Curriculum vitae

Summary

Nicholas obtained his first degree on Biology at the University of Athens, studying for his final year thesis with Prof Hamodrakas on a new multiple sequence alignment algorithm. Being charmed by this computational work, he naturally decided to abandon Biology for Physics and computational Biology, and obtained a PhD on biological crystallography at the (then) Astbury Department of Biophysics (UK) with Prof Simon Phillips. Coming back to Greece, and following a year-long tour of duty, he spent six lovely years as a postdoc with Prof Mike Kokkinidis at Crete writing code, avoiding the wet lab, and occasionally solving a structure. In 2003 —and after a short visit to beautiful Ioannina— he decided to take-up Einstein's advice and got a (mostly) teaching job at the Department of Molecular Biology & Genetics at Alexandroupolis, where he still serves as an Assistant Professor. He has authored ∼45 research articles in journals of the Science Citation Index, with most of them revolving around structural biology, crystallography and computational biology.

Personal details

Full name	Nicholas Menelaou Glykos.
Place of birth	Athens, Greece.
Nationality	Greek.
Home address	Petrina Alexandroupolis, 68100 Alexandroupolis, Greece.
Work address	Department of Molecular Biology & Genetics, Democritus University of Thrace, University campus (Dragana), 68100 Alexandroupolis, Greece.
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Positions and qualifications

2003-present	Assistant Professor (since 2008) and Lecturer (since 2003) of Structural and Computational Biology at the Department of Molecular Biology and Genetics of Democritus University of Thrace, Greece.
2003-present	Speaker for the Postgraduate programs "Protein Biotechnology" (University of Crete) and "Translational Reasearch in Biomedicine" (Democritus University of Thrace).
2002-2003	Visiting lecturer, Department of Biological Applications & Technologies, University of Ioannina, Greece.

1996-2001	Postdoctoral research fellow at the macromolecular crystallography group of the Institute of Molecular Biology and Biotechnology, Foundation for Research and Technology–Hellas, Crete, Greece.
1997-1998	EMBO short-term fellowship at the University of Leeds.
1991-1995	PhD, Department of Biophysics, University of Leeds, Thesis title : "Structural studies of the arginine repressor/activator from *Bacillus subtilis*".
1986-1990	BSc, Department of Biology, University of Athens.

Teaching

The undergraduate courses that are —or have been— taught include *'Bioinformatics'* (mainly algorithms), *'Introduction to computational biology'* (unix and C programming), *'Advanced themes of bioinformatics'* (perl), *'Advanced themes of computational biology'* (structural computational biology), *'Structural biology'* (basic stuff based on the Branden and Tooze book), and finally, the *'Advanced themes of Structural biology'* (essentially methods of macromolecular crystallography). Final year (diploma thesis) students are trained on structural computational biology projects. See http://utopia.duth.gr/glykos/people.html for PDF copies (in Greek) of students' theses. See the links given in http://utopia.duth.gr/glykos/teaching.html for more details (again in Greek) of the undergraduate courses taught.

At the postgraduate level, and other than tormenting the occasional PhD student, the courses of *'Bioinformatics'*, *'Introduction to crystallography'* and *'Crystallographic computing'* are —or have been— taught at the MSc level at Democritus University of Thrace and the University of Crete.

Publications

Only research articles published in journals of the Science Citation Index are shown in the list the follows, with the exception of an arXiv electronic preprint (reference number 41), a letter to the Editor (reference number 29) and NMG's thesis (reference number 0) which are also included in the list for completeness. Articles whose reference numbers are shown in bold are those for which NMG serves as the corresponding author. In the electronic version of this document the articles that follow are active links to electronic (PDF) offprints.

44. Fadouloglou, V.E., Balomenou, S., Aivaliotis, M., Kotsifaki, D., Arnaouteli, S., Tomatsidou, A., Efstathiou, G., Kountourakis, N., Miliara, S., Griniezaki, M., Tsalafouta, A., Pergantis, S.A., Boneca, I.G., **Glykos, N.M.**, Bouriotis, V. & Kokkinidis, M. (2017), "An unusual -carbon hydroxylation of proline promotes active-site maturation", *J. Am. Chem. Soc.*, **139**, 5330–5337.

43. Serafeim A.-P., Salamanos, G., Patapati, K.K. & **Glykos*, N.M.** (2016), "Sensitivity of Folding Molecular Dynamics Simulations to Even Minor Force Field Changes", *J. Chem. Inf. Model.*, **56**, 2035–2041.

42. Baltzis, A.S. & **Glykos*, N.M.** (2016), "Characterizing a partially ordered miniprotein through folding molecular dynamics simulations: Comparison with the experimental data", *Prot. Sci.*, **25**, 587–596.

41. Baltzis, A.S., Koukos, P.I. & **Glykos*, N.M.** (2015), "Clustering of molecular dynamics trajectories via peak-picking in multidimensional PCA-derived distributions", *arXiv:***1512.04024** [q-bio.BM].

40. Koukos, P.I. & **Glykos*, N.M.** (2014), "Folding Molecular Dynamics Simulations Accurately Predict the Effect of Mutations on the Stability and Structure of a Vammin-Derived Peptide", *J. Phys. Chem. B*, **118**, 10076–10084.

39. Koukos, P.I. & **Glykos*, N.M.** (2014), "On the application of Good-Turing statistics to quantify convergence of biomolecular simulations", *J. Chem. Inf. Model.*, **54**, 209–217.

38. Koukos, P.I. & **Glykos*, N.M.** (2013), "grcarma: A Fully Automated Task-Oriented Interface for the Analysis of Molecular Dynamics Trajectories", *J. Comput. Chem.*, **34**, 2310–2312.

37. Kontopoulos, D.-G. & **Glykos*, N.M.** (2013), "Pinda: A Web service for detection and analysis of intraspecies gene duplication events", *Comput. Methods Programs Biomed.*, **111**, 711–714.

36. Georgoulia, P.S. & **Glykos*, N.M.** (2013), "On the Foldability of Tryptophan-Containing Tetra- and Pentapeptides: An Exhaustive Molecular Dynamics Study", *J. Phys. Chem. B*, **117**, 5522–5532.

35. Patmanidis, I. & **Glykos*, N.M.** (2013), "As good as it gets? Folding molecular dynamics simulations of the LytA choline-binding peptide result to an exceptionally accurate model of the peptide structure", *J. Mol. Graph. Model.*, **41**, 68–71.

34. Fadouloglou, V.E., Kapanidou, M., Agiomirgianaki, A., Arnaouteli, S., Bouriotis, V., **Glykos*, N.M.** & Kokkinidis*, M. (2013), "Structure determination through homology modelling and torsion-angle simulated annealing: application to a polysaccharide deacetylase from Bacillus cereus", *Acta Crystallogr.*, D**69**, 276–283.

33. Kokkinidis, M., **Glykos, N.M.** & Fadouloglou, V.E. (2012), "Protein Flexibility and Enzymatic Catalysis", *Adv. Protein Chem. Struct. Biol.*, **87**, 181–218.

32. Georgoulia, P.S. & **Glykos*, N.M.** (2011), "Using J-coupling constants for force field validation: Application to hepta-alanine", *J. Phys. Chem. B*, **115**, 15221-15227.

31. Patapati, K.K. & **Glykos*, N.M.** (2011), "Three Force Fields' Views of the 3_{10} Helix", *Biophys. J.*, **101**, 1766–1771.

30. Glykos*, N.M. (2011), "On the application of structure-specific bulk-solvent models", *Acta Cryst.*, D**67**, 739–741.

29. Glykos*, N.M. (2011), "The 11th Misconception ?", A letter to the Editor, *CBE Life Sci. Educ.*, **10**, 1-2.

28. Patapati, K.K. & **Glykos*, N.M.** (2010), "Order through Disorder: Hyper-Mobile C-Terminal Residues Stabilize the Folded State of a Helical Peptide. A Molecular Dynamics Study",

PLoS ONE, **5**, e15290.

27. Fadouloglou, V.E., Stavrakoudis, A., Bouriotis, V., Michael Kokkinidis, M. & **Glykos*, N.M.** (2009), "Molecular Dynamics Simulations of BcZBP, A Deacetylase from Bacillus cereus: Active Site Loops Determine Substrate Accessibility and Specificity", *J. Chem. Theory Comput.*, **5**, 3299–3311.

26. Fadouloglou, V.E., Bastaki, M.N., Ashcroft, A.E., Phillips, S.E.V., Panopoulos, N.J., **Glykos*, N.M.**, & Kokkinidis*, M. (2009), "On the quaternary association of the type III secretion system HrcQB-C protein: Experimental evidence differentiates among the various oligomerization models", *J. Struct. Biol.*, **166**, 214–225.

25. Fadouloglou, V.E., Kokkinidis, M. & **Glykos*, N.M.** (2008), "Determination of protein oligomerization state: Two approaches based on glutaraldehyde crosslinking", *Anal. Biochem.*, **373**, 404–406.

24. Mizas, Ch., Sirakoulis, G.Ch., Mardiris, V., Karafyllidis, I., **Glykos, N.M.,** & Sandaltzopoulos, R. (2008), "Reconstruction of DNA sequences using genetic algorithms and cellular automata: Towards mutation prediction ?", *BioSystems*, **92**, 61–68.

23. Fadouloglou, V.E., Deli, A., **Glykos, N.M.,** Psylinakis, E., Bouriotis, V. & Kokkinidis, M. (2007), "Crystal structure of the BcZBP, a zinc-binding protein from Bacillus cereus. Functional insights from structural data", *FEBS J.*, **274**, 3044–3054.

22. Glykos*, N.M. (2007), "On the application of molecular-dynamics simulations to validate thermal parameters and to optimize TLS-group selection for macromolecular refinement", *Acta Cryst.*, D**63**, 705–713.

21. Glykos*, N.M. (2006), "Carma : a molecular dynamics analysis program", *J. Comput. Chem.*, **27**, 1765–1768.

20. **Glykos, N.M.**, Papanikolau, Y., Vlassi, M., Kotsifaki, D., Cesareni G. & Kokkinidis, M. (2006), "Loopless Rop: Structure and Dynamics of an Engineered Homotetrameric Variant of the Repressor of Primer Protein", *Biochemistry*, **45**, 10905–10919.

19. Glykos*, N.M. (2005), "Qs v.1.3: a parallel version of Queen of Spades", *J. Appl. Cryst.*, **38**, 574–575.

18. **Glykos, N.M.** & Kokkinidis, M. (2004), "Structural polymorphism of a marginally stable 4-α-helical bundle : Images of a trapped molten globule ?", *Proteins*, **56**, 420–425.

17. Papanikolau, Y., Kotsifaki, D., Fadouloglou, V.E., **Glykos, N.M.,** Cesareni, G. & Kokkinidis, M. (2004), "Ionic strength reducers: an efficient approach to protein purification and crystallization. Application to two Rop variants.", *Acta Cryst.*, D**60**, 1334–1337.

16. Glykos*, N.M. & Kokkinidis, M. (2004), "Molecular Replacement with multiple different models", *J. Appl. Cryst.*, **37**, 159–161.

15. Fadouloglou, V.E., Tampakaki, A.P., **Glykos, N.M.**, Bastaki, N., Hadden, J.M., Phillips, S.E., Panopoulos, N.J. & Kokkinidis, M. (2004), "Structure of $HrcQ_B$-C, a conserved component of the bacterial type III secretion systems", *Proc. Natl. Acad. Sci. USA*, **101**, 70–75.

14. Glykos*, N.M. & Kokkinidis, M. (2003), "Structure determination of a small protein through a 23-dimensional molecular-replacement search", *Acta Cryst.*, D**59**, 709–718.

13. Dennis, C.A., **Glykos, N.M.,** Parsons, M.R. & Phillips, S.E.V. (2002), "The structure of the arginine repressor/activator protein from *Bacillus subtilis*.", *Acta Cryst.*, D**58**, 421–430.

12. Glykos*, N.M. & Kokkinidis, M. (2001), "Multidimensional Molecular Replacement", *Acta Cryst.*, D**57**, 1462–1473.

11. Fadouloglou, V.E., **Glykos, N.M.** & Kokkinidis, M. (2001), "Side-chain conformations in 4-α-helical bundles", *Protein Engng.*, **14**, 321–328.

10. Fadouloglou, V.E., **Glykos*, N.M.** & Kokkinidis, M. (2000), "A fast and inexpensive procedure for drying polyacrylamide gels.", *Anal. Biochem.*, **287**, 185-186.

9. Spyridaki, A., **Glykos, N.M.,** Kotsifaki, D., Fadouloglou, V. & Kokkinidis, M. (2000), "Crystallization and diffraction to ultrahigh resolution (0.8A) of a designed variant of the Rop protein.", *Acta Cryst.*, D**56**, 1015–1016.

8. **Glykos, N.M.** & Kokkinidis, M. (2000), "On the distribution of the bulk solvent correction parameters", *Acta Cryst.*, D**56**, 1070–1072.

7. Glykos*, N.M. & Kokkinidis, M. (2000), "GraphEnt : a maximum entropy program with graphics capabilities", *J. Appl. Cryst.*, **33**, 982–985.

6. Andreeva, A.E., Borissova, B.E., Mironova, R., **Glykos, N.M.,** Kotsifaki, D., Ivanov, I., Krysteva, M. & Kokkinidis, M. (2000), "Crystallization of type I chloramphenicol acetyltransferase : An approach based on the concept of ionic strength reducers", *Acta Cryst.*, D**56**, 101–103.

5. Glykos*, N.M. & Kokkinidis, M. (2000), "A stochastic approach to Molecular Replacement", *Acta Cryst.*, D**56**, 169–174.

4. Glykos*, N.M. (1999), "Pepinsky's Machine : an interactive, graphic-based Fourier synthesis program with applications in teaching and research", *J. Appl. Cryst.*, **32**, 821–823.

3. **Glykos, N.M.** & Kokkinidis, M. (1999), "Meaningful refinement of poly-alanine models using rigid-body simulated annealing : application to the structure determination of the A31P Rop mutant", *Acta Cryst.*, D**55**, 1301-1308.

2. **Glykos, N.M.,** Cesareni, G. & Kokkinidis, M. (1999), "Protein plasticity to the extreme : Changing the topology of a 4-α-helical bundle with a single amino-acid substitution", *Structure*, **7**, 597–603.

1. **Glykos, N.M.,** Holzenburg, A.K.H. & Phillips, S.E.V. (1998), "Low resolution structural characterisation of the Arginine repressor/activator from *Bacillus subtilis* : A combined X-ray crystallographic and electron microscopical approach", *Acta Cryst.*, D**54**, 215–225.

0. **Glykos, N.M.** (1995), "Structural studies of the arginine repressor/activator from *Bacillus subtilis*", PhD thesis, Astbury Department of Biophysics, University of Leeds.

Other publications and textbooks

More than approximately thirty conference abstracts and papers have been published in various conference proceedings and conference-related publications. In some cases (eg. the Erice and the European Crystallographic Association meetings), these have appeared in the form of articles in dedicated volumes.

A free and open access electronic textbook entitled "A non-mathematical introduction to protein crystallography" (in Greek) has been written as part of the 'Kallipos : Hellenic Academic Open Access E-textbooks' project.

Together with Professors Kokkinidis & Hamodrakas, we served as scientific advisors for the translation to Greek of Branden & Tooze's book "Introduction to protein structure".

Publication statistics

As of July 2017, and based on the Google Scholar database, NMG has authored 44 publications in journals of the Science Citation Index of which 42 were research articles, 1 letter, and 1 review. These research articles were cited a total of 898 times, giving an overall h-factor of 14 and an i10-index of 20. Of these 44 papers, NMG serves as the corresponding author for 27, of which five are single-author papers.

Other contributions

Nicholas serves as a reviewer for the following SCI journals : *Acta Crystallographica section D Biological Crystallography, Journal of Applied Crystallography, PLOS One, Nature communications, Journal of Computational Chemistry, Biopolymers, Proteins : Structure, Function, and Bioinformatics, Journal of Molecular Graphics and Modeling, Journal of Physical Chemistry, Journal of Biomolecular Structure and Dynamics, Molecular simulation, International Journal of Peptide Research & Therapeutics, Structural chemistry, International Journal of Molecular Sciences, Computer Methods & Programs in Biomedicine.*

He contributed as a partner in several successful grant applications, including three FP7 grants, amounting collectively to a grant total of ∼1.3 million Euros. He has also been involved in the organisation of several meetings and science events, notably the 2008 "European Researchers' Night in Greece".