Supporting Information

Explanation for Eq. (5)

The Langmuir isotherm is described mathematically as Eq. (S1).

$$Q_{EQ} = \frac{Q_{Max} b_1 C_{EQ}}{1 + b_1 C_{EQ}} \qquad \text{(S1)}$$

where Q_{EQ} (M) is the equilibrium amount of carboxylic acid adsorbed in the adsorbate, Q_{Max} (mol/kg) is the maximum adsorption capacity, C_{EQ} (M) is the equilibrium concentration of unionized carboxylic acid, and b is the apparent equilibrium constant (L/mol).

For a monocaroxylic acid, HA, there is only one dissociation reaction and corresponding equilibrilum constant, K_a as Eq. (S2).

$$HA \leftrightarrow H^+ + A^- \qquad K_a = \frac{[H+]C_{EQ}}{C_{EQ,T}} \qquad \text{(S2)}$$

where $C_{EQ,T}$ (M) is the equilibrium concentration of total (unionized + ionized) carboxylic acid.

C_{EQ}, the concentration of unionized carboxylic acid is then expressed as Eq. (S3).

$$C_{EQ} = \frac{C_{EQ,T}}{1 + 10^{pH-pKa}} \qquad \text{(S3)}$$

Therefore, Eq. (S1) is expressed as Eq. (5).

$$Q_{EQ} = \frac{Q_{Max} b_1 \frac{C_{EQ,T}}{1+10^{pH-pK_a}}}{1 + b_1 \frac{C_{EQ,T}}{1+10^{pH-pK_a}}} \qquad \text{(5)}$$

Table S1. Langmuir isotherm parameters for acetic acid adsorption at 35°C of amine-functionalized MSN and pure MSN

N density (mol N/kg)	Q_{Max}[a]		b (L/mol)[a]	R^2
	(mol/kg)	(mol/mol N)[b]		
0	0.33	-	15.8	0.972
0.84	1.18	1.01	33.2	0.958
1.38	2.06	1.25	24.0	0.974
3.14	3.98	1.16	30.1	0.984
3.49	3.81	1.00	30.5	0.973
3.65	3.85	0.97	30.7	0.921

[a]As defined at Eq (S1).

[b] Assuming that silica atoms in amine-functionalized MSN had same adsorption capacity of pure MSN.

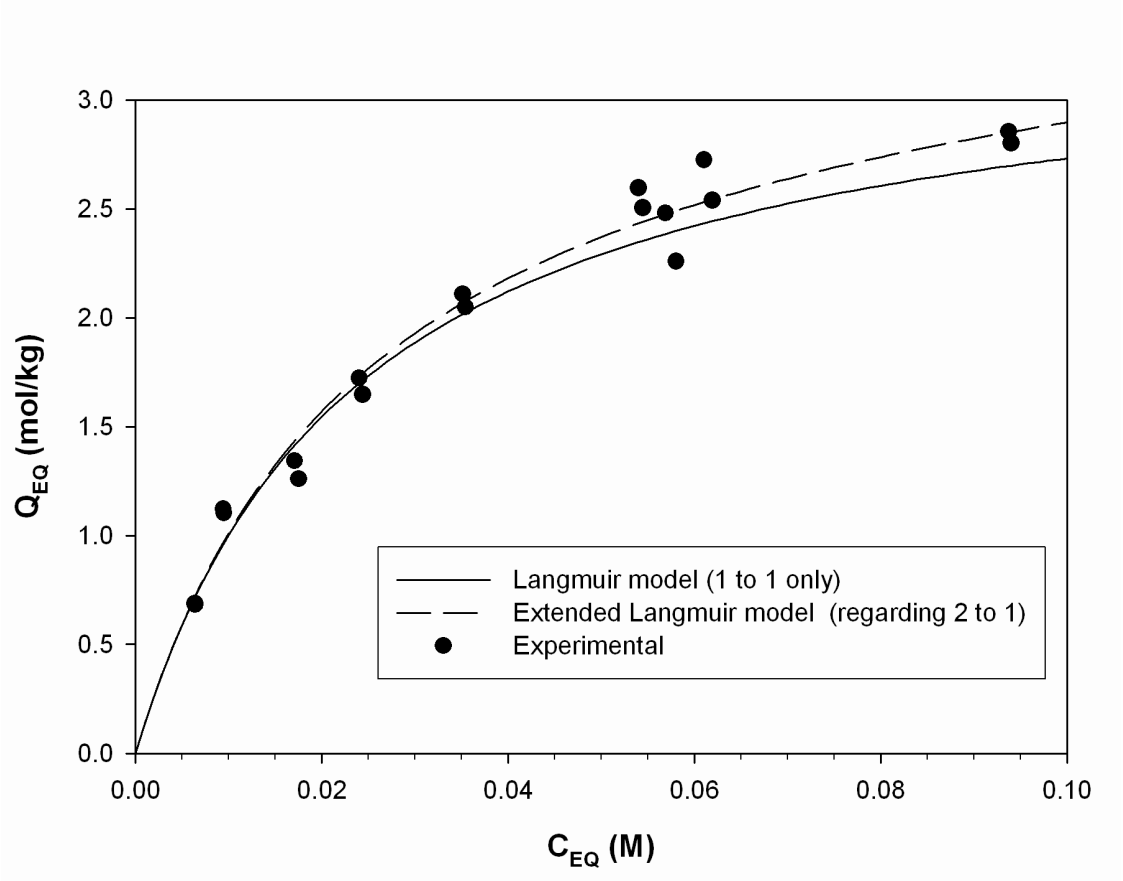

Figure S1. Comparison of Langmuir models with or without regarding 2 to 1 complexation for acetic acid adsorption onto the 3.14 mol N/kg MSN at 35°C.

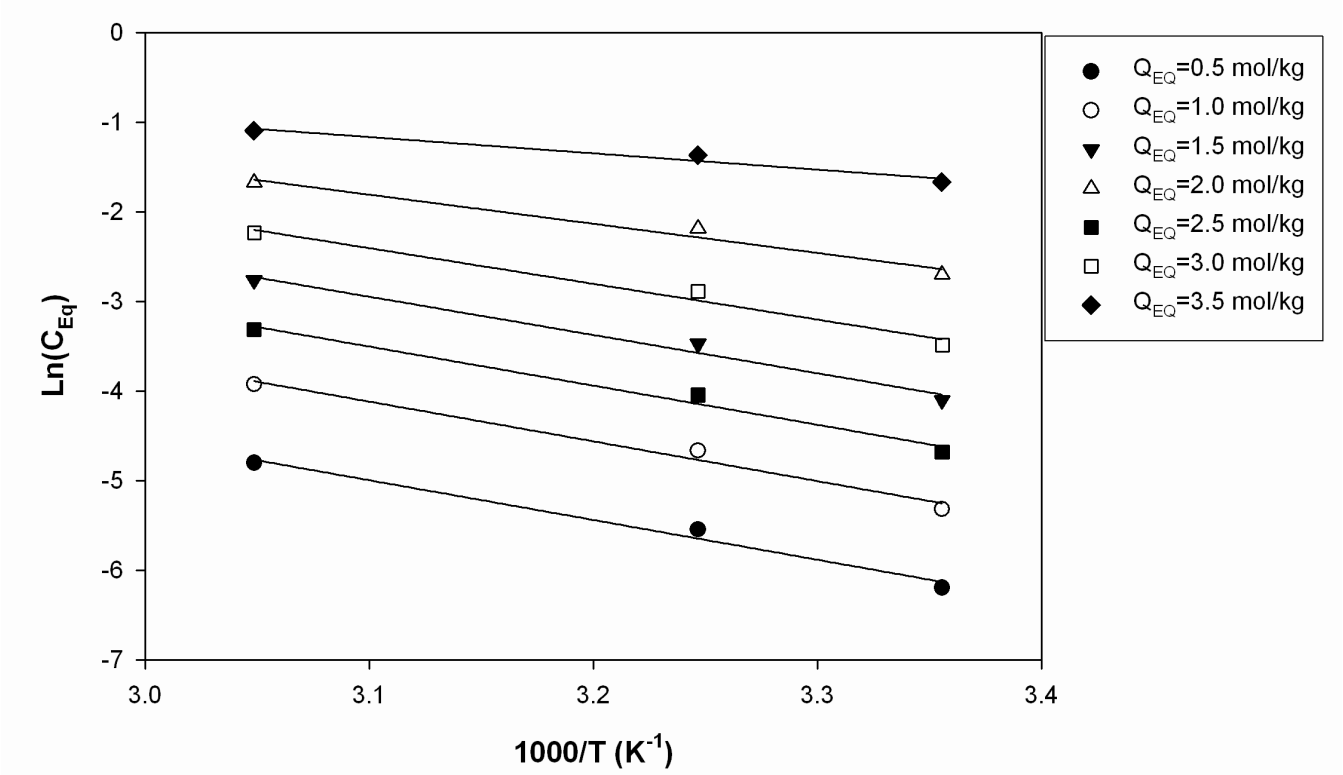

Figure S2. Effect of temperature on acetic acid adsorption onto the 3.14 mol N/kg MSN.

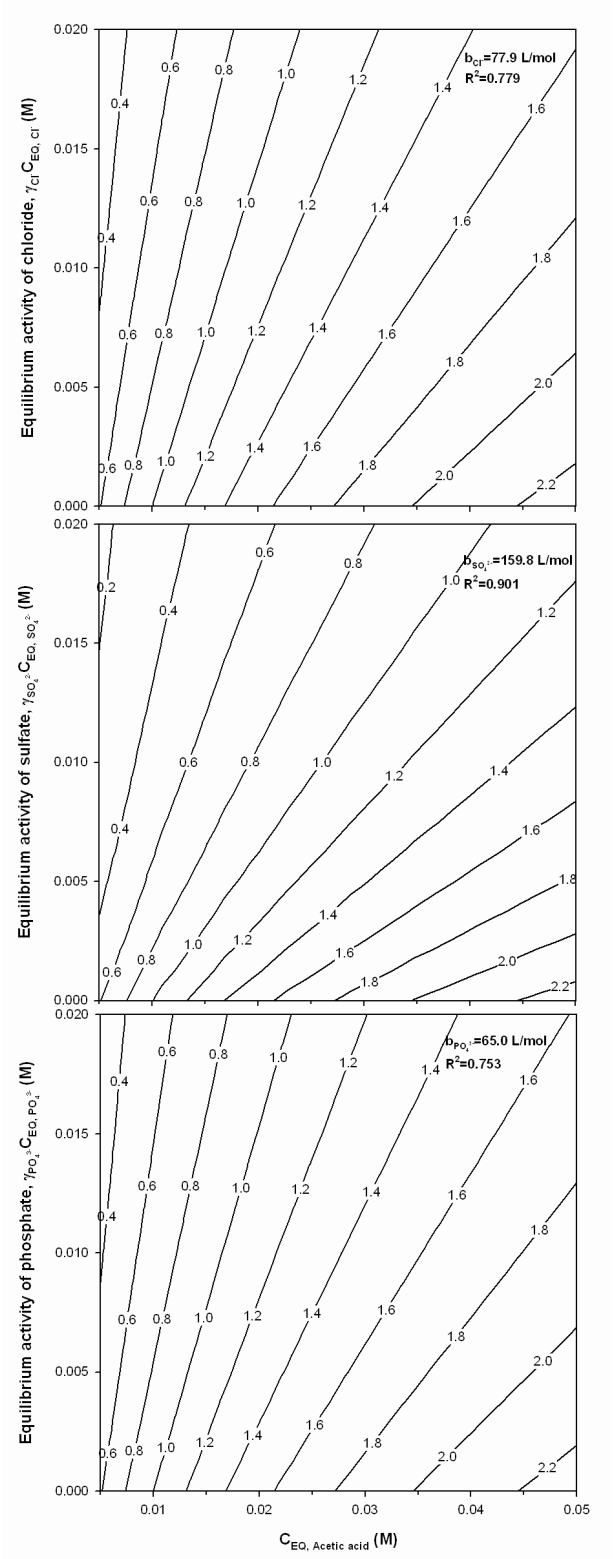

Figure S3. Contour lines of constant acetic acid adsorption onto the 3.14 mol N/kg MSN vs. equilibrium concentration of acetic acid and equilibrium activity of chloride, sulfate, and phosphate.