Supporting Information

The Vilsmeier reagent: an efficient reagent for the transformation of 2-aminobenzamides into quinazolin-4(3*H*)-one derivatives

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3-Butylquinazolin-4(3H)-one (5a). Yield: 80%, yellow crystals. Mp 72-74 °C (70-72 °C)^[15a]; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.42 (s, 1H, H₂), 8.16 (dd, *J* = 8.0, 1.5 Hz, 1H, H₅), 7.81 (dt, *J* = 8.0, 1.5 Hz, 1H, H₇), 7.68 (d, *J* = 8.0 Hz, 1H, H₈), 7.54 (t, *J* = 8.0 Hz, 1H, H₆), 3.98 (t, *J* = 7.4 Hz, NCH₂CH₂CH₂CH₃), 1.68 (quintet, *J* = 7.4 Hz, NCH₂CH₂CH₂CH₃), 1.31 (sextet, *J* = 7.4 Hz, NCH₂CH₂CH₂CH₃), 0.91 (t, *J* = 7.4 Hz, NCH₂CH₂CH₂CH₃); Anal. Calcd for C₁₂H₁₄N₂O: C, 71.26; H, 6.98; N, 13.85; Found: C, 71.51; H, 7.14; N, 13.98.

3-Isopropylquinazolin-4(3H)-one (5b). Yield: 80%, yellow crystals. Mp 85-87 °C (87-88 °C)^[15f]; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.49 (s, 1H, H₂), 8.15 (d, *J* = 7.5 Hz, 1H, H₅), 7.81 (t, *J* = 7.5 Hz, 1H, H₇), 7.68 (d, *J* = 7.5 Hz, 1H, H₈), 7.54 (t, *J* = 7.5 Hz, 1H, H₆), 5.00 (m, 1H, NCH(CH₃)₂), 1.43 (d, *J* = 6.0 Hz, 6H, NCH(CH₃)₂); ¹³C NMR (DMSO-*d*₆, 125 MHz): δ_C = 159.6, 147.2, 145.3, 134.2, 126.9, 126.8, 126.2, 121.3, 46.1, 21.1; Anal. Calcd for C₁₁H₁₂N₂O: C, 70.19; H, 6.43; N, 14.88; Found: C, 69.92; H, 6.67; N, 14.65.

3-Allylquinazolin-4(3H)-one (5c). Yield: 75%, yellow crystals. Mp 68-70 °C (65 °C)^[15e]; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.67 (s, 1H, H₂), 8.15 (d, *J* = 8.0 Hz, 1H, H₅), 7.81 (t, *J* = 8.0 Hz, 1H, H₇), 7.68 (d, *J* = 8.0 Hz, 1H, H₈), 7.54 (t, *J* = 8.0 Hz, 1H, H₆), 6.01 (ddt, *J* = 17.1, 10.4, 5.4 Hz, 1H, CH), 5.22 (dd, *J* = 10.4, 1.2 Hz, 1H, CH), 5.19 (dd, *J* = 17.1, 1.2 Hz, 1H, CH), 4.65 (d, *J* = 5.4 Hz, 2H, NCH₂); ¹³C NMR (DMSO-*d*₆, 125 MHz): δ_C = 159.5, 148.5, 145.7, 134.8, 132.7, 127.6, 126.3, 125.7, 121.2, 117.9, 48.1; Anal. Calcd for C₁₁H₁₀N₂O: C, 70.95; H, 5.41; N, 15.04; Found: C, 71.17; H, 5.74; N, 14.82.

3-Phenylquinazolin-4(3H)-one (5d). Yield: 65%, yellow crystals. Mp 145-147 °C (141-142 °C)^[15a]; 8.36 (s, 1H, H₂), 8.21 (d, *J* = 8.0 Hz, 1H, H₅), 7.89 (t, *J* = 8.0 Hz, 1H, H₇), 7.75 (d, *J* = 8.0 Hz, 1H, H₈), 7.62 (m, 6H, H₆, Ph); Anal. Calcd for C₁₄H₁₀N₂O: C, 75.66; H, 4.54; N, 12.60; Found: C, 75.32; H, 4.71; N, 12.86.

3-Benzylquinazolin-4(3H)-one (5e). Yield: 82%, yellow crystals. Mp 155-156 °C (154-155 °C)^{15h}; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.60 (s, 1H, H₂), 8.16 (d, *J* = 8.0 Hz, 1H, H₅), 7.85 (t, *J* = 8.0 Hz, 1H, H₇), 7.71 (d, *J* = 8.0 Hz, 1H, H₈), 7.57 (t, *J* = 8.0 Hz, 1H, H₆), 7.38-7.28 (m, 5H, Ph), 5.21 (s, 2H, NCH₂); Anal. Calcd for C₁₅H₁₂N₂O: C, 76.25; H, 5.12; N, 11.86; Found: C, 76.42; H, 5.39; N, 11.61.

3-(2-Chlorobenzyl)quinazolin-4(3H)-one (5f). Yield: 75%, yellow crystals. Mp 117-119 °C (116 °C)^{15c}; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.50 (s, 1H, H₂), 8.13 (d, *J* = 7.5 Hz, 1H, H₅), 7.85 (t, *J* = 7.5 Hz, 1H, H₇), 7.71 (d, *J* = 7.5 Hz, 1H, H₈), 7.56-7.47 (m, 2H, H₆, H_{3'}), 7.31-7.27 (m, 2H, H_{4'}, H_{5'}), 7.07 (d, *J* = 7.9 Hz, 1H, H_{6'}), 5.25 (s, 2H, NCH₂); Anal. Calcd for C₁₅H₁₁ClN₂O: C, 66.55; H, 4.10; N, 10.35; Found: C, 66.27; H, 4.32; N, 10.59.

3-(4-Methoxybenzyl)quinazolin-4(3H)-one (5g). Yield: 80%, yellow crystals. Mp 137-138 °C (134-135 °C)^{15a}; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.59 (s, 1H, H₂), 8.16 (d, *J* = 7.7 Hz, 1H, H₅), 7.84 (t, *J* = 7.7 Hz, 1H, H₇), 7.70 (d, *J* = 7.7 Hz, 1H, H₈), 7.56 (t, *J* = 7.7 Hz, 1H, H₆), 7.36 (d, *J* = 8.0 Hz, 2H, H_{2'}, H_{6'}), 6.91 (d, *J* = 8.0 Hz, 2H, H_{3'}, H_{5'}), 5.13 (s, 2H, NCH₂), 3.72 (s, 3H, OCH₃); Anal. Calcd for C₁₆H₁₄N₂O₂: C, 72.16; H, 5.30; N, 10.52; Found: C, 71.97; H, 5.61; N, 10.32.

4-((4-Qxoquinazolin-3(4H)-yl)methyl)benzoic acid (5h). Yield: 75%, white crystals. Mp 269-270 °C; IR (KBr): 3300-2500, 1720, 1690, 1655, 1598 Cm⁻¹. ¹H NMR (DMSO-*d*₆, 400 MHz): δ_H = 12.90 (bs, 1H, OH), 8.60 (s, 1H, H₂), 8.15 (d, *J* = 7.5 Hz, 1H, H₅), 7.91 (d, *J* = 8.0 Hz, 2H, H_{3'}, H_{5'}), 7.85 (t, *J* = 7.5 Hz, 1H, H₇), 7.71 (d, *J* = 7.5 Hz, 1H, H₈), 7.56 (t, *J* = 7.5 Hz, 1H, H₆), 7.45 (d, *J* = 8.0 Hz, 2H, H_{2'}, H_{6'}), 5.28 (s, 2H, NCH₂); ¹³C NMR (DMSO-*d*₆, 100 MHz): δ_C = 167.5, 160.6, 148.5, 148.4, 142.2, 135.0, 130.5, 130.1, 128.0, 127.8, 127.7, 126.6, 122.1, 49.2; MS: *m/z* (%) = 280 (100) [M]⁺, 135 (65), 107 (45), 77 (38), 51 (12); Anal. Calcd for C₁₆H₁₂N₂O₃: C, 68.56; H, 4.32; N, 9.99; Found: C, 68.39; H, 4.57; N, 10.15.

3-(3,4-Dimethoxyphenethyl)quinazolin-4(3H)-one (5i). Yield: 80%, yellow crystals. Mp 109-110 °C (107-109 °C)^{15g}; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.18 (dd, *J* = 8.0, 1.0 Hz, 1H, H₅), 8.13 (s, 1H, H₂), 7.82 (dt, *J* = 8.0, 1.0 Hz, 1H, H₇), 7.64 (d, *J* = 8.0 Hz, 1H, H₈), 7.55 (t, *J* = 8.0 Hz, 1H, H₆), 6.83 (d, *J* = 8.1 Hz, 1H, H₅'), 6.80 (d, *J* = 1.6 Hz, 1H, H₂'), 6.68 (dd, *J* = 8.1, 1.6 Hz, 1H, H₆'), 4.20 (t, *J* = 7.3 Hz, NCH₂CH₂), 3.70 (s, 3H, OCH₃), 3.65 (s, 3H, OCH₃), 2.97 (t, *J* = 7.3 Hz, NCH₂CH₂); Anal. Calcd for C₁₈H₁₈N₂O₃: C, 69.66; H, 5.85; N, 9.03; Found: C, 69.85; H, 5.97; N, 8.81.

3-(2-Methoxyphenethyl)quinazolin-4(3H)-one (5j). Yield: 77%, yellow crystals. Mp 120-122 °C; ¹H NMR (DMSO-*d*₆, 500 MHz): δ_H = 8.18 (d, *J* = 7.5 Hz, 1H, H₅), 8.00 (s, 1H, H₂), 7.82 (t, *J* = 7.5 Hz, 1H, H₇), 7.64 (d, *J* = 7.5 Hz, 1H, H₈), 7.57 (t, *J* = 7.5 Hz, 1H, H₆), 7.21 (t, *J* = 7.2 Hz, 1H, H₄'), 7.09 (d, *J* = 7.2 Hz, 1H, H₆'), 6.90 (d, *J* = 7.2 Hz, 1H, H₃'), 6.84 (t, *J* = 7.2 Hz, 1H, H₅'), 4.19 (t, *J* = 6.6 Hz, 2H, NCH₂CH₂), 3.54 (s, 3H, OCH₃), 3.00 (t, *J* = 6.6 Hz, 2H, NCH₂CH₂); ¹³C NMR (DMSO-*d*₆, 125 MHz): δ_C = 160.0, 157.3, 148.1, 146.7, 134.5, 130.5, 129.9, 128.3, 127.2, 126.2, 125.6, 121.3, 120.4, 110.6, 55.0, 46.6, 28.9; Anal. Calcd for C₁₇H₁₆N₂O₂: C, 72.84; H, 5.75; N, 9.99; Found: C, 73.02; H, 5.50; N, 10.18.

3-Butylquinazolin-4(3*H*)-one **5a**

3-Isopropylquinazolin-4(3*H*)-one **5b**

(Integrals should be divided by 2)

3-Benzylquinazolin-4(3*H*)-one **5e**

3-(2-Chlorobenzyl)quinazolin-4(3*H*)-one **5f**

(Integrals should be divided by 2)

3-(4-Methoxybenzyl)quinazolin-4(3H)-one **5g**

4-((4-Oxoquinazolin-3(4H)-yl)methyl)benzoic acid **5h**

3-(3,4-Dimethoxyphenethyl)quinazolin-4(3H)-one **5i**

3-(2-Methoxyphenethyl)quinazolin-4(3*H*)-one **5j**

(Integrals should be divided by 3)