Supporting Information

Sulfur Functionalized Biocarbon Sorbents for Low-Concentration Mercury Isolation

Douglas Austin, Kousar Jahan, Xu Feng, Jared Carney, Dale K. Hensley, Jihua Chen, Brianna E Altidor, Zhiyong Guo, Elizabeth Michaelis, Mariana K Kebaso, Yanfeng Yue

Physical Measurements

The gas sorption isotherms were collected on a Quantachrome NOVA 4200e. Ultrahigh-purity-grade (>99.99%) gases were used in this adsorption measurement. To maintain the experimental temperatures, liquid nitrogen (77 K) were used, respectively. X-ray powder diffraction data were collected by a Rigaku MiniFlex 600 X-ray diffractometer at 20 kV, 10 mA for Cu Kα (λ = 1.5406 Å) at room temperature in the range of 5-80 degrees (2 theta) with a scan speed of 0.1 degrees per step.

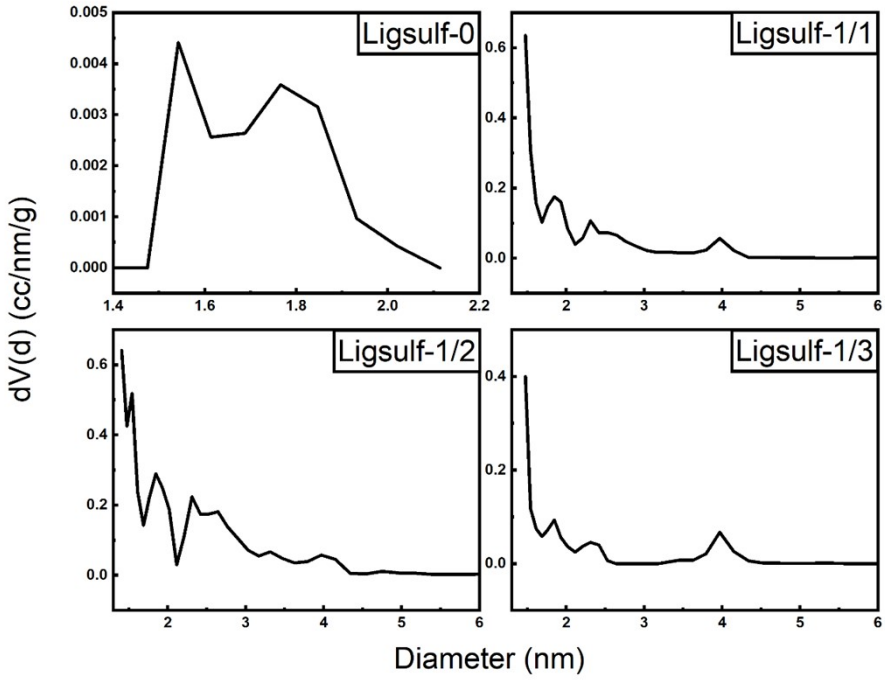

Figure S1. BJH pore size distribution of as-synthesized samples of Ligsulf-0, Ligsulf-1/1, Ligsulf-1/2, and Ligsulf-1/3.

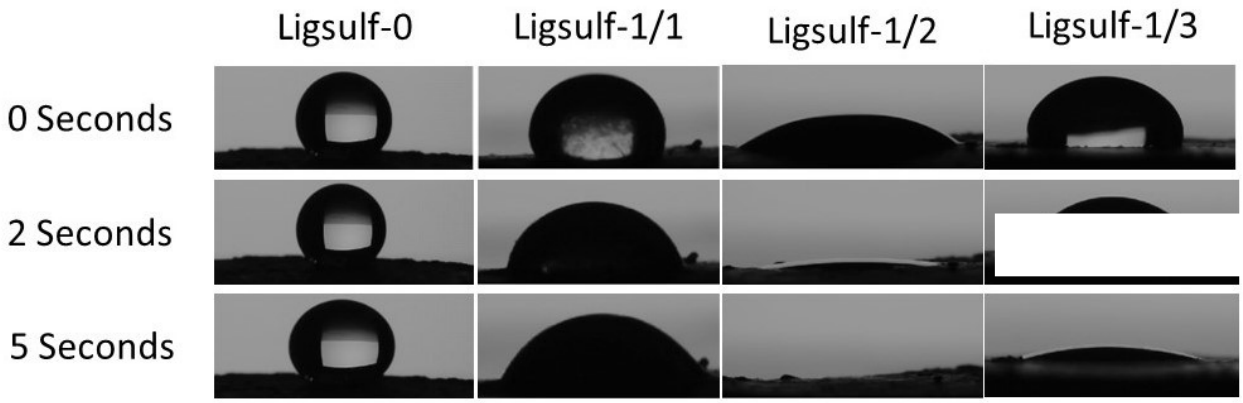

Figure S2. Wettability study using goniometer.

XPS study

The high-resolution C 1s XPS spectra was deconvoluted into four peaks for ligsulf-0, namely, C-S (283.98 eV), C-C/C=C (284.58 eV), C-N/C-O (285.3 eV), O-C=O (286 eV). After functionalization, all the peaks are shifted slightly towards higher binding energy which could be due to the increased amount of bonding of carbon atom with sulfur, nitrogen and oxygen, as could be visualized by increased integral area of the C-S and C-N/C=O peaks. Also, a new peak appeared in the C 1s spectra of ligsulf-1/2 at the higher binding energy that was attributed to carbon atom having three bonds to oxygen atoms, COOR (289.08 eV). The nitrogen spectra of ligsulf-0 and ligsulf-1/2 showed a significant difference and was deconvoluted into two and four peaks, respectively. Sodium thiocyanate functionalization increased the nitrogen content of ligsulf-1/2 and N 1s was divided into pyridine-N (N-6; 398.3 eV), pyrrolic-N (N-5; 400.18eV), quaternary-N (N-Q; 400.98 eV) and oxidized-N (N-X; 405 eV). Similarly, O 1s spectra could be further deconvoluted into five peaks which clearly showed the presence of oxygen functional groups present on both ligsulf-0 and ligsulf-1/2 samples.

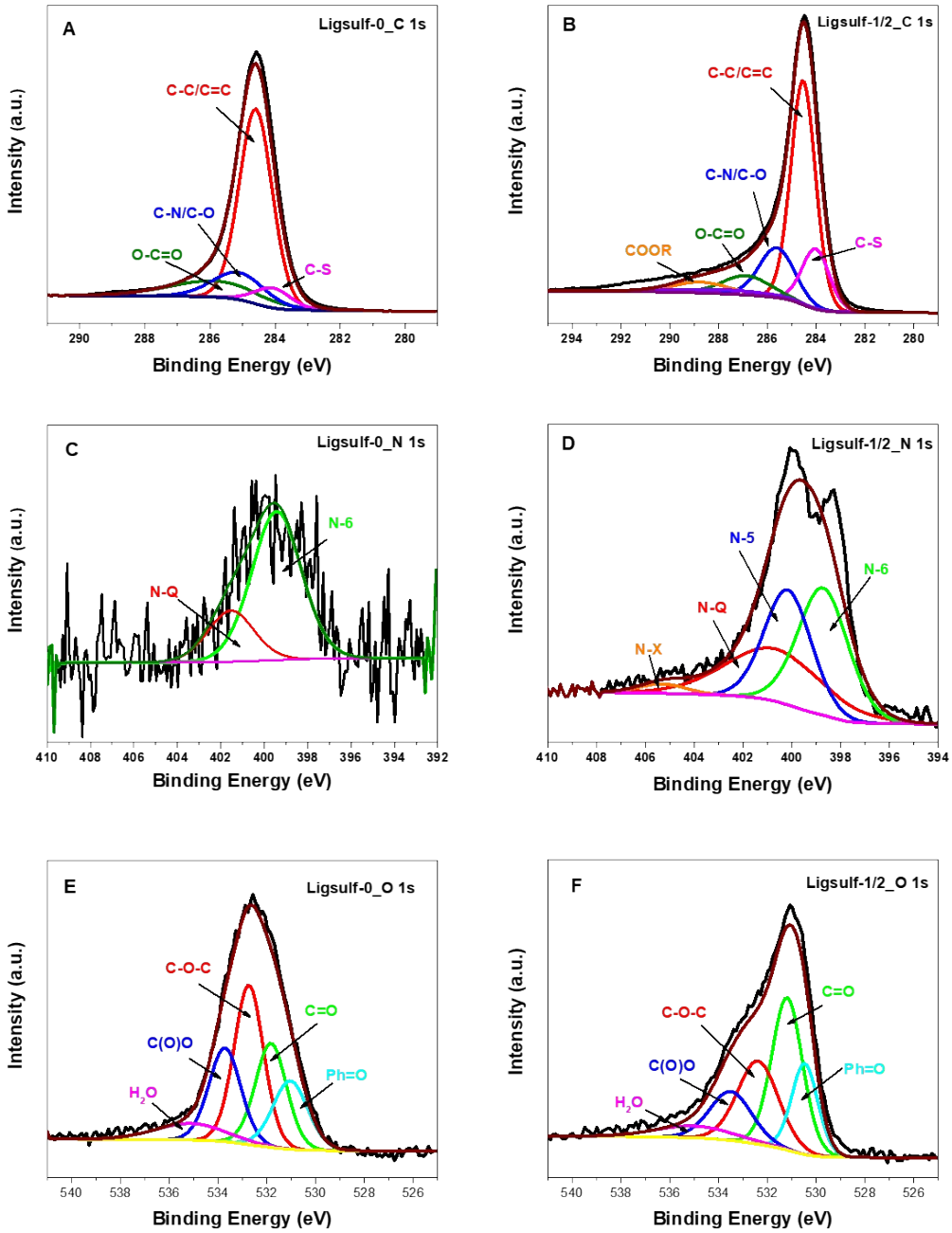

Figure S3. High resolution XPS spectra of Ligsulf-0 and Ligsulg-1/2, (A,B) C 1s, (C,D) N 1s, (E,F) O 1s.

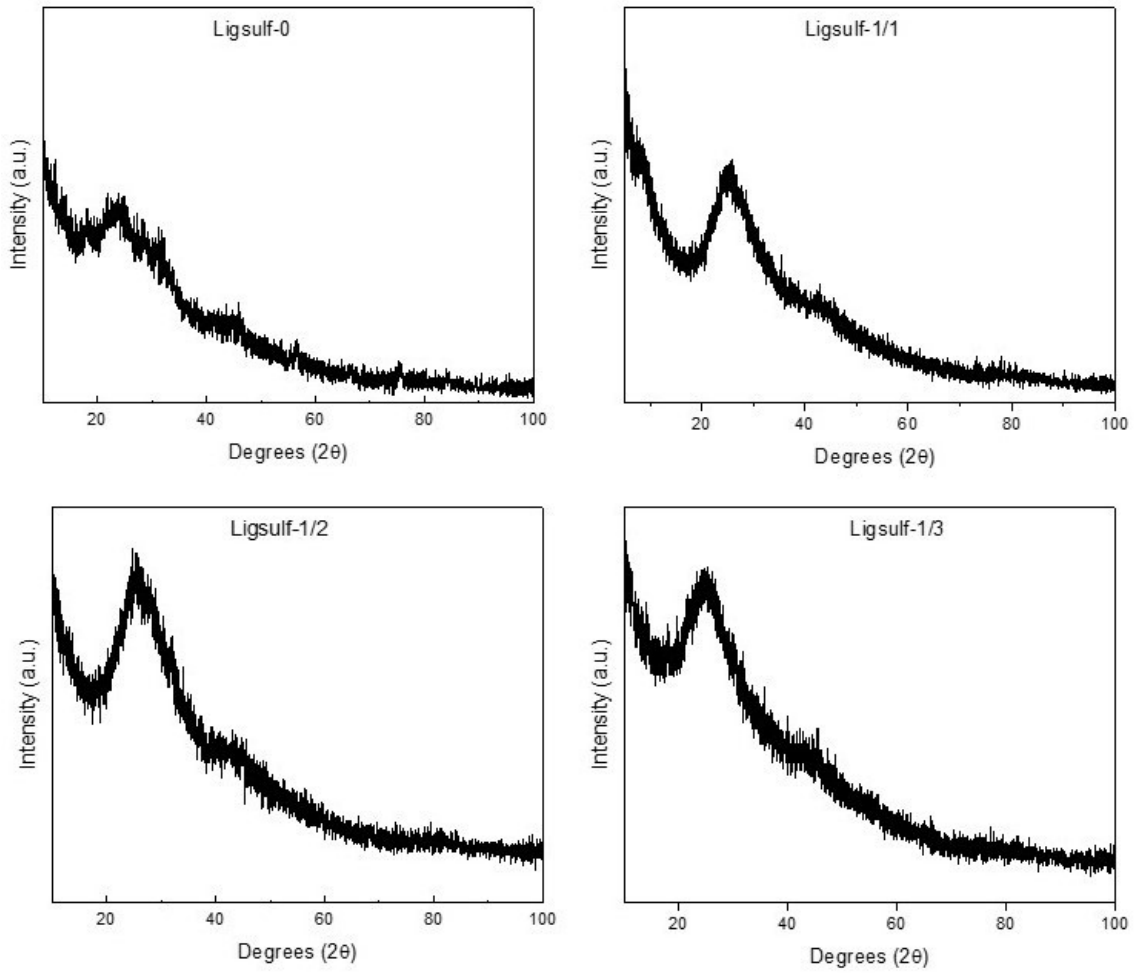

Figure S4. A comparison of XRD patterns from the as-synthesized samples of Ligsulf-0, Ligsulf-1/1, Ligsulf-1/2, and Ligsulf-1/3.

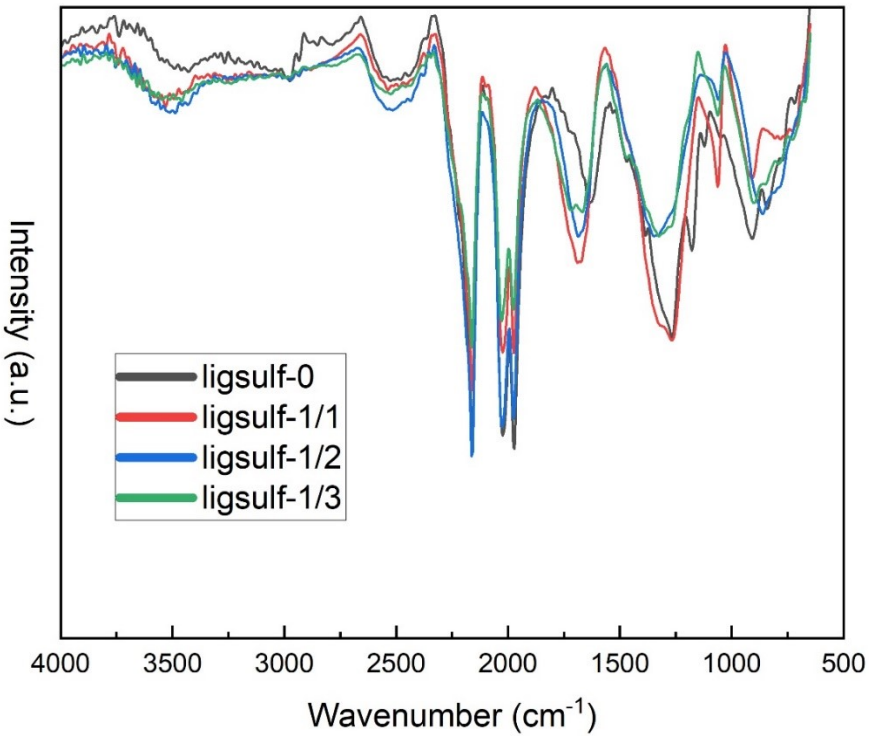

Figure S5. ATR FTIR of Ligsulf-0, Ligsulf-1/1, Ligsulf-1/2, and Ligsulf-1/3.

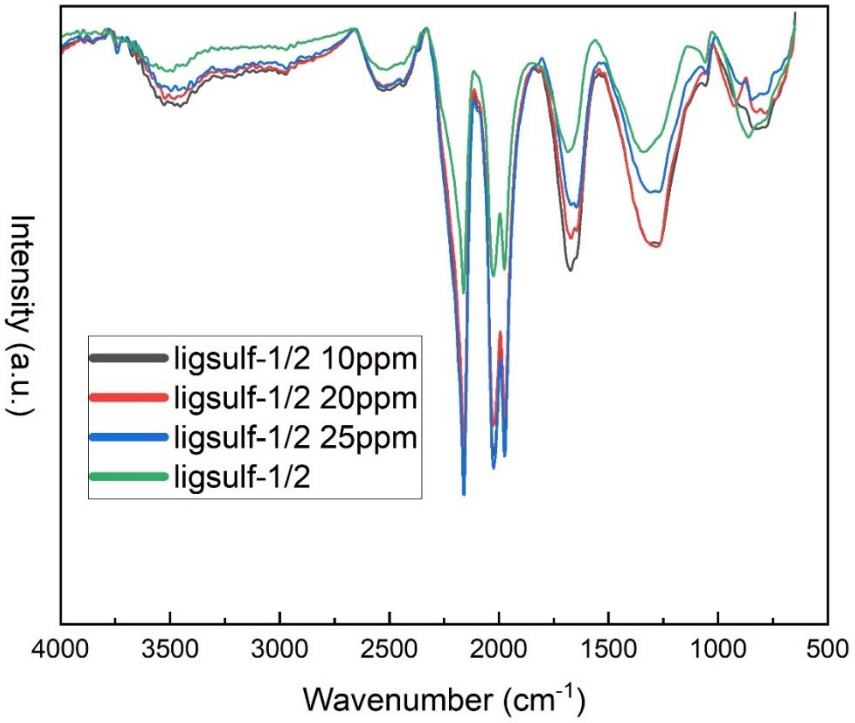

Figure S6. ATR FTIR of Ligsulf-1/2 after adsorption at different concentrations: 10ppm, 20ppm, and 25 ppm.

Sample	Nitrogen%	Carbon%	Hydrogen%	Sulfur%	Other%
Ligsulf-0	0.69	67.26	1.129	4.44	26.481
Ligsulf-1/1	4.27	49.92	1.523	8.065	36.222
Ligsulf-1/2	6.615	62.41	1.468	6.427	23.08
Ligsulf-1/3	2.78	63.53	1.639	8.273	23.778

Table S1. Elemental % of Nitrogen, Carbon, Hydrogen, and Sulfur for samples Ligsulf-0, Ligsulf-1/1, Ligsulf-1/2, and Ligsulf-1/3.