Supporting Information

Copper Catalyzed Aerobic Oxidative Cyclization and Ketonization: One Pot Synthesis of Benzoimidazo[1,2-a]imidazolones

Manikandan Selvaraju,\textsuperscript{a} Tzuen-Yang Ye,\textsuperscript{a} Chia-Hsin Li,\textsuperscript{a,\textit{b}} Pei-Heng Ho,\textsuperscript{a} and Chung-Ming Sun\textsuperscript{* a,\textit{b}}

\textsuperscript{a} Department of Applied Chemistry, 1001 Ta-Hseuh Road, National Chiao Tung University, Hsinchu 300-10, Taiwan, ROC.

\textsuperscript{b} Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, 100, Shih-Chuan 1\textsuperscript{st} Road, Kaohsiung 807-08, Taiwan, ROC.

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General Remarks:

Methanol and acetone were distilled before use. All reactions were performed under an inert atmosphere with unpurified reagents and dry solvents. Analytical thin-layer chromatography (TLC) was performed using 0.25mm silica gel coated plates. Flash chromatography was performed using the indicated solvent and silica gel 60 (230-400 mesh). $^1$H NMR (300 MHz) and $^{13}$C NMR (75 MHz) spectra were recorded on a 300 MHz spectrometer. Chemical shifts are reported in parts per million (ppm) on the scale from an internal standard.

Preparation of 2-aminobenzimidazoles 1.

The preparation of 2-aminobenzimidazoles 1 is accomplished by following literature methods.$^{15}$ The synthesis of 2-aminobenzimidazoles 1 from 1-fluoro-2-nitrobenzene $\mathbf{1s}$ involves a sequential three steps as shown in Scheme 6. Reaction of 1-fluoro-2-nitrobenzene $\mathbf{1s}$ with primary amines furnished ortho nitro anilines $\mathbf{2s}$. Subsequent steps involved a nitro group reduction to $\mathbf{3s}$ followed by ring closure with cyanogen bromide to deliver 2-aminobenzimidazole 1.

![Scheme 6. Preparation of 2-aminobenzimidazoles 1](image-url)
Table 2(continued). Three component synthesis of benzoimidazo[1,2-a]imidazolones

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\(^b\) Isolated Yields
Experimental Procedure for the synthesis of methyl 3-benzoyl-9-isopropyl-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5a)

A solution of methyl 2-amino-1-isopropyl-1H-benzo[d]imidazole-5-carboxylate 1a (0.12 g, 0.52 mmol) in toluene (10 mL) was added benzaldehyde (0.065 g, 0.62 mmol), phenyl acetylene (0.063 g, 0.62 mmol), Cs₂CO₃ (0.25 g, 0.78 mmol) followed by CuI (0.0098 g, 10 mol %) and the resulting reaction mixture was allowed to reflux at 110 °C under oxygen atmosphere. Upon completion (8-10 h) of the reaction, the mixture was filtered through a pad of celite and washed with ethyl acetate (25 mL x 2). The filtrate was concentrated under reduced pressure to give the crude mixture, which was purified by column chromatography on silica gel to afford compound 5a (0.18 g, 77 %).

Spectral Data of compounds 5 and 6:

**Methyl 3-benzoyl-9-isopropyl-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5a):**

- **¹H NMR (300 MHz, CDCl₃)**: δ 9.28 (s, 1H), 8.15 (d, J = 8.6 Hz, 1H), 7.57 (d, J = 8.2 Hz, 2H), 7.49 (d, J = 8.6 Hz, 1H), 7.28-7.26 (m, 3H), 7.08-6.99 (m, 5H), 4.99 (m, 1H), 3.95 (s, 3H), 1.80 (d, J = 6.8 Hz, 6H); **¹³C NMR (75 MHz, CDCl₃)**: δ 185.5, 167.0, 154.9, 150.0, 138.5, 137.5, 134.4, 131.4, 130.1, 129.5, 128.0, 127.7, 127.6, 125.9, 125.4, 122.8, 117.6, 109.7, 52.2, 48.3, 20.7; **MS (ESI-MS)** m/z: 460 (M+Na); **HRMS calcd for C₂₇H₂₃N₃O₃(M+Na):** 460.1637; Found 460.1635; **IR (cm⁻¹, neat):** 3063, 2984, 2937, 1716, 1618, 1568.

**Methyl 3-benzoyl-9-pentyl-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5b):**

- **¹H NMR (300 MHz, CDCl₃)**: δ 9.27 (s, 1H), 8.15 (d, J = 8.6 Hz, 1H), 7.55-7.50 (m, 5H), 7.45 (m, 1H), 7.27-7.23 (m, 3H), 7.14-7.03 (m, 5H), 4.35 (t, J = 7.0 Hz, 2H), 3.96 (s, 3H), 2.04-2.02 (m, 2H), 1.42-1.39 (m, 4H), 0.91 (t, J = 6.8 Hz, 3H); **¹³C NMR (75 MHz, CDCl₃)**: δ 185.5, 167.0, 155.0, 150.6, 138.4, 134.3, 131.4, 130.1, 129.5, 128.1, 127.6, 126.1, 125.4, 123.0, 121.9, 117.6, 109.1, 52.2, 43.6, 28.9, 28.4, 22.3, 13.9; **MS (ESI-MS)** m/z: 488 (M+Na); **HRMS (ESI)** calcd for C₂₉H₂₇N₃O₃(M+Na): 488.1950; Found 488.1952; **IR (cm⁻¹, neat):** 3052, 2940, 2843, 1717, 1618, 1588.
Methyl 3-(4-methylbenzoyl)-9-pentyl-2-(p-tolyl)-9H-benzo[d]imidazo[1,2-a]
imidazole-6-carboxylate (5c): \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 9.19 (s, 1H), 8.15 (d, \(J = 8.3\) Hz, 1H), 7.45 (d, \(J = 8.3\) Hz, 2H), 7.39 (d, \(J = 8.6\) Hz, 1H), 7.18 (d, \(J = 7.8\) Hz, 2H), 6.90-6.87 (m, \(J = 7.3\) Hz, 4H), 4.34 (t, \(J = 7.1\) Hz, 2H), 3.95 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H), 1.96-1.94 (m, 2H), 1.68-1.65 (m, 4H), 1.41 (m, 2H), 0.90 (t, \(J = 6.8\) Hz, 3H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 185.4, 167.1, 154.5, 149.9, 142.0, 137.8, 137.5, 135.8, 131.6, 130.0, 129.7, 128.3, 125.7, 125.4, 122.6, 121.3, 117.4, 109.6, 52.7, 48.2, 21.4, 21.1, 20.7; MS (ESI-MS) \(m/z\): 449.4 (M+H); HRMS (ESI) calcd for C\(_{31}\)H\(_{31}\)N\(_3\)O\(_3\)(M+H): 494.2438; Found 494.2451; IR (cm\(^{-1}\), neat): 2954, 2926, 2855, 1717, 1621, 1605, 1583.

Methyl 3-benzoyl-2-phenyl-9-propyl-9H-benzo[d]imidazo[1,2-a]imidazole
-6-carboxylate (5d): \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 9.28 (d, \(J = 1.6\) Hz, 1H), 8.18 (d, \(J = 8.6\) Hz, 1H), 7.61 – 7.52 (m, 2H), 7.43 (d, \(J = 8.6\) Hz, 1H), 7.32 – 7.27 (m, 2H), 7.24 (t, \(J = 8.6\) Hz, 1H), 7.16 – 7.03 (m, 5H), 4.34 (t, \(J = 7.4\) Hz, 2H), 3.97 (s, 3H), 2.05 (sextet, \(J = 7.4\) Hz, 2H), 1.07 (t, \(J = 7.4\) Hz, 3H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 186.0, 167.5, 155.5, 151.1, 138.9, 138.8, 134.8, 131.9, 130.6, 129.9, 128.5, 128.1, 126.6, 125.9, 123.5, 122.4, 118.1, 109.6, 52.7, 45.6, 22.6, 11.8; MS (ESI-MS) \(m/z\): 437.5 (M+H); HRMS (ESI) calcd for C\(_{27}\)H\(_{23}\)N\(_3\)O\(_3\)(M+H): 437.1734; Found 437.2538; IR (cm\(^{-1}\), neat): 2973, 2934, 2867, 1714, 1620, 1584.

Methyl 9-isopropyl-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo[d]imidazo
[1,2-a]imidazole-6-carboxylate (5e): \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 9.19 (d, \(J = 1.4\) Hz, 1H), 8.13 (dd, \(J = 8.6, 1.4\) Hz, 1H), 7.47-7.44 (m, 3H), 7.18 (dd, \(J = 8.0, 1.4\) Hz, 2H), 6.92-6.86 (m, 4H), 4.97 (m, 1H), 3.95 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H), 1.78 (d, \(J = 6.9\) Hz, 6H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 185.4, 167.1, 154.5, 149.9, 142.0, 137.8, 137.5, 135.8, 131.6, 130.0, 129.7, 128.3, 125.7, 125.4, 122.6, 121.3, 117.4, 109.6, 52.1, 48.2, 21.4, 21.1, 20.7; MS (ESI-MS) \(m/z\): 466.3 (M+H); HRMS (ESI) calcd for C\(_{29}\)H\(_{27}\)N\(_3\)O\(_3\)(M+H): 466.2125; Found 466.2132; IR (cm\(^{-1}\), neat): 3025, 2979, 2947, 1717, 1619, 1604, 1571.

Methyl 9-isopropyl-3-(4-methoxybenzoyl)-2-(4-methoxyphenyl)-9H-benzo
[d]imidazo[1,2-a]imidazole-6-carboxylate (5f): \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 9.14 (s, 1H), 8.13 (dd, \(J = 8.7, 1.7\) Hz, 1H), 7.63 (d, \(J = 8.5\) Hz, 2H), 7.46 (d, \(J = 8.5\) Hz,
1H), 7.30-7.26 (m, 2H), 6.68-6.63 (m, 4H), 4.99 (m, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 1.79 (d, J = 6.9 Hz, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 184.9, 167.5, 162.9, 159.9, 154.1, 150.3, 138.0, 132.3, 131.9, 131.5, 127.7, 126.1, 125.9, 123.1, 121.3, 117.7, 113.8, 113.6, 110.1, 55.8, 55.7, 52.6, 48.6, 21.2; MS (ESI-MS) $m/z$: 498.4 (M+H)$^+$; HRMS (ESI) calcd for C$_{29}$H$_{27}$N$_3$O$_5$ (M+H)$^+$: b498.2023; Found 498.2018; IR (cm$^{-1}$, neat): 2952, 2931, 2839, 1716, 1599, 1571.

Methylbenzoyl-9-cyclopentyl-2-phenyl-9H-benzo[d]imidazo[1,2-a]
imidazole-6-carboxylate (5g): $^1$H NMR (300 MHz, CDCl$_3$) δ 9.28 (s, 1H), 8.15 (d, J = 8.6 Hz, 1H), 7.55-7.48 (m, 3H), 7.28-7.23 (m, 3H), 7.12-7.05 (m, 5H), 5.08 (m, 1H), 3.96 (s, 3H), 2.47-2.40 (m, 2H), 2.26-2.20 (m, 2H), 2.10-2.06 (m, 2H), 1.89-1.80 (m, 2H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 185.5, 167.0, 154.8, 150.2, 138.5, 137.8, 134.4, 131.4, 130.2, 129.5, 128.0, 127.7, 127.6, 125.8, 125.4, 123.8, 117.6, 109.8, 56.6, 52.2, 29.9, 24.6; MS (ESI-MS) $m/z$: 486 (M+Na)$^+$; HRMS calcd for C$_{29}$H$_{25}$N$_3$O$_3$ (M+Na)$^+$: m/z: 486.1797; Found 486.1794; IR (cm$^{-1}$, neat): 3066, 2948, 2872, 1715, 1617, 1569.

Methyl 9-cyclopentyl-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo]
imidazo[1,2-a]imidazole-6-carboxylate (5h): $^1$H NMR (400 MHz, CDCl$_3$) δ 9.17 (d, J = 1.4 Hz, 1H), 8.14-8.12 (m, 1H), 7.48-7.44 (m, 3H), 7.21 (d, J = 6.6 Hz, 2H), 5.08 (m, 1H), 6.91-6.88 (m, 4H), 3.95 (s, 3H), 2.44-2.38 (m, 3H), 2.26 (s, 3H), 2.24 (s, 3H), 2.10 (m, 3H), 1.82 (m, 2H); $^{13}$C NMR (150 MHz,CDCl$_3$) δ 185.1, 166.5, 143.0, 140.3, 139.0, 136.8, 134.7, 131.5, 130.1, 129.7, 129.6, 128.9, 128.6, 128.6, 126.3, 125.4, 123.8, 117.8, 110.8, 57.5, 52.3, 29.9, 24.8, 21.5, 21.2; MS (ESI-MS) $m/z$: 492.2 (M+H)$^+$; HRMS (ESI) calcd for C$_{31}$H$_{29}$N$_3$O$_3$ (M+H)$^+$: m/z: 492.2282; Found 492.2282; IR (cm$^{-1}$, neat): 3066, 2948, 2872, 1715, 1617, 1569.

Methyl 9-cyclopentyl-3-(4-methoxybenzoyl)-2-(4-methoxyphenyl)-9H-benzo[d]
imidazo[1,2-a]imidazole-6-carboxylate (5i): $^1$H NMR (400 MHz, CDCl$_3$) δ 9.12 (s, 1H), 8.11 (d, J = 8.5 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.41 (m, 1H), 7.28-7.25 (m, 2H), 6.64 (d, J = 8.2 Hz, 4H), 5.08 (s, 1H), 3.95 (s, 3H), 3.75 (s, 3H), 3.73 (s, 3H), 2.47-2.43 (m, 2H), 2.24-2.20 (m, 2H), 2.11-2.08 (m, 2H), 1.85-1.81 (m, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 184.3, 166.9, 162.5, 159.5, 137.5, 131.8, 130.8, 125.7, 125.4, 125.4, 122.8, 117.2, 113.3, 113.1, 109.9, 109.8, 56.7, 55.3, 55.2, 52.1, 29.9, 29.1, 25.2, 24.6; MS (ESI-MS) $m/z$: 524.2 (M+H)$^+$; HRMS (ESI) calcd for
Methyl3-benzoyl-9-[2-(cyclohex-1-en-1-yl)ethyl]-2-phenyl-9H-benzo-[d]imidazo[1,2-ajimidazole-6-carboxylate (5j): ¹H NMR (400 MHz, CDCl₃) δ 9.26 (d, J = 1.6 Hz, 1H), 8.16 (dd, J = 8.6, 1.6 Hz, 1H), 7.55-7.50 (m, 2H), 7.40 (d, J = 8.6 Hz, 1H), 7.27-7.23 (m, 3H), 7.12-7.04 (m, 5H), 5.30 (s, 1H), 4.46 (t, J = 7.1 Hz, 2H), 3.96 (s, 1H), 2.58 (t, J = 7.0 Hz, 2H), 2.09-2.05 (m, 2H), 1.81-1.76 (m, 2H), 1.60-1.57 (m, 2H), 1.49-1.45 (m, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 185.8, 166.8, 138.4, 137.5, 133.6, 133.1, 131.9, 130.8, 128.6, 127.5, 125.8, 125.6, 125.1, 120.8, 118.5, 111.0, 52.9, 44.4, 37.1, 28.8, 25.7, 23.2, 22.4; MS (ESI-MS) m/z: 504.4 (M+H)⁺; HRMS (ESI) calcd for C₃₂H₂₉N₃O₃ (M+H)⁺; m/z: 504.2282; Found 504.2276; IR (cm⁻¹, neat): 3063, 3022, 2929, 2852, 1717, 1676, 1622.

Methyl9-(2-methoxyethyl)-3-(3-methylbenzoyl)-2-phenyl-9H-benzo-[d]imidazo[1,2-ajimidazole-6-carboxylate (5k): ¹H NMR (300 MHz, CDCl₃) δ 9.17 (d, J = 1.6 Hz, 1H), 8.14 (dd, J = 8.6, 1.6 Hz, 1H), 7.56-7.46 (m, 3H), 7.30-7.25 (m, 2H), 7.14-7.11 (m, 3H), 6.90 (t, J = 8.6 Hz, 2H), 4.53 (t, J = 5.2 Hz, 2H), 3.95 (s, 3H), 3.89 (t, J = 5.4 Hz, 2H), 3.34 (s, 3H), 2.25 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 185.6, 167.0, 155.0, 154.2, 150.4, 139.1, 138.4, 138.0, 135.5, 134.4, 131.3, 130.1, 129.9, 129.7, 129.5, 128.3, 127.9, 127.6, 126.0, 125.4, 125.3, 70.5, 59.0, 52.2, 43.7, 21.4; MS (ESI-MS) m/z: 468.4 (M+H)⁺; HRMS (ESI) calcd for C₂₈H₂₅N₃O₄ (M+H)⁺; m/z: 468.1918; Found 468.1933; IR (cm⁻¹, neat): 2990, 2949, 2902, 2852, 1715, 1620, 1584.

Methyl 9-(2-methoxyethyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo-[d]imidazo[1,2-ajimidazole-6-carboxylate (5l): ¹H NMR (300 MHz, CDCl₃) δ 9.16 (s, 1H), 8.15 (d, J = 8.7 Hz, 1H), 7.517.47 (m, 3H), 7.18 (d, J = 8.0 Hz, 2H), 6.93-6.87 (m, 4H), 4.53 (t, J = 5.4 Hz, 2H), 3.96 (s, 3H), 3.90 (t, J = 5.4 Hz, 2H), 3.35 (s, 3H), 2.26 (d, J = 6.2 Hz, 6H); ¹³C NMR (75 MHz, CDCl₃) δ 185.3, 166.9, 154.2, 150.2, 142.0, 139.0, 137.8, 135.6, 131.4, 129.9, 129.6, 128.3, 127.9, 127.6, 126.0, 125.4, 125.3, 70.5, 59.0, 52.2, 43.7, 21.4; MS (ESI-MS) m/z: 482.3 (M+H)⁺; HRMS (ESI) calcd for C₂₉H₂₇N₃O₄ (M+H)⁺; m/z: 482.2074; Found 482.2089; IR (cm⁻¹, neat): 3034, 2984, 2948, 1717, 1678, 1621, 1605, 1584.

Methyl 3-benzoyl-9-(3-methoxypropyl)-2-phenyl-9H-benzo[d]imidazo-[1,2-ajimidazole-6-carboxylate (5m): ¹H NMR (300 MHz, CDCl₃) δ 9.26 (s, 1H), C₃₁H₂₉N₃O₃ (M+H)⁺; m/z: 524.2180; Found 524.2177; IR (cm⁻¹, neat): 3010, 2958, 2873, 1719, 1604.
8.17 (d, J = 8.4 Hz, 1H), 7.57 (d, J = 7.5 Hz, 2H), 7.50 (d, J = 8.5 Hz, 1H), 7.27 (t, J = 8.4 Hz, 3H), 7.24-7.05 (m, 5H), 4.49 (t, J = 6.2 Hz, 2H), 3.97 (s, 3H), 3.43-3.40 (m, 2H), 3.34 (s, 3H), 2.28 (t, J = 6.2 Hz, 2H); ^13^C NMR (75 MHz, CDCl₃) δ 185.5, 167.0, 154.9, 150.4, 138.8, 138.3, 134.3, 131.5, 130.1, 129.5, 128.1, 127.7, 126.1, 125.2, 123.0, 121.9, 117.5, 109.2, 68.7, 58.7, 52.2, 40.4, 28.8; MS (ESI-MS) m/z: 468.1 (M+H)^+; HRMS (ESI) calcd for C₂₈H₂₅N₃O₄ (M+H)^+: m/z: 468.1918; Found 468.1922; IR (cm⁻¹, neat): 3056, 3010, 2975, 2952, 2923, 2857, 1715, 1657, 1619, 1584.

Methyl 9-(3-methoxypropyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo-[d]imidazo[1,2-a]imidazole-6-carboxylate (5n): ^1H NMR (400 MHz, CDCl₃) δ 9.17 (s, 1H), 8.15 (d, J = 8.5 Hz, 1H), 7.48 (d, J = 8.2 Hz, 3H), 7.18 (d, J = 8.0 Hz, 2H), 6.92-6.87 (m, 4H), 4.47 (t, J = 6.7 Hz, 2H), 3.96 (s, 3H), 3.40 (m, 2H), 3.33 (s, 3H), 2.28-2.16 (m, 8H); ^13^C NMR (75 MHz, CDCl₃) δ 185.4, 167.0, 154.5, 150.3, 142.1, 137.9, 135.6, 129.9, 129.7, 128.3, 126.0, 125.3, 122.9, 121.7, 117.3, 109.1, 68.7, 58.6, 52.2, 40.3, 28.8, 21.4, 21.1; MS (ESI-MS) m/z: 496.3 (M+H)^+; HRMS (ESI) calcd for C₃₀H₂₉N₃O₄ (M+H)^+: m/z: 496.2231; Found 496.2229; IR (cm⁻¹, neat): 3022, 2984, 2946, 2923, 2863,2807, 1716, 1620, 1605, 1583.

Methyl 3-benzoyl-9-(furan-2-ylmethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5o): ^1H NMR (300 MHz, CDCl₃) δ 9.23 (s, 1H), 8.14 (d, J = 8.5 Hz, 1H), 7.54-7.50 (m, 3H), 7.38 (s, 1H), 7.27-7.23 (m, 3H), 7.09-7.04 (m, 5H), 6.51 (d, J = 7.2 Hz, 1H), 6.36 (d, J = 7.2 Hz, 1H), 5.53 (s, 2H), 3.95 (s, 3H); ^13^C NMR (75 MHz, CDCl₃) δ 185.6, 166.9, 154.8, 150.2, 148.0, 143.1, 138.3, 138.1, 134.2, 131.5, 130.1, 129.5, 128.1, 127.7, 126.2, 125.6, 123.5, 122.1, 117.5, 110.7, 109.8, 109.7, 52.2, 40.0; MS (ESI-MS) m/z: 476.3 (M+H)^+; HRMS (ESI) calcd for C₂₉H₂₁N₃O₄ (M+H)^+: m/z: 476.1605; Found 476.1610 IR (cm⁻¹, neat): 3122, 3060, 2951, 1717, 1620, 1585.

Methyl 9-(furan-2-ylmethyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5p): ^1H NMR (300 MHz, CDCl₃) δ 9.14 (s, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.49 (t, J = 7.6 Hz, 3H), 7.37 (m, 1H), 7.20 (d, J = 8.0 Hz, 2H), 6.90 (t, J = 7.2 Hz, 4H), 6.50 (d, J = 7.2 Hz, 1H), 6.34 (m, 1H), 5.52 (s, 2H), 3.94 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H); ^13^C NMR (75 MHz, CDCl₃) δ 185.5, 166.9, 154.4, 150.1, 148.1, 143.1, 142.1, 138.1, 137.9, 135.6, 131.4, 129.9, 129.7, 128.3, 126.1, 125.6, 123.4, 121.9, 117.3, 110.7, 109.7, 109.6, 52.2, 40.0, 21.4, 21.2; S-8
MS (ESI-MS) \( m/z \): 504.3 (M+H); HRMS (ESI) calcd for C\(_{31}H_{25}N_3O_4\) (M+H); \( m/z \): 504.1918; Found 504.1922; IR (cm\(^{-1}\), neat): 3034, 2952, 2922, 2852, 1717, 1621, 1605, 1585.

**Methyl 3-benzoyl-2-phenyl-9-(thiophen-2-ylmethyl)-9H-benzo[d]imidazole-1,2-ajimidazole-6-carboxylate (5q):** \(^1\)H NMR (300 MHz, CDCl\(_3\)) \( \delta \) 9.23 (d, \( J = 1.6 \) Hz, 1H), 8.14 (dd, \( J = 8.6, 1.6 \) Hz, 1H), 7.59-7.53 (m, 2H), 7.45 (d, \( J = 8.6 \) Hz, 1H), 7.32-7.27 (m, 4H), 7.27-7.23 (m, 2H), 7.18-7.10 (m, 4H), 6.98 (m, 1H), 5.72 (s, 2H), 3.95 (s, 3H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \( \delta \) 186.2, 167.0, 146.5, 141.8, 136.8, 136.5, 133.4, 132.8, 131.2, 130.1, 129.5, 128.3, 125.6, 123.5, 121.9, 110.4, 52.0, 32.1; MS (ESI-MS) \( m/z \): 492.4 (M+H); HRMS (ESI) calcd for C\(_{29}H_{21}N_3O_3S\) (M+H); \( m/z \): 492.1376; Found 492.1369; IR (cm\(^{-1}\), neat): 3060, 2949, 2852, 1716, 1621, 1586.

**Methyl 9-(4-methoxyphenyl)-3-(4-methylbenzoyl)-2-(p-tolyl)-9H-benzo[d]imidazo[1,2-ajimidazole-6-carboxylate (5r):** \(^1\)H NMR (300 MHz, CDCl\(_3\)) \( \delta \) 9.20 (s, 1H), 8.09 (dd, \( J = 8.6, 1.6 \) Hz, 1H), 7.66 (d, \( J = 8.9 \) Hz, 2H), 7.51 (d, \( J = 8.0 \) Hz, 2H), 7.44 (d, \( J = 8.6 \) Hz, 1H), 7.18 (d, \( J = 8.0 \) Hz, 2H), 7.10 (d, \( J = 8.9 \) Hz, 2H), 6.92 (d, \( J = 8.1 \) Hz, 2H), 6.85 (d, \( J = 8.1 \) Hz, 2H), 3.95 (s, 3H), 3.89 (s, 3H), 2.26 (s, 3H), 2.21 (s, 3H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \( \delta \) 185.5, 166.9, 159.5, 154.4, 149.9, 142.2, 138.6, 137.9, 135.6, 131.4, 130.0, 129.7, 128.4, 128.2, 126.7, 126.6, 126.2, 125.4, 123.7, 121.6, 117.4, 115.3, 110.0, 55.6, 52.2, 21.4, 21.1; MS (ESI-MS) \( m/z \): 530.3 (M+H); HRMS (ESI) calcd for C\(_{33}H_{27}N_3O_4\) (M+H); \( m/z \): 530.2074; Found 530.2092; IR (cm\(^{-1}\), neat): 3031, 3005, 2949, 2839, 1717, 1621, 1564.

**Methyl 9-(2-methoxyethyl)-2-(1-methyl-1H-pyrrol-2-yl)-3-picolinoyl-9H-benzo[d]imidazo[1,2-ajimidazole-6-carboxylate (5s):** \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 9.30 (s, 1H), 8.26 (d, \( J = 8.6 \) Hz, 1H), 8.14 (d, \( J = 8.6 \) Hz, 1H), 7.67 – 7.63 (m, 2H), 7.50 (d, \( J = 8.6 \) Hz, 1H), 7.15 (m, 1H), 6.45 (m, 1H), 5.75-5.68 (m, 2H), 4.49 (t, \( J = 6.2 \) Hz, 2H), 3.94 (s, 3H), 3.86 (t, \( J = 6.2 \) Hz, 2H), 3.74 (s, 3H), 3.31 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 183.6, 167.0, 148.1, 138.9, 136.1, 126.2, 125.4, 124.9, 123.8, 123.5, 123.3, 117.5, 114.0, 110.0, 107.8, 70.3, 59.0, 52.2, 43.7; MS (ESI): \( m/z \) 458.3 [M+H]; HRMS (ESI) calcd for C\(_{25}H_{23}N_3O_4\) (M+H); 458.1823; Found 458.1815.

**Methyl 3-(1,1'-biphenyl)-4-carbonyl)-9-(2-methoxyethyl)-2-(naphthalen-2-yl)-9H-benzo[d]imidazo[1,2-ajimidazole-6-carboxylate (5t):** \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \( \delta \) 10.15 (d, \( J = 7.2 \) Hz, 1H), 8.70 (d, \( J = 7.2 \) Hz, 1H), 8.28 – 8.05 (m, 3H), S-9
7.92 – 7.83 (m, 2H), 7.78 – 7.59 (m, 6H), 7.44 – 7.33 (m, 2H), 7.26 (d, J = 7.4 Hz, 1H), 7.09 (m, 1H), 6.94 – 6.82 (m, 2H), 4.51 (t, J = 6.2 Hz, 2H), 3.90 (t, J = 6.2 Hz, 2H), 3.71 (s, 3H), 3.28 (t, J = 6.2 Hz, 2H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 166.3, 152.0, 149.3, 148.8, 140.0, 137.5, 133.6, 133.3, 128.3, 127.9, 127.6, 126.6, 126.0, 124.9, 124.8, 124.3, 123.6, 121.3, 121.1, 118.2, 117.8, 112.9, 110.8, 102.8, 69.7, 58.6, 52.4; MS (ESI): m/z 580.3 [M+H]$^+$; HRMS (ESI) calcd for C$_{37}$H$_{29}$N$_3$O$_4$ (M+H)$^+$; 580.2231; Found 580.2221.

**Methyl 3-(3-methoxybenzoyl)-9-(2-methoxyethyl)-2-(3-(trifluoromethyl)phenyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5u):** $^1$H NMR (400 MHz, Acetone-$d_6$) δ 9.26 (s, 1H), 8.14 (m, 1H), 7.77 (d, J = 8.5 Hz, 1H), 7.64 (d, J = 7.9 Hz, 1H), 7.42 (m, 1H), 7.32 – 7.23 (m, 2H), 7.08 – 6.96 (m, 3H), 6.77 (m, 1H), 4.59 (t, J = 6.2 Hz, 2H), 3.93 (t, J = 6.2 Hz, 2H), 3.85 (s, 3H), 3.68 (s, 3H), 3.29 (s, 3H); $^{13}$C NMR (100 MHz, Acetone-$d_6$) δ 184.2, 166.2, 158.9, 151.8, 150.3, 140.2, 139.2, 133.7, 130.8, 128.6, 128.5, 126.0, 125.9, 125.7, 125.2, 123.4, 122.7, 121.1, 117.2, 117.1, 113.5, 110.6, 69.4, 57.9, 54.6, 51.5, 43.4; MS (ESI): m/z 530.2 [M+H]$^+$; HRMS (ESI) calcd for C$_{33}$H$_{27}$F$_3$N$_3$O$_5$ (M+H)$^+$; 530.2074; Found 530.2074.

**Methyl 3-([1,1'-biphenyl]-4-carbonyl)-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5v):** $^1$H NMR (400 MHz, CDCl$_3$) δ 9.19 (s, 1H), 8.17 (m, 1H), 7.62 – 7.20 (m, 12H), 7.07 – 7.01 (m, 3H), 4.51 (t, J = 6.2 Hz, 2H), 3.91 (s, 3H), 3.88 (t, J = 6.2 Hz, 2H), 3.32 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 180.1, 179.6, 161.6, 145.1, 138.8, 135.3, 135.1, 134.8, 133.8, 133.1, 131.7, 129.0, 127.9, 126.1, 125.2, 124.8, 124.2, 123.6, 123.5, 122.7, 122.2, 121.8, 121.6, 121.0, 120.7, 117.7, 116.7, 112.0, 104.9, 65.1, 53.3, 46.9, 38.4; MS (ESI): m/z 530.3 [M+H]$^+$; HRMS (ESI) calcd for C$_{33}$H$_{27}$F$_3$N$_3$O$_5$ (M+H)$^+$; 530.2074; Found 530.2074.

**Methyl 3-([1,1'-biphenyl]-4-carbonyl)-9-(2-methoxyethyl)-2-(4-methoxyphenyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5w):** $^1$H NMR (400 MHz, CDCl$_3$) δ 9.19 (s, 1H), 8.07 (d, J = 7.0 Hz, 1H), 7.58 (t, J = 7.0 Hz, 2H), 7.42 – 7.15 (m, 5H), 7.33 – 7.15 (m, 5H), 6.55 (t, J = 6.6 Hz, 2H), 4.48 (t, J = 6.2 Hz, 2H), 3.91 (s, 3H), 3.85 (t, 6.2 Hz, 2H), 3.57 (s, 3H), 3.29 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 184.5, 167.0, 162.6, 153.3, 150.4, 140.6, 140.6, 139.1, 133.5, 131.8, 130.9, 130.5, 128.7, 127.4, 126.9, 126.4, 126.0, 125.3, 123.1, 121.8, 117.1, 113.1, 111.3, 110.0, 77.2, 70.5,
Methyl3-benzoyl-9-(2-methoxyethyl)-2-(4-(trifluoromethyl)phenyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5x): \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 9.24 (d, \(J = 1.6\) Hz, 1H), 8.19 (dd, \(J = 8.6, 1.6\) Hz, 1H), 7.61 – 7.52 (m, 3H), 7.42 (d, \(J = 8.1\) Hz, 2H), 7.38 – 7.31 (m, 3H), 7.14 (t, \(J = 7.6\) Hz, 2H), 4.57 (t, \(J = 6.2\) Hz, 2H), 3.99 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 185.4, 167.0, 152.8, 150.6, 139.2, 138.2, 138.1, 131.9, 130.4, 130.1, 129.5, 129.5, 128.1, 127.9, 126.4, 125.3, 124.6, 124.5, 124.5, 123.4, 117.6, 110.3, 77.3, 70.5, 59.2, 52.3, 43.9; MS (ESI): \(m/z\) 522.2 [M+H]\(^+\); HRMS (ESI): calcd for C\(_{28}\)H\(_{23}\)N\(_3\)O\(_4\)[M+H]\(^+\); 522.1635, Found; 522.1633.

Methyl9-(2-methoxyethyl)-2-(4-methoxyphenyl)-3-(4-methylbenzoyl)-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5y): \(^1\)H NMR (400 MHz, Acetone-\(d_6\)) \(\delta\) 9.26 (s, 1H), 8.10 – 8.03 (m, 2H), 7.83 – 7.71 (m, 3H), 7.31 – 7.18 (m, 3H), 7.13 – 7.05 (m, 3H), 4.61 (t, \(J = 6.4\) Hz, 2H), 3.95 – 3.92 (m, 5H), 3.30 (s, 3H); \(^{13}\)C NMR (100 MHz, Acetone-\(d_6\)) \(\delta\) 183.7, 166.3, 156.3, 150.7, 148.1, 136.3, 135.5, 129.6, 127.5, 127.3, 125.5, 123.7, 122.7, 116.9, 110.6, 69.7, 57.9, 51.5, 43.4; MS (ESI): \(m/z\) 455.3 [M+H]\(^+\); HRMS (ESI): calcd for C\(_{26}\)H\(_{22}\)N\(_4\)O\(_4\)[M+H]\(^+\); 455.1714, Found; 455.1719.

(9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazo[3-yl](phenyl)methanone (5aa): \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.57 (d, \(J = 8.2\) Hz, 1H), 7.58 – 7.52 (m, 2H), 7.47 (dd, \(J = 8.2, 1.2\) Hz, 1H), 7.37 (dt, \(J = 8.2, 1.2\) Hz, 1H), 7.31 – 7.20 (m, 4H), 7.11 – 7.00 (m, 5H), 4.49 (t, \(J = 6.2\) Hz, 2H), 3.88 (t, \(J = 6.2\) Hz, 2H), 3.34 (s,
13C NMR (100 MHz, CDCl₃) δ 185.3, 154.9, 150.1, 138.6, 135.8, 134.7, 131.3, 130.1, 129.6, 127.9, 127.6, 125.8, 124.0, 121.1, 115.9, 110.3, 70.5, 59.0, 43.4; MS (ESI): m/z 396.3 [M+H]+; HRMS (ESI): calcd for C₂₅H₂₁N₃O₂ [M+H]+: 396.1707; Found: 396.1717.

(7-chloro-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5ba): ¹H NMR (400 MHz, CDCl₃) δ 8.51 (d, J = 8.0 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.27 – 7.19 (m, 4H), 7.12 – 7.00 (m, 5H), 4.45 (t, J = 6.6 Hz, 2H), 3.86 (t, J = 6.6 Hz, 2H), 3.34 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 185.5, 154.8, 150.2, 138.3, 136.6, 134.4, 131.4, 130.1, 129.8, 129.5, 128.0, 127.6, 124.4, 121.7, 121.4, 116.8, 110.7, 70.5, 59.1, 43.7; MS (ESI): m/z 430.2 [M+H]+; HRMS (ESI): calcd for C₂₅H₂₀ClN₃O₂ [M+H]+: m/z 430.1321, found 430.1317.

3-benzoyl-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carbonitrile (5ca): ¹H NMR (400 MHz, CDCl₃) δ 8.97 (s, 1H), 7.64 (d, J = 8.5 Hz, 1H), 7.57 (d, J = 8.5 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.28 – 7.22 (m, 4H), 7.01 – 7.22 (m, 5H), 4.52 (t, J = 6.4 Hz, 2H), 3.91 (t, J = 6.4 Hz, 2H), 3.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 185.6, 155.0, 150.2, 138.7, 137.9, 134.0, 131.7, 130.1, 129.5, 128.3, 128.0, 127.7, 125.4, 120.0, 119.2, 111.4, 104.2, 70.6, 59.1, 44.0; MS (ESI): m/z 421.1 [M+H]+; HRMS (ESI): calcd for C₂₆H₂₁N₄O₂ [M+H]+: 421.1659, found 421.1664.

2-methoxyethyl 3-benzoyl-9-(2-methoxyethyl)-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazole-6-carboxylate (5da): ¹H NMR (300 MHz, CDCl₃) δ 9.24 (s, J = 1.6 Hz, 1H), 8.17 (dd, J = 8.6, 1.6 Hz, 1H), 7.55 (dd, J = 9.3, 7.9 Hz, 3H), 7.29 (m, 2H), 7.24 (d, J = 1.3 Hz, 1H), 7.09 (m, 5H), 4.54 (m, 4H), 3.90 (t, J = 5.2 Hz, 2H), 3.78-3.70 (m, 2H), 3.46 (s, 3H), 3.35 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 185.4, 166.4, 154.6, 139.2, 138.3, 134.3, 131.5, 130.1, 129.5, 128.1, 127.7, 126.2, 125.4, 123.1, 122.0, 117.6, 110.0, 70.6, 70.5, 64.0, 59.1, 59.0, 43.7; MS (ESI-MS) m/z: 498.4 (M+H)+; HRMS (ESI) calcd for C₂₉H₂₁N₃O₅ (M+H)+: 498.2023, found 498.2016; IR (cm⁻¹, neat): 3061, 2926, 2854, 1713, 1620, 1584.

(9-(2-methoxyethyl)-6-methyl-2-phenyl-9H-benzo[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5ea): ¹H NMR (400 MHz, CDCl₃) δ 8.38 (s, 1H), 7.57 (dd, J = 8.3, 1.2 Hz, 2H), 7.34 (d, J = 8.3 Hz, 1H), 7.25 – 7.20 (m, 3H), 7.20 (m, 1H), 7.04 (m, 6H), 4.45 (t, J = 6.2 Hz, 2H), 3.85 (t, J = 6.2 Hz, 2H), 3.33 (s, 3H), 2.50 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 185.4, 154.9, 138.7, 134.7, 133.8, 131.3, 131.1, 130.1,
129.6, 127.9, 127.6, 125.9, 125.0, 116.1, 109.9, 70.6, 59.0, 43.3, 21.6; MS (ESI): m/z 410.3 [M+H]+; HRMS (ESI): calcd for C_{26}H_{24}N_{3}O_{2}[M+H]+; 410.1863, Found: 410.1859.

(9-(2-methoxyethyl)-6-nitro-2-phenyl-9H-benza[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5fa): ^1^H NMR (400 MHz, CDCl$_3$) δ 9.49 (d, J = 2.2 Hz, 1H), 8.31 (dd, J = 9.0, 2.2 Hz, 1H), 7.61 – 7.49 (m, 3H), 7.26 (m, 3H), 7.08 (m, 5H), 4.55 (t, J = 6.2 Hz, 2H), 3.89 (t, J = 6.2 Hz, 2H), 3.32 (s, 3H); ^1^C NMR (100 MHz, CDCl$_3$) δ 185.5, 154.8, 141.8, 140.2, 137.9, 133.9, 131.7, 130.1, 129.5, 128.4, 127.8, 127.7, 125.0, 120.1, 112.4, 110.4, 70.6, 59.1, 44.2; MS (ESI): m/z 441.1 [M+H]+; HRMS (ESI): calcd for C$_{25}$H$_{20}$N$_{4}$O$_{4}$[M+H]+; 441.1557, Found: 441.1566.

(6-methoxy-9-(2-methoxyethyl)-2-phenyl-9H-benza[d]imidazo[1,2-a]imidazol-3-yl)(phenyl)methanone (5ga): ^1^H NMR (400 MHz, CDCl$_3$) δ 8.22 (d, J = 2.2 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.37 (d, J = 8.9 Hz, 1H), 7.24 – 7.18 (m, 3H), 7.10 – 7.03 (m, 4H), 7.03 – 6.95 (m, 2H), 4.46 (t, J = 6.2 Hz, 2H), 3.92 (s, 3H), 3.86 (t, J = 6.2 Hz, 2H), 3.34 (s, 3H); ^1^C NMR (100 MHz, CDCl$_3$) δ 185.4, 155.4, 154.9, 150.6, 138.8, 134.7, 131.2, 130.1, 129.9, 129.5, 127.9, 127.6, 127.5, 126.2, 121.4, 112.9, 110.9, 100.2, 70.7, 59.0, 56.1, 43.4; MS (ESI): m/z 426.3 [M+H]+; HRMS (ESI): calcd for C$_{26}$H$_{23}$N$_{3}$O$_{3}$[M+H]+; 426.1816, found 426.1812.

9-(2-methoxyethyl)-2-phenyl-6-(trifluoromethyl)-9H-benza[d]imidazo[1,2-a]imidazol-3-carboxylate (5ha): ^1^H NMR (300 MHz, CDCl$_3$) δ 9.24 (s, 1H), 7.65 (d, J = 8.6 Hz, 1H), 7.57 (d, J = 8.6 Hz, 1H), 7.26 – 7.50 (m, 2H), 7.28 – 7.20 (m, 3H), 7.13 – 7.01 (m, 5H), 4.52 (t, J = 6.4 Hz, 2H), 3.87 (t, J = 6.4 Hz, 2H), 3.32 (s, 3H); ^1^C NMR (75 MHz, CDCl$_3$) δ 185.6, 167.0, 154.8, 150.4, 150.4, 139.1, 138.2, 138.0, 134.2, 131.6, 130.1, 129.5, 128.2, 127.7, 125.4, 121.9, 121.2, 113.7, 113.6, 110.7, 70.6, 59.1, 43.8; MS (ESI): m/z 464.2 [M+H]+; HRMS (ESI): calcd for C$_{26}$H$_{23}$F$_{3}$N$_{3}$O$_{2}$ [M+H]+; 464.1580, found 464.1585.

Methyl 3-benzoyl-9-(2-methoxyethyl)-2-phenyl-9H-benza[d]imidazo-[1,2-a]imidazole-6-carboxylate (5ia): ^1^H NMR (300 MHz, CDCl$_3$) δ 9.24 (s, 1H), 8.15 (dd, J = 8.6, 1.4 Hz, 1H), 7.55 (t, J = 7.9 Hz, 3H), 7.26 (t, J = 8.1 Hz, 3H), 7.08 (m, 5H), 4.53 (t, J = 6.2 Hz, 2H), 3.96 (s, 3H), 3.90 (t, J = 6.2 Hz, 2H), 3.34 (s, 3H); ^1^C NMR (75 MHz, CDCl$_3$) δ 185.5, 167.0, 154.8, 150.4, 150.4, 139.1, 138.3, 134.3, 131.5, 130.1, 129.5, 128.1, 127.7, 126.1, 125.4, 123.2, 122.0, 117.4, 110.1, 70.5, 59.0,
52.2, 43.7; MS (ESI-MS) m/z: 476 (M+Na); HRMS calcd for C_{27}H_{23}N_{3}O_{4} (M+Na): 476.1586, found 476.1588; IR (cm\(^{-1}\), neat): 3066, 2925, 2851, 1711, 1623, 1586.

**Phenyl(2-phenylimidazo[1,2-a]pyridin-3-yl)methanone (6a):** \(^1\)H NMR (400 MHz, Acetone-\(d_6\)) \(\delta\) 9.46 (d, 1.2 Hz, 1H), 7.79 (dd, \(J = 9.0, 1.2\) Hz, 1H), 7.65 (dd, \(J = 9.0, 1.2\) Hz, 1H), 7.56 – 7.51 (m, 2H), 7.39 – 7.34 (m, 2H), 7.33 – 7.23 (m, 2H), 7.18 – 7.06 (m, 5H); \(^{13}\)C NMR (100 MHz, Acetone-\(d_6\)) \(\delta\) 186.7, 154.1, 147.2, 134.5, 131.5, 130.2, 129.5, 129.1, 128.0, 127.9, 127.7, 117.3, 114.5; MS (ESI): m/z 299.3 [M+H]; HRMS (ESI): calcd for C_{20}H_{14}N_{2}O [M+H]: 299.1179, found 299.1181.

**(2-(4-nitrophenyl)imidazo[1,2-a]pyrazin-3-yl)(phenyl)methanone (6b):** \(^1\)H NMR (400 MHz, Acetone-\(d_6\)) \(\delta\) 9.33 (d, \(J = 1.5\) Hz, 1H), 9.23 (dd, \(J = 7.2, 1.5\) Hz, 1H), 8.28 (d, \(J = 7.2\) Hz, 1H), 8.07 – 8.04 (m, 2H), 7.74 (d, \(J = 7.4, 2\)H), 7.64 (d, \(J = 7.4, 2\)H), 7.42 (m, 1H), 7.27 – 7.23 (m, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 187.0, 162.5, 151.3, 147.7, 144.3, 139.5, 137.4, 133.4, 132.6, 131.0, 129.6, 128.5, 123.2, 121.0, 120.2; MS (ESI): m/z 325.2 [M+H]; HRMS (ESI): calcd for C_{19}H_{12}N_{4}O_{3} [M+H]: 345.0982, found 345.0984.

**Phenyl(2-phenylimidazo[1,2-a]pyrazin-3-yl)methanone (6c):** \(^1\)H NMR (400 MHz, Acetone-\(d_6\)) \(\delta\) 9.24 (s, 1H), 9.18 (dd, \(J = 7.4, 1.5\) Hz, 1H), 8.21 (d, \(J = 7.4\) Hz, 1H), 7.65 – 7.56 (m, 2H), 7.47 – 7.30 (m, 3H), 7.27 – 7.10 (m, 5H); \(^{13}\)C NMR (100 MHz, Acetone-\(d_6\)) \(\delta\) 187.2, 153.4, 143.6, 141.3, 137.9, 133.7, 132.3, 131.7, 130.2, 129.5, 128.5, 127.9, 127.7, 120.3, 120.1. MS (ESI): m/z 300.2 [M+H]; HRMS (ESI): calcd for C_{19}H_{14}N_{3}O_{3}[M+H]: 300.1131, found 300.1132.
$^1$H NMR spectrum (300MHz) of compound 5a in CDCl$_3$
$^{13}$C NMR spectrum (75MHz) of compound 5a in CDCl$_3$

S-16
ESI$^+$ Mass spectrum of compound 5a
High resolution mass (ESI\textsuperscript{+}) spectrum of compound 5a
IR spectrum of compound 5a
S-19
$^1$H NMR spectrum (300MHz) of compound 5b in CDCl$_3$

S-20
$^{13}$C NMR spectrum (75MHz) of compound 5b in CDCl$_3$
Tony-n-pentyl ESI+

Chemical Formula: C_{20}H_{27}N_{2}O_{3}
Exact Mass: 465.21

ESI\textsuperscript{+} Mass spectrum of compound 5b
Tony-\(n\)-pentyl ESI+
Molecular Formula: C_{29}H_{27}N_{3}O_{3}Na
Exact Mass: 488.1950
Measured Mass: 488.1952

High resolution mass (ESI\(^+\)) spectrum of compound **5b**
IR spectrum of compound 5b
$^1$H NMR spectrum (300MHz) of compound 5c in CDCl$_3$

S-25
\[ ^{13}C \text{ NMR spectrum (75MHz) of compound 5c in CDCl}_3 \]

S-26
ESI\textsuperscript{+} Mass spectrum of compound 5c

S-27
High resolution mass (ESI\(^+\)) spectrum of compound \textit{5c}
IR spectrum of compound 5c
1H NMR spectrum (300MHz) of compound 5d in CDCl3
$^{13}$C NMR spectrum (150MHz) of compound 5d in CDCl3

S-19
ESI$^+$ Mass spectrum of compound $5d$

Chemical Formula: C$_2$H$_2$N$_2$O$_3$
Exact Mass: 437.17
High resolution mass (ESI+) spectrum of compound 5d
IR spectrum of compound 5d
$^1$H NMR spectrum (300MHz) of compound 5e in CDCl$_3$
$^{13}$C NMR spectrum (75MHz) of compound 5e in CDCl$_3$
Chemical Formula: C_{23}H_{27}N_{3}O_{3}
Exact Mass: 465.21

ESI\(^+\) Mass spectrum of compound 5e

S-25
High resolution mass (ESI⁺) spectrum of compound 5e
IR spectrum of compound $5e$
$^1$H NMR spectrum (300MHz) of compound 5f in CDCl$_3$
$^{13}$C NMR spectrum (150MHz) of compound 5f in CDCl$_3$
ESI⁺ Mass spectrum of compound 5f
S-30
High resolution mass (ESI\textsuperscript{+}) spectrum of compound 5f

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<th>Delta Mass (ppm)</th>
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IR spectrum of compound 5f
$^1$H NMR spectrum (300MHz) of compound 5g in CDCl$_3$

S-33
$^{13}$C NMR spectrum (75MHz) of compound 5g in CDCl$_3$
ESI⁺ Mass spectrum of compound 5g

S-35
Tony-cyclopentyl ESI+
Molecular Formula: C29H25N3O3Na
Exact Mass: 486.1794
Measured Mass: 486.1797

Chemical Formula: C29H25N3O3
Exact Mass: 463.1896

High resolution mass (ESI+) spectrum of compound 5g
IR spectrum of compound 5g

S-37
$^1$H NMR spectrum (300MHz) of compound 5h in CDCl$_3$

S-38
\(^{13}\)C NMR spectrum (150MHz) of compound 5h in CDCl\(_3\)
ESI$^{+}$ Mass spectrum of compound 5h

Chemical Formula: C$_{31}$H$_{52}$N$_{2}$O$_{3}$

Exact Mass: 491.2209
High resolution mass (ESI⁺) spectrum of compound 5h
IR spectrum of compound 5h

S-42
$^1$H NMR spectrum (400MHz) of compound 5i in CDCl$_3$
$^{13}$C NMR spectrum (150MHz) of compound 5i in CDCl$_3$

S-44
cyclopentyl-PhOMe

Chemical Formula: C₃₁H₂₉N₃O₅
Exact Mass: 523.2107

ESI⁺ Mass spectrum of compound 5i
High resolution mass (ESI$^+$) spectrum of compound 5i

S-46
IR spectrum of compound 5i
$^1$H NMR spectrum (400 MHz) of compound 5j in CDCl$_3$

S-48
$^{13}\text{C}$ NMR spectrum (150MHz) of compound 5j in CDCl$_3$
ESI⁺ Mass spectrum of compound 5j
S-50
High resolution mass (ESI⁺) spectrum of compound 5j

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Chemical Formula: C₉₂H₃₀N₄O₃N₂
Exact Mass: 503.2209
IR spectrum of compound 5j
S-52
$^1$H NMR spectrum (300MHz) of compound 5k in CDCl$_3$
$\text{\textsuperscript{13}C NMR spectrum (75MHz) of compound 5k in CDCl}_3$

S-54
Expanding $^{13}$C NMR spectrum (75MHz) of compound 5k in CDCl$_3$
Chemical Formula: C_{20}H_{20}N_{2}O_{6}
Exact Mass: 467.18
High resolution mass (ESI⁺) spectrum of compound 5k
IR spectrum of compound 5k

S-58
$^1$H NMR spectrum (300MHz) of compound 51 in CDCl$_3$
$^{13}$C NMR spectrum (75 MHz) of compound 51 in CDCl$_3$
Expanding $^{13}$C NMR spectrum (75MHz) of compound 5I in CDCl$_3$
ESI\textsuperscript{+} Mass spectrum of compound 51

Chemical Formula: C\textsubscript{29}H\textsubscript{37}N\textsubscript{5}O\textsubscript{4}
Exact Mass: 481.20
60-Cu-2-methoxy-Phme-H#1-20 RT: 0.01-0.43 AV: 20
T: FTWS + p ESI Full ms [150.00-700.00]
m/z= 445.7723-498.4735
Isotope  Min  Max
C-12   0   29
H-1    0   80
O-16   0   9
N-14   0   4
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

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Chemical Formula: C_{25}H_{27}N_{3}O_{4}
Exact Mass: 481.20

High resolution mass (ESI⁺) spectrum of compound 51
IR spectrum of compound 51

S-64
$^1$H NMR spectrum (300MHz) of compound 5m in CDCl$_3$
$^{13}$C NMR spectrum (75MHz) of compound 5m in CDCl$_3$

S-66
ESI$^+$ Mass spectrum of compound 5m
High resolution mass (ESI+) spectrum of compound 5m
IR spectrum of compound 5m

S-69
$^1$H NMR spectrum (400MHz) of compound 5n in CDCl$_3$

S-70
$^{13}$C NMR spectrum (75MHz) of compound 5n in CDCl$_3$
ESI$^+$ Mass spectrum of compound 5n

S-72
High resolution mass (ESI⁺) spectrum of compound 5n

S-73
IR spectrum of compound 5n
S-74
$^1$H NMR spectrum (300MHz) of compound 5o in CDCl$_3$

S-75
$^{13}$C NMR spectrum (75MHz) of compound 5o in CDCl$_3$
ESI⁺ Mass spectrum of compound 5o
High resolution mass (ESI⁺) spectrum of compound 5o

Chemical Formula: C_{29}H_{21}N_{2}O_{4}
Exact Mass: 476.15
IR spectrum of compound 5o
S-79
$^1$H NMR spectrum (300MHz) of compound 5p in CDCl$_3$

S-80
$^{13}$C NMR spectrum (75MHz) of compound 5p in CDCl$_3$

S-81
ESI$^+$ Mass spectrum of compound 5p

Chemical Formula: $C_{31}H_{27}N_3O_4$
Exact Mass: 503.18

S-82
High resolution mass (ESI⁺) spectrum of compound 5p

Chemical Formula: C₃₃H₂₅N₅O₄
Exact Mass: 503.18

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Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00

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109-Tony-furul-phen-phen-H#1-20 RT: 0.01-0.28 AV: 20
T: FIMS + p ESI Full ms [500.00-510.00]
IR spectrum of compound 5p

S-84
$^1$H NMR spectrum (300MHz) of compound 5q in CDCl$_3$

S-85
$^{13}$C NMR spectrum (75MHz) of compound $5q$ in CDCl$_3$
ESI$^+$ Mass spectrum of compound 5q
High resolution mass (ESI\textsuperscript{+}) spectrum of compound 5q
IR spectrum of compound 5q
$^1$H NMR spectrum (300MHz) of compound 5r in CDCl$_3$

S-90
'\textsuperscript{13}C NMR spectrum (75MHz) of compound 5r in CDCl₃
ESI⁺ Mass spectrum of compound 5r

S-92
High resolution mass (ESI⁺) spectrum of compound 5r
IR spectrum of compound 5r
$^1$H NMR spectrum (400MHz) of compound 5s in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5s in CDCl$_3$
ESI⁺ Mass spectrum of compound 5s
High resolution mass (ESI⁺) spectrum of compound 5s
$^1$H NMR spectrum (400MHz) of compound 5t in DMSO-$d_6$
$^{13}$C NMR spectrum (75MHz) of compound 5t in DMSO-$d_6$
ESI$^+$ Mass spectrum of compound 5t
High resolution mass (ESI⁺) spectrum of compound 5t
$^1$H NMR spectrum (400MHz) of compound 5u in Acetone-$d_6$
$^{13}$C NMR spectrum (100MHz) of compound 5u in Acetone-$d_6$
High resolution mass (ESI+) spectrum of compound 5u
$^1$H NMR spectrum (400MHz) of compound 5v in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5v in CDCl$_3$
High resolution mass (ESI⁺) spectrum of compound 5v

S-110
\(^1\)H NMR spectrum (400MHz) of compound 5w in CDCl\(_3\)
$^{13}$C NMR spectrum (100MHz) of compound 5w in CDCl$_3$
Mass spectrum of compound 5w
High resolution mass (ESI\(^+\)) spectrum of compound 5w

C\(_{56}\)H\(_{50}\)N\(_x\)O\(_y\)S, 560.2180
$^1$H NMR spectrum (400MHz) of compound 5x in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5x in CDCl₃

S-116
ESI⁺ Mass spectrum of compound 5x
High resolution mass (ESI$^+$) spectrum of compound 5x
$^1$H NMR spectrum (400MHz) of compound 5y in CDCl$_3$
$\text{C NMR spectrum (100MHz) of compound 5y in CDCl}_3$
ESI$^+$ Mass spectrum of compound 5y
High resolution mass (ESI⁺) spectrum of compound 5y
1H NMR spectrum (400MHz) of compound 5z in Acetone-d$_6$
$^{13}$C NMR spectrum (100MHz) of compound 5z in Acetone-$d_6$
ESI$^+$ Mass spectrum of compound 5z
High resolution mass (ESI\(^+\)) spectrum of compound 5z
$^1$H NMR spectrum (400MHz) of compound 5aa in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5aa in CDCl$_3$
ESI$^+$ Mass spectrum of compound 5aa
High resolution mass (ESI⁺) spectrum of compound 5aa
$^1$H NMR spectrum (400MHz) of compound 5ba in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5ba in CDCl$_3$
E SI^+ Mass spectrum of compound 5ba
High resolution mass (ESI⁺) spectrum of compound 5ba
$^1$H NMR spectrum (400MHz) of compound 5ca in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5ca in CDCl$_3$
ESI⁺ Mass spectrum of compound 5ca
High resolution mass (ESI+) spectrum of compound 5ca
$^1$H NMR spectrum (300MHz) of compound 5da in CDCl$_3$
$^{13}$C NMR spectrum (75MHz) of compound 5da in CDCl$_3$
ESI⁺ Mass spectrum of compound 5da

S-141
High resolution mass (ESI⁺) spectrum of compound 5da
IR spectrum of compound 5da
$^1$H NMR spectrum (400MHz) of compound 5ea in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5ea in CDCl$_3$
High resolution mass (ESI⁺) spectrum of compound 5ea
$^1$H NMR spectrum (400MHz) of compound 5fa in CDCl$_3$
$^{13}$C NMR spectrum (100MHz) of compound 5fa in CDCl$_3$
ESI^+ Mass spectrum of compound 5fa
High resolution mass (ESI$^+$) spectrum of compound 5fa
\(^1\)H NMR spectrum (400MHz) of compound 5ga in CDCl\(_3\)
$^{13}$C NMR spectrum (100MHz) of compound 5ga in CDCl$_3$
ESI+ Mass spectrum of compound 5ga
High resolution mass (ESI$^+$) spectrum of compound 5ga
$^{1}$H NMR spectrum (400MHz) of compound 5ha in CDCl$_3$
$^1$H NMR spectrum (100MHz) of compound 5ha in CDCl$_3$
ESI$^+$ Mass spectrum of compound 5ha
High resolution mass (ESI\textsuperscript{+}) spectrum of compound 5ha
$^1$H NMR spectrum (300MHz) of compound 5ia in CDCl$_3$
$^{13}$C NMR spectrum (75MHz) of compound 5ia in CDCl$_3$
ESI$^+$ Mass spectrum of compound 5ia

S-162
Tony-2-methoxy ESI+
Molecular Formula: C27H23N3O4Na
Exact Mass: 476.1586
Measured Mass: 476.1588

High resolution mass (ESI⁺) spectrum of compound 5ia
S-163
$^1$H NMR spectrum (400MHz) of compound 6a in Acetone-$d_6$
$^{13}$C NMR spectrum (100MHz) of compound 6a in Acetone-$d_6$
ESI$^+$ Mass spectrum of compound 6a
High resolution mass (ESI⁺) spectrum of compound 6a
$^1$H NMR spectrum (400MHz) of compound 6b in Acetone-$d_6$
$^{13}$C NMR spectrum (100MHz) of compound 6b in Acetone-$d_6$
Mass spectrum of compound 6b
High resolution mass (ESI$^+$) spectrum of compound 6b
$^1$H NMR spectrum (400MHz) of compound 6c in Acetone-$d_6$
$^{13}$C NMR spectrum (100MHz) of compound 6c in Acetone-$d_6$
ESI⁺ Mass spectrum of compound 6c
High resolution mass (ESI\(^+\)) spectrum of compound 5r
$^1$H NMR spectrum (300MHz) of compound 4a in CDCl$_3$

S-177
$^{13}$C NMR spectrum (75MHz) of compound 4a in CDCl$_3$
ESI$^+$ Mass spectrum of compound 4a
High resolution mass (ESI⁺) spectrum of compound 4a
IR spectrum of compound 4a

S-181
Table 1. Crystal data and structure refinement for 121122LT_0m.

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Final R indices [I>2sigma(I)]

R1 = 0.0937, wR2 = 0.2148

R indices (all data)

R1 = 0.2285, wR2 = 0.3196

Extinction coefficient

0.0107(7)

Largest diff. peak and hole

1.705 and -1.228 e.Å⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for 121122LT_0m. U(eq) is defined as one third of the trace of the orthogonalized Uᵢᵣ tensor.

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\text{C(116)} & \text{-} & \text{C(111)} & \text{-} & \text{C(100)} & 121.7(5) \\
\text{C(113)} & \text{-} & \text{C(112)} & \text{-} & \text{C(111)} & 120.7(5) \\
\text{C(113)} & \text{-} & \text{C(112)} & \text{-} & \text{H(112)} & 119.7 \\
\text{C(111)} & \text{-} & \text{C(112)} & \text{-} & \text{H(112)} & 119.7 \\
\text{C(114)} & \text{-} & \text{C(113)} & \text{-} & \text{C(112)} & 120.1 \\
\text{C(112)} & \text{-} & \text{C(113)} & \text{-} & \text{H(113)} & 120.1 \\
\text{C(115)} & \text{-} & \text{C(114)} & \text{-} & \text{C(113)} & 119.6(6) \\
\text{C(115)} & \text{-} & \text{C(114)} & \text{-} & \text{H(114)} & 120.2 \\
\text{C(113)} & \text{-} & \text{C(114)} & \text{-} & \text{H(114)} & 120.2 \\
\text{C(114)} & \text{-} & \text{C(115)} & \text{-} & \text{C(116)} & 121.1(5) \\
\text{C(114)} & \text{-} & \text{C(115)} & \text{-} & \text{H(115)} & 119.4 \\
\text{C(116)} & \text{-} & \text{C(115)} & \text{-} & \text{H(115)} & 119.4 \\
\text{C(115)} & \text{-} & \text{C(116)} & \text{-} & \text{C(111)} & 119.5(5) \\
\text{C(115)} & \text{-} & \text{C(116)} & \text{-} & \text{H(116)} & 120.2 \\
\text{C(111)} & \text{-} & \text{C(116)} & \text{-} & \text{H(116)} & 120.2 \\
\end{array} \]

Symmetry transformations used to generate equivalent atoms: Table 4. Anisotropic displacement parameters (\(\text{Å}^2 \times 10^3\)) for 121122LT_0m. The anisotropic displacement factor exponent takes the form: 

\[ -2\pi^2 [h^2 a^* a^* U_{11} + ... + 2hk a^* b^* U_{12} ] \]

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S-209
Table 5. Hydrogen coordinates (x 10$^4$) and isotropic displacement parameters (Å$^2$ x 10$^3$) for 121122LT_0m.

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| H(91B) | 5555 | 5292 | 2104 | 38 |
| H(92A) | 4518 | 6132 | 2124 | 27 |
| H(92B) | 5380 | 6179 | 1916 | 27 |
| H(97)  | 1698 | 5935 | -1448 | 38 |
| H(98)  | 408  | 5672 | -1769 | 51 |
| H(99)  | -183 | 5082 | -1163 | 54 |
| H(10A) | 4507 | 5563 | -740  | 23 |
| H(10B) | 6930 | 5111 | -1690 | 47 |
| H(10C) | 7716 | 5337 | -1325 | 47 |
| H(10D) | 7070 | 5702 | -1678 | 47 |
| H(106) | 6702 | 5537 | 228   | 29 |
| H(107) | 6195 | 5674 | 1184  | 28 |
| H(109) | 1744 | 5042 | 104   | 37 |
| H(110) | 482  | 4769 | -244  | 48 |
| H(112) | 1863 | 5627 | 1709  | 32 |
| H(113) | 602  | 5841 | 1927  | 43 |
| H(114) | -206 | 6328 | 1208  | 42 |
| H(115) | 238  | 6578 | 266   | 39 |
| H(116) | 1501 | 6377 | 44    | 32 |
Compound Name: 5h

Formula: C$_{31}$ H$_{29}$ N$_{3}$ O$_{3}$

Unit Cell Parameters: a 15.4841(5) b 28.1687(10) c 17.1022(5) P21/c

Table 1. Crystal data and structure refinement for 140616LT_0M.
Identification code: 140616LT_0m
Empirical formula: C31 H29 N3 O3
Formula weight: 491.57
Temperature: 100(2) K
Wavelength: 0.71073 Å
Crystal system: Monoclinic
Space group: P 21/c
Unit cell dimensions:

\[a = 15.4841(5) \, \text{Å}\]
\[b = 28.1687(10) \, \text{Å}\]
\[c = 17.1022(5) \, \text{Å}\]
\[\alpha = 90^\circ\]
\[\beta = 98.999(2)^\circ\]
\[\gamma = 90^\circ\]

Volume: 7367.6(4) Å³
Z: 12
Density (calculated): 1.330 Mg/m³
Absorption coefficient: 0.086 mm⁻¹
F(000): 3120
Crystal size: 0.30 x 0.25 x 0.03 mm³
Theta range for data collection: 1.331 to 26.411°.
Index ranges: -19 ≤ h ≤ 13, -28 ≤ k ≤ 35, -21 ≤ l ≤ 19
Reflections collected: 59484
Independent reflections: 15029 [R(int) = 0.0510]
Completeness to theta = 25.242°: 99.9 %
Absorption correction: Semi-empirical from equivalents
Max. and min. transmission: 0.9485 and 0.8258
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 15029 / 0 / 1009
Goodness-of-fit on F²: 1.041
Final R indices [I>2σ(I)]: R1 = 0.0789, wR2 = 0.2033
R indices (all data): R1 = 0.1260, wR2 = 0.2424
Extinction coefficient: n/a
Largest diff. peak and hole: 1.072 and -0.417 e.Å⁻³
Table 2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for 140616LT_0M. U(eq) is defined as one third of the trace of the orthogonalized U^ij tensor.

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Symmetry transformations used to generate equivalent atoms:
Table 4. Anisotropic displacement parameters (Å² x 10³) for 140616LT_0M. The anisotropic displacement factor exponent takes the form: -2π² [h²a²U₁¹ + ... + 2hkab*U₁²].

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| C(72) | 16(1) | 19(2) | 18(1) | 0(1)  | 0(1)  | -1(1) |
| C(73) | 26(2) | 14(2) | 19(1) | -2(1) | -2(1) | -3(1) |
| C(74) | 32(2) | 17(2) | 40(2) | -6(1) | 0(1)  | -6(1) |
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