Electronic Supplementary Material (ESI) for New Journal of Chemistry

Mesoporous silica-supported copper-catalysts for homocoupling reaction of terminal alkynes at room-temperature

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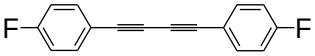
Supporting information

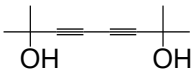
Characterization data of products 2a–2h:

1,4-Diphenylbutadiyne (**2a**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.54-7.52 (m, 4 H), 7.37-7.32 (m, 6 H).

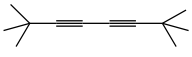


1,4-bis(4-Fluorophenyl)buta-1,3-diyne (**2b**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.47-7.42 (m, 4 H), 7.00-6.94 (m, 4 H).

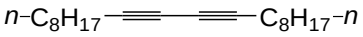
1,4-bis(*p*-methylphenyl)buta-1,3-diyne (**2c**)[2]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.43-7.41 (d, *J* = 8.0 Hz, 4 H), 7.15-7.13 (d, *J* = 8.0 Hz, 4 H), 2.36 (s, 6 H).



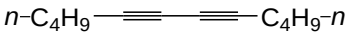
2,7-Dimethyl-3,5-octadiyne-2,7-diol (**2d**)[3]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.01 (s, 2 H), 1.54 (s, 12 H).



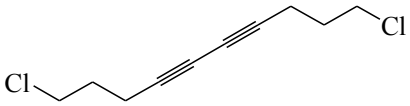
2,2,7,7-Tetramethylocta-3,5-diyne (**2e**)[2]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.22 (s, 18 H).



Icosa-9,11-diyne (**2f**)[2]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.27-2.24 (t, *J* = 7.0 Hz, 4 H), 1.55-1.48 (m, 4 H), 1.41-1.36 (m, 4 H), 1.32-1.27 (m, 16 H), 0.90-0.86 (t, *J* = 6.8 Hz, 6 H).

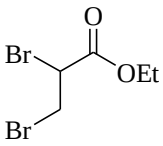


Dodeca-5,7-diyne (**2g**)[4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.26-2.22 (t, *J* = 7.0 Hz, 4 H), 1.56-1.50 (m, 4 H), 1.48-1.37 (m, 4 H), 0.92-0.89 (t, *J* = 7.2 Hz, 6 H).

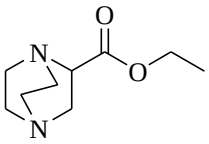


1,10-dichlorodeca-4,6-diyne (**2h**)[5]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.66-3.63 (t, *J* = 6.2 Hz, 4 H), 2.48-2.46 (t, *J* = 6.8 Hz, 4 H), 2.04-1.95 (m, 4 H).

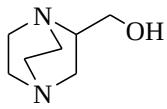
Characterization data of products 2–4:



ethyl 2,3-dibromopropanoate **2**[6]: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.43 (dd, J = 11.2, 4.4 Hz, 1 H), 4.30 (q, J = 7.2 Hz, 2 H), 3.93 (dd, J = 10.6, 4.4 Hz, 1 H), 3.68 (dd, J = 10.0, 4.4 Hz, 1 H), 1.33 (t, J = 7.2 Hz, 3 H).



ethyl 1,4-diaza-bicyclo[2.2.2]octane-2-carboxylate **3**: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.25 (q, J = 7.2 Hz, 2 H), 3.47 (t, J = 8.4 Hz, 1 H), 2.66-3.13 (m, 10 H), 1.31 (t, J = 7.2 Hz, 3 H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 171.71, 60.92, 57.11, 49.23, 48.60, 46.68, 46.12, 42.69, 14.13; LRMS (EI, 70 eV): m/z (%) = 184 (M^+, 100).



1,4-diaza-bicyclo[2.2.2]octan-2-ylmethanol **4**: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.79 (s, 1 H), 3.64-3.59 (m, 2 H), 3.48 (dd, J = 12.0, 4.4 Hz, 1 H), 2.98-2.56 (m, 10 H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 61.48, 56.23, 49.86, 49.14, 47.10, 46.29, 40.26; LRMS (EI, 70 eV): m/z (%) = 142 (M^+, 100).

References

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