

**S2 Table. Summary of small-molecule inhibitor binding sites of AlphaFold-predicted NOX1 structure model.**

| <b>Molecules</b> | <b>Binding Sites</b>                                  |
|------------------|---|
| Heme1            | ARG54, ARG57, PRO260, ALA174, THR169, ASN122          |
| Heme2            | HIS208, HIS101, PHE204, ARG73, TRP337                 |
| FAD              | TRP337, PRO339, ARG356, PHE564, ILE405, PRO533        |
| NADPH            | LEU451, TRP418, ASN450, ALA345                        |
| GKT136901        | LEU68, ARG73, TRP205, HIS208, PHE211, TYR280, ARG284  |
| GKT137831        | VAL71, ARG73, TYR280, ARG284, ARG287                  |
| VAS2870          | VAL71, ARG73, TRP205, PHE211, TYR280, ARG284, ARG287  |
| VAS3947          | VAL71, ARG73, TRP205, TYR280, ARG284, ARG287, TRP337  |
| ML090            | LEU60, HIS115, GLY178, MET181, THR182, TYR214, HIS221 |
| ML171            | ILE67, HIS101, LEU185, HIS208, PHE211, TYR214, TYR280 |