RICC Usage Report for Fiscal Year 2011

Project Title:

Methane hydrate under pressure

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Description of the project

Use Performing large-scale molecular dynamics simulations f6r nanosystem (methane hydrates under high pressure) and radiobiological problems (extended biological structures - proteins). The objects of radiation genetics and radiobiology research include the mechanism of the induction of mutations of different nature by ionizing radiation. High-power beams of particle accelerators provide a wide basis for the investigation of the mutagenic effect of ionizing radiation. In some aspects, computer molecular simulation and analysis is an extremely efficient tool for supporting various biophysical and radiobiological experiments. Specially mentioned should be the modern molecular dynamics approach, which is widely applied in today's biophysical, radiobiological, and materials science research. Based on advanced molecular dynamics methods and visualization techniques, we simulate here the behavior of wild-type and mutated proteins in water and ionic solvents at physiological temperatures and conditions. The obtained molecular dynamics (MD) simulation results are discussed in terms of their strong correlation with different diseases of a radiobiological nature. The experimental studies of mutation transitions for protein structures by the traditional X-ray or NMR measurement represent themselves as the extremely difficult, expensive and time consuming task. Using the adequate computational methods (molecular dynamics), based on their efficient implementation in the parallel/vector and special-purpose machines (say, MDGRAPE-2 and 3), would allow ones to simulate the valid behavior of the wild-type and mutated proteins in water or ionic solvents at reliable physiological temperatures and conditions. Thus, the molecular simulation studies between the wild-type and mutant proteins represent themselves as a fundamental problem of great importance. You can omit items not applicable to you.

1.
2. Molecular dynamics method
3. Result: 5 papers published
4. Conclusion: ricc usage should be extended
5. Schedule and prospect for the future: april.2012-april.2013
6. If you wish to extend your account, provide usage situation (how far you have achieved, what calculation you have completed and what is yet to be done) and what you will do specifically in the next usage term: we achieved significant scientific results in 2011; multiple calculations on ricc were completed; yet md simulation to be done on the specified objects and systems; in the next usage term we plan to increase the amount of models and develop new data analysis

Fiscal Year 2011 List of Publications Resulting from the Use of RICC

[Publication]

All cited publications contain the acknowledgement of RIKEN and RICC:

(1) Roman Eremin, Kholmirzo Kholmurodov, Mikhail Avdeev, Viktor Petrenko, Kenji Yasuoka, "Molecular Dynamics Simulation on trans- and cis-Decalins: The Effect of Partial Atomic Charges and Adjustment of "Real Densities"", International Journal of Chemistry, Canadian Center of Science and Education, No. 1, (2012).

(2) Kholmirzo Kholmurodov, "On the Correlation Effects Between the Molecular Mechanisms of Protein Structure Changes and Diseases of a Radiobiological Nature", International Seminar on Radioactivity, Curies and Social Commitments of the Scientists, Invited Talk at The Asiatic Society, Kolkata, India. (2011).

(3) Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, Hagar Khalil, Ahmed Galal, Sameh Ahmed, Nasser Sweilam, Hatem Moharram, "Molecular Dynamics Simulation of the Interaction of Ethanol-Water Mixture with a Pt Surface", Natural Science, www.scirp.org/ns/ (2011).

(4) Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, "MD Simulations of the P53 oncoprotein structure: the effect of the Arg273 → His mutation on the DNA binding domain, Advances in Bioscience and Biotechnology", Volume 2, Number 5, ISSN Print: 2156-8456 ISSN Online: 2156-8502 (2011).

[Proceedings, etc.]

All cited publications contain the acknowledgement of RIKEN and RICC:

(1) Kholmurodov Kh.T. (Editor) MOLECULAR DYNAMICS OF NANOBIOSTRUCTURES, Nova Science Publishers (N.Y.), ISBN: 978-1-61324-320-6 (2011).

(2) Robert A. Selwyne, Kholmirzo T. Kholmurodov, Natalia A. Koltovaya, "Homology Modelling and Molecular Dynamics of Cyclin-Dependent Protein Kinases" by has been published by IT for Real Rorld Problems, (Universities Press Series in Systems, Models, Informatics and Control), Ed. Sree Hari Rao (Ed.), pp. 1-72 (2011).

(3) Kh.T. Kholmurodov, E.A. Krasavin, V.A. Krylov, E.B. Dushanov, V.V. Korenkov, K. Yasuoka, T. Narumi, Y. Ohno, M. Taiji, T. Ebisuzaki, "MD Simulations on the Structure of Onco-Proteins P53: Wild-Type and Radioresistant Mutant Systems", In: "MOLECULAR DYNAMICS OF NANOBIOSTRUCTURES", Nova Science Publishers (N.Y.), ISBN: 978-1-61324-320-6 (2011).

(4) Kh.T. Kholmurodov, T.B. Feldman, M.A. Ostrovsky, "Chromophore Rearrangement in Binding Pocket of Rhodopsin Makes Sense for its Physiological Dark-Adapted State: Computer Molecular Simulation Study" In: "MOLECULAR DYNAMICS OF NANOBIOSTRUCTURES", Nova Science Publishers (N.Y.), ISBN: 978-1-61324-320-6 (2011).

[Oral presentation at an international symposium]

International Seminar on Radioactivity, Curies and Social Commitments of the Scientists, Invited Talk at The Asiatic Society, Kolkata, India, December 21-22 (2011).

[Others]