# Amine-Type Distribution vs Catalyst Combination (Ullmann Dataset)

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| --- | --- | --- | --- | --- | --- | --- | --- |
| Catalyst combo | Reactions | primary\_alkyl % | primary\_aryl % | secondary\_alkyl % | secondary\_aryl % | tertiary\_alkyl % | tertiary\_aryl % |
| 7681-65-4 | 371 | 0.0 | 0.0 | 2.7 | 0.0 | 0.0 | 2.2 |
| 147-85-3 + 7681-65-4 | 109 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.9 |
| 66-71-7 + 7681-65-4 | 99 | 0.0 | 0.0 | 0.0 | 0.0 | 9.1 | 0.0 |
| 110-70-3 + 7681-65-4 | 85 | 0.0 | 0.0 | 9.4 | 0.0 | 2.4 | 0.0 |
| 7787-70-4 | 74 | 0.0 | 0.0 | 2.7 | 0.0 | 1.4 | 0.0 |
| 7440-50-8 | 58 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1317-39-1 | 53 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 2903-48-2 + 7681-65-4 | 42 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 110-18-9 + 7681-65-4 | 41 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1317-38-0 | 40 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 2.5 |
| 51-35-4 + 7681-65-4 | 36 | 0.0 | 0.0 | 0.0 | 0.0 | 2.8 | 0.0 |
| 1127-45-3 + 7787-70-4 | 36 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1121-22-8 + 7681-65-4 | 33 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1118-71-4 + 7681-65-4 | 33 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 67579-81-1 + 7681-65-4 | 32 | 0.0 | 0.0 | 0.0 | 0.0 | 3.1 | 3.1 |
| 110-70-3 + 1317-39-1 | 32 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1317-39-1 + 92149-07-0 | 30 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 39207-65-3 + 7681-65-4 | 28 | 0.0 | 0.0 | 0.0 | 0.0 | 3.6 | 0.0 |
| 106129-86-6 + 7681-65-4 | 27 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 614-65-3 + 7681-65-4 | 24 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 107-15-3 + 7681-65-4 | 22 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1317-39-1 + 66-71-7 | 21 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 30754-24-6 + 7681-65-4 | 21 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 25322-68-3 + 7681-65-4 | 20 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1655-07-8 + 7787-70-4 | 19 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 602-09-5 + 7681-65-4 | 19 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1118-68-9 + 7681-65-4 | 18 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 107-97-1 + 7681-65-4 | 18 | 0.0 | 0.0 | 100.0 | 0.0 | 0.0 | 0.0 |

## Key Take-aways

* Primary amines are virtually absent across all catalyst systems in this corpus.
* CuI alone (7681‑65‑4) couples a small set of secondary alkyl (≈3 %) and tertiary aryl (≈2 %) amines.
* Phenanthroline‑ligated CuI (66‑71‑7 + CuI) skews strongly toward tertiary alkyl amines (≈9 %).
* Diamine‑ligated CuI (110‑70‑3 + CuI) shows the highest share of secondary alkyl amines (~9 %).
* The mixed CuCl / TMEDA / CuI system (CuCl+TMEDA+CuI) is the only one with measurable double‑ortho reactivity and handles the broadest amine set (secondary alkyl ≈11 %, tertiary aryl ≈6 %).