Supplementary information

Computationally exploring novel xanthine oxidase inhibitors using docking-based 3D-QSAR, molecular dynamics, and virtual screening

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Supplementary Table

Table S1 The partial modeling results with the different division of training set and test set compounds.

NO.	Training set compounds	Test set compounds	q^2			ONC			R^2			F			SEE		
			CoMFA	CoMSIA	Topomer CoMFA	CoMFA	CoMSIA	Topomer CoMFA	CoMFA	CoMSIA	Topomer CoMFA	CoMFA	CoMSIA	Topomer CoMFA	CoMFA	CoMSIA	Topomer CoMFA
1	44	9	0.742	0.848	0.950	6	6	7	0.987	0.980	0.983	462.029	309.740	291.873	0.080	0.097	0.092
2	43	10	0.741	0.844	0.949	6	6	7	0.987	0.982	0.983	458.164	325.694	281.583	0.080	0.094	0.094
3	42	11	0.741	0.846	0.947	6	6	7	0.988	0.982	0.983	477.620	309.759	271.451	0.078	0.097	0.096
4	41	12	0.739	0.845	0.947	6	6	7	0.988	0.981	0.983	463.207	289.884	222.561	0.079	0.100	0.100
5	40	13	0.709	0.835	0.948	6	6	7	0.988	0.981	0.984	450.178	282.564	286.130	0.079	0.099	0.091
6	39	14	0.697	0.829	0.937	5	7	7	0.978	0.988	0.980	298.437	358.903	222.561	0.102	0.079	0.100
7	38	15	0.694	0.846	0.944	4	6	7	0.959	0.984	0.984	193.045	309.462	268.198	0.143	0.093	0.093

Supplementary Figure

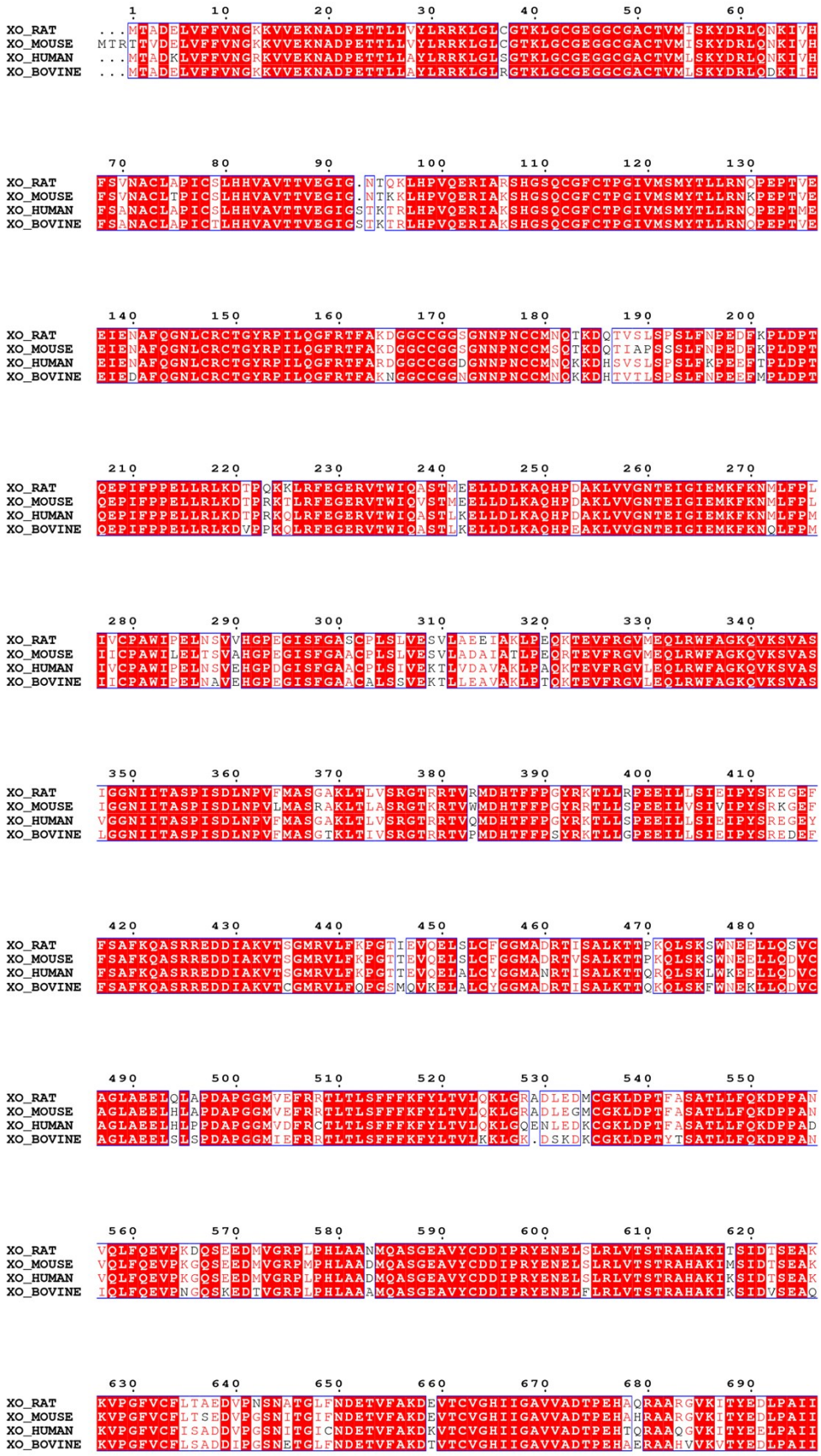

Fig. S1 The sequence alignment of the rat (*Rattus norvegicus*), mouse (*Mus musculus*), human (*Homo sapiens*) and bovine (*Bos taurus*) XO enzymes. The key residues were marked by black frames.

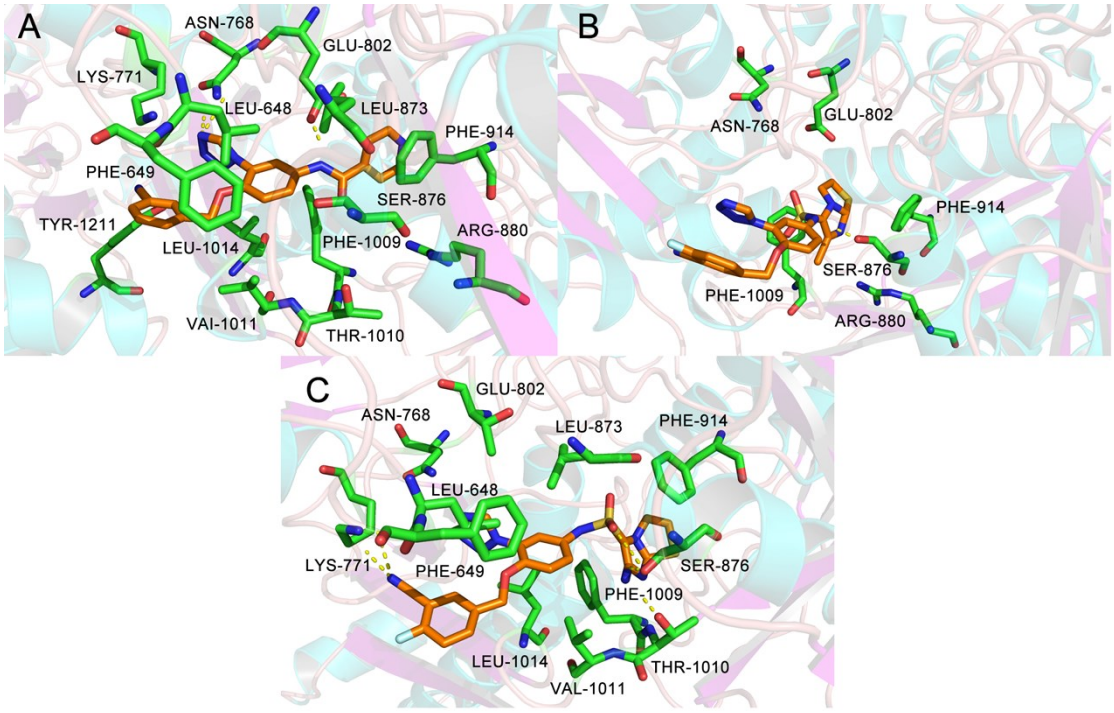

Fig. S2 Binding modes of compounds **19** (**A**), **N1** (**B**), and **N6** (**C**) in the XO protein (PDB ID: 1N5X) at the moment of 10 ns during the 10 ns MD simulation.