Metallovesicles as smart nanoreactors for green catalytic synthesis of benzimidazole derivatives in water

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Supplementary Information

S1: Spectroscopic data (^{1}H NMR) of (entries 1a-1i, Table 1).

Entry 1a: *2-Phenyl-benzimidazole,* white solid, m.p. 292-294 °C; ^{1}H NMR (DMSO-d6, 400 MHz) δ(ppm): 7.22 (q, J = 4.2 Hz, 2H), 7.51-7.62 (m, 5H), 8.24 (dd, J = 8.8, 1.8 Hz, 2H), 11.81 (s, 1H).
Entry 1b: *2-(2-Methoxyphenyl)benzimidazole*, light yellow solid, m.p. 200-205 °C; ^{1}H NMR (DMSO-d_6, 400 MHz,) δ(ppm): 12.75 (s, 1H), 8.11(m, 4H), 7.56 (s, 1H), 7.09 (m, 4H), 3.83 (s, 3H).

Entry 1c: *2-(4-Methoxyphenyl)benzimidazole*, light yellow solid, m.p. 221-223 °C; ^{1}H NMR (DMSO-*d*6, 400 MHz) δ(ppm): 12.33 (br s, 1H), 8.24 (d, J = 4.5 Hz, 2H), 7.78–7.63 (m, 4H), 7.34 (br s, 2H), 3.40 (s, 3H).

Entry 1d: *2-(4-Nitrophenyl)benzimidazole*, light red solid, m.p. 318-320 °C, ^{1}H NMR (DMSO-*d*6, 400 MHz) δ(ppm): 12.70 (s, 1H), 8.44-8.40 (m, 4H), 7.57 (d, J = 6.4 Hz, 2H), 7.19 (d, J = 6.4 Hz, 2H).
Entry 1e: *2-(3-Nitrophenyl)benzimidazole*, yellow solid, m.p. 201-203 °C, ^{1}H NMR (DMSO-d_6, 400 MHz) δ(ppm): 13.87 (s, 1H), 9.03 (t, J = 1.9 Hz, 1H), 8.60-8.64 (m, 1H), 8.30-8.34 (m, 1H), 7.97 (s, 1H), 7.85 (t, J = 8.03, 1H), 7.59 -7.75 (m, 1H) 7.25-7.30 (m, 2H).

Entry 1f: *2-(4-Chlorophenyl) benzimidazole*, white solid, m.p. 288-290 ºC, ^{1}H NMR (DMSO-d6, 400 MHz) δ(ppm): 7.19-7.26 (m, 2H), 7.52-7.64 (m, 4H), 7.17-7.20 (d, J = 11.6 Hz, 2H), 12.99 (s, 1H).

Entry 1g: *2-(4-Bromophenyl)benzimidazole*, white solid, m.p. 294-296 °C, ^{1}H NMR (400MHz, DMSO-d_6): δ = 12.50 (s, 1H), 8.19 (d, J=8.5 Hz, 2H), 7.67-7.55 (m, 4H), 7.25-7.19 (m, 2H) ppm.

Entry 1h: *2-(4-Cyanophenyl) benzimidazole*, white solid, m.p. 248-250 °C, ^{1}H NMR (400MHz, DMSO-d_6,): δ =13.18 (s, 1H), 8.33 (d, J=8.3 Hz, 2H), 8.00 (d, J=8.3 Hz, 2H), 7.71 (d, J=7.1 Hz, 1H), 7.57 (d, J=7.1 Hz, 1H), 7.23 (m, 2H) ppm.

Entry 1i: *2-(4-Methylphenyl)benzimidazole*, yellow solid, m.p. 275-276 °C, ^{1}H NMR (DMSO-d6, 400 MHz) *δ*(ppm): 2.5 (s, 3H), 6.88 (d, *J* = 11.0 Hz, 2H), 7.11 (q, *J* = 4.0 Hz, 2H), 7.56 (q, *J* = 3.5 Hz, 2H), 8.10 (d, *J* = 10.0 Hz, 2H), 12.56 (br, 1H).

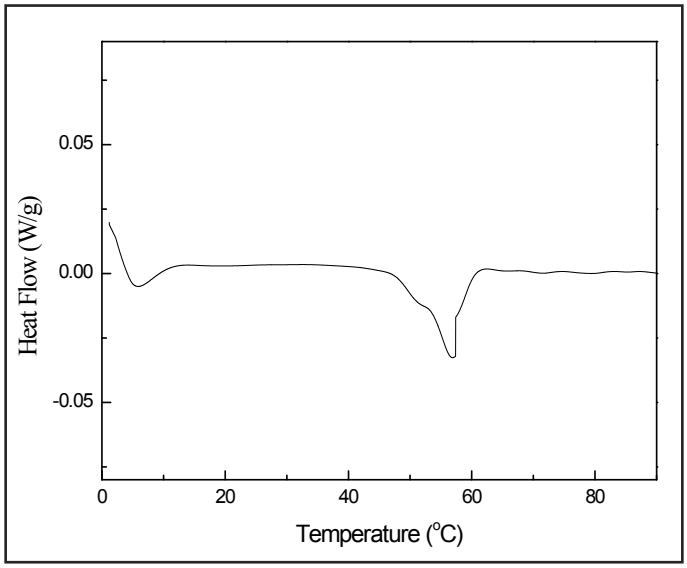


Figure S1 DSC curve showing phase transition temperature of metallosurfactant complex.

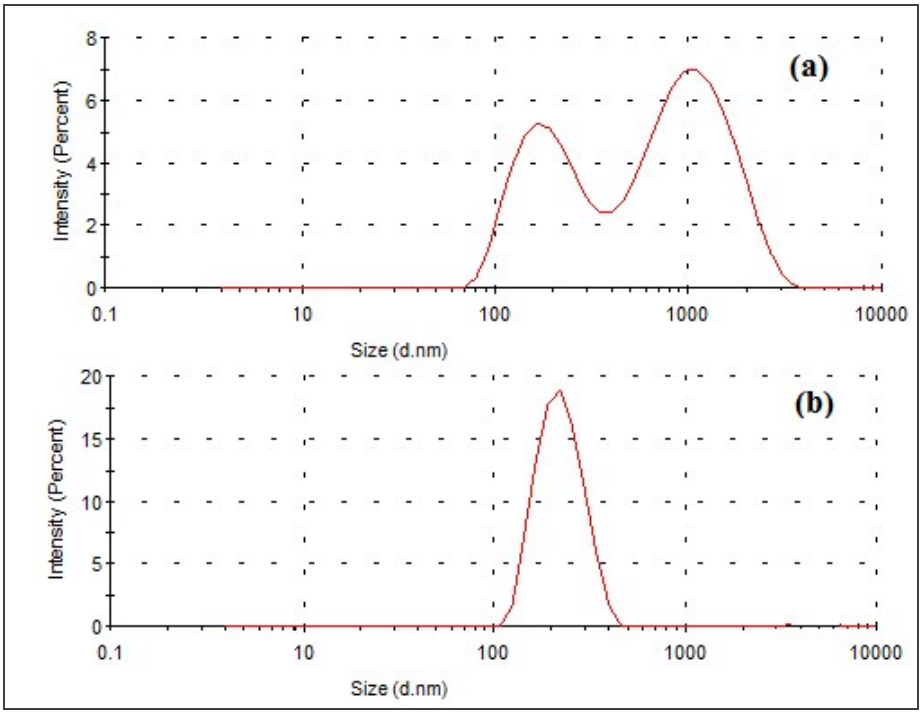


Figure S2 DLS analysis of CuMVs (a) before extrusion and (b) after extrusion.

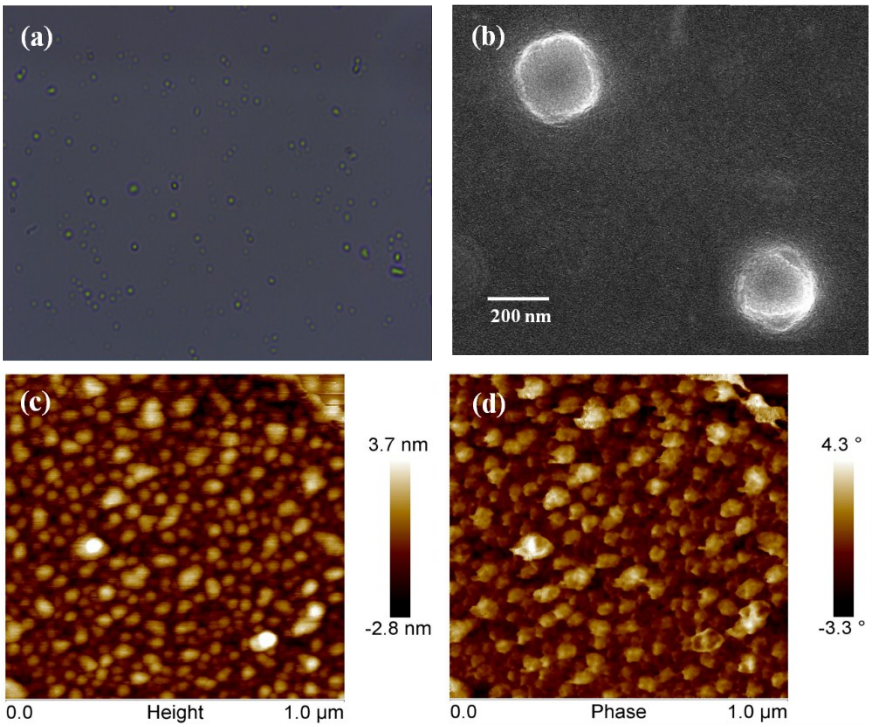


Figure S3 Structural investigations of CuMVs showing (a) Conventional light microscope (b) FESEM image (c) AFM height images[58] and (d) AFM phase contrast image.

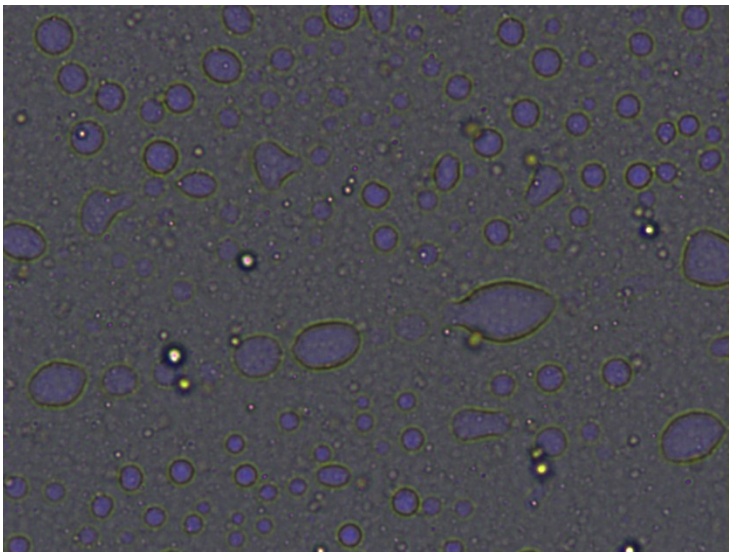
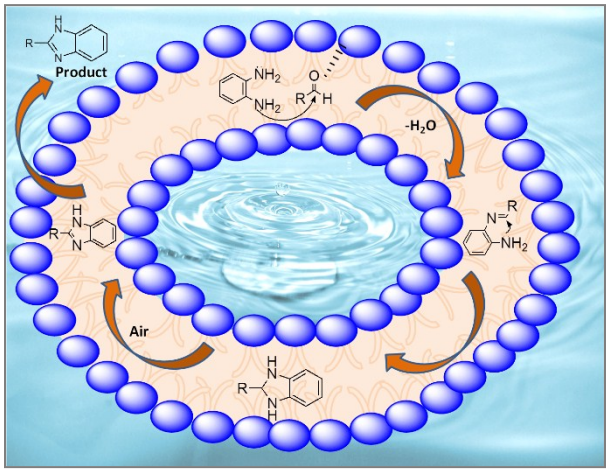


Figure S4 Conventional light microscope images of CuMVs recovered after 6 reaction cycles.



Scheme S1 Proposed mechanism for catalytic action of CuMVs in water.