Supplementary Information for

Hydrophobicity Enhances Membrane Affinity and Anti-Cancer Effects of Schiff Base Vanadium(V) Catecholate Complexes

Debbie C. Crans,^{*a,b} Jordan T. Koehn,^a Stephanie M. Petry,^a Caleb M. Glover,^a Asanka Wijetunga,^c Ravinder Kaur,^c Aviva Levina,^c and Peter A. Lay^{*c}

^aChemistry Department, Colorado State University, Fort Collins, Colorado 80523, United States; ^bCell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado 80523, United States; and ^cSchool of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia.

Table of Contents

1.	NMR Spectra
	1.2. 1D ¹ H NMR Spectra of ¹ H NMR Spectra of [VO(Hshed)(cat)] in D ₂ O, d ₆ -DMSO, and in a Series of Reverse MicellesS3
2.	Dynamic Light Scattering Data for [V(O)2(Hshed)], H2shed, [VO(Hshed)(cat)], H2cat, [VO(Hshed)(dtb)], and H2dtbS4
3.	ReferencesS5

1. NMR Spectra

1.1 ¹H NMR Spectra of [VO(Hshed)(dtb)] in D₂O, d₆-DMSO, and in a Series of Reverse Micelles.



Figure S1: ¹H NMR spectra of [VO(Hshed)(dtb)] in d₆-DMSO, *iso*-octane, and in a series of RMs ($w_0 = 8, 12, 16, and 20$ prepared from 0.750 M AOT/*iso*-octane stock solution). The spectrum in D₂O was recorded after 60 min. and the spectra in RMs was recorded after 50 min. once equilibrium had been established. Proton labeling scheme is found in Figure 1. SalA = Salicylaldehyde.



1.2 ¹H NMR Spectra of [VO(Hshed)(cat)] in D₂O, d₆-DMSO, and in a Series of Reverse Micelles.

Figure S2: ¹H NMR spectra of [VO(Hshed)(cat)] in d₆-DMSO, D₂O, and in a series of RMs ($w_0 = 8, 12, 16, and 20$ prepared from 0.750 M AOT/*iso*-octane stock solution). The spectrum in D₂O was recorded after 50 min. and the spectra in RMs was recorded after 40 min. once equilibrium had been reached. Proton labeling scheme is found in Figure 1. SalA = Salicylaldehyde.

2. Dynamic Light Scattering Data for [V(O)₂(Hshed)], H₂shed, [VO(Hshed)(cat)], H₂cat,

[VO(Hshed)(dtb)], and H₂dtb.

Table S1. Dynamic Light Scattering measurements on [V(O)₂(Hshed)], H₂shed, [VO(Hshed)(cat)], H₂cat, [VO(Hshed)(dtb)], and H₂dtb in 0.1 M AOT/isooctane RMs.

	$w_0 = 12$	$w_o = 20$
N(probe)/N(micelle)	2.3	1.4
[V(O) ₂ (Hshed)] r _h ^a (nm)	3.9 (± 0.3)	4.5 (± 0.3)
PDI [V(O) ₂ (Hshed)]	0.33 (±0.16)	0.52 (±0.17)
H ₂ shed r _h ^a (nm)	4.0 (± 0.3)	4.3 (± 0.3)
PDI H ₂ shed	0.20 (±0.08)	0.60 (±0.20)
[VO(Hshed)(cat)] r _h ^a (nm)	3.5 (±0.3)	4.3 (± 0.4)
PDI [VO(Hshed)(cat)]	0.27 (±0.12)	0.46 (±0.18)
H₂cat r _h ª (nm)	3.8 (±0.2)	4.4 (± 0.3)
PDI H ₂ cat	0.43 (±0.16)	0.23 (±0.09)
[VO(Hshed)(dtb)] r _h ^a (nm)	3.6 (±0.5)	4.1 (±0.3)
PDI [VO(Hshed)(dtb)]	0.45 (±0.08)	0.16 (±0.05)
H ₂ dtb r _h ^a (nm)	3.8 (±0.2)	4.3 (±0.3)
PDI H ₂ dtb	0.22 (±0.08)	0.48 (±0.11)
Blank r _h ª (nm)	3.6 (± 0.3)	4.6 (± 0.3)
PDI Blank	0.42 (±0.17)	0.50 (±0.19)
Lit. r _h ^b (nm)	3.7	4.4

^aRadius measurements were taken from the volume distribution ^bRef. 1.

Interpretation of DLS measurements on [V(O)₂(Hshed)], H₂shed, [VO(Hshed)(cat)], H₂cat, [VO(Hshed)(dtb)], and H₂dtb Containing AOT/isooctane RMs. DLS established the formation of RMs. Samples of [V(O)₂(Hshed)], H₂shed, [VO(Hshed)(cat)], H₂cat, [VO(Hshed)(dtb)], or H₂dtb RMs were prepared using 0.10 M AOT/isooctane and the results are shown in Table S1. The average radius obtained from w_0 sizes 12, and 20 compared favorably with those reported previously in the literature.^{1, 2, 3} These results were observed with RMs prepared with and without [V(O)₂(Hshed)], H₂shed, [VO(Hshed)(cat)], H₂cat, [VO(Hshed)(dtb)], or H₂dtb. These results showed that RMs formed, and that the presence of [V(O)₂(Hshed)], H₂shed, [VO(Hshed)(cat)], H₂cat, [VO(Hshed)(dtb)], or H₂dtb did not significantly affect the size or stability of the RM.

3. References:

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