

Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2013

Supplementary Material

Enantioselective recognition of alcohol by UV-*vis* through hydrogen bond interaction

Su-Ying Xu,^a Bin Hu,^b Stephen E. Flower,^a Yun-Bao Jiang,^c John S. Fossey,^{b,d} Wei-Ping Deng*^b
and Tony D. James*^a

^a Department of Chemistry, University of Bath, Bath, BA2 7AY UK

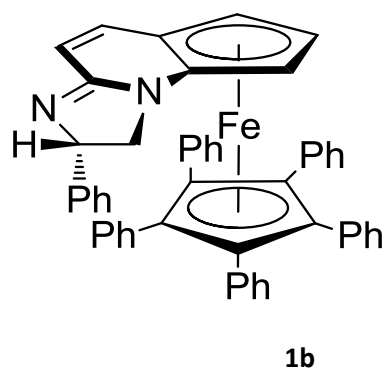
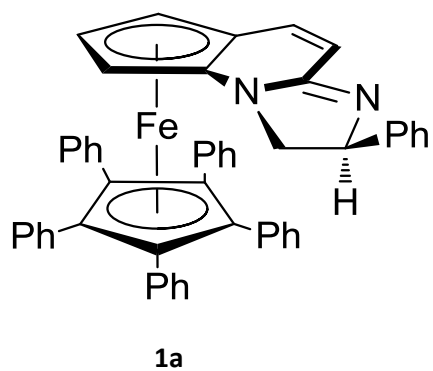
^b Shanghai Key Laboratory of Functional Materials Chemistry & School of Pharmacy, East China University of Science and Technology, Shanghai, 20023, China

^c Department of Chemistry, College of Chemistry and Chemical Engineering, and the MOE Key Laboratory of Analytical Sciences, Xiamen University, Xiamen 361005, China

^d School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, U.K.

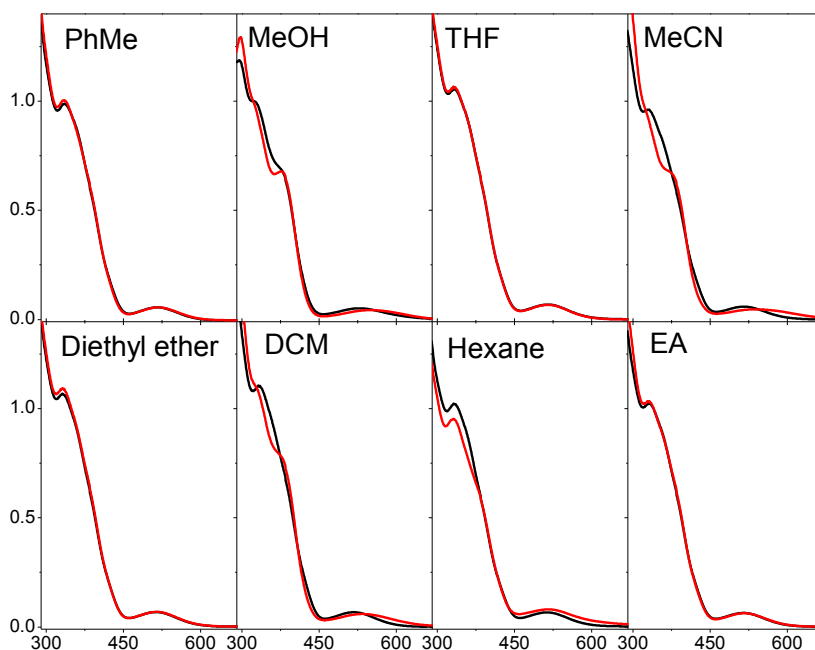
S1 Structures of compounds 1a and 1b	2
S2 different solvent effects of 1a after addition of alcohols	3
S3 Binding constant calculation of D/L-dimethyl tartrate (D/L-DT)	4
S4 Absorption spectra of compound 1a with D/L-tartaric acid	5
S5 Colour changes of compound 1a with D/L-tartaric acids (D/L-TA)	5
S6 Binding constant calculation of tartaric acids	6
S7 ¹ H-NMR investigation of compound 1a	7
S8 NMR photos	11
S9 Proposed hydrogen binding structure	12

S1 Structures of compounds 1a and 1b



S 1 structures of compound 1a and 1b

S2 different solvent effects of 1a after addition of alcohols



S 2 Absorption changes of 1a before (black line) and after (red line) addition of dimethyl-D-tartrate (D-DT) in different solvents and the exact absorption values were shown in Table 1

Table 1 The ratio values of absorption at 576 nm to 516 nm of compound 1a in different solvent before and after addition of dimethyl D-tartrate

	Δ^a	A1 ^b	A2 ^c
Toluene	0.046	0.246	0.292
Methanol	0.456	0.650	1.106
THF	-0.009	0.331	0.322
Acetonitrile	0.571	0.354	0.925
Diethyl ether	0.018	0.319	0.337
Dichloromethane	0.438	0.363	0.801
Hexane	0.210	0.328	0.538
Ethyl acetate	0.042	0.331	0.373

^a $\Delta = A2 - A1$

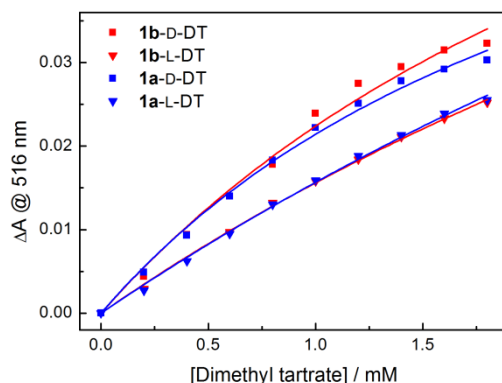
^b A1: ratio values of absorption at 576 nm to 516 nm when 1a was 0.1 mM in each solvent

^c A2: ratio values of absorption at 576 nm to 516 nm when 0.6 mM dimethyl-D-tartrate was added to the prepared solution

S3 Binding constant calculation of D/L-dimethyl tartrate (D/L-DT)

Table 2 calculated binding constant for **1a** and **1b**

	1b -D-DT	1b -L-DT	1a -D-DT	1a -L-DT
<i>b</i>	0.0974 ± 0.019	0.126 ± 0.020	0.0760 ± 0.008	0.155 ± 0.035
<i>K</i>	298.3 ± 84.7	141.4 ± 26.1	392.5 ± 63.2	112.5 ± 29.3
R-sq.	0.988	0.998	0.994	0.998



S3 Absorption difference at 516 nm of compound **1a** and **1b** in MeCN versus concentrations of dimethyl tartrate; [**1a**] = [**1b**] = 0.1 Mm; $\Delta A = A_0 - A$

The binding constants were calculated using non-linear curve fitting of eqn. (1), which was derived from eqn. (2).¹

$$y = \frac{b * K * x}{1 + K * x} \quad \text{eqn. (1)}$$

Derivation of eqn (1) from eqn (2) ¹:

$$A = \frac{A_0 + A_{lim} * K * [Guest]}{1 + K * [Guest]} \quad \text{eqn. (2) } \rightarrow \rightarrow \rightarrow$$

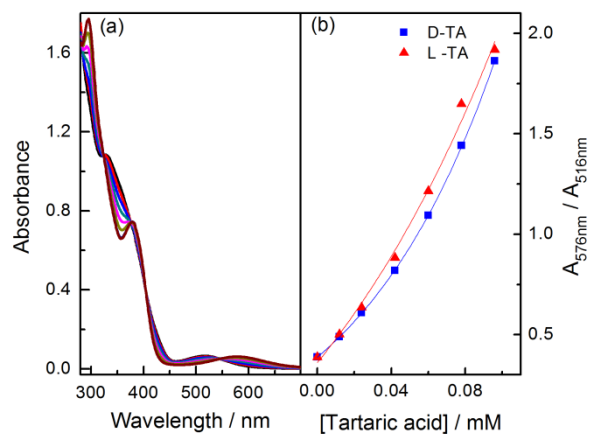
$$A - A_0 = \frac{A_0 + A_{lim} * K * [Guest]}{1 + K * [Guest]} - A_0 \rightarrow \rightarrow \rightarrow$$

$$A - A_0 = \frac{(A_{lim} - A_0) * K * [Guest]}{1 + K * [Guest]} \rightarrow \rightarrow \rightarrow$$

$$y = \frac{b * K * x}{1 + K * x} \quad \text{eqn. (1) when } y = A - A_0, b = A_{lim} - A_0, x = [Guest]$$

1. C. J. Ward, P. Patel and T. D. James, *J. Chem. Soc., Perkin Trans. 1*, 2002, **4**, 462-470.

S4 Absorption spectra of compound **1a** with D/L-tartaric acid



S4 (a): Absorption changes of **1a** with addition of D-tartaric acid; (b): ratio of absorbance of compound **1a** at 576 nm to 516 nm against concentration of D/L-tartaric acids

S5 Colour changes of compound **1a** with D/L-tartaric acids (D/L-TA)

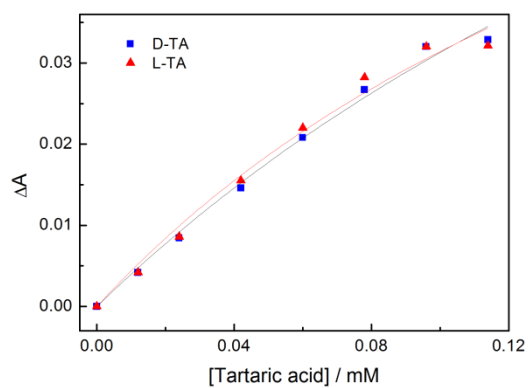


S5 From left to right: 0.1 mM compound **1a**; with 1 eq. L-tartaric acid; with 1 eq. D-tartaric acid

S6 Binding constant calculation of tartaric acids

Table 3 calculated binding constants for tartaric acids with **1a**

	1a-D-TA	1a-L-TA
b	0.131 ± 0.038	0.0991 ± 0.027
K	3131 ± 1157	4636 ± 1755
R-sq.	0.992	0.986

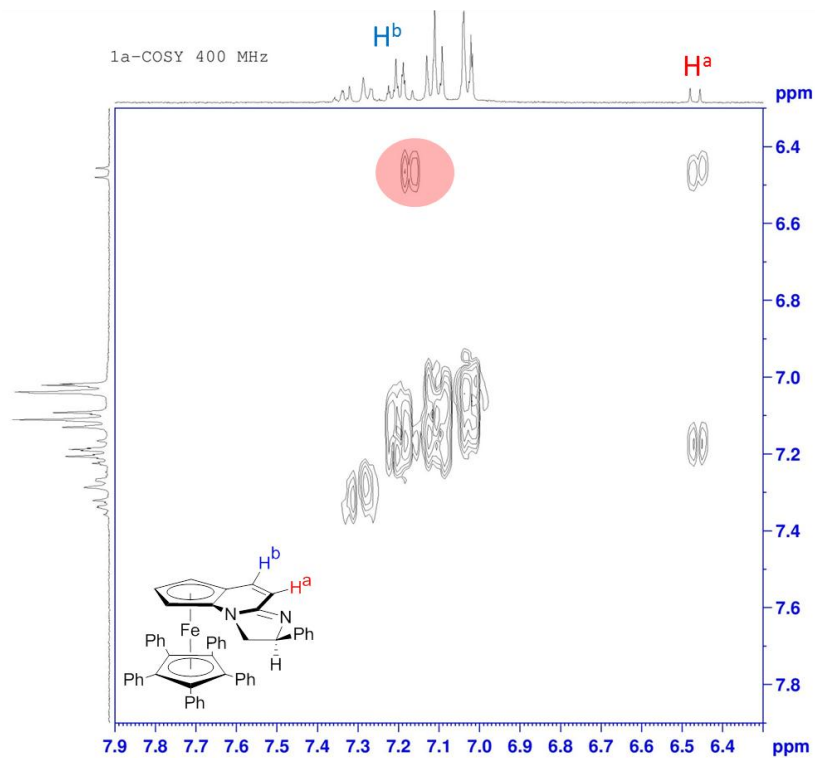


S 6 Absorption difference at 516 nm of compound **1a** in MeCN *versus* concentrations of tartaric acids; [**1a**] = 0.1 mM;
 $\Delta A = A_0 - A$

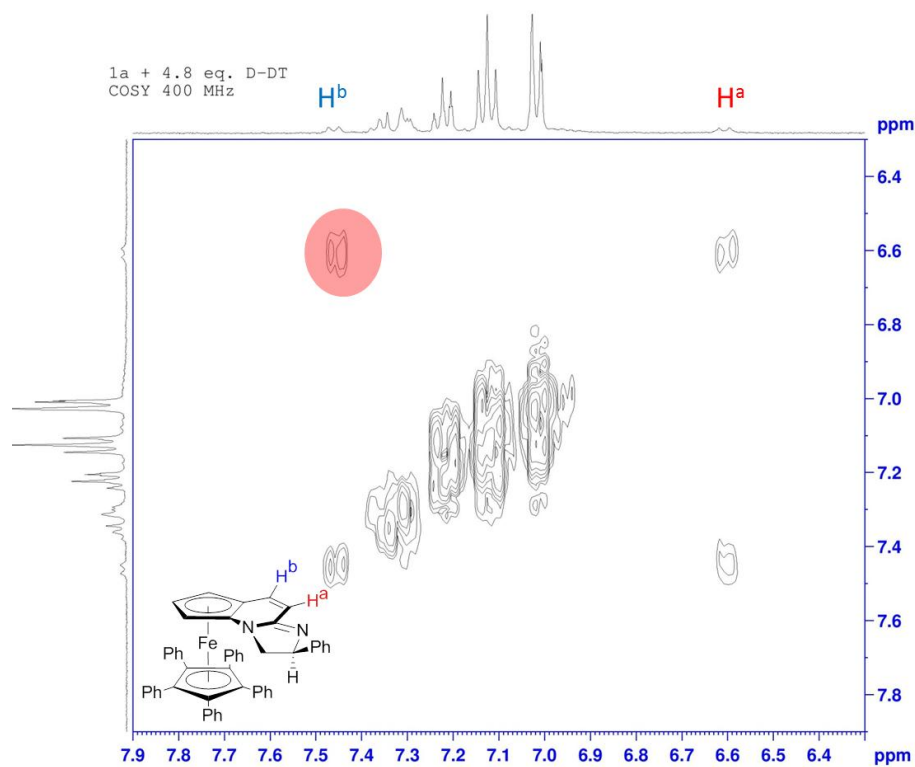
S7 ^1H -NMR investigation of compound **1a**

All NMR investigations were carried out in $\text{MeCN-}d_3$ solvent with 2.5 mM of **1a**. Protons a and b are down-shifted upon addition of either tartaric acid or dimethyl tartrate, shown as below.

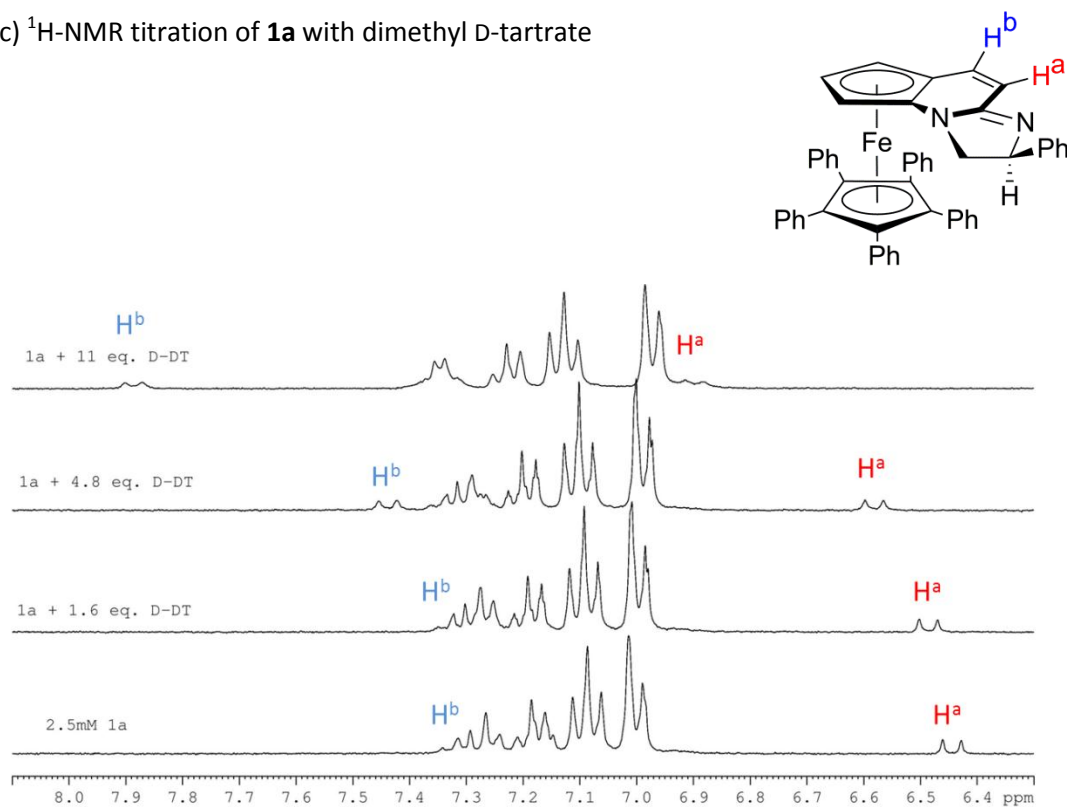
(a) COSY ^1H -NMR spectrum of **1a**



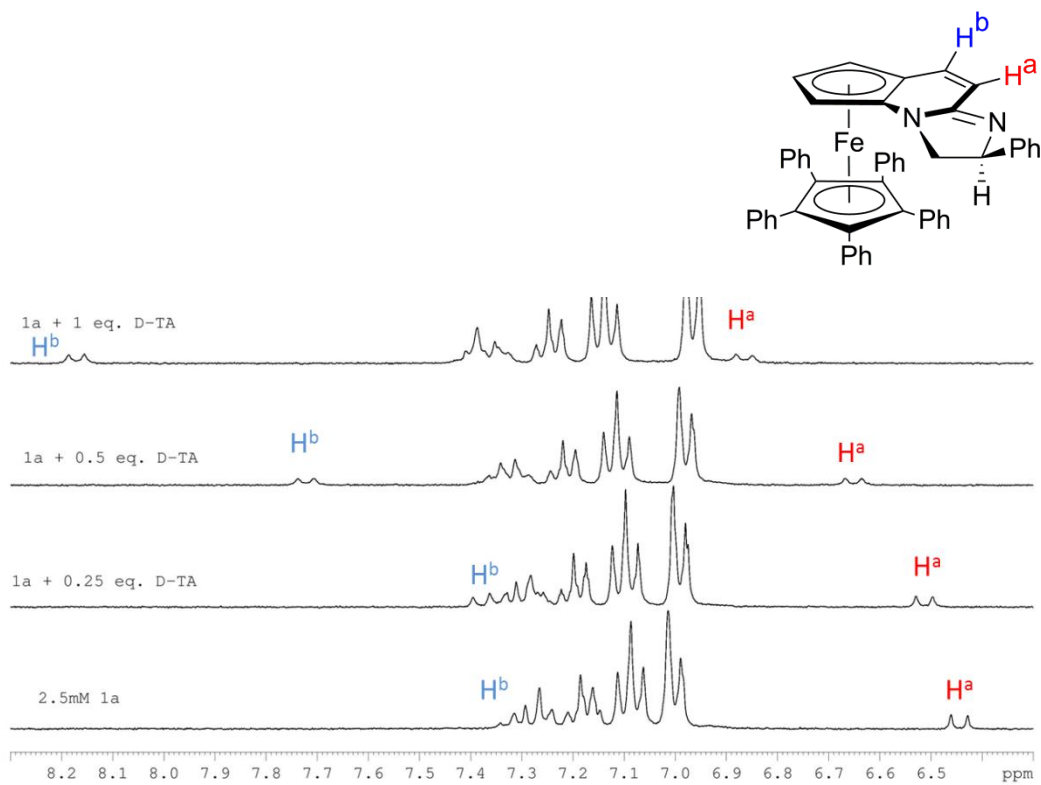
(b) COSY $^1\text{H-NMR}$ spectrum of **1a** with 4.8 eq. D-DT



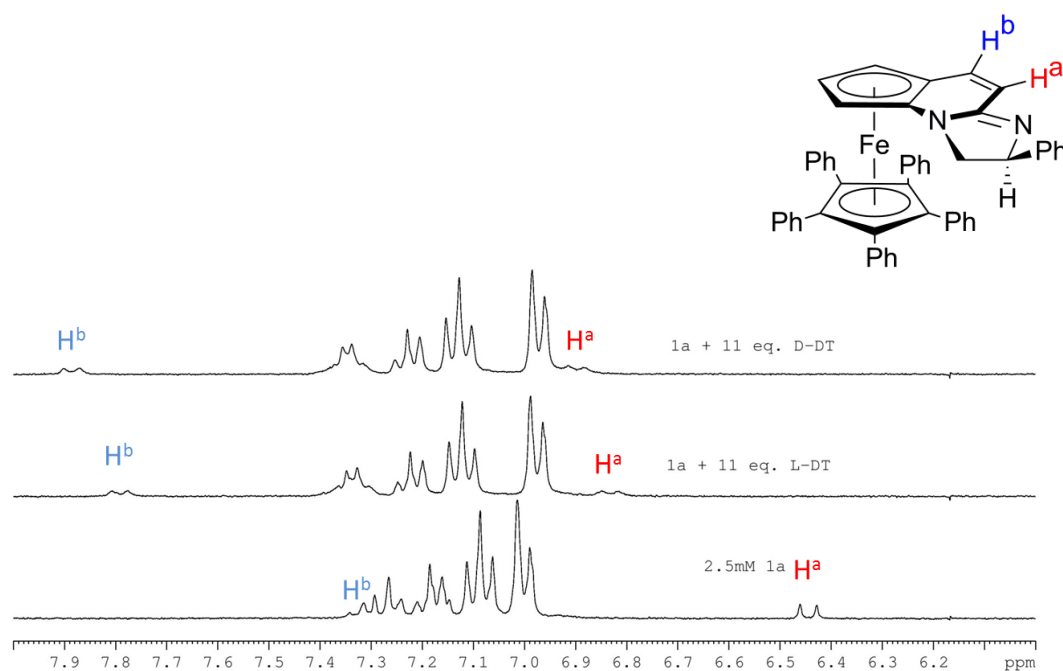
(c) $^1\text{H-NMR}$ titration of **1a** with dimethyl D-tartrate



(d) $^1\text{H-NMR}$ titration of **1a** with D-tartaric acid



(e) $^1\text{H-NMR}$ comparison of dimethyl tartrates with **1a**



S 7 $^1\text{H-NMR}$ spectra changes of **1a** (2.5 mM in $\text{MeCN-}d_3$) with different concentration of (a) 0, 1.6 eq., 4.8 eq. and 11 eq. of D-DT (b) 0, 0.25eq., 0.5 eq. and 1 eq. of D-TA; (c) comparison of **1a**, **1a** + 11 eq. of D-DT and **1a** + 11 eq. of L-DT

S8 NMR photos



S8 (a) [1a] = 2.5 mM in MeCN- d_3 ; from left to right: **1a**, **1a** + 0.25 eq. D-TA, **1a** + 0.5 eq. D-TA, **1a** + 1 eq. D-TA

(b)



S8 (b) NMR titration of **1a** with dimethyl D-tartrate: [1a] = 2.5 mM in MeCN- d_3 ; from left to right: **1a**, **1a** + 4.8 eq. D-DT, **1a** + 11 D-DT

S9 Proposed hydrogen bonding structure

