

Simplifying Levulinic Acid Conversion Towards a Sustainable

Biomass Valorisation

Chiara Defilippi¹, Daily Rodríguez-Padrón², Rafael Luque^{2,3}, Cristina Giordano^{*,1}

¹*School of Biological and Chemical Sciences, Chemistry Department, Queen Mary University of London, Mile End Road, London E1 4NS, United Kingdom*

²*Departamento de Química Orgánica, Facultad de Ciencias, Universidad de Córdoba, Campus de Rabanales, Edificio Marie Curie (C-3), Ctra Nnal IV-A, Km 396, E14014 Córdoba, Spain*

³*Peoples Friendship University of Russia (RUDN University), 6 Miklukho Maklaya str., 117198, Moscow, Russia*

*c.giordano@qmul.ac.uk

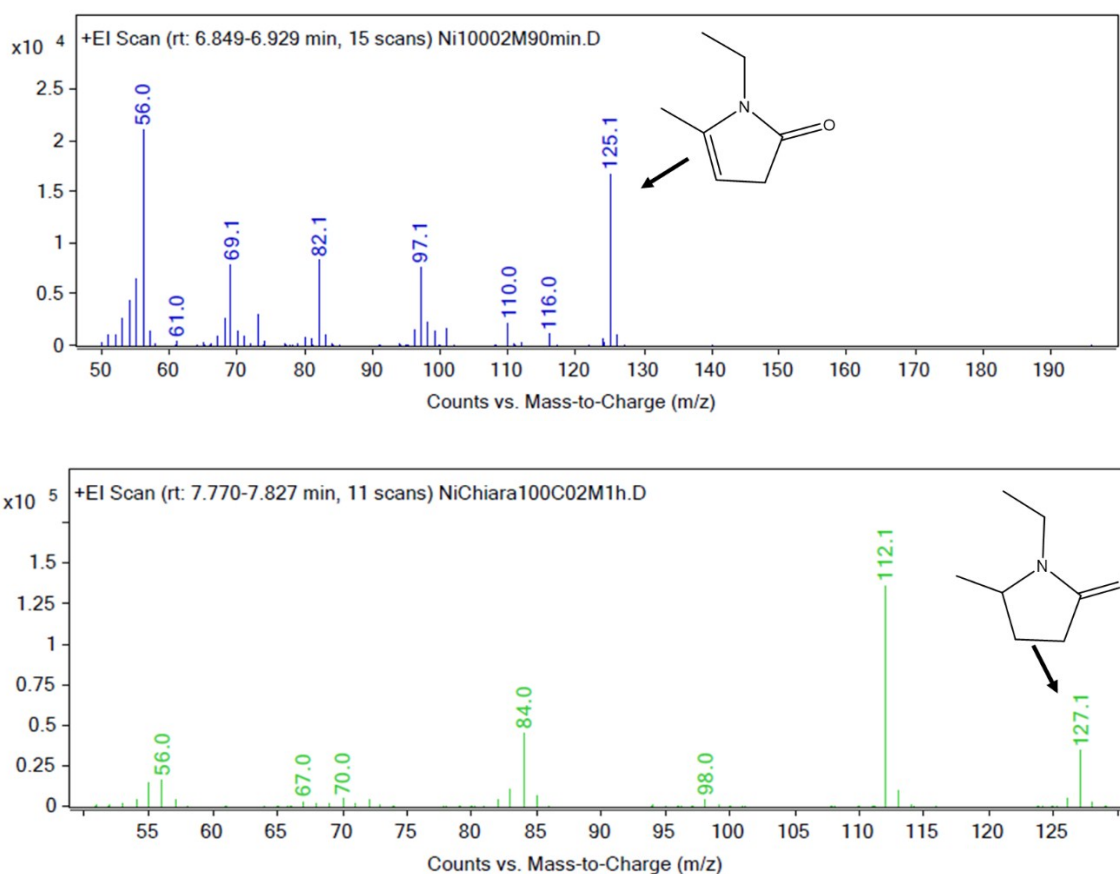


Figure SI 1. GC-MS spectra of the two products obtained (P1 and P2) from the continuous flow conversion of levulinic acid to nitrogen-heterocycles using Ni-based catalysts.

Table S11. Peak assignment in the Nickel region for Ni⁰, Ni₃N and Ni₃N + Ni⁰ before and after the reaction.

Ni 2p _{3/2}	Position (eV)	Assignment	Comment/reference
Ni ⁰	852.5/855.2	Ni ⁰ /Ni ²⁺	1,2
Ni ₃ N	852.3/855.5	Ni ⁰ /Ni ²⁺	
Ni ₃ N + Ni ⁰	852.5/855.4	Ni ⁰ /Ni ²⁺	
Ni ⁰ -tested	852.8/856.1	Ni ⁰ /Ni ²⁺	
Ni ₃ N -tested	852.6/855.6	Ni ⁰ /Ni ²⁺	
Ni ₃ N + Ni ⁰ -tested	852.1/855.6	Ni ⁰ /Ni ²⁺	

Table S12. Peak assignment in the carbon region for Ni⁰, Ni₃N and Ni₃N + Ni⁰ before and after the reaction

C 1s	Position (eV)	Assignment	Comment/reference
Ni ⁰	284.6	C-C/C = C	3
Ni ₃ N	284.6	C-C/C = C	
Ni ₃ N + Ni ⁰	284.6	C-C/C = C	
Ni ⁰ -tested	284.6	C-C/C = C	
Ni ₃ N -tested	284.6	C-C/C = C	
Ni ₃ N + Ni ⁰ -tested	284.6	C-C/C = C	

Table S13. Peak assignment in the oxygen region for Ni⁰, Ni₃N and Ni₃N + Ni⁰ before and after the reaction

O 1s	Position (eV)	Assignment	Comment/reference
Ni ⁰	531.0	O-O	4
Ni ₃ N	530.8	O-O	
Ni ₃ N + Ni ⁰	531.0	O-O	
Ni ⁰ -tested	531.5	O-O	
Ni ₃ N -tested	531.1	O-O	
Ni ₃ N + Ni ⁰ -tested	531.2	O-O	

Table S14. Peak assignment in the nitrogen region for Ni⁰, Ni₃N and Ni₃N + Ni⁰ before and after the reaction

N 1s	Position (eV)	Assignment	Comment/reference
Ni ⁰	-	N-Ni	5
Ni ₃ N	398.4	N-Ni	
Ni ₃ N + Ni ⁰	398.7	N-Ni	
Ni ⁰ -tested	-	N-Ni	
Ni ₃ N -tested	399.0	N-Ni	
Ni ₃ N + Ni ⁰ -tested	398.7	N-Ni	

References

- 1 H. W. Nesbitt, D. Legrand and G. M. Bancroft, *Physics and Chemistry of Minerals*, 2000, **27**, 357.
- 2 S. Oswald and W. Brückner, *Surface and Interface Analysis*, 2004, **36**, 17.
- 3 D. Rodríguez-Padrón, A. R. Puente-Santiago, A. M. Balu, A. A. Romero and R. Luque, *Chemical Communications*, 2017, **53**, 7635.
- 4 D. Rodríguez-Padrón, M. Algarra, L. A. C. Tarelho, J. Frade, A. Franco, G. de Miguel, J. Jiménez, E. Rodríguez-Castellón and R. Luque, *ACS Sustainable Chemistry & Engineering*, 2018, **6**, 7200.
- 5 D. Rodríguez-Padrón, A. D. Jodlowski, G. de Miguel, A. R. Puente-Santiago, A. M. Balu and R. Luque, *Green Chemistry*, 2018, **20**, 225.