Supporting Information

for

Chan–Evans–Lam N1-(het)arylation and N1-alkenylation of 4-fluoroalkylpyrimidin-2(1H)-ones

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1. General methods

All chemicals (including starting pyrimidin-2(1H)-ones 1a–c,e–h, boronic acids 2a–w, boronic acid pinacol esters 6a–d and 7a–h) were obtained from Enamine Ltd. and used without further purification. All solvents were purified by standard methods. Melting points are uncorrected. $^{19}$F NMR, $^1$H NMR and $^{13}$C NMR spectra were recorded on a Varian VXR-300, Varian Mercury-400 or Bruker Avance DRX-500 spectrometers with TMS or CCl$_3$F as an internal standard. Multiplets were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), q (quartet), m (multiplet) and br s (broad singlet). LC-MS spectra were recorded on an Agilent 1100 Series high performance liquid chromatograph equipped with a diode matrix with an Agilent LC/MSD SL mass selective detector. Mass spectrometric detections of samples were performed with an Infinity 1260 UHPLC system (Agilent Technologies, Waldbronn, Germany) coupled to an 6224 Accurate Mass TOF LC/MS system (Agilent Technologies, Singapore). Infrared (IR) spectra were recorded on a Bruker Vertex 70 (ATR) or FT-IR spectrometer. The samples were prepared as neat fine powders and the wave numbers are reported in cm$^{-1}$. UV absorbance data were measured on a Shimadzu UV-3100 spectrophotometer. Fluorescence spectra were determined using a Solar CM-2203 fluorescence spectrophotometer. Compound 1d was prepared according to the literature procedure [1].

2. General procedure 1 (GP1) for the synthesis of compounds 3a–w, 5a and 9a–g by Chan–Evans–Lam reaction of pyrimidin-2(1H)-ones 1a–h with boronic acids 2a–w and 4

To a suspension of compound 1a–h, corresponding boronic acid 2a–w, 4 and copper(II) acetate monohydrate (599 mg, 3 mmol, 1 equiv) in acetonitrile (20 mL) pyridine (0.475 g, 0.48 mL, 6 mmol, 2 equiv) was added. The mixture was vigorously stirred with an open air condenser at room temperature for 48 h and then heated at 80 °C for 8 h. After cooling to room temperature the mixture was filtered, the solid material was washed with acetonitrile (2 × 10 mL). The combined filtrates were concentrated under reduced pressure, the residue was treated with 2 N ammonium hydroxide solution (20 mL) and was extracted with ethyl acetate (2 × 30 mL). The organic layers were combined, washed with brine (2 × 30 mL), dried over anhydrous sodium sulfate, filtered and the solvent was evaporated under reduced pressure. The obtained residue was treated as specified below.
1-Phenyl-4-(trifluoromethyl)pyrimidin-2(1H)-one (3a). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and phenylboronic acid 2a (366 mg, 3 mmol, 1 equiv). The obtained residue was refluxed with methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (658 mg, 90%). Mp 162-164 °C. IR (neat): \( \nu_{\text{max}} \) 3060, 1670, 1530, 1456, 1325, 1308, 1204, 1155, 1055, 790, 696. \(^1\)H NMR (400 MHz, DMSO-\( d_6 \)): \( \delta \) 8.60 (d, \( J = 6.6 \) Hz, 1H), 7.55 (bs, 5H), 6.95 (d, \( J = 6.6 \) Hz, 1H). \( ^{13} \)C NMR (125 MHz, DMSO-\( d_6 \)): \( \delta \) 162.5 (q, \( J = 35.3 \) Hz), 155.1, 154.5, 140.3, 129.7, 129.6, 126.9, 120.0 (q, \( J = 277.6 \) Hz), 99.5. \(^{19} \)F NMR (376 MHz, DMSO-\( d_6 \)): \( \delta \) –70.97 (s). HRMS (ESI+): calcd for C\(_{11}\)H\(_7\)F\(_3\)N\(_2\)O [M+H]+ : 241.0583, found 241.0582.

1-(4-Methoxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3b). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and 4-methoxyphenylboronic acid 2b (456 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (699 mg, 85%). Mp 127-129 °C. IR (neat): \( \nu_{\text{max}} \) 3030, 1670, 1513, 1464, 1316, 1262, 1208, 1170, 1027, 836, 798. \(^1\)H NMR (400 MHz, DMSO-\( d_6 \)): \( \delta \) 8.55 (d, \( J = 6.6 \) Hz, 1H), 7.46 (d, \( J = 8.8 \) Hz, 2H), 7.08 (d, \( J = 8.8 \) Hz, 2H), 6.92 (d, \( J = 6.6 \) Hz, 1H), 3.81 (s, 3H). \( ^{13} \)C NMR (126 MHz, DMSO-\( d_6 \)): \( \delta \) 162.2 (q, \( J = 35.5 \) Hz), 160.0, 155.3, 154.7, 133.1, 128.1, 120.0 (q, \( J = 277.6 \) Hz), 114.8, 99.4, 56.0. \(^{19} \)F NMR (376 MHz, DMSO-\( d_6 \)): \( \delta \) –71.01 (s). HRMS (ESI+): calcd for C\(_{12}\)H\(_9\)F\(_3\)N\(_2\)O\(_2\) [M+H]+ : 271.0689, found 271.0688.

1-(Benzo[d][1,3]dioxol-5-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3c). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and benzo[d][1,3]dioxol-5-ylboronic acid 2c (498 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. Light brown solid (767 mg, 90%). Mp 168-170 °C. IR (neat): \( \nu_{\text{max}} \) 3102, 2905, 1669, 1527, 1494, 1450, 1199, 1145, 1038, 933, 806. \(^1\)H NMR (400 MHz, DMSO-\( d_6 \)): \( \delta \) 8.54 (d, \( J = 6.6 \) Hz, 1H), 7.18 (s, 1H), 7.06 (d, \( J = 8.2 \) Hz, 1H), 7.00 (d, \( J = 8.3 \) Hz, 1H), 6.92 (d, \( J = 6.7 \) Hz, 1H), 6.13 (s, 2H). \( ^{13} \)C NMR (126 MHz, DMSO-\( d_6 \)): \( \delta \) 162.3 (d, \( J = 35.2 \) Hz), 155.4, 154.6,
148.2, 147.9, 134.1, 120.0 (d, J = 277.5 Hz), 120.6, 108.7, 108.2, 102.5, 99.3. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –70.93 (s). HRMS (ESI+): calcd for C$_{12}$H$_7$F$_3$N$_2$O$_3$ [M+H]$^+$: 285.0482, found 285.0484.

1-(4-(Trifluoromethoxy)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3d).

Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-(trifluoromethoxy)phenyl)boronic acid 2d (618 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (651 mg, 67%). Mp 147-148 °C. IR (neat): $\nu_{\text{max}}$ 3103, 3036, 1679, 1528, 1505, 1466, 1314, 1212, 1152, 1056, 803. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.65 (d, $J$ = 6.7 Hz, 1H), 7.72 (d, $J$ = 8.7 Hz, 2H), 7.58 (d, $J$ = 8.4 Hz, 2H), 6.99 (d, $J$ = 6.7 Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$): $\delta$ 162.69 (q, $J$ = 35.5 Hz), 155.08, 154.39, 148.84, 139.09, 129.35, 122.32, 120.49 (q, $J$ = 257.1 Hz), 119.97 (q, $J$ = 277.6 Hz), 99.65. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –57.43 (s, 3F), -71.03 (s, 3F). HRMS (ESI+): calcd for C$_{12}$H$_6$F$_6$N$_2$O$_2$ [M+H]$^+$: 325.0406, found 325.0404.

1-[4-(1H-Pyrazol-1-yl)phenyl]-4-(trifluoromethyl)pyrimidin-2(1H)-one (3e).

Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-(1H-pyrazol-1-yl)phenyl)boronic acid 2e (564 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether, cooled and filtered off. White solid (753 mg, 82 %). Mp 226-227 °C. IR (neat): $\nu_{\text{max}}$ 3119, 3072, 1676, 1623, 1533, 1512, 1455, 1311, 1207, 1141, 1061, 936, 812, 744. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.62 (d, $J$ = 4.7 Hz, 1H), 8.56 (s, 1H), 8.01 (d, $J$ = 6.6 Hz, 2H), 7.80 (s, 1H), 7.69 (d, $J$ = 6.6 Hz, 2H), 6.95 (d, $J$ = 4.9 Hz, 1H), 6.59 (s, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$): $\delta$ 162.5 (q, $J$ = 35.3 Hz), 155.10, 154.48, 142.07, 140.37, 137.82, 128.62, 128.26, 119.24, 120.00 (q, $J$ = 277.8 Hz), 108.84, 99.62. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –70.91 (s). HRMS (ESI+): calcd for C$_{14}$H$_9$F$_3$N$_4$O [M+H]$^+$: 307.0801, found 307.0798.
1-(4-((1H-1,2,4-Triazol-1-yl)methyl)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3f). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-((1H-1,2,4-triazol-1-yl)methyl)phenyl)boronic acid 2f (619 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (685 mg, 70%). Mp 163-165 °C. IR (neat): νmax 3092, 3035, 1675, 1509, 1465, 1316, 1215, 1151, 1059, 805. 1H NMR (400 MHz, DMSO-d6): δ 8.72 (s, 1H), 8.59 (d, J = 6.6 Hz, 1H), 8.01 (s, 1H), 7.54 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 6.6 Hz, 1H), 5.51 (s, 2H). 13C NMR (150 MHz, DMSO-d6): δ 162.5 (q, J = 35.4 Hz), 155.0, 154.4, 152.3, 144.9, 139.7, 137.9, 129.1, 127.2, 119.9 (q, J = 277.5 Hz), 99.5, 51.9. 19F NMR (376 MHz, DMSO-d6): δ –70.98 (s). HRMS (ESI+): calcd for C14H10F3N5O [M+H]+ : 322.0910, found 322.0909.

1-(4-Bromophenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3g). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-bromophenyl)boronic acid 2g (600 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (632 mg, 66%). Mp 164-166 °C. IR (neat): νmax 3081, 3065, 1672, 1516, 1433, 1304, 1152, 1063, 846. 1H NMR (400 MHz, DMSO-d6): δ 8.57 (d, J = 6.6 Hz, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 6.6 Hz, 1H), 5.51 (s, 2H). 13C NMR (126 MHz, DMSO-d6): δ 162.6 (q, J = 35.4 Hz), 155.0, 154.4, 152.3, 144.9, 139.7, 137.9, 129.1, 127.2, 119.9 (q, J = 277.6 Hz), 99.6. 19F NMR (376 MHz, DMSO-d6): δ –70.59 (s). HRMS (ESI+): calcd for C11H6BrF3N2O [M+H]+ : 318.9689, found 318.9693.

4-(Trifluoromethyl)-1-(4-(trifluoromethyl)phenyl)pyrimidin-2(1H)-one (3h). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-(trifluoromethyl)phenyl)boronic acid 2h (570 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (795 mg, 86%). Mp 165-166 °C. IR (neat): vmax 3116, 3056, 1433, 1304, 1152, 1063, 846. 1H NMR (400 MHz, DMSO-d6): δ 8.63 (d, J = 6.3 Hz, 1H), 7.95 (d, J = 8.2 Hz, 2H), 7.82 (d, J = 8.1 Hz, 2H), 6.99 (d, J = 6.4 Hz, 1H). 13C NMR (126 MHz, DMSO-d6): δ 162.84 (q, J = 35.3 Hz), 154.9, 154.2, 143.5, 130.0 (q,
\( J = 32.2 \text{ Hz}, 128.3, 126.9, 124.3 \text{ (q, } J = 277.2 \text{ Hz)}, 120.0 \text{ (q, } J = 289.8 \text{ Hz}), 99.8. \)

**19F NMR** (376 MHz, DMSO-\(d_6\)): \( \delta -61.70 \text{ (s, 3F), -71.02 \text{ (s, 3F). HRMS (ESI+): calcd for C}_{12}\text{H}_{6}\text{F}_{6}\text{N}_{2}\text{O} \ [M+H]^+: 309.0457, \text{ found 309.0462.} \)

**4-(2-Oxo-4-(trifluoromethyl)pyrimidin-1(2H)-yl)benzamide (3i).** Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-carbamoylphenyl)boronic acid 2i (495 mg, 3 mmol, 1 equiv). The obtained residue was purified by reverse phase HPLC method (eluent CH\(_3\)CN/H\(_2\)O). White solid (365 mg, 43%). Mp > 260 °C. **IR** (neat): \( \nu_{\text{max}} 3385, 3183, 1681, 1645, 1459, 1305, 1208, 1152, 1123, 1047, 790. \)

**1H NMR** (400 MHz, DMSO-\(d_6\)): \( \delta 8.62 \text{ (d, } J = 6.7 \text{ Hz, 1H)}, 8.12 \text{ (s, 1H)}, 8.02 \text{ (d, } J = 8.4 \text{ Hz, 2H)}, 7.64 \text{ (d, } J = 8.4 \text{ Hz, 2H)}, 7.52 \text{ (s, 1H)}, 6.97 \text{ (d, } J = 6.7 \text{ Hz, 1H)}. \)

**13C NMR** (126 MHz, DMSO-\(d_6\)): \( \delta 167.4, 162.6 \text{ (q, } J = 35.4 \text{ Hz), 154.9, 154.2, 142.3, 135.4, 128.8, 126.9, 119.9 \text{ (q, } J = 277.6 \text{ Hz), 99.6. 19F NMR (376 MHz, DMSO-\(d_6\)): \( \delta -70.93 \text{ (s). HRMS (ESI+): calcd for C}_{12}\text{H}_{8}\text{F}_{3}\text{N}_{3}\text{O}_{2} \ [M+H]^+: 284.0642, \text{ found 284.0643.} \)

**1-(4-(Methylsulfonyl)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3j).** Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-(methylsulfonyl)phenyl)boronic acid 2j (610 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (553 mg, 57 %). Mp 220-222 °C. **IR** (neat): \( \nu_{\text{max}} 3107, 1687, 1532, 1460, 1306, 1201, 1147, 1057, 792.1H NMR** (400 MHz, DMSO-\(d_6\)): \( \delta 8.66 \text{ (d, } J = 6.7 \text{ Hz, 1H)}, 8.12 \text{ (d, } J = 8.4 \text{ Hz, 2H)}, 7.86 \text{ (d, } J = 8.4 \text{ Hz, 2H)}, 7.03 \text{ (d, } J = 6.7 \text{ Hz, 1H)}, 3.32 \text{ (s, 3H). 13C NMR** (125 MHz, DMSO-\(d_6\)): \( \delta 162.9 \text{ (q, } J = 35.6 \text{ Hz), 154.8, 154.2, 144.2, 141.8, 128.6, 128.3, 119.9 \text{ (q, } J = 277.8 \text{ Hz), 99.9, 43.8. 19F NMR (376 MHz, DMSO-\(d_6\)): \( \delta -70.99 \text{ (s). HRMS (ESI+): calcd for C}_{12}\text{H}_{9}\text{F}_{3}\text{N}_{2}\text{O}_{3}\text{S} \ [M+H]^+: 319.0359, \text{ found 319.0362.} \)

**4-(2-Oxo-4-(trifluoromethyl)pyrimidin-1(2H)-yl)benzaldehyde (3k).** Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-formylphenyl)boronic acid 2k (450 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (572 mg, 70 %). Mp 160-162
°C. IR (neat): $v_{\text{max}}$ 3023, 1716, 1683, 1523, 1456, 1313, 1216, 1152, 1058, 831, 815. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 10.10 (s, 1H), 8.63 (d, $J = 6.6$ Hz, 1H), 8.09 (d, $J = 8.1$ Hz, 2H), 7.80 (d, $J = 8.1$ Hz, 2H), 6.99 (d, $J = 6.6$ Hz, 1H). $^{13}$C NMR (150 MHz, DMSO-$d_6$): $\delta$ 192.8, 162.7 (q, $J = 35.4$ Hz), 154.7, 154.1, 144.7, 136.7, 130.7, 127.9, 119.9 (q, $J = 277.8$ Hz), 99.7. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –71.02 (s). HRMS (ESI+): calcd for C$_{12}$H$_7$F$_3$N$_2$O$_2$ [M+H]$^+$: 269.0534, found 269.0535.

1-(3-Hydroxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3l). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (3-hydroxyphenyl)boronic acid 2l (414 mg, 3 mmol, 1 equiv). The obtained residue was purified by reverse phase HPLC method (eluent CH$_3$CN/H$_2$O). Slightly brown solid (576 mg, 75 %). Mp 192-195 °C. IR (neat): $v_{\text{max}}$ 3342, 3038, 1657, 1615, 1587, 1457, 1313, 1214, 1155, 1067, 963. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 9.98 (s, 1H), 8.54 (d, $J = 6.3$ Hz, 1H), 7.33 (t, $J = 7.4$ Hz, 1H), 6.91 (bs, 4H). $^{13}$C NMR (125 MHz, DMSO-$d_6$): $\delta$ 162.4 (q, $J = 35.3$ Hz), 158.4, 155.0, 154.3, 141.2, 130.6, 120.0 (q, $J = 276.1$ Hz), 117.2, 116.7, 114.0, 99.4. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –70.33 (s). HRMS (ESI+): calcd for C$_{11}$H$_7$F$_3$N$_2$O$_2$ [M+H]$^+$: 257.0532, found 257.0536.

1-(4-Hydroxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3m). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-hydroxyphenyl)boronic acid 2m (414 mg, 3 mmol, 1 equiv). The obtained residue was purified by reverse phase HPLC method (eluent CH$_3$CN/H$_2$O). Slightly brown solid (668 mg, 87 %). Mp 213-215 °C. IR (neat): $v_{\text{max}}$ 3335, 3025, 1664, 1620, 1454, 1323, 1216, 1152, 1073, 957. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 9.94 (s, 1H), 8.53 (d, $J = 5.0$ Hz, 1H), 7.32 (d, $J = 7.2$ Hz, 2H), 6.88 (bs, 3H). $^{13}$C NMR (150 MHz, DMSO-$d_6$): $\delta$ 162.0 (q, $J = 35.2$ Hz), 158.4, 155.3, 154.6, 131.6, 127.9, 120.0 (d, $J = 277.5$ Hz), 115.9, 99.3. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –70.42 (s). HRMS (ESI+): calcd for C$_{11}$H$_7$F$_3$N$_2$O$_2$ [M+H]$^+$: 257.0532, found 257.0535.
1-(4-(Hydroxymethyl)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3n). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (4-(hydroxymethyl)phenyl)boronic acid 2n (456 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (486 mg, 60%). Mp 145-146 °C. IR (neat): νmax 3288, 3030, 2920, 2875, 1668, 1529, 1463, 1313, 1133, 1056, 798. 1H NMR (400 MHz, DMSO-d6): δ 8.57 (d, J = 6.6 Hz, 1H), 7.64 – 7.38 (m, 5H), 6.94 (d, J = 6.7 Hz, 1H), 5.35 (t, J = 5.7 Hz, 1H), 4.57 (d, J = 5.6 Hz, 3H). 13C NMR (126 MHz, DMSO-d6): δ 162.3 (q, J = 35.2 Hz), 155.1, 154.4, 144.2, 138.7, 127.4, 126.5, 119.94 (q, J = 277.8 Hz), 99.5, 62.7. 19F NMR (376 MHz, DMSO-d6): δ –70.42 (s). HRMS (ESI+): calcd for C12H9F3N2O2 [M+H]+: 271.0689, found 271.0692.

1-(2-Methoxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3o). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (2-methoxyphenyl)boronic acid 2o (456 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (421 mg, 52%). Mp 156-158 °C. IR (neat): νmax 3104, 1673, 1531, 1502, 1450, 1296, 1202, 1150, 759. 1H NMR (400 MHz, DMSO-d6): δ 8.49 (d, J = 6.1 Hz, 1H), 7.61 – 7.35 (m, 2H), 7.22 (d, J = 8.0 Hz, 1H), 7.07 (t, J = 7.2 Hz, 1H), 6.89 (d, J = 6.1 Hz, 1H), 3.75 (s, 3H). 13C NMR (100 MHz, DMSO-d6): δ 162.7 (q, J = 35.5 Hz), 156.2, 154.0, 131.5, 128.6, 128.5, 121.1, 119.9 (q, J = 277.9 Hz), 113.1, 99.2, 56.5. 19F NMR (376 MHz, DMSO-d6): δ –71.03 (s). HRMS (ESI+): calcd for C12H9F3N2O2 [M+H]+: 271.0689, found 271.0694.

1-(o-Tolyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3p). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and o-tolylboronic acid 2p (612 mg, 4.5 mmol, 1.5 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (267 mg, 35%). Mp 145-147 °C. IR (neat): νmax 3053, 1672, 1542, 1452, 1330, 1312, 1206, 1147, 1060, 792, 685. 1H NMR (400 MHz, DMSO-d6): 8.56 (d, J = 6.4 Hz, 1H), 7.56 – 7.27 (bs, 4H), 6.98 (d, J = 6.4 Hz, 1H), 2.10 (s, 3H). 13C NMR (100 MHz, DMSO-d6): δ 162.8 (q, J = 35.2 Hz), 155.4, 154.0, 139.5, 134.7, 131.4, 130.0, 127.7, 127.6, 120.0 (q, J = 276.3 Hz), 99.6, 17.4. 19F NMR (376 MHz, DMSO-d6): δ –70.88 (s). HRMS (ESI+): calcd for C12H9F3N2O [M+H]+: 255.0740, found 255.0740.
1-(Pyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3q). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and pyridin-3-ylboronic acid 2q (562 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. White solid (94 mg, 13%). Mp 152-154 °C. IR (neat): ν max 3113, 1676, 1533, 1459, 1305, 1156, 1062, 793, 707. 1H NMR (400 MHz, DMSO-d6): 8.77 (s, 1H), 8.74 – 8.64 (m, 2H), 8.05 (d, J = 7.4 Hz, 1H), 7.65 – 7.55 (m, 1H), 7.02 (d, J = 6.6 Hz, 1H). 13C NMR (125 MHz, DMSO-d6): δ 162.90 (q, J = 35.2 Hz), 155.1, 154.4, 150.5, 147.7, 136.9, 135.0, 124.4, 120.0 (q, J = 276.2 Hz), 99.8. 19F NMR (376 MHz, DMSO-d6): δ –71.08 (s). HRMS (ESI+): calcd for C10H6F3N3O [M+H]+ : 242.0536, found 242.0537.

1-(Pyridin-4-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3r). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and pyridin-4-ylboronic acid 2r (562 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. White solid (123 mg, 17%). Mp 135-137 °C. IR (neat): ν max 3110, 1679, 1524, 1453, 1335, 1307, 1151, 1057, 798, 704. 1H NMR (400 MHz, DMSO-d6): δ 8.80 (bs, 2H), 8.66 (d, J = 6.8 Hz, 1H), 7.66 (d, J = 4.5 Hz, 2H), 7.04 (d, J = 6.8 Hz, 1H). 13C NMR (150 MHz, DMSO-d6): δ 162.9 (q, J = 35.5 Hz), 154.4, 153.7, 151.4, 147.2, 121.8, 119.9 (q, J = 276.2 Hz), 99.9. 19F NMR (376 MHz, DMSO-d6): δ –71.07 (s). HRMS (ESI+): calcd for C10H6F3N3O [M+H]+ : 242.0536, found 242.0541.

1-(6-Methoxypyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3s). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (6-methoxypyridin-3-yl)boronic acid 2s (700 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. White solid (372 mg, 45%). Mp 128-130 °C. IR (neat): ν max 3104, 1671, 1529, 1501, 1455, 1323, 1312, 1207, 1154, 1022, 806. 1H NMR (400 MHz, DMSO-d6): δ 8.62 (d, J = 6.4 Hz, 1H), 8.34 (s, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.15 – 6.85 (m, 2H), 3.91 (s, 3H). 13C NMR (125 MHz, DMSO-d6): δ 163.9, 162.6 (q, J = 35.3 Hz), 155.3, 154.6, 144.9, 138.2, 131.3, 120.0 (q, J = 276.3 Hz), 111.0, 99.7, 54.2. 19F NMR (376 MHz, DMSO-d6): δ –71.07 (s). HRMS (ESI+): calcd for C10H6F3N3O [M+H]+ : 242.0536, found 242.0537.
MHz, DMSO-d$_6$): $\delta$ –70.48 (s). HRMS (ESI+): calcd for C$_{11}$H$_8$F$_3$N$_3$O$_2$ [M+H]$^+$: 272.0641, found 272.0644.

1-(6-(Pyrrolidin-1-yl)pyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3t). Following the GP, using compound 1a (492 mg, 3 mmol, 1 equiv) and (6-(pyrrolidin-1-yl)pyridin-3-yl)boronic acid 2t (878 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. Yellow solid (595 mg, 63 %). Mp 230-232°C. IR (neat): $\nu_{\text{max}}$ 3093, 2865, 1692, 1615, 1520, 1463, 1306, 1203, 1147, 1057, 806, 790. $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 8.56 (d, $J$ = 6.6 Hz, 1H), 8.16 (d, $J$ = 1.5 Hz, 1H), 7.66 (d, $J$ = 10.5 Hz, 1H), 6.93 (d, $J$ = 6.6 Hz, 1H), 6.53 (d, $J$ = 9.0 Hz, 1H), 3.42 (bs, 4H), 1.96 (bs, 4H). $^{13}$C NMR (125 MHz, DMSO-d$_6$): $\delta$ 162.2 (q, $J$ = 35.6 Hz), 157.0, 155.3, 154.8, 145.5, 135.5, 125.9, 120.0 (q, $J$ = 277.1 Hz), 106.1, 99.5, 47.1, 25.5. $^{19}$F NMR (376 MHz, DMSO-d$_6$): $\delta$ –70.89 (s). HRMS (ESI+): calcd for C$_{14}$H$_{13}$F$_3$N$_4$O $[M+H]^+$: 311.1114, found 311.1117.

1-(Thiophen-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3u). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and thiophen-3-ylboronic acid 2u (585 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. White solid (352 mg, 47 %). Mp 148-150 °C. IR (neat): $\nu_{\text{max}}$ 3095, 1663, 1514, 1458, 1338, 1299, 1204, 1146, 1052, 795. $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 8.64 (d, $J$ = 6.7 Hz, 1H), 7.94 (br s, 1H), 7.69 (dd, $J$ = 5.0, 3.2 Hz, 1H), 7.38 (d, $J$ = 0.9 Hz, 1H), 6.94 (d, $J$ = 6.7 Hz, 1H). $^{13}$C NMR (125 MHz, DMSO-d$_6$): $\delta$ 162.1 (q, $J$ = 35.6 Hz), 154.8, 153.8, 137.8, 126.9, 125.4, 122.6, 120.0 (q, $J$ = 276.3 Hz), 99.6. $^{19}$F NMR (376 MHz, DMSO-d$_6$): $\delta$ –70.96 (s). HRMS (ESI+): calcd for C$_9$H$_5$F$_3$N$_2$OS $[M+H]^+$: 247.0147, found 247.0155.

4-(Trifluoromethyl)-1-(5-(trifluoromethyl)thiophen-3-yl)pyrimidin-2(1H)-one (3v). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (5-(trifluoromethyl)thiophen-3-yl)boronic acid 2v (896 mg, 4.5 mmol, 1.5 equiv). The obtained residue was purified by reverse phase HPLC method (elucent CH$_3$CN/H$_2$O). White solid (191 mg, 20 %). Mp 142-144 °C. IR (neat): $\nu_{\text{max}}$ 3082,
1684, 1471, 1293, 1220, 1161, 1138, 801. \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): 8.71 (d, \(J = 6.8\) Hz, 1H), 8.33 (d, \(J = 1.6\) Hz, 1H), 8.03 (d, \(J = 0.9\) Hz, 1H), 7.01 (d, \(J = 6.8\) Hz, 1H). \(^{13}\)C NMR (125 MHz, DMSO-\(d_6\)): \(\delta\) 162.6 (q, \(J = 35.4\) Hz), 154.9, 153.8, 137.1, 129.1 (q, \(J = 38.8\) Hz), 128.6 (q, \(J = 3.7\) Hz), 127.8, 122.6 (q, \(J = 267.3\) Hz), 119.9 (q, \(J = 276.3\) Hz), 99.8. \(^{19}\)F NMR (376 MHz, DMSO-\(d_6\)): \(\delta\) –55.26 (s, 3F), –71.04 (s, 3F). HRMS (ESI+): calcd for C\(_{10}\)H\(_4\)F\(_6\)N\(_2\)OS [M+H]\(^+\): 315.0021, found 315.0024.

1-(Furan-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3w). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and furan-3-ylboronic acid 2w (512 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. Beige solid (97 mg, 14 %). Mp 138-140 °C. IR (neat): \(\nu\) max 3122, 1664, 1526, 1460, 1338, 1212, 1151, 1065, 793. \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): 8.83 (d, \(J = 6.8\) Hz, 1H), 8.47 (s, 1H), 7.85 (s, 1H), 7.10 (s, 1H), 7.02 (d, \(J = 6.8\) Hz, 1H). \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)): \(\delta\) 160.9 (q, \(J = 35.3\) Hz), 152.8, 152.5, 143.9, 138.1, 127.1, 120.0 (q, \(J = 275.8\) Hz), 106.9, 100.0. \(^{19}\)F NMR (376 MHz, DMSO-\(d_6\)): \(\delta\) –70.76 (s). HRMS (ESI+): calcd for C\(_9\)H\(_5\)F\(_3\)N\(_2\)O\(_2\) [M+H]\(^+\) : 231.0376, found 231.0375.

(E)-1-Styryl-4-(trifluoromethyl)pyrimidin-2(1H)-one (5a). Following the GP1, using compound 1a (492 mg, 3 mmol, 1 equiv) and (E)-styrylboronic acid 4 (444 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. Yellow solid (694 mg, 87%). Mp 147-148 °C. IR (neat): \(\nu\) max 3099, 3030, 1669, 1528, 1461, 1326, 1204, 1150, 1045, 955, 805, 749. UV-vis (CH\(_2\)Cl\(_2\)): \(\lambda\) max 370 nm. Fluorescence emission (CH\(_2\)Cl\(_2\)): \(\lambda\) max 490 nm. \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 8.86 (d, \(J = 6.6\) Hz, 1H), 7.69 (d, \(J = 14.6\) Hz, 1H), 7.58 (d, \(J = 7.1\) Hz, 2H), 7.49 – 7.33 (m, 3H), 7.30 (d, \(J = 14.7\) Hz, 1H), 6.96 (d, \(J = 6.4\) Hz, 1H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)): \(\delta\) 161.6 (q, \(J = 35.5\) Hz), 153.4, 150.5, 134.4, 129.4, 129.3, 127.4, 126.21, 126.1, 120.0 (q, \(J = 277.5\) Hz), 100.1. \(^{19}\)F NMR (376 MHz, DMSO-\(d_6\)): \(\delta\) –70.36 (s). HRMS (ESI+): calcd for C\(_{13}\)H\(_9\)F\(_3\)N\(_2\)O [M+H]\(^+\) : 267.0740, found 267.0741.
4-(Difluoromethyl)-1-phenylpyrimidin-2(1H)-one (9a). Following the GP1, using 4-(difluoromethyl)pyrimidin-2(1H)-one 1b (438 mg, 3 mmol, 1 equiv) and phenylboronic acid 2a (336 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (266 mg, 40 %). Mp 118-119 °C. IR (neat): $\nu_{\text{max}}$ 3100, 3059, 1667, 1526, 1453, 1079, 1062, 783, 690. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.45 (d, $J = 6.7$ Hz, 1H), 7.59 – 7.47 (m, 5H), 6.77 (t, $J = 54.1$ Hz, 2H), 6.75 (d, $J = 6.7$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$): $\delta$ 168.6 (t, $J = 26.1$ Hz), 154.8, 153.4, 140.5, 129.7, 129.4, 126.9, 112.5 (t, $J = 242.1$ Hz), 99.6. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –121.84 (d, $J = 54.1$ Hz). HRMS (ESI+): calcd for C$_{11}$H$_8$F$_2$N$_2$O [M+H]$^+$: 223.0678, found 223.0677.

4-(Chlorodifluoromethyl)-1-phenylpyrimidin-2(1H)-one (9b). Following the GP1, using 4-(chlorodifluoromethyl)pyrimidin-2(1H)-one 1c (542 mg, 3 mmol, 1 equiv) and phenylboronic acid 2a (336 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. Light yellow solid (596 mg, 74%). Mp 151-152 °C. IR (neat): $\nu_{\text{max}}$ 3058, 2963, 1669, 1526, 1453, 1283, 1148, 1058, 966, 887, 762. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.57 (d, $J = 6.7$ Hz, 1H), 7.66 – 7.47 (m, 5H), 6.90 (d, $J = 6.7$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$): $\delta$ 166.4 (t, $J = 29.9$ Hz), 154.9, 154.5, 140.3, 129.7, 129.6, 126.9, 123.0 (t, $J = 292.8$ Hz), 98.6. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –59.59 (s). HRMS (ESI+): calcd for C$_{11}$H$_7$ClF$_2$N$_2$O [M+H]$^+$: 257.0288, found 257.0287.

4-(Perfluoroethyl)-1-phenylpyrimidin-2(1H)-one (9c). Following the GP1, using 4-(perfluoroethyl)pyrimidin-2(1H)-one 1d (642 mg, 3 mmol, 1 equiv) and phenylboronic acid 2a (366 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (679 mg, 78%). Mp 154-156 °C. IR (neat): $\nu_{\text{max}}$ 3113, 3062, 1675, 1529, 1453, 1234, 1210, 1174, 1129, 1081, 767, 697. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.61 (d, $J = 6.7$ Hz, 1H), 7.66 – 7.23 (m, 5H), 6.97 (d, $J = 6.7$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$): $\delta$ 162.9 (t, $J = 287.2$ Hz), 112.9 (tq, $J = 256.8$, 36.3 Hz), 100.9 (tq, $J = 256.8$, 37.5 Hz), 100.5. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –82.18 (s, 3F), –119.04 (s, 2F). HRMS (ESI+): calcd for C$_{12}$H$_7$F$_5$N$_2$O [M+H]$^+$: 291.0552, found 291.0554.
Ethyl 2-oxo-1-phenyl-4-(trifluoromethyl)-1,2-dihydropyrimidine-5-carboxylate (9f). To a mixture of ethyl 2-oxo-4-(trifluoromethyl)-1,2-dihydropyrimidine-5-carboxylate 1g (708 mg, 3 mmol, 1 equiv), phenylboronic acid 2a (402 mg, 3.3 mmol, 1.1 equiv) and copper(II) acetate monohydrate (599 mg, 3 mmol, 1 equiv) in dichloromethane (25 mL) pyridine (0.475 g, 0.48 mL, 6 mmol, 2 equiv) was added. The reaction mixture was vigorously stirred at room temperature for 96 h. The solvent was evaporated and the residue was treated with 2 N hydrochloric acid (20 mL) and was extracted with ethyl acetate (2 × 30 mL). The organic layer was washed with brine (2 × 50 mL), dried over anhydrous sodium sulfate and the solvent was evaporated. The obtained residue was refluxed in toluene (25 mL) and acetic acid (0.2 mL) for 5 h, cooled and the precipitate was filtered off. White solid (609 mg, 65%). Mp 140-142 °C. IR (neat): ν_{max} 2993, 1718, 1680, 1623, 1492, 1269, 1206, 1147, 792, 701. ¹H NMR (400 MHz, DMSO-d₆): δ 8.88 (s, 1H), 7.58 (s, 5H), 4.26 (q, J = 6.4 Hz, 2H), 1.27 (t, J = 6.2 Hz, 3H). ¹³C NMR (125 MHz, DMSO-d₆): δ 161.6, 159.4 (q, J = 35.6 Hz), 157.6, 153.3, 139.5, 130.0, 129.8, 127.00, 119.7 (q, J = 277.9 Hz), 106.3, 62.1, 14.2. ¹⁹F NMR (376 MHz, DMSO-d₆): δ –67.47 (s). HRMS (ESI+): calcd for C₁₄H₁₁F₃N₂O₃ [M+H]⁺: 313.0795, found 313.0798.

5-Bromo-1-phenyl-4-(trifluoromethyl)pyrimidin-2(1H)-one (9g). Following the GP1, using 5-bromo-4-(trifluoromethyl)pyrimidin-2(1H)-one 1h (729 mg, 3 mmol, 1 equiv) and phenylboronic acid 2a (366 mg, 3 mmol, 1 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (785 mg, 82%). Mp 189-192 °C. IR (neat): ν_{max} 3058, 1699, 1675, 1487, 1452, 1294, 1216, 1148, 1049, 780, 700. ¹H NMR (400 MHz, DMSO-d₆): δ 8.95 (s, 1H), 7.58 (bs, 5H). ¹³C NMR (125 MHz, DMSO-d₆): δ 158.5 (q, J = 34.2 Hz), 155.7, 152.8, 139.5, 129.9, 129.7, 127.0, 120.7 (q, J = 277.3 Hz), 90.7. ¹⁹F NMR (376 MHz, DMSO-d₆): δ –69.19 (s). HRMS (ESI+): calcd for C₁₁H₆BrF₃N₂O [M+H]⁺: 318.9688, found 318.9686.
3. General procedure 2 (GP2) for the synthesis of compounds 3a,g,q,s, 5a–h and 8 by Chan–Evans–Lam reaction of pyrimidin-2(1H)-one 1a with boronic acid pinacol esters 6a–d and 7a–h

To a suspension of compound 1a, corresponding boronic acid pinacol esters 6b–d or 7a–h, copper(II) acetate monohydrate (599 mg, 3 mmol, 1 equiv) and boric acid (371 mg, 6 mmol, 2 equiv) in acetonitrile (20 mL) pyridine (0.475 g, 0.48 mL, 6 mmol, 2 equiv) was added. The mixture was vigorously stirred and heated at 80 °C for 8 h with an open air condenser. After cooling to room temperature the mixture was filtered, the solid material was washed with acetonitrile (2 × 10 mL). The combined filtrates were concentrated under reduced pressure, the residue was treated with 2 N ammonium hydroxide solution (20 mL) and was extracted with ethyl acetate (2 × 30 mL). The organic layers were combined, washed with brine (2 × 30 mL), dried over anhydrous sodium sulfate, filtered and the solvent was evaporated under reduced pressure. The obtained residue was treated as specified below.

1-Phenyl-4-(trifluoromethyl)pyrimidin-2(1H)-one (3a). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and 4,4,5,5-tetramethyl-2-phenyl-1,3,2-dioxaborolane 6a (933 mg, 4.5 mmol, 1.5 equiv). The obtained residue was refluxed with methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (629 mg, 86%). Physico-chemical and spectral characteristics of this product was identical with the compound obtained according to GP1.

1-(4-Bromophenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3g). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and 2-(4-bromophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 6b (1.27 g, 4.5 mmol, 1.5 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (680 mg, 71%). Physico-chemical and spectral characteristics of this product was identical with the compound obtained according to GP1.
1-(Pyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3q). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine 6c (937 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. White solid (109 mg, 15%). Physico-chemical and spectral characteristics of this product was identical with the compound obtained according to GP1.

1-(6-Methoxypyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3s). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and 2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine 6d (860 mg, 4.5 mmol, 1.5 equiv). The obtained residue was recrystallized from toluene. White solid (372 mg, 45 %). Physico-chemical and spectral characteristics of this product was identical with the compound obtained according to GP1.

(E)-1-Styryl-4-(trifluoromethyl)pyrimidin-2(1H)-one (5a). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and (E)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane 7a (1035 mg, 4.5 mmol, 1.5 equiv). The obtained residue was refluxed with methyl tert-butyl ether (20 mL), cooled and filtered off. White solid (654 mg, 82 %). Physico-chemical and spectral characteristics of this product was identical with the compound obtained according to GP1.

(E)-1-(3,5-Difluorostyryl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5b). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and (E)-2-(3,5-difluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 7b (1.197 g, 4.5 mmol, 1.5 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. Yellow solid (680 mg, 75%). Mp 236-237 °C. IR (neat): \( \nu_{\text{max}} \) 3098, 3033, 1667, 1528, 1459, 1309, 1209, 1161, 940, 810, 671. UV-vis (CH\(_2\)Cl\(_2\)): \( \lambda_{\text{max}} \) 369 nm. Fluorescence emission (CH\(_2\)Cl\(_2\)): \( \lambda_{\text{max}} \) 491 nm. \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \( \delta \) 8.81 (d, \( J = 6.8 \) Hz, 1H), 7.85 (d, \( J = 14.6 \) Hz, 1H), 7.38 (d, \( J = 6.8 \) Hz, 2H), 7.32 (d, \( J = 14.6 \) Hz, 1H), 7.23 (t, \( J = 9.2 \) Hz, 1H), 7.03 (d, \( J = 6.9 \) Hz, 1H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)): ...
DMSO-\textsubscript{d6}): \( \delta \) 163.1 (dd, \( J = 246.0, 13.6 \) Hz), 162.0 (q, \( J = 35.6 \) Hz), 153.3, 150.6, 138.4 (t, \( J = 10.2 \) Hz), 128.9, 124.1, 119.9 (q, \( J = 277.5 \) Hz), 110.5 (dd, \( J = 20.0, 6.2 \) Hz), 104.3 (t, \( J = 26.1 \) Hz), 100.2. \textit{\textsuperscript{19}F NMR} (376 MHz, DMSO-\textsubscript{d6}): \( \delta \) –70.85 (s, 3F), –109.97 (s, 2F). HRMS (ESI+): calcd for C\textsubscript{13}H\textsubscript{7}F\textsubscript{5}N\textsubscript{2}O \([M+H]^+\): 303.0552, found 303.0550.

\begin{align*}
\text{(E)-1-(3-Methoxystyryl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5c). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and (E)-2-(3-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 7c (1.17 g, 4.5 mmol, 1.5 equiv). The reaction was carried out in darkness. The obtained residue was refluxed in methyl \textit{tert}-butyl ether (20 mL), cooled and filtered off. Yellow solid (498 mg, 56%). Mp 187-188 \degree C. IR (neat): \( \nu_{\text{max}} \) 3060. UV-vis (CH\textsubscript{2}Cl\textsubscript{2}): \( \lambda_{\text{max}} \) 372 nm. Fluorescence emission (CH\textsubscript{2}Cl\textsubscript{2}): \( \lambda_{\text{max}} \) 493 nm.} \\
\textit{\textsuperscript{1}H NMR} (400 MHz, DMSO-\textsubscript{d6}): \( \delta \) 8.86 (d, \( J = 6.7 \) Hz, 1H), 7.72 (d, \( J = 14.6 \) Hz, 1H), 7.33 (t, \( J = 7.7 \) Hz, 1H), 7.27 (d, \( J = 14.6 \) Hz, 1H), 7.15 (d, \( J = 7.5 \) Hz, 2H), 7.00 (d, \( J = 6.7 \) Hz, 1H), 6.93 (d, \( J = 7.6 \) Hz, 1H). \textit{\textsuperscript{13}C NMR} (126 MHz, DMSO-\textsubscript{d6}): \( \delta \) 161.2 (q, \( J = 35.7 \) Hz), 159.6, 153.0, 150.1, 135.4, 130.0, 126.0, 125.8, 119.6 (d, \( J = 277.3 \) Hz), 119.5, 114.7, 112.0, 99.7, 55.2. \textit{\textsuperscript{19}F NMR} (376 MHz, DMSO-\textsubscript{d6}): \( \delta \) –70.35 (s). HRMS (ESI+): calcd for C\textsubscript{14}H\textsubscript{11}F\textsubscript{3}N\textsubscript{2}O\textsubscript{2} \([M+H]^+\): 297.0844, found 297.0846.
\end{align*}

\begin{align*}
\text{(E)-1-(4-Fluorostyryl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5d). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and (E)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 7d (1.116 g, 4.5 mmol, 1.5 equiv). The obtained residue was refluxed in methyl \textit{tert}-butyl ether, cooled and filtered off. Yellow-green solid (780 mg, 91.5%). Mp 235-236 \degree C. IR (neat): \( \nu_{\text{max}} \) 3110, 3029, 1659, 1512, 1458, 1322, 1206, 1170, 1043, 956, 817. UV-vis (CH\textsubscript{2}Cl\textsubscript{2}): \( \lambda_{\text{max}} \) 368 nm. Fluorescence emission (CH\textsubscript{2}Cl\textsubscript{2}): \( \lambda_{\text{max}} \) 493 nm.} \\
\textit{\textsuperscript{1}H NMR} (400 MHz, DMSO-\textsubscript{d6}): \( \delta \) 8.85 (d, \( J = 6.8 \) Hz, 1H), 7.82 – 7.48 (m, 3H), 7.35 – 7.17 (m, 3H), 7.00 (d, \( J = 6.8 \) Hz, 1H). \textit{\textsuperscript{13}C NMR} (126 MHz, DMSO-\textsubscript{d6}): \( \delta \) 162.77 (d, \( J = 246.5 \) Hz), 161.68 (q, \( J = 35.3 \) Hz), 153.5, 150.6, 131.0 (d, \( J = 3.2 \) Hz), 129.6 (d, \( J = 8.3 \) Hz), 126.1, 125.2, 120.0 (q, \( J = 277.2 \) Hz), 116.4 (d, \( J = 21.8 \) Hz), 100.1. \textit{\textsuperscript{19}F NMR} (376 MHz, DMSO-\textsubscript{d6}): \( \delta \) –70.77 (s, 3F), –112.89 (s, 1F). HRMS (ESI+): calcd for C\textsubscript{13}H\textsubscript{8}F\textsubscript{4}N\textsubscript{2}O \([M+H]^+\): 285.0646, found 285.0652.
\end{align*}
(E)-1-(4-Methoxystyril)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5e). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and (E)-2-(4-methoxystyril)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 7e (1.17 g, 4.5 mmol, 1.5 equiv). The obtained residue was refluxed in methyl tert-butyl ether (20 mL), cooled and filtered off. Yellow-green solid (542 mg, 61%). Mp 234-236 °C. IR (neat): \( \nu_{\text{max}} \) 3098, 3036, 2961, 2938, 1666, 1528, 1459, 1328, 1257, 1206, 1146, 814. UV-vis (CH\(_2\)Cl\(_2\)): \( \lambda_{\text{max}} \) 383 nm. Fluorescence emission (CH\(_2\)Cl\(_2\)): \( \lambda_{\text{max}} \) 532 nm. \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \( \delta \) 8.54 (d, \( J = 6.6 \) Hz, 1H), 7.18 (s, 1H), 7.06 (d, \( J = 8.2 \) Hz, 1H), 7.00 (d, \( J = 8.3 \) Hz, 1H), 6.92 (d, \( J = 6.7 \) Hz, 1H), 6.13 (s, 2H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)): \( \delta \) 161.3 (q, \( J = 35.1 \) Hz), 160.3, 153.5, 150.5, 129.0, 126.9, 126.1, 124.2, 120.0 (d, \( J = 277.5 \) Hz), 114.9, 100.0, 55.7. \(^{19}\)F NMR (376 MHz, DMSO-\(d_6\)): \( \delta \) –70.70 (s). HRMS (ESI+): calcd for C\(_{14}\)H\(_{11}\)F\(_3\)N\(_2\)O\(_2\) [M+H]\(^+\): 297.0846, found 297.0846.

4-(Trifluoromethyl)-1-vinylpyrimidin-2(1H)-one (5f). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and vinylboronic acid pinacol ester 7f (939 mg, 6.0 mmol, 2 equiv). The obtained residue was washed with water (2\(\times\)10 mL), dried and recrystallized from toluene. White solid (336 mg, 58 %). Mp 136-138 °C. IR (neat): \( \nu_{\text{max}} \) 3037, 1685, 1623, 1526, 1470, 1336, 1200, 1145, 1113, 958, 814, 790. \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \( \delta \) 8.77 (d, \( J = 6.4 \) Hz, 1H), 7.22 (dd, \( J = 15.7, 8.9 \) Hz, 1H), 6.94 (d, \( J = 8.3 \) Hz, 1H), 5.84 (d, \( J = 15.8 \) Hz, 1H), 5.39 (d, \( J = 8.6 \) Hz, 1H). \(^{13}\)C NMR (125 MHz, DMSO-\(d_6\)): \( \delta \) 162.1 (q, \( J = 35.5 \) Hz), 153.2, 150.1, 132.7, 119.9 (q, \( J = 277.5 \) Hz), 110.3, 100.0. \(^{19}\)F NMR (376 MHz, DMSO-\(d_6\)): \( \delta \) –71.04 (s). HRMS (ESI+): calcd for C\(_7\)H\(_5\)F\(_3\)N\(_2\)O \([M+H]^+\): 191.0427, found 191.0429.

(E)-1-(Prop-1-en-1-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5g). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and propen-1-ylboronic acid pinacol ester 7g (1.024 g, 6.0 mmol, 2 equiv). The obtained residue was washed with water (2\(\times\)10 mL), dried and recrystallized from toluene. White solid (367 mg, 60 %). Mp 202-204 °C. IR (neat): \( \nu_{\text{max}} \) 3030, 1682, 1530, 1467, 1332, 1206, 1147, 1110, 952, 812,
794. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.67 (d, $J = 6.5$ Hz, 1H), 6.95 (d, $J = 14.2$ Hz, 1H), 6.90 (d, $J = 6.5$ Hz, 1H), 6.21 – 6.30 (m, 1H), 1.83 (d, $J = 6.6$ Hz, 1H). $^{13}$C NMR (150 MHz, DMSO-$d_6$): $\delta$ 161.5 (q, $J = 35.4$ Hz), 153.3, 151.1, 127.4, 123.7, 119.9 (q, $J = 277.5$ Hz), 99.7, 15.5. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –70.91 (s). HRMS (ESI+): calcd for C$_8$H$_7$F$_3$N$_2$O [M+H]$^+$: 205.0583, found 205.0587.

(E)-1-(2-Cyclopropylvinyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5h). Following the GP2, using compound 1a (492 mg, 3 mmol, 1 equiv) and 2-cyclopropylvinylboronic acid pinacol ester 7h (1.164 g, 6.0 mmol, 2 equiv). The obtained residue was washed with water (2 x 10 mL), dried and recrystallized from toluene. White solid (428 mg, 62 %). Mp 150-152 °C. IR (neat): $\nu_{\max}$ 3095, 2083, 1664, 1534, 1460, 1331, 1303, 1201, 1150, 1096, 1042, 945, 808. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.64 (d, $J = 6.7$ Hz, 1H), 7.04 (d, $J = 14.0$ Hz, 1H), 6.88 (d, $J = 6.7$ Hz, 1H), 5.83 (dd, $J = 14.0$, 9.6 Hz, 1H), 1.75 – 1.60 (m, 1H), 0.90 – 0.75 (m, 2H), 0.60 – 0.45 (m, 2H). $^{13}$C NMR (150 MHz, DMSO-$d_6$): $\delta$ 161.2 (q, $J = 35.3$ Hz), 153.2, 150.7, 133.0, 124.3, 119.9 (q, $J = 277.4$ Hz), 99.7, 12.4, 7.5. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –70.96 (s). HRMS (ESI+): calcd for C$_{10}$H$_9$F$_3$N$_2$O [M+H]$^+$: 231.0740, found 231.0742.

1,1’-(2,4-Bis(3-methoxyphenyl)cyclobutane-1,3-diyl)bis(4-(trifluoromethyl)pyrimidin-2(1H)-one) (8). Compound 5c (100 mg) was exposed to sunlight in an open air Petri dish at room temperature for 12 h. The solid was washed with ethyl acetate (2x20 mL) and air-dried. White solid (76 mg, 76%). Mp >260 °C. IR (neat): $\nu_{\max}$ 3099, 3024, 2944, 1662, 1588, 1531, 1466, 1317, 1205, 1142, 1051, 792. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 8.65 (d, $J = 6.7$ Hz, 2H), 7.19 (t, $J = 8.1$ Hz, 2H), 6.91 – 6.61 (m, 8H), 6.06 – 5.94 (m, 2H), 5.20 – 4.91 (m, 2H), 3.68 (s, 6H). $^{13}$C NMR (126 MHz, DMSO-$d_6$): $\delta$ 161.1 (q, $J = 35.6$ Hz), 159.7, 154.4, 152.6, 136.9, 130.0, 120.4, 119.9 (q, $J = 277.3$ Hz), 114.1, 113.4, 99.0, 58.7, 55.5, 45.2. $^{19}$F NMR (376 MHz, DMSO-$d_6$): $\delta$ –70.89 (s). HRMS (ESI+): calcd for C$_{28}$H$_{22}$F$_6$N$_4$O$_4$ [M+H]$^+$: 593.1618, found 593.1617.
4. References

1. Gorbunova, M. G.; Gerus, I. I.; Kukhar, V. P. Synthesis and Properties of β-Ethoxyvinyl Polyfluoroalkyl Ketones. *Synthesis (Stuttg).* **2000**, **2000** (05), 738–742. https://doi.org/10.1055/s-2000-6386.
5. Copies of the $^1$H and $^{13}$C NMR spectra

1-Phenyl-4-(trifluoromethyl)pyrimidin-2(1H)-one (3a)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
1-(4-Methoxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3b)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
NOE experiment

$^1$H NMR (600 MHz, DMSO-$d_6$):
1-(Benzo[d][1,3]dioxol-5-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3c)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
1-(4-(Trifluoromethoxy)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3d)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
1-[4-(1H-Pyrazol-1-yl)phenyl]-4-(trifluoromethyl)pyrimidin-2(1H)-on (3e)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
1-(4-((1H-1,2,4-Triazol-1-yl)methyl)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3f)

$^1$H NMR (400 MHz, DMSO-$d_6$):

13C NMR (150 MHz, DMSO-$d_6$):
1-(4-Bromophenyl)-4-(trifluoromethyl)pyrimidin-2(1\textit{H})-one (3g)

\textbf{\textit{1}H NMR} (400 MHz, DMSO-\textit{d}_6):

\textbf{\textit{13}C NMR} (125 MHz, DMSO-\textit{d}_6):
4-(Trifluoromethyl)-1-(4-(trifluoromethyl)phenyl)pyrimidin-2(1H)-one (3h)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
4-(2-Oxo-4-(trifluoromethyl)pyrimidin-1(2H)-yl)benzamide (3i)

$^1$H NMR (400 MHz, DMSO-$d_6$):

1-(4-(Methylsulfonyl)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3j)

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
4-(2-Oxo-4-(trifluoromethyl)pyrimidin-1(2H)-yl)benzaldehyde (3k)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (150 MHz, DMSO-$d_6$):
1-(3-Hydroxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3l)

$^1$H NMR (400 MHz, DMSO-d$_6$):

$^{13}$C NMR (125 MHz, DMSO-d$_6$):
1-(4-Hydroxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3m)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (150 MHz, DMSO-$d_6$):
1-(4-(Hydroxymethyl)phenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3n)

$^1$H NMR (400 MHz, DMSO-d$_6$):

$^{13}$C NMR (125 MHz, DMSO-d$_6$):
1-(2-Methoxyphenyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3o)

$^1$H NMR (400 MHz, DMSO-$d_6$):

13C NMR (100 MHz, DMSO-$d_6$):
1-(o-Tolyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3p)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (100 MHz, DMSO-$d_6$):
1-(Pyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3q)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
1-(Pyridin-4-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3r)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (150 MHz, DMSO-$d_6$):
1-(6-Methoxypyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3s)

\(^1\)H NMR (400 MHz, DMSO-\(d_6\)):

\[
\begin{align*}
2.80 & \text{ (s, CH)} \\
1.86 & \text{ (s, CH)} \\
0.96 & \text{ (t, CH)} \\
0.95 & \text{ (t, CH)} \\
1.00 & \text{ (t, CH)} \\
3.91 & \text{ (s, OMe)} \\
6.98 & \text{ (d, ArH)} \\
6.99 & \text{ (d, ArH)} \\
7.00 & \text{ (d, ArH)} \\
7.92 & \text{ (d, ArH)} \\
7.94 & \text{ (d, ArH)} \\
8.34 & \text{ (s, NH)} \\
8.61 & \text{ (s, NH)} \\
8.63 & \text{ (s, NH)}
\end{align*}
\]

\(^{13}\)C NMR (125 MHz, DMSO-\(d_6\)):

\[
\begin{align*}
54.2 & \text{ (CH)} \\
99.7 & \text{ (C)} \\
111.0 & \text{ (C)} \\
116.7 & \text{ (C)} \\
118.9 & \text{ (C)} \\
121.1 & \text{ (C)} \\
123.3 & \text{ (C)} \\
131.3 & \text{ (N)} \\
138.2 & \text{ (C)} \\
144.9 & \text{ (C)} \\
154.6 & \text{ (C)} \\
155.3 & \text{ (C)} \\
162.2 & \text{ (C)} \\
162.5 & \text{ (C)} \\
162.8 & \text{ (C)} \\
163.1 & \text{ (C)} \\
163.8 & \text{ (C)}
\end{align*}
\]
1-(6-(Pyrrolidin-1-yl)pyridin-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3t)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
1-(Thiophen-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3u)

\(^1\)H NMR (400 MHz, DMSO-d₆):

\[^{13}\text{C} \text{NMR} \text{ (125 MHz, DMSO-d₆):}\]
4-(Trifluoromethyl)-1-(5-(trifluoromethyl)thiophen-3-yl)pyrimidin-2(1\textit{H})-one (3v).

\textit{\textsuperscript{1}H NMR} (400 MHz, DMSO-\textit{d}_6):

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{hnmr.png}
\end{figure}

\textit{\textsuperscript{13}C NMR} (125 MHz, DMSO-\textit{d}_6):

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{cnmr.png}
\end{figure}
1-(Furan-3-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (3w)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (100 MHz, DMSO-$d_6$):
(E)-1-Styryl-4-(trifluoromethyl)pyrimidin-2(1H)-one (5a)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
NOE experiment

1H NMR (600 MHz, DMSO-d6):

[Chemical structure image]

- Chemical labels:
  - CF₃
  - N
  - O
  - Ph
  - Ha
  - Hb
  - H6
  - 5a

[Graphical representation of NMR spectrum with peak assignments]
(E)-1-(3,5-Difluorostyryl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5b)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
(E)-1-(3-Methoxystyryl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5c)

$^1$H NMR (400 MHz, DMSO-$d_6$):

13C NMR (125 MHz, DMSO-$d_6$):
(E)-1-(4-Fluorostyryl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5d)

$^1$H NMR (400 MHz, DMSO-d$_6$):

$^{13}$C NMR (125 MHz, DMSO-d$_6$):
(E)-1-(4-Methoxystyryl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5e)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
4-(Trifluoromethyl)-1-vinylpyrimidin-2(1H)-one (5f)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
(E)-1-(Prop-1-en-1-yl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5g)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (150 MHz, DMSO-$d_6$):
(E)-1-(2-Cyclopropylvinyl)-4-(trifluoromethyl)pyrimidin-2(1H)-one (5h)

$^1$H NMR (400 MHz, DMSO-d$_6$):

$^{13}$C NMR (150 MHz, DMSO-d$_6$):
1,1'-[(2,4-bis(3-Methoxyphenyl)cyclobutane-1,3-diyl)bis(4-(trifluoromethyl)pyrimidin-2(1H)-one) (8)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
4-(Difluoromethyl)-1-phenylpyrimidin-2(1H)-one (9a)

**^1^H NMR (400 MHz, DMSO-d6):**

![NMR spectrum of 4-(Difluoromethyl)-1-phenylpyrimidin-2(1H)-one (9a)](image)

**^1^C NMR (125 MHz, DMSO-d6):**

![NMR spectrum of 4-(Difluoromethyl)-1-phenylpyrimidin-2(1H)-one (9a)](image)
4-(Chlorodifluoromethyl)-1-phenylpyrimidin-2(1H)-one (9b)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):
4-(Perfluoroethyl)-1-phenylpyrimidin-2(1H)-one (9c)

$^{1}H$ NMR (400 MHz, DMSO-$d_6$):

$^{13}C$ NMR (125 MHz, DMSO-$d_6$):
Ethyl 2-oxo-1-phenyl-4-(trifluoromethyl)-1,2-dihydropyrimidine-5-carboxylate (9f)

$^1$H NMR (400 MHz, DMSO-$d_6$):

13C NMR (125 MHz, DMSO-$d_6$):

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5-Bromo-1-phenyl-4-(trifluoromethyl)pyrimidin-2(1H)-one (9g)

$^1$H NMR (400 MHz, DMSO-$d_6$):

$^{13}$C NMR (125 MHz, DMSO-$d_6$):