Supplementary Information

Ferrocene-appended Anthraquinone and Coumarin as Redox-active Cytotoxins

Aryan Houshmand,[a] Devon Heroux,[b] Dennis Y. Liu,[a] Wen Zhou,[a] Roger G. Linington,[a] Marcel Bally,[b] Jeffrey J. Warren,[a] and Charles J. Walsby[a,*]

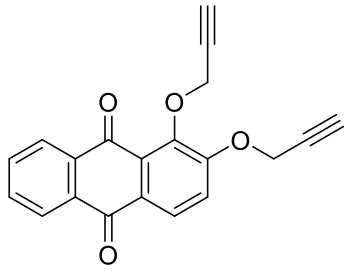
a) Department of Chemistry, Simon Fraser University, 8888 University Dr., Burnaby, BC, V5A 1S6, Canada.

b) BC Cancer Research Institute, 675 West 10th Ave., Vancouver, BC, V5Z 1L3, Canada.

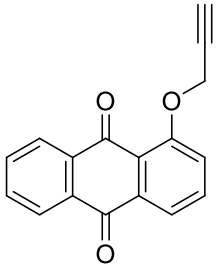
Table of Contents

Synthesis of Starting Materials

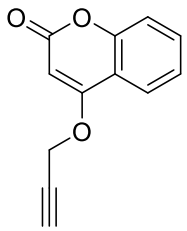
1,2-bis(prop-2-yn-1-yloxy)anthracene-9,10-dione (1,2-DiPAQ). Synthesis followed the literature.[1] In a 100 mL round bottom flask, alizarin (240 mg, 1 mmol), and K_2CO_3 (830 mg, 6 mmol) were combined with 40 mL of dry acetone to obtain a deep purple solution. Propargyl bromide (0.15 mL, 2 mmol) was added, and the solution was refluxed for 60 h. The solution was concentrated, and the crude solid was added to DCM (50 mL) and the resulting suspension was washed with a 0.5 M solution of HCl (2 × 10 mL) and finally with brine (2 × 20 mL). The organic solution was dried over Na_2SO_4 and concentrated to afford an orange gummy residue. The reaction mixture was not purified and reacted crude in the next step.



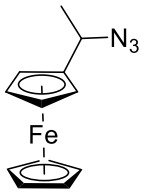
1-(prop-2-yn-1-yloxy)anthracene-9,10-dione (1-PAQ). Synthesis followed the literature.[2] In a 100 mL round bottom flask, 1-hydroxyanthracene-9,10-dione (224 mg, 1 mmol), and K_2CO_3 (830 mg, 6 mmol) were combined with 40 mL of dry acetone to obtain a deep purple solution. Propargyl bromide (0.090 mL, 1.2 mmol) was added, and the solution was refluxed for 60 h. The solution was concentrated, and the crude solid was added with DCM (50 mL) and the resulting suspension was washed with a 0.5 M solution of HCl (2 x 10 mL) and finally with brine (2 x 20 mL). The organic solution was dried over Na_2SO_4 and concentrated to afford an orange gummy residue. The reaction mixture was not purified and reacted crude in the next step.



4-(prop-2-yn-1-yloxy)-2H-chromen-2-one (4-PC). Synthesis followed the literature.[3] 4-Hydroxycoumarin (162mg, 1mmol), K_2CO_3 (414 mg, 3 mmol) in DMF were heated to 50 °C for half an hour. After cooling the solution, propargyl bromide (0.090 mL, 1.2 mmol) was added and stirred for 4 h at room temperature. The resulting solution is poured into ice water. The precipitate formed was filtered and washed with water to afford a white flaky precipitate. The crude reaction mixture was not purified and reacted crude in the next step.



(1-Azidoethyl)ferrocene (Fc-EtAzide). Synthesis followed the literature.[4] 1-hydroxyethylferrocene (1.018 g, 4.4 mmol) and sodium azide (1.730 g, 26.6 mmol) were combined in a 100 mL round bottom flask with glacial acetic acid (50.6 mL, 885.5 mmol). The solution was allowed to react at 50 °C under N_2 for 4 hours. The reaction was then allowed to cool to room temperature and then diluted with DCM (200 mL). The solution was then washed with saturated $NaHCO_3$ (3 x 50 mL) followed by water (2 x 50 mL). The organic layer was then dried over Na_2SO_4 to yield a crude orange solid. The crude product was not purified any further and reacted as is.



$^{1}H/^{13}C$ NMR and Mass Spectrometry Data

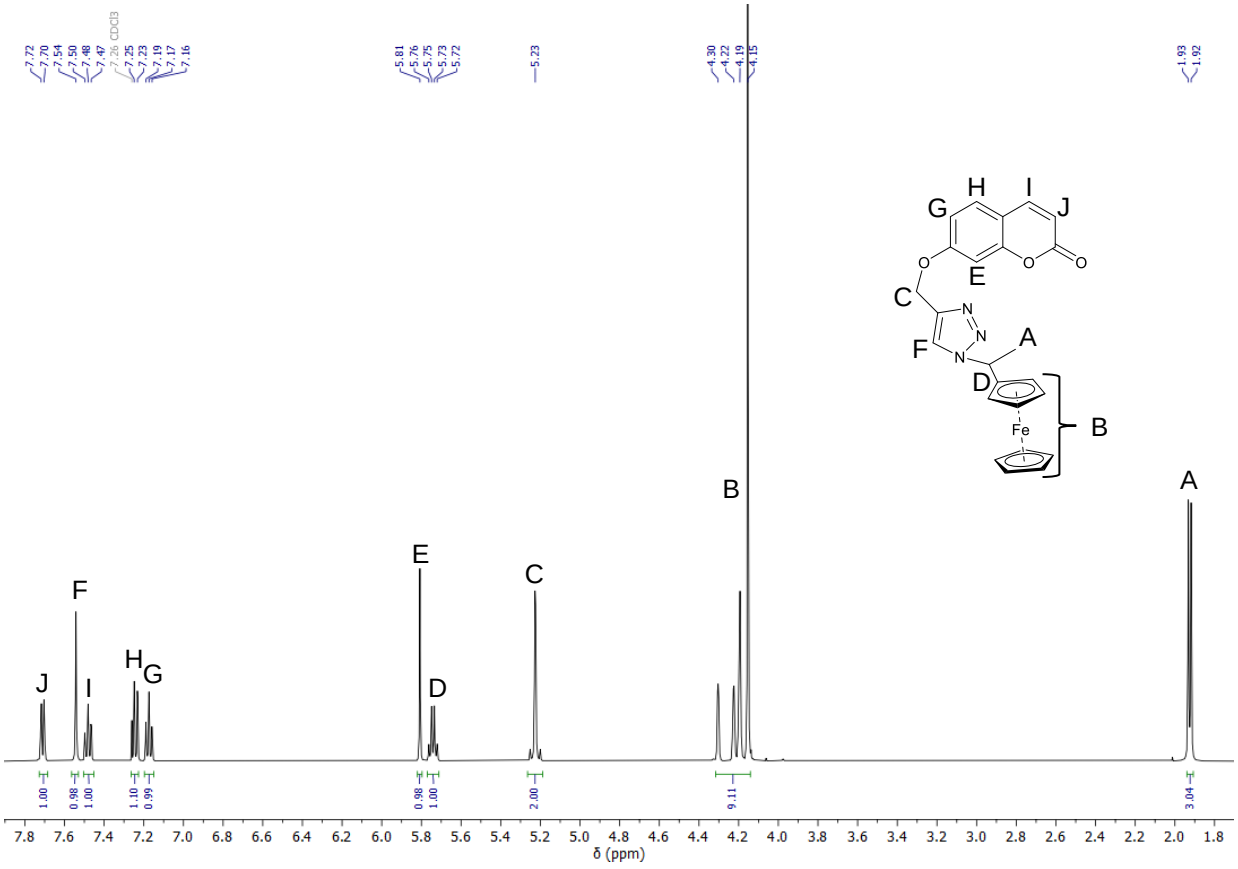


Figure S1. ^{1}H NMR spectrum for **4-FcC** (500 MHz, $CDCl_3$) δ 7.72 – 7.70 (dd, J = 7.9, 1.6 Hz, 1H), 7.54 (s, 1H), 7.48 (ddd, J = 8.7, 7.3, 1.6 Hz, 1H), 7.25 – 7.23 (m, 1H), 7.19 – 7.16 (m, 1H), 5.81 (s, 1H), 5.76 – 5.72 (q, J = 7.0 Hz, 1H), 5.23 (d, J = 1.7 Hz, 2H), 4.30 – 4.15 (m, 9H), 1.93 (d, J = 7.0 Hz, 3H).

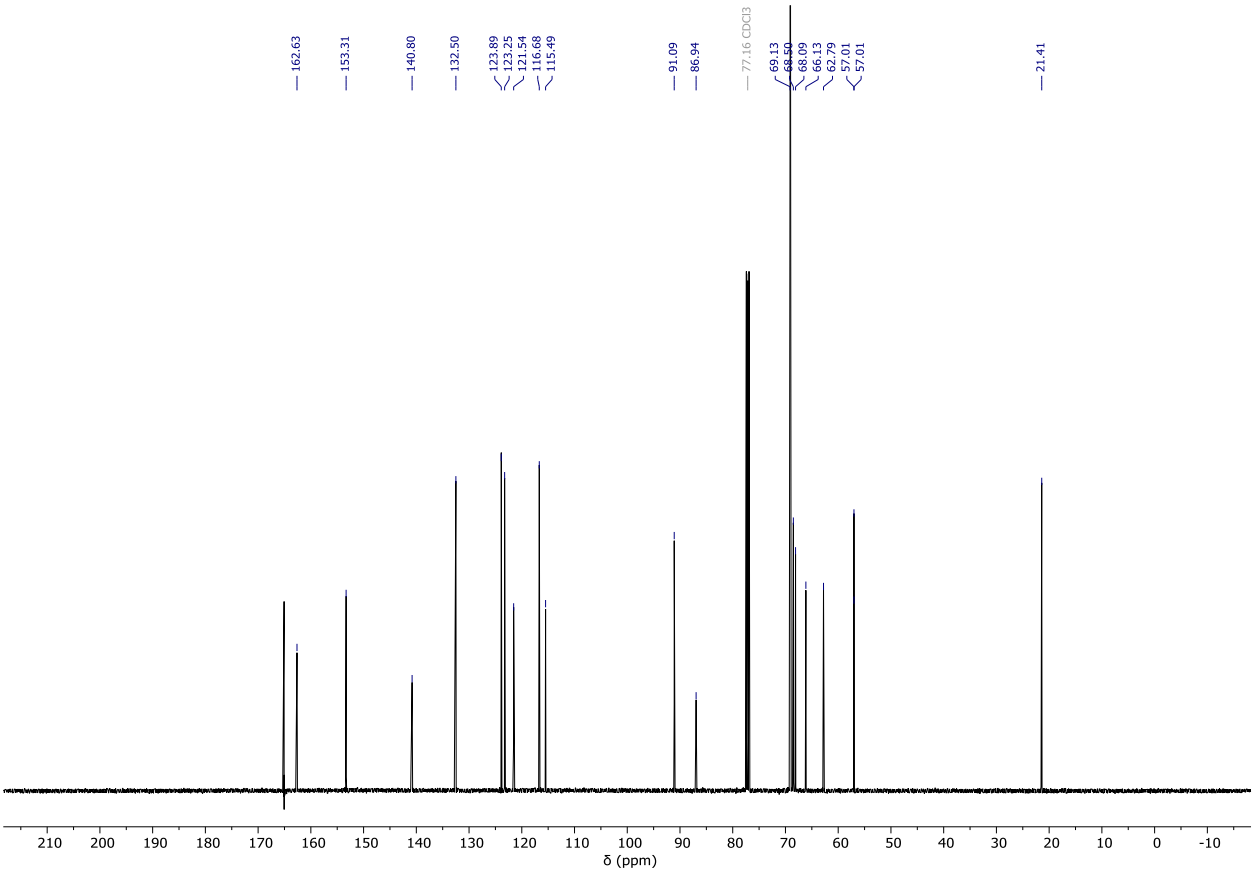


Figure S2. ^{13}C NMR spectrum for **4-FcC** (500 MHz, $CDCl_3$)

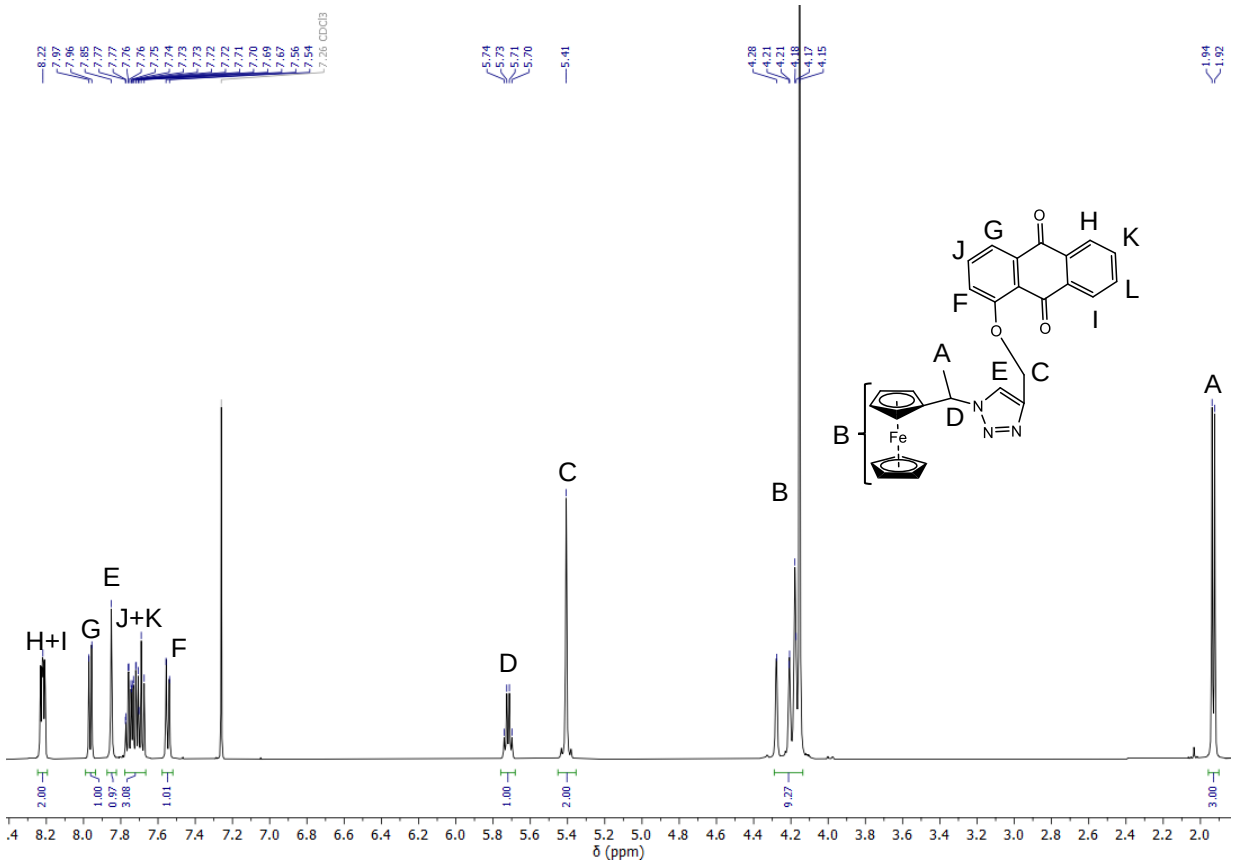


Figure S3. ^{1}H NMR spectrum for **1-FcAQ** (500 MHz, $CDCl_3$) δ 8.22 (ddd, J = 7.3, 4.3, 1.5 Hz, 2H), 7.96 (dd, J = 7.7, 1.0 Hz, 1H), 7.85 (s, 1H), 7.77 – 7.67 (m, 3H), 7.56 (dd, J = 8.4, 1.1 Hz, 1H), 5.72 (q, J = 7.0 Hz, 1H), 5.41 (s, 2H), 4.28 – 4.15 (m, 9H), 1.93 (d, J = 7.0 Hz, 3H).

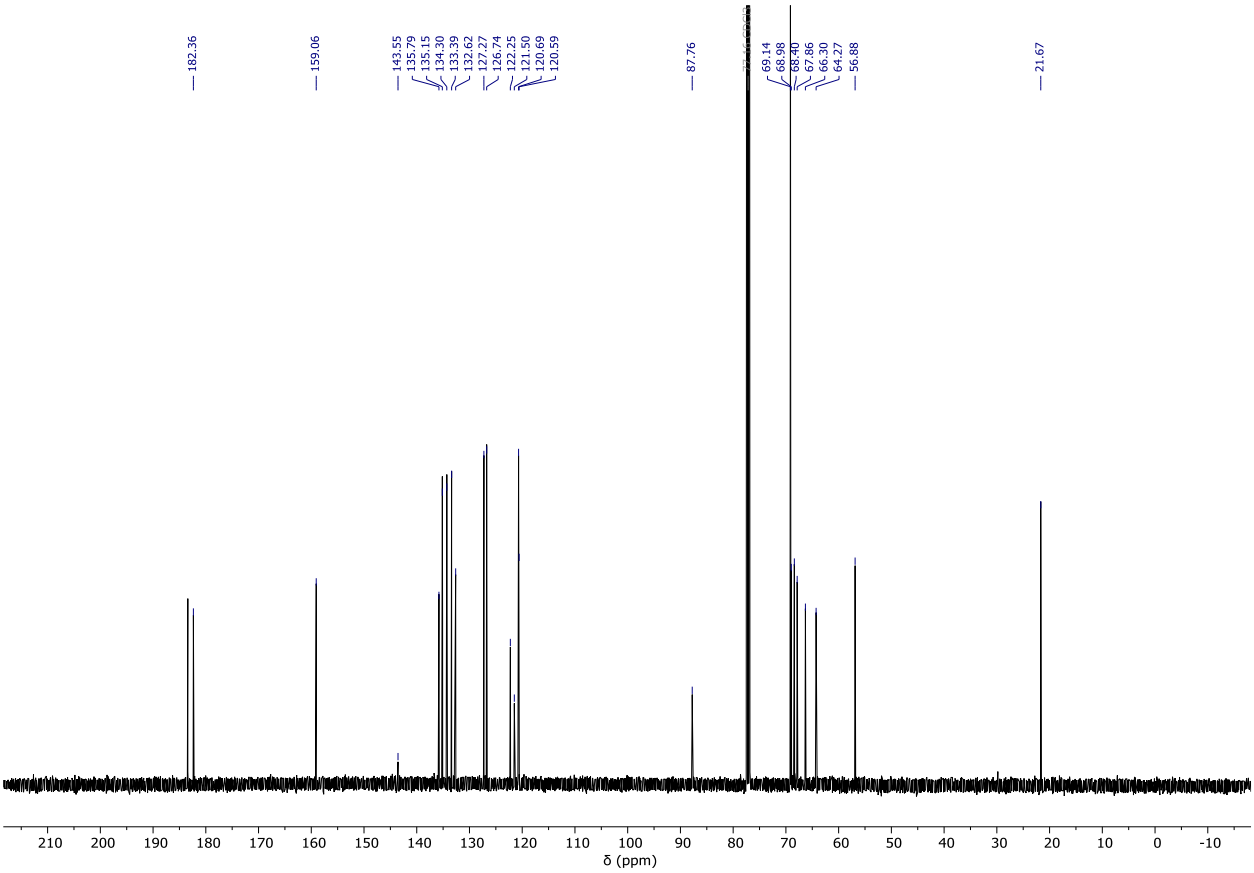


Figure S4. ^{13}C NMR spectrum for **1-FcAQ** (500 MHz, $CDCl_3$).

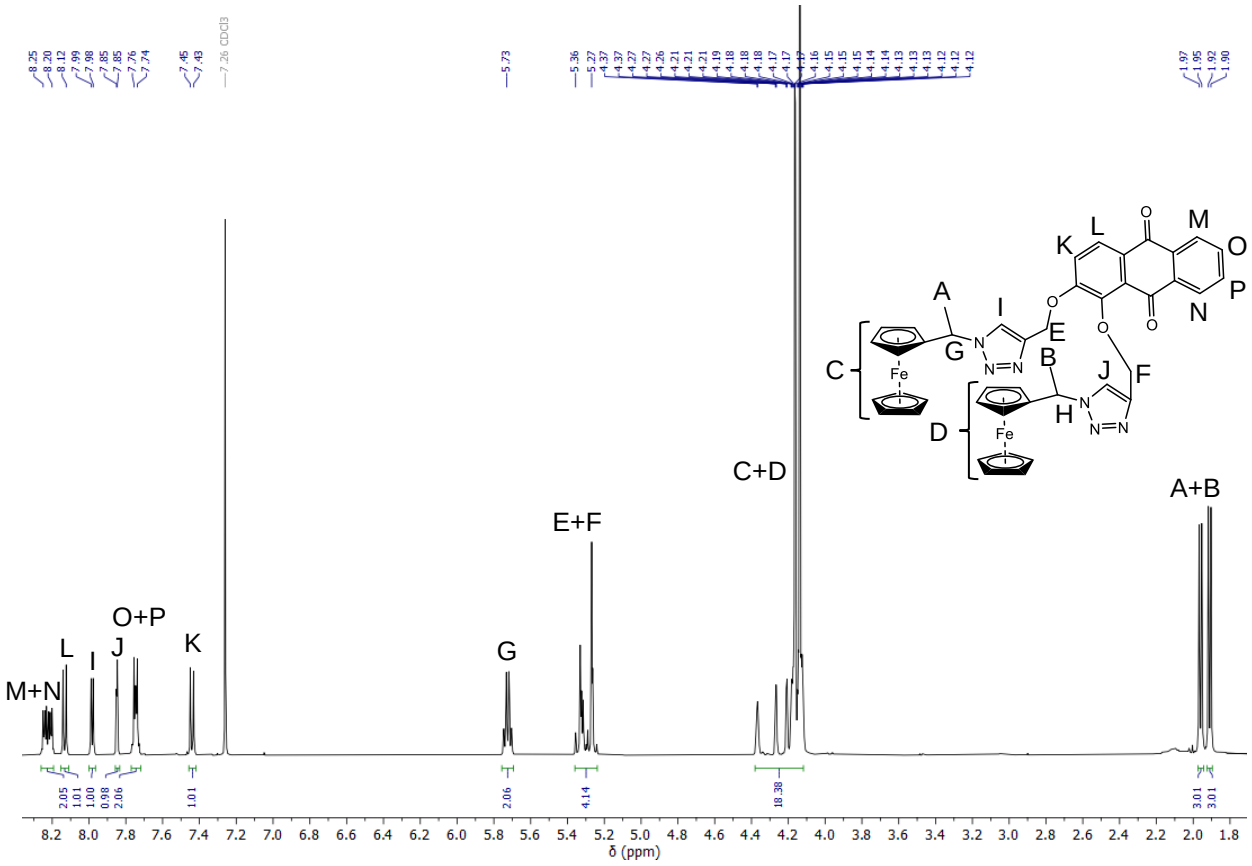


Figure S5. ^{1}H NMR spectrum for **1,2-DiFcAQ** (500 MHz, $CDCl_3$) δ 8.25 – 8.20 (m, 2H), 8.12 (d, J = 8.7 Hz, 1H), 7.99 – 7.98 (d, J = 5.7 Hz, 1H), 7.85 (d, J = 2.2 Hz, 1H), 7.76 – 7.74 (m, 2H), 7.45 – 7.43 (d, J = 8.7 Hz, 1H), 5.73 (m, 2H), 5.36 – 5.27 (m, 4H), 4.37 – 4.12 (m, 18H), 1.96 (d, J = 7.1 Hz, 3H), 1.91 (d, J = 7.1 Hz, 3H).

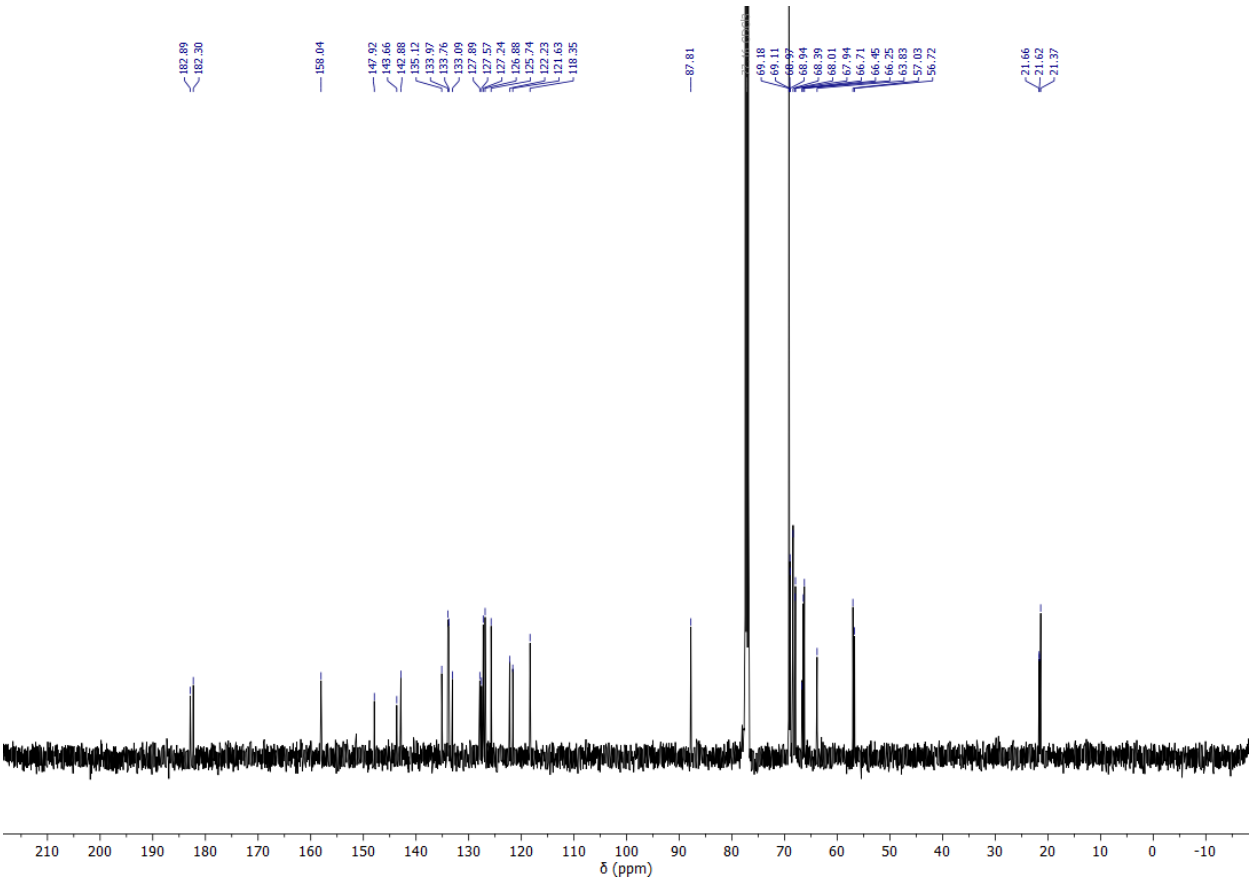


Figure S6. ^{13}C NMR spectrum for **1,2-DiFcAQ** (500 MHz, $CDCl_3$).

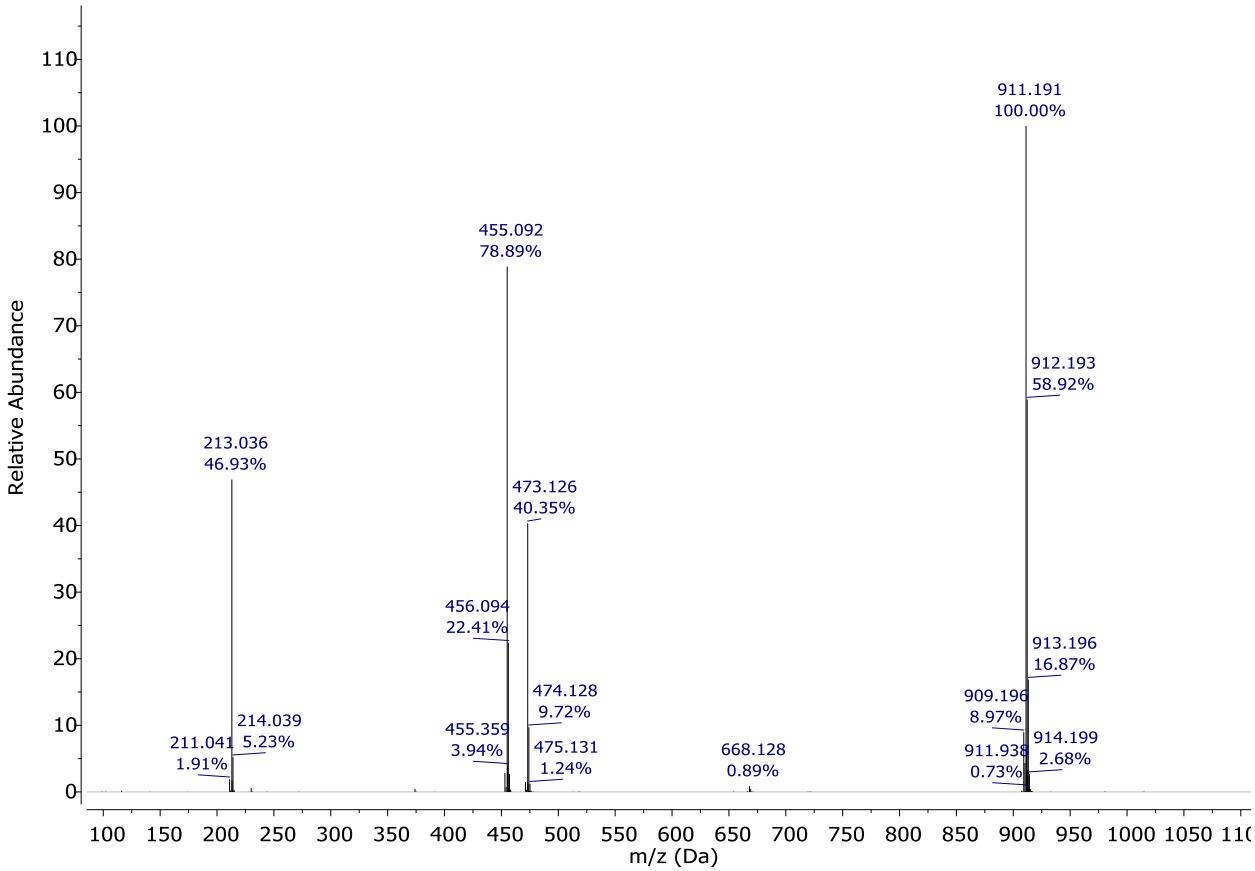


Figure S7. Mass Spectrum scan for **4-FcC** using an ESI-ToF in positive mode.

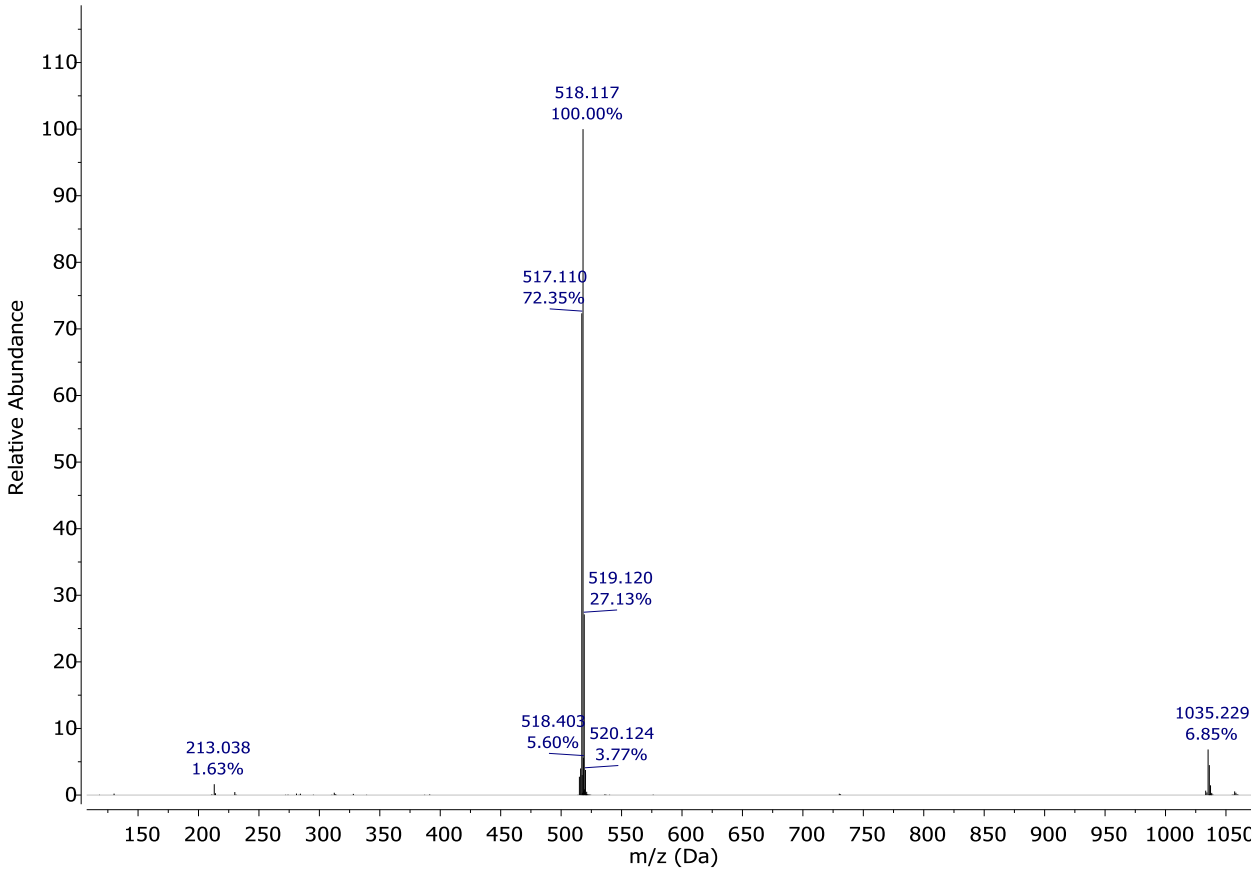


Figure S8. Mass Spectrum scan for **1-FcAQ** using an ESI-ToF in positive mode**.**

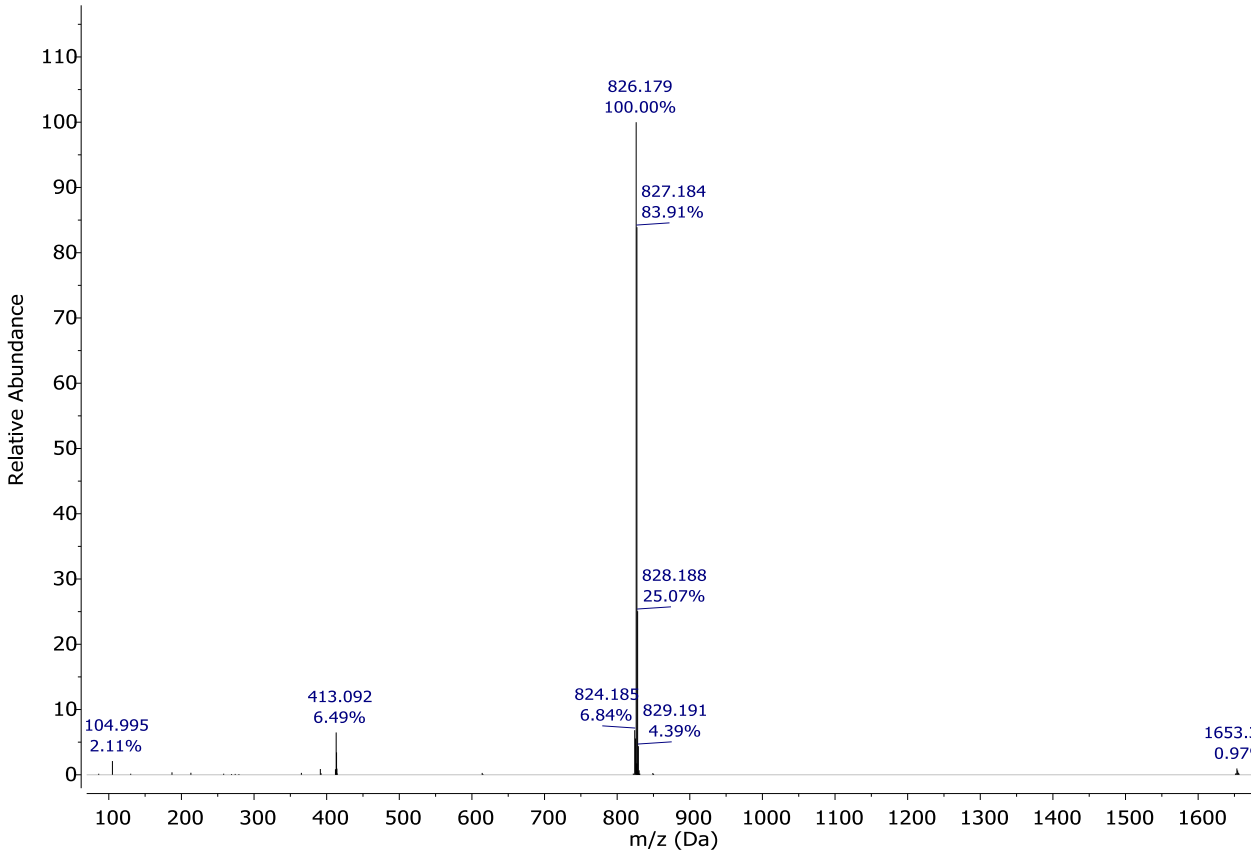


Figure S9. Mass Spectrum scan for **1,2-DiFcAQ** using an ESI-ToF in positive mode**.**

EPR Spin Trapping

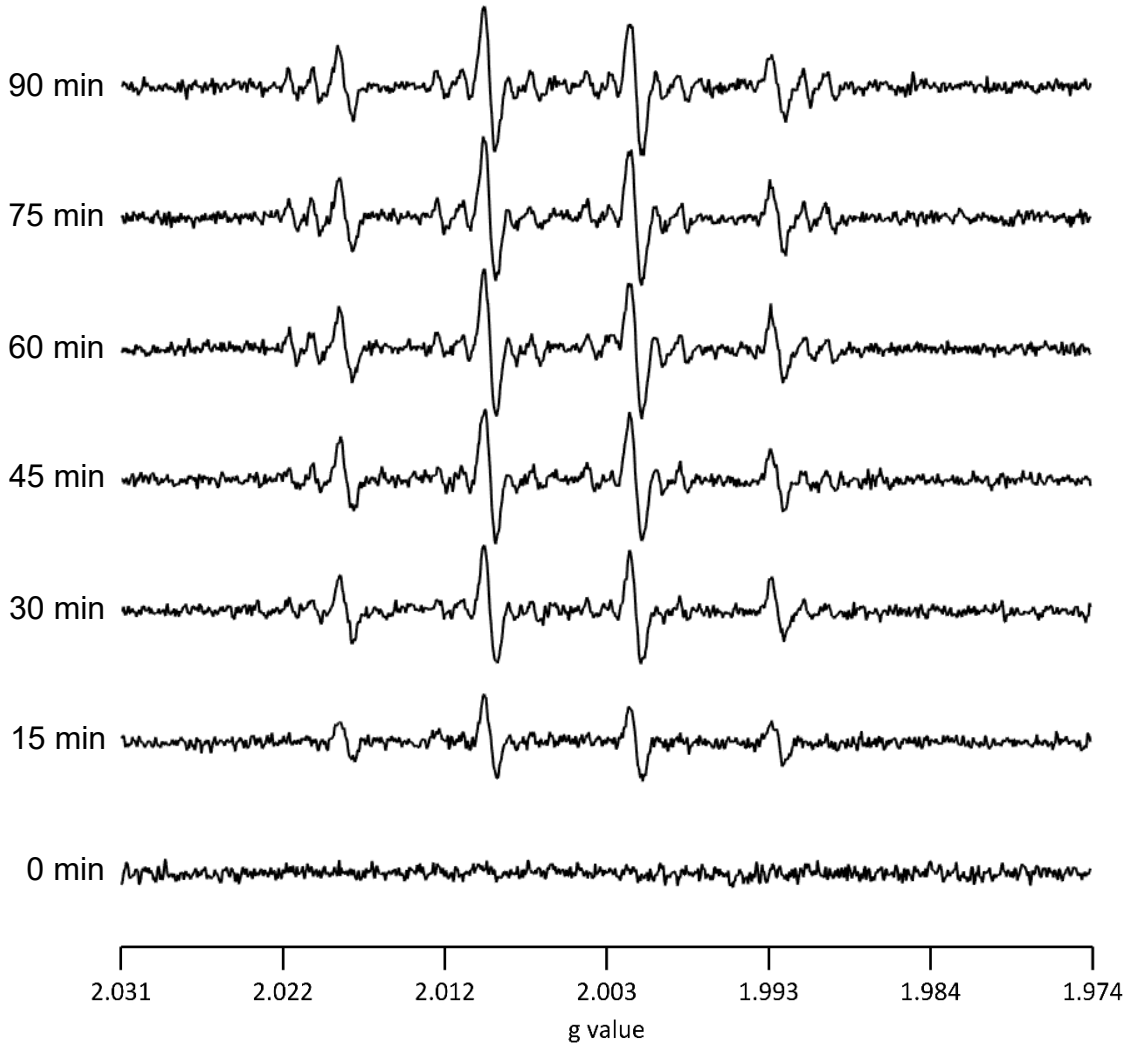


Figure S10. Time dependent spin trapping experiment using 100 μM of **1,2-DiFcAQ** with 50 mM DMPO, 10% MeCN and 100 μM of H_2O_2 as a radical initiator in Milli-Q® H_2O.

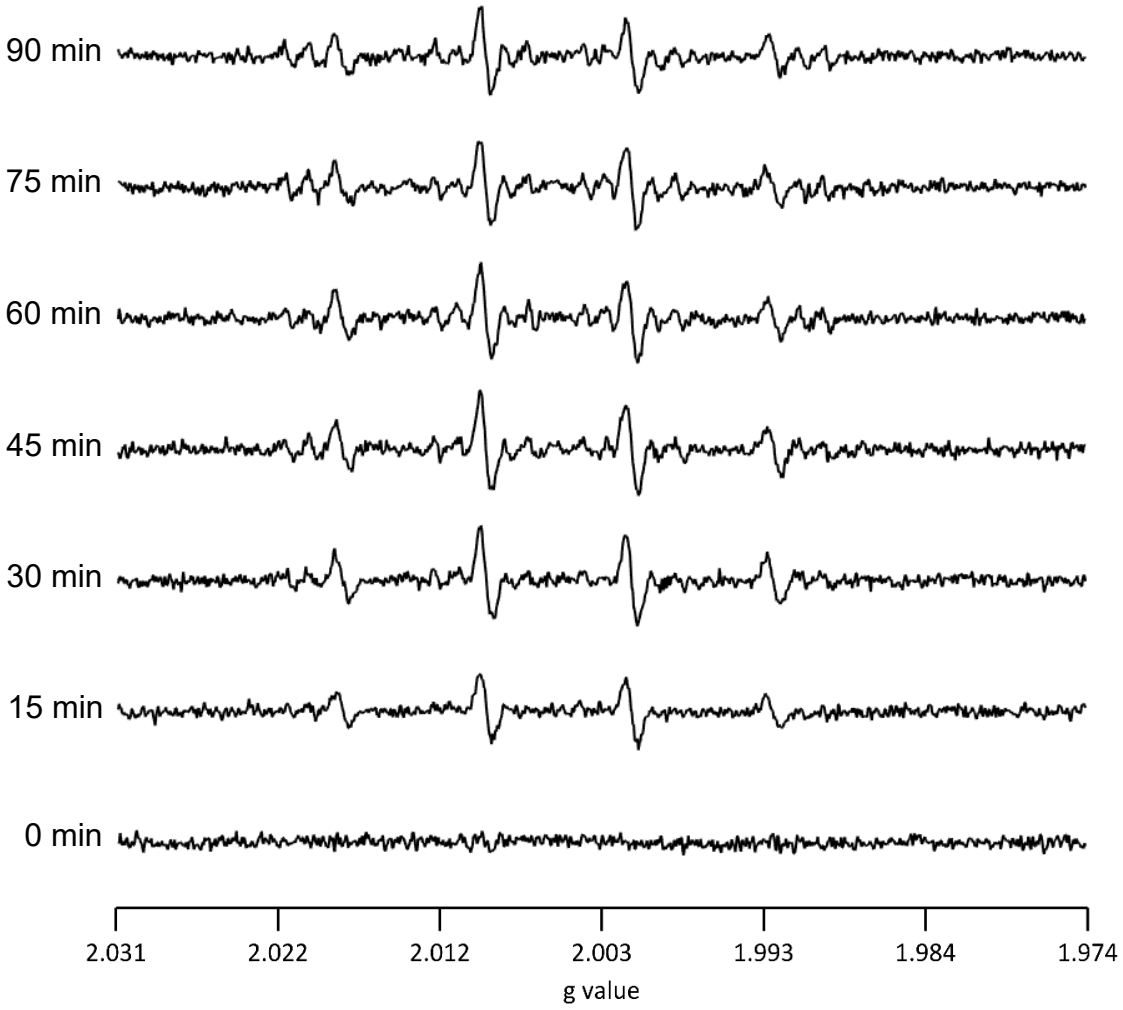


Figure S11. Time dependent spin trapping experiment using 100 μM of **4-FcC** with 50 mM DMPO, 10% MeCN and 100 μM of H_2O_2 as a radical initiator in Milli-Q® H_2O.

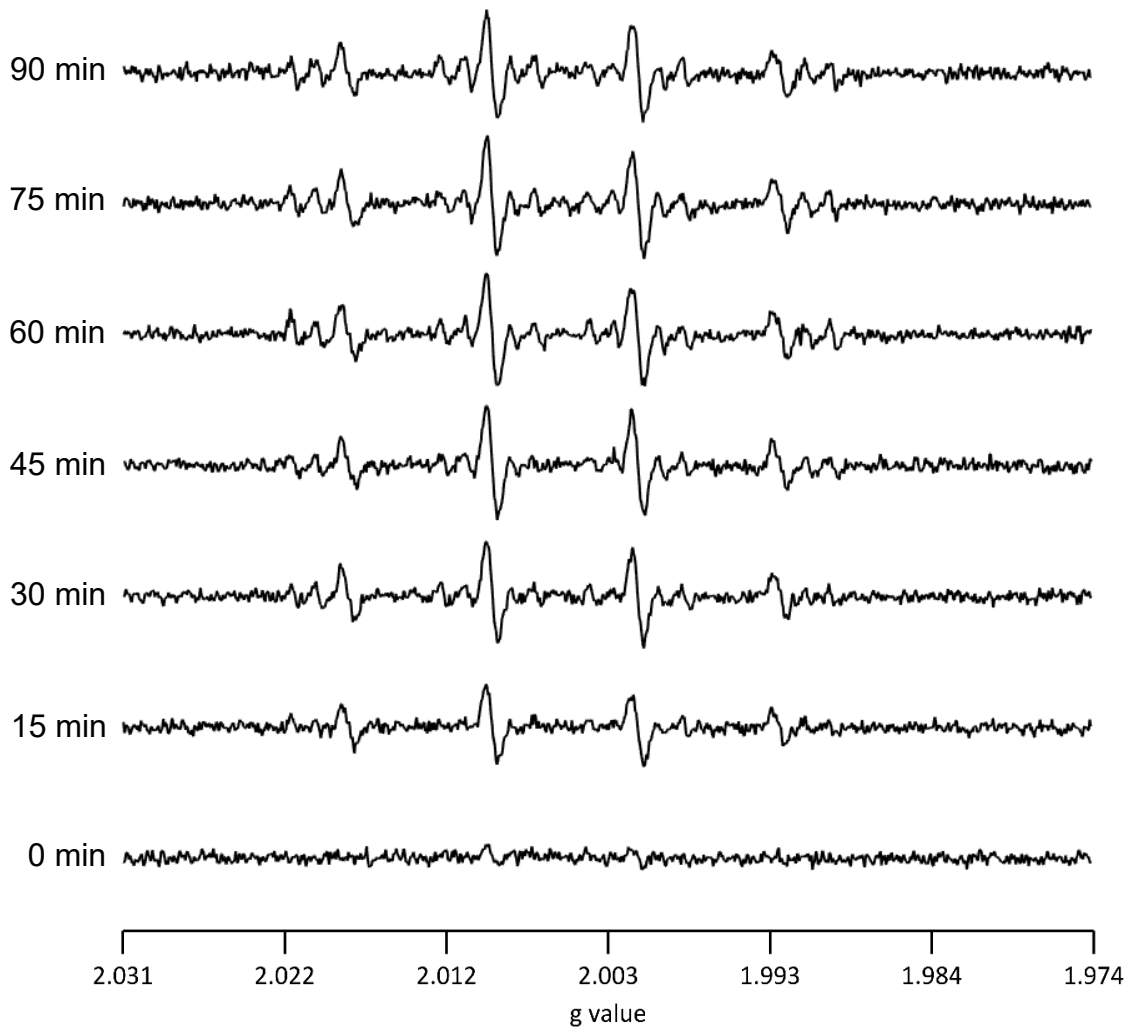


Figure S12. Time dependent spin trapping experiment using 100 μM of **1-FcAQ** with 50 mM DMPO, 10% MeCN and 100 μM of H_2O_2 as a radical initiator in Milli-Q® H_2O.

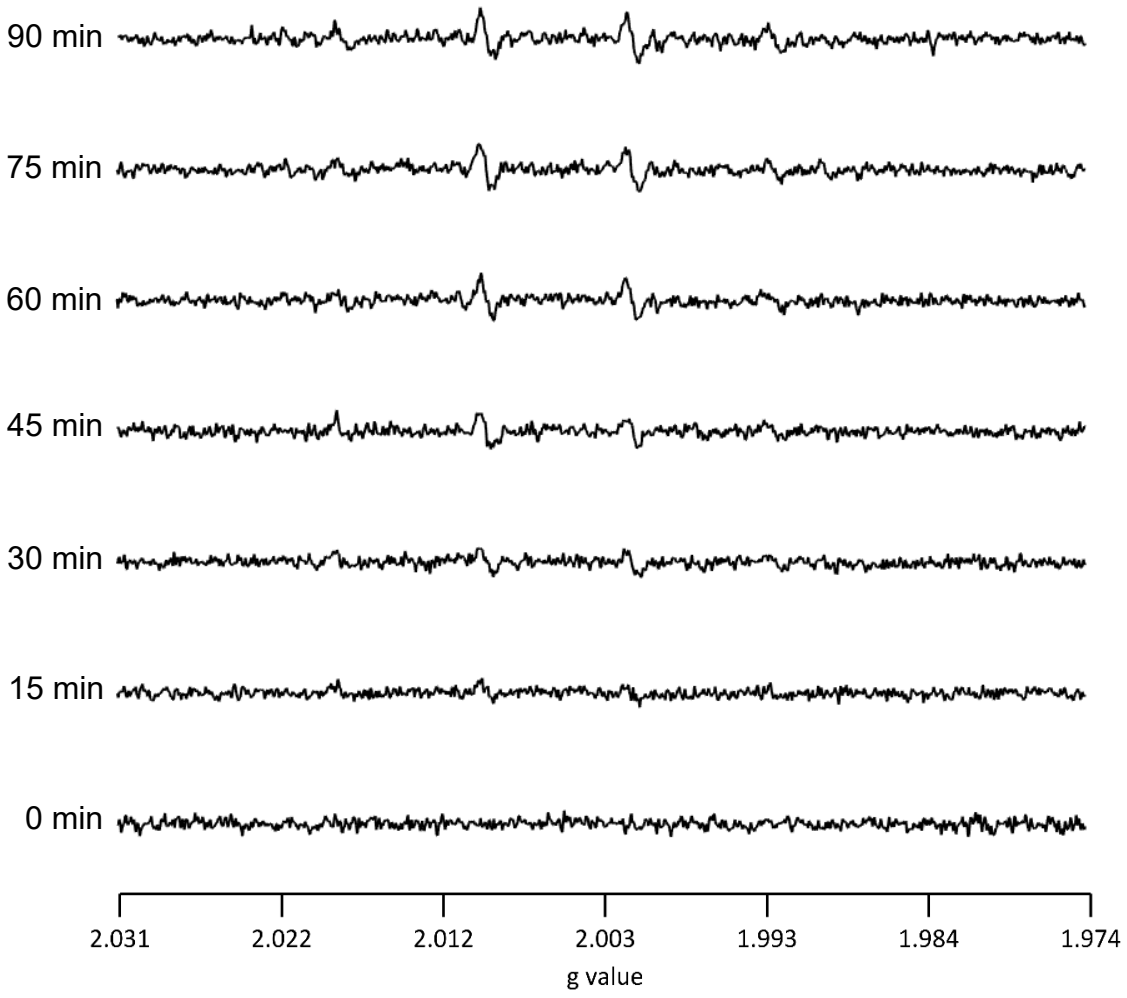


Figure S13. Time dependent spin trapping experiment control using 50 mM DMPO, 10% MeCN and 100 μM of H_2O_2 in Milli-Q® H_2O.

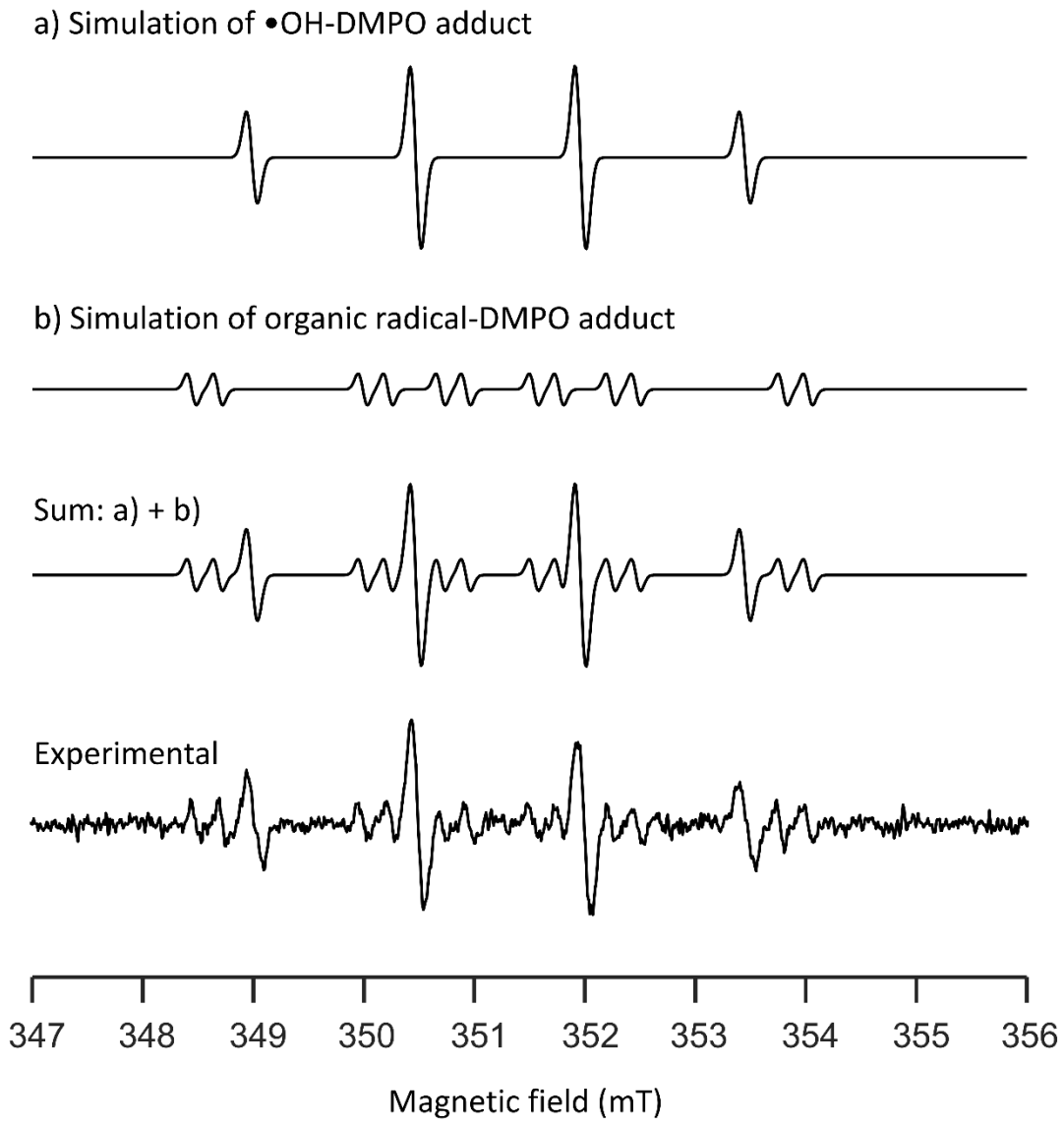


Figure S14. Deconvolution of EPR spectrum from DMSO spin-trapping experiment with **4-FcC** at 90 min timepoint. Solution: 100 μM **4-FcC**, 50 mM DMPO, 10% MeCN and 100 μM of H_2O_2 as a radical initiator in Milli-Q® H_2O. Simulation performed using the Matlab-based Toolbox EasySpin.[5] Simulation parameters:

(i) •OH-DMPO radical adduct: g = 2.0052, $a(^{14}N)$ = 1.49 mT, $a(^{1}H)$ = 1.49 mT, peak-to-peak linewidth = 0.1 mT

(ii) organic radical-DMPO adduct: g = 2.0052. $a(^{14}N)$ = 1.55 mT, $a(^{1}H)_1$ = 2.25 mT, $a(^{1}H)_2$ = 0.23 mT, peak-to-peak line width = 0.85 mT

Spectral weighting, •OH-DMPO radical adduct : organic radical-DMPO adduct = 2:1

Antibacterial Screening Results

Table S1. Antibacterial screening results for **1,2-DiFcAQ**, **1-FcAQ**, **4-FcC** and positive control, enrofloxacin. Listed values are MIC_{90} in μM.

Strain	1,2-DiFcAQ	1-FcAQ	4-FcC	Enrofloxacin
E. coli	>256	>256	>256	0.06
K. aerogenes	>256	>256	>256	0.25
K. pneumoniae	>256	>256	>256	3.33
P. alcalifaciens	>256	>256	>256	0.25
S. enterica	>256	>256	>256	0.06
S. sonnei	>256	>256	>256	0.10
Y. pseudotuberculosis	>256	>256	>256	0.06
A. baumanii	>256	>256	>256	0.83
P. aeruginosa	>256	>256	>256	3.00
V. cholerae	>256	>256	>256	0.01
O. anthropi	>256	>256	>256	0.21
B. subtilis	>256	>256	>256	0.33
L. ivanovii	>256	>256	>256	4.00
MSSA	>256	>256	>256	0.67
MRSA	>256	>256	>256	13.3
S. epidermidis	>256	>256	>256	3.33
E. faecium	>256	>256	>256	3.33
E. faecalis	>256	>256	>256	3.33
S. pneumoniae	>256	>256	>256	3.33

Table S2. Antibacterial screening growth conditions and strain designations.

Strain Name	Strain Designation	BSL	Growth Medium	Growth Condition
Gram-Positive				
Bacillus subtilis	ATCC 6051	1	NB	37 °C
Enterococcus faecalis	ATCC 29212	2	BHI	37 °C
Enterococcus faecium	ATCC 6569	2	BHI	37 °C
Listeria ivanovii	BAA-139	1	BHI-A; HTM	37 °C; 5% CO_2
Staphylococcus aureus (Methicillin-Resistant)	BAA-44	2	TSB	37 °C
Staphylococcus aureus (Methicillin-Sensitive)	ATCC 29213	2	TSB	37 °C
Staphylococcus epidermidis	ATCC 14990	1	TSB	37 °C
Streptococcus pneumoniae	ATCC 49619	2	BHI	37 °C; 5% CO_2
Gram-Negative				
Acinetobacter baumanii	ATCC 19606	2	TSB	37 °C
Escherichia coli	K-12 MG1655	1	NB	37 °C
Klebsiella aerogenes	ATCC 35029	1	NB	37 °C
Klebsiella pneumoniae	ATCC 700603	2	NB	37 °C
Ochrobactrum anthropi	ATCC 49687	1	TSB	37 °C
Providencia alcalifaciens	ATCC 9886	1	TSB	37 °C
Pseudomonas aeruginosa	ATCC 27853	2	TSB	37 °C
Salmonella enterica	ATCC 13311	2	NB	37 °C
Shigella sonnei	ATCC 25931	2	NB	37 °C
Vibrio cholerae	A1552 El Tor	2	TSB	37 °C
Yersinia pseudotuberculosis	ATCC 6904	2	BHI	37 °C

X-ray Crystallography

Table S3. Crystal data and details of data collection and refinement for **1-FcAQ.**

Identification code	AH_1HAQ_Fc_0m_a
Empirical formula	$C_{29}H_{23}FeN_3O_3$
Formula weight	517.35
Temperature/K	150(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.5846(11)
b/Å	10.9289(12)
c/Å	12.3271(14)
α/°	96.266(2)
β/°	104.325(2)
γ/°	106.238(2)
Volume/Å^3	1178.9(2)
Z	2
ρ_{calc}g/cm^3	1.455
μ/mm^{-1}	0.678
F(000)	536.0
Crystal size/mm	0.142 × 0.134 × 0.060
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.474 to 50.728
Index ranges	$-11 \leq h \leq 11$, $-13 \leq k \leq 13$, $-14 \leq l \leq 14$
Reflections collected	12982
Independent reflections	4299 [R_{int} = 0.0466, R_{sigma} = 0.0604]
Data/restraints/parameters	4299/18/382
Goodness-of-fit on F^2	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0486, wR_2 = 0.0887
Final R indexes [all data]	R_1 = 0.0813, wR_2 = 0.0977
Largest diff. peak/hole / e Å^{-3}	0.36/-0.35

Table S4. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1-FcAQ**. U_{eq} defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe1	-2143.5(5)	7141.0(4)	935.9(4)	37.67(16)
O1	5185(2)	7073.9(17)	4195.5(16)	43.5(5)
O2	4784(2)	4904.7(19)	2885.3(17)	53.8(6)
O3	9382(3)	4139(2)	5919.7(19)	68.6(7)
N3	3211(3)	9274(2)	3184(2)	54.4(7)
C1	5412(4)	2619(3)	2440(3)	47.2(8)
C2	5776(4)	1506(3)	2237(3)	57.5(9)
C3	6973(4)	1294(3)	3001(3)	60.4(10)
C4	7787(4)	2199(3)	3975(3)	56.0(9)
C5	7426(3)	3337(3)	4193(3)	40.7(7)
C6	6228(3)	3548(3)	3418(2)	36.6(7)
C7	5812(3)	4753(3)	3610(2)	34.7(7)
C8	6687(3)	5724(3)	4669(2)	32.8(7)
C9	7899(3)	5506(3)	5456(2)	38.6(7)
C10	8316(4)	4306(3)	5241(3)	44.8(8)
C11	6382(3)	6890(3)	4934(2)	35.5(7)
C12	7272(3)	7797(3)	5918(2)	43.3(8)
C13	8442(4)	7539(3)	6651(3)	53.8(9)
C14	8755(4)	6405(3)	6430(3)	50.2(8)
C15	4988(3)	8322(3)	4333(2)	38.6(7)
C36	1730(20)	7410(20)	-355(16)	52(6)
C37	-490(20)	6792(17)	477(17)	21(5)
C30	964(14)	7810(20)	505(12)	33(5)
N4	2090(30)	8210(20)	1680(20)	30(5)
N5	2100(30)	9310(20)	2230(30)	43(6)
C35	3010(30)	7630(20)	2200(20)	27(5)
C16	3744(3)	8267(3)	3314(2)	36.5(7)
C31	1269(7)	7935(7)	-286(6)	53.2(19)
C22	-530(6)	6393(7)	541(5)	30.3(13)
C18	1086(4)	7031(6)	539(4)	34.9(16)
N1	2073(11)	7683(7)	1694(8)	36.9(17)
N2	2208(9)	8894(8)	2158(10)	53(2)
C17	3025(10)	7238(7)	2412(6)	31.4(16)
C20	-2542(4)	5231(3)	977(3)	47.6(8)
C21	-971(4)	5897(3)	1392(3)	45.9(8)
C23	-1831(3)	6167(3)	-441(2)	40.8(7)
C24	-3069(3)	5394(3)	-152(3)	41.1(8)
C25	-2612(4)	8780(3)	556(3)	64.7(10)
C26	-3799(4)	7987(3)	884(4)	63.2(10)
C27	-3205(5)	7800(4)	1995(4)	73.9(11)
C28	-1624(5)	8500(4)	2350(3)	76.0(12)
C29	-1272(4)	9097(3)	1455(4)	70.1(12)

Table S5. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1-FcAQ**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	34.2(3)	33.3(2)	40.6(3)	-1.54(18)	6.45(19)	10.30(18)
O1	42.0(12)	35.8(11)	42.6(13)	-7.0(9)	-2.8(10)	15.7(9)
O2	64.2(15)	44.8(12)	40.6(13)	-4.8(10)	-9.5(12)	25.4(11)
O3	76.3(17)	81.9(17)	51.9(15)	15.1(13)	-0.5(13)	47.8(14)
N3	41.9(16)	49.8(16)	56.3(19)	-4.7(14)	-9.9(15)	17.7(13)
C1	53(2)	35.9(17)	48(2)	2.6(15)	11.2(17)	12.1(15)
C2	66(2)	44(2)	61(2)	-1.4(17)	21(2)	18.2(18)
C3	76(3)	40(2)	78(3)	7(2)	37(2)	28.1(19)
C4	58(2)	59(2)	65(2)	18(2)	24(2)	32.1(19)
C5	48.7(19)	40.5(17)	42.8(19)	13.4(15)	22.2(16)	19.6(15)
C6	41.7(17)	34.1(16)	36.5(18)	7.6(14)	17.6(15)	10.3(14)
C7	39.5(17)	33.5(16)	30.2(16)	5.5(13)	10.7(14)	9.8(13)
C8	34.1(16)	35.2(16)	27.0(16)	4.0(13)	8.6(13)	8.8(13)
C9	38.4(17)	43.9(18)	33.7(18)	8.0(14)	9.7(14)	13.8(14)
C10	51(2)	55(2)	37.2(19)	17.2(16)	14.1(16)	25.5(16)
C11	31.6(16)	38.4(17)	31.7(17)	4.8(14)	5.1(14)	8.1(13)
C12	47.3(19)	38.2(17)	39.0(19)	-1.1(14)	8.3(16)	12.1(15)
C13	52(2)	55(2)	37.0(19)	-5.2(16)	-5.1(16)	11.5(17)
C14	51(2)	55(2)	38.2(19)	3.6(16)	-0.9(16)	20.8(17)
C15	36.2(16)	32.3(16)	41.9(18)	-2.8(13)	6.3(14)	10.6(13)
C36	41(10)	77(13)	36(9)	-14(9)	8(8)	29(8)
C37	21(5)	21(5)	21(5)	4.0(14)	6.1(17)	6.6(18)
C30	32(7)	40(11)	29(8)	9(7)	6(6)	16(6)
N4	28(7)	34(17)	27(9)	-5(12)	5(6)	14(13)
N5	37(7)	40(10)	49(8)	-1(8)	-4(6)	27(7)
C35	35(8)	17(8)	30(9)	-5(6)	7(7)	14(8)
C16	25.8(15)	37.3(17)	38.9(18)	-4.8(14)	4.0(14)	7.7(13)
C31	37(3)	63(4)	51(4)	15(3)	11(3)	3(3)
C22	31(3)	20(3)	35(3)	1(2)	2.8(18)	9(2)
C18	32(2)	30(3)	34(3)	-4(2)	-1.3(19)	11(2)
N1	30(3)	27(4)	45(3)	-5(4)	1(2)	9(4)
N2	49(3)	40(6)	66(5)	-1(4)	-7(3)	34(4)
C17	29(3)	28(3)	39(3)	9(3)	8(2)	13(3)
C20	55(2)	34.0(17)	49(2)	6.3(15)	14.7(17)	6.5(15)
C21	52(2)	46.8(19)	36.2(19)	5.6(16)	3.0(16)	20.5(16)
C23	35.5(17)	48.2(18)	31.6(17)	-0.5(14)	2.8(14)	11.7(15)

Table S6. Bond Lengths for **1-FcAQ**.

Atom	Atom	Length/Å
Fe1	C37	1.93(2)
Fe1	C22	2.071(6)
Fe1	C20	2.023(3)
Fe1	C21	2.034(3)
Fe1	C23	2.035(3)
Fe1	C24	2.033(3)
Fe1	C25	2.039(3)
Fe1	C26	2.040(3)
Fe1	C27	2.029(4)
Fe1	C28	2.021(3)
Fe1	C29	2.028(3)
O1	C11	1.355(3)
O1	C15	1.427(3)
O2	C7	1.218(3)
O3	C10	1.221(3)
N3	N5	1.39(3)
N3	C16	1.345(3)
N3	N2	1.325(10)
C1	C2	1.371(4)
C1	C6	1.385(4)
C2	C3	1.385(5)
C3	C4	1.369(5)
C4	C5	1.397(4)
C5	C6	1.392(4)
C5	C10	1.473(4)
C6	C7	1.491(4)
C7	C8	1.480(4)
C8	C9	1.413(4)
C8	C11	1.408(4)
C9	C10	1.490(4)

Atom	Atom	Length/Å
C9	C14	1.373(4)
C11	C12	1.390(4)
C12	C13	1.373(4)
C13	C14	1.369(4)
C15	C16	1.484(4)
C36	C30	1.52(3)
C37	C30	1.51(2)
C37	C21	1.641(19)
C37	C23	1.422(19)
C30	N4	1.51(3)
N4	N5	1.31(3)
N4	C35	1.32(3)
C35	C16	1.38(2)
C16	C17	1.375(7)
C31	C18	1.501(10)
C22	C18	1.511(7)
C22	C21	1.338(7)
C22	C23	1.447(6)
C18	N1	1.472(10)
N1	N2	1.341(8)
N1	C17	1.339(11)
C20	C21	1.408(4)
C20	C24	1.408(4)
C23	C24	1.401(4)
C25	C26	1.401(5)
C25	C29	1.400(5)
C26	C27	1.407(5)
C27	C28	1.422(5)
C28	C29	1.406(5)

Table S7. Bond Angles for **1-FcAQ**.

Atom	Atom	Atom	Angle/°
C37	Fe1	C20	77.5(5)
C37	Fe1	C21	48.8(5)
C37	Fe1	C23	41.9(6)
C37	Fe1	C24	74.3(5)
C37	Fe1	C25	116.6(5)
C37	Fe1	C26	154.7(6)
C37	Fe1	C27	157.3(6)
C37	Fe1	C28	117.8(6)
C37	Fe1	C29	100.1(5)
C20	Fe1	C22	65.6(2)
C20	Fe1	C21	40.62(12)
C20	Fe1	C23	68.06(12)
C20	Fe1	C24	40.61(11)
C20	Fe1	C25	157.73(14)
C20	Fe1	C26	121.58(15)
C20	Fe1	C27	106.05(15)
C20	Fe1	C29	159.69(15)
C21	Fe1	C22	38.0(2)
C21	Fe1	C23	68.42(12)
C21	Fe1	C25	161.09(14)
C21	Fe1	C26	156.28(15)
C23	Fe1	C22	41.26(16)
C23	Fe1	C25	109.84(14)
C23	Fe1	C26	125.33(14)
C24	Fe1	C22	66.94(17)
C24	Fe1	C21	68.42(12)
C24	Fe1	C23	40.29(11)
C24	Fe1	C25	123.29(13)
C24	Fe1	C26	108.39(13)
C25	Fe1	C22	128.5(2)
C25	Fe1	C26	40.16(14)
C26	Fe1	C22	164.2(2)
C27	Fe1	C22	155.0(2)
C27	Fe1	C21	120.14(16)
C27	Fe1	C23	160.37(15)
C27	Fe1	C24	123.21(15)
C27	Fe1	C25	68.09(17)
C27	Fe1	C26	40.47(15)
C28	Fe1	C22	121.61(19)
C28	Fe1	C20	122.62(17)
C28	Fe1	C21	106.13(14)
C28	Fe1	C23	157.89(16)
C28	Fe1	C24	159.59(17)
C28	Fe1	C25	68.00(16)
C28	Fe1	C26	68.23(15)
C28	Fe1	C27	41.11(16)

Atom	Atom	Atom	Angle/°
C14	C9	C10	117.8(3)
O3	C10	C5	121.0(3)
O3	C10	C9	120.3(3)
C5	C10	C9	118.6(3)
O1	C11	C8	117.0(2)
O1	C11	C12	122.3(3)
C12	C11	C8	120.8(3)
C13	C12	C11	119.6(3)
C14	C13	C12	121.2(3)
C13	C14	C9	120.0(3)
O1	C15	C16	105.4(2)
C30	C37	Fe1	124.9(11)
C30	C37	C21	133.0(14)
C21	C37	Fe1	68.9(8)
C23	C37	Fe1	73.0(8)
C23	C37	C30	130.1(15)
C23	C37	C21	96.4(11)
C37	C30	C36	113.8(16)
N4	C30	C36	109.2(15)
N4	C30	C37	111.8(16)
N5	N4	C30	113(2)
N5	N4	C35	118(2)
C35	N4	C30	130(2)
N4	N5	N3	92.1(18)
N4	C35	C16	110.5(17)
N3	C16	C15	121.6(2)
N3	C16	C35	93.9(10)
N3	C16	C17	112.6(4)
C35	C16	C15	142.5(11)
C17	C16	C15	125.8(4)
C18	C22	Fe1	132.2(4)
C21	C22	Fe1	69.5(3)
C21	C22	C18	126.4(4)
C21	C22	C23	110.3(4)
C23	C22	Fe1	68.0(3)
C23	C22	C18	123.1(5)
C31	C18	C22	115.3(5)
N1	C18	C31	110.5(5)
N1	C18	C22	111.4(5)
N2	N1	C18	123.0(8)
C17	N1	C18	127.6(6)
C17	N1	N2	109.3(8)
N3	N2	N1	111.1(7)
N1	C17	C16	103.2(6)
C21	C20	Fe1	70.08(17)
C24	C20	Fe1	70.08(16)

Table S7. Bond Angles for **1-FcAQ**.

Atom	Atom	Atom	Angle/°
C28	Fe1	C29	40.63(15)
C29	Fe1	C22	110.5(2)
C29	Fe1	C21	123.74(13)
C29	Fe1	C23	123.34(16)
C29	Fe1	C24	158.58(16)
C29	Fe1	C25	40.27(13)
C29	Fe1	C26	67.89(15)
C29	Fe1	C27	68.62(17)
C11	O1	C15	118.5(2)
C16	N3	N5	124.8(10)
N2	N3	C16	103.6(4)
C2	C1	C6	120.6(3)
C1	C2	C3	120.6(3)
C4	C3	C2	119.6(3)
C3	C4	C5	120.3(3)
C4	C5	C10	119.8(3)
C6	C5	C4	119.8(3)
C6	C5	C10	120.4(3)
C1	C6	C5	119.1(3)
C1	C6	C7	119.3(3)
C5	C6	C7	121.7(3)
O2	C7	C6	118.8(3)
O2	C7	C8	122.9(3)
C8	C7	C6	118.3(2)
C9	C8	C7	120.0(3)
C11	C8	C7	122.8(2)
C11	C8	C9	117.2(3)
C8	C9	C10	121.0(3)
C14	C9	C8	121.2(3)

Atom	Atom	Atom	Angle/°
C24	C20	C21	108.6(3)
C37	C21	Fe1	62.3(7)
C22	C21	Fe1	72.5(3)
C22	C21	C20	107.6(3)
C20	C21	Fe1	69.30(17)
C20	C21	C37	108.2(7)
C37	C23	Fe1	65.0(8)
C22	C23	Fe1	70.7(3)
C24	C23	Fe1	69.80(17)
C24	C23	C37	116.0(8)
C24	C23	C22	105.3(4)
C20	C24	Fe1	69.32(17)
C23	C24	Fe1	69.91(16)
C23	C24	C20	107.9(3)
C26	C25	Fe1	69.96(19)
C29	C25	Fe1	69.45(19)
C29	C25	C26	108.4(4)
C25	C26	Fe1	69.88(19)
C25	C26	C27	108.4(3)
C27	C26	Fe1	69.4(2)
C26	C27	Fe1	70.2(2)
C26	C27	C28	107.2(4)
C28	C27	Fe1	69.1(2)
C27	C28	Fe1	69.8(2)
C29	C28	Fe1	70.0(2)
C29	C28	C27	107.9(4)
C25	C29	Fe1	70.28(18)
C25	C29	C28	108.0(4)
C28	C29	Fe1	69.4(2)

Table S8. Hydrogen-Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1-FcAQ**.

Atom	*x*	*y*	*z*	U(eq)
H1	4593.22	2754.61	1905.25	57
H2	5201.99	873.67	1565.02	69
H3	7226.46	524.83	2850.71	72
H4	8602.16	2052.9	4504.9	67
H12	7072.26	8590.07	6081.19	52
H13	9046.14	8158.99	7324.07	65
H14	9563.27	6239.75	6951.04	60
H15A	5933.53	9009.69	4368.89	46
H15B	4706.89	8502.43	5040.09	46
H36A	1000.83	7130.86	-1117.42	78
H36B	2098.48	6692.63	-143	78
H36C	2591.9	8150.13	-355.81	78
H30	693.76	8596.96	306.43	39
H35	3159.65	6868.03	1856.68	33
H31A	2351.96	8345.19	-191.29	80
H31B	806.37	8606.35	-137.75	80
H31C	767.81	7445.19	-1067.66	80
H18	1467.88	6313.18	298.47	42
H17	3168.74	6411.83	2320.52	38
H20	-3176.95	4726.02	1412.08	57
H21	-297.02	5948.19	2169.29	55
H23	-1831.61	6442.96	-1187.94	49
H24	-4139.45	5028.49	-656.89	49
H25	-2702.82	9062.5	-195.7	78
H26	-4881.75	7607.56	405.74	76
H27	-3787.6	7280.19	2451.65	89
H28	-892.9	8559.51	3105.52	91
H29	-244.28	9651.4	1459.69	84

Table S9. Crystal data and details of data collection and refinement for **4-FcC**.

Identification code	AH_Coum_Fc_0m_a
Empirical formula	$C_{24}H_{21}FeN_3O_3$
Formula weight	455.29
Temperature/K	150(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.7127(6)
b/Å	29.914(3)
c/Å	12.0899(14)
α/°	90
β/°	91.627(2)
γ/°	90
Volume/Å^3	2065.2(4)
Z	4
ρ_{calc}g/cm^3	1.464
μ/mm^{-1}	0.762
F(000)	944.0
Crystal size/mm	0.476 × 0.374 × 0.172
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.634 to 52.922
Index ranges	$-7 \leq h \leq 7$, $-37 \leq k \leq 37$, $-15 \leq l \leq 15$
Reflections collected	16206
Independent reflections	4232 [R_{int} = 0.0390, R_{sigma} = 0.0428]
Data/restraints/parameters	4232/18/316
Goodness-of-fit on F^2	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.0478, wR_2 = 0.1033
Final R indexes [all data]	R_1 = 0.0727, wR_2 = 0.1078
Largest diff. peak/hole / e Å^{-3}	0.58/-0.40

Table S10 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4-FcC**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe1	4877.2(6)	2099.2(2)	4838.1(3)	33.25(14)
O1	6655(4)	4682.1(6)	7088.5(17)	48.2(5)
O2	7588(5)	5527.4(8)	10386(2)	69.3(7)
O3	4794(4)	5701.5(7)	9171.4(19)	60.0(6)
N3	10439(4)	3858.7(9)	6182(2)	48.2(7)
C1	6673(6)	5436.9(10)	9503(3)	50.8(8)
C2	7326(6)	5082.2(9)	8782(3)	43.5(7)
C3	6175(5)	5006.5(9)	7814(3)	41.2(7)
C4	4219(5)	5287.2(9)	7468(3)	44.6(7)
C5	3600(6)	5628.8(10)	8186(3)	50.5(8)
C6	1725(7)	5906.4(12)	7938(3)	64.7(10)
C7	480(7)	5846.4(13)	6971(4)	68.3(11)
C8	1061(7)	5509.7(13)	6235(3)	68.0(11)
C9	2918(6)	5230.7(11)	6487(3)	56.6(9)
C10	8346(6)	4351.9(10)	7450(3)	49.1(8)
C31	5550(60)	3124(7)	5010(20)	21(7)
N4	6900(60)	3478(11)	5710(30)	31(7)
N5	9210(80)	3465(10)	5510(30)	27(7)
C11	8393(5)	3992.9(9)	6608(2)	39.1(7)
C12	6635(5)	3740.4(11)	6155(3)	45.1(8)
C13	4924(7)	3288.2(13)	3968(3)	68.3(11)
N1	7769(10)	3458.5(10)	5445(3)	34.1(9)
N2	10090(8)	3537.4(14)	5485(3)	43.1(11)
C14	6834(8)	3105.9(11)	4695(3)	39.4(12)
C16	6174(5)	2701.0(9)	5383(2)	33.7(6)
C15	4060(6)	2610.5(11)	5903(3)	45.7(8)
C17	7765(5)	2347.2(10)	5638(3)	43.4(8)
C18	6547(6)	2036.5(10)	6330(3)	54.6(9)
C19	4295(7)	2208.8(12)	6467(3)	52.0(9)
C20	4572(6)	2095.2(12)	3138(3)	54.7(9)
C21	5957(6)	1739.9(15)	3510(3)	65.3(12)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4-FcC**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	30.4(2)	38.1(2)	30.9(2)	-9.36(18)	-4.77(16)	-1.15(18)
O1	63.4(13)	35.0(11)	44.9(12)	-3.3(10)	-17.5(11)	9.9(10)
O2	81.7(17)	64.3(16)	61.0(16)	-19.4(13)	-15.5(14)	-11.4(13)
O3	75.6(16)	43.9(13)	60.2(15)	-8.8(11)	-4.3(13)	4.3(12)
N3	45.5(15)	44.7(15)	53.9(17)	1.1(13)	-6.5(13)	-0.5(12)
C1	58(2)	39.6(18)	54(2)	-1.3(15)	-3.4(17)	-12.8(16)
C2	49.4(18)	32.1(16)	48.7(19)	-0.2(13)	-5.9(15)	-4.7(13)
C3	50.3(17)	27.3(14)	45.6(19)	4.8(13)	-6.4(15)	-4.8(13)
C4	51.6(18)	32.4(16)	49.7(19)	8.3(14)	-1.9(15)	0.0(14)
C5	56(2)	37.5(17)	58(2)	8.8(15)	4.9(17)	0.0(15)
C6	74(2)	47(2)	74(3)	11.4(19)	12(2)	14.2(19)
C7	62(2)	59(2)	84(3)	26(2)	6(2)	17.8(19)
C8	66(2)	72(3)	65(2)	24(2)	-12(2)	4(2)
C9	65(2)	50(2)	54(2)	7.4(16)	-9.4(18)	6.6(17)
C10	60(2)	35.9(16)	49.7(19)	-2.3(14)	-18.0(16)	8.3(15)
C31	20(7)	21(7)	20(7)	-0.1(10)	0.6(10)	-0.1(10)
N4	30(8)	31(8)	31(8)	-0.1(10)	0.9(11)	-0.1(10)
N5	27(7)	27(7)	27(7)	-0.2(10)	0.7(11)	0.0(10)
C11	43.7(17)	32.1(15)	40.8(17)	2.6(12)	-9.6(14)	2.4(13)
C12	41.4(17)	43.6(18)	49.8(19)	-1.5(16)	-5.7(15)	1.2(14)
C13	78(3)	75(3)	51(2)	11.1(19)	-14.7(19)	-16(2)
N1	30(2)	32.0(16)	40(2)	-3.3(13)	3.9(19)	1.5(15)
N2	30(2)	45(2)	55(2)	-0.6(15)	0.6(17)	-0.3(17)
C14	37(3)	44(2)	37(2)	-5.6(15)	3.1(18)	-3.2(16)
C16	31.1(14)	38.1(15)	31.4(15)	-10.3(12)	-4.9(12)	-0.7(12)
C15	45.8(18)	46.7(19)	44.7(18)	-16.1(15)	3.8(15)	-2.3(15)
C17	31.9(15)	46.3(18)	51.0(18)	-19.2(15)	-15.4(14)	3.2(13)
C18	79(2)	35.0(17)	48.3(19)	-3.1(14)	-34.9(18)	-1.4(16)
C19	58(2)	64(2)	33.9(18)	-9.2(16)	4.6(16)	-15.4(18)
C20	64(2)	70(2)	30.3(16)	-11.9(16)	2.3(16)	-15.8(19)
C21	37.4(17)	102(3)	56(2)	-51(2)	-2.1(17)	2(2)
C22	82(3)	38.3(18)	62(2)	-25.6(17)	-38(2)	16.2(18)
C23	46.1(18)	48.7(18)	43.4(18)	-7.2(15)	-8.6(15)	-15.0(15)
C24	44.1(17)	51.1(19)	40.8(17)	-8.0(15)	-13.9(14)	4.4(14)

Table S12. Bond Lengths for **4-FcC**.

Atom	Atom	Length/Å
Fe1	C16	2.049(3)
Fe1	C15	2.062(3)
Fe1	C17	2.029(3)
Fe1	C18	2.025(3)
Fe1	C19	2.033(3)
Fe1	C20	2.058(3)
Fe1	C21	2.042(3)
Fe1	C22	2.031(3)
Fe1	C23	2.041(3)
Fe1	C24	2.047(3)
O1	C3	1.342(3)
O1	C10	1.441(3)
O2	C1	1.206(4)
O3	C1	1.384(4)
O3	C5	1.373(4)
N3	N5	1.58(3)
N3	C11	1.352(4)
N3	N2	1.290(5)
C1	C2	1.430(4)
C2	C3	1.345(4)
C3	C4	1.450(4)
C4	C5	1.393(4)
C4	C9	1.392(4)
C5	C6	1.382(5)
C6	C7	1.363(5)
Fe1	C16	2.049(3)
Fe1	C15	2.062(3)

Atom	Atom	Length/Å
C7	C8	1.390(5)
C8	C9	1.377(5)
C10	C11	1.481(4)
C31	N4	1.55(4)
C31	C13	1.38(2)
C31	C16	1.39(2)
N4	N5	1.35(4)
N4	C12	0.97(3)
N5	C12	1.87(4)
C11	C12	1.359(4)
C12	N1	1.378(6)
C13	C14	1.486(5)
N1	N2	1.346(5)
N1	C14	1.481(4)
C14	C16	1.523(5)
C16	C15	1.404(4)
C16	C17	1.423(4)
C15	C19	1.386(5)
C17	C18	1.443(5)
C18	C19	1.400(5)
C20	C21	1.392(5)
C20	C24	1.394(5)
C21	C22	1.411(5)
C22	C23	1.409(5)
C23	C24	1.402(4)
C7	C8	1.390(5)
C8	C9	1.377(5)

Table S13. Bond Angles for **4-FcC**.

Atom	Atom	Atom	Angle/°
C16	Fe1	C15	39.93(11)
C16	Fe1	C20	110.25(13)
C17	Fe1	C16	40.84(11)
C17	Fe1	C15	68.07(12)
C17	Fe1	C19	68.45(14)
C17	Fe1	C20	121.52(14)
C17	Fe1	C21	107.92(13)
C17	Fe1	C22	124.70(13)
C17	Fe1	C23	161.64(13)
C17	Fe1	C24	156.42(13)
C18	Fe1	C16	68.76(11)
C18	Fe1	C15	67.77(13)
C18	Fe1	C17	41.70(13)
C18	Fe1	C19	40.36(14)
C18	Fe1	C20	156.01(16)
C18	Fe1	C21	120.45(15)
C18	Fe1	C22	106.12(13)
C18	Fe1	C23	123.67(13)
C18	Fe1	C24	161.29(14)
C19	Fe1	C16	67.31(13)
C19	Fe1	C15	39.57(14)
C19	Fe1	C20	163.10(15)
C19	Fe1	C21	155.23(17)
C19	Fe1	C23	107.50(14)
C19	Fe1	C24	126.21(14)
C20	Fe1	C15	127.87(15)
C21	Fe1	C16	126.94(15)
C21	Fe1	C15	163.82(17)
C21	Fe1	C20	39.68(15)
C21	Fe1	C24	66.85(13)
C22	Fe1	C16	163.01(14)
C22	Fe1	C15	154.73(16)
C22	Fe1	C19	119.99(16)
C22	Fe1	C20	67.44(15)
C22	Fe1	C21	40.52(15)
C22	Fe1	C23	40.49(13)
C22	Fe1	C24	67.37(12)
C23	Fe1	C16	155.79(12)
C23	Fe1	C15	121.00(13)
C23	Fe1	C20	67.42(13)
C23	Fe1	C21	67.80(14)

Atom	Atom	Atom	Angle/°
C6	C7	C8	121.1(3)
C9	C8	C7	119.6(4)
C8	C9	C4	120.3(4)
O1	C10	C11	108.3(2)
C13	C31	N4	111.4(18)
C13	C31	C16	132.8(18)
C16	C31	N4	108.8(17)
N5	N4	C31	111(3)
C12	N4	C31	141(3)
C12	N4	N5	107(3)
N3	N5	C12	78.7(14)
N4	N5	N3	108(3)
N4	N5	C12	29.6(15)
N3	C11	C10	120.7(3)
N3	C11	C12	108.6(3)
C12	C11	C10	130.7(3)
N4	C12	N5	43.5(18)
N4	C12	C11	123(2)
C11	C12	N5	80.3(11)
C11	C12	N1	103.6(3)
C12	N1	C14	130.5(4)
N2	N1	C12	110.5(3)
N2	N1	C14	119.0(4)
N3	N2	N1	106.7(3)
C13	C14	C16	115.2(3)
N1	C14	C13	110.3(3)
N1	C14	C16	108.8(3)
C31	C16	Fe1	127.4(9)
C31	C16	C15	96.1(14)
C31	C16	C17	154.9(14)
C14	C16	Fe1	128.0(2)
C15	C16	Fe1	70.53(16)
C15	C16	C14	128.8(3)
C15	C16	C17	108.2(3)
C17	C16	Fe1	68.83(15)
C17	C16	C14	122.9(3)
C16	C15	Fe1	69.54(16)
C19	C15	Fe1	69.10(19)
C19	C15	C16	108.3(3)
C16	C17	Fe1	70.33(15)
C16	C17	C18	106.8(3)

Table S13. Bond Angles for **4-FcC**.

Atom	Atom	Atom	Angle/°
C23	Fe1	C24	40.10(12)
C24	Fe1	C16	122.47(12)
C24	Fe1	C15	110.14(13)
C24	Fe1	C20	39.69(13)
C3	O1	C10	116.4(2)
C5	O3	C1	121.5(3)
C11	N3	N5	92.3(15)
N2	N3	C11	110.5(3)
O2	C1	O3	116.2(3)
O2	C1	C2	126.3(3)
O3	C1	C2	117.5(3)
C3	C2	C1	121.7(3)
O1	C3	C2	125.9(3)
O1	C3	C4	113.6(3)
C2	C3	C4	120.5(3)
C5	C4	C3	116.9(3)
C9	C4	C3	124.3(3)
C9	C4	C5	118.8(3)
O3	C5	C4	121.9(3)
O3	C5	C6	117.1(3)
C6	C5	C4	121.0(3)
C7	C6	C5	119.3(4)

Atom	Atom	Atom	Angle/°
C18	C17	Fe1	69.02(16)
C17	C18	Fe1	69.28(16)
C19	C18	Fe1	70.11(18)
C19	C18	C17	106.9(3)
C15	C19	Fe1	71.33(19)
C15	C19	C18	109.7(3)
C18	C19	Fe1	69.53(19)
C21	C20	Fe1	69.55(19)
C21	C20	C24	107.9(3)
C24	C20	Fe1	69.74(17)
C20	C21	Fe1	70.77(19)
C20	C21	C22	108.2(3)
C22	C21	Fe1	69.32(18)
C21	C22	Fe1	70.16(19)
C23	C22	Fe1	70.14(17)
C23	C22	C21	107.7(3)
C22	C23	Fe1	69.37(17)
C24	C23	Fe1	70.18(16)
C24	C23	C22	107.2(3)
C20	C24	Fe1	70.57(17)
C20	C24	C23	108.9(3)
C23	C24	Fe1	69.72(16)

Table S14. Hydrogen-Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4-FcC**.

Atom	*x*	*y*	*z*	U(eq)
H2	8606.75	4895.1	8991.67	52
H6	1307.31	6136.75	8435.91	78
H7	-805.69	6037.68	6796.37	82
H8	183.2	5472.34	5562.45	82
H9	3312.64	4998.6	5989.83	68
H10A	7906.92	4226.66	8172.69	59
H10B	9914.29	4490.39	7536.76	59
H102	3210(60)	2061(11)	6880(30)	59(10)
H101	2670(70)	2823(12)	5840(30)	73(11)
H31	3990.99	3148.42	5357.86	25
H12	5008.49	3754.94	6294.43	54
H13A	4320.97	3051.7	3476.71	103
H13B	3657.12	3399.39	4423.72	103
H13C	5533.46	3533.86	3523.68	103
H13D	4686.73	3604.93	4139.37	103
H13E	5350.58	3257.25	3192.35	103
H13F	3474.24	3122.77	4092.39	103
H14	8132.18	3012.5	4208.37	47
H17	9419.49	2322.09	5396.73	52
H18	7197.46	1754.91	6661.9	66
H20	5068.3	2340.09	2632.76	66
H21	7619.4	1683.74	3312.19	78
H22	5133.42	1189.6	4584.01	74
H23	1014.59	1548.84	4681.66	55
H24	1025.55	2259.59	3477.63	55

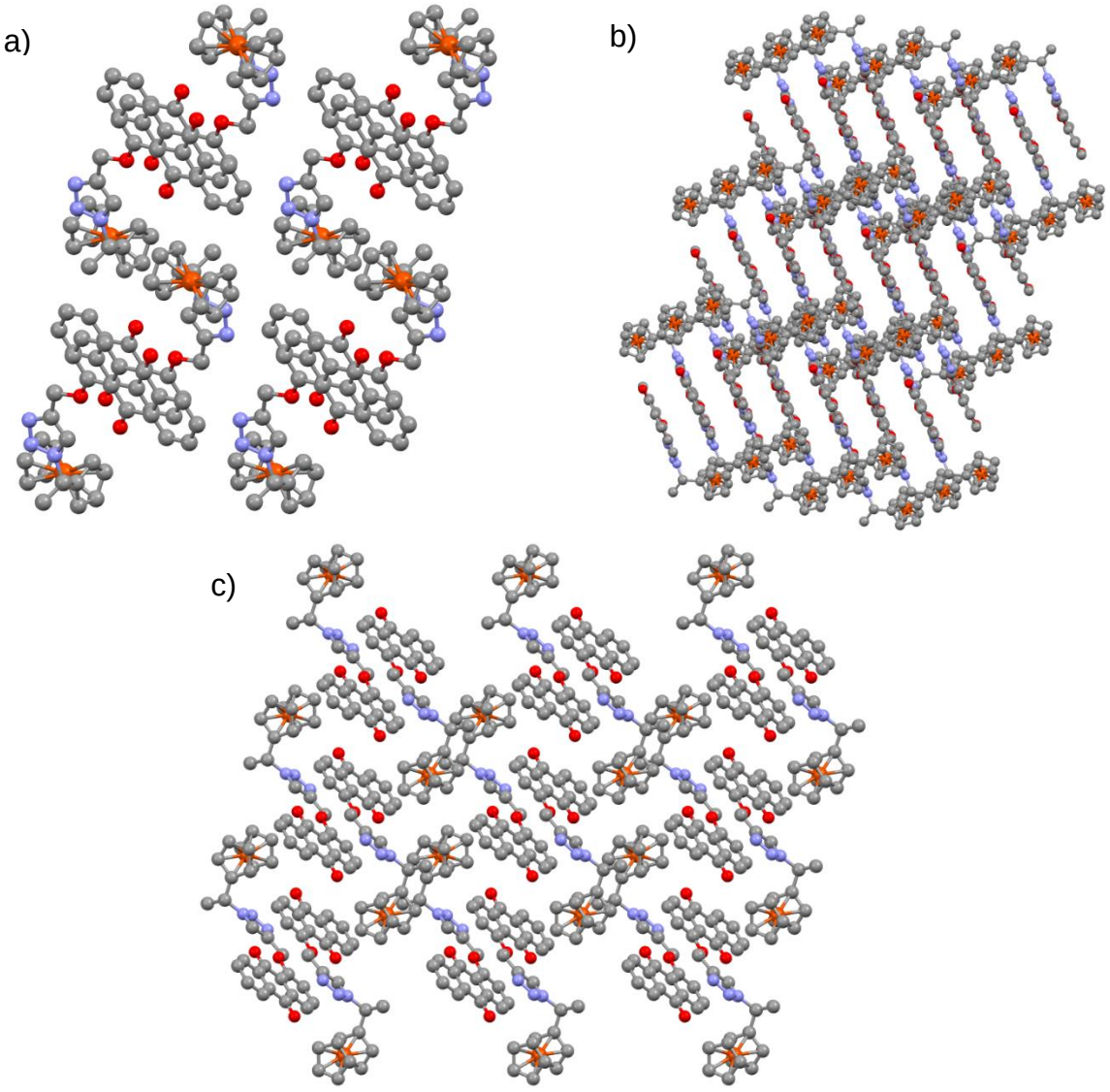


Figure S15. Extended crystal lattice from X-ray crystal structure of **1-FcAQ** viewed along: a) the crystallographic *a* axis, b) the anthraquinone molecular plane, and c) crystallographic *b* axis.

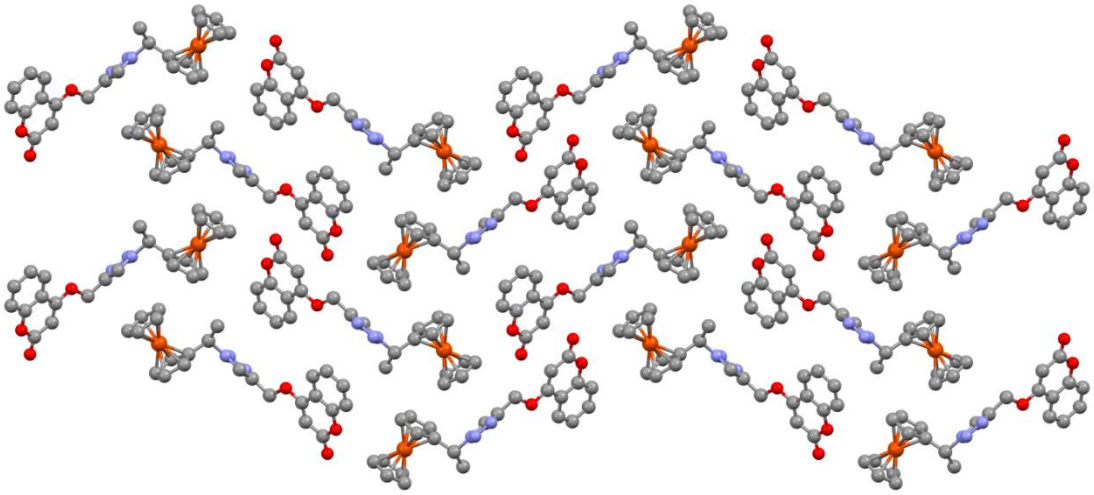


Figure S16. Extended crystal lattice from X-ray crystal structure of **4-FcC** viewed along the crystallographic *a*-axis.

Calculations of logP

Due to limited aqueous solubility and modest extinction coefficients, experimental evaluation of logP for **1,2-DiFcAQ**, **1-FcAQ**, and **4-FcC** using the octanol/water "shake flask" method and UV-Vis measurements was not successful. Furthermore, software to directly calculate logP values of metal-containing compounds is not widely available. However, an approximate calculated value (clogP) can be obtained using the approach of Rekker.[6] This method deconvolutes molecules of interest into smaller substructures and the sum of contributions from each component is used to estimate the logP of the whole compound. Initially, a theoretical logP was calculated for substructures of the Fc compounds where Fc was replaced by a methyl group. This was done using ChemDraw, which utilizes a combination of Crippen's[7] and Viswanadhan's[8] fragmentation. The logP value for ferrocene has been reported previously to be 2.66,[9] and the contribution from the methyl group were determined from tables published by Rekker.[6] Using these values, the final value of clogP resulting from changing the methyl group of the organic fragments to Fc was calculated as described by Ahmedi *et al*.,[9] and outlined in the calculations below.

1,2-DiFcAQ:

$$cLogP = (\ cLogP\ Organic\ Fragment) - \left(f_{CH_3}\right) + (f_{Fc}) - (f_{Fc-H})$$

$$cLogP = (3.0307) - (2 \times 0.724) + (2 \times 2.660) - (2 \times 0.204)$$

$$cLogP = 6.49$$

1-FcAQ:

$$cLogP = (cLogP\ Organic\ Fragment) - \left(f_{CH_3}\right) + (f_{Fc}) - (f_{Fc-H})$$

$$cLogP = (3.4719) - (0.724) + (2.660) - (0.204)$$

$$cLogP = 5.20$$

4-FcC:

$$cLogP = (\ cLogP\ Organic\ Fragment) - \left(f_{CH_3}\right) + (f_{Fc}) - (f_{Fc-H})$$

$$cLogP = (1.8175) - (0.724) + (2.660) - (0.204)$$

$$cLogP = 3.55$$

UV-Vis Characterization

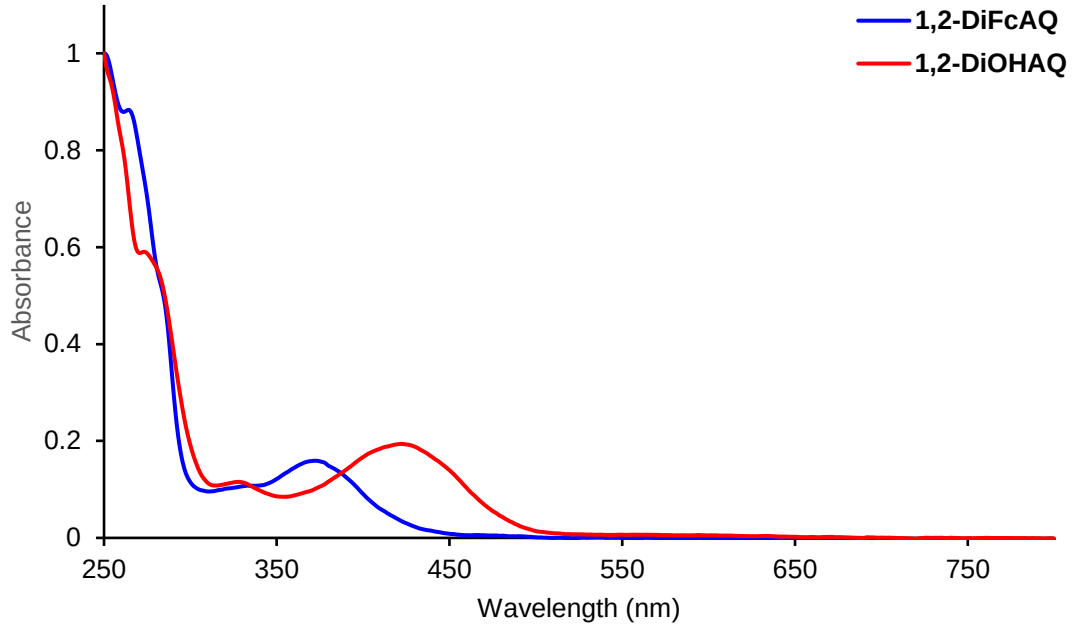


Figure S17. UV-Vis spectrum of **1,2-DiFcAQ** and **1,2-DiOHAQ** in acetonitrile. Concentration = 25 μM.

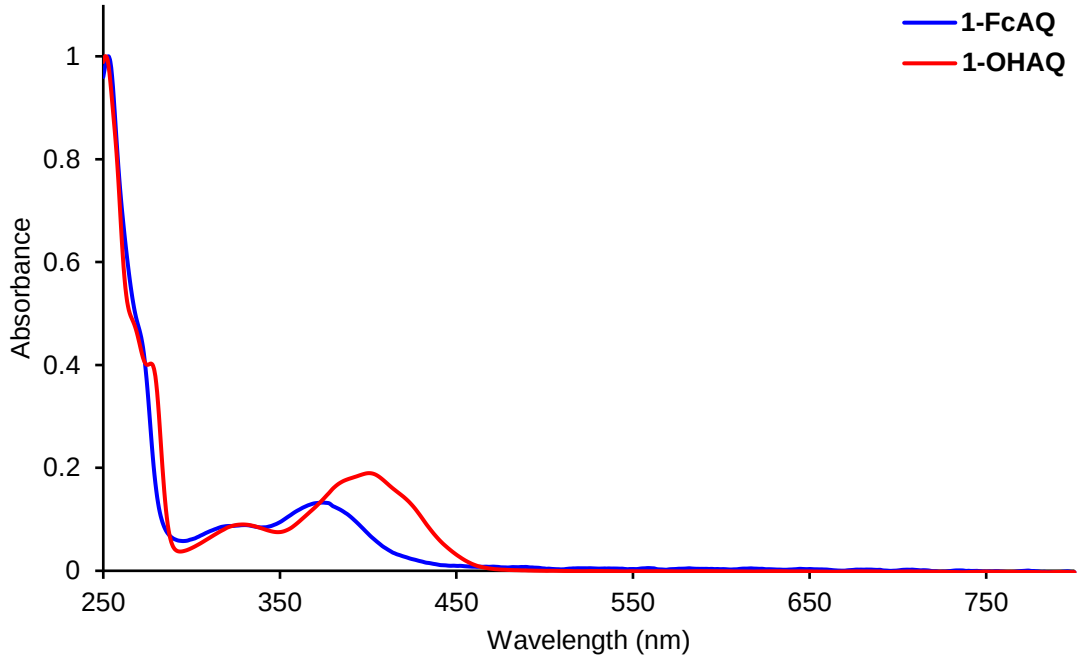


Figure S18. UV-Vis spectrum of **1-FcAQ** and **1-OHAQ** in acetonitrile. Concentration = 25 μM.

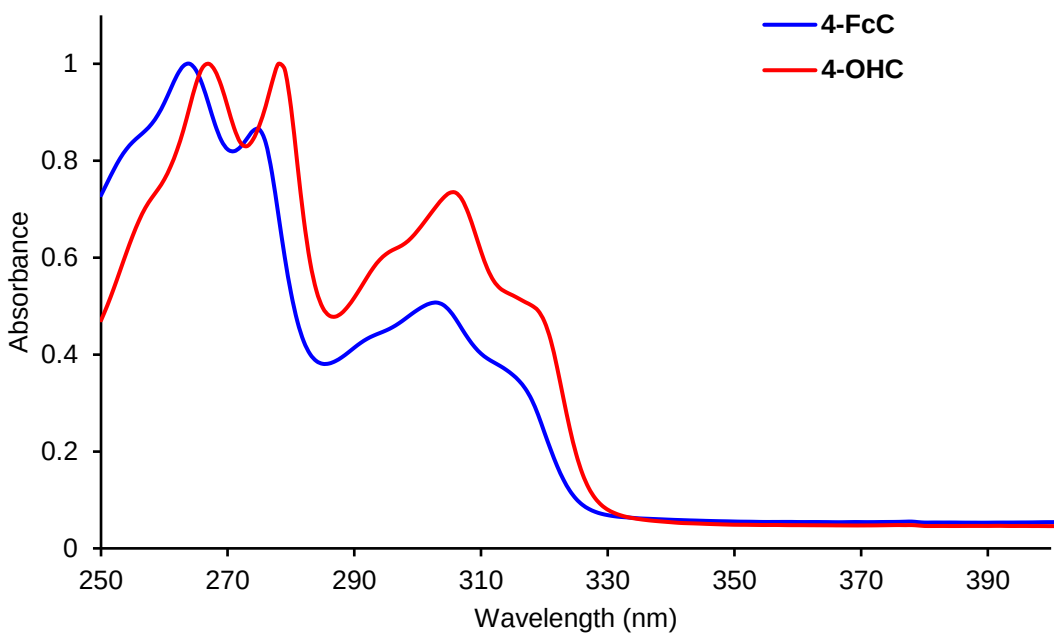


Figure S19. UV-Vis spectrum of **4-FcC** and **4-OHC** in acetonitrile. Concentration = 100 μM.

References

1 R. G. Balasingham, C. F. Williams, H. J. Mottram, M. P. Coogan and S. J. A. Pope, *Organometallics*, 2012, **31**, 5835-5843.
2 S. Nadali, G. Aghapour and Z. Rafieepour, *Can. J. Chem.*, 2017, **95**, 1045-1051.
3 P. Thasnim and D. Bahulayan, *New J. Chem.*, 2017, **41**, 13483-13489.
4 B. M. Upton, R. M. Gipson, S. Duhovic, B. R. Lydon, N. M. Matsumoto, H. D. Maynard and P. L. Diaconescu, *Inorg. Chem. Front.*, 2014, **1**, 271-277.
5 S. Stoll and A. Schweiger, *J. Magn. Reson.*, 2006, **178**, 42-55.
6 R. Mannhold and R. F. Rekker, *Perspect. Drug Discov. Des*., 2000, **18**, 1-18.
7 A. K. Ghose and G. M. Crippen, *J. Chem. Inf. Comput. Sci*., 1987, **27**, 21-35.
8 V. N. Viswanadhan, A. K. Ghose, G. R. Revankar and R. K. Robins, *J. Chem. Inf. Comput. Sci.*, 1989, **29**, 163-172.
9 R. Ahmedi and T. Lanez, *Asian J. Chem.*, 2010, **22**, 299-306.