

Supporting Information

Synthesis of renewable C-C cyclic oxygenated compounds dedicated for high-density biofuels from biomass-derived cyclopentanone

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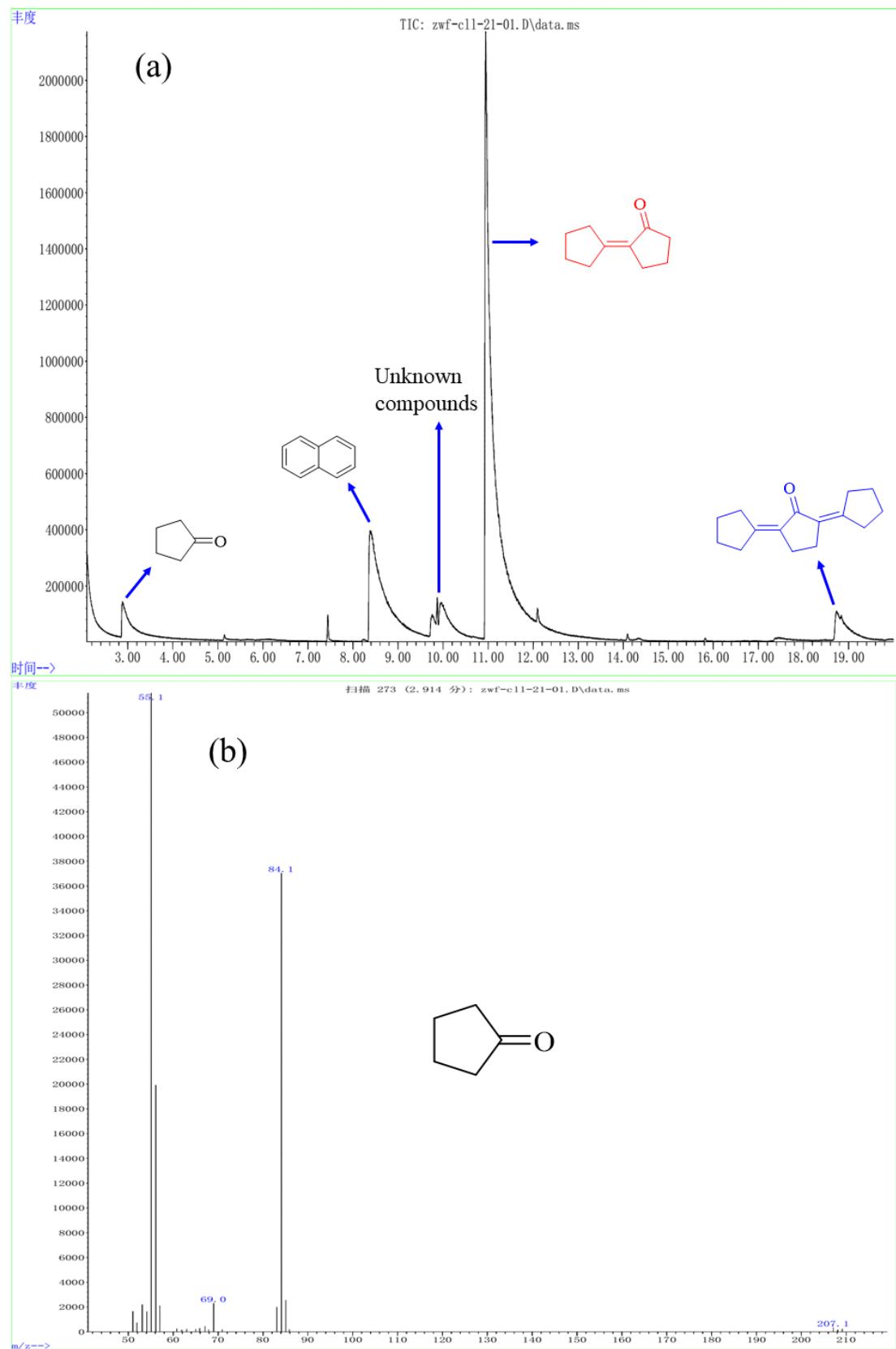
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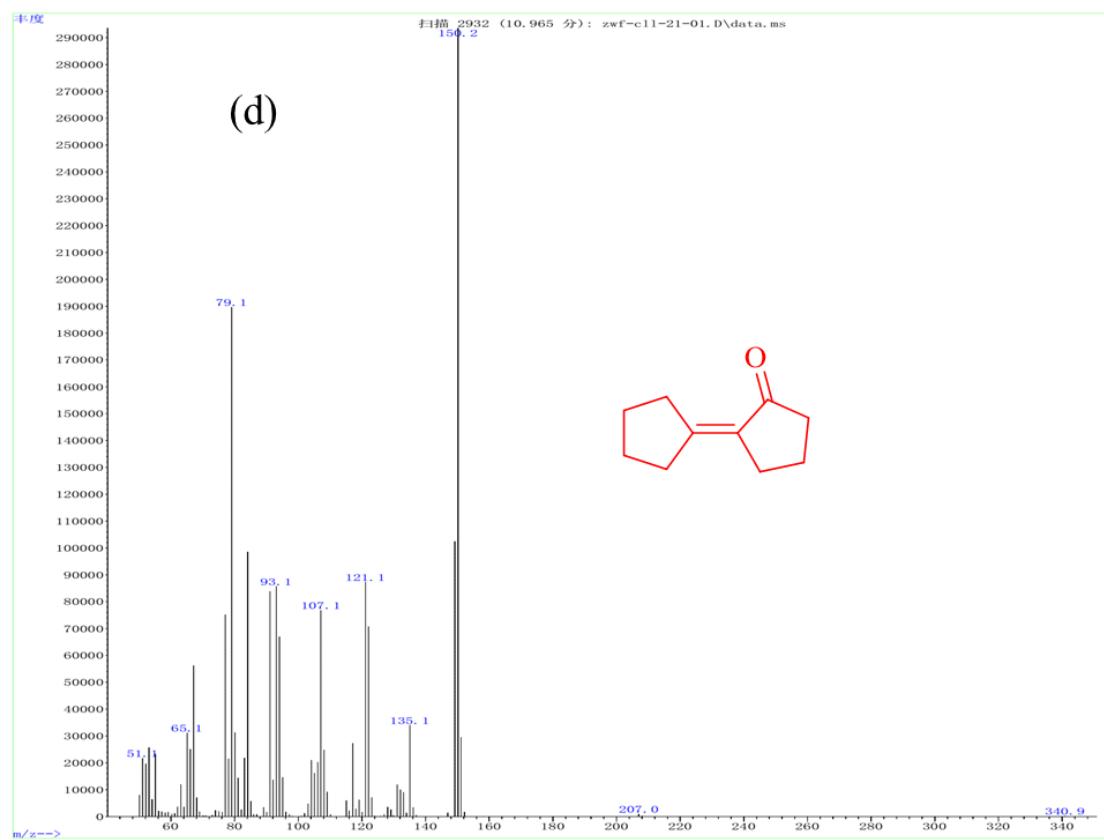
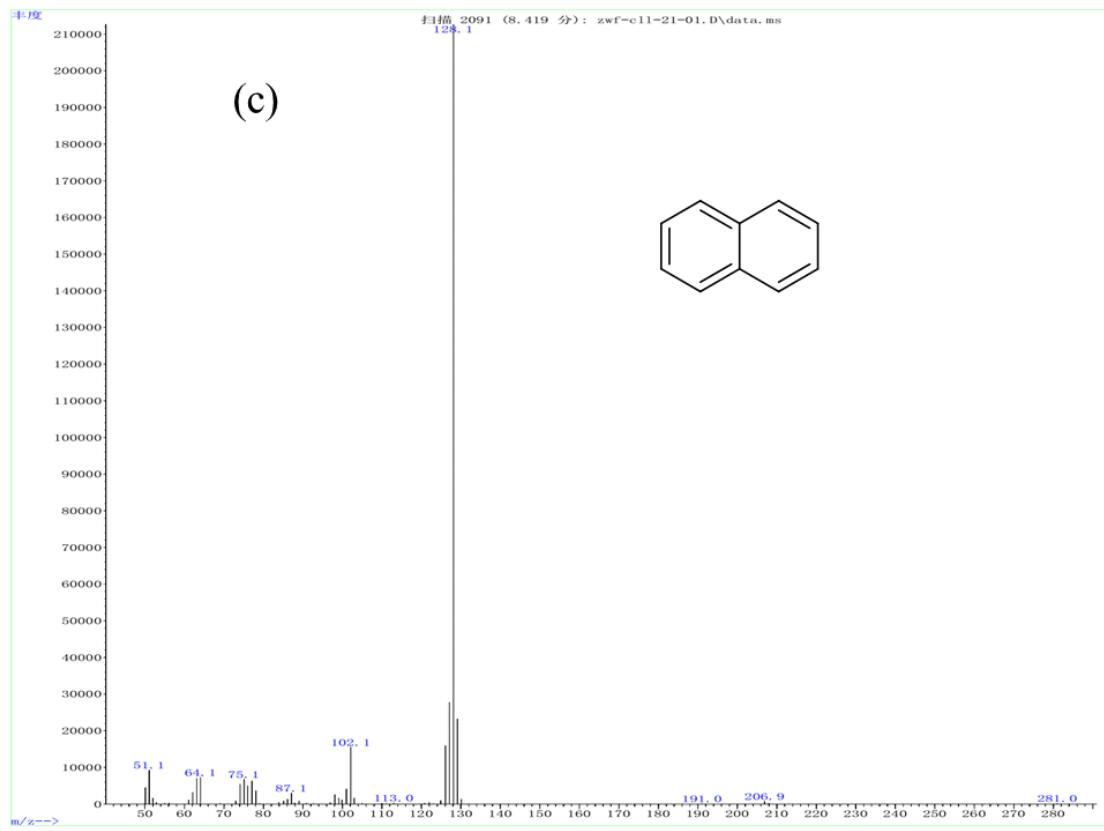
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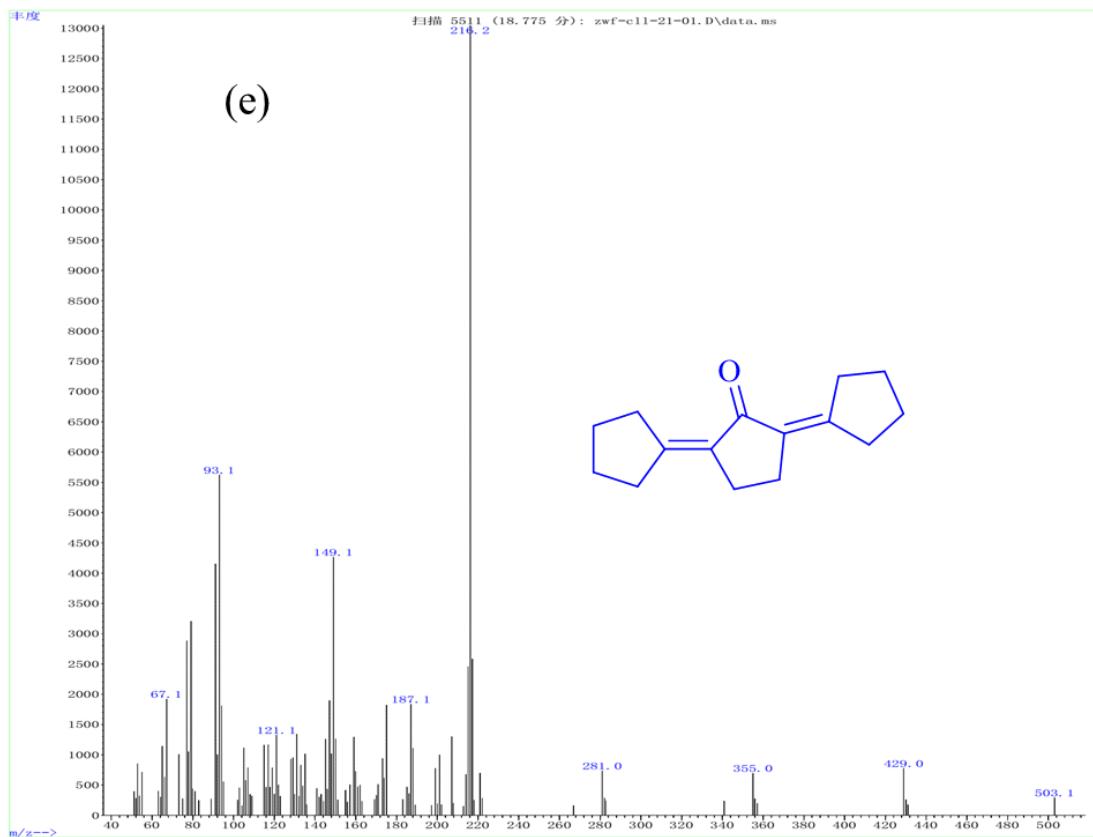


Figure S1 GC chromatograms of reaction mixture (from GC-MS) catalyzed by $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O}$ at 180°C .

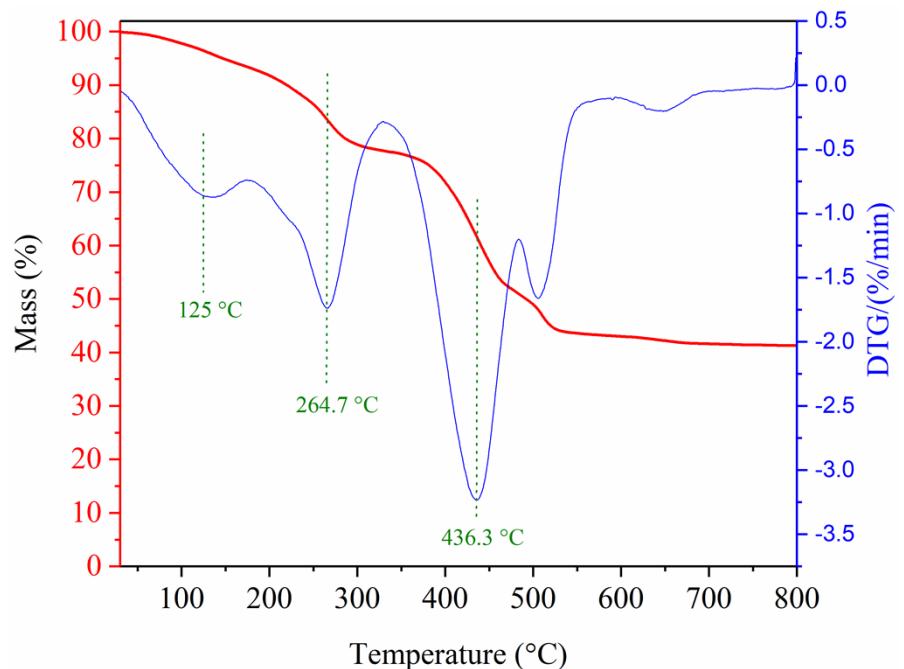


Figure S2 TGA and DTG curves of $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O}$ catalyst

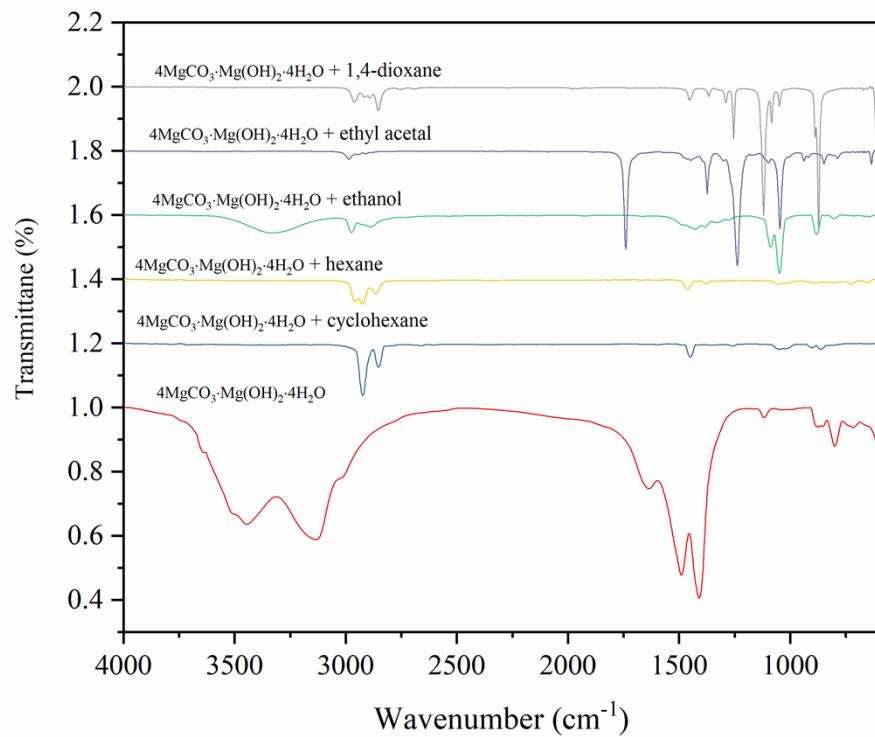


Figure S3 FT-IR spectra of basic magnesium carbonate/reaction solvents

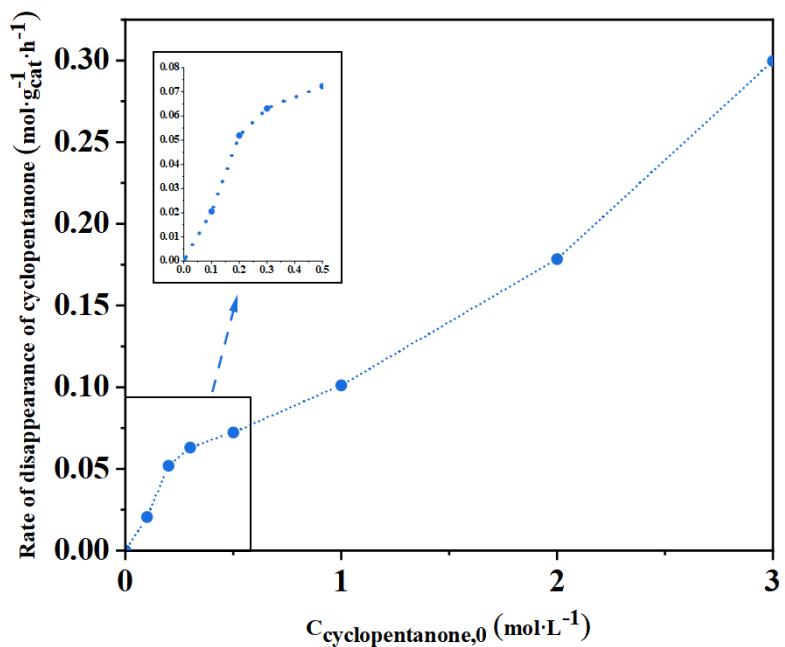


Figure S4 Initial rates of cyclopentanone conversion over $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O}$ catalyst as a plot of initial cyclopentanone concentration. Reaction condition: 0.05 g $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O}$, 10 mL of total liquid volume, 120 °C and 0.5 h

Table S1 Linearization of cyclopentanone self-condensation initial rates derived from Langmuir-Hinshelwood and Eley-Rideal reaction models

Model	Initial rate expression	Linearized function
Langmuir-Hinshelwood Deprotonation	$r = k_{DP} \frac{K_{ads}C}{1 + K_{ads}C}$	$\frac{1}{r} = \frac{1}{k_{DP}K_{ads}C} + \frac{1}{k_{DP}}$
Langmuir-Hinshelwood C-C coupling	$r = k_{LH}K_{DP} \left(\frac{K_{ads}C}{1 + K_{ads}C + K_{ads}K_{DP}C} \right)^2$	$\frac{1}{\sqrt{r}} = \frac{1}{K_{ads}\sqrt{k_{LH}K_{DP}C}} + \frac{1 + k_{DP}}{\sqrt{k_{LH}K_{DP}}}$
Eley-Rideal C-C coupling	$r = k_{ER}K_{DP} \frac{K_{ads}C}{1 + K_{ads}C + K_{ads}K_{DP}C} C$	$\frac{C^2}{r} = \frac{1 + K_{DP}}{k_{ER}K_{DP}} C + \frac{1}{k_{ER}K_{DP}K_{ads}}$

* k_{DP} , k_{LH} , and k_{ER} are the rate constants of the different kinetic models; K_{ads} is the adsorption constant of cyclopentanone; K_{DP} is the equilibrium constant for deprotonation; and C is the initial concentration of the cyclopentanone.

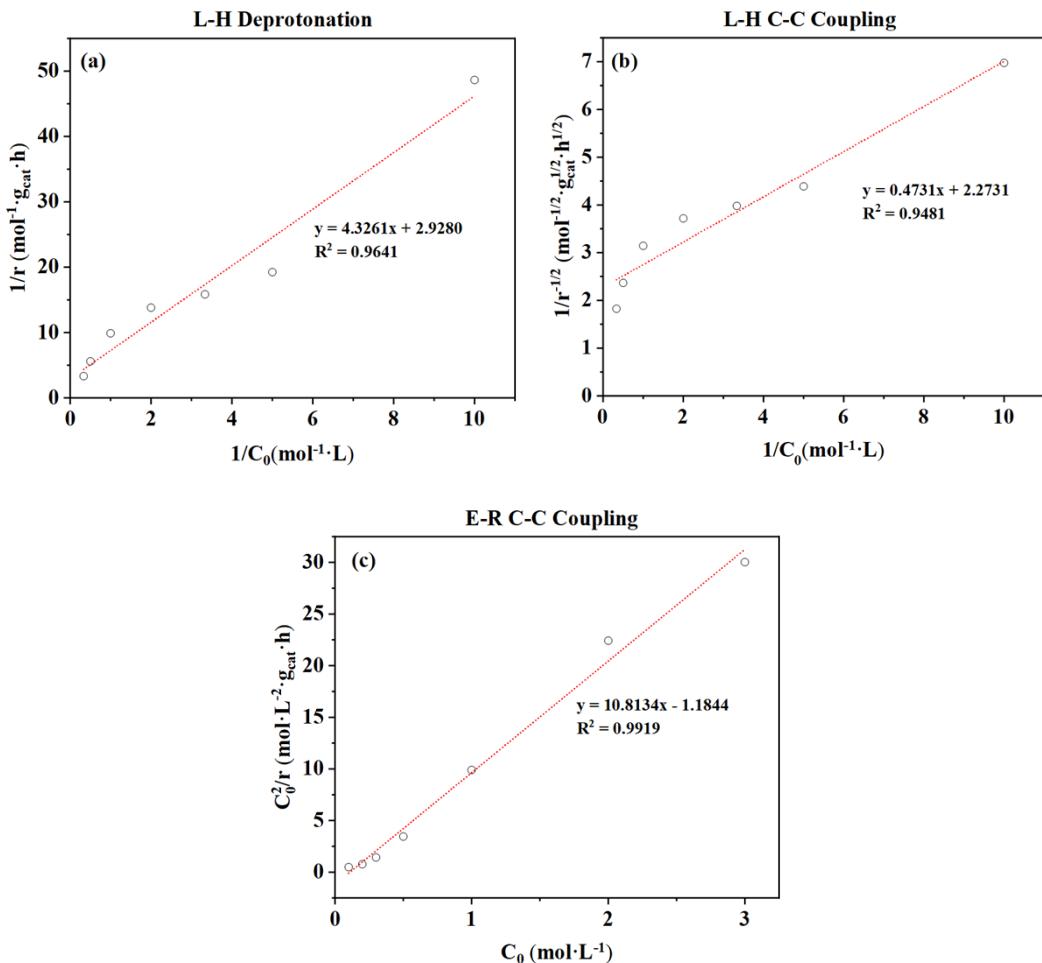


Figure S5 Linearization of initial rates over $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O}$. Reaction condition: 0.05 g $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O}$, 10 mL of total liquid volume, 120 °C and 0.5 h