

## Alexander Tomoaki Taguchi

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### Education

University of California at San Diego (2006-2010)

Degrees: Biophysics (*Bachelor of Science*) and Japanese Studies (*Bachelor of Arts*)

University of Illinois Urbana-Champaign (2010-2014)

Ph.D. in *Biophysics and Computational Biology*

Research: Pulsed EPR spectroscopy and simulations of photosynthetic membrane proteins

Advisors: Professors Colin A. Wraight and Sergei A. Dikanov

Nippon Medical School of Tokyo JSPS Postdoctoral Fellowship (2014-2015)

Research: Electronic structure and function of iron-sulfur clusters

Advisor: Professor Toshio Iwasaki

Massachusetts Institute of Technology NIH F32 Postdoctoral Fellowship (2016-present)

Research: Solid-state protein NMR structural investigations by fast spinning MAS

Advisors: Professors Robert G. Griffin and JoAnne Stubbe

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### Awards

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| 2018      | Best Poster Award European Chemistry Conference at Rome, Italy                               |
| 2018      | MIT Medicine Dermatology Hackathon Winner (\$20000)  |
| 2018      | MIT BASF Coding Chemistry Hackathon Top Team (\$1000)  |
| 2017-2019 | F32 Postdoctoral Fellowship from National Institutes of Health (NIH)                         |
| 2015      | Travel grant for 17 <sup>th</sup> International Conference on Biological Inorganic Chemistry |
| 2014-2016 | Postdoctoral Fellowship from Japan Society for the Promotion of Science (JSPS)               |
| 2010-2013 | Molecular Biophysics Training Grant from National Institutes of Health (NIH)                 |
| 2013      | Travel grant for 6 <sup>th</sup> Advanced EPR School at the Weizmann Institute in Israel     |
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### Oral Presentations

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| July, 2018 | European Chemistry Conference 2018 at Rome, Italy<br>Talk title: <i>The Unpaired Electron Spin Density Distribution in Reduced [2Fe-2S] Clusters by <sup>13</sup>C<sub>β</sub>-Cysteine Labeling</i>   |
| May, 2017  | MIT Chemistry Student Seminar Series at Massachusetts Institute of Technology<br>Talk title: <i>Structural Modeling of Ribonucleotide Reductases: A Combination of Electron Microscopy, EPR, and NMR</i>   |
| Oct., 2015 | High school outreach JSPS Science Dialogue lecture at Kamaishi High school, Japan<br>Talk title: <i>How Magnets Have Changed the World We Live In</i>  |
| July, 2015 | 17 <sup>th</sup> International Conference on Biological Inorganic Chemistry in Beijing, China<br>Talk title: <i>Mapping the Electron Spin Distribution in [2Fe-2S] Proteins by <sup>13</sup>C<sub>β</sub> Cysteine Labeling: Implications in Electron Transport Pathways</i> |
| Apr., 2014 | 10 <sup>th</sup> Illinois Biophysical Society Symposium at Univ. of Illinois Urbana-Champaign<br>Talk title: <i>Structural Determination of Q<sub>B</sub> by high frequency pulsed EPR</i>   |

- Nov., 2013 Molecular Biophysics Training Grant Symposium at Univ. of Illinois Urbana-Champaign  
Talk title: *Pulsed EPR Investigation of the  $^{13}\text{C}$  couplings in  $Q_A$  and  $Q_B$*
- Aug., 2013 16<sup>th</sup> International Congress on Photosynthesis Symposium in St. Louis, Missouri  
Talk title:  *$Q_A$  and  $Q_B$  Methoxy Dihedral Angles determined by pulsed EPR*

## Publications

1. Blaesi, E. J., Palowitch, G. M., Hu, K., Kim, A. J., Rose, H. R., Alapati, R. B., Lougee, M. G., Kim, H. J., **Taguchi, A. T.**, Tan, K. O., Laremore, T. N., Griffin, R. G., Krebs, C., Matthews, M. L., Silakov, A., Bollinger, M. J. Jr., Allen, B. D., Boal, A. K. Metal-free class I ribonucleotide reductase from pathogens initiates catalysis with a tyrosine-derived dihydroxyphenylalanine radical. *PNAS*, September, 2018.
2. **Taguchi, A. T.**, Ohmori, D., Dikanov, S. A., and Iwasaki, T. g-Tensor Directions in the Protein Structural Frame of Hyperthermophilic Archaeal Reduced Rieske-Type Ferredoxin Explored by <sup>13</sup>C Pulsed Electron Paramagnetic Resonance. *Biochemistry*, Vol. 57, No. 28, pp. 4074-4082, June, 2018.
3. Dikanov, S. A. and **Taguchi, A. T.** Two-dimensional Pulsed EPR Resolves Hyperfine Coupling Strain in Nitrogen Hydrogen Bond Donors of Semiquinone Intermediates. *J. Phys. Chem. B.*, Vol. 122, No. 20, pp. 5205-5211, April, 2018.
4. **Taguchi, A. T.**, Miyajima-Nakano, Y., Fukazawa, R., Lin, M. T., Baldansuren, A., Gennis, R. B., Hasegawa, K., Kumasaka, T., Dikanov, S. A., and Iwasaki, T. Unpaired Electron Spin Density Distribution across Reduced [2Fe-2S] Cluster Ligands by <sup>13</sup>C<sub>β</sub>-Cysteine Labeling. *Inorg. Chem.*, Vol. 57, No. 2, pp. 741-746, December, 2017.
5. **Taguchi, A. T.**, O'Malley, P. J., Wraight, C. A., and Dikanov, S. A. Determination of the Complete Spin Density Distribution in <sup>13</sup>C-Labeled Protein-Bound Radical Intermediates Using Advanced 2D Electron Paramagnetic Resonance Spectroscopy and Density Functional Theory. *J. Phys. Chem. B*, Vol. 121, No. 44, pp. 10256-10268, October, 2017. (4 minute LiveSlides presentation narrated by **Taguchi, A. T.** available at <http://pubs.acs.org/doi/suppl/10.1021/acs.jpcc.7b10036>)
6. Greene, B. L., **Taguchi, A. T.**, Stubbe, J., and Nocera, D. G. Conformationally Dynamic Radical Transfer within Ribonucleotide Reductase. *J. Am. Chem. Soc.*, Vol. 139, No. 46, pp. 16657-16665, October, 2017.
7. Lin, Q.,\* Parker, M. J.,\* **Taguchi, A. T.**,\* Ravichandran, K.,\* Kim, A., Kang, G., Shao, J., Drennan, C. L., and Stubbe, J. Glutamate 52-β at the α/β Subunit Interface of *E. coli* Class Ia Ribonucleotide Reductase is essential for Conformational Gating of Radical Transfer. *J. Biol. Chem.*, Vol. 292, No. 22, pp. 9229-9239, April, 2017. (\*authors contributed equally to this paper)
8. Ravichandran, K. R., Zong, A. B., **Taguchi, A. T.**, Nocera, D. G., Stubbe, J., and Tommos, C. Formal Reduction Potentials of Difluorotyrosine and Trifluorotyrosine Protein Residues: Defining the Thermodynamics of Multistep Radical Transfer. *J. Am. Chem. Soc.*, Vol. 139, No. 8, pp. 2994-3004, February, 2017.
9. Ravichandran, K., Minnihan E. C., Lin Q., Yokoyama K., **Taguchi A. T.**, Shao J., Nocera, D. G., and Stubbe, J. Glutamate 350 Plays an Essential Role in Conformational Gating of Long-Range Radical Transport in *Escherichia coli* Class Ia Ribonucleotide Reductase. *Biochemistry*, Vol. 56, No. 6, pp. 856-868, January, 2017.
10. **Taguchi, A. T.**, Baldansuren, A., and Dikanov, S. A. Basic and Combination Cross-Features in X- and Q-band HYSCORE of the <sup>15</sup>N Labeled Bacteriochlorophyll *a* Cation Radical. *Z. Phys. Chem.*, Vol. 231, pp. 725-744, February, 2017.
11. Sun, C., **Taguchi, A. T.**, Vermaas, J. V., Beal, N. J., O'Malley, P. J., Tajkhorshid, E., Gennis, R. B., Dikanov, S. A. Q-Band Electron-Nuclear Double Resonance Reveals Out-of-Plane Hydrogen Bonds Stabilize an Anionic Ubisemiquinone in Cytochrome *bo*<sub>3</sub> from *Escherichia coli*. *Biochemistry*, Vol. 55, No. 40, pp. 5714-5725, October, 2016.
12. Ravichandran, K. R., **Taguchi, A. T.**, Wei, Y., Tommos, C., Nocera, D. G., and Stubbe, J. A >200 meV Uphill Thermodynamic Landscape for Radical Transport in *Escherichia coli* Ribonucleotide Reductase Determined Using Fluorotyrosine-Substituted Enzymes. *J. Am. Chem. Soc.*, Vol. 138, No. 41, pp. 13706-13716, September, 2016.
13. Sun, C., **Taguchi, A. T.**, Beal, N., O'Malley, P. J., Dikanov, S. A., and Wraight, C. A. Regulation of the Primary Quinone Binding Conformation by the H Subunit in Reaction Centers from *Rhodobacter sphaeroides*. *J. Phys. Chem. Lett.*, Vol. 6, No. 22, pp. 4541-4546, October, 2015.
14. Yi, S., **Taguchi, A. T.**, Samoiloa, R. I., O'Malley, P. J., Gennis, R. B., and Dikanov, S. A. Plasticity in the High Affinity Menaquinone Binding Site of the Cytochrome *aa*<sub>3</sub>-600 Menaquinol Oxidase from *Bacillus subtilis*. *Biochemistry*, Vol. 54, No. 32, pp. 5030-5044, July, 2015.

15. **Taguchi, A. T.**, O'Malley, P. J., Wraight, C. A., and Dikanov, S. A. Hydrogen Bond Network around the Semiquinone of the Secondary Quinone Acceptor Q<sub>B</sub> in Bacterial Photosynthetic Reaction Centers. *J. Phys. Chem. B*, Vol. 119, No. 18, pp. 5805-5814, April, 2015.
16. Vermaas, J. V., **Taguchi, A. T.**, Dikanov, S. A., Wraight, C. A., and Tajkhorshid, E. Redox Potential Tuning through Differential Quinone Binding in the Photosynthetic Reaction Center of *Rhodobacter sphaeroides*. *Biochemistry*, Vol. 54, No. 12, pp. 2104-2116, March, 2015.
17. Hong, S., De Almeida, W., **Taguchi, A. T.**, Samoilova, R. I., Gennis, R. B., O'Malley P. J., Dikanov, S. A., and Crofts, A. R. The Semiquinone at the Q<sub>i</sub> Site of the bc<sub>1</sub> Complex Explored Using HYSCORE Spectroscopy and Specific Isotopic Labeling of Ubiquinone in *Rhodobacter sphaeroides* via <sup>13</sup>C Methionine and Construction of a Methionine Auxotroph. *Biochemistry*, Vol. 53, No. 38, pp. 6022-6031, September, 2014.
18. Samoilova, R. I., **Taguchi, A. T.**, O'Malley P. J., Dikanov, S. A., and Lugtenburg, J. Hyperfine Interaction Tensors of <sup>13</sup>C Nuclei for Ring Carbons of Ubisemiquinone-10 Hydrogen Bonded in Alcohol Solvents. *Appl. Magn. Reson.*, Vol. 45, No. 9, pp. 941-953, September, 2014.
19. **Taguchi, A. T.**, O'Malley, P. J., Wraight, C. A., and Dikanov, S. A. Hyperfine and Nuclear Quadrupole Tensors of Nitrogen Donors in the Q<sub>A</sub> Site of Bacterial Reaction Centers: Correlation of the Histidine N<sub>δ</sub> Tensors with Hydrogen Bond Strength. *J. Phys. Chem. B*, Vol. 118, No. 31, pp. 9225-9237, July, 2014.
20. De Almeida, W., **Taguchi, A. T.**, Dikanov, S. A., Wraight, C. A., and O'Malley, P. J. The 2-Methoxy Group Orientation Regulates the Redox Potential Difference between the Primary (Q<sub>A</sub>) and Secondary (Q<sub>B</sub>) Quinones of Type II Bacterial Photosynthetic Reaction Centers. *J. Phys. Chem. Lett.*, Vol. 5, No. 15, pp.2506-2509, June, 2014. (5 minute LiveSlides presentation narrated by **Taguchi, A. T.** available at <http://pubs.acs.org/doi/suppl/10.1021/jz500967d>)
21. **Taguchi, A. T.**, O'Malley, P. J., Wraight, C. A., and Dikanov, S. A. Nuclear hyperfine and quadrupole tensor characterization of the nitrogen hydrogen bond donors to the semiquinone of the Q<sub>B</sub> site in bacterial reaction centers: A combined X- and S-band <sup>14,15</sup>N ESEEM and DFT study. *J. Phys. Chem. B*, Vol. 118, No. 6, pp. 1501-1509, February, 2014.
22. **Taguchi, A. T.**, Mattis, A. J., O'Malley, P. J., Dikanov, S. A., and Wraight, C. A. Tuning Cofactor Redox Potentials: The 2-Methoxy Dihedral Angle Generates a Redox Potential Difference of >160 mV between the Primary (Q<sub>A</sub>) and Secondary (Q<sub>B</sub>) Quinones of the Bacterial Photosynthetic Reaction Center. *Biochemistry*, Vol. 52, No. 41, pp. 7164-7166, September, 2013.
23. **Taguchi, A. T.**, O'Malley, P. J., Wraight, C. A., and Dikanov, S. A. Conformational Differences between the Methoxy Groups of Q<sub>A</sub> and Q<sub>B</sub> Site Ubisemiquinones in Bacterial Reaction Centers: A Key Role for Methoxy Group Orientation in Modulating Ubiquinone Redox Potential. *Biochemistry*, Vol. 52, No. 27, pp. 4648-4655, June, 2013.

## Patents

1. Woodbury, N. W., **Taguchi, A. T.** Methods, Systems, and Media for Predicting Functions of Molecular Sequences. M18-149L / 0118090.200-US1. *Patent pending.*

## Poster Abstracts and Other Publications

1. Iwasaki, T., Fukazawa, R., Miyajima-Nakano, Y., **Taguchi, A. T.**, Hasegawa, K., Kumasaka, T., Lin, M. T., Dikanov, S. A., Gennis, R. B. *Escherichia coli* Amino Acid Auxotrophic Expression Strains for the Structure-function Studies of Metalloenzymes. **14<sup>th</sup> European Biological Inorganic Chemistry Conference (EuroBIC 14)**, Birmingham, United Kingdom, August, 2018. (*conference abstract*)
2. **Taguchi, A. T.**, Kang, G., Ni, Q. Z., Can, T. V., Lin, Q., Drennan, C. L., Stubbe, J., Griffin, R. G. Structural Studies of the *E. coli* Class Ia Ribonucleotide Reductase. **European Chemistry Conference 2018**, Rome, Italy, July, 2018. (*conference abstract*)
3. **Taguchi, A. T.**, Miyajima-Nakano, Y., Fukazawa, F., Matsushita, S., Lin, M. T., Baldansuren, A., Samoilova, R. I., Gennis, R. B., Hasegawa, K., Kumasaka, T., Dikanov, S. A., and Iwasaki, T. The Spin Density Distribution is a Sensitive Probe of the Cysteine Ligand Geometries in Rieske, mitoNEET, and Plant-Type

[2Fe-2S] Ferredoxins. **17<sup>th</sup> International Conference on Biological Inorganic Chemistry (ICBIC 16)**, Beijing, China, July, 2015. (*conference abstract*)

4. **Taguchi, A. T.** Investigation of the Quinone Sites in Reaction Centers from *Rhodobacter Sphaeroides* by Pulsed EPR and Spectral Simulations. Thesis. University of Illinois at Urbana-Champaign, Ann Arbor: ProQuest LLC, 2014. (*dissertation*)
5. **Taguchi, A. T.**, Mattis, A. J., O'Malley, P. J., Dikanov, S. A., and Wraight, C. A. Methoxy dihedral angles of Ubiquinone contribute more than 160 mV to the redox potential difference between the primary (Q<sub>A</sub>) and secondary (Q<sub>B</sub>) quinones of the photosynthetic reaction center. ***Biophysical Journal***, Vol. 106, No. 2, pp. 370a, San Francisco, USA, January, 2014. (*conference abstract*)
6. Matsushita, S., Fukazawa, R., Iwasaki, T., **Taguchi, A. T.**, Baldansuren, A., Dikanov, S. A. 2D pulsed EPR analysis of histidine ligand residue(s) of the thermophile Rieske and mitoNEET type iron-sulfur proteins. **16<sup>th</sup> International Conference on Biological Inorganic Chemistry (ICBIC 16)**, #1714640, Mz76, Grenoble, France, July, 2013. (*conference abstract*)
7. **Taguchi, A.**, Nick, T., Doll, A., and Smith, G. Impressions from the 6th EF-EPR School in Rehovot. ***EPR Newsletter***, Vol. 22, No. 4, pp. 17–19, 2013. (*invited article, non-refereed*)
8. **Taguchi, A. T.**, Kokhan, O., and Wraight, C. A. Pyrazole Cytochrome C Complexes. ***Biophysical Journal***, Vol. 102, No. 3, pp. 466a–467a, San Diego, USA, January, 2012. (*conference abstract*)