

Byungkook Lee, Ph.D.

Bibliography (June 2014)

Patents Issued:

1. Pastan, I., **Lee, B.**, Jung, S.-H., and Brinkmann, U.: Recombinant disulfide-stabilized polypeptide fragments having binding specificity. Patent ID: US5747654. Issue date: May 5, 1998.
2. Pastan, I., Benhar, I., Padlan, E. A., Jung, S.-H., and **Lee, B.**: Humanized B3 antibody fragments, fusion proteins, and uses thereof. Patent ID: US5889157. Issue date: March 30, 1999.
3. Pastan, I., **Lee, B.**, Jung, S.-H., and Brinkmann, U.: Recombinant disulfide-stabilized polypeptide fragments having binding specificity. Patent ID: US6147203. Issue date: November 14, 2000.
4. Pastan, I., Benhar, I., Padlan, E., Jung, S.-H. and **Lee, B.**: Methods of inhibiting the growth of cells bearing Lewis Y antigens using B1, B3, or B5 targeted immunoconjugates. Patent ID: US6287562. Issue date: September 11, 2001.
5. Pastan, I., **Lee, B.**, Jung, S.-H., and Brinkmann, U.: Methods of making recombinant disulfide-stabilized polypeptide fragments having binding specificity. Patent ID: US6558672. Issue date: May 6, 2003.
6. Pastan, I., Essand, M., **Lee, B.**, Vasmatzis, G., Wolfgang, C., Brinkmann, U: T-cell receptor gamma. alternate reading frame protein, (TARP) and uses thereof. Patent ID: US7052703. Issue date: May 30, 2006.
7. Pastan, I., Brinkmann, U., Vasmatzis, G., **Lee, B.**: Page-4, an X-linked GAGE-like gene expressed in normal and neoplastic prostate, testis, and uterus, and uses therefor. Patent ID: US7399827. Issue date: July 15, 2008.
8. Pastan, I., Onda, M., Nagata, S., Tsutsumi, Y., Vincent, J., Kreitman, R., Vasmatzis, G., **Lee, B.**: Reduction of the nonspecific animal toxicity of immunotoxins by mutating the framework regions of the Fv to lower the isoelectric point. Patent ID: US7521054. Issue date: April 21, 2009.
9. Ira H. Pastan, Masanori Onda, Satoshi Nagata, David Fitzgerald, Robert Kreitman and **Byungkook Lee**: Mutated Pseudomonas exotoxins with reduced antigenicity. European patent numbers: 10179520.1-2405, 10179539.1-2405. Issue date: 3/12/2010.
10. Pastan, I., Bera, T., **Lee, B.**: Gene Expressed In Prostate Cancer, Methods And Use Thereof. Patent number: US7897355. Issue date: March 1, 2011.

11. Mitchell Ho, Ira Pastan, Osamu Kaneko, **Byungkook Lee**: Blocking mesothelin peptide fragments. Patent number: US8623828. Issue Date: Jan. 7, 2014.

Patents Pending:

1. Pastan, I., Tsutsumi, Y., Onda, M., Nagata, S., **Lee, B.**, Kreitman, R.: PEGylation of linkers improves antitumor activity and reduces toxicity of immunoconjugates. Application ID: US 20040018203. Application number: 10/297337. Publication date: January 29, 2004.
2. Pastan, I., Liu, X.-F., Bera, T. K., **Lee, B.**, Egland, K. A.: *XAGE-1*, a gene expressed in multiple cancers, and uses thereof. Application ID: US20040087772. Application Number: 10/363233. Publication date: May 6, 2004.
3. Pastan, I., Bera, T., Wolfgang, C., **Lee, B.**, Vincent, J.: Gene expressed in prostate cancer and methods of use. Application ID: US20040241702. Application Number: 10/495663. Publication date: December 2, 2004.
4. Pastan, I., Egland, K., **Lee, B.**, Vincent, J.: Gene expressed in breast cancer and methods of use. Application ID: US20050053988. Application Number: 10/913196. Publication date: March 10, 2005.
5. Pastan, I., Olsson, P., Bera, T. K., Essand, M., **Lee, B.**: GHEP, a gene highly expressed in normal and neoplastic prostate, and uses thereof. Application number: 60/239,413. Filing date: 10/10/2001.
6. Tapan K. Bera, Hiroshi Maeda, Curt D. Wolfgang, Dennis Gately, Kandasamy Hariharan, Vasantha Kumar, **Byungkook Lee** and Ira Pastan: NGEP, a novel gene specifically expressed in prostate cancer and normal prostate. Application number: 60/336,308.
7. Ira Pastan, Kristi Egland, James Vincent, **Byungkook Lee** and Robert Strausberg: BASE: a new cancer gene, and methods and uses thereof. Application number: 60/432,531. Filing date: 12/10/2002.
8. Ira H. Pastan, Tapan K. Bera and **Byungkook Lee**: MRP9 and its use in detecting and treating cancer. Application numbers: 60/350,053 and 60/375,121. Filing date: 1/15/2003.
9. Ira H. Pastan, Tapan K. Bera, and **Byungkook Lee**: Antibodies that bind POTE and uses thereof. Application number: 60/546,058. Filing date: 2/17/2005.
10. Ira H. Pastan, Masanori Onda, Satoshi Nagata, David Fitzgerald, Robert Kreitman and **Byungkook Lee**: Mutated *Pseudomonas* exotoxins with reduced antigenicity. Application numbers: 11/997,202, 60/703,798. Filing date: 7/29/2005.
11. Mitchell Ho, Ira Pastan, Osamu Kaneko, Byungkook Lee: Blocking mesothelin peptide fragments. Application number: 13/133,136. Filing date: 6/7/2011.
12. Ira H. Pastan, Ronit Mazur, Masanori Onda, and **Byungkook Lee**: Modified *Pseudomonas* Exotoxin A. Application Number 61/982,051. Filing date: April 21, 2014.

Presentations and activities at scientific meetings in the past 6 years:

2012

May 14 - 16. First Pre-CASP10 meeting, Annapolis, MD.

BL was invited as a CASP10 assessor and reported on his experience in CASP6 and his plan for CASP10 on the New Fold target prediction assessment.

July 13-14. 3DSIG 2012: an ISMB satellite meeting on Structural Bioinformatics and Computational Biophysics, Long Beach, CA.

BL and CHT attended and presented a poster:

Chin-Hsien Tai, Dukka K.C., Byungkook Lee, “Internally symmetric proteins with multiple axes”.

October 21-22. CASP10 Planning meeting, Rome, Italy.

BL and CHT were invited as CASP10 assessor team members.

BL presented four talks:

- (1) “Overview of CASP10 targets”
- (2) “Template-free modeling assessment”
- (3) “CASP Roll assessment”
- (4) “Assessment of Contact-assisted predictions”

CHT presented one talk:

“EvalScore plugin in Chimera for rapid visual inspection of many models.”

December 9-12. CASP10 meeting, Gaeta, Italy.

BL, CHT, and TT were invited as members of CASP10 assessor team.

BL presented four talks and organized and chaired two roundtable discussions.

Talks:

- (1) Domain definition and classification
- (2) Template free modeling assessment in CASP10
- (3) Roll target assessment in CASP10
- (4) Contact-assisted prediction assessment in CASP10

Roundtable discussions organized and chaired:

- (1) FM (template-free modelling) roundtable
- (2) Contact-assisted modeling roundtable

2011

June 28 – July 1. JOBIM 2011, Paris, France.

Jean Garnier attended and presented a paper:

Franck Samson, Richard Shrager, Chin-Hsien Tai, Vichetra Sam, Jean-Francois Gibrat, Peter Munson, Byungkook Lee and Jean Garnier, “DOMIRE, a web server for structural domain identification in proteins”.

July 15-16. 3DSIG 2011: an ISMB satellite meeting on Structural Bioinformatics and Computational Biophysics, Vienna, Austria.

BL, CHT, DKC, and TT attended and presented two posters:

(1) Chin-Hsien Tai, Rohit Paul, Dukka K.C., Jeffery Shilling, Byungkook Lee, “SymD server: a platform for detecting internally symmetric protein structures”.

(2) Dukka B KC, Todd Taylor, & Byungkook Lee, “Slip symmetry- a new type of symmetry in protein structures”.

July 17 – July 19. The 19th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) and the 10th European Conference on Computational Biology (ECCB), Vienna, Austria.

BL, CHT, DKC, and TT attended and presented two posters:

(1) Chin-Hsien Tai, Rohit Paul, Dukka K.C., Jeffery Shilling, Byungkook Lee, “SymD server: a platform for detecting internally symmetric protein structures”.

(2) Dukka B KC, Todd Taylor, & Byungkook Lee, “Slip symmetry- a new type of symmetry in protein structures”.

2010

February 20-24. The 54th Annual Meeting of the Biophysical Society, San Francisco, CA.

Jean Garnier attended and presented a poster on:

Chin-Hsien Tai, Vichetra Sam, Jean-Francois Gibrat, Peter Munson, Byungkook Lee, Jean Garnier, “*Using structure recurrence to define protein domains*”.

July 9-10. 3DSIG 2010: an ISMB satellite meeting on Structural Bioinformatics and Computational Biophysics, Boston, MA.

BL, CHT, DKC, and TT attended and presented two posters:

(1) Changhoon Kim, Jodi Basner & Byungkook Lee, “*Detecting Internally Symmetric Protein Structures*”.

(2) Chin-Hsien Tai, Vichetra Sam, Jean Garnier, Jean-Francois Gibrat, Peter J. Munson, & Byungkook Lee, “*Protein domain assignment from the recurrence of locally similar structures*”.

In addition, BL presented a talk on “*Detecting Internally Symmetric Protein Structures*”.

BL also participated in a panel discussion on “*Epistemology of domains, families, and assemblies: How do we know?*” as one of three panel members.

July 11 – July 13. The 18th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB), Boston, MA.

BL and DKC attended and presented two posters:

(1) Changhoon Kim, Jodi Basner & Byungkook Lee, “*Detecting Internally Symmetric Protein Structures*”.

(2) Chin-Hsien Tai, Vichetra Sam, Jean Garnier, Jean-Francois Gibrat, Peter J. Munson, & Byungkook Lee, “*Protein domain assignment from the recurrence of locally similar structures*”.

2009

January 13-16. The Seventh Asia Pacific Bioinformatics Conference, Beijing, China.

BL chaired a session on “Protein structure, location and function”.

BL presented a paper (#17), a talk, and a poster on:

Chin-Hsien Tai, James J. Vincent, Changhoon Kim, Byungkook Lee, “*SE: An algorithm for deriving sequence alignment from a pair of superimposed structures*”.

May 18-21. 13th Annual International Conference on Research in Computational Molecular Biology (RECOMB), Tucson, AZ.

CK attended and presented a poster on:

Changhoon Kim, Chin-Hsien Tai and Byungkook Lee, “*Iterative refinement of structure-based sequence alignments by Seed Extension*”.

June 27 – July 2. 17th Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) & 8th European Conference on Computational Biology (ECCB), Stockholm, Sweden.

CHT attended and presented a poster on:

Changhoon Kim, Chin-Hsien Tai and Byungkook Lee, “*Iterative refinement of structure-based sequence alignments by Seed Extension*”.

July 14. US - Korea Workshop on Biomedical Sciences, Vienna, VA.

BL presented an invited talk on “*Targeted delivery of anti-cancer agents*”.

July 24-29. The Protein Society annual meeting, Boston, MA.

BL attended.

October 11-15. The 17th Annual Microbial Genomics Conference, Rocky Gap, MD.

BL attended and presented a poster on:

Inbal Yomtovian, Nuttinee Teerakulkittipong, Byungkook Lee, John Moulton and Ron Unger, “*Composition bias and the origin of ORFan genes*”.

November 7. Annual Bioscience and Engineering Symposium (ABES), Bethesda, MD.

BL delivered the Keynote lecture on “*Targeted delivery of anti-cancer agents*”.

2008

February 2-6. 16th International Biophysics Congress (IUPAB) and Biophysical Society 52nd Annual Meeting (USA), Long Beach, California.

JG attended and presented a poster on:

Vichetra Sam, Chin-Hsien Tai, Jean Garnier, Jean-Francois Gibrat, Byungkook Lee, Peter J. Munson, “*Towards an automatic classification of protein structural domains based on structural similarity*”.

July 19-23. 16th International Conference on Intelligent Systems for Molecular Biology (ISMB) and 3DSIG: Structural Bioinformatics & Computational Biophysics Satellite Meeting, Toronto, Canada.

BL and CHT attended and presented 3 posters, first two at the main ISMB meeting and the 3rd at the 3DSIG.

1. Vichetra Sam, Chin-Hsien Tai, Jean Garnier, Jean-Francois Gibrat, Byungkook Lee, Peter J. Munson, “*Towards an automatic classification of protein structural domains based on structural similarity*”.

2. Changhoon Kim and BK Lee, “*Accuracy of structure-based sequence alignments of automatic methods*”.
 3. Chin-Hsien Tai, James J. Vincent, Changhoon Kim and Byungkook Lee, “*SE: An algorithm for deriving sequence alignment from superimposed structures*”.
- BL chaired the 3DSIG session on “Residue level structure prediction”.

October 9-11. 8th KIAS-Yonsei Conference on Protein Structure and Function, Seoul, Korea.
BL attended and presented an invited lecture on “*Assessment and improvement of the accuracy of structure-based sequence alignments*”.

2007

January 3-7. Pacific Symposium on Biocomputing, Wailea, Maui, Hawaii.

CHT attended and presented a poster on:

Chin-Hsien Tai, James J. Vincent, Byungkook Lee, “*SE: A New Algorithm for Deriving Sequence Alignment from Superimposed Structures*”.

July 21-25. 21st Annual Symposium of The Protein Society, Boston, MA.

CK attended and presented a poster on:

Changhoon Kim and BK Lee, “*Accuracy of structure-based sequence alignments of automatic methods*”.

November 30 – December 2. 5th Annual Rocky Mountain Bioinformatics Conference, Aspen/Snowmass, Colorado.

BL attended and presented a talk on:

Changhoon Kim and BK Lee, “*Accuracy of structure-based sequence alignments of automatic methods*”.

BIBLIOGRAPHY

Reviews and Book Chapters

1. Feldmann, R.J., Brooks, B.R., and **Lee, B.**: Understanding protein architecture through simulated unfolding. Research Publication of Division of Computer Research and Technology, National Institutes of Health, Bethesda, Maryland, 1986.
2. **Lee, B.**: Analyzing solvent reorganization and hydrophobicity. In *Methods in Enzymology*. Vol. 259, Chap. 25, 1995, pp. 555-576.
3. Reiter, Y., Brinkmann, U., **Lee, B.**, and Pastan, I.: Engineering antibody Fv fragments for cancer detection and therapy: Disulfide-stabilized Fv fragments. *Nat. Biotechnol* 14: 1239-1245, 1996.
4. **Lee, B.** and Vasmatzis, G.: Stabilization of protein structures. *Curr. Opin. Biotechnol.* 8: 423-428, 1997.
5. Bera, T.K., Eglund, K.A., **Lee, B.**, and Pastan, I.: Identification of novel cancer target antigens utilizing EST and genome sequence databases. In Larochelle, W.J. and Shimkets, R.A. (Eds.): *Oncogenomics Handbook, Cancer Drug Discovery and Development*. Totowa, New Jersey, Humana Press, 2005, pp. 31-42.
6. Tapan K. Bera and **Byungkook Lee**: Mining of Genome Sequence Databases to Identify New Targets for Prostate and Breast Cancer Therapy. In *Genomics: Fundamentals and Applications*, Supratim Choudhuri and David B. Carlson eds., Informa Healthcare USA, Inc., New York, NY, 6:191-205, 2009.

Conference Proceedings

7. Hoard, J.L., Lind, M.D., and **Lee, B.**: Stereochemistry of the ethylenediaminetetraacetato complexes of lanthanum and other rare earth(III) ions. *Proc. Conf. Rare Earth Res.* 4: 403-414, 1965.
8. * Richards, F.M., Wyckoff, H.W., Carlson, W.A., Allewell, N.M., **Lee, B.**, and Mitsui, Y.: Protein structure, ribonuclease-S and nucleotide interactions. *Cold Spring Harbor Symposium Quant. Biol.* 36: 35-43, 1971.
9. ** **Lee, B.**: An anatomy of hydrophobicity. In Eisenfeld, J. and DeLisi, C. (Eds.): *Mathematics and Computers in Biomedical Applications*. North-Holland, Elsevier, 1985, pp. 3-11.
10. * Syi, J.L. and **Lee, B.**: GEMM - an interactive geometry manipulator for molecular modeling. *J. Mol. Graph.* 6: 226-226, 1988.
11. **Lee, B.**: Computer modeling of biological macromolecules. *Proceedings of the International Conference of Korean Scientists and Engineers. 1988 Fall Workshop*: 182-185, 1988.

12. **Lee, B.** and Kang, H.S.: Chorus: A protein tertiary structure prediction program. In Byun, S.M., Lee, S.Y., and Yang, C.H. (Eds.): *Recent Advances in Biochemistry: The Proceedings of 5th FAOB Congress*. 1991, pp. 43-51.
13. Kang, H.S. and **Lee, B.**: Chorus: A protein tertiary structure prediction program. *The Proceedings of the KSEA 20th Anniversary Symposium, Washington, DC*, 1992, pp. 305-309.
14. Suh, E., **Lee, B.**, Narahari, B., Choudhary, A.N., and Martino, R.: Parallel computation of solvent accessible surface area of protein molecules. *Proceeding of the Seventh International Parallel Processing Symposium*, 1993, pp. 685-689.
15. * Kurochkina, N.A., Kang, H.S., and **Lee, B.**: Experiences with dihedral angle space Monte Carlo search for small protein structures. In Doniach, S. (Ed.): *Statistical Mechanics, Protein Structure, and Protein Substrate Interactions*. New York, Plenum. 1994, pp. 147-157.
16. Greenwood, G.W., Shin, J.-M., **Lee, B.**, and Fogel, G.B.: A survey of recent work on evolutionary approaches to the protein folding problem. *Proceedings of the 1999 Congress on Evolutionary Computation*, 1999, pp. 488-495.
17. Chin-Hsien Tai, James J. Vincent, Changhoon Kim, **Byungkook Lee**: SE: An algorithm for deriving sequence alignment from a pair of superimposed structures. *BMC Bioinformatics*, 10 Suppl 1:S4, 2009.

Peer-reviewed Articles

Stars indicate my sense of the degree of importance of an article.

Crystallography and small molecule structures

18. Lind, M.D., **Lee, B.**, and Hoard, J.L.: Structure and bonding in a ten-coordinate lanthanum(III) chelate of ethylenediaminetetraacetic acid. *J. Am. Chem. Soc.* 87: 1611-1612, 1965.
19. *Hoard, J.L., **Lee, B.**, and Lind, M.D.: On the structure-dependent behavior of ethylenediaminetetraacetato complexes of the rare earth Ln³⁺ ions. *J. Am. Chem. Soc.* 87: 1612-1613, 1965.
20. ***Lee, B.**, Burlitch, J.M., and Hoard, J.L.: The crystal and molecular structure of Zn[Co(CO)₄]₂. *J. Am. Chem. Soc.* 89: 6362-6363, 1967.
21. Cella, R.J., **Lee, B.**, and Hughes, R.E.: Lorentz and orientation factors in fiber x-ray diffraction analysis. *Acta Cryst.* A26: 118-124, 1970.
22. **Lee, B.** and Yang, H.J.: Crystallographic studies of L-asparaginase from *P. vulgaris* I. Preliminary crystal data. *J. Biol. Chem.* 248: 7620-7621, 1973.

23. Yang, H.J., **Lee, B.**, and Haslam, J.L.: Studies on histidinol dehydrogenase. Preliminary crystallographic data. *J. Mol. Biol.* 81: 517-519, 1973.
24. **Lee, B.**, Seymour, J.P., and Burgstahler, A.W.: Crystal structure of carbocamphenilone and the visible region Cotton effects of cyclic α -diketones. *Chem. Comm.* 235-236, 1974.
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27. **Lee, B.**, and Henry, G.M.: (-)-3(α)-Trimethylammonium-2(α)-acetoxy-*trans*-decalin iodide. *Acta Cryst.* B32: 938-940, 1976.
28. **Lee, B.** and Ruble, J.R.: A semi-empirical absorption correction technique for symmetrical crystals in single-crystal x-ray crystallography I. *Acta Cryst.* A33: 629-637, 1977.
29. **Lee, B.** and Ruble, J.R.: A semi-empirical absorption correction technique for symmetrical crystals in single-crystal x-ray crystallography II. *Acta Cryst.* A33: 637-641, 1977.
30. Seymour, J.P., **Lee, B.**, and Burgstahler, A.W.: (\pm)-Carbocamphenilone. *Acta Cryst.* B33: 2667-2669, 1977.
31. Jain, N.B., **Lee, B.**, Mertes, K.B., and Pitman, I.H.: Sodium 5,6-dihydro-2-thiouracil-6-sulfonate monohydrate. *Acta Cryst.* B34: 927-930, 1978.
32. Walters, D.E., Grunewald, G.L., Staples, M., Rodgers, J., Ruble, J.R., and **Lee, B.**: (\pm)-9-exo-amino-5,6,7,8-tetrahydro-5,8-methano-9*H*-benzocyclo-hepten-8-ol hydrochloride. *Acta Cryst.* B34: 947-949, 1978.
33. Mitcham, R.V., **Lee, B.**, Mertes, K.B., and Ziolo, R.F.: The nature of triphenylselenonium chloride. Crystal and molecular structure of the monohydrate: $(C_6H_5)_3SeCl \cdot H_2O$. *Inorg. Chem.* 18: 3498-3502, 1979.
34. Sheldon, R.I. and **Lee, B.**: 4-[(4-Chlorophenyl)methyl]-6,7-dihydro-6,6-dimethyl-1*H*-imidazo[1, 2- α]-pyrin-9(4*H*)-one hydrochloride dihydrate, $C_{16}H_{16}ClN_5O \cdot HCl \cdot 2H_2O$. *Cryst. Struct. Comm.* 10: 1087-1092, 1981.
35. Brouillette, C.B., Brouillette, W.J., Grunewald, G.L., Cole, C.L., Ruble, J.R., and **Lee, B.**: 1-Ethoxycarbonyl-3-hydroxy-3-phenyl-2-piperidinone, $C_{13}H_{17}NO_4$. *Cryst. Struct. Comm.* 10: 1239-1243, 1981.
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37. **Lee, B.**, Griffith, J.P., Park, C.H., Sheldon, R.I., McLinden, J., Murdock, A.L., and Amelunxen, R.E.: Preliminary crystallographic data for glyceraldehyde-3-phosphate dehydrogenase from the thermophile *Bacillus coagulans*. *J. Mol. Biol.* 158: 153-156, 1982.
38. Jackman, D.E., Burgstahler, A.W., **Lee, B.**, and Sheldon, R.I.: 3,4-Dihydro-2,4,4,5,7-pentamethylpyrrolo-[1,2- β]-pyridazine, C₁₂H₁₈N₂. *Cryst. Struct. Comm.* 11: 1111-1114, 1982.
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Hydrophobicity and statistical thermodynamics

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57. Graziano, G. and Lee, B.: On the intactness of hydrogen bonds around nonpolar solutes dissolved in water. *J. Phys. Chem. B* 109: 8103-8107, 2005.

Immunotoxin

58. Brinkmann, U., Lee, B., and Pastan, I.: Cytotoxicity of recombinant immunotoxins containing the VH or VL domain of monoclonal antibody B3 fused to *Pseudomonas* exotoxin. *J. Immunol.* 150: 2774-2782, 1993.
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