

SUPPORTING INFORMATION

Amoxidation of Lignocellulosic Materials: Formation of *non*-Heterocyclic Nitrogenous Compounds from Monosaccharides

Karl Michael Klinger, Falk Liebner,* Takashi Hosoya, Antje Potthast, Thomas Rosenau

University of Natural Resources and Life Sciences Vienna, Austria

Department of Chemistry, UFT Tulln, Konrad-Lorenz-Straße 24, A-3430 Tulln

*To whom correspondence should be addressed: Tel, +43-1-47654-6458; Fax, +43-1-47654-6059; E-mail: falk.liebner@boku.ac.at

Table S1. Relative Amount of Other Nitrogenous Compounds in the Crude Products Obtained by Amoxidation of D-Glucose at 70 °C, 100 °C and 140 °C (0.2 MPa O₂, 3 h).

Rt (min)	Compound	70 °C	100 °C	140 °C
		Relative percentage [%] ^d		
8.56 ^{a,b} , 16.7 ^b	Urea (10)	1.10	0.34	0.36
11.41 ^b , 15.53 ^c	Ammonium carbamate (34)	0.14	0.16	0.05
13.6 ^b	Ammonium oxalate (37)	1.94	0.81	3.36
7.16 ^b	Acetamide (86)	0.09	0.07	0.00

Numbers in parentheses refer to peak numbering as given in Table 1. ^a carbodiimide derivative; ^b bis TMS derivative; ^c tris TMS derivative; ^d Values were calculated as ratio of the relative peak areas of the analytes and that obtained from 200 µg of the internal standard phenyl α -glucopyranoside.

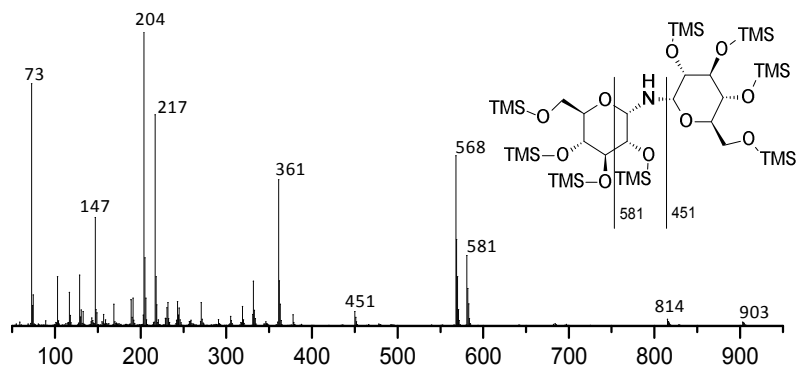


Figure S1. EI-MS (70 eV) spectrum of octakis-*O*-TMS di(glucopyranosyl) amine. Assignment in accordance with literature:¹⁻⁴ m/z 903 ($M^+ - CH_3$), 814 ($M^+ - [CH_2O-TMS]$), 581 ([tetra-*O*-TMS glucopyranosylamine-CH=CH-O-TMS]⁺), 568 (tetra-*O*-TMS glucopyranosylamine-CH⁺-O-TMS), 451 ([tetra-*O*-TMS glucopyranosyl]⁺), 361 (451 - [HO-TMS]).

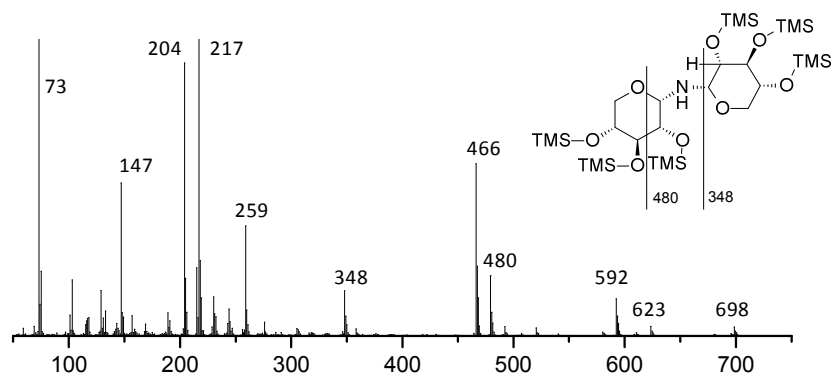


Figure S2. EI-MS (70 eV) spectrum of hexakis-*O*-TMS di(xylopyranosyl) amine.

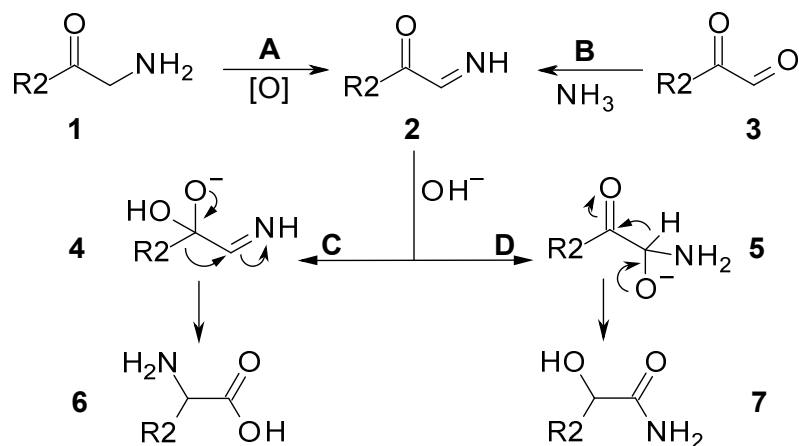


Figure S3. Proposed reaction mechanisms for the formation of α -amino acids and α -hydroxyamides.

EI-MS (70 eV) fragmentation pattern of persilylated commercial *N*-heterocyclic compounds.

***N,O*-bis(trimethylsilyl)-lactamide:** m/z 233 (M^+ ; 0.7%), 218 ($M^+ - \text{CH}_3$; 11.8%), 188 (29.4%), 147 ($(\text{SiMe}_3)\text{O}^+(\text{SiMe}_2)$; 44.5%), 133 (6.0%), 117 ($\text{CH}_3\text{C}^+\text{HOSiMe}_3$; 39.6%), 103 (3.9%), 90 (SiMe_3OH ; 6.4%), 73 (SiMe_3 ; 100%), 59 (5.2%).

***N,O*-bis(trimethylsilyl)-glycolamide:** m/z 219 (M^+ ; 1.5%), 204 ($M^+ - \text{CH}_3$; 26.0%), 188 (44.6%), 177 (3.8%), 158 (1.9%), 147 ($(\text{SiMe}_3)\text{O}^+(\text{SiMe}_2)$; 38.7%), 133 (6.8%), 116 (12.4%), 104 (28.9%), 95 (2.4%), 89 (10.6%), 73 (100%), 66 (7.4%).

Tris(trimethylsilyl)carbamate: m/z 262 ($M^+ - \text{CH}_3$; 23.2%), 174 ($\text{SiMe}_3\text{NHC}^+\text{OSiMe}_2$; 7.0%), 147 ($(\text{SiMe}_3)\text{O}(\text{SiMe}_2)$; 100%), 131 (5.1%), 117 (1.4%), 100 (5.3%), 73 (31.5%).

References

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