

Electronic Supplementary Information

Oxygenase mimicking immobilized iron complex catalysts for alkane hydroxylation with H₂O₂

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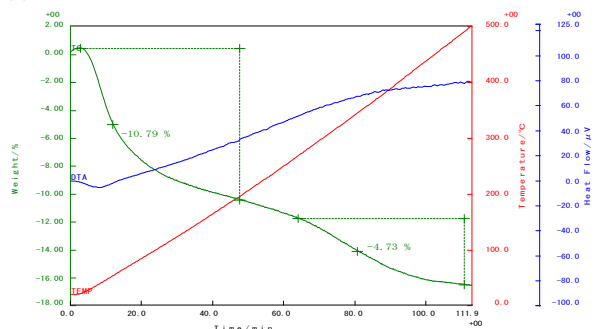
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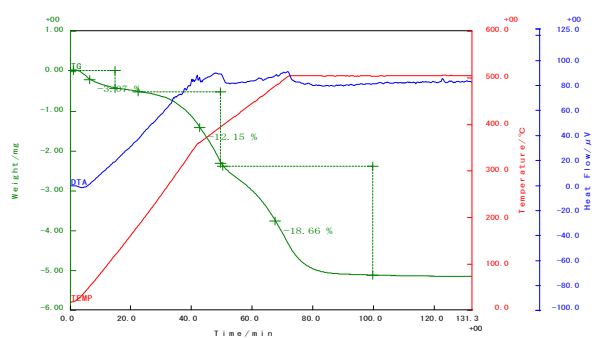
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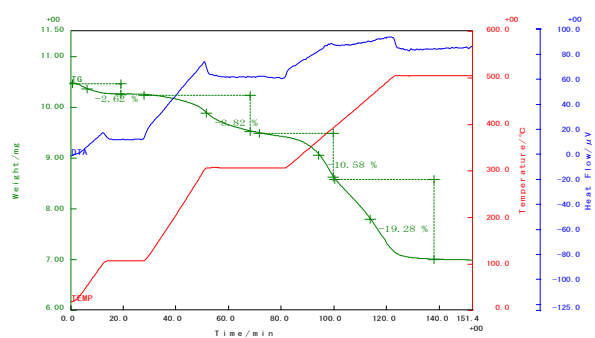
(a) L-SBA



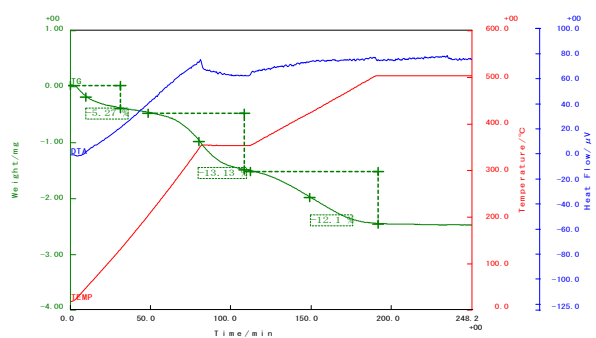
(b-1) L-SBA-FC(8)



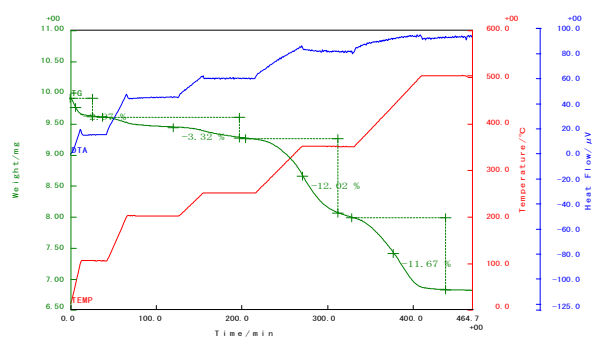
(b-2) L-SBA-FC(8)TMS



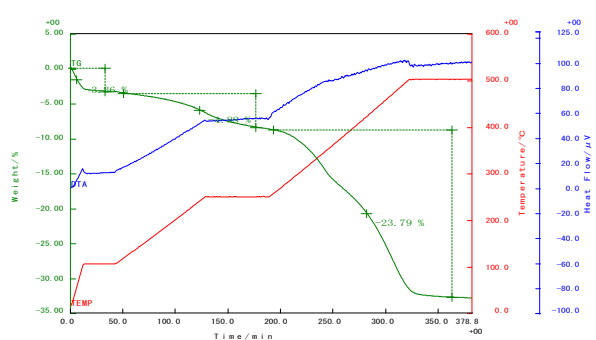
(c-1) L-SBA-FC(6)



(c-2) L-SBA-FC(6)TMS



(d-1) L-SBA-FC(4)



(d-2) L-SBA-FC(6)TMS

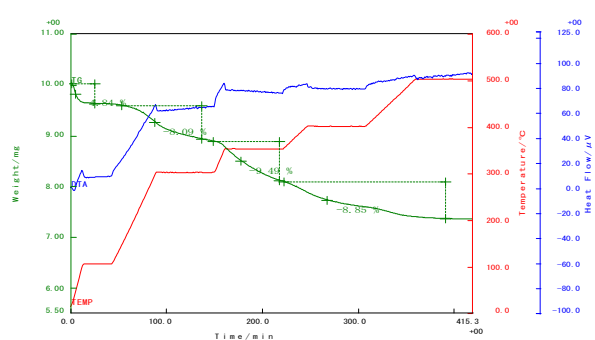
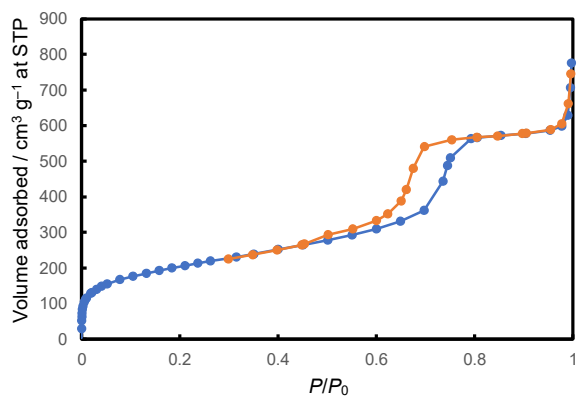
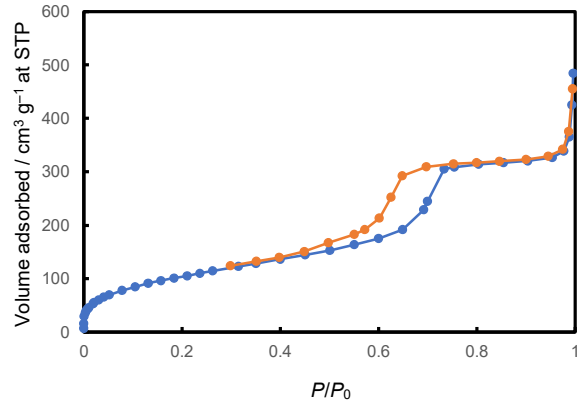


Fig. S1 TG curves of the supports.

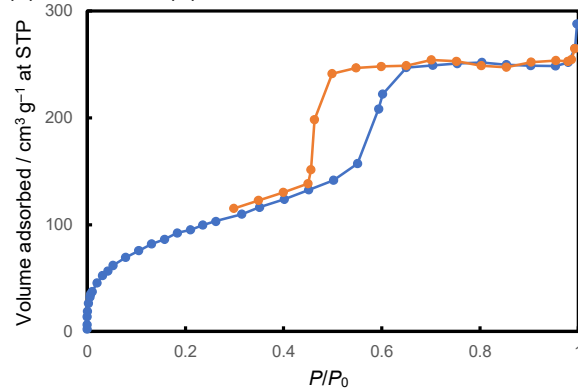
(a) N₃-SBA



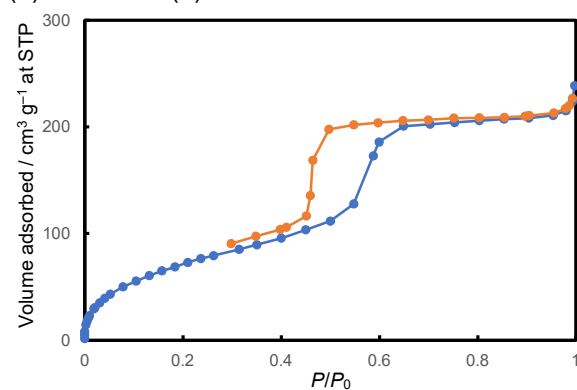
(b) L-SBA



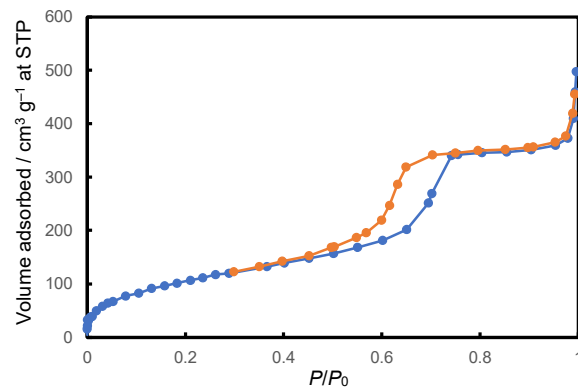
(c) L-SBA-FC(8)



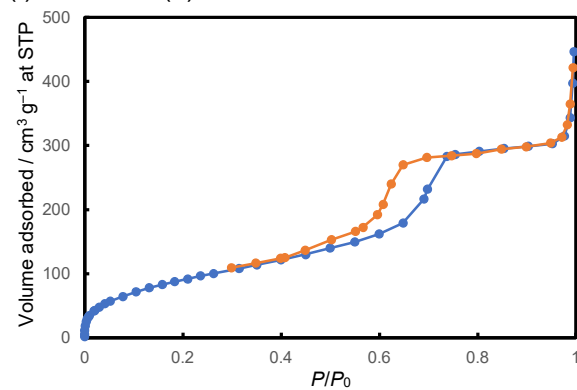
(d) L-SBA-FC(8)TMS



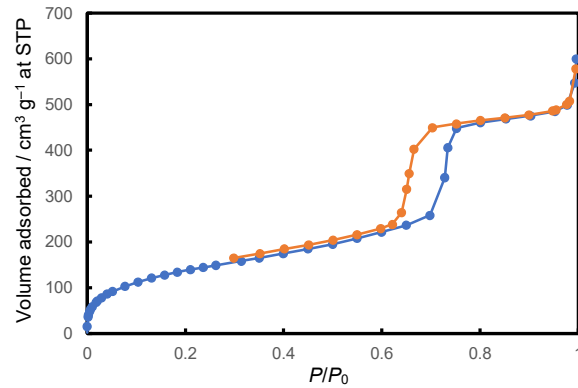
(e) L-SBA-FC(6)



(f) L-SBA-FC(6)TMS



(g) L-SBA-FC(4)



(h) L-SBA-FC(4)TMS

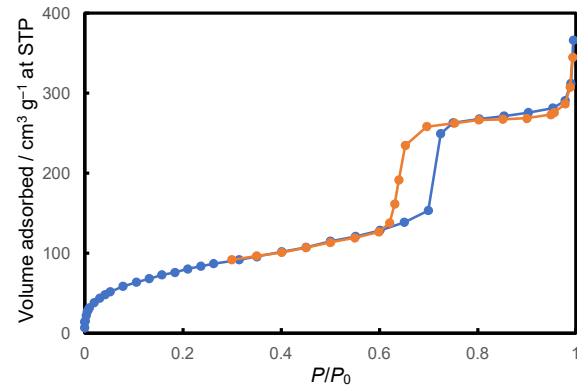


Fig. S2 N₂ isotherm adsorption curves of the supports.

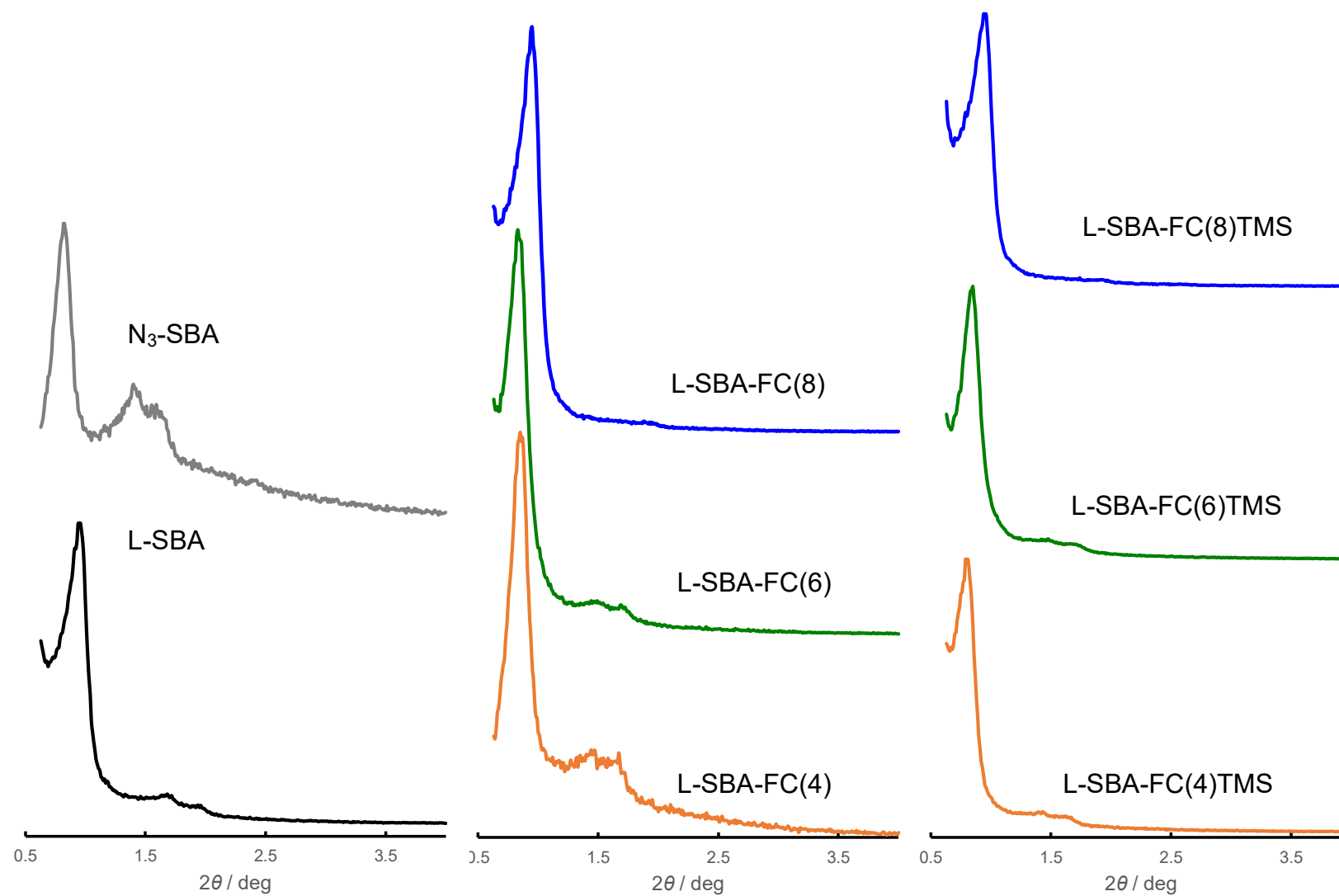


Fig. S3 PXRD of the supports.

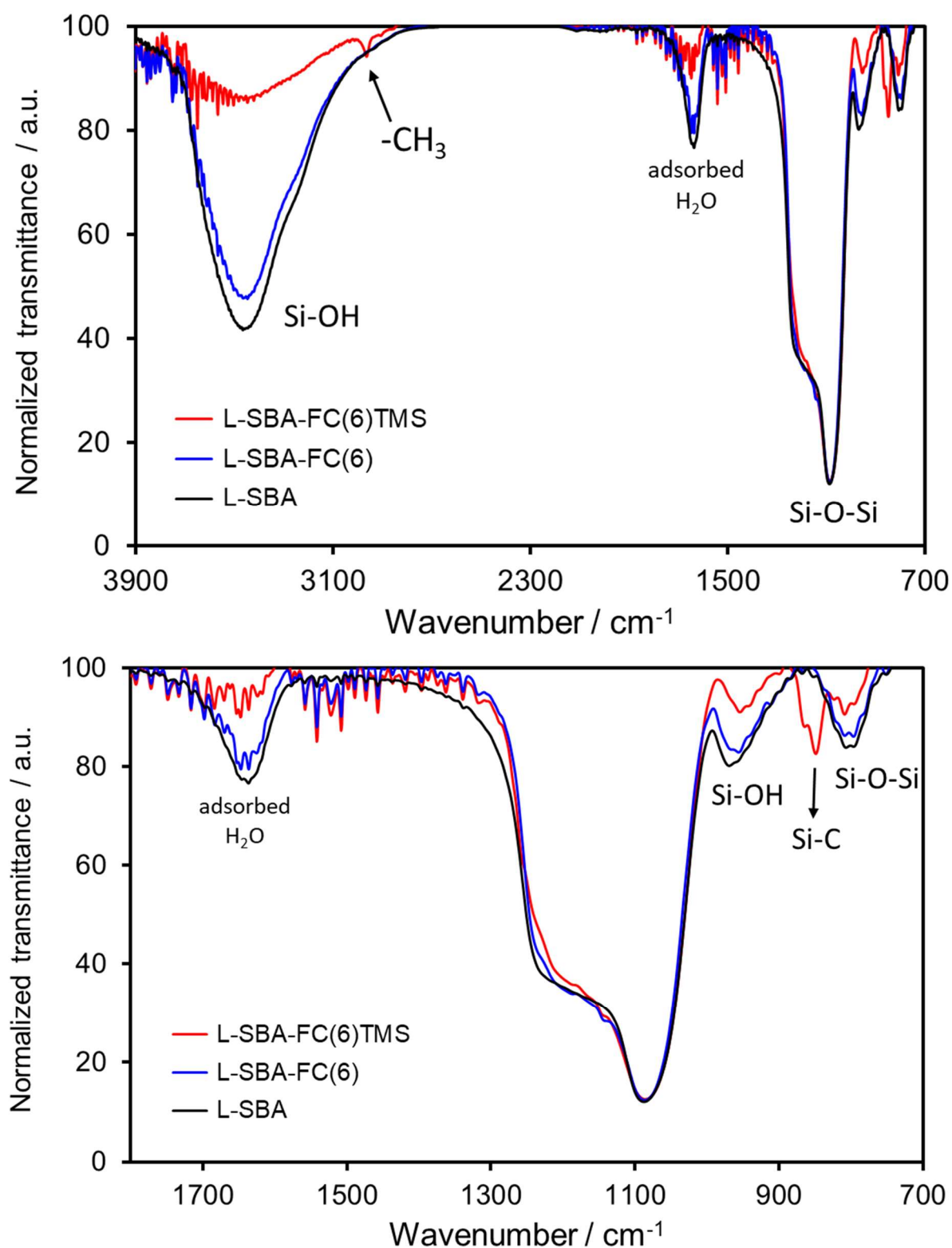


Fig. S4 IR spectra of L-SBA, L-SBA-FC(6) and L-SBA-FC(6)TMS.

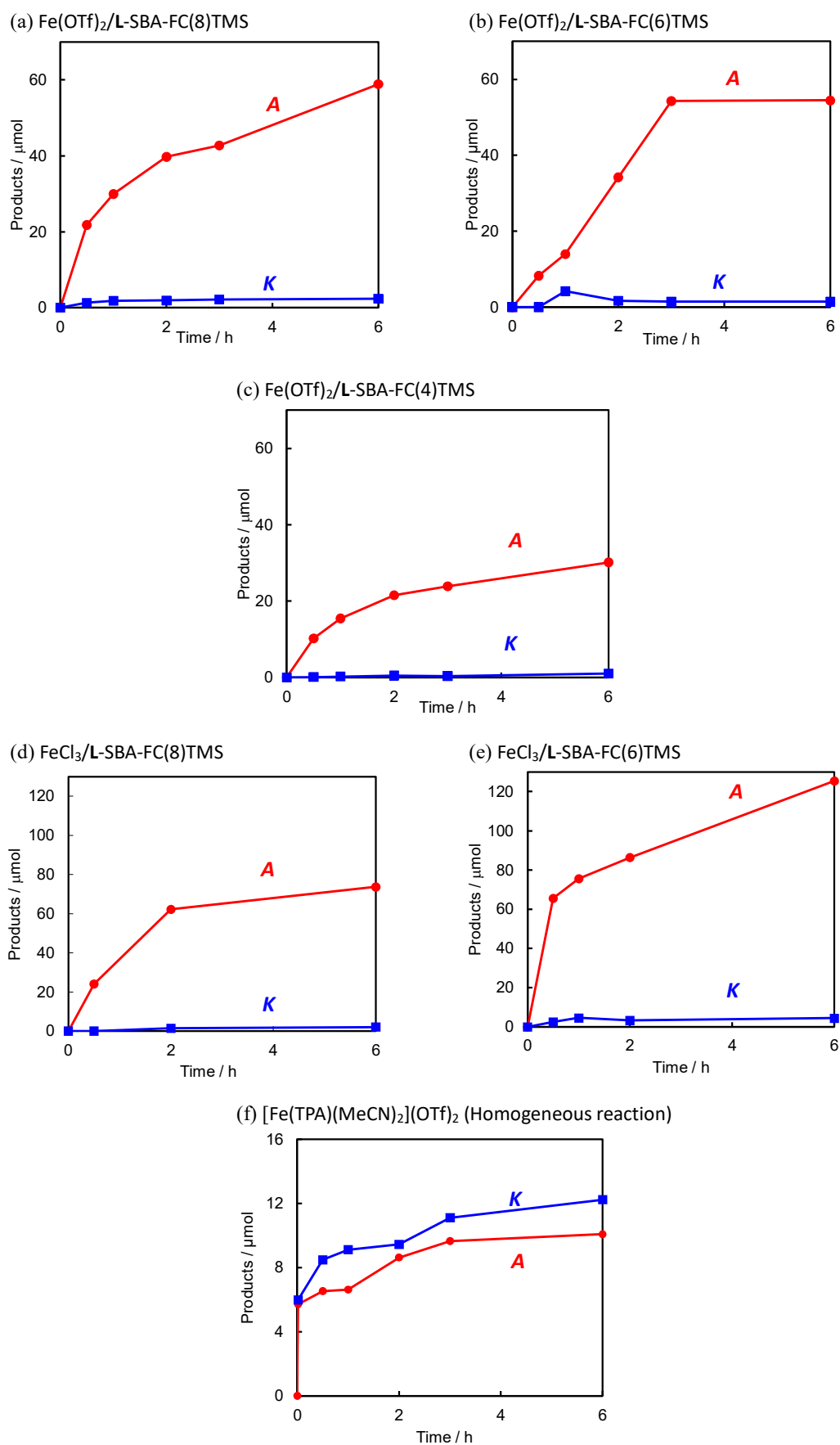
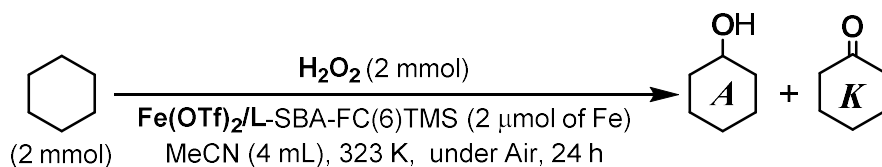


Fig. S5 Time course of the cyclohexane oxidation with H_2O_2 catalyzed by $\text{Fe}(\text{OTf})_2/\text{L-SBA-FC}(n)\text{TMS}$ ($n = 8$ (a), 6 (b), and 4 (c)), $\text{FeCl}_3/\text{L-SBA-FC}(n)\text{TMS}$ ($n = 8$ (d) and 6 (e)), and $[\text{Fe}(\text{TPA})(\text{MeCN})_2](\text{OTf})_2$ (homogeneous reaction, (f)).

Table S1 Recycle test for Fe(OTf)₂/L-SBA-FC(6)TMS



Trial	Products / TON		<i>A</i> / <i>K</i>	Relative activity
	<i>A</i>	<i>K</i>		
First	39.2	1.4	28.5	1
Second	32.9	3.1	10.5	0.89
Third	32.9	3.1	10.5	0.89

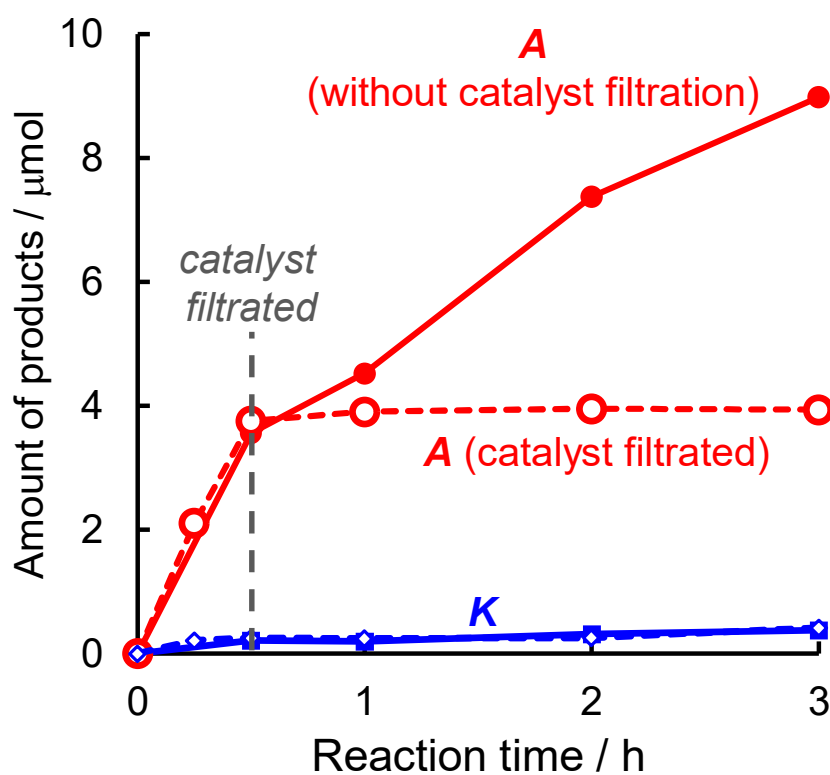
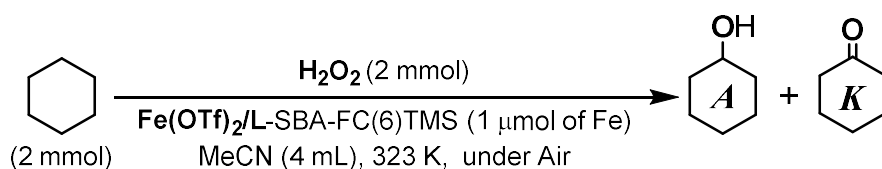
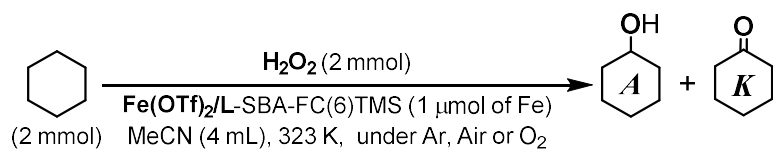


Fig. S6 Catalyst filtration test.

Table S2 Cyclohexane oxidation catalyzed by $\text{Fe}(\text{OTf})_2/\text{L-SBA-FC(6)TMS}$ under various under different atmospheres (argon, air, O_2).



Reaction Time /h	under Ar			under Air			under O_2		
	Yield / μmol		A / K	Yield / μmol		A / K	Yield / μmol		A / K
	A	K		A	K		A	K	
0.5	1.27	0.28	4.5	3.56	0.21	16.9	2.71	0.30	9.0
1	4.44	0.29	15.2	4.52	0.20	22.5	4.39	0.34	13.0
2	7.02	0.46	15.4	7.37	0.32	23.3	6.97	0.44	15.8
3	9.07	0.50	18.2	8.98	0.38	23.6	8.83	0.48	18.3
6	13.33	0.57	23.4	12.14	0.42	29.0	12.06	0.63	19.0

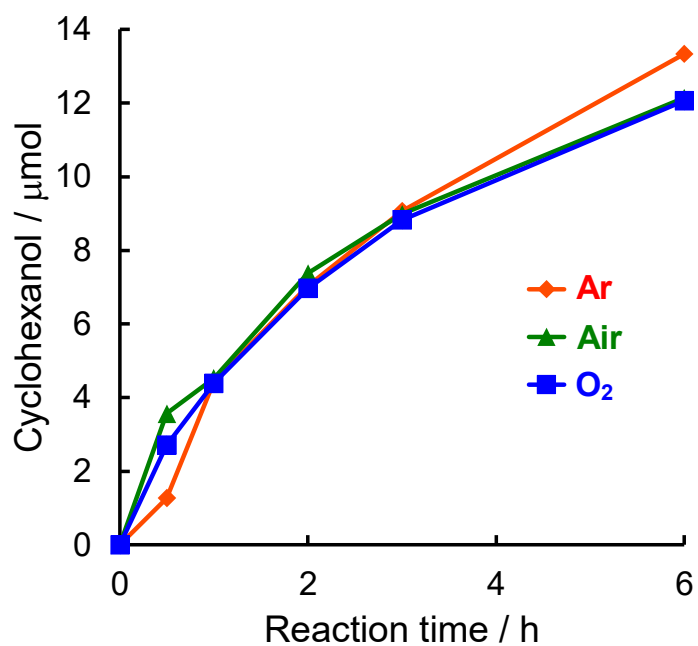


Fig. S7 Time course of the cyclohexanol production catalyzed by $\text{Fe}(\text{OTf})_2/\text{L-SBA-FC(6)TMS}$.

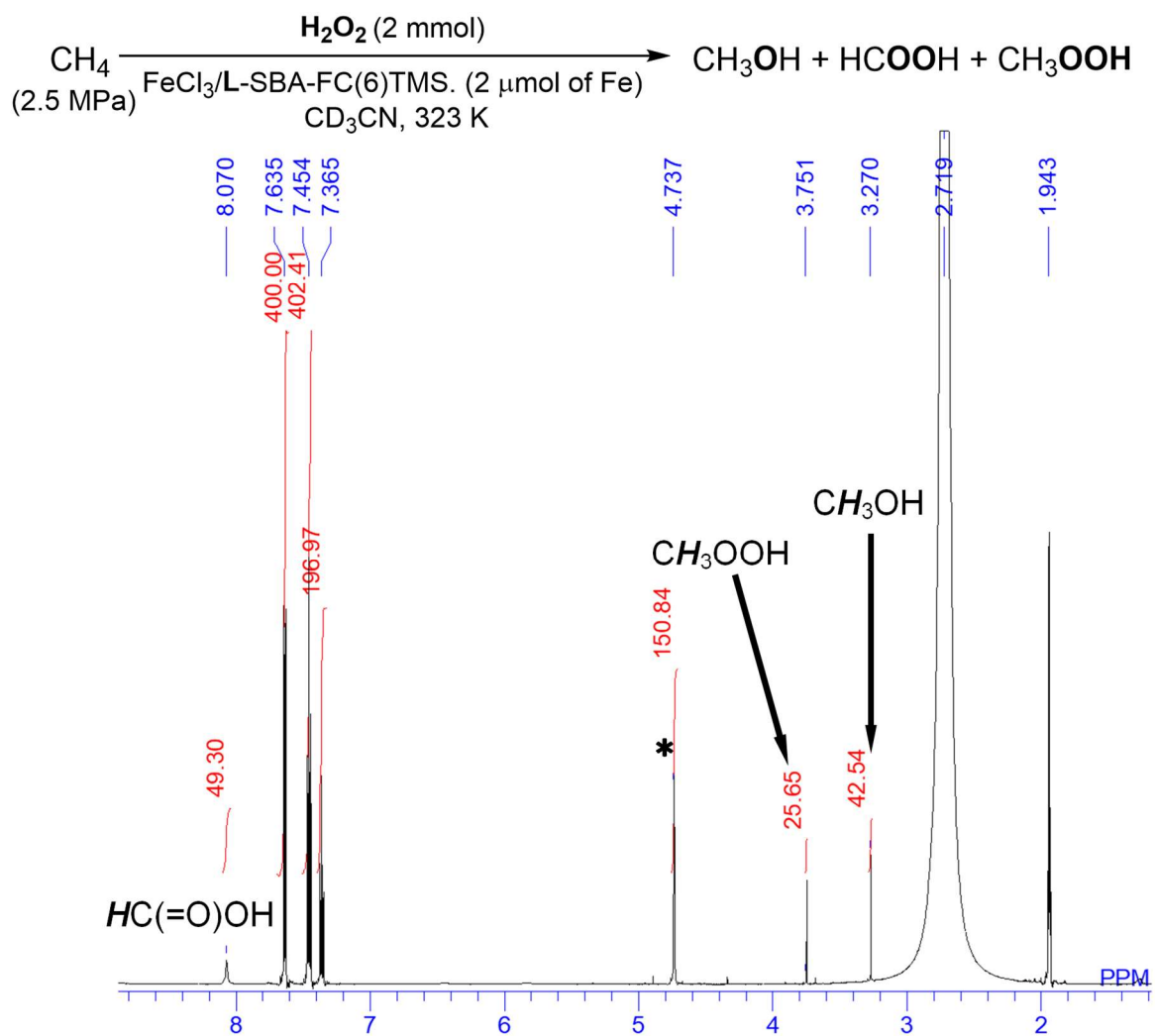


Fig. S8 ^1H NMR spectrum of the reaction solution of methane oxidation with H_2O_2 catalyzed by $\text{FeCl}_3/\text{L-SBA-FC(6)TMS}$.