

Supplementary Materials: The Efficient Recyclable Molybdenum- and Tungsten-Promoted Mesoporous ZrO_2 Catalysts for Aminolysis of Epoxides

Xolani Sibusiso Hlatshwayo, Morena S. Xaba, Matumuene Joe Ndolomingo, Ndzondelelo Bingwa * and Reinout Meijboom *

Center for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, P.O. Box 524, Auckland Park, Johannesburg 2006, South Africa; mrsbuda.mhayise@outlook.com (X.S.H.); xabams@gmail.com (M.S.X.); joe_ndol@yahoo.fr (M.J.N.)

* Correspondence: nbingwa@uj.ac.za (N.B.); rmeijboom@uj.ac.za (R.M.); Tel.: +27-(0)11-559-2367 (R.M.); Fax: +27-(0)11-559-2819 (R.M.)

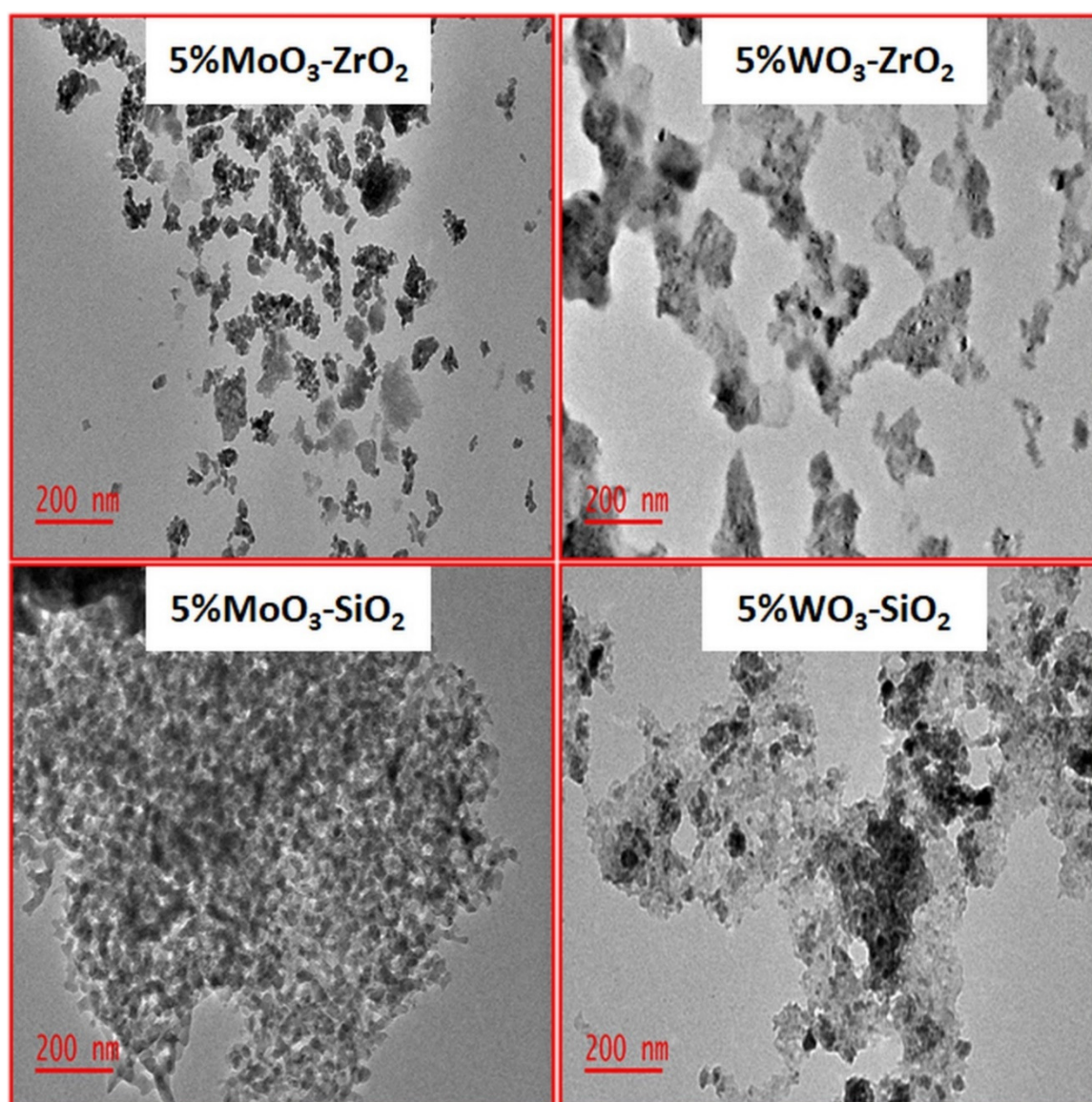


Figure S1. TEM analyses of the as-synthesized catalysts.

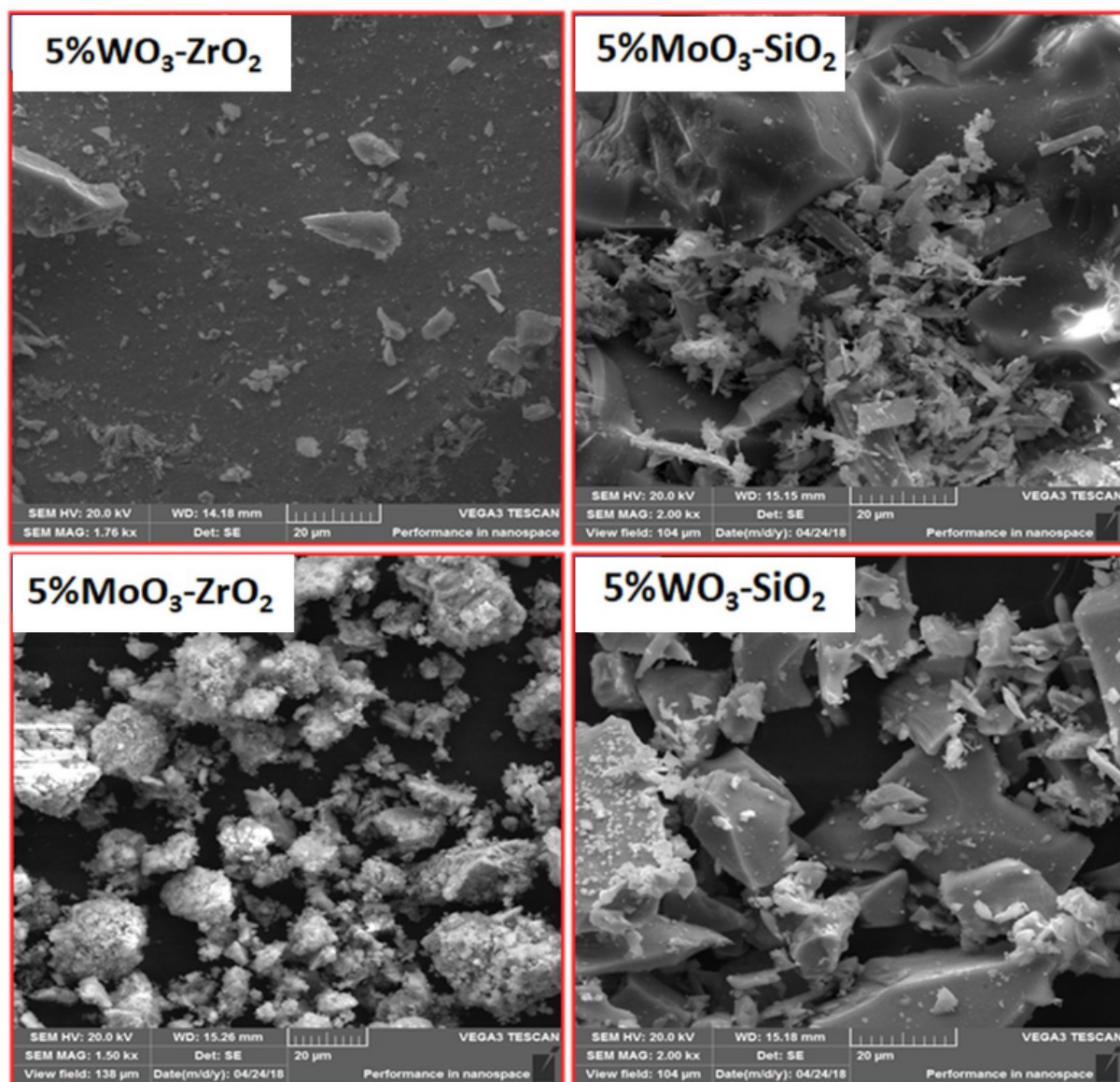


Figure S2. SEM images of the as-synthesized catalysts.

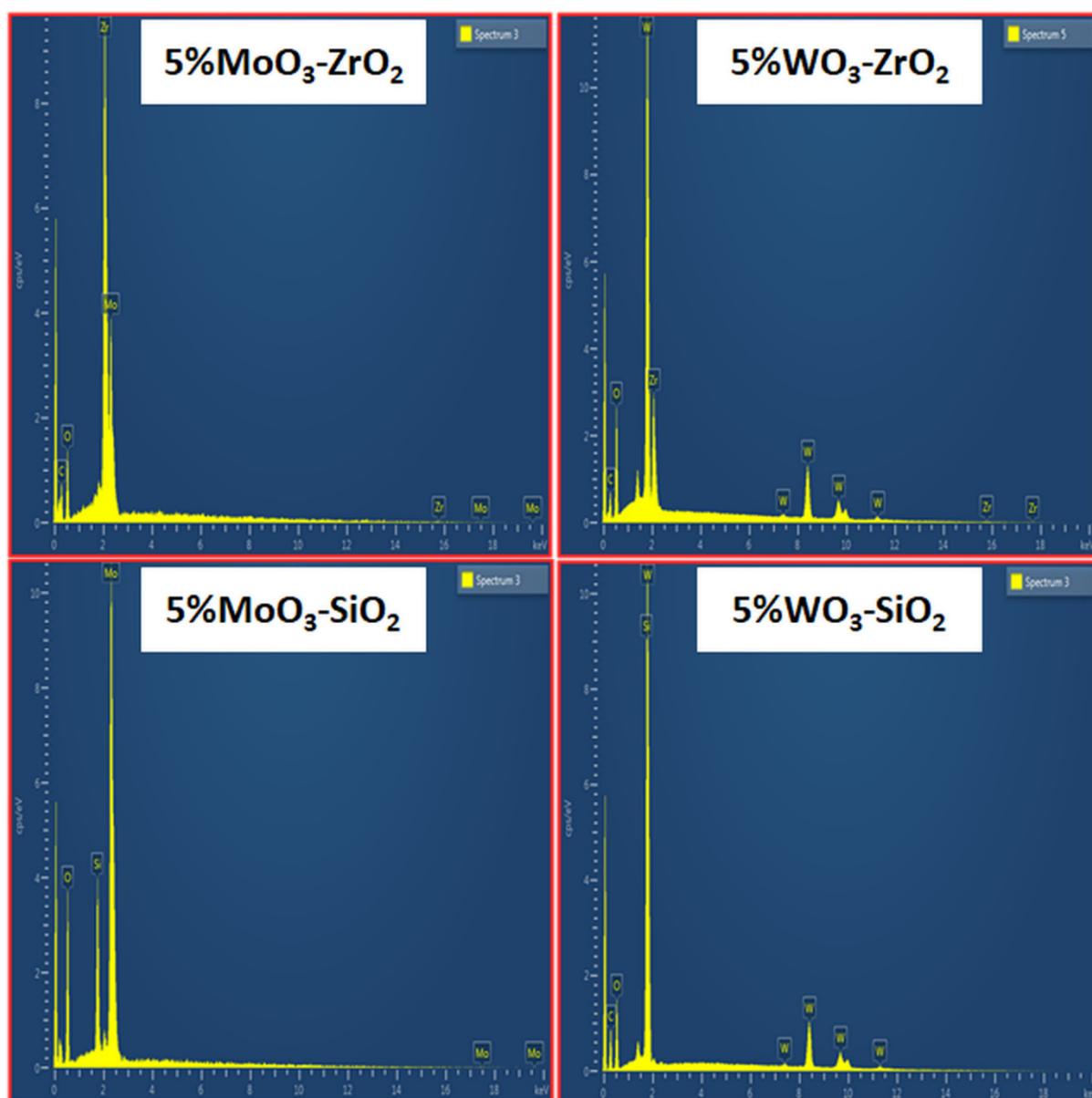


Figure S3. EDX characterization of the as-synthesized materials.

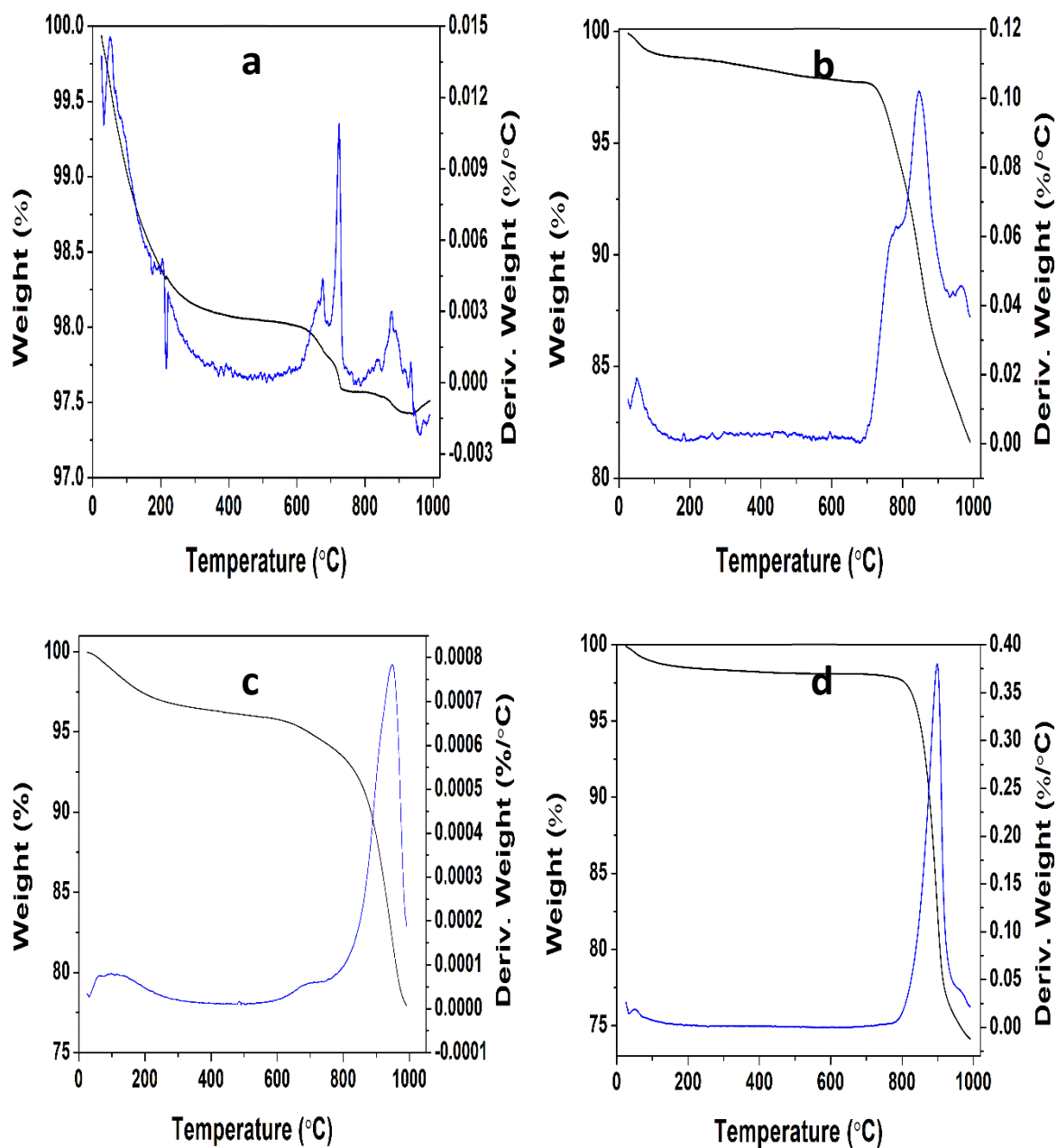


Figure S4. Thermal gravimetric analysis plots of mesoporous metal oxides: (a) 5%MoO₃-ZrO₂, (b) 5%WO₃-ZrO₂, (c) 5%MoO₃-SiO₂, and (d) 5%WO₃-SiO₂.

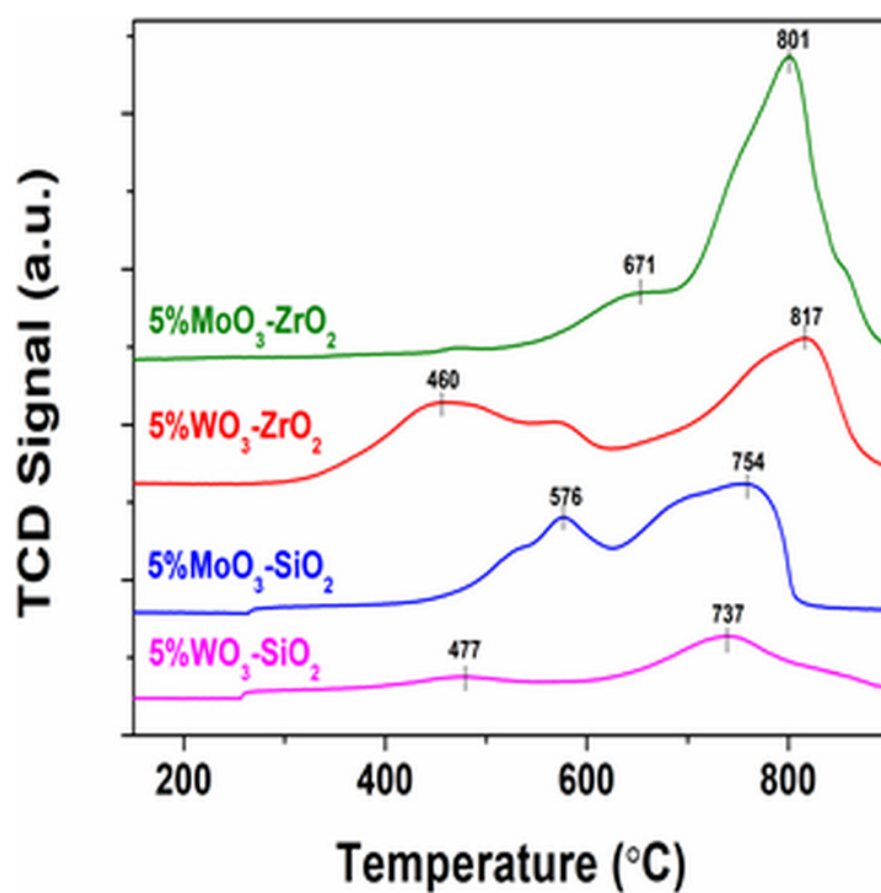


Figure S5. Temperature-programmed reduction of the synthesized materials.

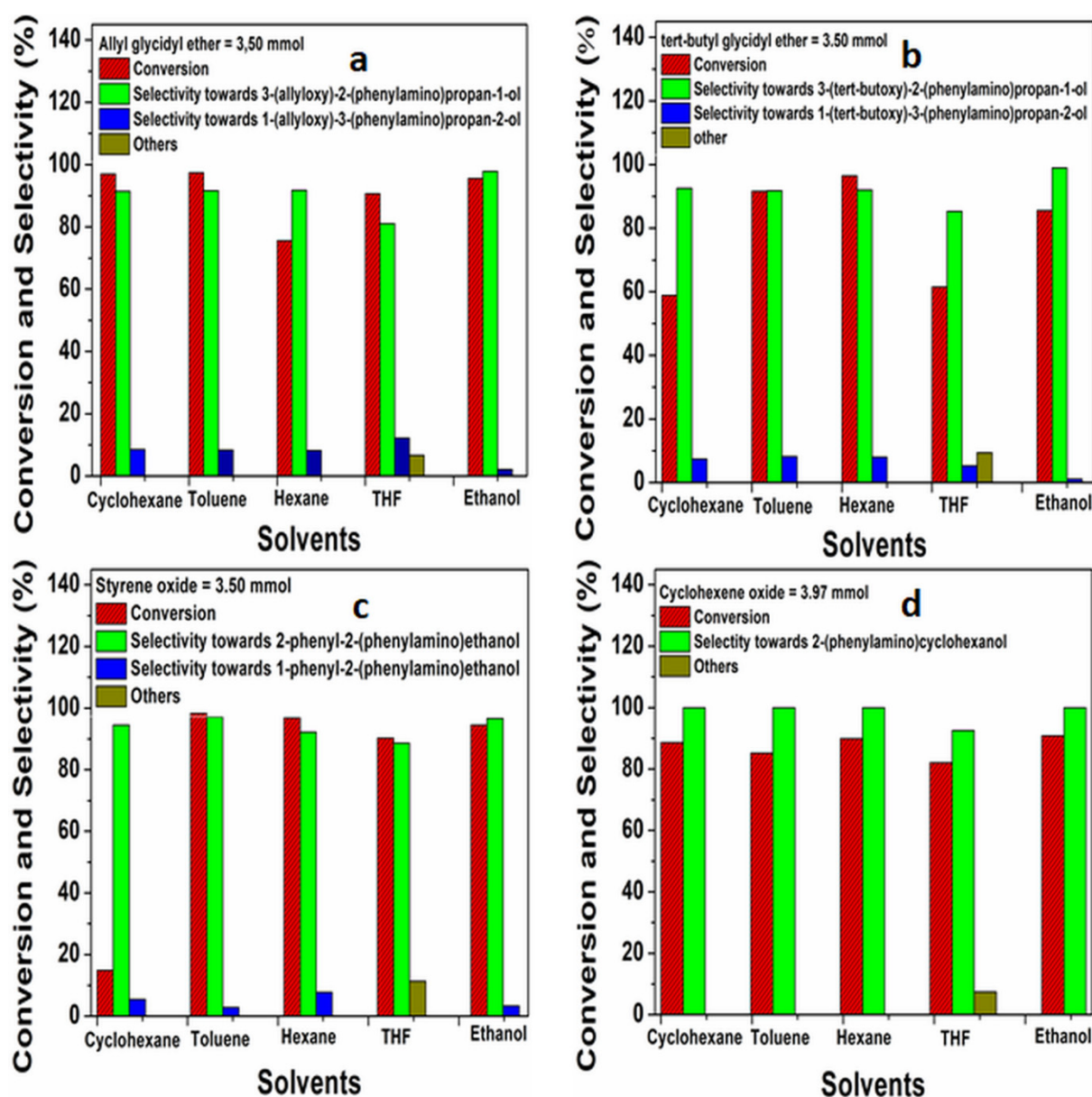


Figure S6. The ring opening efficacy of different substrates under various solvents. The reaction conditions: time = 3 hours; catalyst amount (5%MoO₃-ZrO₂) = 25 mg; stirring speed = 450 rpm.

Equation (S1) Conversion equations

$$R_{IS} = \frac{IS_t}{IS_i}$$

$$C_S = \frac{S}{R_{IS}}$$

$$C_P = \frac{P}{R_{IS}}$$

$$C_{SP} = \frac{SP}{R_{IS}}$$

$$S_{rem} = \frac{C_{P_t}}{C_{P_i}} \times 100$$

$$\text{Conversion (\%)} = 100 - S_{rem}$$

$$PS = \frac{C_P}{C_P + C_{SP}} \times 100$$

$$SPS = \frac{C_{SP}}{C_P + C_{SP}} \times 100$$

Abbreviations and acronyms for conversion calculations: The internal standard = (IS); The substrate = (S); Product = (P); Product selectivity = (PS); Side product selectivity = (SPS); The ratio of internal standard = (R_{IS}); Corrected substrate = (C_S); Corrected product = (C_P); Corrected side product = (C_{SP}); Amount of substrate remaining = (S_{rem}).

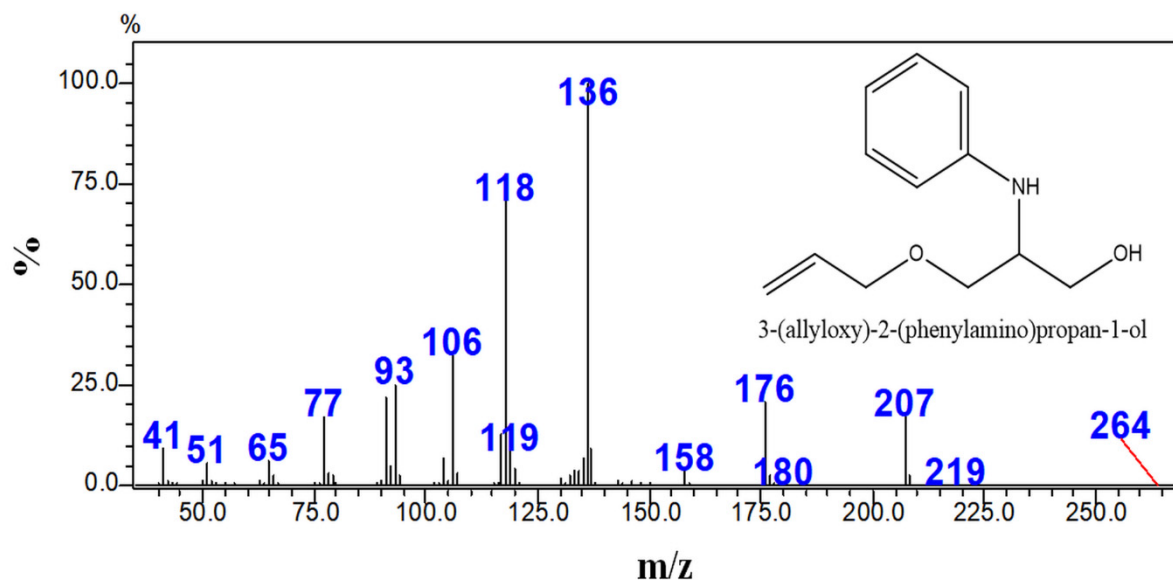


Figure S7. GC-MS spectra for the ring opening of ally glycidyl ether into β -amino alcohol after 4 hours of reaction time.

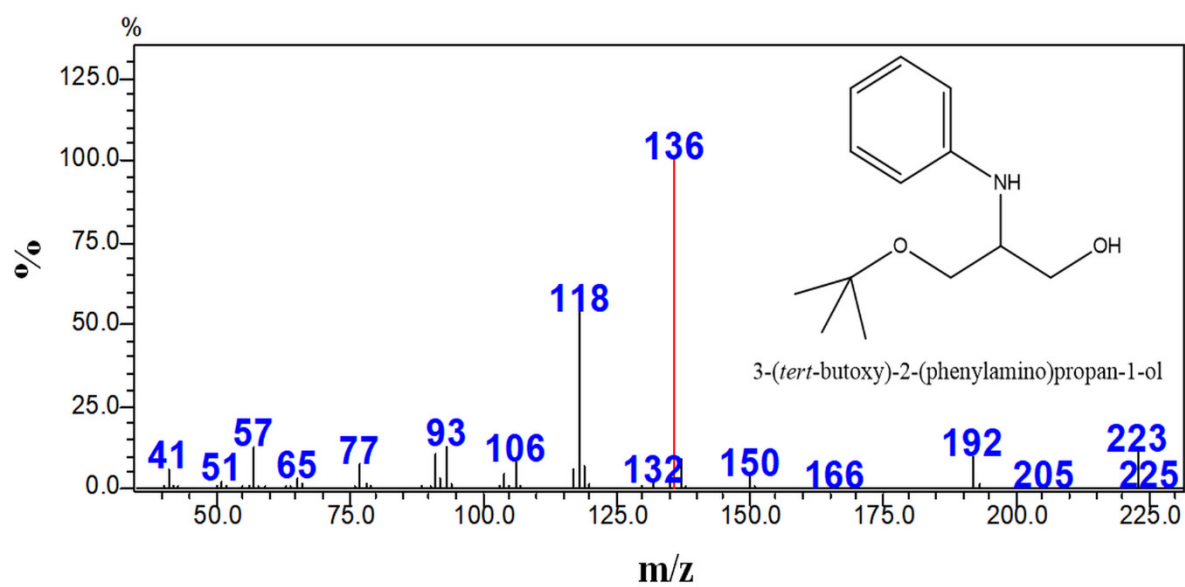
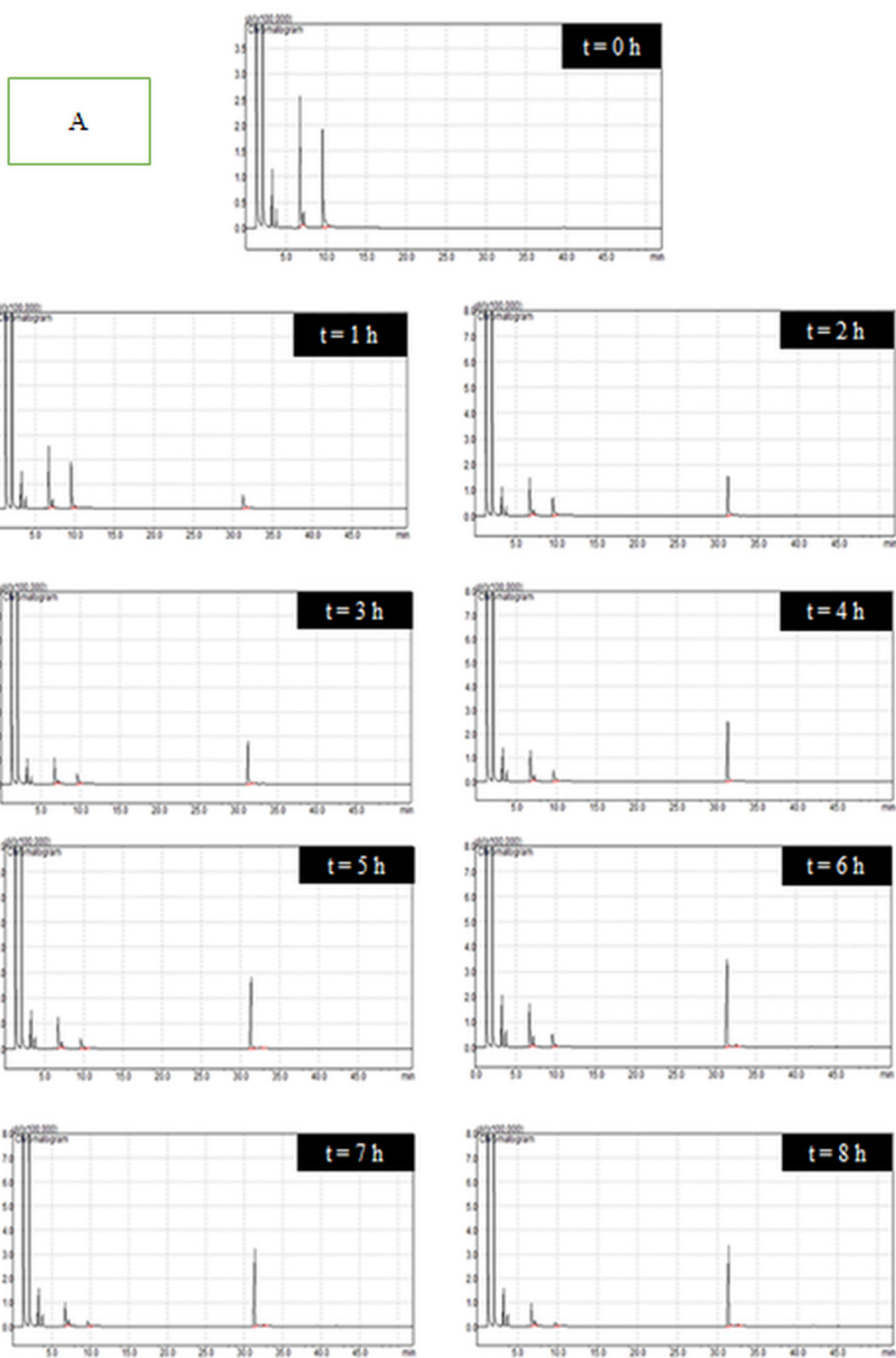
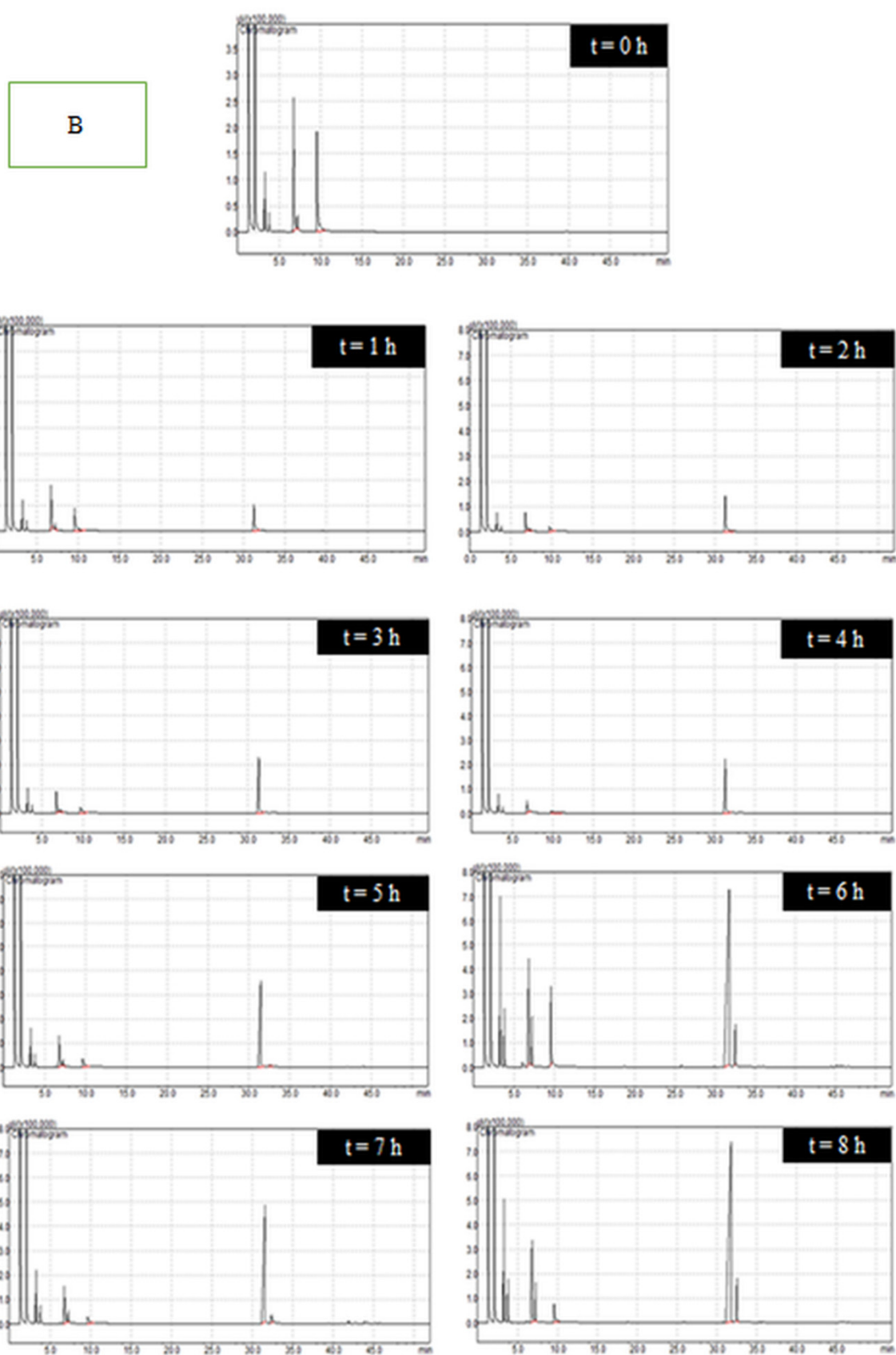
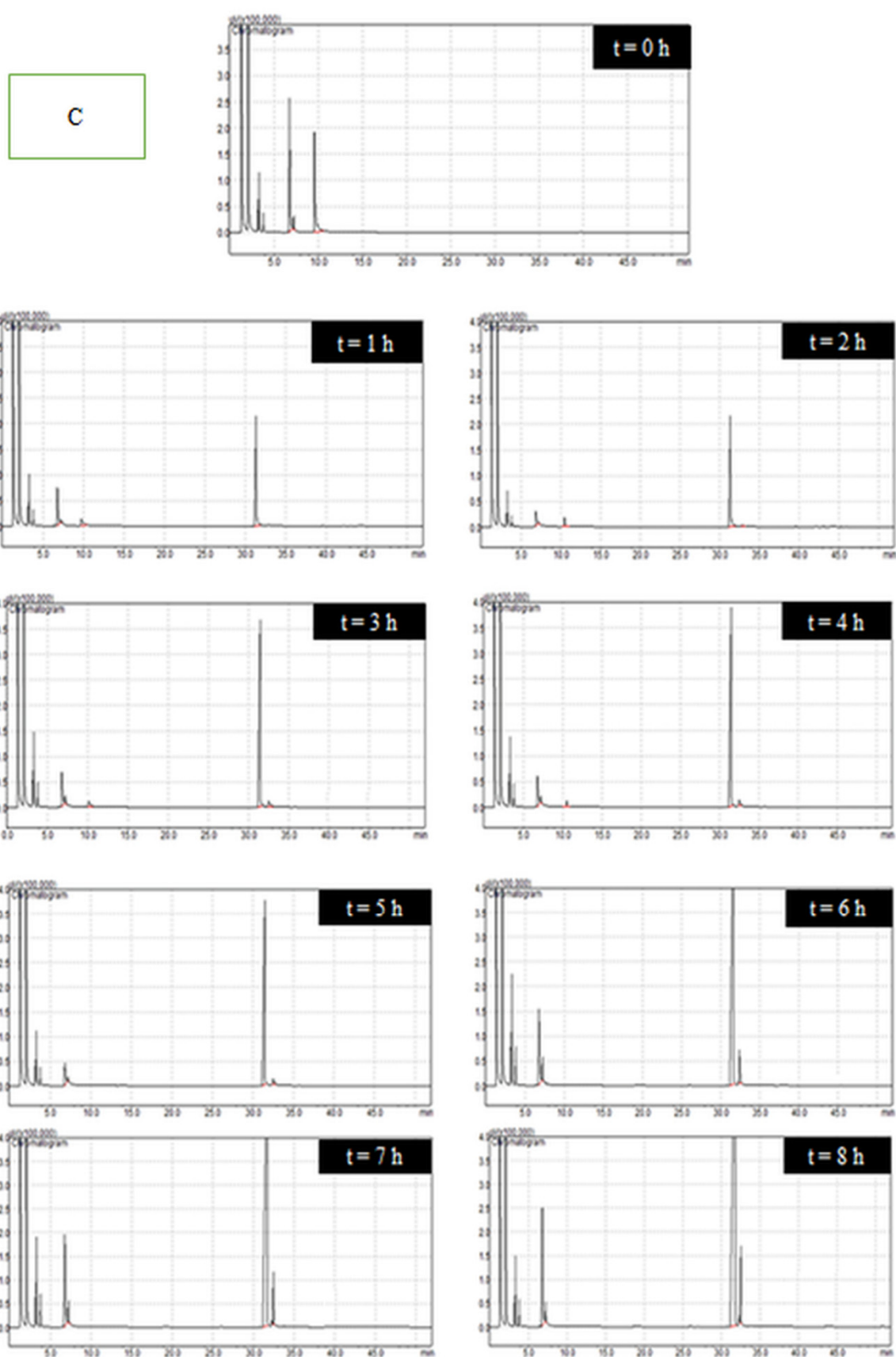
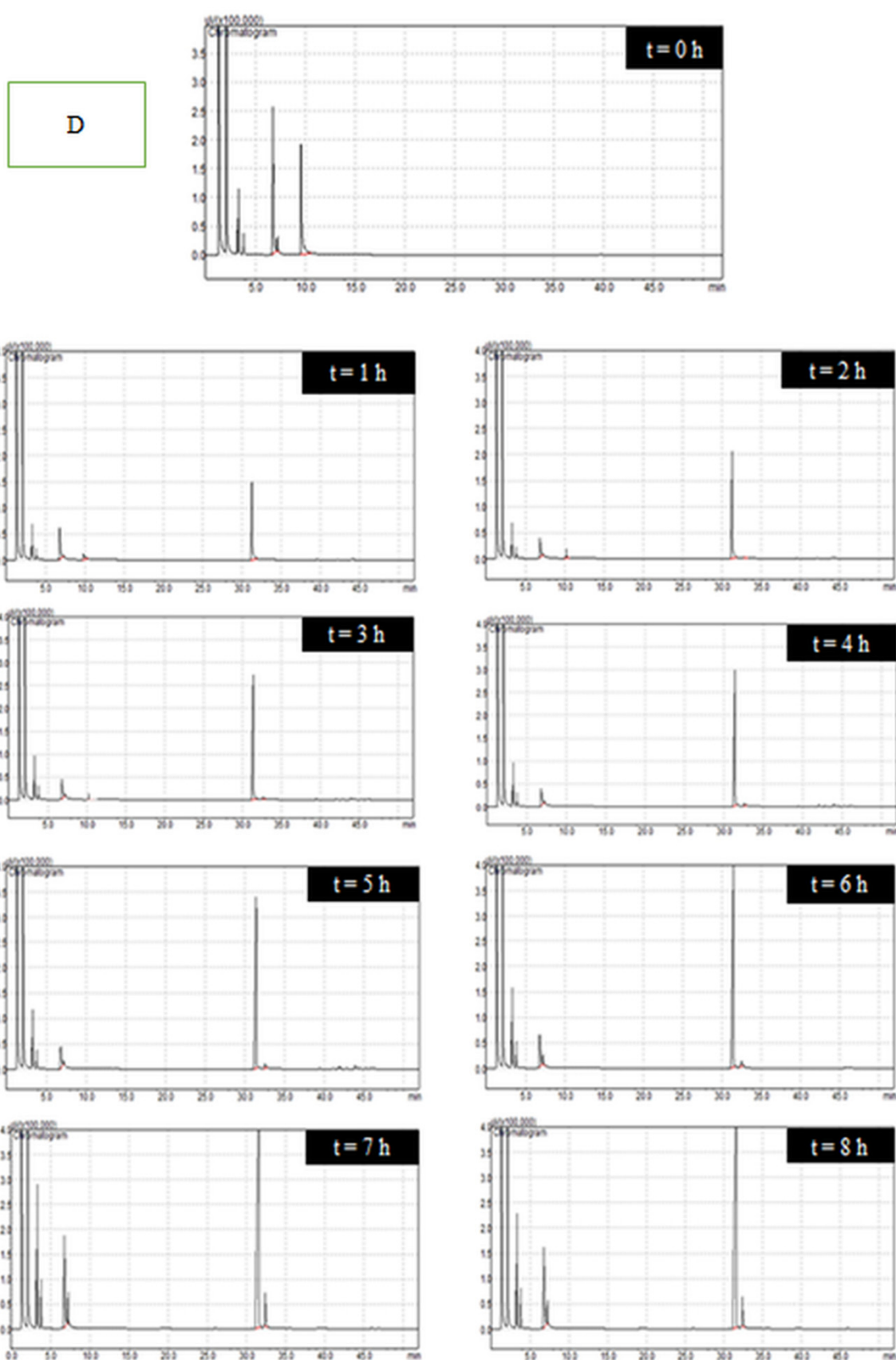


Figure S8. GC-MS spectra for the ring opening of tert-butyl glycidyl ether into β -amino alcohol after 4 hours of reaction time.









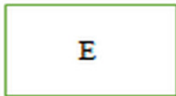


Figure S9. Catalyst variation of **A:** 5%MoO₃-ZrO₂ = 10 mg, **B:** 5%MoO₃-ZrO₂ = 15 mg, **C:** 5%MoO₃-ZrO₂ = 35 mg, **D:** 5%MoO₃-ZrO₂ = 45 mg and **E:** 5%MoO₃-ZrO₂ = 65 mg at different time intervals. The reaction conditions are as follows: stirring speed = 450 rpm, toluene = 10 mL, decane = 0.237 mmol, aniline = 4.20 mmol, styrene oxide = 3.50 mmol and temperature = 120 °C.

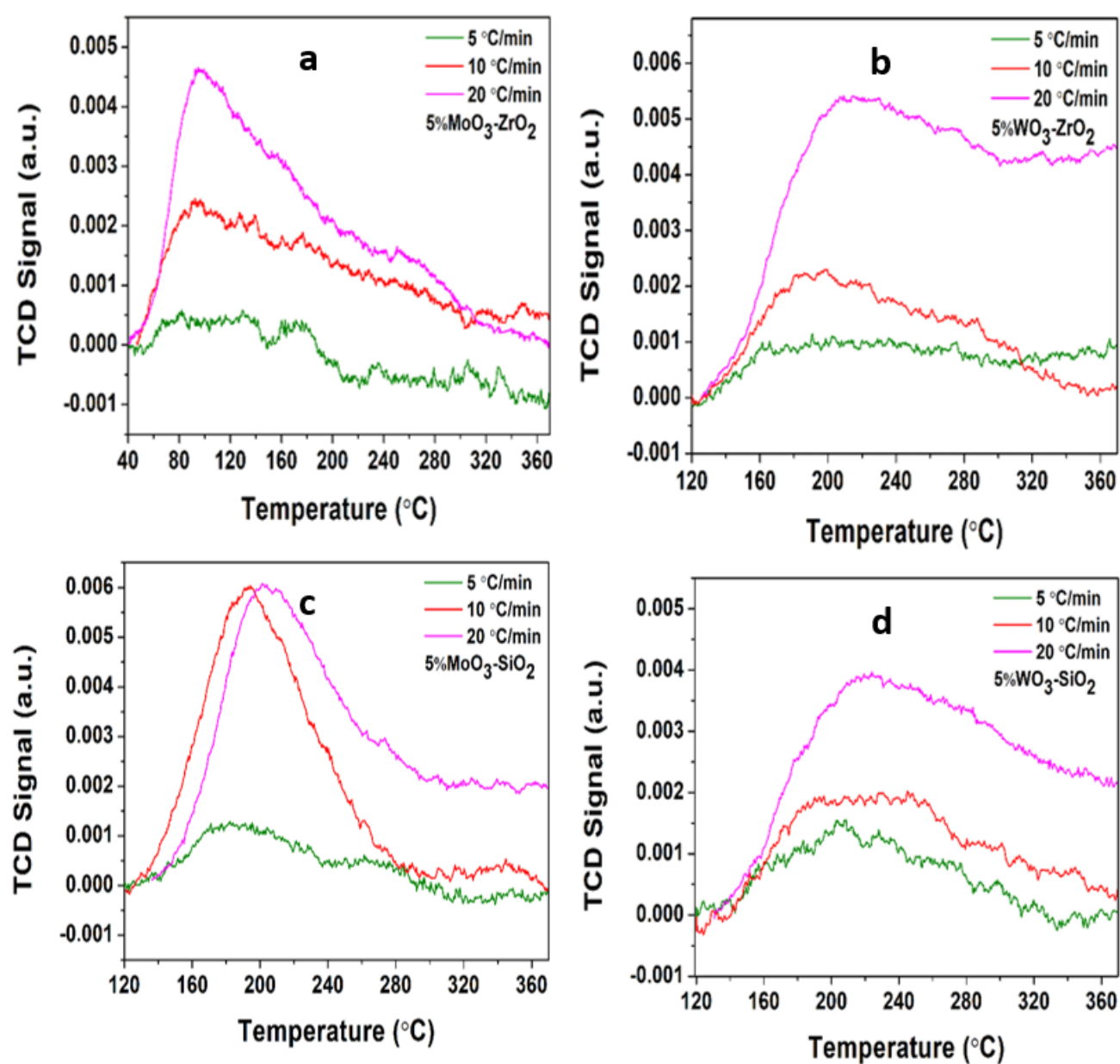


Figure S10. NH₃-TPD profiles of MMOs. (a) 5%MoO₃-ZrO₂, (b) 5%WO₃-ZrO₂, (c) 5%MoO₃-SiO₂, and (d) 5%WO₃-SiO₂.