

Supporting Information

Fast Synthesis of [1,2,3]-Triazole Derivatives through an Efficient Method Executed by a Fe/Cu-Based Hybrid Nanocatalyst

Nima Khaleghi, Zahra Sadat Mojtatabpour, Zahra Rashvandi, Adibeh Mohammadi, Mohadeseh Forouzandeh-Malati, Fatemeh Ganjali, Simindokht Zarei-Shokat, Reza Taheri-Ledari* and Ali Maleki*

¹Endocrinology and Metabolism Research Center, Endocrinology and Metabolism Clinical Sciences Institute, Tehran University of Medical Sciences, Tehran, Iran.

²Catalysts and Organic Synthesis Research Laboratory, Department of Chemistry, Iran University of Science and Technology, Tehran16846-13114, Iran.

*Corresponding authors. R. Taheri-Ledari, E-mail address: Rezataheri13661206@gmail.com, R_taheri94@alumni.iust.ac.ir; A. Maleki: E-mail address: maleki@iust.ac.ir, Tel.: +98 21 77240640-50; fax: +98 2173021584.

 Author's ORCID numbers:

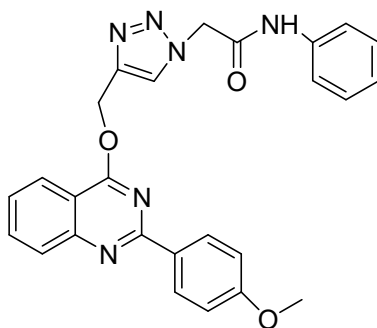
Reza Taheri-Ledari: <https://orcid.org/0000-0002-6511-9411>

Ali Maleki: <https://orcid.org/0000-0001-5490-3350>

Content	Page
¹ H-NMR and ¹³ C-NMR spectral data of the product 2a	2
¹ H-NMR and ¹³ C-NMR spectral data of the product 2b	3
¹ H-NMR and ¹³ C-NMR spectral data of the product 2c	4
¹ H-NMR and ¹³ C-NMR spectral data of the product 2d	5
¹ H-NMR and ¹³ C-NMR spectral data of the product 2e	6

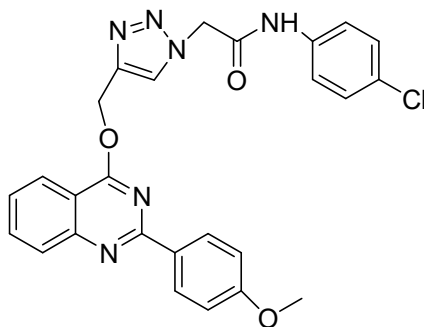
2-(4-(((2-(4-methoxyphenyl)quinazolin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-phenylacetamide (2a)

Yield 72% (335 mg), light brown solid: m.p. 218-220 °C. IR: (KBr) 3370, 1666, 1560, 1340, 1250 cm^{-1} . ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 10.46 (s, 1H), 8.54 (dd, $J = 9.0, 1.4$ Hz, 2H), 8.34 (d, $J = 4$ Hz, 1H), 8.07 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.96 – 7.83 (m, 2H), 7.67 – 7.42 (m, 3H), 7.33 (td, $J = 9.0, 1.4$ Hz, 2H), 7.18 – 6.90 (m, 3H), 5.87 (s, 2H), 5.35 (s, 2H), 3.84 (s, 3H). ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 176.01, 165.47, 158.66, 157.85, 150.13, 142.90, 138.35, 132.41, 130.27, 128.58, 128.23, 127.80, 126.99, 125.97, 123.01, 121.64, 121.44, 117.44, 114.84, 65.52, 56.25, 55.28. Anal. Calcd for $\text{C}_{26}\text{H}_{22}\text{N}_6\text{O}_3$: C 66.94, H 4.75, N 18.02. Found: 67.12, H 4.70, N 17.89.



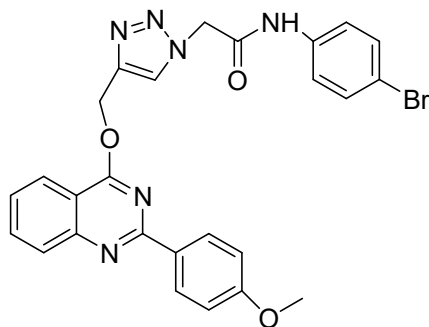
***N*--(4-chlorophenyl)-2-(4-(((2-(4-methoxyphenyl)quinazolin-4-yl)oxy)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (2b)**

Yield 74% (370 mg), brown solid: m.p. 242-243 °C. IR: (KBr) 3365, 1671, 1549, 1332, 1231, 763 cm^{-1} . ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 10.60 (s, 1H), 8.56 (d, $J = 8.6$ Hz, 2H), 8.33 (s, 1H), 8.08 (d, $J = 8.4$ Hz, 1H), 7.96 – 7.84 (m, 2H), 7.65 – 7.51 (m, 3H), 7.36 (d, $J = 8.9$ Hz, 2H), 7.11 (d, $J = 8.7$ Hz, 2H), 5.89 (s, 2H), 5.35 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 175.92, 165.54, 158.66, 157.55, 150.05, 142.48, 138.35, 133.02, 132.40, 130.28, 129.44, 127.97, 127.06, 126.92, 122.90, 121.45, 120.58, 117.45, 114.40, 65.57, 56.27, 55.54. Anal. Calcd for $\text{C}_{26}\text{H}_{21}\text{ClN}_6\text{O}_3$: C 62.34, H 4.23, N 16.78. Found: 67.22, H 4.03, N 17.91.



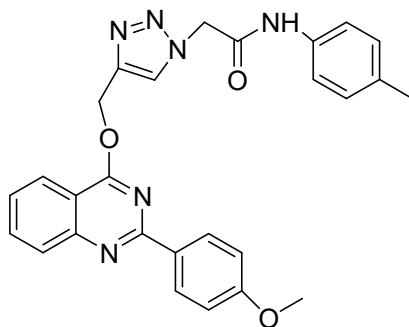
***N*-(4-bromophenyl)-2-(4-(((2-(4-methoxyphenyl)quinazolin-4-yl)oxy)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (2c)**

Yield 79% (429 mg), brown solid: m.p. 258-260 °C. IR: (KBr) 3349, 1658, 1569, 1325, 1212, 683 cm^{-1} . ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 10.58 (s, 1H), 8.52 (dd, $J = 9.0, 1.4$ Hz, 2H), 8.35 (s, 1H), 8.09 (d, $J = 8.2$ Hz, 1H), 7.98 – 7.78 (m, 2H), 7.65 – 7.45 (m, 5H), 7.10 (dd, $J = 9.0, 1.4$ Hz, 2H), 5.90 (s, 2H), 5.36 (s, 2H), 3.84 (s, 3H). ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 175.93, 165.53, 158.78, 157.65, 150.15, 142.47, 138.39, 132.56, 130.26, 129.43, 127.80, 127.08, 126.96, 122.88, 122.28, 121.89, 121.34, 117.22, 114.81, 65.58, 56.30, 55.45. Anal. Calcd for $\text{C}_{26}\text{H}_{21}\text{BrN}_6\text{O}_3$: C 57.26, H 3.88, N 15.41. Found: 57.42, H 3.99, N 15.53.



2-(4-(((2-(4-methoxyphenyl)quinazolin-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(p-tolyl)acetamide (2d)

Yield 70% (336 mg), light brown solid: m.p. 232-234 °C. IR: (KBr) 3363, 1650, 1578, 1319, 1262 cm^{-1} . ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 10.37 (s, 1H), 8.55 (d, $J = 8.7$ Hz, 2H), 8.33 (s, 1H), 8.08 (d, $J = 8.2$ Hz, 1H), 7.95 – 7.80 (m, 2H), 7.61 – 7.50 (m, 1H), 7.45 (d, $J = 8.1$ Hz, 2H), 7.20 – 6.90 (m, 4H), 5.87 (s, 2H), 5.34 (s, 2H), 3.85 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 175.38, 165.11, 158.08, 157.30, 150.05, 142.50, 138.71, 136.80, 132.41, 130.10, 129.45, 127.97, 126.98, 126.26, 122.28, 121.61, 121.06, 117.44, 114.40, 65.57, 56.27, 55.42, 21.27. Anal. Calcd for $\text{C}_{27}\text{H}_{24}\text{N}_6\text{O}_3$: C 67.49, H 5.03, N 17.49. Found: 67.30, H 4.89, N 17.67.



***N*-(3-methoxyphenyl)-2-(4-(((2-(4-methoxyphenyl)quinazolin-4-yl)oxy)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (2e)**

Yield 73% (362 mg), light brown solid: m.p. 253-255 °C. IR: (KBr) 3356, 1661, 1565, 1343, 1241 cm^{-1} . ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 10.43 (s, 1H), 8.54 (d, $J = 8.7$ Hz, 2H), 8.31 (s, 1H), 8.09 (d, $J = 8.2$ Hz, 1H), 7.93 – 7.92 (m, 2H), 7.59 (t, $J = 8.7$ Hz, 1H), 7.51 (d, $J = 8.1$ Hz, 1H), 7.37 (t, $J = 8.6$ Hz, 1H), 7.15 (d, $J = 8.1$ Hz, 1H), 7.11 (d, $J = 8.6$ Hz, 1H), 7.01 (s, 1H), 5.87 (s, 2H), 5.42 (s, 2H), 3.84 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 175.18, 165.04, 160.23, 158.22, 157.02, 149.68, 142.87, 140.34, 132.32, 130.33, 129.54, 12.56, 127.81, 125.97, 122.63, 121.44, 117.43, 116.76, 114.48, 110.71, 110.19, 65.03, 57.92, 57.66, 57.03. Anal.Calcd for $\text{C}_{27}\text{H}_{24}\text{N}_6\text{O}_4$: C 65.31, H 4.87, N 16.93. Found: 65.56, H 4.69, N 16.66.

