

# Environmentally Friendly Homocoupling Reaction of Functionalized Potassium Aryltrifluoroborates Salts in Aqueous Media

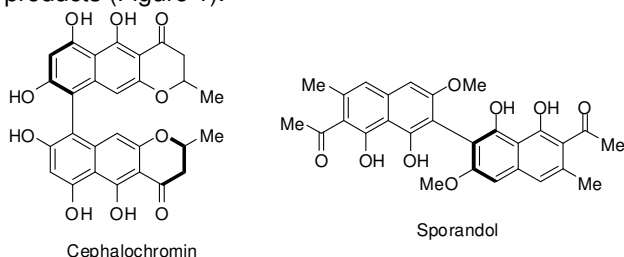
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## INTRODUCTION

The biaryl bond is present in a wide range of natural products (Figure 1).



**Figure 1:** Biaryl natural products

In addition, the widespread application of biaryls as ligands and components in new materials make these compounds interesting synthetic targets.

Herein, we wish to describe an environmentally benign reaction for the synthesis of symmetrical biaryl compounds based on the palladium (II) catalyzed homocoupling of potassium aryl trifluoroborates under aerobic conditions.<sup>2</sup>

## RESULTS AND DISCUSSION

Our initial studies focused on the development of an optimum set of reaction conditions. For this purpose, potassium 3-formylphenyl trifluoroborate (**2a**) was used as standard substrate. The results are depicted in Table 1

**Table 1:** Optimization of reaction conditions.

	Catalyst (mol %)	Solvent	Yield (%) <sup>a</sup>
1	Pd(OAc) <sub>2</sub> (5)	H <sub>2</sub> O	82
2	PdCl <sub>2</sub> (5)	H <sub>2</sub> O	80
3	Pd(OAc) <sub>2</sub> (15)	H <sub>2</sub> O	84
4	-	H <sub>2</sub> O	5
5	Pd(OAc) <sub>2</sub> (5)	H <sub>2</sub> O:THF (1:1)	85
6	Pd(OAc) <sub>2</sub> (5)	THF	- <sup>b</sup>
7	Pd(OAc) <sub>2</sub> (5)	H <sub>2</sub> O	50 <sup>c</sup>

<sup>a</sup> Isolated yield; <sup>b</sup> The product was not observed under the reaction conditions; <sup>c</sup> The reaction was performed without K<sub>2</sub>CO<sub>3</sub>.

By extending the optimum set of conditions for the coupling reaction to other potassium aryl trifluoroborates, various biaryls were obtained in moderate to good yields (Table 2).

**Table 2:** Ar-Ar (**2**) prepared from the homocoupling reaction of ArBF<sub>3</sub>K (**1**) catalyzed by Pd(OAc)<sub>2</sub>

		Pd(OAc) <sub>2</sub> K <sub>2</sub> CO <sub>3</sub> , H <sub>2</sub> O, 25°C, 24h	Ar-Ar <b>2</b>	Yield (%) <sup>a</sup>
	ArBF <sub>3</sub> K, <b>1</b>			
1	3-CHO			82
2	2-CHO			80
3	4-CHO			80
4	3-CN			75
5	3-NO <sub>2</sub>			70
6	3,5-(CF <sub>3</sub> ) <sub>2</sub>			85
8	2,6-(Me) <sub>2</sub>			80 <sup>b</sup>
9	3-Th			75

<sup>a</sup> Isolated yield.

## CONCLUSION

In summary, we have demonstrated that the potassium aryl trifluoroborates are useful substrates for the synthesis of biaryl compounds in good yields and under mild conditions. The green methodology is simple, uses water as solvent, low catalyst loadings, and is synthetically useful while it could be applied for the synthesis of more complex biaryl compounds.

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## REFERENCES

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