

## Supplementary material

### **Pore characteristics influence on MOFs adsorption of pyrethroid pesticides revealed by GCMC simulation and DFT calculation**

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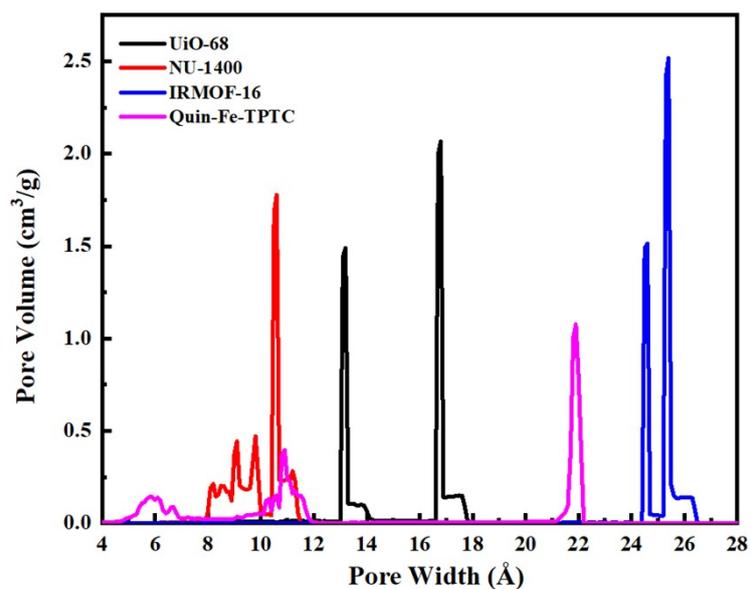


Fig. S1. Aperture distribution of MOFs calculated using Zeo ++.

Table S1. Distribution of PYs in MOFs channels.

MOFs	Cavity shape	binding energy (kcal/mol)	The quantity of lambda-cyhalothrin	binding energy (kcal/mol)	The quantity of bioresmethrin
UiO-68	regular octahedron	-63.47	3	-77.66	4
	regular tetrahedron	-59.33	3	-50.95	2
NU-1400	Rhombic channel	-57.66	/	-87.72	/
IRMOF-16	cube	-75.40	7	-95.46	10
Quin-Fe-TPTC	Hexagonal channel	-83.41	/	-144.84	/