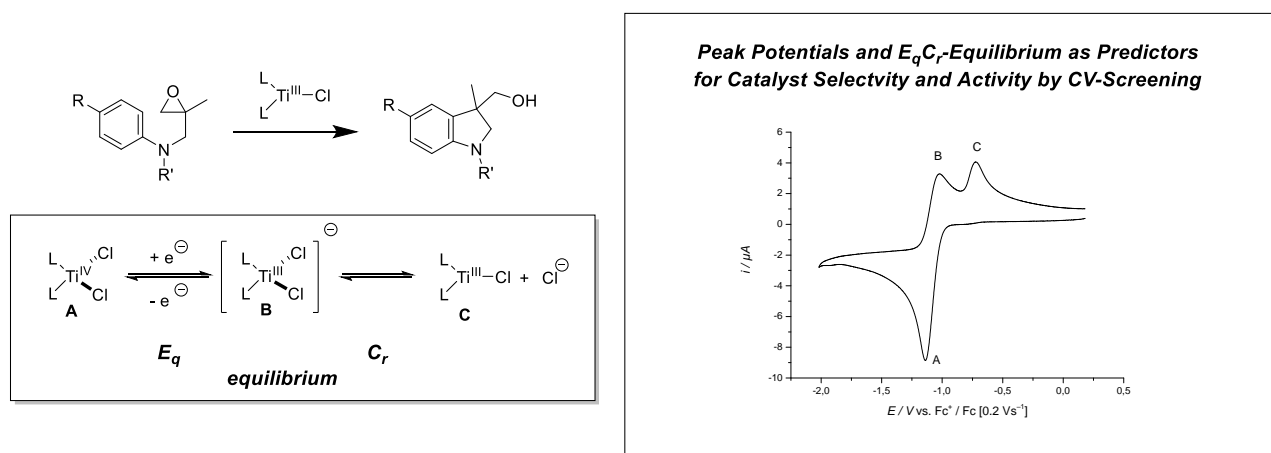


# Discovery of new catalysts for the radical arylation reaction by predictor-based cyclic voltammetry (CV) screening

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The radical arylation reaction with titanocene halides suffers mainly from two aspects. Firstly, electron poor titanocenes are required to facilitate the rate determining step of the reaction.<sup>1</sup> This requires additional synthetic effort to modify the electronic properties of the titanocene complexes for substrates with electron-deficient arenes. The second aspect is the requirement of halide abstracting supramolecular H-bond donors especially during electrochemical reduction of titanocene halides.<sup>2</sup> Cyclic voltammetry can visualize these properties in the form of peak potentials for the different species that are present during catalysis. These peak-potentials as well as the position of the  $E_qC_r$  equilibrium<sup>2</sup> can be used as predictors for the efficiency of catalysis for this system. Our CV screening, by employing those predictors, is advantageous to classical methods, since only the catalysts are required, saving time and resources. This makes the whole process more sustainable and more efficient.



**Figure 1.** Predictor-based CV-screening approach for the radical arylation reaction.

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2 T. Liedtke, T. Hilche, S. Klare, A. Gansäuer, *ChemSusChem*, **2019**, 12, 3166.