

Electronic supplementary information (ESI)

Bis- and tris(pyridyl)amine-oxidovanadium complexes: Characteristics and insulin-mimetic potential

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Table S1. Calculated (BHandHLYP functional, 6-311g(d,p) basis set) EPR parameters for V^{IV}O complexes.^a

	$A_{\text{iso}}^{\text{calcd}}$	T_x^{calcd}	T_y^{calcd}	T_z^{calcd}	A_x^{calcd}	A_y^{calcd}	A_z^{calcd}	$ A_x - A_y ^{\text{calcd}}$	A_z^{exptl}	Dev. (%) ^b
[VO(bp-OH)Cl ₂] ^c	-88.8	32.4	34.9	-67.3	-56.4	-53.9	-156.1	2.4		
[VO(bp-OH)(CH ₃ OH) ₂] ^d	-96.1	32.2	33.7	-65.9	-63.9	-62.4	-162.0	1.5	-164.1	-1.3
[VO(bp-OH)(CH ₃ OH) ₃] ^e	-109.6	32.0	33.1	-65.1	-77.6	-76.5	-174.7	1.1	-175.6	-0.5
[VO(bp-O)HSO ₄] ^f	-93.7	32.0	35.7	-67.7	-61.7	-58.0	-161.4	3.8		
[VO(bp-O)(H ₂ O)] ^g	-96.5	30.8	34.7	-65.5	-65.7	-61.7	-162.0	3.9	-162.4	-0.2

^aAll values provided in 10⁻⁴ cm⁻¹. ^bPercentage deviation from the experimental value calculated as: $(|A_z|^{\text{calcd}} - |A_z|^{\text{exptl}})/|A_z|^{\text{exptl}}$. ^c[(N_{pyr}, N_{amine}^{ax}, N_{pyr}); Cl; Cl] coordination. ^dPredominant species with [(N_{pyr}, N_{amine}^{ax}, N_{pyr}); CH₃OH; CH₃OH] coordination. ^eMinor species with [(N_{pyr}, N_{amine}^{ax}); CH₃OH; CH₃OH; CH₃OH] coordination. ^f[(N_{pyr}, N_{amine}^{ax}, N_{pyr}, O⁻); HSO₄⁻] coordination. ^g[(N_{pyr}, N_{amine}^{ax}, N_{pyr}, O⁻); H₂O] coordination.

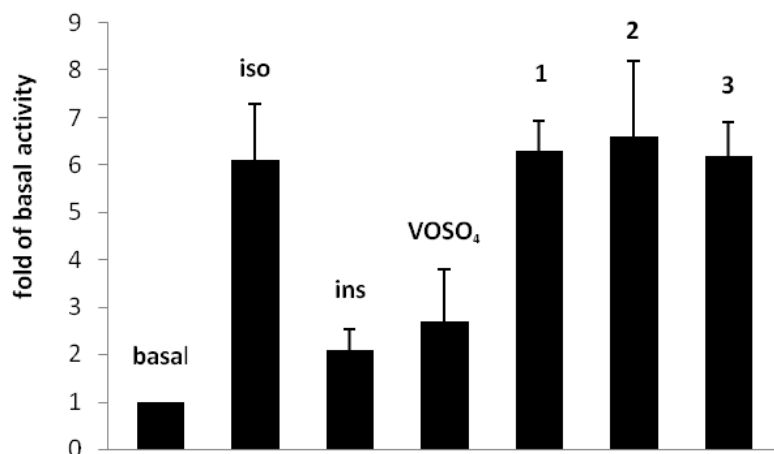


Fig. S1 Results of the glycerol release lipolysis assay for VO(SO₄), **1**, **2** and **3** are shown as the fold of the basal activity. All samples, except the basal, were treated with isoprenaline. The concentrations used were as follows, insulin 1.67 nM, VO(SO₄) 0.5 mM, **1**, **2** and **3** 0.25 mM. Data are expressed as mean $\pm$ SEM, $n=3$.