

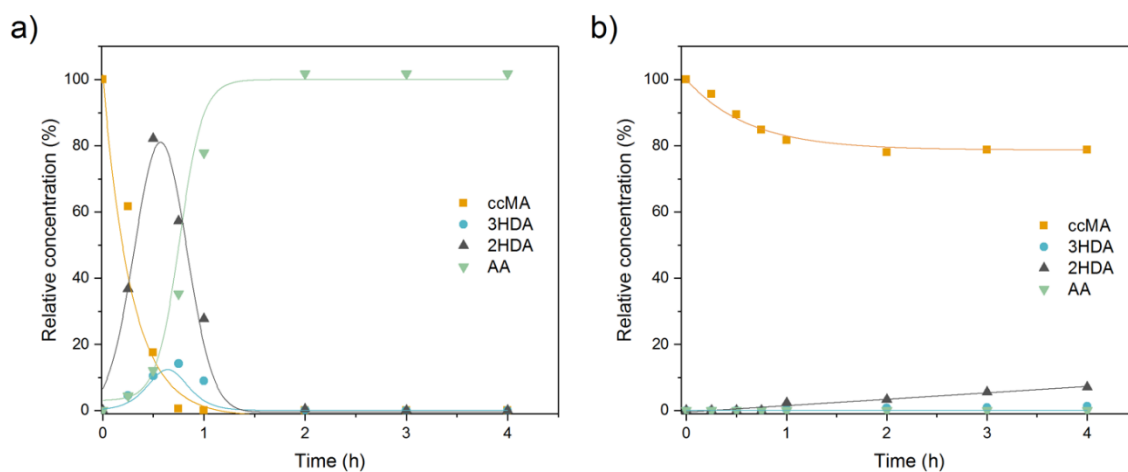
## Supplementary Information

### Electrochemical hydrogenation of bioprivileged *cis,cis*-muconic acid to *trans*-3-hexenedioic acid: from lab synthesis to bench-scale production and beyond

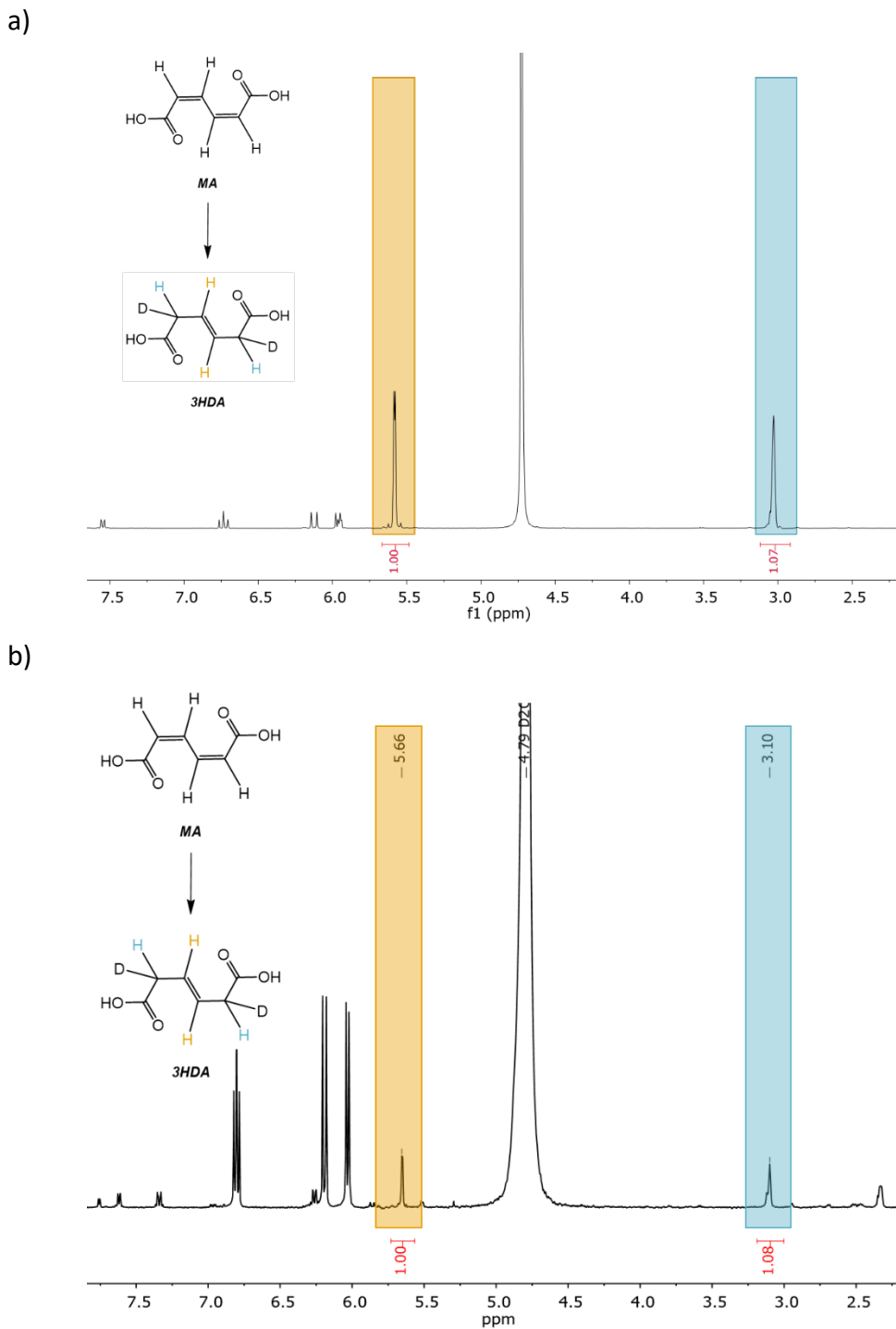
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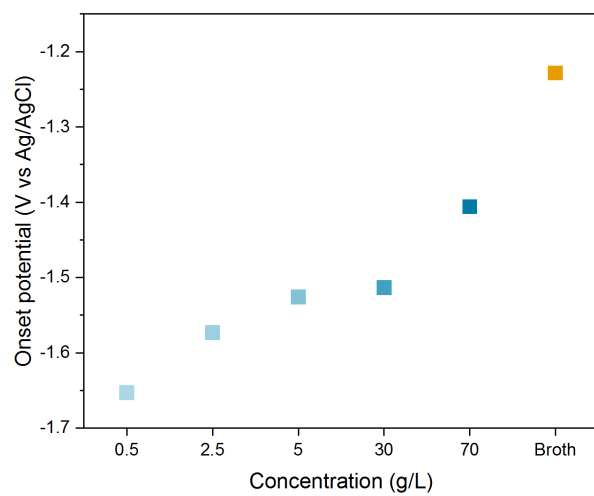
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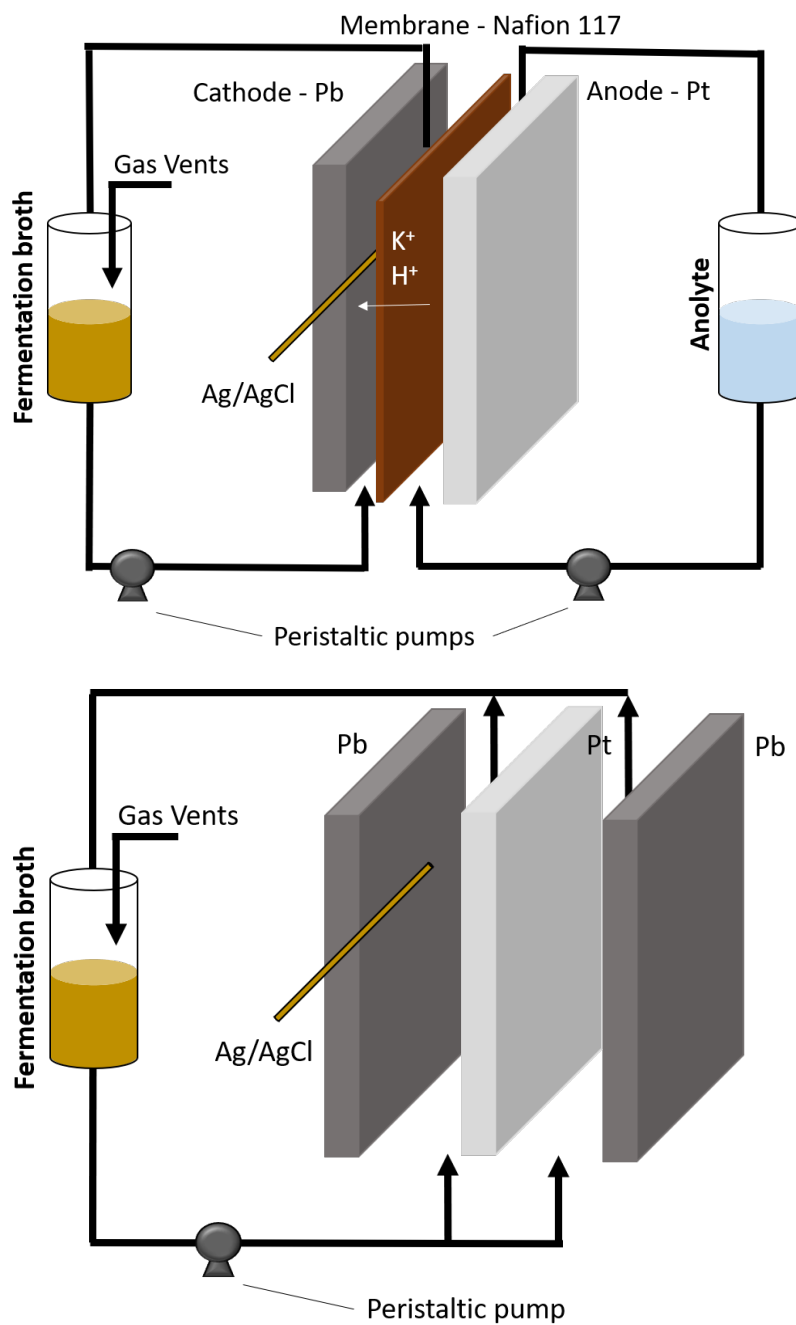
**Figure S1.** Relative concentrations of *ccMA*, 2HDA, 3HDA, and AA during the catalytic hydrogenation of a *ccMA* model solution with (a) 0.4 g/L glutamic acid, 1 mg/L alanine, and 0.6 g/L tyrosine, and (b) 600 mg/L of Peptone. 2HDA and 3HDA indicate a mixture of *cis* and *trans* isomers where the *trans* isomer is the major product.



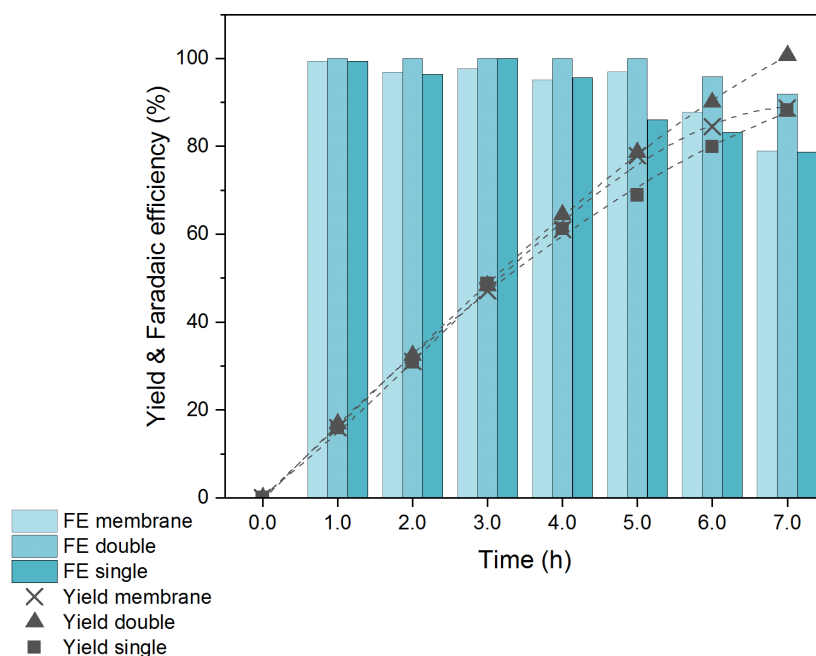
**Figure S2.**  $^1\text{H}$  NMR spectra collected after the electrohydrogenation of 5 g/L of *ct*MA in 0.1 M  $\text{D}_2\text{SO}_4/\text{D}_2\text{O}$  (pD 1) using (a) a lead (Pb) electrode and (b) a palladium (Pd) electrode at -1.2 V vs Ag/AgCl.  $\text{H}_2$  gas was bubbled during each of the reactions to study the possible contribution of hydrogen formed through HER. The signals at 3.10 and 5.66 ppm correspond to the protons in  $\alpha$  and  $\beta$  of the carboxylic functional groups of *t*3HDA. The ratio between the integrated areas of the peaks is 1:1, which indicates a 2,5-addition of deuterium during the electrohydrogenation reaction.



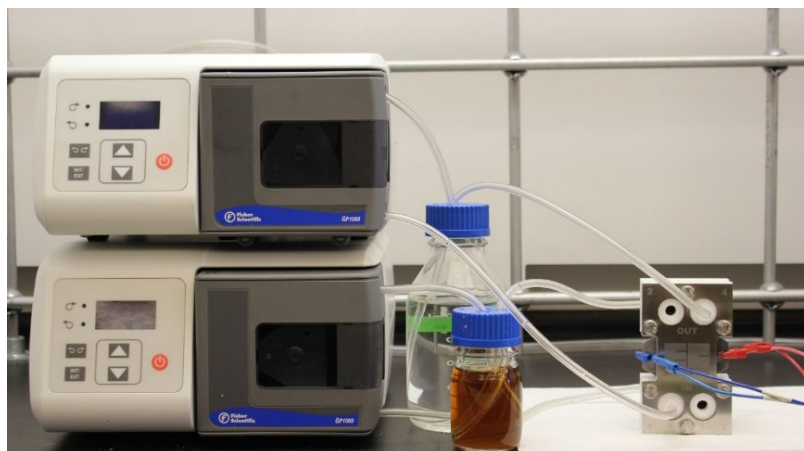
**Figure S3.** Onset potentials for the electrohydrogenation of *ccMA* at pH 7 for model solutions with different *ccMA* concentrations (blue) and for the fermentation broth (orange). The onset potentials were recorded at a current of 0.1 mA.



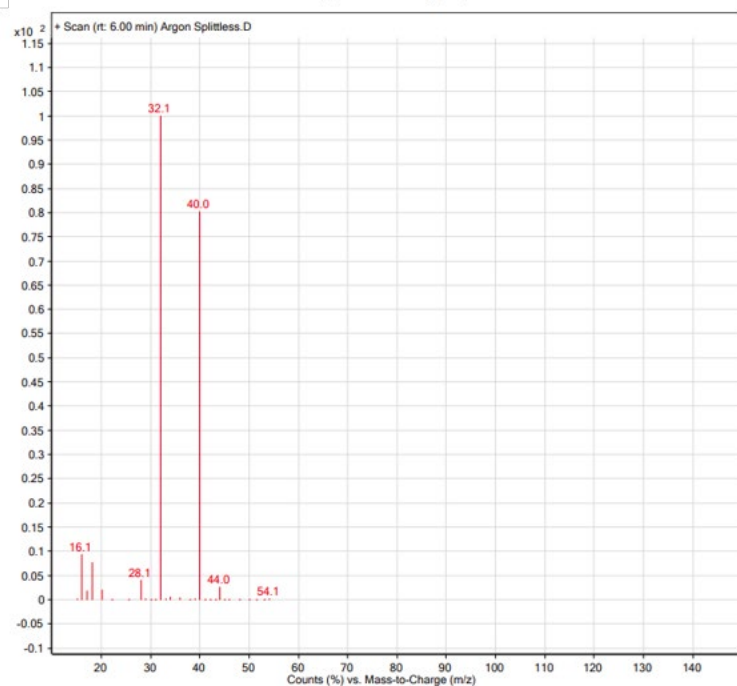
**Figure S4.** Schematics of the electrochemical flow reactors with (top) a divided cell configuration using a Nafion membrane and (bottom) an undivided cell configuration with two modules.



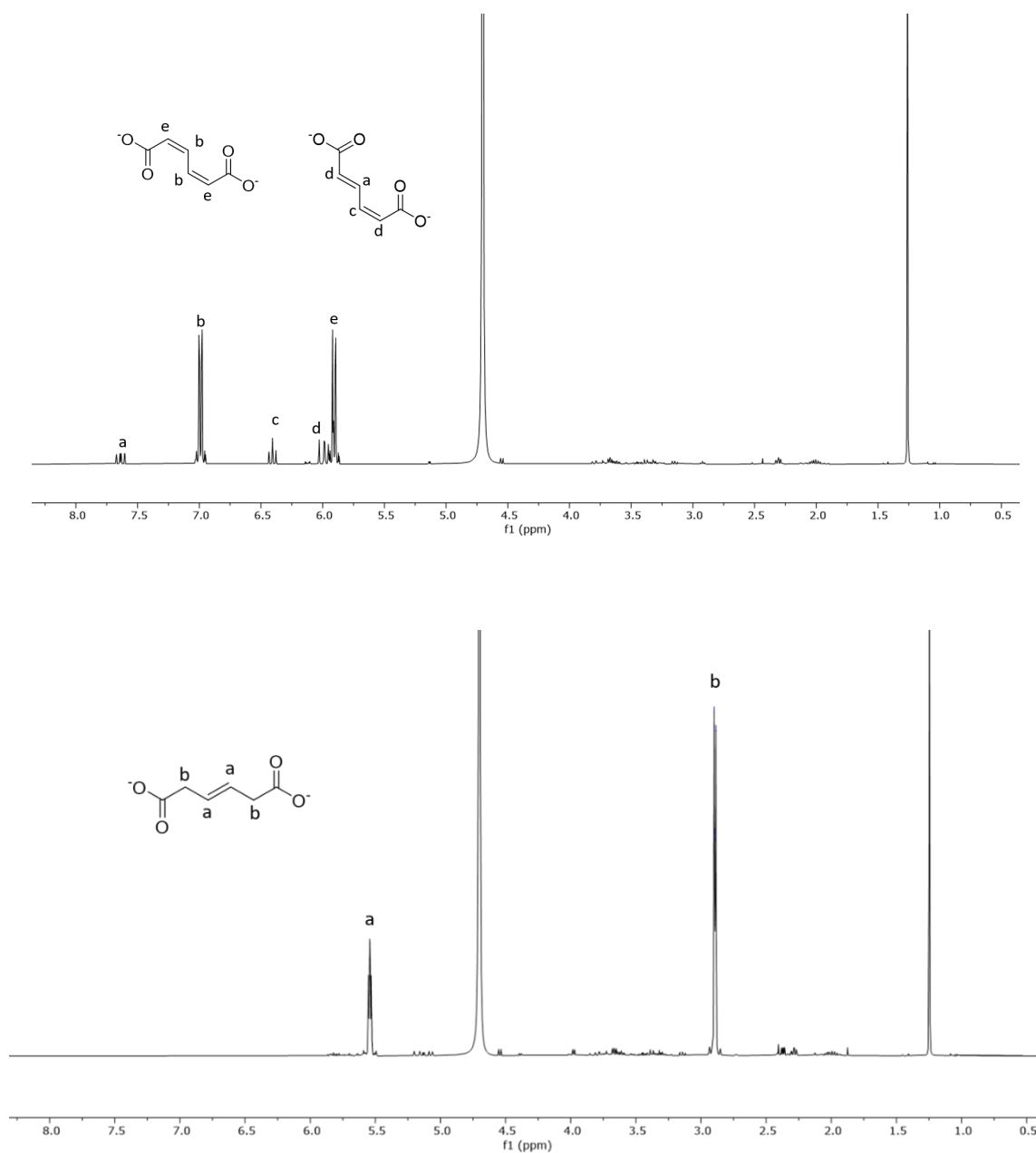
**Figure S5.** Comparison between three different reactor configurations: undivided single-compartment cell (single), undivided double-compartment cell (double), and divided cell equipped with a Nafion membrane (divided). Schematics of the divided and double-compartment configurations are provided in Figure S4. The bars and symbols represent the faradaic efficiency (FE) and the *t*3HDA yield, respectively. The lines that connect the symbols are meant to guide the eye. These results indicate that the addition of a membrane to keep anolyte and catholyte separate did not provide any advantage in terms of selectivity/yield and faradaic efficiency of the reaction. Actually, the membrane adds in complexity as a different feed (0.1 M K<sub>2</sub>SO<sub>4</sub>) needs to be supplied to the anode side to perform the other half reaction. Additionally, a significant gradient in pH between the anolyte and catholyte was observed due to the impermeability of the membrane to OH<sup>-</sup> ions. From an economic perspective, the membrane and anolyte would likely increase the overall capital and operation costs of the reactor system.



**Figure S6.** (top) Looped flow reactor system used for the bench-scale production of *t*3HDA. (bottom) ElectroCell® Micro Flow Cell reactor.

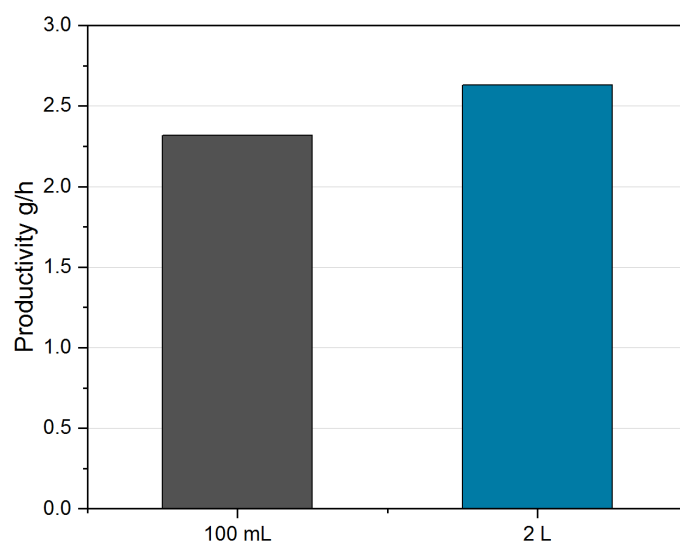


**Figure S7.** Mass spectrum of the gas phase collected during the electrochemical hydrogenation of *cc*MA. The spectrum indicates the presence of O<sub>2</sub> (m/z=32 and 16) and Ar, used here as a sweep gas (m/z=40). Traces of N<sub>2</sub> (m/z=28) and CO<sub>2</sub> (m/z=44) are likely due to the contamination of the sample with air.

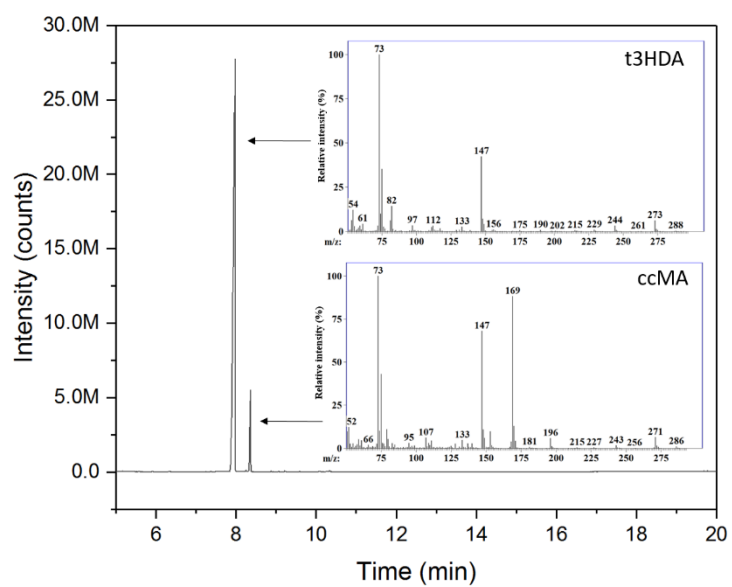


**Figure S8.** <sup>1</sup>H NMR spectra of (top) *cis,cis*-muonic acid and *cis,trans*-muonic acid present in the fermentation broth before reaction, and (bottom) *t*3HDA in the fermentation broth after electrochemical hydrogenation in the flow reactor using a current density of 100 mA/cm<sup>2</sup>. The peaks at 4.75 and 1.25 ppm correspond to water and to the internal standard (dimethyl malonic acid), respectively.

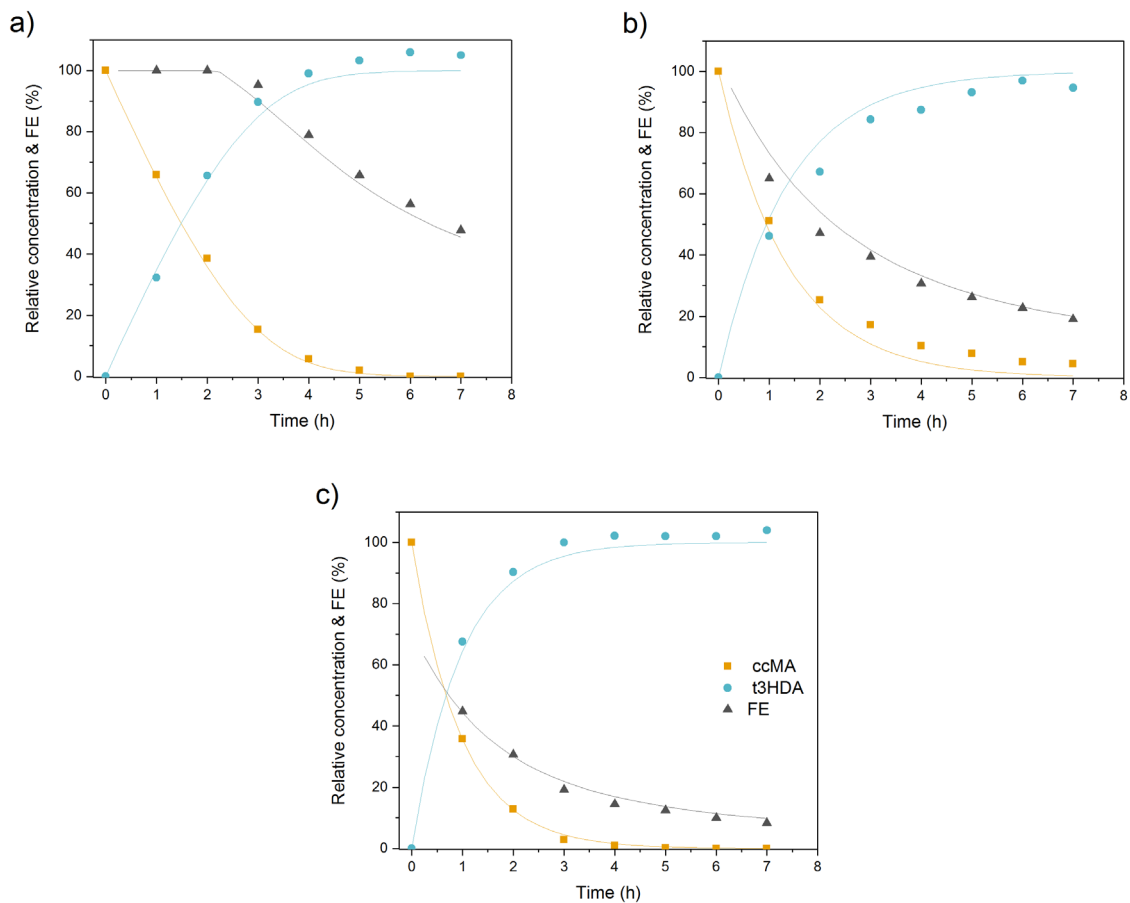




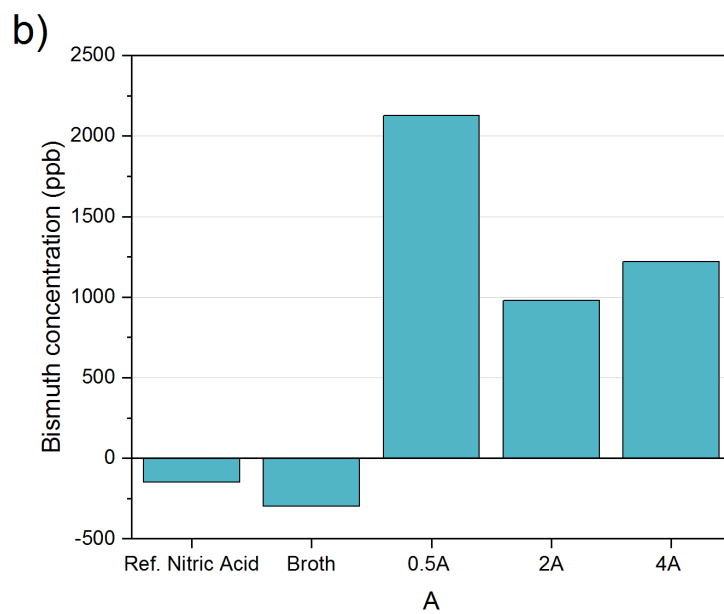
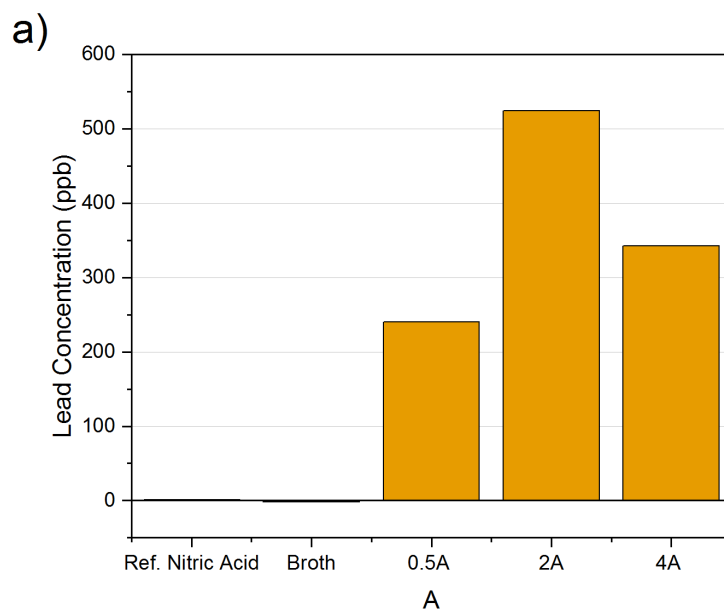
**Figure S9.** Average productivity in  $\text{g}_{\text{B}_{\text{HDA}}}/\text{h}$  calculated when processing a 100 mL batch and a 2 L batch of fermentation broth.



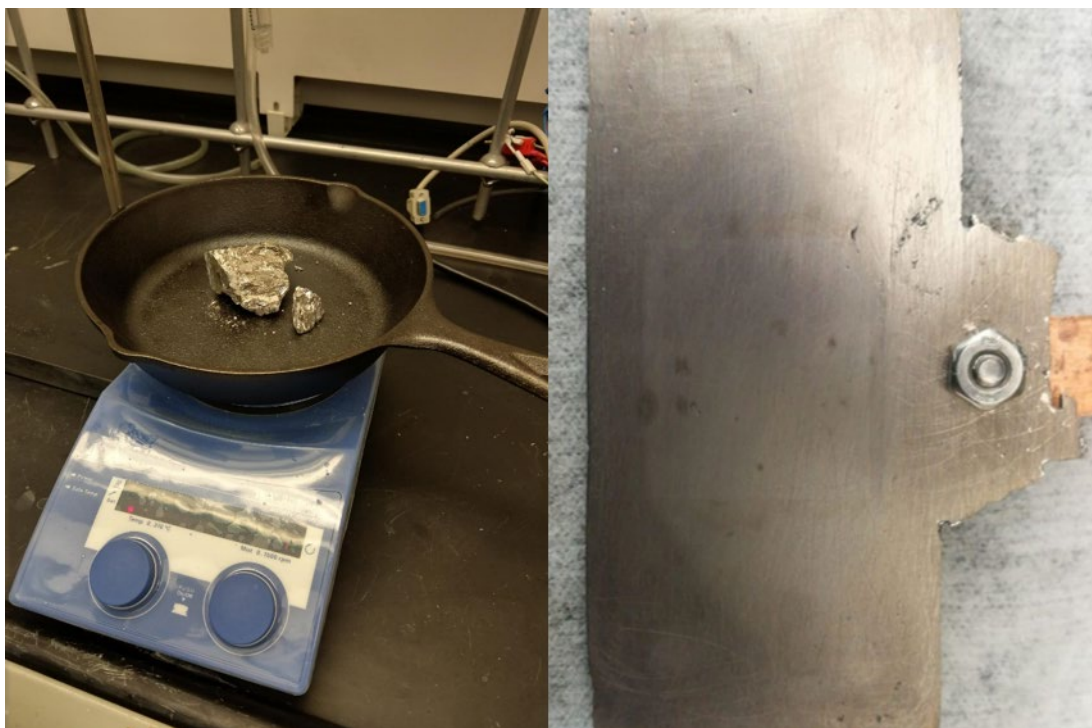
**Figure S10.** GC-MS chromatogram and mass spectra (insets) of the recovered *t*3HDA product.



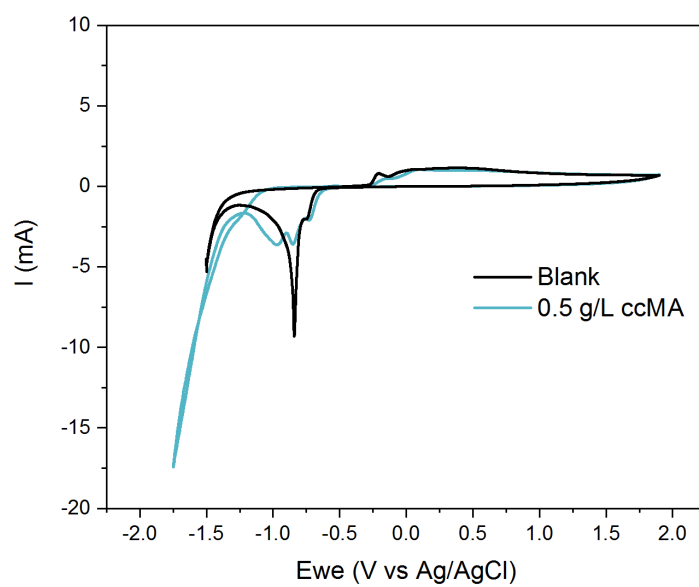
**Figure S11.** Experimental results (symbols) and simulations (lines) based on the proposed kinetic model for the reactions performed at (a) 100, (b) 200, and (c) 300 mA/cm<sup>2</sup>. The model used is based on a mole balance for the reacting volume. The system is considered as a perfectly mixed batch reactor since the flow is looped. The rate law is expressed per units of surface since the reaction occurs at the proximity of the electrode and is a function of the electrode's surface area. The reaction is of zeroth order for high *ccMA* concentration as the term  $k_2C_{MA} \gg 1$  and the rate becomes equal to  $k_1/k_2$  (kinetically or current limited). At low *ccMA* concentration, the reaction is of first order since  $k_2C_{MA} \ll 1$  and the rate is equal to  $k_1C_{MA}$ . The change in the rate law is due to mass transfer limitations at low *ccMA* concentrations.



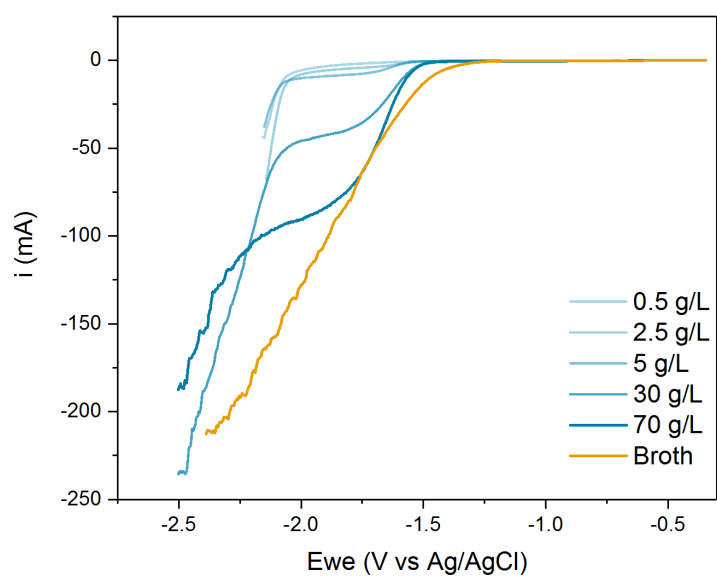
**Figure S12.** Concentrations of the metal impurities in solution determined by ICP-OES for reactions performed with (a) lead and (b) bismuth electrodes for different values of the current.



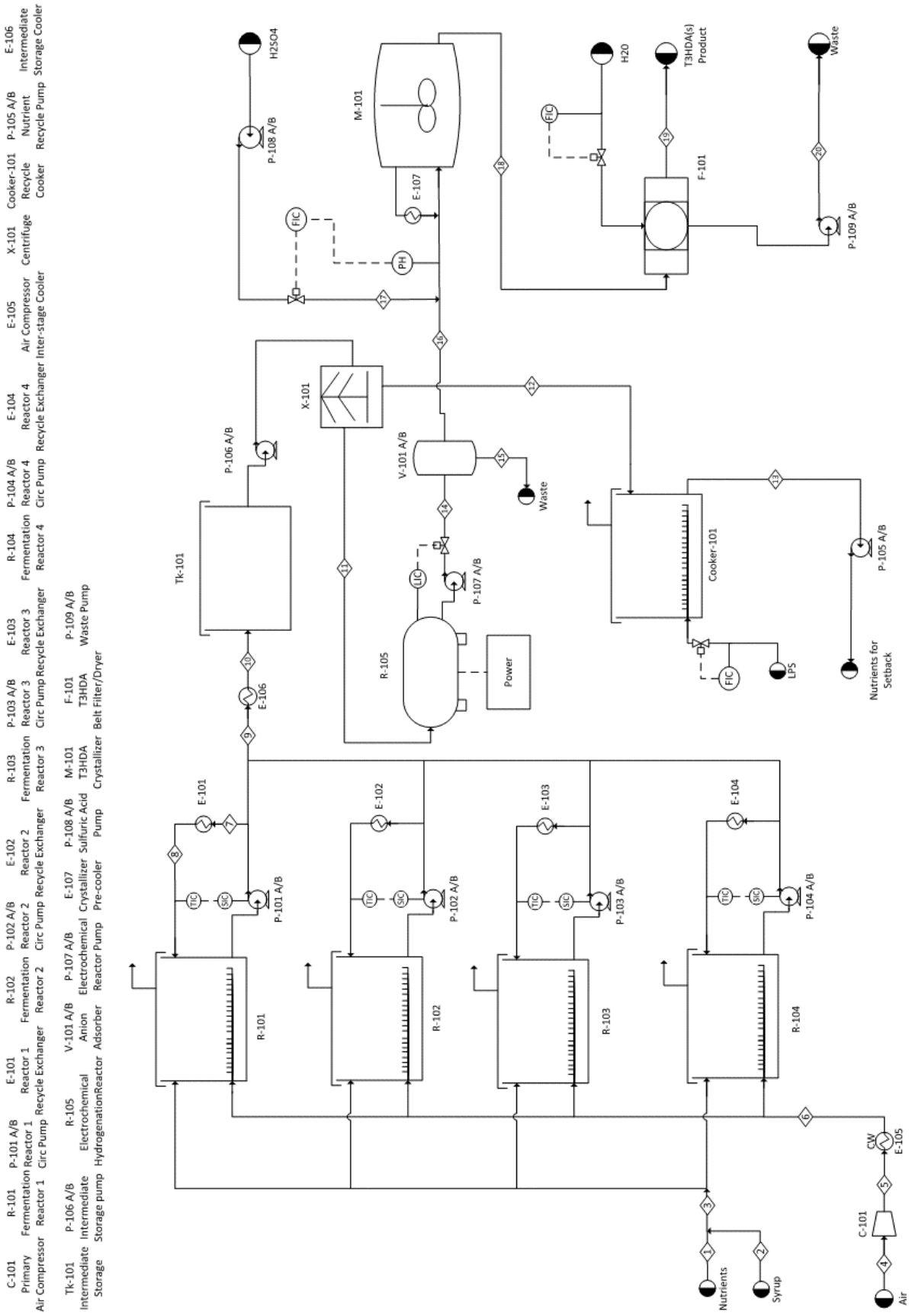
**Figure S13.** Laboratory production of bismuth electrodes by melting bismuth ingots (left). After cooling, the obtained plate was cut to reactor dimensions, sanded, and polished (right).



**Figure S14.** Cyclic voltammograms recorded for a blank and a 0.5 g/L *ccMA* solutions at pH 7 using a bismuth RDE.

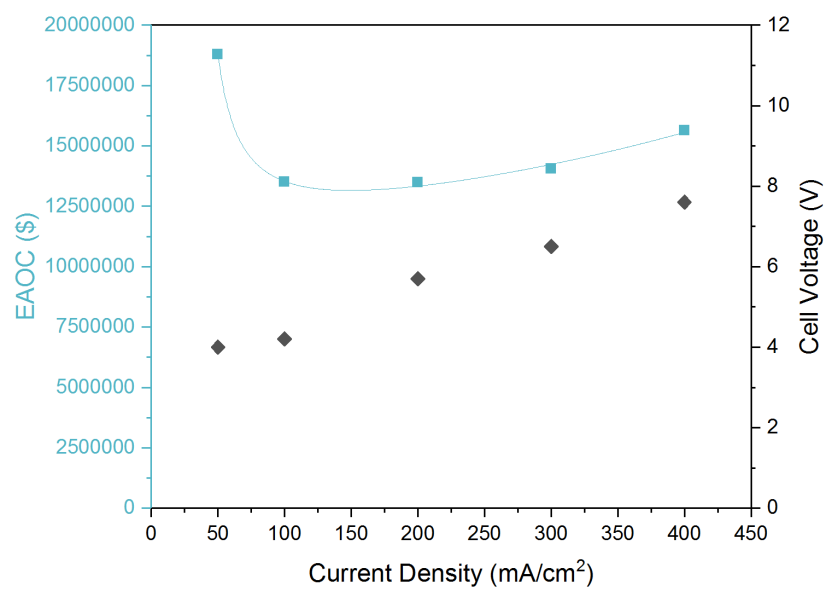


**Figure S15.** Linear sweep voltammograms recorded for model solutions with various concentrations of *ccMA* at pH 7 and for the fermentation broth using a bismuth RDE.



**Figure S16.** Aspen flow diagram for a glucose to t3HDA plant





**Figure S17.** Graph of the equivalent annual operating costs (EAOAC) and cell voltage of the electrochemical reactor at different current densities.

**Table S1:** Results obtained for the production of *t*3HDA using broths with a high concentration of muconic acid (above 70 g/L) at pH 7. The tests were performed using an undivided single-compartment flow reactor. The values provided for the faradaic efficiency, rate, and productivity are average values calculated for the whole duration of the tests.

<b>Current density [mA/cm<sup>2</sup>]</b>	<b>Yield [%]</b>	<b>Faradaic efficiency [%]</b>	<b>Productivity [g/h]</b>	<b>t3HDA in a month [g]</b>
<b>50</b>	98	88.50	1.176	846.72
<b>100</b>	99	78.87	2.079	1496.88
<b>200</b>	94	40.85	2.318	1669.44
<b>300</b>	89	30.71	3.159	2274.84
<b>400</b>	90	24.00	3.195	2300.4
<b><sup>a</sup>0.07</b>	98	99	0.061	44

<sup>a</sup> Productivity of *t*3HDA for experiments run in batch reactor at pH 1, 5 g/L of muconic acid<sup>1</sup>.

## **Technoeconomic analysis for the electrochemical production of *t*3HDA from glucose, via biologically-produced muconic acid**

### ***1. Summary***

Promising preliminary results for the conversion of glucose to *t*3HDA using a biological-electrochemical conversion scheme has prompted further investigation into technoeconomic considerations for the commercialization of this process. The following section outlines an industrial design for the conversion of glucose into muconic acid through biological fermentation for the production *t*3HDA via electrochemical hydrogenation with the goal of minimizing operating cost. The final Aspen flowsheet design was sized to produce 83ktonne/year of *t*3HDA at a cost of manufacturing not considering depreciation (Comd) \$131,698,253 and a product cost \$1.75/kg *t*3HDA.

Non-conventional components and components outside of Aspen databanks were used in this simulation and required the use of several functional group estimation techniques. Specifically, *t*3HDA was not present in Aspen's database and required the use of both the UNIFAC and JOBACK functional group methods to estimate key parameters. Furthermore, while solubility data was provided, the crystallization of *t*3HDA required the addition of the MOFASA functional group method to estimate the solid heat capacities. The results of this design are dependent on these models and prompt further investigation to ensure their validity.

In the final design (Figure S16), glucose and water are fed into a large fermentation reactor and allowed to ferment for approximately 72 hours. Compressed air is fed into the reactor to promote growth of aerobic bacteria and assist in the agitation of the vessels. A recycle cooling loop is utilized to maintain the fermenter temperature at 45 °C and to promote further mixing. Following fermentation, the mixture is cooled to 25 °C prior to entering an intermediate storage tank meant to accommodate process overflows. The cooled fermentation broth enters a centrifuge where cells and nutrients are recycled to save on raw material costs. The clarified broth continues to the electrochemical reactor where muconic acid is converted to *t*3HDA and concentrated via an anion adsorption unit. The concentrated *t*3HDA is desorbed and sent to agitated crystallization reactors where the product is allowed to crystallize. Finally, the stream enters a vacuum drum filter that removes residual moisture leaving dry *t*3HDA crystals.

Special consideration was given to the electrochemical reactor because it was found to represent the majority of both utility costs and capital costs. A parametric optimization was done investigating the impact of voltage vs the equivalent annual operating costs on this unit operation. For the purpose of this analysis, a minimum cost operating point was discovered at approximately 5.7 volts with a current density of 0.2 A/cm<sup>2</sup>. However, Figure S17 prompts further investigation to determine the true operating minimum that may occur between two sets of data points.

Prior to moving forward with this design, a small-scale pilot plant should be created to investigate the scale-up of crystallization kinetics as well as the impact of amino acids/other components not considered in this report. Additionally, key properties of *t*3HDA such as the heat of fusion and solid heat capacities should be measured to increase understanding of interactions within this system. A heat integration study should also be conducted to optimize the use of chilled water

throughout the plant. For this analysis, a refrigeration loop was not considered but would need to be included in the final design. Furthermore, desorption of the anion adsorbent was not modeled and would also need to be considered. Finally, a detailed profitability analysis should be performed given the current and future market for adipic acid and other diacids.

## ***2. Equipment Summary***

The proposed design for the overall process is shown in Figure S16.

All compressors and pumps were sized using Aspen's results for power output. All exchangers were sized using Aspen Exchanger Design and Rating (EDR).

### C-101: Primary Air Compressor

This block serves as the inlet air compressor for the four fermentation reactors. Since the system is aerobic, air must be introduced into the system to promote growth of the cultures and to promote mixing within the vessels. To model the humidity within this air stream, a 0.4 wt% water content was also introduced and a calculator block was used to determine the amount of air required. Within Aspen, the compressor was modeled as isentropic with an efficiency of 0.65 and a mechanical efficiency of 0.9.

### D-101: Primary Air Compressor Drive

The drive was specified as Electric- Explosion proof within Capcost to account for the electricity required to run C-101.

### E-101: Reactor 1 Recycle Exchanger

This exchanger serves as the recycle cooler for fermenter, R-101. Since R-101 is an extremely large reactor, a cooling jacket would be an inefficient/impractical method of cooling the broth. The reaction temperature is maintained via a recycle loop where the bottom of R-101 is pumped through a chilled water exchanger before re-entering R-101. This serves to both cool and assist in the mixing/even heat distribution within the system. E-101 is modeled as a typical shell and tube heat exchanger and specified as a floating head within Capcost. To size E-101, a recycle loop was created within Aspen to model the function of this exchanger and the process conditions were input into Aspen EDR to determine the necessary heat transfer area.

### E-102: Reactor 2 Recycle Exchanger

Similar to E-101, but serves as the recycle cooler for R-102.

E-103: Reactor 3 Recycle Exchanger

Similar to E-101, but serves as the recycle cooler for R-103.

E-104: Reactor 4 Recycle Exchanger

Similar to E-101, but serves as the recycle cooler for R-104.

E-105: Air Compressor Inter-stage cooler

This exchanger serves as an inter-stage cooler for C-101 so that the outlet air stream of the compressor does not enter the reactors at a high temperature. E-105 is also modeled as a shell and tube exchanger with a floating head (sized using Aspen EDR).

E-106: Intermediate Storage Cooler

This exchanger serves as a pre-cooler for the rest of the process prior to entering intermediate storage, Tk-101. E-106 cools the stream down to 25 degrees Celsius using chilled water to prepare the reactor effluent for separation via centrifugation and the electrochemical reaction (sized using Aspen EDR).

E-107: Crystallizer Pre-cooler

Another recycle loop was created for this exchanger. Since the crystallization of t3HDA occurs at such low temperatures (approximately 4 degrees Celsius), refrigerant liquid ammonia was modeled. Although this estimate is sufficient for this stage in design, further optimization on this refrigerant should be done moving forward.

P-101: Reactor 1 Circulation Pump

A centrifugal pump was chosen to model the outlet/recycle pump for R-101. An approximation of a 3 bar pressure drop was used when sizing this pump.

P-102: Reactor 2 Circulation Pump

Similar to P-101, but for R-102.

P-103: Reactor 3 Circulation Pump

Similar to P-101, but for R-103.

P-104: Reactor 4 Circulation Pump

Similar to P-101, but for R-104.

P-105: Nutrient Recycle Pump

The primary function of this pump is to discharge Cooker-101 and can be re-purposed to recycle nutrients from the centrifugation. (2 bar pressure drop accounted for)

P-106: Intermediate Storage Pump

This pump is the outlet of the intermediate storage tank Tk-101 and was sized from Aspen (3 bar pressure drop accounted for)

P-107: Electrochemical Reactor Pump

A dual-purpose pump used to both empty the electrochemical reactor and serve as a recycle pump for the crystallization step within the process. (3 bar pressure drop accounted for)

P-108: Sulfuric Acid Pump

This pump feeds sulfuric acid into the crystallization unit operation to promote growth. (3 bar pressure drop accounted for)

Cooker-101: Recycle Cooker

A jacketed agitated reactor block within Capcost. This unit operation sterilizes the cells using low pressure steam and leaves nutrients that can be recycled to save on raw material costs.

M-101A: t3HDA Crystallizer

The crystallizer was costed as a jacketed agitated vessel with a max volume of 35 m<sup>3</sup>. An approximate volumetric flowrate of 90 m<sup>3</sup>/h was determined from the Aspen flowsheet. From this it can be determined that just over 4 vessels would be needed to handle the crystallization volume required; however, to account for liquid holdup and an operating liquid level of 90% 4 crystallizers were costed. Additionally, Towler mentions the use of a circulating magma crystallizer which can

handle large crystallization volumes and could be explored in further profitability analysis as an alternative crystallization approach.<sup>2</sup>

M-101B: t3HDA Crystallizer

See M-101A.

M-101C: t3HDA Crystallizer

See M-101A.

M-101D: t3HDA Crystallizer

See M-101A.

R-101: Fermentation Reactor 1

The fermenters were sized as follows:

$$83000 \frac{\text{tonnes}}{\text{year}} * \frac{1 \text{ year}}{8000 \text{ hours}} * \frac{1 \text{ L}}{0.08 \text{ kg}} * \frac{1 \text{ m}^3}{1000 \text{ L}} * \frac{1000 \text{ kg}}{1 \text{ tonne}} * 72 \frac{\text{h}}{\text{run}} = 9338 \text{ m}^3$$

This is equivalent to approximately 2.47 million gallons. It was assumed that there would be four fermenters where three would be in operation while one was on standby. Ultimately, this resulted in a reactor volume of 825,000 gallons per vessel; however, it was also assumed that the reactors would also operate at 90% capacity to prevent overflow and allow for venting. Thus, R-101 was sized as an API Fixed Roof tank with a volume capacity of 925,000 gallons.

Assuming an L/D of approximately 2, the Length (L) and diameter (D) of the fermenters were back calculated using the volume equation:

$$V = \pi * D^2 * 0.25 * L$$

R-102: Fermentation Reactor 2

Similar to R-101.

R-103: Fermentation Reactor 3

Similar to R-101.

#### R-104: Fermentation Reactor 4

Similar to R-101.

#### Tk-101: Intermediate Storage

A tank to serve as an intermediate storage before the reacted broth proceeds downstream. Since the fermenters will operate on a staggered schedule to promote a continuous process, this tank was sized as an API fixed roof tank with a volume 1.25 times the volume of the fermenters resulting in a total volume of 1,125,000 gallons. The length and diameter were calculated in a similar manner as R-101.

#### X-101: Centrifuge

According to Towler, because this system deals with particles approximately 1 micrometer in diameter it is acceptable to use a high speed disk as a means of separation.<sup>2</sup> The following equation can be found:

$$C_e = a + bS^n$$

Where, a and b are cost constants, S is a size parameter and n is the exponent for this type of equipment. The largest diameter given for this type of centrifuge was 0.49 meters resulting in a cost of:

$$C_e = 63000 + 260000 * 0.49^{0.8} \sim \$210,000$$

This was then brought to present day using the CEPCI index:

$$C_2 = C_1 * \frac{CPI_2}{CPI_1} = 210,000 * \frac{610}{478.6} \sim \$268,000$$

Towler also mentions that this type of centrifuge can process approximately 110 m<sup>3</sup>/h of material at the cost of reduced efficiency. Therefore, with an approximate flowrate of 90 m<sup>3</sup>/h determined from Aspen, one centrifuge was costed.<sup>2</sup>

#### V-101: Anion Adsorber

The amount of adsorbent required was found as follows:<sup>3</sup>

$$90 \frac{m^3}{h} * \frac{m^3 \text{ bed}}{25m^3 \text{ flow}} * \frac{1090kg}{m^3} = 3924 \text{ kg sorbent per bed}$$



Assuming 2 beds:

$$3924 \frac{kg}{bed} * \frac{\$450}{kg} * 2 beds = \$3.5 \text{ million sorbent}$$

The vessels were sized accordingly:

$$\frac{3924kg}{bed} * \frac{m^3}{1090kg} = 3.6 \frac{m^3}{bed}$$

Assuming an L/D of 5:

$$V = \pi * D^2 * 0.25 * L$$

The length of these vessels was found to be 5m and the diameter to be 1m.

Finally, the cycle time for these beds was back calculated as follows:

The anion absorbent was found to have a 1.25 eq/L capacity:

$$\frac{1196mol}{h} * \frac{1eq}{mol} * \frac{1L}{1.25eq} * t * \frac{1090kg}{m^3sorbent} * \frac{m^3}{1000L} = \frac{3924kg}{vessel}$$
$$t \sim 3.8 \frac{hours}{cycle}$$

This number is reasonable.<sup>4</sup>

#### F-101: t3HDA Belt Filter/Dryer

Towler describes a vacuum drum filter that would be desirable for this system. It is estimated that this type of filter can process 10 m<sup>3</sup>/h/m<sup>2</sup>. Therefore, a 20 m<sup>2</sup> filter could process approximately 200 m<sup>3</sup>/h which would be more than sufficient for this process. Thus, using a similar sizing equation as for centrifuge X-101A.<sup>2</sup>

$$C_e = a + bS^n = \$118,000$$

R-105: Electrochemical Hydrogenation Reactor

The reaction rate was first converted into a current (Amps) as follows:

$$64.75 \frac{\text{kmol (MA)}}{\text{hr}} * 2 \frac{\text{mol } e^-}{\text{mol MA}} * 6.022E23 \frac{e^-}{\text{mol } e^-} * \frac{1}{6.2415E18} \frac{\text{coulomb}}{e^-} * \frac{1}{3600} \frac{\text{h}}{\text{s}} \\ * \frac{1}{1} \frac{\text{Amp}}{\text{coulomb}} * \frac{1000}{1} \frac{\text{mol}}{\text{kmol}} = 3.48E6 \text{ Amps}$$

Then the electrode area was found given a current density of 0.2 A/cm<sup>2</sup>.

$$0.2 \frac{\text{A}}{\text{cm}^2} * \frac{100^2 \text{cm}^2}{\text{m}^2} = 2000 \frac{\text{A}}{\text{m}^2} \\ A = \frac{3.48E6}{2000} \frac{\text{A}}{\frac{\text{A}}{\text{m}^2}} \sim 1736 \text{ m}^2$$

Finally, the cost was estimated assuming \$10,000/m<sup>2</sup> of electrode area:<sup>1</sup>

$$C = 1736 \text{ m}^2 * \frac{\$10,000}{\text{m}^2} \sim \$17.4 \text{ million}$$

Furthermore, an optimization study was done where several voltages and current densities were considered. Results were obtained as follows:

$$P = I * V = 3.48E6 \text{ Amps} * 5.7 \text{ Volts} \sim 20,000 \text{ kW}$$

Where V is the voltage.

There are 8000 operating hours in one year, so:

$$9900 \text{ kW} * 8000 \text{ hours} \sim 1.58E8 \text{ kWh}$$

The yearly operating costs or YOC is given by:

$$YOC = 1.58E8 \text{ kWh} * \frac{0.0036 \text{ GJ}}{\text{kWh}} * \frac{\$18.72}{\text{GJ}} = \$10.7 \text{ million}$$

To compare the different YOC values combined with their associated capital costs, these values were converted to an equivalent annual operating cost EAOE given by the following equation:<sup>5</sup>

$$EAOE = P \frac{i(1+i)^n}{(1+i)^n - 1} + YOC \sim \$13.5 \text{ million}$$

Where n was assumed to be 10 years with an interest rate, i, of 10%.

The results of the optimization are shown in Fig S17 and summarized in the Table S2 below:

**Table S2:** Summary of EAOOC at each voltage and current density

Voltage (Volts)	Current Density (Amps/cm <sup>2</sup> )	EAOOC (\$)
4	0.05	18,781,611
4.2	0.1	13,507,418
5.7	0.2	13,489,985
6.5	0.3	14,045,530
7.6	0.4	15,633,134

It was found that operating at 5.7 volts with a current density of 0.2 A/cm<sup>2</sup> produced the cheapest result for the givens. However, it can be seen from Figure S17 that there may exist a true operating minimum between 4.2 and 5.7 volts. Therefore, it is recommended that additional experiments be done to determine the true minimum because for each million dollars saved it equates to approximately \$0.012/kg of t3HDA which is significant.

### ***3. Utility Summary***

Duties and power requirements were found for most equipment from Aspen. The following equipment required additional calculations:

#### Cooker-101:

In order to kill the cells in the centrifuge waste stream, it was assumed that the temperature would be brought to 100 degrees Celsius with low pressure steam. A heat exchanger on Aspen was input on the outlet stream of the separator block to determine the required duty for the required temperature increase. Consideration could also be given to injection of live steam, obviating the heat exchanger.

#### R-105:

The power requirement was calculated as shown in the equipment summary section and input as a custom electric utility within Capcost.

#### E-107:

This exchanger utilized ammonia refrigerant to achieve the desired temperature. However, within Aspen and Capcost it was specified as a “medium-cold” refrigeration utility and costed accordingly to the duty output by Aspen and cost from Turton.<sup>5</sup>

#### 4. Cost of Manufacturing, without Depreciation

##### Cost of Land:

The land was assumed to be purchased in Iowa and was sized using an estimate based on an ethanol plant that produced 10 times as much ethanol as the designated scope of this site. From Aspen, it was estimated that approximately 14 million gallons/year would be produced while the ethanol plant produced 140 million.<sup>6</sup> This ethanol plant spanned approximately 270 acres of land. 50 acres was chosen as the size of this plant to account for expansion if necessary. The average cost of land in Iowa was determined to be approximately \$7300/acre resulting in a Cost of Land of \$365,000.<sup>7</sup>

##### Cost of Operating Labor:

From the PFD, there are approximately 12 non-particulate processing steps and 3 solids processing steps. According to Turton, the number of operators per shift can be calculated from the following:<sup>5</sup>

$$N_{ol} = (6.029 + 31.7P^2 + 0.23N_{np})^{0.5} = 17.1566 \sim 18 \frac{\text{operators}}{\text{shift}}$$

Where, P = solid processing steps, and  $N_{np}$  = non-particulate processing steps.

Assuming 3 shifts and a salary of \$52,000/year:<sup>8</sup>

$$18 \frac{\text{operators}}{\text{shift}} * 3 \text{shifts} * \frac{\$52,000}{\text{year}} = \$2,808,000$$

##### Raw Materials:

Sulfuric acid – determined from Turton’s cost data and flowrate from Aspen.

Feedstock- cost from paper and flowrate from Aspen only including glucose flow.

##### *Key Metric:*

$$Com_d = \$131,698,253$$

Cost per kg:

$$\frac{Com_d}{kg/year} = \frac{\$131,698,253}{\frac{9412kg}{h} * \frac{8000h}{year}} = \frac{\$1.75}{kg}$$

**Table S3: Equipment Summary Table**

<b>Equipment</b>	<b>R-101</b>	<b>R-102</b>	<b>R-103</b>	<b>R-104</b>	<b>Tk-101</b>	<b>X-101A</b>	<b>C-101</b>	<b>F-101</b>
MOC	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel
Volume m <sup>3</sup>	3500	3500	3500	3500	4260	-	-	-
Area m <sup>2</sup>	-	-	-	-	-	-	-	20
Orientation	Vertical	Vertical	Vertical	Vertical	Horizontal	-	-	-
Pressure (barg)	3	3	3	3	3	4	-	4
Diameter (m)	13	13	13	13	13.5	0.49	-	-
Length (m)	26.5	26.5	26.5	26.5	30	-	-	-
Power (shaft) (kW)	-	-	-	-	-	-	1740	-
Efficiency	-	-	-	-	-	-	0.75	-
Type/drive	-	-	-	-	-	-	Centrifugal /Electric	-
Temperature (°C)	-	-	-	-	-	-	200	2
Discharge P (barg)	-	-	-	-	-	-	4	-
<b>Equipment</b>	<b>E-101</b>	<b>E-102</b>	<b>E-103</b>	<b>E-104</b>	<b>E-105</b>	<b>E-106</b>	<b>E-107</b>	<b>R-105</b>
MOC	-	-	-	-	-	-	-	Stainless Steel
Type	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	-
Duty (kW)	11361	11361	11361	11361	3083	2339	1561	20,000
Pressure (barg)	-	-	-	-	-	-	-	4
Area (m <sup>2</sup> )	105	105	105	105	80.3	60.3	187	1736
<b>Shell</b>								
Temperature (°C)	90	90	90	90	200	50	-25	-
Pressure (barg)	3	3	3	3	3	2.5	1	-
Phase	V+L	V+L	V+L	V+L	V	V+L	V+L	-
MOC	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Stainless Steel	-
<b>Tube</b>								
Temperature (°C)	45	45	45	45	45	25	2	-
Pressure (barg)	0	0	0	0	0	0	3	-
Phase	L	L	L	L	L	V+L	S+L	-
MOC	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Stainless Steel	-

<b>Equipment</b>	<b>P-101</b>	<b>P-102</b>	<b>P-103</b>	<b>P-104</b>	<b>P-105</b>	<b>P-106</b>	<b>P-107</b>
MOC	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel
Power (kW)	58	58	58	58	1	12	17
Efficiency	0.75	0.75	0.75	0.75	0.75	0.75	0.75
Type/drive	Centrifugal	Centrifugal	Centrifugal	Centrifugal	Centrifugal	Centrifugal	Centrifugal
Temperature (°C)	90	90	90	90	100	25	25
Pressure in (barg)	1	1	1	1	4	4	0
Pressure out (barg)	4	4	4	4	6	6	3
<b>Equipment</b>	<b>P-108</b>	<b>P-109</b>	<b>Cooker-101</b>	<b>M-101A</b>	<b>M-101B</b>	<b>M-101C</b>	<b>M-101D</b>
MOC	Stainless Steel	Carbon Steel	Carbon Steel	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel
Power (kW)	1	4.2	-	-	-	-	-
Efficiency	0.75	0.75	-	-	-	-	-
Type/drive	Centrifugal	Centrifugal	-	-	-	-	-
Temperature (°C)	25	25	-	-	-	-	-
Pressure in (barg)	0	0	-	-	-	-	-
Pressure out (barg)	3	2	-	-	-	-	-
Volume (m <sup>3</sup> )	-	-	35	35	35	35	35
Orientation	-	-	Horizontal	Vertical	Vertical	Vertical	Vertical
Pressure (barg)	-	-	3	0	0	0	0
Power/duty (MJ/h)	-	-	245	-	-	-	-
<b>Equipment</b>	<b>V-101 A/B</b>						
MOC	Stainless Steel						
Pressure (barg)	0						
Diameter (m)	1						
Length (m)	5						
Orientation	Vertical						

**Table S4: Utility Summary Table**

<b>Equipment</b>	<b>Cooker-101</b>	<b>C-101</b>	<b>E-101</b>	<b>E-102</b>	<b>E-103</b>	<b>E-104</b>	<b>E-105</b>
Utility	LPS	Electricity	Refrigerated Water	Refrigerated Water	Refrigerated Water	Refrigerated Water	Cooling Water
Usage	245 MJ/h	3860 kW	40900 MJ/h	40900 MJ/h	40900 MJ/h	40900 MJ/h	11100 MJ/h
Cost/hr	\$1.11	\$261.25	\$195.13	\$195.13	\$195.13	\$195.13	\$4.20
Annual Cost	\$8,899	\$2,090,000	\$1,561,000	\$1,561,000	\$1,561,000	\$1,561,000	\$33,600
<b>Equipment</b>	<b>E-106</b>	<b>E-107</b>	<b>P-101</b>	<b>P-102</b>	<b>P-103</b>	<b>P-104</b>	<b>P-105</b>
Utility	Refrigerated Water	Ammonia	Electricity	Electricity	Electricity	Electricity	Electricity
Usage	8420 MJ/h	5620 MJ/h	77.3 kW	77.3 kW	77.3 kW	77.3 kW	1.33 kW
Cost/hr	\$40.18	\$47.68	\$5.21	\$5.21	\$5.21	\$5.21	\$0.09
Annual Cost	\$321,400	\$381,400	\$41,700	\$41,700	\$41,700	\$41,700	\$719
<b>Equipment</b>	<b>P-106</b>	<b>P-107</b>	<b>P-108</b>	<b>P-109</b>	<b>R-105</b>		
Utility	Electricity	Electricity	Electricity	Electricity	Electricity		
Usage	16 kW	22.7 kW	1.33 kW	5.6 kW	20,000 kW		
Cost/hr	\$1.08	\$1.53	\$0.09	\$0.38	\$1,347.88		
Annual Cost	\$8,630	\$12,200	\$719	\$3,020	\$10,783,000		





Stream Number	Units	7	8	9	10	11	12
Temperature	C	86.9744	45.0000	45.0000	25.0000	25.0000	25.0000
Pressure	bar	1.0000	1.0000	1.0000	5.9000	5.9000	6.0000
Mass Vapor Fraction		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Mass Flows	kg/hr	21833	21833	21833	87335	79803	7532
<b>Mole Flows</b>	kmol/hr	1031.6787	1031.6787	1031.6787	4126.7144	3875.8568	250.8577
MA	kmol/hr	16.4864	16.4864	16.4864	65.9457	65.9457	0.0000
GLUCOSE	kmol/hr	0.3056	0.3056	0.3056	1.2222	1.2222	0.0000
H2O	kmol/hr	1012.7582	1012.7582	1012.7582	4051.0359	3800.1782	250.8577
H2	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
t3HDA	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
t3HDA(S)	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H3O+	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
OH-	kmol/hr	0.0006	0.0006	0.0006	0.0024	0.0024	0.0000
E-	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
NH4+	kmol/hr	0.6741	0.6741	0.6741	2.6985	2.6985	0.0000
H2SO4	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON(S)	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SALT1	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HSO4-	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SO4--	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
O2	kmol/hr	0.0002	0.0002	0.0002	0.0007	0.0007	0.0000
CO2	kmol/hr	0.0145	0.0145	0.0145	0.0575	0.0575	0.0000
SALT2	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HCO3-	kmol/hr	0.6380	0.6380	0.6380	2.5474	2.5474	0.0000
CO3--	kmol/hr	0.0100	0.0100	0.0100	0.0416	0.0416	0.0000
N2	kmol/hr	0.0030	0.0030	0.0030	0.0120	0.0120	0.0000
AMMONIA	kmol/hr	0.7726	0.7726	0.7726	3.0851	3.0851	0.0000
SALT3	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
NH2COO-	kmol/hr	0.0155	0.0155	0.0155	0.0655	0.0655	0.0000

<b>Stream Number</b>	<b>Units</b>	<b>13</b>	<b>14</b>	<b>15</b>	<b>16</b>	<b>17</b>	<b>18</b>
Temperature	C	100.0000	25.0000	25.0000	25.0000	20.0117	2.0000
Pressure	bar	5.9000	1.0000	1.0000	1.0000	1.2000	1.0000
Mass Vapor Fraction		0.0000	0.0128	0.1010	0.0000	0.0000	0.0000
Mass Flows	kg/hr	7532	79803	10395	69407	405	69812
<b>Mole Flows</b>	kmol/hr	250.8577	3843.4244	447.6363	3395.7924	13.3051	3409.0975
MA	kmol/hr	0.0000	1.1957	0.0120	1.1837	0.0000	1.1837
GLUCOSE	kmol/hr	0.0000	1.2222	1.2222	0.0000	0.0000	0.0000
H2O	kmol/hr	250.8577	3735.3060	404.8061	3330.5061	9.1096	3338.7279
H2	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
t3HDA	kmol/hr	0.0000	64.7500	0.6475	64.1025	0.0000	0.0000
t3HDA(S)	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	64.1025
H3O+	kmol/hr	0.0000	0.0000	0.0000	0.0000	2.1308	3.0186
OH-	kmol/hr	0.0000	0.0025	0.0003	0.0000	0.0000	0.0000
E-	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
NH4+	kmol/hr	0.0000	5.3771	5.3628	0.0000	0.0000	0.0000
H2SO4	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON(S)	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SALT1	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HSO4-	kmol/hr	0.0000	0.0000	0.0000	0.0000	1.9985	1.1107
SO4--	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0662	0.9540
O2	kmol/hr	0.0000	32.3757	32.3757	0.0000	0.0000	0.0000
CO2	kmol/hr	0.0000	0.0002	0.0044	0.0000	0.0000	0.0000
SALT2	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HCO3-	kmol/hr	0.0000	0.0484	0.0521	0.0000	0.0000	0.0000
CO3--	kmol/hr	0.0000	2.6627	2.6550	0.0000	0.0000	0.0000
N2	kmol/hr	0.0000	0.0120	0.0120	0.0000	0.0000	0.0000
AMMONIA	kmol/hr	0.0000	0.4711	0.4857	0.0000	0.0000	0.0000
SALT3	kmol/hr	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
NH2COO-	kmol/hr	0.0000	0.0008	0.0005	0.0000	0.0000	0.0000

Stream Number	Units	19	20
Temperature	C	2.0000	2.0000
Pressure	bar	1.0133	0.9000
Mass	Vapor	0.0000	0.0000
Fraction			
Mass Flows	kg/hr	9412	60400
<b>Mole Flows</b>	kmol/hr	73.6616	3335.4359
MA	kmol/hr	0.0036	1.1802
GLUCOSE	kmol/hr	0.0000	0.0000
H2O	kmol/hr	9.5392	3329.1887
H2	kmol/hr	0.0000	0.0000
t3HDA	kmol/hr	0.0000	0.0000
t3HDA(S)	kmol/hr	64.1025	0.0000
H3O+	kmol/hr	0.0096	3.0090
OH-	kmol/hr	0.0000	0.0000
E-	kmol/hr	0.0000	0.0000
NH4+	kmol/hr	0.0000	0.0000
H2SO4	kmol/hr	0.0000	0.0000
AMMON(S)	kmol/hr	0.0000	0.0000
SALT1	kmol/hr	0.0000	0.0000
HSO4-	kmol/hr	0.0037	1.1070
SO4--	kmol/hr	0.0030	0.9510
O2	kmol/hr	0.0000	0.0000
CO2	kmol/hr	0.0000	0.0000
SALT2	kmol/hr	0.0000	0.0000
HCO3-	kmol/hr	0.0000	0.0000
CO3--	kmol/hr	0.0000	0.0000
N2	kmol/hr	0.0000	0.0000
AMMONIA	kmol/hr	0.0000	0.0000
SALT3	kmol/hr	0.0000	0.0000
NH2COO-	kmol/hr	0.0000	0.0000

Note: Ammonium sulfate is defined as SALT1, Ammonium-Hydrogen-Carbonate is defined as SALT2, and Ammonium-Carbamate is defined as SALT3.

## 5. Aspen Flowsheet Assumptions

A stoichiometric balance was performed on the fermentation reaction to ensure enough *t*3HDA was produced to meet the design specification of 83,000 Mg/y. Water, glucose and compressed air streams were fed into an adiabatic RSTOIC reactor to simulate the fermentation. Ammonium hydroxide was added to increase the pH to 11.5. Additionally, a nutrient stream was added such that the fermentation broth consisted of 3 wt% of these nutrients to help promote the fermentation (2/3 of the nutrients converted to cells within fermenter). Furthermore, the fermentation reaction was assumed to produce 0.43 g MA/g glucose with a 99.9 % conversion. The fermenters were sized such that the fermentation cycle time could be 72 hours as described in literature.<sup>1</sup>

A sep block was used to simulate the centrifugation of the fermentation broth. It was assumed that two-thirds of the nutrients would be recovered as cells and could then be recycled to save on raw material costs. Furthermore, this stream would contain 60 wt% water with 40 wt % cells dry weight with an assumed 100 % cell recovery from within the broth.

The electrochemical process was simulated using an RSTOIC reactor where muconic acid was driven to *t*3HDA and water with a 99.9 % conversion. Furthermore, the Electrolyte NRTL thermodynamic package was used to capture the ionic behavior present in these aqueous solutions.

*t*3HDA was not present within Aspen's database, so the UNIFAC and JOBACK functional group methods were used to simulate its properties. A separator block was used to simulate an anion adsorbent bed that would concentrate the *t*3HDA to promote crystallization. *t*3HDA and muconic acid were selectively adsorbed while all other components were treated as a waste stream. Additionally, given the solubility limitations of *t*3HDA in solution prior to the crystallizer, engineering judgement was used to determine an amount of water that would be involved in desorption to stay below the limit of solubility. The solubility data that was provided was also used to simulate the crystallization of *t*3HDA. The MOFASA functional group method was used to simulate the solid heat capacities of *t*3HDA. Enough sulfuric acid was added such that the pH of the solution within the crystallizers would be at 1.5 to promote crystal growth.

Capcost software by Turton is a Microsoft Excel macro-enabled file that uses heuristics and equipment correlations to help determine Cost of Manufacturing, equipment costs and annual utility costs. Furthermore, the software can be used to conduct profitability analysis generating cash flow diagrams and Monte Carlo simulations.<sup>5</sup>

**Table S6:** Capcost Equipment Summary Table with CPI: 610<sup>5</sup>

Compressors	Compressor Type	Power (kilowatts)	# Spares	MOC		Purchased Equipment Cost	Bare Module Cost	
C-101	Centrifugal	1740	0	Carbon Steel		\$ 1,280,000	\$ 3,500,000	
Drives	Drive Type	Power (kilowatts)	# Spares			Purchased Equipment Cost	Bare Module Cost	
D-101	Electric - Explosion Proof	3474	0			\$ 455,000	\$ 683,000	
Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost	
E-105	Floating Head	3	0	Carbon Steel / Carbon Steel	80.3	\$ 35,700	\$ 117,000	
E-106	Floating Head	2.5	0	Carbon Steel / Carbon Steel	60.3	\$ 32,500	\$ 107,000	
E-101	Floating Head	3	0	Carbon Steel / Carbon Steel	105	\$ 39,700	\$ 131,000	
E-102	Floating Head	3	0	Carbon Steel / Carbon Steel	105	\$ 39,700	\$ 131,000	
E-103	Floating Head	3	0	Carbon Steel / Carbon Steel	105	\$ 39,700	\$ 131,000	
E-104	Floating Head	3	0	Carbon Steel / Carbon Steel	105	\$ 39,700	\$ 131,000	
E-107	Floating Head	1	3	Stainless Steel / Stainless Steel	187	\$ 53,600	\$ 330,000	
Pumps (with drives)	Pump Type	Power (kilowatts)	# Spares	MOC	Discharge Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	
P-101	Centrifugal	58	1	Carbon Steel	3	\$ 28,200	\$ 112,000	
P-102	Centrifugal	58	1	Carbon Steel	3	\$ 28,200	\$ 112,000	
P-103	Centrifugal	58	1	Carbon Steel	3	\$ 28,200	\$ 112,000	
P-104	Centrifugal	58	1	Carbon Steel	3	\$ 28,200	\$ 112,000	
P-105	Centrifugal	1	1	Carbon Steel	5	\$ 7,530	\$ 30,000	
P-106	Centrifugal	12	1	Carbon Steel	5	\$ 13,000	\$ 51,700	
P-107	Centrifugal	17	1	Carbon Steel	3	\$ 15,000	\$ 59,700	
P-108	Centrifugal	1	1	Stainless Steel	2	\$ 7,530	\$ 37,400	
P-109	Centrifugal	4.2	1	Carbon Steel	3	\$ 9,330	\$ 37,200	
Reactors	Type	Volume (cubic meters)				Purchased Equipment Cost	Bare Module Cost	
Cooker-101	Jacketed Agitated	35				\$ 129,000	\$ 194,000	
M-101A	Jacketed Agitated	35				\$ 129,000	\$ 194,000	
M-101B	Jacketed Agitated	35				\$ 129,000	\$ 194,000	
M-101C	Jacketed Agitated	35				\$ 129,000	\$ 194,000	
M-101D	Jacketed Agitated	35				\$ 129,000	\$ 194,000	
Storage Tanks	Tank Type	Volume (cubic meters)				Purchased Equipment Cost	Bare Module Cost	
R-101	Fixed Roof	3500				\$ 278,000	\$ 306,000	
R-102	Fixed Roof	3500				\$ 278,000	\$ 306,000	
R-103	Fixed Roof	3500				\$ 278,000	\$ 306,000	
R-104	Fixed Roof	3500				\$ 278,000	\$ 306,000	
Tk-101	Fixed Roof	4260				\$ 315,000	\$ 347,000	
Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
V-101	Vertical	5	1	Stainless Steel		4	\$ 9,730	\$ 77,000
V-102	Vertical	5	1	Stainless Steel		4	\$ 9,730	\$ 77,000
User Added Equipment	Description	BMF <sub>e</sub>	Actual BMF				Purchased Equipment Cost	Bare Module Cost
X-101A	High Speed Disk Centrifuge	1.5	1.5				\$ 268,000	\$ 402,000
F-101	Belt Filter/Dryer	1.5	1.5				\$ 118,000	\$ 177,000
R-105	Electrochemical Reactor	1.5	1.5				\$ 17,400,000	\$ 26,100,000
Z-101	Absorbent	1.5	1.5				\$ 3,500,000	\$ 5,250,000

Total Bare Module Cost \$ 40,549,000

**Table S7: Annual Utility Costs for each Piece of Equipment** <sup>5</sup>

Name	Total Module Cost	Grass Roots Cost	Utility Used	Efficiency	Actual Usage	Annual Utility Cost
C-101	\$ 4,120,000	\$ 5,870,000	NA			
Cooker-10	\$ 229,000	\$ 294,000	Low-Pressure Steam		245 MJ/h	\$ 8,899
D-101	\$ 806,000	\$ 1,150,000	Electricity	0.9	3860 kilowatts	\$ 2,080,000
E-101	\$ 154,290	\$ 220,000	Refrigerated Water		40900 MJ/h	\$ 1,561,000
E-102	\$ 154,000	\$ 220,000	Refrigerated Water		40900 MJ/h	\$ 1,561,000
E-103	\$ 154,000	\$ 220,000	Refrigerated Water		40900 MJ/h	\$ 1,561,000
E-104	\$ 154,000	\$ 220,000	Refrigerated Water		40900 MJ/h	\$ 1,561,000
E-105	\$ 139,000	\$ 197,000	Cooling Water		11100 MJ/h	\$ 33,600
E-106	\$ 126,000	\$ 180,000	Refrigerated Water		8420 MJ/h	\$ 321,400
E-107	\$ 389,504	\$ 478,000	Refrigeration (-20°C)		5620 MJ/h	\$ 381,400
F-101	\$ 139,000	\$ 228,000	Custom		0 MJ/h	\$ -
M-101A	\$ 229,000	\$ 294,000	Custom		0 MJ/h	\$ -
M-101B	\$ 229,000	\$ 294,000	Custom		0 MJ/h	\$ -
M-101C	\$ 229,000	\$ 294,000	Custom		0 MJ/h	\$ -
M-101D	\$ 229,000	\$ 294,000	Custom		0 MJ/h	\$ -
P-101	\$ 132,000	\$ 178,000	Electricity	0.75	77.3 kilowatts	\$ 41,700
P-102	\$ 132,000	\$ 178,000	Electricity	0.75	77.3 kilowatts	\$ 41,700
P-103	\$ 132,000	\$ 178,000	Electricity	0.75	77.3 kilowatts	\$ 41,700
P-104	\$ 132,000	\$ 178,000	Electricity	0.75	77.3 kilowatts	\$ 41,700
P-105	\$ 35,400	\$ 47,600	Electricity	0.75	1.33 kilowatts	\$ 719
P-106	\$ 61,100	\$ 82,000	Electricity	0.75	16 kilowatts	\$ 8,630
P-107	\$ 70,000	\$ 95,000	Electricity	0.75	22.7 kilowatts	\$ 12,200
P-108	\$ 44,100	\$ 56,300	Electricity	0.75	1.33 kilowatts	\$ 719
P-109	\$ 43,800	\$ 59,000	Electricity	0.75	5.6 kilowatts	\$ 3,020
R-101	\$ 361,000	\$ 514,000	NA			
R-102	\$ 361,000	\$ 514,000	NA			
R-103	\$ 361,000	\$ 514,000	NA			
R-104	\$ 361,000	\$ 514,000	NA			
R-105	\$ 10,240,000	\$ 16,700,000	Custom		72000 MJ/h	\$ 10,783,000
Tk-101	\$ 417,000	\$ 593,000	NA			
V-101	\$ 91,000	\$ 111,000	NA			
V-102	\$ 91,000	\$ 111,000	NA			
X-101	\$ 316,000	\$ 517,000	Custom		0 MJ/h	\$ -
Z-101	\$ 4,130,000	\$ 6,760,000	Custom		0 MJ/h	\$ -
<b>Totals</b>	<b>\$ 25,000,000</b>	<b>\$ 38,400,000</b>				<b>\$ 20,000,000</b>

The following table translates raw material costs and costs associated with waste streams into annual utility costs. For the purpose of this analysis, fresh water costs associated with treatment were not considered.

**Table S8: Raw Material Costs** <sup>5</sup>

Material Name	Classification	Price (\$/kg)	Flowrate (kg/h)	Annual Cost
Sulfuric Acid	Raw Material	\$ 0.09	405.00	\$ 304,560
Sugar Feedstock	Raw Material	\$ 0.30	22019.50	\$ 52,846,800
Waste Water		\$ 0.04	60400.00	\$ 17,395,200
Nutrients		\$ 0.10	4497.00	\$ 3,597,600

**Table S9: Cost of Manufacturing Input Table <sup>5</sup>**

**Economic Options**

Cost of Land	\$	365,000
Taxation Rate		28%
Annual Interest Rate		10%
Salvage Value		0
Working Capital	\$	10,520,000
FCIL	\$	38,400,000
Total Module Factor		1.18
Grass Roots Factor		0.50

**Economic Information Calculated From Given Information**

Revenue From Sales	\$	-
C <sub>RM</sub> (Raw Materials Costs)	\$	63,945,360
C <sub>UT</sub> (Cost of Utilities)	\$	20,000,000
C <sub>WT</sub> (Waste Treatment Costs)	\$	-
C <sub>OL</sub> (Cost of Operating Labor)	\$	2,808,000

**Factors Used in Calculation of Cost of Manufacturing (COM<sub>d</sub>)**

$$\text{Comd} = 0.18 \cdot \text{FCIL} + 2.76 \cdot \text{COL} + 1.23 \cdot (\text{CUT} + \text{CWT} + \text{CRM})$$

Multiplying factor for FCIL		0.18
Multiplying factor for C <sub>OL</sub>		2.76
Factors for C <sub>UT</sub> , C <sub>WT</sub> , and C <sub>RM</sub>		1.23
COM <sub>d</sub>	\$	117,914,873

**Factors Used in Calculation of Working Capital**

$$\text{Working Capital} = A \cdot \text{C}_{\text{RM}} + B \cdot \text{FCIL} + C \cdot \text{C}_{\text{OL}}$$

A		0.10
B		0.10
C		0.10

Project Life (Years after Startup)	10
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Construction period	2
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**Distribution of Fixed Capital Investment (must sum to one)**

End of year One	60%
End of year Two	40%
End of year Three	
End of year Four	
End of year Five	

**Table S10:** Summary table from CAPCOST of common utility costs used in analysis.

<b>Hours per Operating Year</b>		8000
		<b><u>Cost (\$/GJ)</u></b>
<b>Common Utilities</b>		
Electricity (110V - 440V)		18.72
Cooling Water (30°C to 45°C)		0.378
Refrigerated Water (15°C to 25°C)		4.77
<b>Steam from Boilers</b>		
Low Pressure (5 barg, 160°C)		4.54
Medium Pressure (10 barg, 184°C)		4.77
High Pressure (41 barg, 254°C)		5.66
<b>Fuels</b>		
Fuel Oil (no. 2)		10.3
Natural Gas		3.16
Coal (FOB mine mouth)		2.04
<b>Thermal Systems</b>		
Moderately High (up to 330°C)		3.51
High (up to 400°C)		3.73
Very High (up to 600°C)		3.95
<b>Refrigeration</b>		
Moderately Low (5°C)		4.77
Low (-20°C)		8.49
Very low (-50°C)		14.12
		<b><u>Cost (\$/tonne)</u></b>
<b>Waste Disposal (solid and liquid)</b>		
Non-Hazardous		36
Hazardous		1100



**Table S11:** Cost category analysis and overall cost of production of t3HDA.

<b>Cost Category</b>	<b>Grass roots cost</b>	<b>Utility Cost</b>	<b>Total ComD</b>	<b>\$/kg T3HDA</b>
<b>Fermentation</b>	\$ 1,955,700	\$ 10,485,012	\$ 12,440,712	\$ 0.17
<b>Electrochem Conversion</b>	\$ 3,006,000	\$ 13,263,090	\$ 16,269,090	\$ 0.22
<b>Separation</b>	\$ 308,448	\$ 417,767	\$ 726,215	\$ 0.01
<b>Purification</b>	\$ 1,633,374	\$ 488,727	\$ 2,122,101	\$ 0.03
<b>Cost of Labor</b>	\$ 7,750,080	\$ -	\$ 7,750,080	\$ 0.10
<b>Raw Materials</b>	\$ 65,376,173		\$ 65,376,173	\$ 0.87
<b>Waste Water Treatment</b>	\$ 27,060,000		\$ 27,060,000	\$ 0.36
<b>Total</b>			\$ 131,744,371	\$ 1.75

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