

## Supplementary Information

### **$\gamma$ -Valerolactone-Introduced Controlled-Isomerization of Glucose for Lactic Acid Production over Sn-Beta Catalyst**

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## 1. Experimental and Computational Methods

### 1.1 Catalyst synthesis and characterization

All chemicals were purchased from the major commercial suppliers: the zeolite beta with  $\text{SiO}_2/\text{Al}_2\text{O}_3=25$  was purchased from Nankai University Catalyst Co., Ltd, tin (IV) chloride pentahydrate ( $\text{SnCl}_4 \cdot 5\text{H}_2\text{O}$ , Macklin, AR),  $\text{HNO}_3$  (65.0 wt % in water, Macklin), L-Lactic acid (1.0 mol/L standard solution, Merck, HPLC), fructose (AR, 99.0 %), glucose (AR, 99.0 %),  $\gamma$ -valerolactone (GVL, Macklin, 98 %) and other reagents were from Sinopharm Chemical Reagent Co, Ltd (Shanghai, China).

For the Synthesis of deAl-Beta catalyst, commercial Beta zeolite with a  $\text{SiO}_2/\text{Al}_2\text{O}_3=25$  was calcinated at 550 °C for 6 h before usage to remove the template and adsorbed impurities. deAl-Beta, short for dealuminated Beta zeolite, was prepared by stirring commercial Beta in a 13.0 mol/L aqueous nitric acid solution at 100 °C for 20 h. Afterwards the powder was washed with water until the PH was neutral and dried at 100 °C.

For the Synthesis of Sn-Beta catalyst, deAl-Beta was pretreated at 373 K overnight to remove physisorbed water. Afterward, 3.0 g of the solid powder was finely ground with appropriate amount of  $\text{SnCl}_4 \cdot 5\text{H}_2\text{O}$  in the mortar for 1 h. After this, the solids were calcined under air (550 °C, 5 °C  $\text{min}^{-1}$ , 6 h). The synthesized catalysts were denoted as x wt% Sn-Beta, where x denotes the content of Sn in catalyst added theoretically.<sup>1</sup>

The phase composition of the samples was determined by X-ray powder diffraction (XRD) by a Rigaku Ultima IV X-ray diffractometer (40 kV, 40 mA) using the CuK $\alpha$  radiation in the 2 Theta range from 5° to 70° at a scanning rate of 4°/min. The morphological information was examined by the scanning electron microscopy (SEM) using SUPRRATM 55 with a 2.0 kV accelerating voltage. UV-vis diffuse reflectance spectra were recorded on a Shimadzu UV-2700 spectrophotometer in the range of 200-800 nm, with  $\text{BaSO}_4$  as the reference.  $\text{N}_2$ -adsorption and desorption were carried out with a Micromeritics ASAP 2020 equipment to determine the specific surface area, micropore area and pore size distribution of the samples. The sample to be tested was first degassed at 300 °C for 10 h, and then tested with  $\text{N}_2$  as the medium at -196 °C. The concentration of Sn and Al was measured by the inductively coupled plasma-atomic emission spectrometry (ICP-AES) on Perkin Elmer Optima 3000. Raman spectra of dehydrated samples were recorded on a high-resolution, dispersive Raman spectrometer system (Horiba-JobinYvon LabRam-IR) with the He-Cd laser with a 325-nm line as the excitation source. FT-IR spectra of

pyridine adsorption were performed with a spectral resolution of  $4\text{ cm}^{-1}$  on a Nicolet Nexus 670 FT-IR spectrometer. In a home-made vacuum infrared cell with  $\text{CaF}_2$  windows, a self-supporting wafer of the sample (about 10 mg) was initially dried under vacuum at  $350\text{ }^\circ\text{C}$  for 1 h, then cooled down to  $50\text{ }^\circ\text{C}$  and saturated with about 25 mbar of pyridine vapor at  $50\text{ }^\circ\text{C}$  for 10 min and then evacuated again for 30 min to fully remove the physisorbed pyridine. Finally, the evacuated sample containing chemisorbed pyridine was heated to 100, 200 and  $350\text{ }^\circ\text{C}$  for 30 min, with a heating rate of  $10\text{ }^\circ\text{C}/\text{min}$ , and the IR spectra were recorded in situ at these temperatures. The amounts of acid sites were determined from the integral intensity of characteristic bands ( $1450\text{ cm}^{-1}$  for Lewis acid sites, and  $1540\text{ cm}^{-1}$  for Brønsted acid sites) using the molar extinction coefficients of Emeis. X-ray photoelectron spectrometry (XPS) was used to probe the Sn state on a K-Alpha spectrometer (Thermo Fisher Scientific). The Thermogravimetric analysis (TGA) was performed under He or air flow on a Netzsch STA449F5 instrument. For the experiment, 10 mg of samples was placed in the crucible and heated from  $40\text{ }^\circ\text{C}$  to  $900\text{ }^\circ\text{C}$  under He to inspect the weight loss of the samples. For the synthesized of Sn-Beta catalyst pre-adsorbed with 16.6 wt% GVL, 0.2g GVL was added to 1g catalyst and 1ml ethanol was added for the dispersion of GVL, then the catalyst was dried at  $100^\circ\text{C}$ , 5h to evacuate ethanol.

## 1.2 Catalytic evaluation and product analysis

The catalytic conversion of stock (glucose, fructose and 1,3-dihydroxyacetone) was carried out in a stainless steel autoclave (Parr, 30 ml) with an initial He pressure of 4 MPa at  $200\text{ }^\circ\text{C}$  for 30 min, and 30 min was needed to warm up from room temperature to  $200\text{ }^\circ\text{C}$ . Generally, a mixture of reactant, the solid acid catalyst, and  $\gamma$ -valerolactone/water mixture were loaded into the sealed autoclave with a stirring speed of 530 rpm. After the reaction, the autoclave was cooled with ice bath and the liquid solution was separated from the solid mixture by centrifugation. The collected liquid solution was filtered through  $0.45\text{ }\mu\text{m}$  pore-size filters prior to analysis. The separated solid catalyst was washed with water and ethanol mixture for six times and dried at  $100\text{ }^\circ\text{C}$  overnight for the recycle of catalyst. Glucose isomerization reaction was conducted at  $100\text{ }^\circ\text{C}$  to avoid further subsequent reactions, and other reaction conditions were same with those of batch lactic acid synthesis reactions.

The liquid products were quantified by HPLC (Shimadzu LC-20AD, Aminex HPX-87H ion exclusion column:  $300\text{ mm} \times 7.8\text{ mm}$ , column temperature:  $50\text{ }^\circ\text{C}$ , mobile phase:  $0.005\text{ M}$  aqueous  $\text{H}_2\text{SO}_4$  with a flow rate of  $0.65\text{ mL}/\text{min}$ ) with a differential refraction detector (RID-10A) for LA and UV detector at  $284\text{ nm}$  for 5-HMF and MF. The conversion of glucose was calculated based on the HPLC data using the equation:

$$\text{Conversion} = (\text{moles of glucose} - \text{moles of glucose in the resultant liquid determined by HPLC}) \div (\text{moles of in glucose}) \times 100\%.$$

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

$$\text{Yield} = (\text{moles of carbon in the products determined by HPLC}) \div (\text{moles of carbon in glucose}) \times 100\%.$$

### 1.3 Computational methods

The Vienna Ab initio Simulation Package (VASP) was used to perform all the DFT calculations with the projector augmented wave (PAW) potentials and the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional.<sup>2–5</sup> Van der Waals interactions were accounted for by the Grimme’s DFT-D3 method.<sup>6</sup> An energy cut-off of 400 eV and the Gaussian smearing width of 0.05 eV were employed. The electronic energy of the supercell was converged to  $10^{-6}$  eV, and the force on all the unconstrained atoms were converged to  $0.01 \text{ eV } \text{Å}^{-1}$ . Brillouin zone sampling was restricted to the  $\Gamma$  point. The periodic model of Sn-Beta polymorph zeolite was used in this study.<sup>7</sup> A complete zeolite Beta unit cell containing an open lattice Sn site (Figure S11) is generated by replacing a Si atom by a Sn atom at the T9 site of Beta.

## 2. Additional table and figures

**Table S1 Physicochemical properties of the synthesized materials**

Samples	Sn content mg/g <sup>a</sup>	S <sub>BET</sub> (m <sup>2</sup> g <sup>-1</sup> ) <sup>1</sup>	Micropore area (m <sup>2</sup> g <sup>-1</sup> )	Micropore volume (mL g <sup>-1</sup> )	Brønsted site density(mmol g <sup>-1</sup> )	Lewis site density(mmol g <sup>-1</sup> ) <sup>b</sup>
Al-Beta	-	592.5	454.1	0.181	0.155	0.072
deAl-beta	-	580.9	444.5	0.177	0.018	0.017
0.5 wt% Sn-beta	5.72	576.4	420.4	0.168	0.017	0.036
0.75 wt% Sn-beta	7.60	574.6	419.3	0.167	0.025	0.072
1.5 wt%	15.92	554.9	401.7	0.161	0.023	0.131

Sn-beta						
3.0 wt%	31.91	535.7	393.3	0.157	0.021	0.131
Sn-beta						
5.0 wt%	47.74	525.0	390.2	0.156	0.029	0.136
Sn-beta						

a. Measured by ICP ; b. Acids calculated from peak areas of FT-IR spectra obtained by pyridine desorption 350 °C.

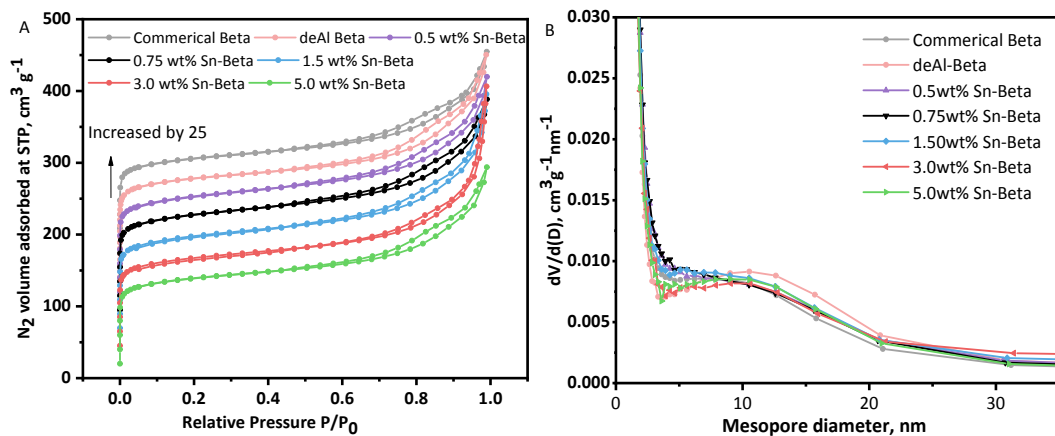
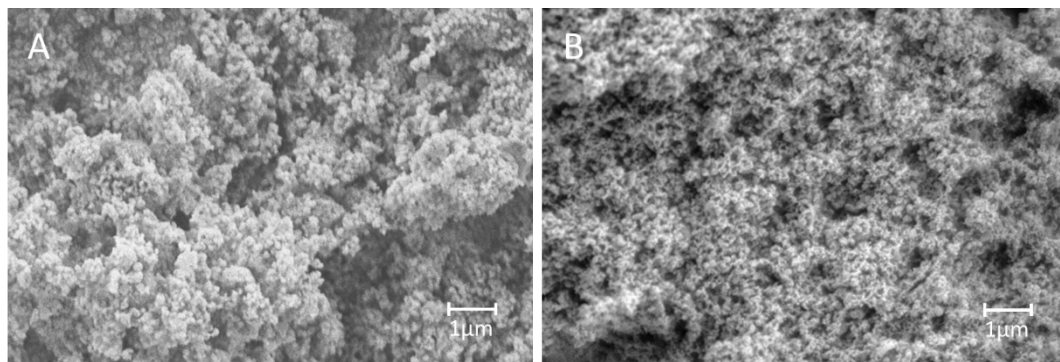
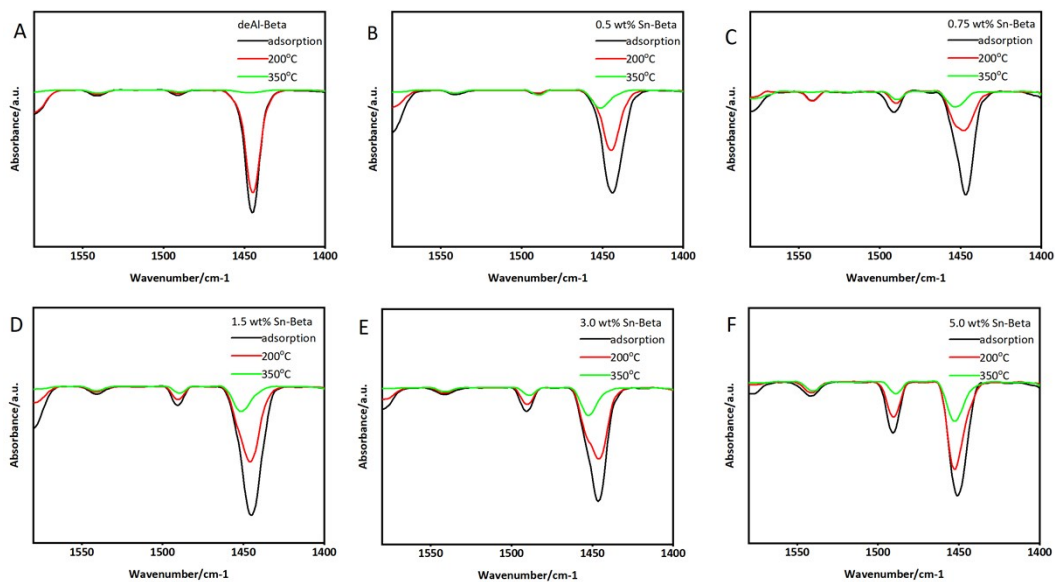


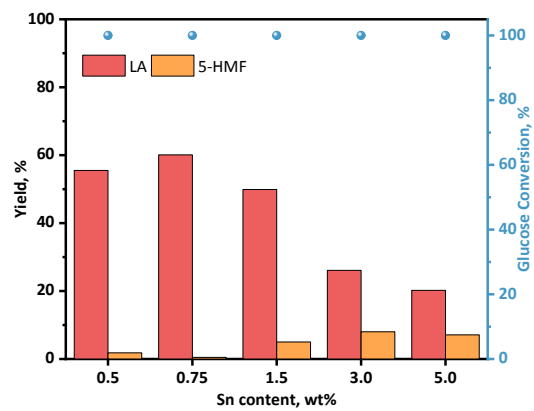
Figure S1. (a) N<sub>2</sub> adsorption-desorption isotherms and (b) the corresponding mesopore size distributions of the samples



**Figure S2. Typical SEM micrograph of (a) commercial Beta; (b) 0.75 wt% Sn-Beta**



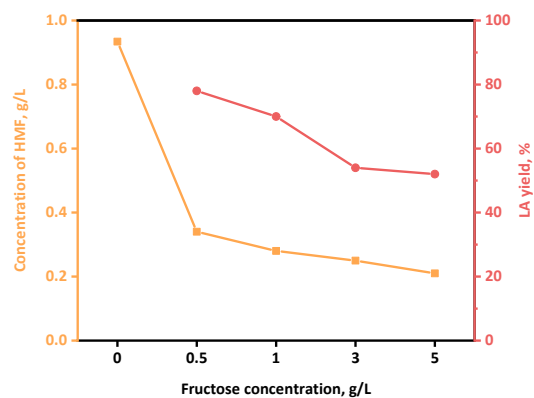
**Figure S3. Py-IR of (a) deAl-Beta; (b) 0.5 wt% Sn-Beta; (c) 0.75 wt% Sn-Beta; (d) 1.5 wt% Sn-Beta; (e) 3.0 wt% Sn-Beta; (f) 5.0 wt% Sn-Beta**



**Figure S4. Product distributions from glucose with different Sn-Beta catalysts**

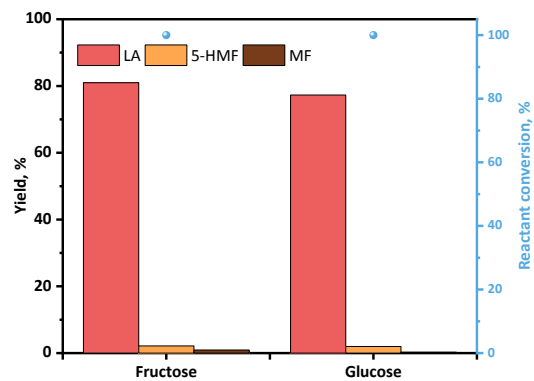
Reaction conditions: 0.5 h, 50.0 mg glucose, 10.0 mL water, 4 MPa N<sub>2</sub>, m(glucose):m(Sn)=50:1, 200 °C, 530 rpm.





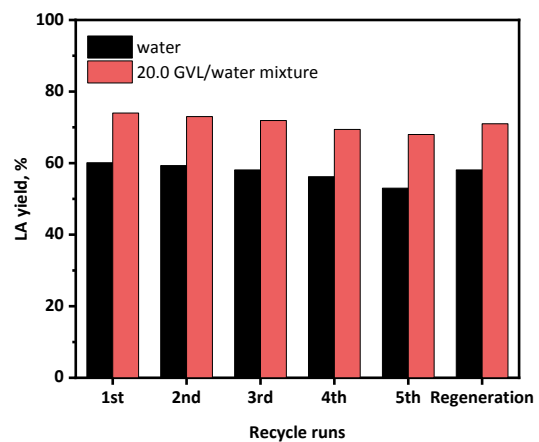
**Figure S5. HMF stability and LA yield at 1g/L HMF and different fructose concentration.**

Reaction conditions: 0.5 h, 10.0 mg HMF; 0, 5.0, 10.0, 30.0, and 50.0 mg fructose was added for different fructose concentration, 10.0 mL water, 4 MPa N<sub>2</sub>, 200 °C, 100.0 mg 0.75 wt% Sn-Beta catalyst, 530 rpm.



**Figure S6. Lactic acid synthesized with fructose or glucose concentration of 1.0 g/L**

Reaction conditions: 0.5 h, 10.0mg fructose or glucose, 10.0 mL water, 4 MPa N<sub>2</sub>, 200 °C, 100.0 mg 0.75 wt% Sn-Beta catalyst, 530 rpm.



**Figure S7. Catalytic recycling results for Sn-Beta catalyst in water and 20.0 wt% GVL/water.**

Reaction conditions: 0.5 h, 50.0 mg glucose, 10.0 mL water, 4 MPa N<sub>2</sub>, 200 °C, 100.0 mg 0.75 wt% Sn-Beta catalyst, 530 rpm.

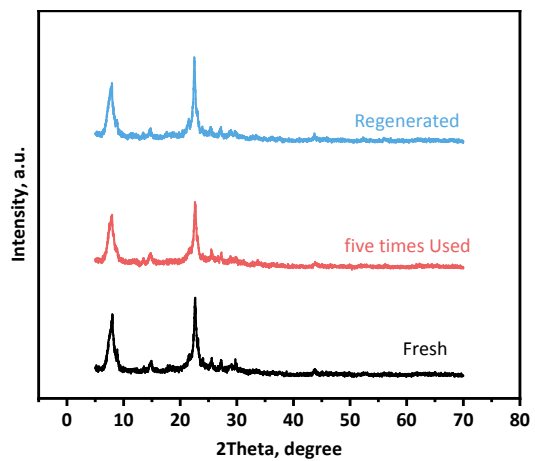


Figure S8. XRD patterns of the fresh, used and regenerated Sn-Beta catalyst by calcination at 550 °C for 3 h.

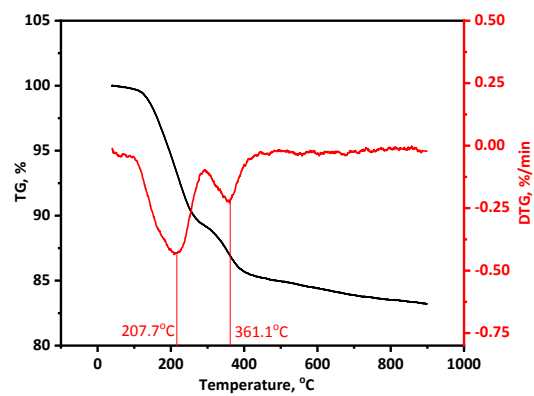
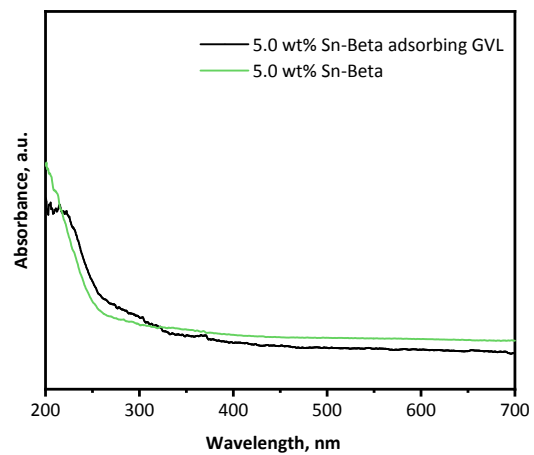
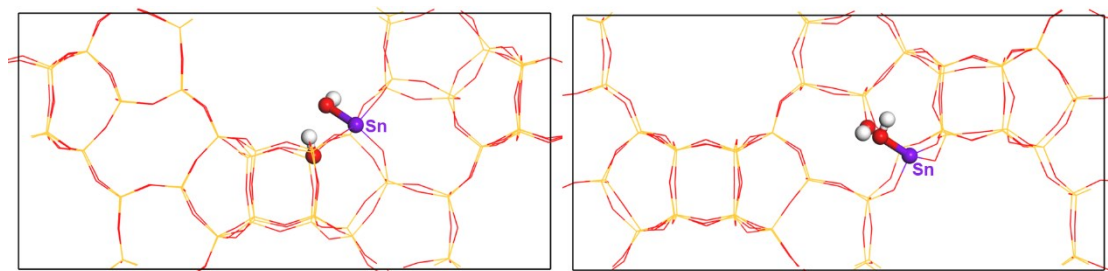


Figure S9. TG and DTG signals of deAl-Beta pre-adsorbed with 16.6 wt% GVL.



**Figure S10. UV-vis spectroscopy of 5.0 wt% Sn-Beta and 5.0 wt% Sn-Beta catalyst pre-adsorbed with 16.6 wt% GVL.**



**Figure S11. Optimized structure of the open Sn site in the Sn-Beta catalyst model.**

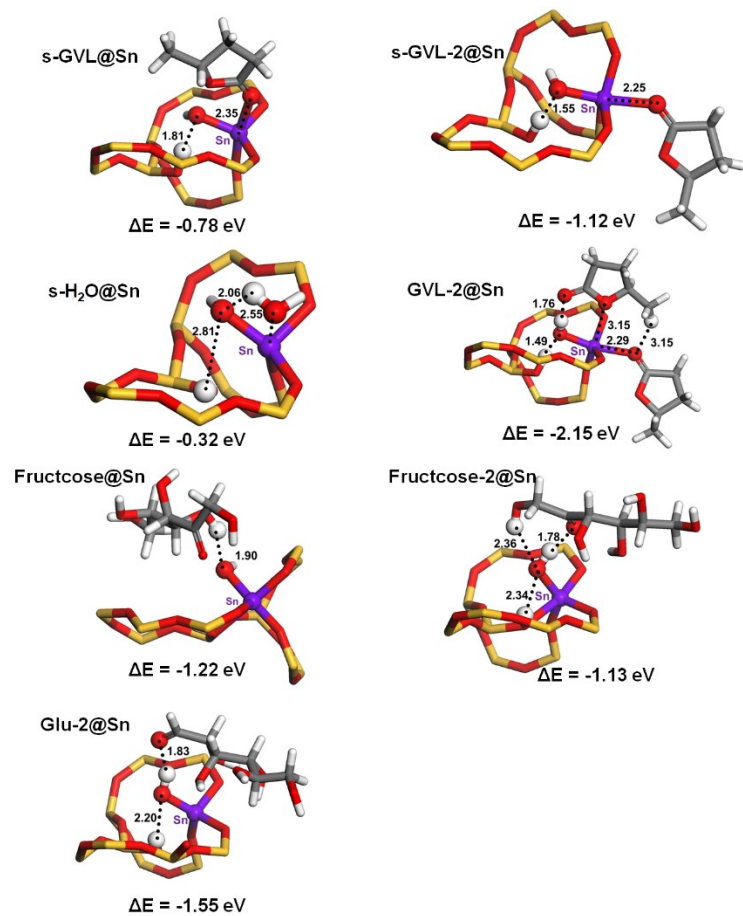
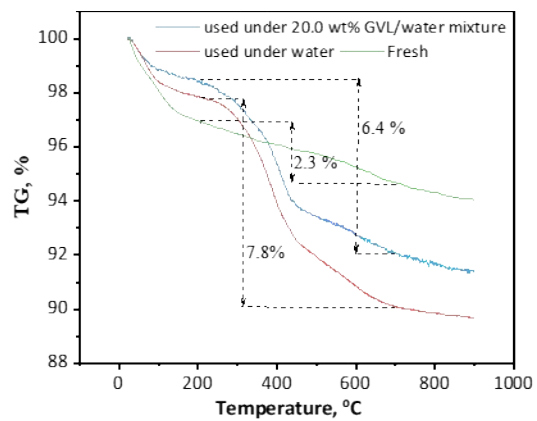


Figure S12. Other possible adsorption configuration of GVL, water, glucose, and fructose





**Figure S13.** TG profile of fresh 0.75 wt% Sn-Beta and 0.75 wt% Sn-Beta after five runs under water and 20.0 wt% GVL/water mixture under a flowing air atmosphere.

**3. List of DFT-optimized fractional coordinates of the isolated molecules and the catalyst models with and without adsorbates.**

**Coordinates of the optimized structures of the open Sn sites**

open Sn site

CONTCAR

1.0

12.6569995880	0.0000000000	0.0000000000
0.0000000000	12.6569995880	0.0000000000
0.0000000000	0.0000000000	26.3959999084

O Si Sn H

129 63 1 2

Cartesian

4.106943190	8.311598336	1.752958292
4.366411736	10.359374468	0.066253960
3.274239218	10.735793331	2.413386297
5.876644993	10.256599627	2.196675049
4.441467826	6.488863732	26.240791476
3.046919543	5.922083466	2.039090897
5.697801635	6.182564438	2.124350122
8.998367330	8.402476038	1.755070086
10.770726563	10.403927257	1.852207319
8.380705856	10.751235472	2.823052188
10.689848645	6.357863927	1.557627929

8.302738475	6.012454577	2.630889321
12.461069463	8.369440917	1.565810690
0.606143711	10.670356799	2.561203842
0.431477130	6.023212926	2.576513466
9.091776097	4.019483370	14.667465875
8.781932934	1.870577967	13.140456408
9.786012300	1.661231120	15.591589309
7.189808956	2.183458975	15.201456828
8.866734569	6.085991651	12.933512357
9.479333157	6.498610032	15.475975154
6.723398076	8.245149378	14.946735640
3.558135753	4.130864966	15.011932622
2.157005945	1.950063988	14.656907297
4.594997133	1.821342329	15.771082001
1.951582815	6.201423706	14.596460181
4.211237048	6.491015327	15.991753306
0.426287739	4.030368461	14.765129975
12.465625382	1.671356703	15.775833440
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4.359703469	3.694198444	8.277257819
2.384072513	4.229589725	6.567324634
1.952468688	2.735050961	8.722294595
2.363314947	5.376693533	8.907066576

6.311919240	4.163013648	6.510309332
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6.258886438	5.489467403	8.780365205
4.330339337	8.894706804	8.481034769
2.172700626	10.397725204	8.091693670
1.950823307	8.007451014	9.188711274
6.488863732	10.440379128	8.194902164
6.665555495	8.055800779	9.345239725
4.326541984	11.946056089	7.982150186
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6.482535691	0.238457873	9.168914135
8.614607245	8.469178480	21.873309582
10.179012472	8.357163552	19.707781436
10.885146569	9.812465141	21.841898165
10.922231394	7.137661462	21.864335341
6.861739104	9.137594042	20.014766880
6.293819669	9.659569167	22.470914752
6.340777159	7.131206679	21.750303950
8.515123166	3.751534812	21.516171283
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10.787814084	4.563860877	22.528721830
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6.138518239	4.557912307	22.337350541

8.523603556	0.473498335	21.440678468
10.781738772	12.366648270	22.603423263
6.207499017	12.364749405	22.430529093
8.234263910	8.534234786	24.872158330
8.701307746	10.525307505	0.192690804
9.913848085	10.463667949	24.243670379
7.295621076	11.018804182	24.460117309
8.496137534	6.420896135	0.033786879
9.898026474	6.499242987	24.212258961
7.250562074	6.210916145	24.101396245
3.867093232	8.528919171	24.612422958
2.195736340	10.562519073	24.900402646
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2.255730515	6.402543458	24.723021356
4.633854082	6.227497076	23.614653791
0.553617169	8.440952761	24.806168393
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4.258700751	4.228830028	11.386970070
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3.055526297	1.906650366	10.995781888
5.712736808	2.016766241	11.005811830
4.368436966	6.034098017	13.382508403

3.157288524	6.621129448	11.099253914
5.823991662	6.371407202	11.256838065
8.749024555	3.926580816	11.443457915
10.710606400	2.129793406	11.324940190
8.269830097	1.507068953	10.552856513
10.730604458	5.707927029	11.072858254
8.295271266	6.280782984	10.334826032
0.033667619	3.947718043	11.457975764
0.469068405	1.512638052	10.582684380
0.552351448	6.377735243	10.605385088
8.611316483	3.759508611	18.109239998
10.571126204	4.189593609	19.897832706
11.031208289	2.886681969	17.627248983
10.607831559	5.511490314	17.661827502
6.587714856	4.262117878	19.751334196
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7.026026759	5.818929154	17.596893266
8.340456256	8.855975843	17.837888773
10.422279935	10.510499074	18.228814210
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6.584298106	10.829582324	17.976467169
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8.635997201	12.505748240	18.303249751

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6.743143405	9.696021037	4.644640258
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6.673656414	4.427165231	3.900800897
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1.942722954	12.329816174	4.021958660
6.503292692	12.238432259	3.897897327
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0.158085920	6.303818699	26.350862811
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12.398037255	6.005113356	13.119075719
2.158271477	12.624091209	6.632259264
6.452032391	12.546756783	6.536705385

10.668584676	12.550301029	19.980979743
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4.331478505	6.725422929	1.445708922
9.213283087	10.010294131	1.643942855
9.129873349	6.804908949	1.483191208
12.286782024	9.979664088	1.480815587
12.251722805	6.767824123	1.405850917
6.864144182	10.738198409	3.395845249
8.698649184	2.423182569	14.667728620
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3.664960676	2.555701391	14.667728620
3.508520455	5.730076682	14.762491510
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0.419579519	5.644768833	14.558712987
6.086624606	2.001198113	16.393764385
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5.940942356	4.058213954	8.086150849
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5.926640139	8.911920314	8.181704334
2.709357251	11.928209625	7.989805195
5.942967586	11.958206713	7.966840955



2.011323884	6.576323929	9.940469962
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10.124207169	3.646228528	21.366769990
6.919961156	3.673567431	21.231885760
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1.926015658	1.581238981	9.876854958
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131 63 1 6

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133 63 1 18 10

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0.0000000000	0.0000000000	26.3959999084

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130 63 1 4

Cartesian

4.221489184	8.311092123	1.817100556
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3.300818801	10.708454806	2.468553927
5.905249806	10.339882623	2.163680080
4.432481223	6.524936132	26.253725775

3.020339771	5.979546199	2.043842336
5.680461384	6.082700888	2.120126730
8.983052686	8.427916453	1.769587738
10.781358547	10.410129311	1.892329249
8.396653455	10.768195497	2.864757866
10.685545456	6.399125953	1.580328539
8.294511569	6.033844910	2.642503600
12.487142834	8.391590570	1.601181378
0.630318593	10.717820880	2.542198676
0.416288709	6.037008931	2.612940052
9.052919148	4.030115355	14.717090094
8.727000890	1.895512169	13.174243545
9.702982788	1.655662022	15.631974968
7.122346818	2.208013517	15.227061106
8.840407715	6.093206131	12.967563026
9.425920507	6.517342181	15.494979337
7.061592946	8.327926161	15.229699571
3.511431369	4.083148156	14.785455750
2.104226249	1.898423460	14.740318652
4.542723651	1.854883286	15.825457658
1.947659098	6.202056284	14.711547273
4.245410960	6.223699723	16.122148842
0.409453937	4.026950957	14.790207189

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12.125152176	6.375963874	15.693213466
4.322871750	3.687616919	8.337704148
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1.881589611	2.757960122	8.670558189
2.337241577	5.394666362	8.892020876
6.258126741	4.185163301	6.556766449
6.792252112	2.855039312	8.781157373
6.223573358	5.474531853	8.847675160
4.337553817	8.888630738	8.432729783
2.182699655	10.420634553	8.167450017
1.993857080	8.023019142	9.261564837
6.503166705	10.427595549	8.198333584
6.652012974	8.049219254	9.351574715
4.345401252	11.947447987	8.006698763
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6.516329754	0.214915851	9.182904134
8.613974290	8.447787770	21.926100902
10.145471138	8.348303691	19.734177096
10.849706370	9.849930193	21.840842464
10.953493637	7.177657578	21.897593841
6.907304319	9.212903616	20.073365340
6.319893039	9.705893325	22.523179009

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8.497276702	3.763558694	21.515906964
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10.760095333	4.596516150	22.535584670
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6.140543469	4.592592432	22.352924877
8.500820949	0.513494452	21.465227045
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6.197246882	12.413984854	22.479361930
8.221354344	8.572712263	24.916768364
8.721938759	10.567202487	0.225949759
9.888027444	10.494424733	24.250533219
7.278154838	11.066647733	24.522411507
8.494492153	6.441779878	0.048040720
9.882078874	6.537087510	24.222024585
7.234108262	6.256354995	24.119873364
3.853929805	8.544993512	24.599488660
2.172827179	10.569100598	24.898555563
4.616767314	11.037663072	23.999770515
2.243453150	6.418491057	24.743874195
4.617146786	6.232686326	23.632075210
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2.981229716	2.064103579	10.975456899
5.648185961	1.957911234	10.997365439
4.358311195	6.168262220	13.452985460
3.126405375	6.527467952	11.142543142
5.803487391	6.420896135	11.303295182
8.755985551	3.940377198	11.464310754
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10.982352311	2.887694395	17.644406083
10.588719185	5.517059413	17.667106005
6.566704372	4.334136312	19.765852832
6.072448752	3.339929234	17.390476278
7.001346041	5.858671787	17.566801867

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10.718453835	8.112250708	17.143409312
6.496331696	10.835404152	18.002600084
5.636415185	8.356277867	17.920771492
8.589546301	12.463094316	18.320935489
11.034625039	0.226307155	17.408426334
6.344700877	0.678162051	17.266943582
4.376284024	8.472848713	4.872965392
2.445332410	8.201862499	6.683203502
2.039802144	9.703489001	4.564924248
2.189407733	7.051720658	4.336070870
6.269011832	8.197432569	6.741801961
6.688971058	9.723739789	4.633817754
6.587968340	7.058176196	4.412883311
4.334136312	3.681794714	4.790346205
2.221683157	2.073216547	5.050610608
1.956772066	4.440708129	3.947521939
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6.717449506	4.443366314	3.963887264
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12.455246881	6.012074729	13.129634298
2.176624155	12.621433402	6.659182774
6.471776965	12.537644193	6.552542860
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6.433299488	0.049615439	19.856391346
6.932618747	5.628314644	14.729231437
4.525130671	8.912805998	15.310208143
4.434885924	9.914101569	1.636288042
4.344768297	6.724537244	1.463658191
9.220877038	10.033582952	1.675618001
9.122279398	6.831362545	1.498500931
12.294503472	9.999409417	1.495333436
12.251975535	6.792758325	1.437526162
6.866295776	10.775916190	3.401124538
8.635744472	2.439636758	14.703891477
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3.619015990	2.482290682	14.654267259
3.503963783	5.697928000	14.794165673
0.566653854	2.412170925	14.608074460
0.418693552	5.644388985	14.593028761

6.039287267	2.030435881	16.439692865
2.736823085	4.031254523	8.121521537
5.903098211	4.054290237	8.134191517
2.744037564	8.894326579	8.124160788
5.938664020	8.901414317	8.170881437
2.728595990	11.946056089	8.028079453
5.961953218	11.946815032	7.980302317
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6.901355749	3.711411953	21.229774359
10.120663678	0.585639392	21.393694287
6.889457855	0.630824853	21.303947155
10.993490509	6.096749999	23.112865638
8.523223331	10.167241319	25.063002555
8.464368324	6.960590227	24.901194028
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0.688034479	6.834906037	24.933134082
6.115862374	11.066647733	23.374978303
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9.158604526	5.513389179	11.476980734
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6.784025206	1.647182009	9.879758528
10.158634188	4.106057129	18.333605468
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9.894356240	8.974445554	18.259168354
6.817819269	9.302261923	18.460042521
10.158001233	12.092876752	18.514153860
6.970842740	12.340448158	18.368712624
10.730098245	6.616953001	16.494597160
2.767452938	8.351974679	5.099179126
5.977141498	8.357417036	5.152499083
2.739227785	3.608257264	5.088357015
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5.918792704	0.484509932	5.142732673
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1.985503432	10.844770226	3.403236333
6.808199711	5.913476712	3.280230897
11.006653558	1.633006156	16.611531334

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10.983111254	10.868185789	23.113129957
6.089156048	6.084219528	22.972702905
5.968281637	7.122979773	16.400889970
7.972391041	8.375263500	15.578919330
6.429629254	5.919552023	13.937616513
5.324040202	9.420098679	15.049942561
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CONTCAR

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133 63 1 18 10

Cartesian

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4.534243638	6.504938073	26.285137192

3.106280763	6.044223411	2.082644444
5.768554159	6.150542498	2.182685247
9.049248160	8.445636175	1.783577737
10.855528952	10.412407647	1.949608477
8.473228185	10.774903764	2.931803700
10.771486259	6.425832278	1.580856389
8.381971766	6.044097046	2.647782693
12.578779478	8.408171124	1.623354039
0.690186168	10.722630282	2.635376638
0.500204613	6.047134702	2.619275042
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8.826484969	1.851465970	13.149694968
9.758420291	1.572758780	15.626432147
7.223476278	2.268767200	15.194065351
9.113166053	6.090168475	13.017451563
9.545149915	6.459626342	15.556746472
6.354699906	7.689506932	15.579975030
3.551174380	4.213768491	14.797070029
2.145994301	2.032587475	14.828744192
4.614742085	1.984364452	15.827833378
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3.773937571	6.387228059	16.227204419
0.402745717	4.129725798	14.862267011

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2.318509240	5.423777388	8.949035785
6.313817728	4.269965313	6.621700685
6.820097606	2.893643154	8.809137371
6.277745328	5.529083672	8.934517936
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2.239655986	10.454175133	8.176688576
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6.575437491	10.483539265	8.234496441
6.754787816	8.103517588	9.382986132
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6.509748229	0.272125500	9.270011228
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6.593916910	2.125869689	21.860110965
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3.223358011	6.593031225	11.145974562
5.864114521	6.547466010	11.366381549
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6.603536468	5.961320263	18.149361338



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8.736114235	0.175046299	18.400388361
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4.470325746	8.454749520	4.830204014
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6.275973205	8.239580280	6.794330536
6.751497053	9.798795879	4.730955184
6.750104401	7.144875942	4.446670054
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6.548605178	0.400467475	19.879619905
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3.360686612	4.707264790	18.914053538
3.862030346	6.900596052	18.945993593
3.565350233	9.439590524	15.984888893
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4.439315855	6.765926013	1.495597361
9.291123726	10.053201539	1.732633500
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12.374242221	10.016749668	1.563698994
12.340068687	6.811617216	1.451252038
6.949072559	10.832999074	3.489023408
8.754087441	2.431789323	14.669312958
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3.660024533	2.619365988	14.674328715

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0.360977619	5.733620928	14.559770261
6.134341415	2.154221395	16.395347149
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5.949422746	4.125548974	8.200709304
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2.789602780	11.980483107	8.051308011
6.019669057	12.001747076	8.041277283
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7.143357302	8.633085910	21.616475420
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11.112719162	6.146618781	23.109434218
8.634605304	10.224197461	25.121336696
8.587647436	7.008307037	24.911225543
3.823679611	10.177873303	25.078310999
3.882281511	6.979196388	24.869782610
0.742079896	10.108892525	25.045581136

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4.477034012	5.935373258	11.942342498
9.204043754	2.389641612	11.658585613
9.246318207	5.523641315	11.506279964
12.350447187	2.450521660	11.692899813
12.268682831	5.556802423	11.592067039
6.859208038	1.708315164	9.932022784
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6.975145929	4.414634759	18.372935427
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6.902368175	9.506545696	18.589646675
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7.124371670	12.606371487	18.423615346
10.807558659	6.700868952	16.532869844
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6.059412067	8.401969825	5.198164424
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2.157132498	11.321432865	15.698229224
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135 63 1 14 6

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6.458233690	12.656366633	19.974908285
6.843765898	5.688308819	14.899749887
5.209747693	10.767689284	10.964370470
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2.815929257	8.912046301	14.744277136
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8.109213429	10.808445098	11.242584535
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9.286187582	10.015737242	1.748734900

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0.681959120	6.748838491	25.020503922
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Cartesian

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8.296156950	10.695038272	3.031052727
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Glu-2@open Sn site

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