Transferrin-inspired iron delivery across the cell membrane using $[(L_2Fe)_2(\mu\text{-}O)]$ (L = chlorquinaldol) to harness anticancer activity of ferroptosis

Nalin Abeydeera, Khalil Mudarmah, Bishnu D. Pant, Jeanette A. Krause, Yao-Rong Zheng, and Songping D.

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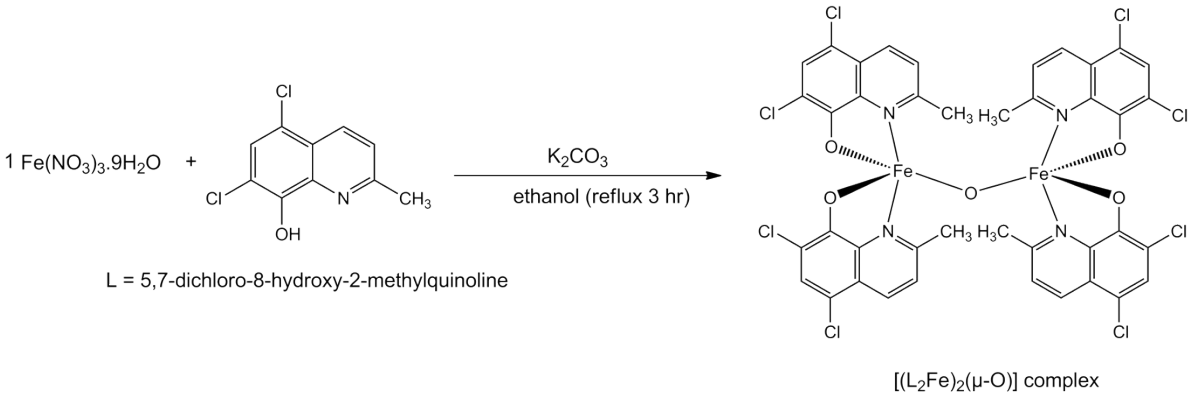

Scheme S1. Synthesis of $[(L_2Fe)_2(\mu\text{-}O)]$ (**1**) in ethanol.

Table S1. Results of elemental analysis of $C_{40}H_{24}N_4O_5Cl_8Fe_2$ (**1**)

Formula $C_{40}H_{24}N_4O_5Cl_8Fe_2$	Calculated	Found
Fe%	10.78	10.61
C%	46.38	46.44
H%	2.34	2.43
N%	5.41	5.31

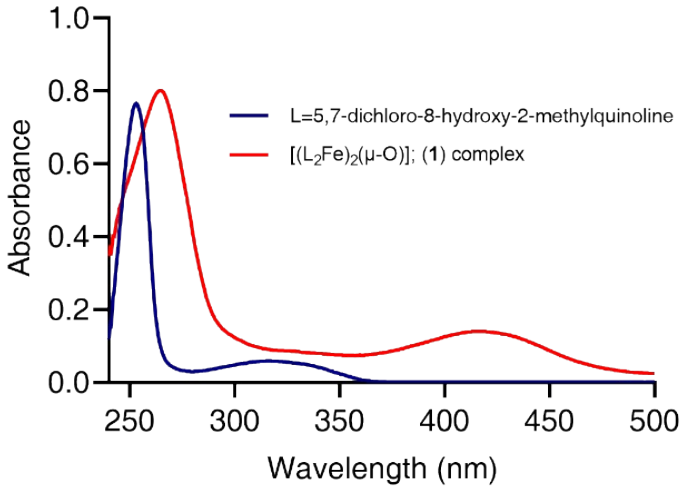

Figure S1. UV-vis spectra of $[(L_2Fe)_2(\mu\text{-}O)]$ (**1**) and the ligand L in chloroform.
(The peak at ~270 nm is due to a π-π* transition in the ligand, while the transition at ~400 nm is a LMCT).

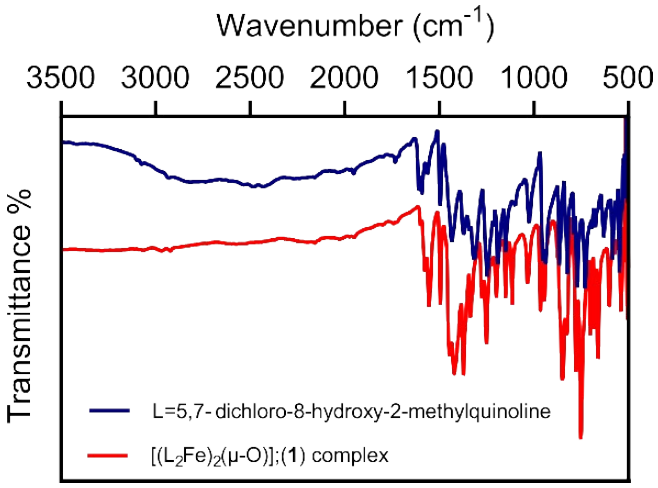

Figure S2. FT-IR spectra of $[(L_2Fe)_2(\mu\text{-}O)]$ (**1**) complex and ligand.
(The IR absorption peaks at 1579 cm^{-1}, 1500 cm^{-1}, and 1387 cm^{-1} correspond to the skeleton vibration of quinoline rings. The IR absorption peak at 1203 cm^{-1} corresponds to the C-O stretching vibration. And the IR absorption peak appearing at 775 cm^{-1} corresponds to the out-of-plane bending vibration of C-H in the quinoline ring.)

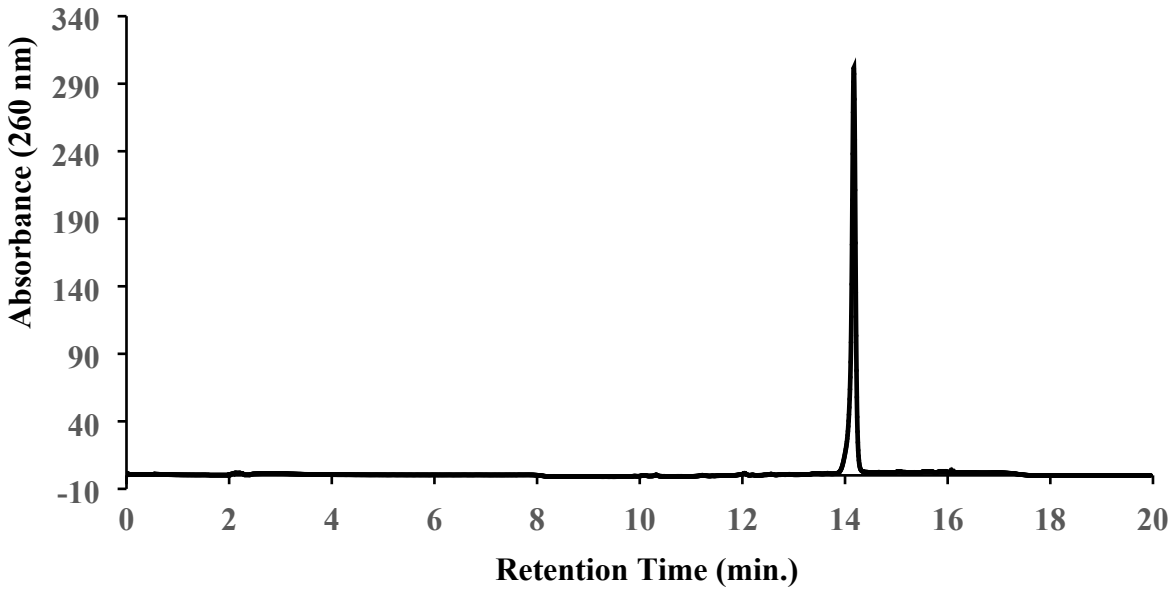

Figure S3. The HPLC trace of $[(L_2Fe)_2(\mu\text{-}O)]$ showing that the sample is about 98.4 % pure. (Gradient: 0 min 5% B, 5 min 5% B, 10 min 85% B, 15 min 90% B, 20 min 98% B, 30 min 5% B: solvent A is 0.1% TFA aqueous solution and solvent B is acetonitrile)

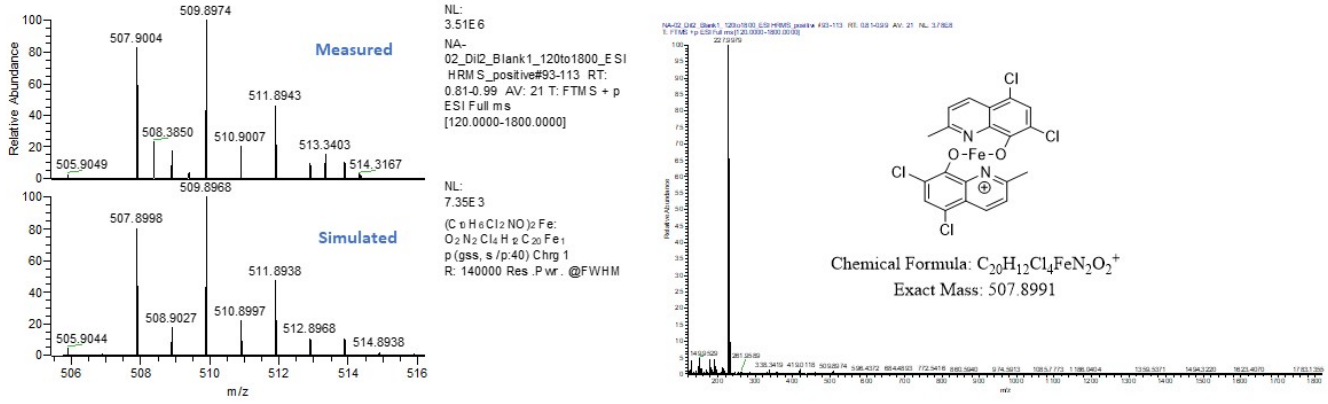

Figure S4. ESI-HRMS of $[(L_2Fe)_2(\mu\text{-}O)]$ showing the major peak for $[(C_{10}H_6Cl_2NO)_2Fe]^+$ at 509.8974. (Bruker Esquire ESI-HRM was used to measure the mass spectrum of $[(L_2Fe)_2(\mu\text{-}O)]$)

Table S2. Crystal data and structure refinement for $C_{40}H_{24}N_4O_5Cl_8Fe_2$ (**1**).

CCDC deposition no.	**CCDC-2260085**	
Empirical formula	$C_{40}H_{24}N_4O_5Cl_8Fe_2$	
Formula weight	1035.93	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.4118(3) Å	α = 83.8140(9)°
	b = 13.9698(4) Å	β = 89.0383(9)°
	c = 14.0458(4) Å	γ=78.4616(9)°
Volume	1990.01(10) Å^3	
Z	2	
Density (calculated)	1.729 Mg/m^3	
Absorption coefficient	1.319mm^{-1}	
F(000)	1040	
Crystal size	0.137 x 0.089 x 0.055 mm^3	
θ range for data collection	2.593 to 28.343°	
Index ranges	$-13 \le h \le 13$, $-18 \le k \le 18$, $-18 \le l \le 18$	
Reflections collected	99839	
Independent reflections	9901[R_{int}=0.0347]	
Completeness to θ = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.862 and 0.809	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9901 / 0 / 536	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2σ(I)]	R1 = 0.0252, wR2 = 0.0629	
R indices (all data)	R1 = 0.0301, wR2 = 0.0665	
Largest diff. peak and hole	0.653 and -0.364 eÅ^{-3}	

Table S3. Atomic coordinates [x10^4] and equivalent isotropic displacement parameters [Å^{2}x10^3] for $C_{40}H_{24}N_4O_5Cl_8Fe_2$ (**1**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	2409(1)	8152(1)	7339(1)	16(1)
Fe(2)	3806(1)	5778(1)	6956(1)	17(1)
Cl(1)	4639(1)	10814(1)	8019(1)	37(1)
Cl(2)	2058(1)	10655(1)	11361(1)	36(1)
Cl(3)	-2176(1)	8155(1)	6565(1)	28(1)
Cl(4)	-767(1)	9158(1)	2939(1)	34(1)
Cl(5)	789(1)	3822(1)	8429(1)	49(1)
Cl(6)	4616(1)	2470(1)	11061(1)	31(1)
Cl(7)	7221(1)	6430(1)	4711(1)	29(1)
Cl(8)	3239(1)	7491(1)	2163(1)	29(1)
O(1)	3367(1)	9136(1)	7637(1)	20(1)
O(2)	578(1)	8225(1)	7027(1)	21(1)
O(3)	3323(1)	6928(1)	7415(1)	24(1)
O(4)	2746(1)	4868(1)	7475(1)	25(1)

O(5)	5171(1)	5827(1)	6021(1)	22(1)
N(1)	1782(1)	8314(1)	8793(1)	18(1)
N(2)	2416(1)	8623(1)	5819(1)	18(1)
N(3)	5108(1)	4928(1)	8106(1)	20(1)
N(4)	2632(1)	6049(1)	5638(1)	18(1)
C(1)	3103(1)	9493(1)	8462(1)	18(1)
C(2)	3603(2)	10256(1)	8769(1)	23(1)
C(3)	3300(2)	10595(1)	9667(1)	28(1)
C(4)	2466(2)	10190(1)	10271(1)	26(1)
C(5)	1908(2)	9408(1)	10016(1)	22(1)
C(6)	2245(1)	9074(1)	9113(1)	18(1)
C(7)	1047(2)	8926(1)	10580(1)	26(1)
C(8)	608(2)	8164(1)	10250(1)	27(1)
C(9)	991(2)	7857(1)	9344(1)	22(1)
C(10)	524(2)	7016(1)	8973(1)	27(1)
C(11)	243(1)	8438(1)	6120(1)	18(1)
C(12)	-992(1)	8443(1)	5764(1)	20(1)
C(13)	-1304(2)	8674(1)	4786(1)	22(1)
C(14)	-377(2)	8915(1)	4152(1)	22(1)
C(15)	908(2)	8937(1)	4458(1)	19(1)
C(16)	1199(1)	8677(1)	5441(1)	17(1)
C(17)	1933(2)	9188(1)	3871(1)	23(1)
C(18)	3139(2)	9138(1)	4262(1)	23(1)
C(19)	3379(2)	8834(1)	5243(1)	20(1)
C(20)	4714(2)	8728(1)	5673(1)	27(1)
C(21)	3125(2)	4354(1)	8295(1)	22(1)
C(22)	2360(2)	3802(1)	8839(1)	27(1)
C(23)	2816(2)	3228(1)	9696(1)	28(1)
C(24)	4050(2)	3216(1)	10023(1)	24(1)
C(25)	4880(2)	3786(1)	9525(1)	22(1)
C(26)	4397(2)	4351(1)	8660(1)	20(1)
C(27)	6148(2)	3856(1)	9817(1)	26(1)
C(28)	6846(2)	4422(1)	9251(1)	27(1)
C(29)	6316(2)	4955(1)	8381(1)	24(1)
C(30)	7115(2)	5543(1)	7749(1)	31(1)
C(31)	4776(1)	6189(1)	5147(1)	19(1)
C(32)	5590(1)	6491(1)	4434(1)	21(1)
C(33)	5123(2)	6884(1)	3508(1)	23(1)
C(34)	3835(2)	6954(1)	3284(1)	22(1)

C(35)	2943(2)	6643(1)	3966(1)	19(1)
C(36)	3423(1)	6292(1)	4899(1)	17(1)
C(37)	1600(2)	6671(1)	3798(1)	22(1)
C(38)	838(2)	6389(1)	4535(1)	22(1)
C(39)	1360(1)	6103(1)	5467(1)	20(1)
C(40)	480(2)	5870(1)	6277(1)	25(1)
H(3A)	3678	11111	9855	33
H(7A)	773	9131	11187	31
H(8A)	36	7835	10636	32
H(10A)	1233	6636	8621	41
H(10B)	-229	7273	8545	41
H(10C)	262	6592	9512	41
H(13A)	-2158	8662	4564	27
H(17A)	1782	9392	3208	27
H(18A)	3826	9309	3867	27
H(20A)	5001	8056	5979	41
H(20B)	4679	9193	6153	41
H(20C)	5334	8867	5169	41
H(23A)	2269	2849	10047	34
H(27A)	6510	3512	10403	31
H(28A)	7704	4460	9443	32
H(30A)	6546	5970	7261	46
H(30B)	7800	5097	7436	46
H(30C)	7520	5946	8136	46
H(30D)	7962	5513	8056	46
H(30E)	6647	6228	7645	46
H(30F)	7258	5272	7132	46
H(33A)	5704	7099	3041	27
H(37A)	1231	6882	3179	27
H(38A)	-58	6386	4419	27
H(40A)	552	6279	6790	38
H(40B)	739	5175	6522	38
H(40C)	-429	6003	6048	38

Table S4. Bond lengths [Å] and angles [°] for $C_{40}H_{24}N_4O_5Cl_8Fe_2$ (**1**).

Fe(1)-O(3)	1.7757(11)	Fe(1)-O(1)	1.9359(10)
Fe(1)-O(2)	1.9438(10)	Fe(1)-N(1)	2.1554(12)
Fe(1)-N(2)	2.1658(12)	Fe(2)-O(3)	1.7718(11)
Fe(2)-O(4)	1.9239(11)	Fe(2)-O(5)	1.9250(11)
Fe(2)-N(4)	2.1924(12)	Fe(2)-N(3)	2.2076(13)
Cl(1)-C(2)	1.7316(16)	Cl(2)-C(4)	1.7394(16)
Cl(3)-C(12)	1.7325(16)	Cl(4)-C(14)	1.7397(15)
Cl(5)-C(22)	1.7372(17)	Cl(6)-C(24)	1.7366(16)
Cl(7)-C(32)	1.7315(15)	Cl(8)-C(34)	1.7374(16)
O(1)-C(1)	1.3137(18)	O(2)-C(11)	1.3131(17)
O(4)-C(21)	1.3114(18)	O(5)-C(31)	1.3163(18)
N(1)-C(9)	1.3287(19)	N(1)-C(6)	1.3702(19)
N(2)-C(19)	1.3359(19)	N(2)-C(16)	1.3676(18)
N(3)-C(29)	1.330(2)	N(3)-C(26)	1.373(2)
N(4)-C(39)	1.3352(19)	N(4)-C(36)	1.3706(19)
C(1)-C(2)	1.387(2)	C(1)-C(6)	1.429(2)
C(2)-C(3)	1.404(2)	C(3)-C(4)	1.366(2)
C(4)-C(5)	1.416(2)	C(5)-C(7)	1.410(2)
C(5)-C(6)	1.413(2)	C(7)-C(8)	1.365(2)
C(8)-C(9)	1.413(2)	C(9)-C(10)	1.502(2)
C(11)-C(12)	1.385(2)	C(11)-C(16)	1.430(2)
C(12)-C(13)	1.406(2)	C(13)-C(14)	1.369(2)
C(14)-C(15)	1.419(2)	C(15)-C(16)	1.412(2)
C(15)-C(17)	1.414(2)	C(17)-C(18)	1.365(2)
C(18)-C(19)	1.410(2)	C(19)-C(20)	1.498(2)
C(21)-C(22)	1.383(2)	C(21)-C(26)	1.428(2)
C(22)-C(23)	1.406(2)	C(23)-C(24)	1.368(2)
C(24)-C(25)	1.417(2)	C(25)-C(27)	1.414(2)
C(25)-C(26)	1.416(2)	C(27)-C(28)	1.363(2)
C(28)-C(29)	1.420(2)	C(29)-C(30)	1.499(2)
C(31)-C(32)	1.387(2)	C(31)-C(36)	1.432(2)
C(32)-C(33)	1.410(2)	C(33)-C(34)	1.365(2)
C(34)-C(35)	1.418(2)	C(35)-C(36)	1.411(2)
C(35)-C(37)	1.415(2)	C(37)-C(38)	1.365(2)
C(38)-C(39)	1.412(2)	C(39)-C(40)	1.499(2)
O(3)-Fe(1)-O(1)	115.72(5)	O(3)-Fe(1)-O(2)	111.98(5)
O(1)-Fe(1)-O(2)	132.22(5)	O(3)-Fe(1)-N(1)	103.07(5)

O(1)-Fe(1)-N(1)	80.03(5)	O(2)-Fe(1)-N(1)	86.93(4)
O(3)-Fe(1)-N(2)	102.88(5)	O(1)-Fe(1)-N(2)	92.32(4)
O(2)-Fe(1)-N(2)	79.70(4)	N(1)-Fe(1)-N(2)	153.73(5)
O(3)-Fe(2)-O(4)	111.01(5)	O(3)-Fe(2)-O(5)	110.57(5)
O(4)-Fe(2)-O(5)	138.28(5)	O(3)-Fe(2)-N(4)	100.28(5)
O(4)-Fe(2)-N(4)	89.34(5)	O(5)-Fe(2)-N(4)	80.09(5)
O(3)-Fe(2)-N(3)	101.72(5)	O(4)-Fe(2)-N(3)	79.41(5)
O(5)-Fe(2)-N(3)	95.50(5)	N(4)-Fe(2)-N(3)	157.69(5)
C(1)-O(1)-Fe(1)	116.39(9)	C(11)-O(2)-Fe(1)	116.78(9)
Fe(2)-O(3)-Fe(1)	151.68(7)	C(21)-O(4)-Fe(2)	116.94(10)
C(31)-O(5)-Fe(2)	115.73(9)	C(9)-N(1)-C(6)	119.87(13)
C(9)-N(1)-Fe(1)	130.51(10)	C(6)-N(1)-Fe(1)	109.43(9)
C(19)-N(2)-C(16)	119.28(13)	C(19)-N(2)-Fe(1)	131.02(10)
C(16)-N(2)-Fe(1)	109.69(9)	C(29)-N(3)-C(26)	119.07(13)
C(29)-N(3)-Fe(2)	132.78(11)	C(26)-N(3)-Fe(2)	107.77(9)
C(39)-N(4)-C(36)	119.14(13)	C(39)-N(4)-Fe(2)	132.95(10)
C(36)-N(4)-Fe(2)	107.58(9)	O(1)-C(1)-C(2)	124.98(14)
O(1)-C(1)-C(6)	119.08(13)	C(2)-C(1)-C(6)	115.94(14)
C(1)-C(2)-C(3)	122.38(15)	C(1)-C(2)-Cl(1)	119.00(12)
C(3)-C(2)-Cl(1)	118.63(12)	C(4)-C(3)-C(2)	120.52(15)
C(3)-C(4)-C(5)	120.89(14)	C(3)-C(4)-Cl(2)	119.63(13)
C(5)-C(4)-Cl(2)	119.47(13)	C(7)-C(5)-C(6)	116.61(14)
C(7)-C(5)-C(4)	126.13(15)	C(6)-C(5)-C(4)	117.26(14)
N(1)-C(6)-C(5)	122.55(14)	N(1)-C(6)-C(1)	114.44(13)
C(5)-C(6)-C(1)	123.01(14)	C(8)-C(7)-C(5)	119.83(15)
C(7)-C(8)-C(9)	120.89(15)	N(1)-C(9)-C(8)	120.24(15)
N(1)-C(9)-C(10)	118.18(14)	C(8)-C(9)-C(10)	121.59(14)
O(2)-C(11)-C(12)	124.26(13)	O(2)-C(11)-C(16)	118.98(13)
C(12)-C(11)-C(16)	116.76(13)	C(11)-C(12)-C(13)	122.19(14)
C(11)-C(12)-Cl(3)	118.10(12)	C(13)-C(12)-Cl(3)	119.71(11)
C(14)-C(13)-C(12)	119.90(14)	C(13)-C(14)-C(15)	121.54(14)
C(13)-C(14)-Cl(4)	119.15(12)	C(15)-C(14)-Cl(4)	119.27(12)
C(16)-C(15)-C(17)	116.62(13)	C(16)-C(15)-C(14)	117.09(14)
C(17)-C(15)-C(14)	126.29(14)	N(2)-C(16)-C(15)	122.87(13)
N(2)-C(16)-C(11)	114.64(13)	C(15)-C(16)-C(11)	122.48(13)
C(18)-C(17)-C(15)	119.69(14)	C(17)-C(18)-C(19)	120.81(14)
N(2)-C(19)-C(18)	120.64(14)	N(2)-C(19)-C(20)	117.90(14)
C(18)-C(19)-C(20)	121.45(14)	O(4)-C(21)-C(22)	123.75(14)
O(4)-C(21)-C(26)	119.25(14)	C(22)-C(21)-C(26)	117.00(14)

C(21)-C(22)-C(23)	122.31(15)	C(21)-C(22)-Cl(5)	117.95(12)
C(23)-C(22)-Cl(5)	119.74(13)	C(24)-C(23)-C(22)	119.82(15)
C(23)-C(24)-C(25)	121.42(14)	C(23)-C(24)-Cl(6)	119.14(13)
C(25)-C(24)-Cl(6)	119.43(12)	C(27)-C(25)-C(26)	116.57(15)
C(27)-C(25)-C(24)	125.98(14)	C(26)-C(25)-C(24)	117.44(14)
N(3)-C(26)-C(25)	123.16(14)	N(3)-C(26)-C(21)	114.88(13)
C(25)-C(26)-C(21)	121.95(14)	C(28)-C(27)-C(25)	119.40(15)
C(27)-C(28)-C(29)	121.23(15)	N(3)-C(29)-C(28)	120.51(15)
N(3)-C(29)-C(30)	118.93(14)	C(28)-C(29)-C(30)	120.55(14)
O(5)-C(31)-C(32)	124.15(14)	O(5)-C(31)-C(36)	119.18(13)
C(32)-C(31)-C(36)	116.67(14)	C(31)-C(32)-C(33)	122.29(14)
C(31)-C(32)-Cl(7)	118.50(12)	C(33)-C(32)-Cl(7)	119.15(12)
C(34)-C(33)-C(32)	119.86(14)	C(33)-C(34)-C(35)	121.36(14)
C(33)-C(34)-Cl(8)	119.99(12)	C(35)-C(34)-Cl(8)	118.57(12)
C(36)-C(35)-C(37)	116.81(14)	C(36)-C(35)-C(34)	117.63(13)
C(37)-C(35)-C(34)	125.55(14)	N(4)-C(36)-C(35)	122.84(13)
N(4)-C(36)-C(31)	115.07(13)	C(35)-C(36)-C(31)	122.08(13)
C(38)-C(37)-C(35)	119.38(14)	C(37)-C(38)-C(39)	120.99(14)
N(4)-C(39)-C(38)	120.65(14)	N(4)-C(39)-C(40)	119.49(14)
C(38)-C(39)-C(40)	119.86(13)		

Table S5. Anisotropic displacement parameters [$Å^2x10^3$] for $C_{40}H_{24}N_4O_5Cl_8Fe_2$ (**1**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+... +2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	15(1)	18(1)	16(1)	-2(1)	-2(1)	-3(1)
Fe(2)	16(1)	17(1)	19(1)	-1(1)	-1(1)	-3(1)
Cl(1)	41(1)	36(1)	40(1)	-6(1)	7(1)	-23(1)
Cl(2)	48(1)	36(1)	24(1)	-14(1)	-2(1)	-1(1)
Cl(3)	17(1)	40(1)	29(1)	-6(1)	2(1)	-9(1)
Cl(4)	33(1)	46(1)	20(1)	-2(1)	-9(1)	2(1)
Cl(5)	30(1)	66(1)	50(1)	32(1)	-16(1)	-26(1)
Cl(6)	37(1)	28(1)	25(1)	6(1)	-9(1)	-2(1)
Cl(7)	16(1)	37(1)	36(1)	-9(1)	3(1)	-9(1)
Cl(8)	33(1)	31(1)	20(1)	0(1)	1(1)	-2(1)
O(1)	21(1)	22(1)	17(1)	-3(1)	1(1)	-7(1)
O(2)	16(1)	30(1)	16(1)	-1(1)	-1(1)	-6(1)
O(3)	23(1)	21(1)	27(1)	-6(1)	-5(1)	0(1)
O(4)	21(1)	27(1)	26(1)	7(1)	-6(1)	-8(1)
O(5)	16(1)	29(1)	21(1)	-2(1)	-3(1)	-3(1)

N(1)	17(1)	20(1)	18(1)	-1(1)	-2(1)	-3(1)
N(2)	16(1)	18(1)	18(1)	-3(1)	0(1)	-3(1)
N(3)	18(1)	18(1)	22(1)	-3(1)	-3(1)	-1(1)
N(4)	16(1)	18(1)	21(1)	-2(1)	-1(1)	-4(1)
C(1)	17(1)	18(1)	19(1)	-1(1)	-4(1)	-2(1)
C(2)	24(1)	22(1)	25(1)	-2(1)	-1(1)	-6(1)
C(3)	32(1)	23(1)	30(1)	-8(1)	-6(1)	-5(1)
C(4)	30(1)	25(1)	20(1)	-8(1)	-5(1)	1(1)
C(5)	22(1)	23(1)	18(1)	-2(1)	-3(1)	2(1)
C(6)	18(1)	18(1)	18(1)	-1(1)	-2(1)	-1(1)
C(7)	27(1)	32(1)	17(1)	-1(1)	1(1)	0(1)
C(8)	26(1)	33(1)	21(1)	4(1)	3(1)	-6(1)
C(9)	21(1)	22(1)	21(1)	3(1)	-2(1)	-3(1)
C(10)	28(1)	28(1)	27(1)	3(1)	0(1)	-12(1)
C(11)	16(1)	18(1)	19(1)	-3(1)	-2(1)	-1(1)
C(12)	15(1)	22(1)	23(1)	-5(1)	0(1)	-2(1)
C(13)	17(1)	23(1)	26(1)	-7(1)	-6(1)	1(1)
C(14)	24(1)	22(1)	18(1)	-3(1)	-6(1)	2(1)
C(15)	21(1)	16(1)	18(1)	-3(1)	-2(1)	1(1)
C(16)	16(1)	15(1)	18(1)	-4(1)	-2(1)	-1(1)
C(17)	30(1)	20(1)	18(1)	-2(1)	2(1)	-2(1)
C(18)	24(1)	22(1)	23(1)	-4(1)	7(1)	-5(1)
C(19)	18(1)	19(1)	24(1)	-6(1)	3(1)	-4(1)
C(20)	18(1)	36(1)	29(1)	-6(1)	3(1)	-9(1)
C(21)	21(1)	21(1)	23(1)	1(1)	-3(1)	-3(1)
C(22)	22(1)	30(1)	30(1)	6(1)	-6(1)	-7(1)
C(23)	29(1)	26(1)	29(1)	6(1)	-2(1)	-6(1)
C(24)	30(1)	19(1)	22(1)	1(1)	-4(1)	1(1)
C(25)	24(1)	18(1)	22(1)	-3(1)	-4(1)	1(1)
C(26)	20(1)	17(1)	21(1)	-4(1)	-2(1)	0(1)
C(27)	26(1)	23(1)	25(1)	-4(1)	-9(1)	2(1)
C(28)	21(1)	28(1)	31(1)	-6(1)	-9(1)	-1(1)
C(29)	20(1)	23(1)	28(1)	-6(1)	-3(1)	-1(1)
C(30)	22(1)	37(1)	35(1)	-3(1)	-3(1)	-10(1)
C(31)	17(1)	17(1)	23(1)	-5(1)	1(1)	-3(1)
C(32)	16(1)	21(1)	27(1)	-8(1)	2(1)	-4(1)
C(33)	24(1)	21(1)	24(1)	-4(1)	6(1)	-5(1)
C(34)	25(1)	20(1)	19(1)	-4(1)	1(1)	-1(1)
C(35)	21(1)	16(1)	21(1)	-5(1)	0(1)	-2(1)

C(36)	16(1)	15(1)	21(1)	-5(1)	0(1)	-2(1)
C(37)	21(1)	22(1)	23(1)	-4(1)	-5(1)	-2(1)
C(38)	16(1)	23(1)	28(1)	-5(1)	-4(1)	-4(1)
C(39)	17(1)	17(1)	27(1)	-3(1)	-1(1)	-4(1)
C(40)	17(1)	31(1)	29(1)	2(1)	-1(1)	-7(1)

Table S6. Torsion angles [°] for $C_{40}H_{24}N_4O_5Cl_8Fe_2$ (**1**).

O(4)-Fe(2)-O(3)-Fe(1)	-94.53(15)	O(5)-Fe(2)-O(3)-Fe(1)	81.92(16)
N(4)-Fe(2)-O(3)-Fe(1)	-1.26(16)	N(3)-Fe(2)-O(3)-Fe(1)	-177.57(15)
O(1)-Fe(1)-O(3)-Fe(2)	-134.34(14)	O(2)-Fe(1)-O(3)-Fe(2)	48.59(16)
N(1)-Fe(1)-O(3)-Fe(2)	140.56(15)	N(2)-Fe(1)-O(3)-Fe(2)	-35.35(16)
Fe(1)-O(1)-C(1)-C(2)	-174.45(12)	Fe(1)-O(1)-C(1)-C(6)	5.96(17)
O(1)-C(1)-C(2)-C(3)	-178.98(15)	C(6)-C(1)-C(2)-C(3)	0.6(2)
O(1)-C(1)-C(2)-Cl(1)	1.0(2)	C(6)-C(1)-C(2)-Cl(1)	-179.41(11)
C(1)-C(2)-C(3)-C(4)	-1.4(3)	Cl(1)-C(2)-C(3)-C(4)	178.65(13)
C(2)-C(3)-C(4)-C(5)	1.2(3)	C(2)-C(3)-C(4)-Cl(2)	-177.56(13)
C(3)-C(4)-C(5)-C(7)	179.45(16)	Cl(2)-C(4)-C(5)-C(7)	-1.8(2)
C(3)-C(4)-C(5)-C(6)	-0.4(2)	Cl(2)-C(4)-C(5)-C(6)	178.41(11)
C(9)-N(1)-C(6)-C(5)	-0.5(2)	Fe(1)-N(1)-C(6)-C(5)	174.90(11)
C(9)-N(1)-C(6)-C(1)	179.00(13)	Fe(1)-N(1)-C(6)-C(1)	-5.62(15)
C(7)-C(5)-C(6)-N(1)	-0.8(2)	C(4)-C(5)-C(6)-N(1)	179.07(14)
C(7)-C(5)-C(6)-C(1)	179.78(14)	C(4)-C(5)-C(6)-C(1)	-0.4(2)
O(1)-C(1)-C(6)-N(1)	0.39(19)	C(2)-C(1)-C(6)-N(1)	-179.23(13)
O(1)-C(1)-C(6)-C(5)	179.88(13)	C(2)-C(1)-C(6)-C(5)	0.3(2)
C(6)-C(5)-C(7)-C(8)	1.4(2)	C(4)-C(5)-C(7)-C(8)	-178.43(16)
C(5)-C(7)-C(8)-C(9)	-0.8(2)	C(6)-N(1)-C(9)-C(8)	1.1(2)
Fe(1)-N(1)-C(9)-C(8)	-173.16(11)	C(6)-N(1)-C(9)-C(10)	-178.96(13)
Fe(1)-N(1)-C(9)-C(10)	6.8(2)	C(7)-C(8)-C(9)-N(1)	-0.5(2)
C(7)-C(8)-C(9)-C(10)	179.62(15)	Fe(1)-O(2)-C(11)-C(12)	174.67(11)
Fe(1)-O(2)-C(11)-C(16)	-5.04(17)	O(2)-C(11)-C(12)-C(13)	-179.87(14)
C(16)-C(11)-C(12)-C(13)	-0.2(2)	O(2)-C(11)-C(12)-Cl(3)	0.2(2)
C(16)-C(11)-C(12)-Cl(3)	179.96(11)	C(11)-C(12)-C(13)-C(14)	-0.8(2)
Cl(3)-C(12)-C(13)-C(14)	179.09(12)	C(12)-C(13)-C(14)-C(15)	0.1(2)
C(12)-C(13)-C(14)-Cl(4)	177.90(12)	C(13)-C(14)-C(15)-C(16)	1.4(2)
Cl(4)-C(14)-C(15)-C(16)	-176.36(11)	C(13)-C(14)-C(15)-C(17)	-179.01(15)
Cl(4)-C(14)-C(15)-C(17)	3.2(2)	C(19)-N(2)-C(16)-C(15)	0.9(2)
Fe(1)-N(2)-C(16)-C(15)	-178.07(11)	C(19)-N(2)-C(16)-C(11)	-179.93(13)
Fe(1)-N(2)-C(16)-C(11)	1.10(15)	C(17)-C(15)-C(16)-N(2)	-2.9(2)
C(14)-C(15)-C(16)-N(2)	176.71(13)	C(17)-C(15)-C(16)-C(11)	177.97(13)

C(14)-C(15)-C(16)-C(11)	-2.4(2)	O(2)-C(11)-C(16)-N(2)	2.36(19)
C(12)-C(11)-C(16)-N(2)	-177.38(13)	O(2)-C(11)-C(16)-C(15)	-178.47(13)
C(12)-C(11)-C(16)-C(15)	1.8(2)	C(16)-C(15)-C(17)-C(18)	2.3(2)
C(14)-C(15)-C(17)-C(18)	-177.30(15)	C(15)-C(17)-C(18)-C(19)	0.2(2)
C(16)-N(2)-C(19)-C(18)	1.8(2)	Fe(1)-N(2)-C(19)-C(18)	-179.50(11)
C(16)-N(2)-C(19)-C(20)	-177.64(13)	Fe(1)-N(2)-C(19)-C(20)	1.1(2)
C(17)-C(18)-C(19)-N(2)	-2.4(2)	C(17)-C(18)-C(19)-C(20)	177.05(15)
Fe(2)-O(4)-C(21)-C(22)	168.38(13)	Fe(2)-O(4)-C(21)-C(26)	-11.77(19)
O(4)-C(21)-C(22)-C(23)	177.39(16)	C(26)-C(21)-C(22)-C(23)	-2.5(3)
O(4)-C(21)-C(22)-Cl(5)	-2.1(2)	C(26)-C(21)-C(22)-Cl(5)	178.10(12)
C(21)-C(22)-C(23)-C(24)	1.0(3)	Cl(5)-C(22)-C(23)-C(24)	-179.61(14)
C(22)-C(23)-C(24)-C(25)	1.2(3)	C(22)-C(23)-C(24)-Cl(6)	-177.86(14)
C(23)-C(24)-C(25)-C(27)	177.48(16)	Cl(6)-C(24)-C(25)-C(27)	-3.5(2)
C(23)-C(24)-C(25)-C(26)	-1.7(2)	Cl(6)-C(24)-C(25)-C(26)	177.40(11)
C(29)-N(3)-C(26)-C(25)	0.8(2)	Fe(2)-N(3)-C(26)-C(25)	-172.99(12)
C(29)-N(3)-C(26)-C(21)	-178.67(14)	Fe(2)-N(3)-C(26)-C(21)	7.52(15)
C(27)-C(25)-C(26)-N(3)	1.4(2)	C(24)-C(25)-C(26)-N(3)	-179.39(14)
C(27)-C(25)-C(26)-C(21)	-179.16(14)	C(24)-C(25)-C(26)-C(21)	0.1(2)
O(4)-C(21)-C(26)-N(3)	1.6(2)	C(22)-C(21)-C(26)-N(3)	-178.58(14)
O(4)-C(21)-C(26)-C(25)	-177.92(14)	C(22)-C(21)-C(26)-C(25)	1.9(2)
C(26)-C(25)-C(27)-C(28)	-2.3(2)	C(24)-C(25)-C(27)-C(28)	178.61(16)
C(25)-C(27)-C(28)-C(29)	1.1(2)	C(26)-N(3)-C(29)-C(28)	-2.1(2)
Fe(2)-N(3)-C(29)-C(28)	169.83(11)	C(26)-N(3)-C(29)-C(30)	176.83(14)
Fe(2)-N(3)-C(29)-C(30)	-11.2(2)	C(27)-C(28)-C(29)-N(3)	1.2(2)
C(27)-C(28)-C(29)-C(30)	-177.71(16)	Fe(2)-O(5)-C(31)-C(32)	164.73(12)
Fe(2)-O(5)-C(31)-C(36)	-14.71(17)	O(5)-C(31)-C(32)-C(33)	-179.36(14)
C(36)-C(31)-C(32)-C(33)	0.1(2)	O(5)-C(31)-C(32)-Cl(7)	-2.2(2)
C(36)-C(31)-C(32)-Cl(7)	177.30(11)	C(31)-C(32)-C(33)-C(34)	-1.6(2)
Cl(7)-C(32)-C(33)-C(34)	-178.75(12)	C(32)-C(33)-C(34)-C(35)	0.3(2)
C(32)-C(33)-C(34)-Cl(8)	176.95(11)	C(33)-C(34)-C(35)-C(36)	2.4(2)
Cl(8)-C(34)-C(35)-C(36)	-174.34(11)	C(33)-C(34)-C(35)-C(37)	-178.83(15)
Cl(8)-C(34)-C(35)-C(37)	4.4(2)	C(39)-N(4)-C(36)-C(35)	3.0(2)
Fe(2)-N(4)-C(36)-C(35)	-171.18(11)	C(39)-N(4)-C(36)-C(31)	-178.57(13)
Fe(2)-N(4)-C(36)-C(31)	7.29(14)	C(37)-C(35)-C(36)-N(4)	-4.4(2)
C(34)-C(35)-C(36)-N(4)	174.44(13)	C(37)-C(35)-C(36)-C(31)	177.18(13)
C(34)-C(35)-C(36)-C(31)	-3.9(2)	O(5)-C(31)-C(36)-N(4)	3.70(19)
C(32)-C(31)-C(36)-N(4)	-175.78(13)	O(5)-C(31)-C(36)-C(35)	-177.81(13)
C(32)-C(31)-C(36)-C(35)	2.7(2)	C(36)-C(35)-C(37)-C(38)	1.8(2)
C(34)-C(35)-C(37)-C(38)	-176.98(15)	C(35)-C(37)-C(38)-C(39)	2.1(2)

C(36)-N(4)-C(39)-C(38)	1.2(2)	Fe(2)-N(4)-C(39)-C(38)	173.55(11)
C(36)-N(4)-C(39)-C(40)	-178.01(13)	Fe(2)-N(4)-C(39)-C(40)	-5.6(2)
C(37)-C(38)-C(39)-N(4)	-3.8(2)	C(37)-C(38)-C(39)-C(40)	175.45(15)

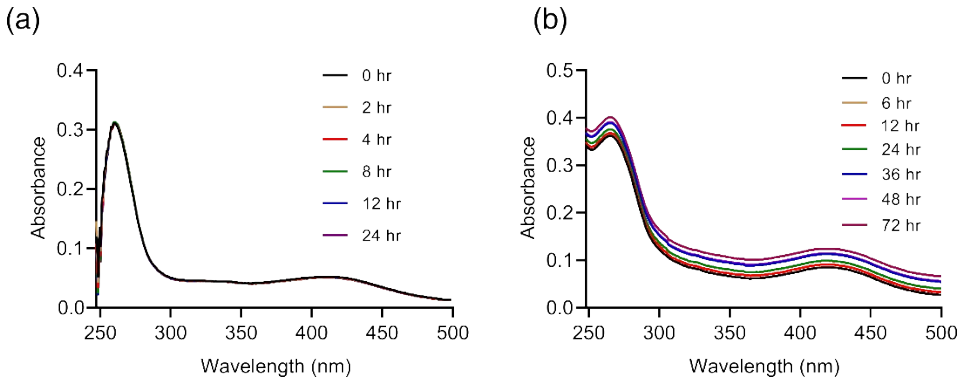

Figure S5. (**a**) UV-Vis absorption spectra of (**1**) in DMSO solution in the time course of 0 hr, 2 hr, 4 hr, 8 hr 12 hr and 24 hr and (**b**) in the cell culture medium containing DMSO under the physiological conditions (RPMI medium with 10% FBS and 1% antibiotics, pH-7.3, containing 1% DMSO) in the time course of 0 hr, 6 hr, 12 hr, 24 hr, 36 hr, 24 hr and 72 hr.

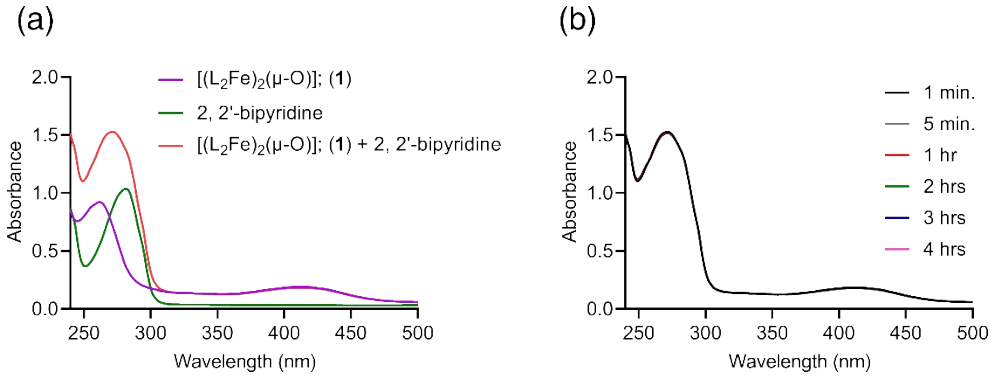

Figure S6. (**a**) UV-Vis absorption spectra of (**1**), 2,2ˈ-bipyridine and mixture of (**1**) and 2,2ˈ-bipyridine in DMSO solution, (b) UV-Vis absorption spectra of mixture (**1**) and 2,2ˈ-bipyridine without adding ascorbic acid in the time course 1 min, 5 min, 1 hr, 2 hrs, 3 hrs,and 4 hrs respectively (no peak shift was observed).

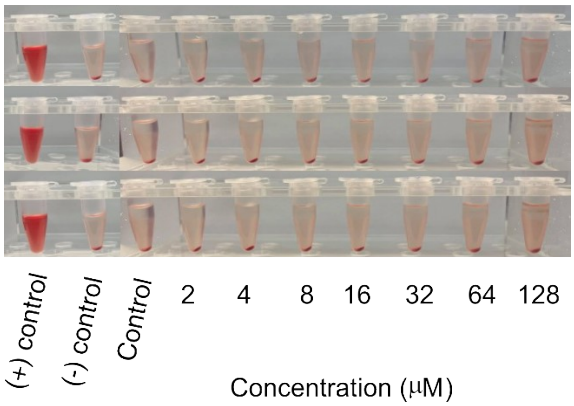

Figure S7. Representative images of hRBCs hemolysis in response to $[(L_2Fe)_2(\mu\text{-}O)]$ (**1**) with the corresponding concentrations.