Supporting Information

Table S1. Force field parameters for the silica model[1].

atom	σ (nm)	ε (kJ/mol)	q (e)
Si	0.33020	0.0000077	1.24
[a]O_b	0.31656	0.65000	-0.620
O	0.31656	0.65000	-0.710
H	0.12950	0.00155	0.400
angle		k (kJ/mol/rad^2)	(deg)
Si-O-H		104.2314	118.5
HO-Si-OH		159.7196	118.5

[a]O_b indicates a bridging, or siloxane, oxygen.

Table S1. Force field parameters for the TIP4P[2, 3].

atom	σ (nm)	ε (kJ/mol)	q (e)
OW	0.31589	0.77490	0.0
HW1	-	-	0.52
HW2	-	-	0.52
[b]MW	-	-	-1.04

[a]MW represents the virtual atom of a water molecule to improve the accuracy.

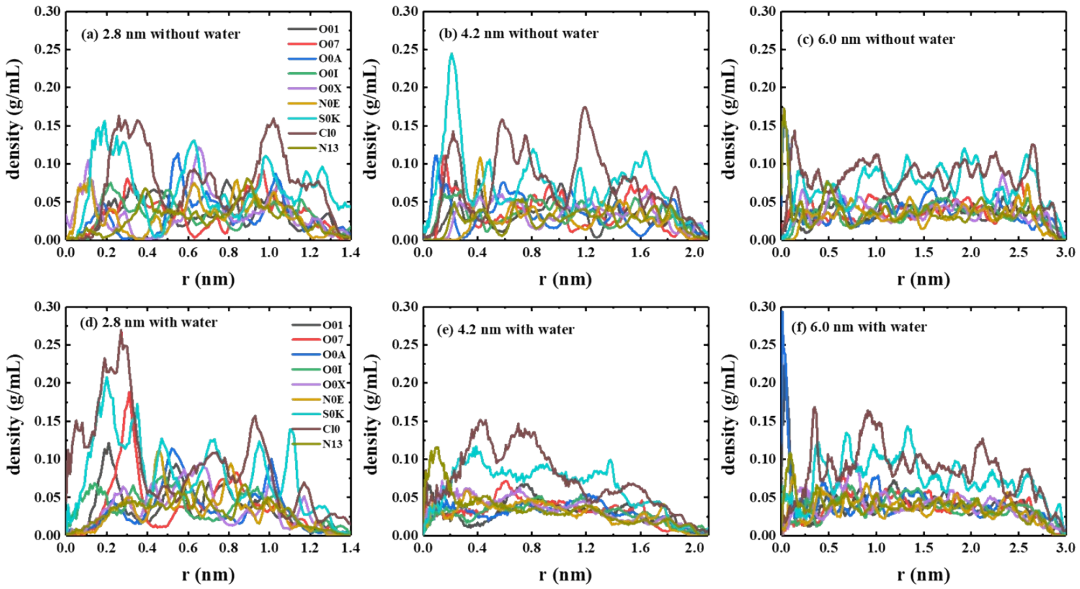
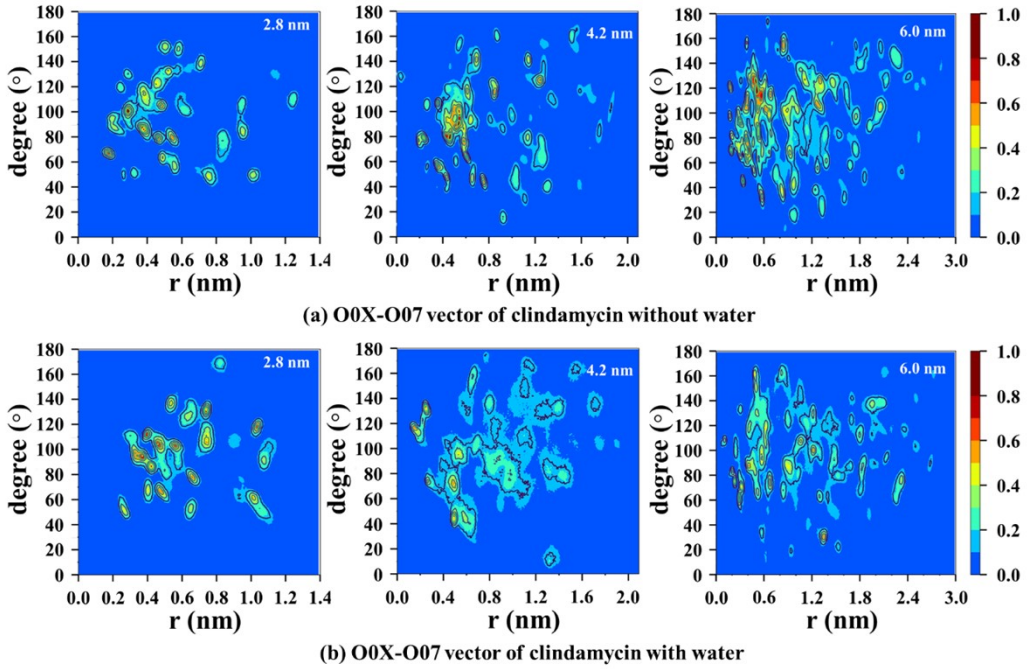


Figure S1 Atomic density profiles of clindamycin as a function of the distance from

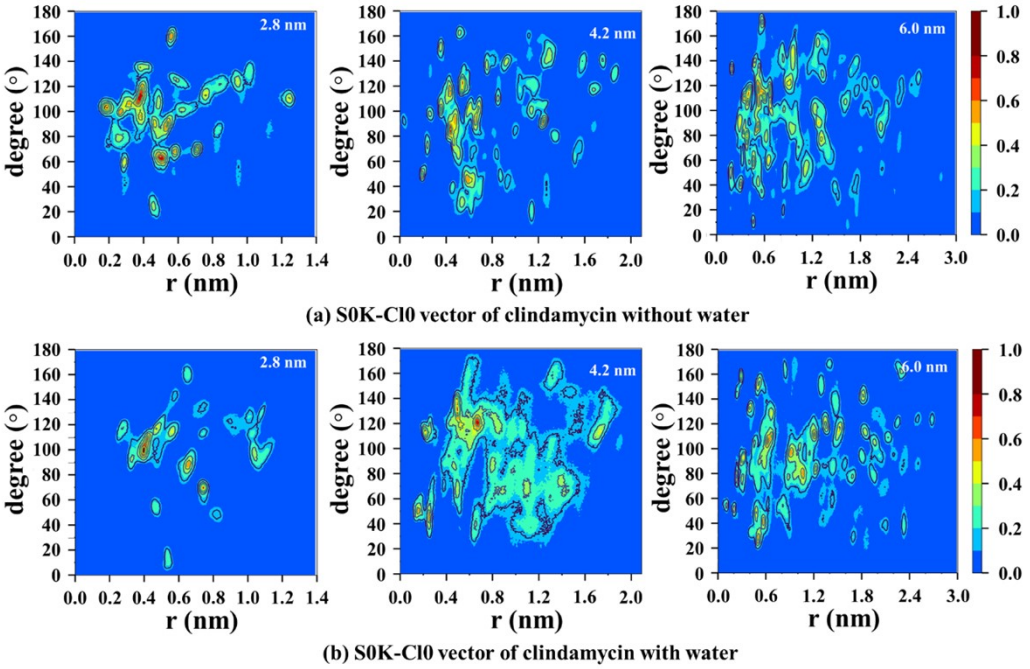
pore surface to pore center in the system with different pore sizes without (a-c) and with (d-f) water.



(a) O0X-O07 vector of clindamycin without water

(b) O0X-O07 vector of clindamycin with water

Figure S2 The orientational distribution with the angle between the O0X-O07 vector and pore center axis along the *z* direction as a function of the distance (r) between the special parts of the clindamycin and the nearest O atom of the silanol groups on pore surface of different mesoporous silica systems without (a) and with water (b).



(a) S0K-Cl0 vector of clindamycin without water

(b) S0K-Cl0 vector of clindamycin with water

Figure S3 The orientational distribution with the angle between the S0K-Cl0 vector and pore center axis along the *z* direction as a function of the distance (r) between the special parts of the clindamycin and the nearest O atom of the silanol groups on pore surface of different mesoporous silica systems without (a) and with water (b).

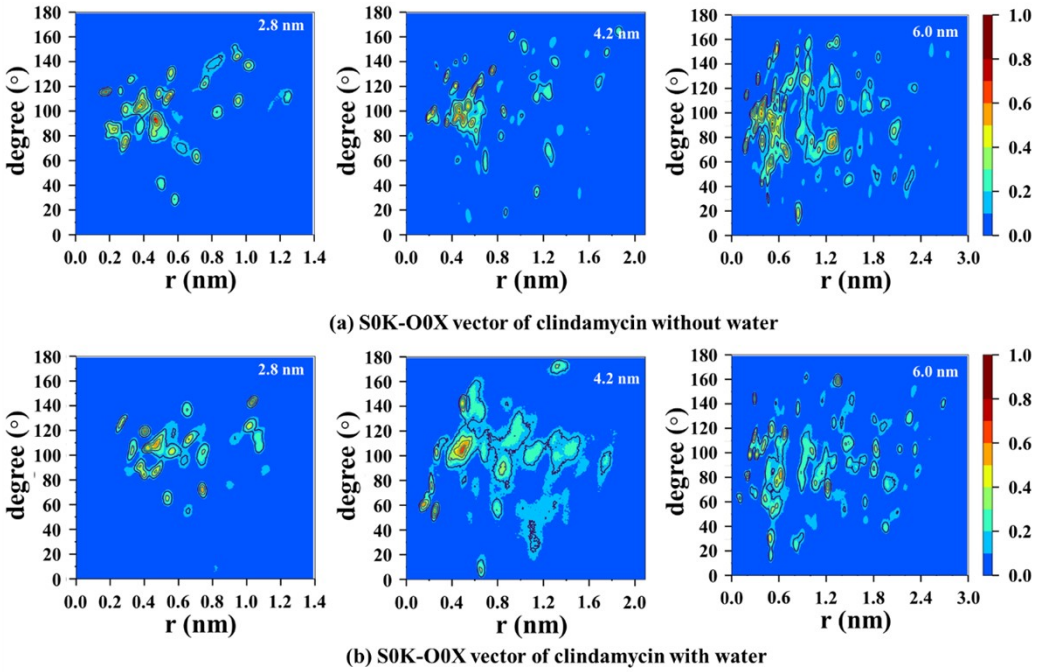


Figure S4 The orientational distribution with the angle between the S0K-O0X vector and pore center axis along the *z* direction as a function of the distance (r) between the special parts of the clindamycin and the nearest O atom of the silanol groups on pore surface of different mesoporous silica systems without (a) and with water (b).

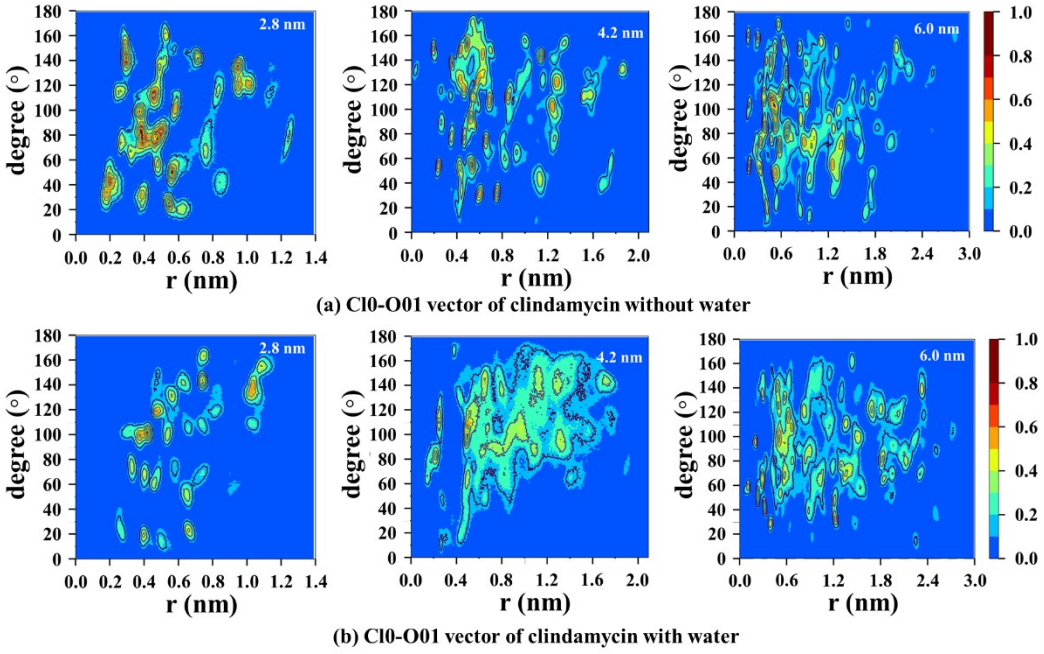


Figure S5 The orientational distribution with the angle between the Cl0-O01 vector and pore center axis along the *z* direction as a function of the distance (r) between the special parts of the clindamycin and the nearest O atom of the silanol groups on pore surface of different mesoporous silica systems without (a) and with water (b).

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2. Abascal, J. L. F.; Vega, C., A general purpose model for the condensed phases of water: TIP4P/2005. *The Journal of Chemical Physics* **2005,** *123* (23), 234505.
3. Harrach, M. F.; Drossel, B., Structure and dynamics of TIP3P, TIP4P, and TIP5P water near smooth and atomistic walls of different hydroaffinity. *J Chem Phys* **2014,** *140* (17), 174501.