

## Supplementary Information

### Direct Conversion of Chitin into a *N*-containing Furan Derivative

Xi Chen<sup>a</sup>, Shu Ling Chew<sup>a</sup>, Francesca M. Kerton<sup>b</sup>, and Ning Yan<sup>a,\*</sup>

<sup>a</sup> Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, 117576, Singapore.

<sup>b</sup> Department of Chemistry, Memorial University of Newfoundland, St. John's, NL, A1B 3X7, Canada.

\* Corresponding author. E-mail: ning.yan@nus.edu.sg

### Content

**Figure S1** 3A5AF HPLC calibration curve

**Figure S2** Solvent screening experiments

**Figure S3** Optimization of reaction temperature

**Figure S4** Optimization of solvent amounts

**Figure S5** Screening and optimization of combined additives

**Table S1** Elemental analysis of chitin, recovered chitin after reaction and chitin-humins

**Figure S6** <sup>1</sup>H NMR of 3A5AF after column chromatography separation

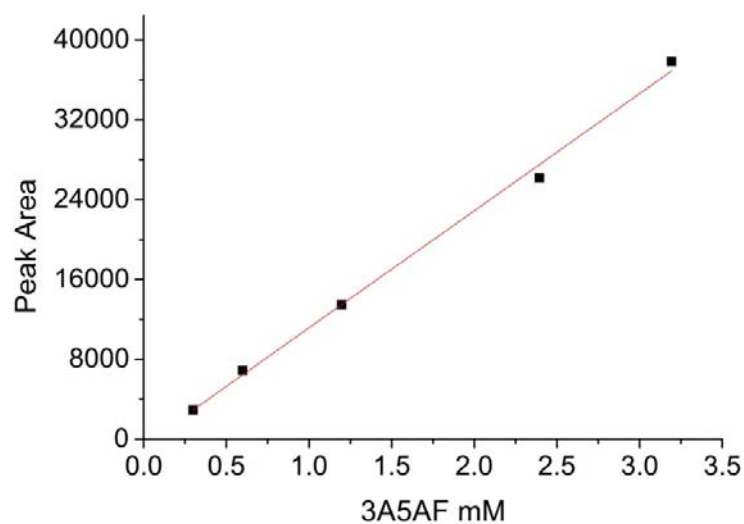
**Figure S7** GPC analysis of chitin-humins fraction

**Figure S8** GPC analysis of the raw filtrate after reaction

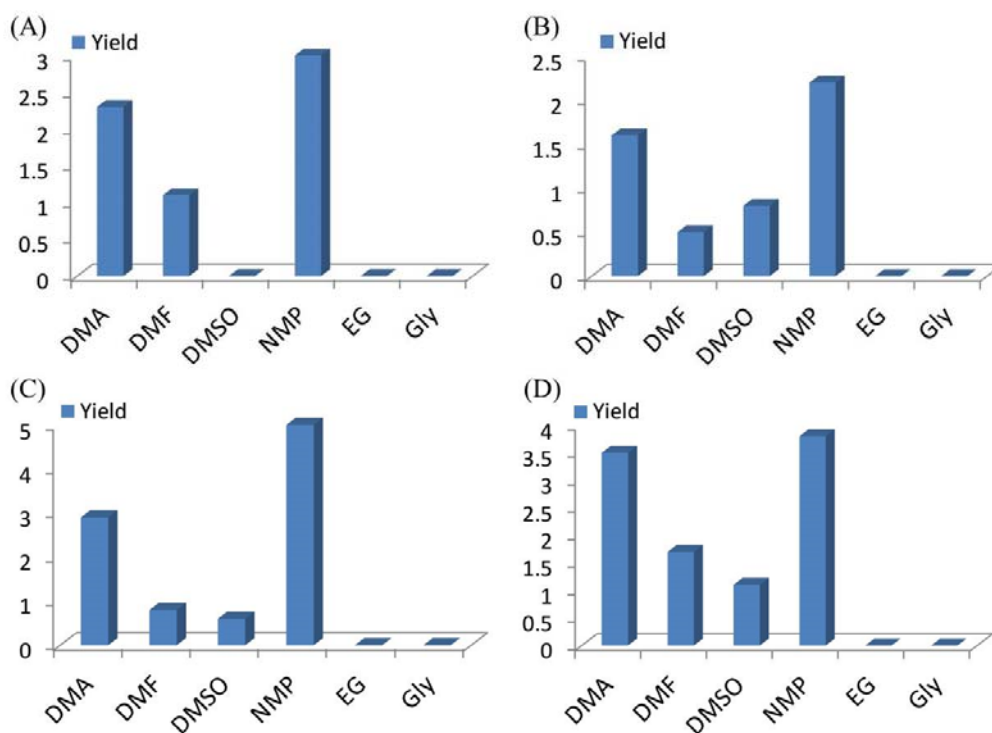
**Figure S9** The influence of water on the reaction

**Figure S10** Poison tests for NAG conversion to 3A5AF

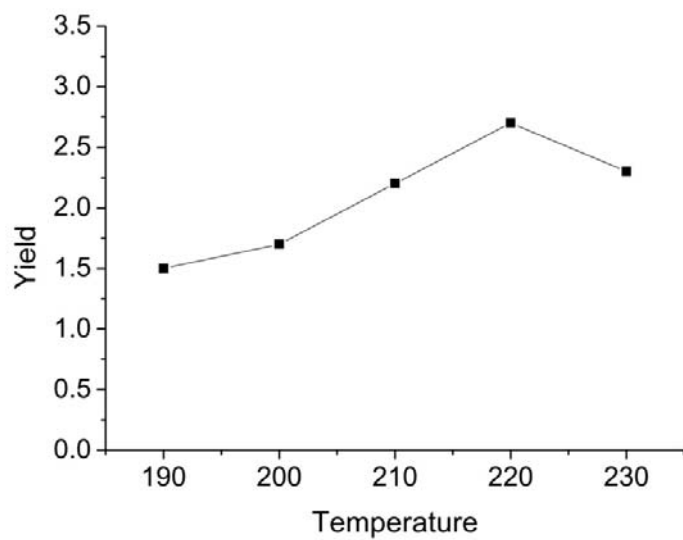
**Figure S11** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) of pure NAG and NAG-boric acid at different temperatures



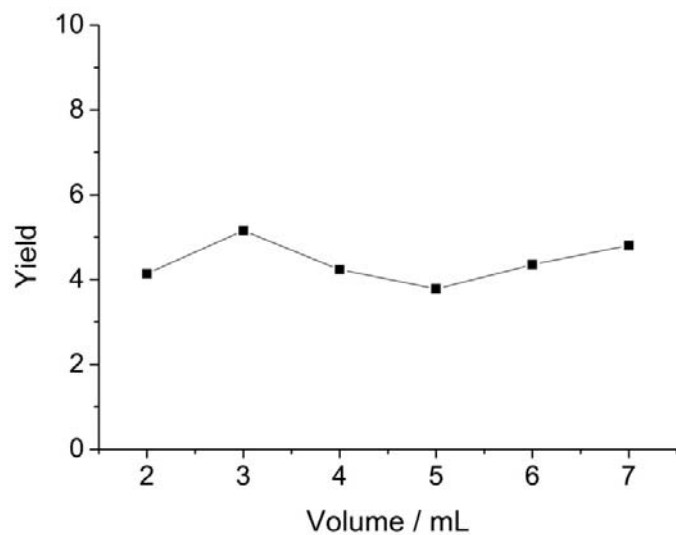
**Figure S1** Calibration curve of 3A5AF on HPLC (230 nm,  $R^2 = 0.995$ )



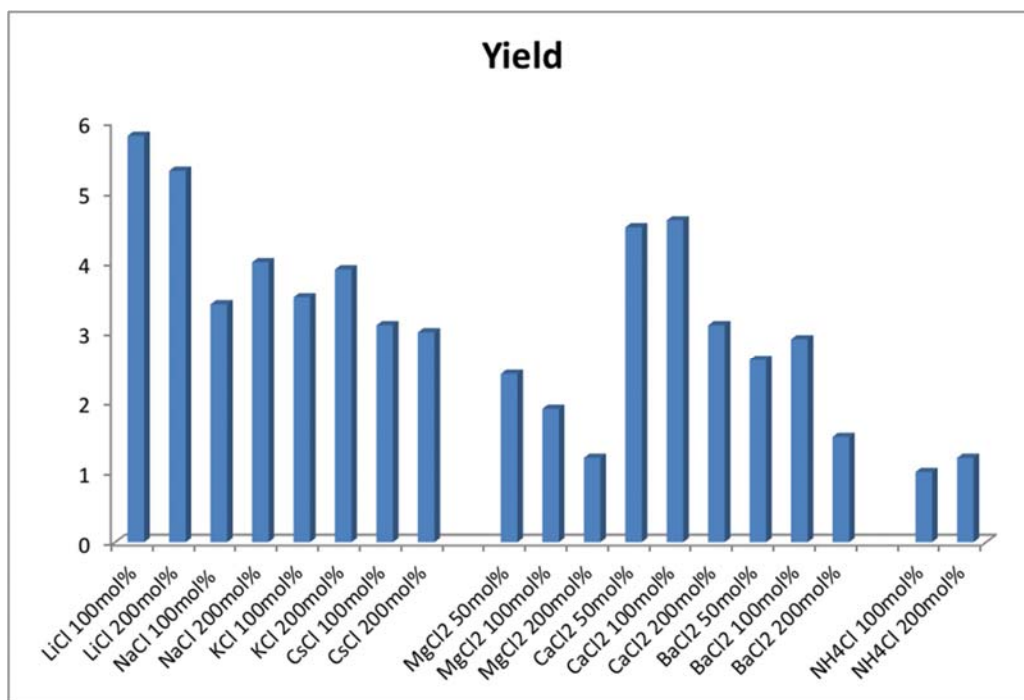
**Figure S2** Solvent screening experiments on chitin to 3A5AF. Reaction conditions: 195°C, 1h, solvent (3 mL), chitin (100 mg). (A) 80  $\mu$ L HCl (fumed); (B) 400 mol% boric acid; (C) 5 wt% in solvent LiCl, 400 mol% boric acid; (D) 80  $\mu$ L HCl (fumed), 400 mol% boric acid.



**Figure S3** Optimization of reaction temperature. Reaction conditions: 1 h, NMP (3 mL), chitin (100 mg), boric acid (400 mol%).



**Figure S4** Optimization of solvent amounts. Reaction conditions: 195 °C, 1 h, chitin (100 mg), boric acid (400 mol%), LiCl (5 wt% in NMP).

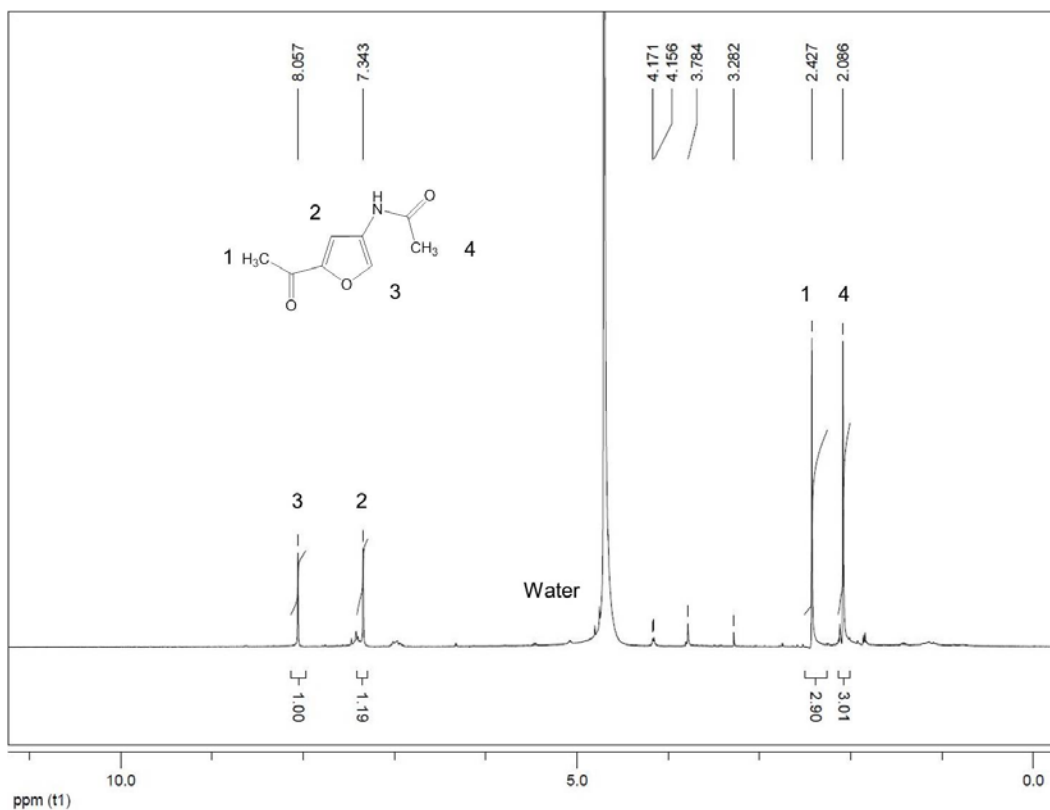


**Figure S5** Screening of combined additives (boric acid plus alkali/alkaline earth chlorides). Reaction conditions: 215 °C, 1 h, chitin (100 mg), boric acid (400 mol%).

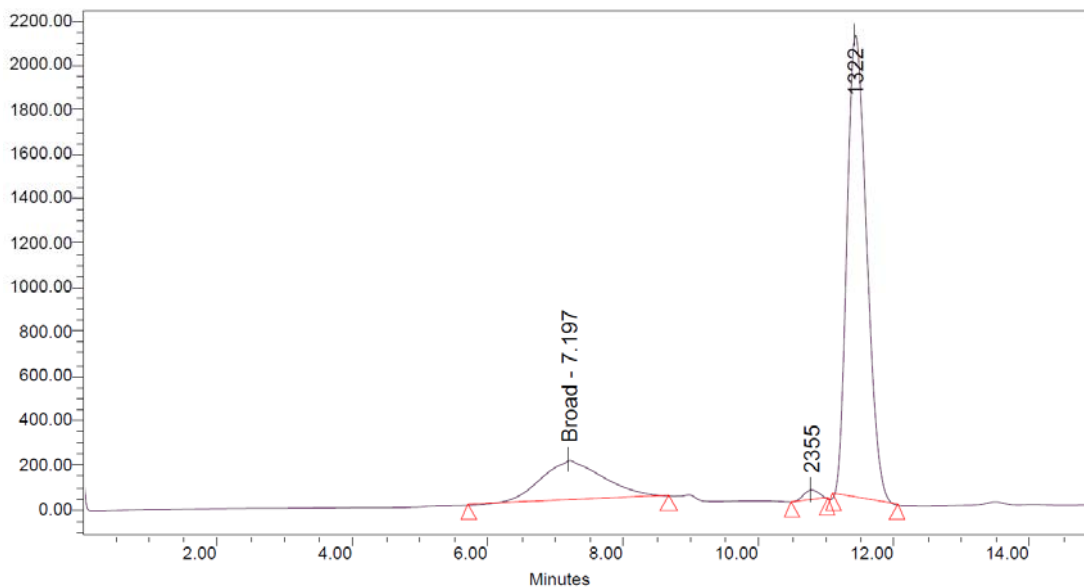
**Table S1** Elemental analysis of chitin, recovered chitin after reaction and chitin-humins

Entry		C wt%	H wt%	N wt%
Chitin	before	47.24	6.40	6.89
Chitin	after reaction	44.15	6.62	6.13
Chitin-humins		54.88	5.39	8.05

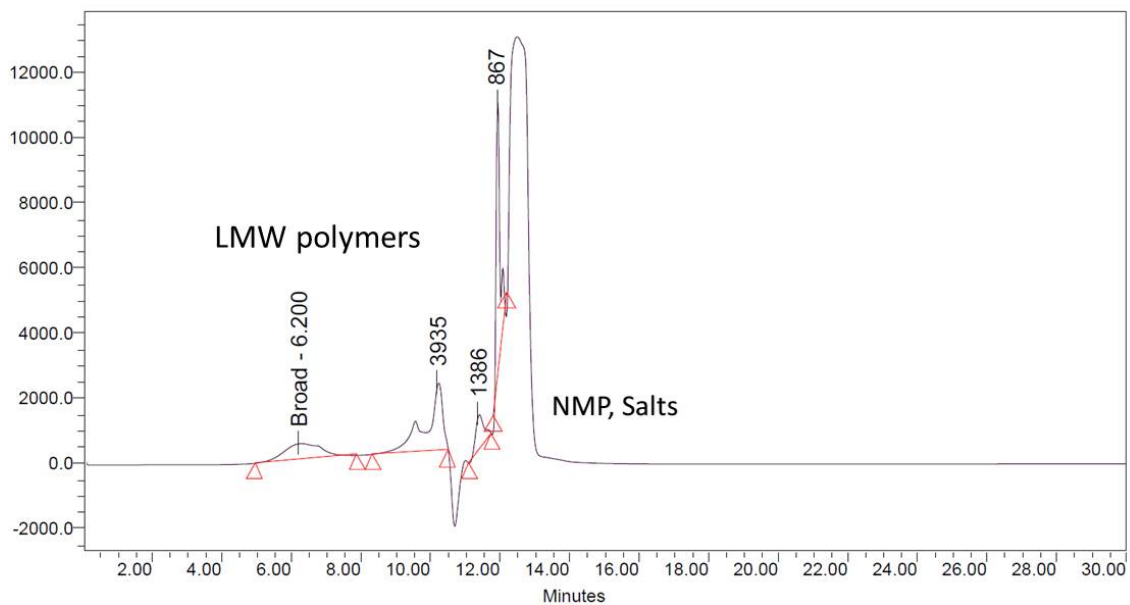
Reaction conditions: 215 °C, 1 h, NMP (3 mL), chitin (100 mg), boric acid (400 mol%), NaCl (200 mol%).



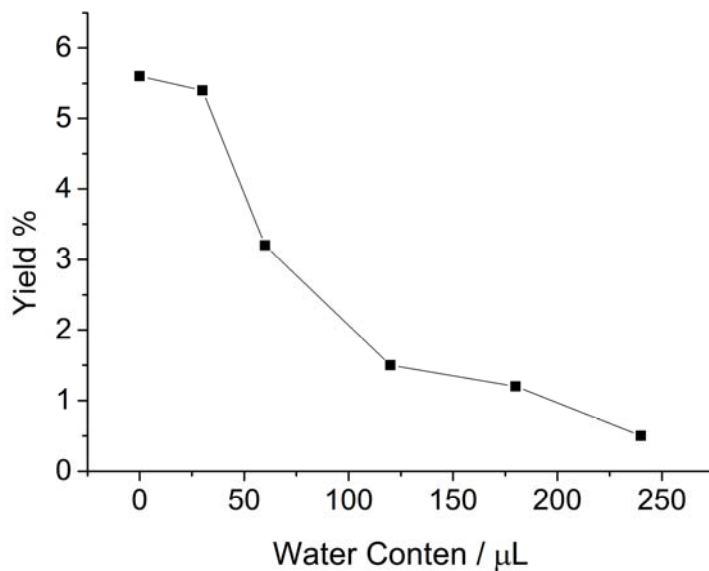
**Figure S6**  $^1\text{H}$  NMR of 3A5AF (400 MHz,  $\text{D}_2\text{O}$ )  $\delta$  8.06 (1H), 7.34 (1H), 2.43 (3H), 2.09 (3H)

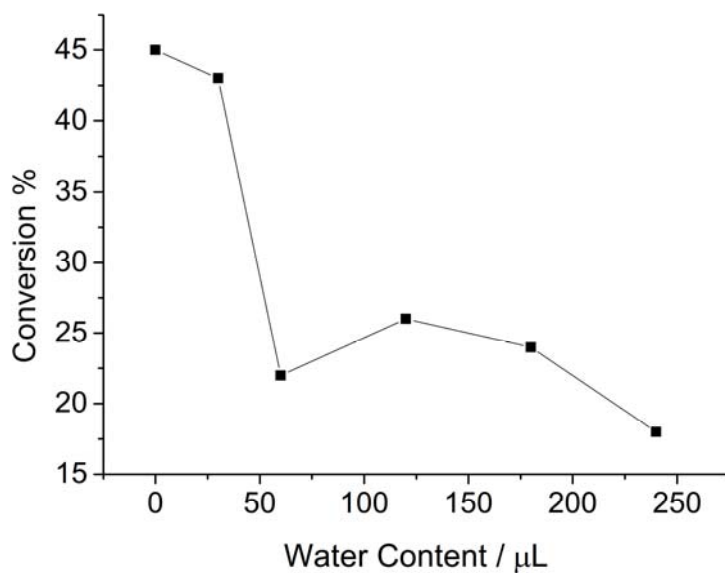


**Figure S7** GPC analysis of chitin-humins fraction after column separation. Reaction conditions: 215 °C, 1 h, NMP (3 mL), chitin (100 mg), boric acid (400 mol%), NaCl (200 mol%).

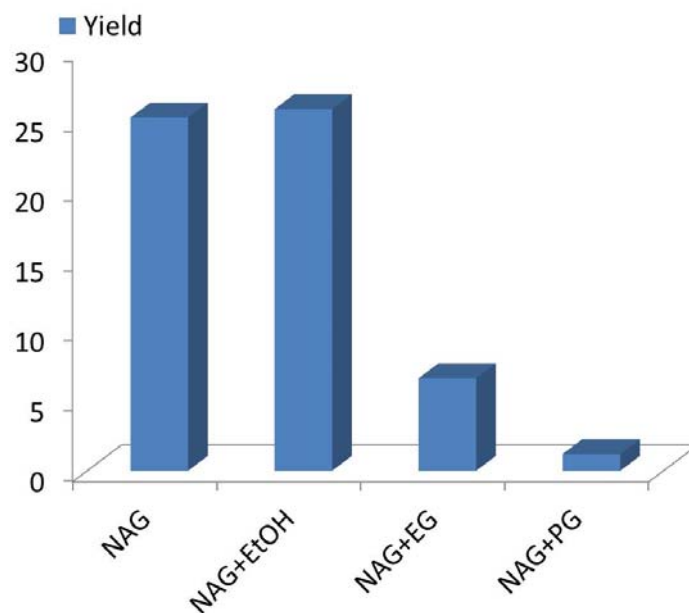


**Figure S8** GPC analysis of the raw filtrate after reaction. Reaction conditions: 215 °C, 1 h, NMP (3 mL), chitin (100 mg), boric acid (400 mol%), NaCl (200 mol%).

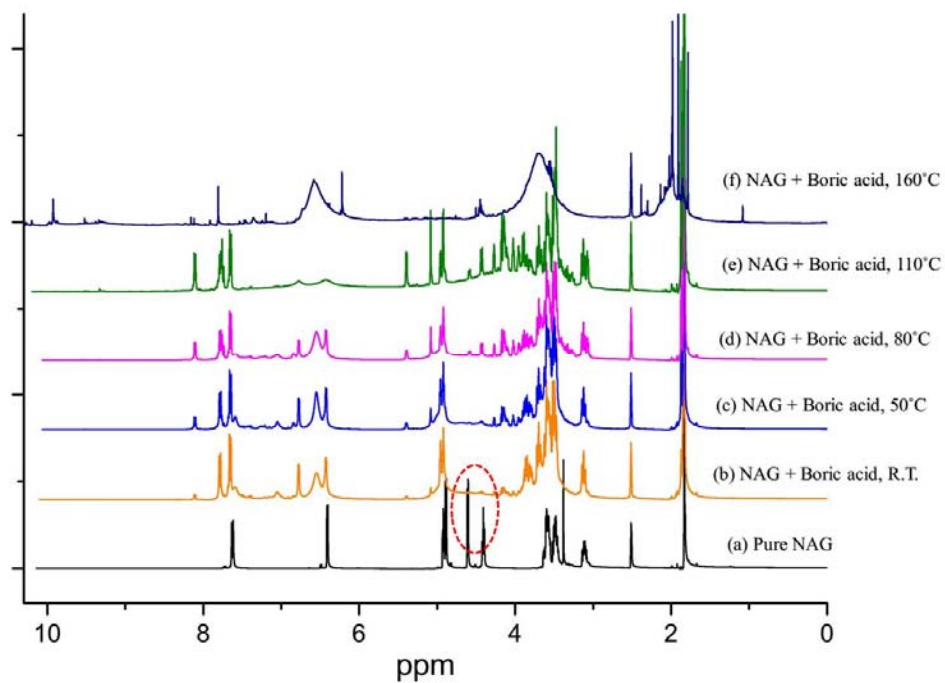




**Figure S9** The influence of water on the reaction. Reaction conditions: 215 °C, 1 h, NMP (3 mL), chitin (100 mg), boric acid (400 mol%), NaCl (200 mol%).



**Figure S10** Poison tests for NAG conversion to 3A5AF. Reaction conditions: 215 °C, 1 h, NMP (3 mL), chitin (100 mg), boric acid (400 mol%), NaCl (200 mol%).



**Figure S11** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) spectra of pure NAG and NAG-boric acid at different temperatures. Note: upon the addition of boric acid, two peaks disappear which are labeled with a red ellipse. The broadening of peaks is probably due to the interaction with boric acid.