Appendix 1. Chemical structure of captopril.

Appendix 2. Docking energies of the best four molecules, and captopril screened against VIM-2 MBL with their ZINC ID, and 2D scheme structures.
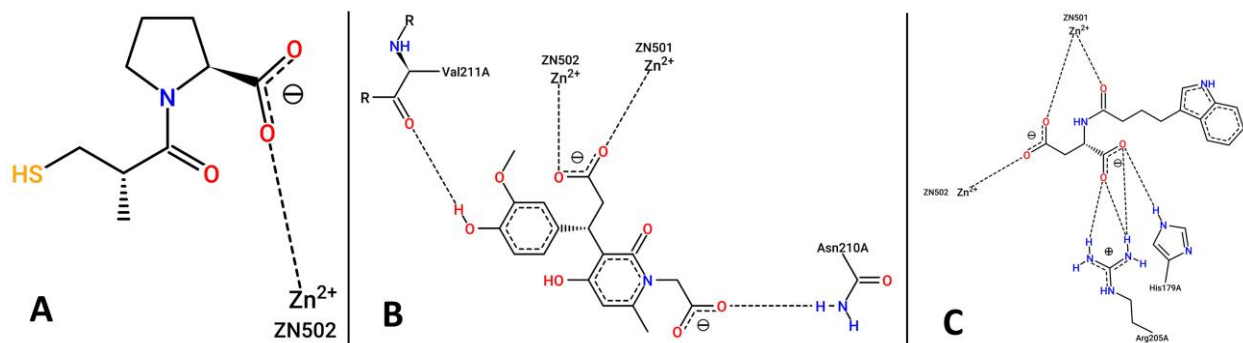
No.	ZINC IDs	2D-structure	Docking energy (kcal/mol)
1	ZINC98363781		-14.1
2	ZINC04090499		-12.7
3	ZINC19893180		-12.3
4	ZINC00518625		-12.2
5	Captopril		-10.8

Appendix 3. Qikprop outcomes and their acceptable range, selected compounds are shown in bold.
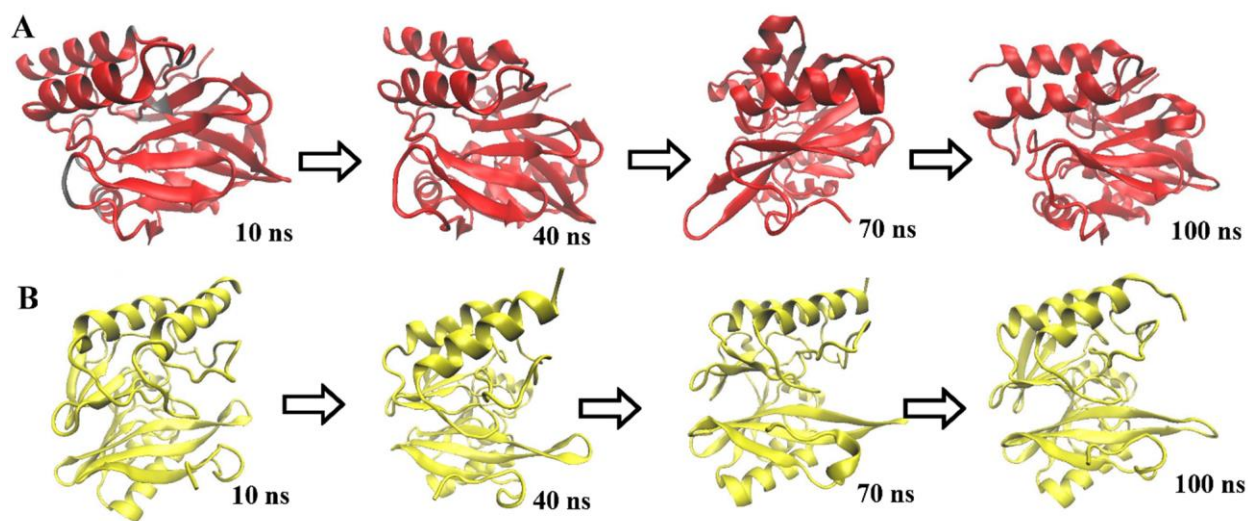
Properties	ZINC98363781	ZINC04090499	ZINC19893180	ZINC00518625	Captopril
MW[a] (g mol^{-1})	374.32	316.31	265.2	228.24	217.29
Log S (ESOL) mol L^{-1}	-2.38	-2.24	-0.79	-1.29	-1.14
Solubility (mg ml^{-1})	1.09e+00	1.82e+00	4.30e+01	1.18e+01	1.58e+01
Log P$_{o/w}$ (iLOGP)[b]	1.51	0.92	0.03	1.42	1.44
Lipinski's rule of five (violation)	0	0	0	0	0
Ghose (violation)	1	1	1	1	0
Veber (violation)	1	0	1	0	0
Egan (violation)	1	0	1	0	0
Muegge (violation)	1	0	0	0	0
Bioavailability score	0.11	0.56	0.56	0.56	0.56
Synthetic accessibility	3.44	2.63	2.23	3.32	2.47
TPSA (Å^2)	154.78	125.15	145.31	89.49	96.41
ABS	55.6	65.82	58.86	78.12	75.73

[a] Molecular weight
[b] Predicted octanol/water partition coefficient

Appendix 4. Interaction of captopril (A), ZINC98363781 (B), and ZINC04090499 (C) within the active cavity of VIM-2 MBL after molecular docking.

Appendix 5. The crystal structure of MBL-ZINC98363781 (A) and MBL-ZINC04090499 (B) during the MD simulation (10 ns, 40 ns, 70 ns, and 100 ns).