Supplementary Material (ESI) for Organic and Biomolecular Chemistry

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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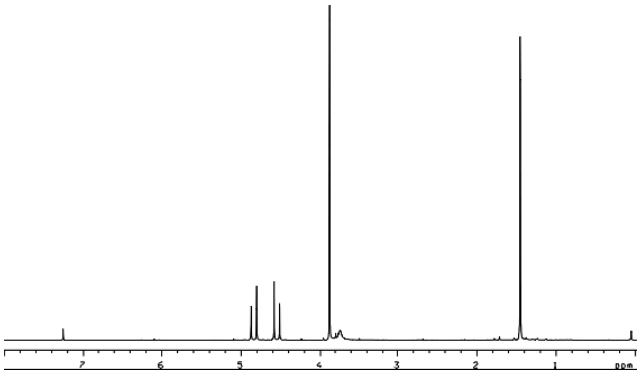
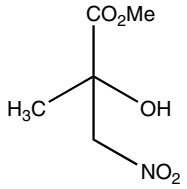
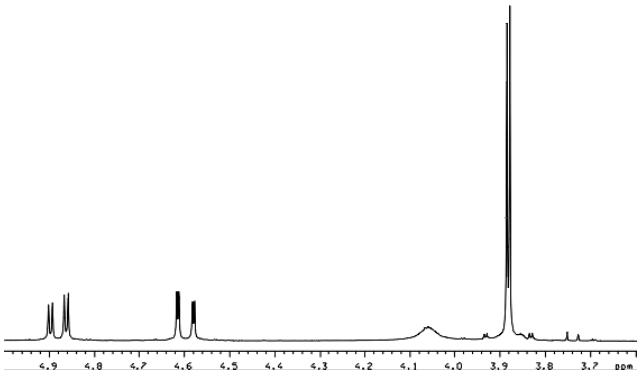


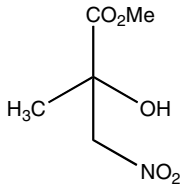
^{1}H NMR spectrum (400 MHz, $CDCl_3$)



Racemic 2a, *Entry 2, Table 1*



Partial ^{1}H NMR spectrum (400 MHz, $CDCl_3$) with 2% $Eu(hcp)_3$



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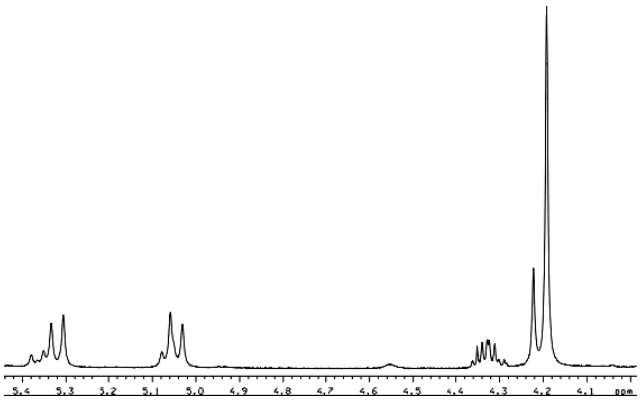
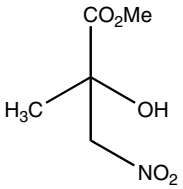
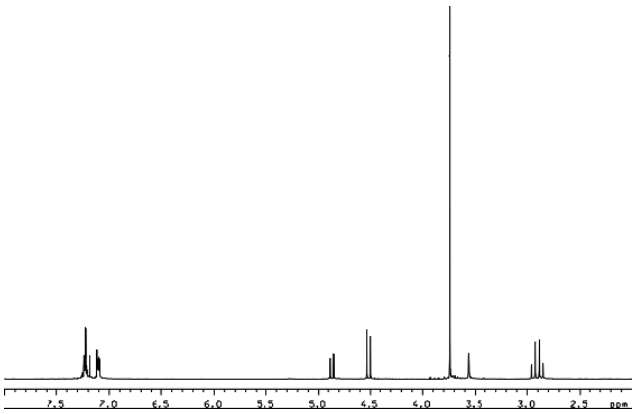


Partial ^{1}H NMR spectrum (400 MHz, $CDCl_3$) with 2% $Eu(hcp)_3$

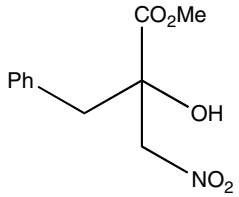


58% ee 2a, *Entry 3, Table 1*

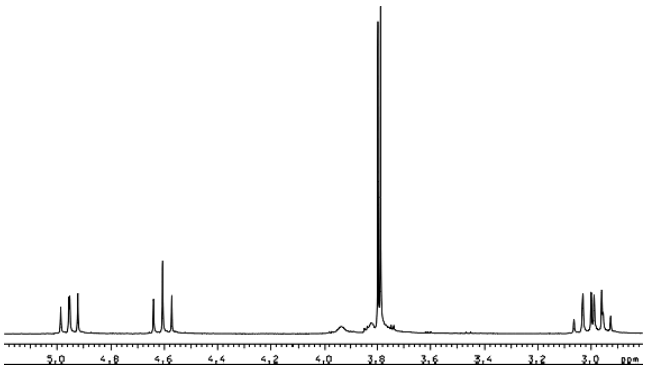
E**S3**



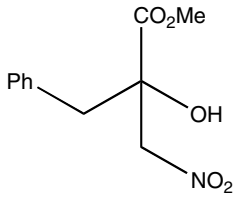
^{1}H NMR spectrum (400 MHz, $CDCl_3$)



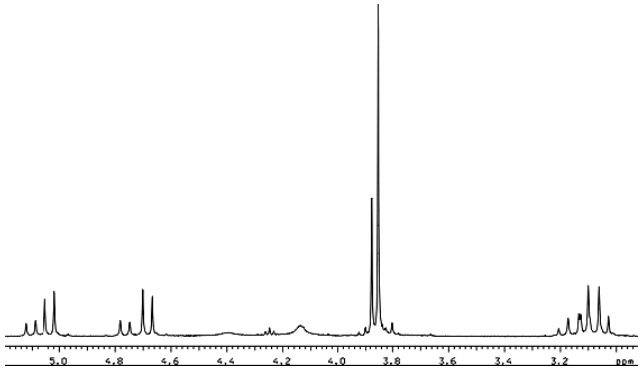
Racemic 2b, *Entry 7, Table1*



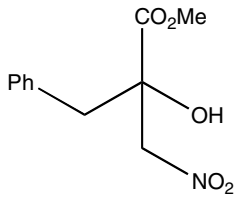
Partial ^{1}H NMR spectrum (400 MHz, $CDCl_3$) with 2% $Eu(hcp)_3$



Racemic 2b, *Entry 7, Table 1*

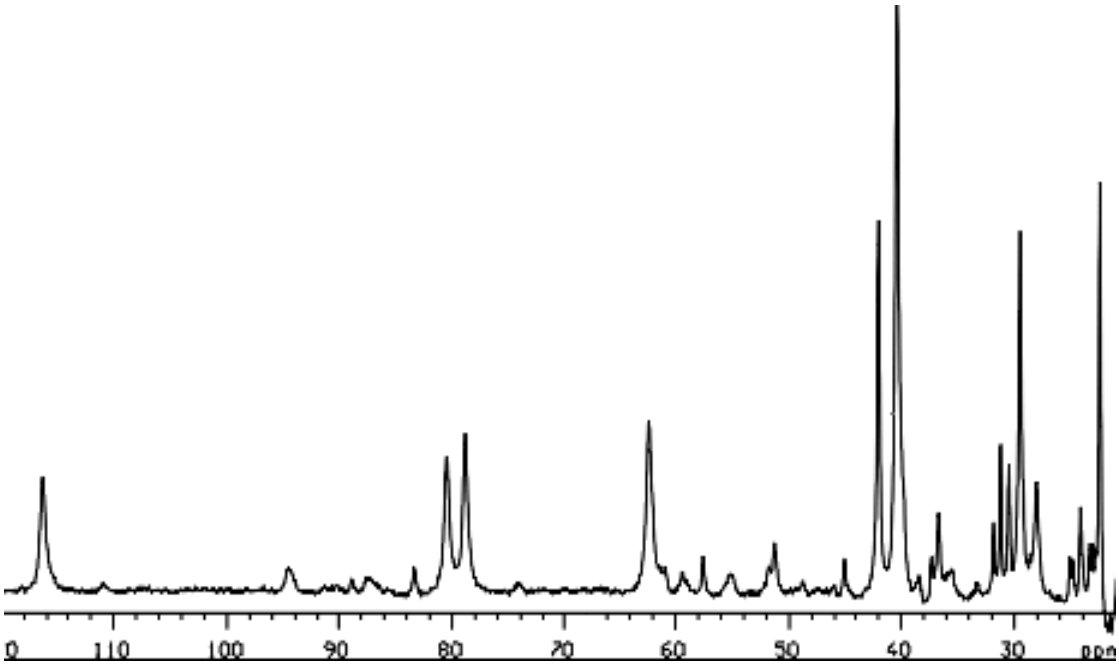


Partial ^{1}H NMR spectrum (400 MHz, $CDCl_3$) with 2% $Eu(hcp)_3$

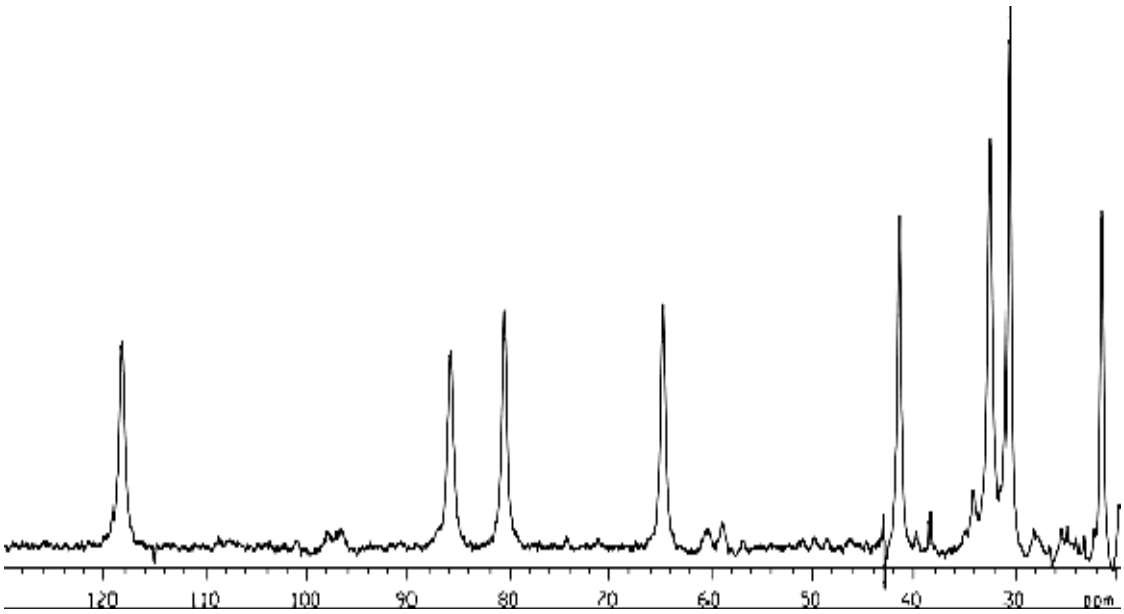


41% ee 2b, *Entry 8, Table 1*

ES4



Partial ^{1}H NMR spectrum (CD_3OD, 300 MHz) of the crude reaction mixture of sodium pyruvate with nitromethane catalyzed by 10 mol % (*RRR*)-[YbL(H_2O)$_2$]OTf$_3$ 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 ^{1}H NMR spectrum (CD_3OD, 200 MHz) of the crude reaction mixture of sodium phenylpyruvate with nitromethane, catalyzed by 10 mol % (*RRR*)-[YbL^1(H_2O)$_2$]OTf_3 after 48 h at RT. The 4 major resonances above 64 ppm are assigned to the axial ring protons of the chelated product adduct.