



J. Serb. Chem. Soc. 88 (11) S318-S325 (2023)

JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS Supplementary material

SUPPLEMENTARY MATERIAL TO Antidiabetic potential of simple carbamate derivatives: Comparative experimental and computational study

RELJA V. SURUČIĆ¹, IVANA I. JEVTIĆ², TATJANA P. STANOJKOVIĆ³ and JELENA B. POPOVIĆ-DJORDJEVIĆ⁴*

¹University of Banja Luka, Faculty of Medicine, Save Mrkalja 14, 78000 Banja Luka, Bosnia and Herzegovina, ²University of Belgrade-Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12, 11000 Belgrade, Serbia, ³University of Belgrade-Institute for Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Serbia and ⁴University of Belgrade-Faculty of Agriculture, Department of Chemistry and Biochemistry, Nemanjina 6, 11080 Belgrade, Serbia

J. Serb. Chem. Soc. 88 (11) (2023) 1089–1102

SPECTROSCOPIC DATA AND YIELDS OF SYNTHESIZED COMPOUNDS 1-5

Methyl dec-9-en-1-ylcarbamate [1] Yield: 0.30 g (92 %); pale yellow oil. ¹H NMR (200 MHz, CDCl₃): δ = 5.81 (ddt, J = 16.9, 10.1, 6.6 Hz, 1H), 5.08 – 4.87 (m, 2H), 4.80 (br s, 1H), 3.66 (s, 3H), 3.16 (dd, J = 13.1, 6.5 Hz, 2H), 2.13 – 1.94 (m, 2H), 1.61 – 1.17 (m, 12H) ppm. ¹³C NMR (50 MHz, CDCl₃): δ =157.1, 139.1, 114.1, 51.9, 41.0, 33.7, 29.9, 29.2, 29.1, 28.9, 28.8, 26.6 ppm. (+)ESI-ToF-HRMS m/z: calculated for [C₁₂H₂₃NO₂ + H+] 214.18016, observed 214.17992.

The spectra are in accordance with the previously reported data.¹

Methyl benzylcarbamate [2] Yield: 0.25 g (86 %); white amorphous solid; mp: 65 °C. ¹H NMR (200 MHz, CDCl₃): δ = 7.46 – 7.10 (m, 5H), 5.19 (br s, 1H), 4.34 (d, *J* = 6.0 Hz, 2H), 3.67 (s, 3H) ppm. ¹³C NMR (50 MHz, CDCl₃): δ = 157.1, 138.5, 128.5, 127.4, 52.0, 44.9 ppm. (+)ESI-ToF-HRMS m/z: calculated for [C₉H₁₁NO₂ + H+] 166.08626, observed 166.08596.

The spectra are in accordance with the previously reported data.¹

Methyl phenylcarbamate **[3]** Yield 0.52 g (90 %); white powder; mp: 47 °C. ¹H NMR (200 MHz, CDCl₃): δ = 7.67 (br. s, 1H), 7.37 (ddd, *J* = 4.4, 3.3, 1.8 Hz, 2H), 7.30 – 7.12 (m, 2H), 7.03 – 6.90 (m, 1H), 3.63 (s, 3H) ppm. ¹³C NMR (50 MHz, CD₃CN): δ = 155.6, 140.2, 130.2, 124.3, 119.9, 52.9 ppm. (+)ESI-ToF-HRMS m/z: calculated for [C₈H₉NO₂ + H+] 152.07060, observed 152.07036.

The spectra are in accordance with the previously reported data.¹

Methyl m-tolylcarbamate [4] Yield 0.33 g (92 %); Yield: 0.33 g (89 %); pale yellow solid; mp: 57-58°C. ¹H NMR (500 MHz, CD₃CN) δ = 7.67 (d; J = 0.7 Hz; 1H); 7.29 – 7.21 (m, 2H); 7.17 (t; J = 7.8 Hz; 1H); 6.91 – 6.82 (m; 1H); 3.69 (s; 3H); 2.30 (s; 3H) ppm. ¹³C NMR (126 MHz, CD₃CN) δ = 155.6 (C=O); 140.2 (C); 140.1 (C); 130.1 (CH); 125.0 (CH);

S318

^{*} Corresponding author. E-mail: jelenadj@agrif.bg.ac.rs

120.5 (CH); 117.1 (CH); 53.0 (CH₃); 21.9 (CH₃) ppm. (+)ESI-ToF-HRMS m/z: calculated for $[C_9H_{11}NO_2 + H+]$ 166.08626, observed 166.08653.

The spectra are in accordance with the previously reported data.¹

Methyl (2-ethoxyphenyl)carbamate [5] Yield: 0.08 g (85 %); colorless oil. ¹H NMR (200 MHz, CDCl₃) δ = 8.20 – 7.95 (m; 1H); 7.26 (d; J = 2.2 Hz; 1H); 7.07 – 6.70 (m; 3H); 4.06 (q; J = 7.0 Hz; 2H); 3.78 (s; 3H); 1.42 (t; J = 7.0 Hz; 3H) ppm. ¹³C NMR (50 MHz, CDCl₃) δ = 153.9 (C=O); 146.8 (C), 127.6 (C); 122.6 (CH); 120.9 (CH); 118.0 (CH); 110.8 (CH); 64.0 (CH₂); 52.1 (CH₃); 14.7 (CH₃) ppm. (+)ESI-ToF-HRMS m/z: calculated for [C₁₀H₁₃NO₃ + H+] 196.09682, observed 196.09680.

The spectra are in accordance with the previously reported data.¹

SURUČIĆ et al.

NMR SPECTRA OF COMPOUNDS 1-5



Available on line at www.shd.org.rs/JSCS/

S320



Available on line at www.shd.org.rs/JSCS/

S321







S324

SURUČIĆ et al.



REFERENCES

1. I. I. Jevtić, Lj. Došen-Mićović, E. R. Ivanović, M. D. Ivanović, *Synthesis* **48** (2016) 1550 (https://doi.org/10.1055/s-0036-1588985).