

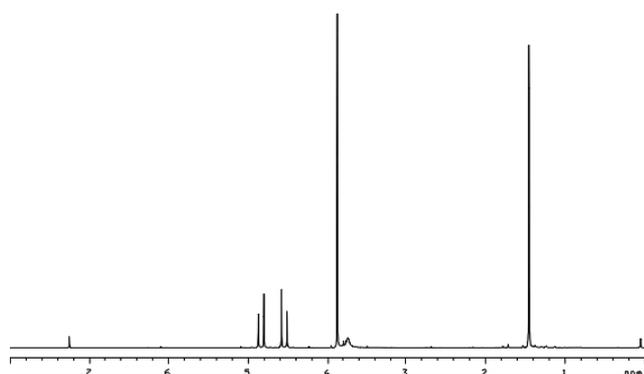
**ESI: Enantioselective Catalysis of the Henry Reaction by a Chiral  
Macrocyclic Ytterbium Complex in Aqueous Media**

Shashi U. Pandya, Rachel S. Dickins and D. Parker

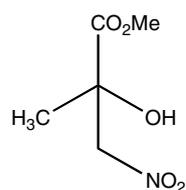
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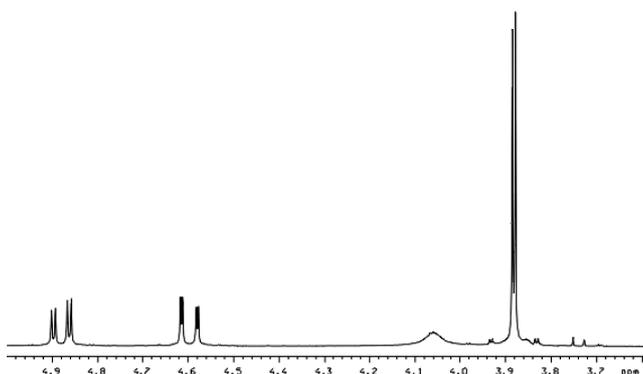
ES2



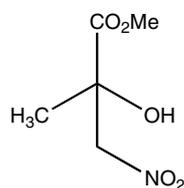
<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>)



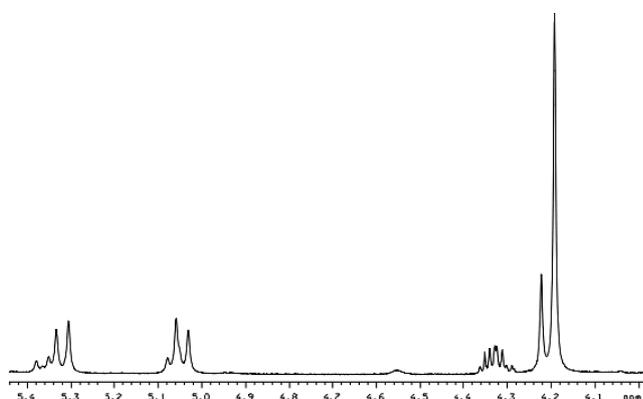
Racemic 2a, Entry 2, Table 1



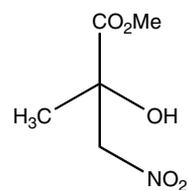
Partial <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>)  
with 2% Eu(hcp)<sub>3</sub>



Racemic 2a, Entry 2, Table 1

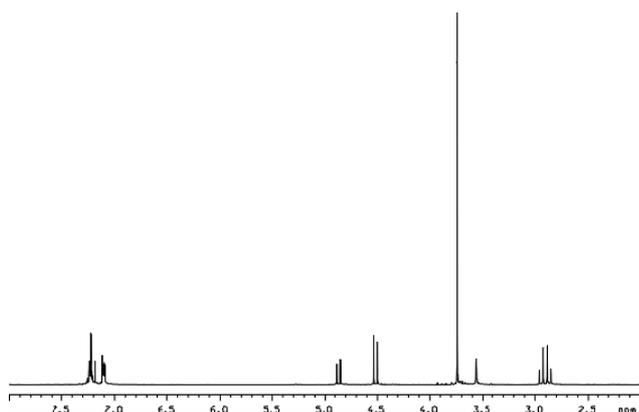


Partial <sup>1</sup>H NMR spectrum (400 MHz,  
CDCl<sub>3</sub>) with 2% Eu(hcp)<sub>3</sub>

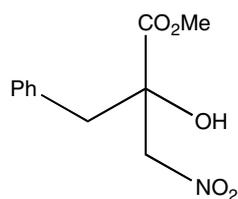


58% ee 2a, Entry 3, Table 1

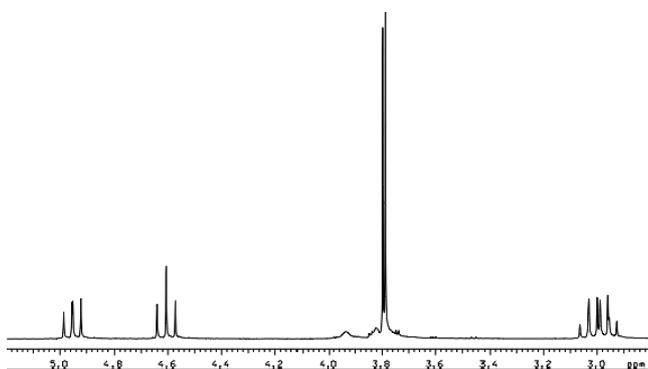
ES3



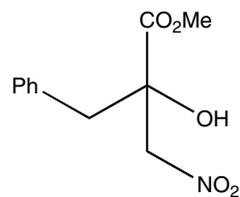
$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ )



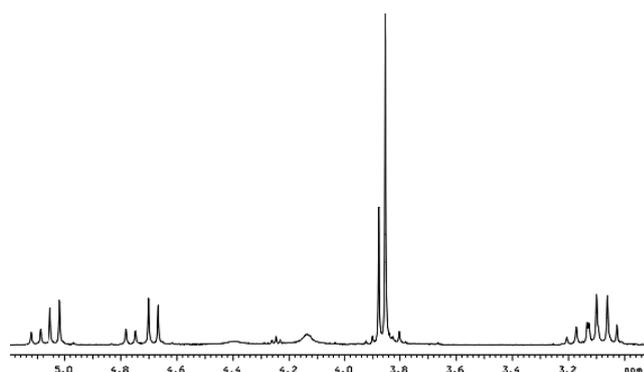
Racemic 2b, *Entry 7, Table 1*



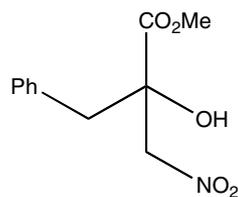
Partial  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) with 2%  $\text{Eu}(\text{hcp})_3$



Racemic 2b, *Entry 7, Table 1*

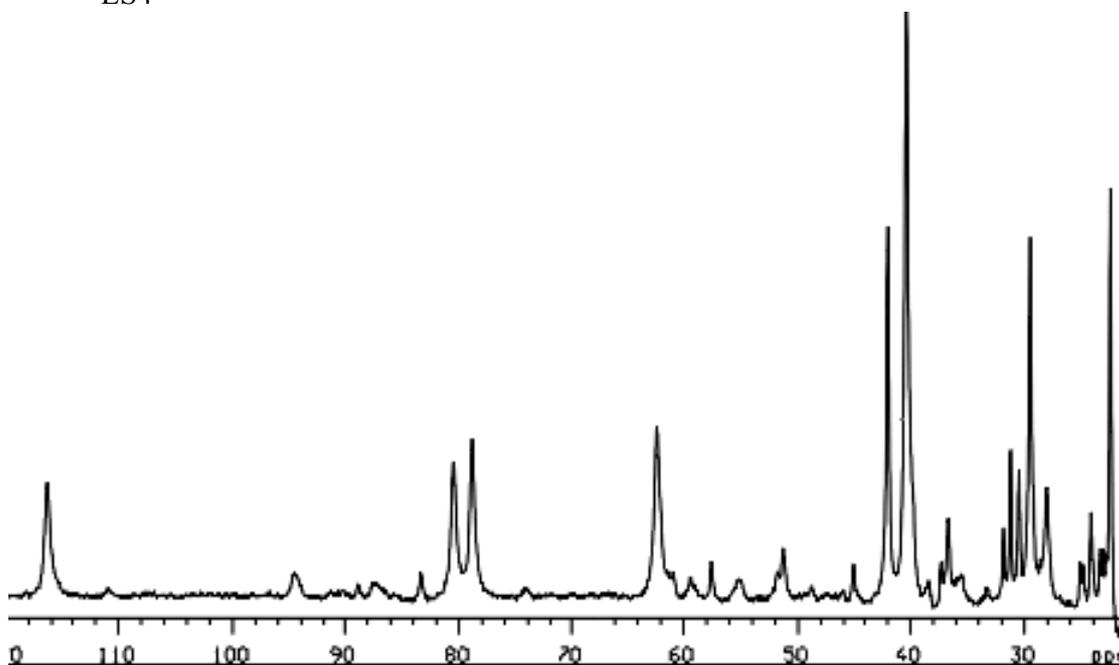


Partial  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) with 2%  $\text{Eu}(\text{hcp})_3$

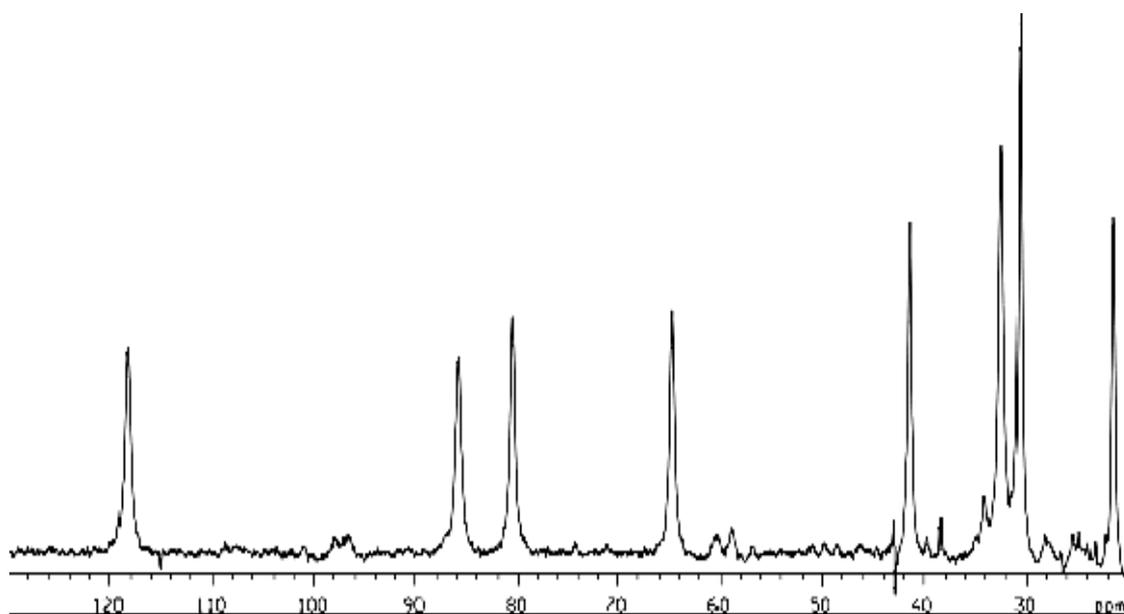


41% ee 2b, Entry 8, Table 1

ES4



Partial <sup>1</sup>H NMR spectrum (CD<sub>3</sub>OD, 300 MHz) of the crude reaction mixture of sodium pyruvate with nitromethane catalyzed by 10 mol % (*RRR*)-[YbL(H<sub>2</sub>O)<sub>2</sub>]OTf<sub>3</sub> after 48 h at RT. The 4 major resonances above 64 ppm are assigned to the axial ring protons of the chelated product adduct.



Partial <sup>1</sup>H NMR spectrum (CD<sub>3</sub>OD, 200 MHz) of the crude reaction mixture of sodium phenylpyruvate with nitromethane, catalyzed by 10 mol % (*RRR*)-[YbL<sup>1</sup>(H<sub>2</sub>O)<sub>2</sub>]OTf<sub>3</sub> after 48 h at RT. The 4 major resonances above 64 ppm are assigned to the axial ring protons of the chelated product adduct.