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Sterol C(14)-demethylase inhibitors as fungicides for use in crop protection

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π-fungicides play an important role in controlling diseases in crops. A particular important class of fungicides are the sterol C(14) demethylase inhibitors, which inhibit the oxidative demethylation of C(14) during the fungal biosynthesis of ergosterol. This talk will discuss design and synthesis of molecules acting as inhibitors of the involved cytochrome P450, 'CYP51'. In the first part of the talk, the synthetic access to pyridyl-isoxazole derivatives will be presented, with a focus on the efficient synthesis of the isoxazole ring. In the second part of the talk CH-pi interactions between C(14) demethylase inhibitors and the enzyme will be discussed and inhibitors which could engage in stronger CH-pi contacts and therefore more selective binding to the targeted P450 will be presented.