Supplementary Material

New Bidentate N-Sulfonyl-Substituted Aromatic Amines as Chelate Ligand Backbones: Pd Catalyst Generation in C-C Coupling via In Situ and Precatalyst Modes


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Fig. S1: An illustration of the peaks at around 4.4 ppm utilized for estimation of catalytic yield.

It is important to clarify that the 1H triplet signal of the bromobenzenealcohol at about 5.3 ppm (bottom spectra) belongs to the OH function and caused the corresponding splitting of its neighbouring –CH₂– group at about 4.4 ppm. Due to fast proton exchange interactions, this methanoyl OH signal as well as the splitting of the –CH₂– is often not observed as is the case for the resultant reaction mixtures after reflux (middle and top spectra). The broad signal of the OH can be seen in the middle and top spectra without splitting.
**Fig. S2**: Comparison of reaction mixture spectra for Heck coupling in the presence of the ligand free Pd(OAc)$_2$ with the starting materials (styrene and bromobenzenemethanol).

It is important to clarify that the 1H triplet signal of the bromobenzenealcohol at about 5.3 ppm (bottom spectra of **Fig. S2**) belongs to the OH function and caused the corresponding splitting of its neighbouring –CH$_2$– group at about 4.4 ppm. Due to fast proton exchange interactions, this methanolyl OH signal as well as the splitting of the –CH$_2$– is often not observed as is the case for the resultant reaction mixture after reflux (topmost spectra).