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Viologen phosphorus dendritic molecule as carrier of ATP and Mant-ATP. Spectrofluorimetric and NMR studies.

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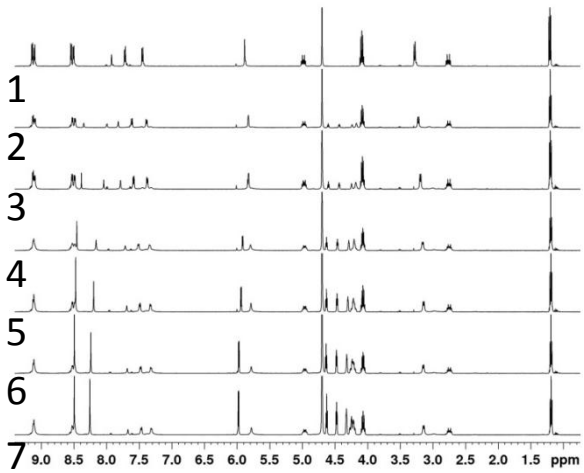

Figure S1. Full ^{1}H NMR titration spectra of the dendrimer when mixed with ATP. The concentration of the dendrimer was kept constant at 1.2 mmol/L. The molar ratio of ATP – dendrimer ranges from 0 to 10 (1-7).

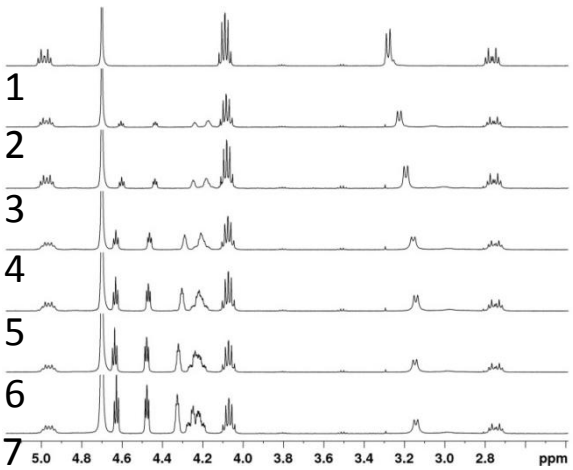

Figure S2. Expanded aliphatic region of the ^{1}H NMR titration spectra of the dendrimer when mixed with ATP. The concentration of the dendrimer was kept constant at 1.2 mmol/L. The molar ratio of ATP – dendrimer ranges from 0 to 10 (1-7)

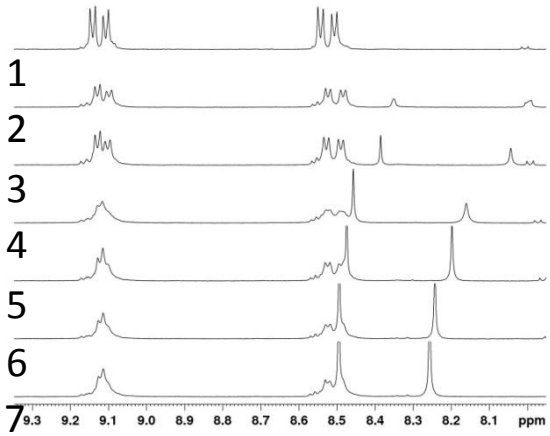

Figure S3. ^{1}H NMR titration spectra of the viologen dendrimer part when mixed with ATP. The concentration of the dendrimer was kept constant at 1.2 mmol/L. The molar ratio of ATP – dendrimer ranges from 0 to 10 (1-7).

Table S1. Comparison of the maximum chemical shift difference (ppm), $\delta_{initial}$ - δ_{final} of the dendrimer ^{1}H resonances on titration with ATP.

Hydrogen position	H1	H2	H3	H4	H5	H6	H7	H8	H9	H10	H11
Chemical shift difference	-0.14	-0.25	-0.25	-0.14	-0.09	-0.01	-0.02	-0.03	-0.01	-0.02	-0.02

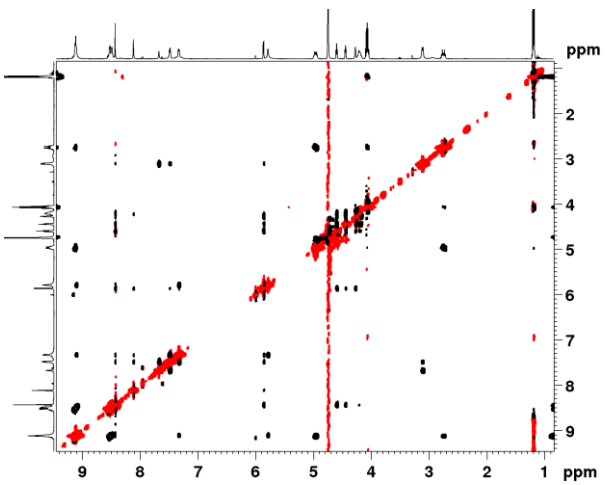

Figure S4. Full ^{1}H-^{1}H ROESY spectrum of the 1/4 dendrimer – ATP mixture.

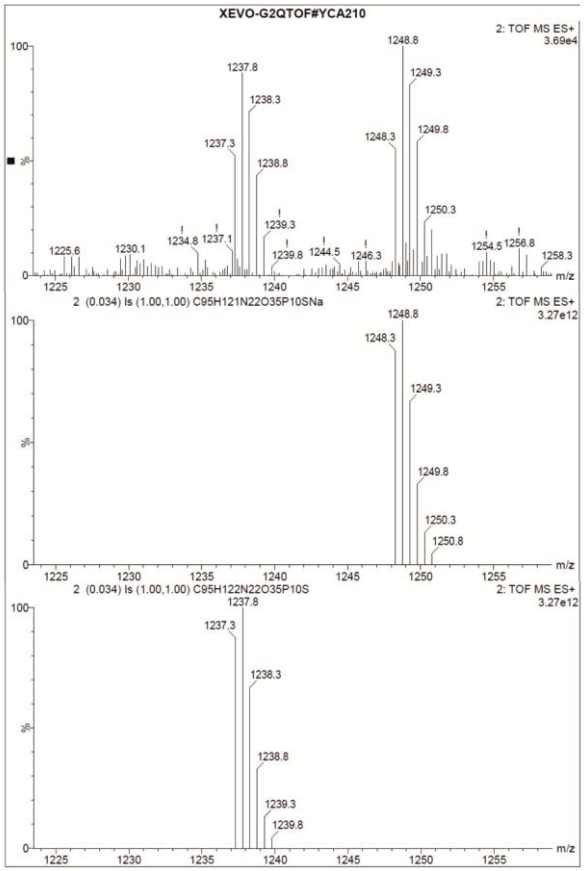

Figure S5. Mass Spectrometry of the ATP – dendrimer complex showing the formation of a 2/1 complex. Spectra were recorded on a Xevo-G2QTOF (Waters) on ESI(+), Flow Injection Analysis (0.15 mL/min) in 100% MeOH (from 100 to 3000 m/z).