

Curriculum Vitae

Netaly Khazanov, PhD

Education:

- 2011 – 2016:** Postdoctoral fellowships in Bar-Ilan University, Department of Chemistry, Hanoch Senderowitz Research Group
- 2008 – 2011:** Postdoctoral fellowships in Weizmann Institute of Science, Department of Structural Biology, Koby Levy Research Group
- 2003- 2007:** Ph.D. Theoretical Biochemistry, Department of Chemistry, Bar-Ilan University.
Supervisor: Prof. A. Albeck, Dr. M. Shokhen.
Thesis title: Catalysis and Inhibition Mechanisms in Serine and Cysteine Proteases and their Implication to Drug Design. A Molecular Modeling Approach.
- 2001 – 2003:** M.Sc. Theoretical Biochemistry, Department of Chemistry, Bar-Ilan University. **(with distinction).**
Supervisor: Prof. A. Albeck, Dr. M. Shokhen.
Thesis title: Study of the catalytic mechanism and inhibition of cysteine proteases by molecular modeling.
- 1999- 2001:** B.Sc. Computer Science, Bar-Ilan University.
- 1994 – 1997:** B.Sc. Chemistry, Bar-Ilan University.

Employment:

- 2019 – current:** Lab Manager in Bar-Ilan University, Department of Chemistry, Hanoch Senderowitz Research Group
- 2016 – 2019:** Research Associate in Bar-Ilan University, Department of Chemistry, Hanoch Senderowitz Research Group
- 2001 – 2007:** T.A. in various undergraduate courses and laboratories, Bar-Ilan University
- 1997 – 2000:** Analytical Laboratory, Teva Kfar-Saba.

Awards and fellowships:

- 2005** – The Israel Chemical Society Prize for Excellence in PhD studies.
- 2008-2009** – Council for Higher Education fellowship

Publication

1. Singh Bahia, M.; **Khazanov**, N.; Zhou, Q.; Yang, Z.; Wang, C.; Hong, J.; Rab, A.; Sorscher, E.; Brouillette, C.; Hunt, J.; Senderowitz, H., Stability Prediction for Mutations in the Cytosolic Domains of CFTR, *Journal of Chemical Information and Modeling*, **2021**, 61, 4, 1762.
2. Bar Aluma, B.; , I.; Senderowitz, H.; Cohen-Cymberknob, M.; **Khazanov**, N.; Dagan, A.; Bezael, Y.; Ashkenazi, M.; Keler, S.; Efrati, O. Phenotypic and molecular characteristics of Cystic Fibrosis patients carrying the I1234V mutation, *Respiratory Medicine*, **2020**, 170, 106027.

3. Rippin, I.; **Khazanov**, N.; Ben Joseph, S.; Kudinov, T.; Berent, E.; Arciniegas Ruiz, S.M.; Marciano, D.; Levy, L.; Gruzman, A.; Senderowitz, H.; Eldar-Finkelman, H. Discovery and Design of Novel Small Molecule GSK-3 Inhibitors Targeting the Substrate Binding Site. *Int. J. Mol. Sci.* **2020**, *21*, 8709. <https://doi.org/10.3390/ijms21228709>
4. Joshi, R.; **Khazanov**, N.; Burdman, S.; Carmi, N.; Yedidia, I. Senderowitz, H. Direct Binding of Salicylic Acid to PectobacteriumN-Acyl-Homoserine Lactone Synthase, *ACS Chemical Biology*, **2020**, *15*, 7, 1883–1891
5. Nassir, M.; Pelletier, J.; Arad, U.; Arguin, G.; **Khazanov**, N.; Gendron, F-P.; Sévigny, J. Senderowitz, H.; Fischer, B. Structure-activity relationship study of NPP1 inhibitors based on uracil-N1-(methoxy)ethyl-β-phosphate scaffold, *European Journal of Medicinal Chemistry*, **2019**, <https://doi.org/10.1016/j.ejmech.2019.111754>
6. Getter, T.; Margalit, R.; Zilber, S.; Kahremany, S.; **Khazanov**, N.; Levy, L.; Blum, E.; Tamir, T. Y.; Major, B. M.; Lahav, R.; Senderowitz, H.; Bradfield, P.; Imhof, B.; Alpert, E.; Gruzman, A. Novel inhibitors of leukocyte transendothelial migration. *Bioorganic Chemistry* **2019**, Sep 9;92:103250. doi: 10.1016/j.bioorg.2019.103250.
7. Kakhlon, O.; Ferreira, I.; Solmesky, L.J.; Weil, M.; **Khazanov**, N.; Senderowitz, H.; Lossos, A.; Alvarez, R.; Yetil, D.; Pampou, S.; Escriba, P.; Yue, W.; Akman, H.; Guaiacol as a drug-candidate for treating Adult Polyglucosan Body Disease, **2018**, *JCI Insight*, **2018** 3(17). pii: 99694.
8. Mei-Zahav, M.; Stafler, P.; Senderowitz, H.; Bentur, L.; Livnat, G.; Shtainberg, M.; Orenstein, N.; Bazak, L.; Prais, D.; Levine, H.; Gur, M.; **Khazanov**, N.; Simhaev, L.; Blau, H.; Mussaffi, H. The Q359K/T360K Mutation Causes Cystic Fibrosis in Georgian Jews, *J. Cyst. Fibros.* **2018**, *17*, e41-e45.
9. Wang, C.; Aleksandrov, A.A.; Yang, Z.; Forouhar, F.; Proctor, E.; Kota, P.; An, J.; Kaplan, A.; **Khazanov**, N.; Boël, G.; Stockwell, B.R.; Senderowitz, H.; Dokholyan, N.V.; Riordan, J.R.; Brouillette, C.G.; Hunt, J.F. Thermodynamic correction of F508del-hCFTR by ligand binding to a remote site in the mutated domain, *J. Biol Chem.*, **2018**, Jun 14. pii: jbc.RA117.000819. doi: 10.1074/jbc.RA117.000819.
10. Yang, Z.; Hildebrandt E.; Jiang, F.; Zhou, Q.; An, J.; Xavier, B.M.; Ding, H.; **Khazanov**, N.; Senderowitz, H.; Kappes, J.C.; Brouillette, C.G.; Urbatsch, I.L. Structural stability of purified human CFTR is systematically improved by mutations in nucleotide binding domain 1, *Biochim Biophys Acta*. **2018**, *1860*, 1193-1204.
11. Solmesky, L.J.; **Khazanov**, N.; Senderowitz, H.; Wang, P.; Minassian, B.; Ferreira, I.M.; Yue, W.; Lossos, A.; Weill, M.; Kakhlon, O. A novel image-based high throughput screening assay discovers therapeutic candidates for adult polyglucosan body disease, *Biochemical Journal*, **2017**, *474*, 3403-3420.
12. Hildebrandt, E.; **Khazanov**, N.; Kappes, J.C.; Dai, Q.; Senderowitz, H.; Urbatsch IL. Specific stabilization of CFTR by phosphatidylserine, *Biochim Biophys Acta*. **2017**, *1859*, 289-293.
13. Raj Joshi, J.; **Khazanov**, N.; Senderowitz, H.; Burdman, S.; Lipsky, A.; Yedidia, I. Plant phenolic volatiles inhibit quorum sensing in Pectobacteria and reduce their virulence by potential binding to ExpI and ExpR proteins, *Scientific Reports*, **2016**, *6*, 38126.
14. Cui, G.; **Khazanov**, N.; Stauffer, B.B.; Infield, d.T.; Imhoff, B.R., Senderowitz, H.; McCarty, N.A. Potentiators exert distinct effects on human, murine, and Xenopus CFTR, *Am J Physiol Lung Cell Mol Physiol*. **2016**, *311*, L192-207.

- 15.** Khazanov, N.; Iline-Vul, T.; Noy, E.; Goobes, G.; Senderowitz, H. Design of Cellulose Binding Peptides as Carriers for Catalytic Degradation of Cellulose Inspired by the Cellulose Binding Domain from T. Reesei, *J. Phys. Chem. B.* **2016**, 120, 309-19.
- 16.** M Shokhen; M Hirsch; N Khazanov; R Ozeri, N.; Perlman, T.; Traube; S. Vijayakumar; Albeck.A, From Catalytic Mechanism to Rational Design of Reversible Covalent Inhibitors of Serine and Cysteine Hydrolases. *Israel Journal of Chemistry*, **2014**, 54 (8-9), 1137-1151.
- 17.** Khazanov, N; Marcovitz, A; Levy, Y. Asymmetric DNA-Search Dynamics by Symmetric Dimeric Proteins., *Biochemistry*, **2013**, 52(32), 5335-5344.
- 18.** Khazanov, N.; Levy, Y. Sliding of p53 along DNA can be modulated by its oligomeric state and by cross-talks between its constituent domains. *JMB*, **2011**, 408(2), 335-355.
- 19.** Shokhen, M.; Khazanov, N.; Albeck, A. The mechanism of papain inhibition by peptidyl aldehydes. *Proteins*, **2011**, 79(3), 975-985.
- 20.** Shokhen, M.; Khazanov, N.; Albeck, A Challenging a paradigm: Theoretical calculations of the protonation state of the Cys25-His159 catalytic diad in free papain. *Proteins*, **2009**, 77(4), 916-926.
- 21.** Shokhen, M.; Khazanov, N.; Albeck, A. Screening of the active site from water by the incoming ligand triggers catalysis and inhibition in serine proteases *Proteins*, **2008**, 70(4), 1578-1587.
- 22.** Ozeri, R.; Khazanov, N.; Perlman, N.; Shokhen, M.; Albeck, A. Enzyme Isoselective Inhibitors: A Tool for Binding Trend Analysis. *ChemMedChem*, **2006**, 1, 631-638.
- 23.** Shokhen, M.; Khazanov, N.; Albeck, A. Enzyme Isoselective Inhibition: Application to Drug Design. *ChemMedChem*, **2006**, 1, 639-643.

Poster Presentation:

1. Tel-Aviv, IL, 2004, The 69th meeting of the Israel chemical society
2. Tel-Aviv, IL, 2005, The 70th meeting of the Israel chemical society
3. Zurich, Switzerland, 2009, VIII European Symposium of the Protein Society.
4. Khazanov, N.; Levy. Y. "Sliding of p53 along DNA can be modulated by its oligomeric state and by cross-talks between its constituent domains" IX European Symposium of the Protein Society. **2011**, Stockholm, Sweden
5. Noy, E.; Zhenin, M.; Khazanov, N. Senderowitz, H. "Replica exchange MD simulations of nucleotide binding domains of CFTR", Presented at the NAIS: State-of-the-Art Algorithms for Molecular Dynamics conference, April **2012**, Edinburgh, UK.
6. Khazanov, N; Senderowitz, H. "Stability prediction of nucleotide binding domain 2 of CFTR using MD simulations", Presented at the 2012 NACFC meeting, October **2012**, Orlando, USA.
7. Khazanov, N; Senderowitz, H. "Conformational predictions of NBD2 of CFTR using computational tools", Presented at the 2013 NACFC meeting, October **2013**, Salt Lake City, USA.
8. Khazanov, N.; Noy, E.; Simchaev, L.; Zhenin, M. Senderowitz, H. "Insight into the structure, dynamics and energetics of the ABC transporter CFTR from atomistic simulations", Presented at the Gordon Research Conference on Biopolymers Mechanisms of Biomolecular Interactions: From Physical Principles to Biological Insights, June **2014**, Newport, RI, USA.

9. Cui, G.; **Khazanov**, N.; Senderowitz, H.; McCarty, N. A. "*Comparative molecular pharmacology of CFTR: toward the identification of novel potentiators and their binding sites*", Presented at the Cystic Fibrosis Foundation Research Conference: Pushing the Frontiers, June **2015**, Chantilly, Virginia, USA.
10. Guiying, C.; **Khazanov**, N.; Senderowitz, H.; McCarty, N.A. "*Comparative molecular pharmacology of CFTR. Towards the identification of novel potentiators and their binding sites*", Presented at the 2015 NACFC meeting, October **2015**, Phoenix, USA.
11. Cui, G.; **Khazanov**, N.; Stauffer, B. B.; Infield, D. T. Imhoff, B. R.; Senderowitz, H. McCarty, N. A. "*CFTR potentiators exert different effects on Human, Murine, and Xenopus CFTR*", Presented at the 60th annual meeting of the biophysics society, February **2016**, Los Angeles, USA.
12. Guiying, C.; **Khazanov**, N.; Imhoff, B.R.; Senderowitz, H.; McCarty, N.A. "*Novel potentiators of cystic fibrosis transmembrane conductance regulator identified with pharmacophore modeling and experimental screening*", Presented at the 2016 NACFC meeting, October **2016**, Orlando, USA.
13. Yang, Z.; An, J.; Zhou, Q.; **Khazanov**, N.; Hildebrandt, E.; Dai, Q.; Ding, H.; Macon, K.; He, L.; Riordan, J.R.; DeLucas, L.J.; Kappes, J.C.; Urbatsch, I.L.; Senderowitz, H.; Brouillette, C.G. "*Identification of "supper" thermostabilizing NBD1 mutations for introduction into heterologously expressed human CFTR destined for large scale purification and biophysical characterization*", Presented at the 2016 NACFC meeting, October **2016**, Orlando, USA.
14. Hildebrandt, E.; Kappes, J.C.; Yang, Z.; Zhou, Q.; An, J.; Dai, Q.; Ding, H.; **Khazanov**, N.; Senderowitz, H.; Brouillette, C.G.; Urbatsch, I. L. "*Thermal stabilization of CFTR by specific phospholipids and by mutations in the nucleotide binding domains*", Presented at the 2016 NACFC meeting, October **2016**, Orlando, USA.
15. Yang, Z.; Zhou, Q.; An, J.; Rab, A.; Hong J. S.; **Khazanov**, N.; Senderowitz, H.; Sorscher, E.; Brouillette, C. "*CFTR2 mutations in NBD1: correlation between in vitro thermal instability and severity of folding defect*", Presented at the 2017 NACFC meeting, November **2017**, Indianapolis, USA.
16. Kakhlon, O.; Ferreira, I.; Solmesky, L.J.; Weil, M.; **Khazanov**, N.; Senderowitz, H.; Lossos, A.; Alvarez, R.; Yetil, D.; Pampou, S.; Escriba, P.; Yue, W.; Akman, H. "*Guaiacol can be a drug-candidate for treating Adult Polyglucosan Body Disease*" Presented at the American Academy of Neurology 70th Annual Meeting, April 2018, Los Angeles, CA, USA.
17. Senderowitz, H.; Zhenin, M.; Simhaev, L.; **Khazanov**, N. "*The dynamics of WT and mutant CFTR*" Presented at the 2018 NACFC meeting, October **2018**, Denver, USA.
18. Urbatsch, I.L.; Yang, Z.; Hildebrandt, E.; Jiang, F.; Aleksandrov, A.; **Khazanov**, N.; Riordan, J.R.; Senderowitz, H.; Brouillette, C.; Kappes, J.C. "*Functional stabilization of purified human CFTR by NBD1 mutations and by conformations*" Presented at the 2018 NACFC meeting, October **2018**, Denver, USA.