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Improving sustainability in the construction of conjugated molecular scaffolds: ionic liquids and (waste)water as solvents

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The synthesis of highly conjugated molecular scaffolds, relevant for applications in optoelectronics and organic electronics, is often performed through Pd-catalysed direct C–H arylation.[1] As highlighted in a recent review,[2] a major critical point in the sustainability of direct C–H arylations is represented by their high *E*-factor values, mainly related to the amount of solvent employed in the process, whose nature should likewise not be overlooked. In this framework, we present here our work on the C–H arylation of thiophene derivatives in two non-conventional solvents, namely water and glycerol-based ionic liquids. In the first case, the use of water allows to streamline the post-reaction treatment, significantly improving the mass-related *green* metrics; moreover, we show that the yield is not dependent on the purity grade of the water, allowing the use of industrial wastewater, thus reducing the environmental impact of the methodology.[3] On the other hand, we show that the thoughtful design of a new ionic liquid, containing a carboxylate anion, eliminates the need to add a super-stoichiometric amount of base, and in addition it enables the successful reuse of the reaction medium for five cycles, again improving the mass efficiency of the process.

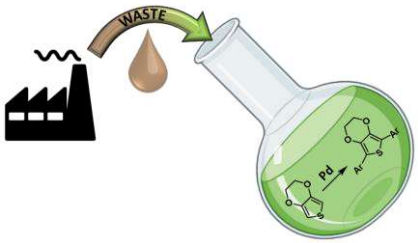

Figure 13. Industrial wastewater as an effective solvent for Pd-catalysed C–H arylation

References:
[1] I. A. Stepek, K. Itami, *ACS Materials Lett.* **2020**, *2*, 951–974
[2] F. Ferlin, G. Brufani, G. Rossini, L. Vaccaro, *Green Chem.* **2023**, *25*, 7916–7933
[3] S. Nejrotti, B. Centrella, D. Gallo, C. Barolo, M. Bonomo, *Green Chem.* **2024**, *26*, 7013–7018