# Curriculum Vitae



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| Name | **Anwar Rayan** |
| Date of Birth | September 8, 1967 |
| Place of Birth | Haifa |
| Current Position | Head of drug discovery informatics laboratory, QRC-Qasemi Research Center, Al-Qasemi Academic College; Senior researcher at the Institute of Applied Research, The Galilee Society |
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| Internet | http://www.qsm.ac.il/mop/staff/anwar_rayan/site.htm |
| Family status | Married+5 |

Fields of expertise (keywords only): Computational Biology, Structural Biology, Combinatorial Optimization Technologies, Molecular Bioactivity Indexing, Homology Modeling, G-Protein Coupled Receptors (GPCRs), Proteases, Kinases, Loop prediction, Conformational ensembles, Docking, Protein-protein interactions, Protein Design, Drug Design, Algorithms development, bioinformatics and chemoinformatics;drug-likeness, molecular bioactivity indexing, protein mechanism of action studies; anti-cancer drugs; DNA/RNA binders; combinatorial chemistry; multi-component reactions.

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PROFESSIONAL EXPERIENCE
2015- :         Associate Professor of Chemistry,  Al-Qasemi Academic College
2008-2014:    Senior Lecturer, Al-Qasemi College, Bakka El-Garbiyye
2003-2010:    Research associate in the Molecular Modeling and Drug Design Laboratory and the Alex Grass Center for Drug Design and Synthesis, Institute of Drug Research, School of Pharmacy of the Faculty of Medicine, The Hebrew University of Jerusalem, Jerusalem

2001-2002:    Research fellow-School of Pharmacy, Hebrew University of Jerusalem
               "Development of New Algorithms to predict 3D of proteins",
               "ADME/TOX prediction and development of new algorithm for predicting druglikeness in the frame of PHARMALOGICA consortium",
               "Developing new drugs – projects with Pharmaceutical Industries"

2000:          Research associate - FMP, Berlin, Germany "Structure-Based Drug Design" (I worked on projects for the pharmaceutical industry)
9-10/1999:    guest scientist – University of Duesseldorf, School of pharmacy, Prof. Dr. Hans-Dieter Höltje group

1998-1999:    Postdoctoral fellow- School of Pharmacy, Hebrew University of Jerusalem "Structure - Function Relationships of the GPCRs"

9/1999-11/1999:    Research guest, Pharmaceutical Department, University of Duesseldorf, Duesseldorf, Germany

1989-1995:    Ph.D. candidate in Pharmaceutical Chemistry, Hebrew University of Jerusalem, Advisor: Prof. A. Goldblum
Thesis title:    "Computerized models for the mechanism of HIV-1 protease as a basis for the design of novel inhibitors"

1986-1988:    B.Sc. in chemistry, Hebrew University of Jerusalem (degree awarded with distinction)


Involvement in important projects connected to the industry (only the name and year of the project):


2011-:         Pepticom LTD (Innovative computational drug discovery company); co-founder
2010-:         Sensetrade LTD (Stock market algo-trading); co-founder and director
2010-:         IDD Therapeutics (novel anti-cancer drugs); founder and director
2009-:         Genearrest LTD (Silencing genes through molecules acting on dsDNA); co-founder
2008-2009:    MedWell Laboratories LTD (anti-inflammation drugs, COX-2 inhibitors)
2007-2009:    Antigene Biotechnologies (DNA/RNA binders)
2000:          design of novel inhibitors (FMP institute, Berlin, Germany – project for the Schering)
2001-2002:    DAAT consortium (development of novel tools in bioinformatics era)
2002:          Project for TEVA ltd
2003-2004:    Pharmalogica consortium (development of novel tools in chemoinformatics era)
2005:          NOFAR (project financed by the industry and trade ministry and aims to commercialize tools for drug and molecular bioactivity indexing)

**Supports and prizes:**

2015,          Leaders organization, PATENT first prize (20,000 euro).

2015,          MOFET, "How integrating chemical drawing and modeling tools in teaching affect college-students' understanding of chemistry" (18,400 NIS).

2013-2014,   The Israeli Industry and Commerce Ministry (330,000 $).

             Development of novel anticancer drug. [IDD Therapeutics, Initiator: Anwar Rayan]). www.idd-therapeutics.com

2013-2014,   Qasemi Research Foundation, Al-Qasemi Academic College, "How integrating modeling tools in teaching affect college-students' understanding of chemistry" (4,000 $).

2013-2014,   EUREKA project in collaboration with BIOSEKA company (Lithuania); "PNA applications for inhibition of streptococci biofilms" (320,000 euro in total for both partners).

2012-2014,   PATENT project (38,500 Euro) "isolation and identification of natural chemicals influencing hH4R" (in collaboration with The Regional R.&D. Center, The Galilee Society).

2010-2012,   The Israeli Industry, Commerce and employment Ministry (600,000 $).

             Development of new anticancer drug: IDD1010, bi-functional drug. [IDD Therapeutics, Initiator: Anwar Rayan].www.idd-therapeutics.com

2009-2010,   Nofar project "in-silico design of targeted" (110,000 $).

2009-2013,   The Israeli Industry, Commerce and employment Ministry (980,000 $)-

             novel technology for silencing genes by small molecules. [GeneArrest, Initiators: Anwar Rayan and Mizied Falah].www.genearrest.com

2007-2008,   Tnufa, ministry of industry (novel DNA binders) (80,000 $).

2008-2013,   Projects for the Industry (90,000 $).

2001-2009,   Chief scientist of several projects in molecular modeling group headed by Prof. Amiram Goldblum (School of Pharmacy, The Hebrew University of Jerusalem). 1- The part of chemoinformatics in The Israeli Consortium of Pharmalogica 2- Nofar project "Indexing molecules by their drug likeness" 3- Hadaseet project "discovery of novel AChE inhibitors by ISE" 4- the part of chemoinformatics in the CancerGrid FP6 project, LSH-2005-2.2.0-8 Small-ligand libraries: improved tools for exploration and prospective anti-tumor therapy.

2001,          Accelrys Award for the annual international meeting of the molecular graphics and modeling society, Erlangen, Germany, september 16th-21st 2001.

1999,          Boehringer Ingelheim Award for short-term visits (University of Duesseldorf, School of pharmacy, Prof. Dr. Hans-Dieter Höltje group, Sep-Oct 1999).

1998-1999,   Postdoctoral Scholarship, Ministry of Science, Israel.

1989-1995,   monthly Scholarship, The Hebrew University of Jerusalem.

1987,          Dean prize for distinction, The Hebrew University of Jerusalem.


**Teaching Activities**

2008-:         Al-Qasemi Academic College. (Courses: 1- "Instrumental chemistry", 2- "science and technology", 3- "Natural products – limited resources", 4- "Chemistry – technological applications"). Supervising 8 final projects of students (subjects: Shelf-life of taxol and docetaxel, bio-active fractions from plants, synthesis of new chemicals by Ugi reaction

(combinatorial chemistry) (co-advisor Mr. Hafiz Mawassi), solid phase synthesis of PNA analogues (co-advisor Mrs. Siba Shadafny), Quality of rural dairy products (Alham Raiyn, West Galillee College).

2009-:        Writing courses programs: 1- general chemistry and analytical 2- introduction to bioinformatics 3- introduction to chemistry lab 4- computerized models in biotechnology 5- programming and bioinformatics applications. Those courses are part of the B.Sc. in biotechnology program to be open in Al-Qasemi college.

2001-2015:    associate supervisor of more than 10 research projects for B.Sc. students, M.Sc. and Ph.D. students at the modeling group, medicinal chemistry department, Hebrew University of Jerusalem. (Dr. Mier Glick (PhD.) [development of novel optimization technique - ISE], Dr. Efrat Noy (PhD.) [protein-protein interaction], Dr. Andrea Scaiewitz (PhD.) [design of bioactive chemicals from scaffolds by ISE], Dr. David Marcus (PhD.) [applications of ISE in chemoinformatics], Mr. Amit Michaeli(PhD.) [peptide-protein interactions], Mr. Beni Daadosh (MSc.) [modeling of ADAMTS13 and design of novel inhibitors], Mrs. Sarah Schneeberger (MSc.) [TACE inhibitors], Mrs. Gloria Boursheh (MSc.) [design of novel inhibitors for beta and gamma secretase], Mr. Nir Shachaf (MSc.) [Ret kinase inhibitors], Mr. Ido Ben-Shalom (MSc.) [in-silico screening for novel HSP90 inhibitors], Mr. Hafiz Mawasi (BSc.) [Ret kinase inhibitors]). Associate supervisor of Mrs. Chiara Platania (MSc.) from the group of Prof. Salvatore Guccione (University of Catania, Italy). Supervisor of Ms. Seba Shdafne (Identification of anticancer drug candidates from natural resources).

2002-2003:    General chemistry course, The Open University.

1990-1995:    Organic chemistry laboratory for pharmacists, course of 6 points,School of Pharmacy, the Hebrew University of Jerusalem.


## Other Scientific Activities

Management Committee member of European Cooperation in Science and Technology (COST)Action BM0806 "Recent advances in histamine receptor H4R research". 2009-2013.http://w3.cost.esf.org/index.php?id=213&action_number=BM0806

Management Committee member of European Cooperation in Science and Technology (COST) Action BM1204 "An integrated European platform for pancreas cancer research: from basic science to clinical and public health interventions for a rare disease". 2012-2016. http://www.cost.eu/domains_actions/bmbs/Actions/BM1204

Management Committee member of European Cooperation in Science and Technology (COST) Action TD1204 "Modelling Nanomaterial Toxicity (MODENA)". 2012-2016. http://www.cost.eu/domains_actions/mpns/Actions/TD1204

Management Committee member of European Cooperation in Science and Technology (COST) Action BM1207"Networking towards clinical application of antisense-mediated exon skipping". 2013-2017. http://www.cost.eu/domains_actions/bmbs/Actions/BM1207

Management Committee member of European Cooperation in Science and Technology (COST) Action CM1207 "GLISTEN: GPCR-Ligand Interactions, Structures, and Transmembrane Signalling: a European Research Network". 2013-2017. http://www.cost.eu/domains_actions/cmst/Actions/CM1207

Management Committee member of The Institute of Applied Research – The Galilee Society.


## Editorial Member and Advisory Function, Reviewer

Editor-in-chief "International Journal of Computational Bioinformatics and In Silico Modeling"
http://bioinfo.aizeonpublishers.net//

Editorial advisory board member of:

         The Open Nutraceuticals Journal "tonutraj",

Steering Committee member of Qasemi Research Center (QRC).

Invited as reviewer forEuropean Journal of Medicinal Chemistry (EJMECH), Journal of Molecular Modeling (JMM), The Open Nutraceuticals Journal (TONUTRAJ), Future Medicinal Chemistry, Interdisciplinary Sciences- Computational Life Sciences, and others.

## Collaboration in Research

- Prof. Amiram Goldblum, Molecular Modeling and Drug Design Lab and the Alex Grass Center for Drug Design and Synthesis, Institute of Drug Research, The Hebrew University of Jerusalem 91120.
- Prof. Abd Al-Roof Higazi , head of Department of Clinical Biochemistry, HebrewUniversity – Hadassah Medical Center, Jerusalem.
- Prof. Holger Stark, Chemie Institut Pharmazeutische, Goethe-Universitaet Johann Wolfgang, Frankfurt am Main 60438, Germany.
- Prof. Salvatore Guccione, Department of Chemical Sciences- University of Catania- V.le A. Doria 6, I-95125 Catania, Italy.
- Prof. Samir Droby, Volcani Center, Bet Dagan 50-250.
- Dr. Ahmed Nasser, Institute of Soils, Water and Environmental Sciences, ARO, Volcani Center, Bet Dagan 50-250.
- Collaborations with Prof. Mohamed Zidan, Prof. Bashar Saad, Dr. Mahmoud Massalha and Dr. Hilal Zaid from QRC – Qasemi Research Center, Al-Qasemi College.
- RAND Biotechnologies LTD.
- GeneArrest LTD.
- IDD Therapeutics LTD.

## Other Activities (educational and social)

1991-1996: Board Member in "ALTAWEYA" association for deepening the consciousness and education, Kabul.

1994: Environmental planning internship program, Geography department, The Hebrew University of Jerusalem

1995: Office manager in 1995 Census of Population and Housing (nine localities in Nazareth distinct)

1996: The head of Environmental Education, Environment Unit "Shaar Hagaleel"

1996-1997:  Aukad company LTD, Founder and General Manager.

1996-1997: Training course for teachers (56 hours) under the title "selected environmental issues"

1997: The author of "Activities notebook, Environmental issues - Rural quality". Produced by The Future Association for health and environmental education and published by Aukad company LTD. The book and the video film "Rural Environment" were recommended by the ministry of education to be part of the environmental education program in elementary schools.

1997: Producer and scientific consultant of video film "Rural Environment". The film is in Arabic and English.

1998: The author of "bad habit called smoking".Produced by The Future Association for health and environmental education and published by Aukad company LTD. The book was authorized by the ministry of education to be used by schools teachers for promotion of health education among teenagers.

1998: Translating to Arabic language the video film "The Killer Image" produced by Farmafilms for the national association of South Africa in conjunction with the department of health, Welfare, Pensions. Written permission was received from the Embassy of South Africa, Tel-Aviv.

1995-1999: dozens of lectures for teachers in training school. Most of these talks focused in health and environmental education.

2002-2003: Advisory board member of "Al-Burhan" magazine, produced and published by "Al-Kalam academic association", Nazareth.

1997-2011: The Future Association for health and environmental education, head of board of directors.

2007-2009: director of Antigene Biotechnologies ltd.

2010-: director and founder in Sensotrade ltd.

2010-: director and founder in IDD Therapeutics.

2009-2010: CSO of GeneArrest ltd.

2010-2012: CEO of GeneArrest ltd.

2015-: CSO of IDD Therapeutics.


**Selected interviews with the media**


- "New Drug Discovery Platform Targeting Specific Gene Expression" Video Interview at BioInvest Israel 2012

http://stocknewsnow.com/dr-anwar-rayan-ceo-genearrest-new-drug-discovery-platform-targeting-specific-gene-expression-video-interview-at-bioinvest-israel-2012/


- BioIsrael.com, Volume VIII Issue 4: "GeneArrest Silences Mutated DNA Sequences With Third Generation Drug Technology"

http://www.genearrest.com/index.php?&tPath=210&itemID=5


**Selected papers from the list of publications in peer reviewed journals**

- Matteo Pappalardo, NirShachaf, Livia Basile, Danilo Milardi, Mouhammed Zeidan, Jamal Raiyn, Salvatore Guccione and **Anwar Rayan**. (2014).Sequential application of ligand and structure based modeling approaches to index chemicals for their $hH_4R$ Antagonism. PLoS ONE 9(10): e109340. doi:10.1371/journal.pone.0109340. **(Thompson Impact Factor = 3.53)**

- **Anwar Rayan**, Mizied Falah, Jamal Raiyn, Beny Da'adoosh, Sleman Kadan, Hilal Zaid and Amiram Goldblum. "Implication of ISE for indexing molecules for their hERG liability". European Journal of Medicinal Chemistry. 65: 304-314, (2013). **(Thompson Impact Factor = 3.43; citations = 4)**

- Hilal Zaid, Siba Ismael, Amit Michaeli and **Anwar Rayan**. "Computerized modeling techniques predict the 3D structure of H4 receptor: facts and fiction", Frontiers in Bioscience. 17, 1: 232-247, (2012). **(Thompson Impact Factor = 3.29; citations = 2)**

- Oleg Ursu, **Anwar Rayan**, Amiram Goldblum, Tudor I. Oprea. "Understanding drug-likeness". WIREs Computational Molecular Science. Volume 1, Issue 5, 760–781 (2011). **(Thompson Impact Factor = 11.885; Citations = 32)**

Curriculum Vitae

- **Anwar Rayan**, David Marcus and Amiram Goldblum. "Predicting Oral Drug-likeness by Iterative Stochastic Elimination". J Chem Inf Model. 22; 50(3): 437-45 (2010).`(Thompson Impact Factor = 4.30; citations = 11)`
- Rami Abu Fanne, Taher Nassar, Sergey Yarovoi, **Anwar Rayan**, Itschak Lamensdorf, Michael Karakoveski, Polianski Vadim, Mahmud Jamal, Douglas B. Cines and Abd Al-Roof Higazi. "Blood brain barrier permeability and tPA-mediated neurotoxicity". Neuropharmacology, 58(7): 972-80 (2010). `(Thompson Impact Factor = 4.11; citations = 35)`
- **Anwar Rayan**, "New vistas in  GPCR 3D structure prediction", J Mol Model, 16(2): 183-191 (2010). `(Thompson Impact Factor = 1.98; citations =17)`
- **A. Rayan**, E. Noy, D. Chema, A. Levitzki and A. Goldblum, Stochastic algorithm for kinase homology model construction, Current Medicinal Chemistry, 11, 675-692 (2004)**. (Thompson Impact Factor = 3.715; citations = 17)**
- **Anwar Rayan**, Hanoch Senderowitz and Amiram Goldblum, Exploring the conformational space of cyclic peptides by a stochastic search method, JOURNAL OF MOLECULAR GRAPHICS & MODELLING, 22, 319-333 (2004)**. (Thompson Impact Factor = 2.006; citations = 24)**
- Meir Glick, **Anwar Rayan** and Amiram Goldblum "A Novel Stochastic Algorithm for Global Optimization and Best Populations: A Test Case of Side Chains in Proteins", **PNAS**, 99:703-8 (2002)**. (Thompson Impact Factor = 9.809; citations = 37)**


**Publications (in peer reviewed journals)**

1. Hilal Zaid, Jamal Raiyn, Midhat Osman, Mizied Falah, Samer Srouji, and **Anwar Rayan** (2016). in-silico modeling techniques for predicting tertiary structure of human $H_4$ receptor. Frontiers in Bioscience (Landmark Ed). 21: 597-619. **(Thompson Impact Factor = 3.52)**
2. Amit Michaeli and **Anwar Rayan** (2016). Modeling ensample of loop conformations by Iterative Stochastic Elimination, Letters in Drug Design and Discovery. 13(): **in press (Thompson Impact Factor = 0.77)**.
3. Mizied Falah, **Anwar Rayan**, and Samer Srouji. (2015). Storage effect on viability and biofunctionality of human adipose tissue-derived stromal cells. Cytotherapy. 17(9): 1220-1229. **(Thompson Impact Factor = 3.293)**
4. **Anwar Rayan**. (2015). Approaches to index chemicals for their hH$_4$R antagonism. In *Inflammation Research*, vol. 64, Suppl 1: 27-28. **(Thompson Impact Factor = 2.347)**
5. Jamal Raiyn, Seba Shdafny, and **Anwar Rayan**. (2015). Natural likeness of chemicals and drug development. In *Inflammation Research*, vol. 64, Suppl 1: 42-43. **(Thompson Impact Factor = 2.347)**
6. Jamal Raiyn, and **Anwar Rayan**. (2015). How Chemicals' Drawing and Modeling Improve Chemistry Teaching in Colleges of Education. World Journal of Chemical Education 3, 1: 1-4. doi: 10.12691/wjce-3-1-1.
7. Matteo Pappalardo, Nir Shachaf, Livia Basile, Danilo Milardi, Mouhammed Zeidan, Jamal Raiyn, Salvatore Guccione and **AnwarRayan**. (2014). Sequential application of ligand and structure based modeling approaches to index chemicals for their hH$_4$R Antagonism. PLoS ONE 9(10): e109340. doi:10.1371/journal.pone.0109340. **(Thompson Impact Factor = 3.234)**

8. **Anwar Rayan**, Mizied Falah, Jamal Raiyn, Beny Da'adoosh, Sleman Kadan, Hilal Zaid and Amiram Goldblum. "Implication of ISE for indexing molecules for their hERG liability". European Journal of Medicinal Chemistry. 65: 304-314, (2013).

9. **Anwar Rayan**. "Glimpse into GPCRs: a 'hot topic' for both academia and industry". International Journal of Computational Bioinformatics and In Silico Modeling 2, 4: 138-140, (2013).

10. Sleman Kadan, Mahmoud Rayan and **Anwar Rayan**. " Anticancer activity of Anise (Pimpinella anisum L.) seed extract", The Open Nutraceuticals Journal. 6: 1-5, (2013).

11. Or Kakhlon, Hava Glickstein, Naomi Feinstein, Hasan Orhan Akman, Salvatore DiMauro, Amit Michaeli, **Anwar Rayan**, Tamar R. Grossman, Leonardo Solmesky, Miguel Weil, Dima Kozakov, Alexander Lossos, "Searching for efficient therapeutic avenues to treat Adult Polyglucosan Body Disease (APBD) and Lafora Disease (LD) using a High-Throughput Screening platform." In *HUMAN GENE THERAPY*, vol. 24, no. 3, pp. A10-A11. (2013).

12. Hilal Zaid, Siba Ismael, Amit Michaeli and **Anwar Rayan**. "Computerized modeling techniques predict the 3D structure of H4 receptor: facts and fiction", Frontiers in Bioscience. 17, 1: 232-247, (2012).

13. Jamal Raiyn, Mohammed Azab, Mahmud Masalha and **Anwar Rayan**. "Tips for loop prediction and conformational search". Journal of Bioinformatics & Research. 1, 4: 41-45, (2012).

14. Falah, M., M. Azab, S. Shdafnay, A. Michaeli, and **A. Rayan**. "Silencing human H4R gene by novel triplex-forming molecule." In *Inflammation Research*, vol. 61, pp. S52-S53, (2012).

15. Oleg Ursu, **Anwar Rayan**, Amiram Goldblum, TudorI. Oprea. "Understanding drug-likeness". WIREs Computational Molecular Science. Volume 1, Issue 5, 760–781 (Sep/Oct 2011).

16. **Anwar Rayan**, David Marcus and Amiram Goldblum. "Predicting Oral Drug-likeness by Iterative Stochastic Elimination". J Chem Inf Model. 22; 50(3): 437-45 (2010).

17. Rami Abu Fanne, Taher Nassar, Sergey Yarovoi, **Anwar Rayan**, Itschak Lamensdorf, Michael Karakoveski, Polianski Vadim, Mahmud Jamal, Douglas B. Cines and Abd Al-Roof Higazi. "Blood brain barrier permeability and tPA-mediated neurotoxicity". Neuropharmacology, 58(7): 972-80 (2010).

18. **Anwar Rayan**, "New vistas in  GPCR 3D structure prediction", J Mol Model, 16(2): 183-191 (2010).

19. **Anwar Rayan**, Mizied Falah, Hafiz Mawasi and Nur-Eldin Raiyn. "Assessing drugs for their cardio-toxicity". Letters in Drug Design & Discovery 7(6):409-414 (2010).

20. Hilal Zaid, Jamal Raiyn, Ahmed Nasser, Bashar Saad and **Anwar Rayan** (2010). "Physicochemical Properties of Natural Based Products versus Synthetic Chemicals". The Open Nutraceuticals Journal, 3: 194-202 (2010).

21. Hilal Zaid, **Anwar Rayan,** Omar Said and Bashar Saad (2010). "Cancer Treatment by Greco-Arab and Islamic herbal medicine". The Open Nutraceuticals Journal, 3: 203-212 (2010).

22. **Anwar Rayan**, "The utility of Intelligent Learning Engine in Drug Discovery Informatics", Proceedings of the British Pharmacological Society, 7(4): 26 (2010).

23. Guccione, Salvatore, Chiara Platania, Nir Shachaf, Danilo Milardi, Matteo Pappalardo, and **Anwar Rayan**. "Is it possible to increase hit rates in virtual screening by multiple focusing? Indexing chemicals for their H4R antagonism." In *INFLAMMATION RESEARCH*, vol. 59, pp. S351-S352. (2010).

24. **Rayan, Anwar**. "Indexing drugs for their cardio-toxicity." In *INFLAMMATION RESEARCH*, vol. 59, pp. S357-S358. (2010).

25. Mizied Falah, Taher Nassar and **Anwar Rayan**, "A Simple Approach for Discriminating 'Cardio-safe' drugs from Non-safe ones". Bioinformation 3(9), 389-393 (2009).

26. **Anwar Rayan**, "New Tips for Structure Prediction by Comparative Modelling", Bioinformation, 3(6), 263-267 (2009)

27. **Anwar Rayan**, Mohamed Hegaze and Jamal Raiyn, "How Much Bovine Rhodopsin Crystal Structure is Useful for Modeling Human GPCRs? B2-Adrenergic Receptor as a Test Case", Proceedings of biosignals 2009, 291-298 (2009).

28. Jamal Raiyn and **Anwar Rayan**, "How Much Sequence Identity Guarantee Good Models in Homology Modeling: Proteins from Serine Protease Family as a Test Case", Proceedings of biosignals 2009, 455-458 (2009).

29. Marcus David, **Anwar Rayan**, Dinorah Barasch, Maayan Elias, and Amiram Goldblum. "CINF 67-Learning from failures: Discontinued compounds as a source for knowledge in drug discovery." In *ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY*, vol. 236. (2008).

30. **Rayan, Anwar**, David Marcus, Ohad Givaty, Dinorah Barasch, and Amiram Goldblum. "Double focusing by molecular bioactivity and drug likeness." In *ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY*, vol. 230, pp. U1013-U1013. (2005).

31. **A. Rayan**, E. Noy, D. Chema, A. Levitzki and A. Goldblum, Stochastic algorithm for kinase homology model construction, Current Medicinal Chemistry, 11, 675-692 (2004).

32. **Anwar Rayan**, Hanoch Senderowitz and Amiram Goldblum, Exploring the conformational space of cyclic peptides by a stochastic search method, JOURNAL OF MOLECULAR GRAPHICS & MODELLING, 22, 319-333 (2004)

33. **Anwar Rayan**, Andrea Scaiewitz, Inbal Geva-Dotan, Dinorah Barasch, Amiram Goldblum, Screening Molecules for their Drug Like Index. EuroQSAR 2004 Proceedings, pp. 197-200 (2004)

34. **Anwar Rayan**, Andrea Scaiewitz, Inbal Geva-Dotan, Dinorah Barasch, Amiram Goldblum, Distinguishing between Databases using Iterative Stochastic Elimination – A Novel Approach to Discriminate between Drugs and Non-drugs. EuroQSAR 2004 Proceedings, pp. 555-556 (2004)

35. **Rayan, A**., Scaiewicz, A., Geva-Dotan, I., Barasch, D. & Goldblum, A., Screening molecules for their drug-like index. Abstracts of Papers of the American Chemical Society, 228, U358-U358 (2004).

36. **Rayan, A**., Barasch, D., Brinker, G., Cycowitz, A., Geva-Dotan, I., Scaiewicz, A. & Goldblum, A. New stochastic algorithm to determine drug-likeness. Abstracts of Papers of the American Chemical Society, 226, pp. U297-U297 (2003).

37. Noy, E., Gorelik, B., **Rayan, A.** and Goldblum, A. Stochastic path to form ensembles and to quantify flexibility in proteins. Abstracts of Papers of the American Chemical Society, 225, pp. U781-U781 (2003).

38. Meir Glick, **Anwar Rayan** and Amiram Goldblum "A Novel Stochastic Algorithm for Global Optimization and Best Populations: A Test Case of Side Chains in Proteins", **PNAS**, 99:703-8 (2002)

39. Cherno-Schwartz, S., **Rayan, A.** and Goldblum, A. Novel measures of variability in multiple alignments as a basis for modeling 3D structures of G-protein coupled receptors. Abstracts of Papers of the American Chemical Society, 223, pp. U503-U503 (2002).

40. Goldblum, A., Glick, M., **Rayan, A.,** Gorelik, B. and Brinker, G. A novel stochastic search method finds global minima and low-energy populations. Abstracts of Papers of the American Chemical Society 223, U499-U500 (2002).

41. **Rayan-A**, Siew-N, Cheno-Schwartzs-S, Matzner-Y, Bautsch-W and Goldblum-A, "A Novel Computational Method for Predicting the Transmembranal structure of G-Protein Coupled Receptors: Application to C5aR and C3aR", Receptors Channels; 7(2):121-37 (2000).

42. Siew N., **Rayan A**., Bautsch W., Matzner Y. and Goldblum-A, "A Novel Computational Method for Predicting the transmembranal structure of G-Protein Coupled Receptors", Molecular Modeling and Prediction of Bioactivity, pp. 440-441 (2000).

43. Amiram Goldblum, Meir Glick and **Anwar Rayan** "Extending Crystallographic Information with Semiempirical Quantum Mechanics and Molecular Mechanics: "A Case of Aspartic Proteinases" J. Chem. Inform. Comp. Sci. 33(2): 270-274 (1993).

44. Amiram Goldblum, Meir Glick and **Anwar Rayan**, "Determining Proton Positions in an Enzyme-Inhibitor Complex is a First Step for Theoretical Mechanistic Studies of Aspartic Proteinases", Theor. Chim. Acta, 85: 231-247 (1993).

45. **Anwar Rayan**, Amit Fliess, Moshe Kotler, Michael Chorev and Amiram Goldblum, "Modeling of Inhibitors for HIV-1 Proreinase" Trends in Medicinal Chemistry '90" 65-71 (Eds. S. Sarel, R. Mechoulam and I Agranat), Blackwell Scientific Publications (1992).

46. **Anwar Rayan**, Amit Fliess, Moshe Kotler, Michael Chorev and Amiram Goldblum, "Theoretical Models of Aspartic Proteases: Active Site Properties, Dimer Stability and Interactions with Model Inhibitors" Adv. Exp. Med. Biol. 306: 555-8 (1991).

**Editorials**

47. **Anwar Rayan**. Editorial. International Journal of Computational Bioinformatics and In Silico Modeling 2(2): 102-103 (2013).
48. **Anwar Rayan**. "Integrating Modeling and In Silico Techniques in Chemistry Teaching". International Journal of Computational Bioinformatics and In Silico Modeling 3(1): 302-303 (2014).

## Submitted manuscripts &in preparation manuscripts
.

49. W. Barriah, B. A. Farkh, M. Rayan, A. Nasser, **Anwar Rayan** (2016). Cytotoxic Activity of *Cuscuta palaestina*, <u>The Open Nutraceuticals Journal</u>. Submitted.
50. Amit Michaeli, **Anwar Rayan** and Amiram Goldblum (2016). From Finance to Chemistry: Risks and return in Protein Interface Design". In preparation**.**
51. **Anwar Rayan** (2016). "Indexing molecules for their Natural Product Likeness". In preparation.
52. Jamal Raiyn and **Anwar Rayan** (2016). "Intelligent Learning Engine – novel optimization technique. Classification of proteins as a test case". In preparation.
53. David Marcus, **Anwar Rayan** and Amiram Goldblum (2016). "Molecular Bioactivity Indexing of molecules: new technique for accelerating drug discovery process". In preparation.

## Patents

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## Selected Abstracts:
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determined structural conserved common motifs", Convegno Congiunto SCICASI, Catanzaro 3-4 December 2015.

66. J. Raiyn, S. Shadafny, Anwar Rayan. "Natural products' databases as a preferred source for drug development", European Histamine Research Society 44th Annual Meeting, Malaga, Spain, May 6th-9th, 2015. (oral presentation).

67. Anwar Rayan, "Sequential application of ligand & structure based modelling approaches to index chemicals for their bioactivity: hH$_4$R antagonism as a test case", European Histamine Research Society 44th Annual Meeting, Malaga, Spain, May 6th-9th, 2015. (oral presentation).

68. **Anwar Rayan**, "Utility of ISE & ILE in drug discovery",MODENA COST Action meeting under the title"Nanosafety forum for young scientists", Siracusa, Italy, October 10th -11th, 2014.

69. **Anwar Rayan**, "Computerized techniques for drug discovery", School of Pharmacy, University of Catania, Catania, Italy (invited by Prof. Salvatore Guccione), February 9th, 2014.

70. **Anwar Rayan**, "Indexing Chemicals for their Bioactivity on GPCRs by Ligand-Structural Combined Approach", TM's 3rd World Molecular & Cell Biology Online Conference, (invited speaker and chairing Session 9: GPCR structure and function), 25th-28th Feb 2014.

71. Anwar Rayan, "Aspects on delivery of PNA based oligonucleotides**,**Workshop on Delivery for COST Action BM1207, September 25-26, 2013, Leiden, Netherlands.

72. Azmi Adawi, Sleman Kaadan, Holger Stark and **Anwar Rayan**, "Natural chemicals influencing the hH$_4$R", COST BM0806 Final Conference, March 21-23, 2013, Athens, Greece.

73. Matteo Pappalardo, Danilo Milardi, **Anwar Rayan**, Nir Shachaf, Livia Basile, Salvatore Guccione, "Compounds Repositioning to H4 Antagonists Combining *in-silico* Approaches", COST BM0806 Final Conference, March 21-23, 2013, Athens, Greece.

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76. **Anwar Rayan**, "GeneArrest novel technology pave the way for the next generation of drugs", The 1st annual BioInvest Israel 2012 partnering conference, (Oral presentation), March 5-6, 2012.

77. **Anwar Rayan**, "A Combined Virtual Screening Approach for Discovery of hH$_4$R Antagonists", 2012 World GPCR Online Symposium, (invited speaker), October 1, 2012 – October 2, 2012.

78. **Anwar Rayan** and Amiram Goldblum, "Assessing chemicals for their drug-likeness and safety by ISE", TM's 2nd world drug discovery online conference, (Oral presentation), October 16-18, 2012.

79. **Anwar Rayan**, "New Tips for GPCR 3D Structure Prediction",2012World GPCR Online Symposium, (invited speaker),Apr 9, 2012 – Apr 10, 2012.

80. **Anwar Rayan**,David Marcus and Amiram Goldblum, "Predicting Oral DrugLikeness", ADME & Predictive Toxicology, 13-14 March 2012, Munich, Germany.

81. Hafiz Mawasi, Azmi Adawi, Jamal Raiyn, Walaa Haj-Yehia, Rawan Badawiand **Anwar Rayan**, "Novel technique for design of MCR Libraries for Drug Discovery", The 77th Israel Chemical Society Conference at the KfarMaccabiahConvention Center in Ramat Gan on February 7-8, 2012.

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