Supporting Information

Highly Selective Conversion of Glyceric Acid to 3-Iodopropionic Acid by Hydriodic Acid Mediated Hydrogenation

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The conversion and yield were calculated as following:

n (GA) = m (GA) / 106

n (DIPA) = m (DIPA) / 200

n (3-IPA) = m (3-IPA) / 326

Conversion of GA= [1 - n (GA after reaction) / n (GA before reaction)] ×100%

Yield of DIPA = n (DIPA after reaction) / n (GA before reaction) × 100%

Yield of 3-IPA = n (3-IPA after reaction) / n (GA before reaction) × 100%

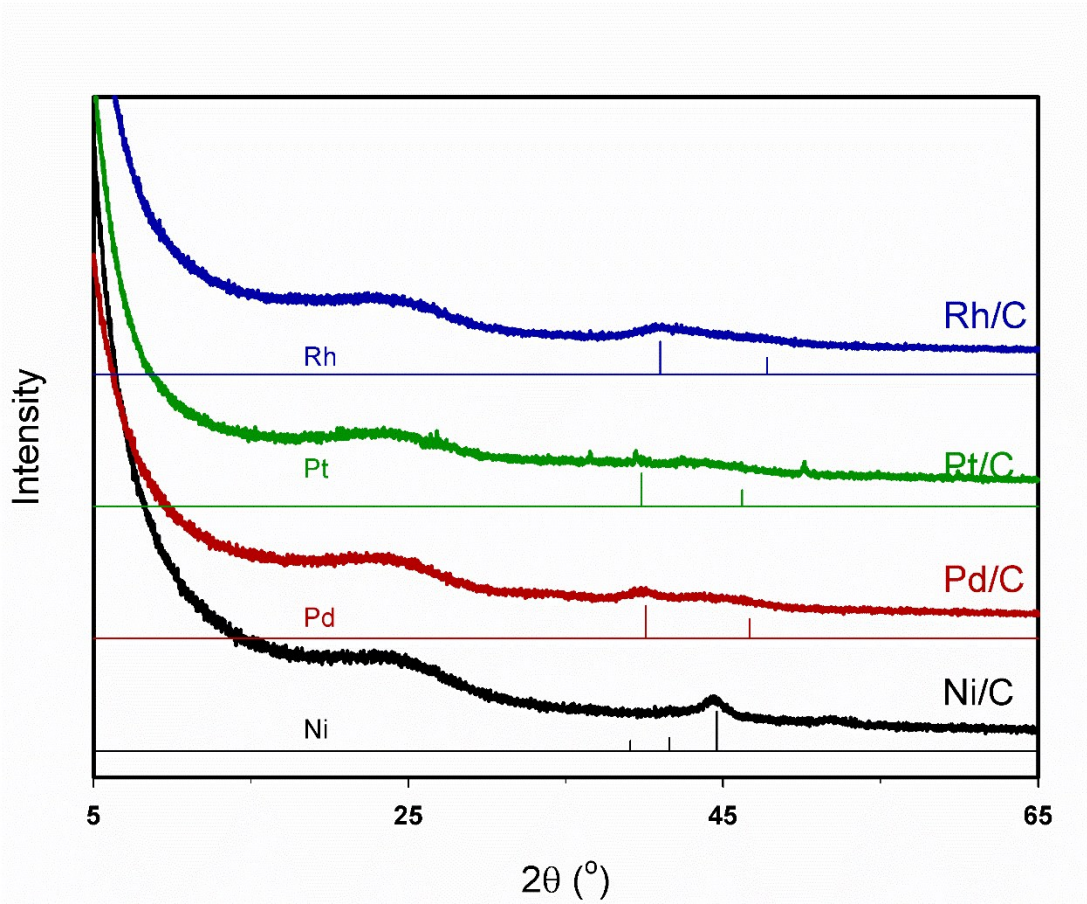

Figure S1. X-ray diffraction patterns of different metal catalysts

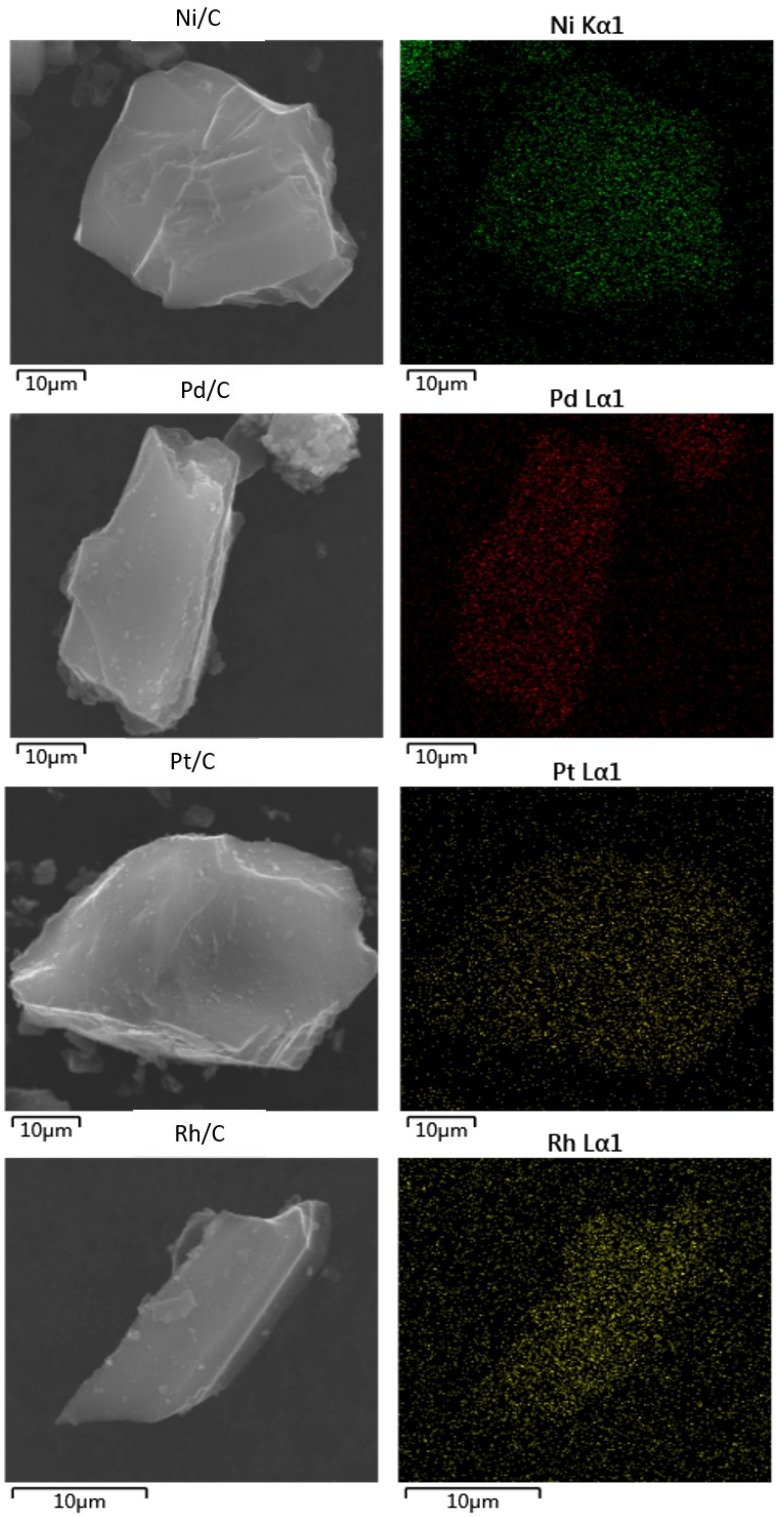

Figure S2. SEM-EDS elemental mapping of different metal catalysts

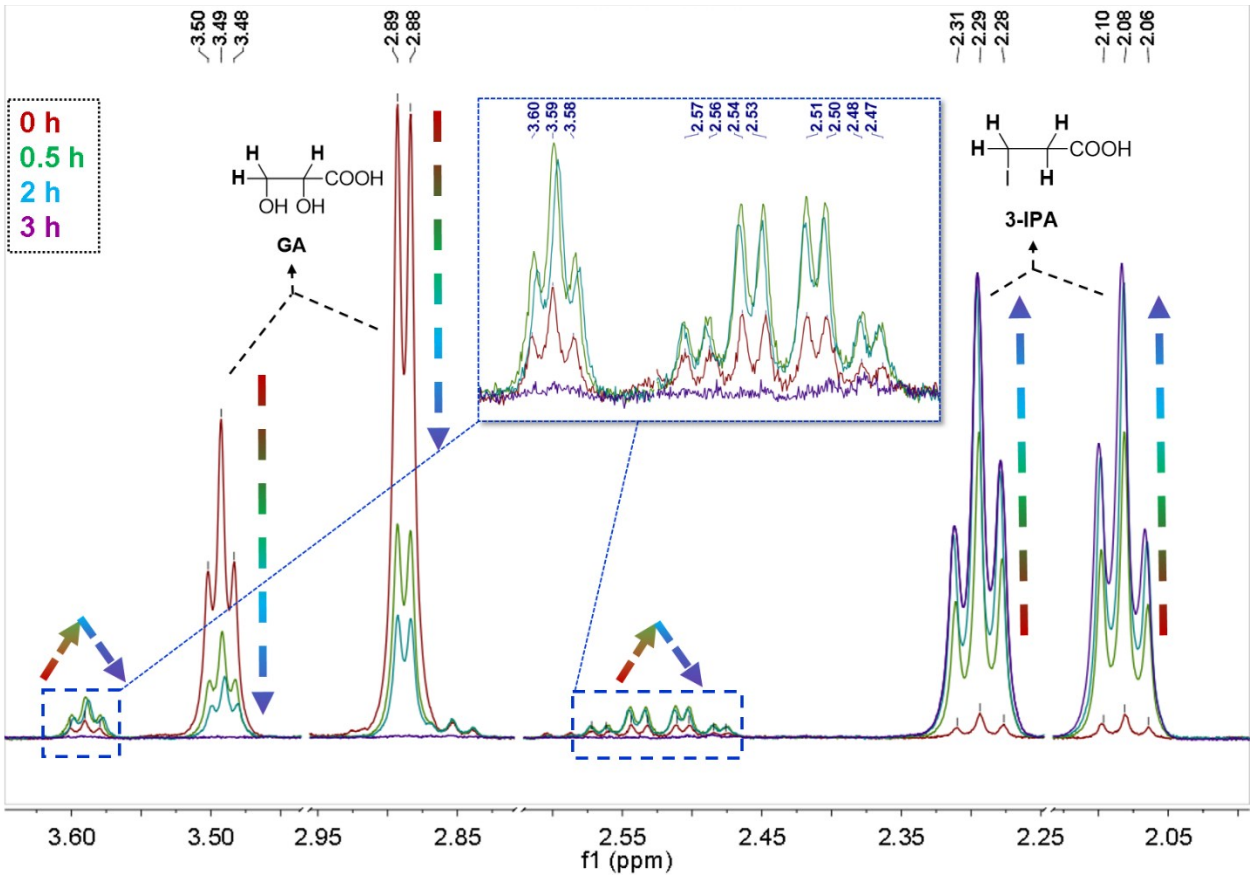

Figure S3. ^{1}H NMR spectrum for reaction liquid in different reaction time (GA: Glyceric acid; 3-IPA: 3-iodopropionic acid). Reaction conditions: 0.56 g 20wt% GA aqueous solution (0.84 mmol GA), 4.5 mL 57wt% hydroiodic acid, I_2 0.65 g, 5wt% Rh/C 0.05 g, 373 K, initial H_2 pressure 400 psi, 400 rpm.

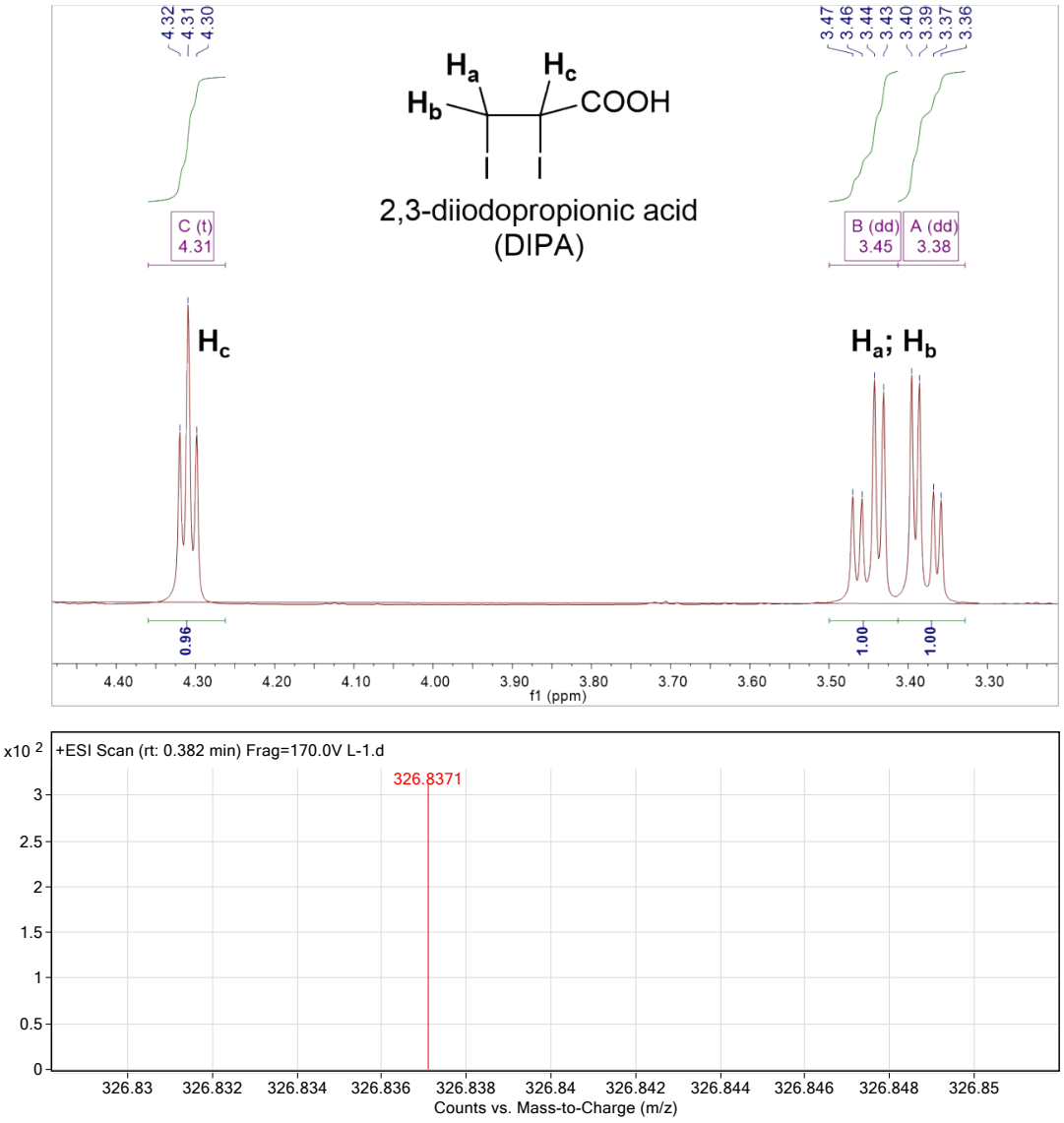

Figure S4. ^{1}H NMR spectrum by 400M NMR (Top) and MS spectrum (Bottom) for intermediate

Table S1. Hydrolysis of 3-IPA and iodination reaction of 3-HPA catalyzed by HI

Entry	Reactant	Solvent	Conversion (%)	Product	Yield (%)
1 [a]	3-IPA	Water	75.8	3-HPA	69.4
2 [b]	3-HPA	Water	N. D.	3-IPA	N. D.
3 [b]	3-HPA	Cyclohexane	5.4	3-IPA	5.0

Reaction conditions: Reactant 0.84 mmol, 5wt% Rh/C 0.1g, solvent 5 mL, 373 K, 1 h, 400 rpm, initial H_2 pressure 400 psi; [a] 22wt% HI; [b] I_2 2 mmol (equal to 9.0wt% HI).

Method for the calculation of the reaction rate constants (*k*) and reaction order (n)

As the conversion is low, the conversion is linearly related with time, and

$r \approx (a\text{-}a_t)/t$,

$r = k * a^n$,

namely $\ln r = \ln k + n * \ln a$,

where r is the reaction rate, a is the initial concentration of reactant, and a_t is the concentration of reactant at t h.

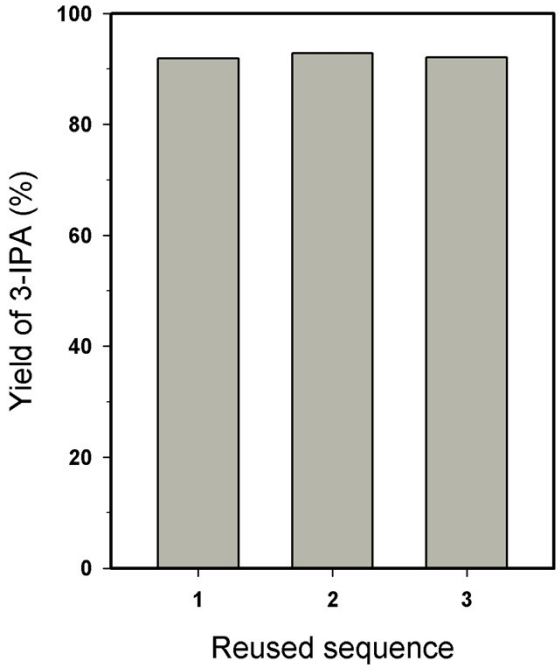

Figure S5. Reused test of HI-Rh reaction system. Reaction conditions: 0.56 g 20wt% GA aqueous solution (0.84 mmol GA), 15 μmol $RhCl_3$, 4.5 ml 57wt% hydroiodic acid, 0.65 g I_2, 373 K, 3 h, initial H_2 pressure 400 psi, 400 rpm.

Table S2. The distribution coefficient of 3-IPA in organic solvent and water

Organic solvent	Hexane	Cyclohexane	CCl_4	$HCCl_3$	Ether	Hexanol	Tributyl phosphate
Distribution coefficient	0	0.033	0.18	0.82	10.1	38.6	49.9