10.0 | 5.0% | CuO | 10.0% | KOPiv | 2.93 | t-AmOH | 12.28 | 118 | 24.0 | 16.89% | 69.40% |
| 10 |  | 5.0% | CuCl | 10.0% | KOPiv | 2.93 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.21% | 74.35% |
| 10 |  | 5.0% | CuO | 10.0% | KOPiv | 3.07 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 75.14% |
| 10 |  | 5.0% | CuCl | 10.0% | KOPiv | 0.00 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.07% | 64.52% |
| 10 |  | 5.0% | CuO | 10.0% | KOPiv | 3.14 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.07% | 72.51% |
| 10 |  | 5.0% | CuCl | 10.0% | KOPiv | 3.28 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.05% | 86.72% |
| 10 |  | 5.0% | CuO | 10.0% | KOPiv | 2.86 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.05% | 75.73% |
| 10 | 10.0 | 5.0% | Cu(OAc)2 | 10.0% | KOPiv | 2.93 | p-Xylene | 12.28 | 118 | 24.0 | 31.32% | 60.64% |
| 10 | 10.0 | 5.0% | CuI | 10.0% | KOPiv | 3.07 | p-Xylene | 12.28 | 118 | 24.0 | 29.43% | 66.76% |
| 10 | 10.0 | 5.0% | Cu(OAc)2 | 10.0% | KOPiv | 3.00 | CPME | 12.28 | 118 | 24.0 | 19.38% | 72.70% |
| 10 | 10.0 | 5.0% | CuI | 10.0% | KOPiv | 3.00 | CPME | 12.28 | 118 | 24.0 | 19.57% | 73.31% |
| 10 | 10.0 | 5.0% | Cu(OAc)2 | 10.0% | KOPiv | 3.00 | t-AmOH | 12.28 | 118 | 24.0 | 17.91% | 68.86% |
| 10 | 10.0 | 5.0% | CuI | 10.0% | KOPiv | 3.36 | t-AmOH | 12.28 | 118 | 24.0 | 10.55% | 81.25% |
| 10 |  | 5.0% | Cu(OAc)2 | 10.0% | KOPiv | 3.14 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.18% | 77.58% |
| 10 |  | 5.0% | CuI | 10.0% | KOPiv | 2.93 | 50:50 p-Xylene:Bromobenzene | 14.73 | 118 | 24.0 | 0.08% | 82.87% |
| 10 |  | 5.0% | Cu(OAc)2 | 10.0% | KOPiv | 3.00 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.05% | 80.76% |
| 10 |  | 5.0% | CuI | 10.0% | KOPiv | 3.00 | 50:50 CPME:Bromobenzene | 14.73 | 118 | 24.0 | 0.06% | 83.89% |
| 10 |  | 5.0% | Cu(OAc)2 | 10.0% | KOPiv | 3.14 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.04% | 80.61% |
| 10 |  | 5.0% | CuI | 10.0% | KOPiv | 2.93 | 50:50 t-AmOH:Bromobenzene | 14.73 | 118 | 24.0 | 0.05% | 84.14% |

| DOE #1 Pd source | Base | Solvent | Time | Phi equiv | Pd mol % | base equiv | HOAc equiv | Vol | Temp | AP Product | AP SM |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 1.97 | 0.3 | 6 | 80 | 40.041 | 55.04 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 2.01 | 0.1 | 12 | 80 | 25.677 | 70.17 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 2.95 | 0.1 | 6 | 80 | 30.999 | 64.517 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 3.03 | 0.3 | 12 | 80 | 24.243 | 72.286 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 2.03 | 0.1 | 6 | 80 | 93.079 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 1.97 | 0.3 | 12 | 80 | 93.915 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 3.02 | 0.3 | 6 | 80 | 93.603 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 2.96 | 0.1 | 12 | 80 | 92.35 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.53 | 0.2 | 9 | 80 | 91.871 | 0.17 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 2.66 | 0.1 | 6 | 80 | 42.568 | 51.857 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 2.07 | 0.3 | 12 | 80 | 29.339 | 66.833 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 3.01 | 0.3 | 6 | 80 | 48.072 | 41.328 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 3.00 | 0.1 | 12 | 80 | 39.851 | 53.511 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 2.00 | 0.3 | 6 | 80 | 87.679 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 1.93 | 0.1 | 12 | 80 | 86.655 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 3.00 | 0.1 | 6 | 80 | 89.423 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 3.03 | 0.3 | 12 | 80 | 85.736 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 3 | 2.45 | 0.2 | 9 | 90 | 83.364 | 11.666 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 5 | 2.44 | 0.2 | 9 | 90 | 31.998 | 63.183 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 1.84 | 0.2 | 9 | 90 | 82.94 | 10.658 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.35 | 0.2 | 6 | 90 | 92.606 | 0.046 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.54 | 0.1 | 9 | 90 | 91.266 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.48 | 0.2 | 9 | 90 | 83.287 | 10.685 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.51 | 0.2 | 9 | 90 | 86.34 | 7.106 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.42 | 0.2 | 9 | 90 | 91.353 | 0.987 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.42 | 0.2 | 9 | 90 | 81.405 | 12.366 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.53 | 0.3 | 9 | 90 | 93.606 | 0.115 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.54 | 0.2 | 12 | 90 | 89.055 | 3.112 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.90 | 0.2 | 9 | 90 | 93.233 | 0.501 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 5 | 2.56 | 0.2 | 9 | 90 | 92.734 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 7 | 2.50 | 0.2 | 9 | 90 | 91.183 | 0.17 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 2.00 | 0.1 | 6 | 100 | 23.748 | 69.384 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 1.87 | 0.3 | 12 | 100 | 22.864 | 72.244 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 2.96 | 0.3 | 6 | 100 | 22.481 | 72.511 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 3 | 3.00 | 0.1 | 12 | 100 | 22.411 | 73.686 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 2.00 | 0.3 | 6 | 100 | 92.974 | 0.056 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 2.01 | 0.1 | 12 | 100 | 90.389 | 0.081 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 2.93 | 0.1 | 6 | 100 | 91.548 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 3 | 2.95 | 0.3 | 12 | 100 | 90.882 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 6 | 5 | 2.42 | 0.2 | 9 | 100 | 93.65 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 2.02 | 0.3 | 6 | 100 | 84.762 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 2.00 | 0.1 | 12 | 100 | 30.603 | 65.995 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 2.94 | 0.1 | 6 | 100 | 32.953 | 60.939 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 2 | 7 | 3.00 | 0.3 | 12 | 100 | 26.315 | 68.967 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 1.93 | 0.1 | 6 | 100 | 90.365 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 2.04 | 0.3 | 12 | 100 | 89.614 | 0 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 2.99 | 0.3 | 6 | 100 | 87.992 | 1.09 |
| Pd(OAc)2 | KHCO3 | Dioxane | 24 | 10 | 7 | 3.07 | 0.1 | 12 | 100 | 87.943 | 0 |

Screen #4

| SM | PhI | Pd | AcOH | | Additive | | | Temp | | PdL | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | equiv | 5 mol % | equiv | Equiv | 1.0 equiv | Name | vol | °C | h | AP | AP |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | None | Anisole | 1.50 | 113 | 24.0 | 10.11% | 87.46% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KI | Anisole | 1.50 | 113 | 24.0 | 10.04% | 87.17% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KPF6 | Anisole | 1.50 | 113 | 24.0 | 11.75% | 0.85425 |
| 10 | 10.0 | Pd(OAc)2 | 0 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 13.87% | 0.83144 |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 12.61% | 0.84418 |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | TBAOTf | Anisole | 1.50 | 113 | 24.0 | 0 | 89.80% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | None | Anisole | 1.50 | 113 | 24.0 | 0 | 75.99% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KI | Anisole | 1.50 | 113 | 24.0 | 19.50% | 77.23% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KPF6 | Anisole | 1.50 | 113 | 24.0 | 22.16% | 74.66% |
| 10 | 10.0 | Pd(OAc)2 | 0 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 23.92% | 72.96% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 23.92% | 73.22% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | TBAOTf | Anisole | 1.50 | 113 | 24.0 | 9.68% | 87.01% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | None | Anisole | 1.50 | 113 | 24.0 | 29.19% | 67.21% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KI | Anisole | 1.50 | 113 | 24.0 | 27.81% | 68.54% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KPF6 | Anisole | 1.50 | 113 | 24.0 | 29.33% | 66.94% |
| 10 | 10.0 | Pd(OAc)2 | 0 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 26.66% | 69.33% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 27.33% | 69.20% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | TBAOTf | Anisole | 1.50 | 113 | 24.0 | 11.55% | 85.41% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | None | Anisole | 1.50 | 113 | 24.0 | 28.45% | 66.98% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KI | Anisole | 1.50 | 113 | 24.0 | 32.16% | 63.64% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KPF6 | Anisole | 1.50 | 113 | 24.0 | 31.37% | 64.09% |
| 10 | 10.0 | Pd(OAc)2 | 0 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 39.50% | 56.59% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 62.41% | 26.23% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | TBAOTf | Anisole | 1.50 | 113 | 24.0 | 17.29% | 73.02% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | None | Anisole | 1.50 | 113 | 24.0 | 61.32% | 28.55% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KI | Anisole | 1.50 | 113 | 24.0 | 62.61% | 27.19% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KPF6 | Anisole | 1.50 | 113 | 24.0 | 64.05% | 25.88% |
| 10 | 10.0 | Pd(OAc)2 | 0 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 60.25% | 27.31% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 63.12% | 25.15% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | TBAOTf | Anisole | 1.50 | 113 | 24.0 | 19.51% | 70.80% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | None | Anisole | 1.50 | 113 | 24.0 | 71.10% | 19.16% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KI | Anisole | 1.50 | 113 | 24.0 | 69.11% | 20.27% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KPF6 | Anisole | 1.50 | 113 | 24.0 | 67.95% | 20.90% |
| 10 | 10.0 | Pd(OAc)2 | 0 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 70.32% | 18.10% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | KOTf | Anisole | 1.50 | 113 | 24.0 | 70.23% | 17.75% |
| 10 | 10.0 | Pd(OAc)2 | 0.2 | 3.00 | TBAOTf | Anisole | 1.50 | 113 | 24.0 | 20.02% | 69.36% |

Screen #5

| SM | PhI | Pd | Additive | Additive | Base | | Additive | | | Temp | | Pdt. | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | equiv | 6 mol % | 6 mol % | Equiv | Name | Equiv | 10 mol % | Name | vol | °C | h | AP | AP |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 16.19% | 74.15% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 4 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 16.51% | 61.79% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 6 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 7.08% | 0.73252 |
| 10 | 10.0 | Pd(OAc)2 | | | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 56.61% | 0.40052 |
| 10 | 10.0 | Pd(OAc)2 | | | TEA | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 3.02% | 0.7397 |
| 10 | 10.0 | Pd(OAc)2 | | | DABCO | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0 | 51.81% |
| 10 | 10.0 | Pd(OAc)2 | | | DIPEA | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0 | 84.83% |
| 10 | 10.0 | Pd(OAc)2 | | | KTOMS | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 2.21% | 75.42% |
| 10 | 10.0 | Pd(OAc)2 | | | 2,6-lutidine | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 8.03% | 86.65% |
| 10 | 10.0 | Pd(OAc)2 | | | DMAP | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 1.91% | 94.60% |
| 10 | 10.0 | Pd(OAc)2 | | | DBU | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.41% | 96.40% |
| 10 | 10.0 | Pd(OAc)2 | | | Cy2NMe | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 2.12% | 72.98% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 51.64% | 26.97% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 4 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 30.03% | 46.81% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 6 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 19.89% | 58.50% |
| 10 | 10.0 | Pd(OAc)2 | | | KHCO3 | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 52.25% | 44.39% |
| 10 | 10.0 | Pd(OAc)2 | | | TEA | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 5.41% | 65.96% |
| 10 | 10.0 | Pd(OAc)2 | | | DABCO | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 3.90% | 49.42% |
| 10 | 10.0 | Pd(OAc)2 | | | DIPEA | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 2.85% | 85.29% |
| 10 | 10.0 | Pd(OAc)2 | | | KTOMS | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 17.49% | 75.42% |
| 10 | 10.0 | Pd(OAc)2 | | | 2,6-lutidine | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 7.81% | 86.34% |
| 10 | 10.0 | Pd(OAc)2 | | | DMAP | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 1.71% | 93.55% |
| 10 | 10.0 | Pd(OAc)2 | | | DBU | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 0.52% | 92.65% |
| 10 | 10.0 | Pd(OAc)2 | | | Cy2NMe | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 2.09% | 74.78% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 66.37% | 16.01% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 4 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 26.39% | 50.83% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 6 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 15.87% | 62.71% |
| 10 | 10.0 | Pd(OAc)2 | | | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 58.48% | 38.24% |
| 10 | 10.0 | Pd(OAc)2 | | | TEA | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 3.30% | 84.84% |
| 10 | 10.0 | Pd(OAc)2 | | | DABCO | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 3.34% | 59.22% |
| 10 | 10.0 | Pd(OAc)2 | | | DIPEA | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 2.98% | 79.45% |
| 10 | 10.0 | Pd(OAc)2 | | | KTOMS | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 38.85% | 47.64% |
| 10 | 10.0 | Pd(OAc)2 | | | 2,6-lutidine | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 17.05% | 75.25% |
| 10 | 10.0 | Pd(OAc)2 | | | DMAP | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 1.16% | 88.72% |
| 10 | 10.0 | Pd(OAc)2 | | | DBU | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.59% | 92.80% |
| 10 | 10.0 | Pd(OAc)2 | | | Cy2NMe | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 2.13% | 69.80% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 40.69% | 37.43% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 4 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 17.35% | 59.49% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 6 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 11.38% | 78.93% |
| 10 | 10.0 | Pd(OAc)2 | | | KHCO3 | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 55.52% | 40.54% |
| 10 | 10.0 | Pd(OAc)2 | | | TEA | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 2.80% | 70.44% |
| 10 | 10.0 | Pd(OAc)2 | | | DABCO | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 3.27% | 49.37% |
| 10 | 10.0 | Pd(OAc)2 | | | DIPEA | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 3.46% | 75.02% |
| 10 | 10.0 | Pd(OAc)2 | | | KTOMS | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 18.29% | 58.85% |
| 10 | 10.0 | Pd(OAc)2 | | | 2,6-lutidine | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 11.18% | 56.39% |
| 10 | 10.0 | Pd(OAc)2 | | | DMAP | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 0.79% | 81.30% |
| 10 | 10.0 | Pd(OAc)2 | | | DBU | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 0.41% | 79.72% |
| 10 | 10.0 | Pd(OAc)2 | | | Cy2NMe | 3.00 | | Anisole | 4.00 | 110 | 24.0 | 1.72% | 56.96% |

:reen #5, cont

| SM | PhI | Pd | Additive | Additive | Base | | Additive | | | Temp | | Pdt. | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | equiv | 5 mol % | 5 mol % | Equiv | Name | Equiv | 10 mol % | Name | vol | °C | h | *AP* | *AP* |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 17.34% | 68.71% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 4 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 15.61% | 62.25% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 6 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 8.42% | 69.75% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 51.07% | 31.17% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | TEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.73% | 59.15% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | DABCO | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.11% | 37.19% |
| 10 | 10.0 | Pd(OPiv)2 | DMPU | 2 | DIPEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.96% | 63.30% |
| 10 | 10.0 | Pd(OPiv)2 | DMPU | 2 | KTOMS | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 4.69% | 56.36% |
| 10 | 10.0 | Pd(OPiv)2 | DMPU | 2 | 2,6-lutidine | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 4.13% | 62.55% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | DMAP | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.53% | 79.81% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | DBU | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.57% | 82.75% |
| 10 | 10.0 | Pd(OAc)2 | DMPU | 2 | Cy2NMe | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.97% | 63.47% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 41.92% | 35.73% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 4 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 23.57% | 51.58% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 6 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 16.89% | 59.33% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 32.96% | 35.50% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | TEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.66% | 58.08% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | DABCO | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.82% | 32.06% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | DIPEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.62% | 63.06% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | KTOMS | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 6.20% | 56.69% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | 2,6-lutidine | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 5.06% | 64.31% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | DMAP | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.22% | 70.02% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | DBU | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 68.41% |
| 10 | 10.0 | Pd(OAc)2 | DMAc | 2 | Cy2NMe | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.40% | 63.00% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 38.94% | 52.92% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 4.00 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 23.09% | 67.58% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 6.00 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 17.37% | 56.46% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 34.90% | 41.39% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | TEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.42% | 58.86% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | DABCO | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.28% | 36.53% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | DIPEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 2.32% | 63.18% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | KTOMS | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 9.38% | 56.51% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | 2,6-lutidine | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 64.75% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | DMAP | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.20% | 68.56% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | DBU | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.52% | 68.88% |
| 10 | 10.0 | Pd(OAc)2 | NMP | 2.00 | Cy2NMe | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.87% | 56.56% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 49.65% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 4.00 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 61.78% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 6.00 | KHCO3 | 3.00 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 12.71% | 77.33% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 50.35% | 38.12% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | TEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.50% | 51.32% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | DABCO | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 28.57% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | DIPEA | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 1.80% | 54.84% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | KTOMS | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 58.39% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | 2,6-lutidine | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 59.97% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | DMAP | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 66.12% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | DBU | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 67.79% |
| 10 | 10.0 | Pd(OAc)2 | DMSO | 2.00 | Cy2NMe | 3.00 | AcOH | Anisole | 4.00 | 110 | 24.0 | 0.00% | 49.83% |

Screen #6

| SM | Electrophile | Pd | Additive | Additive | Base | | Ligand | Additive | | | Temp | | Pdt. | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| umol | 10 equiv | 5 mol % | 6 mol % | Equiv | Name | Equiv | 5 mol % | 10 mol % | Name | vol | °C | h | AP | AP |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | DABCO | AcOH | Dioxane | 4.00 | 110 | 24.0 | 26.22% | 62.29% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 4 | KHCO3 | 3.00 | COD | AcOH | Dioxane | 4.00 | 110 | 24.0 | 87.54% | 5.83% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 6 | KHCO3 | 3.00 | Pyridine | AcOH | Dioxane | 4.00 | 110 | 24.0 | 90.25% | 0.04851 |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DBU | AcOH | Dioxane | 4.00 | 110 | 24.0 | 7.55% | 0.8506 |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DABCO | AcOH | Anisole | 4.00 | 110 | 24.0 | 58.30% | 0.2029 |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | COD | AcOH | Anisole | 4.00 | 110 | 24.0 | 0 | 44.18% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | Pyridine | AcOH | Anisole | 4.00 | 110 | 24.0 | 1 | 18.81% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DBU | AcOH | Anisole | 4.00 | 110 | 24.0 | 13.21% | 45.22% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DABCO | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 48.61% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | COD | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 51.70% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | Pyridine | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 65.24% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DBU | AcOH | Dioxane | 4.00 | 110 | 24.0 | 2.40% | 48.18% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | IPrNHC | AcOH | Dioxane | 4.00 | 110 | 24.0 | 26.12% | 54.66% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 4 | KHCO3 | 3.00 | Ph2POEt | AcOH | Dioxane | 4.00 | 110 | 24.0 | 60.32% | 28.32% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 6 | KHCO3 | 3.00 | dba | AcOH | Dioxane | 4.00 | 110 | 24.0 | 88.27% | 5.56% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | 2,6-lutideni | AcOH | Dioxane | 4.00 | 110 | 24.0 | 88.65% | 5.00% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | IPrNHC | AcOH | Anisole | 4.00 | 110 | 24.0 | 13.36% | 62.44% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | Ph2POEt | AcOH | Anisole | 4.00 | 110 | 24.0 | 55.56% | 22.16% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | dba | AcOH | Anisole | 4.00 | 110 | 24.0 | 73.59% | 17.36% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | 2,6-lutideni | AcOH | Anisole | 4.00 | 110 | 24.0 | 60.96% | 18.86% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | IPrNHC | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 49.30% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | Ph2POEt | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 61.49% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | dba | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.13% | 54.83% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | 2,6-lutideni | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 50.21% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 2 | KHCO3 | 3.00 | StBu | AcOH | Dioxane | 4.00 | 110 | 24.0 | 23.63% | 68.50% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 4 | KHCO3 | 3.00 | P(O-tol)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 33.56% | 48.62% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 6 | KHCO3 | 3.00 | styrene | AcOH | Dioxane | 4.00 | 110 | 24.0 | 90.61% | 4.38% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DFPE | AcOH | Dioxane | 4.00 | 110 | 24.0 | 90.03% | 5.41% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | StBu | AcOH | Anisole | 4.00 | 110 | 24.0 | 21.85% | 55.68% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | P(O-tol)3 | AcOH | Anisole | 4.00 | 110 | 24.0 | 73.37% | 20.22% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | styrene | AcOH | Anisole | 4.00 | 110 | 24.0 | 52.65% | 25.58% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DFPE | AcOH | Anisole | 4.00 | 110 | 24.0 | 49.59% | 30.70% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | StBu | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.08% | 68.95% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | P(O-tol)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 69.69% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | styrene | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.54% | 51.97% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | DFPE | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 46.05% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 2 | KHCO3 | 3.00 | F-AcAc | AcOH | Dioxane | 4.00 | 110 | 24.0 | 59.30% | 36.49% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 4 | KHCO3 | 3.00 | P(OiPr)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 28.98% | 60.22% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 6 | KHCO3 | 3.00 | CF3-styren | AcOH | Dioxane | 4.00 | 110 | 24.0 | 23.20% | 61.30% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | CF3-P | AcOH | Dioxane | 4.00 | 110 | 24.0 | 30.66% | 57.40% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | F-AcAc | AcOH | Anisole | 4.00 | 110 | 24.0 | 46.35% | 35.74% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | P(OiPr)3 | AcOH | Anisole | 4.00 | 110 | 24.0 | 64.32% | 19.16% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | CF3-styren | AcOH | Anisole | 4.00 | 110 | 24.0 | 54.68% | 23.85% |
| 10 | Iodobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | CF3-P | AcOH | Anisole | 4.00 | 110 | 24.0 | 26.15% | 47.22% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | F-AcAc | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 66.84% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | P(OiPr)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 54.18% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | CF3-styren | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 49.15% |
| 10 | Bromobenzene | Pd(OAc)2 | | | KHCO3 | 3.00 | CF3-P | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.15% | 64.53% |

reen #6, cont

| SM | Electrophile | Pd | Additive | Additive | Base | | Ligand | Additive | | | Temp | | PdL | SM |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| µmol | 10 equiv | 5 mol % | 5 mol % | Equiv | Name | Equiv | 5 mol % | 10 mol % | Name | vol | °C | h | AP | AP |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | tBu-pyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 30.75% | 58.18% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 4 | KHCO3 | 3.00 | P(OMe)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 45.63% | 41.34% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 6 | KHCO3 | 3.00 | CF3-pyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 13.48% | 85.37% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | PMe3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 43.79% | 44.98% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | tBu-pyr | AcOH | Anisole | 4.00 | 110 | 24.0 | 19.01% | 59.23% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | P(OMe)3 | AcOH | Anisole | 4.00 | 110 | 24.0 | 29.47% | 49.09% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | CF3-pyr | AcOH | Anisole | 4.00 | 110 | 24.0 | 53.40% | 30.13% |
| 10 | Iodobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | PMe3 | AcOH | Anisole | 4.00 | 110 | 24.0 | 40.27% | 37.58% |
| 10 | Bromobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | tBu-pyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 44.52% |
| 10 | Bromobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | P(OMe)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 63.97% |
| 10 | Bromobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | CF3-pyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 46.29% |
| 10 | Bromobenzene | Pd(OAc)2 | DMAc | 2 | KHCO3 | 3.00 | PMe3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 61.50% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | QNOL | AcOH | Dioxane | 4.00 | 110 | 24.0 | 53.76% | 40.95% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 4.00 | KHCO3 | 3.00 | PnBu3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 28.35% | 52.37% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 6.00 | KHCO3 | 3.00 | OMe-pyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 19.72% | 64.07% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | AcAc | AcOH | Dioxane | 4.00 | 110 | 24.0 | 18.83% | 64.46% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | QNOL | AcOH | Anisole | 4.00 | 110 | 24.0 | 75.17% | 18.43% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | PnBu3 | AcOH | Anisole | 4.00 | 110 | 24.0 | 19.54% | 57.25% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | OMe-pyr | AcOH | Anisole | 4.00 | 110 | 24.0 | 78.44% | 17.88% |
| 10 | Iodobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | AcAc | AcOH | Anisole | 4.00 | 110 | 24.0 | 46.88% | 32.87% |
| 10 | Bromobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | QNOL | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 86.42% |
| 10 | Bromobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | PnBu3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.05% | 58.03% |
| 10 | Bromobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | OMe-pyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.11% | 64.76% |
| 10 | Bromobenzene | Pd(OAc)2 | NMP | 2.00 | KHCO3 | 3.00 | AcAc | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.11% | 54.09% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Dioxane | 4.00 | 110 | 24.0 | 14.08% | 39.88% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 4.00 | KHCO3 | 3.00 | Blank | AcOH | Dioxane | 4.00 | 110 | 24.0 | 24.53% | 62.06% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 6.00 | KHCO3 | 3.00 | Mepyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 15.35% | 33.90% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Dioxane | 4.00 | 110 | 24.0 | 18.98% | 55.32% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Anisole | 4.00 | 110 | 24.0 | 48.08% | 44.04% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Anisole | 4.00 | 110 | 24.0 | 47.45% | 34.20% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Mepyr | AcOH | Anisole | 4.00 | 110 | 24.0 | 13.98% | 66.91% |
| 10 | Iodobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Anisole | 4.00 | 110 | 24.0 | 47.08% | 35.90% |
| 10 | Bromobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 44.56% |
| 10 | Bromobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 84.37% |
| 10 | Bromobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Mepyr | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 52.21% |
| 10 | Bromobenzene | Pd(OAc)2 | DMSO | 2.00 | KHCO3 | 3.00 | Blank | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 61.02% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | 2-pyrMeOH | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 32.55% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 4 | KHCO3 | 3.00 | P(OEt)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 98.10% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 6 | KHCO3 | 3.00 | OMe-sty | AcOH | Dioxane | 4.00 | 110 | 24.0 | 88.96% | 4.88% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | DMSO | AcOH | Dioxane | 4.00 | 110 | 24.0 | 87.23% | 4.79% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | 2-pyrMeOH | AcOH | Anisole | 4.00 | 110 | 24.0 | 52.38% | 27.69% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | P(OEt)3 | AcOH | Anisole | 4.00 | 110 | 24.0 | 47.89% | 32.44% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | OMe-sty | AcOH | Anisole | 4.00 | 110 | 24.0 | 52.47% | 26.87% |
| 10 | Iodobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | DMSO | AcOH | Anisole | 4.00 | 110 | 24.0 | 50.78% | 28.50% |
| 10 | Bromobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | 2-pyrMeOH | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 50.07% |
| 10 | Bromobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | P(OEt)3 | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 53.73% |
| 10 | Bromobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | OMe-sty | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 51.84% |
| 10 | Bromobenzene | Pd(OAc)2 | DMPU | 2 | KHCO3 | 3.00 | DMSO | AcOH | Dioxane | 4.00 | 110 | 24.0 | 0.00% | 55.17% |

Standard conditions: 5 mol % Pd(OAc)2, 3.0 equiv base, 10 mol % pyridine, 5/3 Anisole/PhI (8 vol total)

| Variation | SM | Product |
|---|---|---|
| KOAc | 43.40 | 40.82 |
| KOPiv | 0.22 | 80.88 |
| CsOAc | 2.95 | 46.36 |
| NaOAc | 85.26 | 7.65 |
| K-Ethylhexanoate | 0.19 | 58.00 |
| CsOPiv (7.5 h) | 0.70 | 51.63 |
| AgOAc | 41.97 | 4.58 |
| 1 equiv KOPiv | 9.64 | 72.53 |
| 3 equiv KOPiv, open to air | 0.04 | 72.53 |
| 3 equiv CsOAc, 110 C (batch 1) | 0.02 | 56.33 |
| 3 equiv CsOAc, 110 C (batch 2) | 0.05 | 60.86 |
| 1 equiv CsOAc, 95 C (batch 1) | 77.42 | 21.38 |
| 1 equiv CsOAc, 95 C (batch 2) | 78.18 | 20.19 |
| 0.50 Cs2CO3, 1.05 PivOH | 0.02 | 87.01 |
| 0.50 Cs2CO3, 1.05 PivOH | 0.02 | 84.92 |
| 0.50 Cs2CO3, 1.25 PivOH | 0.02 | 86.88 |
| 0.47 Cs2CO3, 1.00 PivOH | 5.80 | 84.05 |
| 0.53 Cs2CO3, 1.00 PivOH | 0.02 | 79.84 |
| 0.53 Cs2CO3, 1.11 PivOH | 0.05 | 85.36 |

| Variation | SM | Product |
|---|---|---|
| 1.05 equiv CsOAc - 110 C | 0.90 | 88.55 |
| 2 equiv CsOAc - 95 C | 82.47 | 14.11 |
| 3 equiv KOPiv - 2MeOEtOH (solv) | 58.29 | 32.95 |
| 1.05 equiv CsOAc - 2MeOEtOH (solv) | 65.23 | 24.44 |
| KOBz (1 equiv) | 59.65 | 18.59 |
| KOBz (2 equiv) | 69.72 | 10.76 |
| KOBz (3 equiv) | 71.90 | 11.08 |
| KOBz (1 equiv) + pyr | 74.06 | 9.76 |
| KOPiv (1 equiv) | 0.51 | 78.99 |
| KOPiv (1 equiv)+pyr | 1.53 | 74.29 |
| KOPiv (2 equiv) | 0.81 | 72.81 |
| KOPiv (2 equiv) + pyr | 0.50 | 77.47 |
| KOPiv (3 equiv) | 1.99 | 79.98 |
| KOPiv (3 equiv) + pyr | 0.14 | 80.85 |
| Diglyme (solv), KOPiv | 44.97 | 39.17 |

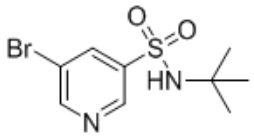
| Amount of water | SM | Product |
|---|---|---|
| 1 equiv | 3.19 | 82.98 |
| 3 equiv | 46.36 | 43.52 |
| 5 equiv | 62.50 | 30.25 |

| Amount of pyr | SM | Product |
|---|---|---|
| 0.00 | 23.94 | 65.14 |
| 0.05 | 0.00 | 78.95 |
| 0.10 | 0.04 | 86.02 |
| 0.20 | 0.07 | 83.12 |
| 0.50 | 12.79 | 75.93 |
| 1.00 | 27.15 | 63.24 |

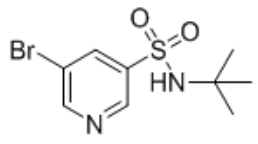
DOE #2

| Reaction ID | Arene µmol | PhI equiv | Pd(OAc)2 mol % | Cs2CO3 equiv | PivOH equiv | Water equiv | KF (wt%) | Solvent Name | vol | Temp °C | Prod AP | SM AP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A1 | 497.19 | 9.05 | 0.07 | 0.51 | 1.01 | 3.02 | 1.01 | Anisole | 4.02 | 108 | 52.54% | 46.97% |
| A2 | 502.32 | 8.96 | 0.03 | 0.57 | 1.14 | 3.00 | 1.14 | Anisole | 3.98 | 108 | 58.45% | 40.69% |
| A3 | 502.75 | 14.92 | 0.03 | 0.53 | 1.00 | 1.01 | 1.00 | Anisole | 3.98 | 108 | 96.90% | |
| A4 | 496.97 | 15.09 | 0.03 | 0.50 | 1.29 | 3.02 | 1.29 | Anisole | 6.04 | 108 | 96.80% | 0.79% |
| A5 | 496.12 | 9.07 | 0.03 | 0.55 | 1.01 | 1.01 | 1.01 | Anisole | 6.05 | 108 | 58.28% | 41.00% |
| A6 | 501.47 | 14.96 | 0.07 | 0.50 | 1.33 | 1.01 | 1.33 | Anisole | 3.99 | 108 | 93.96% | |
| B1 | 496.76 | 15.10 | 0.07 | 0.56 | 1.26 | 3.02 | 1.26 | Anisole | 6.04 | 108 | 96.40% | |
| B2 | 496.54 | 15.10 | 0.03 | 0.59 | 1.31 | 1.01 | 1.31 | Anisole | 4.03 | 108 | 96.07% | |
| B3 | 504.25 | 14.87 | 0.07 | 0.58 | 0.99 | 2.99 | 0.99 | Anisole | 5.95 | 108 | 98.05% | 0.13% |
| B4 | 496.54 | 9.06 | 0.07 | 0.58 | 1.12 | 1.01 | 1.12 | Anisole | 6.04 | 108 | 61.36% | 38.11% |
| B5 | 498.68 | 12.03 | 0.05 | 0.58 | 1.16 | 2.01 | 1.16 | Anisole | 5.01 | 119 | 94.95% | |
| B6 | 504.03 | 11.90 | 0.05 | 0.54 | 1.10 | 2.00 | 1.10 | Anisole | 4.96 | 119 | 94.91% | |
| C1 | 499.54 | 12.01 | 0.05 | 0.60 | 1.15 | 2.01 | 1.15 | Anisole | 5.00 | 119 | 95.21% | |
| C2 | 500.18 | 12.00 | 0.05 | 0.66 | 1.10 | 2.01 | 1.10 | Anisole | 5.00 | 119 | 94.55% | |
| C3 | 497.19 | 15.08 | 0.07 | 0.51 | 1.01 | 1.01 | 1.01 | Anisole | 6.04 | 130 | 93.25% | |
| C4 | 504.68 | 14.86 | 0.03 | 0.58 | 1.04 | 2.99 | 1.04 | Anisole | 3.96 | 130 | 94.98% | |
| C5 | 499.75 | 15.01 | 0.03 | 0.56 | 1.12 | 1.01 | 1.12 | Anisole | 6.00 | 130 | 93.68% | |
| C6 | 501.68 | 8.97 | 0.03 | 0.57 | 1.35 | 1.01 | 1.35 | Anisole | 3.99 | 130 | 94.04% | 2.09% |
| D1 | 501.47 | 8.97 | 0.07 | 0.52 | 1.03 | 1.01 | 1.03 | Anisole | 3.99 | 130 | 91.67% | |
| D2 | 503.39 | 14.90 | 0.07 | 0.66 | 1.13 | 3.00 | 1.13 | Anisole | 3.97 | 130 | 84.04% | |
| D3 | 500.61 | 8.99 | 0.07 | 0.61 | 1.29 | 1.01 | 1.29 | Anisole | 3.99 | 130 | 90.81% | |
| D4 | 495.69 | 9.08 | 0.03 | 0.59 | 1.09 | 3.03 | 1.09 | Anisole | 6.05 | 130 | 95.01% | |
| D5 | 499.75 | 9.00 | 0.03 | 0.57 | 1.27 | 3.01 | 1.27 | Anisole | 6.00 | 130 | 96.64% | |
| D6 | 499.33 | 9.01 | 0.07 | 0.68 | 1.49 | 3.01 | 1.49 | Anisole | 6.01 | 130 | 92.88% | |

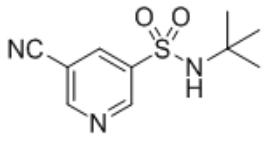
$^{1}$H NMR (500 MHz, DMSO-d$_6$) of 5-bromo-N-tertbutylpyridine-3-sulfonamide (**4**)



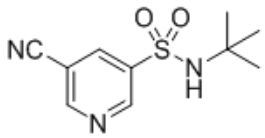
$^{13}C\{1H\}$NMR (125.8 MHz, DMSO-$d_6$) of 5-bromo-N-tertbutylpyridine-3-sulfonamide (**4**)



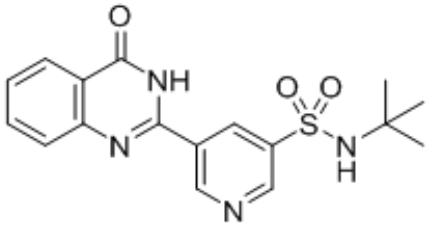
$^{1}$H NMR (500 MHz, DMSO-d$_6$) of N-(tert-butyl)-5-cyanopyridine-3-sulfonamide (**9**)



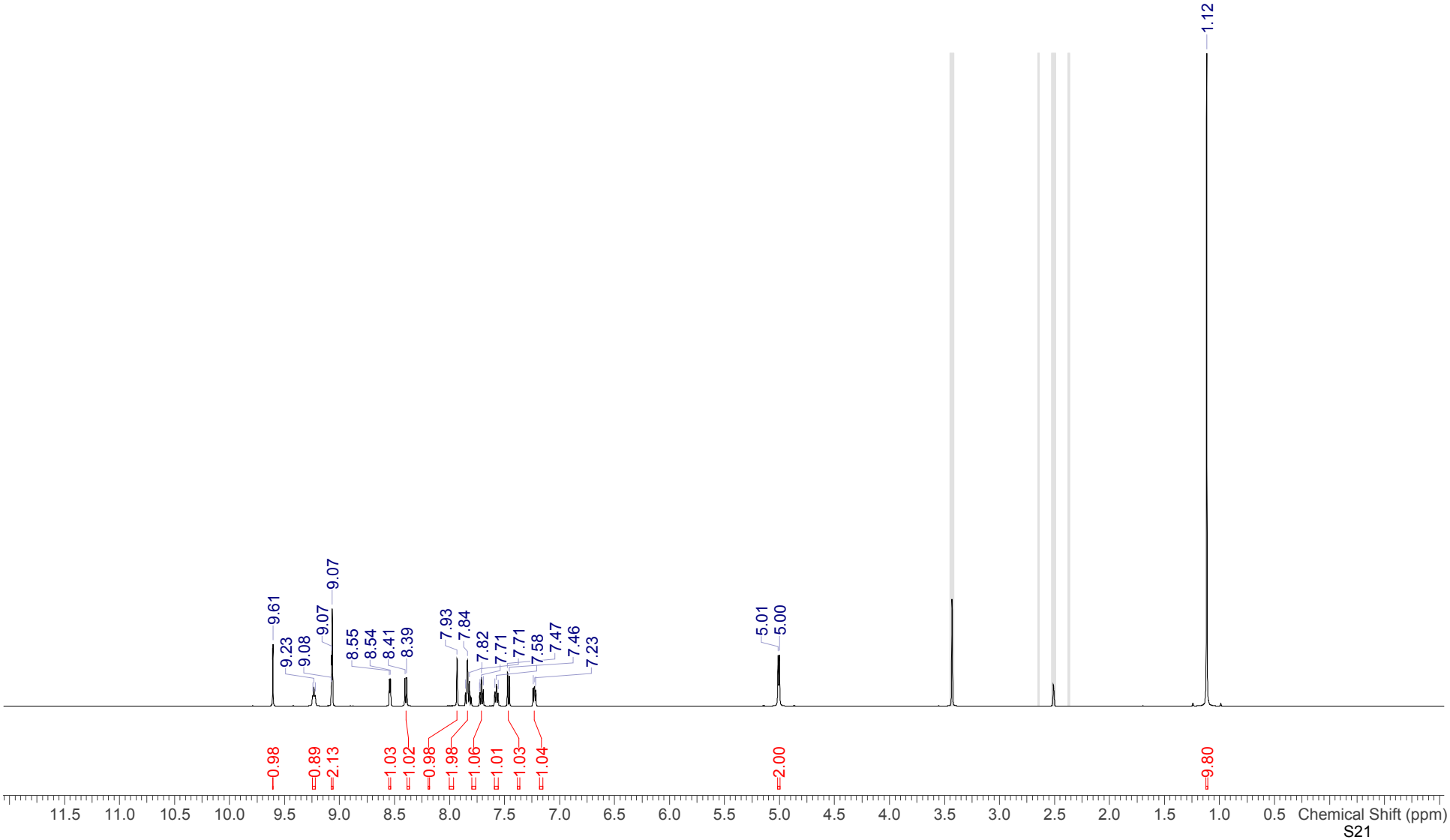
$^{13}C\{1H\}$NMR (125.8 MHz, DMSO-$d_6$) of N-(tert-butyl)-5-cyanopyridine-3-sulfonamide (**9**)



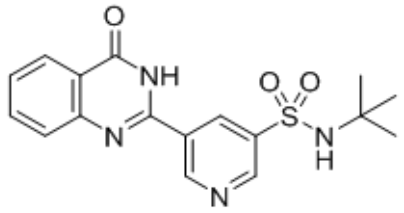
$^{1}$H NMR (500 MHz, DMSO-d$_6$) of N-(tert-butyl)-5-(4-oxo-3,4-dihydroquinazolin-2-yl)pyridine-3-sulfonamide

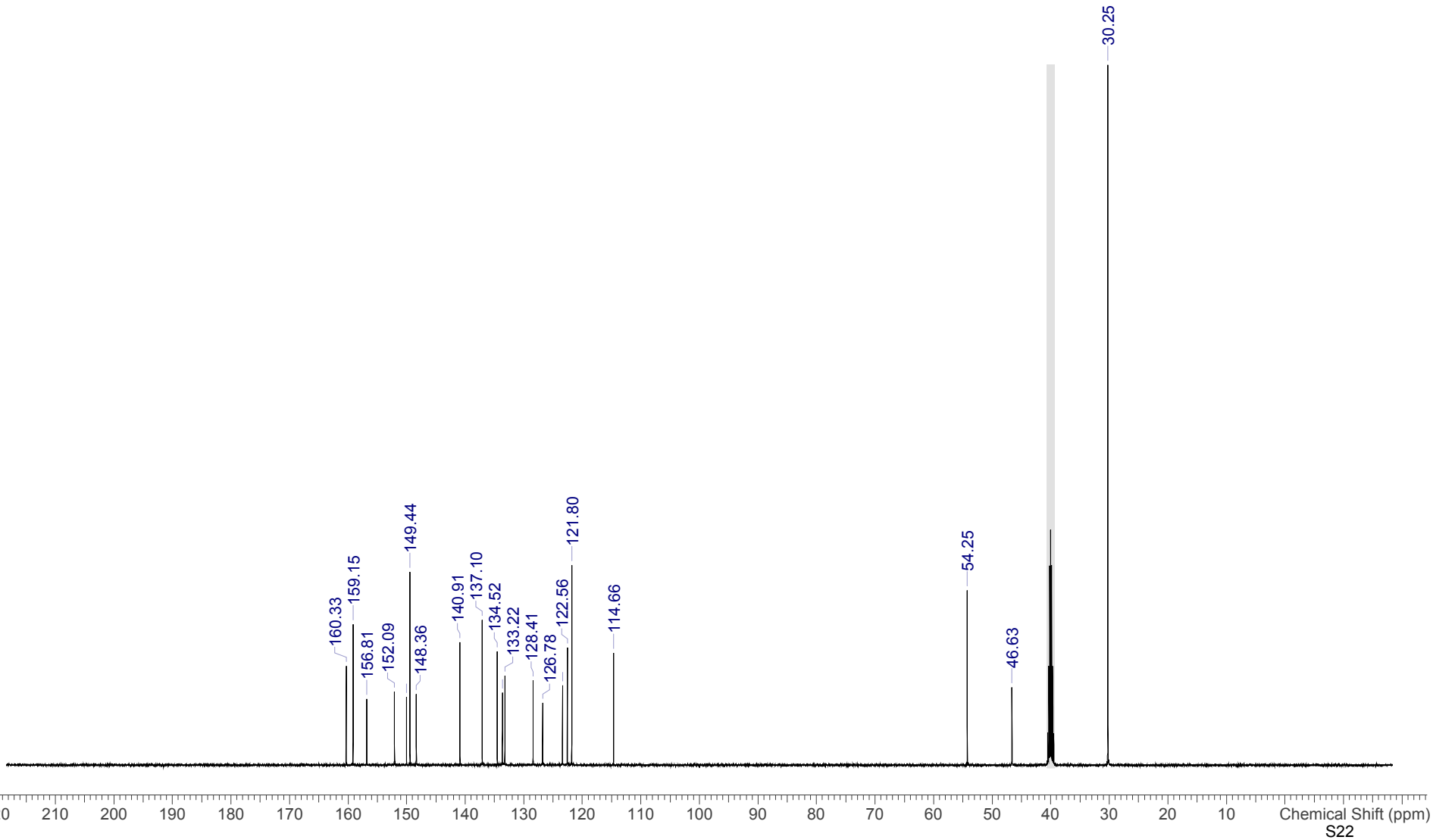


(**10**)

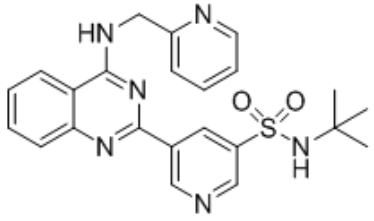


$^{13}C\{1H\}$NMR (125.8 MHz, DMSO-$d_6$) of N-(tert-butyl)-5-(4-oxo-3,4-dihydroquinazolin-2-yl)pyridine-3-sulfonamide (**10**)

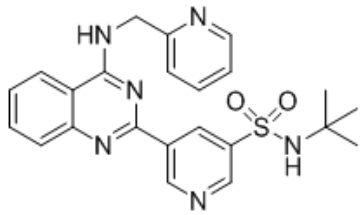


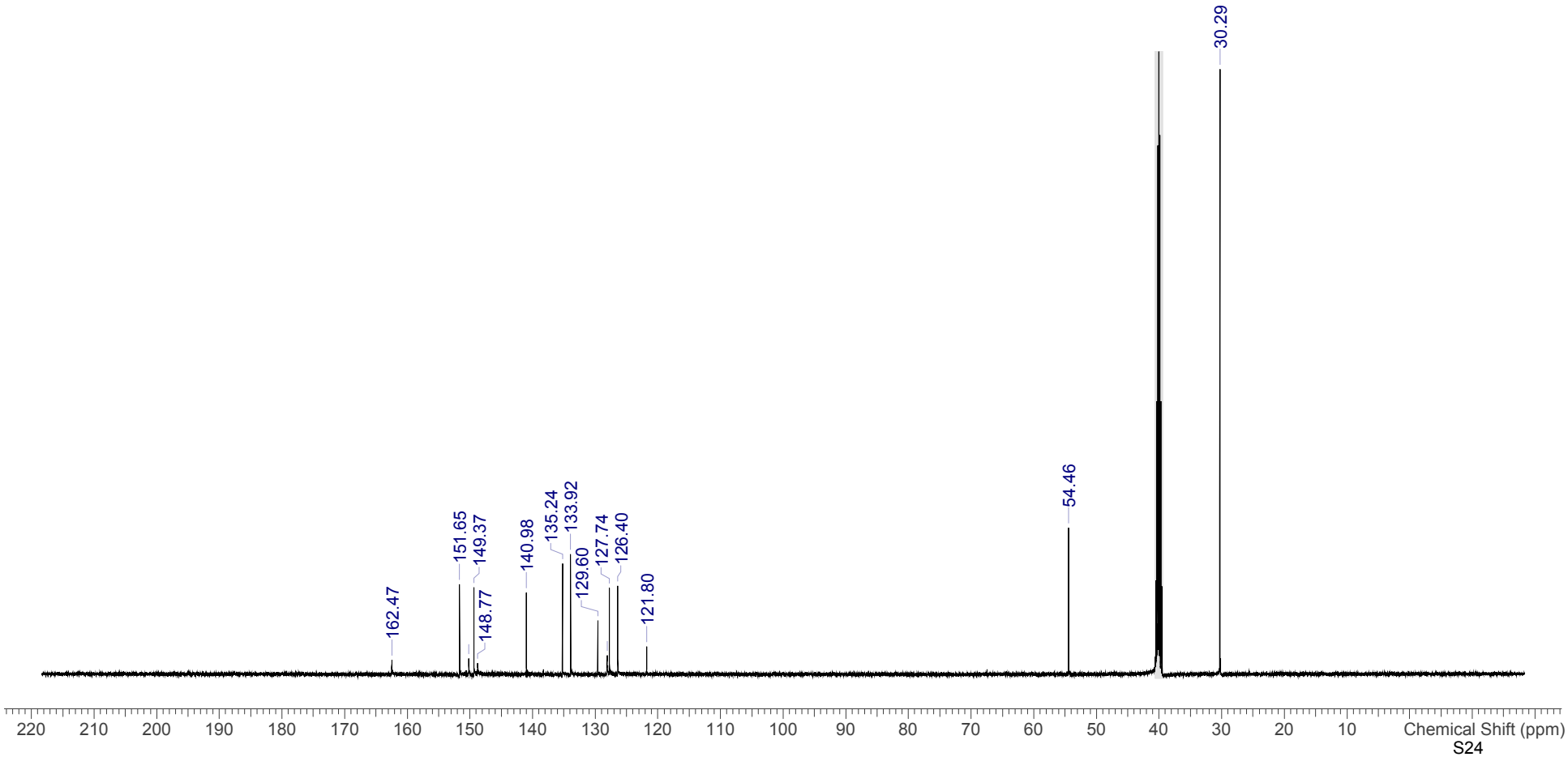
$^{1}$H NMR (500 MHz, DMSO-d$_6$) of N-(tert-butyl)-5-(4-((pyridin-2-ylmethyl)amino)quinolin-2-yl)pyridine-3-sulfonamide (**6**)



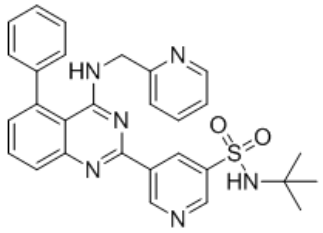
$^{13}C\{1H\}$NMR (125.8 MHz, DMSO-$d_6$) of N-(tert-butyl)-5-(4-((pyridin-2-ylmethyl)amino)quinolin-2-



yl)pyridine-3-sulfonamide (**6**)

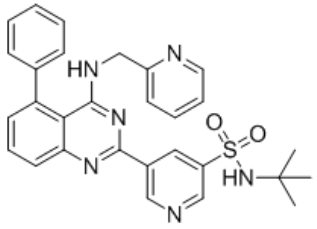


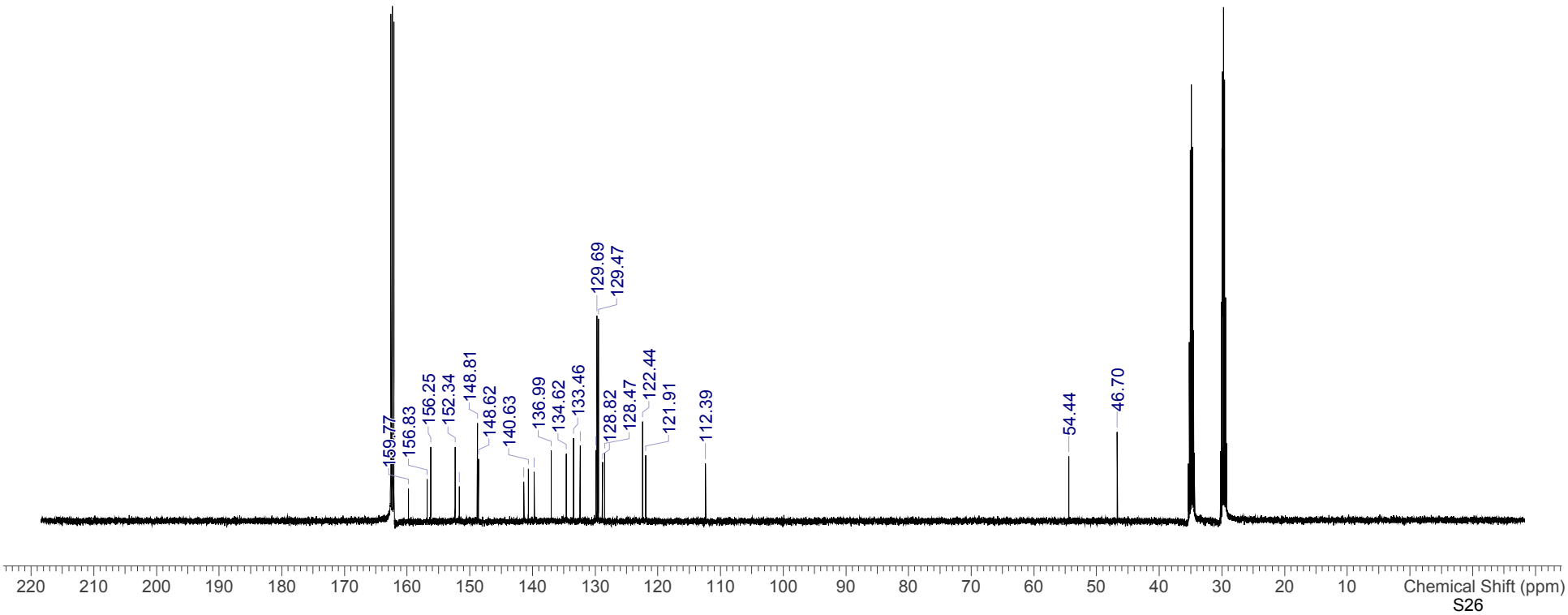
$^{1}$H NMR (500 MHz, DMF-d$_7$) of N-(tert-butyl)-5-(5-phenyl-4-((pyridin-2-ylmethyl)amino)quinazolin-2-



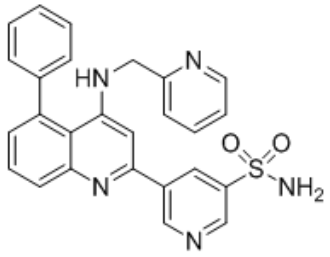

yl)pyridine-3-sulfonamide (**8**)

$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(5-phenyl-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**8**)

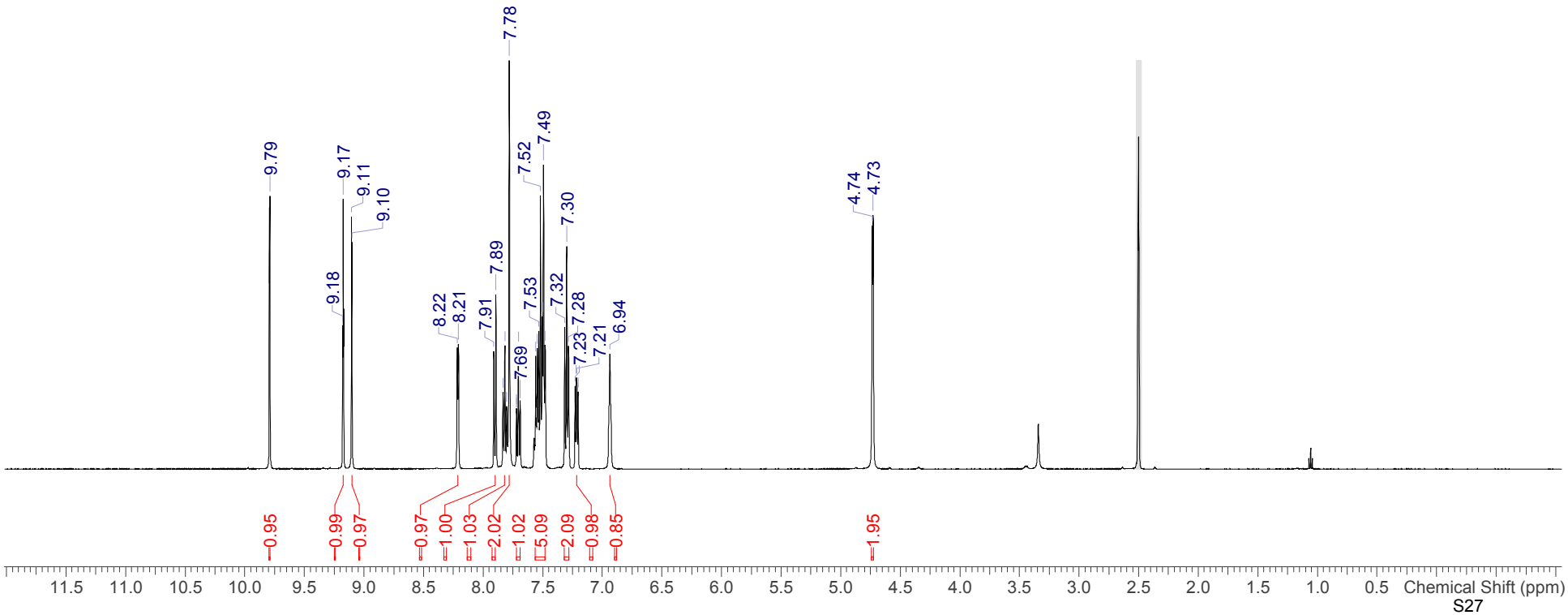


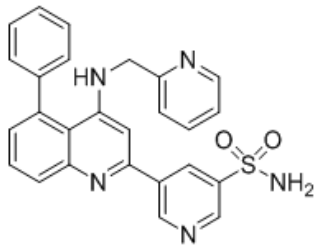
$^{1}$H NMR (500 MHz, DMSO-d$_6$) of 5-(5-phenyl-4-((pyridin-2-ylmethyl)amino)quinolin-2-yl)pyridine-3-



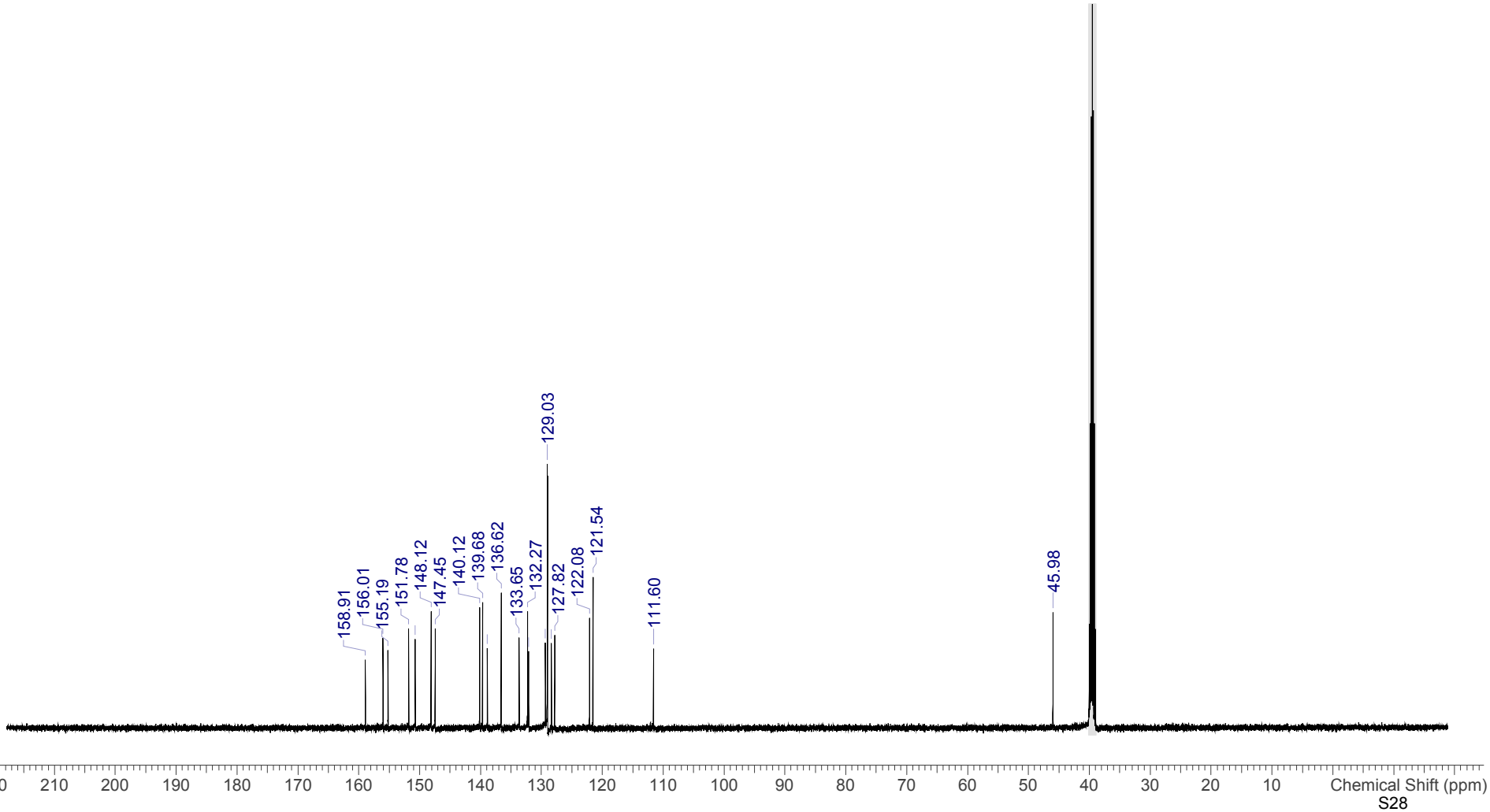

sulfonamide (**1**)



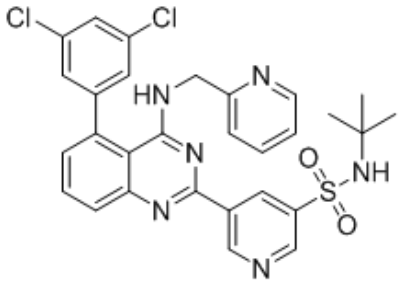
$^{13}C\{1H\}$NMR (125.8 MHz, DMSO-$d_6$) of 5-(5-phenyl-4-((pyridin-2-ylmethyl)amino)quinolin-2-yl)pyridine-3-



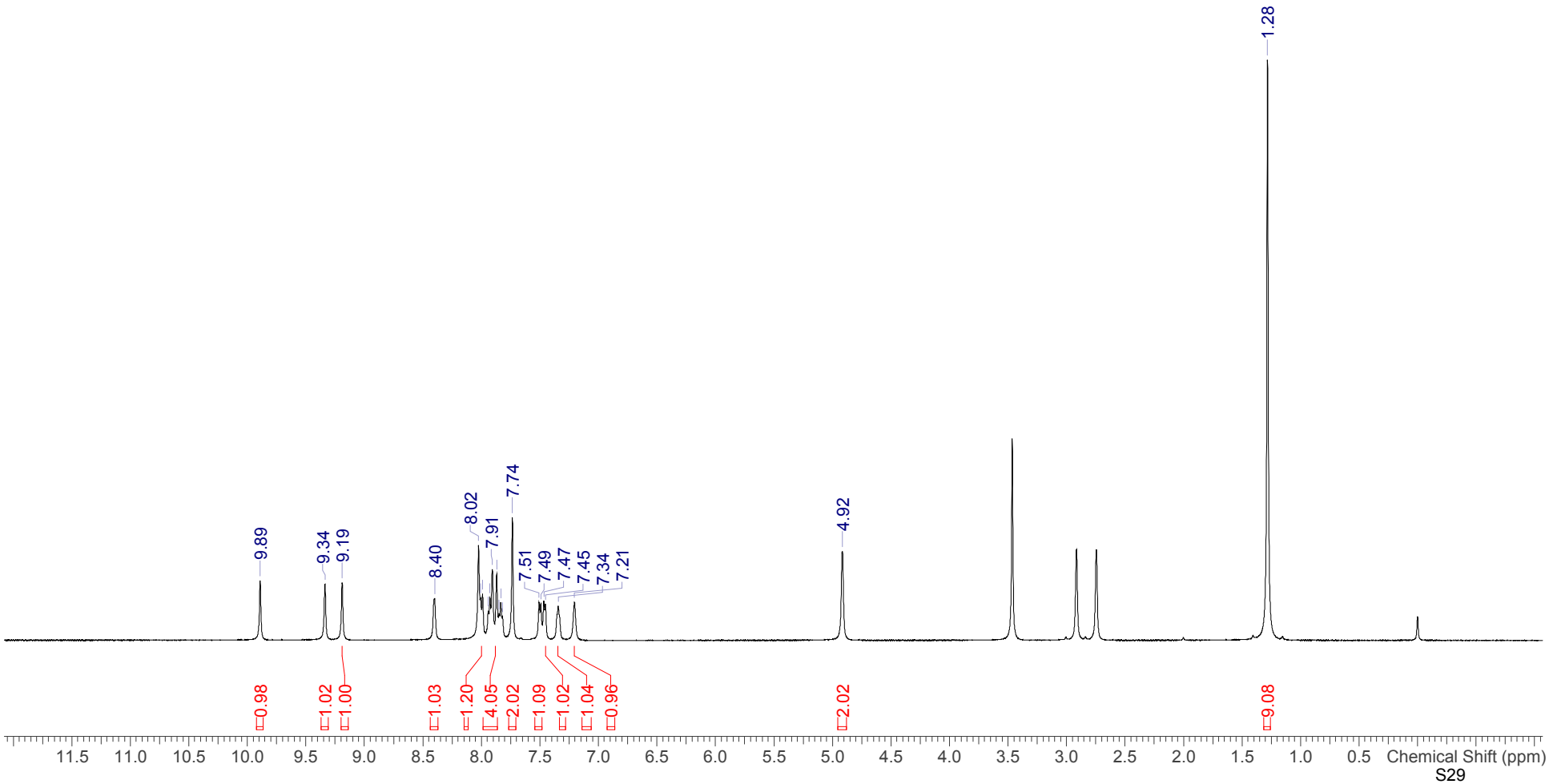

sulfonamide (**1**)



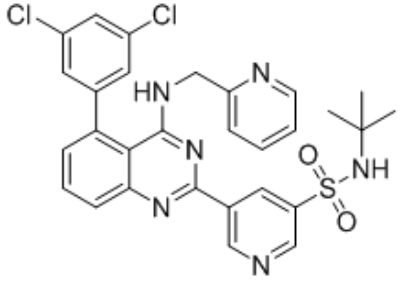
$^1$H NMR (500 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(5-(3,5-dichlorophenyl)-4-((pyridin-2-



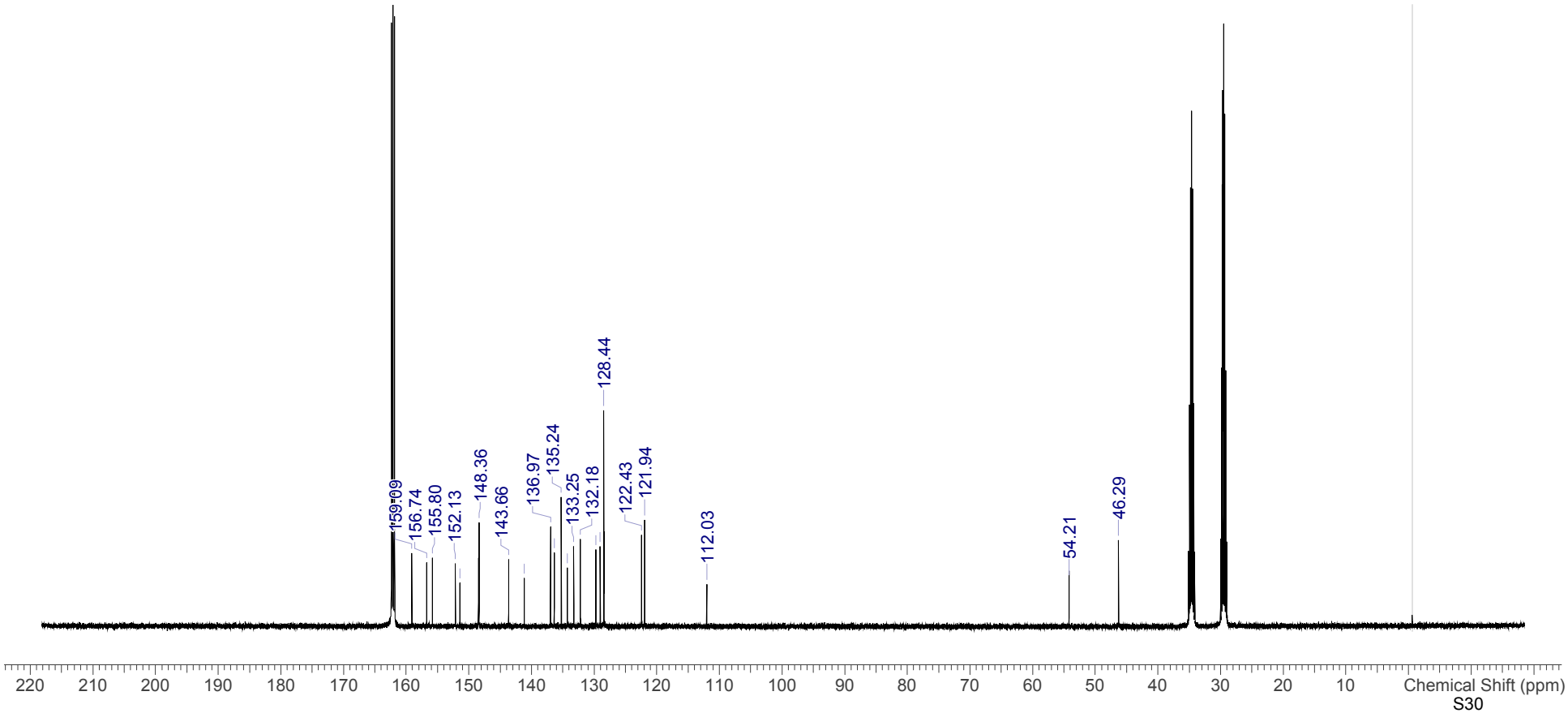

ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19a**)



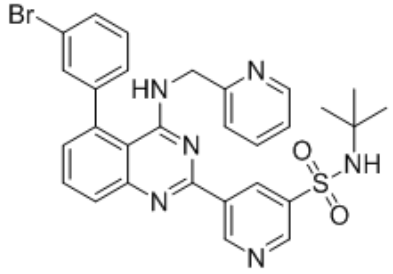
$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(5-(3,5-dichlorophenyl)-4-((pyridin-2-



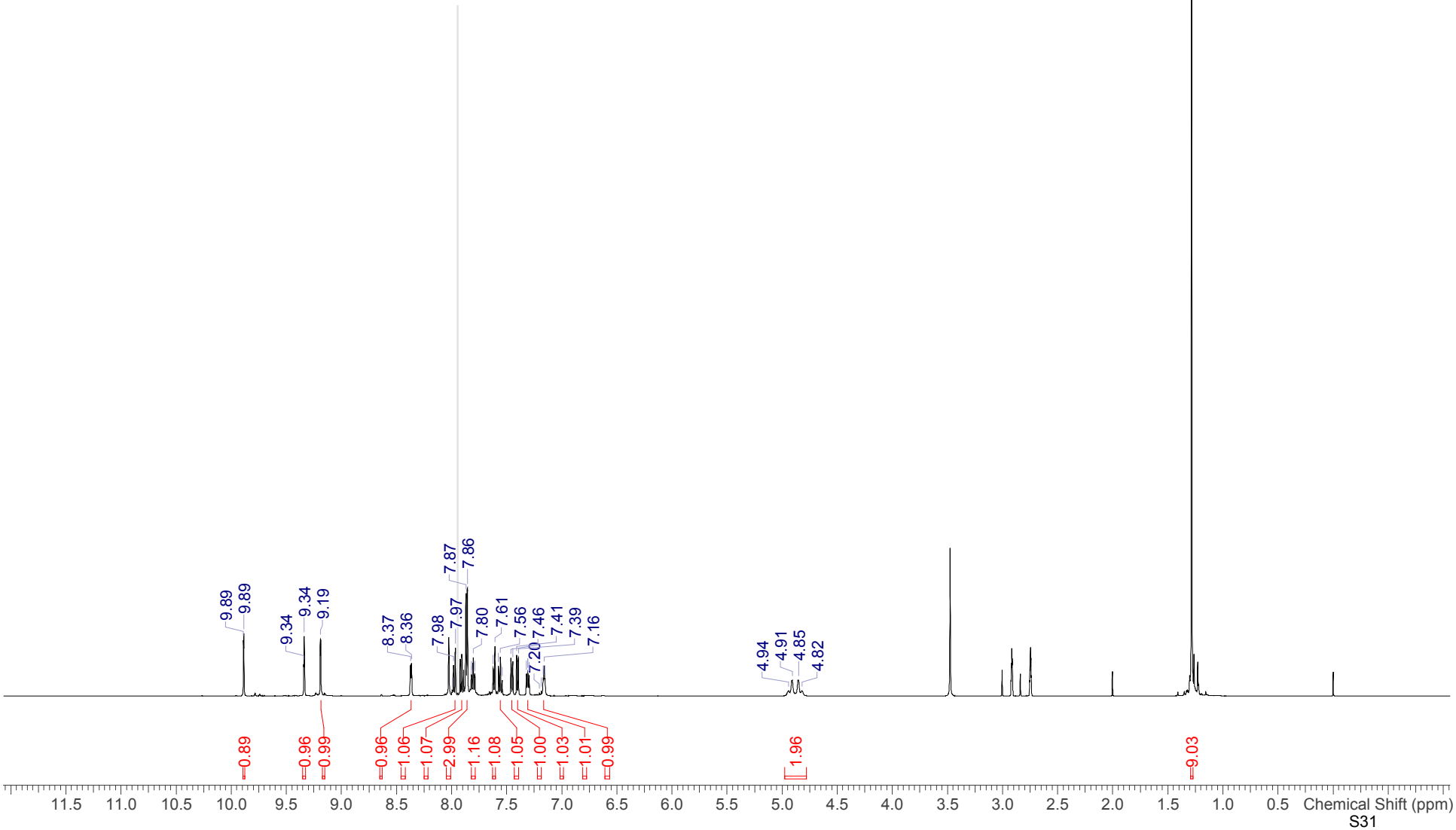

ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19a**)



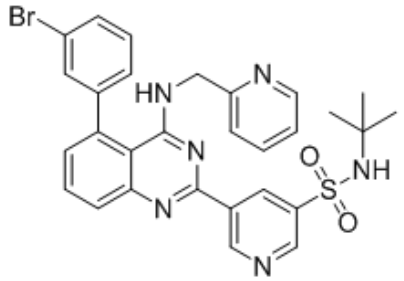
$^{1}$H NMR (500 MHz, DMF-$d_7$) of 5-(5-(3-bromophenyl)-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)-N-(tert-



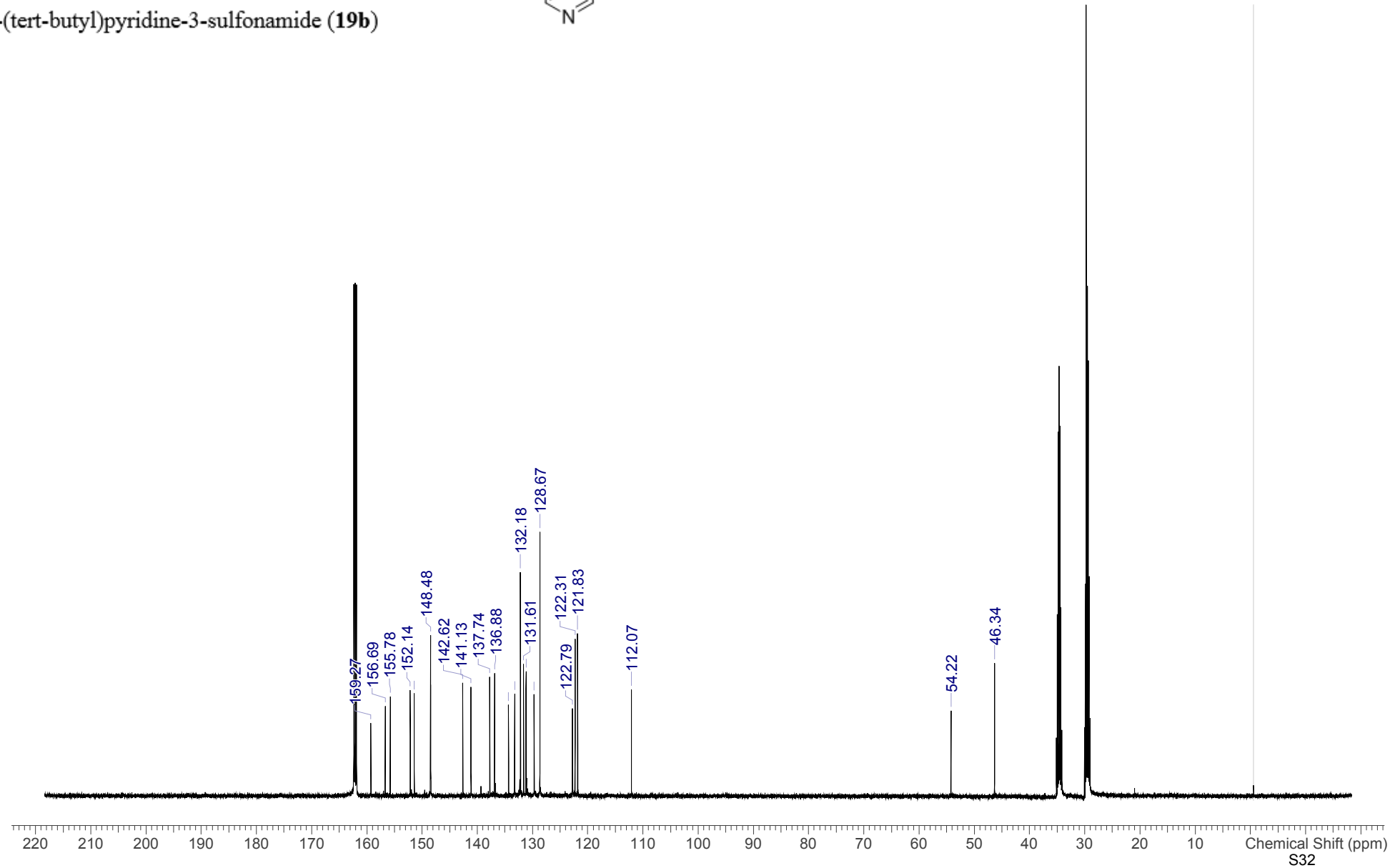

butyl)pyridine-3-sulfonamide (**19b**)



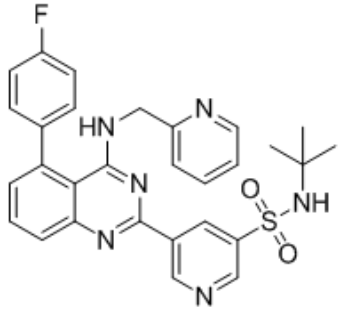
$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of 5-(5-(3-bromophenyl)-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)-



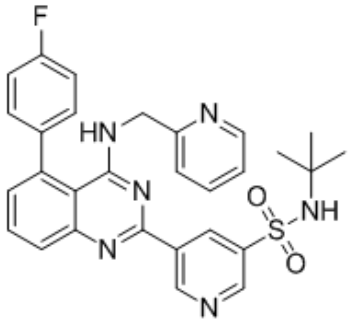

N-(tert-butyl)pyridine-3-sulfonamide (**19b**)

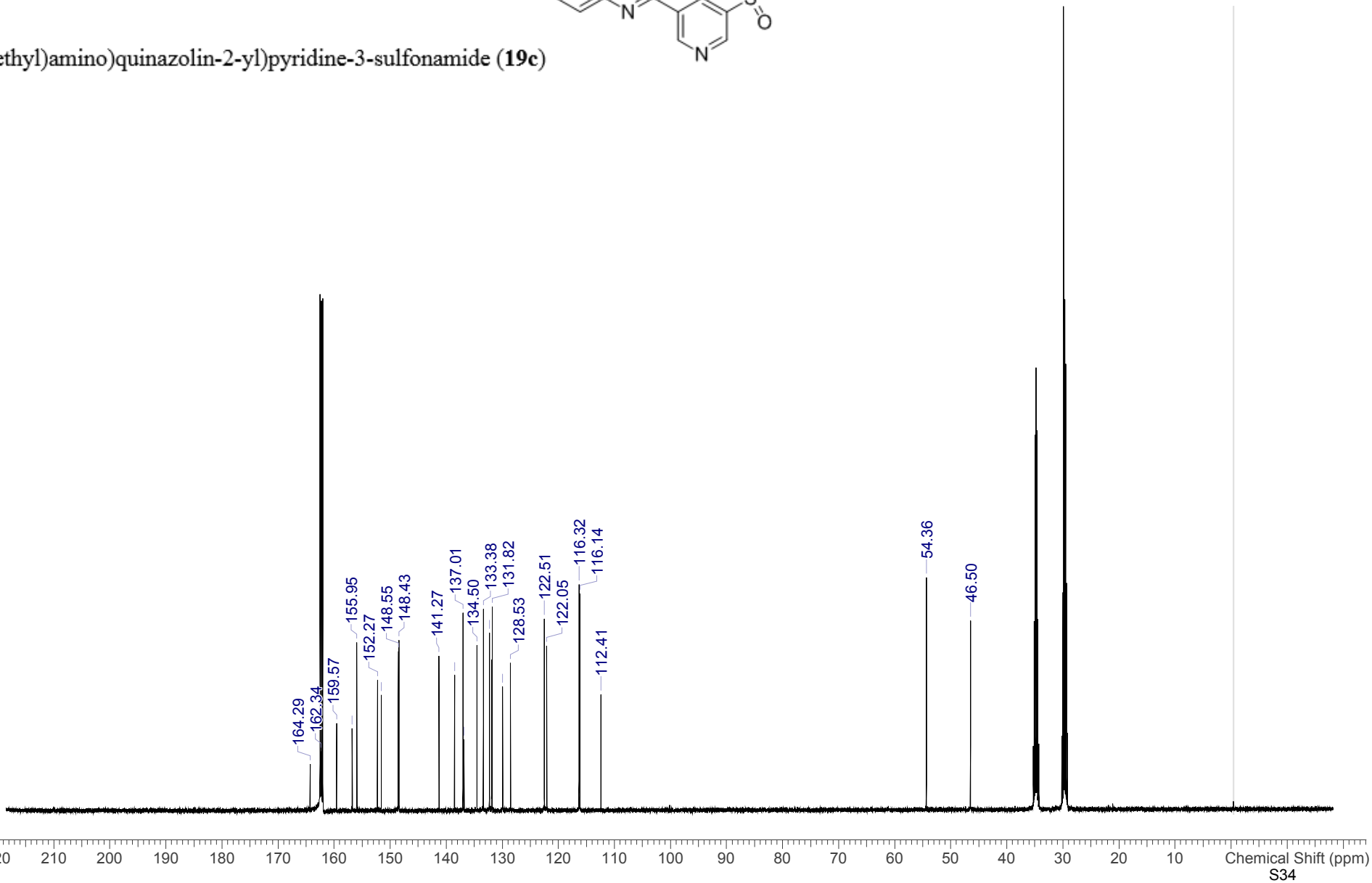


$^{1}$H NMR (500 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(5-(4-fluorophenyl)-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19c**)

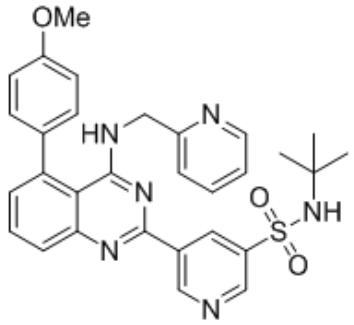


$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(5-(4-fluorophenyl)-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19c**)



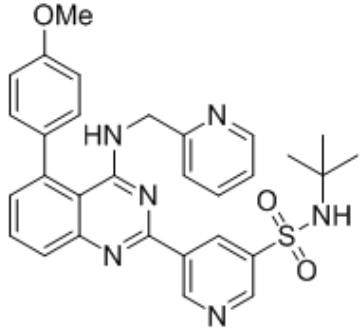



$^{1}$H NMR (500 MHz, DMF-d$_7$) of N-(tert-butyl)-5-(5-(4-methoxyphenyl)-4-((pyridin-2-

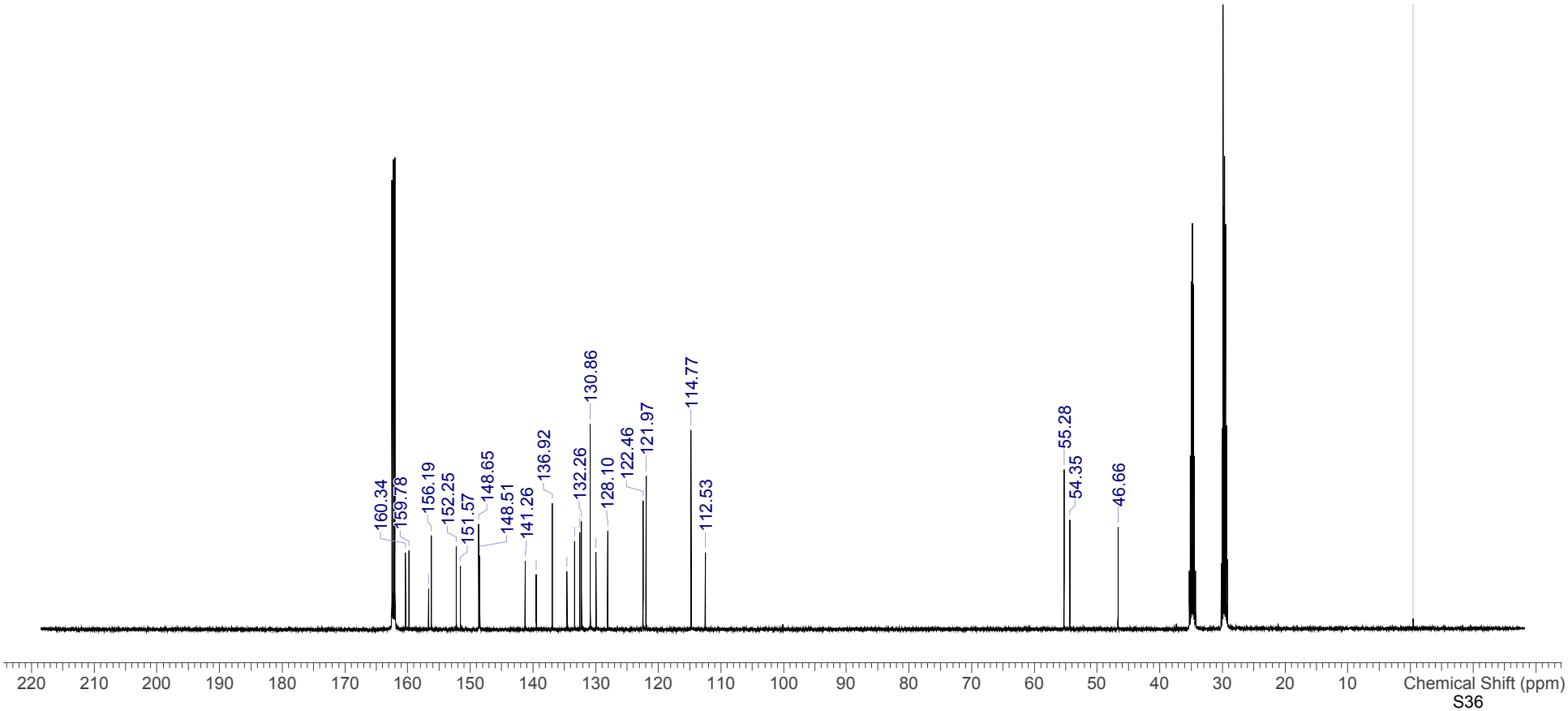



ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19d**)

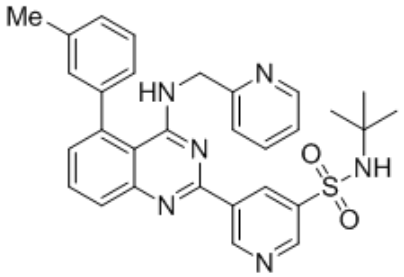
$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(5-(4-methoxyphenyl)-4-((pyridin-2-



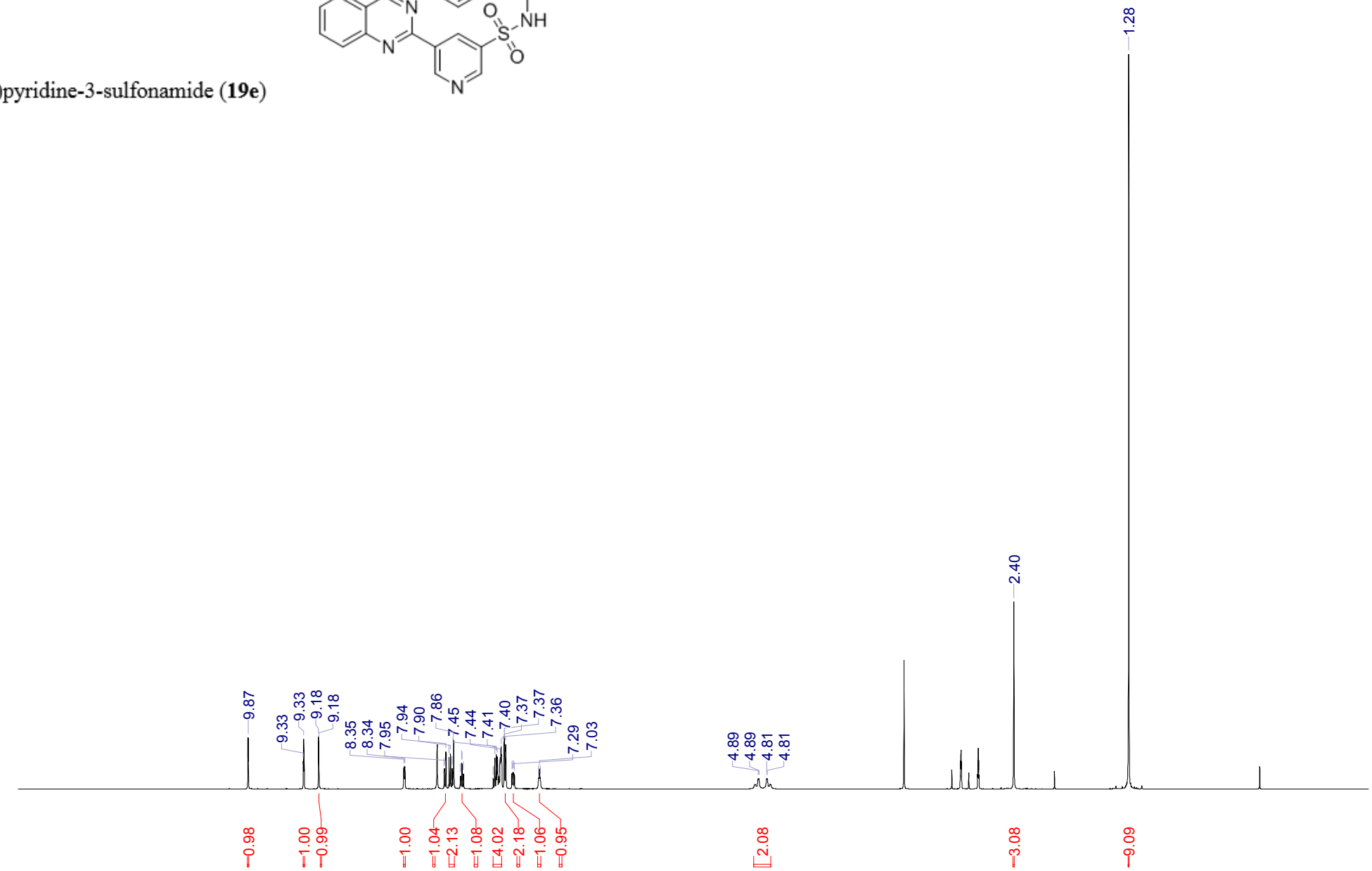

ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19d**)



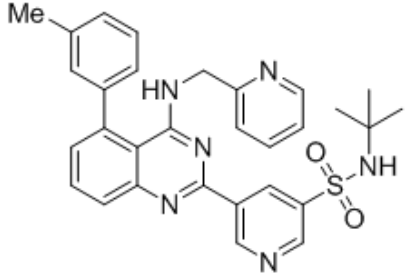
$^{1}$H NMR (500 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(4-((pyridin-2-ylmethyl)amino)-5-(m-tolyl)quinazolin-2-



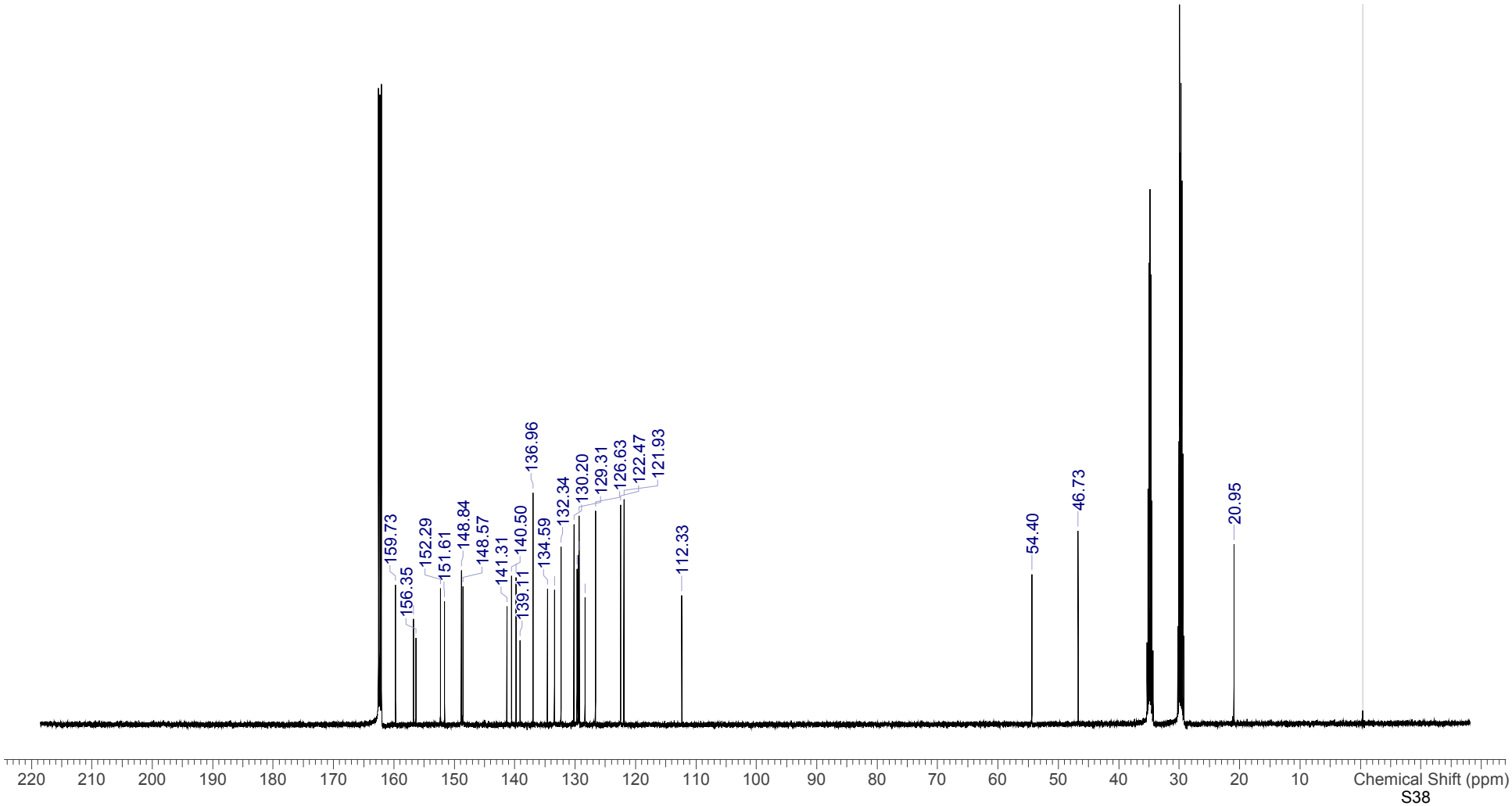

yl)pyridine-3-sulfonamide (**19e**)



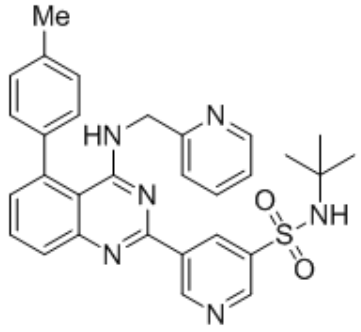
$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(4-((pyridin-2-ylmethyl)amino)-5-(m-tolyl)quinazolin-



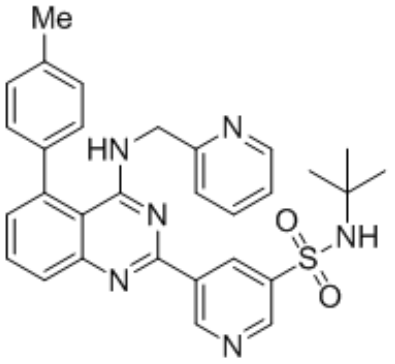

2-yl)pyridine-3-sulfonamide (**19e**)



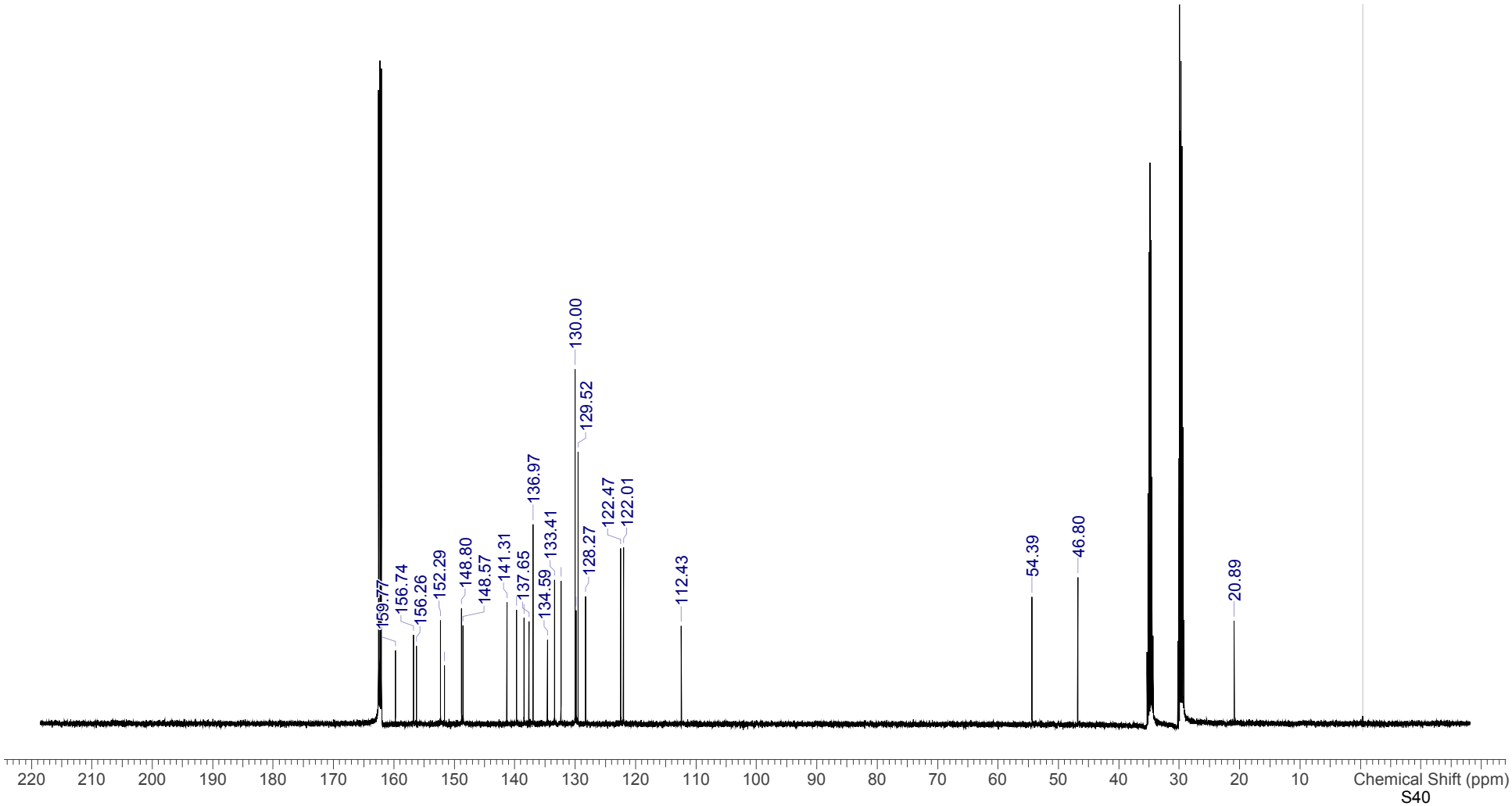
$^{1}$H NMR (500 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(4-((pyridin-2-ylmethyl)amino)-5-(p-tolyl)quinazolin-2-yl)pyridine-3-sulfonamide (**19f**)



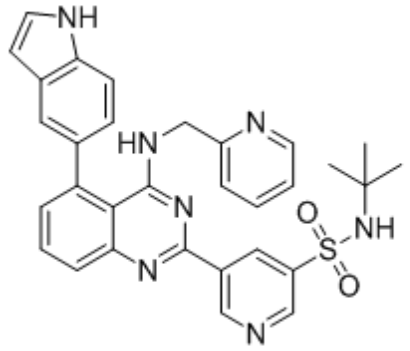
$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(4-((pyridin-2-ylmethyl)amino)-5-(p-tolyl)quinazolin-




2-yl)pyridine-3-sulfonamide (**19f**)

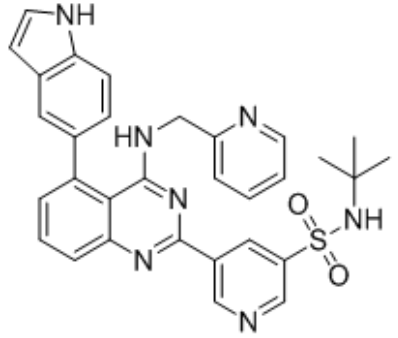


$^{1}$H NMR (500 MHz, DMF-d$_7$) of 5-(5-(1H-indol-5-yl)-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)-N-(tert-

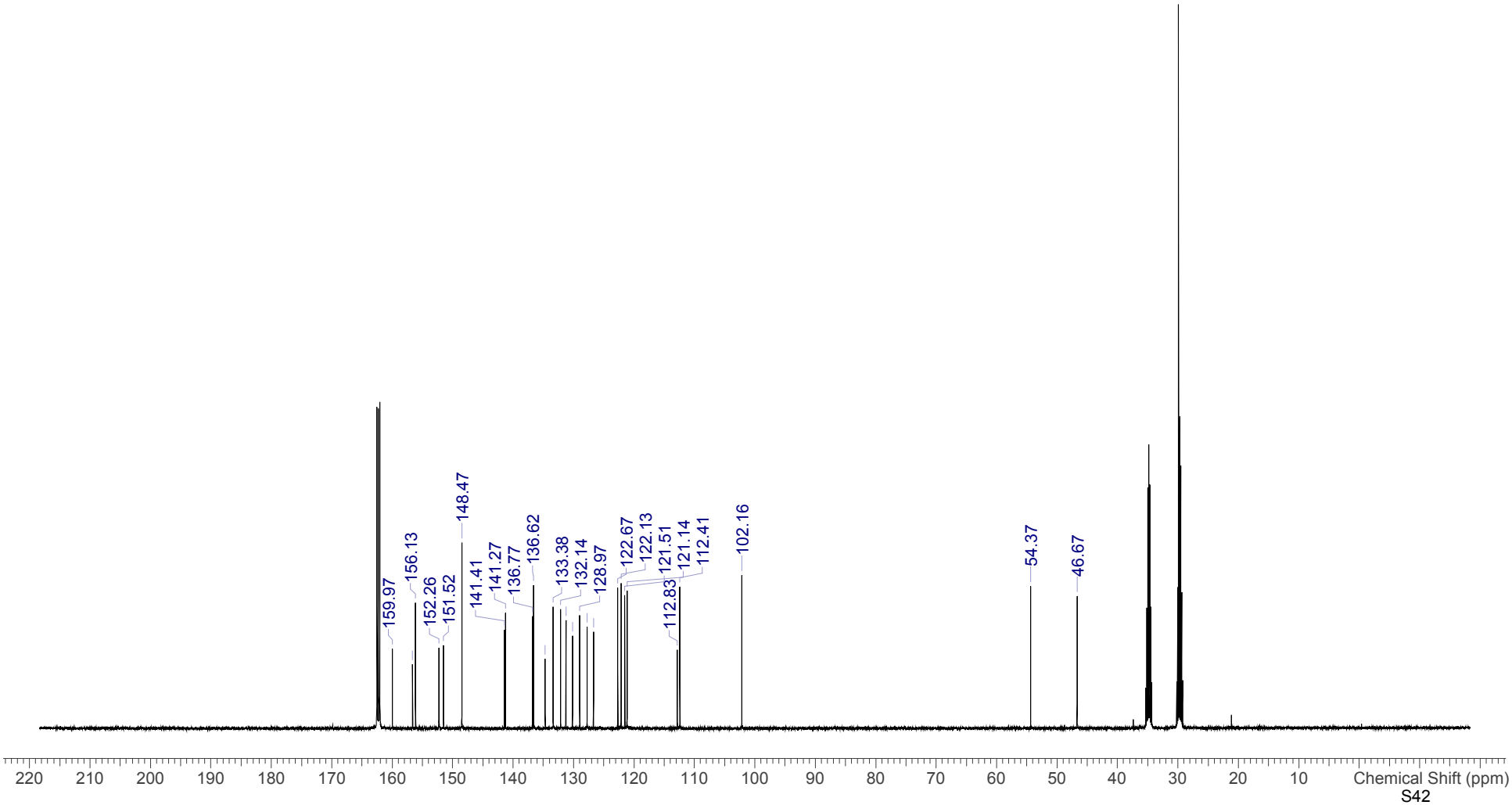



butyl)pyridine-3-sulfonamide (**19g**)

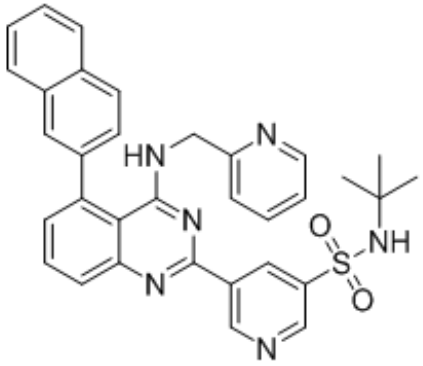
$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of 5-(5-(1H-indol-5-yl)-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)-

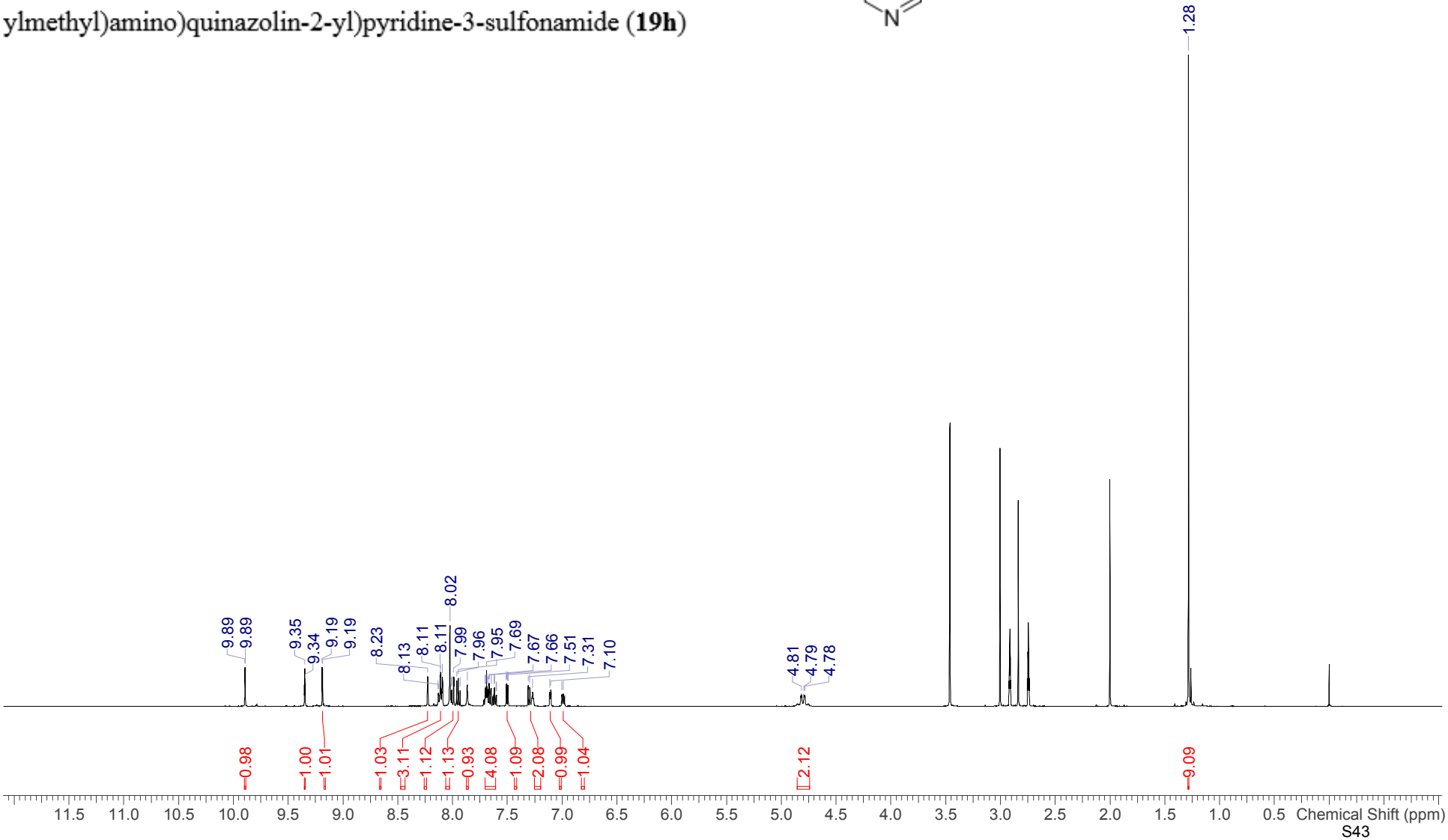



N-(tert-butyl)pyridine-3-sulfonamide (**19g**)

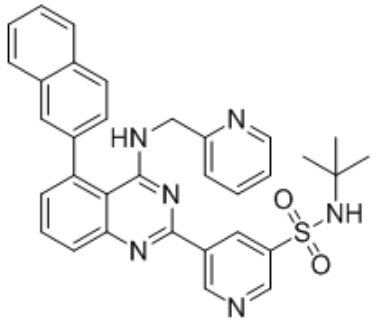


$^1$H NMR (500 MHz, DMF-d$_7$) of N-(tert-butyl)-5-(5-(naphthalen-2-yl)-4-((pyridin-2-ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19h**)

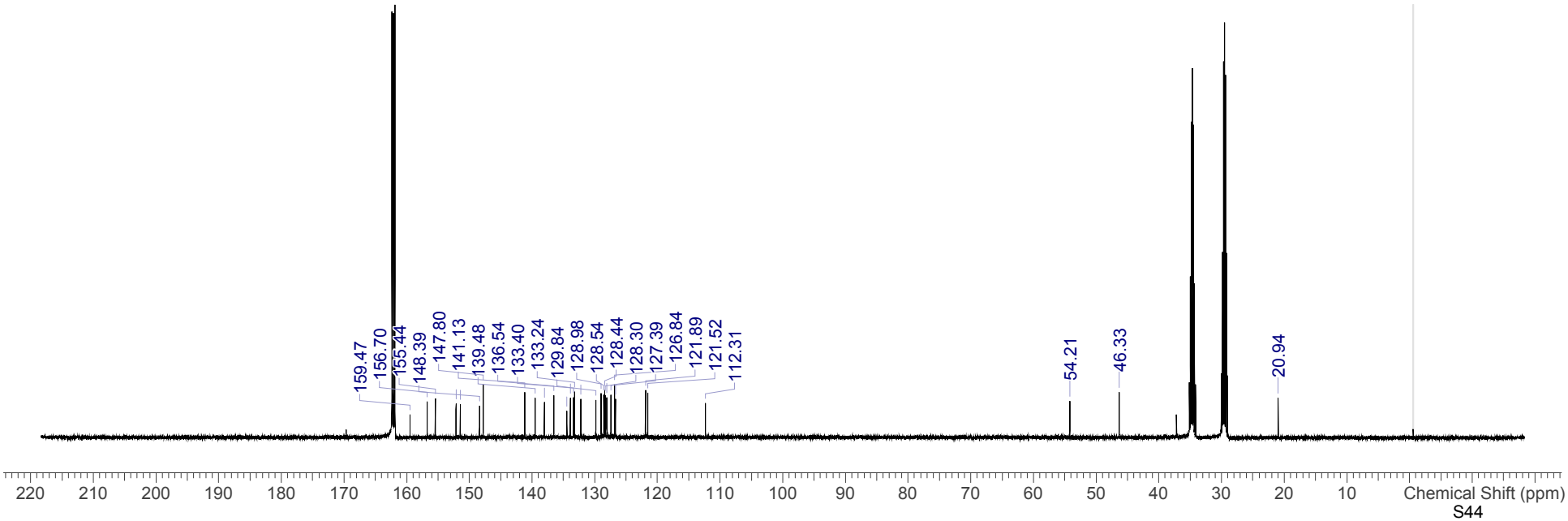


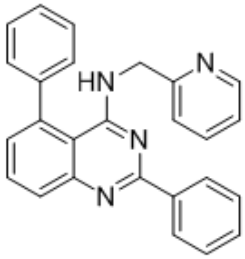
$^{13}C\{1H\}$NMR (125.8 MHz, DMF-$d_7$) of N-(tert-butyl)-5-(5-(naphthalen-2-yl)-4-((pyridin-2-

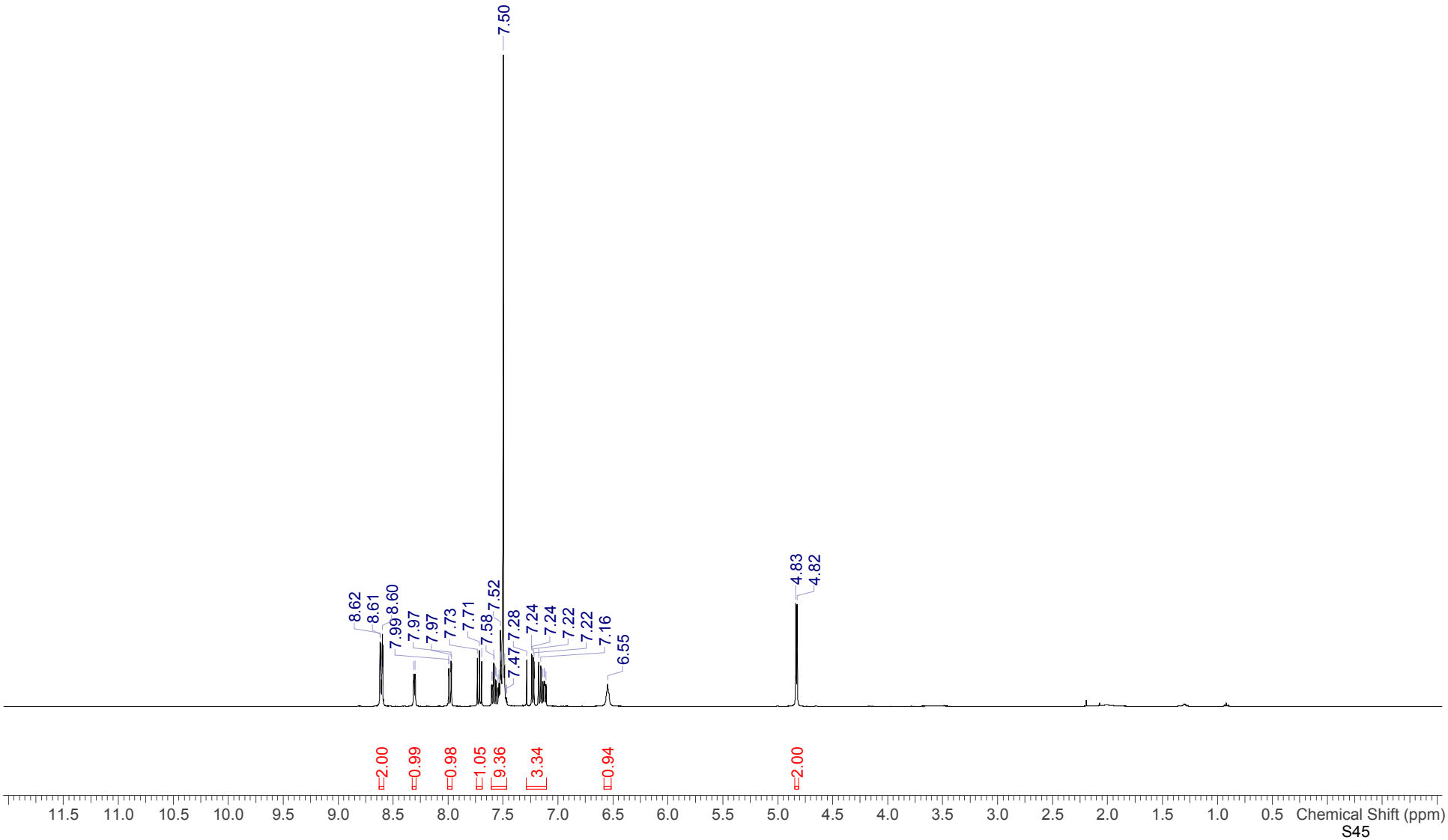



ylmethyl)amino)quinazolin-2-yl)pyridine-3-sulfonamide (**19h**)

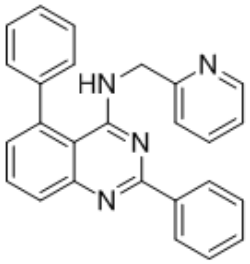


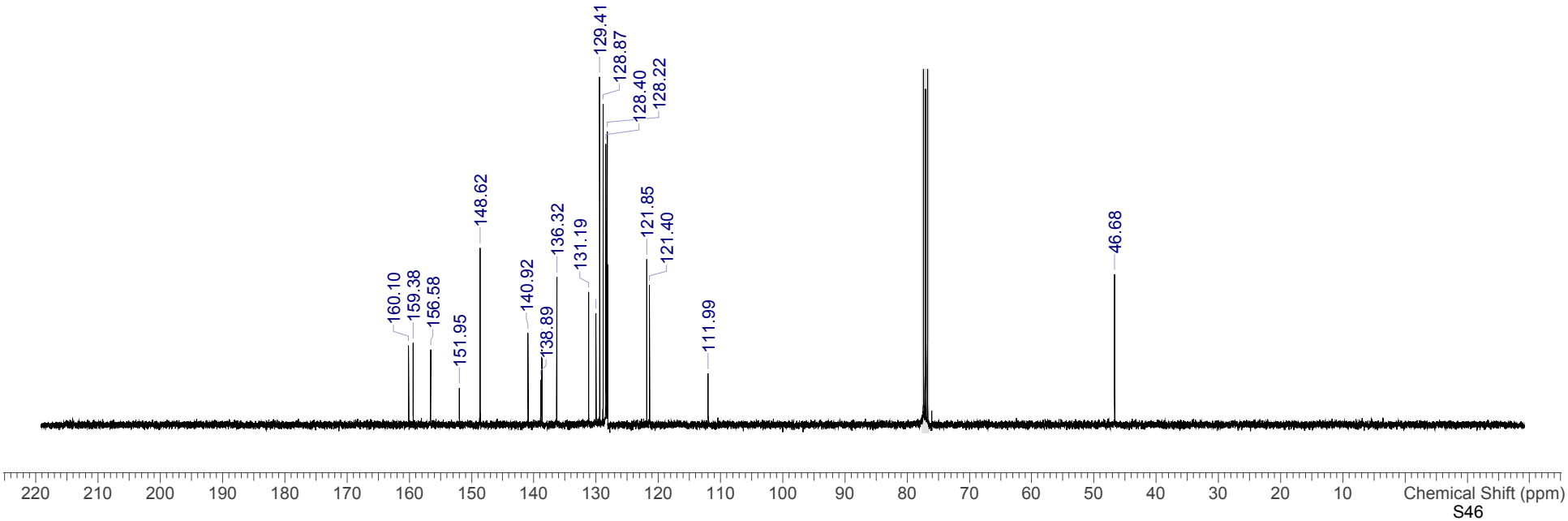
$^{1}$H NMR (400 MHz, $CDCl_3$) of 2,5-diphenyl-N-(pyridin-2-ylmethyl)quinazolin-4-amine (**20a**).



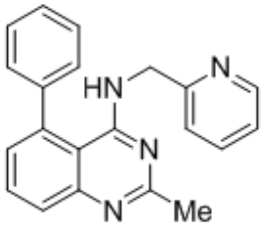



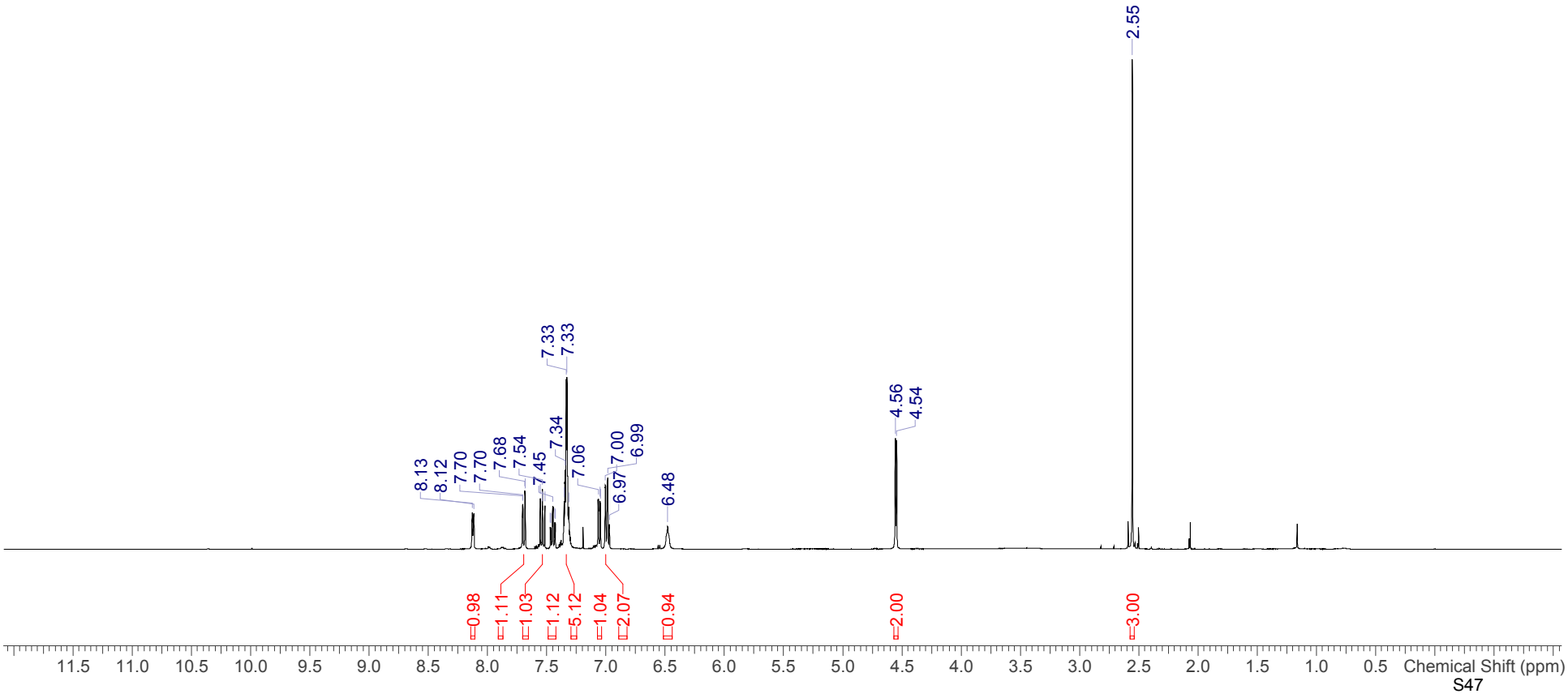
$^{13}C\{1H\}$NMR (125.8 MHz, $CDCl_3$) of 2,5-diphenyl-N-(pyridin-2-ylmethyl)quinazolin-4-amine (**20a**).



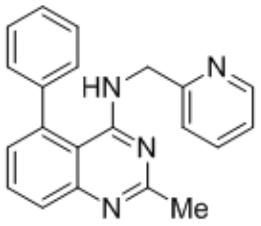



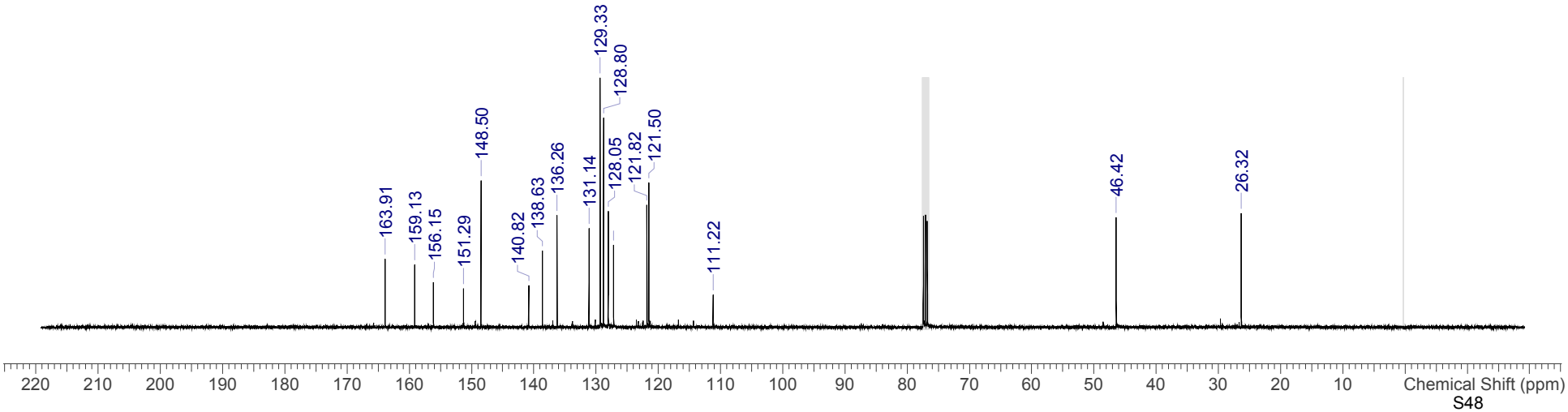
$^{1}$H NMR (400 MHz, $CDCl_3$) of 2-methyl-5-phenyl-N-(pyridin-2-ylmethyl)quinazolin-4-amine (**20b**)



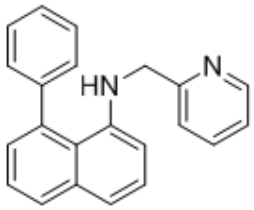



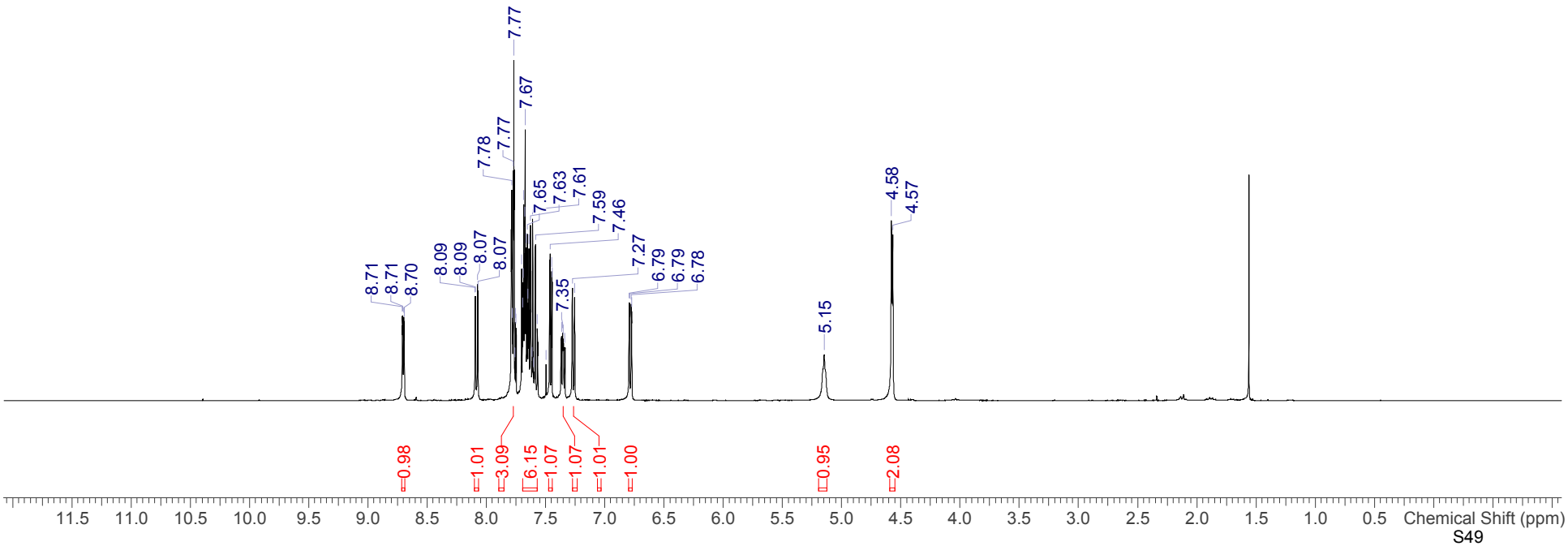
$^{13}C\{1H\}$NMR (125.8 MHz, $CDCl_3$) of 2-methyl-5-phenyl-N-(pyridin-2-ylmethyl)quinazolin-4-amine (**20b**)



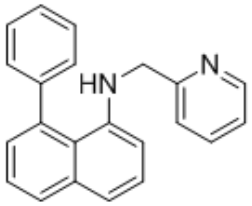



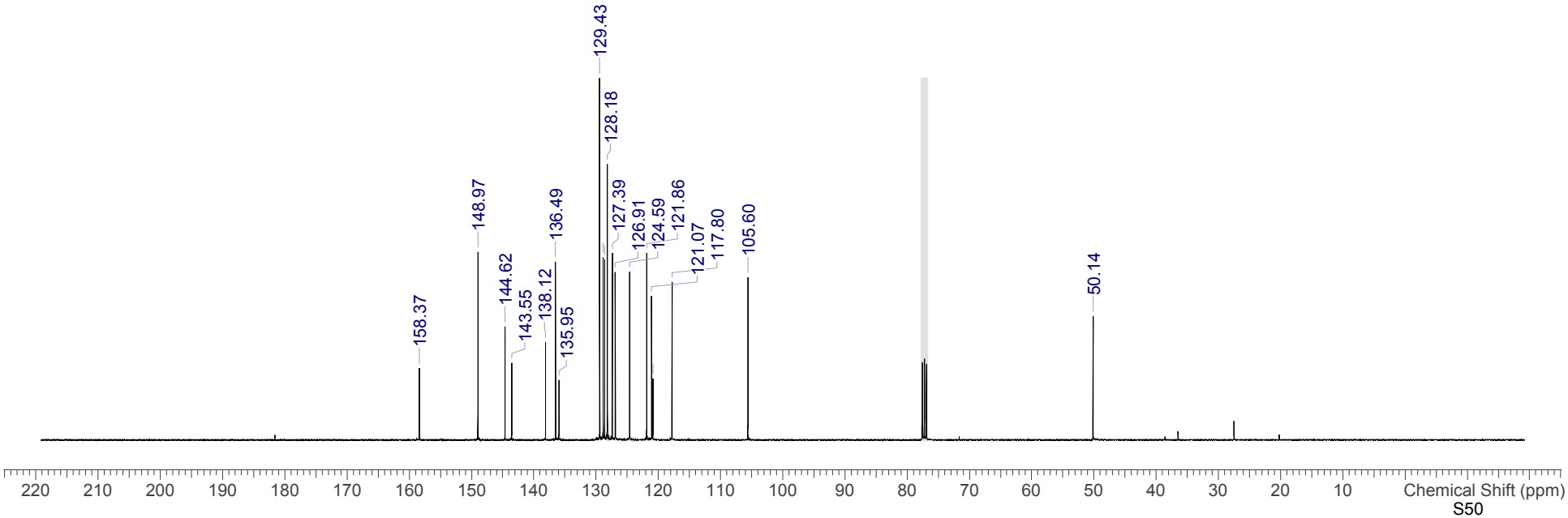
$^1$H NMR (400 MHz, $CDCl_3$) of 8-phenyl-N-(pyridin-2-ylmethyl)naphthalen-1-amine (**20c**)



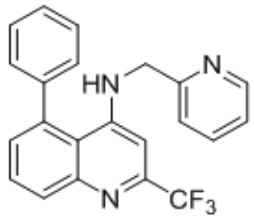



$^{13}C\{1H\}$NMR (125.8 MHz, $CDCl_3$) of 8-phenyl-N-(pyridin-2-ylmethyl)naphthalen-1-amine (**20c**)

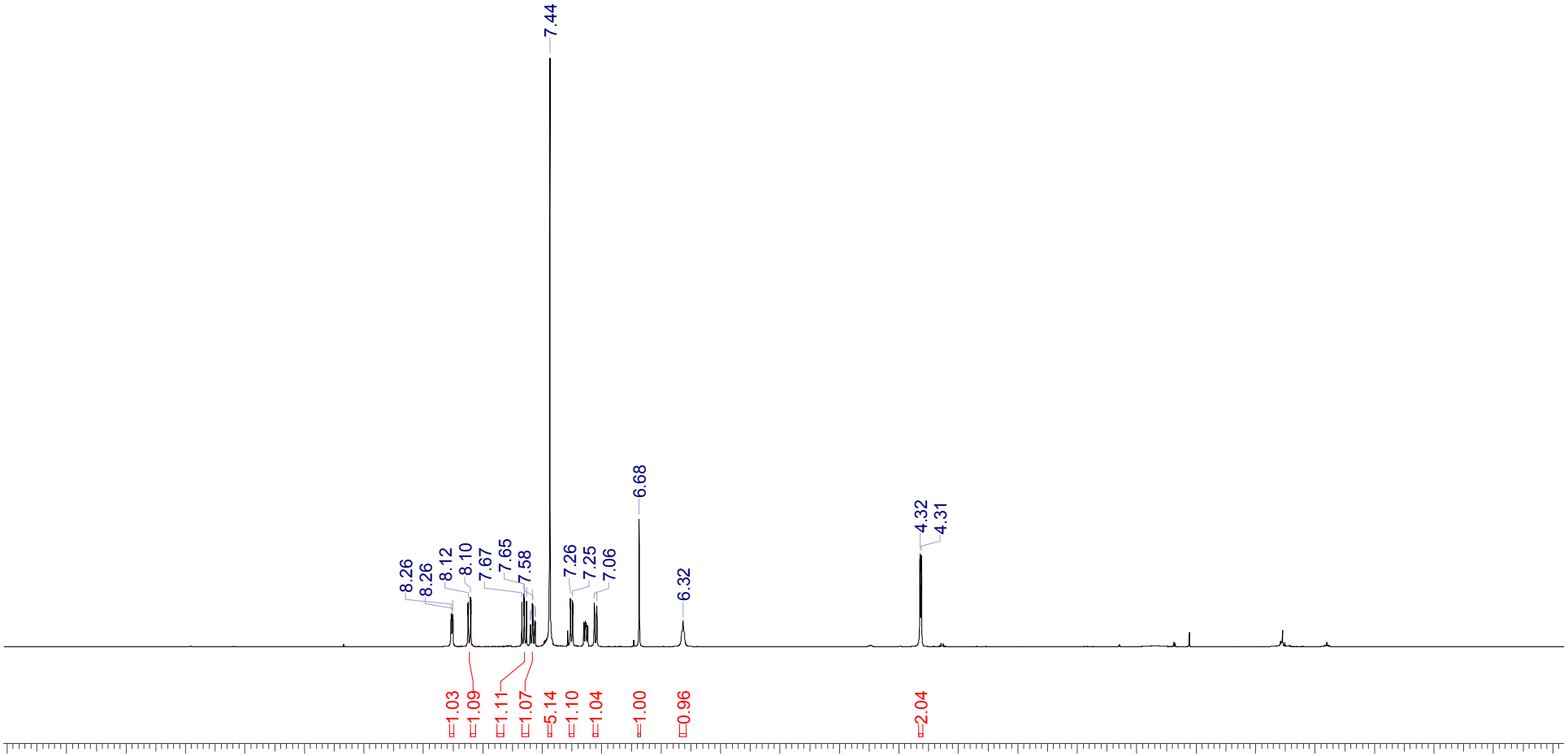


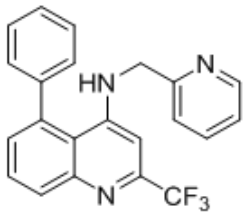
$^1$H NMR (400 MHz, $CDCl_3$) of 5-phenyl-N-(pyridin-2-ylmethyl)-2-(trifluoromethyl)quinolin-4-amine




(**20d**)



$^{13}C\{1H\}$NMR (125.8 MHz, $CDCl_3$) of 5-phenyl-N-(pyridin-2-ylmethyl)-2-(trifluoromethyl)quinolin-4-amine




(**20d**)