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SUPPLEMENTARY MATERIAL TO

Solvent effects on the absorption spectra of potentially pharmacologically active 5-alkyl-5-arylhydantoins: a structure–property relationship study

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PHYSICAL AND SPECTRAL DATA FOR COMPOUNDS **7**–**12**

*5-Ethyl-5-phenylhydantoin (**7**)*. Yield: 76 %; m.p.: 198–199 °C (lit**. 194–196 °C); IR (KBr, cm^{-1}): 3285 (NH), 3214 (NH), 1771 (C=O), 1737 (C=O); ^{1}H--NMR (200 MHz, DMSO-d_6, δ / ppm): 0.83 (3H, *t*, J = 7.3 Hz, CH_3), 1.82–2.18 (2H, *m*, CH_2), 7.28–7.55 (5H, *m*, Ph), 8.67 (1H, *s*, N1),10.80 (1H, *s*, N3); ^{13}C--NMR (50 MHz, DMSO-d_6, δ / ppm): 8.2, 31.4, 68.3, 125.7, 128.0, 128.7, 139.4, 157.0, 176.6.

*5-Ethyl-5-(4-hydroxyphenyl)hydantoin (**8**)*. Yield: 48 %; m.p.: 265–267 °C; Anal. Calcd. for $C_{11}H_{12}N_2O_3$: C, 59.99; H, 5.49; N, 12.72 %. Found: C, 60.10; H, 5.36; N, 12.70 %; IR (KBr, cm^{-1}): 3420 (OH), 3269 (NH), 3148 (NH), 1753 (C=O), 1728 (C=O); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 0.81 (3H, *t*, J = = 7.1 Hz, CH_3), 1.76–2.13 (2H, *m*, CH_2), 6.78 (2H, *d*, J = 8.4 Hz, Ar-H), 7.29 (2H, *d*, J = 8.4 Hz, Ar-H), 8.51 (1H, *s*, N1), 10.11 (1H, *bs*, N3), 10.08 (1H, *bs*, **H**O–C_6H_4) (signal at 10.11 is partly covered by the signal at 10.08); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 8.3, 31.2, 67.9, 115.4, 127.0, 129.6, 157.1, 157.3, 177.1; HRMS (*m*/*z*): 221.0924, corresponding to the molecular formula $C_{11}H_{12}N_2O_3H^+$ (error in ppm: 1.32).

*5-Ethyl-5-(4-methylphenyl)hydantoin (**9**)*. Yield: 58 %; m.p.: 196–198 °C; Anal. Calcd. for $C_{12}H_{14}N_2O_2$: C, 66.04; H, 6.47; N, 12.84 %. Found: C, 66.12; H, 6.42; N, 12.78 %; IR (KBr, cm^{-1}): 3268 (NH), 3206 (NH), 1779 (C=O), 1746 (C=O); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 0.92 (3H, *t*, J = 7.1 Hz, CH_3), 1.90–2.26 (2H, *m*, CH_2), 2.39 (3H, *s*, C**H**$_3$–C_6H_4), 7.30 (2H, *d*, J = 8.0 Hz, Ar-H), 7.50 (2H, *d*, J = 8.4 Hz, Ar-H), 8.72 (1H, *s*, N1), 10.82 (1H, *bs*, N3); ^{13}C-NMR

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(50 MHz, DMSO-d_6, δ / ppm): 8.2, 20.8, 31.3, 68.1, 125.6, 129.3, 136.5, 137.3, 157.0, 176.8; HRMS (*m*/*z*): 219.1124, corresponding to the molecular formula $C_{12}H_{14}N_2O_2H^+$ (error in ppm: –1.68).

5-Ethyl-5-(4-methoxyphenyl)hydantoin ***(10)***. Yield: 44 %; m.p.: 210–212 °C; Anal. Calcd. for $C_{12}H_{14}N_2O_3$: C, 61.53; H, 6.02; N, 11.96 %. Found: C, 61.55; H, 6.00; N, 11.92 %; IR (KBr, cm^{-1}): 3277 (NH), 3202 (NH), 1772 (C=O), 1721 (C=O); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 0.81 (3H, *t*, *J* = 7.3 Hz, CH_3), 1.78–2.11 (2H, *m*, CH_2), 3.71 (1H, *s*, CH_3O–C_6H_4), 6.96 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.42 (2H, *d*, *J* = 9.0 Hz, Ar-H), 8.61 (1H, *s*, N1), 10.74 (1H, *s*, N3); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 8.2, 31.3, 55.4, 67.9, 114.1, 126.9, 131.3, 157.0, 159.1, 176.9; HRMS (*m*/*z*): 235.1075 corresponding to the molecular formula $C_{12}H_{14}N_2O_3H^+$ (error in ppm: –0.76).

5-(4-Chlorophenyl)-5-ethylhydantoin ***(11)***. Yield: 72 %; m.p.: 213–215 °C; Anal. Calcd. for $C_{11}H_{11}ClN_2O_2$: C, 55.36; H, 4.65; N, 11.74 %. Found: C, 55.42; H, 4.58; N, 11.72 %; IR (KBr, cm^{-1}): 3282 (NH), 3204 (NH), 1772 (C=O), 1730 (C=O); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 0.83 (3H, *t*, *J* = 7.3 Hz, CH_3), 1.81–2.16 (2H, *m*, CH_2), 7.47 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.55 (2H, *d*, *J* = 9.0 Hz, Ar-H), 8.69 (1H, *s*, N1), 10.95 (1H, *s*, N3); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / / ppm): 8.2, 31.5, 68.0, 127.7, 128.7, 132.9, 138.5, 157.3, 176.6; HRMS (*m*/*z*): 239.0583 corresponding to the molecular formula $C_{11}H_{11}ClN_2O_2H^+$ (error in ppm: 0.39).

5-(4-Bromophenyl)-5-ethylhydantoin ***(12)***. Yield: 68 %; m.p.: 222–224 °C; Anal. Calcd. for $C_{11}H_{11}BrN_2O_2$: C, 46.67; H, 3.92; N, 9.89 %. Found: C, 46.55; H, 3.88; N, 9.82 %; IR (KBr, cm^{-1}) 3252 (NH), 3222 (NH), 1772 (C=O), 1733 (C=O); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 0.82 (3H, *t*, *J* = 7.1 Hz, CH_3), 1.80–2.16 (2H, *m*, CH_2), 7.47 (2H, *d*, *J* = 9.0 Hz, Ar-H), 7.62 (2H, *d*, *J* = 8.6 Hz, Ar-H), 8.73 (1H, *s*, N1), 10.87 (1H, *s*, N3); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / / ppm): 8.2, 31.5, 68.0, 121.5, 130.1, 132.0, 138.8, 156.8, 176.2; HRMS (*m*/*z*): 283.0080 corresponding to the molecular formula $C_{11}H_{11}BrN_2O_2H^+$ (error in ppm: 1.20).