

Druckfreigabe/approval for printing	
Without corrections/ ohne Korrekturen	<input type="checkbox"/>
After corrections/ nach Ausführung der Korrekturen	<input type="checkbox"/>
Date/Datum:	
Signature/Zeichen:	

22 | 1 Metalloenzyme Informatics and Drug Design

- 3 Shakespear, M.R., Halili, M.A., Irvine, K.M. et al. (2011). Histone deacetylases as regulators of inflammation and immunity. *Trends in Immunology* 32: 335–343.
- 4 Shen, M., Pan, P., Li, Y. et al. (2015). Farnesyltransferase and geranylgeranyltransferase I: structures, mechanism, inhibitors and molecular modeling. *Drug Discovery Today* 20: 267–276.
- 5 Chen, A.Y., Adamek, R.N., Dick, B.L. et al. (2019). Targeting metalloenzymes for therapeutic intervention. *Chemical Reviews* 119: 1323–1455.
- 6 Boswell-Smith, V., Spina, D., and Page, C.P. (2006). Phosphodiesterase inhibitors. *British Journal of Pharmacology* 147: S252–S257.
- 7 Moretto, J., Pudlo, M., and Demougeot, C. (2021). Human-based evidence for the therapeutic potential of arginase inhibitors in cardiovascular diseases. *Drug Discovery Today* 26: 138–147.
- 8 Peng, T., Gong, J., Jin, Y. et al. (2018). Inhibitors of phosphodiesterase as cancer therapeutics. *European Journal of Medicinal Chemistry* 150: 742–756.
- 9 Li, G., Su, Y., Yan, Y.H. et al. (2020). MeLAD: an integrated resource for metalloenzyme-ligand associations. *Bioinformatics* 36: 904–909.
- 10 Andreini, C., Cavallaro, G., Lorenzini, S., and Rosato, A. (2013). MetalPDB: a database of metal sites in biological macromolecular structures. *Nucleic Acids Research* 41: D312–D319.
- 11 Li, G., Dai, Q.Q., and Li, G.B. (2022). MeCOM: a method for comparing three-dimensional metalloenzyme active sites. *Journal of Chemical Information and Modeling* 62: 730–739.
- 12 Yu, J.-L., Wang, Y.-G., Peng, J. et al. (2024). Geometric deep learning-enabled metal-binding site identification and grafting. *Fundamental Research*.
- 13 Cheng, Y., Wang, H., Xu, H. et al. (2023). Co-evolution-based prediction of metal-binding sites in proteomes by machine learning. *Nature Chemical Biology* 19: 548–555.
- 14 Dai, Q., Yan, Y., Ning, X. et al. (2021). AncPhore: a versatile tool for anchor pharmacophore steered drug discovery with applications in discovery of new inhibitors targeting metallo- β -lactamases and indoleamine/tryptophan 2,3-dioxygenases. *Acta Pharmaceutica Sinica B* 11: 1931–1946.
- 15 Li, G.-B., Abboud, M.I., Brem, J. et al. (2017). NMR-filtered virtual screening leads to non-metal chelating metallo- β -lactamase inhibitors. *Chemical Science* 8: 928–937.
- 16 Yu, J.L., Zhou, C., Ning, X.L. et al. Knowledge-guided diffusion model for 3D ligand-pharmacophore mapping. *Nature* 16: <https://diffphore.ddtmlab.org/>.
- 17 Jiang, D., Ye, Z., Hsieh, C.Y. et al. (2023). MetalProGNet: a structure-based deep graph model for metalloprotein-ligand interaction predictions. *Chemical Science* 14: 2054–2069.
- 18 Putignano, V., Rosato, A., Banci, L., and Andreini, C. (2018). MetalPDB in 2018: a database of metal sites in biological macromolecular structures. *Nucleic Acids Research* 46: D459–D464.
- 19 Lin, Y.F., Cheng, C.W., Shih, C.S. et al. (2016). MIB: metal ion-binding site prediction and docking server. *Journal of Chemical Information and Modeling* 56: 2287–2291.

Druckfreigabe/approval for printing	
Without corrections/ ohne Korrekturen	<input type="checkbox"/>
After corrections/ nach Ausführung der Korrekturen	<input type="checkbox"/>
Date/Datum:	
Signature/Zeichen:	

- 20 Lu, C.H., Lin, Y.S., Chen, Y.C. et al. (2006). The fragment transformation method to detect the protein structural motifs. *Proteins* 63: 636–643.
- 21 Lu, C.H., Chen, C.C., Yu, C.S. et al. (2022). MIB2: metal ion-binding site prediction and modeling server. *Bioinformatics* 38: 4428–4429.
- 22 Dürr, S.L., Levy, A., and Rothlisberger, U. (2023). Metal3D: a general deep learning framework for accurate metal ion location prediction in proteins. *Nature Communications* 14: 2713.
- 23 Abramson, J., Adler, J., Dunger, J. et al. (2024). Accurate structure prediction of biomolecular interactions with AlphaFold 3. *Nature* 630: 493–500.
- 24 Jumper, J., Evans, R., Pritzel, A. et al. (2021). Highly accurate protein structure prediction with AlphaFold. *Nature* 596: 583–589.
- 25 O’Boyle, N.M., Vandermeersch, T., Flynn, C.J. et al. (2011). Confab - systematic generation of diverse low-energy conformers. *Journal of Cheminformatics* 3: 8.
- 26 Judson, R.S., Jaeger, E.P., Treasurywala, A.M., and Peterson, M.L. (1993). Conformational searching methods for small molecules. II. Genetic algorithm approach. *Journal of Computational Chemistry* 14: 1407–1414.
- 27 Li, G.-B., Yang, L.-L., Wang, W.-J. et al. (2013). ID-Score: a new empirical scoring function based on a comprehensive set of descriptors related to protein–ligand interactions. *Journal of Chemical Information and Modeling* 53: 592–600.
- 28 Zhou, C., Cai, C.-P., Huang, X.-T. et al. (2024). TarKG: a comprehensive biomedical knowledge graph for target discovery. *Bioinformatics* 40: btae598.
- 29 Zhang, Y., Wang, Y., Zhao, Z. et al. (2022). Glutaminyl cyclases, the potential targets of cancer and neurodegenerative diseases. *European Journal of Pharmacology* 931: 175178.
- 30 Vijayan, D.K. and Zhang, K.Y.J. (2019). Human glutaminyl cyclase: structure, function, inhibitors and involvement in Alzheimer’s disease. *Pharmacological Research* 147: 104342.
- 31 Coimbra, J.R.M., Moreira, P.I., Santos, A.E., and Salvador, J.A.R. (2023). Therapeutic potential of glutaminyl cyclases: current status and emerging trends. *Drug Discovery Today* 28: 103644.

Druckfreigabe/approval for printing	
Without corrections/ ohne Korrekturen	<input type="checkbox"/>
After corrections/ nach Ausführung der Korrekturen	<input type="checkbox"/>
Date/Datum:	
Signature/Zeichen:	

Page Proof
WILEY-VCH