Supporting Information

for

Regiodivergent synthesis of functionalized pyrimidines and imidazoles through phenacyl azides in deep eutectic solvents

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*Beilstein J. Org. Chem.* **2020**, *16*, 1915–1923. doi:10.3762/bjoc.16.158

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1. Compound characterization data

2-Azido ketones 2a, 2b, 2c, 2g, 2h, 2i and 2j were prepared as reported [1]. Spectroscopic data of α-azido ketones 2d, 2e, 2f, 2k, 2l and 2m are in agreement with those reported in the literature [2-5].

1.1 Spectroscopic data of α-azido ketones 2d, 2e, 2f, 2k, 2l and 2m

**2-Azido-1-(4-bromophenyl)ethanone** (2d) [2]. Orange solid (yield: 86%). $^1$H NMR (600 MHz, CDCl$_3$) δ 7.77 (d, $J = 8.5$ Hz, 2 H), 7.64 (d, $J = 8.5$ Hz, 2 H), 4.53 (s, 2 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 192.3, 133.0, 132.3, 129.4, 129.3, 54.7. FT-IR (KBr): 2905, 2851, 2104, 1694, 1584, 1568, 1485, 1401, 1342, 1283, 1219, 1178, 1069, 996, 911, 806, 721 cm$^{-1}$. HRMS calcd for C$_{11}$H$_9$BrNO$_2$Na [M +Na]$^+$. Found: 261.9586. 261.9579.

**4-(2-Azidoacetyl)benzonitrile** (2e) [3]. Brown solid (yield: 83%). $^1$H NMR (600 MHz, CDCl$_3$) δ 8.02 (d, $J = 7.3$ Hz, 2 H), 7.82 (d, $J = 7.3$ Hz, 2 H), 4.58 (s, 2 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 192.1, 137.2, 132.8, 132.7, 129.4, 128.4, 117.5, 117.4, 55.1. FT-IR (KBr): 3097, 2954, 2914, 2231, 2107, 1694, 1606, 1402, 1342, 1293, 1273, 1217, 1004, 914, 832, 765 cm$^{-1}$. GC-MS (70 eV) m/z (%): 158 [(M+28)$^+$, 1], 131 (15), 130 (100), 102 (43), 75 (11), 51 (6). HRMS calcd for C$_{12}$H$_{11}$N$_3$O [M-H]: 185.0469. Found: 185.0365.

**2-Azido-1-(4-methoxyphenyl)ethanone** (2f) [3]. Yellow solid (yield: 79%). $^1$H NMR (600 MHz, CDCl$_3$) δ 7.90 (d, $J = 8.9$ Hz, 2 H), 6.97 (d, $J = 8.9$ Hz, 2 H), 4.51 (s, 2 H), 3.89 (s, 3 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 191.6, 164.2, 130.3, 127.4, 114.2, 55.6, 54.6. FT-IR (KBr): 3031, 2922, 2851, 2124, 1683, 1600, 1517, 1454, 1421, 1361, 1302, 1272, 1240, 1178, 1025, 945, 825, 770 cm$^{-1}$. GC MS (70 eV) m/z (%): 163 [(M+28)$^+$, 1], 135 (100), 92 (17), 77 (21), 64 (10), 63 (9). HRMS calcd for C$_{14}$H$_{13}$N$_3$O$_2$ [M+Na]$^+$. Found: 214.0587. 214.0582.

**2-Azido-1-[[1,1'-biphenyl]-4-yl]ethanone** (2k) [4,5]. Dark yellow solid (yield: 67%). $^1$H NMR (600 MHz, CDCl$_3$) δ 8.08 (d, $J = 8.4$ Hz, 2 H), 7.73 (d, $J = 8.4$ Hz, 2 H), 7.84 (m, 2 H), 7.49 (m, 2 H), 7.43 (t, $J = 7.3$ Hz, 1 H), 4.5 (s, 2 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 192.8, 146.7, 139.4, 133.0, 129.1, 128.9, 128.5, 127.5, 127.2, 54.9 FT-IR (KBr): 3080, 2960, 2100, 1684 1604, 1581, 1460, 1447, 1420, 1276, 1226, 1191, 1116, 1075, 911, 847, 832, 809 cm$^{-1}$. HRMS calcd for C$_{14}$H$_{13}$N$_3$O [M+Na]$^+$. Found: 260.0794. 260.0800.
2-Azido-1-[2-(trifluoromethyl)phenyl]ethanone (2l) [2]. Colourless oil (yield: 71%). $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.77–7.75 (m, 1 H), 7.68–7.61 (m, 2 H), 7.47–7.42 (m, 1 H), 4.33 (s, 2 H). $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 197.9, 136.9, 132.2, 131.2, 127.3, 127.2 (q, $^3J_{C-F} = 9$ Hz), 127.2 (q, $^3J_{C-F} = 19$ Hz), 126.5 (q, $^1J_{C-F} = 273$ Hz), 57.8. FT-IR (film): 3083, 2110, 1702, 1583, 1310, 1271, 1165, 1110, 1033, 765 cm$^{-1}$. HRMS calcd for C$_9$H$_6$F$_3$N$_3$ONa [M+Na]$^+$: 252.0355. Found: 252.0354.

2-Azido-1-[4-(trifluoromethyl)phenyl]ethanone (2m) [2]. Orange solid (yield: 93%). $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 8.02 (d, $J = 8.1$ Hz, 2 H), 7.77 (d, $J = 8.1$ Hz, 2 H), 4.59 (s, 2 H). $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 192.5, 137.0, 135.4 (q, $^2J_{C-F} = 33$ Hz), 128.3, 126.0 (q, $^3J_{C-F} = 4$ Hz), 124.3 (q, $^1J_{C-F} = 271$ Hz), 55.1. FT-IR (KBr): 2918, 2108, 1704, 1620, 1585, 1514, 1412, 1325, 1218, 1169, 1130, 1068, 1016, 1005, 915, 846, 775, 700 cm$^{-1}$. GC-MS (70 eV) m/z (%): 201 [(M-28)$^+$, 1], 174 (11), 173 (100), 145 (63), 125 (7), 95 (9), 75 (8), 50 (4). HRMS calcd for C$_9$H$_6$F$_3$N$_3$O [M-H]: 228.0390. Found: 228.0300.
2.4 Spectroscopic data of 2-aryl-4-aryl-1H-imidazoles 3a–3k and 2-aryl-5-aryl-1H-imidazoles 3a’–3c’, 3f’, 3g’, 3i’, and 3k’

2-Benzoyl-4-phenyl-1H-imidazole (3a) and 2-benzoyl-5-phenyl-1H-imidazole (3a’) [6]. Light yellow solid (yield: 88%); 3a:3a’ = 57:43.1H NMR (600 MHz, CDCl3) δ 10.98–10.85 (bs, 1 H, minor), 10.78–10.65 (bs, 1 H, major), 8.78 (d, J = 7.5 Hz, 2 H, major), 8.60 (d, J = 7.6 Hz, 2 H, minor), 8.35–8.25 (m, 1 H, minor), 7.92 (d, J = 7.5 Hz, 2 H, major), 7.68–7.63 (m, 2 H, both tautomers), 7.59–7.53 (m, 2 H major + 2 H imidazolic protons of both tautomers), 7.48 (t, J = 7.5 Hz, 2 H, major), 7.45 (t, J = 7.5 Hz, 2 H, minor), 7.41 (t, J = 7.3 Hz, 1 H, minor), 7.34 (t, J = 7.3 Hz, 1 H, major). 13C NMR (150 MHz, CDCl3) (both tautomers): δ: 181.4, 145.6, 145.1, 144.6, 135.7, 135.5, 133.5, 133.3, 131.3, 130.9, 129.3, 128.9, 128.7, 128.3, 127.7, 125.3, 115.7. FT-IR (KBr): 3409, 3272, 3060, 2917, 2888 1669, 1620, 1597, 1571, 1454, 1438, 1291, 1273, 1168, 903, 868, 763, 732, 689 cm−1. GC-MS (70 eV) m/z (%): 248 (M+, 93), 220 (100), 193 (6), 116 (10), 105 (53), 89 (12), 77 (59), 51 (11). HRMS calcd for C16H12N2O [M-H]: 247.0871. Found: 247.0892.

2-(4-Methylbenzoyl)-4-(p-tolyl)-1H-imidazole (3b) and 2-(4-methylbenzoyl)-5-(4-tolyl)-1H-imidazole (3b’) [7].Yellow solid (yield: 78%); 3b:3b’ = 93:7.1H NMR (600 MHz, CDCl3) δ 11.43–11.41 (bs, 1 H, minor), 10.83–10.80 (bs, 1 H, major), 8.65–8.55 (m, 2 H, major), 8.27 (d, J = 8.2 Hz, 2 H, minor), 8.01 (bs, 1 H, minor), 7.92 (d, J = 8.1 Hz, 2 H, minor), 7.75–7.60 (m, 2 H, major), 7.57 (s, 1 H, major), 7.35 (d, J = 8.0 Hz, 2 H, major), 7.33–7.30 (m, 4 H, minor), 7.26 (m, 2 H, major), 6.99 (s, 1 H, minor), 2.47 (s, 3 H, major), 2.45 (s, 3 H, minor), 2.44 (s, 3 H, minor), 2.41 (s, 3 H, major). 13C NMR (150 MHz, CDCl3) (both tautomers) δ 181.1, 145.3, 144.3, 133.1, 131.3, 129.7, 129.9, 129.3, 129.1, 128.1, 125.3, 21.8, 21.3. FT-IR (KBr): 3272, 3096, 3023, 2917, 2850, 1617, 1603, 1566, 1454, 1411, 1372, 1289, 1270, 1168, 905, 821, 762 cm−1. GC-MS (70 eV) m/z (%): 276 (M+, 100), 248 (96), 221 (3), 184 (2), 119 (53), 103 (6), 91 (45), 77 (5), 65 (13). HRMS calcd for C18H16N2O [M-H]: 275.1263. Found: 275.1188.

2-(4-Chlorobenzoyl)-4-(4-chlorophenyl)-1H-imidazole (3c) and 2-(4-chlorobenzoyl)-5-(4-chlorophenyl)-1H-imidazole (3c’) [8]. Yellow solid (yield: 86%); 3c:3c’ = 88:12.1H NMR [600 MHz, (CD3)2CO] δ 12.80–12.55 (bs, 1 H major), 8.78 (d, J = 8.3 Hz, 2 H, major), 8.66 (d, J = 7.8 Hz, 2 H, minor), 8.06 (s, 1 H, major), 8.02 (d, J = 8.2 Hz, 2 H, major), 7.98 (m, 2 H, minor), 7.78 (s, 1 H, minor), 7.64 (d, J = 8.3 Hz, 2 H major), 7.61 (d, J = 8.4 Hz, 2 H minor), 7.52 (d, J = 7.9 Hz, 2 H minor), 7.46 (d, J = 8.3 Hz, 2 H major). 13C NMR [150 MHz, (CD3)2CO] (both tautomers) δ 179.3, 145.0, 142.5, 138.9, 138.8, 134.6, 132.8, 132.7, 132.5, 132.3, 129.1, 129.0, 128.4, 128.3, 127.3, 126.6, 117.9. FT-IR (KBr): 3429, 2923, 2851, 1658, 1587, 1488, 1400, 1290, 1251, 1166, 1091, 1013, 956, 929, 832, 760 cm−1. GC-MS (70 eV)
m/z (%): 316 (M⁺, 98), 288 (100), 150 (11), 139 (99), 123 (13), 113 (26), 111 (82), 75 (26). HRMS calcd for C₁₆H₁₀Cl₂N₂O [M+H]⁺: 317.0170. Found: 317.0238.

2-(4-Bromobenzoyl)-4-(4-bromophenyl)-1H-imidazole (3d). Yellow solid (yield: 86%). ¹H NMR [600 MHz, (CD₃)₂SO] δ 8.50 (d, J = 8.0 Hz, 2 H), 8.15 (s, 1 H), 7.88 (d, 2H, J = 7.8 Hz), 7.82 (d, J = 8.0 Hz, 2 H), 7.61 (d, J = 7.8 Hz, 2 H). ¹³C NMR [150 MHz, (CD₃)₂SO] δ 180.1, 145.0, 142.3, 135.3, 133.3, 133.1, 132.0, 131.9, 128.4, 127.9, 127.3, 125.7, 120.6, 119.9. FT-IR (KBr): 3436, 3250, 2922, 2852, 1617, 1581, 1558, 1462, 1451, 1412, 1389, 1292, 1247, 1172, 1130, 1070, 1010, 947, 905, 831, 792, 765 cm⁻¹. GC-MS (70 eV) m/z (%): 408 (41), 406 (M⁺, 100), 404 (44), 378 (70), 327 (7), 299 (13), 195 (11), 185 (78), 183 (84), 157 (67), 155 (65), 142 (17), 115 (38), 104 (18), 89 (11), 88 (18), 76 (46), 75 (26), 63 (12), 51 (12), 50 (13). HRMS calcd for C₁₆H₁₀Br₂N₂O [M-H]: 404.9061. Found: 404.9047.

2-(4-Cyanobenzoyl)-4-(4-cyanophenyl)-1H-imidazole (3e). Yellow waxy solid (yield: 78%). ¹H NMR (400 MHz, CDCl₃) δ 10.89 (bs, 1 H), 8.82 (d, 2H, J = 8.3 Hz), 7.98 (d, 2 H, J = 8.3 Hz), 7.85 (d, 2 H, J = 8.4 Hz), 7.73–7.71 (m, 3 H). ¹³C NMR [100 MHz, (CD₃)₂SO] δ 179.8, 144.7, 141.4, 139.3, 137.9, 132.8, 132.4, 131.2, 125.4, 121.6, 119.1, 118.3, 115.1, 109.4. FT-IR (KBr): 3430, 3275, 2920, 2850, 2228, 2106, 1642, 1609, 1472, 1420, 1385, 1290, 1169, 1085, 1016, 909, 845, 771 cm⁻¹. GC-MS (70 eV) m/z (%): 298 (M⁺, 67), 270 (100), 243 (6), 207 (3), 168 (2), 130 (69), 102 (89), 75 (23), 51 (12). HRMS calcd for C₁₈H₁₉N₄O [M-H]: 297.0782; Found: 297.0776.

2-(4-Methoxybenzoyl)-4-(4-methoxyphenyl)-1H-imidazole (3f) and 2-(4-Methoxybenzoyl)-5-(4-methoxyphenyl)-1H-imidazole (3f') [9]. Yellow solid (yield: 98%); 3f:3f' = 50:50. ¹H NMR (600 MHz, CDCl₃) (both tautomers) δ 10.95 (bs, 1 H), 10.71 (bs, 1 H), 8.92–8.60 (m, 2 H), 7.92–7.55 (m, 2 H), 7.50 (bs, 2 H), 7.04–7.02 (m, 4 H), 7.00–6.96 (m, 4 H), 3.92 (s, 6 H), 3.87 (s, 6 H). ¹³C NMR (150 MHz, CDCl₃) (both tautomers) δ 180.0, 179.7, 164.0, 163.9, 160.0, 159.3, 145.5, 145.2, 144.3, 133.8, 133.4, 129.3, 128.7, 128.5, 127.8, 126.8, 126.6, 126.4, 121.2, 114.7, 114.5, 114.2, 114.1, 113.8, 113.7, 55.5, 55.3. FT-IR (KBr): 3436, 3264, 2923, 1611, 1598, 1452, 1286, 1249, 1162, 1027, 904, 833, 825 cm⁻¹. GC-MS (70 eV) m/z (%): 308 (M⁺, 78), 280 (15), 265 (28), 200 (11), 135 (100), 92 (16), 77 (26). HRMS calcd for C₁₈H₁₆N₂O₃ [M+Na]⁺: 331.1053. Found: 331.1057.

2-(2,5-Dimethoxybenzoyl)-4-(2,5-dimethoxyphenyl)-1H-imidazole (3g) and 2-(2,5-Dimethoxybenzoyl)-5-(2,5-dimethoxyphenyl)-1H-imidazole (3g'). Yellow solid (yield: 94%); 3g:3g' = 93:7. ¹H NMR (600 MHz, CDCl₃) δ 11.43 (bs, 1 H, major), 10.64 (bs, 1 H, minor), 7.70–7.60 (m, 1 H, major), 7.55–7.53 (m, 1 H, minor), 7.44–7.43 (m, 1 H, minor), 7.35–7.28 (m, 1 H, minor).
H, major), 7.27–7.23 (m, 1 H, major), 7.23–7.21 (m, 1 H, minor), 7.10–7.06 (m, 1 H, minor),
7.06–7.02 (m, 1 H, major), 7.00–6.95 (m, 2 H, major), 6.92–6.85 (m, 2 H, minor), 6.90–6.85
(m, 1 H, major), 4.03–3.95 (bs, 3 H, minor), 3.87 (s, 3 H, minor), 3.83 (bs, 3 H, major), 3.81
(bs, 6 H, major), 3.77 (s, 3 H, minor), 3.60 (s, 3 H, minor), 3.50 (s, 3 H, minor). 13C NMR
(150 MHz, CDCl3) (both tautomers) δ 183.3, 154.0, 153.1, 152.5, 150.0, 144.6, 127.2, 121.8,
120.9, 118.5, 115.8, 114.8, 113.5, 112.7, 56.7, 56.2, 55.9, 55.8. FT-IR (KBr): 3431, 2922,
1627, 1513, 1469, 1378, 1270, 1137, 1022, 853, 768, 608, 452 cm−1. GC-MS (70 eV) m/z (%):
368 (M+, 72), 337 (100), 323 (19), 319 (10), 307 (38), 218 (12), 217 (15), 203 (15), 187
(8), 184 (8), 176 (11), 169 (11), 165 (46), 162 (19), 135 (11), 122 (11), 107 (17), 77 (11).
HRMS calcd for C20H20N2O5 [M+H]+: 369.1445. Found: 369.3906.

4-(2-Hydroxyphenyl)-2-(2-hydroxybenzoyl)-1H-imidazole (3h). Brown solid (yield: 71%).
1H NMR (300 MHz, CDCl3) δ 12.24 (bs, 1 H), 9.45 (bs, 1 H), 8.47–8.45 (m, 1 H), 8.11–8.10 (m, 1 H), 7.89–7.86 (m, 1 H), 7.68–7.67 (m, 1 H), 7.55–7.51 (m, 2 H), 7.17–7.15 (m, 1 H), 7.10–7.08 (m, 1 H). 13C NMR [75 MHz, (CD3)2SO] δ 175.5, 161.1,
155.6, 154.7, 139.8, 136.0, 134.9, 131.3, 129.3, 127.6, 127.3, 125.5, 123.2, 120.2, 119.4, 118.3. FT-IR (KBr): 3344, 2927,
2873, 1634, 1471, 1110, 1042, 956, 924, 864, 753 cm−1. HRMS calcd for C16H12N2O3 [M+H]+: 281.0842. Found: 281.0833.

4-(4-Fluorophenyl)-2-(4-fluorobenzoyl)-1H-imidazole (3i) and 5-(4-fluorophenyl)-2-(4-
fluorobenzoyl)-1H-imidazole (3i') [9,10]. Yellow solid (yield: 87%); 3i:3i′ = 90:10. 1H NMR
[600 MHz, (CD3)2CO] δ 8.90–8.87 (m, 2 H, major), 8.78–8.73 (m, 2 H, minor), 8.04–8.01
(m, 2 H, both tautomers), 7.98 (s, 1 H), 7.72 (s, 1 H, minor), 7.37–7.30 (m, 2 H, both
tautomers), 7.29–7.25 (m, 2 H, minor), 7.22–7.19 (m, 2 H, major). 13C NMR [150
MHz,(CD3)2CO] (both tautomers) δ 180.6, 167.4 (d, 1JCF = 253 Hz), 163.8 (d, 1JCF = 244 Hz), 146.7, 144.5, 135.6 (d, 3JCF = 9 Hz),
134.3, 132.1, 128.6 (d, 3JCF = 8 Hz), 118.8, 116.9 (d, 2JCF = 22 Hz), 116.8 (d, 2JCF = 22 Hz).
FT-IR (neat) 3435, 3276, 3128, 3096, 2922, 2618, 1598, 1583, 1565, 1510, 1452, 1291,
1241, 1170, 1160, 1101, 907, 842, 775 cm−1. GC-MS (70 eV) m/z (%): 284 (M+, 100), 256
(87), 229 (5), 201 (2), 189 (1), 160 (3), 142 (2), 134 (10), 123 (79), 107 (13), 95 (53), 81 (2),
75 (12), 57 (3). HRMS calcd for C15H10F2O2 [M+Na]+: 307.0653. Found: 307.0653.

4-(2-Naphthyl)-2-(2-naphthyl-1H-imidazole (3j) [10]. Light brown solid (yield: 67%). 1H NMR
[600 MHz, (CD3)2SO] δ 9.50–9.40 (bs, 1 H), 8.57–8.46 (m, 2 H), 8.30–8.20 (m, 2 H),
8.17–8.09 (m, 3 H), 8.05 (d, J = 8.0 Hz, 1 H), 8.01–7.95 (m, 3 H), 7.92 (d, J = 7.8 Hz, 1 H), 7.73–7.70 (m, 1 H), 7.69–7.64 (m, 1 H), 7.56–7.46 (m, 2 H). 13C NMR [150 MHz,
(CD3)2SO] δ 180.7, 145.2, 135.0, 133.3, 133.0, 132.4, 132.0, 130.0, 129.4, 128.8, 128.3, 127.9, 127.7, 127.3,
126.9, 126.5, 125.9, 123.8, 123.0, 119.3. FT-IR (KBr): 3279, 3053, 2921, 2851, 1632, 1611, 1480, 1447, 1360,
1279, 1269, 1230, 1160, 1125, 925, 860, 823, 806, 781, 738 cm−1. HRMS calcd for
C24H16N2O [M-H]−: 347.1184. Found: 347.1177.
4-[1,1'-Biphenyl-4-yl]-2-(4-phenybenzoyl)-1H-imidazole (3k) and 5-[1,1'-biphenyl-4-yl]-2-(4-phenybenzoyl)-1H-imidazole (3k') [10]. Brown solid (yield: 32%); 3k:3k' = 79:21. 

$^1$HNMR [600 MHz, (CD$_3$)$_2$SO] $\delta$ 10.21 (bs, 1 H, minor), 8.71 (d, $J = 8.2$ Hz, 2 H, major), 8.59 (d, $J = 7.2$ Hz, 2 H, minor), 8.15 (s, 1 H), 8.08–8.05 (m, 2 H, minor), 8.03 (d, $J = 8.1$ Hz, 2 H, major), 8.03–7.90 (m, 2 H, minor), 7.93 (d, $J = 8.2$ Hz, 2 H, major), 7.90–7.87 (m, 2 H, minor), 7.82 (d, $J = 7.6$ Hz, 2 H, major), 7.80-7.76 (m, 2 H, minor), 7.74 (d, $J = 8.2$ Hz, 2 H, major), 7.72 (d, $J = 7.8$ Hz, 2 H, major), 7.53 (t, $J = 7.6$ Hz, 2 H, major), 7.50–7.43 (m, 3 H, major + minor), 7.37 (t, $J = 7.3$ Hz, 1 H, major). 

$^{13}$CNMR [150 MHz, (CD$_3$)$_2$SO] $\delta$ 180.6, 145.3, 144.9, 143.0, 140.3, 139.5, 139.3, 135.2, 133.3, 131.9, 129.6, 129.4, 128.9, 127.8, 127.6, 127.5, 127.4, 127.0, 126.9, 125.9, 119.3. FT-IR (KBr): 3421, 3271, 3055, 3031, 2923, 2852, 1670, 1615, 1600, 1485, 1458, 1404, 1294, 1275, 1170, 1115, 1076, 1006, 907, 840, 749, 723, 695 cm$^{-1}$. HRMS calcd for C$_{28}$H$_{20}$N$_2$O [M-H]: 399.1503; Found: 399.1489.
Spectroscopic data of 2,4-diaryl-6-arylpurimidines 7a–h

2,4-Dibenzoyl-6-phenylpyrimidine (7a). Yellow waxy solid (yield: 57%). 1H NMR (600 MHz, CDCl3) δ 9.21 (s, 1 H), 8.14–8.12 (m, 2 H), 8.06–8.04 (m, 3 H), 7.66–7.63 (m, 2 H), 7.56–7.50 (m, 8 H). 13C NMR (150 MHz, CDCl3) δ 192.4, 192.2, 152.9, 151.4, 149.8, 140.0, 133.8, 133.7, 131.1, 130.7, 130.6, 129.3, 128.5, 128.4, 127.5. FT-IR (KBr): 3059, 3033, 2922, 2851, 1674, 1663, 1596, 1581, 1450, 1319, 1290, 1249, 1168, 1121, 1067, 957, 938, 766, 717, 704, 693 cm−1. GC-MS (70 eV) m/z (%): 364 (M+, 50), 336 (4), 308 (3), 287 (9), 259 (26), 232 (3), 204 (1), 128 (3), 105 (100), 77 (59), 51 (7). HRMS calcd for C24H18N2O2 [M+Na]+: 387.1109. Found: 387.1117.

2,4-Bis(4-methylbenzoyl)-6-tolypyrimidine (7b). Light yellow oil (yield: 52%). 1H NMR (600 MHz, CDCl3) δ 9.15 (s, 1 H), 8.03 (d, J = 8.1 Hz, 2 H), 7.95–7.92 (m, 4 H), 7.34 (d, J = 8.1 Hz, 2 H), 7.31–7.28 (m, 4 H), 2.45–2.44 (m, 9 H). 13C NMR (150 MHz, CDCl3) δ 192.1, 191.9, 153.0, 151.3, 149.5, 144.7, 144.6, 141.5, 139.6, 133.0, 132.9, 132.1, 130.8, 130.7, 130.0, 129.2, 129.1, 127.4, 21.8, 21.5. FT-IR (neat): 3032, 2918, 2850, 1660, 1606, 1548, 1519, 1447, 1410, 1315, 1296, 1256, 1181, 1119, 1068, 957, 931, 825, 773, 751, 737 cm−1. GC-MS (70 eV) m/z (%): 406 (M+, 44), 391 (1), 378 (3), 377 (2), 350 (3), 287 (25), 260 (2), 203 (2), 142 (2), 119 (100), 91 (42), 65 (10), 51 (7). HRMS calcd for C27H22N2O2 [M+Na]+: 429.1579. Found: 429.1592.

2,4-Bis(4-chlorobenzoyl)-6-(4-chlorophenyl)pyrimidine (7c). Light brown solid (yield: 45%). 1H NMR (600 MHz, CDCl3) δ 9.15 (s, 1 H), 8.04 (d, J = 8.6 Hz, 2 H), 7.99 (d, J = 8.6 Hz, 2 H), 7.94 (d, J = 8.6 Hz, 2 H), 7.51 (d, J = 8.6 Hz, 2 H), 7.48–7.46 (m, 4 H). 13C NMR (150 MHz, CDCl3) δ 190.9, 190.6, 152.6, 150.5, 149.6, 140.6, 140.5, 139.8, 137.8, 133.5, 133.4, 132.9, 132.1, 131.9, 129.7, 129.0, 128.9, 128.7. FT-IR (KBr): 2918, 2850, 1660, 1588, 1401, 1092, 833 cm−1. GC-MS (70 eV) m/z (%): 470 [M+Cl][Cl]2+ (3), 468 [M+Cl][Cl]2+ (10), 466 [M+Cl][Cl]2+ (10), 355 (1), 329 (4), 327 (6), 142 (2), 141 (33), 139 (100), 136 (2), 113 (12), 111 (38), 75 (10). HRMS calcd for C24H12Cl3N2O2 [M+35Cl][35Cl]3-H]: 464.9970. Found: 464.9964 [M+35Cl][35Cl]3-H], 466.9580 [M+35Cl][35Cl]2-H], 468.9550 [M+35Cl][35Cl]2-H].

2,4-Bis(4-bromobenzoyl)-6-(4-bromophenyl)pyrimidine (7d). Brown solid (yield: 82%). 1H NMR (600 MHz, CDCl3) δ 9.18 (s, 1 H), 7.99 (d, J = 8.4 Hz, 2 H), 7.93 (d, J = 8.4 Hz, 2 H), 7.88 (d, J = 8.4 Hz, 2 H), 7.70 (d, J = 8.4 Hz, 2 H), 7.68–7.66 (m, 4 H). 13C NMR (150 MHz, CDCl3) δ 191.1, 190.8, 152.6, 150.6, 149.6, 139.8, 133.9, 133.4, 132.7, 132.2, 132.0, 131.9, 131.8. FT-IR (KBr): 2918, 2849, 2849, 1660, 1584, 1483, 1396, 1290, 1167, 1070, 1009, 955, 928, 829, 756 cm−1. HRMS calcd for C24H14N2Br3O2 [M+H]+: 598.8605. Found: 598.8460.
2,4-Bis-(2-hydroxybenzoyl)-6-(2-hydroxyphenyl)pyrimidine (7e). Yellow pale solid (yield: 75%). $^1$H NMR (600 MHz, CDCl$_3$) δ 12.24 (bs, 1 H), 11.37 (bs, 2 H), 9.46 (s, 1 H), 8.47–8.45 (m, 1 H), 8.11–8.10 (m, 1 H), 7.89–7.86 (m, 1 H), 7.68–7.67 (m, 1 H), 7.55–7.51 (m, 2 H), 7.17–7.15 (m, 1 H), 7.10–7.07 (m, 1 H), 6.89–6.88 (m, 2 H), 6.80–6.79 (m, 2 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 175.6, 161.2, 155.6, 154.8, 154.7, 139.8, 136.1, 135.0, 132.8, 131.3, 130.2, 129.3, 127.7, 127.4, 125.6, 123.2, 122.3, 120.9, 120.2, 119.5, 118.4, 117.2, 115.9, 115.6. FT IR (KBr): 3341, 2918, 2850, 1614, 1469, 1157, 1038, 886, 754 cm$^{-1}$. HRMS calcd for C$_{24}$H$_{18}$N$_2$O$_5$ [M+H]$^+$: 413.1132. Found: 413.1126.

2,4-Bis(4-fluorobenzoyl)-6-(4-fluorophenyl)pyrimidine (7f). Orange solid (yield: 61%). $^1$H NMR (600 MHz, CDCl$_3$) δ 9.15 (s, 1 H), 8.12–8.10 (m, 4 H), 8.07–8.05 (m, 2 H), 7.24–7.20 (m, 3 H), 7.19–7.17 (m, 3 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 190.7, 190.4, 166.3 (d, $^1$JC-F = 257 Hz), 164.8 (d, $^1$JC-F = 253 Hz), 152.8, 150.5, 149.5, 139.6, 133.6 (d, $^3$JC-F = 9 Hz), 133.3 (d, $^3$JC-F = 9 Hz), 131.6, 130.8 (m), 130.7 (d, $^3$JC-F = 9 Hz), 129.6 (d, $^2$JC-F = 9 Hz), 116.6 (d, $^2$JC-F = 22 Hz), 116.2 (d, $^2$JC-F = 22 Hz), 115.9 (d, $^2$JC-F = 17 Hz), 115.7 (d, $^2$JC-F = 17 Hz). FT-IR (KBr): 2919, 2805, 1668, 1598, 1506, 1411, 1294, 1236, 1156, 1120, 1106, 958, 932, 489, 785, 751 cm$^{-1}$. GC-MS (70 eV) m/z (%): 418 (M$^+$, 25), 323 (2), 295 (9), 146 (2), 124 (7), 123 (100), 120 (2), 95 (36), 75 (6), 77 (46). HRMS calcd for C$_{24}$H$_{12}$F$_3$N$_2$O$_2$ [M+H]$^+$: 417.0856. Found: 417.0849.

2,4-Bis[2-(trifluoromethyl)benzoyl]-6-[2-(trifluoromethyl)phenyl]pyrimidine (7g). Yellow solid (yield: 88%). $^1$H NMR (600 MHz, CDCl$_3$) δ 8.81 (s, 1 H), 7.90–7.53 (m, 12 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 204.4, 183.0, 143.9, 135.7, 135.3, 134.5, 132.0, 131.7, 131.6, 131.5, 131.2, 130.6, 130.0, 127.1, 127.0, 122.8, 122.7, 122.2, 122.1, 119.8. FT-IR (KBr): 2919, 2851, 1693, 1583, 1449, 1365, 1320, 1141, 1061, 1036, 961, 934, 872, 768 cm$^{-1}$. GC-MS (70 eV) m/z (%): 568 (M$^+$, 5), 499 (9), 395 (2), 375 (3), 173 (100), 145 (42), 125 (2), 95 (2). HRMS calcd for C$_{27}$H$_{13}$N$_2$F$_9$O$_2$ [M+Na]$^+$: 591.0726. Found: 591.0731.

2,4-Bis[4-(trifluoromethyl)benzoyl]-6-[4-(trifluoromethyl)phenyl]pyrimidine (7h). Brown solid (yield: 69%). $^1$H NMR (600 MHz, CDCl$_3$) δ 9.29 (s, 1 H), 8.25 (d, $J = 8.2$ Hz, 2 H), 8.19 (d, $J = 8.2$ Hz, 2 H), 8.16 (d, $J = 8.1$ Hz, 2 H), 7.81–7.80 (m, 6 H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ 190.9, 190.8, 152.5, 150.5, 150.0, 140.7, 137.8, 137.7, 137.6, 135.3, 131.0, 130.8, 127.9, 126.4, 125.7, 125.6, 125.4, 121.9, 120.8. FT-IR (KBr): 2918, 2850, 1661, 1411, 1325, 1127, 842 cm$^{-1}$. GC-MS (70 eV) m/z (%): 568 (M$^+$, 20), 549 (4), 423 (2), 395 (7), 196 (1), 173 (100), 145 (44), 95 (3), 75 (1). HRMS calcd for C$_{27}$H$_{13}$N$_2$F$_9$O [M+Na]$^+$: 591.0726. Found: 591.0729.
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2. NMR spectra

2.1 NMR spectra of 2-azido ketones 2d, 2e, 2f, 2k, 2l, and 2m

$^1$H and $^{13}$C NMR spectra of 2-azido-1-(4-bromophenyl)ethanone (2d)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 4-(2-azidoacetyl)benzonitrile (2e)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
\(^1\text{H}\) and \(^{13}\text{C}\) NMR spectra of \(2\text{-azido-1-(4-methoxyphenyl)ethanone (2f)}\)

\(\text{\(^1\text{H NMR (600 MHz, CDCl}_3\)}}\)

\(\text{\(^{13}\text{C NMR (150 MHz, CDCl}_3\)}}\)
$^1\text{H}$ and $^{13}\text{C}$ NMR spectra of 2-azido-1-([1,1'-biphenyl]-4-yl)ethanone (2k)

$^1\text{H}$ NMR (600 MHz, CDCl$_3$)

$^{13}\text{C}$ NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2-azido-1-[2-(trifluoromethyl)phenyl]ethanone (2l)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
\(^1\)H and \(^{13}\)C NMR spectra of 2-azido-1-[4-(trifluoromethyl)phenyl]ethanone (2m)

\(^1\)H NMR (600 MHz, CDCl\(_3\))

\(^{13}\)C NMR (150 MHz, CDCl\(_3\))
2.2 NMR spectra of 2-aroyl-4-aryl-1H-imidazoles 3a–3k and 2-aroyl-5-aryl-1H-imidazoles 3a′–3c′, 3f′, 3g′, 3i′, and 3k′

$^1$H and $^{13}$C NMR spectra of 2-benzoyl-4-phenyl-1H-imidazole (3a) and 2-benzoyl-5-phenyl-1H-imidazole (3a′)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2-(4-methylbenzoyl)-4-(p-tolyl)-1H-imidazole (3b) and 2-(4-methylbenzoyl)-5-(p-tolyl)-1H-imidazole (3b')

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2-(4-chlorobenzoyl)-4-(4-chlorophenyl)-1$H$-imidazole (3c) and 2-(4-chlorobenzoyl)-5-(4-chlorophenyl)-1$H$-imidazole (3c’)

$^1$H NMR [600 MHz, (CD$_3$)$_2$CO]

$^{13}$C NMR [150 MHz, (CD$_3$)$_2$CO]
$^1$H and $^{13}$C NMR spectra of 2-(4-bromobenzoyl)-4-(4-bromophenyl)-1H-imidazole (3d)

$^1$H NMR [600 MHz, (CD$_3$)$_2$SO]

$^{13}$C NMR [150 MHz, (CD$_3$)$_2$SO]
$^1$H and $^{13}$C NMR spectra of $2$-(4-cyanobenzoyl)$-4$-(4-cyanophenyl)$-1$H-imidazole (3e) and $2$-(4-cyanobenzoyl)$-5$-(4-cyanophenyl)$-1$H-imidazole (3e').

$^1$H NMR [600 MHz, CDCl$_3$]

$^{13}$C NMR [100 MHz, (CD$_3$)$_2$SO $\delta$]
\(^1\text{H}\) and \(^{13}\text{C}\) NMR spectra of 2-(4-methoxybenzoyl)-4-(4-methoxyphenyl)-1\(^H\)-imidazole (3f) and 2-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-1\(^H\)-imidazole (3f’)

\(^1\text{H}\) NMR (600 MHz, CDCl\(_3\))

\(^{13}\text{C}\) NMR (150 MHz, CDCl\(_3\))
$^1$H and $^{13}$C NMR spectra of 2-(2,5-dimethoxybenzoyl)-4-(2,5-dimethoxyphenyl)-1H-imidazole (3g) and 2-(2,5-dimethoxybenzoyl)-5-(2,5-dimethoxyphenyl)-1H-imidazole (3g')

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2-(2-hydroxybenzoyl)-4-(2-hydroxyphenyl)-1H-imidazole (3h).

$^1$H NMR [300 MHz, CDCl₃]

$^{13}$C NMR [75 MHz, CDCl₃]
$^1$H and $^{13}$C NMR spectra of 2-(4-fluorobenzoyl)-4-(4-fluorophenyl)-1H-imidazole (3i) and 2-(4-fluorobenzoyl)-5-(4-fluorophenyl)-1H-imidazole (3i').

$^1$H NMR [600 MHz, (CD$_3$)$_2$CO]

$^{13}$C NMR [150 MHz, (CD$_3$)$_2$CO]
$^1$H and $^{13}$C NMR spectra of $4\text{-}(2\text{-naphtyl})\text{-}2\text{-}(2\text{-naphtyloyl})\text{-}1\text{H-imidazole (3j)}$

$^1$H NMR [600 MHz, (CD$_3$)$_2$SO, $\delta$]

$^{13}$C NMR [150 MHz, (CD$_3$)$_2$CO, $\delta$]
$^1$H and $^{13}$C NMR spectra of 4-[1,1'-biphenyl-4-yl]-2-(4-phenybenzoyl)-1H-imidazole (3k) and 5-[1,1'-biphenyl-4-yl]-2-(4-phenybenzoyl)-1H-imidazole (3k')

$^1$H NMR [600 MHz, (CD$_3$)$_2$SO]

$^{13}$C NMR [150 MHz, (CD$_3$)$_2$SO]
2.3 NMR spectra of 2,4-diaroyl-6-arylpyrimidines 7a–h

$^1$H and $^{13}$C NMR spectra of 2,4-dibenzoyl-6-phenylpyrimidine (7a)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$, δ)
$^1$H and $^{13}$C NMR spectra of 2,4-bis-(4-methylbenzoyl)-6-tolylpyrimidine (7b)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2,4-bis(4-chlorobenzoyl)-6-(4-chlorophenyl)pyrimidine (7c)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$, δ)
$^1$H and $^{13}$C NMR spectra of 2,4-bis(4-bromobenzoyl) 6-(4-bromophenyl)pyrimidine (7d)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2,4-bis-[2-(hydroxybenzoyl)]-6-(2-hydroxyphenyl) pyrimidine (7e)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2,4-bis(4-fluorobenzoyl)-6-(4-fluorophenyl)pyrimidine (7f)

$^1$H NMR (600 MHz, CDCl$_3$)

$^{13}$C NMR (150 MHz, CDCl$_3$)
$^1$H and $^{13}$C NMR spectra of 2,4-bis[2-(trifluoromethyl)benzoyl]-6-[2-(trifluoromethyl)phenyl]pyrimidine (7g)

$^1$H NMR (600 MHz, CDCl₃)

$^{13}$C NMR (150 MHz, CDCl₃)
\(^1\)H and \(^{13}\)C NMR spectra of 2,4-bis-[4-(trifluoromethyl)benzoyl]-6-(4-trifluoromethyl)phenylpyrimidine (7h)

\(^1\)H NMR (600 MHz, CDCl\(_3\))

\(^{13}\)C NMR (150 MHz, CDCl\(_3\))