

Supporting Information

Bis(allixinato)oxovanadium(IV) Complex Is A Potent Anti-Diabetic Agent: Studies on Structure-Activity Relationship For A Series of Hydroxypyrrone Vanadium Complexes

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1) Results of oral glucose tolerance tests (OGTT) in STZ-mice treated with vanadyl complex

Time (min)	0	15	30	60	90	120	AUC ($\text{mg}\cdot\text{h}\cdot\text{mL}^{-1}$)
Control	318 ± 116 (mg/dL)	460 ± 143	461 ± 134	473 ± 136	414 ± 147	377 ± 187	868 ± 267
Complex 2	286 ± 99	422 ± 120	450 ± 108	370 ± 83	393 ± 118	332 ± 118	776 ± 199
Complex 3	$174 \pm 26^{*\#}$	$284 \pm 32^{*\#}$	$316 \pm 40^{*\#}$	$283 \pm 70^*$	$222 \pm 62^{*\#}$	197 ± 51	$514 \pm 92^{*\#}$

Significance; * $p < 0.05$ vs. control mice, # $p < 0.05$ vs. complex 2

2) Analytical and spectroscopic data of compounds

Bis(3-hydroxy-4-pyronato)oxovanadium(IV) complex (1). The yield: 49% based on V; ESR (H_2O): $g_0 = 1.968$, $g_{\perp} = 1.982$, $g_{\parallel} = 1.942$, $A_0 = 95 \times 10^{-4}$, $A_{\perp} = 56 \times 10^{-4}$, $A_{\parallel} = 172 \times 10^{-4} \text{ cm}^{-1}$; IR (cm^{-1} , KBr disk): 1600, 1560, 1465 ($\nu_{\text{C=O}}$, $\nu_{\text{C=C}}$); 959 cm^{-1} ($\nu_{\text{V=O}}$); UV/Vis (H_2O): $\lambda_{\max} = 270$ ($\varepsilon = 9077 \text{ M}^{-1}\cdot\text{cm}^{-1}$), and 820 (25) nm; HRMS (m/z): $[\text{M}]^+$ calcd for $\text{C}_{10}\text{H}_6\text{O}_7\text{V}$, 289.9631; found: 289.9642.

Bis(maltolato)oxovanadium(IV) complex (2). The yield: 74% based on V; ESR (H_2O): $g_0 = 1.969$, $g_{\perp} = 1.982$, $g_{\parallel} = 1.942$, $A_0 = 94 \times 10^{-4}$, $A_{\perp} = 56 \times 10^{-4}$, $A_{\parallel} = 171 \times 10^{-4} \text{ cm}^{-1}$; IR (cm^{-1} , KBr disk): 1610, 1550, 1460 ($\nu_{\text{C=O}}$, $\nu_{\text{C=C}}$); 993 ($\nu_{\text{V=O}}$); UV/Vis (H_2O): $\lambda_{\max} = 275$ nm ($\varepsilon = 12000 \text{ M}^{-1}\cdot\text{cm}^{-1}$), 327 (7600), 633 (19), and 873 (27); HRMS (m/z): $[\text{M}]^+$ calcd for $\text{C}_{12}\text{H}_{10}\text{O}_7\text{V}$, 317.9944; found: 317.9950.

Bis(allxinato)oxovanadium(IV) complex (3). The yield: 67% based on V; ESR (DMSO): $g_0 = 1.969$, $g_{\perp} = 1.981$, $g_{\parallel} = 1.944$, $A_0 = 97 \times 10^{-4}$, $A_{\perp} = 57 \times 10^{-4}$, $A_{\parallel} = 176 \times 10^{-4} \text{ cm}^{-1}$; IR (cm^{-1} , KBr disk): 1610, 1550, 1430 ($\nu_{\text{C=O}}$, $\nu_{\text{C=C}}$); 997 cm^{-1} ($\nu_{\text{V=O}}$); UV/Vis (DMSO): $\lambda_{\max} = 277$ nm ($\varepsilon = 13600 \text{ M}^{-1}\cdot\text{cm}^{-1}$), 327 (5300), and 819 (27) nm; HRMS (m/z): $[\text{M}]^+$ calcd for $\text{C}_{24}\text{H}_{34}\text{O}_9\text{V}$, 517.1643; found: 517.1635.

Bis(ethylmaltolato)oxovanadium(IV) complex (4). The yield: 80% based on V; ESR (DMSO): $g_0 = 1.970$, $g_{\perp} = 1.983$, $g_{\parallel} = 1.943$, $A_0 = 95 \times 10^{-4}$, $A_{\perp} = 56 \times 10^{-4}$, $A_{\parallel} = 174 \times 10^{-4} \text{ cm}^{-1}$; IR (cm^{-1} , KBr disk): 1600, 1550, 1470 ($\nu_{\text{C=O}}$, $\nu_{\text{C=C}}$); 992 cm^{-1} ($\nu_{\text{V=O}}$); UV/Vis (H_2O): $\lambda_{\max} = 277$ ($\varepsilon = 13000 \text{ M}^{-1}\cdot\text{cm}^{-1}$), 329 (9000), 631 (23), and 873 (32) nm; HRMS (m/z): $[\text{M}]^+$ calcd for $\text{C}_{14}\text{H}_{14}\text{O}_7\text{V}$, 346.0257; found: 346.0251.

Bis(kojato)oxovanadium(IV) complex (5). The yield: 56% based on V; ESR (H_2O): $g_0 = 1.972$, $g_{\perp} = 1.987$, $g_{\parallel} = 1.940$, $A_0 = 94 \times 10^{-4}$, $A_{\perp} = 54 \times 10^{-4}$, $A_{\parallel} = 175 \times 10^{-4} \text{ cm}^{-1}$; IR (cm^{-1} , KBr disk): 1620, 1560, 1470 ($\nu_{\text{C=O}}$, $\nu_{\text{C=C}}$); 950 cm^{-1} ($\nu_{\text{V=O}}$); UV/Vis (H_2O): $\lambda_{\max} = 262$ ($\varepsilon = 14453 \text{ M}^{-1}\cdot\text{cm}^{-1}$), 627 (14), and 857 (32) nm; HRMS (m/z): $[\text{M}]^+$ calcd for $\text{C}_{12}\text{H}_{10}\text{O}_9\text{V}$, 349.9843; found: 349.9837.

3) Elemental analysis of compounds

Compound	Formula		Calcd.	Found
1	$C_{10}H_6O_7V \cdot H_2O$	C	39.09	38.78
		H	2.61	2.54
		N	0.00	0.00
2	$C_{12}H_{10}O_7V$	C	45.45	45.17
		H	3.18	3.31
		N	0.00	0.00
3	$C_{24}H_{34}O_9V$	C	55.71	55.49
		H	6.62	6.47
		N	0.00	0.00
4	$C_{14}H_{14}O_7V$	C	48.71	49.01
		H	4.09	4.27
		N	0.00	0.00
5	$C_{12}H_{10}O_9V \cdot 1.5H_2O$	C	38.32	38.60
		H	3.48	3.36
		N	0.00	0.00