Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Reaction pathways and kinetics of *N*-acetyl-D-glucosamine hydrolysis in sub- and supercritical water

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Supplementary Data

1. Experimentation
2. Identification and quantification of compounds using HPLC
3. HR-MS of compounds present in reaction mixture during SCW hydrolysis
4. Effect of pressure
5. Characterization of solids
6. Kinetic plots of NAG hydrolysis on normal scale

1. Experimentation

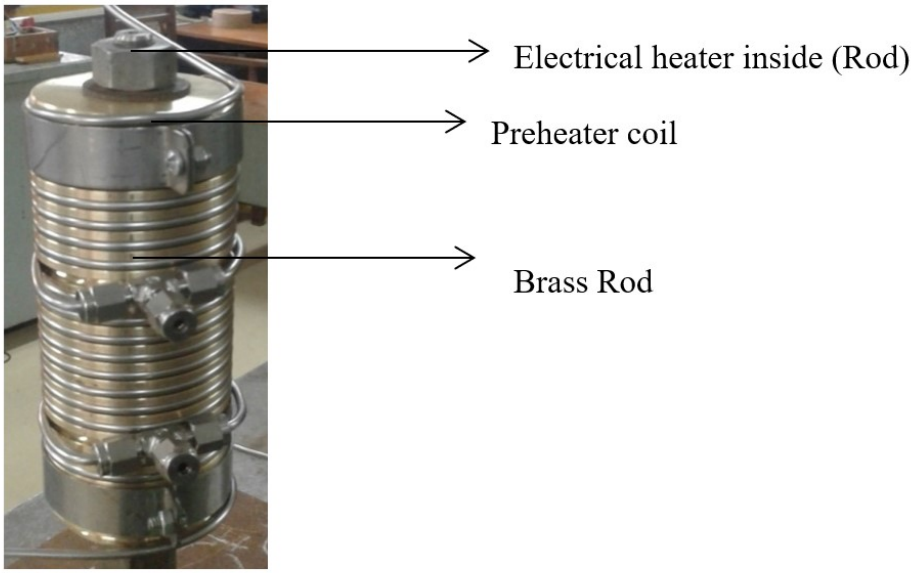

Figure S1. Actual photograph of preheater used to heat water to Subcritical and Supercritical temperatures

2. Identification and quantification of compounds using HPLC

Method: HPLC equipped with Biorad Aminex HPX-87H column (300 x 7.8 mm) and RI detector; Mobile phase: 5 mM aqueous sulphuric acid; Flow rate: 0.6 mL/min; Column Temperature: 50 ^{o}C

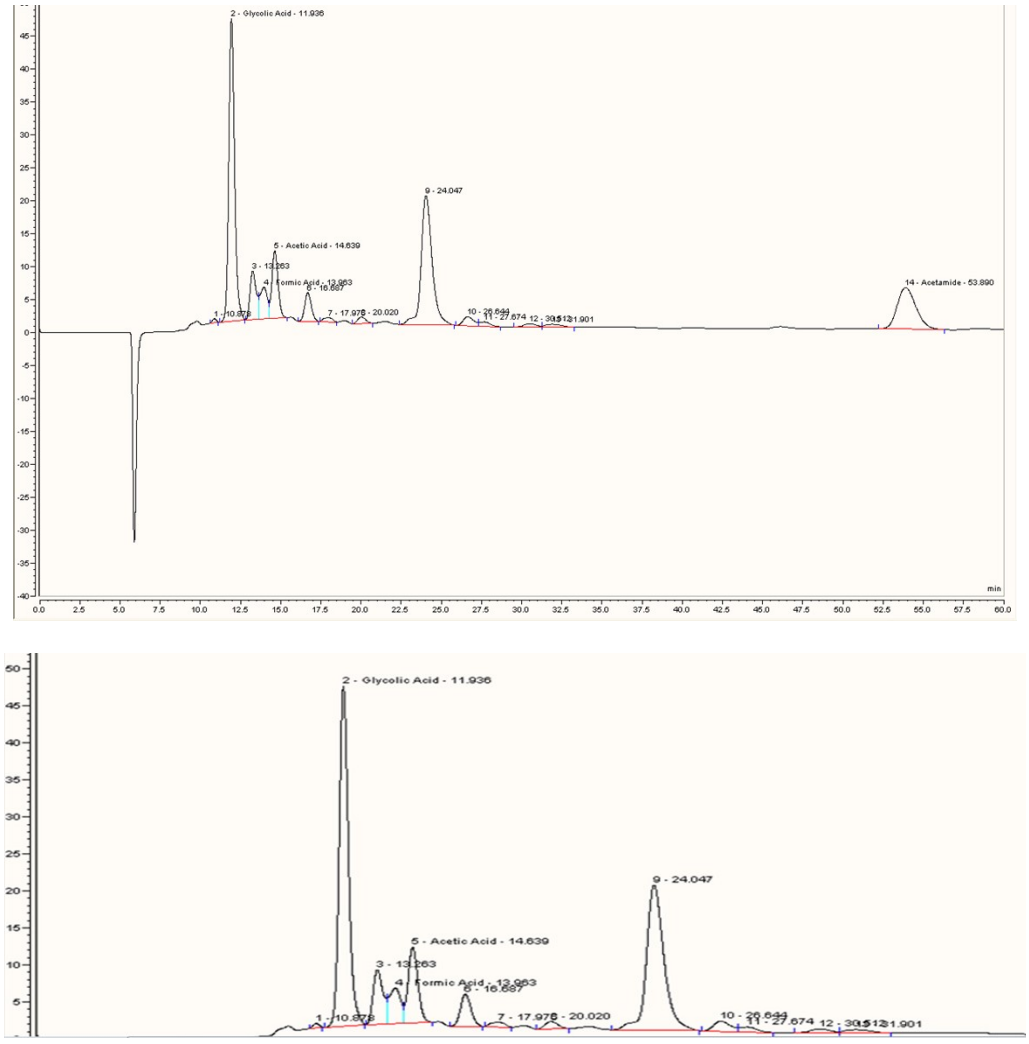

Figure S2a. HPLC chromatogram of reaction mixture
(Temperature: 400 ^{o}C; Pressure: 25 MPa ; NAG concentration: 1 % (w/w); Residence time: 8 s)
(Below picture - zoomed in image of chromatogram)

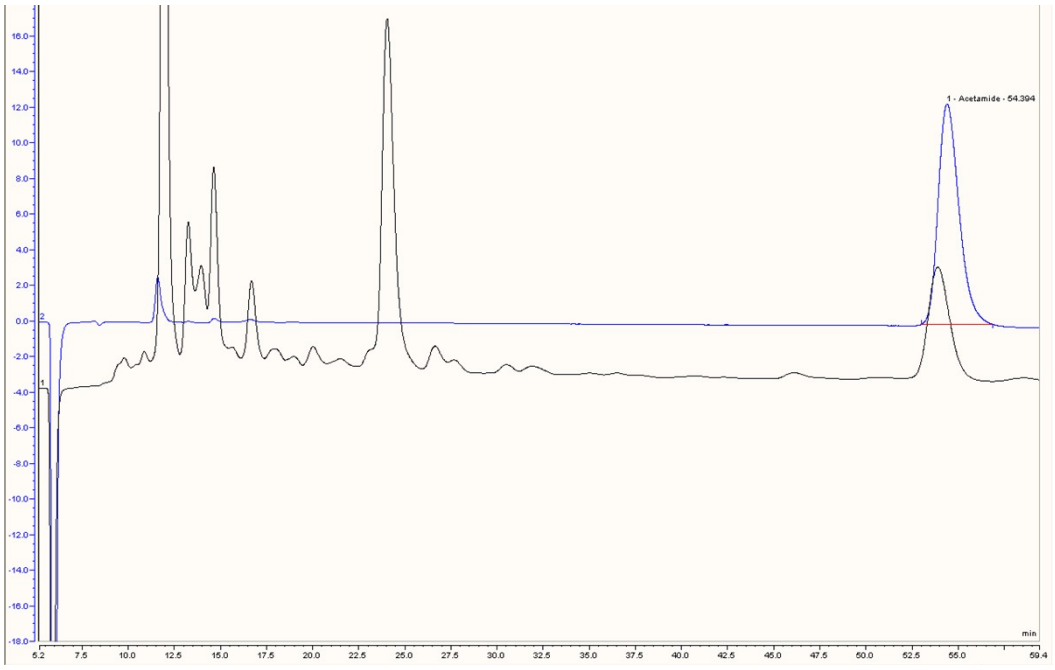

Figure S2b. HPLC chromatogram of reaction mixture confirming Acetamide
(Temperature : 400 ^{o}C ; Pressure: 25 MPa; NAG concentration: 1% (w/w); Residence time: 8 s)

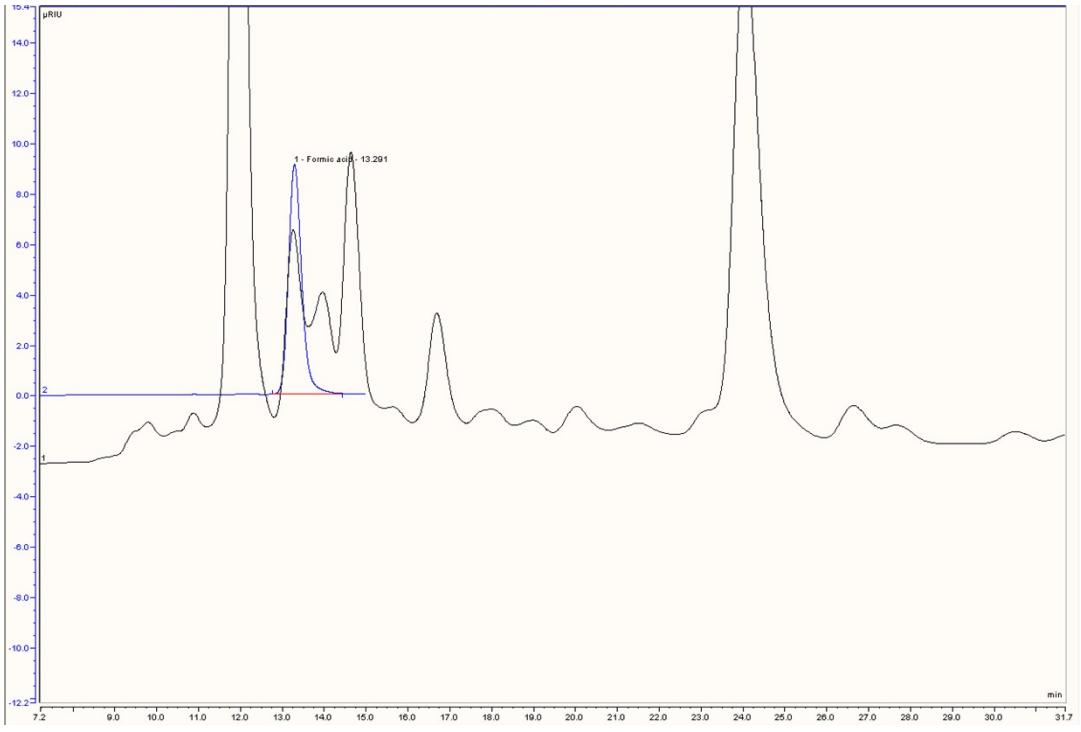

Figure S2c. HPLC chromatogram of reaction mixture confirming Formic acid
(Temperature: 400 ^{o}C ; Pressure-25 MPa ; NAG concentration: 1 % (w/w); Residence time: 8 s)

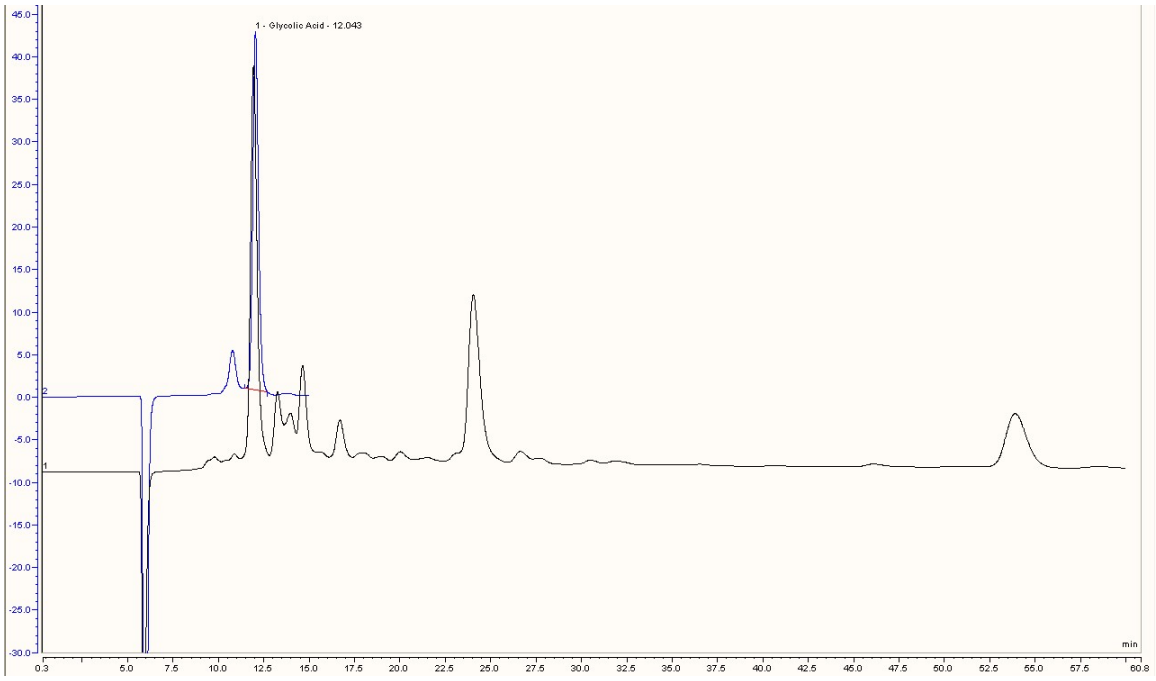

Figure S2d. HPLC chromatogram of reaction mixture confirming Glycolic acid (Temperature: 400 ^{o}C; Pressure: 25 MPa; NAG concentration: 1 % (w/w); Residence time: 8 s)

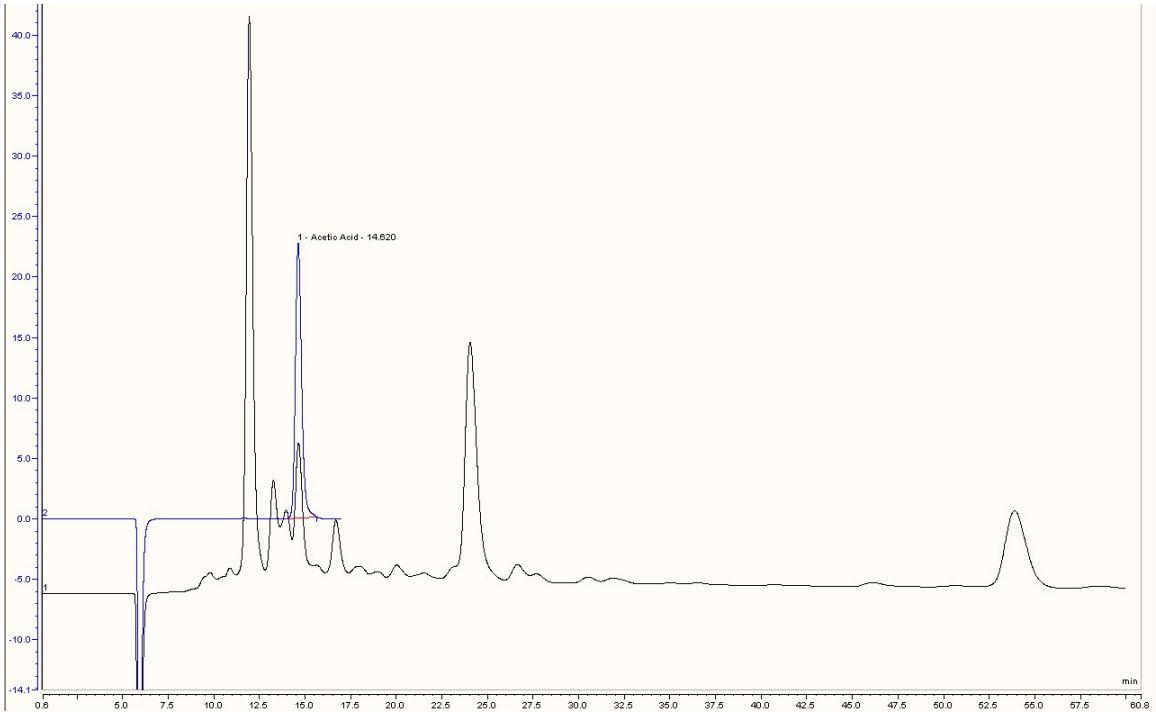

Figure S2e. HPLC chromatogram of reaction mixture confirming Acetic acid (Temperature: 400^{o}C; Pressure: 25 MPa; NAG concentration: 1 % (w/w); Residence time: 8 s)

3. HR-MS of compounds present in reaction mixture during SCW hydrolysis

There were several unknown peaks present in the reaction chromatogram. Most of these compounds were collected separately. The confirmation of the products was done by HR-MS and standards. The possible products were identified based on the literature reported.

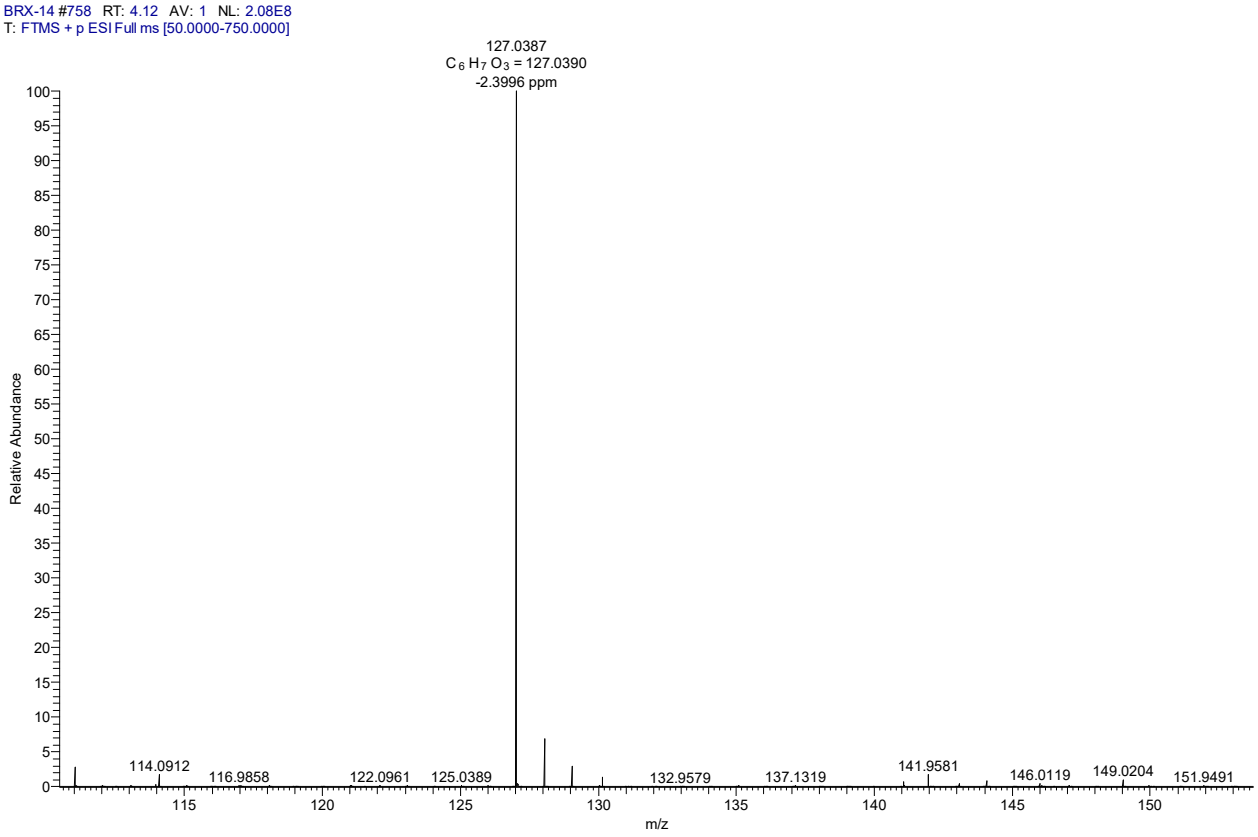

Figure S3a. HR-MS of separated reaction mixture confirming 5-Hydroxymethylfurfural (126+1) (Temperature: 400 ^{o}C; Pressure: 25 MPa ; NAG concentration: 1 % (w/w); Residence time: 8 s)

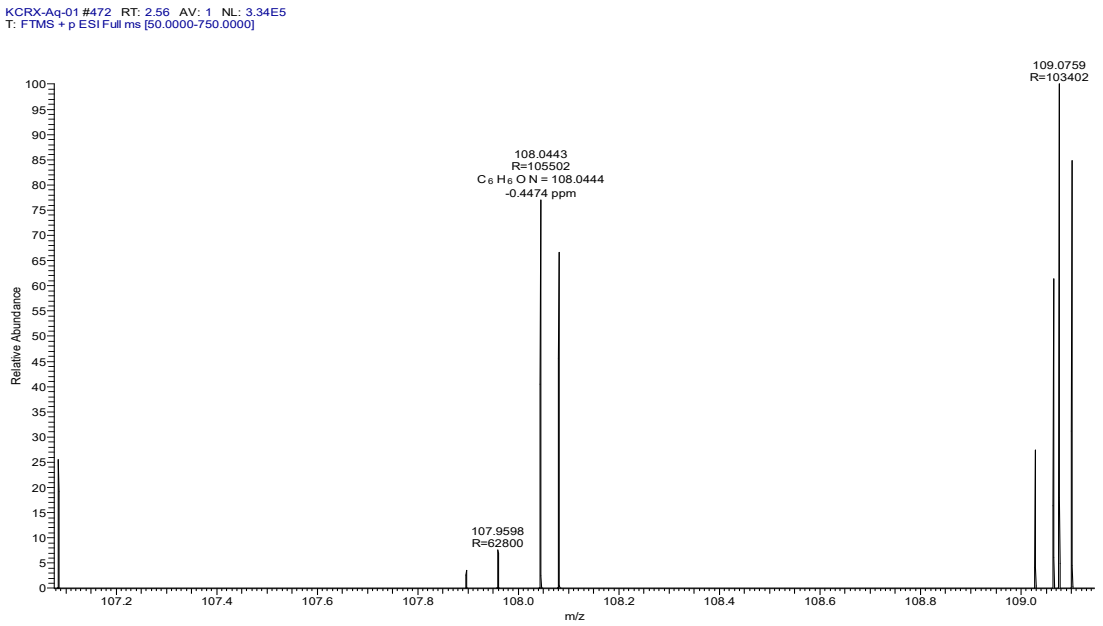

Figure S3b. HR-MS of separated reaction mixture confirming 3-Pyridine carboxyldehyde (107+1) (Temperature: 400 °C; Pressure: 25 MPa; NAG concentration: 1% (w/w); Residence time: 8 s)

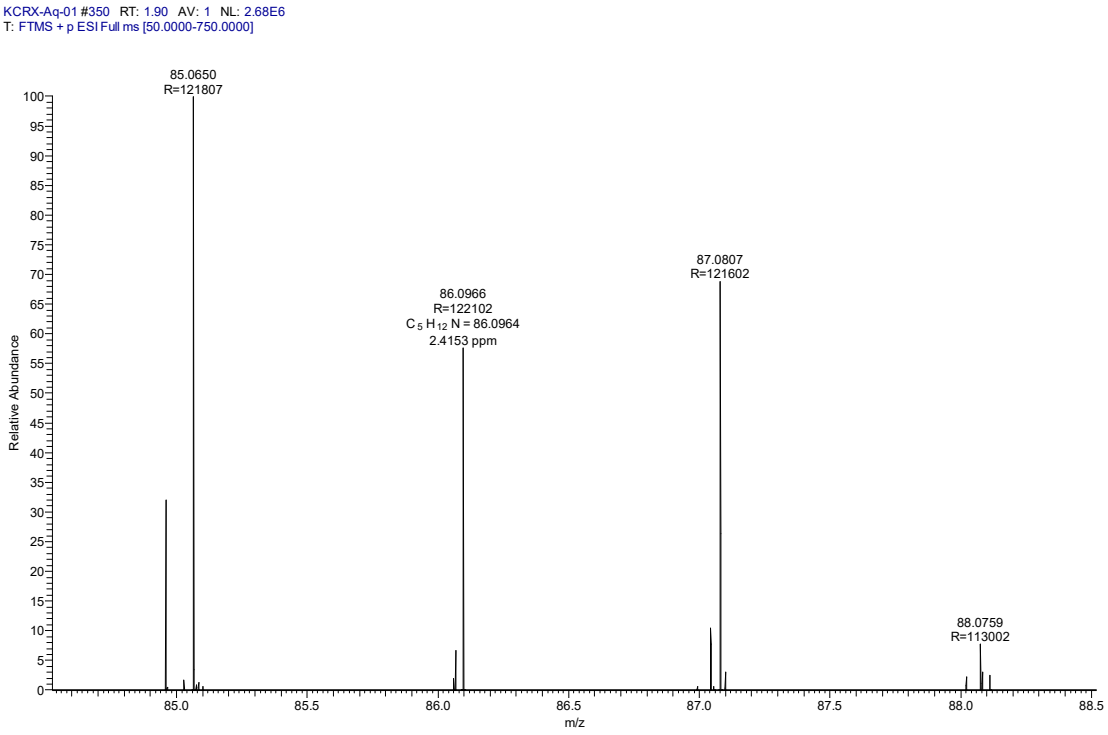

Figure S3c. HR-MS of separated reaction mixture confirming Piperidine (85+1) (Temperature: 400 °C; Pressure: 25 MPa; NAG concentration: 1 % (w/w); Residence time: 8 s)

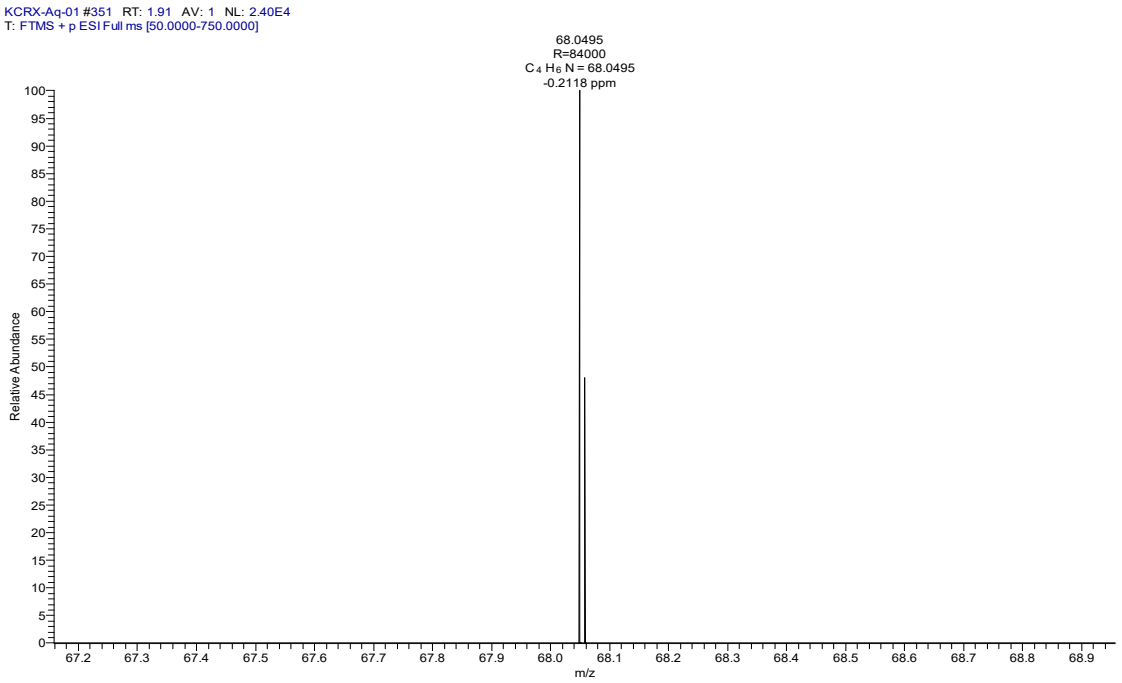

Figure S3d. HR-MS of separated reaction mixture confirming Pyrrole (67+1)
(Temperature: 400 °C; Pressure: 25 MPa; NAG concentration: 1 % (w/w); Residence time: 8 s)

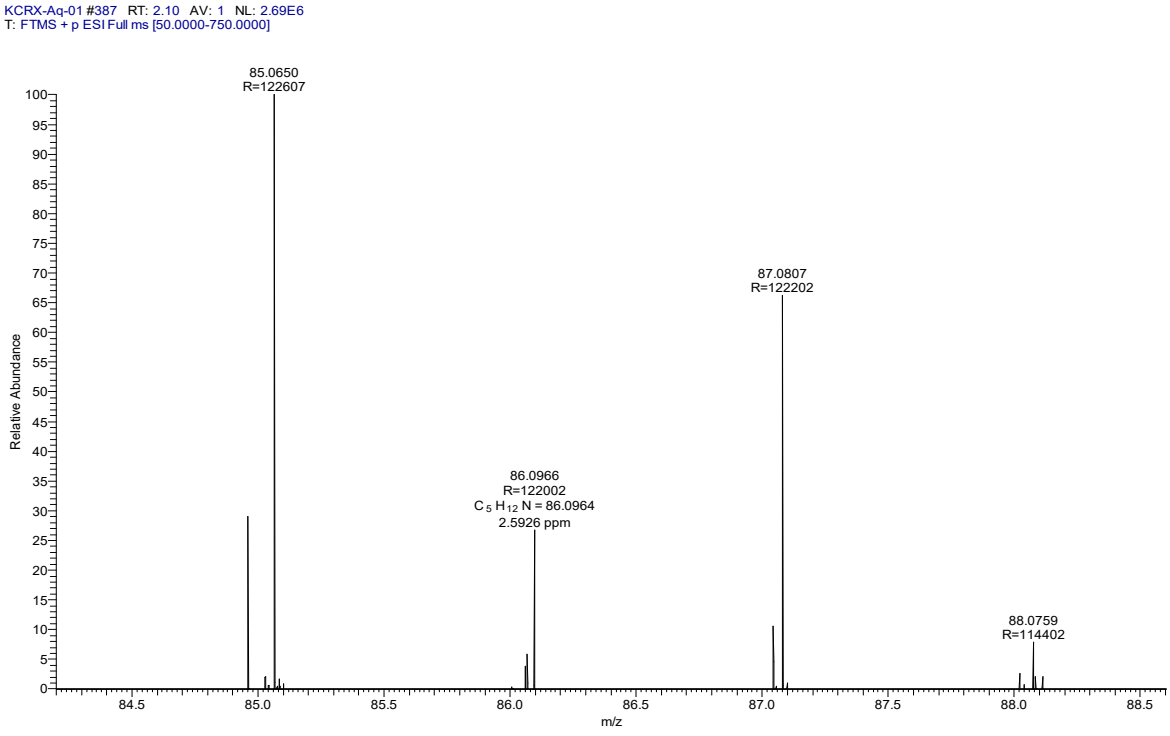

Figure S3e. HR-MS of separated reaction mixture confirming *N*-methyl pyrrolidine (85+1) (Temperature: 400 °C; Pressure: 25 MPa; NAG concentration: 1 % (w/w); Residence time: 8 s)

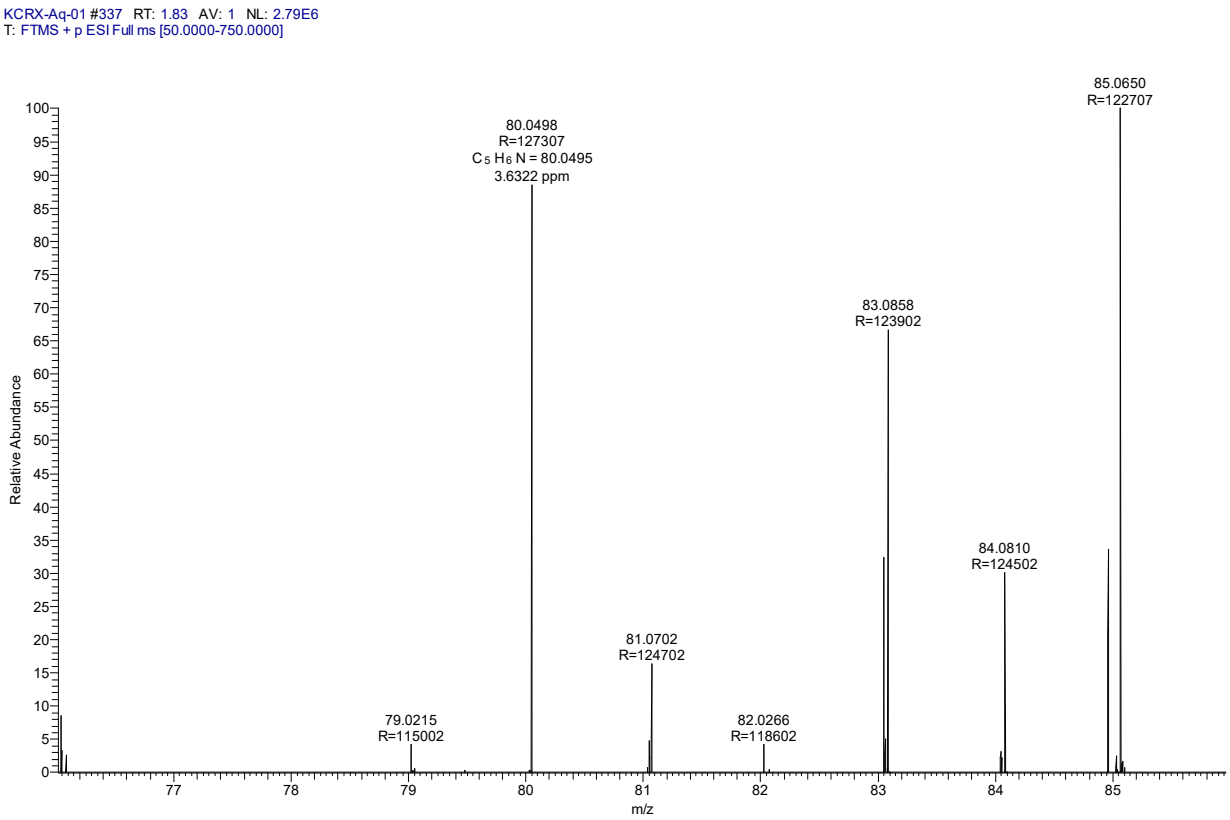

Figure S3f. HR-MS of separated reaction mixture confirming Pyridine (79+1) (Temperature: 400 °C; Pressure: 25 MPa; NAG concentration: 1% (w/w); Residence time: 8 s)

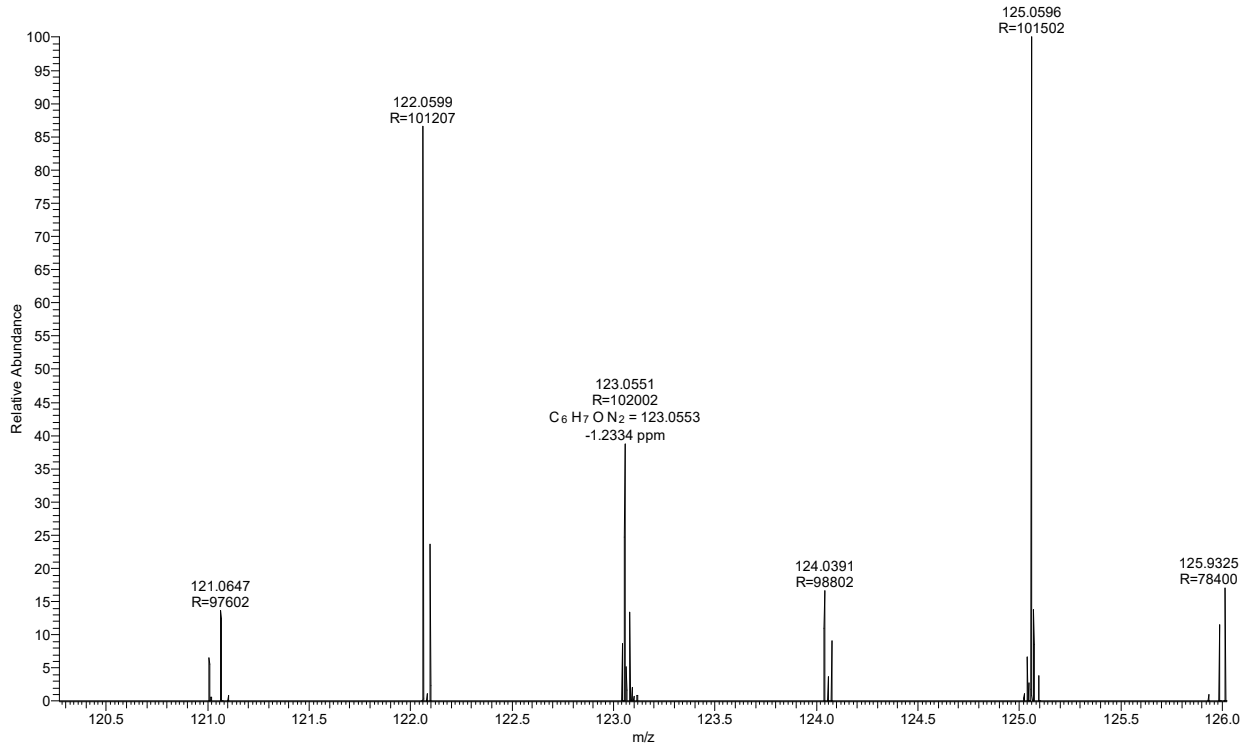

Figure S3g. HR-MS of separated reaction mixture confirming 2-acetyl pyrazine (122+1) (Temperature: 400 ^{o}C; Pressure: 25 MPa; NAG concentration: 1 % (w/w); Residence time: 8 s)

4. Effect of pressure

Figure S4. Reaction mixture of NAG hydrolysis in subcritical water at 250 °C at 5 MPa, 12.5 MPa and 25 MPa (from left to right)

5. Characterization of solids

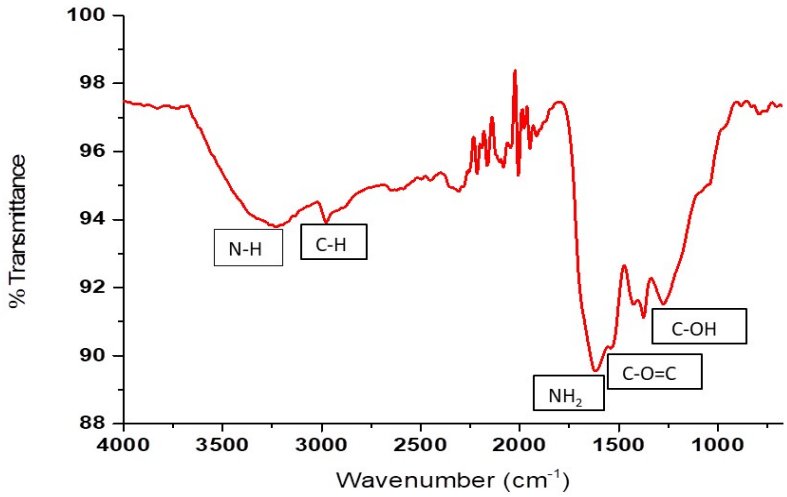

Figure S5. FT-IR spectra of solids formed during continuous flow hydrolysis of NAG in subcritical conditions (250 °C; 25 MPa; 1 % NAG (w/w))

6. Kinetic plots of NAG hydrolysis on normal scale

The kinetic plots (figure 6a-c) are plotted on a log x-axis to capture the change in concentration. Followings are the plots on normal x-axis.

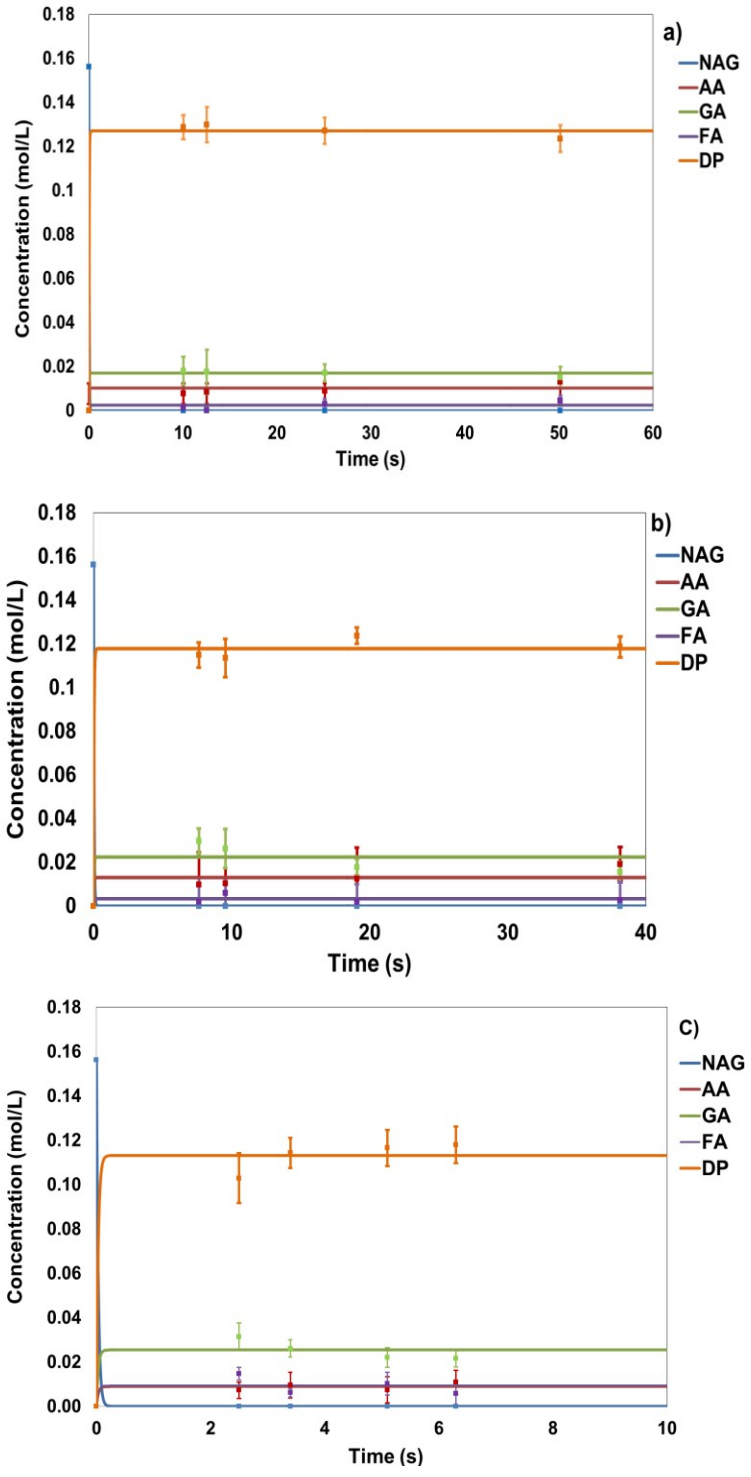

Figure S6. Kinetics of NAG hydrolysis in sub- and supercritical water: concentration of compounds with reaction time (a) 250 °C (b) 350 °C (c) 400 °C at 25 MPa