

Conversion of chitin derived N-acetyl-D-glucosamine (NAG) to polyols over transition metal catalysts and hydrogen in water

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Figure S1. ¹H-NMR spectrum of the crude products in D₂O, obtained after the hydrogenation of NAG.....S2

Figure S2. ¹H-NMR spectrum of the crude products in D₂O, obtained after the hydrogenation of NAG.....S3

Figure S3. A typical FTIR spectrum of gas phase product.....S4

Figure S4. GC-FID chromatogram of glucosamine after reaction, and followed by silylation of the products.....S5

Table S1. Recycle experiments over Ru/C.S6

Table S2. Recycle experiments over Ru/C.S6

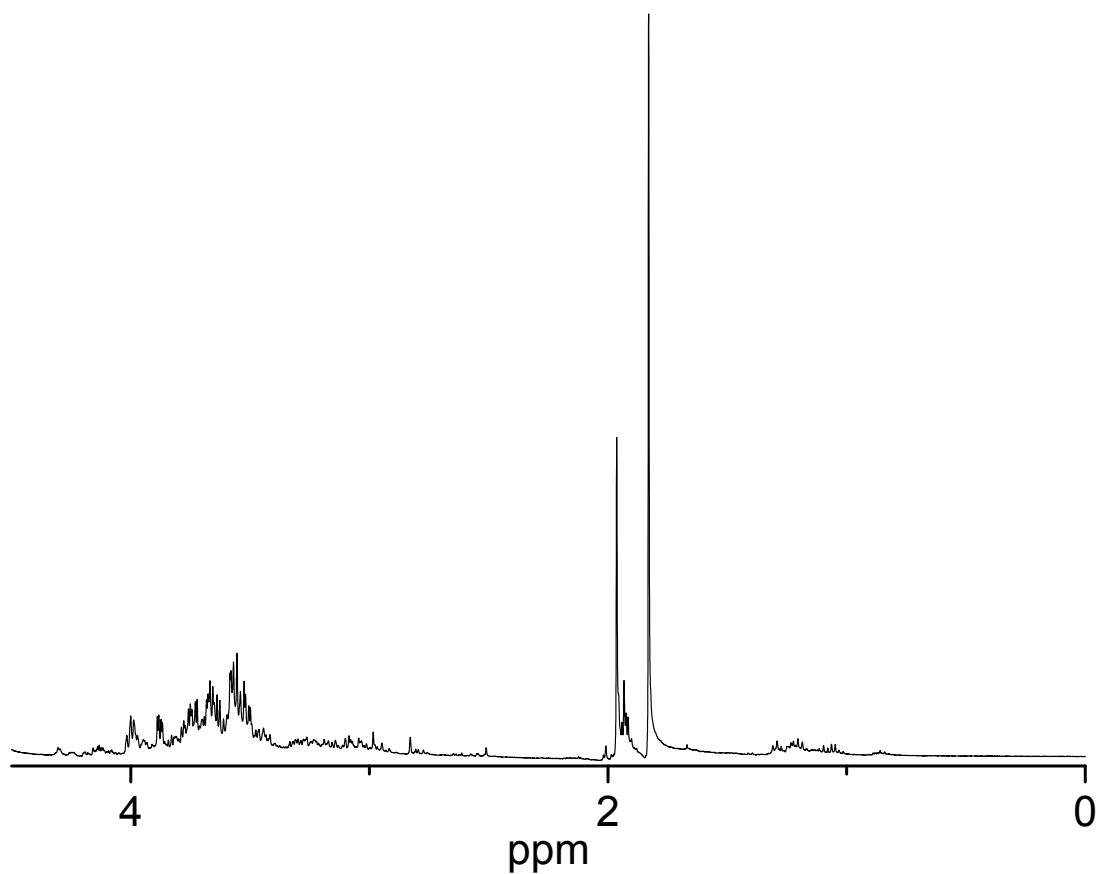


Figure S1. ¹H-NMR spectrum of the crude products in D₂O, obtained after the hydrogenation of NAG. Reaction conditions: 1 g NAG, 5 mol% Ru/C, 25 mL H₂O, 40 bar H₂, 150 °C, 1 h. No peaks were observed above 4.5 ppm.

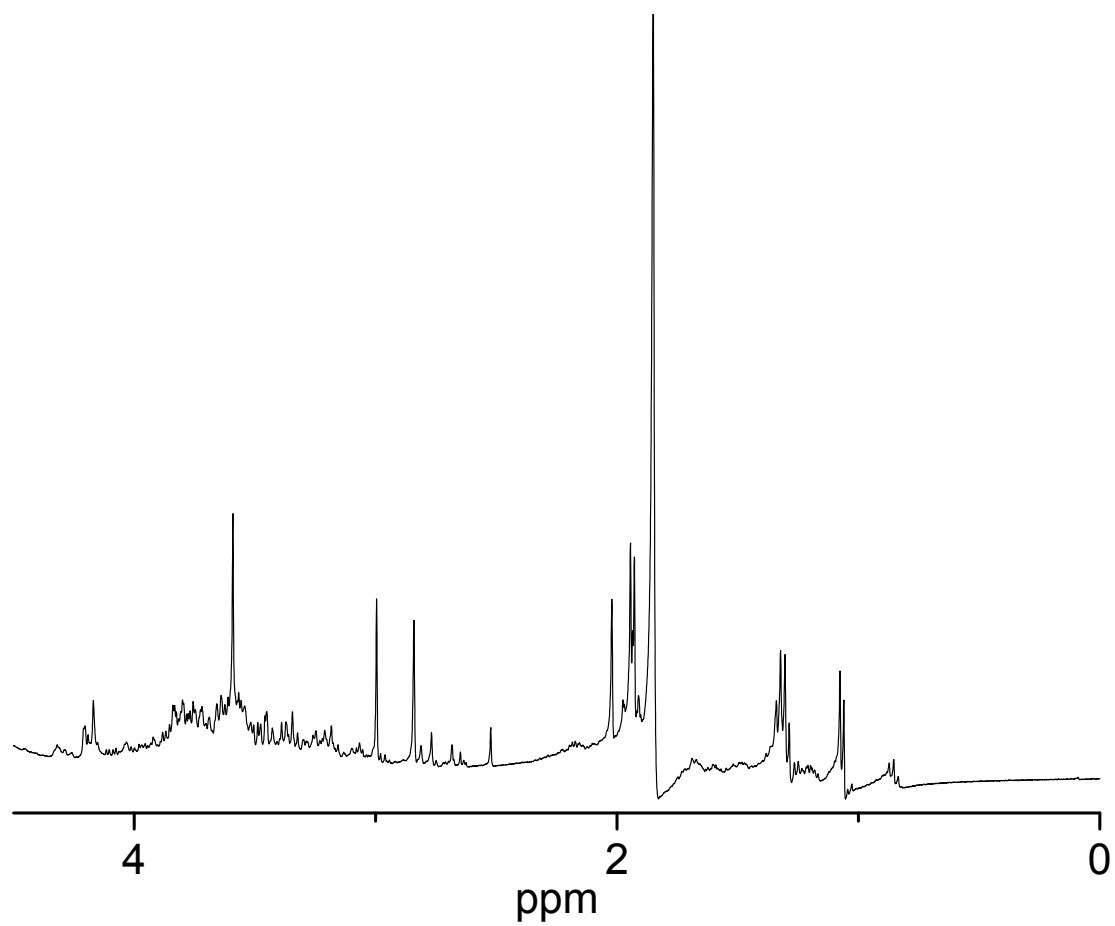


Figure S2. ¹H-NMR spectrum of the crude products in D₂O, obtained after the hydrogenation of NAG. Reaction conditions: 1 g NAG, 5 mol% Ru/C, 25 mL H₂O, 40 bar H₂, 150 °C, 1 h. No peaks were observed above 4.5 ppm.

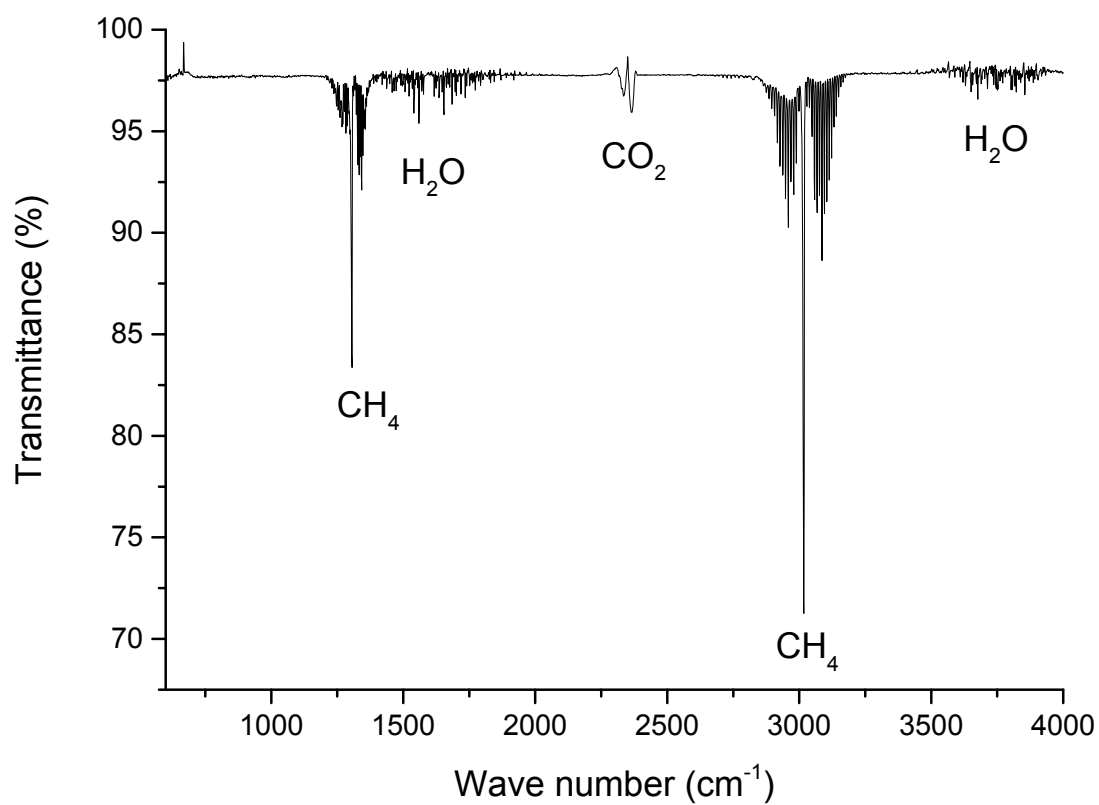


Figure S3. A typical FTIR spectrum of gas phase product. Reaction conditions: 500 mg NAG, 1 mol% Ru/C, 5 mL H₂O, 40 bar H₂, 180 °C, 1 h.

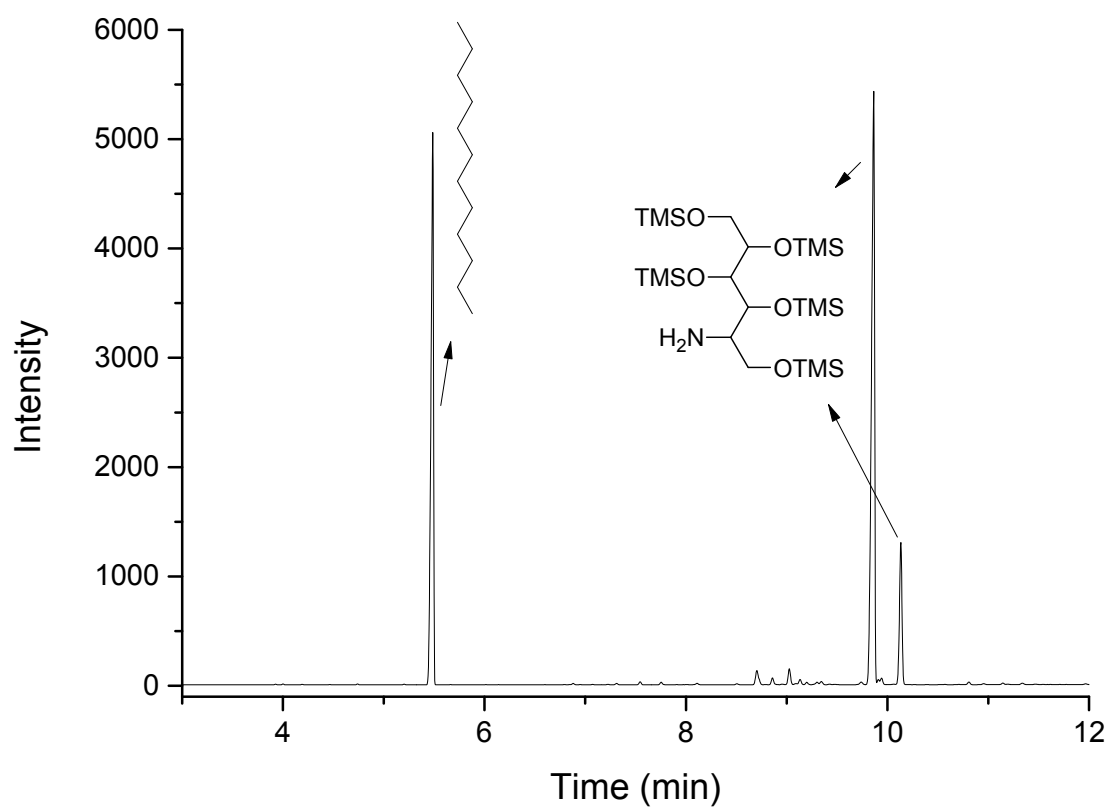


Figure S4. GC-FID chromatogram of glucosamine after reaction, and followed by silylation of the products. The two peaks around 10 min are assigned as two diastereomers generated during the reaction. Reaction conditions: 500 mg glucosamine hydrochloride, 1 mol% Ru/C, 5 mL H₂O, 40 bar H₂, 180 °C, 1 h.

Table S1. Recycle experiments over Ru/C.^[a]

Entry ^[b]	Conv. [%]	Yield [%]		C2 EG	MEA	NMEA	C3 PG	GLY	C4 BDO	BTO	C6-8				Total
		AcOH									HTO	rNAG	rGlcNH	rDNAG	
1	100	2.7	0.5	0.1	6.9	<0.1	<0.1	0.3	5.8	2.4	39.5	9.7	31.7	100	
2	100	3.4	0.7	0.2	11.3	0.1	0.1	0.7	7.9	4.7	14.0	9.1	49.8	102	
3	100	3.3	0.6	0.1	8.4	0.1	0.1	0.3	5.7	3.8	32.4	9.1	36.1	100	
4	100	3.2	0.5	0.1	8.1	0.1	0.1	0.4	6.5	4.2	30.2	9.1	38.4	101	

[a] Reaction conditions: 500 mg NAG, 1 mol% Ru/C (45.7 mg 5 wt% Ru/C), 40 bar H₂, 5 mL H₂O, 180 °C, 1 h. [b] Entry 1-4 represent the data from 1st to 4th use of Ru/C.

Table S2. Recycle experiments over Ru/C.^[a]

Entry	Conv. [%] ^[d]	Yield [%]		AcOH	C2 EG	MEA	NMEA	C3 PG	GLY	C4 BDO	BTO	C6–8 HTO		rNAG	rGlcNH	rDNAG	Total
		CH ₄	CO ₂														
1 ^[b]	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2 ^[b]	67	7.1	3.6	2.2	1.2	<0.1	2.4	0.2	<0.1	0.4	<0.1	<0.1	-	-	-	-	17
3 ^[c]	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
4 ^[c]	89	5.4	2.0	1.8	3.9	0.4	-	0.9	<0.1	2.1	0.1	0.1	-	-	-	-	17

[a] Reaction conditions: 1 g chitin or chitosan, 91.4 mg 5 wt% Ru/C, 40 bar H₂, 25 mL H₂O, 180 °C, 1 h. [b] Chitin as starting material. [c] Chitosan as starting material.