

Supplementary Material

# ***In-Silico* Analysis of Glucose Oxidase from *Aspergillus niger*: Potential Cysteine Mutation Sites for Enhancing Protein Stability**

Sirawit Ittisoponpisan<sup>1\*</sup> and Itthipon Jeerapan<sup>2,3,4\*</sup>

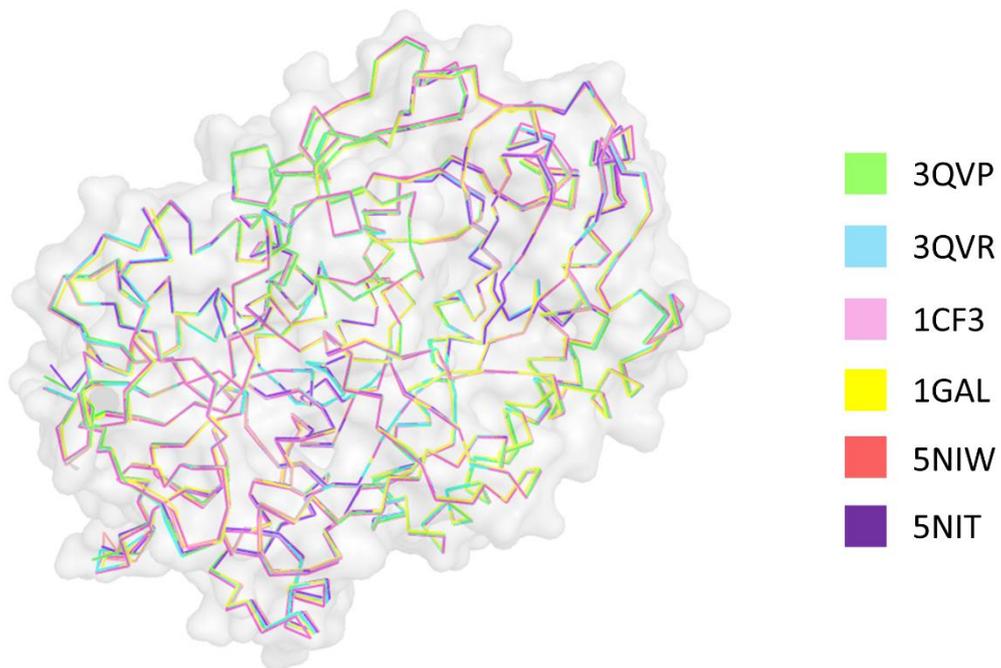
1. Center for Genomics and Bioinformatics Research, Division of Biological Science, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90110, Thailand
2. Center of Excellence for Trace Analysis and Biosensor, Prince of Songkla University, Hat Yai, Songkhla 90110, Thailand
3. Division of Physical Science, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90110, Thailand
4. Center of Excellence for Innovation in Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90110, Thailand

\* Correspondence: sirawit.i@psu.ac.th (S.I.); itthipon.j@psu.ac.th (I.J.)

ORCID of Sirawit Ittisoponpisan: <https://orcid.org/0000-0002-3340-0962>

ORCID of Itthipon Jeerapan: <https://orcid.org/0000-0001-8016-6411>





**Figure S2. Superposition of all PDB coordinates of all GOx used in this study.** The structures are displayed as  $C\alpha$  traces. To give a general outlook of GOx, the protein surface (based on PDB 3QVP) is shown in light grey.

```

3QVP_1|Chain      SNGIEASLLTDPKDVSGRTVDYIIAGGGLTGLTTAARLTENPNISVLVIESGSYSDRGP 60
3QVR_1|Chain      SNGIEASLLTDPKDVSGRTVDYIIAGGGLTGLTTAARLTENPNISVLVIESGSYSDRGP 60
1CF3_1|Chain      SNGIEASLLTDPKDVSGRTVDYIIAGGGLTGLTTAARLTENPNISVLVIESGSYSDRGP 60
1GAL_1|Chain      SNGIEASLLTDPKDVSGRTVDYIIAGGGLTGLTTAARLTENPNISVLVIESGSYSDRGP 60
5NIW_1|Chain      --GIEASLLTDPKDVSGRTVDYIIAGGGLVGLTTAAKL TENPNISVLVIESGSYSDRGP 58
5NIT_1|Chain      --GIEASLLTDPKDVSGRTVDYIIAGGGLVGLTTAARLTENPNISVLVIESGSYSDRGP 58
*****.*****.*****

3QVP_1|Chain      IIEDLNAYGDI FGSSVDHAYETVELATNNQTALIRSGNGLGGSTLVNGGTWTRPHKAQVD 120
3QVR_1|Chain      IIEDLNAYGDI FGSSVDHAYETVELATNNQTALIRSGNGLGGSTLVNGGTWTRPHKAQVD 120
1CF3_1|Chain      IIEDLNAYGDI FGSSVDHAYETVELATNNQTALIRSGNGLGGSTLVNGGTWTRPHKAQVD 120
1GAL_1|Chain      IIEDLNAYGDI FGSSVDHAYETVELATNNQTALIRSGNGLGGSTLVNGGTWTRPHKAQVD 120
5NIW_1|Chain      IIEDLNAYGDI FGSSVDHAYETVELATNNQTALVRSNGNGLGGSTLVNGGTWTRPHKAQVD 118
5NIT_1|Chain      IIEDLNAYGDI FGSSVDHAYETVELATNNQTALVRSNGNGLGGSTLVNGGTWTRPHKAQVD 118
*****.*****.*****

3QVP_1|Chain      SWETVFGNEGWNWDNVAAYS LQAERARAPNAKQIAAGHYFNASCHGVNGTVHAGPRDTGD 180
3QVR_1|Chain      SWETVFGNEGWNWDNVAAYS LQAERARAPNAKQIAAGHYFNASCHGVNGTVHAGPRDTGD 180
1CF3_1|Chain      SWETVFGNEGWNWDNVAAYS LQAERARAPNAKQIAAGHYFNASCHGVNGTVHAGPRDTGD 180
1GAL_1|Chain      SWETVFGNEGWNWDNVAAYS LQAERARAPNAKQIAAGHYFNASCHGVNGTVHAGPRDTGD 180
5NIW_1|Chain      SWETVFGNEGWNWDNVAAYS LQAERARAPNAKQIAAGHYFN T SCHGVNGTVHAGPRDTGD 178
5NIT_1|Chain      SWETVFGNEGWNWDNVAAYS LQAERARAPNAKQIAAGHYFN T SCHGVNGTVHAGPRDTGD 178
*****.*****.*****

3QVP_1|Chain      DYSPIVKALMSAVEDRGPVTKKDFGCGDPHGVSMPFNTLHEDQVRSDAAREWLLPNYQRP 240
3QVR_1|Chain      DYSPIVKALMSAVEDRGPVTKKDFGCGDPHGVSMPFNTLHEDQVRSDAAREWLLPNYQRP 240
1CF3_1|Chain      DYSPIVKALMSAVEDRGPVTKKDFGCGDPHGVSMPFNTLHEDQVRSDAAREWLLPNYQRP 240
1GAL_1|Chain      DYSPIVKALMSAVEDRGPVTKKDFGCGDPHGVSMPFNTLHEDQVRSDAAREWLLPNYQRP 240
5NIW_1|Chain      DYSPIVKALMSAVEDRGPVTKKDFGCGDPHGVSMPFNTLHEDQVRSDAAREWLLPNYQRP 238
5NIT_1|Chain      DYSPIVKALMSAVEDRGPVTKKDFGCGDPHGVSMPFNTLHEDQVRSDAAREWLLPNYQRP 238
*****.*****.*****

3QVP_1|Chain      NLQVLTGQYVGVKLLSQNGTTPRAVGVEFGTHKGNTHNVYAKHEVLLAAGSAVSPTILEY 300
3QVR_1|Chain      NLQVLTGQYVGVKLLSQNGTTPRAVGVEFGTHKGNTHNVYAKHEVLLAAGSAVSPTILEY 300
1CF3_1|Chain      NLQVLTGQYVGVKLLSQNGTTPRAVGVEFGTHKGNTHNVYAKHEVLLAAGSAVSPTILEY 300
1GAL_1|Chain      NLQVLTGQYVGVKLLSQNGTTPRAVGVEFGTHKGNTHNVYAKHEVLLAAGSAVSPTILEY 300
5NIW_1|Chain      NLQVLTGQYVGVKLLSQNGTTPRAVGVEFGTHKGNTHNVYAKHEVLLAAGSAVSPTILEY 298
5NIT_1|Chain      NLQVLTGQYVGVKLLSQNGTTPRAVGVEFGTHKGNTHNVYAKHEVLLAAGSAVSPTILEY 298
*****.*****.*****

3QVP_1|Chain      SGIGMKSILEPLGIDTVVDLPVGLNLQDQTATVRSRITSAGAGQGQAAWFATFNETFGD 360
3QVR_1|Chain      SGIGMKSILEPLGIDTVVDLPVGLNLQDQTATVRSRITSAGAGQGQAAWFATFNETFGD 360
1CF3_1|Chain      SGIGMKSILEPLGIDTVVDLPVGLNLQDQTATVRSRITSAGAGQGQAAWFATFNETFGD 360
1GAL_1|Chain      SGIGMKSILEPLGIDTVVDLPVGLNLQDQTATVRSRITSAGAGQGQAAWFATFNETFGD 360
5NIW_1|Chain      SGIGMKSILEPLGIDTVVDLPVGLNLQDQTATVRSRITSAGAGQGQAAWFATFNETFGD 358
5NIT_1|Chain      SGIGMKSILEPLGIDTVVDLPVGLNLQDQTATVRSRITSAGAGQGQAAWFATFNETFGD 358
*****.*****.*****

3QVP_1|Chain      YSEKAHELLNNTKLEQWAEAEAVARGGFHNTTALLIQYENYRDWIVNHNVAyselFLDTAGV 420
3QVR_1|Chain      YSEKAHELLNNTKLEQWAEAEAVARGGFHNTTALLIQYENYRDWIVNHNVAyselFLDTAGV 420
1CF3_1|Chain      YSEKAHELLNNTKLEQWAEAEAVARGGFHNTTALLIQYENYRDWIVNHNVAyselFLDTAGV 420
1GAL_1|Chain      YSEKAHELLNNTKLEQWAEAEAVARGGFHNTTALLIQYENYRDWIVNHNVAyselFLDTAGV 420
5NIW_1|Chain      YSEKAHELLNNTKLEQWAEAEAVARGGFHNTTALLIQYENYRDWIVNHNVAyselFLDTAGV 418
5NIT_1|Chain      YSEKAHELLNNTKLEQWAEAEAVARGGFHNTTALLIQYENYRDWIVNHNVAyselFLDTAGV 418
*****.*****.*****

3QVP_1|Chain      ASFDVWDL L PPFTRGYVHILDKDPYLHFFAYDPQYFLNELDLLGQAAATQLARNISNSGAM 480
3QVR_1|Chain      ASFDVWDL L PPFTRGYVHILDKDPYLHFFAYDPQYFLNELDLLGQAAATQLARNISNSGAM 480
1CF3_1|Chain      ASFDVWDL L PPFTRGYVHILDKDPYLHFFAYDPQYFLNELDLLGQAAATQLARNISNSGAM 480
1GAL_1|Chain      ASFDVWDL L PPFTRGYVHILDKDPYLHFFAYDPQYFLNELDLLGQAAATQLARNISNSGAM 480
5NIW_1|Chain      ASFDVWDL L PPFTRGYVHILDKDPYLHFFAYDPQYFLNELDLLGQAAATQLARNISNSGAM 478
5NIT_1|Chain      ASFDVWDL L PPFTRGYVHILDKDPYLHFFAYDPQYFLNELDLLGQAAATQLARNISNSGAM 478
*****.*****.*****

3QVP_1|Chain      QTYFAGETIPGDNLAYDADLSAWTEYIPYHFRPNYHGVGTCSMMPKEMGGVVDNAARVYG 540
3QVR_1|Chain      QTYFAGETIPGDNLAYDADLSAWTEYIPYHFRPNYHGVGTCSMMPKEMGGVVDNAARVYG 540
1CF3_1|Chain      QTYFAGETIPGDNLAYDADLSAWTEYIPYHFRPNYHGVGTCSMMPKEMGGVVDNAARVYG 540
1GAL_1|Chain      QTYFAGETIPGDNLAYDADLSAWTEYIPYHFRPNYHGVGTCSMMPKEMGGVVDNAARVYG 540
5NIW_1|Chain      QTYFAGETIPGDNLAYDADLSAWTEYIPYHFRPNYHGVGTCSMMPKEMGGVVDNAARVYG 538
5NIT_1|Chain      QTYFAGETIPGDNLAYDADLSAWTEYIPYHFRPNYHGVGTCSMMPKEMGGVVDNAARVYG 538
*****.*****.*****

3QVP_1|Chain      VQGLRVIDGSIPPTQMSSHVMVFYAMALKISDAILEDYASMQ 583
3QVR_1|Chain      VQGLRVIDGSIPPTQMSSHVMVFYAMALKISDAILEDYASMQ 583
1CF3_1|Chain      VQGLRVIDGSIPPTQMSSHVMVFYAMALKISDAILEDYASMQ 583
1GAL_1|Chain      VQGLRVIDGSIPPTQMSSHVMVFYAMALKISDAILEDYASMQ 583
5NIW_1|Chain      VQGLRVIDGSIPPTQVSSHVMVFYAMALKISDAILEDYASMQ 581
5NIT_1|Chain      VQGLRVIDGSIPPTQVSSHVMVFYAMALKISDAILEDYASMQ 581
*****.*****.*****

```

**Figure S3. Multiple sequence alignment profile of six GOx structures. Amino acid variants are highlighted in yellow.**