Electronic supplementary materials

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Synthesis of 3,4-dihydro-4-oxo-benzofuro[3,2-*d*]pyrimidine-2-carboxylate and its derivatives

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Experimental

`Amines used in the work:

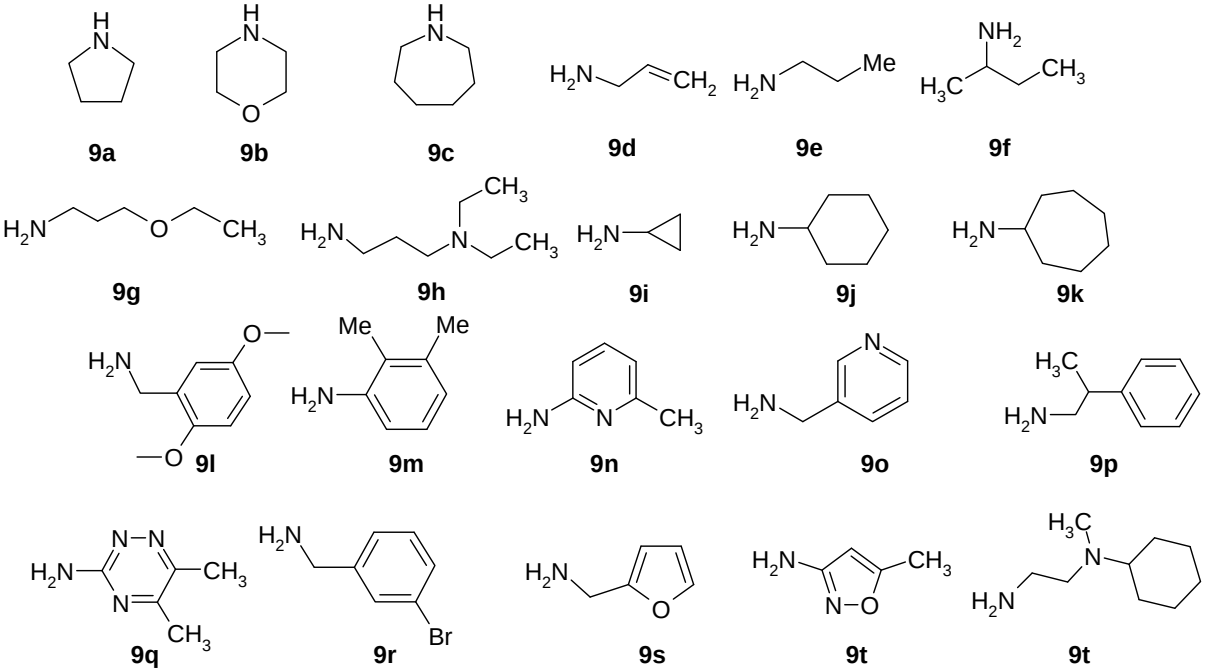
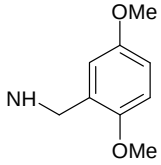
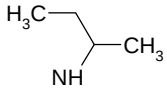
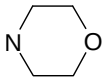
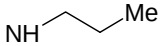
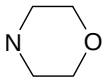
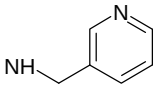
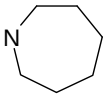
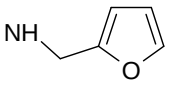
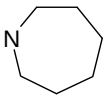
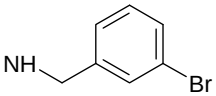


Table 1. Structures and yields of representative compounds from combinatorial libraries **11a-t**, **12a-t** and **13a-t**

Compound	NR^1R^2	NR^3R^4	yield
11l			76%
11f			68%
12e			61%
12o			70%
13s			57%
13r			84%

***N*-(2,5-Dimethoxybenzyl)-4-(1-pyrrolidinyl)-benzofuro[3,2-*d*]pyrimidine-2-carboxamide 11l**. This compound was obtained in 76% yield; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 8.95 (t, *J* = 8.0 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.71 (t, *J* = 8.5 Hz, 1H), 7.52 (t, *J* = 8.5 Hz, 1H), 6.94 (d, *J* = 9.0 Hz, 1H), 6.87-6.77 (m, 2H), 4.47 (d, *J* = 7.0 Hz, 2H), 3.98-3.88 (m, 4H), 3.82 (s, 3H), 3.67 (s, 3H), 2.08-1.98 (m, 4H); Anal. Calcd. for $C_{24}H_{24}N_4O_4$: C, 66.65; H, 5.59; N, 12.96. Found: C, 66.69; H, 5.54; N, 13.01.

***N*-(*Sec*-butyl)-4-pyrrolidin-1-yl-benzofuro[3,2-*d*]pyrimidine-2-carboxamide 11f**. This compound was obtained in 68% yield; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 8.15 (d, *J* = 7.9 Hz, 1H, NH), 7.99 (d, *J* = 7.5 Hz, 1H, Ar-H), 7.76-7.63 (m, 2H, Ar-H), 7.50 (t, *J* = 7.5 Hz, 1H, Ar-H), 4.03-3.88 (m, 5H), 2.12-2.04 (m, 4H, $(CH_2)_2$), 1.60 (qd, *J* = 7.4 Hz, *J* = 2.8 Hz, 2H, Me-**CH_2**-CH), 1.23 (d, *J* = 6.7 Hz, 3H, CH_3), 0.96 (t, *J* = 7.4 Hz, 3H, CH_3); Anal. Calcd. for $C_{19}H_{22}N_4O_2$: C, 67.44; H, 6.55; N, 16.56. Found: C, 67.41; H, 6.58; N, 16.52.

4-(4-Morpholinyl)-*N*-propyl-benzofuro[3,2-*d*]pyrimidine-2-carboxamide 12e. This compound was obtained in 61% yield; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 8.60 (t, *J* = 6.2 Hz, 1H), 8.16 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 7.9 Hz, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 4.15-4.10 (m, 4H), 3.84-3.79 (m, 4H), 3.26 (q, *J* = 6.9 Hz, 2H), 1.59 (q, *J* = 6.7 Hz, 2H), 0.94 (t, *J* = 7.1 Hz, 3H); Anal. Calcd. for $C_{18}H_{20}N_4O_3$: C, 63.52; H, 5.92; N, 16.46. Found: C, 63.55; H, 5.96; N, 16.41.

***N*-(2-Furylmethyl)-4-hexahydro-1*H*-azepin-1-yl-benzofuro[3,2-*d*]pyrimidine-2-carboxamide 13s.** This compound was obtained in 57% yield; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 8.99 (t, *J* = 6.1 Hz, 1H, NH), 8.14 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.83 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.72 (t, *J* = 7.7 Hz, 1H, Ar-H), 7.59 (d, *J* = 1.5 Hz, 1H, Ar-H), 7.53 (t, *J* = 7.7 Hz, 1H, Ar-H), 6.42 (dd, *J* = 3.1 Hz, *J* = 1.5 Hz, 1H, Ar-H), 6.29 (d, *J* = 3.1 Hz, 1H, Ar-H), 4.51 (d, *J* = 7.3 Hz, 2H, CH_2), 4.12-3.98 (m, 4H, $N(CH_2)_2$), 1.95-1.86 (m, 4H, $(CH_2)_2$), 1.61-1.48 (m, 4H, $(CH_2)_2$); Anal. Calcd. for $C_{22}H_{22}N_4O_3$: C, 67.68; H, 5.68; N, 14.35. Found: C, 67.65; H, 5.63; N, 14.39.

***N*-(3-Bromobenzyl)-4-hexahydro-1*H*-azepin-1-yl-benzofuro[3,2-*d*]pyrimidine-2-carboxamide 13r.** This compound was obtained in 84% yield; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 9.21 (t, *J* = 6.4 Hz, 1H), 8.14 (d, *J* = 7.7 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.56 (s, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 7.7 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 4.52 (d, *J* = 6.4 Hz, 2H), 4.15-4.01 (m, 4H), 1.95-1.84 (m, 4H), 1.62-1.49 (m, 4H); Anal. Calcd. for $C_{24}H_{23}BrN_4O_2$: C, 60.13; H, 4.84; N, 16.67. Found: C, 65.17; H, 5.61; N, 12.81.