Supporting information

Vanadyl complexes with dansyl-labelled di-picolinic acid ligands: synthesis, phosphatase inhibition activity and cellular uptake studies

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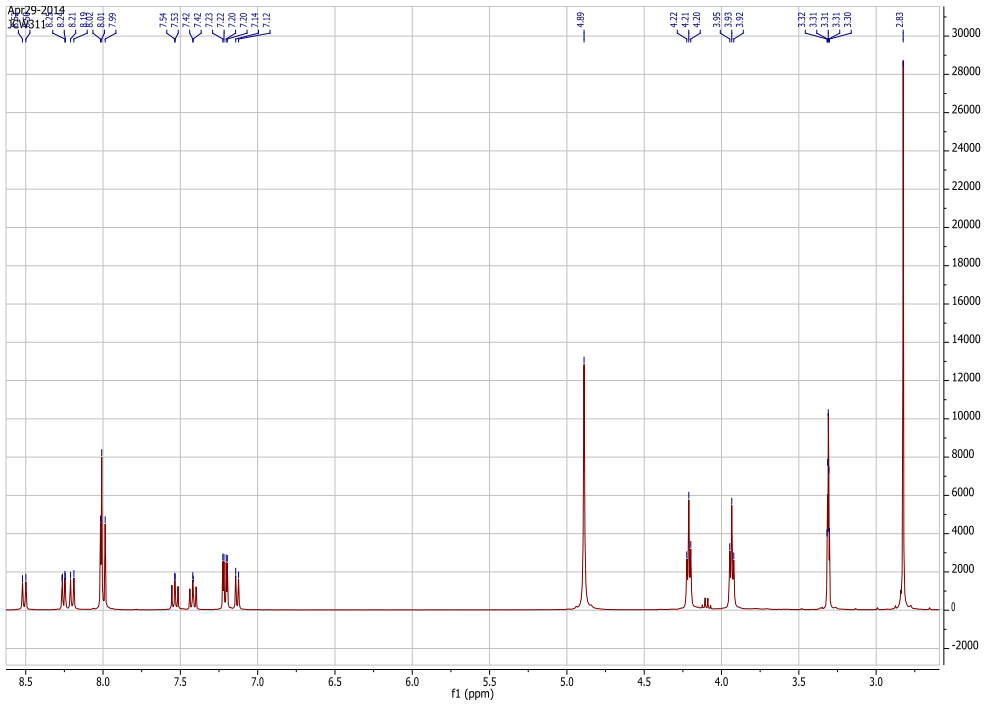

Figure S1: ^{1}H NMR spectrum of **8** (400MHz, CD_3OD)

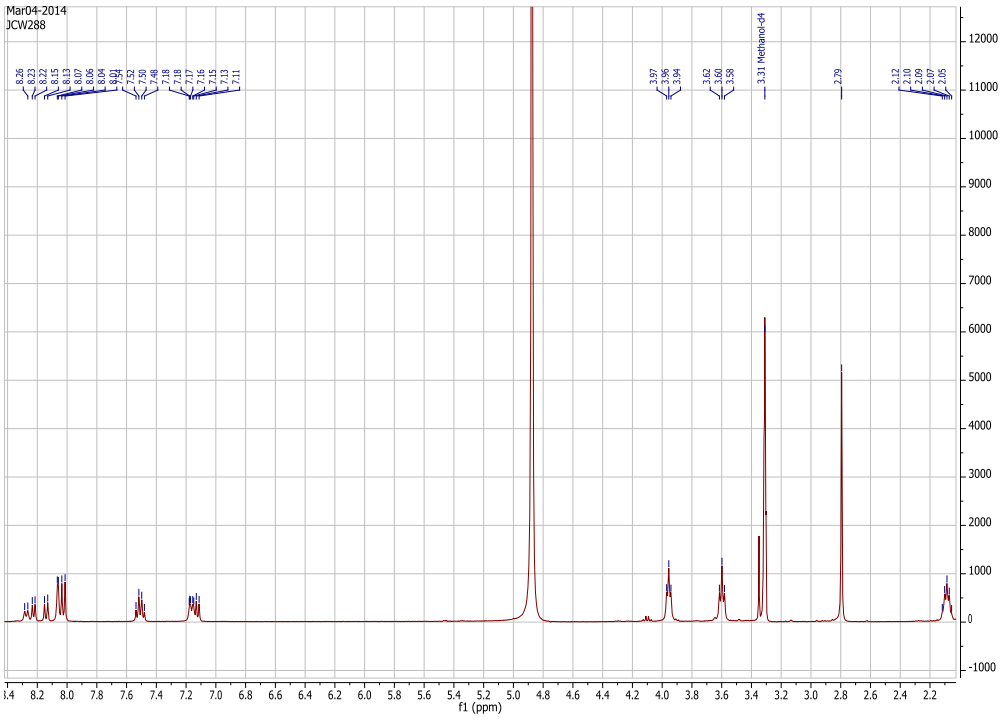

Figure S2: ^{1}H NMR spectrum of **13** (400MHz, CD_3OD)

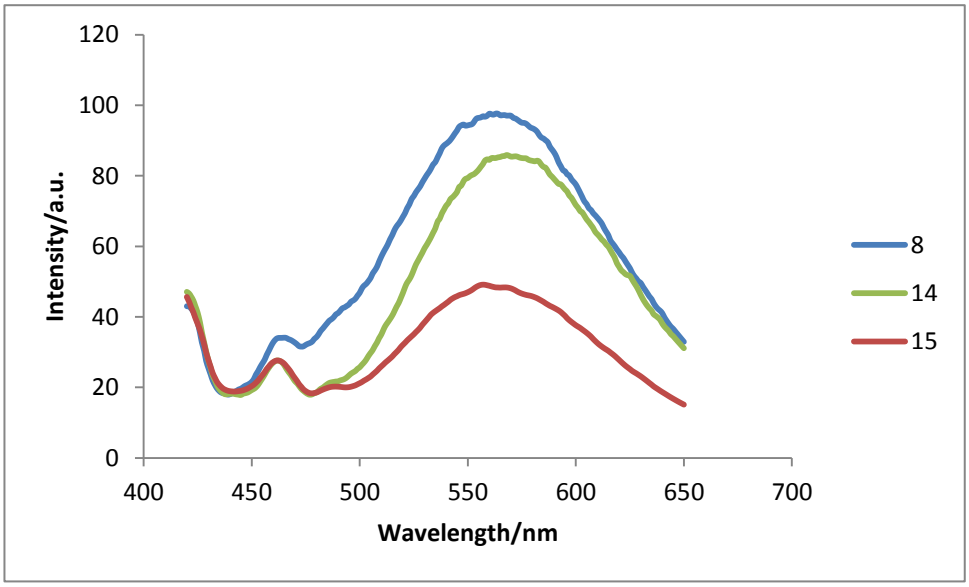

Figure S3. Fluorescence spectra of **8**, **14**, and **15** at 30µM in 100 mM Tris buffer containing 1 mM DTT. Readings were taken using a Varian fluorescence spectrometer in a 96-well plate with excitation of 340 nm and emission recorded from 400-650 nm.

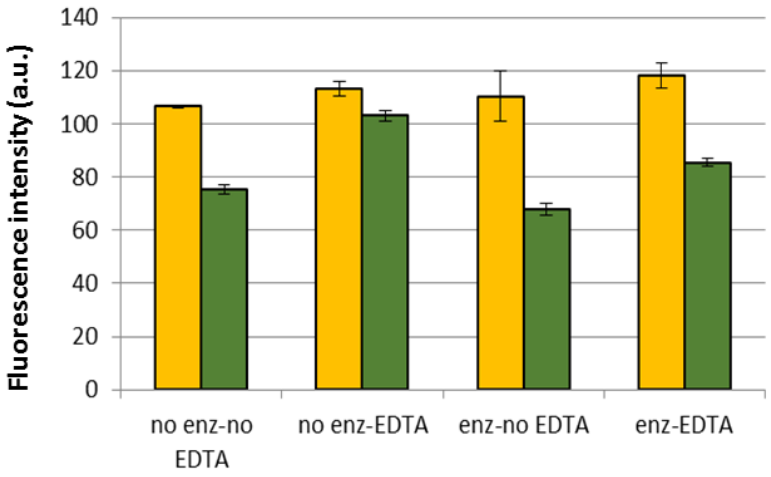

Figure S4. Fluorescence intensity at 560 nm of a 30 µM solution of ligand **8** (yellow bars) and complex **14** (green bars) in the presence or absence of LMW-PTP (Enz) and 1mM EDTA in Tris buffer containing 1mM DTT. Reading was taken after 5 minutes incubation at room temperature. Intensity is recorded ±standard deviation of triplicate repeats.

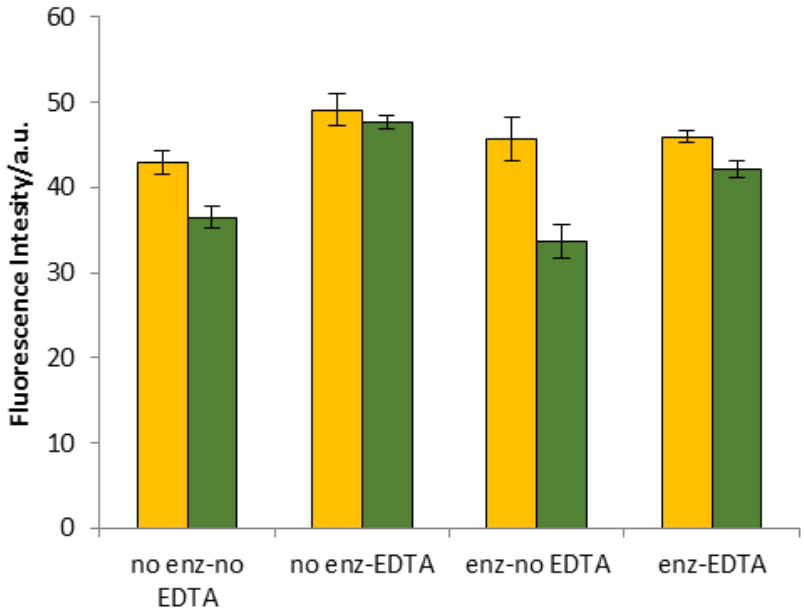

Figure S5. Fluorescence intensity at 560 nm of a 30 µM solution of ligand **13** (yellow bars) and complex **15** (green bars) in the presence or absence of LMW-PTP (Enz) and 1mM EDTA in Tris buffer containing 1mM DTT. Reading was taken after 2 hours incubation at room temperature. Intensity is recorded ±standard deviation of triplicate repeats.

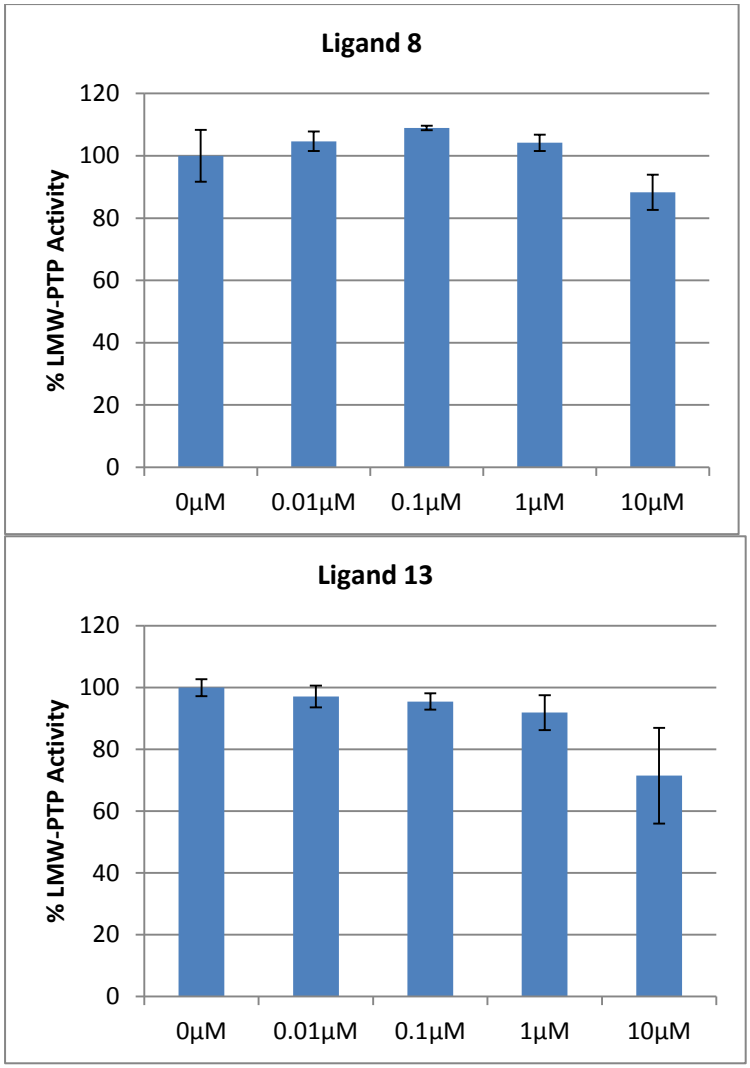

Figure S6. Activity of LMW-PTP in the presence of increasing amounts of ligands **8** and **13**. LMW-PTP activity was measured using the OMFP method (see Experimental Details – Phosphatase inhibition assays). The ligand solutions (prepared from 10 mM stock solution in DMSO and further diluted in water containing 1% DMSO to the required concentrations) were incubated with the enzyme in the buffer (100 mM Tris, pH = 7.4, containing 1 mM DTT) for 10 minutes at room temperature before reaction was initiated by addition of OMFP. Reading was taken over 30 minutes at 60 s intervals.

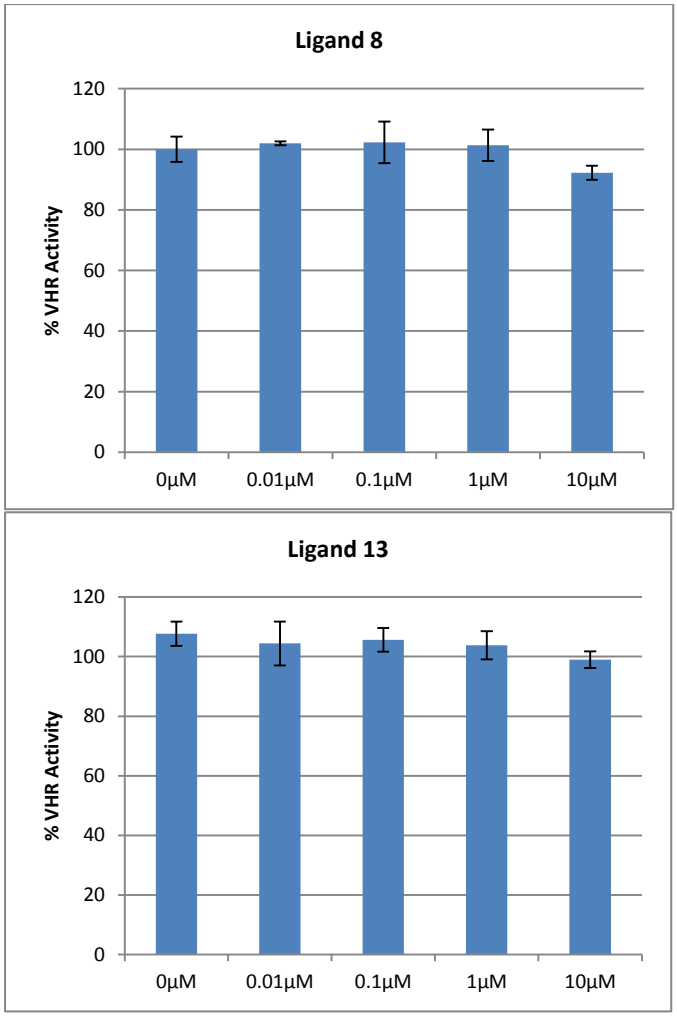

Figure S7. Activity of VHR in the presence of increasing amounts of ligands **8** and **13**. VHR activity was measured using the OMFP method (see Experimental Details – Phosphatase inhibition assays). The ligand solutions (prepared from 10 mM stock solution in DMSO and further diluted in water containing 1% DMSO to the required concentrations) were incubated with the enzyme in the buffer (100 mM Tris, pH = 7.4, containing 1 mM DTT) for 10 minutes at room temperature before reaction was initiated by addition of OMFP. Reading was taken over 30 minutes at 60 s intervals.