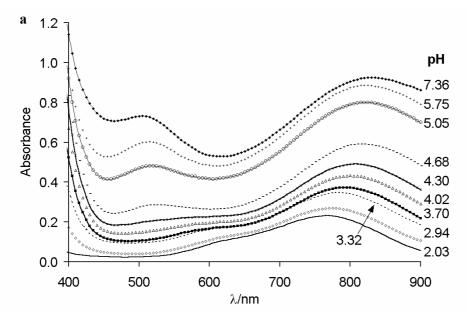
## **Supporting Information**

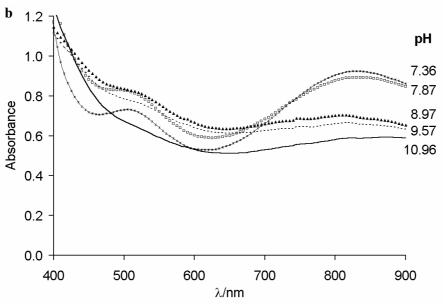
## Oxovanadium(IV) complexes of Salicyl-L-aspartic acid and Salicyl-glycyl-L-aspartic acid

by

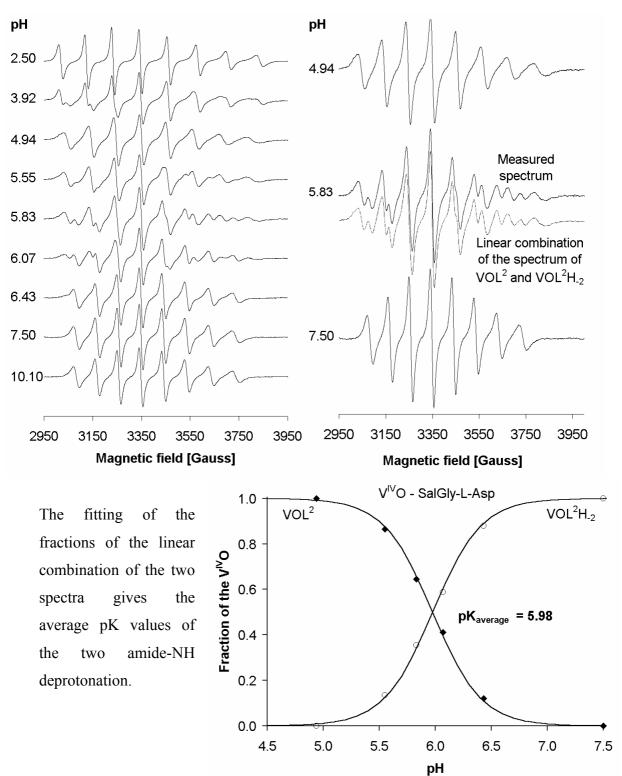
Tamás Jakusch<sup>a</sup>, Susana Marcão<sup>b</sup>, Lígia Rodrigues<sup>c</sup>, Isabel Correia<sup>b</sup>, João Costa Pessoa<sup>b</sup>\*, Tamás Kiss<sup>ad</sup>\*,

**SI-1** UV-Vis spectra of solutions containing  $V^{IV}O^{2+}$  and Sal-L-Asp at different pH values at  $c_{(VO)} \sim 3$  mol dm<sup>-3</sup> and a ligand-to-metal ratio (L<sup>1</sup>:M) of 2.64.

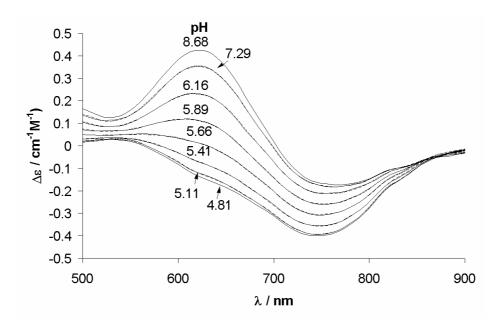




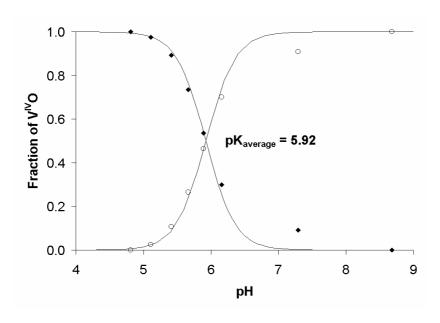
SI-2 The RT - EPR spectra of solutions containing  $V^{IV}O^{2+}$  and SalGly-L-Asp at different pH values at  $c_{(VO)}=1$  mol dm<sup>-3</sup> and  $L^2:M=4$ . The spectra between pH 4.5 and 7.5 can be fitted by a linear combination of the spectra of  $VOL^2$  (spectrum at pH = 4.94) and  $VOL^2H_{-2}$  (spectrum at pH = 7.50).



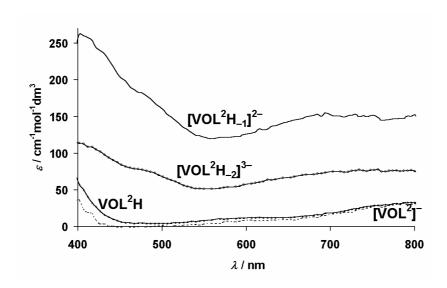
SI-3 Average pK values of the two amide-NH deprotonations as determined from the CD measurements. The CD spectra were measured with solutions containing  $V^{IV}O^{2+}$  (2.7 mol dm<sup>-3</sup>) and SalGly-L-Asp (7.2 mol dm<sup>-3</sup>) for several pH values. The spectra between pH  $\sim$  4.5 and  $\sim$  8.5 can be fitted by a linear combination of the spectra of VOL<sup>2</sup> (spectrum at pH = 4.814) and VOL<sup>2</sup>H<sub>-2</sub> (spectrum at pH = 8.68). For all CD spectra between 4.8 and 8.7, the experimental CD (full lines) and calculated CD (dotted lines) almost coincide.



The fitting of the fractions of the linear combination of the two spectra gives the average pK values of the two amide-NH deprotonations.



SI-4 Calculated Vis spectra for each individual species (except  $VOL^2H_2$ ) formed in the  $V^{IV}O$ -Sal-L-Asp system, using the program PSEQUAD and the formation constants listed in Table 1.



## **SI-5** Determination the two pK values of the amide NH deprotonations from the LN-EPR measurements.

