Supplementary Material (ESI) for Chemical Communications

Supplementary material for the paper

Manganese and iron flavonolates as flavonol 2,4-dioxygenase mimics

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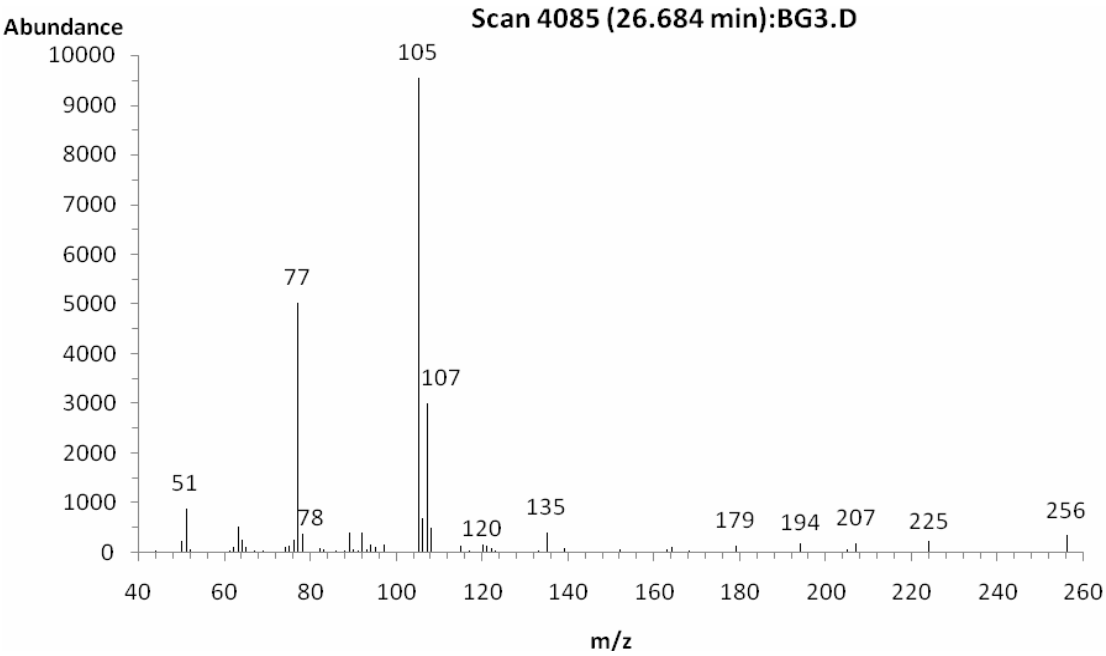
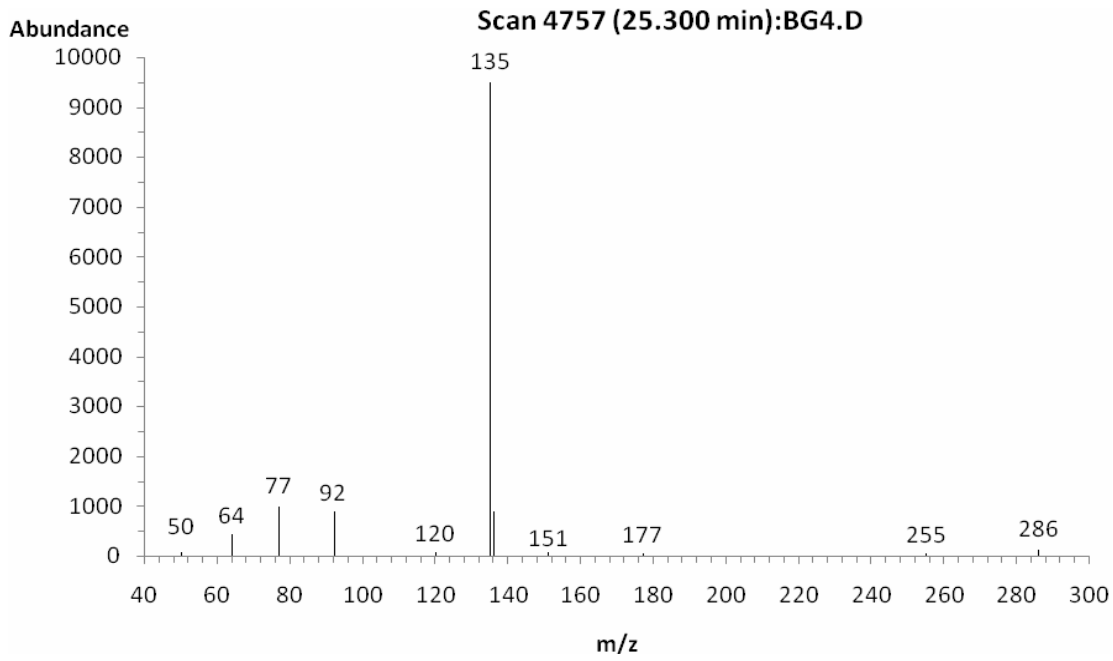
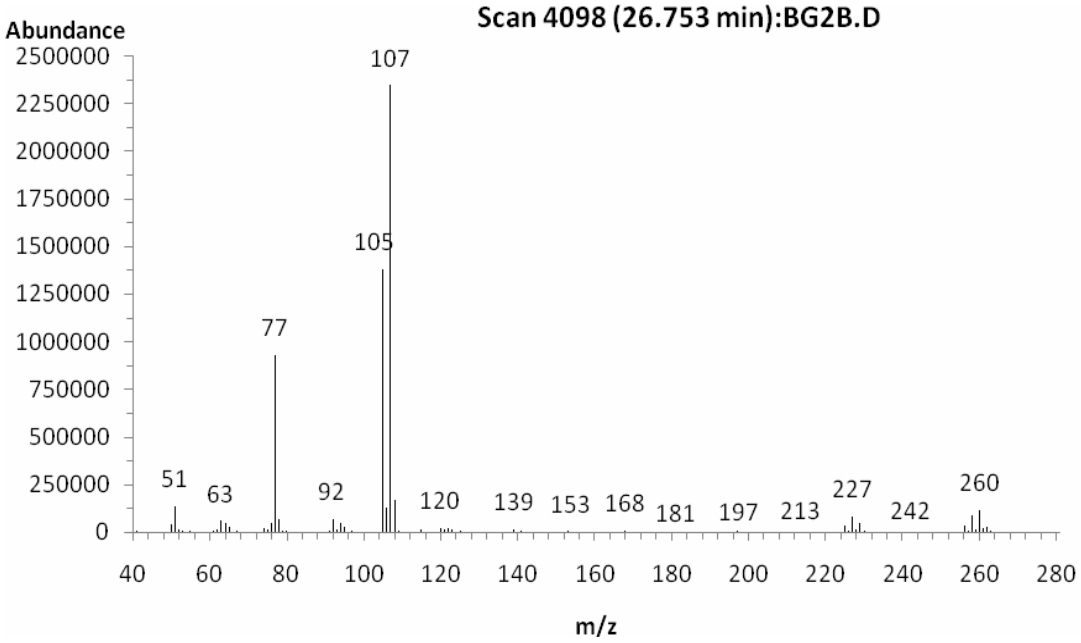
SFigure 1. MS spectrum of the *O*-benzoylsalicylic acid methylester as a main product of the dioxygenation of $[Mn^{II}(fla)_2(py)_2]$ (**1**) under $^{16}O_2$ atmosphere



SFigure 2. MS spectrum of the 4'-methoxy-*O*-benzoylsalicylic acid methylester as a main product of the dioxygenation of [Fe^{III}(4'-MeOfla)$_3$] (**2**) under $^{16}O_2$ atmosphere



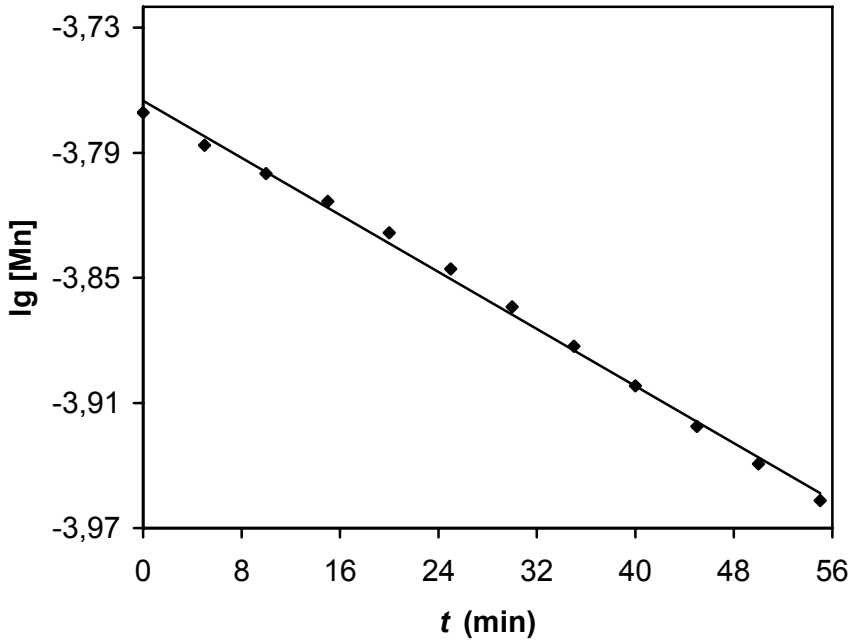
SFigure 3. MS spectrum of the *O*-benzoylsalicylic acid methylester as a main product of the dioxygenation of $[Mn^{II}(fla)_2(py)_2]$ (**1**) under $^{18}O_2$: $^{16}O_2$ (60 : 40%) atmosphere



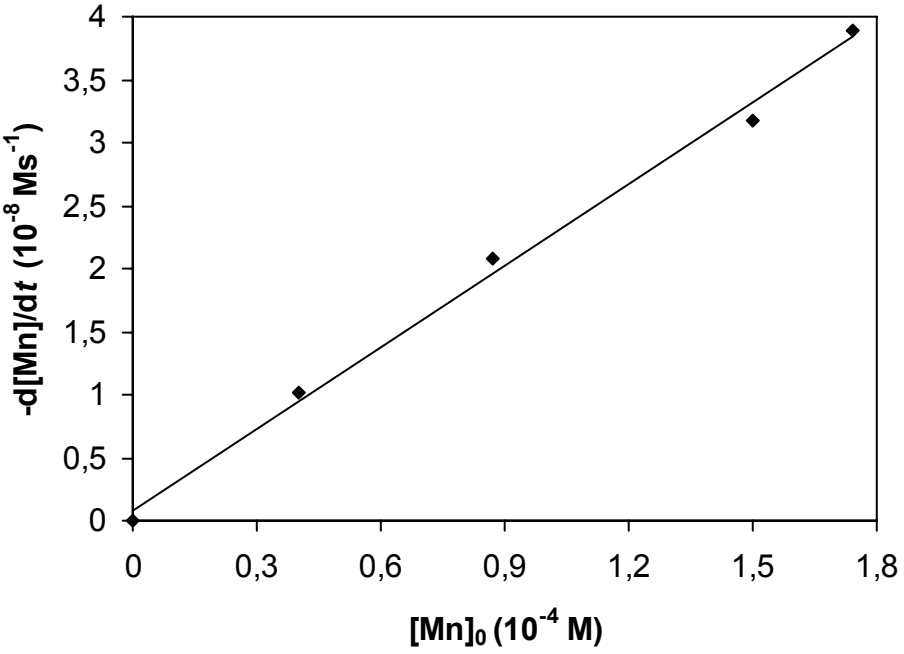
STable 1. Kinetic data for the stoichiometric dioxygenation of $[Mn^{II}(fla)_2(py)_2]$ (**1**) in DMF solution

Expt.[a] **no.**	**Temp (°C)**	**10^4[1]**[a] **mol dm^{-3}**	**10^3[O_2] mol dm^{-3}**	**10^{-8}-d[1]/dt mol dm^{-3} s^{-1}**	***k*** **s^{-1} mol^{-1} dm^3**
1	110	0.40	1.69	1.01	0.15±0,007
2	110	0.87	1.69	2.14	0.15±0,007
3	110	1.50	1.69	3.18	0.13±0,005
4	110	1.74	1.69	3.89	0.13±0,006
5	110	1.50	4.03	6.01	0.10±0,004
6	110	1.50	8.45	11.9	0.09±0,004
7	100	1.50	1.64	1.96	0.08±0,003
8	105	1.50	1.65	2.36	0.09±0,005
9	115	1.50	1.65	3.69	0.15±0,006

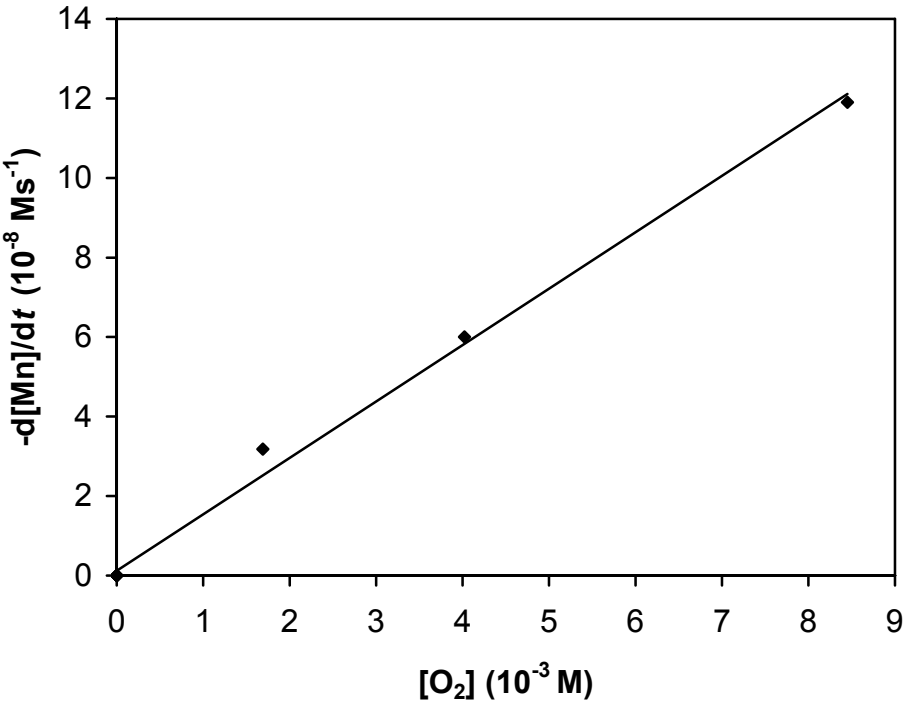
[a]In 50 mL of DMF



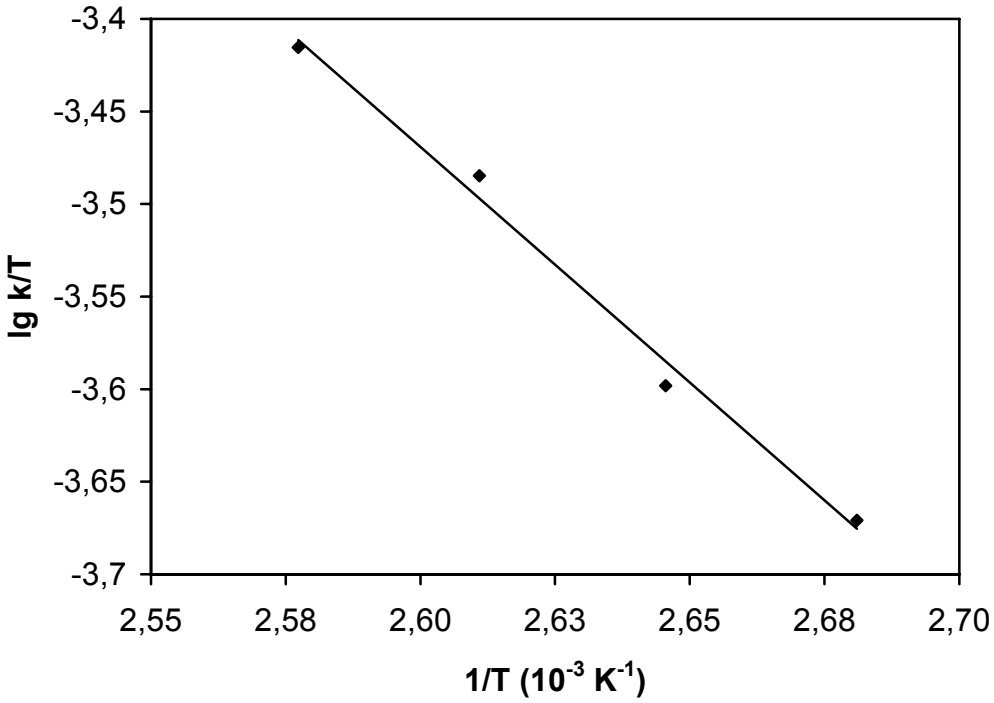
SFigure 4. Plot of log $[Mn^{II}(fla)_2(py)_2]$ (**1**) versus time in DMF: $[Mn^{II}(fla)_2(py)_2]_0 = 1.50 \times 10^{-4}$; $[O_2] = 1.64 \times 10^{-3}$ M; DMF; T = 100 °C



SFigure 5. Plot of oxygenation rate of $[Mn^{II}(fla)_2(py)_2]$ (**1**) versus its initial concentration in DMF: $[O_2] = 1.69 \times 10^{-3}$ M; DMF; T = 110 °C



SFigure 6. Plot of oxygenation rate of $[Mn^{II}(fla)_2(py)_2]$ (**1**) versus initial concentration of dioxygen in DMF: $[Mn^{II}(fla)_2(py)_2]_0 = 1.50 \times 10^{-4}$ M, DMF, T = 110 °C

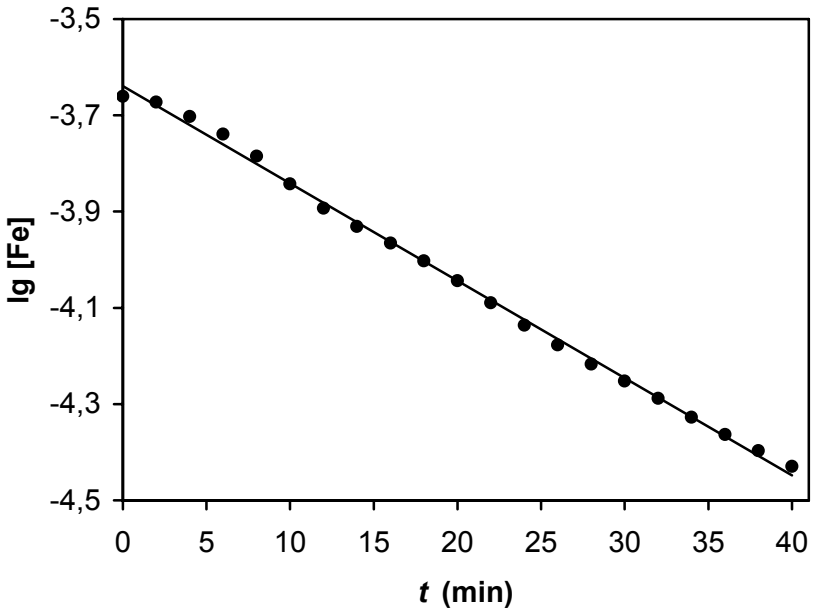


SFigure 7. Eyring plot for the dioxygenation of $[Mn^{II}(fla)_2(py)_2]$ (**1**): $[Mn^{II}(fla)_2(py)_2]_0 = 1.50 \times 10^{-4}$ M, DMF

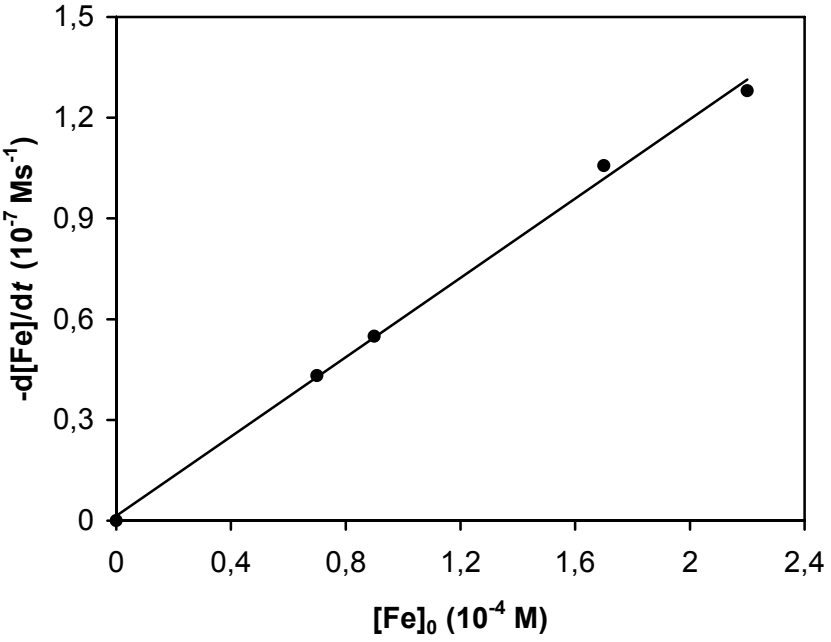
STable 2. Kinetic data for the stoichiometric dioxygenation of [Fe^{III}(4'-MeOfla)$_3$] (**2**) in DMF solution

Expt.[a] **no.**	**Temp (°C)**	**10^4[2]**[a] **mol dm^{-3}**	**10^3[O_2] mol dm^{-3}**	**10^{-7}-d[2]/dt mol dm^{-3} s^{-1}**	***k*** **s^{-1} mol^{-1} dm^3**
1	90	2.2	1.56	1.28	0.37±0.019
2	90	1.7	1.56	1.05	0.39±0.018
3	90	0.9	1.56	0.54	0.39±0.017
4	90	0.7	1.56	0.43	0.39±0.019
5	90	2.2	3.72	3.33	0.40±0.021
6	90	2.2	7.44	6.28	0.38±0.020
7	80	2.2	1.45	1.11	0.25±0.011
8	85	2.2	1.56	1.23	0.28±0.013
9	95	2.2	1.61	1.38	0.44±0.021

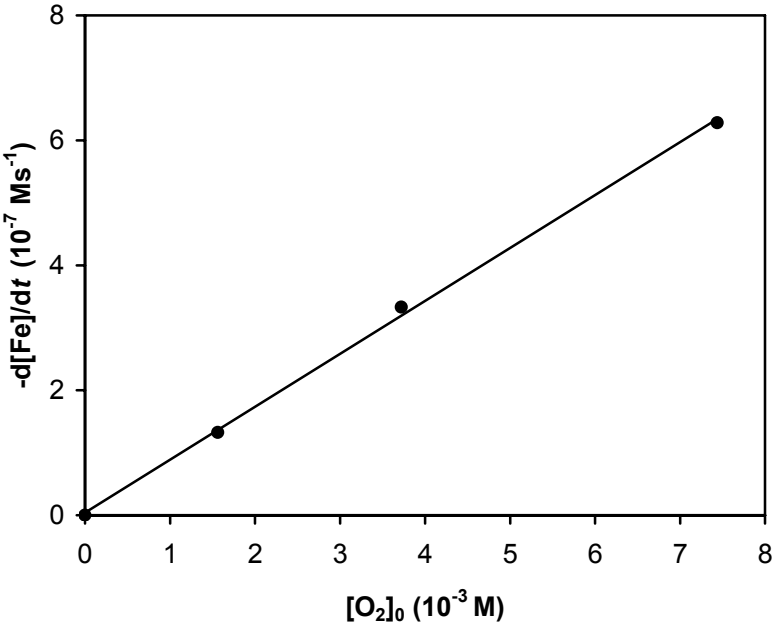
[a]In 50 mL of DMF



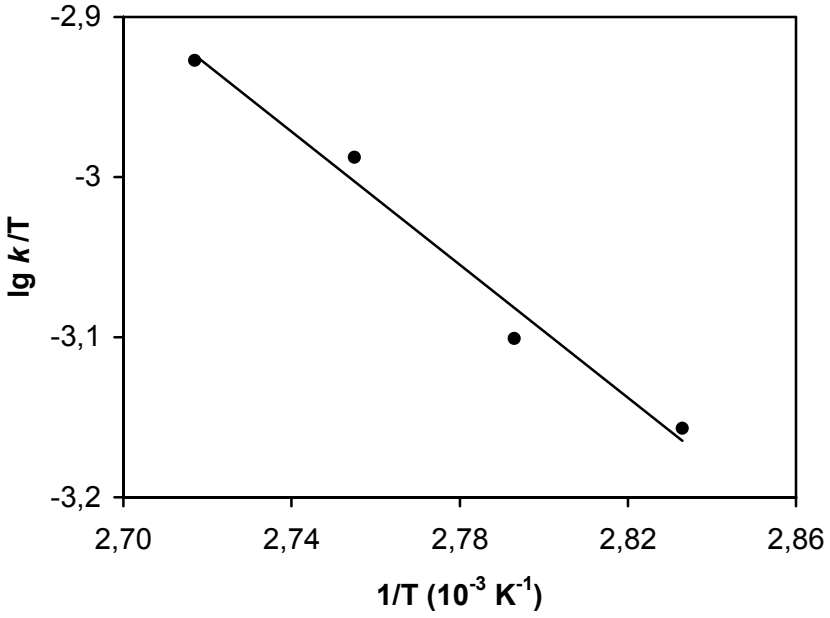
SFigure 8. Plot of log [Fe^{III}(4'-MeOfla)$_3$] (**2**) versus time in DMF: [Fe^{III}(4'-MeOfla)$_3$]$_0$ = 2.20 × 10^{-4} M; [O_2] = 1.56 ×10^{-3} M; DMF; T = 90 °C



SFigure 9. Plot of oxygenation rate of [Fe^{III}(4'-MeOfla)$_3$] (**2**) versus its initial concentration in DMF: [O_2] = 1.56 × 10^{-3} M; DMF; T = 90 °C



SFigure 10. Plot of oxygenation rate of [Fe^{III}(4'-MeOfla)$_3$] (**2**) versus initial concentration of dioxygen in DMF: [Fe^{III}(4'-MeOfla)$_3$]$_0$ = 2.20 ×10^{-4} M; DMF; T = 90 °C



SFigure 11. Eyring plot for the dioxygenation of $[Fe^{III}(4'\text{-MeOfla})_3]$ (**2**): $[Fe^{III}(4'\text{-MeOfla})_3]_0 = 2.20 \times 10^{-4}$ M, DMF