

# Theoretical study of the regioselective cyclization of enaminones in the construction of benzofurans and indoles

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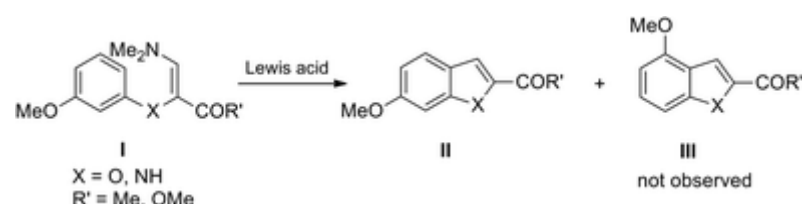
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## Abstract

A theoretical study was undertaken regarding the regioselective Lewis acid-promoted intramolecular cyclization of novel enaminones **1-3** leading to the corresponding benzofurans **4-5** and indoles **6**. The density functional theory (DFT) and hard and soft acids and bases (HSAB) principle provided data to describe the electronic effects of the substituents in the reactivity of the benzene ring and the enaminone moiety. The condensed and local Fukui functions for nucleophilic and electrophilic attacks of the reactants accounted for the experimentally observed preference, in regard to precursors **1-3**, of the cyclization between the C6' carbon (rather than the C2' carbon) of the benzene ring and the C3 center of the enaminone moiety.



Graphical Abstract

A theoretical study (DFT/HSAB) describes the electronic effects of the substituents in the reactivity of the benzene ring and the enaminone moiety of enaminones **I** to explain their Lewis acid-promoted regioselective intramolecular cyclization, which exclusively leads to the corresponding benzofurans and indoles **II**

## Keywords

Cyclization DFT/HSAB theory Enaminones Fukui function Lewis acid catalysis

## Electronic supplementary material

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## Notes

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## Supplementary material

894\_2016\_2985\_MOESM1\_ESM.doc (1.2 mb)

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