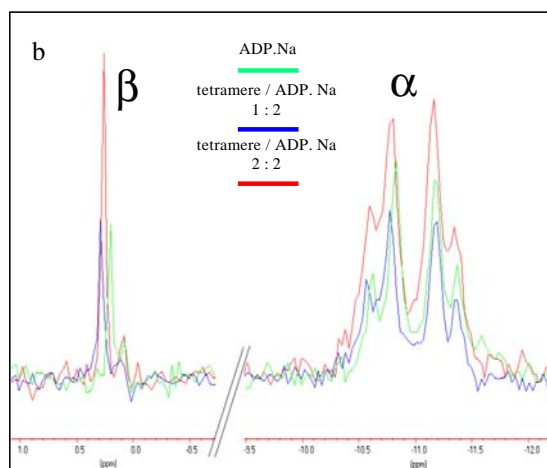
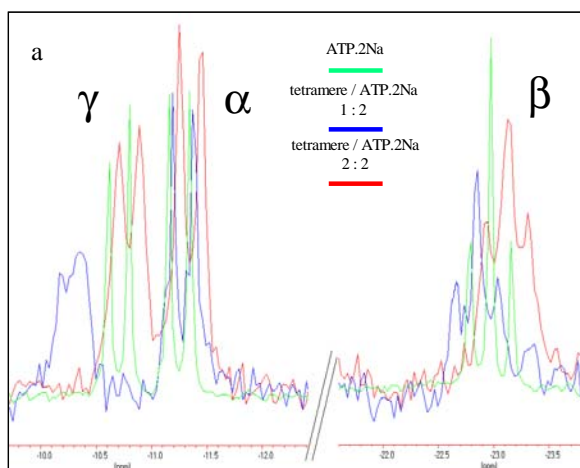


## Molecular Recognition of Nucleotides by a new Bis-guanidinium-tetrakis- $\beta$ -Cyclodextrin Tetrapode.

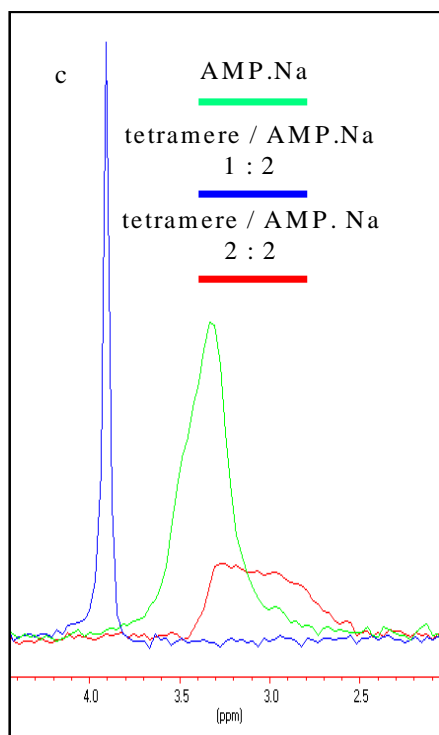
*Stephane Manuel, Raphaël E. Duval, Diana Cuc, Pierre Mutzenhardt and Alain Marsura\**

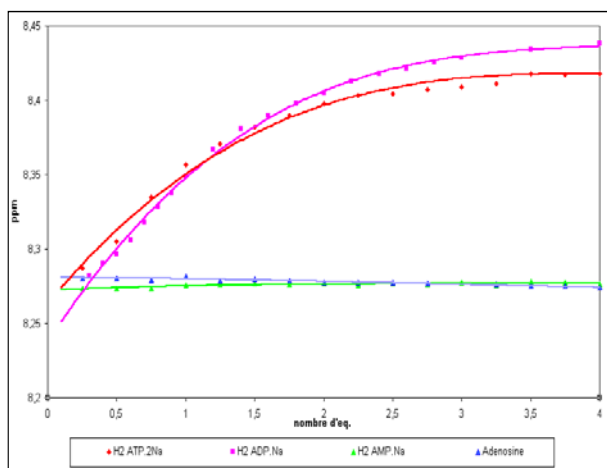
### Supplementary Material

#### 1] $^{31}\text{P}$ NMR spectra and $^1\text{H}$ NMR

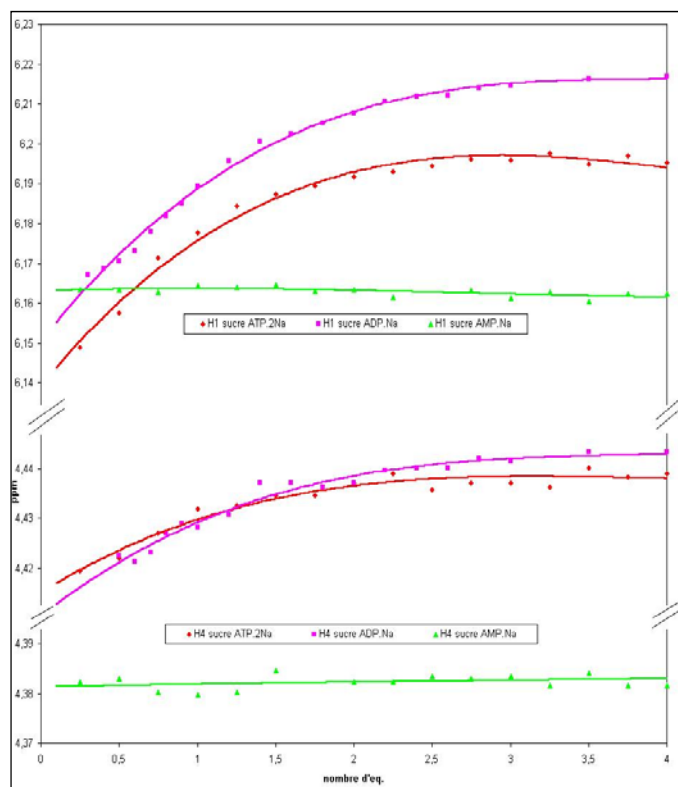


$^{31}\text{P}$  NMR CIS of a) ATP.2Na; b) ADP.Na and c) AMP.Na in  $\text{D}_2\text{O}$  after complexation with tetrapode **5**.

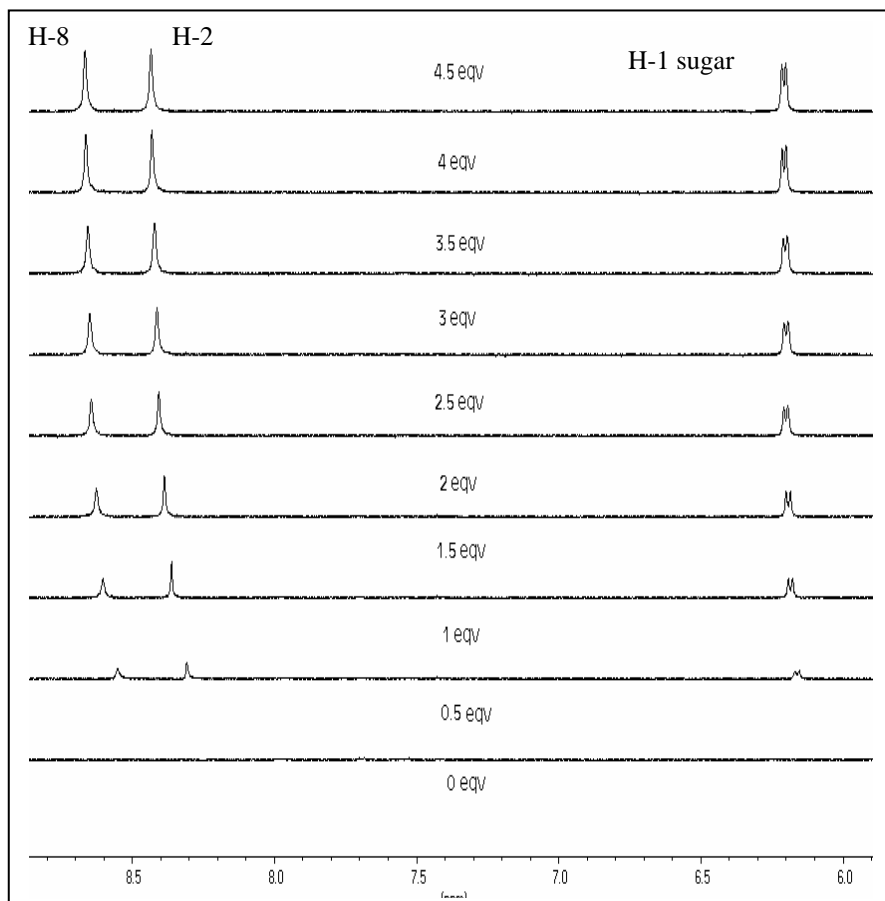




$^1\text{H}$  NMR CIS of the nucleobase H-2 protons in  $\text{D}_2\text{O}$  after complexation with **5**.

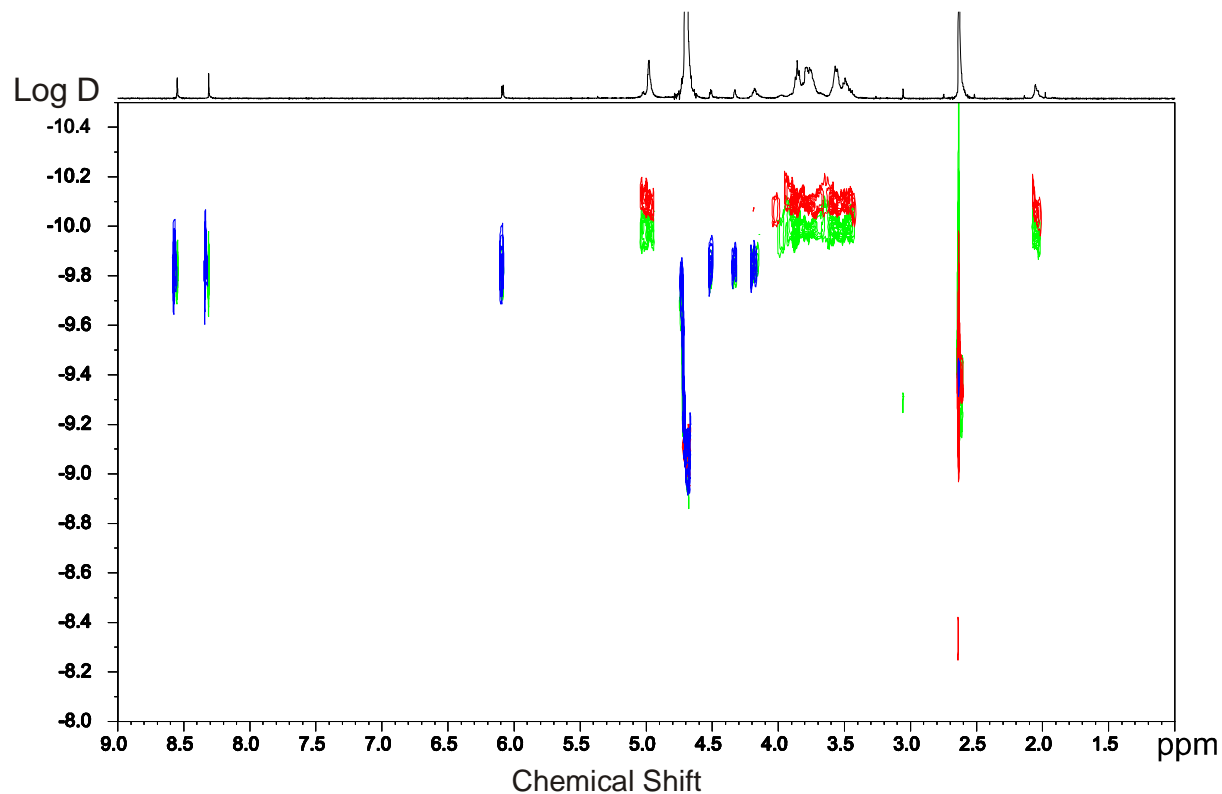


$^1\text{H}$  NMR CIS of the sugar H-1 and H-4 protons in  $\text{D}_2\text{O}$  after complexation with **5**.



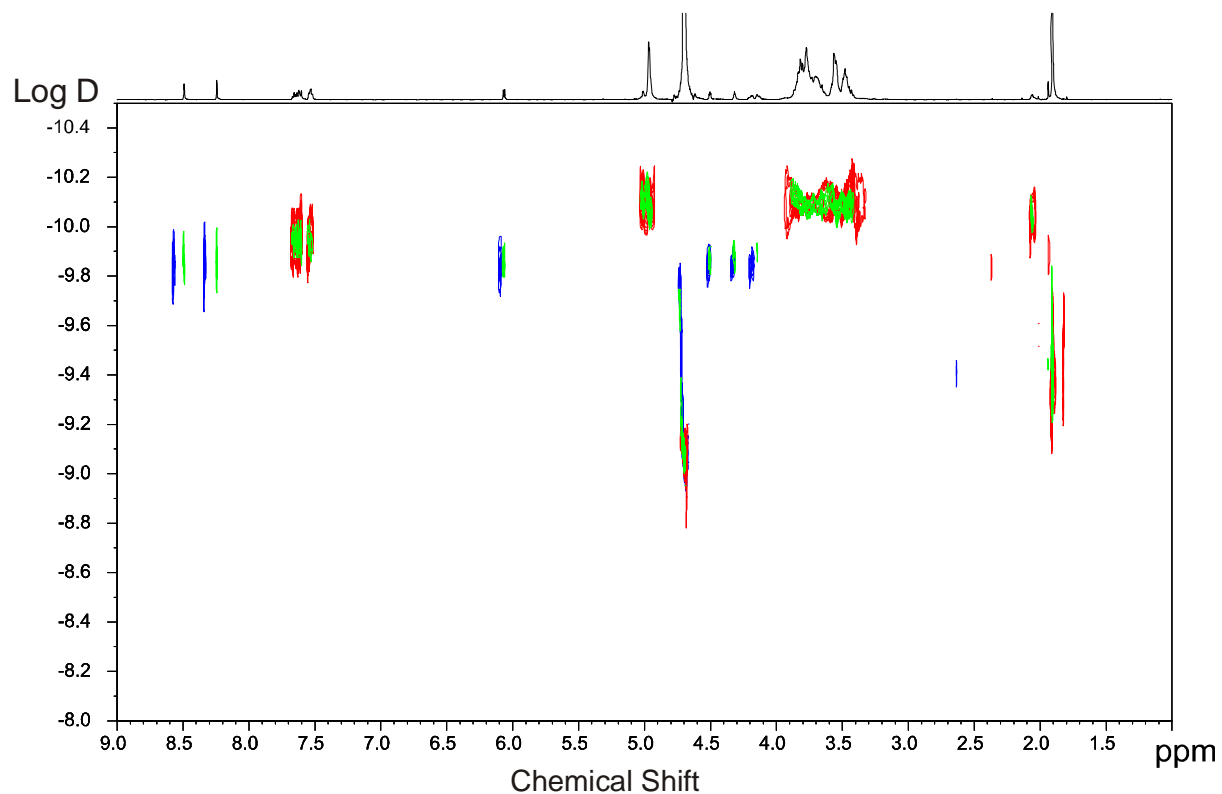
$^1\text{H}$  NMR titration of ATP. 2Na by the tetrapode **5** in  $\text{D}_2\text{O}$  at  $20^\circ\text{C}$  : Part of the spectrum between 9.0 to 6.0 ppm.

## Diffusion NMR experiments



Dosy map of [ATP : Tetrapode **5**] for a diffusion time  $\Delta=200\text{ms}$ . The projection shows the  $^1\text{H}$  spectrum along with the corresponding assignment. It can be noticed that the observed diffusion coefficient of tetrapode **5** increase when it complex the ATP.

blue : ATP ,  $D = 3.21 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ ; red : tetrapode **5** free,  $D = 1.75 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ ; green : [ATP : Tetrapode **5**] complex,  $D = 2.23 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ .



Dosy map of [ATP : Dipode **4**] for a diffusion time  $\Delta=200$ ms. The projection shows the  $^1\text{H}$  spectrum along with the corresponding assignment.

blue : ATP ,  $D = 3.21 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ ; red : dipode **4** ,  $D = 2.40 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ ; green : [ATP : Dipode **4**] ,  $D = 2.42 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ .

	<b>IC<sub>50</sub> (M)</b>
24 h	$6.9 \times 10^{-4}$
48 h	$6.7 \times 10^{-4}$
168 h	$3.9 \times 10^{-4}$

**Table 2 :** IC<sub>50</sub> values obtained for tetrapode **5** at 24h, 48h and 168h, on MRC-5 cells. Values were means of three independent experiments.