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Supplementary Information

Synthesis, crystal structure, and insulin-mimetic activity of zinc(II) complexes with 4-alkyl- and 4,5-dialkyl-3-hydroxythiazole-2(3*H*)-thiones as a new class of hypoglycemic agent candidates

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Contents

Table S1. Crystallographic data and refinement statistics for Zn(**4**)$_2$, Zn(**5f**)$_2$, Zn(**5h**)$_2$, Zn(**6**)$_2$, and Zn(**5h**)$_2$ with pyridine

Complex		Zn(**4**)$_2$	Zn(**5f**)$_2$
Formula		$C_{10}H_{12}N_2O_2S_6Zn$	$C_{10}H_{12}N_2O_2S_4Zn$
Formula weight		441.93	385.83
Temperature /K		120	120
Wavelength /Å		0.71073	0.71073
Crystal system		Monoclinic	Monoclinic
Space group		$P2_1/n$	$P2_1/c$
Unit cell dimensions	a /Å	8.6523(3)	11.6997(5)
	b /Å	21.5296(8)	7.5824(3)
	c /Å	10.1015(4)	17.5946(7)
	α /deg	90	90
	β /deg	103.2029(6)	108.7288(6)
	γ /deg	90	90
Volume /Å^3		1831.97(12)	1432.83(10)
Z		4	4
Density (calculated)		1.602 Mg/m^3	1.789 Mg/m^3
Absorption coefficient		1.805 mm^{-1}	2.293 mm^{-1}
F(000)		912	784
Crystal size		0.354x0.241x0.203 mm^3	0.403x0.263x0.203 mm^3
Theta range for data collection		2.596 to 25.998°	2.522 to 25.999°
Index ranges		–10<=h<=9, –26<=k<=17, –12<=l<=12	–14<=h<=14, –9<=k<=9, –10<=l<=21
Reflections collected		10590	7993
Independent reflections		3608 [R(int) = 0.0229]	2810 [R(int) = 0.0176]
Completeness to theta = 25.242°		99.9%	99.7%
Absorption correction		Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission		0.7457 and 0.6775	0.7457 and 0.6564
Refinement method		Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters		3608 / 0 / 208	2810 / 0 / 172
Goodness-of-fit on F^2		1.030	1.045
Final R indices [I>2sigma(I)]		R_1 = 0.0223, wR_2 = 0.0553	R_1 = 0.0299, wR_2 = 0.0855
R indices (all data)		R_1 = 0.0249, wR_2 = 0.0570	R_1 = 0.0312, wR_2 = 0.0865
Extinction coefficient		n/a	n/a
Largest diff. peak and hole		0.308 and –0.370 e.Å^{-3}	0.756 and –0.747 e.Å^{-3}

Table S1. (continued)

Complex		Zn(**5h**)$_2$	Zn(**6**)$_2$
Formula		$C_{12}H_{16}N_2O_2S_4Zn$	$C_{14}H_{16}N_2O_2S_4Zn$
Formula weight		413.88	437.90
Temprature /K		120	120
Wavelength /Å		0.71073	0.71073
Crystal system		Triclinic	Monoclinic
Space group		*P*-1	*C*2/*c*
Unit cell dimensions	*a* /Å	7.5733(16)	11.9955(7)
	b /Å	8.7066(19)	10.9525(7)
	c /Å	13.442(3)	12.7788(8)
	α /deg	78.741(2)	90
	β /deg	74.963(2)	94.2060(10)
	γ /deg	88.673(3)	90
Volume /Å^3		839.1(3)	1674.37(18)
Z		2	4
Density (calculated)		1.638 Mg/m^3	1.737 Mg/m^3
Absorption coefficient		1.964 mm^{-1}	1.974 mm^{-1}
F(000)		424	896
Crystal size		0.209x0.145x0.109 mm^3	0.292x0.179x0.050 mm^3
Theta range for data collection		1.60 to 26.00°	2.521 to 25.994°
Index ranges		–9<=h<=9, –10<=k<=10, –16<=l<=16	–9<=h<=14, –13<=k<=13, –13<=l<=15
Reflections collected		8842	4733
Independent reflections		3303 [R(int) = 0.0413]	1642 [*R*(int) = 0.0281]
Completeness to theta = 25.242°		100.0%	99.9%
Absorption correction		Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission		0.7457 and 0.6376	0.7457 and 0.6427
Refinement method		Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters		3303 / 0 / 190	1642 / 0 / 105
Goodness-of-fit on F^2		1.006	1.033
Final *R* indices [*I*>2sigma(*I*)]		R_1 = 0.0376, wR_2 = 0.0844	R_1 = 0.0232, wR_2 = 0.0568
R indices (all data)		R_1 = 0.0609, wR_2 = 0.0963	R_1 = 0.0262, wR_2 = 0.0600
Extinction coefficient		n/a	n/a
Largest diff. peak and hole		0.562 and –0.496 e.Å^{-3}	0.320 and –0.218 e.Å^{-3}

Table S1. (continued)

Complex		Zn(**3**)$_2$ (with pyridine)	Zn(**5f**)$_2$ (with pyridine)
Formula		$C_{25}H_{19}Cl_2N_3O_2S_4Zn$	$C_{15}H_{17}N_3O_2S_4Zn$
Formula weight		657.97	464.93
Temprature /K		93	120
Wavelength /Å		0.71073	0.71073
Crystal system		Monoclinic	Monoclinic
Space group		$P2_1/c$	$P2_1$
Unit cell dimensions	a /Å	13.8856(3)	8.3806(3)
	b /Å	15.5863(4)	13.3652(4)
	c /Å	12.3909(3)	9.0229(3)
	α /deg	90	90
	β /deg	92.948(2)	103.7934(4)
	γ /deg	90	90
Volume /Å^3		2678.15(11)	981.50(6)
Z		4	2
Density (calculated)		1.632 Mg/m^3	1.573 Mg/m^3
Absorption coefficient		1.459 mm^{-1}	1.690 mm^{-1}
F(000)		1336	476
Crystal size		0.111x0.091x0.053 mm^3	0.40x0.22x0.18 mm^3
Theta range for data collection		2.612 to 27.499	2.32 to 27.90°
Index ranges		–17<= h<=17, –20<=k<=20, –16<=l<=13	–7<= h<=11, –17<=k<=17, –11<=l<=9
Reflections collected		41661	25560
Independent reflections		6106[R(int) = 0.0486]	4202 [R(int) = 0.0103]
Completeness to theta = 25.242°		99.9%	99.70%
Absorption correction		multi-scan	Empirical
Max. and min. transmission		0.926 and 0.655	0.7518 and 0.5505
Refinement method		Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters		6106 / 0 / 336	4202 / 1 / 230
Goodness-of-fit on F^2		1.027	1.064
Final R indices [I>2sigma(I)]		R_1 = 0.0317 and wR_2 = 0.0662	R_1 = 0.0168, wR_2 = 0.0444
R indices (all data)		R_1 = 0.0442 and wR_2 = 0.0696	R_1 = 0.0169, wR_2 = 0.0445
Extinction coefficient		n/a	n/a
Largest diff. peak and hole		0.46 and –0.40 eÅ^{-3}	0.217 and –0.249 e.Å^{-3}

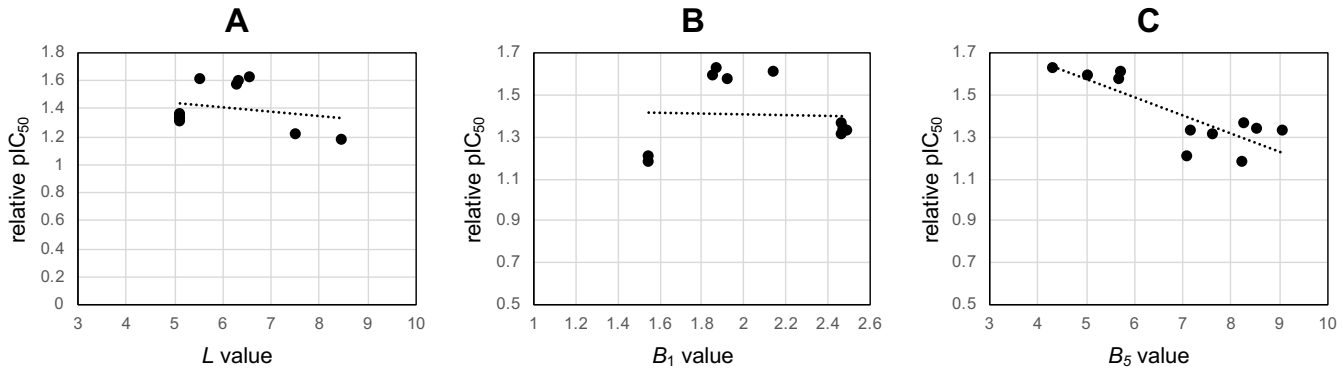

Fig. S1. Plots of the relative pIC_{50} values (in Table 3) of the zinc(II) complexes, Zn(**1a**–**e**)$_2$, Zn(**2a**)$_2$, Zn(**2f**)$_2$, Zn(**4**)$_2$, Zn(**5f**)$_2$, Zn(**5h**)$_2$, and Zn(**6**)$_2$, against (**A**) the Verloop's sterimol length, *L*, (**B**) the V sterimol minimum width, B_1, and (**C**) the sterimol maximum width, B_5.

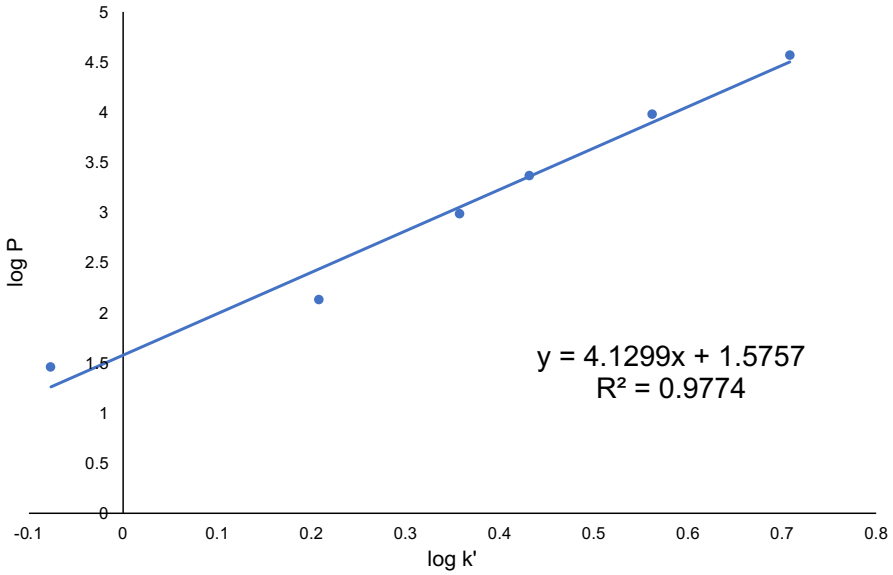

Fig. S2. Calibration curve generating by plotting log*P* against log*k*' obtained by the RP-HPLC for a series of standards (phenol, benzene, bromobenzene, naphthalene, biphenyl, and phenanthrene).