

## **Supplementary Material**

# **Structural Analysis of Spermidine Synthase from *Kluyveromyces lactis***

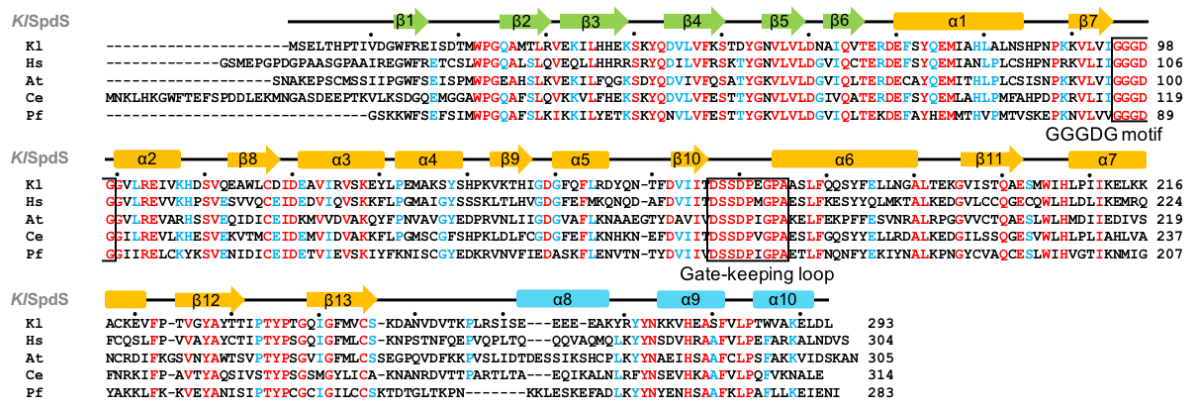
Seongjin Kim 1 and Jeong Ho Chang 1,2,3,\*

1 Department of Biology Education, Kyungpook National University, 80 Daehak-ro, Buk-gu, Daegu 41566, Republic of Korea

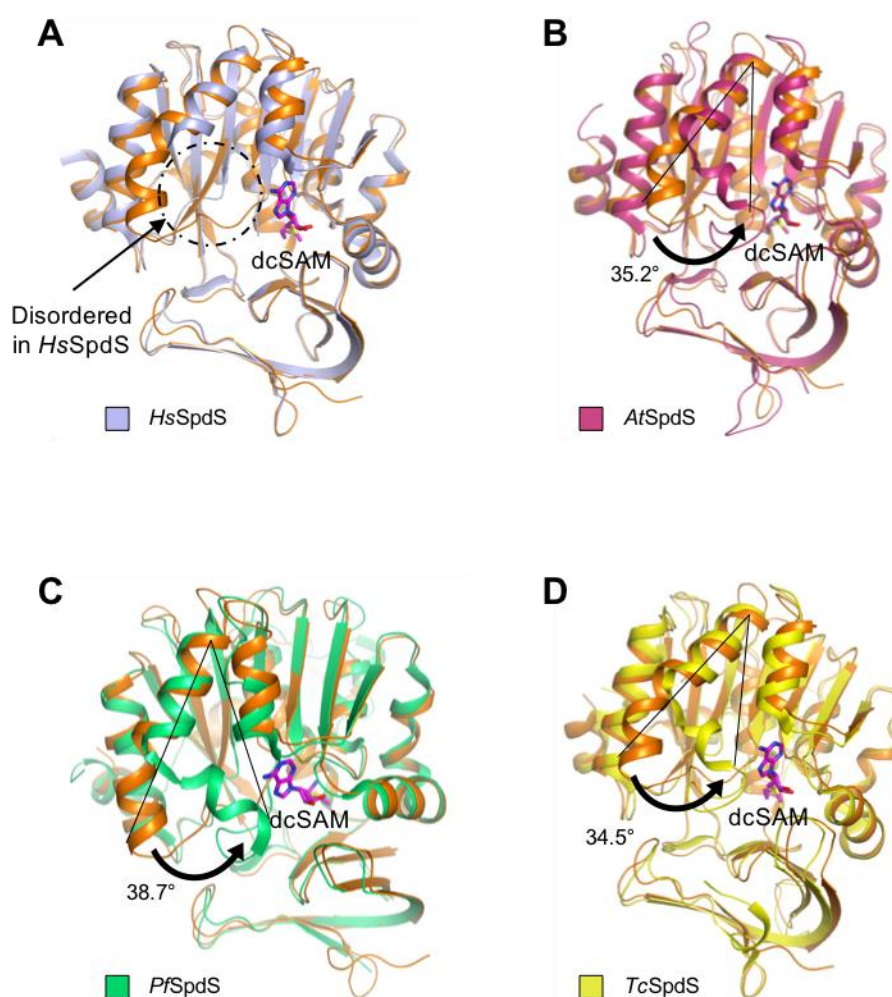
2 Department of Biomedical Convergence Science and Technology, Kyungpook National University, 80 Daehak-ro, Buk-gu, Daegu 41566, Republic of Korea

3 Science Education Research Institute, Kyungpook National University, 80 Daehak-ro, Buk-gu, Daegu 41566, Republic of Korea

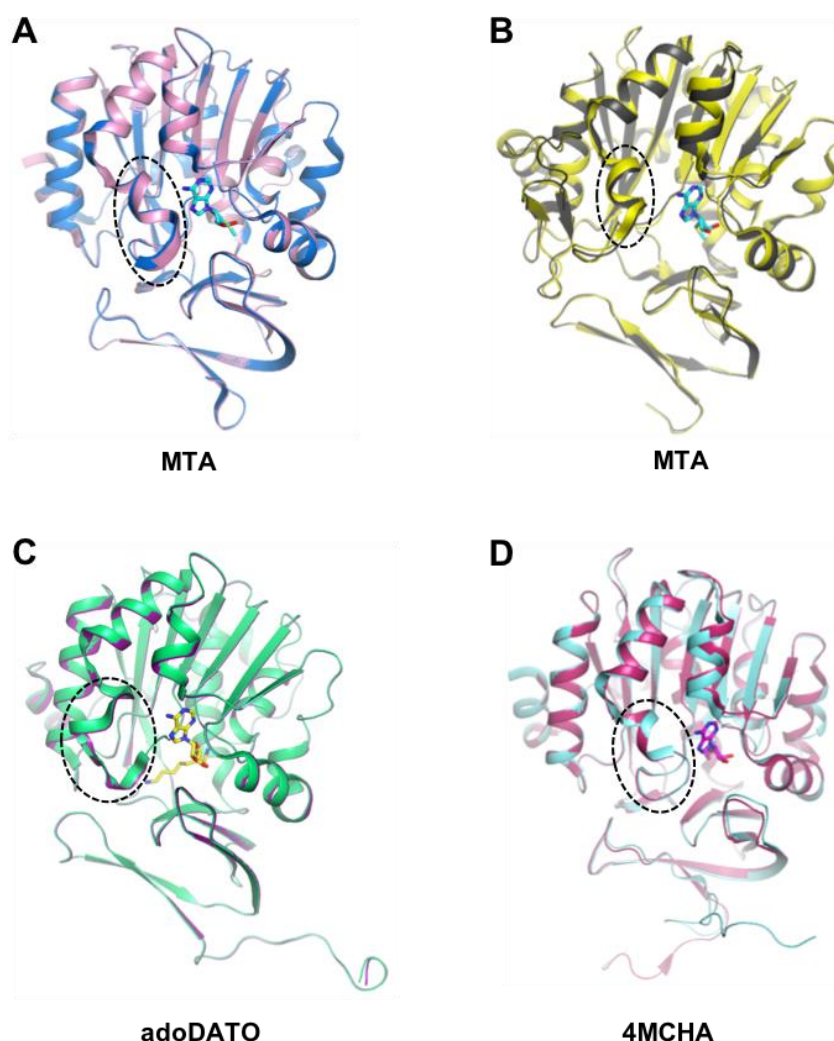
\* Correspondence: [jhcbio@knu.ac.kr](mailto:jhcbio@knu.ac.kr); Tel.: +82-53-950-5913; Fax: +82-53-950-6809



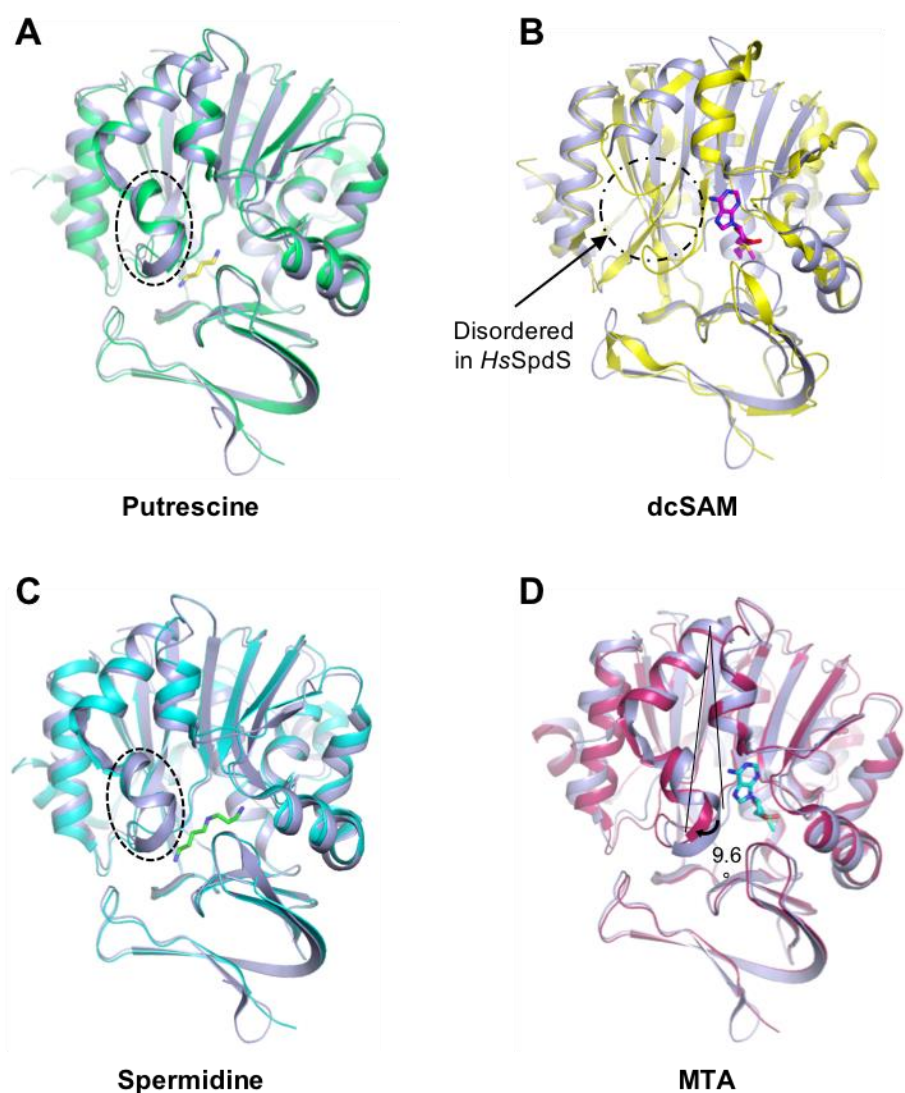
**Supplemental Figure S1. Structure-based amino acid sequence alignment of spermidine synthase (SpdS) from *Kluyveromyces lactis* (KlsSpdS) with other homologs.** Residues with 100% identity are shown in red. Residues with 80% identity are shown in cyan. Black stars indicate three critical aspartic residues (Asp 98, Asp 167, and Asp 170 in KlsSpdS) involved in the aminopropyltransferase reaction. Abbreviations: Hs: *Homo sapiens*. At: *Arabidopsis thaliana*. Ce: *Caenorhabditis elegans*. Pf: *Plasmodium falciparum*.



**Supplemental Figure S2. Comparison of the gate-keeping loop between the apo structures of spermidine synthase (SpdS) from *Kluyveromyces lactis* (KlSpdS) and SpdS complex structures from four other species.** Each figure represents monomer superposition to compare the gate-keeping loop. In (A)–(D), the monomer of apo-KlSpdS is shown in orange. (A) Superposition of apo-KlSpdS and the SpdS complex structures from *Homo sapiens* (HsSpdS; PDB code 2O06). The monomer of apo-HsSpdS is shown in light blue. (B) Superposition of apo-KlSpdS and the SpdS complex structures from *Arabidopsis thaliana* (AtSpdS; PDB code 6O65). The monomer of apo-AtSpdS is shown in warm pink. (C) Superposition of apo-KlSpdS and the SpdS complex structures from *Plasmodium falciparum* (PfSpdS; PDB code 2HTE). The monomer of apo-PfSpdS is shown in lime green. (D) Superposition of apo-KlSpdS and the SpdS complex structures from *Trypanosoma cruzi* (TcSpdS; PDB code 4YUV). The monomer of apo-TcSpdS is shown in yellow.



**Supplemental Figure S3. Comparisons of the gate-keeping loops between apo structures of spermidine synthase (SpdS) and SpdS-substrate complex structures from four species.** (A) Superposition of apo-SpdS (PDB code 2O0L) and the SpdS (PDB code 2O05) complex in *Homo sapiens*. The apo monomer is shown in marine and that of the complex structure is shown in pink. (B) Superposition of apo-SpdS (PDB code 1UIR) and the complex structure of SpdS (PDB code 3ANX) in *Thermus thermophilus*. The apo monomer is shown in yellow and that of the complex structure is shown in dark gray. (C) Superposition of the apo-SpdS (PDB code 1INL) and the complex structure of SpdS (PDB code 1JQ3) in *Thermotoga maritima*. The apo monomer is shown in lime green and that of the complex structure is shown in purple. (D) Superposition of apo-SpdS (PDB code 6O63) and the complex structure of SpdS (PDB code 6O65) in *Arabidopsis thaliana*. The apo monomer is shown in warm pink and that of the complex structure is shown in aquamarine.



**Supplemental Figure S4. Comparison of the gate-keeping loop in spermidine synthase (SpdS) complex structures from different species.** In (A) to (D), the monomer of the *HsSpdS* complex structure is shown in light blue. (A) Superposition of putrescine complex of *HsSpdS* (PDB code 2O06) and *PfSpdS* (PDB code 2HTE). The monomer of the *PfSpdS* complex is shown in lime green. (B) Superposition of the dcSAM complex of *AtSpdS* (PDB code 6O65) and *PfSpdS* (PDB code 2PT6). The monomer of the *PfSpdS* complex is shown in yellow. (C) Superposition of the spermidine complex of *HsSpdS* (PDB code 2O07) and *PfSpdS* (PDB code 2PWP). The monomer of the *PfSpdS* complex is shown in cyan. (D) Superposition of the MTA complex of *HsSpdS* (PDB code 2O05) and *PfSpdS* (PDB code 4BP1). The monomer of the *PfSpdS* complex is shown in warm pink.