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## Reaction of H<sub>2</sub> with mitochondria-relevant metabolites using a single-metal-site (PNNP)iridium complex

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cycle

The Krebs cycle occurs in mitochondrial matrix in cells to produce and transfer electrons to generate energy-rich NADH, GTP and FADH<sub>2</sub>, and conversely to produce not only C<sub>4</sub>-dicarboxylic acids (succinic acid (SucA), fumaric acid (FumA), malic acid (MliA), oxaloacetic acid (OacA)), but also C<sub>5</sub>- (2-oxoglutaric acid (OglA)) and C<sub>6</sub>-polycarboxylic acids (aconitic acid (AcoA) and citric acid (CitA)) as metabolites. Those polycarboxylic acids are in highly oxidized or oxygenated states and thus energy-poor molecules, which are potential candidates as bio-renewable carbon feedstock if hydrogen atoms and electrons could be back into these molecules (Figure 1).

We report herein that those C<sub>4</sub>, C<sub>5</sub>, and C<sub>6</sub> resources, in addition to mitochondria-relevant metabolites (aspartic acid (AspA), tartaric acid (TarA), itaconic acid (ItaA)), sugar-derived artificial feedstock (levulinic acid (LevA)), and petrochemical product (phthalic acid (PhtA)) are convergently reduced and dehydrated to corresponding diols or triols upon reaction with H<sub>2</sub> catalyzed by iridium (Ir) complex (**IrPCY2**, Figure 2) comprising sterically confined Ir-bipyridyl frameworks.<sup>1</sup>



Figure 1. Summary of this work

Figure 2. IrPCY2

1) S. Yoshioka, S. Nimura, M. Naruto, S. Saito, Sci. Adv. 2020, 6, eabc0274.