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## Synthesis of 2-phenyl-1H-benzo[d]imidazole-derived fluorescent Gquadruplexes ligands

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## ABSTRACT

This work presents the unprecedented results of the synthesis, structural characterization and determination of the photophysical properties of a series of 1-ethyl-2-aryl-1H-benzo[d]imidazoles iodide salts with potential application as fluorescent ligands for G-quadruplexes. The products were obtained by a condensation reaction of benzene-1,2-diamine with substituted benzaldehydes (1a-e) and two subsequent alkylations, obtaining the compounds (3a-e, 4a). The synthetic route and the yield of products 3a-e and 4a are shown in Scheme 1. The UV-vis emission properties were investigated, all compounds absorbed in the ultraviolet region presenting fluorescence. Thermal stability was evaluated by thermogravimetric analysis and the results are shown in **Table 1**. The chemical structure of the compounds was determined by <sup>1</sup>H, <sup>13</sup>C NMR and two-dimensional experiments: COSY, HSQC, HMBC.

Scheme 1. Synthesis of salts derived from 1-ethyl-2-phenyl-1H-benzo[d]imidazole.



**Table 1.** Decomposition temperature  $(T_d)$  and melting point  $(T_m)$  of compounds **3a-e** and **4a**.

Compound	<b>T</b> d <sup>a</sup> (°C)	T <sub>m</sub> <sup>b</sup> (°C)	Compound	T <sub>d</sub> ª (°C)	Т <sub>m</sub> <sup>b</sup> (°С)
3a	261	198	3d	270	160
3b	233	150	3e	266	244
3c	273	171	4a	243	248

<sup>a</sup>Decomposition temperature. <sup>b</sup>Melting temperature.

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- SHI, Hong et al. Synthesis and Optical Properties of Novel Fluorescence-Traced Benzimidazolium Bromides. Journal of 1. Heterocyclic Chemistry, v. 51, n. S1, p. E71-E76, 2014.
- LEE, Ye-Sol et al. Significant facilitation of metal-free aerobic oxidative cyclization of imines with water in synthesis of 2. benzimidazoles. Tetrahedron, v. 71, n. 4, p. 532-538, 2015.
- 3. VARSHNEY, Dhaval et al. The regulation and functions of DNA and RNA G-quadruplexes. Nature reviews Molecular cell biology, v. 21, n. 8, p. 459-474, 2020.