Synthesis of imidazoles and imidazolines from 1,2-diamines and ethyl (*E*)- and (*Z*)-3-aryl-3-chloro-2-cyanopropenoates

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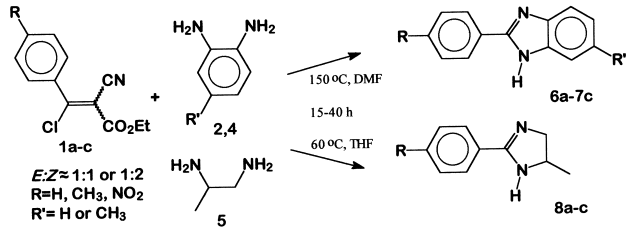
Ethyl (*E*)- and (*Z*)-3-aryl-3-chloro-2-cyanopropenoates react stereoselectively with 1,2-diamines at room temperature to give ethyl (*Z*)-3-(2-aminophenylamino)-3-aryl-2-cyanopropenoates, whereas at higher temperatures cyclisation takes place and imidazoles and imidazolines are formed in moderate to high yields.

Keywords: benzimidazoles, imidazolines, 3-chloro-2-cyanocinnamates

Several molecules containing imidazole,[4] imidazoline[5] or dibenzodiazepine[9] ring systems have proven to be pharmaceutically active. Imidazoles,[15] imidazolines[17] and dibenzodiazepines[21] have earlier been synthesised starting from 1,2-disubstituted diamines. In the present study, we have synthesised some new 2-arylbenzimidazoles **(6a–7c)** and 2-arylimidazolines **(8a–c)**. (Table 1, Scheme 1)



Scheme 1

Table 1 Yields of the reaction products (6a-8c)

Product	R	R′	Yield/%
6a	H	H	88
6b	CH_3	H	86
6c	NO_2	H	95
7a	H	CH_3	66
7b	CH_3	CH_3	90
7c	NO_2	CH_3	92
8a	H		82
8b	CH_3		90
8c	NO_2		73

When analysing the imidazoles and imidazolines by ^{13}C-NMR at room temperature a tautomeric effect was observed and the imidazole and imidazoline carbon signals were observed as multiplets in some spectra. When the analyses were carried out at –40°C, all carbon signals could be observed. By adding a small amount of trifluoroacetic acid (TFA) to the samples sharp peaks were observed at room temperature.

Techniques used: IR, ^{1}H-NMR, ^{13}C-NMR, HRMS

References: 28

Tables: 2

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