

Supplementary material for the paper

RSC NJC (08. 27. 2015)

Oxoiron(IV)-mediated Baeyer-Villiger oxidation of cyclohexanones generated by dioxygen
with co-oxidation of aldehydes.

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Materials

Analytical and physical measurements

Determination of products

Catalytic oxidations

Stoichiometric oxidations

I. Iron-catalyzed Baeyer-Villiger oxidation of cyclohexanones with O₂ in the presence of aldehydes

II. Fe^{IV}=O formation with O₂ in the presence of aldehydes

III. Fe^{IV}=O mediated Baeyer-Villiger oxidation

Materials

[Fe^{II}(N₄Py)(CH₃CN)](ClO₄)₂ was prepared according to the literature. All other chemicals were commercial products and they were used without further purification.

Analytical and physical measurements

UV-vis spectra were recorded on an Agilent 8453 diode-array spectrophotometer using quartz cells. GC analyses were performed on an Agilent 7820A gas chromatograph equipped with a flame ionization detector and a 30 m HP-5 column. GC-MS analyses were carried out on Shimadzu QP2010SE equipped with a secondary electron multiplier detector with conversion dynode and a 30 m HP-5MS column.

Determination of products

All reactions were carried out in a 20 mL Schlenk tube equipped with a condenser. Cyclohexanone (1.00×10^{-2} M), $[\text{Fe}^{\text{II}}(\text{N}_4\text{Py})(\text{CH}_3\text{CN})](\text{ClO}_4)_2$ (1.00×10^{-5} M), acetonitrile (5 mL) and the initiator isobutyraldehyde or benzaldehyde derivatives (1.50×10^{-1} M) were added and then the mixture was stirred at 25°C or 60°C under oxygen atmosphere for 2-24 hours. The products were identified by GC (Agilent 7820A) and GC-MS (Shimadzu QP2010SE) and the yields were calculated based on the amount of cyclohexanone consumed in the reactions.

Catalytic oxidations

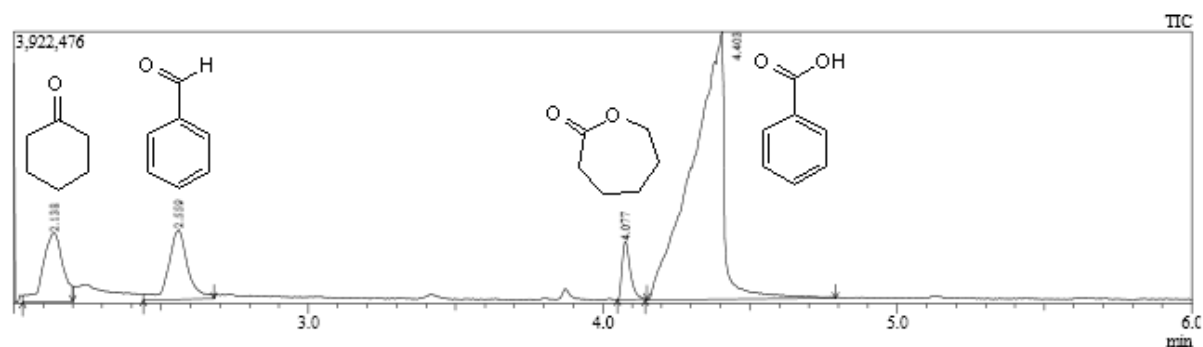
$[\text{Fe}^{\text{II}}(\text{N}_4\text{Py})(\text{CH}_3\text{CN})](\text{ClO}_4)_2$ complex (2.00×10^{-3} M) was dissolved in acetonitrile (1.5 mL) then the benzaldehyde was added to the solution and the progress of the reaction was monitored with UV-vis spectrophotometer (Agilent 8453) at 693 nm ($\epsilon = 400 \text{ M}^{-1} \text{ cm}^{-1}$).

Stoichiometric oxidations

$[\text{Fe}^{\text{II}}(\text{N}_4\text{Py})(\text{CH}_3\text{CN})](\text{ClO}_4)_2$ complex (2.00×10^{-3} M) was dissolved in acetonitrile (1.5 mL), then iodosobenzene (4.00×10^{-3} M) was added to the solution. The mixture was stirred for one hour then excess iodosobenzene was removed by filtration. Cyclohexanone (1.00×10^{-1} M) was added to the solution and the reaction was monitored with UV-vis spectrophotometer (Agilent 8453) at 693 nm ($\epsilon = 400 \text{ M}^{-1} \text{ cm}^{-1}$).

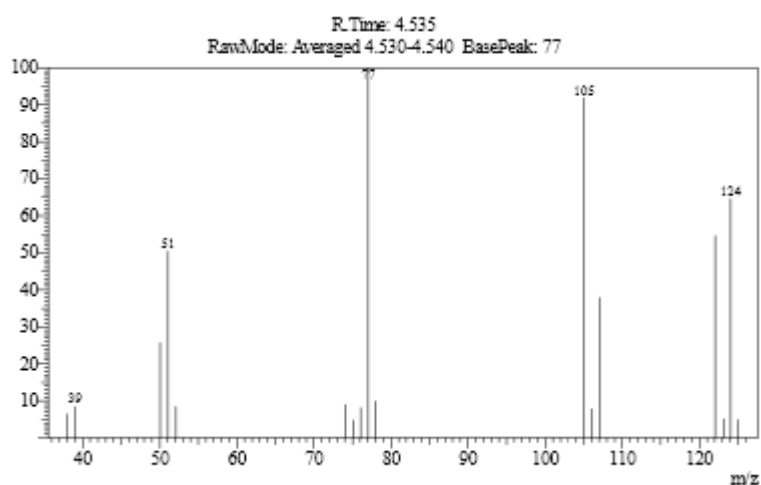
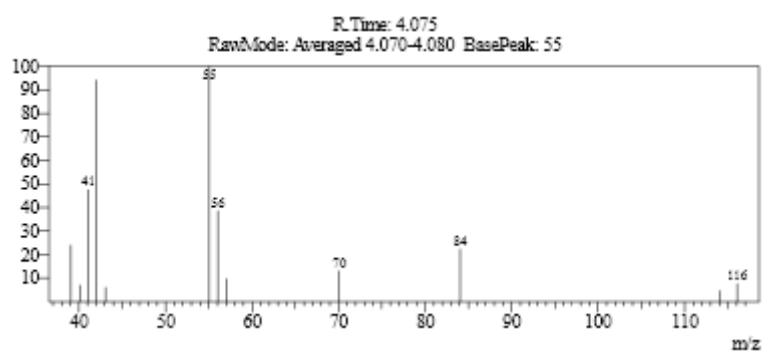
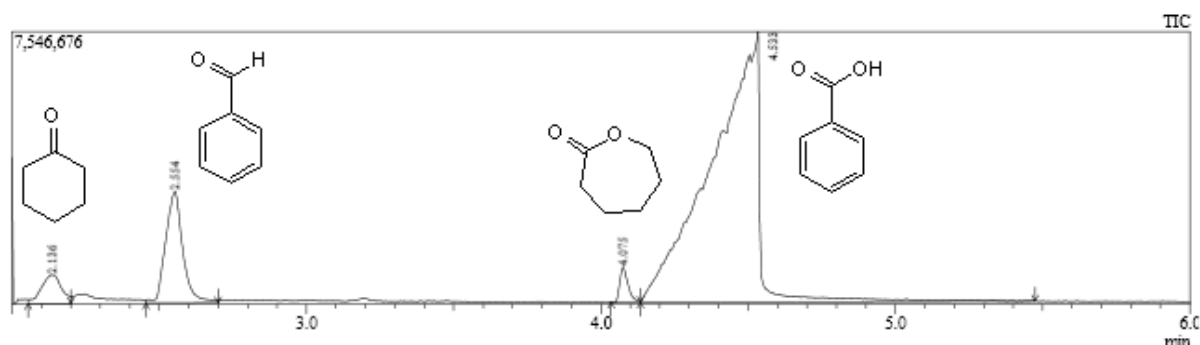
I. Iron-catalyzed Baeyer-Villiger oxidation of cyclohexanones with O_2 in the presence of aldehydes

Fig. S1. GC-MS chromatogram of the reaction of cyclohexanone, benzaldehyde and **1** in MeCN at 60°C under oxygen atmosphere. $[\mathbf{1}]_0 = 1.00 \times 10^{-5}$ M, $[\text{cyclohexanone}]_0 = 1.00 \times 10^{-2}$ M, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1}$ M.



ϵ -caprolactone: m/z (relative intensity) 114 (M^+ , 12.6); 84 (24.1); 70 (15.3); 56 (39.6); 55 (100); 42 (99.8); 41 (49.6); 39 (23.5).

Fig. S2. GC-MS chromatogram of the reaction of cyclohexanone, benzaldehyde and **1** in MeCN at 25°C under ^{18}O atmosphere. $[\mathbf{1}]_0 = 1.00 \times 10^{-5} \text{ M}$, $[\text{cyclohexanone}]_0 = 1.00 \times 10^{-2} \text{ M}$, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1} \text{ M}$.



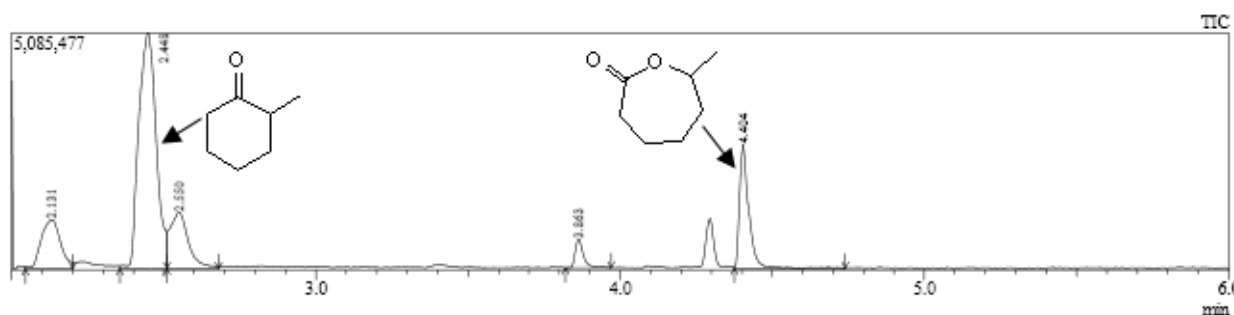
cyclohexanone: m/z (relative intensity) 98 (M^+ , 39.4); 83 (9.2); 70 (22.8); 69 (30.9); 57 (12); 56 (10.2); 55 (100); 43 (11.7); 42 (77.9); 41 (36); 39 (27.4).

benzaldehyde: m/z (relative intensity) 107 (13.6); 106 (M^+ , 86.7); 105 (80.3); 94 (7.7); 78 (17.2); 77 (100); 74 (8.7); 66 (5.3); 52 (12.4); 51 (51.1); 50 (27.5); 39 (9.9).

ϵ -caprolactone: m/z (relative intensity) 116 (7.7); 114 (M^+ , 4.8); 84 (22.4); 70 (13.1); 57 (9.7); 56 (38.7); 55 (100); 42 (94.3); 41 (47.7); 39 (24).

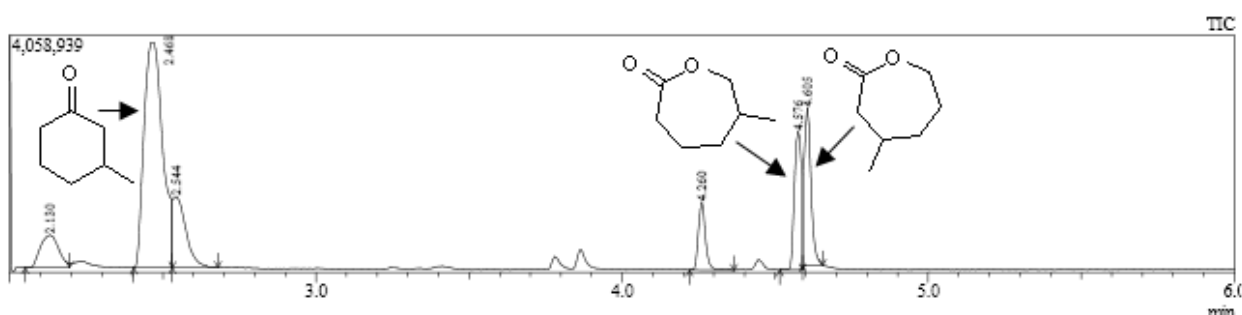
benzoic acid: m/z (relative intensity) 124 (64.6); 122 (M^+ , 54.7); 107 (37.9); 105 (91.9); 78 (10); 77 (100); 51 (50.5); 50 (25.7).

Fig. S3. GC-MS chromatogram of the reaction of 2-methyl-cyclohexanone, benzaldehyde and **1** in MeCN at 60°C under oxygen atmosphere. $[\mathbf{1}]_0 = 1.00 \times 10^{-5}$ M, $[2\text{-methyl-cyclohexanone}]_0 = 1.00 \times 10^{-2}$ M, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1}$ M.



6-methyl-ε-caprolactone: m/z (relative intensity) 128 (M^+ , 10.1); 98 (16.5); 96 (54.4); 83 (26.3); 82 (16.2); 70 (25.2); 69 (28.3); 56 (100); 55 (54.2); 54 (34.7); 43 (16.3); 42 (29.5); 41 (56.2); 39 (24.8).

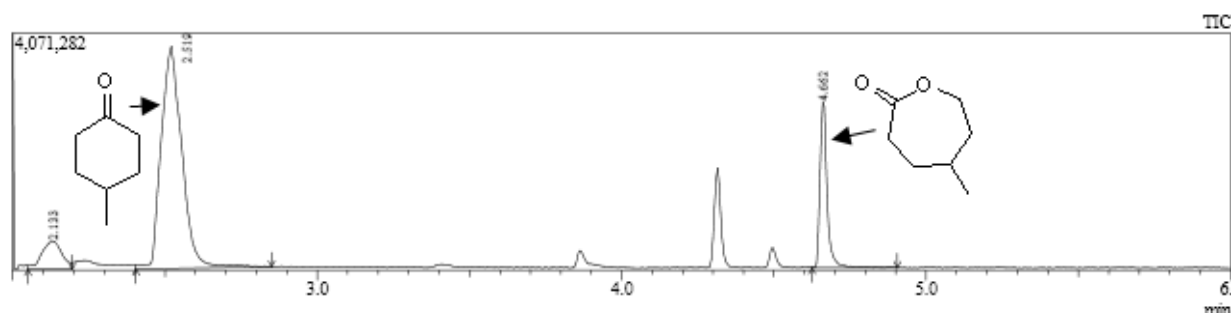
Fig. S4. GC-MS chromatogram of the reaction of 3-methyl-cyclohexanone, benzaldehyde and **1** in MeCN at 60°C under oxygen atmosphere. $[\mathbf{1}]_0 = 1.00 \times 10^{-5}$ M, $[3\text{-methyl-cyclohexanone}]_0 = 1.00 \times 10^{-2}$ M, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1}$ M.



5-methyl-ε-caprolactone: m/z (relative intensity) 128 (M^+ , 7); 100 (13); 98 (31.9); 72 (16.5); 70 (18); 69 (100); 57 (11.3); 56 (61.7); 55 (72.6); 43 (23.4); 42 (90); 41 (59.3); 39 (27.7).

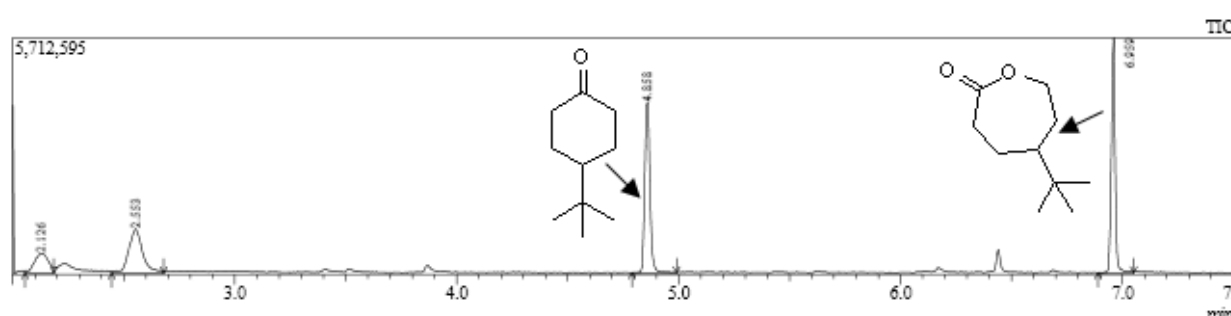
3-methyl-ε-caprolactone: m/z (relative intensity) 128 (M^+ , 12.1); 98 (100); 83 (18.6); 80 (73.9); 70 (11.1); 69 (25.2); 56 (47.5); 55 (52.2); 42 (24.7); 41 (59.6); 39 (25.8).

Fig. S5. GC-MS chromatogram of the reaction of 4-methyl-cyclohexanone, benzaldehyde and **1** in MeCN at 60°C under oxygen atmosphere. $[1]_0 = 1.00 \times 10^{-5}$ M, $[4\text{-methyl-cyclohexanone}]_0 = 1.00 \times 10^{-2}$ M, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1}$ M.



4-methyl- ϵ -caprolactone: m/z (relative intensity) 128 (M^+ , 8.1); 98 (13.2); 70 (9.5); 69 (51.3); 57 (6); 56 (100); 55 (51.4); 43 (11.3); 42 (20.7); 41 (41.4); 39 (14.4).

Fig. S6. GC-MS chromatogram of the reaction of 4-tert-butyl-cyclohexanone, benzaldehyde and **1** in MeCN at 60°C under oxygen atmosphere. $[1]_0 = 1.00 \times 10^{-5}$ M, $[4\text{-tert-butyl-cyclohexanone}]_0 = 1.00 \times 10^{-2}$ M, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1}$ M.



4-tert-butyl- ϵ -caprolactone: m/z (relative intensity) 170 (M^+ , 4.1); 114 (69.2); 86 (79.6); 83 (12.7); 69 (12.5); 68 (16.8); 57 (100); 56 (12.1); 55 (75.8); 54 (12.8); 43 (9.5); 42 (6.8); 41 (46.8); 39 (14.0).

Table S1. Calculated yields, TON and TOF values for the reaction of **1** with different benzaldehyde and cyclohexanone derivatives in MeCN under oxygen atmosphere.

N_0	t (h)	T (K)	substrate	$[\text{Fe}]_0$ (10^{-3} M)	$[\text{S}]_0$ (M)	co-reductant	$[\text{co-reductant}]_0$	yield (%)	TON	TOF (1/h)
1	17	298	cyclohexanone ^A	0.01	0.01	benzaldehyde	0.15	21.5	215	12.65
2	5	333	cyclohexanone	-	0.01	benzaldehyde	0.15	9.8	-	-
2	5	333	cyclohexanone	0.01	0.01	benzaldehyde	0.15	33.6	336	67.20
3	5	333	cyclohexanone	0.01	0.01	isobutyraldehyde	0.15	6.2	62	12.40
4	15	333	cyclohexanone	0.01	0.01	benzaldehyde	0.15	73.0	730	48.67
5	15	333	cyclohexanone	0.01	0.01	isobutyraldehyde	0.15	16.4	164	10.93
6	15	333	cyclohexanone	0.01	0.01	4-methylbenzaldehyde	0.15	79.5	795	53.00
7	15	333	cyclohexanone	0.01	0.01	4-chlorobenzaldehyde	0.15	54.7	547	36.47
8	15	333	cyclohexanone	0.01	0.01	4-cyanobenzaldehyde	0.15	36.4	364	24.27
9	15	333	cyclohexanone	0.01	0.01	4-nitrobenzaldehyde	0.15	29.4	294	19.60
10	15	333	cyclohexanone	-	0.01	benzaldehyde	0.15	28.3	-	-
11	15	333	cyclohexanone	-	0.01	4-methylbenzaldehyde	0.15	32.9	-	-

12	15	333	cyclohexanone	-	0.01	4-chlorobenzaldehyde	0.15	18.2	-	-
13	15	333	cyclohexanone	-	0.01	4-cyanobenzaldehyde	0.15	10.3	-	-
14	15	333	cyclohexanone	-	0.01	4-nitrobenzaldehyde	0.15	8.9	-	-
15	15	333	2-methyl-cyclohexanone	-	0.01	benzaldehyde	0.15	25.2	-	-
16	15	333	3-methyl-cyclohexanone ^C	-	0.01	benzaldehyde	0.15	2.2	-	-
17	15	333	4-methyl-cyclohexanone	-	0.01	benzaldehyde	0.15	18.5	-	-
18	15	333	4-tert-butyl-cyclohexanone	-	0.01	benzaldehyde	0.15	3.8	-	-
19	24	298	cyclohexanone ^B	0.01	0.01	benzaldehyde	0.15	33.1	331	13.79
20	15	333	2-methyl-cyclohexanone ^C	0.01	0.01	benzaldehyde	0.15	62.5	625	41.67
21	15	333	3-methyl-cyclohexanone ^D	0.01	0.01	benzaldehyde	0.15	15.5	155	10.33
22	15	333	4-methyl-cyclohexanone	0.01	0.01	benzaldehyde	0.15	53.0	530	35.33
23	15	333	4-tert-butyl-cyclohexanone	0.01	0.01	benzaldehyde	0.15	18.0	180	12.00
24	15	333	cyclohexanone	-	0.01	<i>m</i> -chloroperoxybenzoic acid	0.15	92.6	-	-
25	15	333	cyclohexanone	0.01	0.01	<i>m</i> -chloroperoxybenzoic acid	0.15	100	1000	66.67
26	5	333	cyclohexanone	-	0.01	<i>m</i> -chloroperoxybenzoic acid	0.15	16.8	-	-
27	5	333	cyclohexanone	0.01	0.01	<i>m</i> -chloroperoxybenzoic acid	0.15	59.1	591	118.2
28	5	323	cyclohexanone	0.01	0.01	<i>m</i> -chloroperoxybenzoic acid	0.15	41.6	416	83.2
29	5	343	cyclohexanone	0.01	0.01	<i>m</i> -chloroperoxybenzoic acid	0.15	73.9	739	147.8
30	5	323	cyclohexanone	0.01	0.01	benzaldehyde	0.15	21.9	219	43.8
31	5	343	cyclohexanone	0.01	0.01	benzaldehyde	0.15	46.8	468	93.6

^A under air

^B under ¹⁸O atmosphere

^C only 6-methyl- ϵ -caprolactone was formed (T. Kawabata, Y. Ohishi, S. Itsuku, N. Fujisaki, T. Shishido, K. Takaki, Q. Zhang, Y. Wang and K. Takehira, *J. Mol. Cat. A.:Chemical*, 2005, **236**, 99-106)

^D two products were formed in 1:1 ratio.

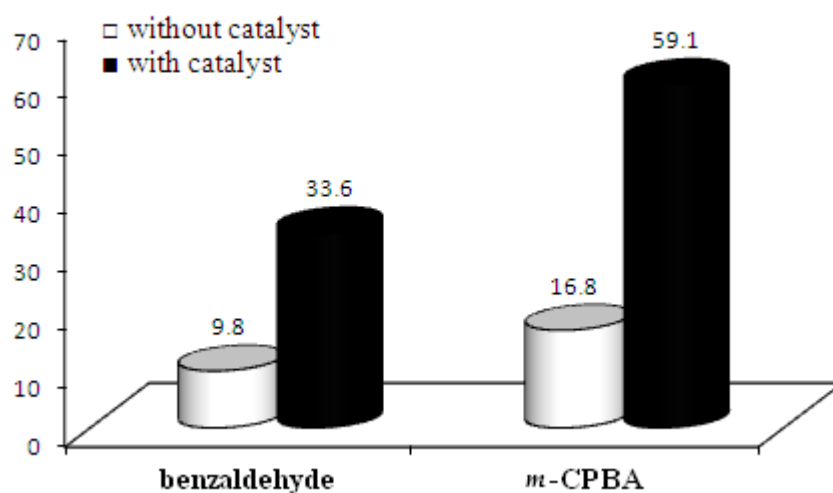


Figure S7. Yields without and with catalyst for the **1**-catalysed B.-V. oxidation of cyclohexanone with benzaldehyde or *m*-CPBA in MeCN at 60°C for 5 hours. $[\mathbf{1}]_0 = 1.00 \times 10^{-5}$ M, $[\text{cyclohexanone}]_0 = 1.00 \times 10^{-2}$ M, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1}$ M, $[\text{m-CPBA}]_0 = 1.50 \times 10^{-1}$ M.

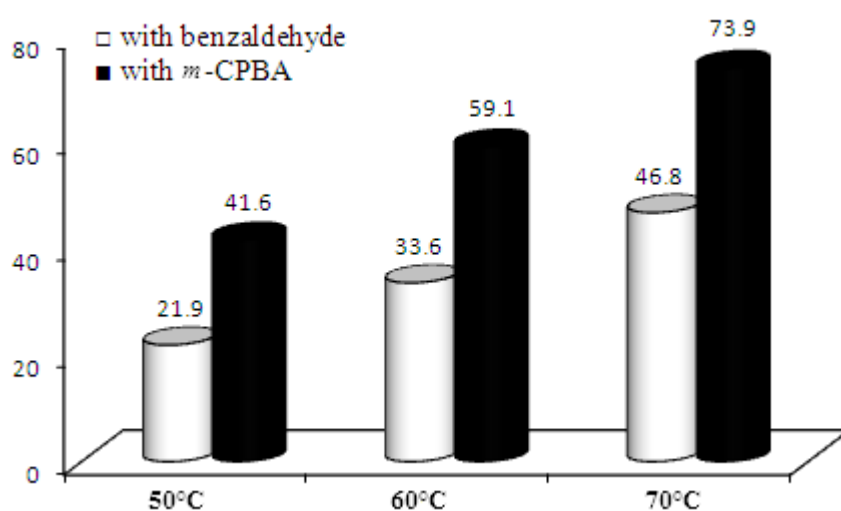


Figure S8. Yields with benzaldehyde (□) and with *m*-CPBA (■) for the **1**-catalysed B.-V. oxidation of cyclohexanone in MeCN at 60°C for 5 hours. $[\mathbf{1}]_0 = 1.00 \times 10^{-5}$ M, $[\text{cyclohexanone}]_0 = 1.00 \times 10^{-2}$ M, $[\text{benzaldehyde}]_0 = 1.50 \times 10^{-1}$ M, $[\text{m-CPBA}]_0 = 1.50 \times 10^{-1}$ M.

Table S2. Calculated yields, TON and relative reaction rate values for the reaction of **1** with different benzaldehyde derivatives and cyclohexanone in MeCN under oxygen atmosphere for 15 h and at 60°C.

N ₀	t (h)	T (K)	aldehyde	[Fe] ₀ (10 ⁻³ M)	[S] ₀ (M)	[aldehyde] ₀	yield (%)	TON	k _{rel}
1	15	333	benzaldehyde	-	0.01	0.15	28.3	-	1
2	15	333	benzaldehyde	0.01	0.01	0.15	73	730	1
3	15	333	4-methylbenzaldehyde	-	0.01	0.15	32.9	-	1.20
4	15	333	4-methylbenzaldehyde	0.01	0.01	0.15	79.5	795	1.21
5	15	333	4-chlorobenzaldehyde	-	0.01	0.15	18.2	-	-0.20
6	15	333	4-chlorobenzaldehyde	0.01	0.01	0.15	54.7	547	-0.22
7	15	333	4-cyanobenzaldehyde	-	0.01	0.15	10.3	-	-0.48
8	15	333	4-cyanobenzaldehyde	0.01	0.01	0.15	36.4	364	-0.50
9	15	333	4-nitrobenzaldehyde	-	0.01	0.15	8.9	-	-0.55
10	15	333	4-nitrobenzaldehyde	0.01	0.01	0.15	29.4	294	-0.58
11	15	333	4-hydroxybenzaldehyde	-	0.01	0.15	-	-	-
12	15	333	4-hydroxybenzaldehyde	0.01	0.01	0.15	-	-	-
13	15	333	4-dimethylaminobenzaldehyde	-	0.01	0.15	-	-	-
14	15	333	4-dimethylaminobenzaldehyde	0.01	0.01	0.15	-	-	-

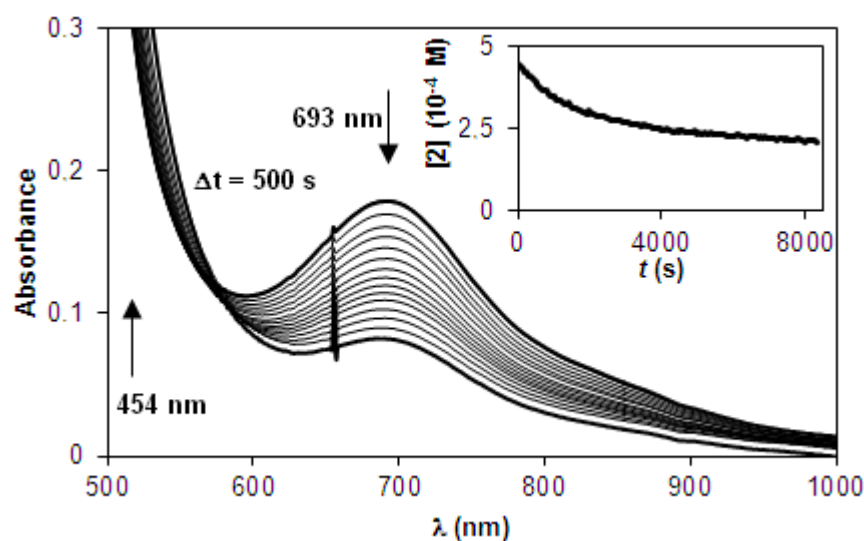


Fig. S9. Visible spectral change for the decay of Fe^{IV}=O species (at 693 nm) derived from the reaction of **1**, benzaldehyde and cyclohexanone in MeCN at 25 °C. Inset: The change of Fe^{IV}=O concentration (at 693 nm) derived from the reaction of Fe^{IV}=O, benzaldehyde and cyclohexanone in MeCN at 25 °C. [1]₀ = 2.00 × 10⁻³ M, [benzaldehyde]₀ = 8.00 × 10⁻² M, [cyclohexanone]₀ = 1.00 × 10⁻¹ M.

II. Fe^{IV}=O formation with O₂ in the presence of aldehydes

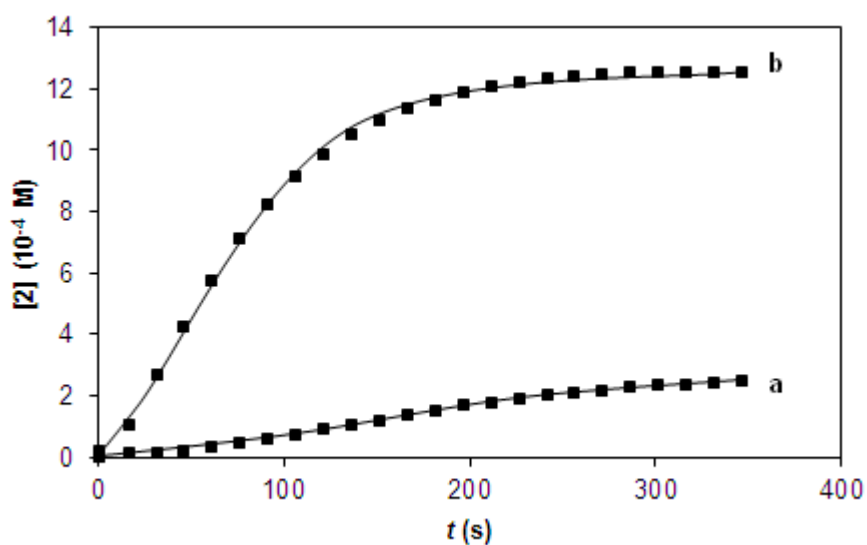


Fig. S10. Fe^{IV}=O formation (at 693 nm) versus time in the reaction of **1** with benzaldehyde (a) and chloroperoxybenzoic acid (b) in MeCN at 25 °C. [1]₀ = 2.00 × 10⁻³ M, [benzaldehyde]₀ = 1.00 × 10⁻² M, [*m*-chloroperoxybenzoic acid]₀ = 1.00 × 10⁻² M.

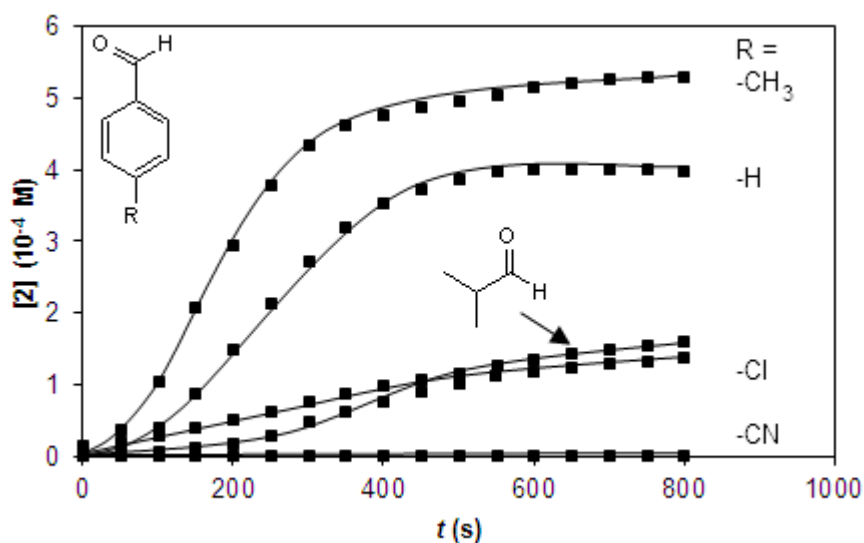


Fig. S11. Formation of Fe^{IV}=O (at 693 nm) versus time in the reaction of **1** with different aldehydes in MeCN at 25 °C. [1]₀ = 2.00 × 10⁻³ M, [aldehyde]₀ = 4.00 × 10⁻² M.

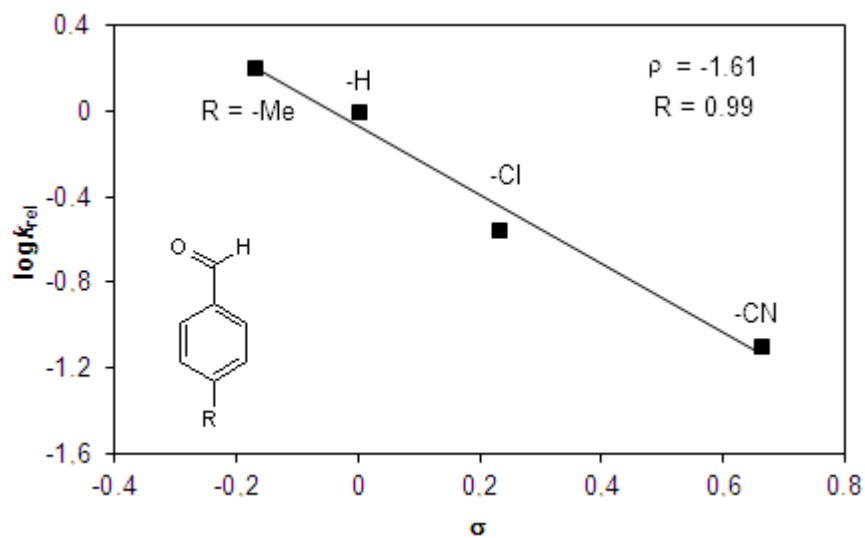


Fig. S12. Hammett plot of para-substituted benzaldehydes in MeCN at 25 °C. $[1]_0 = 2.00 \times 10^{-3}$ M, $[\text{aldehyde}]_0 = 4.00 \times 10^{-2}$ M.

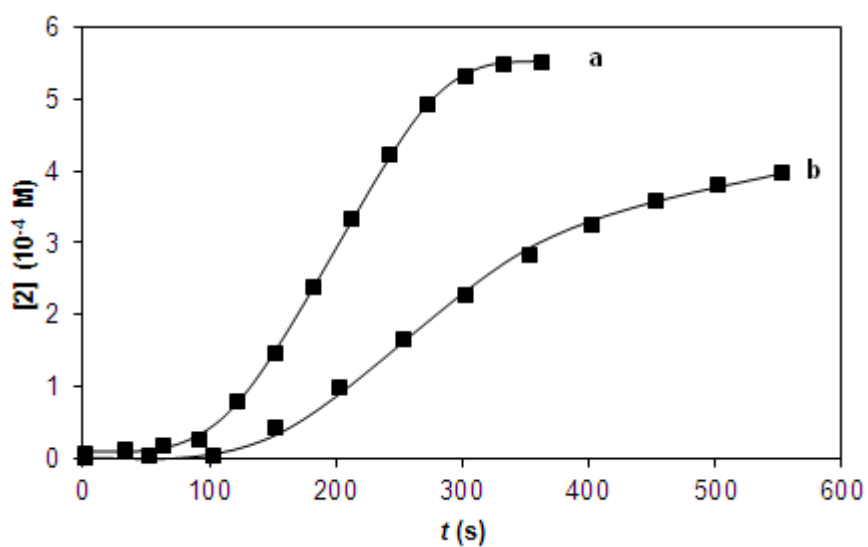


Fig. S13. Formation of $\text{Fe}^{\text{IV}}=\text{O}$ (at 693 nm) versus time in the reaction of **1** with benzaldehyde under oxygen (a) and under air (b) in MeCN at 25 °C. $[1]_0 = 1.00 \times 10^{-3}$ M, $[\text{benzaldehyde}]_0 = 8.00 \times 10^{-2}$ M.

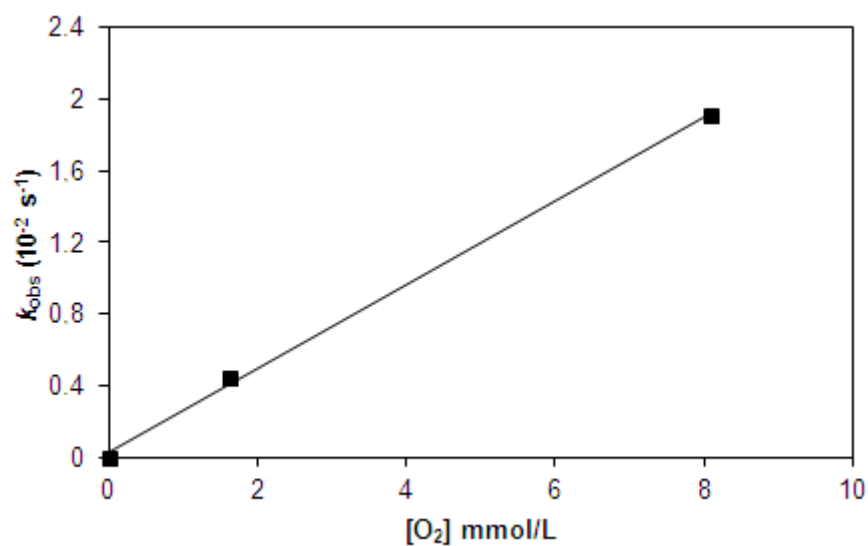


Fig. S14. Reaction rates versus dioxygen concentration in MeCN at 25 °C. $[1]_0 = 1.00 \times 10^{-3}$ M, $[\text{benzaldehyde}]_0 = 8.00 \times 10^{-2}$ M.

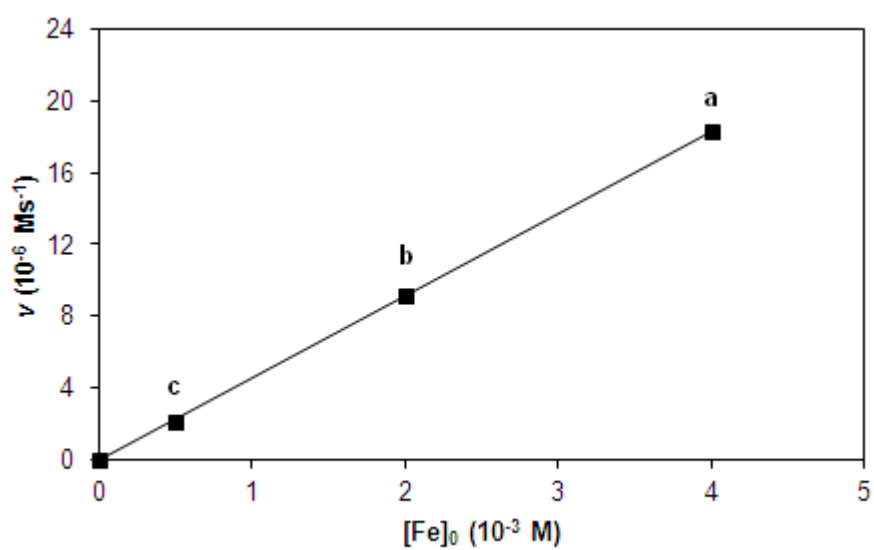


Fig. S15. Reaction rates versus iron concentration in MeCN at 25 °C. $[\text{benzaldehyde}]_0 = 8.00 \times 10^{-2}$ M, $[1]_0 = 4.00 \times 10^{-3}$ M (a); 2.00×10^{-3} M (b); 5.00×10^{-4} M (c).

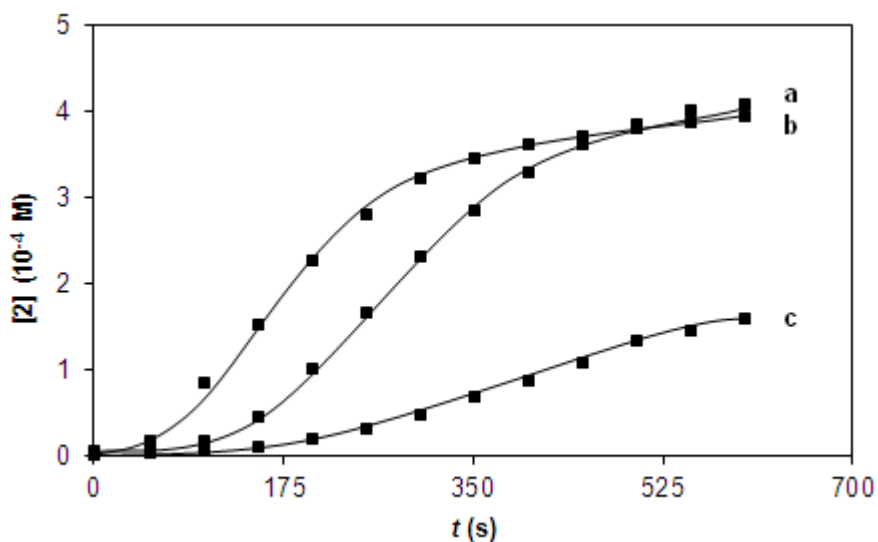


Figure S16. $\text{Fe}^{\text{IV}}=\text{O}$ formation (at 693 nm) versus time in the reaction of **1** with benzaldehyde in MeCN at 25 °C. $[\text{benzaldehyde}]_0 = 8.00 \times 10^{-2} \text{ M}$, $[\mathbf{1}]_0 = 4.00 \times 10^{-3} \text{ M}$ (a); $2.00 \times 10^{-3} \text{ M}$ (b); $5.00 \times 10^{-4} \text{ M}$ (c).

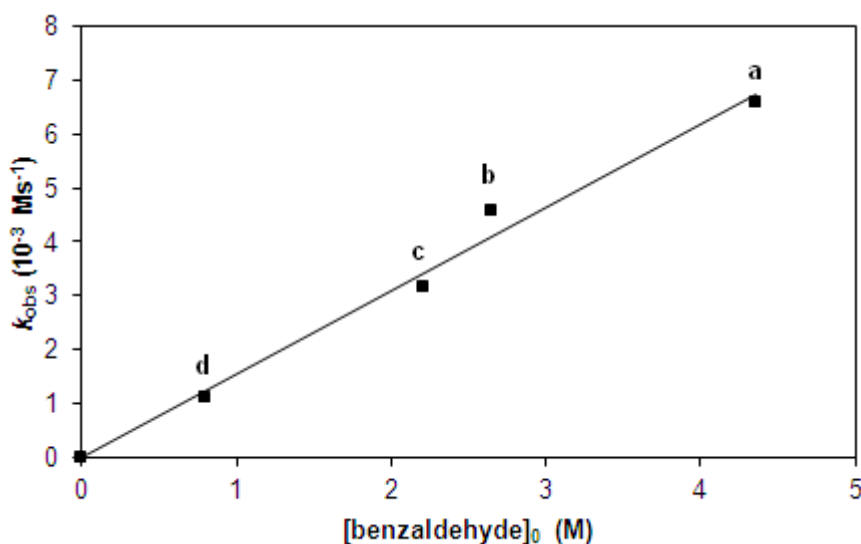


Fig. S17. Observed reaction rates versus benzaldehyde concentration in the reaction of **1** with benzaldehyde in MeCN at 25 °C. $[\mathbf{1}]_0 = 2.00 \times 10^{-3} \text{ M}$, $[\text{benzaldehyde}]_0 = 1.20 \times 10^{-1} \text{ M}$ (a); $8.00 \times 10^{-2} \text{ M}$ (b); $6.00 \times 10^{-2} \text{ M}$ (c); $2.00 \times 10^{-2} \text{ M}$ (d).

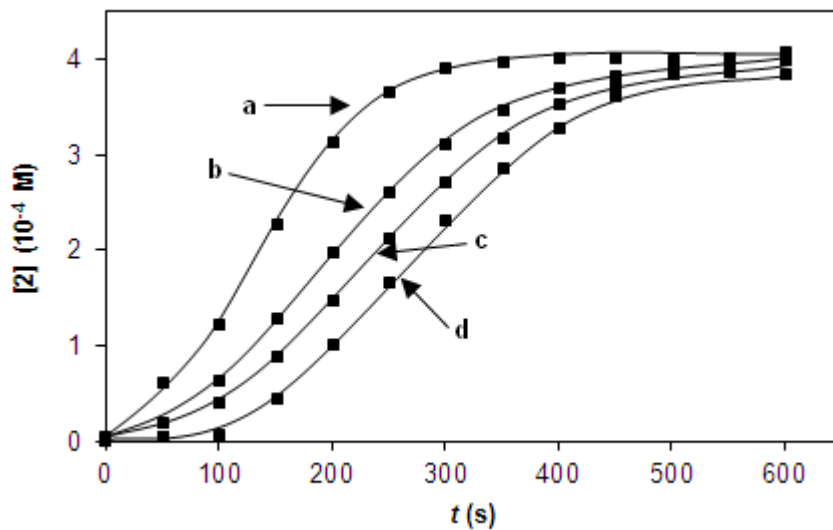


Figure S18. $\text{Fe}^{\text{IV}}=\text{O}$ formation (at 693 nm) versus time in the reaction of **1** with benzaldehyde in MeCN at 25 °C. $[\mathbf{1}]_0 = 2.00 \times 10^{-3} \text{ M}$, $[\text{benzaldehyde}]_0 = 1.20 \times 10^{-1} \text{ M}$ (a); $8.00 \times 10^{-2} \text{ M}$ (b); $6.00 \times 10^{-2} \text{ M}$ (c); $2.00 \times 10^{-2} \text{ M}$ (d).

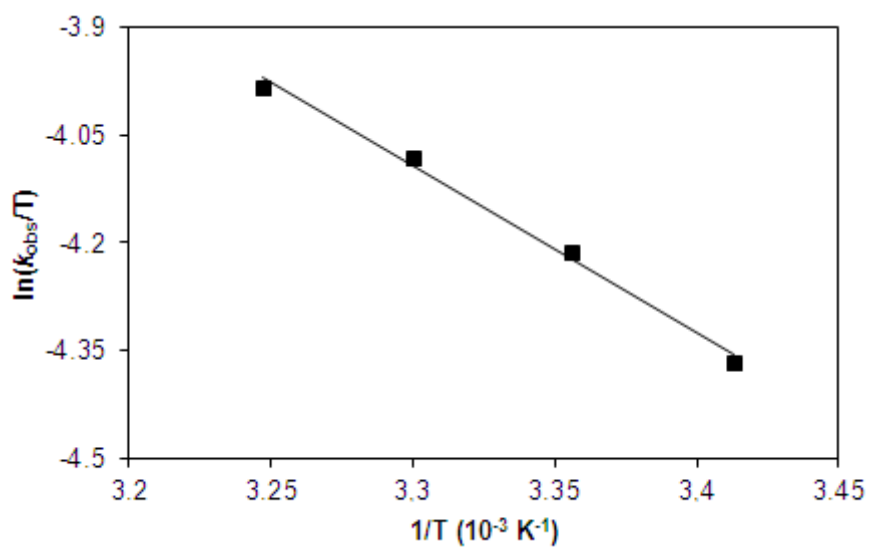


Fig. S19. Eyring plot of of **1** and benzaldehyde in MeCN under O_2 . $[\mathbf{1}]_0 = 2.00 \times 10^{-3} \text{ M}$, $[\text{benzaldehyde}]_0 = 1.20 \times 10^{-1} \text{ M}$.

Table S3. The k_{obs} , k_3 and ν values for the reaction of **1** with different benzaldehyde derivatives in MeCN in cuvette under air.

N ₀	T (K)	aldehyde	[Fe] ₀ (10 ⁻³ M)	[aldehyde] ₀ (10 ⁻² M)	k_{obs} (10 ⁻³ s ⁻¹)	k_3 (M ⁻² s ⁻¹)	ν (10 ⁻⁶ Ms ⁻¹)
1	298	benzaldehyde	0.5	8	4.21	32.48	2.11
2	298	benzaldehyde	1	8	4.39	33.87	4.39
3	298	benzaldehyde	2	8	4.56	35.18	9.12
4	298	benzaldehyde	4	8	4.57	35.26	18.28
5	293	benzaldehyde	2	8	3.14	24.23	6.28
6	303	benzaldehyde	2	8	6.28	48.46	12.56
7	308	benzaldehyde	2	8	7.99	61.65	15.98
8*	298	benzaldehyde	1	8	19.1	29.48	19.10
9	298	benzaldehyde	2	2	1.12	34.57	2.24
10	298	benzaldehyde	2	6	3.15	32.41	6.30
11	298	benzaldehyde	2	12	6.58	33.85	13.16
12	298	isobutyraldehyde	2	4	0.97	14.96	1.94
13	298	4-methylbenzaldehyde	2	4	5.23	80.71	10.46
14	298	4-chlorobenzaldehyde	2	4	0.55	8.49	1.10
15	298	4-cyanobenzaldehyde	2	4	0.05	0.69	0.093

*under O₂ atmosphere

III. $\text{Fe}^{\text{IV}}=\text{O}$ mediated Baeyer-Villiger oxidation of cyclohexanones

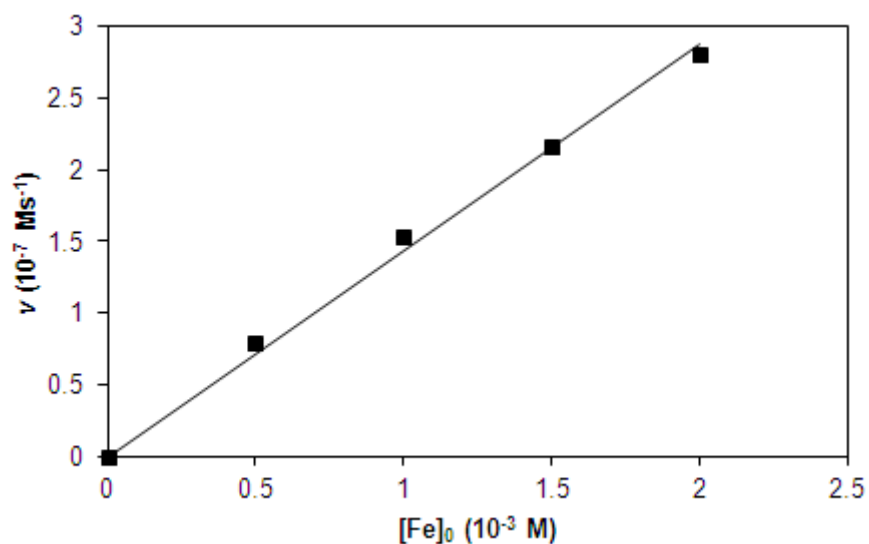


Fig. S20. Dependence on the reaction rate values on the iron concentrations for the decay of **2**, in the presence of cyclohexanone MeCN at 25 °C: $[\text{PhIO}]_0 = 4.00 \times 10^{-3} \text{ M}$, $[\text{cyclohexanone}]_0 = 1.00 \times 10^{-1} \text{ M}$.

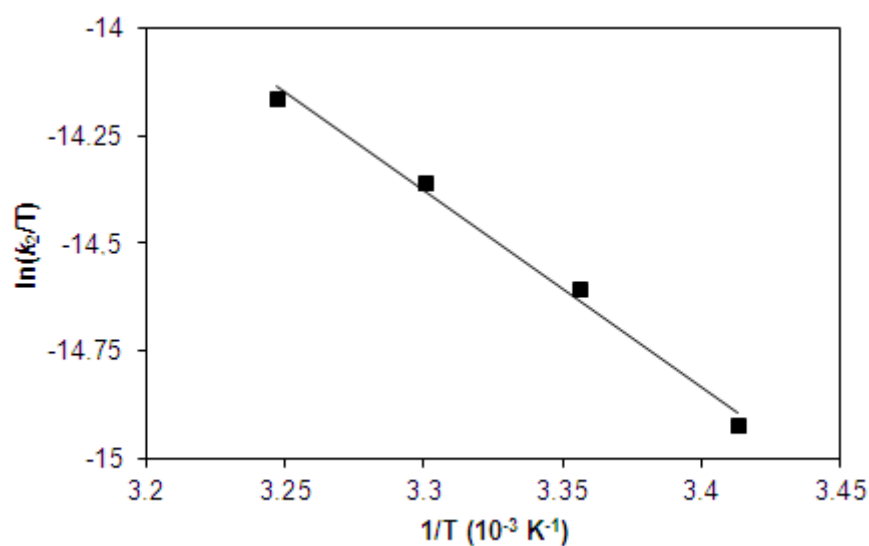


Fig. S21. Eyring plot of the reaction of **1** and cyclohexanone in MeCN. $[\mathbf{1}]_0 = 2.00 \times 10^{-3} \text{ M}$, $[\text{PhIO}]_0 = 4.00 \times 10^{-3} \text{ M}$, $[\text{cyclohexanone}]_0 = 1.00 \times 10^{-1} \text{ M}$.

Table S4. The k_{obs} and k_2 values for the reaction of **1** with cyclohexanone derivatives in MeCN in cuvette under air.

N ₀	T (K)	substrate	[Fe] ₀ (10 ⁻³ M)	[S] ₀ (M)	k_{obs} (10 ⁻⁴ s ⁻¹)	k_2 (10 ⁻³ M ⁻¹ s ⁻¹)	ν (10 ⁻⁷ Ms ⁻¹)
1	298	cyclohexanone	0.5	0.1	1.59	1.59	0.80
2	298	cyclohexanone	1	0.1	1.53	1.53	1.53
3	298	cyclohexanone	1.5	0.1	1.44	1.44	2.16
4	298	cyclohexanone	2	0.1	1.35	1.35	2.70
5	293	cyclohexanone	2	0.1	0.97	0.97	1.94
6	303	cyclohexanone	2	0.10	1.76	1.76	3.52
7	308	cyclohexanone	2	0.10	2.18	2.18	4.36
8	298	cyclohexanone	2	0.15	2.41	1.60	4.82
9	298	cyclohexanone	2	0.20	3.02	1.51	6.03
10	298	cyclohexanone	2	0.25	3.82	1.53	7.64
11	298	2-methyl-cyclohexanone	2	0.10	1.03	1.03	2.06
12	298	2-methyl-cyclohexanone	2	0.15	1.66	1.10	3.32
13	298	2-methyl-cyclohexanone	2	0.20	1.99	1.00	3.98
14	298	2-methyl-cyclohexanone	2	0.25	2.61	1.04	5.22
15	298	3-methyl-cyclohexanone	2	0.10	0.28	0.28	0.56
16	298	3-methyl-cyclohexanone	2	0.15	0.37	0.25	0.74
17	298	3-methyl-cyclohexanone	2	0.20	0.49	0.25	0.98
18	298	3-methyl-cyclohexanone	2	0.25	0.63	0.25	1.25
15	298	4-methyl-cyclohexanone	2	0.10	0.86	0.86	1.71
16	298	4-methyl-cyclohexanone	2	0.15	1.28	0.86	2.56
17	298	4-methyl-cyclohexanone	2	0.20	1.81	0.91	3.62
18	298	4-methyl-cyclohexanone	2	0.25	2.23	0.89	4.46
19	298	4- <i>tert</i> -butyl-cyclohexanone	2	0.10	0.40	0.40	0.80
20	298	4- <i>tert</i> -butyl-cyclohexanone	2	0.15	0.73	0.48	1.46
21	298	4- <i>tert</i> -butyl-cyclohexanone	2	0.20	0.89	0.45	1.78
22	298	4- <i>tert</i> -butyl-cyclohexanone	2	0.25	1.17	0.47	2.34