Supplement Figure 1
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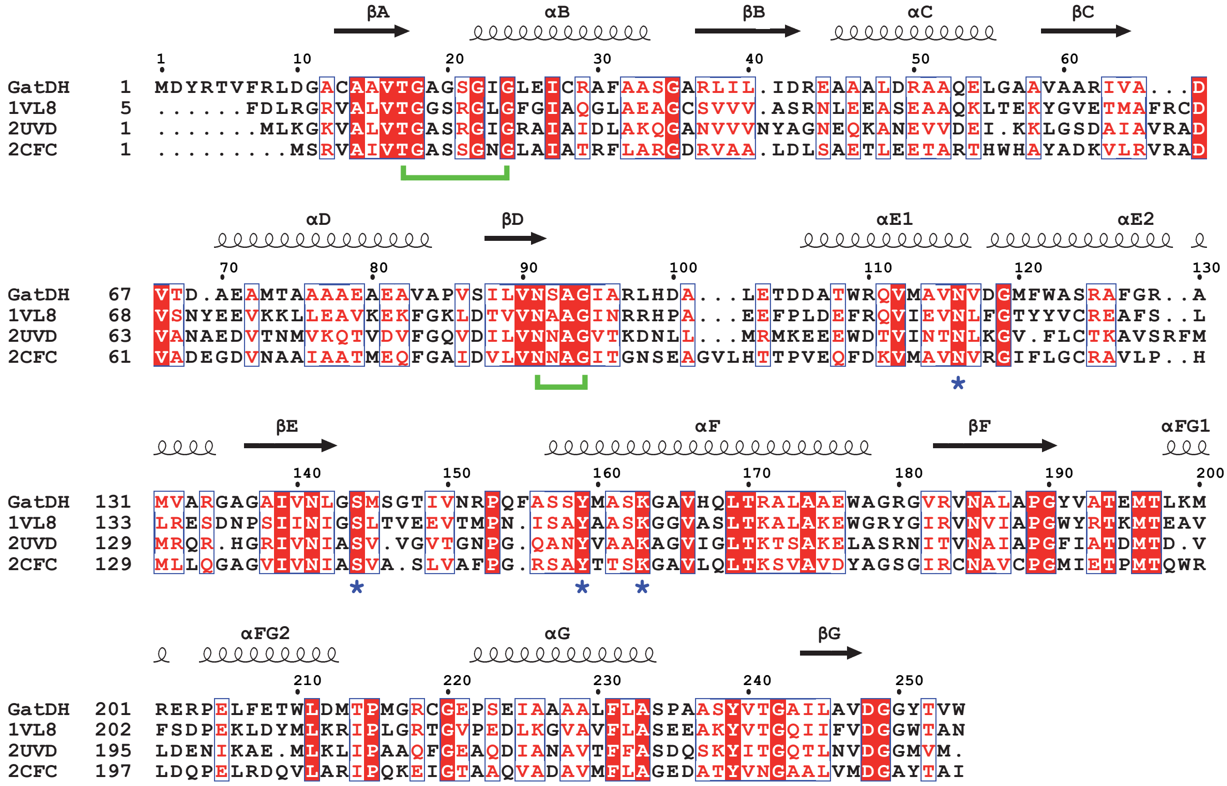

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GatDH    1 MDYRTVFRLDGACAAVTGAGSGIGLEICRAFAASGARLIL.IDREAAALDRAAQELGAAVAARIVA...D
1VL8     5 ......FDLRGRVALVTGGSRGLGFGIAQGLAEAGCSVVV.ASRNLEEASEAAQKLTEKYGVETMAFRCD
2UVD     1 .......MLKGKVALVTGASRGIGRAIAIDLAKQGANVVVNYAGNEQKANEVVDEI.KKLGSDAIAVRAD
2CFC     1 .........MSRVAIVTGASSGNGLAIATRFLARGDRVAA.LDLSAETLEETARTHWHAYADKVLRVRAD

GatDH   67 VTD.AEAMTAAAAEAEAVAPVSILVNSAGIARLHDA...LETDDATWRQVMAVNVDGMFWASRAFGR..A
1VL8    68 VSNYEEVKKLLEAVKEKFGKLDTVVNAAGINRRHPA...EEFPLDEFRQVIEVNLFGTYYVCREAFS..L
2UVD    63 VANAEDVTNMVKQTVDVFGQVDILVNNAGVTKDNLL...MRMKEEEWDTVINTNLKGV.FLCTKAVSRFM
2CFC    61 VADEGDVNAAIAATMEQFGAIDVLVNNAGITGNSEAGVLHTTPVEQFDKVMAVNVRGIFLGCRAVLP..H

GatDH  131 MVARGAGAIVNLGSMSGTIVNRPQFASSYMASKGAVHQLTRALAAEWAGRGVRVNALAPGYVATEMTLKM
1VL8   133 LRESDNPSIINIGSLTVEEVTMPN.ISAYAASKGGVASLTKALAKEWGRYGIRVNVIAPGWYRTKMTEAV
2UVD   129 MRQR.HGRIVNIASV.VGVTGNPG.QANYVAAKAGVIGLTKTSAKELASRNITVNAIAPGFIATDMTD.V
2CFC   129 MLLQGAGVIVNIASVA.SLVAFPG.RSAYTTSKGAVLQLTKSVAVDYAGSGIRCNAVCPGMIETPMTQWR

GatDH  201 RERPELFETWLDMTPMGRCGEPSEIAAAALFLASPAASYVTGAILAVDGGYTVW
1VL8   202 FSDPEKLDYMLKRIPLGRTGVPEDLKGVAVFLASEEAKYVTGQIIFVDGGWTAN
2UVD   195 LDENIKAE.MLKLIPAAQFGEAQDIANAVTFFASDQSKYITGQTLNVDGGMVM.
2CFC   197 LDQPELRDQVLARIPQKEIGTAAQVADAVMFLAGEDATYVNGAALVMDGAYTAI
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Supplement Figure 1.

Structure-based sequence alignment of GatDH with the structurally closest SDR relatives as identified by the *DALI* server (1). The DALI server identified 2-(*R*)-hydroxypropyl-COM-dehydrogenase (PDB-entry 2CFC (2) from *Xantho-bacter autotrophicus* and 3-oxoacylreductase (PDB-entry 2UVD (3) from *Bacillus anthracis* as the closest structural homologues of GatDH. The structure of gluconate 5-dehydrogenase (PDB-entry 1VL8) from *Thermotoga maritima* was used as the template for homology modeling with *SwissModel* (4). The four conserved catalytic key residues and further GatDH positions discussed in the text are labeled by blue asterisks and the main binding motifs for the NAD(H) cofactor are underlined in green. The alignment was prepared with *SuperPose* (5) and *ESPript* (6). The secondary structure elements of GatDH as determined by *DSSP* (7) are shown above its sequence and are labeled according to (8).

References

1. Holm, L., and Sander, C. (1996) *Science* **273**, 595-603
2. Krishnakumar, A. M., Nocek, B. P., Clark, D. D., Ensign, S. A., and Peters, J. W. (2006) *Biochemistry* **45**, 8831-8840
3. Zaccai, N. R., Carter, L. G., Berrow, N. S., Sainsbury, S., Nettleship, J. E., Walter, T. S., Harlos, K., Owens, R. J., Wilson, K. S., Stuart, D. I., and Esnouf, R. M. (2008) *Proteins* **70**, 562-567
4. Arnold, K., Bordoli, L., Kopp, J., and Schwede, T. (2006) *Bioinformatics* **22**, 195-201
5. Maiti, R., Van Domselaar, G. H., Zhang, H., and Wishart, D. S. (2004) *Nucleic Acids Res* **32**, W590-594
6. Gouet, P., Courcelle, E., Stuart, D. I., and Metoz, F. (1999) *Bioinformatics* **15**, 305-308
7. Kabsch, W., and Sander, C. (1983) *Biopolymers* **22**, 2577-2637
8. Ghosh, D., Weeks, C. M., Grochulski, P., Duax, W. L., Erman, M., Rimsay, R. L., and Orr, J. C. (1991) *Proc Natl Acad Sci U S A* **88**, 10064-10068