Electronic Supplementary Information (ESI)

A Common Tattoo Chemical for Energy Storage: Henna Plant-Derived Napthoquinone Dimer as a Green and Sustainable Cathode Material for Li-Ion Batteries


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Material Characterization:

Lawsone (LS):

$^1$H NMR [300 MHz, DMSO-d$_6$, δ]: 11.63 (1H, br s) 8.00 (1H, d), 7.94 (1H, d), 7.82 (2H, m). $^{13}$C NMR (125 MHz, δ): 182.30, 180.19, 156.41, 134.96, 133.56, 132.06, 130.18, 126.13, 125.98, 115.50. FTIR (ATR, cm$^{-1}$): 3300, 1670, 1630, 1583, 1219; MS (ESI+) m/z: 197.2 (100%. M + Na) 175 (57.8, M + H).

Bislawsone (BL):

$^1$H NMR [300 MHz, DMSO-d$_6$, δ]: 11.37 (2H, br s) 8.10 (2H, d), 8.01 (2H, d), 7.86 (4H, m). $^{13}$C NMR (125 MHz, δ): 182.30, 180.19, 156.41, 134.96, 133.56, 132.06, 130.18, 126.13, 125.98,
115.50. FTIR (ATR, cm$^{-1}$): 3300, 1670, 1630, 1583, 1219. MS (ESI–) $m/z$: 345.2 (100%, M – H) 346.2 (70.9, M).

**Lithiated Bislawsone (Li-BL):**

$^1$H NMR [300 MHz, DMSO-d6, δ]: 7.99 (1H, d), 7.87 (1H, d), 7.72 (1H, t), 7.62 (1H, t). $^{13}$C NMR (125 MHz, δ): 188.94, 181.28, 167.77, 136.18, 134.19, 131.47, 131.11, 125.86, 125.33, 117.10. FTIR (ATR, cm$^{-1}$): 1660, 1583, 1510, 1219, 663.
Figure S1: Expanded $^1$H NMR spectrum of pure lawsone (LS) in DMSO with TMS at 0.00 ppm as a reference.
Figure S2: Expanded $^1$H NMR spectrum of pure bislawsone (BL) in DMSO with TMS at 0.00 ppm as a reference.
Figure S3: Expanded $^1$H NMR spectrum of fully lithiated bislawsone (Li-BL) in DMSO with Li metal as lithium source.
Figure S4: Annotated $^{13}$C NMR spectrum of lawsone (LS) in DMSO. Carbons 1 and 4 (carbonyl), as well as carbon 2 (hydroxyl), have been labeled to highlight the significant downfield chemical shift upon subsequent dimerization to bislawsone (BL) and lithium coordination to form lithiated bislawsone (Li – BL).
Figure S5: Annotated $^{13}$C NMR spectrum of bislawsone (BL) in DMSO. Carbons 1 and 4 (carbonyl), as well as carbon 2 (hydroxyl), have been labeled to highlight the significant downfield chemical shift upon lithium coordination to form lithiated bislawsone (Li – BL).
Figure S6: Annotated $^{13}$C NMR spectrum of Li-BL in DMSO. Carbons 1 and 4 (carbonyl), as well as carbon 2 (hydroxyl), have been labeled to highlight the chemical shift of peaks upon lithium coordination compared to bislawsone (BL).
Fig S7: Capacity retention of lawsone molecule tested at current density of 50 mA/g.

Fig S7 represents galvanostatic discharge capacity conducted at current density of 50 mA/g on lawsone molecules. Although greater initial discharge (220 mAh/g) was observed for lawsone molecule than bislawsone (130 mAh/g), more pronounced capacity fade was observed for lawsone molecule than bislawsone molecule.