Supporting Information

Amino-functionalized Ordered Mesoporous Carbon for the Separation of Toxic Microcystin-LR

Wei Teng,[ab] Zhangxiong Wu,[c] Jianwei Fan,[a] Wei-xian Zhang*[a] and Dongyuan Zhao*[b]

[a] College of Environmental Science and Engineering, State Key Laboratory for Pollution Control, Tongji University, Shanghai, China 200092

[b] Department of Chemistry, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, and Advanced Materials Laboratory, Fudan University, Shanghai, China 200433

[c] College of Chemistry, Chemical Engineering and Material Science, Soochow University, Suzhou City, Jiangsu, China 215123

EXPERIMENTAL

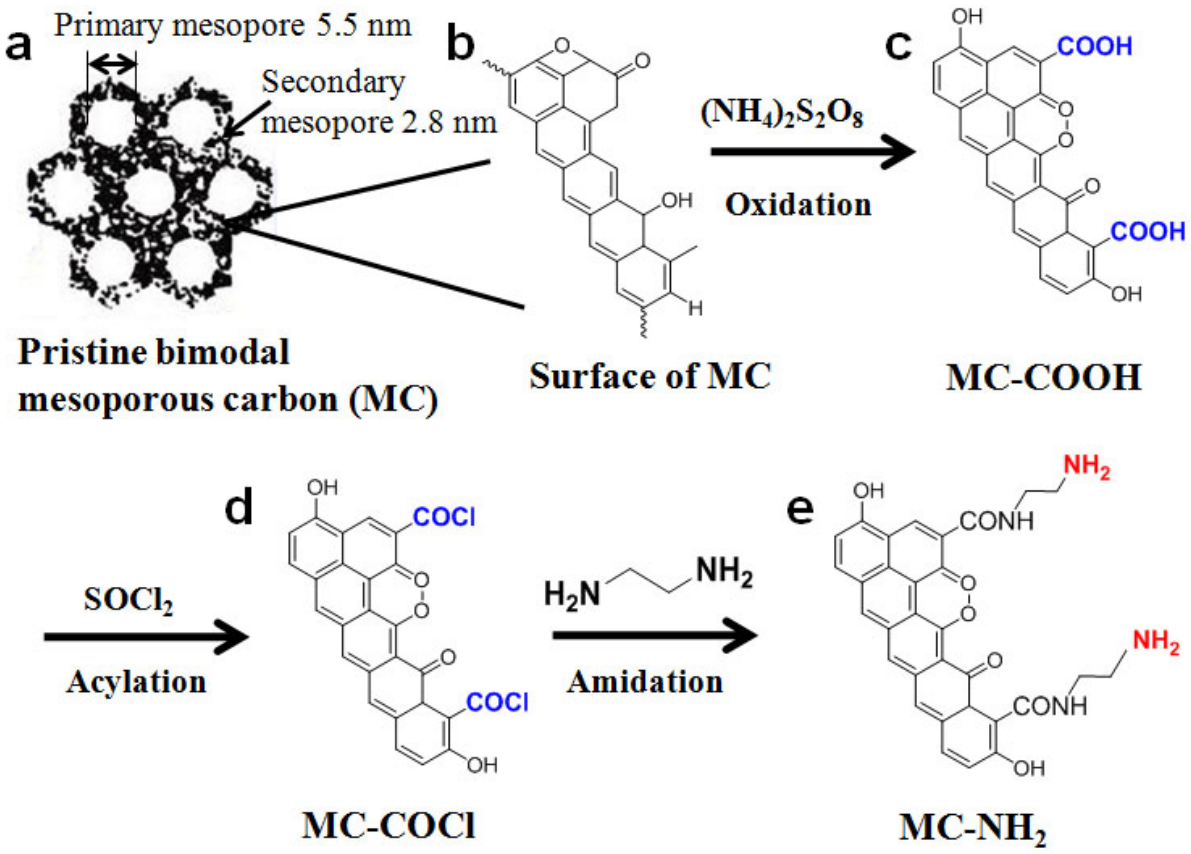
Adsorption Calculation and Modeling

The adsorbed percentage (P) of MC-LR at time (t) is calculated with the equation (1), where C_0 and C_t are the initial solution concentration and the concentration at time t (mg/L), respectively. The adsorbed amount of MC-LR is calculated by using the equation (2), where Q_e is the equilibrium adsorption capacity (mg/g), C_e is the concentration at equilibrium point (mg/L), W is the weight of the dry sorbents (g), and V is the volume of the solution (L). The adsorption isotherms were obtained by plotting Q_e *vs* C_e, and then fitted by Langmuir model equation (3), where Q_{max} is the saturated adsorption capacity (mg/g) and K_L represents the Langmuir equilibrium constant (L/g).

$$P = \frac{(C_0 - C_t)}{C_0} \times 100\% \quad (1)$$

$$Q_e = \frac{(C_0 - C_e) \times V}{W} \quad (2)$$

$$Q_e = \frac{Q_{\max} K_L C_e}{1 + K_L C_e} \quad (3)$$



Scheme S1. Process flow of amino-functionalized mesoporous carbon formation. (a) The frameworks and (b) surface chemistry of the pristine bimodal mesoporous carbon MC, (c) carboxylic groups generated on the MC surface, (d) acyl-chloride groups generated on the MC surface, and (e) amino groups generated on the MC surface.

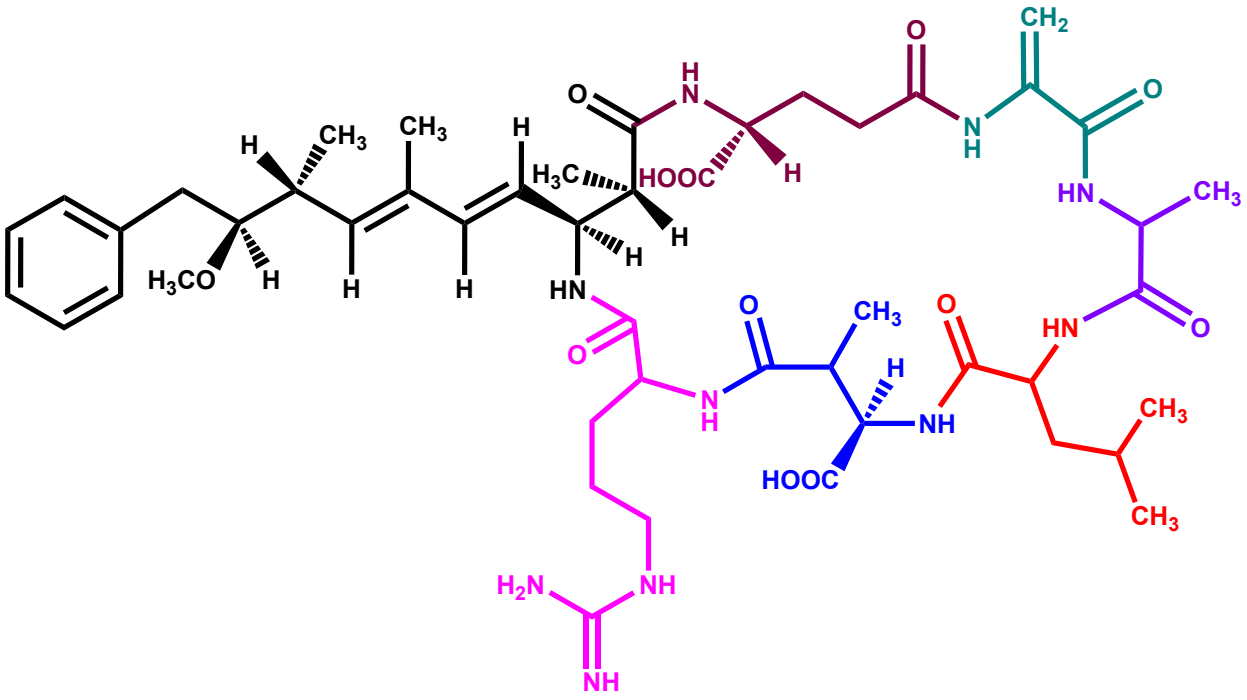


Figure S1. Structure of Microcystin-LR (MC-LR).

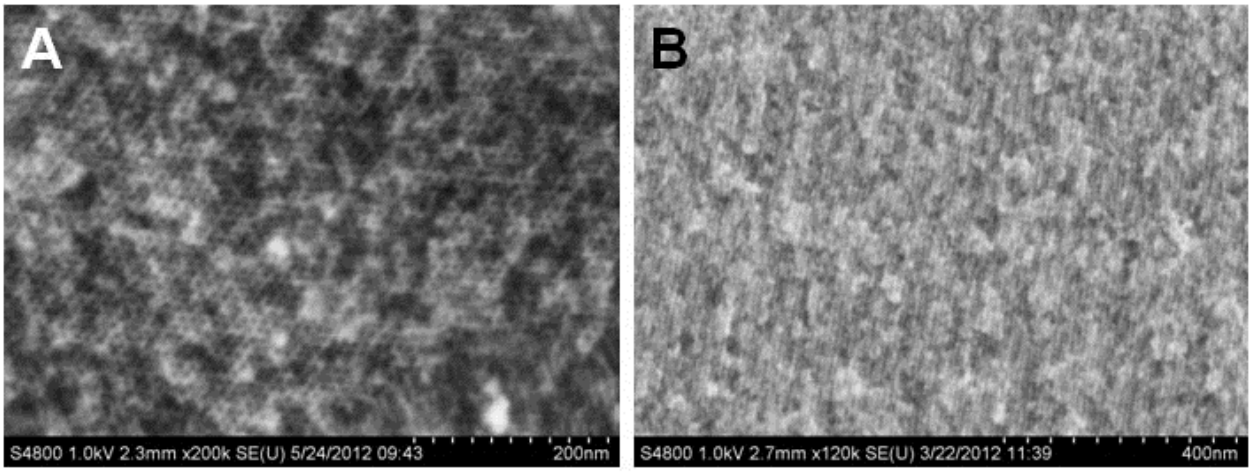


Figure S2. SEM images of pristine ordered mesoporous carbon MC (A) and amino functionalized MC-NH_2 mesoporous carbon (B).

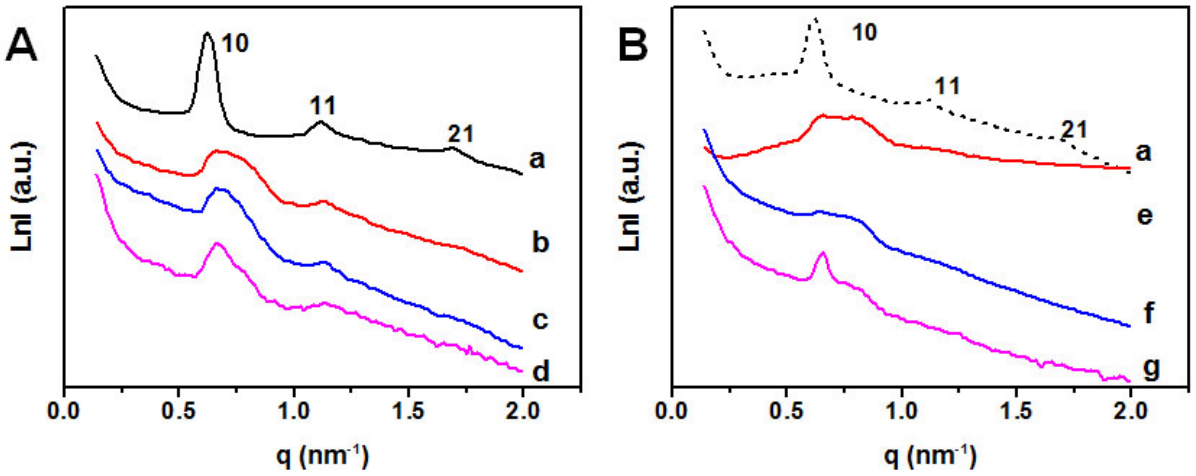


Figure S3. SAXS patterns of pristine and different functionalized ordered mesoporous carbon samples after treatment of oxidation, acylation and amidation. (A) MC (a), MC-COOH-1 (b), MC-COCl-1 (c), MC-NH_2-1-a (d), (B) MC-COOH-2 (e), MC-NH_2-2-b (f), MC-NH_2-1-b (g), where 1 and 2 stand for the oxidation time of 4 and 16 h, and a, b for the added amount of the EDA with 4 and 8 μL, respectively.

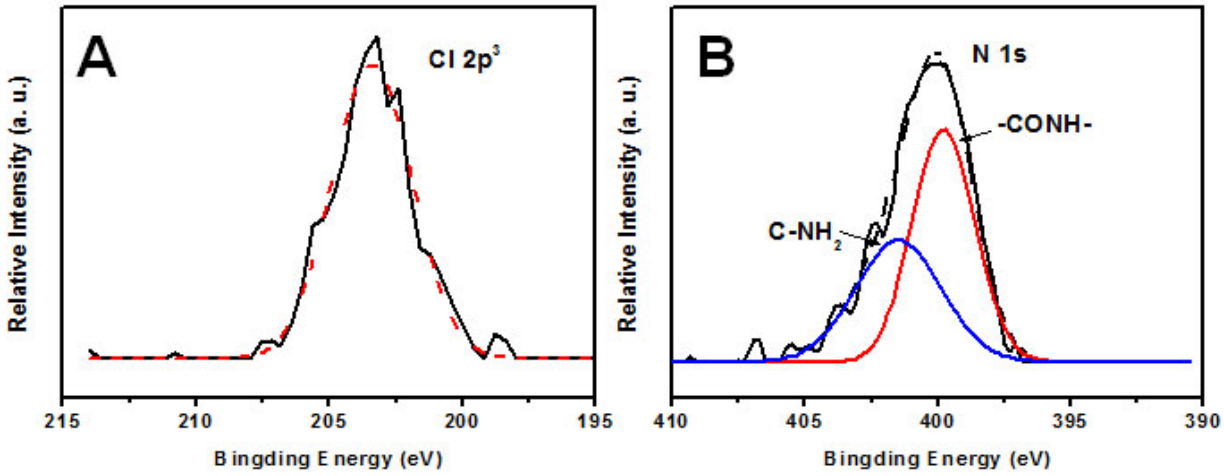


Figure S4. XPS Cl 2p3 spectra of MC-COCl (A) and N 1s spectra of amino functionalized MC-NH_2 mesoporous carbon.

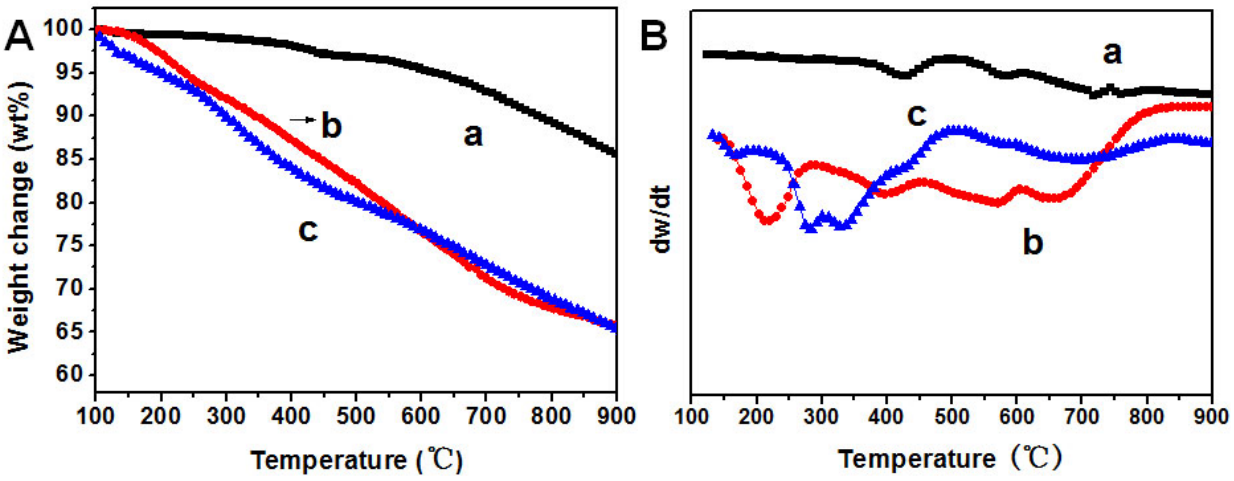


Figure S5. TG curves (A) of pristine mesoporous carbon MC (a), MC-COOH sample treated with surface oxidation (b), MC-COCl sample further treated with thionyl chloride and MC-NH_2 sample last treated by amidation (c). DTG curves (B), the first differential results corresponding to TG data.

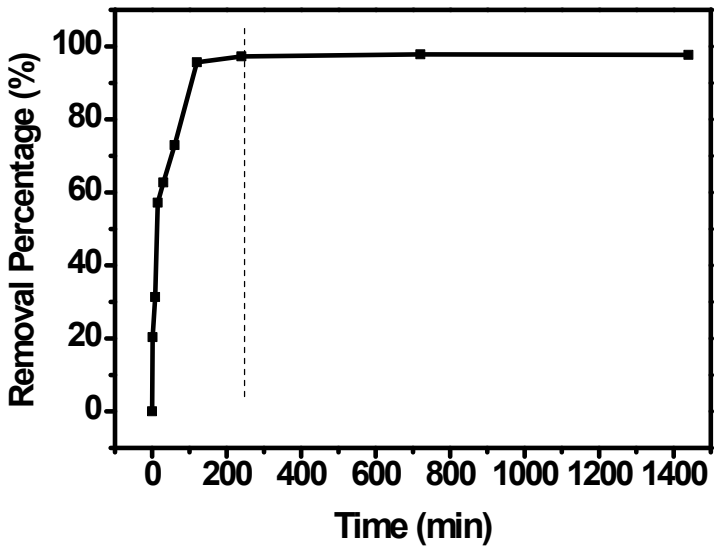


Figure S6. Time-dependent adsorption curve of MC-LR on pristine mesoporous carbon MC with an initial concentration of 2 mg/L.

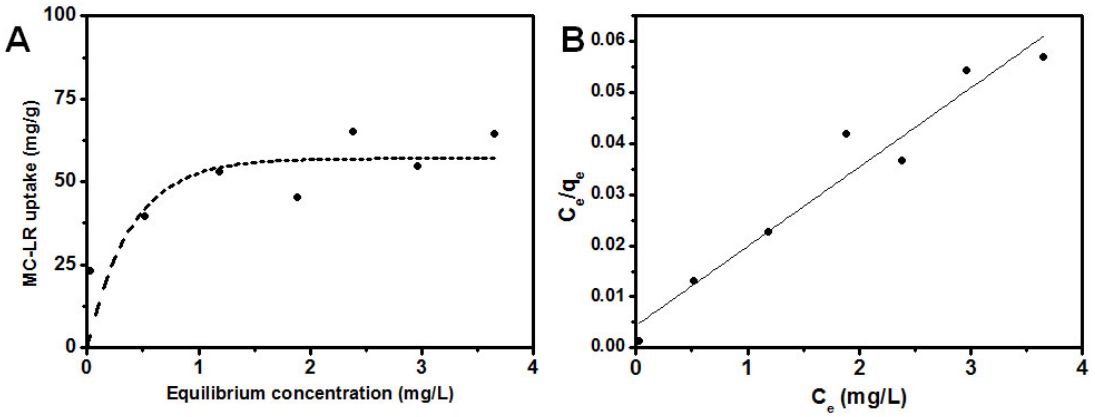


Figure S7. Adsorption isotherms (A) and the corresponding linear Langmuir modeling curves (B) of the powder activated carbon towards MC-LR.

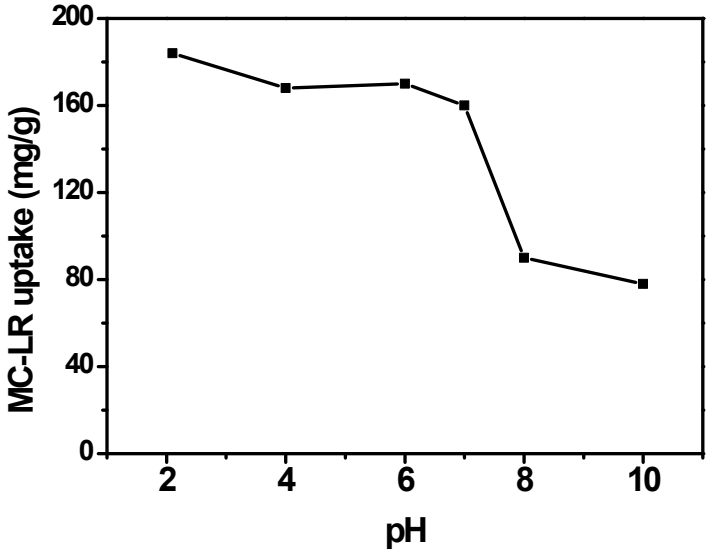


Figure S8. MC-LR uptake versus pH on amino modified MC-NH_2-1-a sorbent.

Table S1. Element analysis results of pristine mesoporous carbon MC and various functionalized mesoporous carbon materials, and the estimated densities of the functional groups.

Sample	N (%)	C (%)	H (%)	O (%)	Grafted amounts (mmol/g)
MC	0.21	92.04	0.57	7.69	--
MC-COOH-1	0.17	62.92	3.28	33.63	2.51 [a]
MC-COOH-2	0.22	60.88	2.98	35.92	--
MC-NH_2-1-a	7.65	65.36	4.54	22.45	2.73
MC-NH_2-2-b	10.96	58.58	4.46	26.00	3.84
MC-NH_2-1-b	9.80	62.36	4.34	23.50	3.43

[a] Calculated from the TG data

Table S2. Langmuir isotherm constants of MC-LR adsorption on different carbon sorbents.

Sorbents	Q_m (mg/g)	K_L (L/g)	R^2
MC	523	0.22	0.948
MC-NH_2-1-a	580	0.27	0.947
PAC	64.5	2.67	0.9773