Design of Experiment Optimisation of the Suzuki Cross-Coupling: A Synthesis of Biphenyl, Catalysed by Palladium Tetrakis, from Phenylboronic Acid and Bromobenzene

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The Suzuki reaction is a widely used method for forming carbon-carbon bonds in organic synthesis. The palladium-catalysed reaction are highly successful due to the high reactivity of boranes, which in turn allows for lower catalyst loading. Furthermore, organoboranes are nontoxic and highly stable and can be worked with at benchtop in a one-pot set up. This reduces the amount of waste and the high atom economy increases reaction efficiency. However, the reaction can be sensitive to various conditions, such as temperature, solvent, and catalyst. In order to optimize the reaction, a Design of Experiments (DOE) approach was used. By using DOE, it is possible to identify the optimal conditions for the Suzuki reaction in an efficient and cost-effective manner. This resulted in improved yield and selectivity, as well as a better understanding of the underlying mechanisms of the reaction. This experiment observes three experimental factors for optimization: residence time, temperature, and catalyst loading. The hypothesis was proven as the yield of biphenyl was the highest when the greatest parameters of reaction temperature, residence time, and catalyst loading were reached. The highest approximate yield was 90% and can be attributed to a temperature of 100 degrees Celsius, 6 hours, and a catalyst load of 5 milligrams. The integrated fluorescence intensity was also highest for these figures, which corresponds to the yield. This experimentation would thus be reliable for an optimization of the Suzuki Cross Coupling in the synthesis of biophenyl. Reaching maximum efficacy could lower the cost of producing pharmaceuticals by millions in large scale production.

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