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Supporting information

The Aminobarbituric Acid–Hydantoin Rearrangement

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1. ^1H NMR data, ^{13}C NMR data, assignments, and elemental analyses

5-Bromo-1,5-dimethylbarbituric acid (**2a**): ^1H NMR (CDCl_3) δ 2.08 (s, 3H, 5- CH_3), 3.33 (s, 3H, 1- CH_3), 8.48 (s, 1H, NH); ^{13}C NMR (CDCl_3) δ 21.7 (5- CH_3), 28.9 (1- CH_3), 45.1 (C-5), 148.7 (C-2), 165.6, 167.1 (CO).

5-Bromo-1-ethyl-5-methylbarbituric acid (**2b**): ^1H NMR (CDCl_3) δ 1.21 (t, $J = 7.0$ Hz, 3H, CH_2CH_3), 2.07 (s, 3H, 5- CH_3), 3.87-4.01 (m, 2H, CH_2), 8.52 (s, 1H, NH); ^{13}C NMR (CDCl_3) δ 12.6 (CH_2CH_3), 21.5 (5- CH_3), 37.7 (CH_2), 45.4 (C-5), 148.4 (C-2), 165.7, 166.6 (CO).

5-Bromo-5-methyl-1-phenylbarbituric acid (**2c**): ^1H NMR (CDCl_3) δ 2.14 (s, 3H, CH_3), 7.22-7.54 (m, 5H, Ph), 8.48 (s, 1H, NH); ^{13}C NMR (CDCl_3) δ 21.2 (CH_3), 45.8 (C-5), 128.0, 129.6, 129.6 (CH-Ph), 133.3 (C-1'), 148.3 (C-2), 165.4, 166.8 (CO).

5-Bromo-1-methyl-5-phenylbarbituric acid (**2d**): ^1H NMR (CDCl_3) δ 3.37 (s, 3H, CH_3), 7.39-7.53 (m, 5H, Ph), 8.44 (s, 1H, NH); ^{13}C NMR (CDCl_3) δ 29.3 (CH_3), 56.2 (C-5), 128.3, 128.9 (C-2', C-3'), 130.0 (C-4'), 132.6 (C-1'), 148.3 (C-2), 164.8, 166.4 (CO).

5-Bromo-1-ethyl-5-phenylbarbituric acid (**2e**): ^1H NMR (CDCl_3) δ 1.24 (t, $J = 7.2$ Hz, 3H, CH_3), 3.99 (q, $J = 7.2$ Hz, 2H, CH_2), 7.39-7.52 (m, 5H, Ph), 8.43 (s, 1H, NH); ^{13}C NMR (CDCl_3) δ 12.8 (CH_3), 38.2 (CH_2), 56.4 (C-5), 128.3, 128.8 (C-2', C-3'), 129.9 (C-4'), 132.6 (C-1'), 148.0 (C-2), 164.8, 165.9 (CO).

5-Bromo-1-propyl-5-phenylbarbituric acid (**2f**): ^1H NMR (CDCl_3) δ 0.92 (t, $J = 7.5$ Hz, 3H, CH_3), 1.64 (sext., $J = 7.5$ Hz, 2H, CH_2CH_3), 3.89 (t, $J = 7.5$ Hz, 2H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 7.37-7.53 (m, 5H, Ph), 8.59 (s, 1H, NH); ^{13}C NMR (CDCl_3) δ 11.0 (CH_3), 20.9 (CH_2CH_3), 44.2 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 56.3 (C-5), 128.3, 128.8 (C-2', C-3'), 129.9 (C-4'), 132.6 (C-1'), 148.4 (C-2), 165.0, 166.2 (CO).

5-Bromo-1,5-diphenylbarbituric acid (**2g**): ^1H NMR (CDCl_3) δ 7.16-7.61 (m, 10H, Ph), 8.54 (s, 1H, NH); ^{13}C NMR (CDCl_3) δ 55.8 (C-5), 128.1, 128.4, 129.0, 129.6, 129.7, 130.1 (CH-Ph), 132.3, 133.3 (C-Ph), 148.1 (C-2), 164.6, 166.0 (CO).

1,5-Dimethyl-5-isopropylaminobarbituric acid (**3a**): ^1H NMR δ 0.84 (d, $J = 6.3$ Hz, 3H, CHCH_3), 0.86 (d, $J = 6.3$ Hz, 3H, CHCH_3), 1.40 (s, 3H, 5- CH_3), 2.68 (sept., $J = 6.3$ Hz, 1H, CH), 3.09 (s, 3H, 1- CH_3), 11.48 (s, 1H, NH); ^{13}C NMR δ 24.1 ($\text{CH}(\text{CH}_3)_2$), 26.2 (5- CH_3), 27.8 (1- CH_3), 45.6 (CH), 62.6 (C-5), 150.3 (C-2), 172.2, 173.2 (CO). Anal. Calcd for $\text{C}_9\text{H}_{15}\text{N}_3\text{O}_3$: C, 50.69; H, 7.09; N, 19.71. Found C, 50.86; H, 7.05; N, 19.20.

5-Benzylamino-1,5-dimethylbarbituric acid (**3b**): ^1H NMR δ 1.46 (s, 3H, 5- CH_3), 3.03 (s, 3H, 1- CH_3), 3.00-3.10 (m, 1H, NHCH_2), 3.44-3.53 (m, 2H, CH_2), 7.18-7.29 (m, 5H, Ph), 11.77 (s,

br, 1H, NH); ^{13}C NMR δ 25.1 (5-CH₃), 27.7 (1-CH₃), 48.5 (CH₂), 63.6 (C-5), 126.9 (C-4'), 128.1, 128.2 (C-2', C-3'), 140.0 (C-1'), 150.3 (C-2), 171.5, 172.4 (CO). Anal. Calcd for C₁₃H₁₅N₃O₃ × 0.3 H₂O: C, 58.55; H, 5.90; N, 15.76. Found C, 58.80; H 5.86; N, 15.40.

5-Cyclohexylamino-1,5-dimethylbarbituric acid (**3c**): ^1H NMR δ 0.90-1.60 (m, 10H, CH₂), 1.40 (s, 3H, 5-CH₃), 2.28-2.44 (m, 2H, NHCH); 3.09 (s, 3H, 1-CH₃), 11.47 (s, br, 1H, NH); ^{13}C NMR δ 24.7, 25.5, 34.1, 34.1 (CH₂), 26.2 (5-CH₃), 27.8 (1-CH₃), 53.2 (CH), 63.3 (C-5), 150.3 (C-2), 172.2, 173.1 (CO). Anal. Calcd for C₁₂H₁₉N₃O₃: C, 56.90; H, 7.56; N, 16.59. Found C, 56.80; H, 7.82; N, 16.50.

1-Ethyl-5-methyl-5-propylaminobarbituric acid (**3d**): ^1H NMR δ 0.80 (t, J = 7.4 Hz, 3H, CH₂CH₂CH₃), 1.07 (t, J = 7.1 Hz, 3H, NCH₂CH₃), 1.29-1.36 (m, 2H, CH₂CH₂CH₃), 1.40 (s, 3H, 5-CH₃), 2.21 (t, J = 7.1 Hz, 2H, CH₂CH₂CH₃), 3.73 (q, J = 7.1 Hz, 2H, NCH₂CH₃), 11.45 (s, 1H, NH); ^{13}C NMR δ 11.8 (CH₂CH₂CH₃), 13.2 (NCH₂CH₃), 23.0 (CH₂CH₂CH₃), 24.4 (5-CH₃), 36.0 (NCH₂CH₃), 46.3 (CH₂CH₂CH₃), 63.5 (C-5), 149.9 (C-2), 171.6, 172.1 (CO). Anal. Calcd for C₁₀H₁₇N₃O₃ × 0.2 H₂O: C, 52.03; H, 7.60; N, 18.20. Found C, 52.36; H, 7.40; N, 17.77.

1-Ethyl-5-isopropylamino-5-methylbarbituric acid (**3e**): ^1H NMR δ 0.84 (d, J = 6.3 Hz, 3H, CHCH₃), 0.87 (d, J = 6.3 Hz, 3H, CHCH₃), 1.07 (t, J = 7.1 Hz, 3H, CH₂CH₃), 1.40 (s, 3H, 5-CH₃), 2.65-2.73 (m, 1H, CH), 3.74 (q, J = 7.1 Hz, 2H, CH₂CH₃), 11.50 (s, 1H, NH); ^{13}C NMR δ 13.0 (CH₂CH₃), 24.0 (CHCH₃), 26.3 (5-CH₃), 36.0 (CH₂CH₃), 45.5 (CH), 62.5 (C-5), 149.8 (C-2), 172.1, 172.7 (CO). Anal. Calcd for C₁₀H₁₇N₃O₃: C, 52.85; H, 7.54, N, 18.49. Found C, 52.92; H, 7.44; N, 17.99.

5-Benzylamino-1-ethyl-5-methylbarbituric acid (**3f**): ^1H NMR δ 1.05 (t, J = 7.1 Hz, 3H, CH₂CH₃), 1.46 (s, 3H, 5-CH₃); 3.01-3.12 (m, 1H, NHCH₂), 3.43-3.55 (m, 2H, NHCH₂), 3.69 (q, J = 7.1 Hz, 2H, CH₂CH₃), 7.18-7.29 (m, 5H, Ph), 11.47 (s, 1H, NH); ^{13}C NMR δ 13.1 (CH₂CH₃), 24.9 (5-CH₃), 35.9 (CH₂CH₃), 48.3 (NHCH₂), 63.5 (C-5), 126.8 (C-4'), 128.0 (C-2'), 128.1 (C-3'), 139.8 (C-1'), 149.7 (C-2), 171.3, 171.8 (CO). Anal. Calcd for C₁₄H₁₇N₃O₃: C, 61.08; H, 6.22; N, 15.26. Found C, 61.29; H, 6.18; N, 15.32.

5-Cyclohexylamino-1-ethyl-5-methylbarbituric acid (**3g**): ^1H NMR δ 0.90-1.65 (m, 10H, CH₂), 1.06 (t, J = 7.1 Hz, 3H, CH₂CH₃), 1.45 (s, 3H, 5-CH₃), 2.28-2.42 (m, 1H, CH), 3.74 (q, J = 7.1 Hz, 2H, CH₂CH₃); 11.51 (s, 1H, NH); ^{13}C NMR δ 12.9 (5-CH₃), 23.8, 24.6, 25.4, 30.5, 34.0 (CH₂), 26.2 (CH₂CH₃), 35.9 (CH₂CH₃), 53.2 (CH), 61.2 (C-5), 149.8 (C-2), 172.1, 172.7 (CO).

Anal. Calcd for $C_{13}H_{21}N_3O_3 \times 0.8 H_2O$: C, 55.42; H, 8.09; N, 14.91. Found C, 55.25; H, 7.50; N, 15.05.

5-Benzylamino-5-methyl-1-phenylbarbituric acid (**3h**): 1H NMR δ 1.60 (s, 3H, CH_3), 3.17 (s, br, 1H, $NHCH_2$), 3.62 (s, br, 2H, CH_2), 7.21-7.47 (m, 10H, Ph), 11.60 (s, 1H, NH); ^{13}C NMR δ 24.5 (CH_3), 48.4 (CH_2), 64.0 (C-5), 126.9, 128.2, 128.3, 128.5, 128.9, 129.1 (CH-Ph), 135.3, 140.2 (C-Ph), 150.0 (C-2), 171.5, 172.1 (CO). Anal. Calcd for $C_{18}H_{17}N_3O_3 \times 0.2 CH_3CO_2C_2H_5$: C, 66.22; H, 5.50; N, 12.32. Found C, 66.60; H, 5.55; N, 12.04.

5-Cyclohexylamino-5-methyl-1-phenylbarbituric acid (**3i**): 1H NMR δ 0.96-1.70 (m, 10H, CH_2), 1.52 (s, 3H, CH_3), 2.43-2.50 (m, 1H, CH), 7.21-7.26 (m, 2H, 2'-H, 6'-H), 7.40-7.52 (m, 3H, 3'-H, 4'-H, 5'-H), 10.83 (s, br, 1H, NH); ^{13}C NMR δ 24.8, 24.8, 25.5, 34.3, 34.3 (CH_2), 25.6 (CH_3), 53.1 (CH), 62.6 (C-5), 128.6 (C-4'), 129.0, 129.1 (C-2', C-3'), 135.2 (C-1'), 150.0 (C-2), 172.2, 172.9 (CO). Anal. Calcd for $C_{17}H_{21}N_3O_3 \times 0.4 H_2O$: C, 63.30; H, 6.81; N, 13.03. Found C, 63.69; H, 6.70; N, 13.00.

1-Methyl-5-phenyl-5-propylaminobarbituric acid (**3k**): 1H NMR δ 0.85 (t, $J = 7.4$ Hz, 3H, CH_2CH_3), 1.44 (sext., $J = 7.4$ Hz, 2H, CH_2CH_3), 2.34-2.36 (m, 2H, $CH_2CH_2CH_3$), 2.83 (s, br, 1H, $NHCH_2$), 3.17 (s, 3H, 1- CH_3), 7.32-7.42 (m, 5H, Ph), 11.75 (s, 1H, NH); ^{13}C NMR δ 11.8 (CH_2CH_3), 23.2 (CH_2CH_3), 28.0 (1- CH_3), 46.6 ($CH_2CH_2CH_3$), 71.3 (C-5), 126.5, 128.8 (C-2', C-3'), 128.9 (C-4'), 138.3 (C-1'), 150.1 (C-2), 169.7, 171.1 (CO). Anal. Calcd for $C_{14}H_{17}N_3O_3 \times 0.3 H_2O$: C, 59.52; H, 6.35; N, 14.87. Found C, 59.50; H, 5.88; N, 14.69.

5-Benzylamino-1-methyl-5-phenylbarbituric acid (**3l**): 1H NMR δ 3.15 (s, 3H, CH_3), 3.26-3.32 (m, 1H, $NHCH_2$), 3.60-3.69 (m, 2H, CH_2), 7.20-7.49 (m, 10H, Ph), 11.73 (s, 1H, NH); ^{13}C NMR δ 28.1 (CH_3), 48.7 (CH_2), 71.2 (C-5), 126.5, 126.9, 128.2, 128.2, 128.9, 129.0 (CH-Ph), 138.2, 140.3 (C-Ph), 150.2 (C-2), 169.7, 171.0 (CO). Anal. Calcd for $C_{18}H_{17}N_3O_3 \times 0.4 H_2O$: C, 65.40; H, 5.43; N, 12.71. Found C, 65.47; H, 5.27; N, 12.64.

1-Ethyl-5-phenyl-5-propylaminobarbituric acid (**3m**): 1H NMR δ 0.85 (t, $J = 7.3$ Hz, 3H, $CH_2CH_2CH_3$), 1.08 (t, $J = 7.0$ Hz, 3H, NCH_2CH_3), 1.44 (sext., $J = 7.3$ Hz, 2H, $CH_2CH_2CH_3$), 2.32-2.39 (m, 2H, $CH_2CH_2CH_3$), 2.86 (s, br, 1H, $NHCH_2$), 3.73-3.87 (m, 2H, NCH_2CH_3), 7.33-7.42 (m, 5H, Ph), 11.76 (s, 1H, NH); ^{13}C NMR δ 11.8 ($CH_2CH_2CH_3$), 13.1 (NCH_2CH_3), 23.2 ($CH_2CH_2CH_3$), 36.4 (NCH_2CH_3), 46.6 ($CH_2CH_2CH_3$), 71.1 (C-5), 126.3, 128.8 (C-2', C-3'), 128.9 (C-4'), 138.2 (C-1'), 149.7 (C-2), 169.7, 170.6 (CO). Anal. Calcd for $C_{15}H_{19}N_3O_3$: C, 62.27; H, 6.62; N, 14.52. Found C, 61.93; H, 6.24; N, 13.93.

5-Benzylamino-1-ethyl-5-phenylbarbituric acid (**3n**): ^1H NMR δ 1.08 (t, $J = 6.9$ Hz, 3H, CH_3), 3.28-3.35 (m, 1H, NHCH_2), 3.59-3.85 (m, 4H, CH_2), 7.20-7.47 (m, 10H, Ph), 11.78 (s, 1H, NH); ^{13}C NMR δ 13.1 (CH_3), 36.5 (CH_2CH_3), 48.6 (NHCH_2), 71.1 (C-5), 126.4, 127.0, 128.2, 128.3, 129.0, 129.1 (CH-Ph), 138.0, 140.2 (C-Ph), 149.7 (C-2), 169.6, 170.5 (CO). Anal. Calcd for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3 \times 0.1 \text{H}_2\text{O}$: C, 67.28; H, 5.71; N, 12.39. Found C, 67.20; H, 6.19; N, 12.60.

5-Benzylamino-5-phenyl-1-propylbarbituric acid (**3o**): ^1H NMR δ 0.77 (t, $J = 7.4$ Hz, 3H, CH_2CH_3), 1.49 (sext., $J = 7.4$ Hz, 2H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 3.30-3.33 (m, 1H, NHCH_2), 3.59-3.77 (m, 4H, $\text{CH}_2\text{CH}_2\text{CH}_3$, CH_2Ph), 7.21-7.45 (m, 10H, Ph), 11.80 (s, 1H, NH); ^{13}C NMR δ 11.1 (CH_2CH_3), 20.8 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 42.7 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 48.6 (NHCH_2), 71.2 (C-5), 126.4, 126.9, 128.2, 128.2, 128.9, 129.1 (CH-Ph), 138.0, 140.2 (C-Ph), 150.0 (C-2), 169.7, 170.6 (CO). Anal. Calcd for $\text{C}_{20}\text{H}_{21}\text{N}_3\text{O}_3$: C, 68.36; H, 6.02; N, 11.96. Found C, 68.28; H, 5.75; N, 11.67.

1,5-Diphenyl-5-propylaminobarbituric acid (**3p**): ^1H NMR δ 0.87 (t, $J = 7.4$ Hz, 3H, CH_3), 1.42-1.50 (m, 2H, CH_2CH_3), 2.44-2.49 (m, 2H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 2.94 (s, br, 1H, NHCH_2), 7.25-7.54 (m, 10H, Ph), 11.90 (s, 1H, NH); ^{13}C NMR δ 11.8 (CH_3), 23.3 (CH_2CH_3), 46.6 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 71.6 (C-5), 126.6, 128.8, 128.9, 129.0, 129.0, 129.2 (CH-Ph), 134.9, 138.0 (C-Ph), 149.8 (C-2), 169.7, 170.8 (CO). Anal. Calcd for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3$: C, 67.64; H, 5.68; N, 12.46. Found C, 67.83; H, 5.69; N, 12.19.

1,5-Diphenyl-5-isopropylaminobarbituric acid (**3r**): ^1H NMR δ 1.00 (d, $J = 6.3$ Hz, 3H, CH_3), 1.04 (d, $J = 6.3$ Hz, 3H, CH_3), 2.97 (sept., $J = 6.3$ Hz, 1H, CH), 7.25-7.56 (m, 10H, Ph), 11.97 (s, 1H, NH); ^{13}C NMR δ 24.5 (CH_3), 46.0 (CH), 70.9 (C-5), 126.5, 128.8, 128.8, 128.9, 129.0, 129.3 (CH-Ph), 134.8, 138.8 (C-Ph), 149.7 (C-2), 170.1, 171.7 (CO). Anal. Calcd for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3 \times 1.1 \text{H}_2\text{O}$: C, 63.89; H, 5.98; N, 11.76. Found C, 64.16; H, 5.59; N, 11.39.

5-Benzylamino-1,5-diphenylbarbituric acid (**3s**): ^1H NMR δ 3.37-3.40 (t, $J = 7.4$ Hz, 1H, NHCH_2), 3.69-3.79 (m, 2H, CH_2), 7.22-7.61 (m, 15H, Ph), 11.95 (s, 1H, NH); ^{13}C NMR δ 48.7 (CH_2), 71.7 (C-5), 126.6, 126.9, 128.2, 128.8, 128.9, 129.1, 129.2 (CH-Ph), 134.9, 137.8, 140.4 (C-Ph), 149.8 (C-2), 169.6, 170.6 (CO). Anal. Calcd for $\text{C}_{23}\text{H}_{19}\text{N}_3\text{O}_3$: C, 71.67; H, 4.97; N, 10.90. Found C, 71.97; H, 5.04; N, 10.94.

1-Isopropyl-5-methyl-5-methylcarbamoylhydantoin (**4a**): ^1H NMR δ 1.21 (d, $J = 6.9$ Hz, 3H, CHCH_3), 1.29 (d, $J = 6.9$ Hz, 3H, CHCH_3), 1.51 (s, 3H, 5- CH_3), 2.59 (d, $J = 4.5$ Hz, 3H, NHCH_3), 3.44 (sept., $J = 6.9$ Hz, 1H, CH), 7.97 (q, $J = 4.5$ Hz, 1H, NHCH_3), 10.83 (s, 1H, NH); ^{13}C NMR δ 18.9 (5- CH_3), 20.5, 20.8 (CHCH_3), 26.6 (NHCH_3), 45.4 (CH), 69.7 (C-5), 155.1 (C-2),

166.6 ($\underline{\text{CONHCH}_3}$), 173.0 (C-4). Anal. Calcd for $\text{C}_9\text{H}_{15}\text{N}_3\text{O}_3$: C, 50.69; H, 7.09; N, 19.71. Found C, 50.75; H, 7.00; N, 19.38.

1-Benzyl-5-methyl-5-methylcarbamoylhydantoin (**4b**): ^1H NMR δ 1.36 (s, 3H, 5- $\underline{\text{CH}_3}$), 2.49 (d, $J = 4.6$ Hz, 3H, NHCH_3), 4.14 (d, $J = 15.9$ Hz, 1H, $\underline{\text{CH}_2}$), 4.60 (d, $J = 15.9$ Hz, 1H, $\underline{\text{CH}_2}$), 7.23-7.34 (m, 5H, Ph), 7.99 (q, $J = 4.6$ Hz, 1H, NHCH_3), 11.16 (s, 1H, NH); ^{13}C NMR δ 18.8 (5- $\underline{\text{CH}_3}$), 26.7 (NHCH_3), 44.1 ($\underline{\text{CH}_2}$), 69.9 (C-5), 127.5 (C-4'), 128.2, 128.6 (C-2', C-3'), 137.9 (C-1'), 156.9 (C-2), 166.1 ($\underline{\text{CONHCH}_3}$), 173.1 (C-4). Anal. Calcd for $\text{C}_{13}\text{H}_{15}\text{N}_3\text{O}_3$: C, 59.76; H, 5.76; N, 16.08. Found C, 59.85; H, 5.76; N, 15.85.

1-Cyclohexyl-5-methyl-5-methylcarbamoylhydantoin (**4c**): ^1H NMR δ 1.00-1.77 (m, 10H, $\underline{\text{CH}_2}$), 1.53 (s, 3H, 5- $\underline{\text{CH}_3}$), 2.58 (d, $J = 4.6$ Hz, 3H, NHCH_3), 2.70-3.05 (m, 1H, CH), 8.01 (q, $J = 4.6$ Hz, 1H, NHCH_3), 10.87 (s, 1H, NH); ^{13}C NMR δ 19.0 (5- $\underline{\text{CH}_3}$), 25.1, 25.7, 25.8, 30.2, 30.4 ($\underline{\text{CH}_2}$), 26.6 (NHCH_3), 53.4 (CH), 69.7 (C-5), 155.2 (C-2), 166.7 ($\underline{\text{CONHCH}_3}$), 173.0 (C-4). Anal. Calcd for $\text{C}_{12}\text{H}_{19}\text{N}_3\text{O}_3 \times 0.5 \text{H}_2\text{O}$: C, 54.95; H, 7.69; N, 16.02. Found C, 55.04; H, 7.32; N, 15.72.

5-Ethylcarbamoyl-5-methyl-1-propylhydantoin (**4d**): ^1H NMR δ 0.82 (t, $J = 7.4$ Hz, 3H, $\underline{\text{CH}_2\text{CH}_2\text{CH}_3}$), 0.98 (t, $J = 7.3$ Hz, 3H, NHCH_2CH_3), 1.50 (s, 3H, 5- $\underline{\text{CH}_3}$), 1.43-1.50 (m, 2H, $\underline{\text{CH}_2\text{CH}_2\text{CH}_3}$), 2.93-3.19 (m, 4H, NHCH_2 , $\underline{\text{CH}_2\text{CH}_2\text{CH}_3}$), 8.06 (t, $J = 5.4$ Hz, 1H, NHCH_2), 10.91 (s, 1H, NH); ^{13}C NMR δ 11.4 ($\underline{\text{CH}_2\text{CH}_2\text{CH}_3}$), 14.5 (NHCH_2CH_3), 18.4 (5- $\underline{\text{CH}_3}$), 21.8 ($\underline{\text{CH}_2\text{CH}_2\text{CH}_3}$), 34.4 (NHCH_2), 42.3 ($\underline{\text{CH}_2\text{CH}_2\text{CH}_3}$), 69.4 (C-5), 156.4 (C-2), 165.7 ($\underline{\text{CONHCH}_2}$), 173.0 (C-4). Anal. Calcd for $\text{C}_{10}\text{H}_{17}\text{N}_3\text{O}_3 \times 0.1 \text{H}_2\text{O}$: C, 52.43; H, 7.57; N, 18.34. Found C, 52.29; H, 7.48; N, 18.30.

5-Ethylcarbamoyl-1-isopropyl-5-methylhydantoin (**4e**): ^1H NMR δ 0.99 (t, $J = 7.2$ Hz, 3H, $\underline{\text{CH}_2\text{CH}_3}$), 1.22 (d, $J = 6.8$ Hz, 3H, CHCH_3), 1.30 (d, $J = 6.8$ Hz, 3H, CHCH_3), 1.51 (s, 3H, 5- $\underline{\text{CH}_3}$), 3.00-3.16 (m, 2H, $\underline{\text{CH}_2\text{CH}_3}$), 3.44 (sept., $J = 6.8$ Hz, 1H, CHCH_3), 8.04 (t, $J = 5.4$ Hz, 1H, NHCH_2), 10.81 (s, 1H, NH); ^{13}C NMR δ 15.3 ($\underline{\text{CH}_2\text{CH}_3}$), 19.6 (5- $\underline{\text{CH}_3}$), 21.2, 21.6 (CHCH_3), 35.1 ($\underline{\text{CH}_2\text{CH}_3}$), 46.1 (CHCH_3), 70.4 (C-5), 155.9 (C-2), 166.6 ($\underline{\text{CONHCH}_2}$), 173.7 (C-4). Anal. Calcd for $\text{C}_{10}\text{H}_{17}\text{N}_3\text{O}_3$: C, 52.85; H, 7.54; N, 18.49. Found C, 52.87; H, 7.50; N, 18.28.

1-Benzyl-5-ethylcarbamoyl-5-methylhydantoin (**4f**): ^1H NMR δ 0.90 (t, $J = 7.3$ Hz, 3H, $\underline{\text{CH}_2\text{CH}_3}$), 1.33 (s, 3H, 5- $\underline{\text{CH}_3}$), 2.94-3.00 (m, 2H, $\underline{\text{CH}_2\text{CH}_3}$), 4.10 (d, $J = 16.1$ Hz, 1H, $\underline{\text{CH}_2\text{Ph}}$), 4.59 (d, $J = 16.1$ Hz, 1H, $\underline{\text{CH}_2\text{Ph}}$), 7.21-7.32 (m, 5H, Ph), 8.01-8.04 (t, $J = 5.5$ Hz, 1H, NHCH_2), 11.11 (s, br, 1H, NH); ^{13}C NMR δ 14.4 ($\underline{\text{CH}_2\text{CH}_3}$), 18.7 (5- $\underline{\text{CH}_3}$), 34.4 ($\underline{\text{CH}_2\text{CH}_3}$), 43.9 ($\underline{\text{CH}_2\text{Ph}}$), 69.7 (C-

5), 127.3 (C-4'), 128.0, 128.4 (C-2', C-3'), 137.8 (C-1'), 157.0 (C-2), 165.2 (CONHCH₂), 173.1 (C-4). Anal. Calcd for C₁₄H₁₇N₃O₃ × 0.8 H₂O: C, 58.04; H, 6.47; N, 14.50. Found C, 57.93; H, 5.98; N, 14.16.

1-Cyclohexyl-5-ethylcarbamoyl-5-methylhydantoin (**4g**): ¹H NMR δ 0.98 (t, *J* = 7.1 Hz, 3H, CH₂CH₃), 1.03-1.96 (m, 10H, CH₂), 1.50 (s, 3H, 5-CH₃), 2.95-3.20 (m, 3H, CH₂CH₃, CH), 8.09 (t, *J* = 5.5 Hz, 1H, NHCH₂), 10.85 (s, 1H, NH); ¹³C NMR δ 14.5 (CH₂CH₃), 19.0 (5-CH₃), 25.1, 25.7, 25.8, 30.3, 30.5 (CH₂), 34.4 (CH₂CH₃), 53.5 (CH), 69.7 (C-5), 155.2 (C-2), 165.9 (CONHCH₂), 173.0 (C-4). Anal. Calcd for C₁₃H₂₁N₃O₃ × 0.4 H₂O: C, 56.87; H, 8.00; N, 15.31. Found C, 56.91; H, 7.79; N, 14.80.

1-Benzyl-5-methyl-5-phenylcarbamoylhydantoin (**4h**): ¹H NMR δ 1.52 (s, 3H, CH₃), 4.34 (d, *J* = 16.0 Hz, 1H, CH₂Ph), 4.59 (d, *J* = 16.0 Hz, 1H, CH₂Ph), 7.06-7.46 (m, 10H, Ph), 9.64 (s, 1H, NHPh), 11.23 (s, 1H, NH); ¹³C NMR δ 19.0 (CH₃), 44.0 (CH₂Ph), 70.4 (C-5), 121.3, 124.4, 127.3, 128.2, 128.4, 128.5 (CH-Ph), 137.5, 138.0 (C-Ph), 156.8 (C-2), 164.3 (CONHPh), 172.6 (C-4). Anal. Calcd for C₁₈H₁₇N₃O₃ × 0.4 H₂O: C, 65.40; H, 5.43; N, 12.71. Found C, 65.52; H, 5.34; N, 12.77.

1-Cyclohexyl-5-methyl-5-phenylcarbamoylhydantoin (**4i**): ¹H NMR δ 1.01-1.99 (m, 10H, CH₂), 1.64 (s, 3H, CH₃), 3.10-3.17 (m, 1H, CH), 7.07-7.12 (m, 1H, 4'-H), 7.29-7.35 (m, 2H, 3'-H, 5'-H), 7.56-7.61 (m, 2H, 2'-H, 6'-H), 9.81 (s, 1H, NHPh), 10.98 (s, 1H, NH); ¹³C NMR δ 19.7 (CH₃), 25.1, 26.6, 25.8, 30.1, 30.7 (CH₂), 53.6 (CH), 70.5 (C-5), 121.1, 124.4 (C-2', C-3'), 128.7 (C-4'), 138.2 (C-1'), 155.3 (C-2), 165.1 (CONHPh), 172.6 (C-4). Anal. Calcd for C₁₇H₂₁N₃O₃ × 0.5 H₂O: C, 62.95; H, 6.84; N, 12.95. Found C, 62.72; H, 6.81; N, 12.85.

5-Methylcarbamoyl-5-phenyl-1-propylhydantoin (**4k**): ¹H NMR δ 0.62 (t, *J* = 7.4 Hz, 3H, CH₂CH₃), 1.08-1.29 (m, 2H, CH₂CH₃), 2.67 (d, *J* = 4.4 Hz, 3H, NHCH₃), 3.10-3.25 (m, 2H, CH₂CH₂CH₃), 7.22-7.45 (m, 5H, Ph), 7.81 (q, *J* = 4.4 Hz, 1H, NHCH₃), 11.25 (s, 1H, NH); ¹³C NMR δ 11.2 (CH₂CH₃), 21.1 (CH₂CH₃), 26.8 (NHCH₃), 43.5 (CH₂CH₂CH₃), 75.8 (C-5), 127.9, 128.9 (C-2', C-3'), 129.1 (C-4'), 134.8 (C-1'), 156.0 (C-2), 165.6 (CONHCH₃), 171.6 (C-4). Anal. Calcd for C₁₄H₁₇N₃O₃ × 0.2 H₂O: C, 60.29; H, 6.29; N, 15.07. Found C, 60.41; H, 6.08; N, 14.70.

1-Benzyl-5-methylcarbamoyl-5-phenylhydantoin (**4l**): ¹H NMR δ 2.45 (d, *J* = 4.6 Hz, 3H, CH₃), 4.45 (d, *J* = 16.3 Hz, 1H, CH₂), 4.64 (d, *J* = 16.3 Hz, 1H, CH₂), 6.97-7.38 (m, 10H, Ph), 7.77 (q, *J* = 4.6 Hz, 1H, NHCH₃), 11.38 (s, 1H, NH); ¹³C NMR δ 26.5 (CH₃), 44.9 (CH₂), 76.1 (C-5),

126.7, 127.3, 127.9, 128.0, 128.9, 129.0 (CH-Ph), 134.2, 137.4 (C-Ph), 156.5 (C-2), 165.5 (CONHCH₃), 171.5 (C-4). Anal. Calcd for C₁₈H₁₇N₃O₃: C, 66.86; H, 5.30; N, 13.00. Found C, 66.51; H, 5.30; N, 12.76.

5-Ethylcarbamoyl-5-phenyl-1-propylhydantoin (**4m**): ¹H NMR δ 0.63 (t, *J* = 7.4 Hz, 3H, CH₂CH₂CH₃), 1.04 (t, *J* = 7.3 Hz, 3H, NHCH₂CH₃), 1.07-1.31 (m, 2H, CH₂CH₂CH₃), 3.11-3.25 (m, 4H, CH₂CH₂CH₃, NHCH₂), 7.23-7.46 (m, 5H, Ph), 7.86 (t, *J* = 5.7 Hz, 1H, NHCH₂), 11.25 (s, 1H, NH); ¹³C NMR δ 11.2 (CH₂CH₂CH₃), 14.4 (NHCH₂CH₃), 21.2 (CH₂CH₂CH₃), 34.6 (NHCH₂), 43.5 (CH₂CH₂CH₃), 75.8 (C-5), 127.9, 128.9 (C-2', C-3'), 129.0 (C-4'), 134.8 (C-1'), 156.1 (C-2), 164.9 (CONHCH₂), 171.7 (C-4). Anal. Calcd for C₁₅H₁₉N₃O₃: C, 62.27; H, 6.62; N, 14.52. Found C, 61.97; H, 6.61; N, 14.27.

1-Benzyl-5-ethylcarbamoyl-5-phenylhydantoin (**4n**): ¹H NMR δ 0.87 (t, *J* = 7.3 Hz, 3H, CH₃), 2.90-3.03 (m, 2H, CH₂CH₃); 4.48 (d; *J* = 16.2 Hz, 1H, CH₂Ph), 4.61 (d, *J* = 16.2 Hz, 1H, CH₂Ph), 6.97-7.39 (m, 10H, Ph), 7.80 (t, *J* = 5.4 Hz, 1H, NHCH₂), 11.33 (s, br, 1H, NH); ¹³C NMR δ 14.1 (CH₃), 34.5 (CH₂CH₃), 44.9 (CH₂Ph), 76.1 (C-5), 126.7, 127.2, 127.9, 128.0, 128.9, 129.0 (CH-Ph), 134.4, 137.5 (C-Ph), 156.6 (C-2), 164.7 (CONHCH₂), 171.6 (C-4). Anal. Calcd for C₁₉H₁₉N₃O₃ × 0.5 H₂O: C, 65.88; H, 5.82; N, 12.13. Found C, 66.19; H, 5.60; N, 12.00.

1-Benzyl-5-phenyl-5-propylcarbamoylhydantoin (**4o**): ¹H NMR δ 0.75 (t, *J* = 7.4 Hz, 3H, CH₃), 1.29-1.36 (m, 2H, CH₂CH₃), 2.82-2.98 (m, 2H, CH₂CH₂CH₃), 4.50 (d, *J* = 16.2 Hz, 1H, CH₂Ph), 4.59 (d, *J* = 16.2 Hz, 1H, CH₂Ph), 6.96-7.40 (m, 10H, Ph), 7.78 (t, *J* = 5.7 Hz, 1H, NHCH₂), 11.38 (s, 1H, NH); ¹³C NMR δ 11.4 (CH₃), 21.9 (CH₂CH₃), 41.3 (CH₂CH₂CH₃), 44.9 (CH₂Ph), 76.3 (C-5), 126.7, 127.2, 127.9, 128.1, 128.9, 129.0 (CH-Ph), 134.4, 137.5 (C-Ph), 156.5 (C-2), 164.9 (CONHCH₂), 171.6 (C-4). Anal. Calcd for C₂₀H₂₁N₃O₃ × 0.1 CH₃CO₂C₂H₅: C, 68.02; H, 6.10; N, 11.67. Found C, 68.57; H, 5.96; N, 11.30.

5-Phenyl-5-phenylcarbamoyl-1-propylhydantoin (**4p**): ¹H NMR δ 0.63 (t, *J* = 7.4 Hz, 3H, CH₃), 1.12-1.19 (m, 1H, CH₂CH₃), 1.25-1.34 (m, 1H, CH₂CH₃), 3.21-3.35 (m, 2H, CH₂CH₂CH₃), 7.11-7.60 (m, 10H, Ph), 9.69 (s, 1H, NHPh), 11.38 (s, 1H, NH); ¹³C NMR δ 11.2 (CH₃), 21.2 (CH₂CH₃), 43.4 (CH₂CH₂CH₃), 76.7 (C-5), 121.4, 124.8, 128.0, 128.7, 129.1, 129.2 (CH-Ph), 134.5, 137.8 (C-Ph), 156.1 (C-2), 164.2 (CONHPh), 171.3 (C-4). Anal. Calcd for C₁₉H₁₉N₃O₃: C, 67.64; H, 5.68; N, 12.45. Found C, 67.30; H, 5.65; N, 12.36.

1-Isopropyl-5-phenyl-5-phenylcarbamoylhydantoin (**4r**): ¹H NMR δ 0.91, (d, *J* = 6.9 Hz, 3H, CH₃), 1.41 (d, *J* = 6.9 Hz, 3H, CH₃), 3.50 (sept., *J* = 6.9 Hz, 1H, CH), 7.11-7.62 (m, 10H, Ph),

9.54 (s, 1H, NHPh), 11.37 (s, 1H, NH); ^{13}C NMR δ 20.0 (CH_3), 20.3 (CH_3), 46.8 (CH), 77.3 (C-5), 121.2, 124.7, 128.2, 128.8, 129.1, 129.4 (CH-Ph), 134.8, 137.7 (C-Ph), 154.8 (C-2), 163.9 (CONHPh), 171.7 (C-4). Anal. Calcd for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3 \times 0.5 \text{H}_2\text{O}$: C, 65.88; H, 5.82; N, 12.13. Found C, 65.91; H, 5.59; N, 11.96.

1-Benzyl-5-phenyl-5-phenylcarbamoylhydantoin (**4s**): ^1H NMR δ 4.39 (d, $J = 16.0$ Hz, 1H, CH_2), 4.56 (d, $J = 16.0$ Hz, 1H, CH_2), 7.02-7.46 (m, 15H, Ph), 10.21 (s, 1H, NH). One NH signal did not appear. ^{13}C NMR δ 45.3 (CH_2), 76.3 (C-5), 120.3, 124.2, 125.1, 127.4, 127.6, 127.6, 128.3, 128.8, 128.8 (CH-Ph), 136.9, 137.8, 139.3 (C-Ph), 165.6 (CONHPh). Two carbonyl signals did not appear. Anal. Calcd for $\text{C}_{23}\text{H}_{19}\text{N}_3\text{O}_3 \times 1.1 \text{H}_2\text{O}$: C, 68.17; H, 5.27; N, 10.37. Found C, 67.91; H, 5.01; N, 9.99.

1-Benzyl-3,5-dimethyl-5-ethylcarbamoylhydantoin (**5a**): ^1H NMR δ 0.88 (t, $J = 7.2$ Hz, 3H, CH_2CH_3), 1.37 (s, 3H, 5- CH_3), 2.91 (s, 3H, 3- CH_3), 2.92-2.98 (m, 2H, CH_2CH_3), 4.22 (d, $J = 16.1$ Hz, 1H, CH_2Ph), 4.59 (d, $J = 16.1$ Hz, 1H, CH_2Ph), 7.21-7.31 (m, 5H, Ph), 7.98 (t, $J = 5.4$ Hz, 1H, NH); ^{13}C NMR δ 14.3 (CH_2CH_3), 18.5 (5- CH_3), 25.2 (3- CH_3), 34.4 (CH_2CH_3), 44.2 (CH_2Ph), 68.6 (C-5), 127.4, 128.0, 128.3 (CH-Ph), 137.4 (C-1'), 156.5 (C-2), 164.9 (CONH), 171.7 (C-4). Anal. Calcd for $\text{C}_{15}\text{H}_{18}\text{N}_3\text{O}_3$: C, 62.27; H, 6.62; N, 14.52. Found C, 61.98; H, 6.72; N 14.16.

1-Cyclohexyl-3,5-dimethyl-5-phenylcarbamoylhydantoin (**5b**): ^1H NMR δ 1.03-2.03 (m, 10H, CH_2), 1.64 (s, 3H, 5- CH_3), 2.88 (s, 3H, 3- CH_3), 3.13-3.20 (m, 1H, CH), 7.08-7.13 (m, 1H, 4'-H), 7.29-7.35 (m, 2H, 3'-H, 5'-H), 7.51-7.57 (m, 2H, 2'-H, 6'-H), 9.76 (s, 1H, NH); ^{13}C NMR δ 19.5 (5- CH_3), 25.0 (3- CH_3), 25.1, 25.5, 25.6, 30.3, 30.7 (CH_2), 53.9 (CH), 69.4 (C-5), 121.2, 128.8 (C-2', C-3'), 121.5 (C-4'), 138.1 (C-1'), 154.9 (C-2), 164.8 (CONH), 171.3 (C-4). Anal. Calcd for $\text{C}_{18}\text{H}_{23}\text{N}_3\text{O}_3 \times 0.3 \text{H}_2\text{O}$: C, 64.57; H, 7.11; N, 12.55. Found C, 64.37; H, 7.04; N, 12.43.

1-Benzyl-3-methyl-5-methylcarbamoyl-5-phenylhydantoin (**5c**): ^1H NMR δ 2.45 (d, $J = 4.6$ Hz, 3H, NHCH_3), 2.98 (s, 3H, 3- CH_3), 4.49 (d, $J = 16.1$ Hz, 1H, CH_2), 4.72 (d, $J = 16.1$ Hz, 1H, CH_2), 6.99-7.40 (m, 10H, Ph), 7.88 (q, $J = 4.6$ Hz, 1H, NH); ^{13}C NMR δ 25.6 (3- CH_3), 26.7 (NHCH_3), 45.4 (CH_2), 75.3 (C-5), 127.1, 127.7, 128.1, 128.4, 129.1, 129.3 (CH-Ph), 134.2, 137.3 (C-Ph), 156.4 (C-2), 165.4 (CONH), 170.5 (C-4). Anal. Calcd for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3 \times 0.5 \text{H}_2\text{O}$: C, 65.88; H, 5.82; N, 12.13. Found C, 65.95; H, 5.58; N, 11.98.

5-Ethylcarbamoyl-3-methyl-5-phenyl-1-propylhydantoin (**5d**): ^1H NMR δ 0.64 (t, $J = 7.4$ Hz, 3H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 1.05 (t, $J = 7.3$ Hz, 3H, NHCH_2CH_3), 1.09-1.36 (m, 2H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 2.94 (s, 3H, 3- CH_3) 3.14-3.31 (m, 4H, $\text{CH}_2\text{CH}_2\text{CH}_3$, NHCH_2), 7.25-7.45 (m, 5H, Ph), 7.92 (t, $J =$

5.7 Hz, 1H, NH); ^{13}C NMR δ 11.1 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 14.4 (NHCH_2CH_3), 21.1 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 25.2 (3- CH_3), 34.7 (NHCH_2), 43.9 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 74.8 (C-5), 128.1, 128.9 (C-2', C-3'), 129.1 (C-4'), 134.5 (C-1'), 155.7 (C-2), 164.6 (CONH), 170.4 (C-4). Anal. Calcd for $\text{C}_{16}\text{H}_{21}\text{N}_3\text{O}_3$: C, 63.35; H, 6.98; N, 13.85. Found C, 63.05; H, 6.95; N, 13.33.

3-Ethyl-5-ethylcarbamoyl-5-phenyl-1-propylhydantoin (**5e**): ^1H NMR δ 0.63 (t, $J = 7.4$ Hz, 3H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 1.03 (t, $J = 7.3$ Hz, 3H, NHCH_2CH_3), 1.10 (t, $J = 7.3$ Hz, 3H, NCH_2CH_3), 1.10-1.34 (m, 2H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 3.14-3.27 (m, 4H, $\text{CH}_2\text{CH}_2\text{CH}_3$, NHCH_2), 3.45-3.51 (m, 2H, NCH_2), 7.22-7.46 (m, 5H, Ph), 7.90 (t, $J = 5.7$ Hz, 1H, NHCH_2); ^{13}C NMR δ 11.1 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 13.2 (NCH_2CH_3), 14.4 (NHCH_2CH_3), 21.1 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 33.9 (NCH_2CH_3), 34.6 (NHCH_2CH_3), 43.8 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 74.7 (C-5), 128.0, 129.0 (C-2', C-3'), 129.2 (C-4'), 134.5 (C-1'), 155.4 (C-2), 164.6 (CONH), 170.1 (C-4). Anal. Calcd for $\text{C}_{17}\text{H}_{23}\text{N}_3\text{O}_3 \times 0.1 \text{ C}_6\text{H}_{14}$: C, 64.84; H, 7.54; N, 12.89. Found C, 64.76; H, 7.39; N, 12.62.

3-Methyl-5-phenyl-5-phenylcarbamoyl-1-propylhydantoin (**5f**): ^1H NMR δ 0.67 (t, $J = 7.4$ Hz, 3H, CH_2CH_3), 1.16-1.19 (m, 1H, CH_2CH_3), 1.25-1.33 (m, 1H, CH_2CH_3), 3.00 (s, 3H, 3- CH_3), 3.27-3.31 (m, 1H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 3.38-3.44 (m, 1H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 7.14-7.62 (m, 10H, Ph), 9.75 (s, 1H, NH); ^{13}C NMR δ 11.2 (CH_2CH_3), 21.2 (CH_2CH_3), 25.4 (3- CH_3), 43.8 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 75.6 (C-5), 121.3, 124.8, 128.2, 128.8, 129.0, 129.3 (CH-Ph), 134.2, 137.8 (C-Ph), 155.8 (C-2), 163.9 (CONH), 170.1 (C-4). Anal. Calcd for $\text{C}_{20}\text{H}_{21}\text{N}_3\text{O}_3 \times 0.5 \text{ H}_2\text{O}$: C, 66.65; H, 6.15; N, 11.66. Found C, 66.62; H, 5.92; N, 11.59.

3-Ethyl-5-phenyl-5-phenylcarbamoyl-1-propylhydantoin (**5g**): ^1H NMR δ 0.63 (t, $J = 7.3$ Hz, 3H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 1.12 (t, $J = 7.3$ Hz, 3H, NCH_2CH_3), 1.08-1.19 (m, 1H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 1.24-1.33 (m, 1H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 3.27-3.39 (m, 2H, $\text{CH}_2\text{CH}_2\text{CH}_3$), 3.48-3.57 (m, 2H, NCH_2CH_3), 7.11-7.60 (m, 10H, Ph), 9.75 (s, 1H, NH); ^{13}C NMR δ 11.2 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 13.2 (NCH_2CH_3), 21.2 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 34.1 (NCH_2CH_3), 43.7 ($\text{CH}_2\text{CH}_2\text{CH}_3$), 75.5 (C-5), 121.4, 124.8, 128.1, 128.8, 129.2, 129.4 (CH-Ph), 134.2, 137.8 (C-Ph), 155.4 (C-2), 163.9 (CONH), 169.8 (C-4). Anal. Calcd for $\text{C}_{21}\text{H}_{23}\text{N}_3\text{O}_3 \times 0.1 \text{ H}_2\text{O}$: C, 68.68; H, 6.37; N, 11.44. Found C, 68.57; H, 6.34; N, 11.40.

1-Benzyl-3-methyl-5-phenyl-5-phenylcarbamoylhydantoin (**5h**): ^1H NMR δ 3.02 (s, 3H, CH_3), 4.59 (d, $J = 16.2$ Hz, 1H, CH_2), 4.77 (d, $J = 16.2$ Hz, 1H, CH_2), 6.95-7.12 (m, 6H, Ph), 7.22-7.45 (m, 9H, Ph), 9.65 (s, 1H, NH); ^{13}C NMR δ 25.4 (CH_3), 45.1 (CH_2), 75.7 (C-5), 121.3, 124.6, 126.7, 127.3, 127.8, 128.2, 128.4, 128.8, 129.1 (CH-Ph), 133.7, 136.9, 137.4 (C-Ph), 156.0 (C-2),

163.4 (CONH), 169.9 (C-4). Anal. Calcd for $C_{24}H_{21}N_3O_3 \times 0.5 H_2O$: C, 70.57; H, 5.43; N, 10.28. Found C, 70.91; H, 5.24; N, 10.37.

5-Bromo-1,3-dimethyl-5-phenylbarbituric acid (**7**): 1H NMR ($CDCl_3$) δ 3.39 (s, 6H, CH_3), 7.36-7.50 (m, 5H, Ph); ^{13}C NMR ($CDCl_3$) δ 30.0 (CH_3), 57.0 (C-5), 128.1, 128.8, 129.8 (CH-Ph), 133.4 (C-Ph), 149.8 (C-2), 165.8 (CO).

5-Benzylamino-1,3-dimethyl-5-phenylbarbituric acid (**8**): 1H NMR δ 3.18 (s, 6H, CH_3), 3.39 (t, $J = 7.3$ Hz, 1H, NH), 3.64 (d, $J = 7.3$ Hz, 2H, CH_2), 7.20-7.46 (m, 10H, Ph); ^{13}C NMR δ 29.0 (CH_3), 48.7 (CH_2), 71.2 (C-5), 126.6, 126.9, 128.2, 128.3, 128.9, 129.0 (CH-Ph), 138.2, 140.2 (C-Ph), 150.7 (C-2), 169.7 (CO). Anal. Calcd for $C_{19}H_{19}N_3O_3$: C, 67.65; H, 5.67; N, 12.56. Found C, 67.25; H, 5.63; N, 12.28.

1-Benzyl-3-methyl-5-phenylhydantoin (**9**): 1H NMR δ 2.95 (s, 3H, CH_3), 3.90 (d, $J = 15.8$ Hz, 1H, CH_2), 4.78 (d, $J = 15.8$ Hz, 1H, CH_2), 4.98 (s, 1H, CH), 7.10-7.40 (m, 10H, Ph); ^{13}C NMR δ 25.0 (CH_3), 44.6 (CH_2), 63.6 (C-5), 127.6, 127.9, 128.1, 128.6, 129.0, 129.0 (CH-Ph), 133.5, 136.2 (C-Ph), 156.6 (C-2), 171.4 (C-4). Anal. Calcd for $C_{17}H_{16}N_2O_2 \times H_2O$: C, 68.44; H, 6.08; N, 9.39. Found C, 68.50; H, 5.58; N, 9.46.

5-Bromo-1,5-dimethylbarbituric acid (2a)

2. ^1H NMR spectra and ^{13}C NMR spectra

5-Bromo-1-ethyl-5-methylbarbituric acid (2b)

S14

5-Bromo-1-ethyl-5-methylbarbituric acid (2b)

5-Bromo-5-methyl-1-phenylbarbituric acid (2c)

5-Bromo-1-methyl-5-phenylbarbituric acid (2d)

5-Bromo-1-ethyl-5-phenylbarbituric acid (2e)

S20

5-Bromo-1-propyl-5-phenylbarbituric acid (2f)

S22

5-Bromo-1,5-diphenylbarbituric acid (2g)

S24

1,5-Dimethyl-5-isopropylaminobarbituric acid (3a)

S26

1,5-Dimethyl-5-isopropylaminoobarbituric acid (3a)

S27

5-Benzylamino-1,5-dimethylbarbituric acid (3b)

5-Cyclohexylamino-1,5-dimethylbarbituric acid (3c)

1-Ethyl-5-methyl-5-propylaminobarbituric acid (3d)

1-Ethyl-5-methyl-5-propylaminobarbituric acid (3d)

1-Ethyl-5-isopropylamino-5-methylbarbituric acid (3e)

1-Ethyl-5-isopropylamino-5-methylbarbituric acid (3e)

5-Benzylamino-1-ethyl-5-methylbarbituric acid (3f)

5-Cyclohexylamino-1-ethyl-5-methylbarbituric acid (3g)

5-Cyclohexylamino-1-ethyl-5-methylbarbituric acid (3g)

5-Benzylamino-5-methyl-1-phenylbarbituric acid (3h)

S40