Supporting Information

Catalytic and stoichiometric flavanone oxidations mediated by nonheme oxoiron(IV) complexes as flavone synthase mimics: kinetic, mechanistic and computational studies

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Materials

All syntheses were done under an argon atmosphere unless stated otherwise. Solvents used for the synthesis and reactions were purified by standard methods and stored under argon. The starting materials for the ligand are commercially available and they were purchased from Sigma-Aldrich.

Instrumentation

The crystal evaluation and intensity data collection for **3** was performed on a Bruker-Nonius Kappa CCD single-crystal diffractometer using Mo Kα radiation (λ = 0.71073 Å) at 293 K. Crystallographic data and selected bond lengths and angles are listed in Table S1, Table S2, and Table S3 whereas details of the structure determination are given in Figure S2. Comparison with similar N4Py-based complexes has been made and data is shown in Table S3. SHELX–2013 [1] was used for structure solution and full matrix least squares refinement on F^2.

The UV-visible spectra were recorded on an Agilent 8453 diode-array spectrophotometer using quartz cells.

IR spectra were recorded using a Thermo Nicolet Avatar 330 FT-IR instrument (Thermo Nicolet Corporation, Madison, WI, USA). Samples were prepared in the form of KBr pellets.

GC analyses were performed on an Agilent 6850 gas chromatograph equipped with a flame ionization detector and a 30 m SUPELCO BETA DEX 225 column.

ESI- MS samples were analyzed using triple quadruple Micromass Quattro spectrometer (Waters, Milford, MA, USA), that was operated in positive electrospray ionization mode.

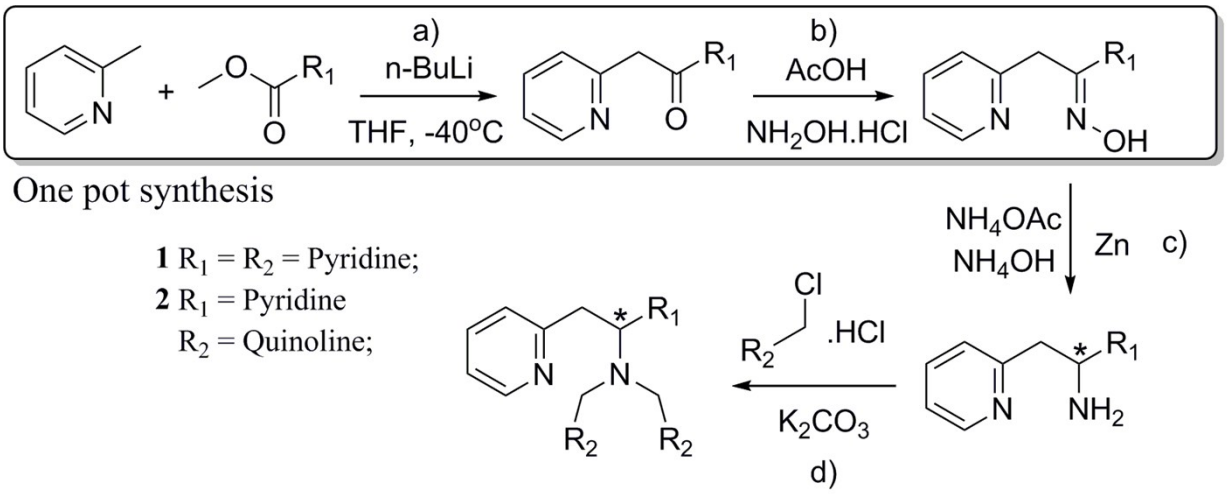
NMR spectrum was recorded on a Bruker Avance 400 spectrometer (Bruker Biospin AG, Fällanden, Switzerland).

Microanalyses (elemental analysis) were done by the Microanalytical Service of the University of Pannonia.

Synthesis and characterization

Preparation of the N4Pys [2,3]. The amine from the previous experiment was used without any purification. It was mixed with 2.2 eq. 2-(chloromethyl)pyridine (or quinoline) hydrochloride (26 mmol) and 20 eq. K_2CO_3 (240 mmol) in 200 ml MeCN and 10 ml water. The mixture was refluxed for 20 hours then (after cooling down) filtered from excess

carbonate. The clear red solution was evaporated partially under reduced pressure. 15 ml water was added and the crude product was extracted with dichloromethane. The organic layer was dried with $NaSO_4$ then solvent was evaporated. The crude brown oil was dissolved in acetone and filtered to result the product as white powder (27-54%).



Scheme S1. Synthesis of asymmetric N4Pys (asN4Py and asN2Py2Q).

Compound Characterization. *1,2-di(2-pyridyl)ethanone oxime*: colorless crystal, 25%; ^{1}H-NMR (400 MHz, $CDCl_3$): 10.22 (s, 1 H), 8.61-8.45 (m, 2 H), 7.97 (d, J = 8, 1 H), 7.67-7.52 (m, 2 H), 7.33 (d, J = 8, 1 H), 7.24-7.17 (m, 1 H), 7.13-7.06 (m, 1 H), 4.62 (s, 2 H). Anal. Calcd. for $C_{12}H_{11}N_3O$: C, 67.59; H, 5.20; N, 19.71. Found C, 67.41; H, 5.22; N, 19.66.

1-(2-quinolyl)-2-(2-pyridyl)ethanone oxime: beige crystal, 20%; ^{1}H-NMR (400 MHz, DMSO): 11.86 (s, 1 H), 8.37 – 8.32 (m, 2 H), 8.10 (d, J = 9 Hz, 1 H), 7.99 – 7.91 (m, 2 H), 7.76 – 7.70 (m, 1 H), 7.66 – 7.56 (m, 2 H), 7.23 (dt, J = 8 Hz, 1 Hz, 1 H), 7.15 – 7.10 (m, 1 H), 4.56 (s, 2 H). Anal. Calcd. for $C_{16}H_{13}N_3O$: C, 72.99; H, 4.98; N, 15.96. Found C, 72.90; H, 4.99; N, 15.89.

N,N-bis(2-pyridylmethyl)-1,2-di(2-pyridyl)ethylamine (**asN4Py**): white solid, 27%; ^{1}H-NMR (400 MHz, DMSO): 8.60-8.56 (m, 1 H), 8.42-8.39 (m, 2 H), 8.38-8.35 (m, 1 H), 7.74 (dt, J = 8, 2, 1 H), 7.63-7.53 (m, 3 H), 7.34-7.29 (m, 1 H), 7.28-7.09 (m, 7 H), 4.46 (t, J = 7, 1 H), 4.03 (d, J = 15, 2 H), 3.64 (d, J = 15, 2 H), 3.53 (dd, J = 14, 7, 1 H), 3.45 (dd, J = 14, 7, 1 H). Anal. Calcd. for $C_{24}H_{23}N_5$: C, 75.56; H, 6.08; N, 18.36. Found C, 75.47; H, 6.10; N, 18.32.

N,N-bis(2-quinolylmethyl)-1,2-di(2-pyridyl)ethylamine (**asN2Py2Q**): light brown solid, 54%; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.67 (d, J = 4, 1 H), 8.43 (d, J = 4, 1 H), 8.14-7.95 (m, 4 H), 7.78-7.63 (m, 6 H), 7.49 (q, J = 7, 3 H), 7.33 (d, J = 9, 3 H), 7.23-7.09 (m, 2 H), 4.49 (t, J = 7, 1 H), 4.34 (d, J = 15, 2 H), 3.86 (d, J = 15, 2 H), 3.81 (dd, J = 14, 7, 1 H), 3.50 (dd, J = 14, 7, 1 H). Anal. Calcd. for $C_{32}H_{27}N_5$: C, 79.81; H, 5.65; N, 14.54. Found C, 79.65; H, 5.66; N, 14.48.

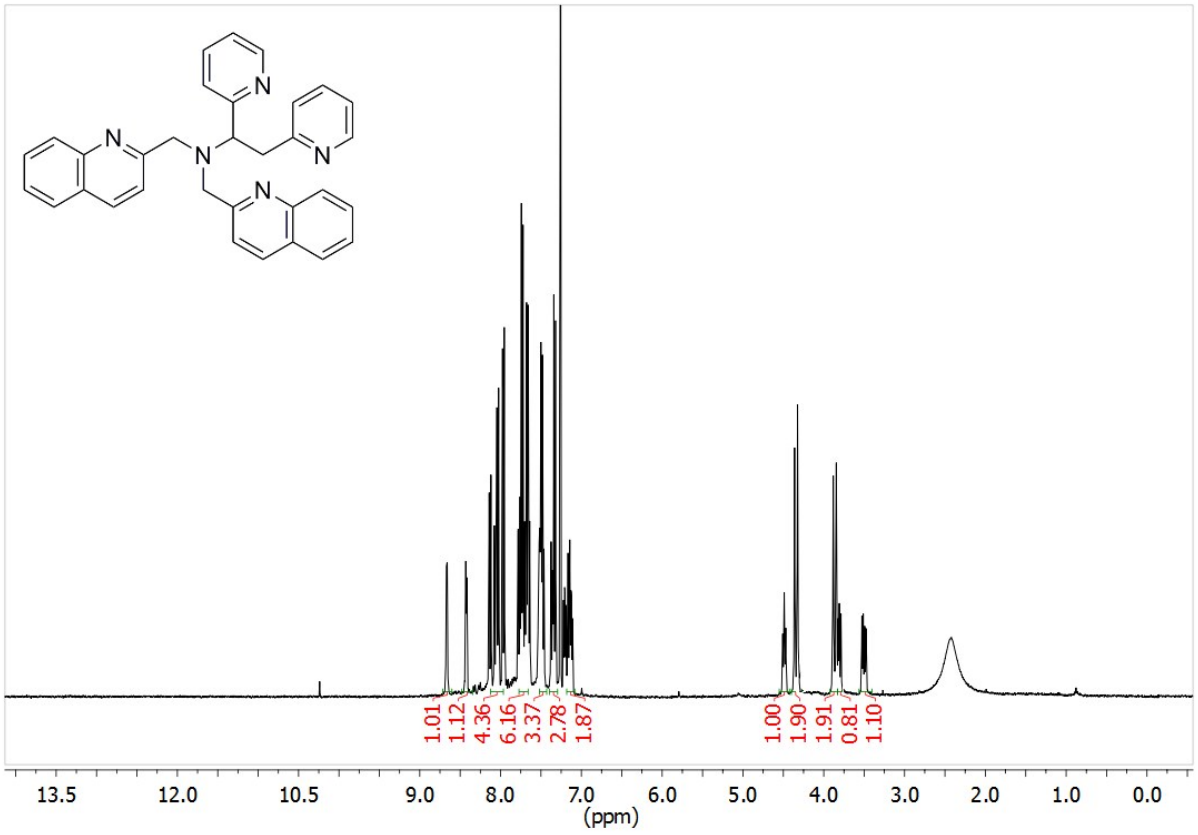


Figure S1. ^{1}H-NMR spectrum of asN2Py2Q in DMSO.

Preparation of [Fe^{II}(asN2Py2Q)(Cl)](ClO_4) (3): 0.407 g (0.786 mmol) ligand, asN2Py2Q.HCl and 0.285 g (0.786 mmol) $Fe^{II}(ClO_4)_2 \times 6H_2O$ were dissolved in 4 ml MeOH-MeCN (1:1) mixture under Ar. The mixture was stirred at RT for 3 hour. 1.5 ml EtOAc was layered onto the surface of the solution and it was placed to the freezer (-40°C). Cubic shaped red crystals formed during overnight. Yield: 0.42 g (80%). FT-IR (KBr, cm^{-1}): 3441 m, 3066 w, 1622 w, 1603 m, 1513 m, 1433 m, 1377 w, 1296 w, 1091 s, 826 m, 784 m, 756 m, 625 m. UV–Vis (MeCN) λmax(log ε, $dm^3mol^{-1}cm^{-1}$): 300 (4.04), 380 (3.00), 440 (2.77). Anal. Calcd. for $C_{32}H_{27}Cl_2FeN_5O_4$ (672.34): C, 57.16; H, 4.05; N, 10.42. Found C, 57.23; H, 4.11; N, 10.37.

[Fe^{II}(asN2Py2Q)(CH_3CN)](ClO_4)$_2$ (3a): It was prepared by reacting $Fe^{II}(ClO_4)_2 \times 6H_2O$ with asN2Py2Q ligand (The free ligand was obtained from asN2Py2Q.HCl and NEt_3, extracted with CH_2Cl_2.) in acetonitrile. $E_{1/2}$ = 0.83 V vs. SCE. Anal. Calcd. for $C_{34}H_{30}Cl_2FeN_6O_8$: C, 52.53; H, 3.89; N, 10.81. Found C, 52.67; H, 3.76; N, 10.74.

Table S1. Summary of crystal data and intensity collection and structure refinement parameters for [Fe^{II}(asN2Py2Q)Cl]ClO_4

Compound	**[Fe^{II}(asN2Py2Q)Cl]ClO_4**
Chemical formula	$C_{39}H_{40.5}Cl_2FeN_5O_{7.5}$
Formula weight	826.01
Crystal system	triclinic
Space group	P-1
a (Å)	12.3536(3)
b (Å)	12.7733(4)
c (Å)	15.3745(3)
α (°)	68.454(3)
β (°)	75.982(2)
γ (°)	61.907(3)
Volume (Å^3)	1983.54(12)
Z	2
Calc. density (g cm^{-1})	1.383
Temperature (K)	173
Abs. coeff. (mm^{-1})	4.755
F (0 0 0)	859
Obs. reflections	7432
Goodness-of-fit	1.063
R_1[a]	0.0556
wR_2	0.1593

[a] $w=1/[\sigma^2(F_o^2)+(\alpha P)^2+bP]$ and $P = (\max F_o^2,0)+2F_c^2)/3$
$R_1 = \Sigma(|F_o|-|F_c|)/\Sigma(|F_o|)$ and $wR_2 = \{\Sigma[w(Fo^2-Fc^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Table S2. Selected bond distances (Å) and angles (°) for [Fe^{II}(asN2Py2Q)Cl]ClO_4 complex

distances		angles	
Fe(1) – Cl(1)	2.321(1)	N(1)-Fe(1)-N(2)	90.0(1)
Fe(1) – N(2)	2.254(2)	N(1)-Fe(1)-N(4)	75.34(9)
Fe(1) – N(3)	2.230(2)	N(2)-Fe(1)-N(3)	80.63(9)
Fe(1) – N(4)	2.292(2)	N(4)-Fe(1)-N(5)	84.38(9)
Fe(1) – N(5)	2.220(3)	N(2)-Fe(1)-N(5)	81.07(9)
Fe(1) – N(1)	2.203(3)	N(1)-Fe(1)-Cl(1)	160.77(7)

Table S3. Comparison of different Fe−N bond distances (Å) between Fe(N4Py) derivates (N_{div} = diverse or nonregular pyridyl moiety)

entry	Fe–N_{py} (av)	Fe–N_{div} (av)	Fe–N_{MeCN}	Fe–N_{amine}	ref.
$[Fe^{II}(asN4Py)(MeCN)](ClO_4)_2$	1.968	2.037(3)	1.944(4)	1.972(4)	[4]
$[Fe^{II}(N3PyBzIM)(MeCN)](ClO_4)_2$	1.953	1.977	1.909(6)	1.980(6)	[5]
$[Fe^{II}(N2Py2BzIM)(MeCN)](ClO_4)_2$	1.974	1.981	1.901(3)	2.028(2)	[5]
$[Fe^{II}(N4Py)(MeCN)](ClO_4)_2$	1.972	-	1.915(3)	1.961(3)	[6]
$[Fe^{II}(asN2Py2Q)Cl](ClO_4)$	2.242	2.256	-	2.203(3)	[this work]

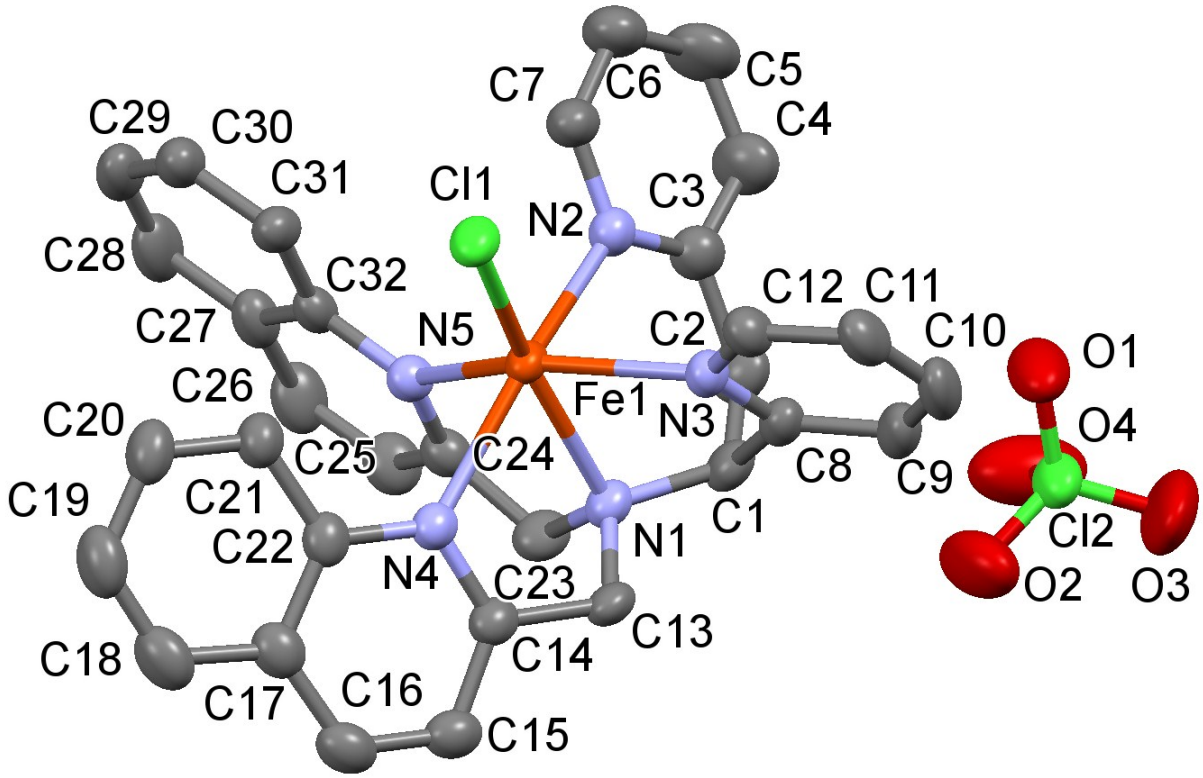


Figure S2. X-ray structure of **3**. Thermal ellipsoids are plotted at 50% probability level. Outer sphere solvent molecules, hydrogen atoms were omitted for clarity. (CCDC 1841256).

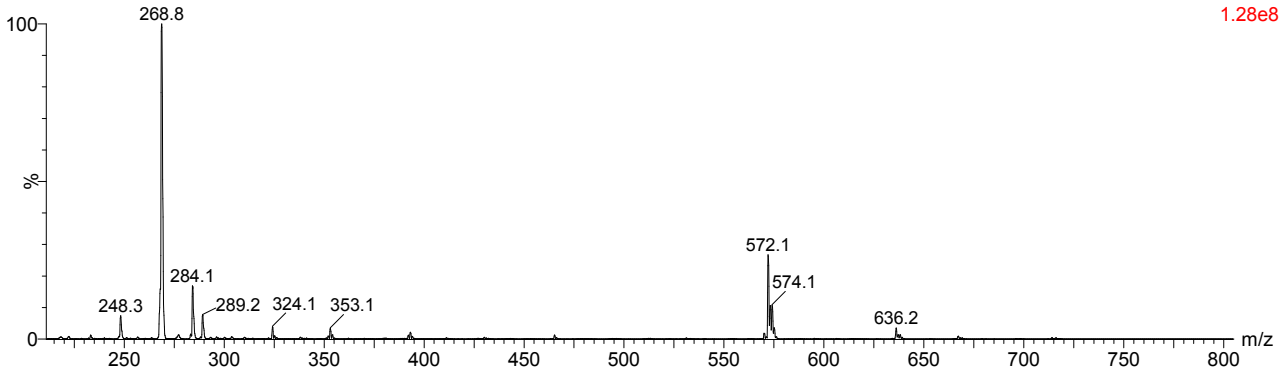


Figure S3. Electrospray ionization mass spectrum of $[Fe^{II}(asN2Py2Q)Cl]ClO_4$ complex. The peaks at m/z = 268.8 and m/z = 289.2 correspond to the formulations $[Fe^{II}(asN2Py2Q)]^{2+}$ (calcd 268.6) and $[Fe^{II}(asN2Py2Q)(CH_3CN)]^{2+}$ (calcd 289.6), respectively, as well as peaks at m/z = 572.1 and m/z = 636.2 correspond to the formulations $[Fe^{II}(asN2Py2Q)(Cl)]^{+}$ (calcd 572.1) and $[Fe^{II}(asN2Py2Q)(ClO_4)]^{+}$ (calcd 636.1), respectively.

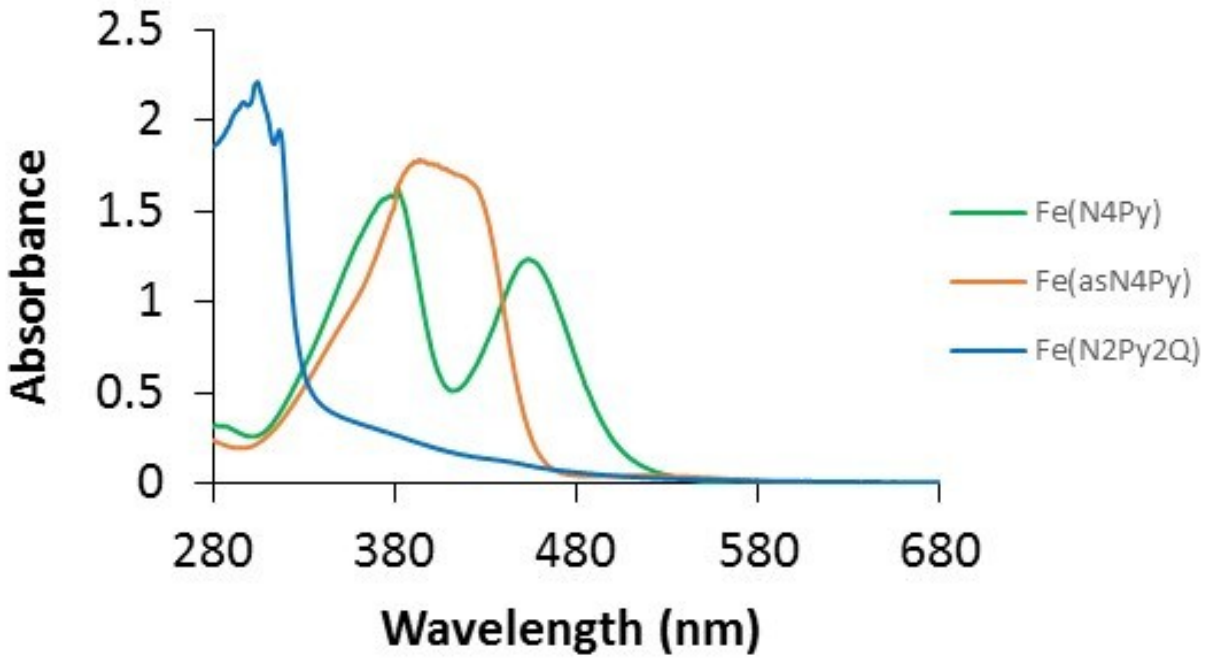


Figure S4. UV−Vis spectra of complexes $[Fe^{II}(asN2Py2Q)(Cl)](ClO_4)$ (blue), $[Fe^{II}(asN4Py)(MeCN)](ClO_4)_2$ (red) (0.20 mM) and $[Fe^{II}(N4Py)(MeCN)](ClO_4)_2$ (green) in acetonitrile recorded at room temperature (298 K).

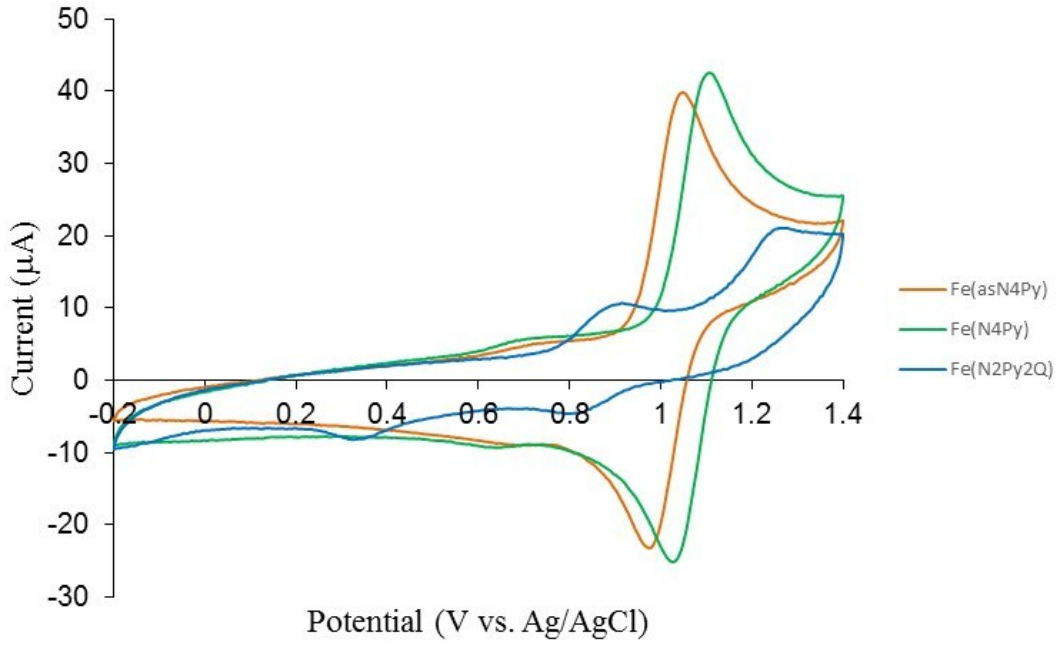


Figure S5. Cyclic voltammograms of 1 mM $[Fe^{II}(N4Py)(MeCN)](ClO_4)_2$ (green), $[Fe^{II}(asN4Py)(MeCN)](ClO_4)_2$ (red) and $[Fe^{II}(asN2Py2Q)(Cl)](ClO_4)$ (blue) in CH_3CN with 0.1 M $(Bu_4N)ClO_4$; scan rate 100 mVs^{-1}; working electrode: glassy carbon electrode (GCE), auxiliary electrode: Pt wire, reference electrode: Ag/AgCl.

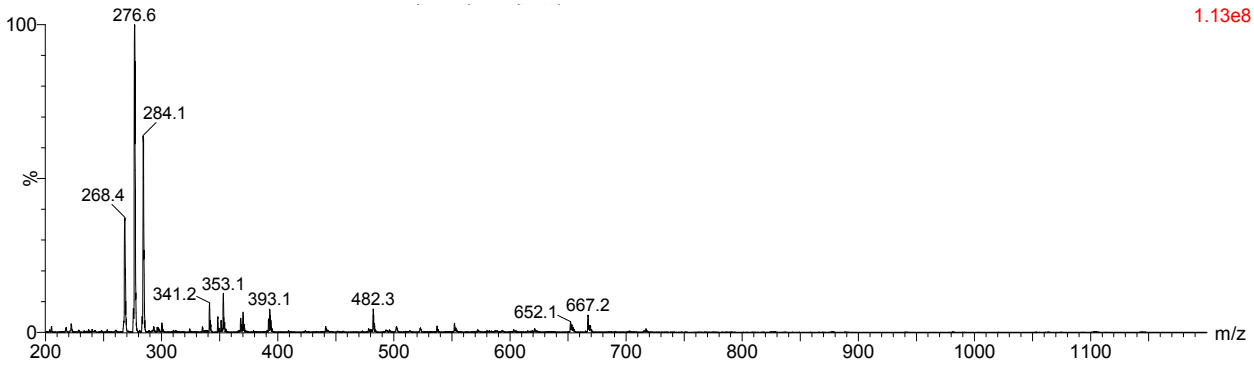


Figure S6. Electrospray ionization mass spectrum of **6**. The peaks at *m*/*z* = 276.6 (z = 2) and 652.1 (z = 1)correspond to the formulae $[Fe^{IV}(O)(asN2Py2Q)]^{2+}$ (*m*/*z* calcd 276.6) and $[Fe^{IV}(O)(asN2PyQ2)(ClO_4)]^{+}$ (*m*/*z* calcd 652.1), respectively.

Oxidation reactions

Reaction conditions for catalysis

In a typical reaction, 2 ml of 337.5 mM mCPBA solution in CH_3CN was delivered by syringe pump in air or under argon to a stirred 1 ml solution of catalyst (9 μmol), and the substrate (3 mmol) inside a vial. The final concentrations of the reagents were 3 mM iron catalyst, 225 mM mCPBA, and 1000 mM flavanone. After syringe pump addition (5 min the solution was stirred for 5 minutes and a known amount of PhBr (0.315 mmol) was added as an internal standard. The iron complex was removed by passing the reaction mixture through a silica column followed by elution with ethyl acetate. The products (1,3-dione (D) and flavone) were identified by GC/MS and confirmed by comparison with authentic samples. Flavone is commercially available and it was purchased from Sigma-Aldrich. 1-(2-hydroxy-phenyl)-3-phenyl-propane-1,3-dione (D): o-Benzoyloxyacetophenone has been prepared by the action of benzoyl chloride on a pyridine solution of o-hydroxyacetophenone. Its rearrangement to 1-(2-hydroxy-phenyl)-3-phenyl-propane-1,3-dione (D) by alkali has been described [7]. Yield: 80–85%; m.p. 117–120 °C. GC-MS spectrum: *m/z*: 240 (13.7 %), 121 (23.1 %), 105 (100 %), 77 (63.3 %), 69 (13.1 %), 65 (24.7 %), 51 (26.4 %), 39 (23.4 %).

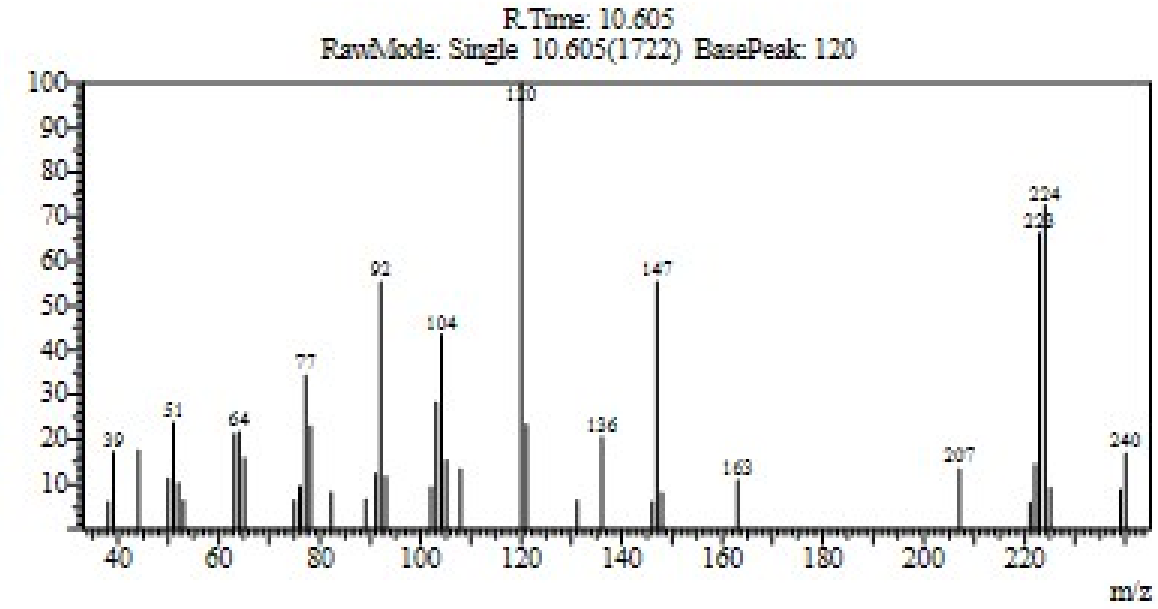


Figure S7. GC-MS spectrum of 2-hydroxy-flavanone (A): *m/z*: 240 (16.9 %), 224 (72,6 %), 163 (11 %), 136 (20.5 %), 120 (100 %), 105 (15,4 %).

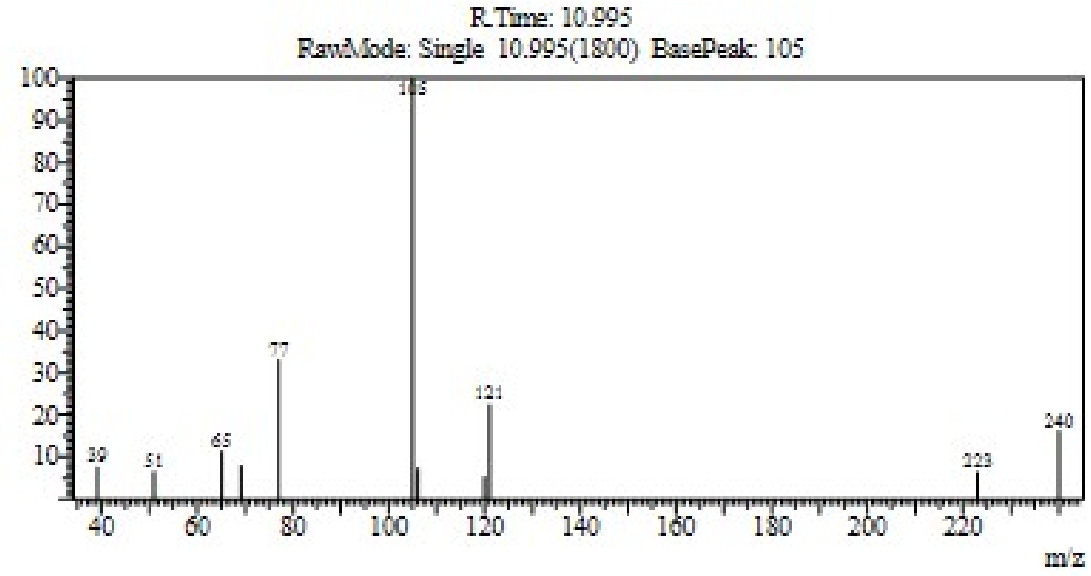


Figure S8. GC-MS spectrum of 1-(2-hydroxy-phenyl)-3-phenyl-propane-1,3-dione (D): *m/z*: 240 (16,1 %), 223 (6,3 %), 121 (22,4 %), 120 (5,3 %), 106 (7,2 %), 105 (100 %), 77 (33 %), 69 (8.0 %), 65 (11,4 %), 51 (6,5 %), 39 (7,5 %).

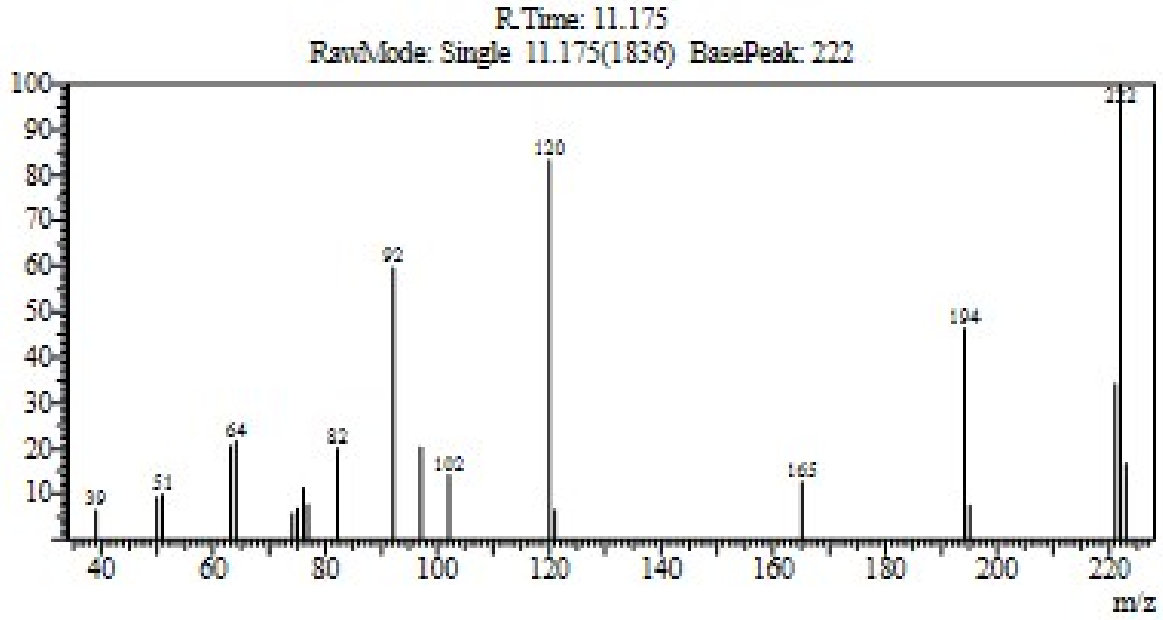


Figure S9. GC-MS spectrum of flavone (F): *m/z*: 223 (72 %), 222 (100 %), 194 (46,4 %), 120 (83,4 %), 92 (59,6 %).

Table S4. Catalytic flavanone oxidation in acetonitrile at 25°C by mCPBA using compound **1**, **2** and **3**.

Entry	Conditions	Product	Yield[a] (%)	TON
1	$[Fe(ClO_4)_2]$: [mCPBA] : $[FlaH_2]$ 3 : 225 :1000	Flavone A D	1.6 - -	1.2 - -
2	[1] : [mCPBA] : $[FlaH_2]$ 3 : 75 :1000	Flavone A D	11.8 0.05 0.59	2.95 0.01 0.15
3	[1] : [mCPBA] : $[FlaH_2]$ 3 : 225 :1000	Flavone A D	14.6 0.13 1.4	10.9 0.10 1.05
4	[1] : [mCPBA] : $[FlaH_2]$ 3 : 450 :1000	Flavone A D	14.4 0.07 0.44	21.6 0.11 0.66
5	[2] : [mCPBA] : $[FlaH_2]$ 3 : 75 :1000	Flavone A D	10.7 - 0.68	2.85 - 0.17
6	[2] : [mCPBA] : $[FlaH_2]$ 3 : 225 :1000	Flavone A D	9.25 0.03 0.14	6.93 0.02 0.11
7	[3] : [mCPBA] : $[FlaH_2]$ 3 : 75 :1000	Flavone A D	22.0 0.02 0.23	5.5 0.01 0.06
8	[3] : [mCPBA] : $[FlaH_2]$ 3 : 225 :1000	Flavone A D	17.9 0.03 0.59	13.4 0.03 0.74
9	[3a] : [mCPBA] : $[FlaH_2]$ 3 : 225 :1000	Flavone A D	25.5 0.02 0.54	19.5 0.02 0.4
10[b]	[3a] : [mCPBA] : $[FlaH_2]$ 3 : 225 :1000	Flavone A D	16.5 0.04 11.1	12.4 0.03 8.31
11	[3] : [mCPBA] : $[FlaH_2]$ 1 : 225 :1000	Flavone A D	5.76 - 0.1	13.0 - 0.23
12	[3] : [mCPBA] : $[FlaH_2]$ 5 : 225 :1000	Flavone A D	25.7 - 0.21	11.7 - 0.10

[a]Based on oxidant. [b]In the presence of $H_2{}^{18}O$ (37 mM) and $H_2{}^{16}O$ (47 mM) coming from the oxidant, mCPBA.

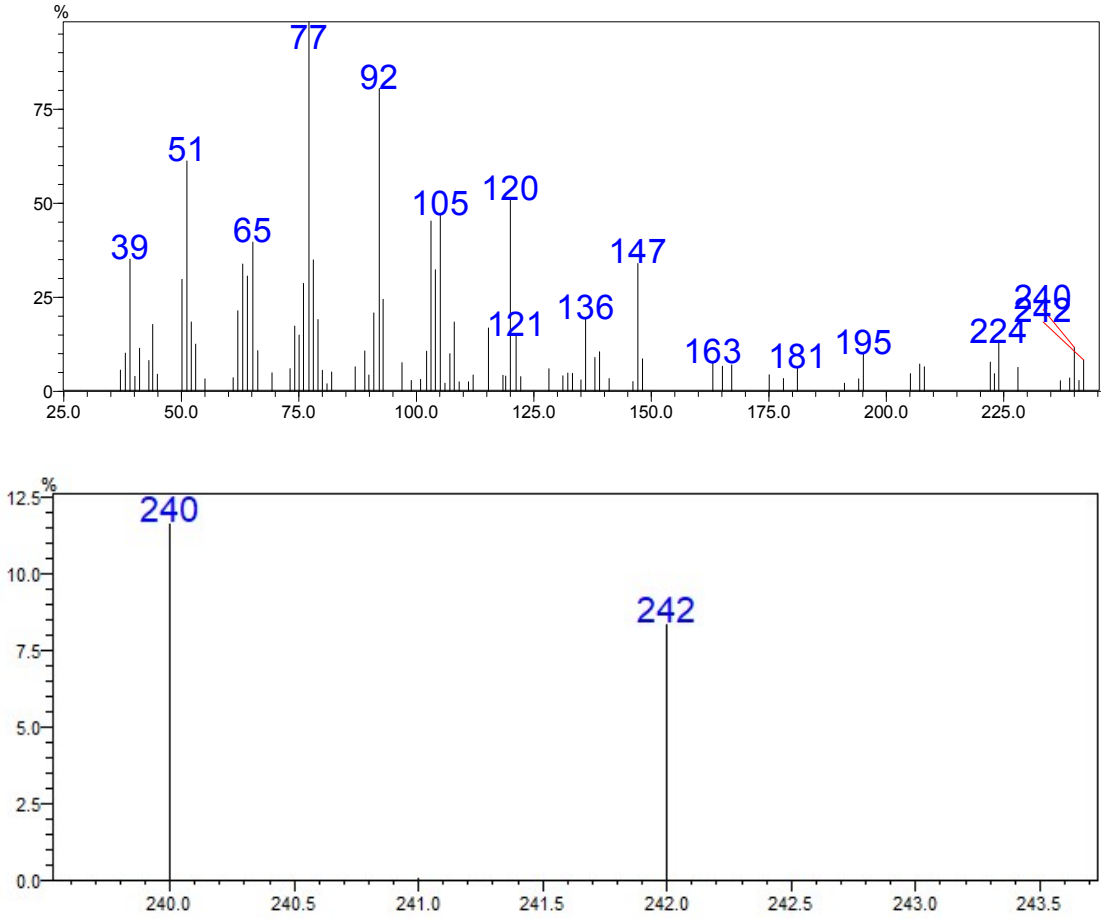
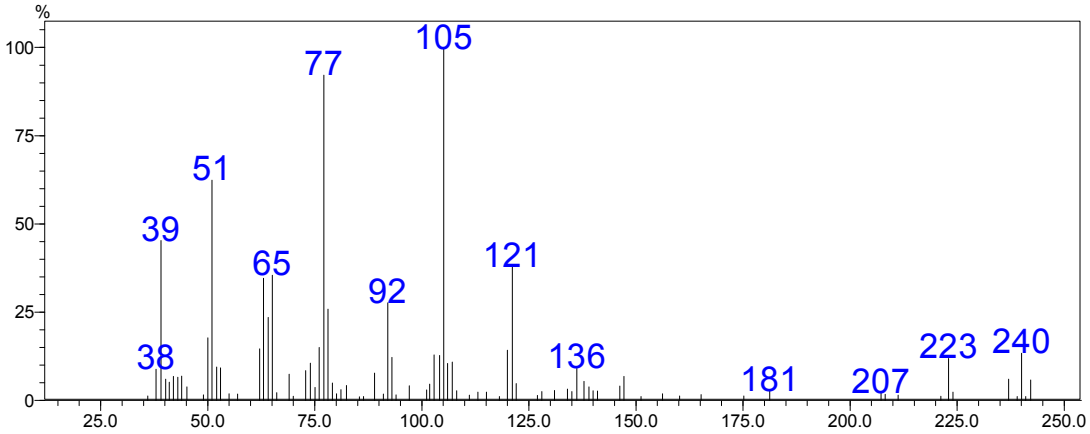


Figure S10. Catalytic flavanone oxidation in acetonitrile at 25°C by mCPBA using compound **3a** (Table S4, Entry 10). GC-MS spectrum of 2-hydroxy-flavanone (A) in the presence of $H_2{}^{18}O$ (37 mM) (and $H_2{}^{16}O$ (47 mM) coming from the oxidant, mCPBA) *m/z*: 242 (8.38 %), 240 (11.67 %), 224 (12.94 %), 163 (7.56 %), 136 (19.17 %), 120 (50.80 %), 105 (46.98 %), 77 (100 %).



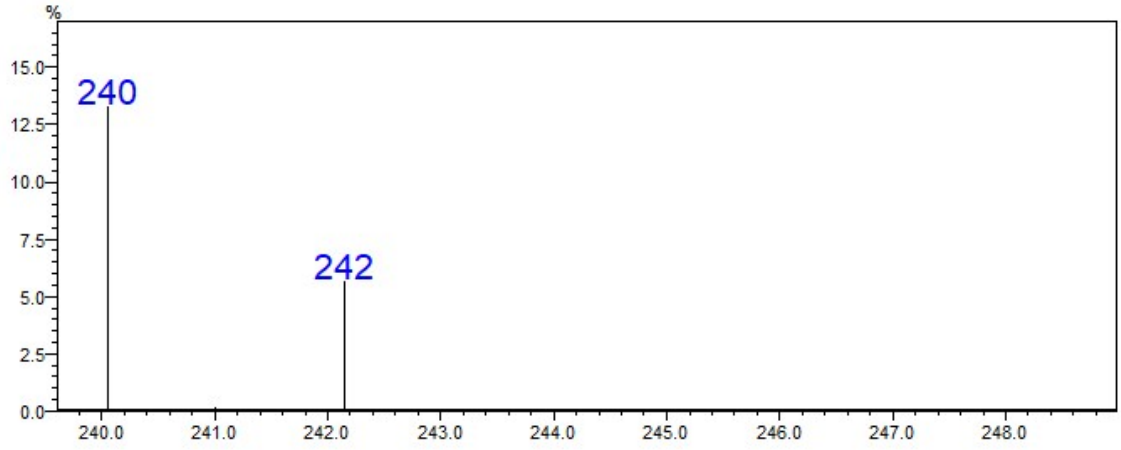


Figure S11. Catalytic flavanone oxidation in acetonitrile at 25°C by mCPBA using compound **3a** (Table S4, Entry 10). GC-MS spectrum of 1-(2-hydroxy-phenyl)-3-phenyl-propane-1,3-dione (D) in the presence of $H_2{}^{18}O$ (37 mM) (and $H_2{}^{16}O$ (47 mM) coming from the oxidant, mCPBA) *m/z*: 242 (5.75 %), 240 (13.34 %), 223 (11.86 %), 121 (37.81 %), 120 (14.25 %), 106 (10.47 %), 105 (100 %), 77 (92.18 %), 69 (7.43 %), 65 (35.49 %), 51 (62.43 %), 39 (45.33 %).

Description of the Fe(IV) intermediate formations with PhIO and their stoichiometric oxidation with flavanone

1, 2 or 3 complex (1.5×10^{-3} M) was dissolved in acetonitrile (1.5 mL), then iodosylbenzene (2.00×10^{-3} M) was added to the solution. The mixture was stirred for 50, 50 or 4 minutes, respectively, then the excess iodosylbenzene was removed by filtration. Flavanone (0.6 M) was added to the solution and the reaction was monitored by UV-vis spectrophotometer (Agilent 8453) at 695, 705 or 805 nm ($\varepsilon = 400, 400, 280$ M^{-1} cm^{-1}).

^{18}O-labeled experiments in the presence of $H_2{}^{18}O$ (18 mM) were also carried out:
Flavone (F, yields 70-80%, based on the intermediates generated) *m/z*: 223 (7.54 %), 222 (49.27 %), 194 (36.41 %), 120 (57.76 %), 105 (100 %), 92 (100 %).
GC-MS spectrum of 1-(2-hydroxy-phenyl)-3-phenyl-propane-1,3-dione (D, yields 5-10% based on the intermediates generated) *m/z*: 242 (2.44 %), 223 (22.79 %), 121 (15.62 %), 120 (62.09 %), 106 (1.43 %), 105 (6.47 %), 77 (53.41 %).

Table S5. The calculated *v, k_{obs}* and *k_2* values in the reaction of **4** and flavanone in MeCN.

N_0	T (K)	$[4]_0$ (10^{-3} M)	Flavanon (M)	k_{obs} ($10^{-4}s^{-1}$)	k_2 (10^{-3} $M^{-1}s^{-1}$)
1	298	1.5	0.3	1.70	0.57±0.03
2	298	1.5	0.45	2.49	0.55±0.03
3	298	1.5	0.6	3.30	0.55±0.03
4	298	1.5	0.75	4.29	0.57±0.04
5	298	1.5	0.9	5.05	0.56±0.03
6	288	1.5	0.75	2.59	0.35±0.01
7	293	1.5	0.75	3.26	0.44±0.01
8	303	1.5	0.75	4.98	0.66±0.02
9	308	1.5	0.75	6.35	0.85±0.04

Table S6. The calculated *v, k_{obs}* and *k_2* values in the reaction of **5** and flavanone in MeCN.

N_0	T (K)	$[Fe]_0$ (10^{-3} M)	Flavanon (M)	k_{obs} ($10^{-4}s^{-1}$)	k_2 (10^{-3} $M^{-1}s^{-1}$)
1	298	1.5	0.3	0.65	0.22±0.01
2	298	1.5	0.6	1.35	0.23±0.01
3	298	1.5	0.75	1.83	0.24±0.01
4	298	1.5	0.9	2.28	0.25±0.01
6	288	1.5	0.75	0.43	0.06±0.003
7	293	1.5	0.75	0.74	0.10±0.006
8	303	1.5	0.75	2.11	0.28±0.01
9	308	1.5	0.75	3.39	0.45±0.02
10	313	1.5	0.75	4.55	0.61±0.03

Table S7. The calculated *v, k_{obs}* and *k_2* values in the reaction of **6** and flavanone in MeCN.

N_0	T (K)	$[Fe]_0$ (10^{-3} M)	Flavanon (M)	k_{obs} ($10^{-3}s^{-1}$)	k_2 (10^{-3} $M^{-1}s^{-1}$)
1	298	1.5	0.15	3.19	21.27±1.3
2	298	1.5	0.3	5.96	19.87±0.79
3	298	1.5	0.45	7.68	17.07±0.68
4	298	1.5	0.6	11.1	18.42±0.92
6	298	1.5	0.75	14.2	19.20±1.1
7	278	1.5	0.75	3.27	4.36±0.17
8	283	1.5	0.75	4.90	6.50±0.32
9	288	1.5	0.75	7.38	9.84±0.39
10	293	1.5	0.75	9.58	12.77±0.63

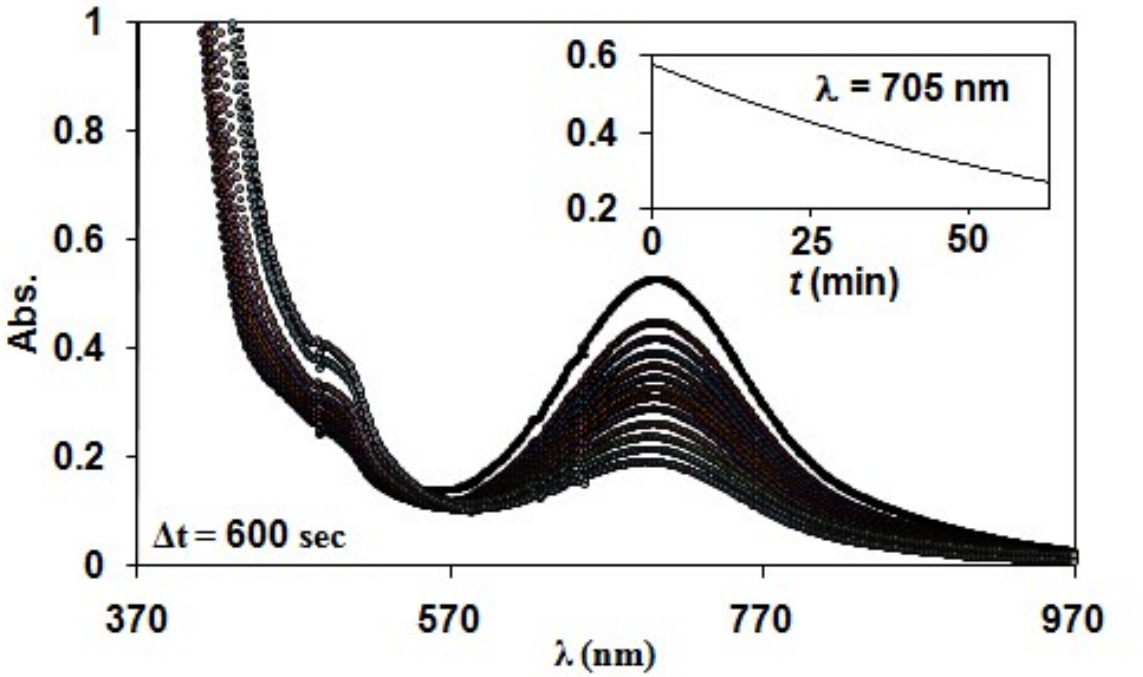


Figure S12. UV-vis spectral change of **6** (1.5 mM) upon addition of flavanone (0.6 M) at 298 K. Inset shows time course of the decay of **6** monitored at 705 nm.

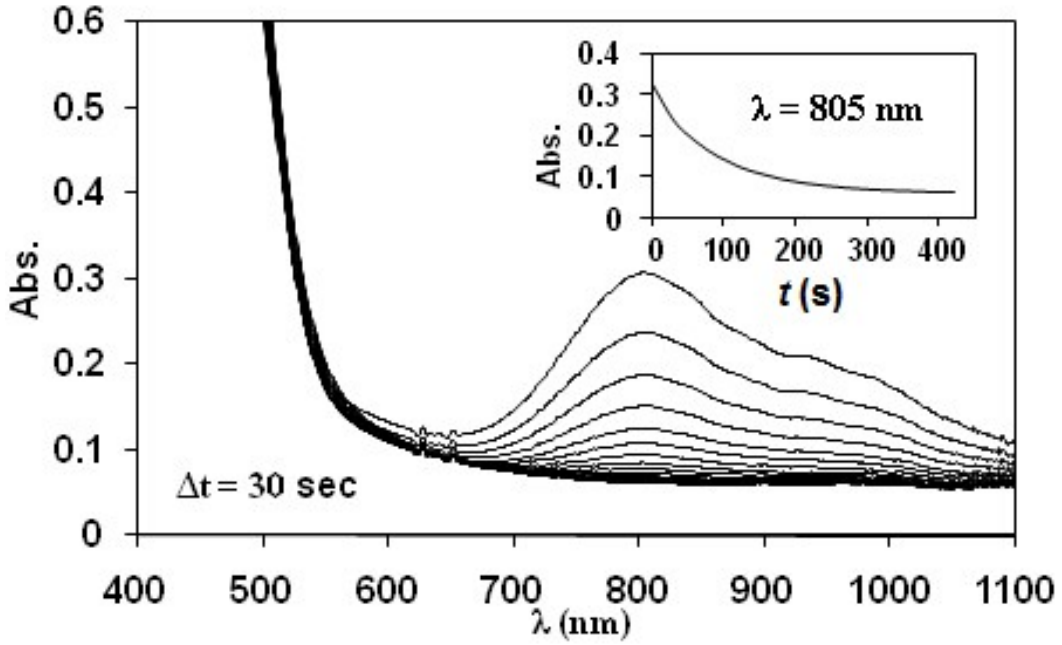


Figure S13. UV-vis spectral change of **6** (1.5 mM) upon addition of flavanone (0.6 M) at 298 K. Inset shows time course of the decay of **6** monitored at 805 nm

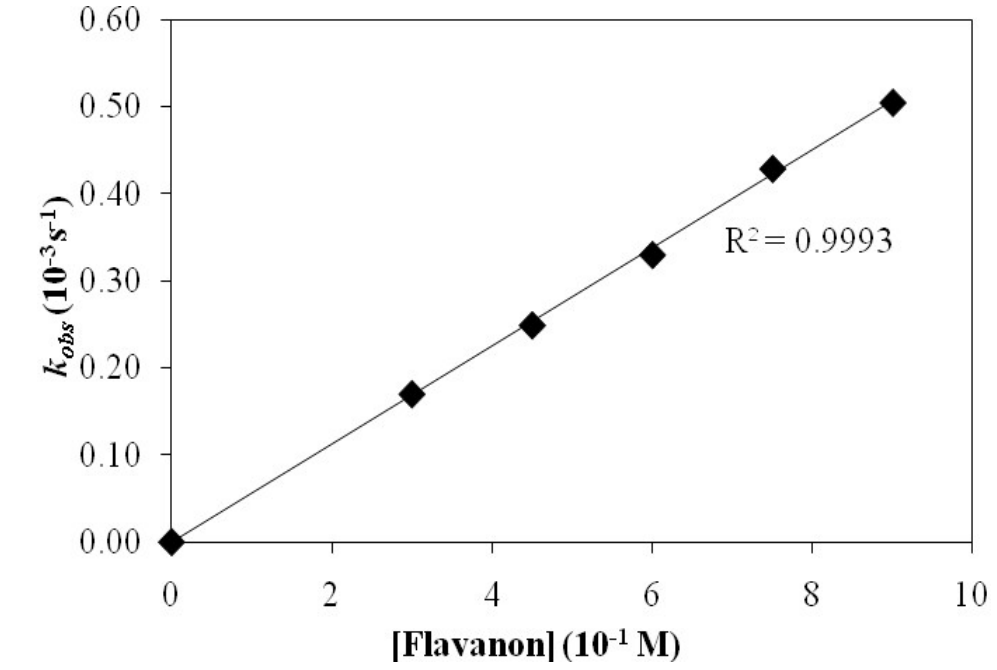


Figure S14. Reaction rates versus flavanone concentration in MeCN at 25 °C. $[\mathbf{4}]_0 = 1.50 \times 10^{-3}$ M.

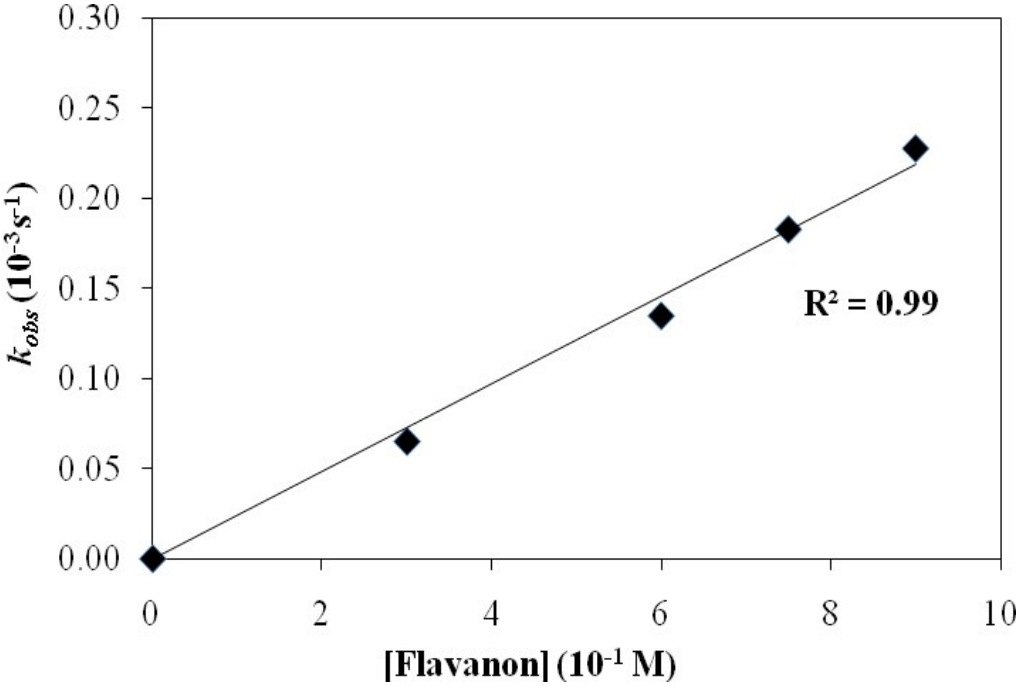


Figure S15. Reaction rates versus flavanone concentration in MeCN at 25 °C. $[\mathbf{5}]_0 = 1.50 \times 10^{-3}$ M.

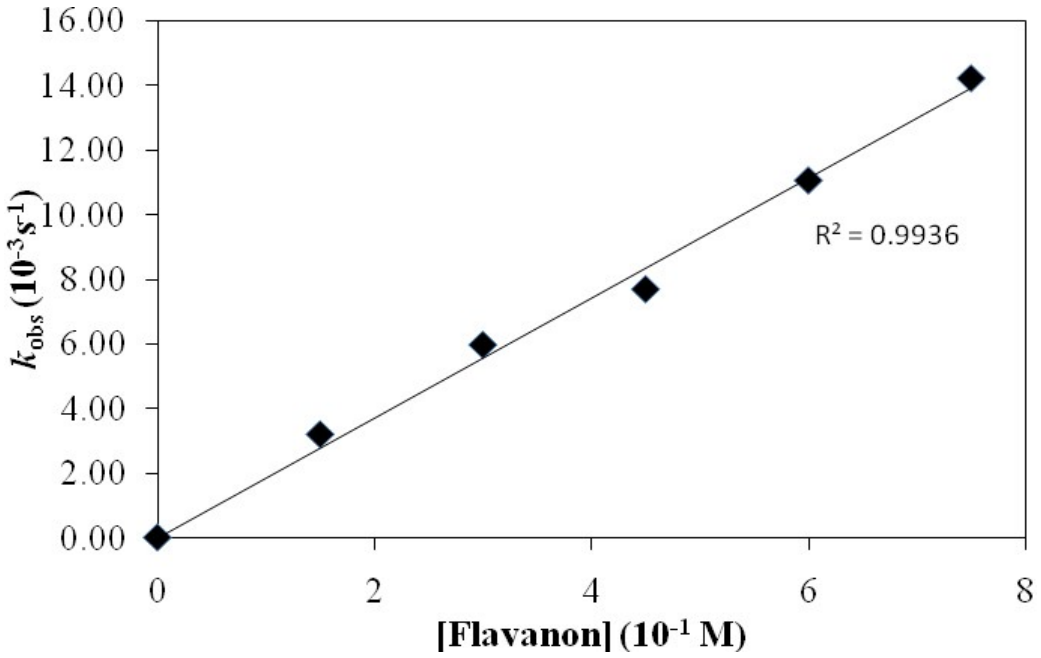


Figure S16. Reaction rates versus flavanone concentration in MeCN at 25 °C. $[\mathbf{6}]_0$ = 1.50×10^{-3} M.

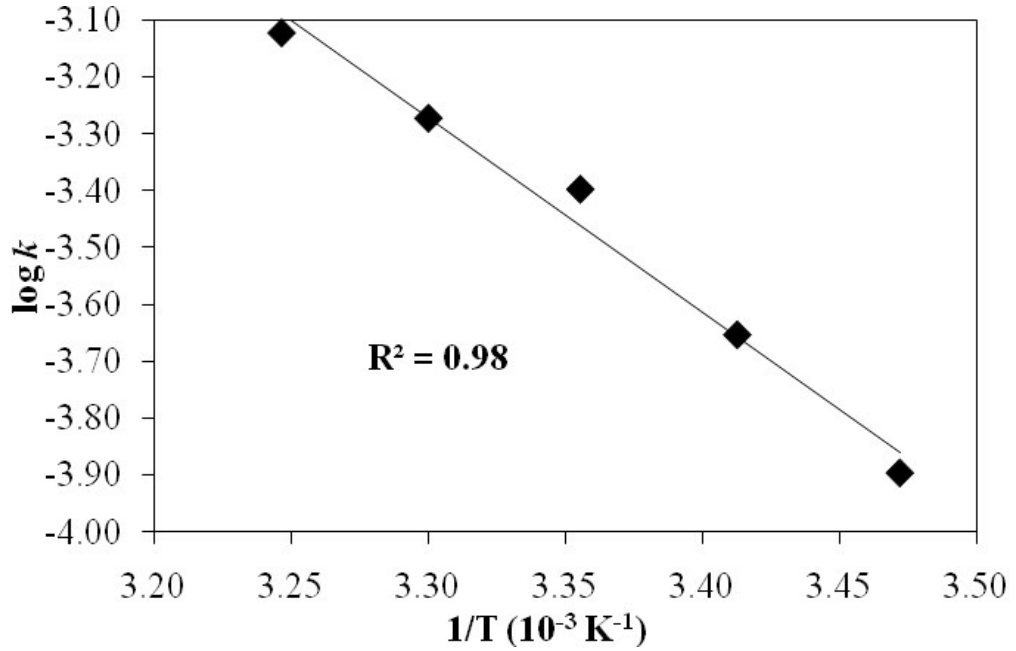


Figure S17. *Arrhenius* plot of the reaction of **4** and flavanone in MeCN. $[\mathbf{4}]_0 = 1.50 \times 10^{-3}$ M, $[\text{flavanone}]_0 = 0.75$ M.

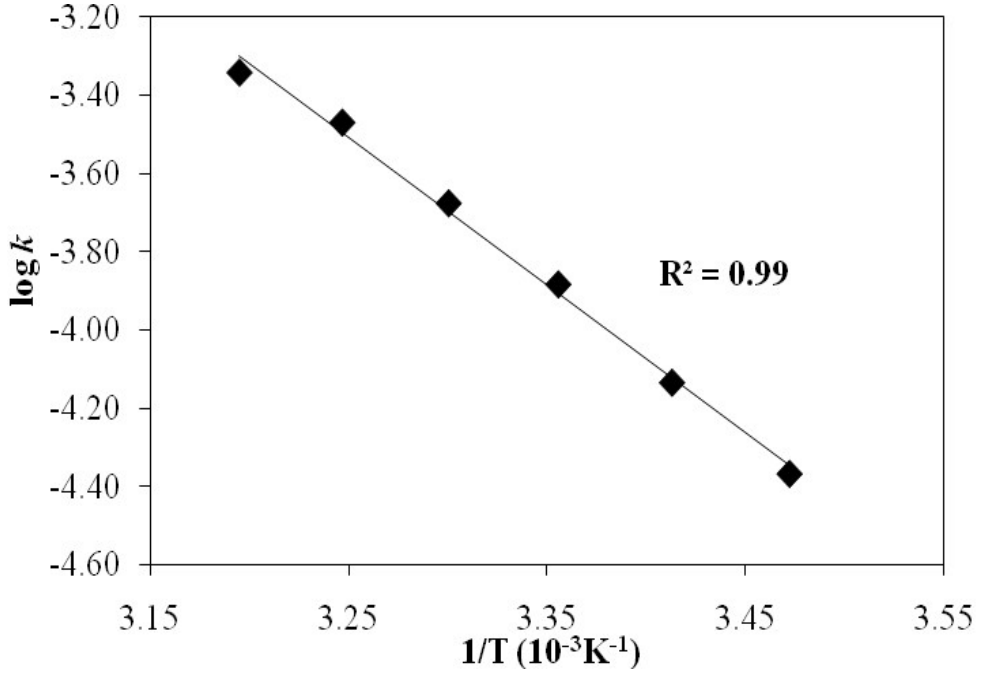


Figure S18. *Arrhenius* plot of the reaction of **5** and flavanone in MeCN. $[\mathbf{5}]_0 = 1.50 \times 10^{-3}$ M, $[\text{flavanone}]_0 = 0.75$ M.

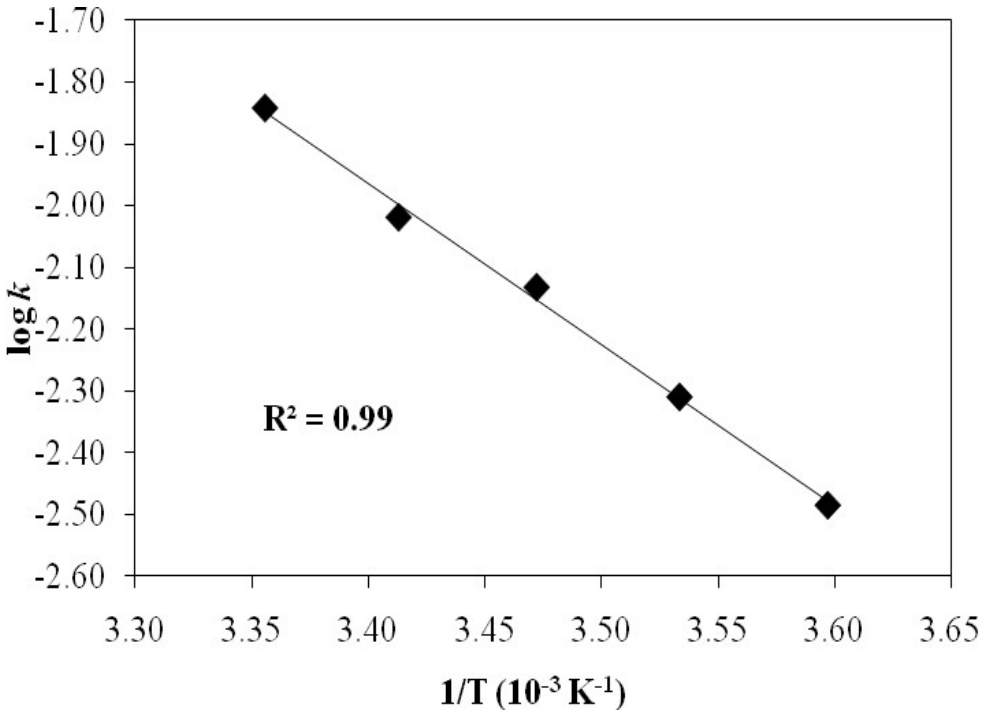


Figure S19. *Arrhenius* plot of the reaction of **6** and flavanone in MeCN. $[\mathbf{6}]_0 = 1.50 \times 10^{-3}$ M, $[\text{flavanone}]_0 = 0.75$ M.

Theoretical methods

Geometry optimizations were carried out on the $[N_4PyFe^{4+}O]^{2+}$ + flavanone model complex without any constraints at the M06L/6-31g(d,p) level of theory [8] as implemented in the Gaussian09 software package [9]. The optimized ($[N_4PyFe^{4+}O]^{2+}$ + flavanone) model complex is depicted in figure 1. Initial calculations on the $[N_4PyFe^{4+}O]^{2+}$ model structure led to an intermediate (*S*=1) ground state and thus, only the *S*=1 spin state was utilized in all further calculations. All transition states were characterized by one imaginary frequency and confirmed using IRC calculations. Single point energy calculations were then performed on the optimized structures by utilizing the same DFT functional and the def2-TZVP basis set. Calculations were performed in water using the CPCM solvation model [10] and accounting for Grimme's empirical dispersion correction [11]. Thus, the final free energies are those obtained with the higher basis set including zero-point corrections, thermal corrections and entropy at (298.15K), as well as solvent and dispersion corrections.

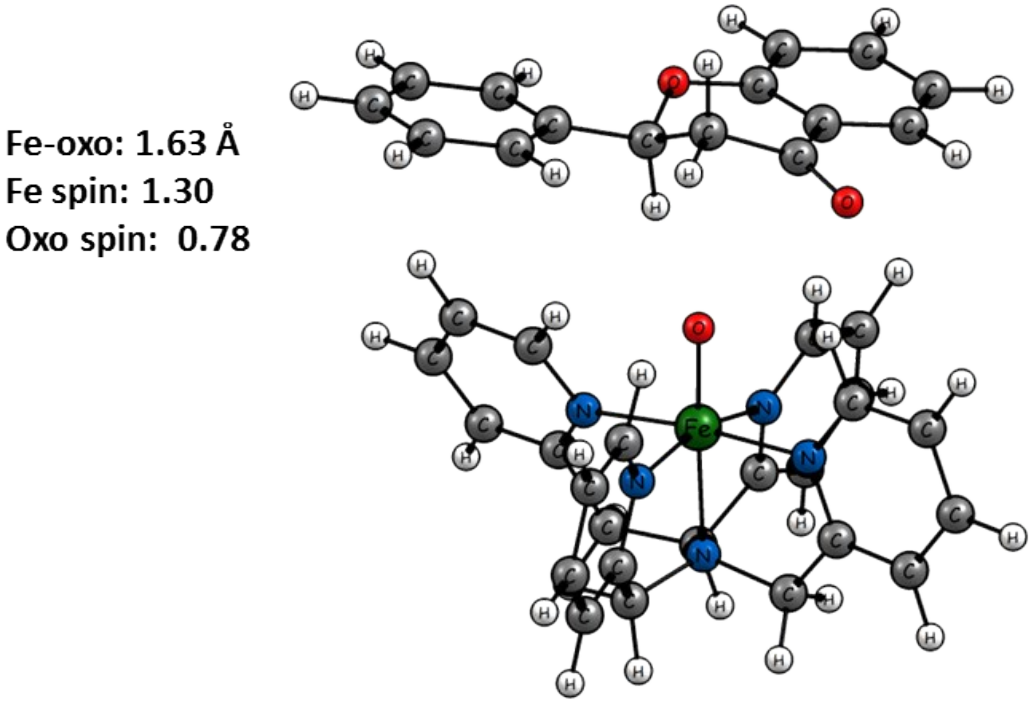


Figure S20. The optimized structure of the $[N_4PyFe^{4+}O]^{2+}$ + flavanone model complex

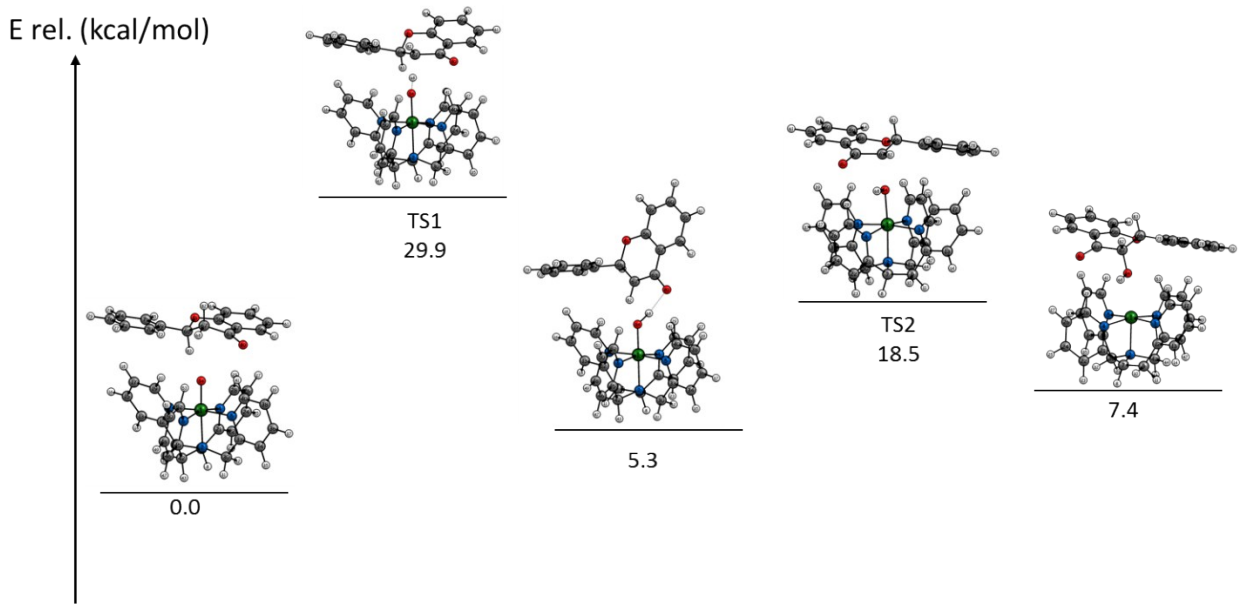


Figure S21. M06-L/def2-TZVP DFT results for the proposed reaction mechanism (1) involving the formation of 3-hydroxy-flavanone through H-atom abstraction from flavanone's C^3 by $[N_4PyFe^{4+}O]^{2+}$ to form the enzyme-like product flavone.

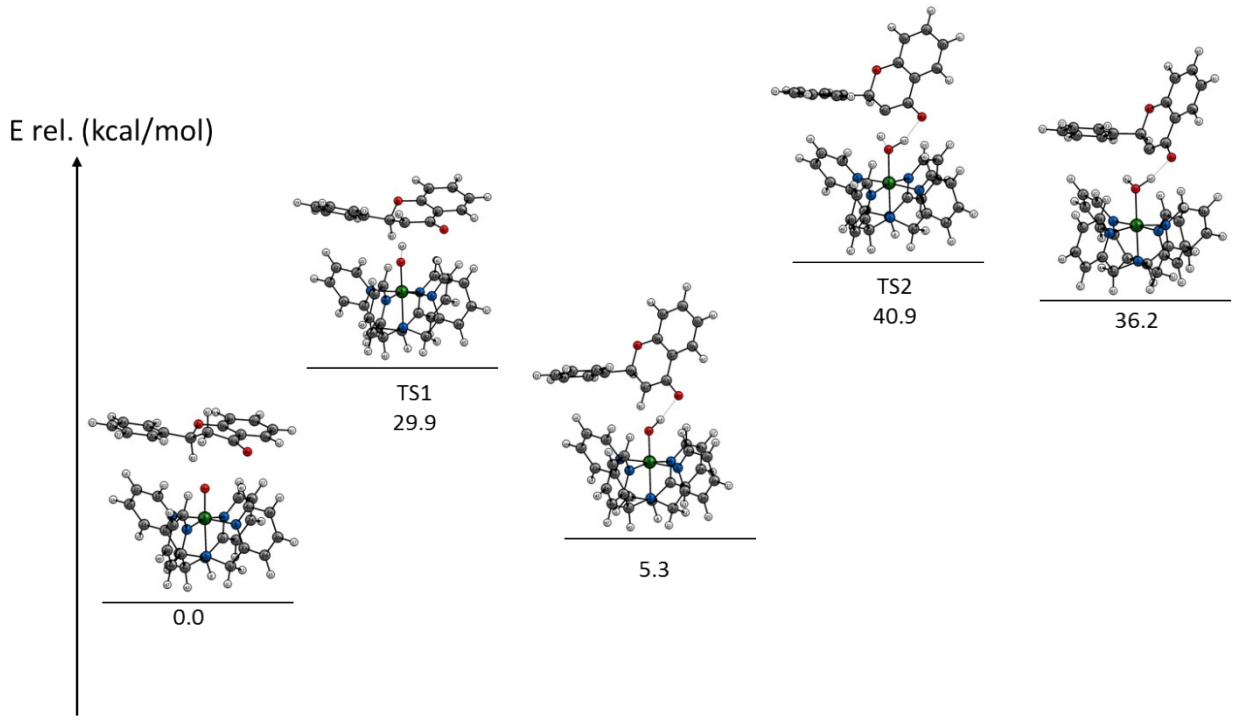


Figure S22. M06-L/def2-TZVP DFT results for the proposed reaction mechanism (2) involving a direct 2 H-atom abstraction step by $[N_4PyFe^{4+}O]^{2+}$ leading to the formation of the enzyme-like product flavone without a hydroxy-flavanone intermediate.

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Cartesian coordinates for all optimized structures including absolute energies and imaginary frequencies for transition states.

Flavanone

E = -729.205900764 a.u.

C	-4.221140	-0.095510	0.149528
C	-2.854391	-0.183367	-0.042386
C	-2.054389	0.968134	-0.063759
C	-2.659507	2.223375	0.131963
C	-4.041968	2.318310	0.311152
C	-4.809922	1.164005	0.316219
H	-4.834780	-0.990446	0.161468
H	-2.354860	-1.135284	-0.201046
C	-0.621668	0.875624	-0.387386
H	-4.483970	3.298430	0.456898
H	-5.883911	1.243827	0.461212
C	-0.544438	3.255019	0.392038
C	0.061990	2.218278	-0.544010
H	1.136131	2.111132	-0.372071
C	0.084376	4.612514	0.252785
C	1.326655	4.849713	0.846134
C	-0.518771	5.624196	-0.494917
C	1.958589	6.078592	0.693248
H	1.798558	4.065673	1.436337
C	0.111650	6.856912	-0.641239
H	-1.488663	5.442150	-0.946519
C	1.350795	7.087193	-0.050946
H	2.923194	6.251587	1.161998
H	-0.370185	7.641293	-1.218382
H	1.839803	8.050351	-0.165624
O	-0.039936	-0.183801	-0.563255
O	-1.956873	3.384862	0.148334

H	-0.064722	2.558019	-1.581640
H	-0.427648	2.897997	1.430162

$[N_4PyFe^{4+}O]^{2+}$ (S=1)

E = -2540.43900076 a.u.

Fe	0.233644	0.003578	-0.032206
N	1.720951	0.462114	1.350460
N	-0.880927	1.565177	0.652555
N	-0.412188	-1.121506	1.445585
N	1.502954	-1.419683	-0.576535
N	1.273042	1.230530	-1.182559
C	0.993535	0.413330	2.666349
H	1.723998	0.339133	3.483816
C	0.140158	1.645978	2.939167
H	-0.405751	1.446088	3.868458
H	0.787527	2.494243	3.193773
C	-0.854820	2.096262	1.897928
C	-1.721459	3.130456	2.253209
H	-1.672201	3.529502	3.261883
C	-2.624636	3.637736	1.332998
H	-3.300891	4.440452	1.608228
C	-2.641038	3.092249	0.053108
H	-3.326112	3.446760	-0.708106
C	-1.765834	2.066061	-0.244770
H	-1.760178	1.589610	-1.218361
C	0.129552	-0.829464	2.648964
C	-0.172050	-1.581008	3.775334
H	0.281489	-1.333649	4.730723
C	-1.063871	-2.645081	3.656233
H	-1.315746	-3.245938	4.523718
C	-1.625221	-2.926676	2.414477
H	-2.327371	-3.742168	2.285124
C	-1.272120	-2.146692	1.322566
H	-1.668544	-2.309656	0.324959
C	2.774655	-0.600047	1.307829

H	3.768597	-0.145718	1.384611
H	2.662761	-1.230161	2.198324
C	2.671269	-1.471955	0.093799
C	3.684116	-2.344969	-0.283783
H	4.617084	-2.360801	0.270963
C	3.477859	-3.194149	-1.364902
H	4.255856	-3.883908	-1.675119
C	2.261095	-3.146130	-2.039996
H	2.056549	-3.793770	-2.884572
C	1.298032	-2.241072	-1.624990
H	0.335148	-2.138678	-2.115624
C	2.270950	1.783565	0.939136
H	3.268054	1.951859	1.361887
H	1.625719	2.573151	1.332138
C	2.270294	1.899639	-0.558997
C	3.153882	2.700202	-1.268803
H	3.948169	3.224019	-0.746856
C	2.997605	2.822482	-2.647109
H	3.675745	3.445802	-3.220508
C	1.965749	2.134029	-3.278023
H	1.813088	2.202995	-4.348847
C	1.126278	1.336223	-2.515384
H	0.310760	0.760060	-2.943317
O	-0.877921	-0.444837	-1.138593

$[N_4PyFe^{4+}O]^{2+}$+Flavanone

E = -3270.63045564 a.u.

Fe	0.19106500	-0.30279800	-1.03267800
N	1.12282400	0.42679500	0.61497700
N	-0.96165100	1.36873200	-1.15572300
N	-1.04461000	-1.09402600	0.30360600
N	1.41429100	-1.83951700	-0.79859200
N	1.66359800	0.59786500	-2.00379100
C	-0.01281900	0.69633400	1.56685100
H	0.38965200	0.80946500	2.58336400
C	-0.79537700	1.96577000	1.25867500
H	-1.61935700	2.00191100	1.98050400
H	-0.18874200	2.84575400	1.50761000
C	-1.36526700	2.14697200	-0.12399200
C	-2.27319100	3.18902600	-0.31782500
H	-2.57627400	3.78388700	0.53845000
C	-2.77232800	3.45598900	-1.58250000
H	-3.48842600	4.25707100	-1.73802300
C	-2.33117600	2.67471900	-2.64548500
H	-2.68327700	2.83748800	-3.65982600
C	-1.43462800	1.65333400	-2.39536500
H	-1.09203400	0.99284900	-3.18379200
C	-0.91921200	-0.51325000	1.52150000
C	-1.61517900	-0.96960500	2.63057200
H	-1.48061700	-0.48378200	3.59270900
C	-2.47636700	-2.05476000	2.48732500
H	-3.03061700	-2.43202900	3.34053300
C	-2.60265400	-2.64860700	1.23703700
H	-3.25644400	-3.49916400	1.08103200
C	-1.86974000	-2.14910900	0.16781200
H	-1.93912800	-2.58778700	-0.82732600
C	2.02229400	-0.62499900	1.19317500

H	2.96416400	-0.16995600	1.51888900
H	1.54757100	-1.02061800	2.09910600
C	2.26481700	-1.75915200	0.24473800
C	3.25603500	-2.70950200	0.45441600
H	3.92922300	-2.61106400	1.30033200
C	3.36272600	-3.77837500	-0.42750500
H	4.12834300	-4.53320000	-0.28280700
C	2.47460400	-3.86252600	-1.49531100
H	2.52108900	-4.68062500	-2.20469400
C	1.51870100	-2.87291500	-1.65864700
H	0.81372000	-2.86728100	-2.48362000
C	1.90273800	1.61311100	0.15951300
H	2.68778100	1.87742100	0.87751500
H	1.22609400	2.46934300	0.09746300
C	2.45293800	1.36383400	-1.21661200
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H	4.24436800	2.53448600	-1.03608100
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H	4.90673100	2.13537400	-3.41214000
C	3.17286000	0.92092000	-3.82310500
H	3.42517700	0.72317700	-4.85855900
C	2.01959200	0.37239200	-3.27890900
H	1.34086600	-0.26627000	-3.83725100
O	-0.45558600	-0.96681100	-2.55528800
C	-4.51504900	-5.46750600	-5.42639400
C	-3.74043500	-4.71693500	-4.56671500
C	-4.07746200	-3.38406700	-4.27586600
C	-5.22487200	-2.81861100	-4.88137900
C	-6.00872700	-3.58044300	-5.75591400
C	-5.65197300	-4.88955800	-6.01978600
H	-4.25323100	-6.49643000	-5.64755200
H	-2.85387700	-5.12596100	-4.09215700
C	-3.26280800	-2.58100600	-3.38229900
H	-6.88174400	-3.12264700	-6.20752600

H	-6.26373800	-5.47869900	-6.69595300
C	-4.95994900	-0.68887000	-3.74777200
C	-3.73319500	-1.25508500	-3.15000900
H	-1.11697800	-1.69731300	-2.52622400
C	-4.71661100	0.64521600	-4.42564500
C	-3.74098600	0.75041600	-5.42216800
C	-5.48237800	1.75964600	-4.08743000
C	-3.54852700	1.95810500	-6.08463700
H	-3.15325900	-0.12558900	-5.69243100
C	-5.28401700	2.97239300	-4.74507500
H	-6.25295300	1.67135600	-3.32460500
C	-4.32107200	3.07138200	-5.74688500
H	-2.80704100	2.03126200	-6.87464500
H	-5.89752000	3.83185100	-4.49198000
H	-4.18013400	4.00982100	-6.27466200
O	-2.20797100	-3.02211400	-2.84587100
O	-5.62847500	-1.54603200	-4.68862100
H	-3.17291400	-0.60689900	-2.47626800
H	-5.69751500	-0.51940900	-2.94125300

$[N_4PyFe^{4+}O]^{2+}$ + Flavanone (TS1 from C^2)

E = -3270.60134020 a.u.

Fe	-0.450841	-0.276145	-1.224223
N	0.396398	0.205115	0.603348
N	-1.418966	1.500710	-1.222293
N	-1.790917	-1.111331	-0.044330
N	0.670552	-1.922765	-1.058513
N	1.175420	0.587482	-1.929398
C	-0.794889	0.445976	1.490138
H	-0.473785	0.430121	2.541262
C	-1.488353	1.782502	1.257219
H	-2.381603	1.783759	1.892188
H	-0.870326	2.590338	1.670354
C	-1.886956	2.173525	-0.143670
C	-2.662127	3.323247	-0.293756
H	-3.026690	3.828383	0.595801
C	-2.943160	3.818807	-1.557732
H	-3.551336	4.709451	-1.678270
C	-2.406830	3.161904	-2.659532
H	-2.569605	3.509474	-3.674609
C	-1.659497	2.019327	-2.448188
H	-1.227588	1.474122	-3.279534
C	-1.752151	-0.695660	1.240096
C	-2.565698	-1.260822	2.210823
H	-2.508940	-0.912038	3.237713
C	-3.442379	-2.279474	1.843051
H	-4.088878	-2.737766	2.584240
C	-3.465546	-2.708799	0.519810
H	-4.122428	-3.507517	0.193357
C	-2.617908	-2.109166	-0.400222
H	-2.568252	-2.409952	-1.443278
C	1.183271	-0.962860	1.108046

H	2.123723	-0.617315	1.552070
H	0.619884	-1.429726	1.925020
C	1.435461	-1.995335	0.050175
C	2.363495	-3.012510	0.232634
H	2.969108	-3.036393	1.133280
C	2.497978	-3.990161	-0.747406
H	3.219041	-4.791818	-0.625465
C	1.698071	-3.916340	-1.883031
H	1.766959	-4.647949	-2.680708
C	0.800938	-2.866738	-2.009833
H	0.175749	-2.748361	-2.887949
C	1.275447	1.376416	0.339964
H	2.014216	1.512798	1.138855
H	0.660963	2.280112	0.317560
C	1.929308	1.225936	-1.004956
C	3.177048	1.742380	-1.322686
H	3.764298	2.245848	-0.561292
C	3.654683	1.602369	-2.623351
H	4.627862	1.998838	-2.893685
C	2.875939	0.936323	-3.564904
H	3.220182	0.794940	-4.582945
C	1.643446	0.429752	-3.180265
H	0.995017	-0.130203	-3.850281
O	-1.086497	-0.851889	-2.725635
C	-3.352616	-5.295817	-2.868590
C	-2.344481	-4.647629	-3.565463
C	-2.512812	-3.329778	-4.009542
C	-3.710809	-2.659472	-3.703537
C	-4.736429	-3.307209	-3.012743
C	-4.554011	-4.624296	-2.611119
H	-3.226261	-6.325501	-2.551314
H	-1.413512	-5.148747	-3.819365
C	-1.487806	-2.658204	-4.820557
H	-5.655995	-2.769217	-2.805670

H	-5.359475	-5.136651	-2.092995
C	-2.858202	-0.594687	-4.534002
C	-1.967459	-1.380200	-5.470999
H	-1.100757	-0.796896	-5.785519
C	-3.326658	0.737070	-4.952359
C	-2.528725	1.547537	-5.781591
C	-4.570678	1.234452	-4.524575
C	-2.979870	2.792505	-6.203402
H	-1.561739	1.191741	-6.128007
C	-5.016019	2.479249	-4.949116
H	-5.199023	0.620721	-3.889095
C	-4.228557	3.262327	-5.794077
H	-2.363803	3.390368	-6.867854
H	-5.992239	2.835069	-4.633660
H	-4.588401	4.226364	-6.139699
O	-0.356815	-3.094571	-4.978097
O	-3.922372	-1.348892	-4.012278
H	-2.529968	-1.639431	-6.381317
H	-2.003532	-0.493015	-3.473420

$[N_4PyFe^{3+}OH]$ + Flavanone

E = -3270.63297698 a.u.

Fe	-0.429350000	-0.284885000	-1.154024000
N	0.422382000	0.189000000	0.643123000
N	-1.420173000	1.473350000	-1.190572000
N	-1.771467000	-1.121671000	0.027191000
N	0.670332000	-1.927413000	-1.032380000
N	1.189041000	0.574933000	-1.887588000
C	-0.761992000	0.443112000	1.537726000
H	-0.430654000	0.442529000	2.585797000
C	-1.457163000	1.777658000	1.289149000
H	-2.341097000	1.789606000	1.936930000
H	-0.833911000	2.591902000	1.681312000
C	-1.879652000	2.150963000	-0.111295000
C	-2.674973000	3.288020000	-0.259263000
H	-3.033211000	3.795605000	0.631508000
C	-2.987377000	3.766875000	-1.522163000
H	-3.612899000	4.645796000	-1.639664000
C	-2.459106000	3.108917000	-2.628094000
H	-2.644915000	3.444075000	-3.643591000
C	-1.689312000	1.981419000	-2.418346000
H	-1.257624000	1.447112000	-3.259283000
C	-1.722331000	-0.700916000	1.309279000
C	-2.526976000	-1.262114000	2.289290000
H	-2.462417000	-0.910360000	3.314687000
C	-3.405970000	-2.282520000	1.930825000
H	-4.045684000	-2.739491000	2.678705000
C	-3.442020000	-2.715176000	0.608736000
H	-4.102856000	-3.514719000	0.293014000
C	-2.603036000	-2.119302000	-0.322132000
H	-2.565675000	-2.420663000	-1.367269000
C	1.202787000	-0.990984000	1.138556000

H	2.145228000	-0.654863000	1.585159000
H	0.635200000	-1.460038000	1.951250000
C	1.446687000	-2.013981000	0.068158000
C	2.376791000	-3.032529000	0.226842000
H	2.991783000	-3.070381000	1.120605000
C	2.503120000	-3.994237000	-0.770926000
H	3.226658000	-4.796357000	-0.668396000
C	1.693563000	-3.903740000	-1.898339000
H	1.758839000	-4.621372000	-2.708996000
C	0.791594000	-2.854628000	-2.000165000
H	0.158084000	-2.728153000	-2.872552000
C	1.311184000	1.354558000	0.379300000
H	2.050796000	1.483418000	1.178413000
H	0.701821000	2.261819000	0.358707000
C	1.959034000	1.200539000	-0.967997000
C	3.210531000	1.701604000	-1.294040000
H	3.811355000	2.195024000	-0.536636000
C	3.674091000	1.559545000	-2.599934000
H	4.650054000	1.943717000	-2.877844000
C	2.877779000	0.908526000	-3.537168000
H	3.210427000	0.768005000	-4.559175000
C	1.642018000	0.415948000	-3.143473000
H	0.981924000	-0.130243000	-3.813565000
O	-1.183638000	-0.860109000	-2.687203000
C	-3.267981000	-5.163284000	-2.737937000
C	-2.277535000	-4.522499000	-3.463796000
C	-2.512702000	-3.269552000	-4.048993000
C	-3.768179000	-2.667986000	-3.863849000
C	-4.775323000	-3.303167000	-3.137781000
C	-4.520993000	-4.552254000	-2.588224000
H	-3.089046000	-6.145696000	-2.313912000
H	-1.306250000	-4.980972000	-3.631451000
C	-1.495286000	-2.600849000	-4.862880000
H	-5.737957000	-2.815071000	-3.026796000

H	-5.311039000	-5.063187000	-2.045584000
C	-3.119963000	-0.693055000	-5.016097000
C	-2.006328000	-1.425793000	-5.673661000
H	-1.167732000	-0.762326000	-5.896214000
C	-3.462326000	0.671957000	-5.233857000
C	-2.629165000	1.521074000	-6.008607000
C	-4.665663000	1.219602000	-4.714401000
C	-3.000801000	2.829716000	-6.273819000
H	-1.706922000	1.137356000	-6.435991000
C	-5.025674000	2.526628000	-4.993862000
H	-5.324103000	0.589105000	-4.127109000
C	-4.204162000	3.341978000	-5.779001000
H	-2.360549000	3.451504000	-6.892087000
H	-5.966615000	2.913157000	-4.613471000
H	-4.503352000	4.358439000	-6.014593000
O	-0.330557000	-2.968593000	-4.931076000
O	-4.055268000	-1.414363000	-4.324972000
H	-2.334704000	-1.825995000	-6.649692000
H	-1.958157000	-0.350483000	-2.977379000

$[N_4PyFe^{2+}]$ + 2-hydroxy flavanone (TS2 from C^2)

E = -3270.61447909 a.u.

Fe	-0.649887000	-0.043072000	-1.225569000
N	0.424830000	0.454257000	0.603823000
N	-1.225326000	1.856523000	-1.434950000
N	-2.109576000	-0.417604000	0.174641000
N	0.033208000	-1.841057000	-0.854785000
N	1.223182000	0.379968000	-1.991113000
C	-0.656641000	1.036268000	1.440367000
H	-0.325242000	1.116941000	2.487882000
C	-1.075682000	2.442952000	1.012469000
H	-1.949899000	2.702973000	1.621130000
H	-0.308904000	3.157409000	1.337348000
C	-1.398306000	2.756380000	-0.432780000
C	-1.812609000	4.062699000	-0.701306000
H	-1.946307000	4.747836000	0.130753000
C	-2.029829000	4.484534000	-2.002875000
H	-2.344477000	5.501883000	-2.210117000
C	-1.813580000	3.571721000	-3.030772000
H	-1.945886000	3.844199000	-4.071883000
C	-1.421702000	2.288683000	-2.706887000
H	-1.262473000	1.537391000	-3.473292000
C	-1.845822000	0.098256000	1.391826000
C	-2.637208000	-0.186399000	2.496673000
H	-2.391612000	0.241608000	3.464605000
C	-3.736509000	-1.027019000	2.340347000
H	-4.369162000	-1.266449000	3.188629000
C	-3.999108000	-1.566244000	1.084474000
H	-4.836163000	-2.236829000	0.925804000
C	-3.158567000	-1.245240000	0.028328000
H	-3.292463000	-1.652367000	-0.972539000
C	0.950060000	-0.812188000	1.169028000

H	2.001439000	-0.687698000	1.456999000
H	0.416413000	-1.034047000	2.102245000
C	0.806570000	-1.993730000	0.244620000
C	1.402741000	-3.211939000	0.549983000
H	2.026073000	-3.296011000	1.435223000
C	1.185405000	-4.308479000	-0.275612000
H	1.644022000	-5.265562000	-0.050013000
C	0.363691000	-4.154119000	-1.387880000
H	0.149709000	-4.981513000	-2.055705000
C	-0.188116000	-2.910641000	-1.642617000
H	-0.846325000	-2.729955000	-2.483932000
C	1.512391000	1.359875000	0.192914000
H	2.284992000	1.456251000	0.968165000
H	1.100006000	2.359583000	0.031782000
C	2.107252000	0.898502000	-1.110961000
C	3.451240000	1.046734000	-1.423167000
H	4.134438000	1.460878000	-0.687891000
C	3.901009000	0.659797000	-2.683161000
H	4.948166000	0.764805000	-2.947733000
C	2.989487000	0.126408000	-3.587713000
H	3.293348000	-0.203458000	-4.574829000
C	1.663212000	-0.004885000	-3.201274000
H	0.930201000	-0.454425000	-3.866588000
O	-1.895056000	-0.609342000	-2.787111000
C	-1.801240000	-5.830859000	-4.363296000
C	-1.030713000	-4.733013000	-4.713446000
C	-1.591460000	-3.448739000	-4.720204000
C	-2.929996000	-3.301280000	-4.339786000
C	-3.710565000	-4.385978000	-3.966060000
C	-3.138102000	-5.653321000	-3.990256000
H	-1.374860000	-6.828198000	-4.389240000
H	0.009704000	-4.833527000	-5.010955000
C	-0.808466000	-2.264911000	-5.081455000
H	-4.744391000	-4.231386000	-3.676504000

H	-3.742531000	-6.512360000	-3.718125000
C	-2.871908000	-0.944435000	-4.582775000
C	-1.648672000	-1.054076000	-5.420318000
H	-1.048583000	-0.145285000	-5.363287000
C	-3.721461000	0.241091000	-4.607175000
C	-3.412210000	1.331505000	-5.436270000
C	-4.874695000	0.293353000	-3.803277000
C	-4.249666000	2.439576000	-5.471405000
H	-2.539222000	1.304351000	-6.082556000
C	-5.693246000	1.412492000	-3.828773000
H	-5.127293000	-0.555729000	-3.174606000
C	-5.385167000	2.486737000	-4.664754000
H	-4.022105000	3.264078000	-6.140096000
H	-6.584111000	1.443409000	-3.210105000
H	-6.037815000	3.353307000	-4.697021000
O	0.410252000	-2.244723000	-5.130743000
O	-3.544399000	-2.058313000	-4.284960000
H	-1.966049000	-1.165232000	-6.470441000
H	-2.628389000	-0.025458000	-2.552016000

$[N_4PyFe^{2+}]$ + 2-hydroxy flavanone (product, from C^2)

E = -3270.64024968 a.u.

Fe	-0.459293000	-0.124164000	-1.268842000
N	0.440623000	0.435472000	0.607669000
N	-1.107822000	1.729543000	-1.578744000
N	-2.013173000	-0.581431000	-0.006409000
N	0.267947000	-1.897393000	-0.850704000
N	1.370034000	0.341272000	-1.977182000
C	-0.734558000	0.992170000	1.330211000
H	-0.499395000	1.105874000	2.400224000
C	-1.183183000	2.370360000	0.844295000
H	-2.085114000	2.617889000	1.416057000
H	-0.452337000	3.120560000	1.172804000
C	-1.463029000	2.621179000	-0.619207000
C	-2.009763000	3.859517000	-0.958558000
H	-2.300899000	4.538124000	-0.162235000
C	-2.153813000	4.226926000	-2.287173000
H	-2.576260000	5.190714000	-2.551542000
C	-1.715256000	3.342027000	-3.267778000
H	-1.773447000	3.584765000	-4.322458000
C	-1.213730000	2.118161000	-2.873945000
H	-0.880553000	1.387991000	-3.605231000
C	-1.869941000	-0.004255000	1.208263000
C	-2.721385000	-0.292931000	2.265853000
H	-2.568215000	0.189148000	3.227145000
C	-3.755114000	-1.205819000	2.077687000
H	-4.433530000	-1.444741000	2.890089000
C	-3.885840000	-1.820494000	0.836697000
H	-4.660399000	-2.555690000	0.651067000
C	-2.993574000	-1.493201000	-0.173226000
H	-3.043737000	-1.966260000	-1.151243000
C	0.957818000	-0.800789000	1.237125000

H	1.984135000	-0.640010000	1.590366000
H	0.370733000	-1.016187000	2.138972000
C	0.917629000	-2.008535000	0.332364000
C	1.506236000	-3.204807000	0.725199000
H	2.023688000	-3.259785000	1.678493000
C	1.424030000	-4.316280000	-0.104767000
H	1.877878000	-5.256590000	0.190436000
C	0.751899000	-4.198133000	-1.317600000
H	0.658846000	-5.034563000	-2.001158000
C	0.193126000	-2.976946000	-1.654757000
H	-0.332938000	-2.836808000	-2.593693000
C	1.514544000	1.366333000	0.218436000
H	2.254781000	1.499282000	1.018998000
H	1.076764000	2.350732000	0.029938000
C	2.182755000	0.912637000	-1.055849000
C	3.531495000	1.119481000	-1.305810000
H	4.156639000	1.571863000	-0.541962000
C	4.062110000	0.742517000	-2.536869000
H	5.114991000	0.895611000	-2.749933000
C	3.223747000	0.158164000	-3.479461000
H	3.593512000	-0.162972000	-4.446390000
C	1.886795000	-0.037390000	-3.162302000
H	1.211577000	-0.529895000	-3.862121000
O	-2.188948000	-0.644672000	-2.968164000
C	-2.037296000	-5.706034000	-4.280888000
C	-1.241598000	-4.618138000	-4.589841000
C	-1.779082000	-3.320258000	-4.595427000
C	-3.129768000	-3.135205000	-4.253713000
C	-3.933741000	-4.226473000	-3.932877000
C	-3.385507000	-5.502454000	-3.959794000
H	-1.630606000	-6.711392000	-4.306003000
H	-0.195931000	-4.731946000	-4.865604000
C	-0.962587000	-2.163376000	-4.954112000
H	-4.975957000	-4.060702000	-3.680930000

H	-4.018053000	-6.353251000	-3.726088000
C	-2.867635000	-0.755473000	-4.261541000
C	-1.770259000	-0.931348000	-5.286179000
H	-1.122143000	-0.052659000	-5.328351000
C	-3.773683000	0.438905000	-4.429916000
C	-3.619093000	1.366345000	-5.459123000
C	-4.779562000	0.633637000	-3.474222000
C	-4.454113000	2.480869000	-5.525195000
H	-2.858611000	1.226276000	-6.222968000
C	-5.602291000	1.751777000	-3.534477000
H	-4.946426000	-0.119137000	-2.704067000
C	-5.437180000	2.680800000	-4.560578000
H	-4.338011000	3.190215000	-6.339027000
H	-6.387055000	1.887672000	-2.797058000
H	-6.087565000	3.547787000	-4.618821000
O	0.263523000	-2.170043000	-4.966272000
O	-3.714800000	-1.896404000	-4.194933000
H	-2.227918000	-1.062068000	-6.274029000
H	-2.802850000	-0.137376000	-2.415939000

$[N_4PyFe^{4+}O]^{2+}$ + Flavanone (TS1 from C^3)

E = -3270.58120434 a.u.

Fe	0.047258000	-0.192076000	-1.305379000
N	0.770304000	0.317850000	0.539598000
N	-1.118229000	1.486279000	-1.297422000
N	-1.275905000	-1.181998000	-0.221853000
N	1.251481000	-1.750530000	-1.133665000
N	1.634735000	0.834955000	-1.932517000
C	-0.467714000	0.424077000	1.391404000
H	-0.178850000	0.389319000	2.451090000
C	-1.252843000	1.710889000	1.184618000
H	-2.149626000	1.629764000	1.809176000
H	-0.703567000	2.555547000	1.619956000
C	-1.674333000	2.081136000	-0.213420000
C	-2.592879000	3.121359000	-0.352816000
H	-3.020421000	3.562606000	0.542588000
C	-2.945170000	3.582687000	-1.611494000
H	-3.671296000	4.381078000	-1.726523000
C	-2.339663000	3.001117000	-2.719153000
H	-2.569588000	3.315390000	-3.732582000
C	-1.442492000	1.968741000	-2.522918000
H	-0.967358000	1.472466000	-3.360675000
C	-1.325270000	-0.777813000	1.068511000
C	-2.129560000	-1.414927000	2.001491000
H	-2.140956000	-1.071620000	3.031810000
C	-2.906035000	-2.498435000	1.596369000
H	-3.546857000	-3.008996000	2.307758000
C	-2.821785000	-2.932622000	0.277878000
H	-3.384326000	-3.790276000	-0.074112000
C	-1.982781000	-2.261477000	-0.600317000
H	-1.822460000	-2.599902000	-1.618061000
C	1.654749000	-0.784066000	1.045374000

H	2.554067000	-0.356784000	1.502261000
H	1.124166000	-1.304100000	1.851972000
C	2.004764000	-1.783837000	-0.015532000
C	2.982090000	-2.752166000	0.171429000
H	3.582559000	-2.748379000	1.075636000
C	3.161974000	-3.724732000	-0.806487000
H	3.918585000	-4.492078000	-0.680552000
C	2.351339000	-3.705600000	-1.936813000
H	2.443393000	-4.457321000	-2.711986000
C	1.407489000	-2.699385000	-2.079410000
H	0.735088000	-2.636970000	-2.931893000
C	1.547254000	1.573875000	0.347460000
H	2.215221000	1.766109000	1.195095000
H	0.848909000	2.412704000	0.291622000
C	2.288858000	1.503939000	-0.955133000
C	3.506519000	2.126059000	-1.187753000
H	4.010768000	2.650775000	-0.382739000
C	4.059544000	2.065936000	-2.464554000
H	5.011190000	2.544783000	-2.670735000
C	3.379873000	1.380298000	-3.465671000
H	3.780158000	1.308106000	-4.470412000
C	2.173037000	0.766314000	-3.161755000
H	1.597623000	0.198740000	-3.887244000
O	-0.359754000	-0.609154000	-2.932393000
C	-5.030543000	-5.484148000	-3.307261000
C	-3.797910000	-4.863579000	-3.316636000
C	-3.678731000	-3.511569000	-3.689816000
C	-4.837729000	-2.797927000	-4.066280000
C	-6.083250000	-3.431057000	-4.072907000
C	-6.169762000	-4.761711000	-3.697200000
H	-5.120725000	-6.526507000	-3.020676000
H	-2.886313000	-5.398622000	-3.064034000
C	-2.362919000	-2.895798000	-3.841805000
H	-6.957565000	-2.866679000	-4.377707000

H	-7.139389000	-5.250720000	-3.706564000
C	-3.649686000	-0.727756000	-4.023632000
C	-2.372093000	-1.472699000	-4.242812000
H	-1.334028000	-0.955582000	-3.368826000
C	-3.788852000	0.626564000	-4.669136000
C	-2.886449000	1.127753000	-5.608752000
C	-4.906316000	1.396305000	-4.326912000
C	-3.101146000	2.372033000	-6.202325000
H	-2.013272000	0.551593000	-5.903903000
C	-5.125302000	2.634247000	-4.919209000
H	-5.620231000	1.002070000	-3.607410000
C	-4.222105000	3.125197000	-5.862902000
H	-2.400676000	2.742494000	-6.944556000
H	-6.006821000	3.211730000	-4.657506000
H	-4.397209000	4.085566000	-6.338075000
O	-1.301526000	-3.503689000	-3.643006000
O	-4.804263000	-1.503363000	-4.461719000
H	-1.801595000	-1.278111000	-5.153091000
H	-3.793573000	-0.615573000	-2.929366000

$[N_4PyFe^{3+}OH]^{2+}$ + Flavanone (product, from C^3)

E = -3270.61016092 a.u.

Fe	0.191065000	-0.302798000	-1.032678000
N	1.122824000	0.426795000	0.614977000
N	-0.961651000	1.368732000	-1.155723000
N	-1.044610000	-1.094026000	0.303606000
N	1.414291000	-1.839517000	-0.798592000
N	1.663598000	0.597865000	-2.003791000
C	-0.012819000	0.696334000	1.566851000
H	0.389652000	0.809465000	2.583364000
C	-0.795377000	1.965770000	1.258675000
H	-1.619357000	2.001911000	1.980504000
H	-0.188742000	2.845754000	1.507610000
C	-1.365267000	2.146972000	-0.123992000
C	-2.273191000	3.189026000	-0.317825000
H	-2.576274000	3.783887000	0.538450000
C	-2.772328000	3.455989000	-1.582500000
H	-3.488426000	4.257071000	-1.738023000
C	-2.331176000	2.674719000	-2.645485000
H	-2.683277000	2.837488000	-3.659826000
C	-1.434628000	1.653334000	-2.395365000
H	-1.092034000	0.992849000	-3.183792000
C	-0.919212000	-0.513250000	1.521500000
C	-1.615179000	-0.969605000	2.630572000
H	-1.480617000	-0.483782000	3.592709000
C	-2.476367000	-2.054760000	2.487325000
H	-3.030617000	-2.432029000	3.340533000
C	-2.602654000	-2.648607000	1.237037000
H	-3.256444000	-3.499164000	1.081032000
C	-1.869740000	-2.149109000	0.167812000
H	-1.939128000	-2.587787000	-0.827326000
C	2.022294000	-0.624999000	1.193175000

H	2.964164000	-0.169956000	1.518889000
H	1.547571000	-1.020618000	2.099106000
C	2.264817000	-1.759152000	0.244738000
C	3.256035000	-2.709502000	0.454416000
H	3.929223000	-2.611064000	1.300332000
C	3.362726000	-3.778375000	-0.427505000
H	4.128343000	-4.533200000	-0.282807000
C	2.474604000	-3.862526000	-1.495311000
H	2.521089000	-4.680625000	-2.204694000
C	1.518701000	-2.872915000	-1.658647000
H	0.813720000	-2.867281000	-2.483620000
C	1.902738000	1.613111000	0.159513000
H	2.687781000	1.877421000	0.877515000
H	1.226094000	2.469343000	0.097463000
C	2.452938000	1.363834000	-1.216612000
C	3.627587000	1.928191000	-1.691784000
H	4.244368000	2.534486000	-1.036081000
C	3.991948000	1.705366000	-3.017647000
H	4.906731000	2.135374000	-3.412140000
C	3.172860000	0.920920000	-3.823105000
H	3.425177000	0.723177000	-4.858559000
C	2.019592000	0.372392000	-3.278909000
H	1.340866000	-0.266270000	-3.837251000
O	-0.455586000	-0.966811000	-2.555288000
C	-4.515049000	-5.467506000	-5.426394000
C	-3.740435000	-4.716935000	-4.566715000
C	-4.077462000	-3.384067000	-4.275866000
C	-5.224872000	-2.818611000	-4.881379000
C	-6.008727000	-3.580443000	-5.755914000
C	-5.651973000	-4.889558000	-6.019786000
H	-4.253231000	-6.496430000	-5.647552000
H	-2.853877000	-5.125961000	-4.092157000
C	-3.262808000	-2.581006000	-3.382299000
H	-6.881744000	-3.122647000	-6.207526000

H	-6.263738000	-5.478699000	-6.695953000
C	-4.959949000	-0.688870000	-3.747772000
C	-3.733195000	-1.255085000	-3.150009000
H	-1.116978000	-1.697313000	-2.526224000
C	-4.716611000	0.645216000	-4.425645000
C	-3.740986000	0.750416000	-5.422168000
C	-5.482378000	1.759646000	-4.087430000
C	-3.548527000	1.958105000	-6.084637000
H	-3.153259000	-0.125589000	-5.692431000
C	-5.284017000	2.972393000	-4.745075000
H	-6.252953000	1.671356000	-3.324605000
C	-4.321072000	3.071382000	-5.746885000
H	-2.807041000	2.031262000	-6.874645000
H	-5.897520000	3.831851000	-4.491980000
H	-4.180134000	4.009821000	-6.274662000
O	-2.207971000	-3.022114000	-2.845871000
O	-5.628475000	-1.546032000	-4.688621000
H	-3.172914000	-0.606899000	-2.476268000
H	-5.697515000	-0.519409000	-2.941253000

N_4PyFe^{2+} + 3-hydroxy-flavanone (TS2, from C^3)

E = -3270.58975061 a.u.

Fe	-0.784043000	-0.192742000	-0.956966000
N	0.947994000	0.218612000	0.163412000
N	-1.455005000	1.715609000	-0.559399000
N	-1.433503000	-0.886549000	0.784162000
N	0.154945000	-1.951313000	-1.269989000
N	0.280775000	0.481896000	-2.457873000
C	0.368097000	0.590560000	1.495591000
H	1.153042000	0.529731000	2.263724000
C	-0.190838000	2.005898000	1.568032000
H	-0.627015000	2.116115000	2.567443000
H	0.638050000	2.725700000	1.560744000
C	-1.207677000	2.450772000	0.549300000
C	-1.815529000	3.691534000	0.744386000
H	-1.595900000	4.247716000	1.650783000
C	-2.673176000	4.206589000	-0.214164000
H	-3.149510000	5.170463000	-0.067531000
C	-2.892496000	3.465852000	-1.371145000
H	-3.532925000	3.823261000	-2.169920000
C	-2.272522000	2.237737000	-1.506533000
H	-2.432262000	1.623697000	-2.387745000
C	-0.698196000	-0.434612000	1.829775000
C	-0.921220000	-0.872446000	3.127092000
H	-0.305288000	-0.492411000	3.937292000
C	-1.928333000	-1.803542000	3.368412000
H	-2.121334000	-2.156337000	4.376143000
C	-2.660833000	-2.288858000	2.291423000
H	-3.437403000	-3.033165000	2.423703000
C	-2.377750000	-1.820696000	1.016379000
H	-2.910457000	-2.219876000	0.153286000
C	1.768797000	-1.017069000	0.277332000

H	2.833410000	-0.774335000	0.175577000
H	1.648454000	-1.417456000	1.291481000
C	1.370068000	-2.084951000	-0.702613000
C	2.176715000	-3.187018000	-0.962152000
H	3.153478000	-3.262412000	-0.494057000
C	1.713182000	-4.182161000	-1.815652000
H	2.328146000	-5.050139000	-2.029039000
C	0.453161000	-4.042758000	-2.390480000
H	0.043635000	-4.790086000	-3.061514000
C	-0.290360000	-2.910972000	-2.099868000
H	-1.268466000	-2.738447000	-2.532343000
C	1.640725000	1.273979000	-0.615395000
H	2.703081000	1.343584000	-0.349911000
H	1.193387000	2.242007000	-0.375580000
C	1.464129000	1.037233000	-2.093209000
C	2.411267000	1.409062000	-3.035707000
H	3.352065000	1.844255000	-2.713232000
C	2.137648000	1.213434000	-4.387387000
H	2.865743000	1.498324000	-5.139728000
C	0.926423000	0.637332000	-4.752949000
H	0.679703000	0.456886000	-5.793525000
C	0.028262000	0.271524000	-3.760502000
H	-0.920988000	-0.206510000	-3.990541000
O	-2.427145000	-0.672404000	-1.909445000
C	-2.636180000	-5.689969000	-4.523301000
C	-3.262075000	-4.889945000	-3.584981000
C	-3.303945000	-3.495277000	-3.750602000
C	-2.686372000	-2.921362000	-4.882119000
C	-2.027600000	-3.722000000	-5.812706000
C	-2.015297000	-5.098964000	-5.632809000
H	-2.627554000	-6.768426000	-4.407105000
H	-3.737170000	-5.308818000	-2.702578000
C	-3.850926000	-2.629070000	-2.708750000
H	-1.559545000	-3.257188000	-6.673914000

H	-1.526680000	-5.724294000	-6.374029000
C	-3.727209000	-0.835503000	-4.491974000
C	-3.944406000	-1.211105000	-3.071145000
H	-3.027491000	-0.921472000	-1.191818000
C	-3.573104000	0.636023000	-4.781385000
C	-2.581539000	1.112927000	-5.638769000
C	-4.499843000	1.535233000	-4.243730000
C	-2.489192000	2.474945000	-5.918022000
H	-1.898480000	0.410869000	-6.105691000
C	-4.421952000	2.890982000	-4.545715000
H	-5.311413000	1.177846000	-3.612813000
C	-3.406336000	3.367822000	-5.372510000
H	-1.712921000	2.833775000	-6.587687000
H	-5.169414000	3.572891000	-4.149792000
H	-3.349195000	4.424701000	-5.613118000
O	-4.116920000	-3.002376000	-1.559190000
O	-2.645849000	-1.567603000	-5.076793000
H	-4.678115000	-0.624928000	-2.523218000
H	-4.654207000	-1.181691000	-4.998022000

N_4PyFe^{2+} + 3-hydroxy-flavanone (product, from C^3)

E = -3270.61858851 a.u.

Fe	-0.706406890	-0.104330791	-0.967448842
N	1.043611290	0.233822426	0.225253156
N	-1.408482740	1.764958629	-0.592822212
N	-1.432325090	-0.807019160	0.724980525
N	0.169543500	-1.873036991	-1.295790239
N	0.390913100	0.574584091	-2.424722990
C	0.396745910	0.603770106	1.517188194
H	1.120324110	0.539915139	2.336608888
C	-0.164006750	2.025159035	1.563889759
H	-0.635715590	2.135347799	2.549377433
H	0.663294490	2.741281054	1.587518687
C	-1.156897940	2.493125362	0.521016733
C	-1.739965870	3.747991784	0.703776097
H	-1.510687750	4.303705976	1.609692351
C	-2.570259720	4.278485118	-0.262709008
H	-3.031605940	5.252759442	-0.121405051
C	-2.809199320	3.541288023	-1.420902213
H	-3.429336040	3.910188263	-2.225098266
C	-2.208916510	2.304125691	-1.550668217
H	-2.354492690	1.699905399	-2.441284148
C	-0.707079670	-0.408798376	1.796680911
C	-0.951034090	-0.883878435	3.075219860
H	-0.335871290	-0.547136562	3.903886365
C	-1.984232010	-1.797113524	3.275911962
H	-2.196124600	-2.180189363	4.268770594
C	-2.725442180	-2.222187881	2.175510135
H	-3.526573300	-2.949207882	2.272858910
C	-2.419567540	-1.717823753	0.920429047
H	-2.949928350	-2.069079413	0.038388294
C	1.783788840	-1.040098962	0.323110169

H	2.867524940	-0.858266288	0.222249285
H	1.650699160	-1.449091919	1.331905570
C	1.341593240	-2.080239476	-0.678239834
C	2.094777330	-3.225203901	-0.924274705
H	3.047817950	-3.364009533	-0.419335687
C	1.615199640	-4.180144115	-1.812743970
H	2.184580500	-5.079674830	-2.012070471
C	0.390685090	-3.959622027	-2.445791410
H	-0.027187800	-4.672240337	-3.149631114
C	-0.291465810	-2.790435265	-2.166710367
H	-1.231331960	-2.553076805	-2.649635196
C	1.767560290	1.271676182	-0.534149282
H	2.838409130	1.303229587	-0.273020099
H	1.357117980	2.251336578	-0.273003723
C	1.591092660	1.087101020	-2.023174716
C	2.558755760	1.477168075	-2.940841611
H	3.503985700	1.875896612	-2.589254315
C	2.295071010	1.351291142	-4.302869437
H	3.038864190	1.655151630	-5.033393888
C	1.079344340	0.821468895	-4.707590383
H	0.837721320	0.697576298	-5.757638708
C	0.150497000	0.432078655	-3.741128064
H	-0.796742620	-0.012026440	-4.006453690
O	-3.030477950	-0.605163689	-2.087366028
C	-2.731129030	-5.781311135	-4.660407939
C	-3.330228870	-5.017771691	-3.674282955
C	-3.301393840	-3.613786486	-3.745323435
C	-2.630763440	-2.995780581	-4.825806474
C	-2.004292030	-3.761783308	-5.800210965
C	-2.062524590	-5.147617723	-5.716386590
H	-2.780182130	-6.864081236	-4.620711380
H	-3.843421520	-5.474544226	-2.829462743
C	-3.777623450	-2.786301322	-2.642457446
H	-1.495896140	-3.264966422	-6.619785078

H	-1.596301260	-5.745683060	-6.492219864
C	-3.682592820	-0.949860435	-4.373337590
C	-3.880817620	-1.270645572	-2.892508572
H	-3.444218640	-0.519258562	-1.219330879
C	-3.587848030	0.516496375	-4.694316734
C	-2.657778680	1.006175716	-5.607531284
C	-4.506774300	1.405785710	-4.120771227
C	-2.618801670	2.364035075	-5.917520936
H	-1.974972430	0.314271436	-6.091349841
C	-4.488340550	2.756273207	-4.454205266
H	-5.268092810	1.041109204	-3.427914639
C	-3.529848730	3.242829070	-5.344845846
H	-1.882141910	2.730586821	-6.631608326
H	-5.225578860	3.427043656	-4.029193204
H	-3.511523680	4.295546301	-5.608843644
O	-3.974786700	-3.200729839	-1.505038094
O	-2.534962120	-1.633161516	-4.905311191
H	-4.921492110	-1.010819114	-2.666596533
H	-4.561060850	-1.379223234	-4.880684631

$N_4PyFe^{2+}OH_2$ + flavone (TS2, mechanism(2))

E = -3270.54878466 a.u.

Fe	0.110605000	-0.264125000	-1.103629000
N	1.022204000	0.385311000	0.543563000
N	-1.018656000	1.405923000	-1.191654000
N	-1.103656000	-1.125300000	0.181297000
N	1.331266000	-1.829466000	-0.977892000
N	1.575954000	0.662092000	-2.048667000
C	-0.112224000	0.611563000	1.513136000
H	0.297128000	0.697189000	2.529796000
C	-0.920536000	1.875932000	1.251038000
H	-1.746292000	1.869575000	1.971627000
H	-0.329710000	2.756850000	1.534540000
C	-1.479662000	2.110069000	-0.128747000
C	-2.400458000	3.145975000	-0.286536000
H	-2.750760000	3.673922000	0.595527000
C	-2.843451000	3.503792000	-1.550502000
H	-3.567247000	4.302114000	-1.679951000
C	-2.319405000	2.827877000	-2.646814000
H	-2.606232000	3.075937000	-3.664145000
C	-1.420318000	1.802006000	-2.425090000
H	-0.992424000	1.261936000	-3.262683000
C	-0.999954000	-0.605772000	1.426618000
C	-1.688373000	-1.134423000	2.507328000
H	-1.570169000	-0.695869000	3.493851000
C	-2.520794000	-2.232918000	2.302575000
H	-3.069899000	-2.667658000	3.131206000
C	-2.619059000	-2.771515000	1.024260000
H	-3.241614000	-3.636005000	0.824034000
C	-1.891935000	-2.199536000	-0.010897000
H	-1.910469000	-2.608128000	-1.018553000
C	1.924034000	-0.689127000	1.074182000

H	2.863439000	-0.249958000	1.427835000
H	1.446573000	-1.131863000	1.956430000
C	2.179409000	-1.775290000	0.073445000
C	3.193891000	-2.706460000	0.257770000
H	3.855640000	-2.620662000	1.114170000
C	3.341917000	-3.739590000	-0.659037000
H	4.124877000	-4.479726000	-0.533190000
C	2.469159000	-3.801266000	-1.739784000
H	2.544041000	-4.585988000	-2.483480000
C	1.490505000	-2.829182000	-1.869886000
H	0.814525000	-2.847775000	-2.717367000
C	1.796117000	1.596476000	0.151682000
H	2.575658000	1.832539000	0.885615000
H	1.112652000	2.449236000	0.125811000
C	2.354015000	1.410339000	-1.230291000
C	3.524491000	2.007124000	-1.675160000
H	4.127258000	2.596223000	-0.991186000
C	3.904577000	1.839996000	-3.004282000
H	4.815836000	2.297305000	-3.375247000
C	3.102841000	1.073305000	-3.843775000
H	3.365036000	0.916047000	-4.883809000
C	1.953451000	0.492230000	-3.328378000
H	1.295998000	-0.128482000	-3.929915000
O	-0.706005000	-0.925804000	-2.726906000
C	-4.931251000	-5.500226000	-4.906812000
C	-3.902801000	-4.796394000	-4.317316000
C	-4.028249000	-3.415355000	-4.077437000
C	-5.225388000	-2.752873000	-4.447980000
C	-6.263173000	-3.473227000	-5.052968000
C	-6.110867000	-4.828871000	-5.275113000
H	-4.831537000	-6.564087000	-5.092963000
H	-2.973387000	-5.277548000	-4.030667000
C	-2.931986000	-2.661988000	-3.484638000
H	-7.167754000	-2.945440000	-5.333312000

H	-6.919923000	-5.380718000	-5.743543000
C	-4.478899000	-0.605132000	-3.561996000
C	-3.204975000	-1.272342000	-3.294736000
H	-0.850878000	-1.916026000	-2.833089000
C	-4.360736000	0.686918000	-4.337499000
C	-3.402036000	0.826596000	-5.345478000
C	-5.254338000	1.728340000	-4.085984000
C	-3.342151000	1.997157000	-6.096000000
H	-2.716187000	0.005537000	-5.550579000
C	-5.196881000	2.898743000	-4.837575000
H	-6.007966000	1.613232000	-3.309924000
C	-4.240993000	3.034099000	-5.843925000
H	-2.606594000	2.096711000	-6.888515000
H	-5.906217000	3.699065000	-4.649396000
H	-4.204208000	3.940974000	-6.439558000
O	-1.832421000	-3.205432000	-3.175719000
O	-5.448823000	-1.438134000	-4.272323000
H	-1.710227000	-0.680921000	-2.912804000
H	-4.969665000	-0.381533000	-2.596948000

$N_4PyFe^{2+}OH_2$ + flavone (product, mechanism(2))

E = -3270.55086281 a.u.

Fe	0.177175000	-0.202935000	-1.060814000
N	1.063993000	0.428026000	0.592533000
N	-0.913797000	1.481619000	-1.184337000
N	-1.095036000	-1.028565000	0.200638000
N	1.334907000	-1.794316000	-0.916626000
N	1.677797000	0.655337000	-1.988257000
C	-0.076756000	0.683910000	1.542325000
H	0.313812000	0.773424000	2.566613000
C	-0.865167000	1.955890000	1.253860000
H	-1.690782000	1.978225000	1.974048000
H	-0.261190000	2.834798000	1.516632000
C	-1.419136000	2.170195000	-0.131011000
C	-2.369158000	3.177431000	-0.305975000
H	-2.758365000	3.687975000	0.570089000
C	-2.793919000	3.529348000	-1.577753000
H	-3.543048000	4.301318000	-1.720204000
C	-2.205352000	2.891242000	-2.665595000
H	-2.466593000	3.147130000	-3.687470000
C	-1.279450000	1.895040000	-2.424344000
H	-0.771492000	1.410653000	-3.253565000
C	-0.988201000	-0.514648000	1.449549000
C	-1.693458000	-1.024187000	2.528529000
H	-1.568248000	-0.585197000	3.514095000
C	-2.550386000	-2.103589000	2.325123000
H	-3.112309000	-2.524224000	3.152395000
C	-2.655238000	-2.639495000	1.046311000
H	-3.296493000	-3.489898000	0.843960000
C	-1.911173000	-2.084051000	0.014417000
H	-1.942451000	-2.495957000	-0.991096000
C	1.937806000	-0.662174000	1.137242000

H	2.885813000	-0.242934000	1.492644000
H	1.446266000	-1.087231000	2.020579000
C	2.173213000	-1.760876000	0.143953000
C	3.159348000	-2.719179000	0.340171000
H	3.815093000	-2.650694000	1.202782000
C	3.288009000	-3.757822000	-0.573906000
H	4.049320000	-4.518602000	-0.439266000
C	2.424990000	-3.797656000	-1.663902000
H	2.487980000	-4.585723000	-2.405351000
C	1.473819000	-2.799886000	-1.805132000
H	0.802361000	-2.791063000	-2.656830000
C	1.869207000	1.618894000	0.200815000
H	2.635204000	1.855601000	0.949262000
H	1.200620000	2.481975000	0.142031000
C	2.458599000	1.395234000	-1.162517000
C	3.662828000	1.940577000	-1.582228000
H	4.265124000	2.521934000	-0.891060000
C	4.079597000	1.729933000	-2.894385000
H	5.017597000	2.146511000	-3.245615000
C	3.279349000	0.969089000	-3.740754000
H	3.570988000	0.774895000	-4.766648000
C	2.094141000	0.441042000	-3.249917000
H	1.439878000	-0.177773000	-3.857699000
O	-0.683560000	-0.901695000	-2.752950000
C	-4.747640000	-5.564686000	-5.245184000
C	-3.829808000	-4.823536000	-4.533300000
C	-4.085031000	-3.472983000	-4.230230000
C	-5.295974000	-2.877284000	-4.672718000
C	-6.218977000	-3.634852000	-5.402455000
C	-5.942403000	-4.961028000	-5.679228000
H	-4.552729000	-6.606565000	-5.474141000
H	-2.893733000	-5.250374000	-4.188342000
C	-3.108462000	-2.681450000	-3.498690000
H	-7.135770000	-3.161182000	-5.734776000

H	-6.665012000	-5.543643000	-6.242191000
C	-4.828634000	-0.731208000	-3.604889000
C	-3.571443000	-1.367802000	-3.231257000
H	-1.063218000	-1.833856000	-2.822075000
C	-4.632192000	0.597197000	-4.300035000
C	-3.715032000	0.701761000	-5.351615000
C	-5.392153000	1.706058000	-3.930196000
C	-3.574071000	1.903407000	-6.037070000
H	-3.140046000	-0.173162000	-5.653084000
C	-5.249497000	2.909955000	-4.615978000
H	-6.113367000	1.619912000	-3.120500000
C	-4.344628000	3.008317000	-5.671367000
H	-2.879824000	1.975673000	-6.868842000
H	-5.859578000	3.764828000	-4.340492000
H	-4.248206000	3.941281000	-6.218531000
O	-1.976821000	-3.120717000	-3.152021000
O	-5.634310000	-1.587110000	-4.465933000
H	-1.422043000	-0.366074000	-3.080209000
H	-5.447010000	-0.570206000	-2.705634000