Supplementary Information

The supplementary information contains:

Supplementary Materials and Methods

Supplementary Figures

Figure S1. Sugarcane bagasse-derived crude xylose production *via* thermal acidic hydrolysis.

Figure S2. Enzymatic synthesis of reduced nicotinamide adenine dinucleotide (NADH) from nicotinamide mononucleotide (NMN).

Figure S3. One-pot enzymatic synthesis of reduced nicotinamide adenine dinucleotide (NADH) from ribose-5-phosphate (R5P).

Figure S4. Time-dependent analysis of polyphosphate (polyP) consumption and nicotinamide adenine dinucleotide (NADH) synthesis in the one-pot, one-step enzymatic synthesis of NADH from commercial xylose with varying concentrations of xylose, ATP, or nicotinamide (NAM).

Figure S5. Optimization of one-pot, one-step enzymatic synthesis of nicotinamide adenine dinucleotide (NADH) from commercial xylose.

Figure S6. Sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) gel images of purified recombinant proteins.

Figure S7. Standard curves of polyphosphate (polyP), xylose, and reduced nicotinamide adenine dinucleotide phosphate (NADH) determined by UV-Vis analysis.

Figure S8. High-performance liquid chromatography (HPLC) chromatograms of dihydrofolate (DHF), folic acid (FA), nicotinamide adenine dinucleotide (NAD(H)), nicotinamide adenine dinucleotide phosphate (NADP(H)), tetrahydrofolate (THF), xylose, and D-xylulose-5-phosphate (Xu5P).

Figure S9. Standard curves of D-xylulose-5-phosphate (Xu5P; 13.5 min), nicotinamide adenine dinucleotide (NAD^+; 36.8 min), nicotinamide adenine dinucleotide phosphate ($NADP^+$; 30.8 min), reduced NAD^+ (NADH; 42 min), and reduced $NADP^+$ (NADPH; 35.8 min) determined by high-performance liquid chromatography (HPLC) analysis.

Figure S10. Standard curves of tetrahydrofolate (THF; 10.0 min) and folic acid (FA; 12.2 min) determined by high-performance liquid chromatography (HPLC) analysis.

Figure S11. Synthesis tree of E-factor analysis for NADH synthesis.

Figure S12. Synthesis tree of E-factor analysis for NADH synthesis.

Supplementary Tables

Table S1. The list of recombinant proteins and commercial enzymes used in this work.

Table S2. Comparison of the NMN/NAD(P)H synthesis strategies.

Table S3. Materials prices.

Supplementary Data

Data S1. Thermodynamic calculation of the *in vitro* one-pot enzymatic NAD(P)H synthesis process.

Data S2. E-factor calculation of the *in vitro* one-pot enzymatic NAD(P)H synthesis process.

Data S3. Cost calculation for chemo-enzymatic NADPH synthesis

Supplementary References