

Supporting Information

Oxidation of biomass-derived furans to maleic acid over nitrogen-doped carbon catalysts under the acid-free condition

Chi Van Nguyen,^{ab} Jing Rou Boo,^a Chia-Hung Liu,^{c,d} Tansir Ahamad,^e Saad M Alshehri,^e Babasaheb

M. Matsagar ^{*a} and Kevin C.-W. Wu ^{*a}

^{a.} *Department of Chemical Engineering, National Taiwan University. No. 1, Sec. 4, Roosevelt Road, Taipei 10607, Taiwan.*

^{b.} *Institute of Research and Development, Duy Tan University, Danang 550000, Vietnam*

^{c.} *Department of Urology, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan*

^{d.} *Department of Urology, Shuang Ho Hospital, Taipei Medical University, New Taipei City, Taiwan*

^{e.} *Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia*

*Corresponding authors Email: matsagar03@ntu.edu.tw; kevinwu@ntu.edu.tw

Procedure to determine the possible active oxygen species generated on the catalyst:

Typically, NC-900 (50 mg) was added into 5 mL H₂O₂ (35 wt%) and 5 mL H₂O. The mixture was treated at 80 °C for 1 h under magnetic stirring, then the solid was filtered from the solution. The resulting solid was characterized using C1s XPS analysis to determine the formation of active oxygen species.

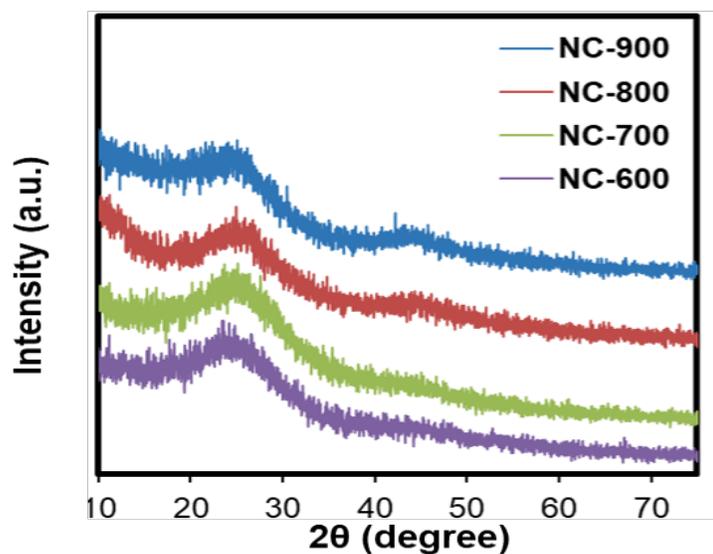


Figure S1. XRD patterns of NC-x catalysts.

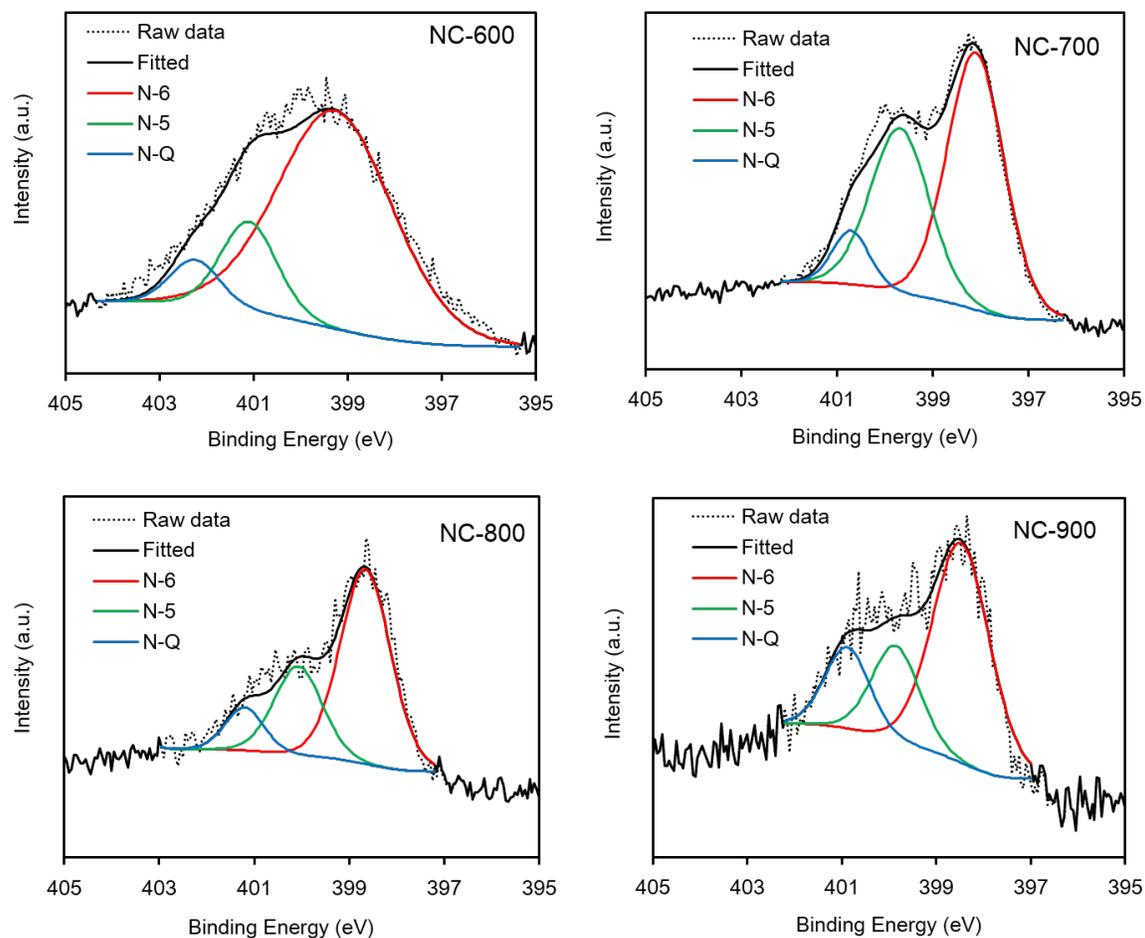


Figure S2. High resolution XPS spectra of N 1s for NC-x catalysts.

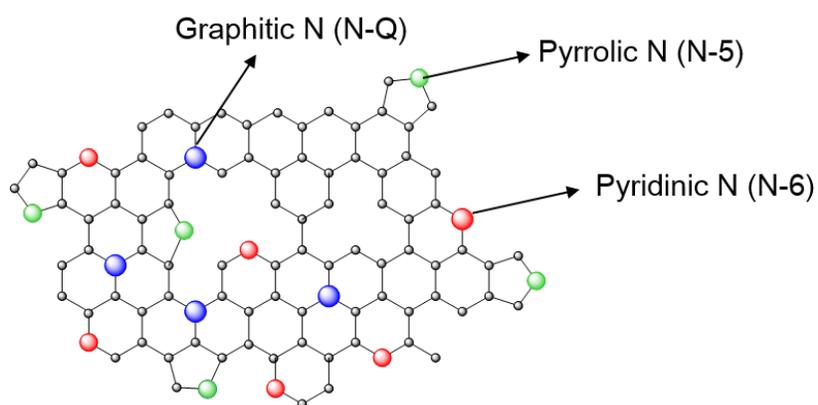
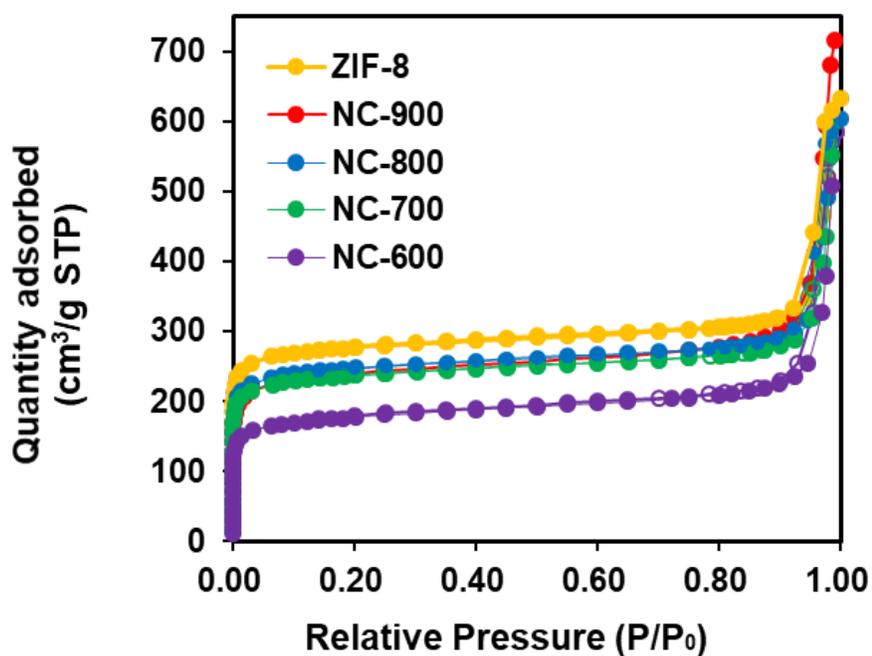


Figure S3. Representation of three chemical bonding configurations in the synthesized NC-x samples.

Table S1 Compositions of NC-x catalysts

Samples	Elemental analysis (wt%)		XPS N 1s (at %)		
	N	C	N-6	N-5	N-Q
NC-900	14.29	63.59	47.56	27.6	24.84
NC-800	22.47	55.63	61.98	23.66	14.37
NC-700	23.71	47.85	58.52	32.78	8.7
NC-600	24.94	44.19	87.3	6.16	6.5
g-C ₃ N ₄	60.81	34.34	80.63	17.52	1.85
biomass-derived NC	4.19	90.57	55.45	39.80	4.71

**Figure S4.** N₂ adsorption-desorption isotherm for ZIF-8 and various ZIF-8-derived NC.

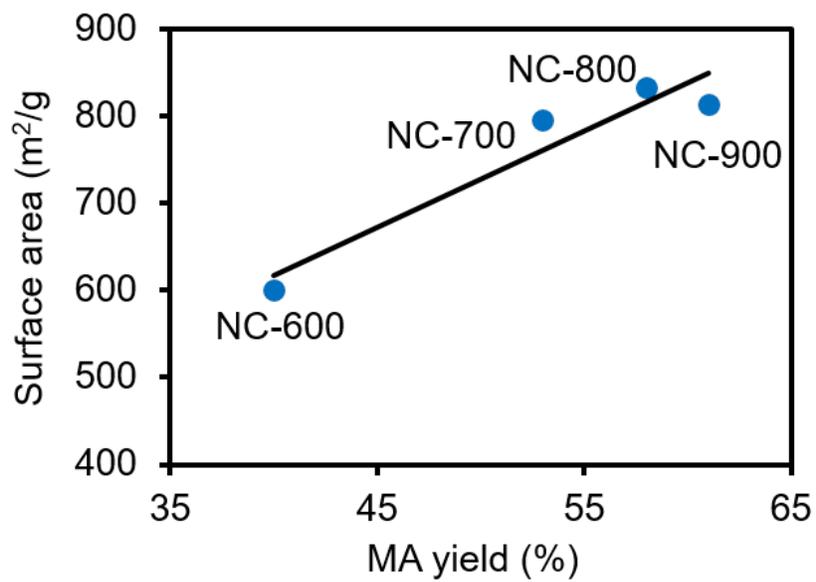


Figure S5 Relationship between the BET specific surface area of the NC-x catalyst with MA yield.

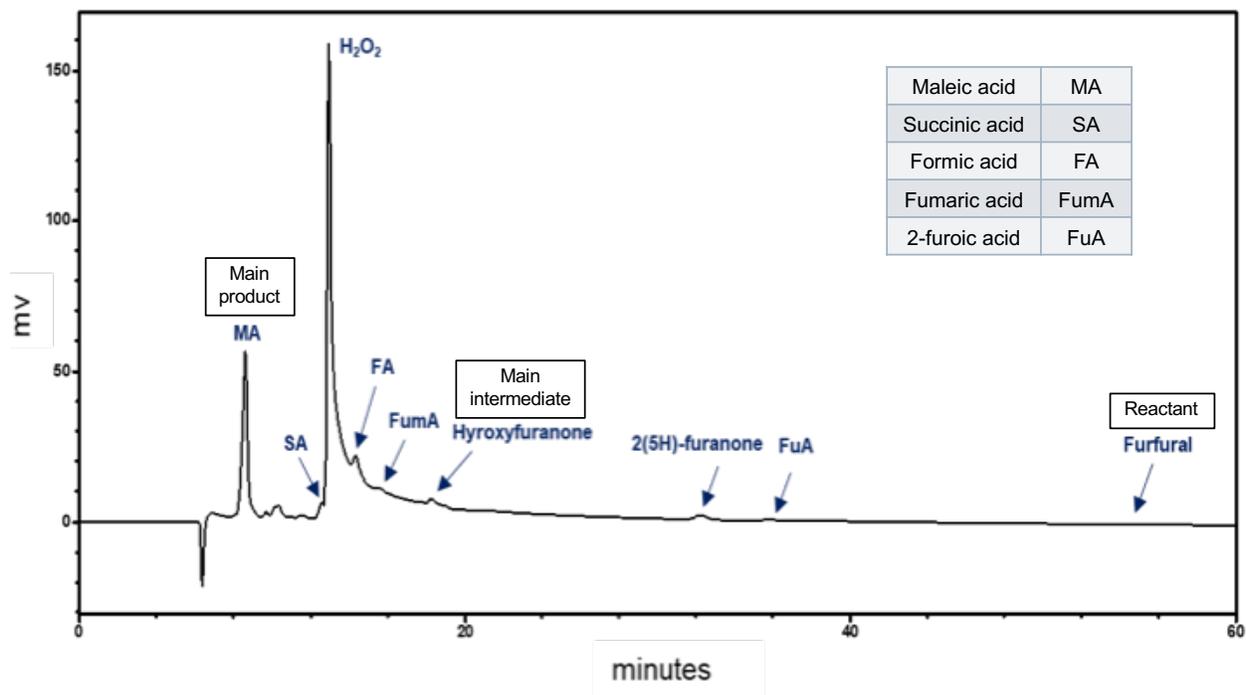


Figure S6. HPLC profile of reaction mixture; Reaction condition: Furfural (1 mmol), H₂O (5 mL), NC-900 (50 mg), H₂O₂ (5 mL; 35 wt%), time 5 h, temperature 80 °C.

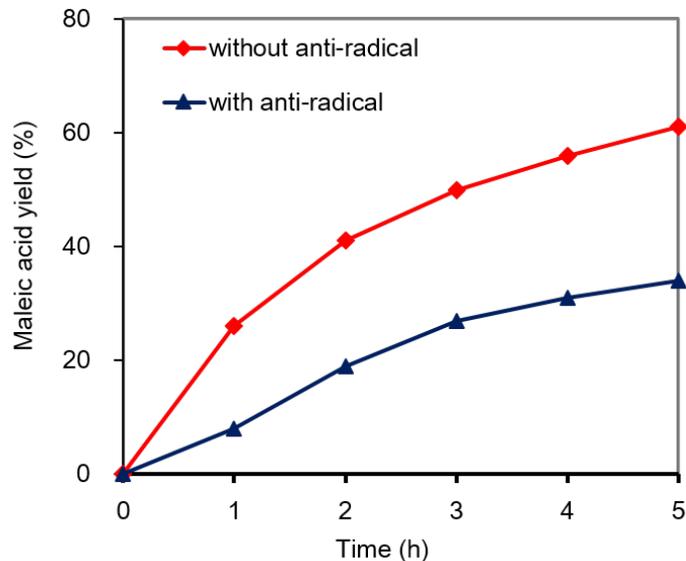


Figure S7. Effect of scavenging agent on the furfural oxidation into MA. Reaction condition without anti-radical agent: furfural (1 mmol), NC-900 catalyst (50 mg), H₂O₂ 5 mL (35 wt%), water 5 mL, temperature 80 °C.

In the presence of anti-radical agent, 2 mmol of Gallic acid was added into the reaction mixture, other parameters remained similar. As shown in the Figure S7, the MA yield significantly decreased in the presence of the Gallic acid. Suggesting that the furfural oxidation could follow a radical mechanism.

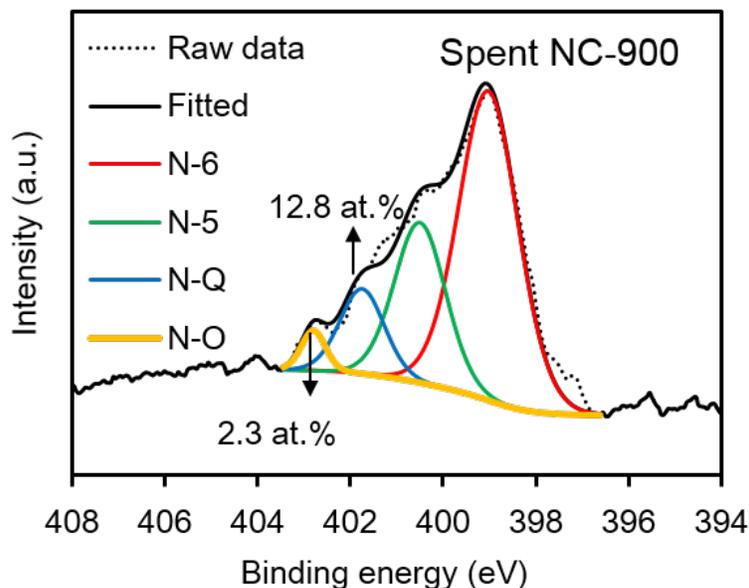


Figure S8. High resolution XPS spectrum of N 1s for spent NC-900 catalyst.

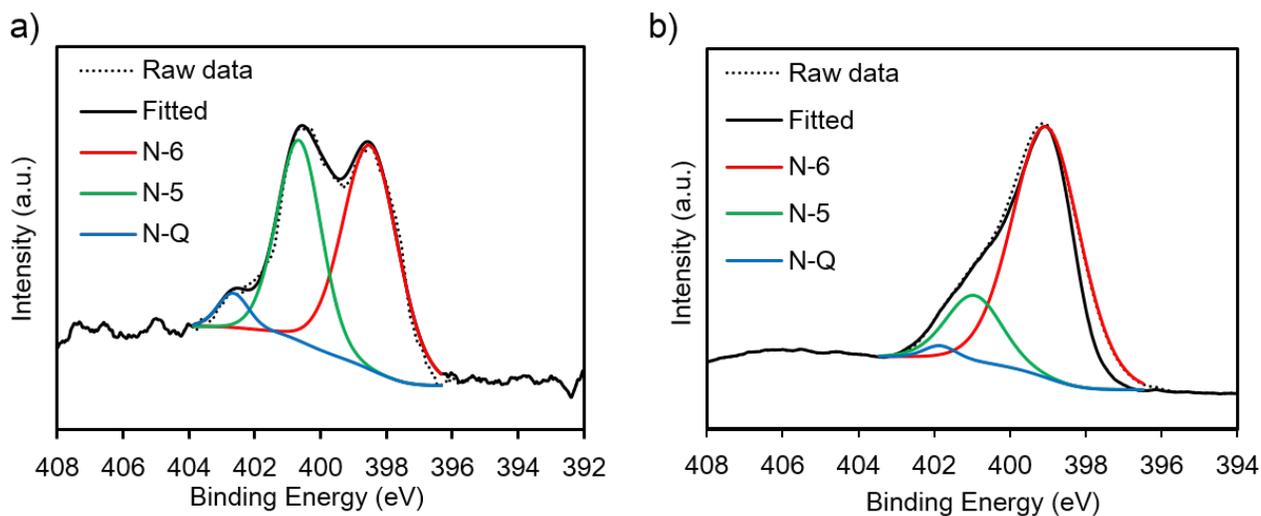


Figure S9. High resolution XPS spectra of N 1s for a) biomass-derived NC and b) g-C₃N₄.

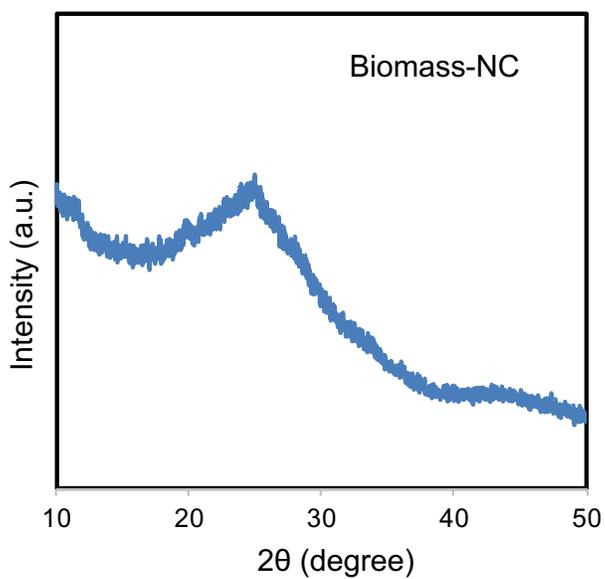


Figure S10. XRD of biomass-derived NC.

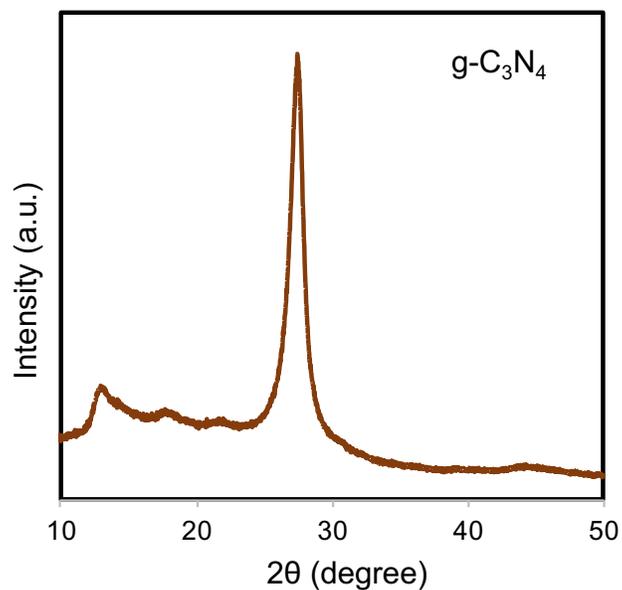


Figure S11. XRD of melamine-derived $g\text{-C}_3\text{N}_4$.

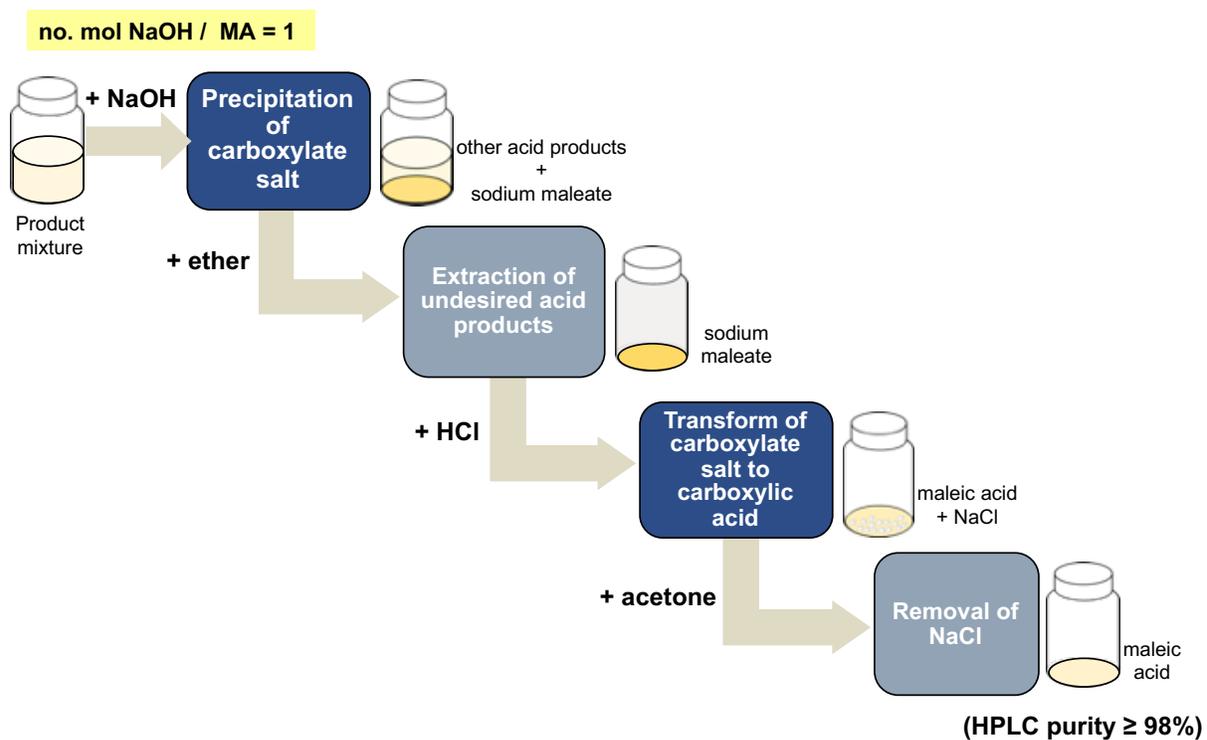


Figure S12. Purification method for the MA.