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Fabrication of Se/C by using carbohydrate as the biomass starting materials: an efficient catalyst for the regio-specific epoxidation of β-ionone with ultrahigh turnover numbers

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Detailed data tables

Table S1 Effect of the catalyst amount (for Fig. 1 in text).[a]

Entry	Catalyst amount (mg)	Conv.[b]	Sel.[c]	Yield[d]
1	1	68%	53%	36%
2	5	76%	51%	39%
3	10	94%	50%	47%
4	20	98%	42%	41%
5	30	100%	40%	40%

[a] 1 mmol of **1**, 4 mmol of H_2O_2 and 1 mL of MeCN were heated in a sealed tube; [b] Unreacted substrate **1** was collected and weight to calculate its conversion ratio. [c] Selectivity of **3** was calculated on the basis of the its isolated amount. [d] Isolated yield of **3** based on **1**.

Table S2 Effect of the reaction solvent (for Fig. 2 in text).[a]

Entry	Solvent	Conv.[b]	Sel.[c]	Yield[d]
1	MeCN	94%	50%	47%
2	EtOH	100%	30%	30%
3	cyclohexanone	100%	47%	47%
4	acetone	70%	40%	28%
5	THF	100%	39%	39%
6	1,4-dioxane	100%	40%	40%
7	EtOAc	100%	62%	62%

[a] 1 mmol of **1**, 4 mmol of H_2O_2, 10 mg of Se/C **6d** and 1 mL of solvent were heated in a sealed tube; [b] Unreacted substrate **1** was collected and weight to calculate its conversion ratio. [c] Selectivity of **3** was calculated on the basis of the its isolated

amount. [d] Isolated yield of **3** based on **1**.

Table S3 Catalyst recycle & reuse (for Fig. 3 in text).[a]

Entry	Condition	Conv.[b]	Sel.[c]	Yield[d]
1	H_2O_2 (4 quiv.)	100%	62%	62%
2	H_2O_2 (4 quiv.) catalyst recycle & reused	80%	61%	49%
3	H_2O_2 (2 quiv.)	79%	63%	50%
4	H_2O_2 (2 quiv.) catalyst recycle & reused	80%	59%	47%
5	O_2	50%	52%	26%
6	O_2 catalyst recycle & reused	50%	48%	24%

[a] 1 mmol of **1**, 10 mg of Se/C **6d** and 1 mL of EtOAc were heated in a sealed tube; [b] Unreacted substrate **1** was collected and weight to calculate its conversion ratio. [c] Selectivity of **3** was calculated on the basis of the its isolated amount. [d] Isolated yield of **3** based on **1**.

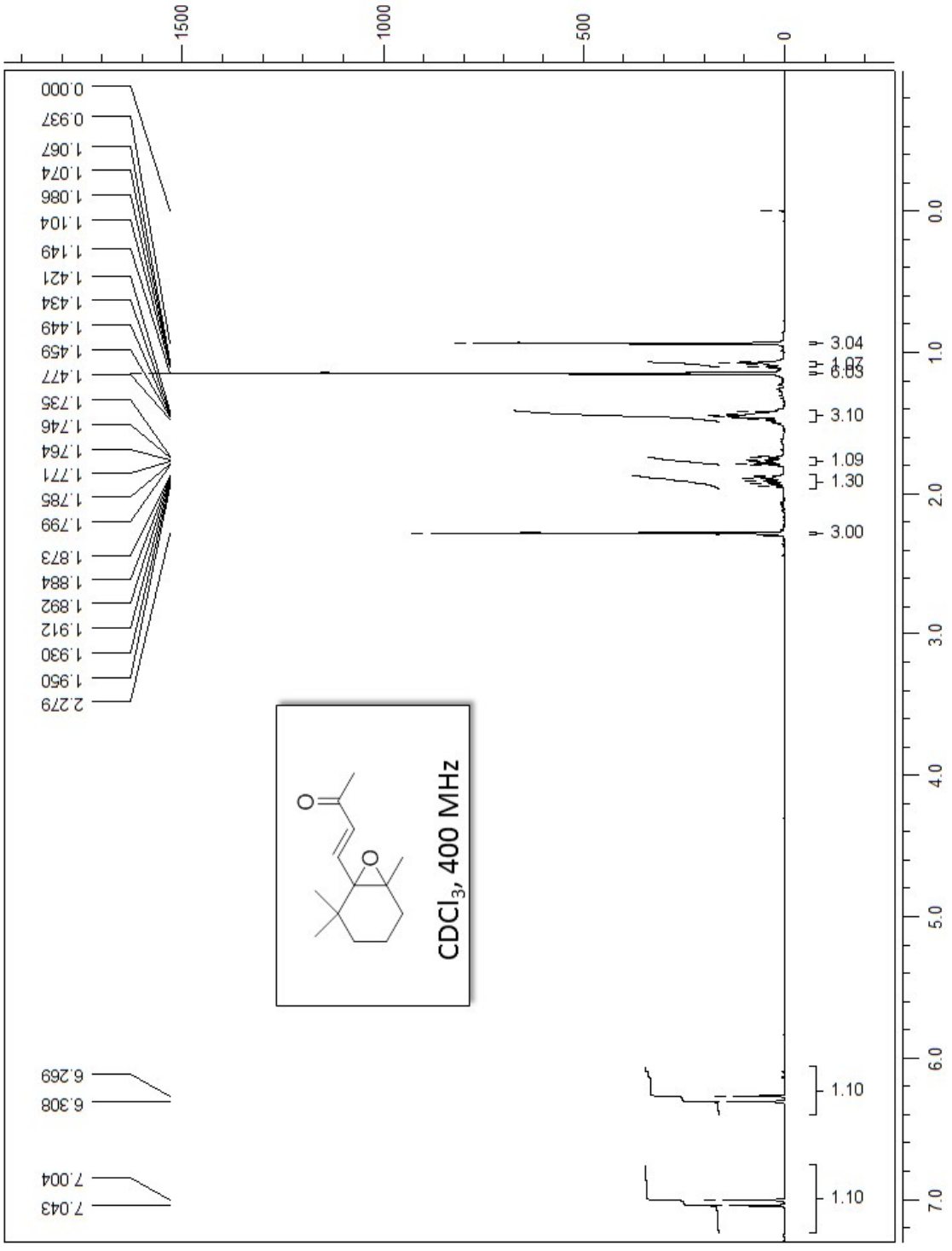
Table S4 Selective epoxidation reaction of β-ionone catalyzed by the S/C fabricated from different carbohydrates (for Fig. 4 in text).[a]

Entry	Carbohydrate	Conv.[b]	Sel.[c]	Yield[d]
1	glocuse	100%	62%	62%
2	fructose	100%	60%	60%
3	sucrose	68%	47%	32%
4	chitosan	79%	48%	38%
5	potato amylum	72%	32%	23%
6	willow sawdust	69%	35%	24%

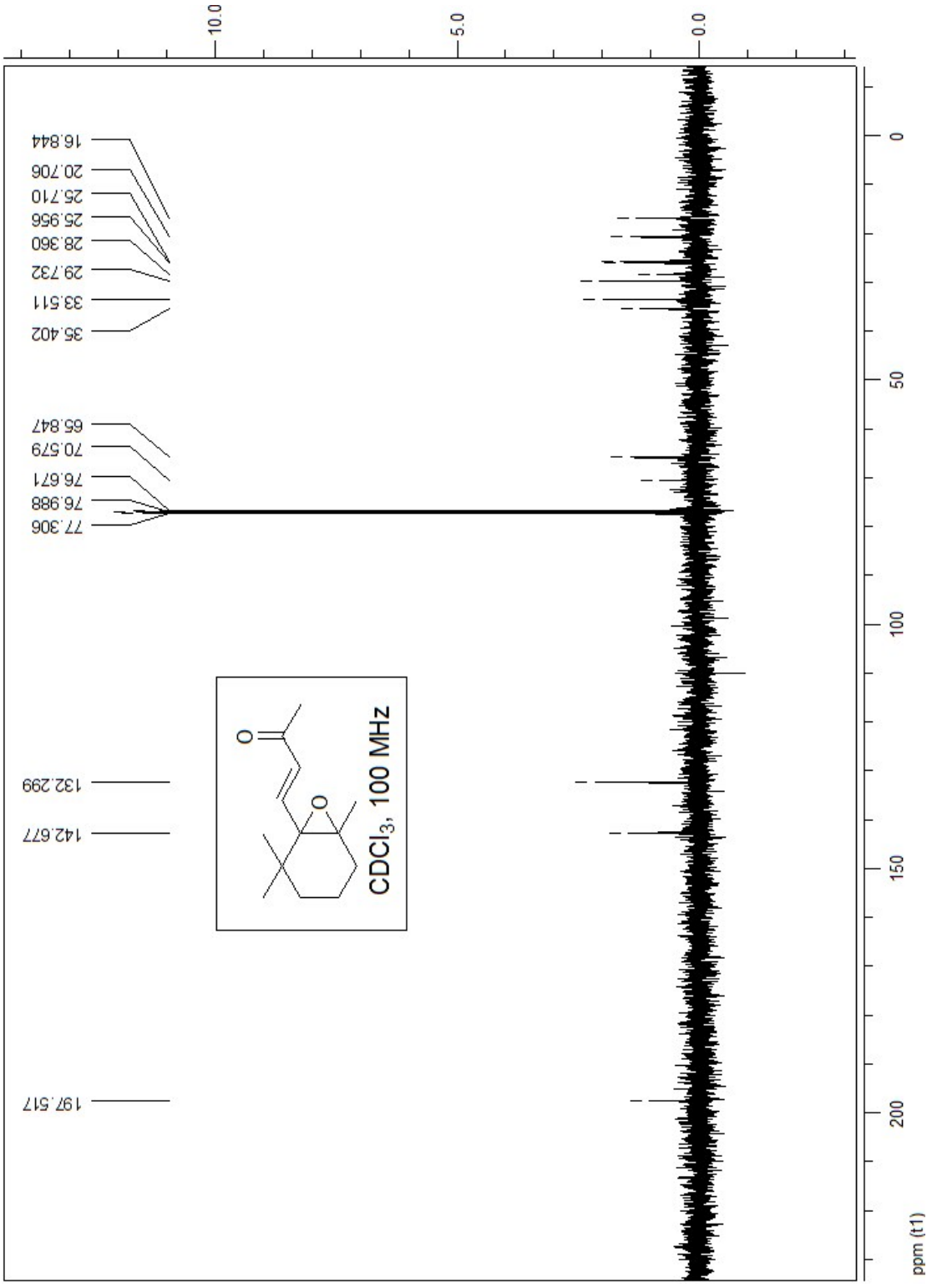
[a] The Se/C catalysts were fabricated under the conditions described in Table 1, entry 4 in text; For catalytic activity evaluation reactions, 1 mmol of **1**, 4 mmol of H_2O_2, 10 mg of Se/C and 1 mL of EtOAc were heated in a sealed tube; [b] Unreacted substrate **1** was collected and weight to calculate its conversion ratio. [c] Selectivity of **3** was calculated on the basis of the its isolated amount. [d] Isolated yield of **3** based on **1**.

NMR spectra of the epoxide 3

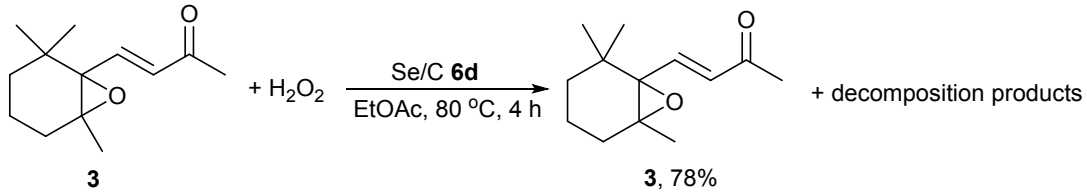
^{1}H NMR of **3**, $CDCl_3$, 400 MHz



^{13}C NMR of **3**, $CDCl_3$, 100 MHz



Decomposition of the epoxide 3 (experimental details)



3 **3**, 78%

52.1 mg of pure epoxide **3** (0.25 mmol), 2.5 mg of Se/C **6d**, 1 mmol of H_2O_2 (30 w/w%), a piece of magnetic bar and 0.25 mL of EtOAc were added into a reaction tube. The tube was sealed and stirred at 80 °C for 4 h. The mixture was cooled to room temperature. Thin layer chromatography indicated that a series of decomposition products were generated (Fig. S1). 78% of **3** was re-obtained after preparative thin layer chromatography separation.

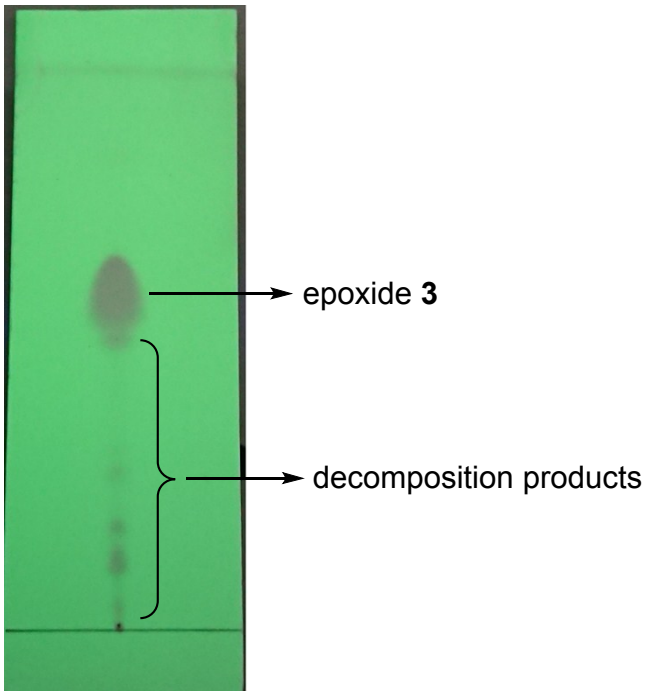


Fig. S1 TLC photograph of the decomposition reaction of epoxide **3**