Electronic Supplementary information for

Ellagic acid – A Novel Organic Electrode Material for High Capacity Lithium Ion Batteries

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Extraction of Ellagic acid:

Pomegranate husk powder (mesh size 50~60, Advait Herbal Extracts, Tumkur, India) was used in the extraction of ellagic acid based on a reported procedure by Jingjing Lu et al.[1] In brief, tannin from finely ground pomegranate husk was extracted thrice using 60% ethanol in water, followed by acid hydrolysis in 5.0 % H_2SO_4 for 5 h. The vacuum dried dark brown crude product was repeatedly recrystallized from methanol to obtain over 90% pure ellagic acid. Subsequently, recrystallization from hot pyridine results in > 99% pure crystalline, ellagic acid. The product was thoroughly characterized by ^{1}H and ^{13}C NMR, FT-IR, LCMS, XRD, SEM techniques (Fig. S1-S5).

Characterization

Solvents and reagents were purchased from Alfa Aesar or Aldrich chemicals and were stored under argon in a glove box. The ^{1}H and ^{13}C-NMR spectra were recorded in DMSO-d_6 at 400 MHz (amx400 FT-NMR spectrometer) with tetramethylsilane as internal standard. The LC system (Thermo LCQ Deca XP MAX, Injector with a 1 μL loop) consisted of a reverse-phase BDS Hypersil C18 analytical column (250 × 4.6 mm i.d., 5 μm particle size). The solvent used was 90% methanol and 10% of H_2O and eluted at a flow rate of 10 μL/min. under isocratic conditions and the run time was kept at 40 minutes. Morphology of EA powder was obtained using scanning electron microscope (Carl-Zeiss FE-SEM). X-ray diffraction patterns were recorded (Philips, The Netherlands) with Cu Kα (1.5418Å) as the source and the spectra were collected at a scan rate 1^0 per minute. Infrared spectra were obtained in transmission mode using FT-IR spectrometer (Perkin-Elmer Spectrum one model) between 4000 and 400 cm^{-1}. Thermogravimetric analysis (TGA) and Differential scanning calorometry (DSC) were carried out on Mettler Toledo TGA/SDTA 851e (temperature rate 10^0C/min under N_2 gas) instruments.

Electrochemical characterization:

Swagelok-type cells were used to follow the electrochemical performance with lithium metal electrode and separator (whatman GF/D borosilicate glass fiber sheet) soaked with 1M $LiPF_6$ in ethylene carbonate and dimethyl carbonate (1:1 in volume ratio) as the electrolyte. The working electrode consisted of EA (50 wt%) with 40 wt% of acetylene black and 10 wt% of polyvinylidene fluoride (PVDF). The mass of each electrode used was ~3-4 mg and the fabrication of cells was carried out in a glove box. Cyclic voltammograms were obtained using a potentiostat (Autolab, PGSTAT30, The Netherlands) and the galvanostatic charge-discharge experiments were conducted using an electrochemical work station (Arbin or Solartron Analytical 1400 cell test system) at 25^0C.

Results and Discussion:

Recrystallized ellagic acid has been characterized using various physicochemical techniques and the NMR and HP-LC show that the compound is highly pure.[2] **^{1}H-NMR**

(DMSO-d$_6$) ppm: δ 7.45 (s, 2H, ArH), 10.67 (s, 4H, -OH), **^{13}C-NMR (DMSO-d$_6$) ppm:** δ 159.08 (C7), 148.08 (C4), 139.55 (C3), 136.35 (C2), 112.27 (C1), 110.21 (C5), 107.59 (C6)

The LC-MS analysis clearly evidences the formation of ellagic acid and the mass spectral data (retention time 13.79 minutes) show molecular ion peak at m/z 301.45, in conformity with the molecular formula $C_{14}H_5O_8$. The ESI-MS (negative mode) m/z is observed at 301.1 [M-H]. The IR spectrum of the compound exhibit broad band in the range, 2800–3700 cm^{-1} which is attributed to the -OH stretching while the band observed at 1725 cm^{-1} corresponds to C=O stretching. The bands observed in the range, 1669 – 1500 cm^{-1} are due to aromatic ring vibrations while the ones at 1190 and 1052 cm^{-1} are due to ester linkage. The band at 751 cm^{-1} is assigned to aromatic C-H bending vibration. The XRD data of the extracted EA reveals that the compound is highly crystalline and the pattern matches well with the reported data for EA.[3] The observed diffraction peaks were at 2 theta values of 10.8, 14.3, 15.8, 17.3, 21.1, 22.8, 24.2, 24.7, 25.4, 26.7, 28.5, 29.7, 32.7 and 34.8 (Fig. S1b). Morphology of the powders shown in figure. S2 reveals highly crystalline material with needle like structures of nanometre sizes.

Supplementary figures:

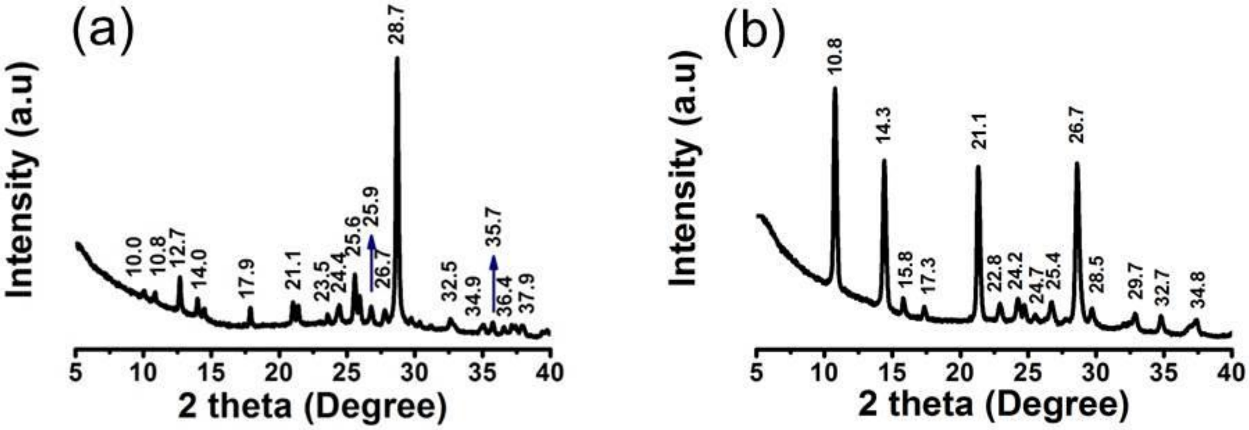

Figure S1. X-ray diffraction patterns of ellagic acid, a) extracted and b) Recrystallized.

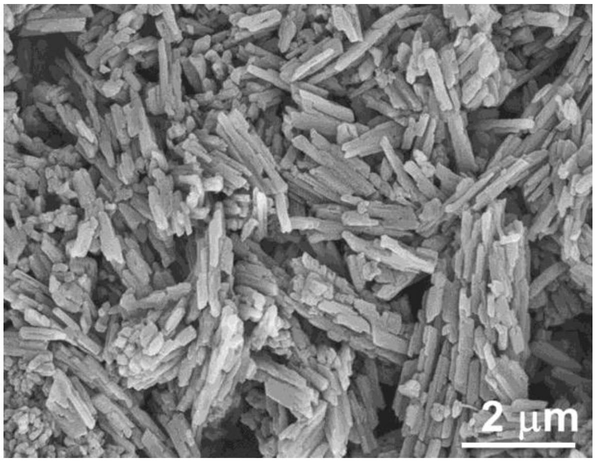

Figure S2. Scanning electron microscopy image of recrystallized ellagic acid.

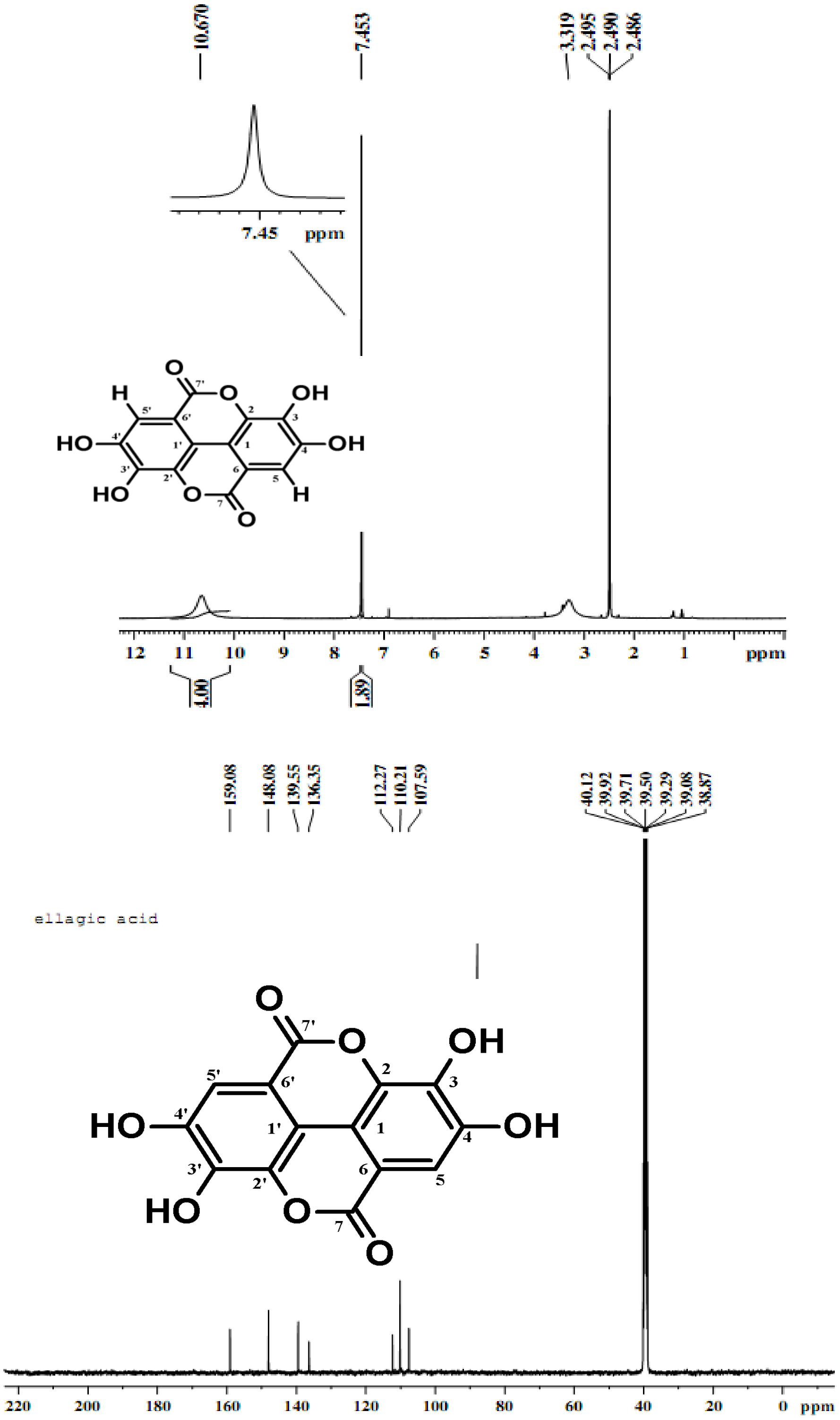

Figure S3. ^{1}H and ^{13}C NMR spectra of ellagic acid, solvent used was DMSO-d6.

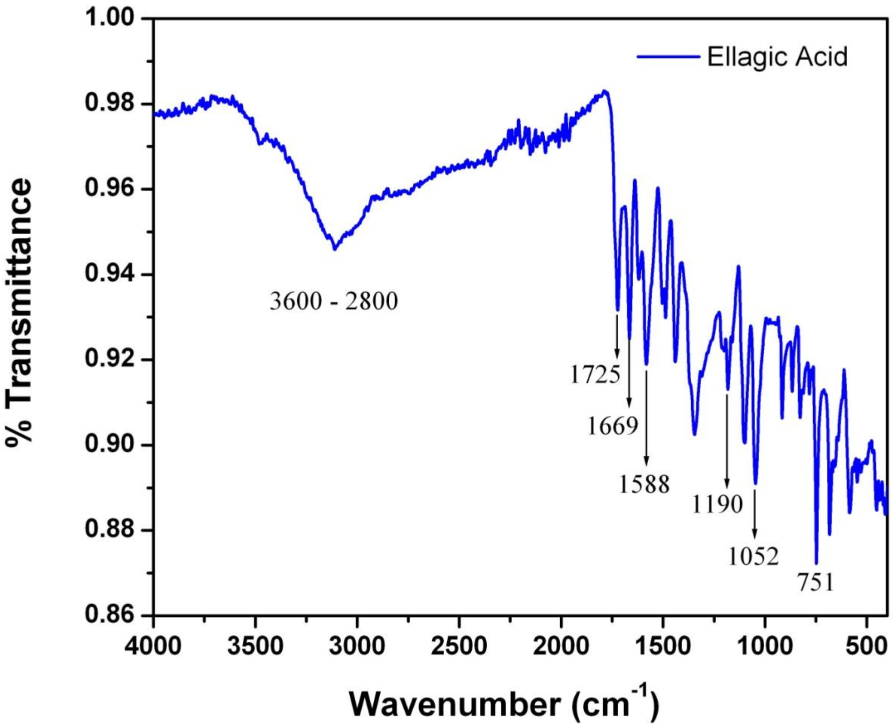

Figure S4. Transmission FT-IR spectrum of ellagic acid

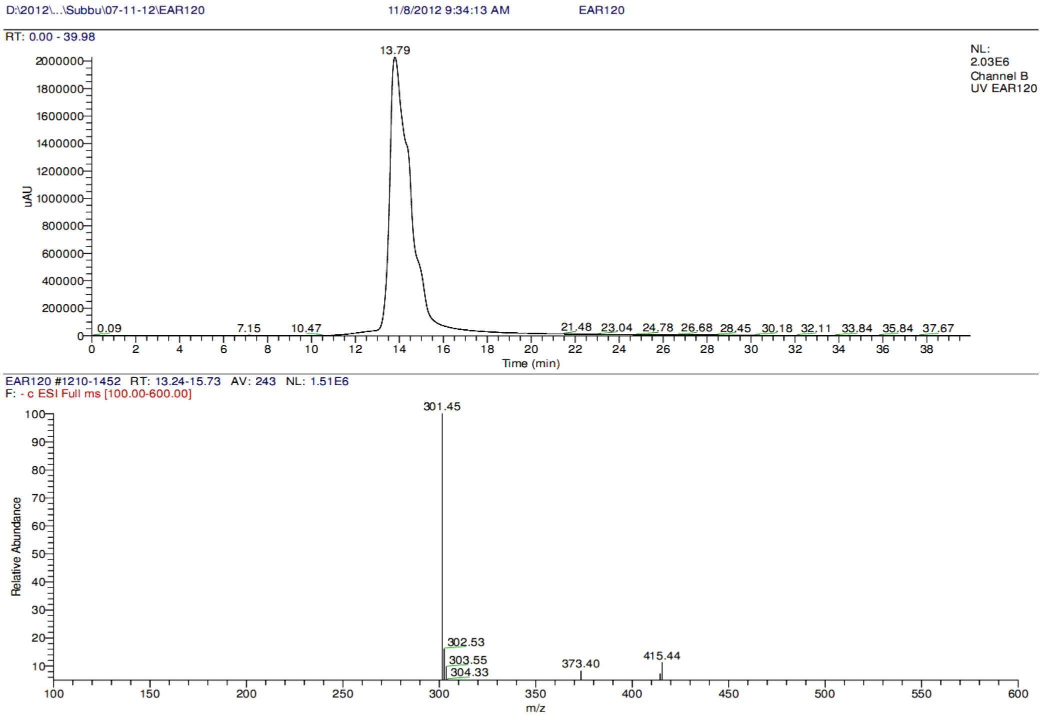

Figure S5. HP-LC and mass spectra of ellagic acid

References:

1. J. Lu and Q. Yuan, *J. Food Proc. Engg*, 2008, **31**, 443.
2. X. C. Li, H. N. Elsohly, C. D. Hufford and A. M. Clark, *Magn. Reson. Chem*. 1999, **37**, 856
3. S. Kim, Y Liu, M. W. Gaber, J. D. Bumgardner, W. O. Haggard and Y. Yang, Biomedical. Mater. Res. Part B: Appl. Biomater., 2008, 145