Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting Information

Zinc-Electrocatalyzed Hydrogenation of Furfural in Near-Neutral Electrolytes

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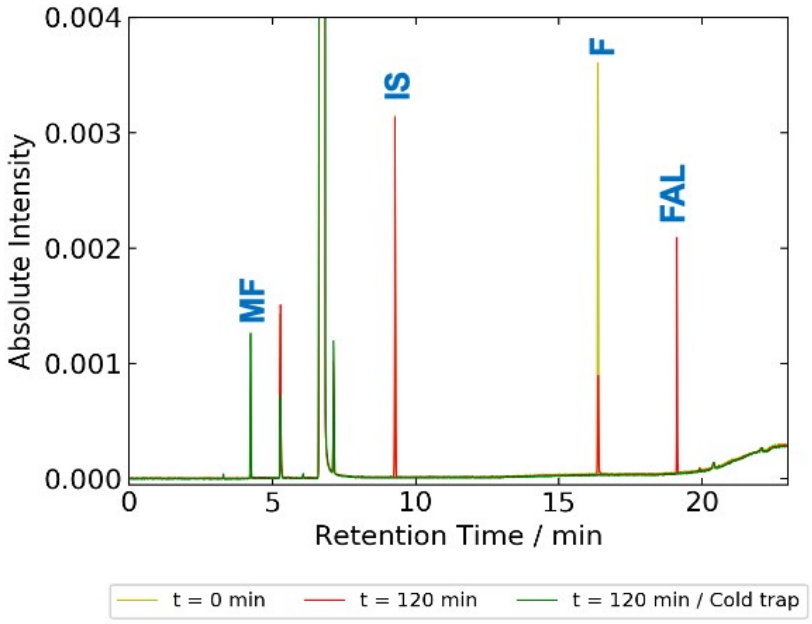

Figure S1. GC chromatogram of reaction mixture containing furfural (F); furfuryl alcohol (FAL), 2-methylfuran (MF), p-xylene (internal standard, IS).

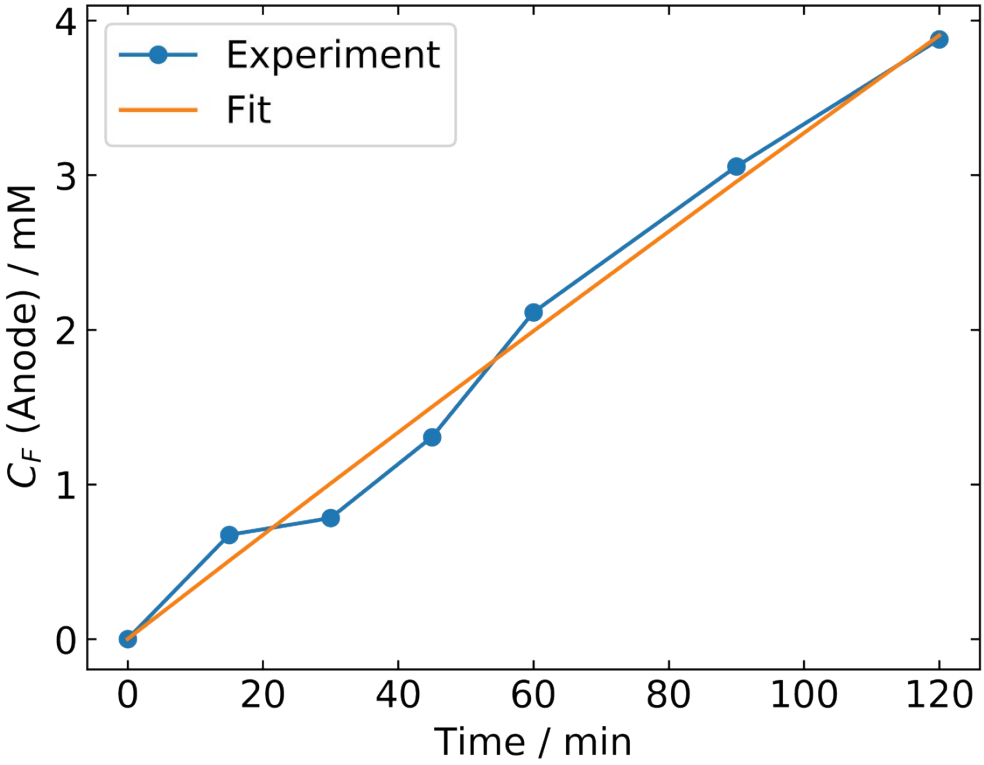

Figure S2. Experimental (Exp.) and fitted (Fit) concentration profile of furfural in anode chamber after permeation

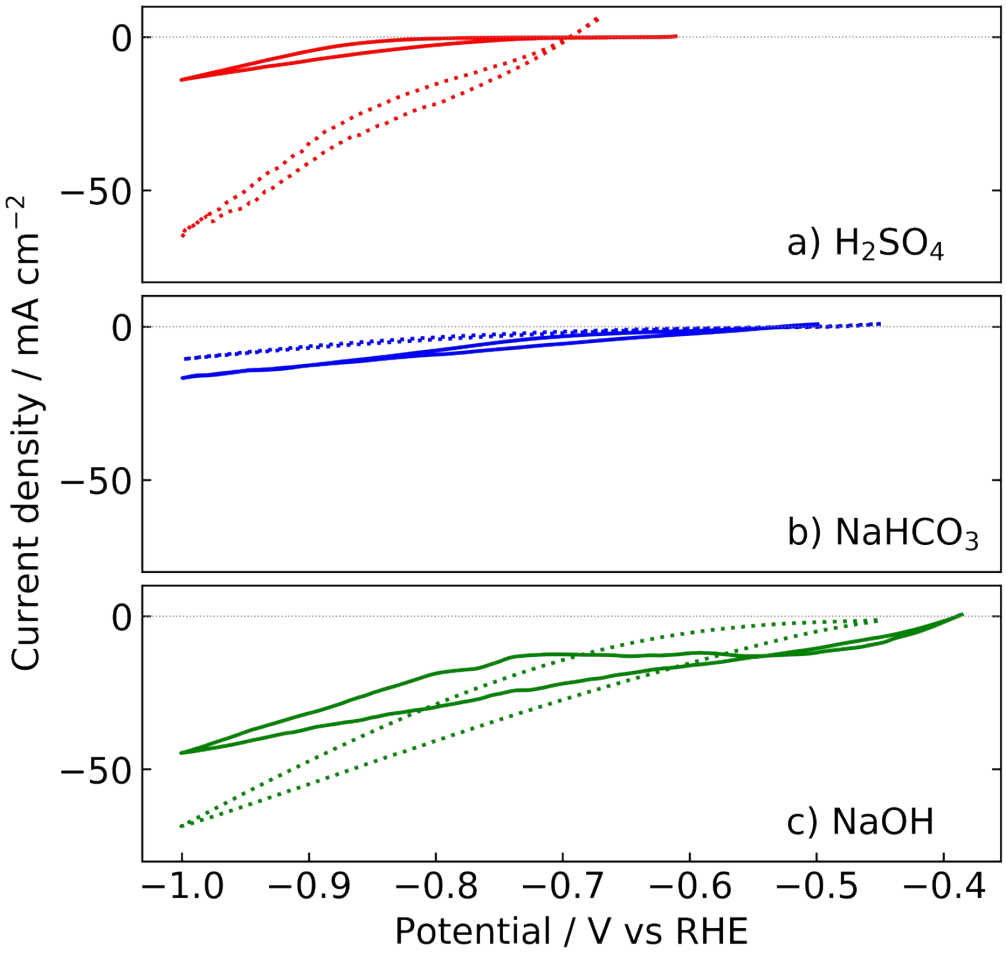

Figure S3. CV showing polarization curves obtained with zinc at different pH (dashed lines = No furfural, bold lines = 100 mM furfural)

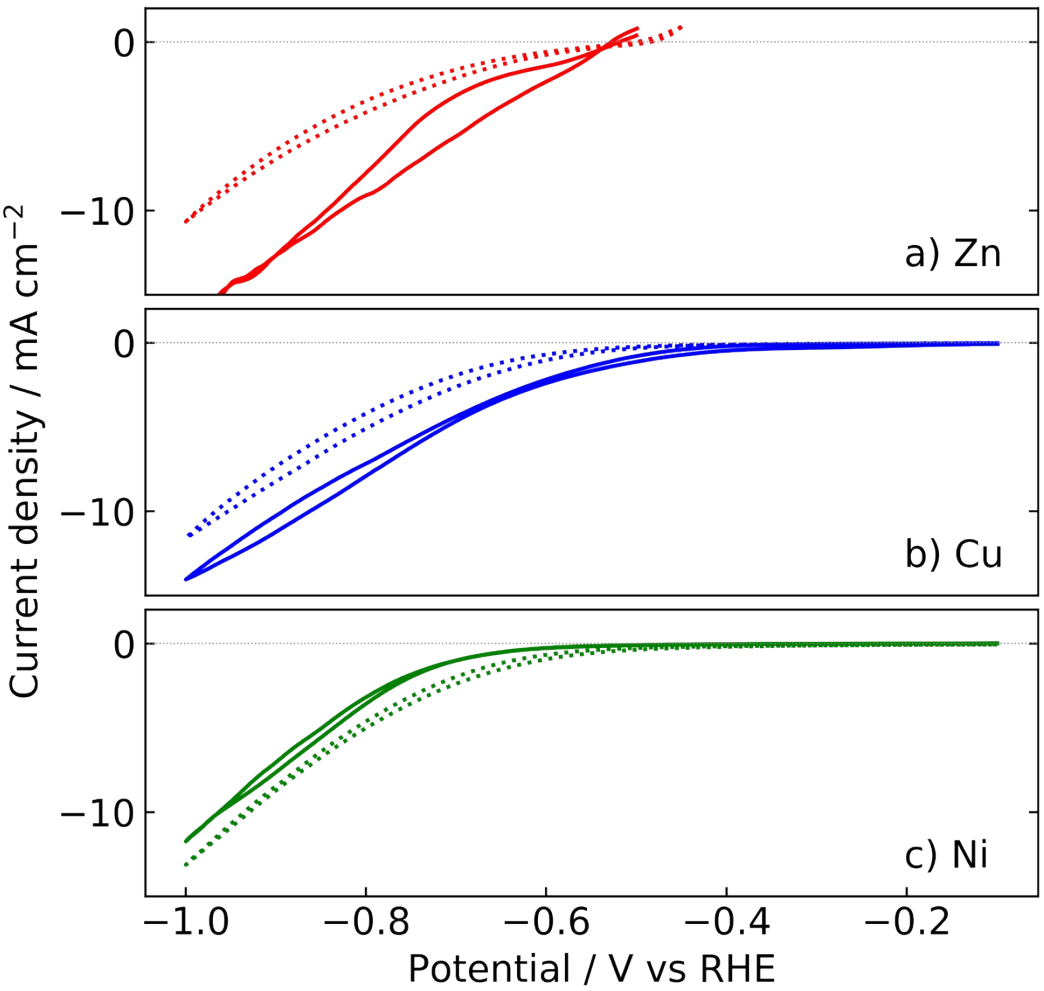

Figure S4. CV showing polarization curves obtained with different catalysts in 0.5 M $NaHCO_3$ (dashed lines = No furfural, bold lines = 100 mM furfural)

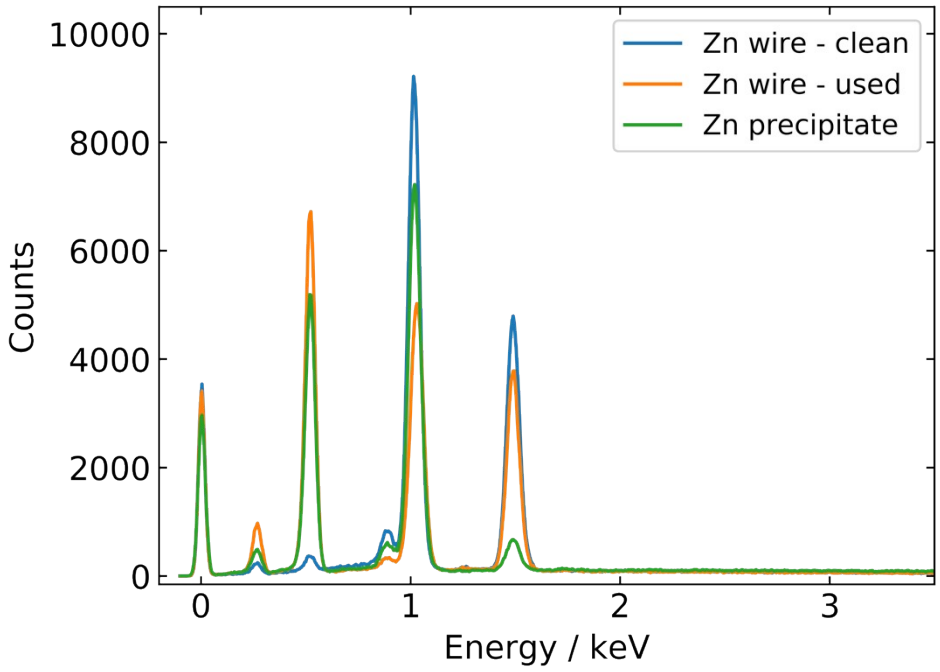

Figure S5. EDS spectra of the clean zinc wire, used zinc wire and zinc precipitates

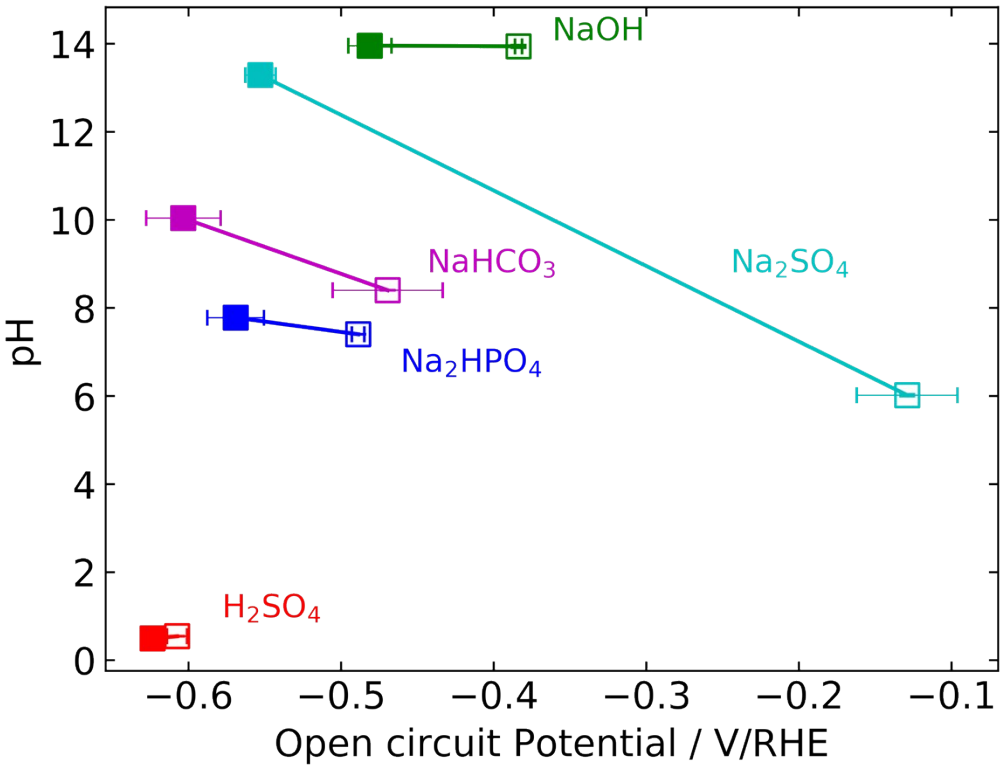

Figure S6. Change in electrolyte pH and Open Circuit potential during two-hour ECH electrolysis. Closed symbols: initial conditions; Open symbols: final conditions.

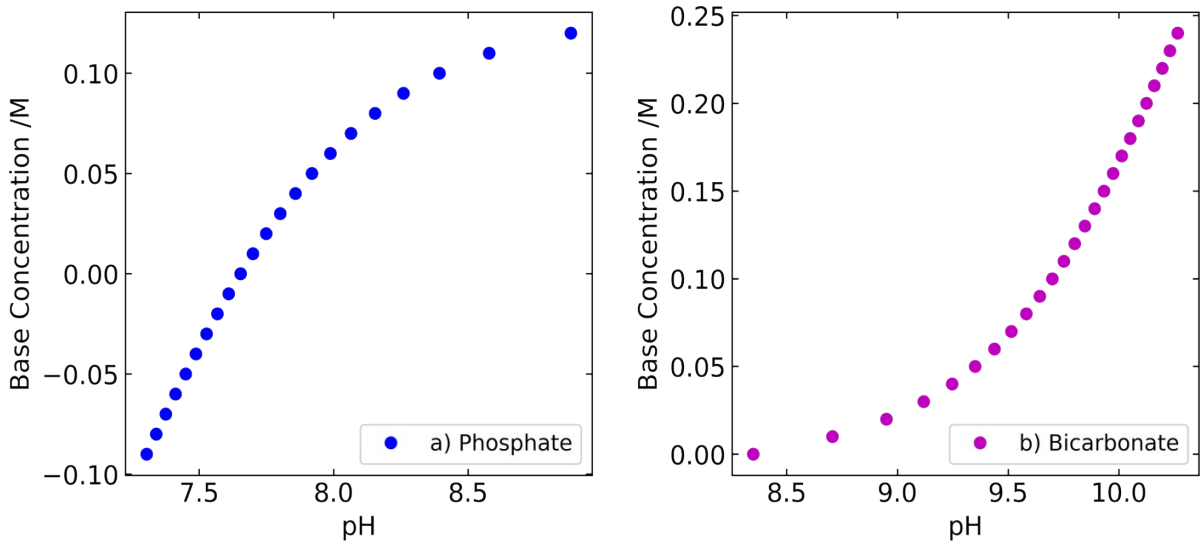

Figure S7. pH as a function of base concentration for a) Phosphate buffer b) Sodium bicarbonate buffer

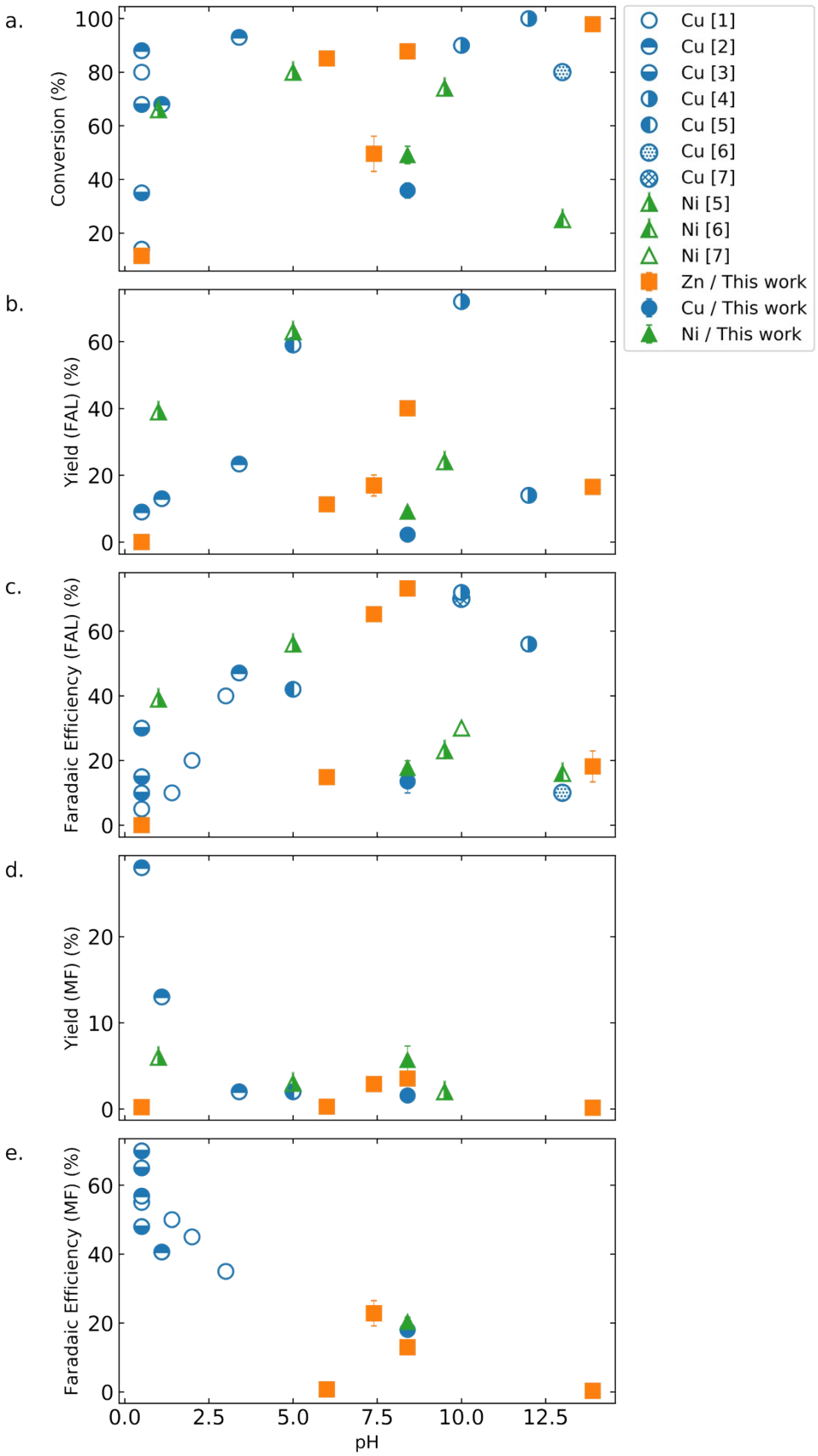

Figure S8. Variation of **(a).** Conversion of furfural, **(b).** Yield of FAL, **(c).** FE of FAL, **(d).** Yield of MF, **(e).** FE of MF with electrolyte pH (Literature vs this work)

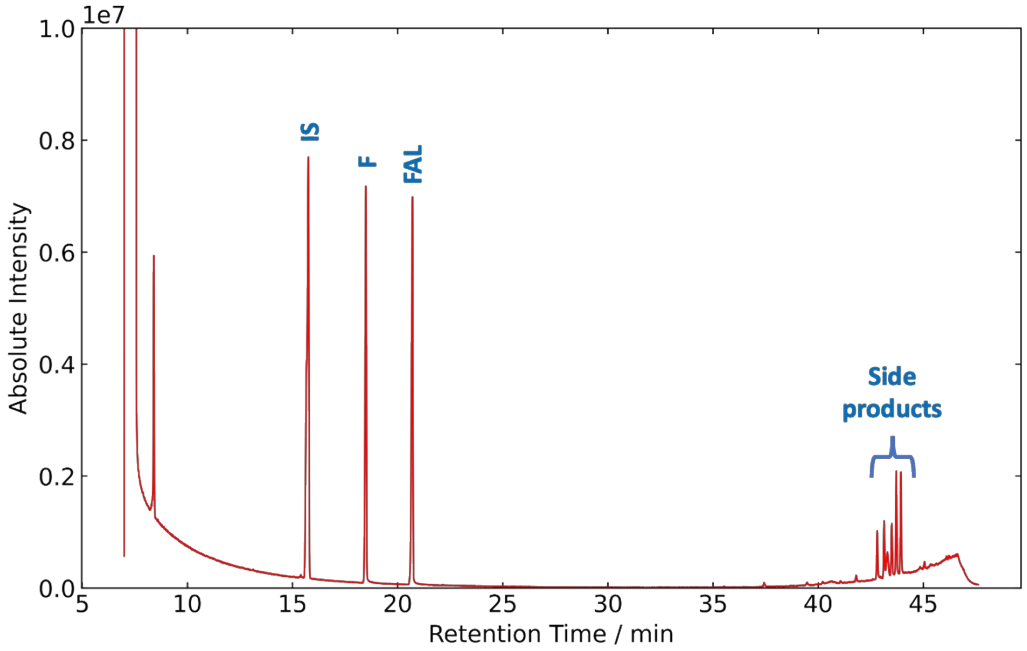

Figure S9. GC chromatogram of reaction mixture containing furfural (F); furfural alcohol (FAL), p-xylene (internal standard, IS) and side products (alpha-furoin (Ethanone,1,2-di-2-furanyl-2-hydroxy); hydrofuroin (1,2-Ethanediol, 1,2-di-2-furanyl-); 4-methyl-5-(2-methyl-2-propenyl)-2(5H)-furanone and 1-(2-furanyl)-3-methyl-butene-1,2-diol [cold trap sample containing MF not analyzed by GC-MS].

Table S1. Similarity indices of probable chemical compounds at respective peak retention times in GC chromatogram [Fig. S9]

		Similarity Index of Chemical Products			
		alpha-furoin	Hydrofuroin	4-methyl-5-(2-methyl-2-propenyl)-2(5H)-furanone	1-(2-furanyl)-3-methyl-butene-1,2-diol
Retention Time / min	42.8	87	-	88	89
	43.1	87	-	89	-
	43.3	80	-	-	-
	43.5	83	82	-	-
	43.7	82	84	85	82
	43.9	82	85	85	

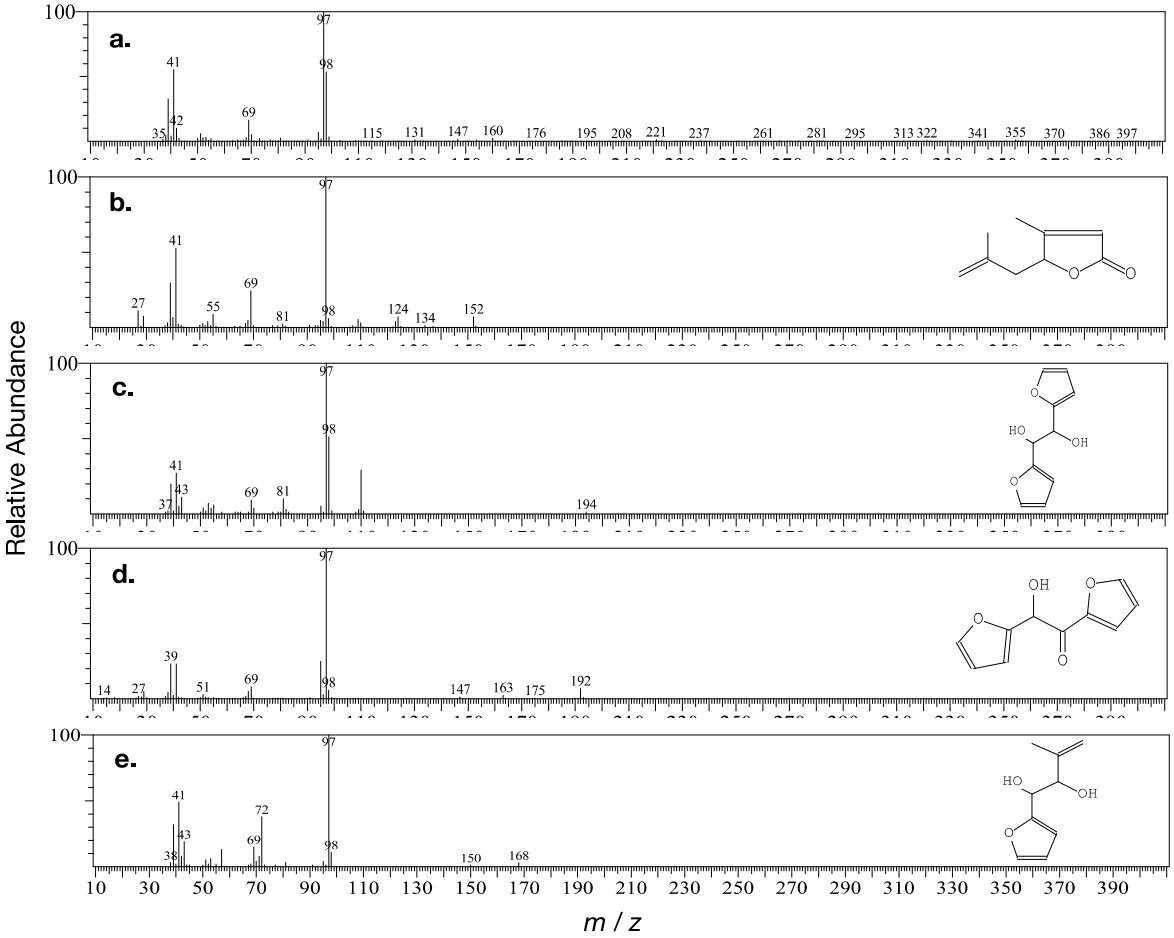

Figure S10. GC Mass spectra with probable chemical side products. (a) Mass spectrum of GC peak at 43.7 min retention time. Reference mass spectrum for (b) 4-methyl-5-(2-methyl-2-propenyl)-2(5H)-furanone; (c) hydrofuroin; (d) alpha-furoin; (e) 1-(2-furanyl)-3-methyl-butene-1,2-diol.

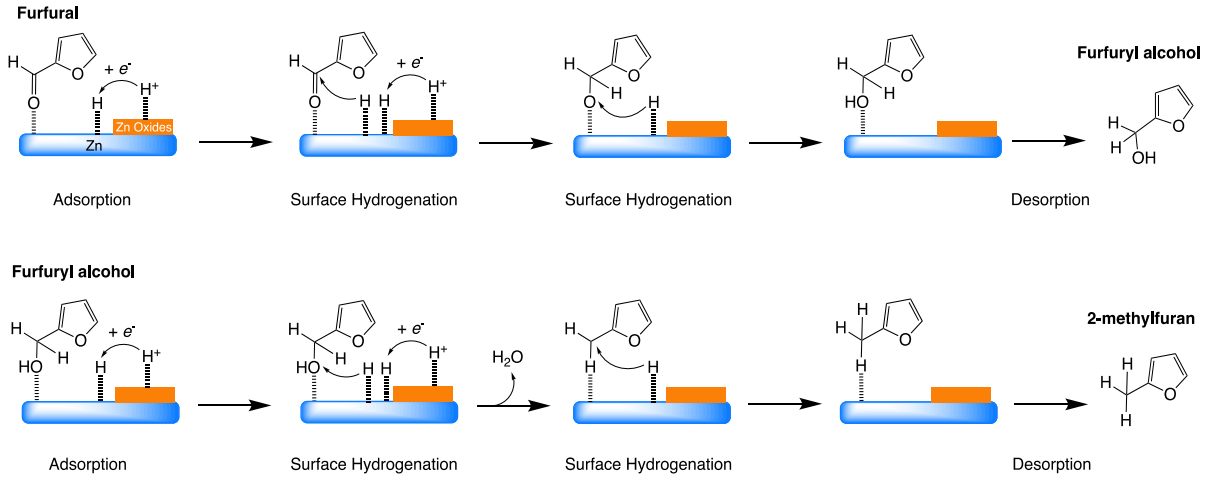

Figure S11. Proposed mechanism for ECH of furfural

References

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