

**XX** REUNIÓN NACIONAL DE  
ESPECTROSCOPIA

**IV** CONGRESO IBÉRICO DE  
ESPECTROSCOPIA



***LIBRO DE RESÚMENES***

**Ciudad Real, 10 – 14 de Septiembre de 2006**



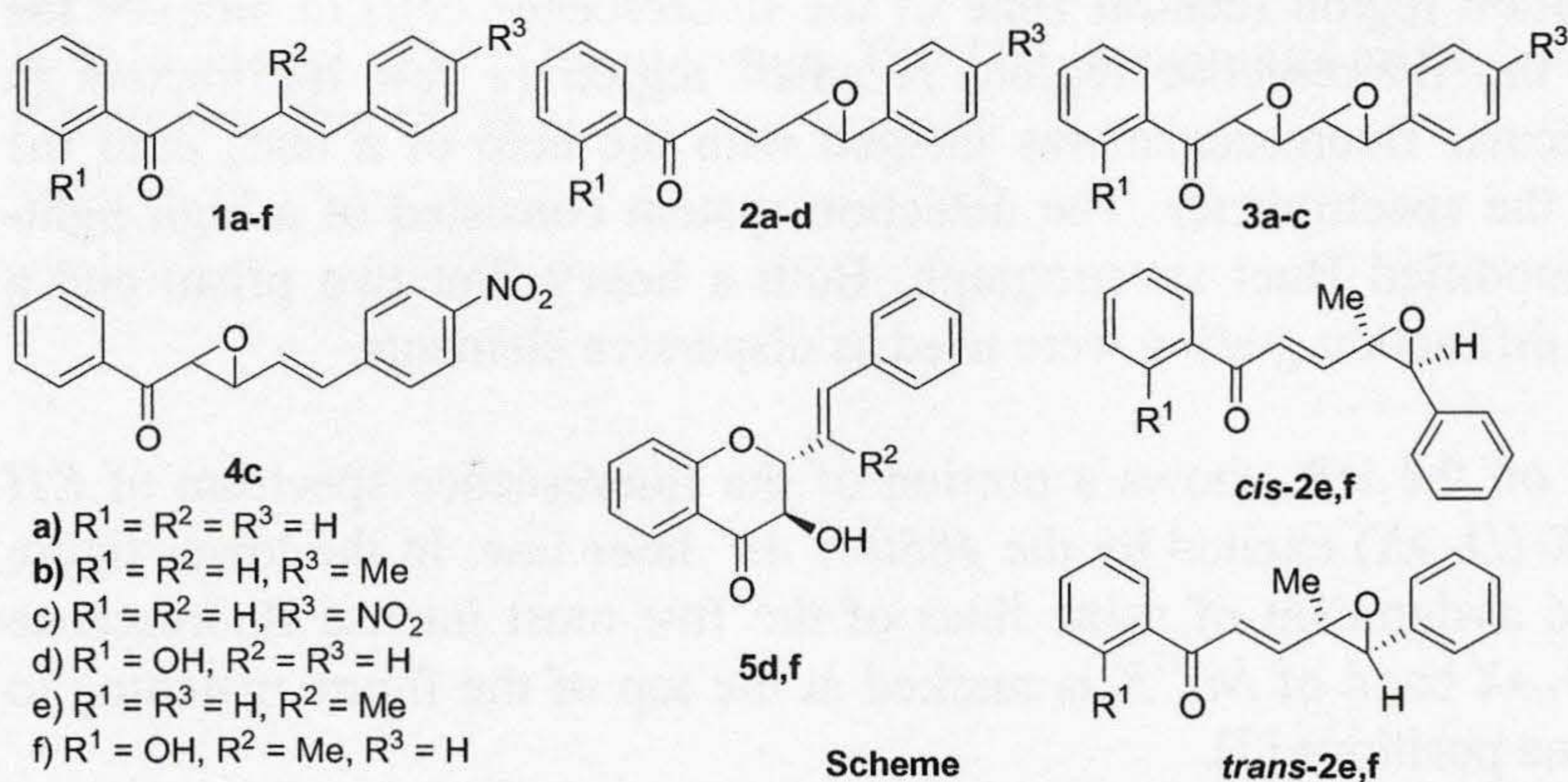
## NMR in the epoxidation of (*E,E*)-cinnamylideneacetophenones

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The epoxidation of cinnamylideneacetophenones have been already performed with hydrogen peroxide as oxidant in Julia's method [1] and with dimethyldioxirane [2], however no studies were performed using salen Mn(III) complexes as catalysts. On these basis, we developed a study on the epoxidation of cinnamylideneacetophenones **1**, catalyzed by commercially available Jacobsen's catalyst [salen Mn(III)] and using iodosylbenzene and hydrogen peroxide as oxidants. The structure of the epoxidation products **2-5**, their stereochemistry and the regiochemistry of the monoepoxides **2** formation were established by 1D and 2D NMR spectroscopy. These studies will be presented and discussed.

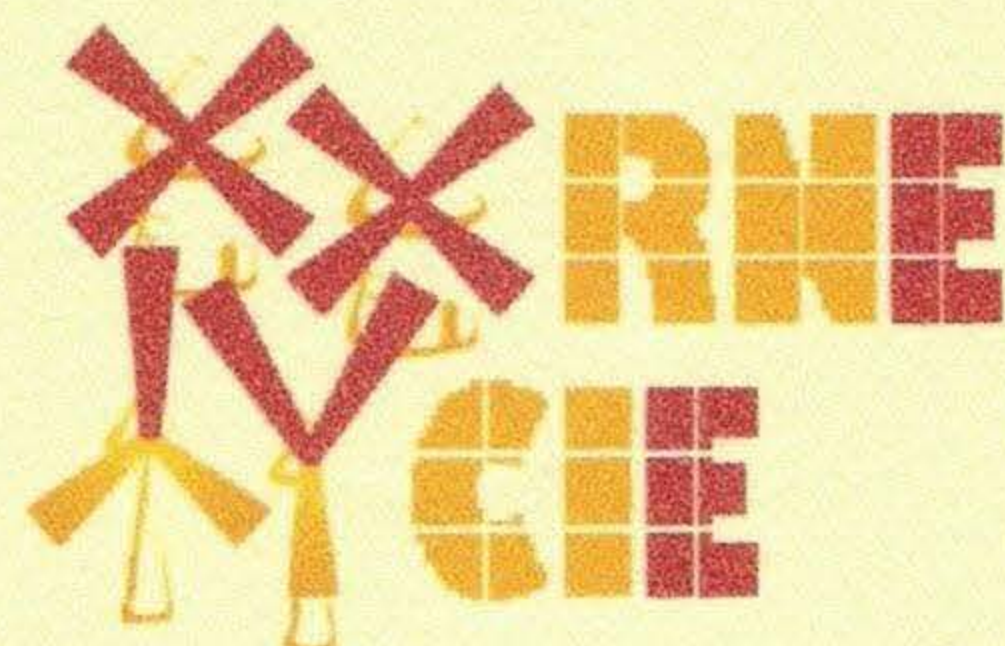


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[1] M. E. Lasterra Sanchez, U. Felper, P. Mayon, S. M. Roberts, A. R. Thornton, C. J. Todd, *J. Chem. Soc., Perkin Trans. I*, **1996**, 343.

[2] A. Lévai, A. M. S. Silva, J. A. S. Cavaleiro, T. Patonay, V. L. M. Silva, *Eur. J. Org. Chem.*, **2001**, 3213.





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**CERTIFICATE**

BARTOLOMÉ M. SIMONET SUAU, Secretary of the Organizing Committee of the Conference "**XX RNE – IV CIE**"

CERTIFY

that **Clementina M. M. Santos** has attended this Conference and has presented the oral communication with the title:

**"NMR in the epoxidation of (*E,E*)-cinnamylideneacetophenones"**

Ciudad Real, September 14, 2006

Dr. Bartolomé M. Simonet Suau  
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Sociedad de Espectroscopía Aplicada  
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## Introduction

The epoxidation of cinnamylideneacetophenones have been already performed with hydrogen peroxide as oxidant in Julia's method [1] and with dimethyldioxirane [2], however no studies were performed using salen Mn(III) complexes as catalysts.

On this basis, we developed a study on the epoxidation of cinnamylideneacetophenones **1**, catalyzed by commercially available Jacobsen's catalyst [salen Mn(III)] and using iodosylbenzene and hydrogen peroxide as oxidants.

The structure of the epoxidation products **2-5**, their stereochemistry and the regiochemistry of the monoepoxides **2** formation were established by 1D and 2D NMR spectroscopy. These studies are presented and discussed.

## Epoxidation of (*E,E*)-cinnamylideneacetophenones

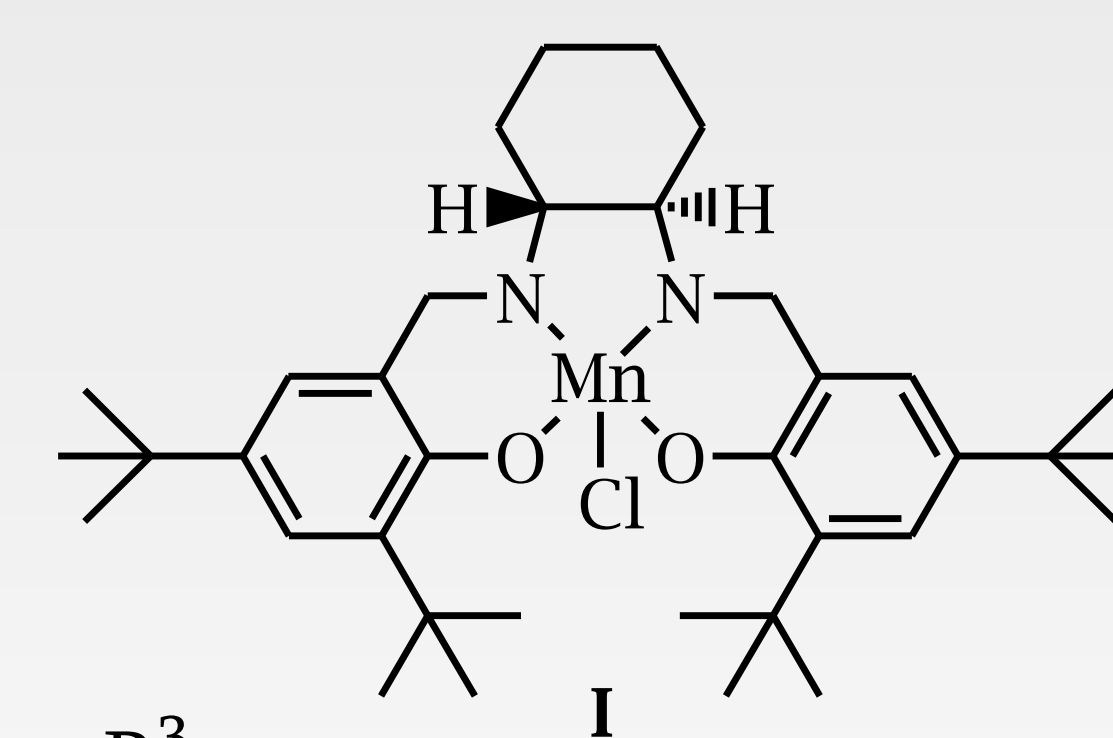
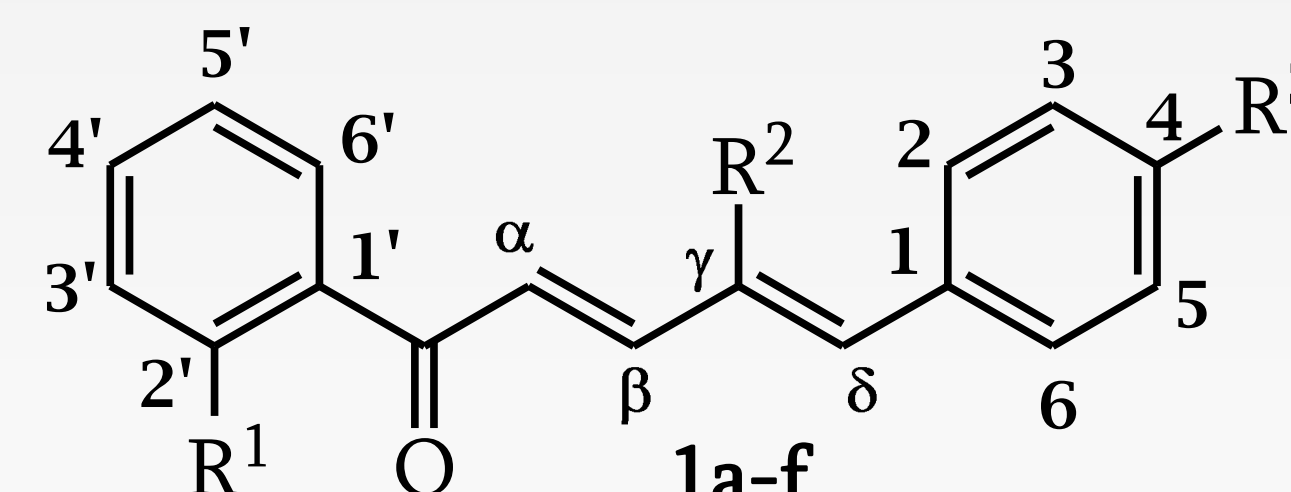
Salen Mn(III) complexes are efficient catalysts for the epoxidation of  $\alpha,\beta$ -unsaturated carbonyl compounds.

We developed a new study on the epoxidation of cinnamylideneacetophenones **1a-f**, catalyzed by commercially available Jacobsen's catalyst **I** and using hydrogen peroxide ( $H_2O_2$ ) and iodosylbenzene (PhIO) as oxidants.

The optimized conditions in the epoxidation of **1a-f** are described in **A** and **B**.

**A:** 0.05 eq. Catalyst **I**, 0.7 eq. 1-MeIm, 10 eq.  $H_2O_2$ ,  $CH_3OH/CH_2Cl_2$  (1:1), 40 °C, 4h

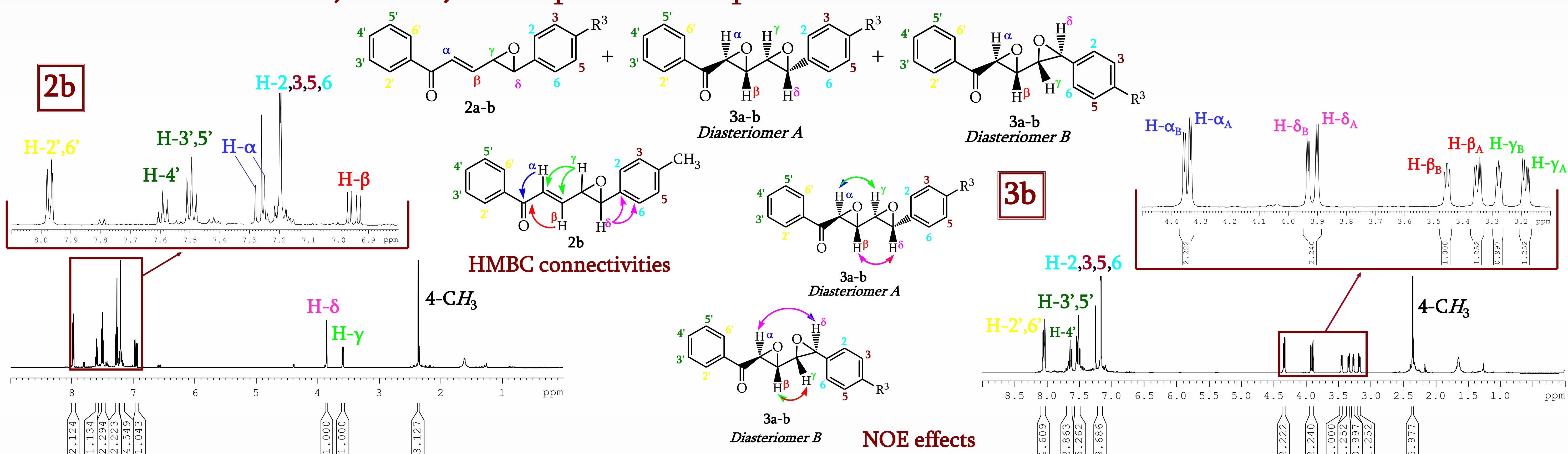
**B:** 0.05 eq. Catalyst **I**, 0.5 eq. PyNO, 2 eq. PhIO,  $CH_3CN$ , r.t., 4h



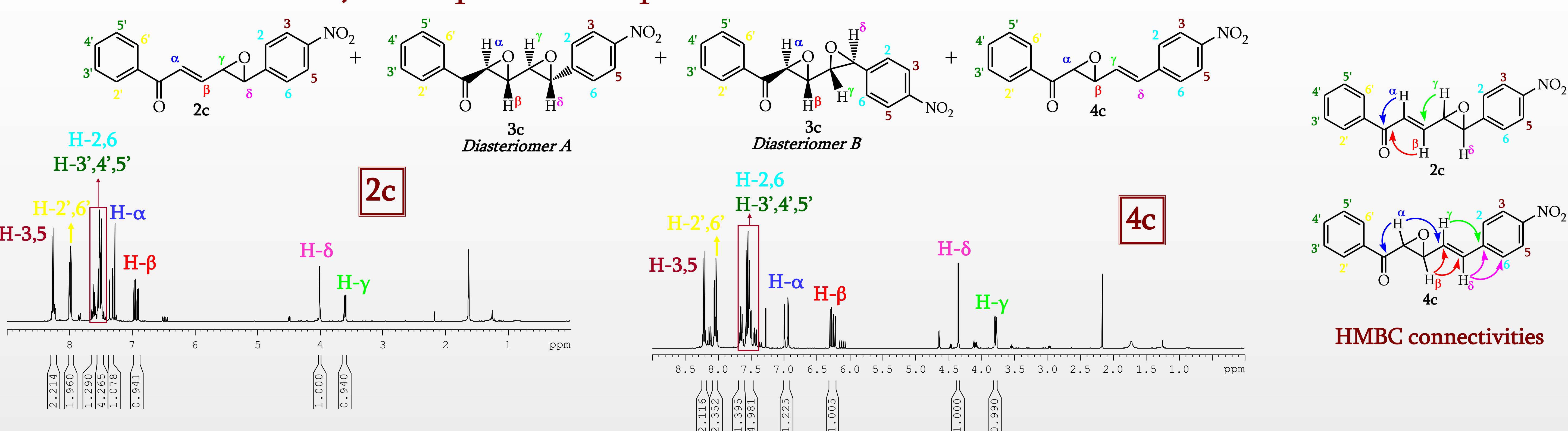
Jacobsen's catalyst

- a)  $R^1 = R^2 = R^3 = H$
- b)  $R^1 = R^2 = H, R^3 = Me$
- c)  $R^1 = R^2 = H, R^3 = NO_2$
- d)  $R^1 = OH, R^2 = R^3 = H$
- e)  $R^1 = R^3 = H, R^2 = Me$
- f)  $R^1 = OH, R^2 = Me, R^3 = H$

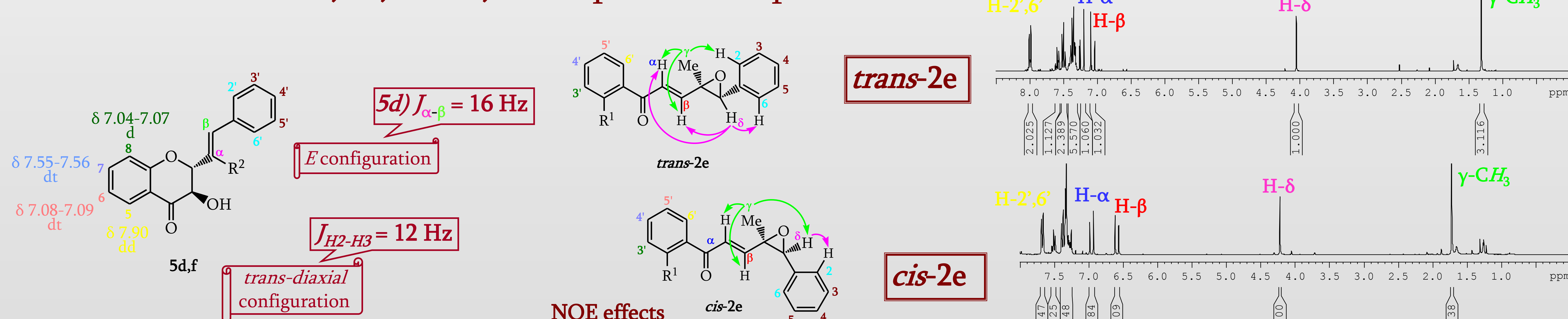
For the derivatives **a)** and **b)**, the epoxidation products are:



For the derivatives **c)**, the epoxidation products are:



For the derivatives **d)**, **e)** and **f)**, the epoxidation products are:



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