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**VICENTE M. REYES, Ph.D.**

Department of Biological Sciences  
School of Biological and Medical Sciences  
College of Science  
Rochester Institute of Technology  
Rochester, NY 14623-5603

Tel: (585) 475-4115  
Cell: (619) 212-9131  
E-mail: vmrsbi@rit.edu  
vicentemreyes@gmail.com

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**FIELDS OF INTEREST:**

- **Computational, Mathematical & Theoretical Biology**
- **Structural Bioinformatics & Biological Data Mining**
- **Structural Biology & Structure-Based Drug Design**

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**EDUCATION:****Degrees:**

**Ph.D. Chemistry**, California Institute of Technology, Pasadena, California, USA  
(conc. in molecular biology & biochemistry)

**B. S. Mathematics** (*magna cum laude*) Univ. of the Philippines, Diliman, Philippines  
(conc. in pure mathematics & operations research)

**B. S. Chemistry** (*magna cum laude*) Univ. of the Philippines, Diliman, Philippines  
(conc. in organic chemistry & biochemistry)

**Certificates/Diplomas:**

**Prof. Cert. in Drug Disc. & Dev.**, UCSD School of Extended Studies, *Ongoing*

**Spec. Cert. in Data Mining**, UCSD School of Extended Studies, *Winter 2007*

**Prof. Cert. in Bioinformatics**, UCSD School of Extended Studies, *Spring 2004*

**Spec. Cert. In Bioinformatics**, UCSD School of Extended Studies, *Spring 2002*

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**CAREER HISTORY:**

**Assistant Professor**, Dept. of Biological Sciences, SBMS, COS, R.I.T. , 9/2008-present  
(*computational biology/bioinformatics*)

**IRACDA Postdoctoral Fellow & Assistant Project Scientist** , UCSD Dept. of Pharmacology, SOM, 2004-'08  
(*computational biology/structural bioinformatics*)

**Structural Bioinformatics Researcher**, San Diego Supercomputer Center, 2002-'04  
(*structural bioinformatics*)

**Bioinformatics studies**, UCSD School of Extended Studies, La Jolla, CA, 2000-'02  
(*general bioinformatics*)

**Senior Research Associate**, The Scripps Research Institute, La Jolla, CA, 1995-'00  
(*protein x-ray crystallography; structure-based drug design*)

**Postdoctoral Biochemist**, Dept. of Chem. & Biochem., UCSD, La Jolla, CA, 1992-'95  
(*protein x-ray crystallography; structural enzymology*)

**Postdoctoral Biologist**, Dept's. of Biol. & Med., UCSD, La Jolla, CA 1990-'92  
(*HIV/AIDS molecular biology*)

**Postdoctoral Research Fellow**, Lab.Tum. Cell Biol., NCI/NIH, Bethesda, MD 1988-'89  
(*HIV/AIDS molecular biology*)

**Graduate Student & Teaching Assistant**, Dept. of Biol., CIT, Pasadena, CA 1983-'88  
(*gene expression molecular biology*)

**Instructor in Mathematics**, Dept. of Math., Univ. of the Phils., Diliman, Phils., 1980-'82  
(*differential and integral calculus I, II, and III; statistics*)

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## **AWARDS:**

- F.E.A.D. Summer Research Funding Award, COS, R.I.T., Summer 2010
- A.R.R.A. Summer Research Funding Award, R.I.T./R.G.H. Alliance, Summer 2009
- F.E.A.D. Summer Research Funding Award, COS, R.I.T., Summer 2009
- IRACDA Postdoctoral Scholars Program, NIGMS, NIH, 2004-'07
- Bioinformatics Career Development WIA Award, State of California, 2002-'03
- Postdoctoral Research Fellowship, NIGMS, NIH, 1992-'95
- John E. Fogarty International Postdoctoral Research Fellowship, NCI, NIH, 1988-'89
- Laszlo Zechmeister Graduate Fellowship in Chemistry, CIT, 1983-'85
- Nat'l. Undergrad. Science & Mathematics Scholarships, NSDB, Philippines, 1976-'80

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## **PATENTS and COPYRIGHTS:**

- "Novel, Analytical Algorithm for High-Throughput Structure-Based Prediction of Ligand Binding Sites in Proteins" (under UCSD review; Docket # SD2007-164).
- "Novel, Analytical Algorithm for High-Throughput Structure-Based Prediction of Protein-Protein Interaction Partners" (under UCSD review; Docket # SD2007-165)
- "Representing Protein Structures in Spherical Coordinates: Two Applications" (under UCSD review; Docket # SD2008-087).
- "Two Algorithms For Quantifying Ligand Binding Site Burial in Proteins" (under UCSD review; Docket # SD2008-086).

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**FORMAL GRANTSMANSHIP TRAINING:**

- NIGMS/UoK Internet Grant Writing Workshop (<http://www.uky.edu/Projects/GrantWriting>), University of Kentucky, Lexington KY, Prof. Donald Frazier, UoK Sch. of Med., Director, May, 2005
- NIGMS/UoK Internet Grant Writing Workshop (<http://www.uky.edu/Projects/GrantWriting>), University of Kentucky, Lexington KY, Prof. Donald Frazier, UoK Sch. of Med., Director, May, 2006
- NIGMS/UoK Internet Grant Writing Workshop (<http://www.uky.edu/Projects/GrantWriting>), University of Kentucky, Lexington KY, Prof. Donald Frazier, UoK Sch. of Med., Director, May, 2007
- Grant Writing Workshop-Seminar, Grant Writers' Seminars and Workshops, LLC (<http://www.grantcentral.com>), Drs. Stephen W. Russell & David C. Morrison, Lecturers, Pasadena Civic Auditorium, Pasadena, CA Sept., 2005

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**PUBLICATIONS:**

- **Reyes, V.M\*** & Sheth, V.N., "Visualization of Protein 3D Structures in 'Double-Centroid' Reduced Representation: Application to Ligand Binding Site Modeling and Screening", Handbook of Research in Computational and Systems Biology: Interdisciplinary Approaches, IGI-Global/Springer (\*corresponding author; *in press*).
- **Reyes, V.M.**, "Modeling Protein-Protein Interface Interactions as a Means for Predicting Protein-Protein Interaction Partners." J. Biomol. Struct. & Dyn., Book of Abstracts, Albany 2009: The 16th Conversation, June 16-20 2009, Vol. 26 (6) June 2009, p. 873
- **Reyes, V.M.**, "Pharmacophore Modeling Using a Reduced Protein Representation as a Tool for Structure-Based Protein Function Prediction", J. Biomol. Struct. & Dyn., Book of Abstracts, Albany 2009: The 16th Conversation, June 16-20 2009, Vol. 26 (6) June 2009, p. 873
- **Reyes, V.M.**, "Pharmacophore Modeling Using a Reduced Protein Representation: Application to the Prediction of ATP, GTP, Sialic Acid, Retinoic Acid, and Heme-Bound and -Unbound Nitric Oxide Binding Proteins", J. Biomol. Struct. & Dyn., Book of Abstracts, Albany 2009: The 16th Conversation, June 16-20 2009, Vol. 26 (6) June 2009, p. 874
- **Reyes, V.M.**, "Representing Protein 3D Structures in Spherical Coordinates – Two Applications: 1. Detection of Invaginations, Protrusions, and Potential Ligand Binding Sites; and 2. Separation of Protein Hydrophilic Outer Layer from the Hydrophobic Core ",

J. Biomol. Struct. & Dyn., Book of Abstracts, Albany 2009: The 16th Conversation, June 16-20 2009, Vol. 26 (6) June 2009, pp. 874-5

- **Reyes, V.M.**, " Two Complementary Methods for Quantifying Ligand Binding Site Burial Depth in Proteins: The "Cutting Plane" and the "Tangent Sphere Methods", J. Biomol. Struct. & Dyn., Book of Abstracts, Albany 2009: The 16th Conversation, June 16-20 2009, Vol. 26 (6) June 2009, p. 875
- Li, W., Byrnes, R.W., Hayes, J., Birnbaum, A., **Reyes, V.M.**, Shahab, A., Mosley, C., Pekurovsky, D., Quinn, G.B., Shindyalov, I.N., Casanova, H., Ang, L., Berman, F., Arzberger, P.W., Miller, M., Bourne, P.E. "The Encyclopedia of Life Project: Grid Software and Deployment." *New Gener. Comp.* (2004) 22:127-136.
- Bourne, P., Miller, M., Baldrige, K., Baru, C., Berman, F., Byrnes, R., Casanova, H., Cotofana, N., Fountwain, T., Greenberg, J., Li, W., Mosley, C., Pekurovsky, D., Quinn, G., **Reyes, V.**, Shin, P., Shindyalov, I., Veretnik, S. "Encyclopedia of Life: to Open New Chapter of Biological Discovery." *SDSC & NPACI EnVision*, (2003) Vol. 19, No. 1, pp. 3-5
- **Reyes, V.M.**, Greasley, S.E., Stura, E.A., Beardsley, G.P., Wilson, I.A. "Crystallization and preliminary crystallographic investigations of avian 5-aminoimidazole-4-carboxamide ribonucleotide transformylase-inosine monophosphate cyclohydrolase expressed in *Escherichia coli*." *Acta Crystallogr D Biol Crystallogr.* (2000) Aug;56 (Pt 8):1051-4.
- Lee, H., \***Reyes, V.M.**, Kraut, J. "Crystal structures of *Escherichia coli* dihydrofolate reductase complexed with 5-formyltetrahydrofolate (folinic acid) in two space groups: evidence for enolization of pteridine O4." *Biochemistry.* (1996) Jun 4;35(22):7012-20. (\*corresponding author)
- **Reyes, V.M.**, Sawaya, M.R., Brown, K.A., Kraut, J. "Isomorphous crystal structures of *Escherichia coli* dihydrofolate reductase complexed with folate, 5-deazafolate, and 5,10-dideazatetrahydrofolate: mechanistic implications." *Biochemistry.* (1995) Feb 28;34(8):2710-23.
- **Reyes, V.M.**, Abelson, J.N. "In vitro synthesis of end-mature, intron-containing transfer RNAs." *Methods Enzymol.* (1989);180:63-9.
- **Reyes, V.M.**, Abelson, J. "Substrate recognition and splice site determination in yeast tRNA splicing." *Cell.* (1988) Nov 18;55(4):719-30.
- **Reyes, V.M.**, Abelson, J. "A synthetic substrate for tRNA splicing." *Anal Biochem.* 1987 Oct;166(1):90-106.
- **Reyes, V.M.**, Newman, A., Abelson, J. "Mutational analysis of the coordinate expression of the yeast tRNA<sup>Arg</sup>-tRNA<sup>Asp</sup> gene tandem." *Mol Cell Biol.* (1986) Jul;6(7):2436-42.

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## PRESENTATIONS (since January 2009):

- Gordon Research Conference on IDRs (Intrinsically Disordered Regions) and Unfoldomics, Davidson, NC (Davidson College), presented one poster; actively participated in post-talk discussions  
**Poster:** "I. Characterizing the Interactions Between Protein & Lipid Moieties at Lipidation & Lipid Binding Sites in Proteolipids/Lipoproteins; and (II.) Determining the Loop Propensities of the 20 Amino Acids"
- Gordon Research Conference on Biopolymers, Newport, RI (Salve Regina University), 6/06/2010-6/11/2010; presented two posters; actively participated in post-talk discussions  
**Poster #1:** Visualization of Protein 3D Structures in 'Double-Centroid' Reduced Representation: Application to Ligand Binding Site Modeling and Screening  
**Poster #2:** Separation of a Protein's Outer Layer from Its Inner Core Using Spherical Coordinate Representation: Potential Application to Computational Epitope Mapping and Detection of Deeply Buried Active Sites
- Gordon Research Conference on Proteins, Holderness, NH (Holderness School), presented two posters; actively participated in post-talk discussions  
**Poster #1:** Two Novel Methods for Protein Structure Analysis: (1.) Spherical Coordinate Representation of Protein Structures; and (2.) Quantification of Ligand Binding Site Burial Using the 'Cutting Plane' and 'Tangent Sphere' Methods  
**Poster #2:** Modeling of, and Screening for, Ligand Binding Sites and Protein-Protein Interface Interactions as Tetrahedral Motifs in Reduced Protein Representation: Applications to Protein Function Prediction
- 6th Conversation on BSDIE (Biological Structure, Dynamics, Interaction and Expression, SUNY-Albany, Albany, NY, June 16-20, 2009  
**Poster #1:** Representing Protein 3D Structures in Spherical Coordinates: Two Applications: (1.) Detection of Invaginations and Protrusions on the Protein Surface; and (2.) Separating the Protein Hydrophobic Inner core from the Hydrophilic Outer layer  
**Poster #2:** Two Complementary Methods for Quantifying Ligand Binding Site Burial Depth In Proteins: (1.) The "Cutting Plane" Method; and (2.) The "Tangent Sphere" Method  
**Poster #3:** Pharmacophore Modeling Using a Reduced Protein Representation as a Tool for Structure-Based Protein Function Prediction  
**Poster #4:** Pharmacophore Modeling Using a Reduced Protein Representation: Application to ATP, GTP, Sialic Acid, Retinoic Acid and Heme-Bound and -Unbound Nitric Oxide  
**Poster #5:** Modeling Protein-Protein Interface Interactions as a Means for Predicting Protein-Protein Interaction Partners
- Pacific Symposium on Biocomputing, Jan. 5-9, 2009, Big Island, Hawaii  
**Poster #1:** Representing Protein 3D Structures in Spherical Coordinates: Two Applications: (1.) Detection of Invaginations and Protrusions on the Protein Surface; and (2.) Separating the Protein Hydrophobic Inner core from the Hydrophilic Outer layer  
**Poster #2:** Two Complementary Methods for Quantifying Ligand Binding Site Burial Depth In Proteins: (1.) The "Cutting Plane" Method; and (2.) The "Tangent Sphere" Method  
**Poster #3:** Pharmacophore Modeling Using a Reduced Protein Representation as a Tool for Structure-Based Protein Function Prediction

**Poster #4:** Pharmacophore Modeling Using a Reduced Protein Representation: Application to ATP, GTP, Sialic Acid, Retinoic Acid and Heme-Bound and -Unbound Nitric Oxide

**Poster #5:** Modeling Protein-Protein Interface Interactions as a Means for Predicting Protein-Protein Interaction Partners

- ISBRA 2009 (5th International Symposium on Bioinformatics Research and Applications), May 13 -16, 2009, Nova Southeastern University, Ft. Lauderdale, FL (with bioinformatics graduate student, Vrunda Sheth)

**Poster:** "Visualization of Protein 3D Structures in Reduced Representation with Simultaneous Display of Intramolecular H-bond and van der Waals Interactions"

- Imagine RIT, May 2, 2009:

- Grad student, Vrunda Sheth (w/ V. Reyes) poster: "Visualization of Protein 3D Structures in Reduced Representation with Simultaneous Display of Intramolecular H-bond and van der Waals Interactions"

- Undergrad student, Wan Munirah Wan Mohamad (w/ V. Reyes) poster: "Building a Library of Protein-Protein Binary Complex (PPBC) Interfacial Interaction Models Using a Reduced Protein Representation"

- RIT's I.T. Collaboratory Access Grid Seminar Series, "Visualization of Protein 3D Structures in Double-Centroid Reduced Representation" Vicente Reyes, and Vrunda Sheth, Dept. of Biological Sciences, Bioinformatics Program, R.I.T. (broadcast over the Access Grid from RIT's I.T. Collaboratory), Jan. 22, 2009.

- R.I.T. Biology Dept. Seminar Series, "Two Structural Proteomics Algorithms and Their Applications", Dec. 15, 2008

- R.I.T. Mathematics Dept. Colloquium Series "Two Structural Proteomics Algorithms and Their Applications", Feb. 4, 2009

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### **COURSES TAUGHT at R.I.T. (since March 2009):**

Perl for Bioinformatics, Spring 2009 and 2010

UNIX Under the Hood, Fall 2010

Bioinformatics, Winter 2010

Bioinformatics Seminar, Fall 2010 and 2011

Proteomics, Spring 2009 and 2010

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### **MISCELLANEOUS:**

- Member, External Faculty, Ph.D. Program of the Golisano Institute of Computing and Information Sciences, R.I.T. (Prof. P.-C. Shi, director)
- Member, Center for Applied and Computational Mathematics, Dept. of Mathematics, R.I.T. (Prof. A. Harkin, director)