Electronic Supporting Information

Photocatalytic selective oxidation of terminal methyl group of dodecane with molecular oxygen over Ti atom dispersed mesoporous TiO$_2$-SiO$_2$ mixed oxides

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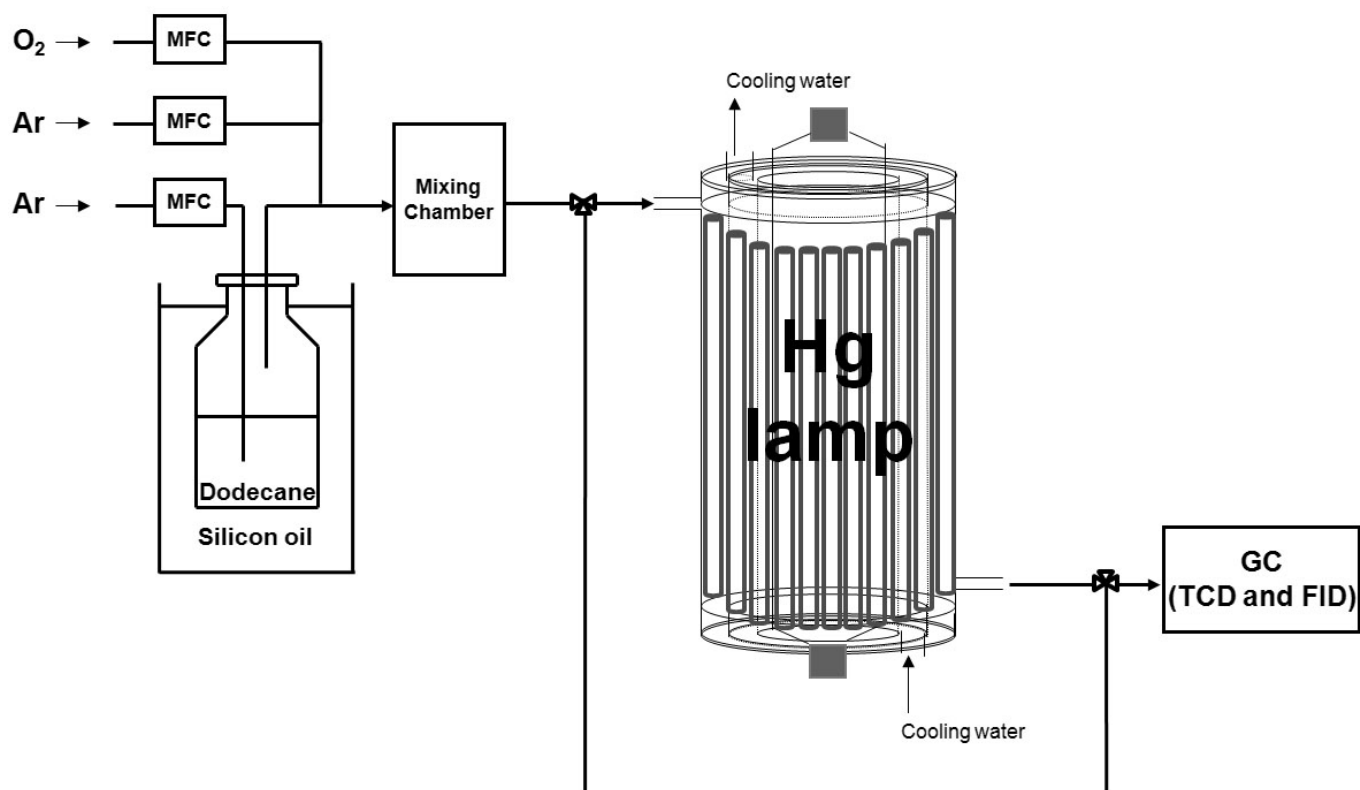
Fig. S1. A lab scale continuous flow system for photocatalytic partial oxdiation of dodecane.
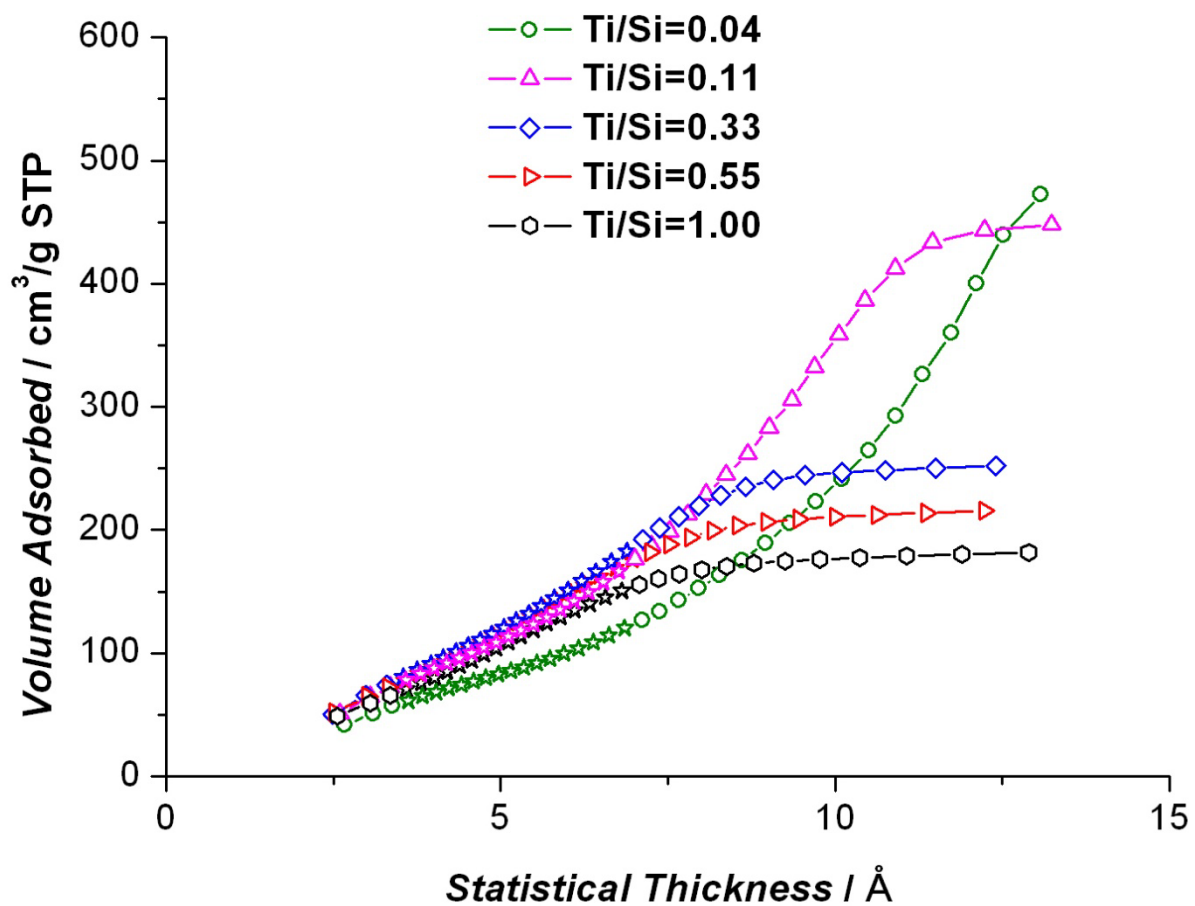Temperature of water for UV-Vis light cooling was 80 °C.

Fig. S2. Profiles based on t-plot method to investigate microporosity of TiO_2-SiO_2 mixed oxide. ☆ indicates parameter ranges for extrapolation.
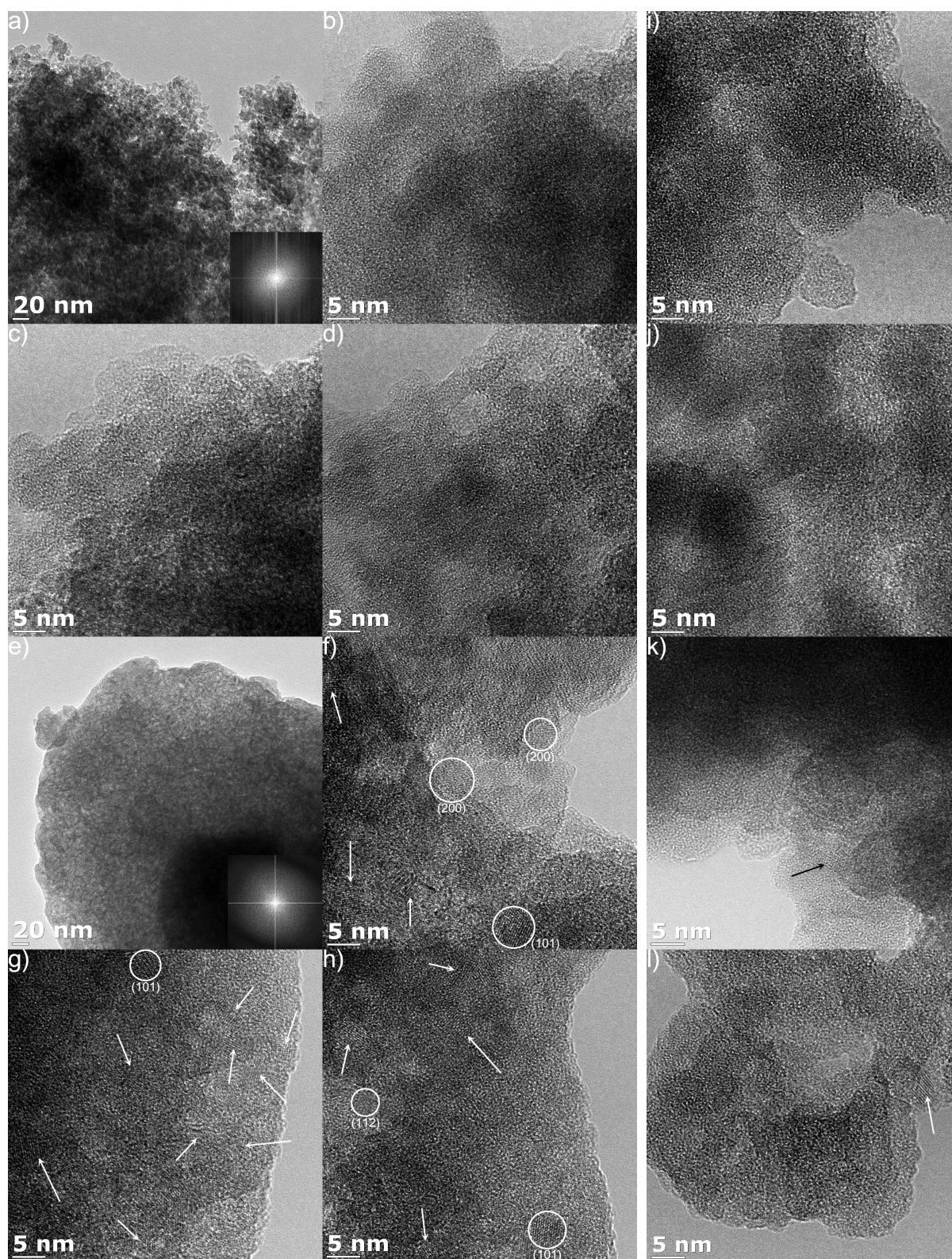
Fig. S3. HRTEM images picked out from more than 30 different spots of TiO_2-SiO_2 mixed oxide with a-d) Ti/Si=0.11 and e-h) 1.00. Images of Ti/Si=0.04 and 0.33 are shown in i, j) and k, l).Circles and arrows indicate phase and lattice fringes of anatase TiO_2 and insets of a, e) represents SAED pattern.
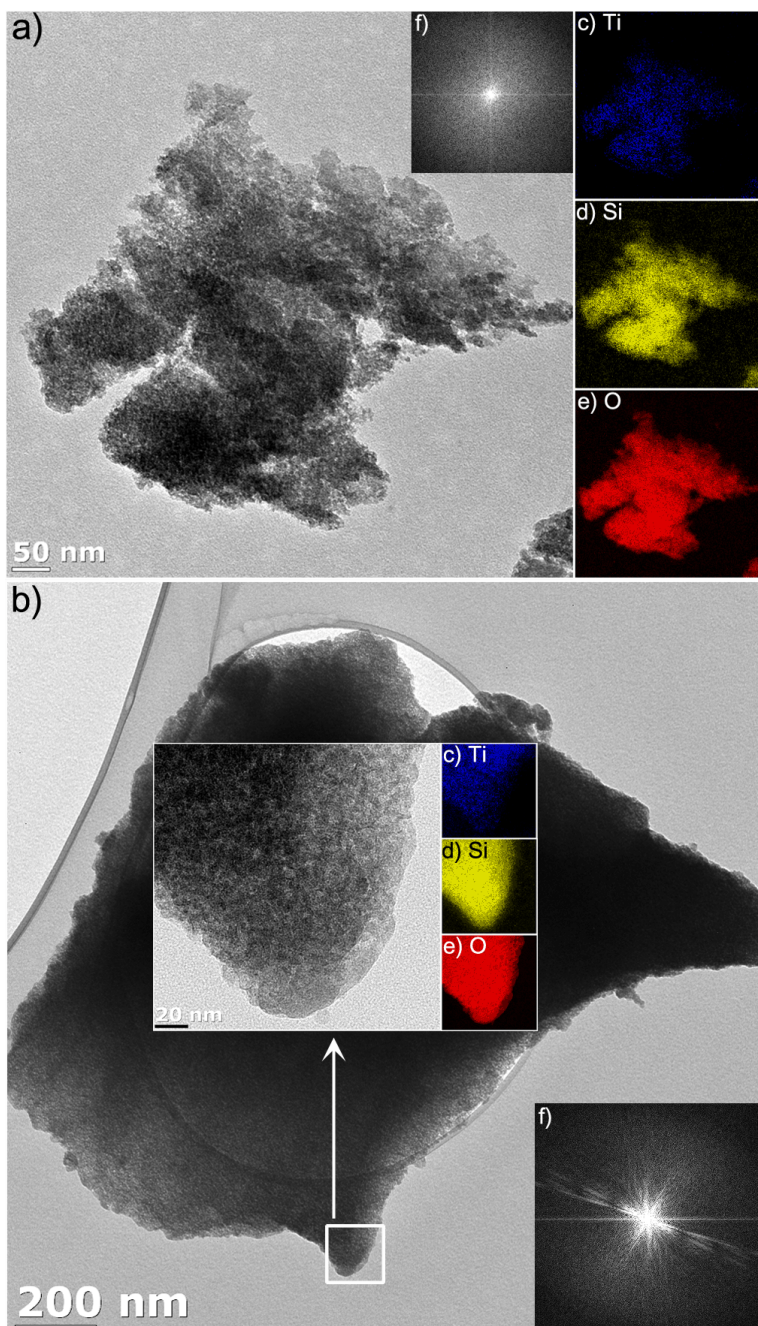
Fig. S4. TEM image of TiO_2-SiO_2 mixed oxide with a) Ti/Si=0.11 and b) 0.33. c-e) EELS mapping of composed atoms. f) SAED pattern for both samples.
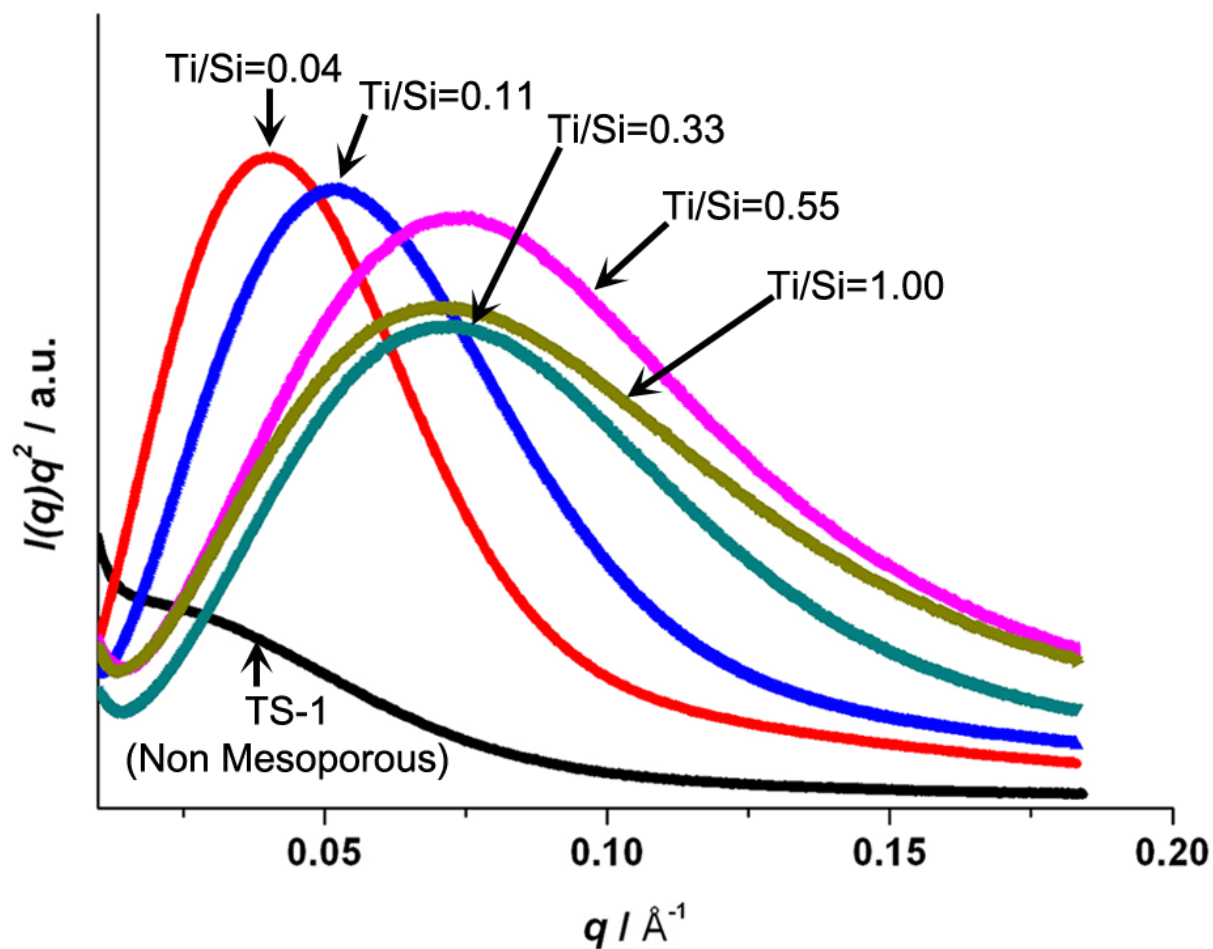
Fig. S5. Lorentz corrected SAXS profiles of series of TiO_2-SiO_2 mixed oxide and TS-1.

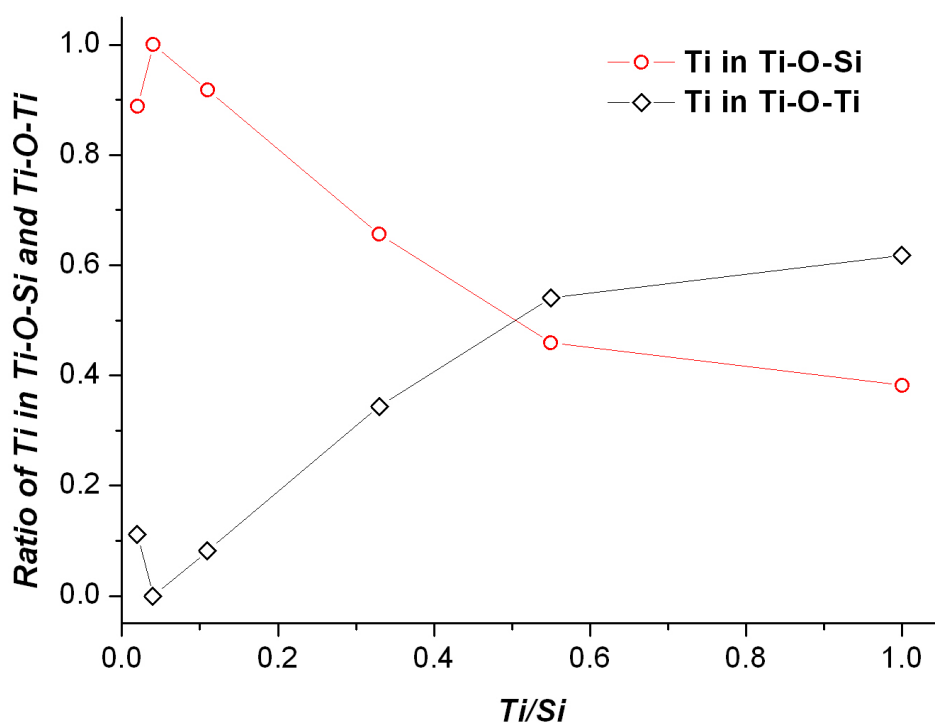Fig. S6. Linear combination fitting of XANES of TiO_2-SiO_2 mixed oxide. Because the intensity of pre-edge peak of sample with Ti/Si=0.02 was smaller than that of one with 0.04 (Fig. 4) due to the octahedral hole formed when bridging O-Si bond is broken by oxide ion from O-Ti when low concentration of Ti are inserted to SiO_2 glass matrix, XANES of the sample with Ti/Si=0.04 and anatase TiO_2 were selected as references spectra of maximum Ti-O-Si and Ti-O-Ti respectively after careful consideration. Fitting range was fixed from 4964.50 to 4976.03 eV to cover both singlet and triplet pre-edge peaks for all cases.

Table S1

Results of preedge fitting for normalized concentration of Ti-O-Si (TOS) and Ti-O-Ti (TOT). [a] C_{TOS}, C_{TOT}: Normalized concentration, [b] $\triangle E_{TOS}$, $\triangle E_{TOT}$: Energy shift correction, [c] X_v^2: Reduced Chi-square, [d] R-factor: a measure of absolute misfit between data and theory.

Ti/Si	C_{TOS}[a] (Uncertainty)	C_{TOT}[a] (Uncertainty)	$\triangle E_{TOS}$[b] (Uncertainty)	$\triangle E_{TOT}$[b] (Uncertainty)	X_v^2[c]	R-factor[d]
0.02	0.888 (0.016)	0.112 (0.016)	0.205 (0.013)	0.377 (0.325)	0.0000159	0.015635
0.11	0.918 (0.007)	0.082 (0.007)	0.042 (0.005)	-0.112 (0.177)	0.0000032	0.002959
0.33	0.656 (0.012)	0.344 (0.012)	0.010 (0.012)	-0.116 (0.073)	0.0000097	0.016549
0.55	0.459 (0.013)	0.541 (0.013)	0.299 (0.017)	0.028 (0.048)	0.0000111	0.038137
1.00	0.382 (0.013)	0.618 (0.013)	0.210 (0.021)	-0.091 (0.042)	0.0000116	0.050538

Table S2. The OHC products identified by GC-MS[a].

Aldehydes [b]		carboxylic acids [c]		Ketones [c]	
RT (min)	Compound	RT (min)	Compound	RT (min)	Compound
4.107	formaldehyde	8.787	acetic acid	9.560	2-butanone
5.000	acetaldehyde	12.653	propanoic acid	13.305	2-pentanone
6.773	propanal	18.058	butanoic acid	19.948	2-hexanone
9.892	butanal	24.313	pentanoic acid	25.926	2-heptanone
14.485	pentanal	30.630	hexanoic acid	33.145	2-octanone
21.365	hexanal	37.248	heptanoic acid	38.895	2-nonanone
27.315	heptanal	41.316	ocatanoic acid	42.586	2-decanone
34.787	octanal	44.357	nonanoic acid		
40.054	nonanal				
43.594	decanal				

[a] Analyzed at a split ratio of 20[b] or 10[c]. Each product at a given retention time (RT) was identified by mass spectroscopy signals.