

David S. Shin, Ph.D.

6820 Fairmount Ave • El Cerrito, CA 94530 • (858) 354-0154 • davidshin444@gmail.com

Curriculum Vitae

Summary

Biochemistry and Molecular Biology Ph.D. with research experience utilizing cross-disciplinary approaches (bioinformatics, biochemistry, molecular biology, small-angle X-ray scattering (SAXS), and X-ray crystallography) to characterize proteins relevant to human diseases. Investigations delve into structure-function relationships, stability, and assembly determinants in proteins and their complexes. Certain components of projects are/were aimed at translating basic research results to applications, such as those in DNA repair, peanut allergy, amyotrophic lateral sclerosis, and biofuels. These projects have led to experience in developing strategies to express and purify difficult target proteins to facilitate structure determination. Experience includes engineering mutants and chimeras, writing scripts to design gene constructs, and initiating a thermophilic eukaryote DNA sequencing project to yield stable proteins.

To support research, I have extensive experience in concept development and writing of government and privately funded grants and fellowships. I have also established collaborations with other laboratories and communicated scientific findings as an invited speaker in the USA and abroad. Current publications include >20 journal articles, 4 cited abstracts, 3 book chapters, and 2 patent publications (Google Scholar citations: 2901, i10-index: 19, h-index: 17). In addition, >140k GenBank, 11 RCSB PDB X-ray crystallographic, and 3 Biolsis SAXS depositions have been contributed.

Education

Ruth L. Kirschstein NSRA and Skaggs Institute Postdoctoral Fellow in Structural Biology

The Scripps Research Institute, La Jolla, CA

Ph.D., Biochemistry and Molecular Biology

University of Arkansas for Medical Sciences, Little Rock, AR

BA, Chemistry, Minor: Sociology

Arizona State University, Tempe, AZ

Science Skills

- **Bioinformatics and Sequencing:** Developed Python-based bioinformatics tools for large-scale gene synthesis. Initiated and developed a large-scale Joint Genome Institute cDNA sequencing project on the deep-sea hydrothermal vent worm *Alvinella pompejana* to supply thermophilic eukaryotic stable homologs of human proteins known to be unstable for structural studies.
- **Cloning, Expression and Purification:** Created recombinant systems specifically tailored to express difficult target proteins including DNA coding segments that enhance expression and suppress mRNA features that down-regulate expression. Made mutants and chimeras to promote folding and alleviate unwanted aggregation and polymerization. Generated a bacterial strain to suppress lethality during toxic gene expression. Developed sparse-matrix and grid screen protocols for protein solubilization.
- **Biochemistry/Biophysics:** Performed and developed enzyme activity assays, DNA-protein and protein-protein binding assays, and various blot analyses to verify activities. Utilized multi-angle light scattering (MALS), dynamic light scattering (DLS), circular dichroism (CD) with SAXS to assess folding and assemblies.
- **Crystallography/SAXS:** Utilize all major crystallization methods. Used 2 θ rotations to collect high-resolution data. Solve phase problems using SAD, MAD, direct methods and molecular replacement. Fit models into very low and very high-resolution data. Collected crystallographic and SAXS data on-site and remotely. Run ALS and SSRL robotics, and develop high-throughput protocols.
- **Computation:** Generated *ab initio* SAXS-based molecular envelope models, and homology-based atomic molecular models. Design and code bioinformatics and structural biology programs to run jobs or use as tools to fetch, retrieve, process, analyze and envision data using UNIX shell scripts, SED, AWK, Python and PyMol.
- **Discovery:** Currently developing a compound screening protocol that uses high-throughput small-angle X-ray scattering to filter leads derived from computational screens and compound libraries.

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Research and Professional Experience

Lawrence Berkeley National Lab, Berkeley, CA

Joint BioEnergy Institute, Emeryville, CA

2010 – Current

Biochemistry Research Scientist, LBNL Life Sciences (Aug 2010 – Current)

Research Scientist, Joint BioEnergy Institute (Aug 2013 – Apr 2014)

Affiliate Scientist, Joint BioEnergy Institute (Mar 2012 – Aug 2012)

- Write, edit and/or aid submission of grant proposals to NIH, DOE and NASA
- Manage structural biology research programs in DNA repair and cancer, amyotrophic lateral sclerosis/free radical detoxification, fuel synthesis, and protein stability
- Develop methodology for protein-ligand interaction screening using small-angle X-ray scattering
- Lead and develop protein design and high-throughput crystallographic techniques for biofuel synthesis
- Program bioinformatic and structural biology tools using shell-scripts, AWK, SED, and Python
- Develop simplified PCR protocol for mutagenesis
- Establish new collaborations from inside and outside of LBNL
- Improve methods with synchrotron beamline 12.3.1 scientists
- Train postdoctoral associates and graduate students
- Solved first amyotrophic lateral sclerosis patient-derived superoxide dismutase mutant X-ray crystal structure
- Solved, as a team, high-resolution (~1 Å) structures of proteins involved in bacterial pathogenesis and DNA repair

The Scripps Research Institute, La Jolla, CA

1998 - 2010

Senior Research Associate (Jan 2008 – Aug 2010)

NSRA and Skaggs Institute for Chemical Biology Fellow / Postdoctoral Associate (Dec 1998 – Dec 2007)

Laboratory of Dr. John A. Tainer

- Wrote proposals and was awarded 2 competitive awards (Incyte and DOE) for sequencing *A. pompejana* cDNA
- Wrote individually, or as part of a team, 2 funded fellowships plus multiple DOE and NIH grants (R01 and P01)
- Wrote proposals and was awarded X-ray crystallography beamtime at the SSRL and ALS synchrotrons
- Initiated EST sequencing project on thermophilic deep-sea hydrothermal vent worm *Alvinella pompejana* to provide thermostable eukaryotic homologs of human proteins for structural and biophysical characterizations
- Dove ~2500 meters in the Pacific Ocean using the Alvin submarine to collect and stabilize *A. pompejana* samples
- Designed a bacterial strain, constructs and solubility screens for proteins difficult to express and purify
- Trained and supervised graduate students and technicians
- Invited speaker at international meetings, and domestic and foreign universities
- Solved first polymeric and full-length structure of homologous recombination enzyme Rad51 (largest structure solved in laboratory and first solved with direct methods via 21 selenium sites) and identified a motif with implications in breast cancer
- Solved highest resolution (first structure below 1 Å) and first reaction ligand complex superoxide dismutase (SOD) crystal structures and first *ab initio* SAXS model using *A. pompejana* SOD, where human SOD is involved in the fatal neurodegenerative disease amyotrophic lateral sclerosis
- Solved (individually and as a team) Rad50 dimer, and Mre11 dimer and DNA complex structures that form a complex involved in cancer prone Ataxia telangiectasia-like disease and Nijmegen Breakage syndrome

University of Arkansas for Medical Sciences, Little Rock, AR

1993 - 1998

Graduate Assistant and Teaching Assistant

Laboratory of Dr. Gary A. Bannon (currently an independent consultant)

- Characterized the major IgE binding epitopes of the major peanut allergen Ara h 1
- Synthesized mutant Ara h 1 epitope peptides and determined relative patient serum IgE reactivities
- Determined a homology-based Ara h 1 structure to identify the locations of epitopes
- Designed and generated mutant Ara h 1 proteins and determined which mutants had diminished IgE binding affinities and were used in patient studies
- Wrote proposal and was awarded grant for supplies and reagents

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University of Arkansas for Medical Sciences, Little Rock, AR 1992 - 1993

Research Technologist I and II

Laboratories of Dr. Charlotte A. Peterson and Dr. Barry K. Hurlburt

- Investigated the specificity and interactions involved in DNA binding of the *E. coli trp* repressor
- Purified proteins and identified DNA binding elements by functional selection
- Characterized muscle transcription factors MyoD, myoglobin and E12

American Interplex Corporation, Little Rock, AR 1992

Chemist

- Analyzed water and ground samples for contaminants
- Utilized gas chromatography and mass spectroscopy

Harris Laboratories Inc., Toxicology Division, Phoenix, AZ 1991 - 1992

Laboratory Technician and Safety Officer

- Analyzed race horse and dog blood and urine samples for pharmaceuticals
- Utilized thin layer chromatography, and gas chromatography and mass spectroscopy

Invited Lectures

LBNL Life Sciences Retreat (2015) "Mechanistic insights into amyotrophic lateral sclerosis and correlations to clinical outcomes using small-angle X-ray scattering and crystallography", Lafayette, CA

Lawrence Berkeley National Laboratory (2009) "Relationships among macromolecular interactions, dynamics & function: Bridging structure resolution gaps with combined structural methods and thermophilic systems", Berkeley, CA

San Diego State University (2008) "Bridging structure-function gaps with combined structural methods and thermophilic systems from *Pyrococcus furiosus* and *Alvinella pompejana*", San Diego, CA

6th International Consortium on Superoxide Dismutase and Amyotrophic Lateral Sclerosis (2006) "Use of a deep-sea thermal vent worm *A. pompejana* for SOD structural biology", Long Beach, CA

2nd Colloquium in Protein Structure, Function and Dynamics (2005) "Use of thermophilic organisms for structural analysis of complex protein systems", San Juan, Puerto Rico

Structural Biology of DNA Repair Machines (2004) "Structural biology of early DNA double-strand break repair events", Berkeley, CA

University of California at Davis (2003) "Structural biochemistry of Rad51 proteins: Mechanisms for Rad51 polymeric assembly and control by BRCA2", Davis, CA

Lawrence Livermore National Laboratory (2003) "Structural biochemistry of Rad51 family proteins", Livermore, CA

Kyoto University (2003) "Structure of full-length and polymeric archaeal Rad51 homolog reveals motifs for self-assembly, DNA contacts and eukaryotic Rad51 interactions with BRCA2", Kyoto, Japan

TSRI Society of Fellows (2003) "Mechanisms for Rad51 polymeric assembly and control by BRCA2", La Jolla, CA

Stanford University (1998) "Modulation of the peanut allergic response through epitope characterization, structural analysis and modification of Ara h 1", Palo Alto, CA

Arkansas Children's Hospital Nutrition Center (1997) "Bioengineering strategies to reduce the type 1 hypersensitivity response to Ara h 1, a major peanut allergen", Little Rock, AR

24th Annual MALTO Medicinal Chemistry and Pharmacognosy Meeting (1997) "Analysis of the Ara h 1 protein, a major peanut allergen: Characterization of the IgE binding epitopes and mutations that lead to decreased binding activity", Little Rock, AR (Session Chair)

Teaching

- Molecular Graphics (2015) Structural Biology of DNA Repair Machines, Berkeley, CA
- Assistant and Guest Instructor of Brazilian Jiu Jitsu (2006-) Gracie Barra San Diego and East Bay Jiu Jitsu
- PyMOL Molecular Graphics Workshop (2004) Structural Biology of DNA Repair Machines, Berkeley, CA
- Teaching Assistant, Molecular Modeling S143 (1998) Biopharmaceutical Sciences, UAMS, Little Rock, AR

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Funding List

Main and Coordinating writer

1. **National Institutes of Health /MSFB R01** (2010) **\$1,442,367 / 4 years** - *Superoxide Dismutase Structures and Lou Gehrig's Disease* [originally Shin, Getzoff, Tainer, remained Getzoff & Tainer due to move to LBNL]
2. **National Institutes of Health/NCI R01** (2005) **\$1,783,544 / 5 years** - *Mre11/Rad50 Structural Biology for DNA Damage Responses* [Tainer, Russell]
3. **US Department of Energy Community Sequence Program** (2005) **Estimated \$852,000** (142,000 x ~\$6/read) - *cDNA Sequences for the Extreme Thermophilic Eukaryote Alvinella Pompejana* [Shin, Cary, Tainer]
4. **Skaggs Institute of Chemical Biology Fellowship** (2002) **Salary supplement, 2 years** [Shin]
5. **Ruth L. Kirschstein NSRA Fellowship** (2001) **\$86,388 / 2 years** - *Structural Biology of Rad51 DNA Recombinational Repair* [Shin]
6. **3rd Annual Incyte Discovery Grant Award** (2001) **\$100,000** - *Alvinella pompejana cDNA sequencing* [Shin]
7. **University of Arkansas for Medical Sciences CAGSRF Grant** (1995) **\$3,000** – *mRNA stability* [Shin]

Co-writer

1. **DOE/ARPA-E** (2014) **\$3,500,000 / 3 years** – *Enzymes for Methane Conversion* [Jansson]
2. **NIH/NCI R01** (2010) **\$1,410,117 / 4 years** - *Mre11/Rad50/Nbs1 Structural Biology for DNA Damage Responses* [Tainer]
3. **NIH/NIGMS R01** (2009) **\$2,454,237 / 4 years** - *Structural Biochemistry of DNA Base Excision Repair* [Tainer]
4. **NIH/NCI P01** (2001) **\$18,871,117 / 5 years** - *Structural Cell Biology of DNA Repair Machines* [Tainer]

Publication List

1. **Shin DS** and Tainer JA (2015) Base excision with a minor twist: a DNA glycosylase that performs DNA repair without flipping out. **Nature** 527, 168-9
2. Pratt AJ*, DiDonato M*, **Shin DS**, Cabelli DE, Bruns CK, Belzer CA, Gorringer AR, Langford PR, Tabatabai LB, Kroll JS, Tainer JA, Getzoff ED (2015) Structural, functional and immunogenic insights on Cu,Zn Superoxide Dismutase pathogenic virulence factors from *Neisseria meningitidis* and *Brucella abortus*. **J Bacteriology** 197, 3834-47
3. Pratt AJ, **Shin DS**, Merz GE, Lancaster WA, Dyer KN, Borbat PP, Poole II FL, Adams MWW, Freed JH, Crane BR, Tainer JA, Getzoff ED (2014) Aggregation propensities of superoxide dismutase G93 hotspot mutants mirror amyotrophic lateral sclerosis clinical phenotypes. **Proc Natl Acad Sci**, 111, E4568-76.
4. **Shin DS**, Pratt AJ, Tainer JA (2014) Archaeal genome guardians give insights into eukaryotic DNA replication and damage response proteins. **Archaea**, 2014, 1-24.
5. Tsutakawa SE, **Shin DS**, Mol CD, Izumi T, Arvai AS, Mantha AK, Szczesny B, Ivanov IN, Hosfield DJ, Maiti BM, Pique ME, Frankel KA, Hitomi K, Cunningham RP, Mitra S, Tainer JA. (2013) Conserved structural chemistry for incision activity in structurally non-homologous apurinic/apyrimidinic endonuclease APE1 and Endonuclease IV DNA repair enzymes. **J Biol Chem**, 288, 8445-55.
6. Hartung S, Arvai AS, Wood T, Kolappan S, **Shin DS**, Craig L, Tainer JA. (2011) Ultra-high resolution and full-length pilin structures with insights for filament assembly, pathogenic functions, and vaccine potential. **J Biol Chem**, 286, 44254-44265.
7. **Shin DS**, Pratt AJ, Getzoff ED, Perry JJP (2011) Amyotrophic lateral sclerosis. In **Advanced Understanding of Neurodegenerative Diseases**. Chang R (Ed.). Intech Publishers.
8. Kashiwagi S, Kuraoka I, Fujiwara Y, Hitomi K, Cheng QJ, Fuss JO, **Shin DS**, Masutani C, Tainer JA, Hanaoka F, Iwai S (2010) Characterization of a Y-Family DNA polymerase eta from the eukaryotic thermophile *Alvinella pompejana*. **J Nucleic Acids**, Sep 20: 1-13.
9. Perry JJP*, **Shin DS***, Getzoff ED, Tainer JA (2009) The structural biochemistry of the superoxide dismutases. **Biochim Biophys Acta**, 1804, 245-262. [*equal contribution] Times cited: 139
10. Perry JJP, **Shin DS**, Tainer JA (2009) Amyotrophic lateral sclerosis. In **Diseases of DNA Repair**. Ahmad. S.I. (Ed.)

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Landes Bioscience and Springer Science+Business Media. Times cited: 24

11. **Shin DS**, DiDonato M, Barondeau DP, Hura GL, Hitomi C, Berglund JA, Getzoff ED, Cary SC, Tainer JA (2009) Superoxide dismutase from the eukaryotic thermophile *Alvinella pompejana*: structures, stability, mechanism and insights into amyotrophic lateral sclerosis. **J Mol Biol**, 385, 1534-1555. [Cover]
12. Williams RS, Moncalian G, Williams JS, Yamada Y, Limbo O, **Shin DS**, Grocock LM, Cahill D, Hitomi C, Guenther G, Moiani D, Carney JP, Russell P, Tainer JA (2008) Mre11 dimers coordinate DNA end bridging and nuclease processing in double-strand-break repair. **Cell**, 135, 97-109. Times cited: 267
13. Fan L, Williams RS, **Shin DS**, Chapados B, Tainer JA (2007) Master keys to DNA replication, repair and recombination from the structural biology of enzymes from thermophiles. In **Thermophiles: Molecular Biology and Technology**. Robb FT, Grogan D, Antranikian G, Driessen A (Eds.) pp. 241-265. Taylor and Francis, Boca Raton, FL.
14. Sarker AH, Tsutakawa SE, Kostek S, Ng C, **Shin DS**, Peris M, Campeau E, Tainer JA, Nogales E, Cooper PK (2005) Recognition of RNA polymerase II and transcription bubbles by XPG, CSB, and TFIIH: insights for transcription-coupled repair and Cockayne Syndrome. **Mol Cell**, 20, 187-198. Times cited: 154
15. Henscheid KL, **Shin DS**, Cary SC, Berglund JA (2005) The splicing factor U2AF65 is functionally conserved in the thermotolerant deep-sea worm *Alvinella pompejana*. **Biochim Biophys Acta**, 1727, 197-207.
16. **Shin DS**, Chahwan C, Huffman JL, Tainer JA (2004) Structure and function of the double-strand break repair machinery. **DNA Repair**, 3, 863-873. [cover photo]
17. **Shin DS**, Pellegrini L, Daniels DS, Yelent B, Craig L, Bates D, Yu DS, Shivji MK, Hitomi C, Arvai AS, Volkmann N, Tsuruta H, Blundell TL, Venkitaraman AR, Tainer JA (2003) Full-length archaeal Rad51 structure and mutants: mechanisms for RAD51 assembly and control by BRCA2. **EMBO J**, 22, 4566-4576. Times cited: 209
18. Craig L, Taylor RK, Pique ME, Adair BD, Arvai AS, Singh M, Lloyd SJ, **Shin DS**, Getzoff ED, Yeager M, Forest KT, Tainer JA (2003) Type IV pilin structure and assembly: X-ray and EM analyses of *Vibrio cholerae* toxin-coregulated pilus and *Pseudomonas aeruginosa* PAK pilin. **Mol Cell**, 11, 1139-1150. Times cited: 191
19. Hopfner KP, Karcher A, **Shin D**, Fairley C, Tainer JA, Carney JP (2000) Mre11 and Rad50 from *Pyrococcus furiosus*: cloning and biochemical characterization reveal an evolutionarily conserved multiprotein machine. **J Bacteriology**, 182, 6036-6041. Times cited: 110
20. Hopfner KP, Karcher A, **Shin DS**, Craig L, Arthur LM, Carney JP, Tainer JA (2000) Structural biology of Rad50 ATPase: ATP-driven conformational control in DNA double-strand break repair and the ABC-ATPase superfamily. **Cell**, 101, 789-800. Times cited: 846
21. Bannon GA, Kopper RA, Maleki SM, **Shin DS**, Sampson HA, Burks AW (2000) Structure plays a critical role in the allergenicity of food proteins. **J Allergy & Clin. Immunol.** 105, S184.
22. Maleki SJ, Kopper RA, **Shin DS**, Park CW, Compadre CM, Sampson H, Burks AW, Bannon GA (2000) Structure of the major peanut allergen Ara h 1 may protect IgE-binding epitopes from degradation. **J Immunol**, 164, 5844-5849. Times cited: 222
23. **Shin DS**, Compadre CM, Sampson HA, Burks AW, Bannon GA (1999) Modulation of the reactivity of the major peanut allergen Ara h 1 through epitope characterization, structural analysis, and mutation. **J Allergy & Clin Immunol**, 103, S99.
24. Bannon GA, **Shin D**, Maleki S, Kopper R, Burks AW (1999) Tertiary structure and biophysical properties of a major peanut allergen, implications for the production of a hypoallergenic protein. **Int Arch Allergy Immunol**, 118, 315-316.
25. **Shin DS**, Compadre CM, Maleki SJ, Kopper RA, Sampson H, Huang SK, Burks AW, Bannon GA (1998) Biochemical and structural analysis of the IgE binding sites on ara h1, an abundant and highly allergenic peanut protein. **J Biol Chem**, 273, 13753-13759. Times cited: 227
26. **Shin D**, Sampson H, Helm R, Huang SK, Burks AW, Bannon GA (1998) Tertiary structure of the major peanut allergen Ara h 1: Implications for the bioengineering of a hypoallergenic protein. **J Allergy & Clin Immunol**, 101, S90.
27. Burks AW, **Shin D**, Cockrell G, Stanley JS, Helm RM, Bannon GA (1997) Mapping and mutational analysis of the IgE-binding epitopes on Ara h 1, a legume vicilin protein and a major allergen in peanut hypersensitivity. **Eur J Biochem**, 245, 334-339. Times cited: 270
28. **Shin D**, Sampson HA, Huang SK, Compadre C, Burks AW, Bannon GA (1997) Characterization of a major peanut allergen: Mutational analysis of the Ara h 1 IgE binding epitopes. **J Allergy & Clin Immunol**, 99, 570.
29. Czernik PJ, **Shin DS**, Hurlburt BK (1994) Functional selection and characterization of DNA binding sites for trp repressor of *Escherichia coli*. **J Biol Chem**, 269, 27869-27875.

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US Patent Publications

1. Caplan MJ, Sosin HB, Sampson HA, Bannon GA, Burks AW, Cockrell G, Compadre CM, Connaughton C, Helm RM, King NE, Kopper RA, Maleki SJ, Rabjohn PA, **Shin DS**, Stanley JS (2003) Methods and reagents for decreasing clinical reaction to allergy. Times cited: 10
2. Bannon G, Burks A, Caplan M, Cockrell G, Compadre C, Connaughton C, Helm R, King N, Kopper R, Maleki S, Rabjohn P, Sampson H, **Shin D**, Sosin H, Stanley J (2002) Methods and reagents for decreasing clinical reaction to allergy. Times cited: 5

RCSB Protein Data Bank Depositions

1. 4L05 (2013) Cu/Zn superoxide dismutase from *Brucella abortus*, 1.01 Å [publication pending]
2. 4HNO (2012) Crystal structure of *T. maritima* Nfo, 0.92 Å, **J Biol Chem**
3. 3SOJ (2011) *Francisella tularensis* pilin PilE, 1.00 Å, **J Biol Chem**
4. 3SOK (2011) *Dichelobacter nodosus* pilin FimA, 2.30 Å, **J Biol Chem**
5. 3GYH (2009) Crystal structure analysis of *S. pombe* ATL in complex with damaged DNA containing POB, 2.80 Å, **Nature**
6. 3F7L (2009) X-ray crystal structure of *Alvinella pompejana* Cu,Zn superoxide dismutase, 0.99 Å, **J Mol Biol**
7. 3F7K (2009) X-ray crystal structure of an *Alvinella pompejana* Cu,Zn superoxide dismutase - hydrogen peroxide complex, 1.35 Å, **J Mol Biol**
8. 3DSC (2008) Crystal structure of *P. furiosus* Mre11 DNA synaptic complex, 2.70 Å, **Cell**
7. 1PZN (2003) Rad51 (RadA), 2.85 Å, **EMBO J**
9. 1OQV (2003) Structure of TcpA, the Type IV pilin subunit from the toxin co-regulated pilus of *Vibrio cholerae* classical biotype, 2.30 Å, **Mol Cell**
10. 1F2U (2000) Crystal structure of RAD50 ABC-ATPase, 1.60 Å, **Cell**
11. 1F2T (2000) Crystal structure of ATP-free RAD50 ABC-ATPase, 1.60 Å, **Cell**

BIOISIS SAXS Data Bank Depositions

1. BASODP (2013) Characterization of Cu,Zn Superoxide Dismutase from the pathogen *Brucella abortus*
2. NMSODP (2013) Characterization of Cu,Zn Superoxide Dismutase from the pathogen *Neisseria meningitides*
3. APSODP (2009) Solution state of superoxide dismutase from *Alvinella Pompejana*, **J Mol Biol**

GenBank Entries

1. EU178106.1 (2009) *Alvinella pompejana* Cu/Zn superoxide dismutase 1 (SOD1) mRNA, complete cds. **J Mol Biol**
2. >142,000 *Alvinella pompejana* EST sequences