# Catalyst Selection Guide for Buchwald C–N Couplings

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| Substrate situation | Recommended Pd / ligand | Rationale | If it stalls… |
| Aryl iodide / easy bromide + aniline | Pd(OAc)₂ + XPhos | Largest dataset; broad scope. | Warm up or move to SPhos |
| Hindered secondary alkyl amine (Br/I) | Pd₂dba₃ + XPhos | 92% alkyl amines success. | For Cl halide → BrettPhos |
| Aryl chloride, moderate sterics | Pd(OAc)₂ + BrettPhos | Highest Cl success (42%). | Very hindered → tBuXPhos |
| Single‑ortho bromide + bulky amine | Pd(OAc)₂ + SPhos | Better with steric Br. | Double‑ortho → tBuXPhos |
| Tough Cl / double‑ortho | Pd₂dba₃ + tBuXPhos | Measurable double‑ortho hits. | Consider Ni if fails |
| Legacy simple anilines | Pd₂dba₃ + P(o‑Tol)₃ | Cheap, documented. | Upgrade to biaryl phosphine |

## Decision Checklist

* Halide: I/Br (easy) → XPhos; tough Br → SPhos; Cl → BrettPhos/tBuXPhos.
* Amine: hindered secondary alkyl → XPhos or BrettPhos; primary aniline → XPhos.
* Sterics: single‑ortho Br → SPhos; double‑ortho/Cl → tBuXPhos.
* Cost: P(o‑Tol)₃ + Pd₂dba₃ fine for simple Br/I on small scale.