Supplementary Material (ESI) for Chemical Communications

Supporting Information for

Stereochemical Control of H_2O_2 Dismutation by a Set of Hangman Porphyrin Xanthene Architectures

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Table S1. Crystal data, structure solution and refinement for the freebase precursor to **3**

Empirical formula	$C_{62}H_{39}F_{15}N_4O_3$
Formula weight	1730.63
Temperature	183(2) K
λ (Å)	0.71073
crystal system	Orthorhombic
space group	$Pca2_1$
a (Å)	23.784(3)
b (Å)	14.5290(16)
c (Å)	16.258(2)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	5618.1(12)
Z	4
ρ_{calcd} (Mg mm^{-3})	1.387
crystal size (mm^3)	$0.15 \times 0.10 \times 0.04$
abs coeff (mm^{-1})	8.903
F(000)	2392
θ range for data collection	2.12 to 20.00°
limiting indices	$-22 \le h \le 22, -9 \le k \le 13, -15 \le \ell \le 15$
no. of reflns collcd	15956
no. of ind reflns (R_{int})	5035 (0.0786)
completeness to $\theta = 23.25°$	99.7 %
absorption corr	SADABS
refinement method	Full–matrix least–squares on F^2
data / restraints / parameters	5035/ 1 / 767
$R1$,[a] $wR2$[b] [$I > 2\sigma$]	0.0708, 0.1712
$R1$,[a] $wR2$[b] (all data)	0.0955, 0.1842
GOF[c] on F^2	1.067
largest diff. peak and hole	0.647 and –0.223 eÅ^{-3}

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = (\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma(w(F_o^2)^2))^{1/2}$. [c] GOF = $(\Sigma\, w(F_o^2 - F_c^2)^2/(n - p))^{1/2}$ where n is the number of data and p is the number of parameters refined.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for the freebase precursor to **3**

Atom	x	y	z	U_{eq} [a]
N(1)	3476(3)	5440(5)	657(5)	45(2)
N(2)	4190(3)	7069(5)	731(5)	43(2)
N(3)	3742(3)	7513(5)	2337(5)	46(2)
N(4)	3005(3)	5897(5)	2236(5)	47(2)
O(1)	5382(3)	8835(4)	2319(4)	57(2)
O(2)	5380(3)	7048(5)	2461(6)	89(3)
O(3)	6159(3)	6398(5)	2816(4)	61(2)
C(1)	4390(4)	8492(6)	1510(6)	39(2)
C(2)	4448(4)	7923(6)	836(6)	41(2)
C(3)	4808(4)	8086(6)	161(6)	41(2)
C(4)	4786(4)	7345(7)	–335(7)	54(3)
C(5)	4382(4)	6708(6)	8(7)	45(2)
C(6)	4204(4)	5877(6)	–339(6)	42(2)
C(7)	3792(4)	5319(6)	–41(6)	47(3)
C(8)	3583(4)	4497(7)	–458(6)	55(3)
C(9)	3144(5)	4189(6)	–5(6)	54(3)
C(10)	3084(4)	4756(6)	701(6)	48(3)
C(11)	2695(4)	4660(6)	1344(7)	48(3)
C(12)	2661(4)	5192(6)	2059(6)	41(2)
C(13)	2284(4)	5051(7)	2731(6)	55(3)
C(14)	2400(4)	5673(7)	3301(6)	51(3)
C(15)	2862(4)	6234(6)	3015(6)	44(2)
C(16)	3099(4)	6971(6)	3397(6)	43(2)
C(17)	3498(4)	7558(6)	3094(6)	44(2)
C(18)	3700(4)	8385(7)	3483(6)	56(3)
C(19)	4045(4)	8836(7)	2937(7)	55(3)
C(20)	4085(4)	8270(7)	2209(7)	47(3)
C(21)	4485(4)	5584(7)	–1116(7)	52(3)

C(22)	4925(5)	4962(8)	–1158(8)	67(3)
C(23)	5184(5)	4688(9)	–1864(11)	82(4)
C(24)	5012(7)	5091(11)	–2599(10)	88(4)
C(25)	4586(6)	5692(9)	–2605(7)	66(3)
C(26)	4321(5)	5948(7)	–1887(7)	56(3)
C(27)	2270(5)	3907(8)	1214(6)	53(3)
C(28)	2411(5)	2995(8)	1290(6)	55(3)
C(29)	2041(6)	2295(7)	1075(6)	61(3)
C(30)	1493(6)	2526(11)	864(7)	72(3)
C(31)	1335(6)	3439(11)	799(8)	79(4)
C(32)	1713(5)	4075(8)	981(7)	61(3)
C(33)	2880(4)	7200(7)	4233(6)	50(3)
C(34)	2417(5)	7739(8)	4354(7)	66(3)
C(35)	2223(5)	8003(8)	5114(9)	72(3)
C(36)	2494(5)	7691(8)	5785(8)	59(3)
C(37)	2937(5)	7158(7)	5721(7)	56(3)
C(38)	3137(4)	6907(7)	4947(7)	54(3)
C(39)	4669(4)	9397(6)	1466(6)	41(2)
C(40)	4438(4)	10119(6)	1021(6)	52(3)
C(41)	4680(4)	10995(7)	976(6)	56(3)
C(42)	5167(4)	11102(7)	1398(7)	54(3)
C(43)	5431(4)	10413(7)	1863(6)	43(3)
C(44)	5158(4)	9579(7)	1862(6)	48(3)
C(45)	5947(4)	10585(7)	2384(9)	75(4)
C(46)	6233(4)	9674(7)	2627(6)	47(3)
C(47)	5935(4)	8868(7)	2579(6)	48(3)
C(48)	6177(4)	8022(6)	2788(5)	43(2)
C(49)	6732(4)	8045(7)	3085(6)	51(3)
C(50)	7038(4)	8836(8)	3157(7)	56(3)
C(51)	6772(4)	9639(8)	2925(6)	56(3)
C(52)	5902(5)	7141(8)	2694(6)	55(3)

C(53)	4416(5)	11782(7)	492(8)	79(4)
C(54)	4802(7)	11984(12)	–237(13)	164(9)
C(55)	3830(5)	11540(7)	151(8)	85(4)
C(56)	4358(7)	12601(8)	1083(13)	151(8)
C(57)	7633(5)	8867(8)	3492(7)	74(3)
C(58)	7653(6)	9550(10)	4256(8)	112(5)
C(59)	8039(4)	9231(9)	2837(8)	83(4)
C(60)	7841(6)	7925(9)	3768(10)	109(5)
C(61)	5769(5)	11086(9)	3218(9)	101(4)
C(62)	6365(5)	11208(9)	1961(10)	124(6)
F(1)	5096(3)	4592(4)	–430(5)	95(2)
F(2)	5615(3)	4118(6)	–1835(5)	131(3)
F(3)	5271(3)	4860(6)	–3294(5)	124(3)
F(4)	4420(3)	6065(5)	–3322(4)	96(2)
F(5)	3899(3)	6560(4)	–1909(4)	74(2)
F(6)	2934(3)	2743(4)	1523(4)	79(2)
F(7)	2208(3)	1407(4)	1159(4)	87(2)
F(8)	1148(3)	1814(5)	670(4)	100(2)
F(9)	825(3)	3609(6)	565(6)	132(3)
F(10)	1548(3)	4942(5)	928(5)	103(2)
F(11)	3608(3)	6404(4)	4877(3)	78(2)
F(12)	3205(3)	6842(4)	6389(4)	92(2)
F(13)	2325(3)	7966(4)	6543(4)	94(2)
F(14)	1775(3)	8560(5)	5181(5)	104(2)
F(15)	2133(2)	8058(5)	3687(4)	87(2)

[a] U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Bond lengths (in Å) for the freebase precursor to **3**

Bond	Distance	Bond	Distance
N(1)–C(10)	1.365(11)	C(11)–C(12)	1.398(13)
N(1)–C(7)	1.372(12)	C(11)–C(27)	1.505(13)
N(2)–C(5)	1.366(12)	C(12)–C(13)	1.429(12)
N(2)–C(2)	1.395(10)	C(13)–C(14)	1.323(12)
N(3)–C(17)	1.362(12)	C(14)–C(15)	1.445(12)
N(3)–C(20)	1.385(12)	C(15)–C(16)	1.360(12)
N(4)–C(12)	1.342(11)	C(16)–C(17)	1.367(12)
N(4)–C(15)	1.400(12)	C(16)–C(33)	1.495(14)
O(1)–C(47)	1.382(11)	C(17)–C(18)	1.440(13)
O(1)–C(44)	1.416(11)	C(18)–C(19)	1.374(13)
O(2)–C(52)	1.305(12)	C(19)–C(20)	1.445(14)
O(3)–C(52)	1.256(11)	C(21)–C(22)	1.385(15)
C(1)–C(2)	1.380(12)	C(21)–C(26)	1.416(15)
C(1)–C(20)	1.384(13)	C(22)–C(23)	1.362(17)
C(1)–C(39)	1.476(12)	C(22)–F(1)	1.363(13)
C(2)–C(3)	1.412(12)	C(23)–F(2)	1.318(14)
C(3)–C(4)	1.347(12)	C(23)–C(24)	1.392(19)
C(4)–C(5)	1.446(13)	C(24)–F(3)	1.331(14)
C(5)–C(6)	1.398(12)	C(24)–C(25)	1.337(17)
C(6)–C(7)	1.362(13)	C(25)–F(4)	1.345(13)
C(6)–C(21)	1.491(13)	C(25)–C(26)	1.377(15)
C(7)–C(8)	1.460(13)	C(26)–F(5)	1.341(11)
C(8)–C(9)	1.354(13)	C(27)–C(28)	1.373(13)
C(9)–C(10)	1.421(13)	C(27)–C(32)	1.399(14)
C(10)–C(11)	1.402(13)	C(28)–F(6)	1.350(11)
C(28)–C(29)	1.390(14)	C(41)–C(42)	1.357(13)
C(29)–F(7)	1.356(12)	C(41)–C(53)	1.524(14)

C(29)–C(30)	1.389(16)	C(42)–C(43)	1.402(13)
C(30)–F(8)	1.358(12)	C(43)–C(44)	1.376(12)
C(30)–C(31)	1.383(16)	C(43)–C(45)	1.511(14)
C(31)–F(9)	1.295(13)	C(45)–C(62)	1.511(16)
C(31)–C(32)	1.322(15)	C(45)–C(46)	1.540(14)
C(32)–F(10)	1.322(11)	C(45)–C(61)	1.596(17)
C(33)–C(34)	1.366(15)	C(46)–C(51)	1.370(13)
C(33)–C(38)	1.378(14)	C(46)–C(47)	1.371(12)
C(34)–F(15)	1.359(12)	C(47)–C(48)	1.400(12)
C(34)–C(35)	1.373(16)	C(48)–C(49)	1.406(13)
C(35)–F(14)	1.342(13)	C(48)–C(52)	1.445(14)
C(35)–C(36)	1.345(16)	C(49)–C(50)	1.365(13)
C(36)–C(37)	1.312(14)	C(50)–C(51)	1.380(13)
C(36)–F(13)	1.356(12)	C(50)–C(57)	1.516(14)
C(37)–F(12)	1.341(11)	C(53)–C(54)	1.53(2)
C(37)–C(38)	1.394(15)	C(53)–C(56)	1.536(19)
C(38)–F(11)	1.342(11)	C(53)–C(55)	1.540(15)
C(39)–C(44)	1.355(12)	C(57)–C(60)	1.522(15)
C(39)–C(40)	1.388(12)	C(57)–C(59)	1.531(15)
C(40)–C(41)	1.399(12)	C(57)–C(58)	1.591(17)

Table S4. Bond angles (in deg) for the freebase precursor to **3**

Bond Angle	Angle	Bond Angle	Angle
C(10)–N(1)–C(7)	108.9(8)	C(11)–C(10)–C(9)	127.7(9)
C(5)–N(2)–C(2)	107.4(7)	C(12)–C(11)–C(10)	127.0(8)
C(17)–N(3)–C(20)	110.5(8)	C(12)–C(11)–C(27)	118.7(9)
C(12)–N(4)–C(15)	108.2(7)	C(10)–C(11)–C(27)	114.3(9)
C(47)–O(1)–C(44)	119.5(7)	N(4)–C(12)–C(11)	124.4(8)
C(2)–C(1)–C(20)	124.4(8)	N(4)–C(12)–C(13)	109.2(8)
C(2)–C(1)–C(39)	116.7(8)	C(11)–C(12)–C(13)	126.3(9)
C(20)–C(1)–C(39)	118.9(9)	C(14)–C(13)–C(12)	107.9(9)
C(1)–C(2)–N(2)	125.8(8)	C(13)–C(14)–C(15)	108.6(9)
C(1)–C(2)–C(3)	125.3(9)	C(16)–C(15)–N(4)	126.0(8)
N(2)–C(2)–C(3)	108.8(8)	C(16)–C(15)–C(14)	127.8(10)
C(4)–C(3)–C(2)	107.9(8)	N(4)–C(15)–C(14)	106.2(8)
C(3)–C(4)–C(5)	107.9(8)	C(15)–C(16)–C(17)	127.9(9)
N(2)–C(5)–C(6)	125.3(9)	C(15)–C(16)–C(33)	116.5(8)
N(2)–C(5)–C(4)	108.0(8)	C(17)–C(16)–C(33)	115.5(9)
C(6)–C(5)–C(4)	126.8(10)	N(3)–C(17)–C(16)	126.2(9)
C(7)–C(6)–C(5)	126.1(9)	N(3)–C(17)–C(18)	107.1(8)
C(7)–C(6)–C(21)	117.0(8)	C(16)–C(17)–C(18)	126.4(10)
C(5)–C(6)–C(21)	116.9(9)	C(19)–C(18)–C(17)	108.3(9)
C(6)–C(7)–N(1)	127.8(8)	C(18)–C(19)–C(20)	107.4(8)
C(6)–C(7)–C(8)	124.5(10)	C(1)–C(20)–N(3)	128.0(9)
N(1)–C(7)–C(8)	107.6(9)	C(1)–C(20)–C(19)	125.1(9)
C(9)–C(8)–C(7)	106.3(9)	N(3)–C(20)–C(19)	106.7(9)
C(8)–C(9)–C(10)	109.0(9)	C(22)–C(21)–C(26)	114.1(10)
N(1)–C(10)–C(11)	124.2(9)	C(22)–C(21)–C(6)	124.6(10)
N(1)–C(10)–C(9)	108.1(9)	C(26)–C(21)–C(6)	121.3(10)
C(23)–C(22)–F(1)	118.9(12)	F(10)–C(32)–C(31)	116.7(12)

C(23)–C(22)–C(21)	125.1(13)	F(10)–C(32)–C(27)	117.7(9)
F(1)–C(22)–C(21)	116.0(11)	C(31)–C(32)–C(27)	125.6(12)
F(2)–C(23)–C(22)	120.3(16)	C(34)–C(33)–C(38)	114.4(10)
F(2)–C(23)–C(24)	121.7(13)	C(34)–C(33)–C(16)	122.7(10)
C(22)–C(23)–C(24)	117.8(12)	C(38)–C(33)–C(16)	122.8(10)
F(3)–C(24)–C(25)	120.7(16)	F(15)–C(34)–C(33)	118.8(11)
F(3)–C(24)–C(23)	119.0(15)	F(15)–C(34)–C(35)	117.1(12)
C(25)–C(24)–C(23)	120.3(12)	C(33)–C(34)–C(35)	124.1(11)
C(24)–C(25)–F(4)	119.4(13)	F(14)–C(35)–C(36)	121.1(12)
C(24)–C(25)–C(26)	121.1(13)	F(14)–C(35)–C(34)	120.5(13)
F(4)–C(25)–C(26)	119.5(12)	C(36)–C(35)–C(34)	118.3(11)
F(5)–C(26)–C(25)	119.9(11)	C(37)–C(36)–C(35)	121.3(11)
F(5)–C(26)–C(21)	118.6(10)	C(37)–C(36)–F(13)	118.9(12)
C(25)–C(26)–C(21)	121.5(11)	C(35)–C(36)–F(13)	119.7(11)
C(28)–C(27)–C(32)	115.1(10)	C(36)–C(37)–F(12)	121.3(11)
C(28)–C(27)–C(11)	121.6(10)	C(36)–C(37)–C(38)	120.0(10)
C(32)–C(27)–C(11)	123.3(10)	F(12)–C(37)–C(38)	118.7(10)
F(6)–C(28)–C(27)	120.9(9)	F(11)–C(38)–C(33)	117.9(10)
F(6)–C(28)–C(29)	117.0(11)	F(11)–C(38)–C(37)	120.2(10)
C(27)–C(28)–C(29)	122.0(11)	C(33)–C(38)–C(37)	121.8(10)
F(7)–C(29)–C(30)	122.0(11)	C(44)–C(39)–C(40)	116.1(9)
F(7)–C(29)–C(28)	119.0(13)	C(44)–C(39)–C(1)	122.5(8)
C(30)–C(29)–C(28)	118.6(11)	C(40)–C(39)–C(1)	121.4(8)
F(8)–C(30)–C(31)	123.3(13)	C(39)–C(40)–C(41)	123.5(9)
F(8)–C(30)–C(29)	116.1(13)	C(42)–C(41)–C(40)	115.4(10)
C(31)–C(30)–C(29)	120.4(11)	C(42)–C(41)–C(53)	121.9(10)
F(9)–C(31)–C(32)	124.7(14)	C(40)–C(41)–C(53)	122.7(9)
F(9)–C(31)–C(30)	117.4(12)	C(41)–C(42)–C(43)	125.0(9)
C(32)–C(31)–C(30)	117.9(12)	C(44)–C(43)–C(42)	114.6(9)
C(44)–C(43)–C(45)	122.0(9)	C(49)–C(48)–C(52)	118.9(9)

C(42)–C(43)–C(45)	123.3(9)	C(50)–C(49)–C(48)	123.4(10)
C(39)–C(44)–C(43)	125.3(9)	C(49)–C(50)–C(51)	116.3(9)
C(39)–C(44)–O(1)	115.0(9)	C(49)–C(50)–C(57)	123.6(11)
C(43)–C(44)–O(1)	119.6(9)	C(51)–C(50)–C(57)	120.1(10)
C(43)–C(45)–C(62)	112.2(10)	C(46)–C(51)–C(50)	123.9(9)
C(43)–C(45)–C(46)	111.2(9)	O(3)–C(52)–O(2)	114.8(10)
C(62)–C(45)–C(46)	109.9(9)	O(3)–C(52)–C(48)	121.6(10)
C(43)–C(45)–C(61)	109.7(9)	O(2)–C(52)–C(48)	123.7(10)
C(62)–C(45)–C(61)	106.7(11)	C(41)–C(53)–C(54)	107.3(10)
C(46)–C(45)–C(61)	107.0(10)	C(41)–C(53)–C(56)	107.2(11)
C(51)–C(46)–C(47)	118.2(9)	C(54)–C(53)–C(55)	113.0(13)
C(51)–C(46)–C(45)	122.4(9)	C(56)–C(53)–C(55)	112.8(9)
C(47)–C(46)–C(45)	119.3(9)	C(50)–C(57)–C(60)	107.9(12)
C(46)–C(47)–O(1)	122.7(9)	C(50)–C(57)–C(59)	108.7(11)
C(46)–C(47)–C(48)	121.5(9)	C(60)–C(57)–C(59)	112.4(10)
O(1)–C(47)–C(48)	115.8(8)	C(50)–C(57)–C(58)	110.4(9)
C(47)–C(48)–C(49)	116.6(9)	C(60)–C(57)–C(58)	108.1(11)
C(47)–C(48)–C(52)	124.4(9)	C(59)–C(57)–C(58)	109.1(10)

Table S5. Anisotropic thermal displacement parameters ($Å^2 \times 10^3$) for the freebase precursor to **3**

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	62(5)	45(5)	29(5)	–7(4)	–6(4)	–1(4)
N(2)	57(5)	38(5)	36(5)	–1(4)	–9(4)	1(4)
N(3)	52(5)	45(5)	41(6)	–6(4)	–7(4)	–10(4)
N(4)	61(5)	38(5)	44(6)	–1(4)	–8(4)	–11(4)
O(1)	41(4)	50(4)	79(5)	1(4)	–11(4)	–7(3)
O(2)	60(5)	52(5)	155(9)	24(5)	–40(5)	–3(4)
O(3)	59(5)	65(5)	60(5)	16(4)	0(4)	–2(4)
C(1)	38(6)	50(7)	29(6)	21(5)	1(5)	–5(5)
C(2)	52(6)	44(7)	26(6)	9(5)	2(5)	–2(5)
C(3)	48(6)	27(6)	47(7)	–5(5)	–13(5)	–11(5)
C(4)	49(7)	57(7)	55(7)	19(7)	15(5)	1(5)
C(5)	53(6)	36(6)	45(6)	6(6)	–11(6)	7(5)
C(6)	55(6)	32(6)	39(6)	–9(5)	0(5)	–8(5)
C(7)	75(7)	41(6)	25(6)	–7(5)	–18(6)	–6(6)
C(8)	65(8)	55(7)	44(6)	7(6)	2(6)	5(5)
C(9)	73(8)	52(6)	38(6)	–6(6)	–19(6)	–7(6)
C(10)	58(7)	43(6)	45(7)	5(6)	–10(6)	–17(5)
C(11)	38(6)	40(6)	66(8)	12(6)	–17(6)	–18(5)
C(12)	49(6)	43(6)	30(6)	–9(5)	–8(5)	–16(5)
C(13)	58(7)	65(7)	41(7)	7(6)	3(6)	–18(5)
C(14)	53(7)	60(7)	40(6)	–10(6)	–5(5)	–10(5)
C(15)	39(6)	38(6)	55(8)	2(6)	–2(5)	–11(5)
C(16)	46(6)	41(6)	42(6)	3(5)	2(5)	–9(5)
C(17)	46(6)	48(7)	38(7)	1(6)	–7(5)	–4(5)
C(18)	53(7)	67(8)	48(7)	–33(6)	5(6)	–4(6)
C(19)	51(6)	44(6)	71(8)	–19(7)	6(6)	–13(5)
C(20)	42(6)	40(6)	60(8)	1(6)	–23(6)	3(5)
C(21)	51(7)	49(7)	55(8)	–7(6)	9(6)	–20(6)

C(22)	65(8)	51(7)	84(10)	8(7)	–2(8)	2(6)
C(23)	65(9)	88(10)	94(12)	–36(9)	42(9)	10(7)
C(24)	104(11)	92(10)	68(11)	–35(10)	37(9)	–7(9)
C(25)	87(9)	71(8)	41(9)	–10(7)	11(8)	–17(7)
C(26)	64(7)	57(7)	48(8)	2(7)	7(7)	–12(6)
C(27)	64(8)	60(8)	35(6)	0(5)	2(5)	–5(7)
C(28)	51(7)	70(9)	44(7)	3(6)	–2(6)	–2(7)
C(29)	104(11)	40(7)	40(7)	–8(5)	20(7)	–23(8)
C(30)	69(10)	101(11)	46(7)	–2(7)	3(6)	–48(9)
C(31)	71(10)	92(11)	73(9)	14(8)	–25(7)	–21(9)
C(32)	65(9)	53(8)	65(8)	–3(6)	–17(6)	–26(8)
C(33)	48(7)	54(7)	48(8)	–8(6)	–1(6)	–14(5)
C(34)	61(8)	85(9)	50(8)	15(7)	–11(7)	–13(7)
C(35)	58(9)	88(9)	71(11)	–13(8)	12(8)	–5(7)
C(36)	57(8)	68(8)	53(9)	–13(7)	13(7)	–4(6)
C(37)	72(8)	63(7)	34(8)	–2(6)	–12(6)	4(6)
C(38)	57(7)	56(7)	47(8)	–6(6)	–21(7)	–4(6)
C(39)	34(6)	31(6)	58(7)	7(5)	–6(5)	–3(5)
C(40)	60(7)	39(6)	57(7)	–1(6)	–10(5)	–4(6)
C(41)	57(7)	58(8)	54(7)	–7(6)	–11(6)	–3(6)
C(42)	59(7)	41(6)	62(7)	1(6)	–8(6)	–9(5)
C(43)	40(6)	35(6)	54(7)	–10(5)	5(5)	–8(5)
C(44)	35(6)	48(7)	61(7)	9(6)	3(6)	11(6)
C(45)	42(7)	64(8)	120(11)	17(8)	–15(7)	–10(6)
C(46)	54(7)	49(7)	38(6)	2(5)	–5(5)	–7(6)
C(47)	44(7)	58(8)	42(7)	–2(5)	16(5)	–7(6)
C(48)	49(7)	43(7)	38(6)	1(5)	1(5)	2(6)
C(49)	51(7)	63(7)	38(6)	0(5)	–2(5)	–3(6)
C(50)	40(6)	72(8)	56(7)	2(6)	–2(6)	–10(7)
C(51)	53(7)	67(8)	47(6)	–3(6)	–5(6)	–6(6)
C(52)	61(8)	64(9)	40(7)	3(6)	–4(6)	6(7)

C(53)	97(10)	44(7)	96(10)	26(7)	–33(9)	2(6)
C(54)	111(13)	184(18)	200(20)	131(16)	–2(13)	15(11)
C(55)	90(9)	69(8)	96(10)	40(7)	–38(8)	5(7)
C(56)	148(14)	54(9)	250(20)	–24(11)	–125(15)	16(8)
C(57)	64(8)	82(9)	76(9)	24(7)	–20(7)	–18(7)
C(58)	96(11)	149(13)	92(11)	–9(10)	–31(9)	–17(9)
C(59)	45(7)	103(10)	102(10)	16(8)	–12(7)	–12(6)
C(60)	90(10)	102(11)	135(13)	38(9)	–56(9)	–31(8)
C(61)	105(10)	99(10)	97(10)	–51(9)	–10(8)	37(8)
C(62)	104(11)	102(11)	165(16)	58(11)	–52(10)	–48(9)
F(1)	105(5)	88(5)	92(6)	9(4)	–4(4)	46(4)
F(2)	113(6)	130(6)	149(8)	–46(6)	34(6)	57(6)
F(3)	129(6)	149(7)	93(6)	–59(5)	57(5)	–28(5)
F(4)	122(6)	122(6)	44(5)	9(4)	7(4)	–32(5)
F(5)	78(4)	82(4)	61(4)	13(4)	0(4)	14(4)
F(6)	87(5)	58(4)	91(5)	7(3)	9(4)	–6(3)
F(7)	124(6)	63(4)	74(5)	–8(4)	16(4)	–34(4)
F(8)	109(5)	106(5)	85(5)	–12(4)	–12(4)	–69(5)
F(9)	77(5)	161(7)	157(8)	–2(6)	–59(6)	–34(5)
F(10)	81(5)	80(5)	148(7)	9(5)	–37(5)	–11(4)
F(11)	102(5)	88(4)	45(4)	–3(3)	–14(3)	40(4)
F(12)	138(6)	93(5)	45(4)	1(4)	–13(4)	0(4)
F(13)	105(5)	108(6)	69(5)	–18(4)	31(4)	–18(4)
F(14)	72(5)	134(6)	107(6)	–11(5)	34(4)	19(5)
F(15)	63(4)	119(5)	80(5)	8(4)	–9(4)	29(4)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

Table S6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for the freebase precursor to **3**

Atom	x	y	z	U_{eq}
H(1)	3519	5886	1018	54
H(3A)	3690	7066	1980	55
H(2)	5268	7541	2246	133
H(3)	5027	8624	73	49
H(4)	4998	7257	–825	64
H(8)	3727	4231	–948	65
H(9)	2913	3677	–139	65
H(13)	2001	4591	2763	66
H(14)	2211	5739	3812	61
H(18)	3610	8585	4023	67
H(19)	4223	9413	3023	66
H(40)	4097	10012	731	62
H(42)	5344	11688	1377	65
H(49)	6903	7481	3243	61
H(51)	6973	10200	2976	67
H(54A)	5168	12192	–34	246
H(54B)	4633	12466	–580	246
H(54C)	4851	11423	–564	246
H(55A)	3667	12083	–116	127
H(55B)	3585	11343	603	127
H(55C)	3864	11041	–251	127
H(56A)	4730	12863	1191	226
H(56B)	4191	12391	1601	226
H(56C)	4116	13070	834	226
H(58A)	7370	9363	4662	168
H(58B)	7573	10178	4069	168
H(58C)	8027	9530	4507	168

H(59A)	8413	9312	3079	125
H(59B)	7902	9824	2630	125
H(59C)	8061	8790	2382	125
H(60A)	7580	7671	4176	164
H(60B)	8215	7986	4013	164
H(60C)	7860	7512	3292	164
H(61A)	6106	11216	3545	151
H(61B)	5516	10686	3531	151
H(61C)	5577	11665	3088	151
H(62A)	6492	10920	1448	185
H(62B)	6689	11308	2323	185
H(62C)	6187	11799	1838	185

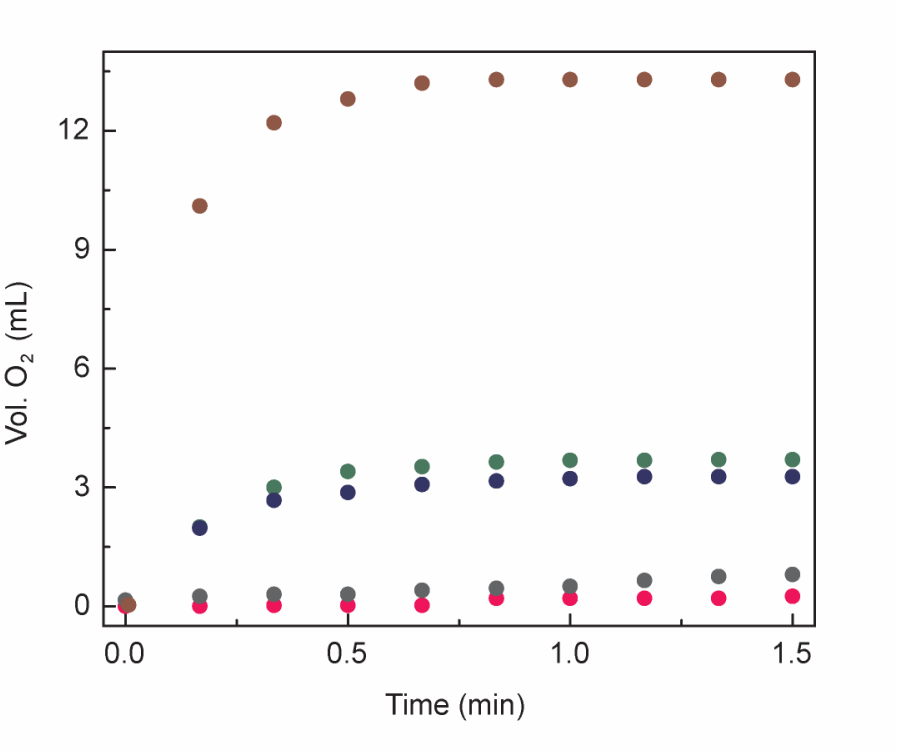

Figure S1. Reaction profiles for H_2O_2 dismutation by Hangman porphyrin xanthene derivatives. Legend: Fe(Cl)TMP (●), Fe(Cl)TMP + $PhCO_2H$ (●), 1 (●), 2 (●), 3 (●).