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Multiscale computational insights into 5-Fluorouracil delivery via Zeolite Imidazole Frameworks (ZIFs)

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Supplementary Information

S.1. Forcefield Parameters

All Forcefield Parameters for bonded and van der Waals interactions for both ZIF compounds except the parameters of Zn and its neighboring atoms were obtained via the General Amber Force Field[1] (68). The MCPB.py Python algorithm, compatible with AmberTools is a tool that performs calculations for organometallic systems using B3LYP/6-31G* (by default)[2] and it was employed for bond, angle and dihedral coefficients between Zn and neighbouring atoms that could not be defined accurately by the GAFF force field. The parameters that were calculated by the MCPB.py algorithm and cannot be directly derived from the General Amber Force Field are presented in the tables below.

Table S1. Bond and Angle Coefficients calculated for bonded interactions between Zn and N atom types for ZIF-8.

Bonded Interaction	ZIF-8
Bond Zn-N K_b	71.9 kcal·mol^{-1}·Å^{-2}
Bond Zn-N B_0	2.011 Å
Angle N-Zn-N K_θ	37.67 kcal·mol^{-1}·rad^{-2}
Angle N-Zn-N Θ_0	109.99°
Angle Zn-N-C K_θ	50.86 kcal·mol^{-1}·rad^{-2}
Angle Zn-N-C Θ_0	127.3°

Table S2. van der Waals coefficients calculated for Zn and N atom types of ZIF-8.

Van der Waals Interactions Atom Types	ε (kcal/mol)	σ (Å)
Zn	0.012	1.373
N	0.17	1.824

Figure S1. Representation of the minimum repetitive unit of the modified ZIF. Atom type N represents the N atom in the 6-atom-ring while atom type N1 represents the N atom in the 5-atom-ring.

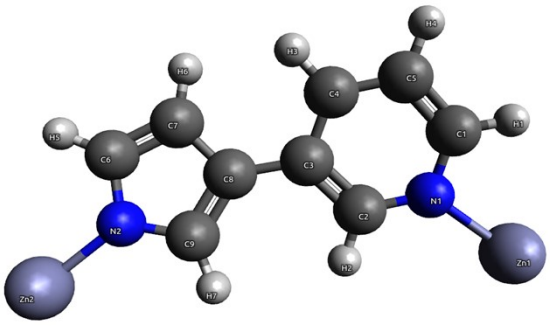

Table S3. Bond and Angle Coefficients calculated for bonded interactions between Zn, N1 and N atom types for the modified ZIF.

Bonded Interaction	Modified ZIF
Bond Zn-N1 K_b	89.2 kcal·mol^{-1}·Å^2
Bond Zn-N1 B_0	1.98 Å
Bond Zn-N K_b	51.7 kcal·mol^{-1}·Å^2
Bond Zn-N B_0	2.07 Å
Angle N-Zn-N K_θ	34.08 kcal·mol^{-1}·rad^{-2}
Angle N-Zn-N Θ_0	107.18°
Angle N-Zn-N1 K_θ	34.11 kcal·mol^{-1}·rad^{-2}
Angle N-Zn-N1 Θ_0	107.78°
Angle N1-Zn-N1 K_θ	27.85 kcal·mol^{-1}·rad^{-2}
Angle N1-Zn-N1 Θ_0	120.65°
Angle Zn-N-C K_θ	36.49 kcal·mol^{-1}·rad^{-2}
Angle Zn-N-C Θ_0	120.19°
Angle Zn-N1-C K_θ	43.72 kcal·mol^{-1}·rad^{-2}
Angle Zn-N1-C Θ_0	126.54°

Table S4. van der Waals coefficients calculated for Zn, N1 and N atom types of the modified ZIF.

Van der Waals Interactions Atom Types	ε (kcal/mol)	σ (Å)
Zn	0.012	1.373
N	0.17	1.824
N1	0.17	1.824

References

1 Wang, J., Wolf, R. M., Caldwell, J. W., Kollman, P. A. & Case, D. A. Development and testing of a general amber force field. *J. Comput. Chem.* **25**, 1157–1174 (2004).
2 P. Li, K. M. Merz, Jr., MCPB.py: A Python Based Metal Center Parameter Builder, *J. Chem. Inf. Model*. **56**, 4, 599–604 (2016).

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