Supporting Information

Combining Click-Multicomponent Reaction; One-pot Synthesis of 1,2,3-Triazol-4-ylmethyl 3-amino-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate Derivatives

Minoo Dabiri,^{*,1} David MaGee,^{*,2} Peyman Salehi,^{*,3} Laleh Torkian,¹ Mahsa Fakharian¹ and Jordan Doanhue²

¹ Department of Chemistry, Faculty of Science, Shahid Beheshti University, G. C., Evin, Tehran 1983963113, Iran. E-mail: m-dabiri@sbu.ac.ir

² Department of Chemistry, University of New Brunswick, P.O. Box 4400 Fredericton, NB Canada E3B 5A3 E-mail address: dmagee@unb.ca

³ Department of Phytochemistry, Medicinal Plants and Drugs Research Institute, Shahid Beheshti University, G. C., Evin, Tehran 1983963113, Iran. E-mail: p-salehi@sbu.ac.ir

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Experimental Section:

Chemicals were purchased from commercial suppliers and were used without purification. Melting points were measured on an Electrothermal 9100 apparatus and were not corrected. High-resolution mass spectra were obtained on a microTOF ESI-MS system (Bruker Daltonics), conditions for HRESITOF-MS were as follows: spectra were recorded in the range of m/z 150–1500 in positive and negative modes. Nitrogen was used as nebulizing gas at a pressure of 2.0 bar and as drying gas at a flow rate of 9.0 L/min (dry gas temperature 240 °C). Capillary voltage was at –4500 V (+4500 V in negative mode), endplate offset at –500 V, hexapole at 250.0 Vpp (negative mode: 230 Vpp), skimmer 1 at 40 V (negative mode: –50 V) and skimmer 2 at 22.5 V (negative mode: –22.5 V). Instrument calibration was performed using a reference solution of sodium formate 0.1% in isopropanol/water (1:1) containing 5 mM sodium hydroxide. Data acquisition and processing were performed using HyStar 3.0 software (Bruker Daltonics). ^1H -NMR and ^{13}C -NMR spectra were recorded on a BRUKER DRX-300 AVANCE spectrometer at 300.13 and 75.47 MHz, respectively, or a Varian Unity 400 spectrometer at 400 and 100.6 MHz, respectively. ^{19}F -NMR spectra were recorded on a Varian Inova 300 spectrometer at 282.2 MHz with α,α,α -trifluorotoluene ($\text{CF}_3\text{C}_6\text{H}_5$) used as an external reference. IR spectra were recorded on a Bomem MB-Series FT-IR spectrometer.

General one-pot procedure for MCR-click reaction to produce 1,2,3-Triazol-4-ylmethyl 3-amino-5,10-dihydro-5,10-dioxo-1H-pyrazolo[1,2-*b*]phthalazine-2-carboxylate **5a-5p**:

A mixture of benzaldehyde derivatives **1a-1n** (1.0 mmol), aryl azide **2a-2e** (1.0 mmol), prop-2-ynyl 2-cyanoacetate (**3**) (1.0 mmol) and phthalhydrazide (**4**) (1.0 mmol) in the presence of $\text{Cu}(\text{OAc})_2$ (0.02 g, 10 mol%), sodium ascorbate (0.04 g, 20 mol%) and $[\text{Hmim}]\text{TFA}$ (0.5 g) were mixed thoroughly and then stirred for 4-5 h at 100 °C. After cooling, ammonia hydroxide (2 mL) and water (5 mL) were added and stirring was continued for 30 min. The solid was filtered and washed with hot ethanol to give the pure products.

(1-(3-Nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl 3-amino-1-(4-chlorophenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (**5a**):

Cream powder; yield: 463 mg (81%); MP 218-219 °C. IR (KBr) (ν_{max} / cm^{-1}): 3463, 3303, 1697, 1672, 1650, 1536, 1391. ^1H NMR (399.939 MHz, $\text{DMSO}-d_6$): δ = 5.17 (d, 1H, J = 12.8 Hz, CH), 5.26 (d, 1H, J = 13.2 Hz, CH), 6.12 (s, 1H, CH), 7.21 (d, 2H, J = 8.4 Hz, H_{Ar}), 7.43 (d, 2H, J = 8.4 Hz, H_{Ar}), 7.88-8.42 (m, 9H, H_{Ar} , NH_2), 8.71 (dd, 1H, J = 2.0 Hz, $\Delta\delta$ = 2.4 Hz, H_{Ar}), 8.78 (s, 1H, H_{Ar}). ^{13}C NMR (100.575 MHz, $\text{DMSO}-d_6$): δ = 55.7,

62.4, 80.7, 114.8, 122.8, 123.2, 126.1, 126.7, 127.3, 127.7, 128.76, 128.8, 129.4, 131.6, 132.0, 133.7, 134.7, 137.1, 138.6, 144.1, 148.5, 150.4, 153.2, 156.9, 163.3. HR-MS (ESI) calcd for $C_{27}H_{18}ClN_7O_6$ [M-H] 570.0934 found 570.0928.

(1-(3-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-5,10-dihydro-1-(4-nitrophenyl)-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5b):

Yellow powder; yield: 437 mg (75%); MP 237 °C decomposed IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3419, 3303, 1702, 1672, 1535, 1348. ^1H NMR (300.13 MHz, $\text{DMSO}-d_6$): δ = 5.13 (m, 1H, CH), 5.25 (m, 1H, CH), 6.22 (s, 1H, CH), 7.70-8.35 (m, 13H, H_{Ar} , NH_2), 8.70 (s, 1H, H_{Ar}), 8.85 (s, 1H, H_{Ar}). ^{13}C NMR (100.757 MHz, $\text{DMSO}-d_6$): δ = 56.0, 62.9, 80.6, 114.6, 115.0, 115.1, 123.3, 123.4, 123.6, 124.5, 124.5, 126.4, 126.7, 127.1, 127.7, 129.0, 129.2, 129.3, 132.0, 132.2, 134.2, 135.1, 137.4, 144.3, 147.1, 147.6, 148.9, 151.0, 157.4, 163.6. HR-MS (ESI) calcd for $C_{27}H_{18}N_8O_8$ [M-H] 581.1175 found 581.1169.

(1-(3-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-1-(3-bromophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5c):

Brown powder; yield: 480 mg (78%); MP 224-226 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3406, 3268, 1706, 1668, 1641, 1534, 1349. ^1H NMR (300.13 MHz, $\text{DMSO}-d_6$): δ = 5.15 (d, 1H, J = 12.7 Hz, CH), 5.24 (d, 1H, J = 12.7 Hz, CH), 6.10 (1H, s, CH), 7.15-8.37 (m, 13H, H_{Ar} , NH_2), 8.17 (s, 1H, H_{Ar}), 8.82 (s, 1H, H_{Ar}). ^{13}C NMR (100.6 MHz, $\text{DMSO}-d_6$): δ = 56.3, 62.9, 80.9, 115.2, 121.5, 123.2, 123.7, 126.6, 126.7, 127.0, 127.2, 127.7, 129.2, 129.3, 130.4, 130.7, 130.8, 131.8, 132.0, 134.1, 135.1, 137.5, 142.8, 148.9, 144.45, 153.7, 157.4, 163.8. HR-MS (ESI) calcd for $C_{27}H_{18}BrN_7O_6$ [M-H] 614.0429 found 614.0423.

(1-(4-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-5,10-dihydro-1-(4-hydroxyphenyl)-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5d):

Yellow powder; yield: 395 mg (74%); MP 244 °C decomposed IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3420, 3312, 1708, 1706, 1644, 1547, 1258. ^1H NMR (300.13 MHz, $\text{DMSO}-d_6$): δ = 5.17 (d, 1H, J = 13.1 Hz, CH), 5.27 (d, 1H, J = 13.1 Hz, CH), 6.06 (s, 1H, CH), 6.61 (d, 2H, J = 7.3 Hz, H_{Ar}), 7.20 (d, 2H, J = 7.3 Hz, H_{Ar}), 7.77-8.43 (m, 11H, H_{Ar} , NH_2), 9.29 (s, 1H, OH). ^{13}C NMR (100.575 MHz, $\text{DMSO}-d_6$): δ = 56.2, 63.0, 81.5, 115.0, 121.0, 121.2, 122.7, 126.0, 127.1, 127.7, 129.0, 129.2, 129.4, 130.2, 134.0, 135.1, 141.1, 145.1, 147.2, 153.4, 157.3, 157.4, 163.9. HR-MS (ESI) calcd for $C_{27}H_{19}N_7O_7$ [M-H] 552.1273 found 552.1296.

(1-(4-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl-3-amino-5,10-dihydro-1-(4-methoxyphenyl)-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5e):

White powder; yield: 442 mg (78%); MP 226-228 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3451, 3341, 1703, 1664, 1528, 1356, 1285. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$): δ = 3.54 (s, 3H, OMe), 5.14 (d, 1H, J = 12.5 Hz, CH), 5.25 (d, 1H, J = 12.5 Hz, CH), 6.07 (s, 1H, CH), 6.70-8.63 (m, 14H, H_{Ar} , NH_2), 8.72 (s, 1H, H_{Ar}). ^{13}C NMR (100.575 MHz, $\text{DMSO-}d_6$): δ = 55.3, 56.1, 63.0, 81.5, 113.5, 115.3, 123.0, 123.6, 126.5, 127.1, 127.7, 129.0, 129.2, 129.3, 131.9, 132.0, 134.0, 135.1, 137.5, 144.7, 148.9, 153.5, 157.3, 159.0, 163.9. HR-MS (ESI) calcd for $\text{C}_{28}\text{H}_{21}\text{N}_7\text{O}_7$ $[\text{M-H}]$ 566.1430 found 566.1423.

(1-(4-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-5,10-dihydro-5,10-dioxo-1-phenyl-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5f):

Yellow powder; yield: 408 mg (76%); MP 248-249 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3338, 3465, 1703, 1526, 1346. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$): δ = 5.17 (d, 1H, J = 12.6 Hz, CH), 5.25 (d, 1H, J = 12.6 Hz, CH), 6.12 (s, 1H, CH), 7.17-8.48 (m, 15H, H_{Ar} , NH_2), 8.58 (s, 1H, H_{Ar}). ^{13}C NMR (100.575 MHz, $\text{DMSO-}d_6$): δ = 56.1, 63.4, 81.5, 121.1, 123.0, 126.1, 127.1, 127.7, 127.8, 128.0, 128.3, 129.1, 129.3, 134.1, 135.1, 140.1, 141.1, 144.9, 147.2, 150.8, 153.6, 157.3, 163.8. HR-MS (ESI) calcd for $\text{C}_{27}\text{H}_{19}\text{N}_7\text{O}_6$ $[\text{M-H}]$ 536.1324 found 536.1318.

(1-(4-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-5,10-dihydro-1-(3-nitrophenyl)-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5g):

Cream powder; yield: 477 mg (82%); MP 242 °C decomposed IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3403, 3294, 1700, 1657, 1529. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$): δ = 5.08 (d, 1H, J = 13.0 Hz, CH), 5.22 (d, 1H, J = 13.0 Hz, CH), 6.25 (s, 1H, CH), 7.46 (m, 1H, CH), 7.89-8.49 (m, 13H, H_{Ar} , NH_2), 8.83 (s, 1H, H_{Ar}). ^{13}C NMR (100.575 MHz, $\text{DMSO-}d_6$): δ = 56.2, 62.9, 80.6, 121.0, 123.0, 123.2, 126.0, 127.1, 127.7, 129.1, 129.4, 129.8, 134.2, 134.5, 135.1, 141.1, 142.4, 144.4, 147.2, 147.7, 151.1, 153.9, 157.5, 163.8. HR-MS (ESI) calcd for $\text{C}_{27}\text{H}_{18}\text{N}_8\text{O}_8$ $[\text{M-H}]$ 581.1175 found 581.1169.

(1-(4-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-1-(3-ethoxy-4-hydroxyphenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5h):

Yellow powder; yield: 388 mg (65%); MP 222-224 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3418, 3319, 1706, 1704, 1647, 1536, 1348. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$): δ = 1.13 (t,

3H, $J = 6.8$ Hz, CH₃), 3.37-3.85 (m, 2H, CH₂), 5.20 (s, 2H, CH), 6.05 (s, 1H, CH), 6.62 (d, 1H, $J = 8.0$ Hz, H_{Ar}), 6.77 (d, 1H, $J = 8.0$ Hz, H_{Ar}), 6.90 (s, 1H, H_{Ar}), 7.87-8.77 (m, 12H, H_{Ar}, NH₂, OH). ¹³C NMR (100.575 MHz, DMSO-*d*₆): $\delta = 15.0, 56.4, 63.3, 64.2, 81.6, 114.1, 115.2, 115.4, 120.1, 122.9, 123.6, 126.5, 127.1, 127.7, 129.1, 129.4, 130.8, 132.0, 133.9, 135.1, 137.4, 144.7, 146.4, 146.8, 149.0, 150.7, 153.5, 157.3, 164.1$. HR-MS (ESI) calcd for C₂₉H₂₃N₇O₈ [M-H] 596.1535 found 596.1602.

(1-(4-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl 3-amino-1-(4-fluorophenyl)-5,10-dihydro-5,10-dioxo-1H-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5i):

Cream powder; yield: 392 mg (72%); MP 213-215 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3454, 3326, 1703, 1624, 1655, 700. ¹H NMR (300.13 MHz, DMSO-*d*₆): $\delta = 5.14$ (d, 1H, $J = 12.8$ Hz, CH), 5.21 (d, 1H, $J = 12.8$ Hz, CH), 6.12 (s, 1H, CH), 6.96-8.25 (m, 14H, H_{Ar}, NH₂), 8.52 (s, 1H, H_{Ar}). ¹³C NMR (100.575 MHz, DMSO-*d*₆): $\delta = 56.2, 62.8, 81.3, 115.0$ (d, $J = 20.8$ Hz), 122.2, 122.8, 127.1, 127.7, 129.2 (d, $J = 5.7$ Hz), 129.9, 130.0, 130.3, 133.5, 134.1, 135.1, 135.7, 136.3 (d, $J = 2.2$ Hz), 144.3, 153.7, 157.4, 161.9 (d, $J = 243.5$ Hz). ¹⁹F NMR (100.6 MHz, CDCl₃): $\delta -49.1$. HR-MS (ESI) calcd for C₂₇H₁₈ClF₂N₆O₄ [M-H] 543.0989 found 543.0983.

(1-(4-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl 3-amino-1-(2,4-dichlorophenyl)-5,10-dihydro-5,10-dioxo-1H-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5j):

Yellow powder; yield: 434 mg (73%); MP 191-192 °C. IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3396, 3303, 1707, 1669, 1647, 710. ¹H NMR (399.939 MHz, DMSO-*d*₆): $\delta = 5.10$ (d, 1H, $J = 12.6$ Hz, CH), 5.20 (d, 1H, $J = 12.6$ Hz, CH), 6.44 (s, 1H, CH), 7.19-8.27 (m, 13H, H_{Ar}, NH₂), 8.55 (s, 1H, H_{Ar}). ¹³C NMR (100.575 MHz, DMSO-*d*₆): $\delta = 55.7, 121.8, 122.4, 126.7, 127.2, 127.3, 128.3, 128.5, 128.7, 129.9, 132.7, 133.0, 133.8, 134.8, 135.3, 143.5, 150.8, 153.1, 156.9, 163.2$. HR-MS (ESI) calcd for C₂₇H₁₇Cl₃N₆O₄ [M-H] 593.0304 found 593.0298.

(1-(4-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl 3-amino-5,10-dihydro-5,10-dioxo-1-p-tolyl-1H-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5k):

Cream powder; yield: 373 mg (69%); MP 199 °C decomposed IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3462, 3330, 1699, 1661, 1620, 695. ¹H NMR (300.13 MHz, DMSO-*d*₆): $\delta = 3.60$ (s, 3H, CH₃), 5.13 (d, 1H, $J = 12.9$ Hz, CH), 5.24 (d, 1H, $J = 12.9$ Hz, CH), 6.10 (s, 1H, CH), 6.74 (d, 2H, $J = 8.0$ Hz, CH), 7.30 (d, 2H, $J = 8.0$ Hz, CH), 7.67-8.24 (m, 10H, H_{Ar}, NH₂), 8.32 (s, 1H, H_{Ar}). ¹³C NMR (100.575 MHz, DMSO-*d*₆): $\delta = 55.3, 56.3,$

63.0, 81.5, 113.6, 122.2, 122.3, 122.6, 127.1, 127.7, 129.1, 129.2, 129.4, 130.3, 131.9, 133.5, 134.0, 135.1, 135.7, 144.4, 153.5, 157.3, 159.1, 163.9. HR-MS (ESI) calcd for $C_{28}H_{21}ClN_6O_4$ [M-H] 539.1240 found 539.1234.

(1-(4-Chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-1-(3-fluorophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5l):

Cream powder; yield: 424 mg (78%); MP 240-242 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3410, 3286, 1704, 1641, 1671, 1531, 1396, 799. ^1H NMR (300.13 MHz, $\text{DMSO}-d_6$): δ = 5.14 (d, 1H, J = 12.9 Hz, CH), 5.21 (d, 1H, J = 12.9 Hz, CH), 6.10 (s, 1H, CH), 6.92-8.07 (m, 13H, H_{Ar} , NH_2), 8.25 (s, 1H, H_{Ar}), 8.58 (s, 1H, H_{Ar}). ^{13}C NMR (100.575 MHz, $\text{DMSO}-d_6$): 56.3, 62.9, 81.0, 114.6, 114.9 (d, J = 21.8 Hz), 122.2, 122.8, 123.9, 127.1, 127.7, 129.2 (d, J = 12.0 Hz), 130.0, 130.2 (d, J = 15.7 Hz), 133.5, 134.1, 135.3 (d, J = 48.9 Hz), 143.1 (d, J = 6.8 Hz), 144.2, 150.8, 153.5, 157.4, 163.2 (d, J = 238.3 Hz), 163.9. ^{19}F NMR (100.6 MHz, CDCl_3): δ -49.1. HR-MS (ESI) calcd for $C_{27}H_{18}ClFN_6O_4$ [M-H] 543.0989 found 543.0983.

(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-5,10-dihydro-1-(4-nitrophenyl)-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5m):

Cream powder; yield: 413 mg (75%); MP 227-230 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3409, 3286, 1706, 1647, 1537, 1349. ^1H NMR (300.13 MHz, $\text{DMSO}-d_6$): δ = 5.05 (s, 2H, CH_2), 5.58 (s, 2H, CH_2), 6.17 (s, 1H, CH), 7.29-8.29 (m, 16H, H_{Ar} , NH_2). ^{13}C NMR (100.6 MHz, $\text{DMSO}-d_6$): δ = 53.2, 56.7, 62.8, 80.7, 123.4, 124.7, 127.1, 127.7, 128.3, 128.6, 129.0, 129.1, 129.2, 129.3, 129.4, 134.3, 135.2, 136.4, 147.3, 147.6, 153.8, 157.4, 163.8. HR-MS (ESI) calcd for $C_{28}H_{21}N_7O_6$ [M-H] 550.1481 found 550.1474.

(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl 3-amino-1-(4-fluorophenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5n):

Yellow powder; yield: 383 mg (73%); MP 202-204 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3396, 3297, 1701, 1670, 1638, 693. ^1H NMR (300.13 MHz, $\text{DMSO}-d_6$): δ = 5.06 (s, 2H, CH_2), 5.59 (s, 2H, CH_2), 6.05 (s, 1H, CH), 6.92-8.06 (m, 15H, H_{Ar} , NH_2), 8.25 (s, 1H, H_{Ar}). ^{13}C NMR (75.47 MHz, $\text{DMSO}-d_6$): δ = 53.2, 56.7, 62.8, 81.3, 115.0 (d, J = 21.3 Hz), 124.6, 127.1, 127.7, 128.4, 128.7, 129.2, 129.8 (d, J = 9.0 Hz), 134.1, 135.1, 136.3 (d, J = 17.3 Hz), 150.6, 153.7, 157.3, 162.5 (d, J = 286.8 Hz). ^{19}F NMR (100.6 MHz, CDCl_3): δ -49.1. HR-MS (ESI) calcd for $C_{28}H_{21}FN_6O_4$ [M-H] 523.1536 found 523.1529.

(1-(3-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 3-amino-1-(2-fluorophenyl)-5,10-dihydro-5,10-dioxo-1H-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5o):

Yellow powder; yield: 377 mg (70%); MP 195 °C decomposed IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3440, 3319, 1708, 1660, 1621, 761, 701. ^1H NMR (300.13 MHz, $\text{DMSO-}d_6$): δ = 5.02 (d, 1H, J = 13.0 Hz, CH), 5.10 (d, 1H, J = 13.0 Hz, CH), 5.61 (s, 2H, CH_2), 6.29 (s, 1H, CH), 6.90-8.27 (m, 15H, H_{Ar} , NH_2). ^{13}C NMR (100.575 MHz, $\text{DMSO-}d_6$): δ = 52.5, 56.6, 57.7, 80.4, 115.2 (d, J = 22.0 Hz), 115.4 (d, J = 21.6 Hz), 115.5 (d, J = 20.9 Hz), 124.4, 124.5, 124.5, 124.6, 126.9 (d, J = 11.2 Hz), 127.0 (d, J = 11.2 Hz), 127.4 (d, J = 62.6 Hz), 129.1, 129.0, 129.1, 129.7 (d, J = 21.52 Hz), 129.8 (d, J = 25.4 Hz), 131.3, 131.4, 134.2, 135.3, 139.1 (d, J = 7.4 Hz), 143.1, 150.9, 153.4, 157.2, 160.5 (d, J = 247.6 Hz), 162.6 (d, J = 244.2 Hz). ^{19}F NMR (100.6 MHz, CDCl_3): δ -49.1. HR-MS (ESI) calcd for $\text{C}_{28}\text{H}_{20}\text{F}_2\text{N}_6\text{O}_4$ [M-H] 541.1514 found 541.1435.

(1-(3-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl 3-amino-1-(3-pyridyl)-5,10-dihydro-5,10-dioxo-1H-pyrazolo[1,2-*b*]phthalazine-2-carboxylate (5p):

Yellow powder; yield: 388 mg (74%); MP 194-196 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 3434, 3323, 1702, 1667, 1526, 1284, 1262, 1137, 727, 701. ^1H NMR (399.939 MHz, CDCl_3): δ = 5.17 (ABq, 2H, J_{AB} = 41.6 Hz, J_{AB} = 12.4 Hz), 5.47 (s, 2H), 6.27 (s, 1H), 6.92-6.97 (m, 1H), 7.02-7.18 (m, 4H), 7.33-7.40 (m, 1H), 7.72 (d, 1 H, J = 7.2 Hz), 7.84-7.88 (m, 2H), 8.22-8.26 (m, 1H), 8.32-8.36 (m, 1H), 8.44 (d, 1H, J = 4.0 Hz), 8.65 (s, 1H). ^{13}C NMR (100.575 MHz, CDCl_3): δ = 53.5 (d, J = 1.8 Hz), 57.0, 61.7, 115.0 (d, J = 22.3 Hz), 115.8 (d, J = 21.0 Hz), 122.9, 123.2, 123.6 (d, J = 2.9 Hz), 127.7, 127.8, 128.7 (d, J = 8.2 Hz), 133.7, 134.1, 134.9, 135.5, 136.8 (d, J = 7.4 Hz), 143.7, 149.2, 149.5, 153.9, 157.3, 163.0 (d, J = 248.2 Hz). ^{19}F NMR (100.6 MHz, CDCl_3): δ -49.1. HR-MS (ESI) calcd for $\text{C}_{27}\text{H}_{20}\text{FN}_7\text{NaO}_4$ [M] $^{+}$ 548.1461 found 548.1453.

(Z)-Prop-2-ynyl 3-(4-chlorophenyl) 2-cyanoacrylate (6a):

White powder; yield: 213 mg (87%); MP 144-146 °C. IR (KBr) ($\nu_{\max}$ / cm^{-1}): 2219, 2116, 1729, 667. ^1H NMR (399.939 MHz, $\text{DMSO-}d_6$): δ = 3.70 (t, 1H, J = 2 Hz, CH), 4.97 (d, 2H, J = 2.4 Hz, CH_2), 7.65-7.71 (m, 2 H, H_{Ar}), 8.05-8.11 (m, 2 H, H_{Ar}), 8.46 (s, 1 H, CH). ^{13}C NMR (100.575 MHz, $\text{DMSO-}d_6$): δ = 54.4, 78.1, 79.2, 102.9, 115.6, 130.0, 130.6, 133.1, 138.7, 155.0, 161.5.

(Z)-(1-(3-Nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl 3-(4-chlorophenyl)-2-cyanoacrylate (7a):

Brown powder; yield: 352 mg (86%); MP 186-188 °C. IR (KBr) (ν_{max} /cm⁻¹): 2235, 1727, 1530, 1354, 738. ¹H NMR (300.13 MHz, DMSO-*d*₆): δ = 5.53 (s, 2H, CH₂), 7.63-8.43 (m, 8H, H_{Ar}), 8.71 (s, 1H, H_{Ar}), 9.16 (s, 1H, CH). ¹³C NMR (75.47 MHz, DMSO-*d*₆): δ = 59.4, 103.2, 115.3, 115.7, 123.7, 124.4, 126.6, 129.9, 130.6, 132.0, 132.9, 137.5, 138.7, 143.2, 148.9, 154.7, 161.9.

expi PROTON

SAMPLE
date Dec 17 2013 satmode n
solvent cdc13 wet n
file exp SPECIAL
ACQUISITION temp 25.0
sw 6410.3 gain 30
at 3.700 spin not used
np 47436 hst 0.008
fb 4800 pw90 13.950
bs 8 alfa 10.000
d1 0
nt 4096 il n
ct 24 in n
TRANSMITTER dp y
tn H1 hs nm
sfrq 399.937 PROCESSING
tof 399.9 fn 131072
tpwr 59 DISPLAY
pw 6.975 sp -24.1
DECOUPLER C13 rf1 3999.4
dn 0 rfp 3708.3
dof 0 rfp 2903.5
dm nnn rp 144.8
decwave W40_AT3 lp 0
dpwr 29412 PLOT
dmf 29412 vc 250
sc 0
vs 29
th 14
al cdc ph

INDEX	FREQUENCY	PPM	HEIGHT
1	1912.1	4.781	72.8
2	1999.7	4.775	71.9
3	1411.3	3.529	139.5
4	1024.3	2.561	21.1
5	1021.8	2.555	39.3
6	1019.3	2.549	19.0

3

expi CARBON

SAMPLE
date Dec 17 2013 satmode n
solvent cdc13 wet n
file exp SPECIAL
ACQUISITION temp 25.0
sw 25000.0 gain 60
at 1.500 spin not used
np 75000 hst 0.008
fb 17000 pw90 9.750
bs 32 alfa 10.000
d1 0.001
nt 1e+09 il n
ct 64 in n
TRANSMITTER C13 dp y
tn H1 hs nm
sfrq 100.575 PROCESSING
tof 1531.3 lb 0.50
tpwr 67 fn 204200
pw 4.875 DISPLAY
DECOUPLER H1 sp -0.1
dn 0 rf1 20114.2
dof 0 rfp 9191.2
dm yyy rfp 7760.1
decwave w rp -138.3
dpwr 43 lp 0
dmf 12046 PLOT
vc 250
sc 0
vs 150
th 16
nm cdc ph

INDEX	FREQUENCY	PPM	HEIGHT
1	16341.0	162.481	49.9
2	11334.8	112.704	16.6
3	7791.9	77.477	33.8
4	7759.8	77.157	34.8
5	7727.8	76.839	34.9
6	7680.9	76.373	133.6
7	7664.3	76.208	54.0
8	5439.2	54.063	150.3
9	2480.1	24.660	135.5

3

Current Data Parameters
NAME Torkian
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110829
Time 1.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TO 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
OW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 19.60 usec
PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 41.43 cm
F1P 12.355 ppm
F1 3708.10 Hz
F2P -0.993 ppm
F2 -298.03 Hz
PPHMC 0.66740 ppm/cm
HZCM 200.30629 Hz/cm

Current Data Parameters
NAME Torkian
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110829
Time 1.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TO 65536
SOLVENT DMSO
NS 406
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
OW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 12.60 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 20.00 cm
CY 198.63 cm
F1P 211.707 ppm
F1 15977.06 Hz
F2P -16.120 ppm
F2 -1216.58 Hz
PPHMC 11.39138 ppm/cm
HZCM 859.68164 Hz/cm

Current Data Parameters
NAME Torkian
EXPNO 42
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110828
Time 23:46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DQ 64.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 19.60 usec
PL1 -2.00 dB
SF01 300.1323866 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 9.26 cm
F1P 12.355 ppm
F1 3708.10 Hz
F2P -0.993 ppm
F2 -298.03 Hz
PPMCH 0.66740 ppm/cm
HZCM 200.30629 Hz/cm

Current Data Parameters
NAME Torkian
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110829
Time 0:53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DQ 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 12.60 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

***** CHANNEL f2 *****
CPOPG2 waltz16
NUC2 1H
PCPD2 87.90 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.30 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 20.00 cm
CY 58.21 cm
F1P 219.155 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCH 11.91609 ppm/cm
HZCM 899.26058 Hz/cm

Current Data Parameters
NAME Hs11289e
EXPNO 37
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110819
Time 23.36
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 64
DM 64.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 19.41 cm
F1P 11.131 ppm
F1 3340.71 Hz
F2P -1.004 ppm
F2 -301.29 Hz
PPHCH 0.60674 ppm/cm
HZCH 182.10017 Hz/cm

Current Data Parameters
NAME Hs11289e
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110819
Time 23.37
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 316
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8215508 sec
RG 2048
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 12.00 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 0.20

1D NMR plot parameters
CX 20.00 cm
CY 67.43 cm
F1P 219.155 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPHCH 11.91609 ppm/cm
HZCH 899.28052 Hz/cm

Current Data Parameters
NAME Fakharian
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110910
Time 0.08
INSTRUM spect
PROBHD 5 mm BBO-BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
OW 64.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 19.60 usec
PL1 -2.00 dB
SFO1 300.132986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 50.24 cm
F1P 10.975 ppm
F1 3293.80 Hz
F2P -0.917 ppm
F2 -275.31 Hz
RPMCN 0.59459 ppm/cm
H2CM 176.45518 Hz/cm