

# Supporting Information

## Size selective recognition of small esters by a negative allosteric hemicarcerand

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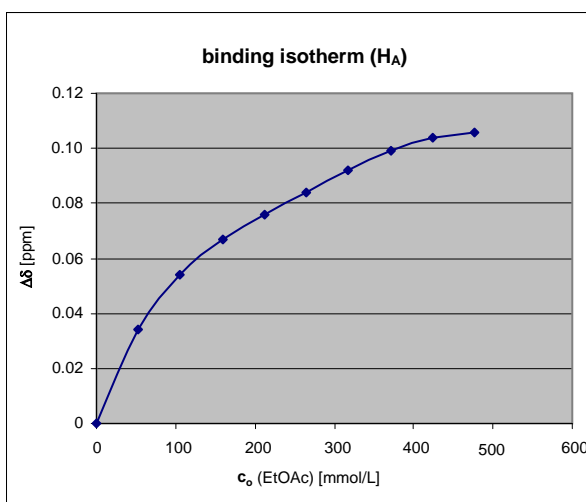
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### NMR Titrations

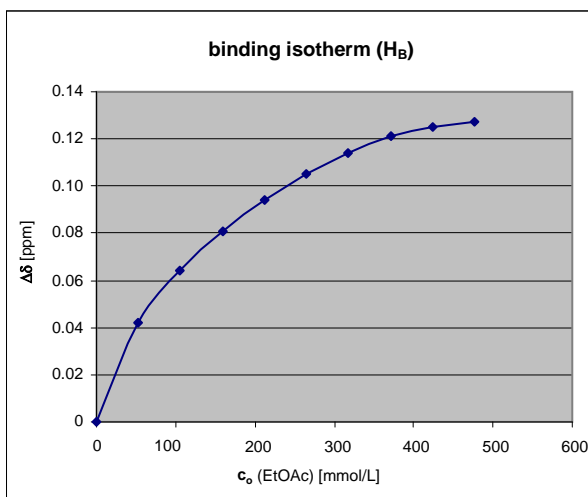
NMR titrations were performed with a 500 MHz NMR spectrometer at 298 K in mesitylene- $d_{12}$ .

**A** Titration of **2** with ethyl acetate,  $c_0$  (**2**) = 5.3 mmol/L.

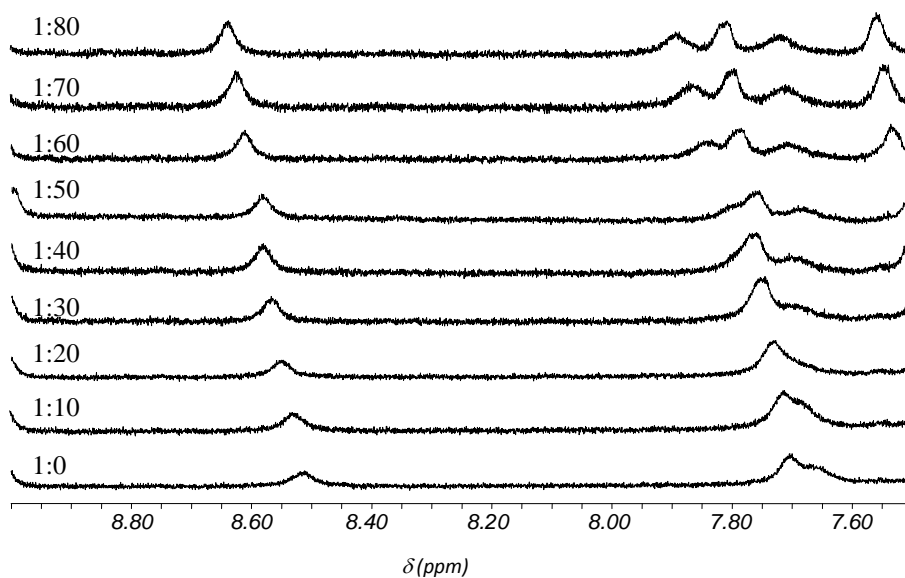
$c_0$ (EtOAc) [mol/L]	$\Delta\delta$ ( $H_A$ )[ppm]
0	0.000
53	0.034
106	0.054
159	0.067
212	0.076
265	0.084
318	0.092
371	0.099
424	0.104
477	0.106



$c_0$ (EtOAc) [mmol/L]	$\Delta\delta$ ( $H_B$ )[ppm]
0	0.000
53	0.042
106	0.064
159	0.081
212	0.094
265	0.105
318	0.114
371	0.121
424	0.125
477	0.127



**B** Titration of  $[(CO)_3Re(2)Cl]$  with ethyl acetate,  $c_0$   $[(CO)_3Re(2)Cl]$  = 5.0 mmol/L.



$c_0$ (EtOAc) [mmol/L]	$\Delta\delta$ ( $H_A$ )[ppm]
0	0.000
50	0.015
100	0.030
150	0.044
200	0.060
250	0.070
300	0.090
350	0.105
400	0.120

