# Supporting Information

# Microwave-assisted controlled-isomerization during glucose conversion into lactic acid over a Sn-Beta catalyst

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**Experimental Procedures**

1. General

All commercial reagents were used directly without further purification, unless otherwise stated. All chemicals were used as received from the commercial suppliers: glucose (AR, 99.0 %), lactic acid (LA) (≥95 %), $SnCl_4 \cdot 5H_2O$ (AR, ≥99.0 %), hydrofluoric acid (HF) (GR, ≥40 %), tetraethyl orthosilicate (TEOS) (99.9 %), tetraethylammonium hydroxide (TEAOH) (99.99 %), fructose (AR, 99.0 %), 1,3-dihydroxyacetone (DHA) (GC, ≥95 %), deuterium water ($D_2O$) (99.9%). D‑Fructose (1-$^{13}$C labeled, AR, 99%) , silicon dioxide ($SiO_2$) (AR,40-60 mesh), silicon carbide (SiC) (99.9%) was purchased from Cambridge Isotope Laboratories, Inc. Deionized water was prepared by HITECH Master touch-D. Microwave heating reaction was performed on Milestone easyCONTROL-640. Centrifugation of the reaction mixture was performed on Thermo LYNX6000.

2. Synthesis of Sn-Beta zeolite and the monolithic catalyst

The Sn-Beta zeolite was synthesized by the rapid synthesis method in literature. In a typical synthesis procedure, 30.6 g TEOS was added to 33.1 g TEAOH with gently stir for 2 h at room temperature until the two-phase system turned into one phase. Then, 0.257 g $SnCl_4 \cdot 5H_2O$ was added into the solution and stirred for another 1 h at room temperature. During the stirring process, add 0.3 wt% of dealuminated molecular sieve seed crystals, and then evaporate the ethanol and part of the water in drying oven set as 70 °C to make the material reach the following ratio: 0.005 $SnCl_4$: 0.55 TEAOH: 0.55 HF: 7.5 $H_2O$. HF was added into sol state and suddenly transformed to solid gel which would be transferred into crystallizing kettle. After that the kettle was heated at 140 °C for 7 days. After taking it out, it was washed with deionized water several times by suction filtration, dried and baked in oven at 550 °C for at least 6 h and cooled naturally.

When 0.15 g Sn-Beta was evenly dispersed in the 25 g mixtures of silicon dioxide ($SiO_2$) and silicon carbide (SiC) by physical mixing the "monolithic" catalyst formed.There were 7 kinds of mass ratio of $SiO_2$:SiC including : ∞ (25 g $SiO_2$) ,250 (24.90 g $SiO_2$+0.099 g SiC) ,50  (24.51 g $SiO_2$+0.49 g SiC) ,7 (21.875 g $SiO_2$+3.125 g SiC) ,3 (18.75 g $SiO_2$+6.25 g SiC) ,1 (12.5 g $SiO_2$+12.5 g SiC) ,0 (25 g SiC ). The "monolithic" catalysts used in different experiments are listed in Table S1.

3. Catalytic reaction and product analysis

*3.1 Catalytic reaction under conventional heating*

The catalytic conversion of feedstock (glucose, fructose and 1,3-dihydroxyacetone) was carried out in a stainless-steel autoclave (Parr, 100 ml) with an initial $N_2$ pressure of 4 MPa at 180/200 °C for 30/60 min. The autoclave was needed to warm up from room temperature to targeted temperature controlled by computer. Generally, a mixture of 0.15 g reactant, 0.15 g solid acid catalyst, and 15 ml deionized water mixture were loaded into the sealed autoclave with a stirring speed of 530 rpm. 0.15 g stock was added into 15 ml deionized water forming 10 g/L glucose solution mixed with 25.15 g "monolithic" catalytic if stirring function was not used. After the reaction, the autoclave was cooled with room temperature water and the liquid solution was separated from the solid mixture by centrifugation in 15 min at a stirring speed of 3600 rpm. The collected liquid solution was filtered through 0.45 μm pore-size filters prior to analysis. The separated solid catalyst was washed with water and ethanol mixture for six times and dried at 100 °C overnight for the recycle of catalyst. Glucose isomerization reaction was conducted at 100 °C to avoid further subsequent reactions, and other reaction conditions were same with those of batch lactic acid synthesis reactions.

*3.2 Catalytic reaction under microwave heating*

The catalytic conversion of stock (glucose, fructose and 1,3-dihydroxyacetone) was carried out in round bottom quartz tubes with a diameter of 25 mm and a height of 115 mm with an initial $N_2$ pressure of 4 MPa. 0.15 g stock was added into 15 ml deionized water forming 10 g/L glucose solution mixed with 25.15 g "monolithic" catalytic. After sealing the autoclave and connecting the inlet and outlet quartz tubes, $N_2$ was fed from the top of the reactor. Temperature of the whole reactor were measures by a temperature probe. The quartz tubes were heated up to 140/160/180 °C from room temperature in 5 min for 15/30/45/60 min and cooled by circulating cooling water controlled by computer. After the reaction, the autoclave was cooled without treatment and the liquid solution was separated from the solid mixture by centrifugation in 15 min at a stirring speed of 3600 rpm. The collected liquid solution was filtered through 0.45 μm pore-size filters prior to analysis. Glucose isomerization reaction was conducted at 100 °C to avoid further subsequent reactions, and other reaction conditions were same with those of batch lactic acid synthesis reactions.

*3.3 Product analysis*

The liquid products were quantified by HPLC (Shimadzu LC-20AD, Aminex HPX-87H ion exclusion column: 300 mm × 7.8 mm, column temperature: 50 °C, mobile phase: 0.005 M aqueous $H_2SO_4$ with a flow rate of 0.65 mL/min) with a differential refraction detector (RID-10A) for LA and 5-HMF. The conversion of feedstock was calculated based on the HPLC data using the equation:

Conversion = (moles of feedstock - moles of feedstock in the resultant liquid determined by HPLC) ÷ (moles of feedstock) × 100%.

The yields of LA, fructose and 5-HMF were calculated based on carbon via the equations:

Yield = (moles of carbon in the products determined by HPLC) ÷ (moles of carbon in feedstock) × 100%.

After the separation of the liquid products and used catalyst, the catalyst was washed by deionized water for 3 times to remove surface soluble substance residues. Then, dichloromethane ($CH_2Cl_2$) was used as extractant to extract carbon deposit from the used catalyst at room tempurature for 4 h. Organic solution was filtered through 0.45 μm pore-size filters and was analysied by gas chromatography-mass spectrometry (GC-MS) by Agilent 7890 GC with Agilent 5975C inert MSD.

Total Organic Carbon (TOC): Shimadzu TOC-LCSH/CPH, Liquid products need to be diluted, range: 4 μg/L~30000 mg/L. According to the TOC results, the carbon balance was 94.1 % and 94.8 %when Sn-Beta as the catalyst in conventional heating and microwave heating.

*3.4 Comparison of heating and cooling processes of two heating methods (Figure S1)*

Microwave heating has a faster heating speed and a slower cooling speed. Conventional heating's heating process is slower and cooling process is faster. Above the reaction temperature of 85 °C (efficient reaction temperature of glucose isomerization), the effective reaction time of the two heating processes is basically the same. Further reaction at the end of the reaction time will not affect subsequent comparisons.

4. Sn-Beta catalyst characterization

The phase composition of the samples was determined by X-ray powder diffraction (XRD) by a Rigaku Ultima IVX-ray diffractometer (40 kV, 40 mA) using the Cu Kα radiation (λ=1.5406 Å) in the 2 Theta range from 5° to 70° at a scanning rate of 4° $min^{-1}$. Ultraviolet and visible spectrophotometer (UV-vis) diffuse reflectance spectra were recorded on a Shimadzu UV-2700 spectrophotometer in the range from 200 to 800 nm, with $BaSO_4$ as the reference. X-ray photoelectron spectrometry (XPS) was used to probe the Sn state on a K-Alpha spectrometer (Thermo Fisher Scientific). The concentration of Sn was measured by the inductively coupled plasmaatomic emission spectrometry (ICP-AES) on Perkin Elmer Optima 3000.

5. H/D exchange experiment and ^{1}H/^{13}C NMR analysis

*5.1 H/D exchange experiment*

In proton/deuterium exchange experiment procedure, Initial reaction solution include 5 ml deionized water ($H_2O$), 2.5 ml $D_2O$ and 0.075 g fructose which concentration still remain 10 g/L. Then solution was transferred into a stainless-steel autoclave and a quartz tube. After sealing the autoclave and connecting the inlet and outlet, $N_2$ was fed from the top of the reactor reaching 4 MPa. The stainless-stell autoclave was heated by conventional way and we set the reaction temperature as 140 °C for 30 min. The quartz tube was heated by microwave and we set the reaction temperature as 140 °C for 30 min as well. After reaction, cooling method is the same as it in catalytic reaction. The liquid solution was collected separately. After diluting with $D_2O$, the solution was filtered through 0.45 μm pore-size filters and transferred into a NMR tube (5 mm×18 cm) prior to analysis.

*5.2 ^{1}H NMR analysis*

The ^{1}H NMR analysis of the samples were recoed on JNM-EZC500R (JEOL) with at room temperature operating at 500 MHz with water peak suppression. The sample were scanned for 16 times.

*5.3 ^{13}C NMR analysis*

The quantitative ^{13}C NMR analysis of the samples were recoed on JNM-EZC500R (JEOL) with at room temperature operating at 126 MHz. The sample were scanned for 1024 times and set the relaxation time to 20 s and turn off noe effect.

6. Density functional theory (DFT) calculations

*6.1 Dipole moment (μ)*

The dipole moments of the molecules at their optimized geometries were calculated with the Gaussian 09W program package [1] with density functional theory (DFT). The B3LYP hybrid functional and the 6-311+G(d,p) triple-zeta basis set were applied for all the atoms.

*6.2 Adsorption energies ($E_{ads}$)*

The adsorption configurations were constructed following the procedures outlined in a previous theoretical study.[2]


*6.3 Calculation of transition state*

DFT calculations were carried out with the B3LYP hybrid exchange–correlation functional to investigate the ring-opening mechanism of β-Pyranose and β-Furanose. The double-zeta basis sets cc-pVDZ were used. The QST2 method was used to calculate the transition state. Analytic harmonic vibrational frequencies were calculated to verify the nature of the stationary states and to obtain the zero-point energy corrections. The conductor polarized continuum model (C-PCM) was utilized to simulate the solvation environment of water. As the ring opening reaction can be expected to be facilitate by proton-containing species such as water or acidic sites, we studied the effect of a water molecule to promote the ring opening reaction, which should provide the correct trend in the energy barriers. These calculations were performed with the Gaussian 09 program package, and visualized with the AGUI graphical interface from the AMPAC program package.
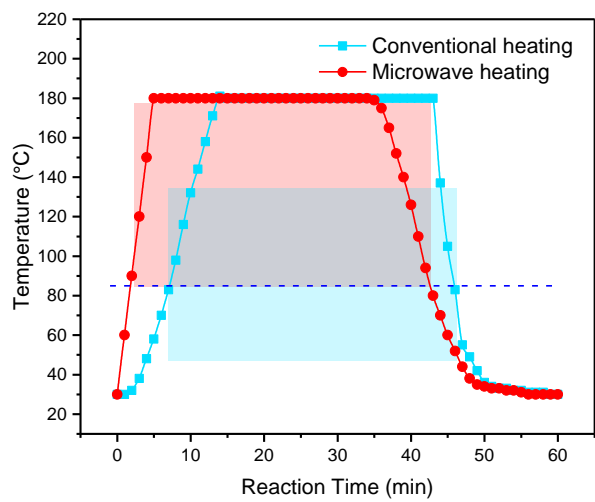
**Results and Discussion**



**Figure S1**. Temperature curve of the whole process of conventional and microwave heating experiment. (Filled with "monolithic" catalyst, 180 °C, 30 min)

From Figure S2 to Figure S4, glucose concentration in solution increases first and then decreases as the mass ration of SiO$_2$:SiC decreases. SiC is shown not to catalyze the conversion from glucose to LA under microwave heating (Figure 1B). Under conventional heating, SiC is shown to not affect the equilibria between glucose and fructose (Figure S6). For these reasons, SiC acts as a microwave absorber and enhances the effect of microwave irradiation. The microwave-absorbing performance of the catalyst further influences the conversion efficiency of the liquid products. As the ratio of SiC increases in the monolithic catalyst, the thermal effect becomes the dominant factor, which increases the temperature to the solution and promotes the reaction to move forward. Thus, SiC only acts as a microwave absorber in this system and has no effect on the isomerization reaction.



**Figure S2.** Product distributions over different mass ratio of SiO$_2$:SiC and conversion rate of glucose under microwave heating. Reaction conditions: 0.5 h, 150.0 mg feedstocks,15.0 mL deionized water, 4 MPa N$_2$, 150.0 mg Sn-Beta catalyst, 25 g SiO$_2$+SiC totally, 140 °C.
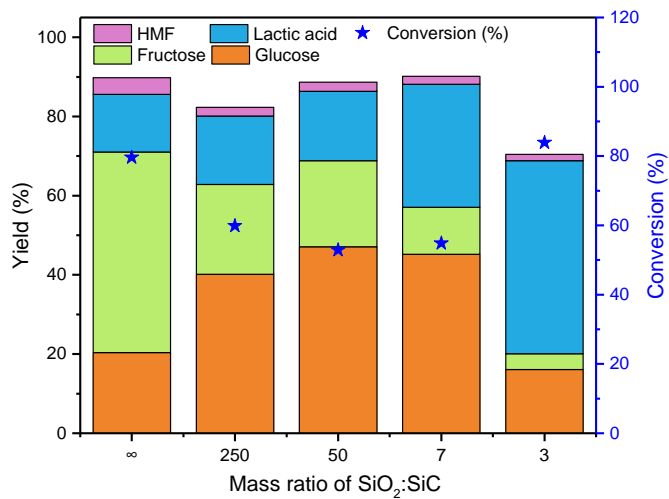
**Figure S3.** Product distributions over different mass ratio of $SiO_2$:SiC and conversion rate of glucose under microwave heating. Reaction conditions: 0.5 h, 150.0 mg feedstocks, 15.0 mL deionized water, 4 MPa $N_2$, 150.0 mg Sn-Beta catalyst, 25 g $SiO_2$+SiC totally, 160 °C.
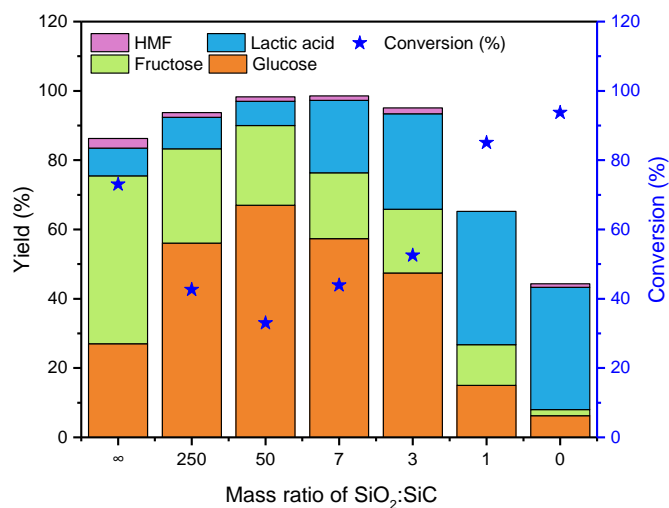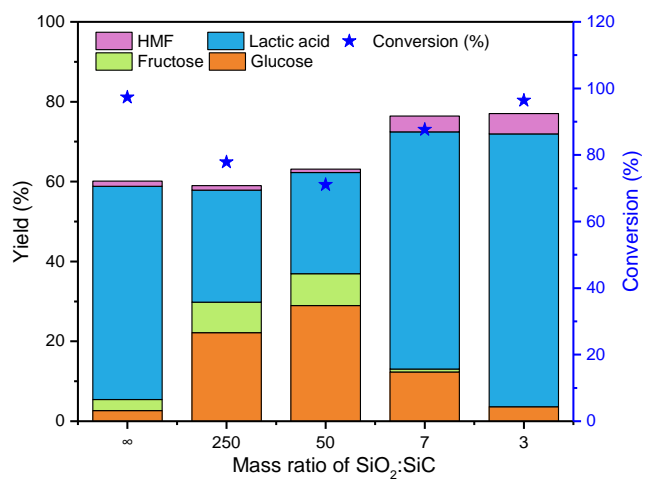
**Figure S4.** Product distributions over different mass ratio of $SiO_2$:SiC and conversion rate of glucose under microwave heating. Reaction conditions: 0.5 h, 150.0 mg feedstocks, 15.0 mL deionized water, 4 MPa $N_2$, 150.0 mg Sn-Beta catalyst, 25 g $SiO_2$+SiC totally, 180 °C.
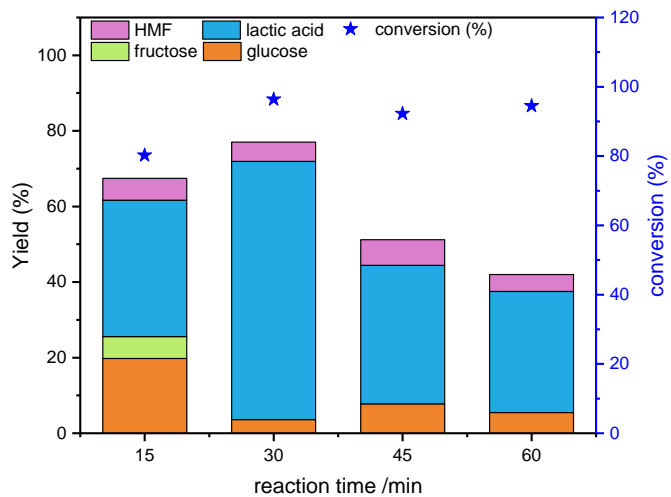
**Figure S5.** Product distributions over different reaction times conversion rate of glucose under microwave heating. Reaction conditions: 150.0 mg feedstocks,15.0 mL deionized water, 4 MPa $N_2$, 150.0 mg Sn-Beta catalyst, 25 g $SiO_2$+SiC totally (18.75 g $SiO_2$+6.25 g SiC), 180 °C.
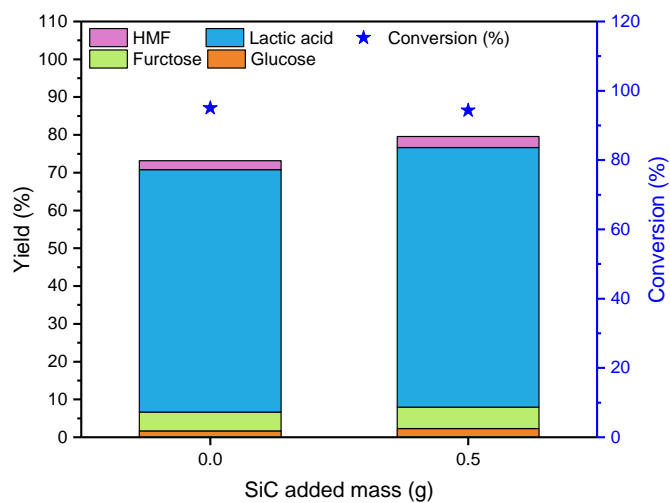
**Figure S6.** Product distributions over different SiC added mass and conversion rate of fructose under conventional heating. Reaction conditions: 150.0 mg feedstocks,15.0 mL deionized water, 4 MPa $N_2$, 150.0 mg Sn-Beta catalyst, 120 °C, 30 min, stirring.
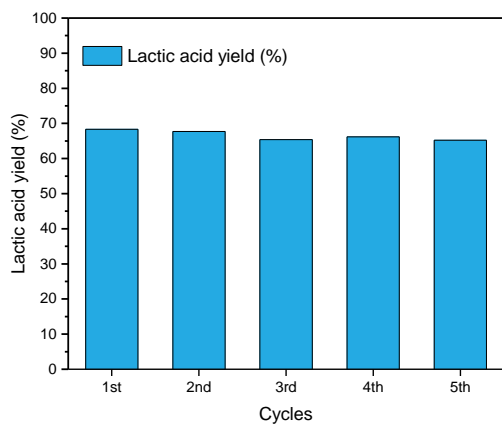
**Figure S7.** Lactic acid yield in catalyst recycling test under microwave heating. Reaction conditions: 180 °C, 0.5 h, 150.0 mg feedstock,15.0 mL deionized water, 4 MPa $N_2$, 150.0 mg Sn-Beta catalyst, mass ratio of $SiO_2$ and SiC is 3:1.
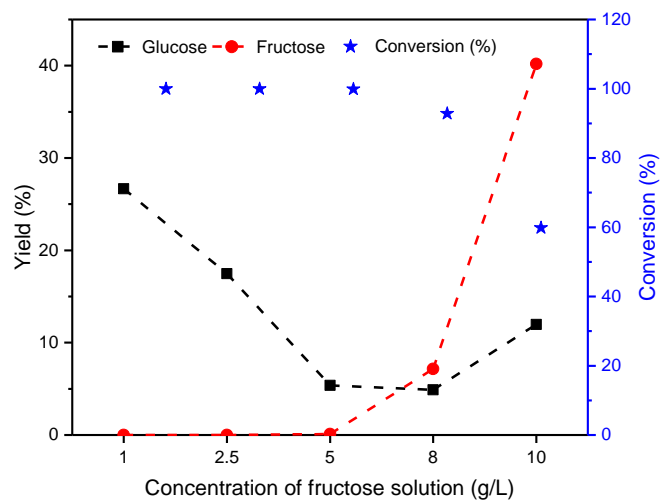
**Figure S8.** Product distributions over different concentration of fructose solution and conversion rate of fructose under microwave heating. Reaction conditions: 0.5 h, 15.0 mL deionized water, 4 MPa $N_2$, 150.0 mg Sn-Beta catalyst, 25 g $SiO_2$+SiC totally (18.75 g $SiO_2$+6.25 g SiC), 180 °C.
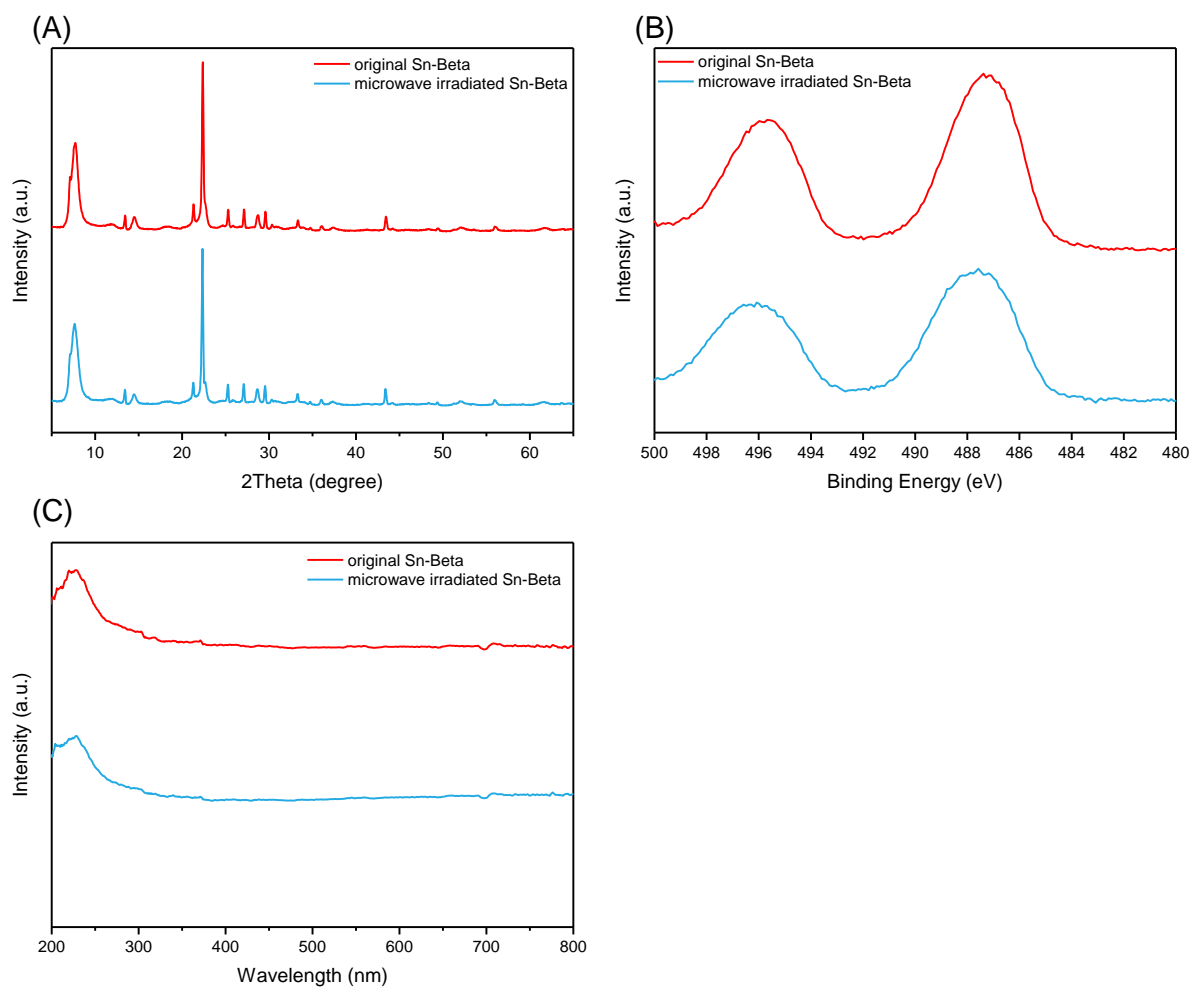
**Figure S9.** (A) XRD patterns, (B) XPS spectra, (C) UV-vis spectra of Sn-Beta catalyst before and after microwave irridation.
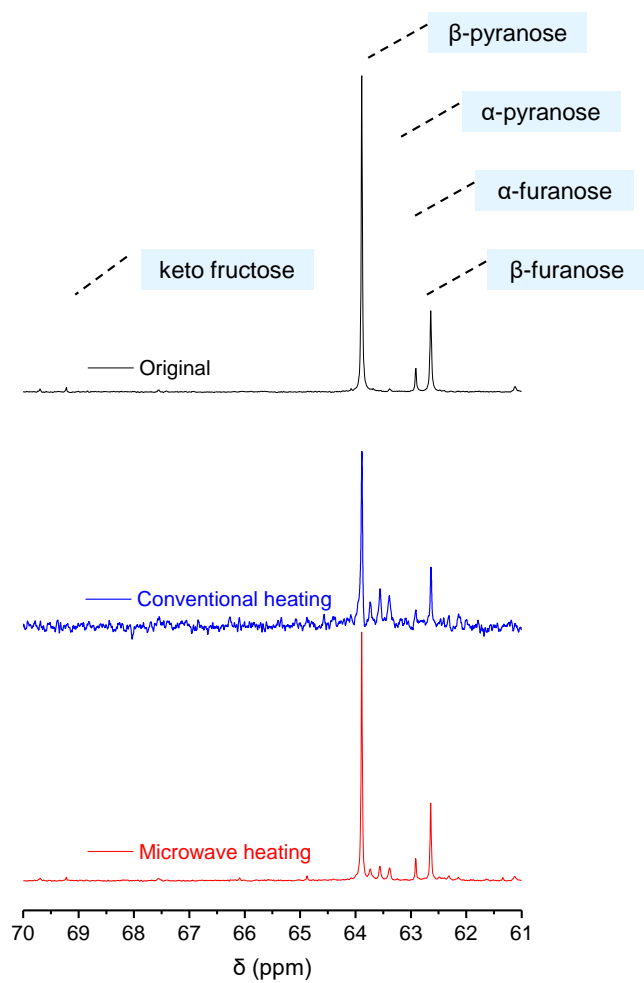
**Figure S10.** Quantitative $^{13}C$ NMR spectrum (126 MHz) for 1-$^{13}C$ labeled D-fructose dissolved in $D_2O$ including the original spectrum and spectrum under conventional heating and microwave heating at 140 °C for 30 min.
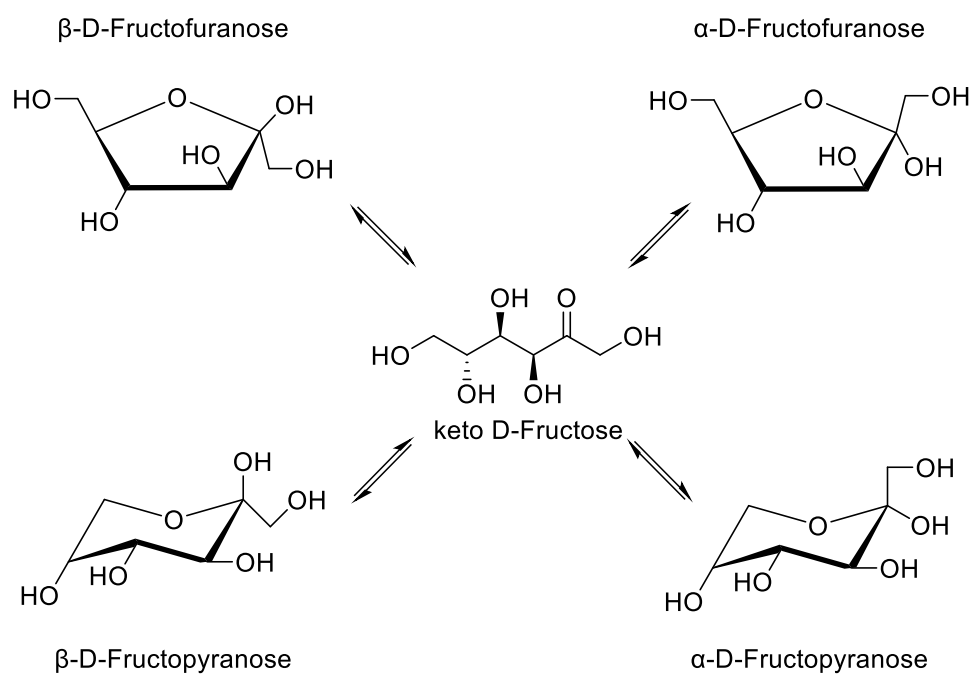
**Figure S11.** Structures of the fructose five tautomers and their inter-conversion via open-chain form.

**(A) β-pyranose-2@Sn**
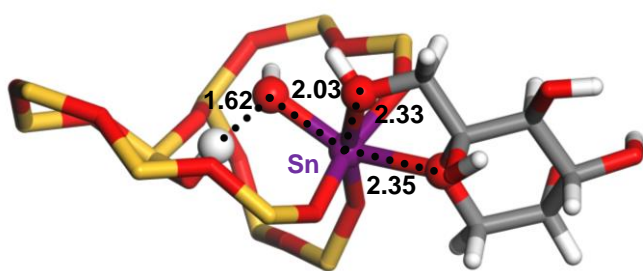
1.62  2.03  2.33  Sn  2.35

ΔE$_{ads}$ = -1.19 eV

**(B) β-furanose-2@Sn**

2.01  1.56  Sn  2.31

ΔE$_{ads}$ = -1.14 eV

**(C) α-pyranose-2@Sn**

1.67  2.02  2.37  Sn  2.39

ΔE$_{ads}$ = -0.97 eV

**(D) α-furanose-3@Sn**

1.62  2.33  Sn  2.35
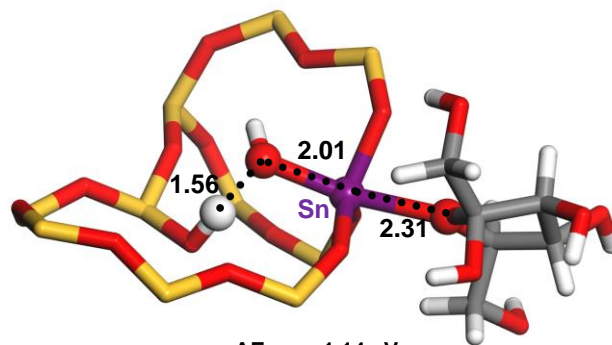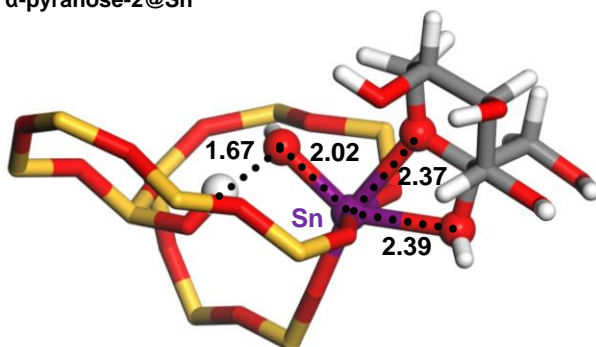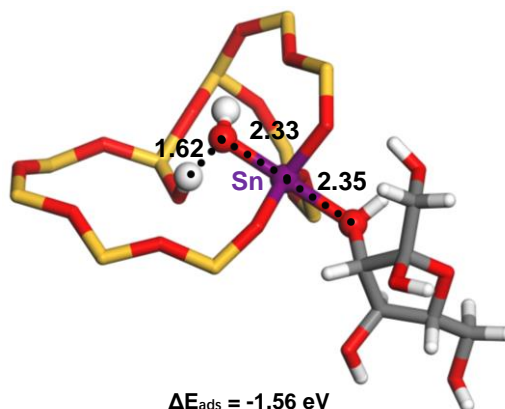
ΔE$_{ads}$ = -1.56 eV

**Figure S12.** Adsorption and adsorption energies (E$_{ads}$) of the four fructose tautomers at the open Sn site on the Sn-Beta catalyst. For clarity, only the relevant part of the periodic zeolite model is shown (bond lengths in Å).
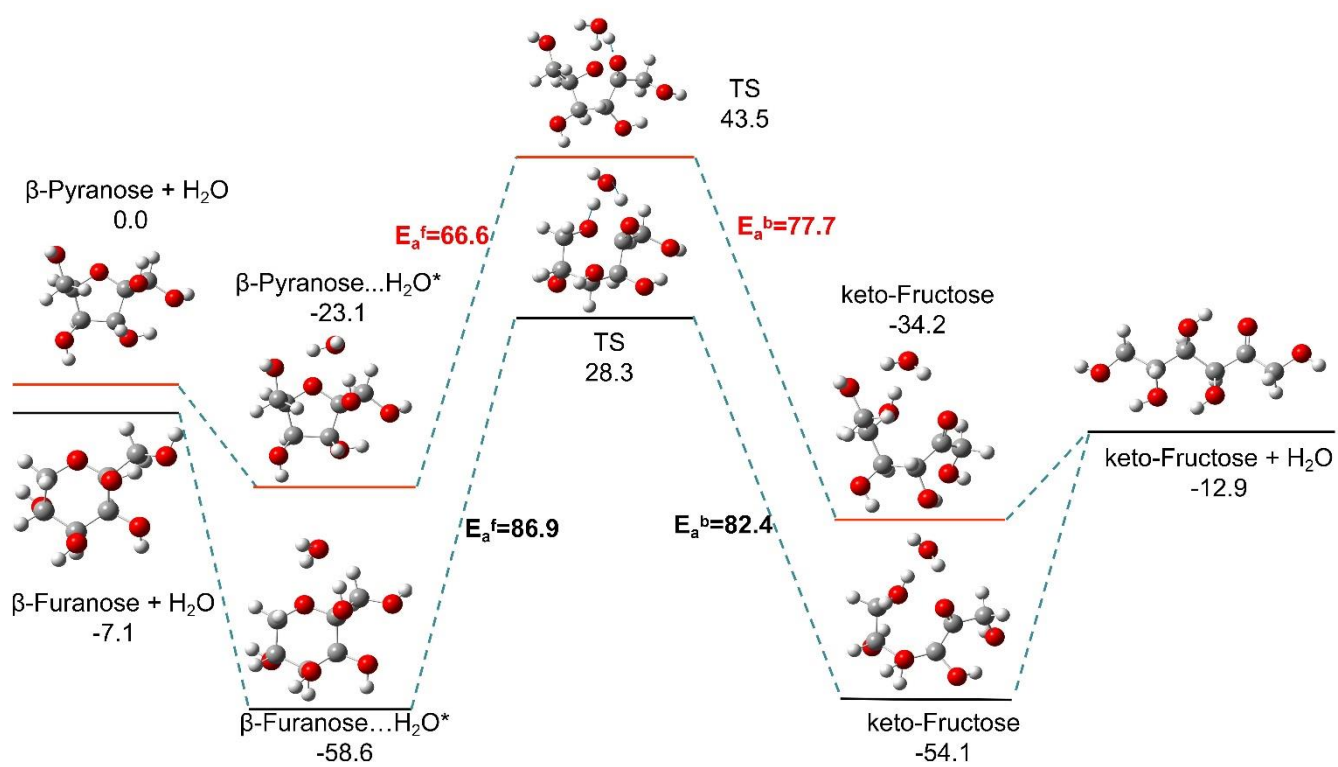
**Figure S13.** The ring-opening reaction pathway of β-Pyranose and β-Furanose in the aqueous solution as facilitated by an $H_2O$ molecule. The energies are shown in kJ/mol.
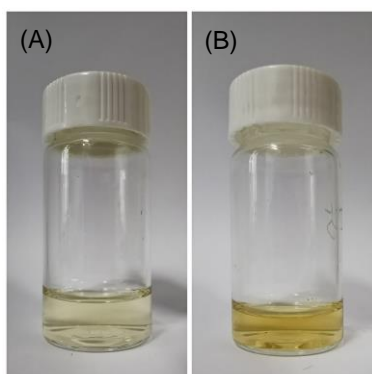
**Figure S14.** Comparison of solution after centrifugation under microwave heating (A) and conventional heating (B).

We analyzed carbon deposition on the catalyst washed by dichloromethane with GC-MS. After microwave heating experiment, main carbon deposit includes 3,4-furandiol, dodecane, cyclooctane, 2-dodecanone, tridecanal, undecanoic acid, dodecanoic acid, and tridecanoic acid. After conventional heating, main carbon deposit includes 2-cyclopenten, indane, dodecane, benzene, decane, tetreadecane, tridecanal,1-octadecene and 9-nonadecene which indicates that the peak substance of conventional heating has longer carbon chain.
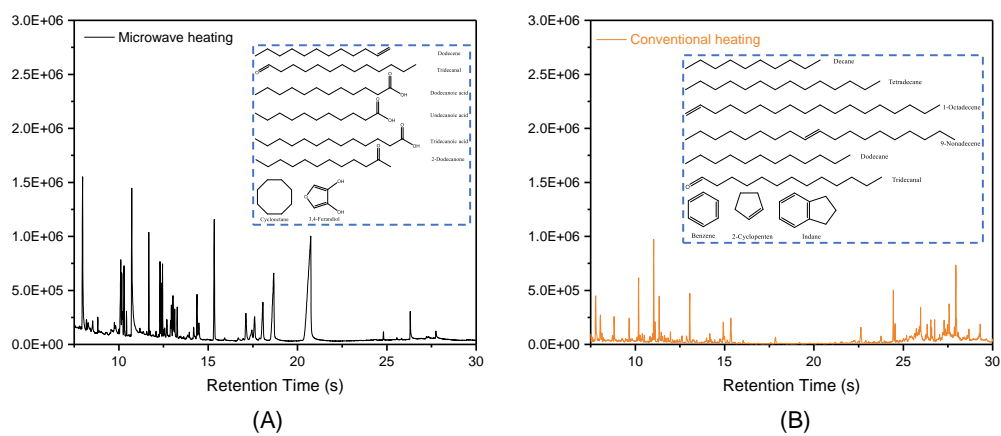


**Figure S15.** Carbon deposit of the catalyst after reaction and containing carbonaceous matter. (A) microwave heating, (B) onventional heating.
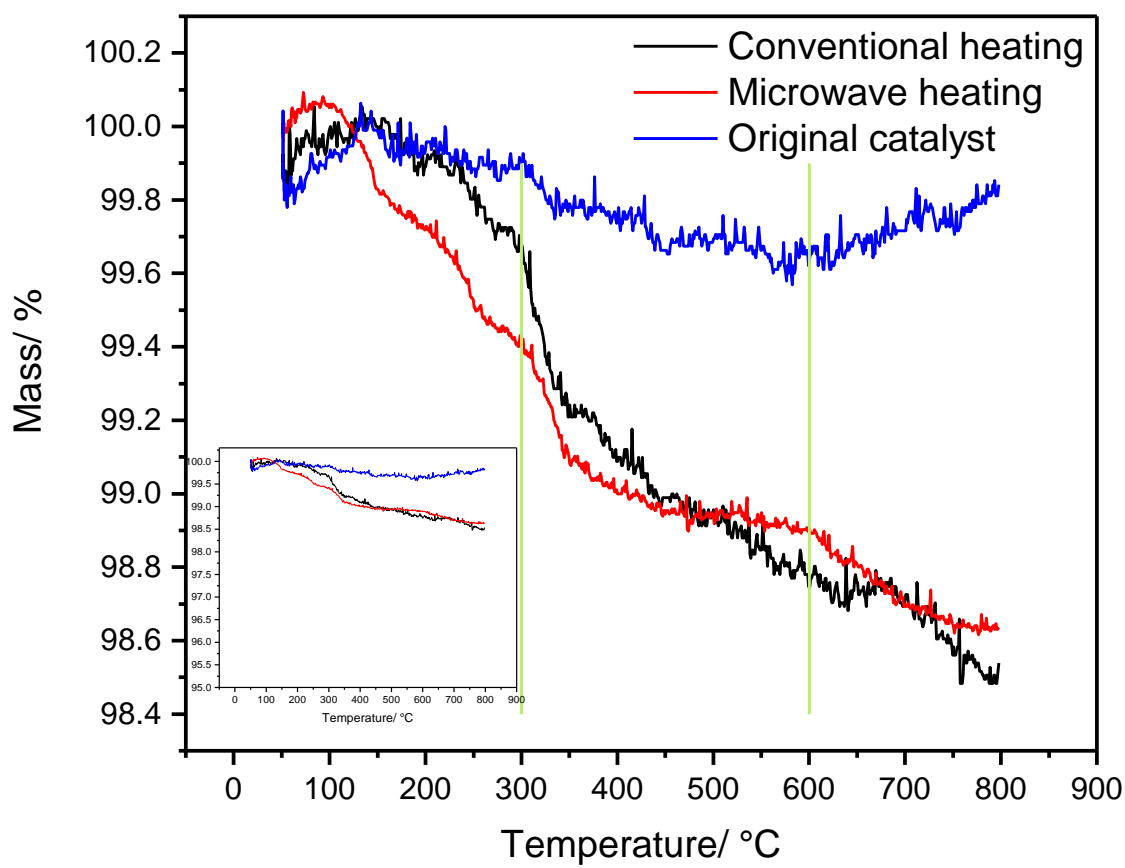
**Figure S16.** The thermogravimetric curve of the catalyst before and after the reaction. Reaction conditions: 0.5 h, 150.0 mg feedstocks,15.0 mL deionized water, 4 MPa $N_2$, "monolithic" catalyst (0.15 g Sn-Beta+ 18.75 g SiC+ 6.25 g $SiO_2$),180 °C.

**Table S1** Catalyst composition in microwave and conventional heating.

| Heating method | Mass ration of $SiO_2$:SiC | Sn-Beta | $SiO_2$ | SiC |
|---|---|---|---|---|
| Microwave heating | ∞ | 0.15 | 25 | 0 |
| | 250 | 0.15 | 24.90 | 0.1 |
| | 50 | 0.15 | 24.51 | 0.49 |
| | 7 | 0.15 | 21.875 | 3.125 |
| | 3 | 0.15 | 18.75 | 6.25 |
| | 1 | 0.15 | 12.5 | 12.5 |
| | 0 | 0.15 | 0 | 25 |
| Conventional heating | / | 0.15 | 0 | 0 |
| | ∞ | 0.15 | 25 | 0 |
| | 3 | 0.15 | 18.75 | 6.25 |

| | | Sn-Beta | $SiO_2$ | SiC |
|---|---|---|---|---|
| | ∞ | 0.15 | 25 | 0 |

**Table S2** Lactic acid yield through two homogeneity providing method under different conditions.

| Reaction number | Heating method | Temperature (°C) | Reaction time (min) | Stirring situation | $SiO_2$ supporting | SiC adding | Lactic acid yield (wt%) |
|---|---|---|---|---|---|---|---|
| 1 | Conventional | 180 | 30 | √ | × | × | 47.3 |
| 2 | Conventional | 180 | 30 | × | √ | √ | 43.8 |
| 3 | Conventional | 200 | 60 | √ | × | × | 56.6 |
| 4 | Microwave | 180 | 30 | × | × | × | 0.0 |
| 5 | Microwave | 180 | 30 | × | √ | × | 53.3 |
| 6 | Microwave | 180 | 30 | × | √ | √ | 68.3 |
| 7 | Microwave | 180 | 60 | × | √ | √ | 32.0 |

**Table S3.** The reaction of 1,3-DHA to LA under mild conditions. ("monolithic" catalyst (0.15 g Sn-Beta+ 18.75 g SiC+ 6.25 g $SiO_2$), 80 °C, 30 min)

| Heating method | Lactic acid yield (wt%) |
|---|---|
| Conventional | 82.1 |
| Microwave | 83.8 |

**Table S4.** ICP tests for Sn-Beta catalyst before and after microwave irradiation.

| Sn-Beta | #Sn (wt%) |
|---|---|
| Original catalyst | 0.76 |
| After microwave irradiation | 0.76 |

**Table S5.** ^{1}H NMR shifts for D-fructose equilibrated in $D_2O$.

| Tautomer | Chemical shift[a] (ppm) | | | | | | |
|---|---|---|---|---|---|---|---|
| | H-1 | H-1′ | H-3 | H-4 | H-5 | H-6 | H-6′ |
| β-Pyranose | 3.529 | 3.376 | 3.613 | 3.718 | 3.814 | 3.857 | 3.521 |
| α-Pyranose | 3.517 | 3.466 | 3.832 | 3.770 | 3.687 | 3.683 | 3.518 |
| β-Furanose | 3.398 | 3.377 | 3.935 | 3.935 | 3.670 | 3.610 | 3.484 |
| α-Furanose | 3.483 | 3.465 | 3.926 | 3.815 | 3.880 | 3.639 | 3.518 |
| keto | 4.470 | 4.360 | 4.460 | 3.760 | 3.590 | 3.671 | 3.483 |

[a] Compared with formerly data, the tiny difference of chemical shift is about 0.2 ppm may be caused by accuracy, test equipment and chemical environment. Assigned on the basis of ref [3]

**Table S6.** Tautomer distributions of fructose equilibrated in $D_2O$ in 20 °C.

| five tautomers | α-furanose | α-pyranose | β-furanose | β-pyranose | keto fructose |
|---|---|---|---|---|---|
| 20 °C | 6.1% | 1.3% | 23.6% | 68.6% | 0.4% |

**Table S7** Correspondence between the peak position in GC-MS and the compound name.

| Heating Method | Retention Time (s) | Compound name |
|---|---|---|
| Microwave heating | 7.97 | 3,4-Furandiol |
| | 10.11/12.30 | Dodecane |
| | 12.36 | Cyclooctane |
| | 13.03 | 2-Dodecanone |
| | 15.34 | Tridecanal |
| | 18.06 | Undecanoic acid |
| | 18.67 | Dodecanoic acid |
| | 20.74 | Tridecanoic acid |
| Conventional heating | 4.61 | 2-Cyclopenten |
| | 7.78 | Indane |
| | 10.18 | Dodecane |
| | 11.03 | Benzene |
| | 11.34 | Decane |
| | 13.05 | Tetradecane |
| | 15.34 | Tridecanal |
| | 24.44 | 1-Octadecene |
| | 27.95 | 9-Nonadecene |

**Coordinates of the adsorption structures at the open Sn site**

α-furanose@Sn
CONTCAR
O Si Sn  H  C
 1.0000000000000000
   12.6569995879999997    0.0000000000000000    0.0000000000000000
    0.0000000000000000   12.6569995879999997    0.0000000000000000
    0.0000000000000000    0.0000000000000000   26.3959999084000003
 135  63   1  14   6
Cartesian
 4.3612224860000000  8.3355201119999993  1.8300346569999999
 4.3028736920000004 10.4597442310000002  0.2161832510000000
 3.5254804810000002 10.7118715560000002  2.6963514069999999
 6.0713095839999998 10.3529196849999998  2.1560252680000001
 4.5463942619999997  6.5267082550000000 26.2819685169999993
 3.0866625530000000  6.0378949920000000  2.0522889240000000
 5.7507076950000000  6.0623229810000003  2.1628883050000001
 9.1005092160000007  8.4750003080000003  1.7957198670000001
10.9303315580000007 10.4297471440000002  2.0462178590000000
 8.5177809740000008 10.7864214319999991  2.9587276039999999
10.7693346650000006  6.4222880320000000  1.6199225209999999
 8.3626059089999991  6.0880168799999996  2.6813057080000000
12.5902971459999993  8.4042474069999997  1.6418311590000001
 0.8666247770000000 10.7390840940000007  2.4141780719999999
 0.4942558550000000  6.0478940220000004  2.6469909170000001
 9.0667151530000005  4.0608717619999997 14.7136586739999995
 8.7132048849999997  1.9460137170000000 13.1576142950000001
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# References

1. Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
2. W. N. van der Graaff, C. H. Tempelman, G. Li, B. Mezari, N. Kosinov, E. A. Pidko and E. J. Hensen, *ChemSusChem*, 2016, **9**, 3145-3149.
3. T. Barclay, M. Ginic-Markovic, M. R. Johnston, P. Cooper and N. Petrovsky, *Carbohydr Res*, 2012, **347**, 136-141.

# Author Contributions

Wang Liu,  carrying out experiments, writing of original draft, synthesis of Sn-Beta catalyst; main equal contributor
Zhimin Zhou, contributions for the DFT calculations; main equal contributor
Zhaohui Guo, contributions for the analysis of NMR data; supporting the contribution
Zhangqian Wei, contributions for the DFT calculation; supporting the contribution
Yanfei Zhang, synthesis of Sn-Beta catalyst; supporting the contribution
Xinpeng Zhao, characteristics of the catalyst; supporting the contribution
Gai Miao, characteristics of the catalyst; supporting the contribution
Lijun Zhu, characteristics of the catalyst; supporting the contribution
Hu Luo,  contributions for the analysis of data; supporting the contribution
Mengya Sun,  contributions for the analysis of data; supporting the contribution
Yingxiong Wang*,  modifying the analysis and presentation of manuscript; supporting the contribution
Shenggang Li*,  modifying the analysis and presentation of manuscript; supporting the contribution
Lingzhao Kong*, supplying the general research idea and design of experiments; leading contributor