



SUPPLEMENTARY MATERIAL TO
Density functional theory: ^1H - and ^{13}C -NMR spectra of some coumarin derivatives

SELMA ŠPIRTOVIĆ-HALILOVIĆ^{1*}, MIRSADA SALIHOVIĆ², SNEŽANA TRIFUNOVIĆ³, SUNČICA ROCA⁴, ELMA VELJOVIĆ¹, AMAR OSMANOVIĆ¹,
MARIJANA VINKOVIĆ⁴ and DAVORKA ZAVRŠNIK¹

¹Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000 Sarajevo, Bosnia and Herzegovina, ²Department of Organic Chemistry, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000 Sarajevo, Bosnia and Herzegovina, ³Faculty of Chemistry, University of Belgrade, Studentski trg 12–16, 11000 Belgrade, Serbia and ⁴NMR Centre, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

J. Serb. Chem. Soc. 79 (11) (2014) 1405–1411

SPECTRAL DATA OF THE PREPARED COMPOUNDS

(E)-3-(3-(4-Bromophenyl)acryloyl)-4-hydroxy-2H-chromen-2-one (**1**). ^1H -NMR (600.133 MHz, DMSO- d_6 , δ / ppm): 7.40 (1H, dd, 3J = 7.57 Hz, H₂₄), 7.79 (1H, dd, 3J = 8.40 Hz, 4J = 1.41 Hz, H₂₅), 7.36 (1H, d, 3J = 8.40 Hz, H₂₆), 8.02 (1H, d, 3J = 7.57 Hz, H₂₇), 8.22 (1H, d, 3J = 15.78 Hz, H₂₉), 7.92 (1H, d, 3J = 15.78 Hz, H₃₀), 7.65 (2H, s, H₃₁, H₃₄), 7.65 (2H, s, H₃₂, H₃₃); ^{13}C -NMR (150.917 MHz, DMSO- d_6 , δ / ppm): 100.5 (C₉), 115.4 (C₅), 116.2 (C₃), 123.2 (C₁₃), 124.0 (C₁), 124.2 (C₂₀), 124.8 (C₆), 130.0 (C₁₈, C₂₂), 131.6 (C₁₉, C₂₁), 132.0 (C₁₇), 135.9 (C₂), 144.0 (C₁₆), 153.8 (C₄), 158.9 (C₈), 179.6 (C₁₀), 190.8 (C₁₂).

(E)-4-Hydroxy-3-(3-(4-methoxyphenyl)acryloyl)-2H-chromen-2-one (**2**). ^1H -NMR (600.133 MHz, DMSO- d_6 , δ / ppm): 7.38 (1H, dd, 3J = 7.95 Hz, 4J = 0.81 Hz, H₂₅), 7.76 (1H, ddd, 3J = 8.43 Hz, 3J = 7.32 Hz, 4J = 1.54 Hz, H₂₆), 7.33 (1H, d, 3J = 8.43 Hz, H₂₇), 8.00 (1H, d, 3J = 7.95 Hz, H₂₈), 8.14 (1H, d, 3J = 15.81 Hz, H₃₀), 7.98 (1H, d, 3J = 15.81 Hz, H₃₁), 7.68 (2H, d, 3J = 8.70 Hz, H₃₂, H₃₅), 7.03 (2H, d, 3J = 8.43 Hz, H₃₃, H₃₄), 3.84 (3H, s, H₃₆, H₃₇, H₃₈); ^{13}C -NMR (150.917 MHz, DMSO- d_6 , δ / ppm): 55.0 (C₂₄), 100.0 (C₉), 114.4 (C₁₉, C₂₁), 115.7 (C₅), 116.1 (C₃), 119.3 (C₁₃), 123.9 (C₁), 124.7 (C₆), 126.7 (C₁₇), 130.5 (C₁₈, C₂₂), 135.7 (C₂), 146.2 (C₁₆), 153.7 (C₄), 159.0 (C₈), 162.0 (C₂₀), 180.1 (C₁₀), 190.4 (C₁₂).

*Corresponding author. E-mail: selmaspirtovic@yahoo.com

(E)-3-(3-(4-Chlorophenyl)acryloyl)-4-hydroxy-2H-chromen-2-one (**3**). ^1H -NMR (600.133 MHz, DMSO- d_6 , δ / ppm): 7.40 (1H, *dd*, $^3J = 7.86$ Hz, $^4J = 0.57$ Hz, H₂₄), 7.78 (1H, *ddd*, $^3J = 8.47$ Hz, $^3J = 7.41$ Hz, $^4J = 1.56$ Hz, H₂₅), 7.35 (1H, *d*, $^3J = 8.47$ Hz, H₂₆), 8.01 (1H, *dd*, $^3J = 7.86$ Hz, $^4J = 1.56$ Hz, H₂₇), 8.21 (1H, *d*, $^3J = 15.81$ Hz, H₂₉), 7.93 (1H, *d*, $^3J = 15.81$ Hz, H₃₀), 7.71 (2H, *d*, $^3J = 8.46$ Hz, H₃₁, H₃₄), 7.49 (2H, *d*, $^3J = 8.46$ Hz, H₃₂, H₃₃); ^{13}C -NMR (150.917 MHz, DMSO- d_6 , δ / ppm): 100.5 (C₉), 115.3 (C₅), 116.2 (C₃), 123.0 (C₁₃), 124.0 (C₁), 124.8 (C₆), 128.6 (C₁₉, C₂₁), 129.8 (C₁₈, C₂₂), 132.8 (C₁₇), 135.0 (C₂), 135.5 (C₂₀), 143.9 (C₁₆), 153.8 (C₄), 158.9 (C₈), 179.6 (C₁₀), 190.8 (C₁₂).