Table 1. Four factor experimental design with ANNs simulated results of dependent variables, where Glu, Xyl, Acetate, Inh, HY, and HER refer to glucose, xylose, acetate, inhibitors, hydrogen yield, and hydrogen evolution rate, respectively.

Runs	Parameters				HY /mol·mol^{-1}	HER /mmol·L^{-1}.h^{-1}
	Glu/ g.L^{-1}	Xyl /g.L^{-1}	Acetate /g.L^{-1}	Inh /g.L^{-1}		
1	20.0	1.4	0.1	1.4	3.1	9.7
2	20.0	1.4	2.5	1.4	2.3	8.4
3	12.5	1.4	1.3	1.4	3.1	9.7
4	12.5	0.1	1.3	2.6	3.1	9.7
5	12.5	0.1	2.5	1.4	2.0	8.5
6	12.5	2.7	1.3	2.6	3.1	9.7
7	12.5	2.7	1.3	0.1	3.0	8.4
8	20.0	1.4	1.3	0.1	3.1	9.6
9	20.0	1.4	1.3	2.6	3.1	9.7
10	20.0	2.7	1.3	1.4	3.1	9.7
11	5.0	1.4	0.1	1.4	0.3	0.4
12	12.5	2.7	0.1	1.4	3.0	9.6
13	12.5	1.4	1.3	1.4	3.1	9.7
14	5.0	1.4	1.3	0.1	2.4	5.9
15	12.5	1.4	2.5	0.1	1.5	4.5
16	12.5	1.4	1.3	1.4	3.1	9.7
17	12.5	1.4	2.5	2.6	2.3	9.1
18	20.0	0.1	1.3	1.4	3.1	9.7
19	5.0	1.4	1.3	2.6	2.7	6.4
20	12.5	1.4	1.3	1.4	3.1	9.7
21	12.5	0.1	1.3	0.1	3.1	9.2
22	5.0	2.7	1.3	1.4	2.5	8.5
23	5.0	0.1	1.3	1.4	2.8	8.8
24	12.5	2.7	2.5	1.4	2.0	8.4
25	12.5	0.1	0.1	1.4	2.9	9.4
26	12.5	1.4	0.1	2.6	0.8	5.7
27	5.0	1.4	2.5	1.4	1.7	8.3
28	12.5	1.4	0.1	0.1	3.1	9.7
29	12.5	1.4	1.3	1.35	3.1	9.7

Table 2. ANOVA analysis for HY (r^2 0.97, Adjust r^2 0.93, Predicted r^2 0.94, adequate precision 16), and HER (r^2 0.95, Adjust r^2 0.94, Predicted r^2 0.92, adequate precision 16), where X_1 is Glucose, X_2 is Xylose, X_3 is Acetate, and X_4 is inhibitors.

Source	HY/mol·mol^{-1}					HER/mmol·L^{-1}.h^{-1}				
	DF	Sum of Squares	Mean Square	F-value	Prob > F	DF	Sum of Squares	Mean Square	F-value	Prob > F
Model	14	12.884	0.920	5.005	0.002	14	101.791	7.271	5.011	0.002
X_1	1	2.430	2.430	13.216	0.003	1	28.521	28.521	19.656	0.001
X_2	1	0.008	0.008	0.041	0.843	1	0.083	0.083	0.057	0.814
X_3	1	0.163	0.163	0.888	0.362	1	0.608	0.608	0.419	0.528
X_4	1	0.100	0.548	0.471	0.100	1	0.75	0.012	0.75	0.516
X_1X_2	1	0.101	0.101	0.548	0.471	1	0.750	0.750	0.517	0.484
X_1X_3	1	1.210	1.210	6.581	0.022	1	21.160	21.160	14.583	0.002
X_2X_3	1	0.023	0.023	0.122	0.732	1	0.023	0.023	0.016	0.903
X_3X_4	1	2.402	2.4025	13.061	0.002	1	18.49	18.49	12.742	0.003
X_1^2	1	0.023	0.023	0.122	0.732	1	0.040	0.040	0.028	0.871
X_2^2	1	0.002	0.002	0.014	0.909	1	0.023	0.023	0.016	0.903
X_3^2	1	0.002	0.002	0.014	0.909	1	0.160	0.160	0.110	0.745
X_4^2	1	0.1301	0.1301	0.708	0.414	1	4.778	4.778	3.293	0.091
Residue	14	2.403	2.403	-	-	14	18.490	18.490	-	-
Lack of fit	10	0.506	0.506	13.066	0.003	10	8.892	8.892	12.743	0.003
Pure Error	4	0.163	0.163	-	-	4	2.671	2.671	-	-

Cor total	28	5.600	5.600	-	-	28	16.519	16.519	-	-

Table 3. The ANNs simulated quadratic coefficients for HY and HER.

Coefficient	Model Coefficient	
-	HY	HER
b0	6.68×10^{-1}	-2.13×10^{-1}
b1	2.64×10^{-1}	1.06×10^{0}
b2	-3.78×10^{-1}	-1.33×10^{0}
b3	1.67×10^{0}	4.40×10^{0}
b4	-4.22×10^{-1}	-2.19×10^{-1}
b5	7.69×10^{-3}	7.69×10^{-3}
b6	-6.11×10^{-2}	-2.56×10^{-1}
b7	-8.00×10^{-3}	-1.07×10^{-2}
b8	-1.60×10^{-2}	-4.81×10^{-2}
b9	1.54×10^{-2}	1.23×10^{-1}
b10	5.17×10^{-1}	1.43×10^{0}
b11	-4.96×10^{-3}	-2.08×10^{-2}
b12	9.37×10^{-2}	3.80×10^{-1}
b13	-6.45×10^{-1}	-1.11×10^{0}
b14	-9.07×10^{-2}	-5.49×10^{-1}

Table 4. *MSE* and *MARR* of the cross validation based upon trained data sets.

	HY **/mol·mol $^{-1}$**	**HER** **/mmol·L^{-1}.h $^{-1}$**
MSE_1	1.193	1.326
MSE_2	1.085	1.064
$MARR_1$	1.261	1.416
$MARR_2$	1.546	1.248